PREPARATION, CHARACTERISATION AND BIOLOGICAL ACTIVITIES OF SOME METAL COMPLEXES OF NEW N [4-BI(5-THION-1,3,4-OXADIAZOLE-2YL)METHANE]METYL DIBUTYL AMINE AND THEORETICAL STUDY

S.K. Ibrahem, F.M. abdul–Hameed and M.F. Alias.

College of Science for Women, University of Baghdad.

Abstract

A new Mannih base N[4-bi(5-thion-1,3,4-oxadiazole-2yl)methane]metyl dibutyl amine (L), have been prepared and characterized by (FTIR) spectroscopy. (L) have been used as a chelating ligand to prepare a number of metal complexes with Co(III), Cu(II), Pd(II), V(IV) and Pt(IV). The complexes were isolated and characterized by (FTIR), UV-Vis spectrophotometer and flame atomic absorption techniques in addition to magnetic susceptibility, and conductivity measurement. The study of the nature of the complexes formed in absolute ethanol following the mole ratio method, gave results which were agreed with those obtained from isolated solid state studies. The antibacterial activity for the ligand and their metal complexes were studied against two selected micro-organisms Bacillus subtilis and Pseudomonas aeruginosa, the antibiotic Ampicillin has been chosen to compare their activity with those of the new compounds. Theoretical treatment of the formation of complexes in the gas phase, this was done by using the HyperChem-6 program for the Molecular mechanics and semi-empirical calculations. The heat of formation (∆H°f) and binding energy (∆Eb) at 298K for the free ligand and their metal complexes were calculated by (PM3, ZINDO/1 and AMBER) methods. Furthermore, the electrostatic potential of the free ligand was calculated to investigate the reactive sites of the molecules. PM3 was used to evaluate the vibrational spectra of the base(L) and compare the theoretically calculated wave numbers with the experimental values by using bis(5-thion-1,3,4-oxadiazole-2yl) methane as authonetic compound. The theoretically obtained frequencies agreed with those values experimentally found, in addition, the calculation helped to assign unambiguously the most diagnostic bands.

Introduction

Interest in substituted of bis ring of 1,3,4-oxadiazole derivatives as a potential antibacterial and antiviral agents has continued, because of their activity against different micro-organisms [1,2]. A number of metal complexes of certain derivatives oxadiazole and bis-oxadiazole nuclei have been reported [3-5], many of these metal complexes have been shown to exhibit the expected syergetic effect of activity. This is expected since the impact of metal ion in the structure of certain active organic molecules have proved to increase their activities [6-8].

Recently, agreat attention has been given to the synthesis and biological evaluation of Mannich bases compounds containing heterocyclic ring. pandeya and Co-workers [9,10] have been able to synthesize an antimicrobial evaluation of Schiff and Mannich base for isatin and it's derivatives with pyrimidine, oxadiazole and triazole ring respectively, they found that these compounds have a highly significaut activity against microbs.

Several intermediates for the synthesis of biologically important compounds were prepared using this novel catalytic asymmetric Mannich–type reaction, and at the same time, absolute and relative stereochemical assignments were made [11]. A new inhibitor of ceramide trafficking from endoplasmic reticulum to the site of sphingomyerin (SM) synthesis has been synthesized efficiently using the present, Mannich–type reaction as a key step [11].

Metal complexes of Mannich bases have been studied [12-15], extensively in recent years due to the selectivity and sensitivity of these ligands towards various metal ions. The
metal complexes of a new Mannich bases, N-(1-morpholinobenzyl) semicarbazide was synthesized and their structural elucidated on the basis of analytical physically [16]. The biological activity of some new complexes of N,N-di (3(5-phenyl 2-thion-1,3,4-oxadiazole) methyl cyclohexyl amine) and cyclopentyl amine, showed a various effect against some bacterial [12].

In present work we synthesis a new ligand derives from the oxadiazole heterocyclic ring and dibutyl amine, was described in an attempt to introduce the amino methyl moiety in the structure of mercaptooxadiazole ring to investigate the coordination behaviour of the new ligand toward some transition metal complexes, and to compare the biological activity of the ligand and their complexes with the main ring structure.

Theoretical study in the gas phase was done by using semi-empirical method in order to show the most stable conformation. The study aims to calculating the heat of formation, and binding energy for all the probable geometries, and to find the most active sites of the mannich base by using the electrostatic potential calculations. Calculation of the vibrational frequencies of the Bis (5-thiol-1,3,4-oxadiazole-2yl) methane and Mannich base ligand have also been carried out in order to compare the results with the experimental vibrational frequencies to make a certain assignment of the most diagnostic bands.

**Experimental**

**A-Materials and Methods :**

The chemicals used in this work were obtained from B.D.H. and they were all pure grade reagents. Flame atomic absorption of elemental analyzer, shimadzu AA-670 was used for metal determination. FTIR spectra were recorded using shimadza-8000 spectrophotometer, for the range of 4000-2000 cm\(^{-1}\). Electronic spectra of the complexes were obtained using, Shimadzu UV-Vis 160A. Electrical conductivity was measured by corning Conductivity Meter 220, and magnetic susceptibility was measured by BM6 using Faraday method.

**B-Preparation of Ligands:**

The method that was used to prepare the bis (5-thiol-1,3,4-oxadiazole -2yl) methane (BTOM) was reported elsewhere [17]. The Mannich base (L) was prepared according to the following:

BTOM (2.16gm) was dissolved in a minimum quantity of ethanol and kept in an ice bath and treated with formaldehyde (0.6gm, 40%). To this mixture, an ethanol solution of dibutyl amine (2.56gm) was added slowly with stirring for one hour, then, left over night in a refrigerator. A crystalline solid precipitate was formed which was filtered off, washed with cold ethanol, dried and recrystallized from aqueous ethanol. The physical data of Mannich base and their corresponding complexes are listed in Table (1).

**C-Preparation of Complexes:**

The salts of [VOSO\(_4\).H\(_2\)O, CoCl\(_2\).6H\(_2\)O, CuCl\(_2\).2H\(_2\)O, PdCl\(_2\). (PhCN)\(_2\), H\(_2\)PtCl\(_6\). 6H\(_2\)O] were dissolved in ethanol and added to an ethanol solution of Mannich base in (2:1) (metal:ligand) mole ratio respectively with stirring. The mixture was heated under reflux for three hours. During this period the precipitation was completed form. The precipitation was then collected by filtration, washed with ethanol and dried under vacuum for 4 hours.

All these complexes were analyzed by using different available techniques the physical properties of these complexes are listed in Table (1).

**D- Study of Complexes Formation in the Solution:**

Complex of Mannich base with metal ions were studied in solution using ethanal as a solvent, in order to determined [M:L] ratio in the complex following molar ratio method [18,19]. Aseries of solutions were prepared having a constant concentration 10-3 M of the metal ion and ligand (L). The [M/L] ratio was determined from the relationship between the absorption of the absorbed light and the mole ratio of [M/L]. The results complexes formation in solution were listed in Table (1).
E-Programs Used in Theoretical Calculation:

1- HyperChem 6:
It is a sophisticated molecular modeler, editor and powerful computational package, that is known for its quality, flexibility and ease of use, uniting 3D visualization and animation with quantum chemical calculations, mechanic and dynamic.

HyperChem can plot orbital were functions resulting from semi-empirical quantum mechanical calculation, as well as the electrostatic potential, the total charge density or the total spin density can also be determined during a semi – empirical calculation. This information is useful in determining reactivity and correlating calculation results with experimental data.

2-Types of Calculation:
- Single point calculation that determines the molecular energy and properties for a given fixed geometry.
- Geometry optimization calculations employ energy minimization algorithms to locate stable structures.
- Vibrational frequency calculations to find the normal vibrational modes of an optimized structure. The vibrational spectrum can be displayed and the vibrational motions associated with specific transitions can be animated[20].

3-Computational Methods:
a-Semi–empirical quantum mechanics:
i- Hyperchem offers ten Semi–empirical molecular orbital methods, with options for organic and main group compounds, for transition metal complexes and spectral simulation [21].
ii- Choose from Zerner’s, INDO method (ZINDO/1) and parameterization model, version3(PM3), [including transition metals] [22]. PM3 were used for the calculation of heat of formation and binding energy for all metal complex except Pt(IV) complex, therefor (ZINDO/1) method was used for the calculation of the heat of formation and binding energy of V(IV) complex.

b-Molecular Mechanics:
It has three important concepts: Functional form, atoms types and parameter sets. Each molecular mechanics method has its own functional form (Assisted Model Building and energy refinement) (AMBER) is based on a force field [23]. AMBER was used for the calculation of the binding energy and heat of formation of Pt (IV).

F-Study of Biological Activity for Mannich Base and their Metal Complexes:
The biological activity of the prepared Mannich and their respective complexes were studied against selected types of bacteria which included Bacillus Subtilis as Gram positive and Pseudomonas aeruginosa as a Gram negative to be cultivated in brain hart broth agar media, wich is used DMFas a solvent and as a control, for the Disc sensitivity test [24], this method involves the exposure of the zone of inhibition toward the diffusion of micro- organis on agar plate. The plates were incubated for 24hr at 37°C, the zone of inhibition of bacteried growth around the disc was observed.

Result and Discussion
A-Elemental Analyses:
The physical and analytical data of the ligand and metal complexes are given in Table (1). The results obtained from elemental analysis are in satisfactory agreement with the calculated values. The suggested molecular formula was also supported by spectral measurement as well as magnetic moments.

B- Infrared Spectroscopic Study:
The infrared spectrum of the ligand exhibited several bands at approximately (2923, 2846), (1288), (1141, 1049), (1450), and (1380) cm⁻¹, and were assigned to stretching mode of [υ CH₂–N, υ C=S, υ N–C=S, υ N–N and υ NCN] respectively. In all complexes (F₁–F₅) ligands behave as ateteradented coordinating with two metal ions through four-donor atoms (through two sulfur of thio carbonyl and two nitrogen of the methylene group); therefore, the bands due to υ (CH₂–N) were shifted to a higher frequency by (23-8, 11) cm⁻¹, and the band due to υ (C=S) was shifted to a lower frequency by (38-8) cm⁻¹. This red shift means a decrease in the double bond character, while for the bands of υ (NCS) one of was them shifted to higher frequency about (23-15) cm⁻¹ and the others
undergo red shifting about (16-15) cm⁻¹, Table (2). These observations were further indicated by the appearance of ν (M-N, M-S and M-X) respectively. The bands due to ν NCN and ν N-N showed a small relative change in the position accompanied by reduction in the intensity in the case of band ν N-N, which ruled out the possibility of bonding with metal ion. In addition, a strong band was observed at (979) cm⁻¹ due to (V=O) stretching mode in (F₃) complexes [25,26] while the band related to sulfate anion was observed at (1203) cm⁻¹, which indicate abidentate behavior[27,28]. A broad band was observed a round (3433-3386) cm⁻¹ in the spectra of all complexes assigned to a (O-H) stretching and suggested the presence of water or ethanol molecules in the crystall lattic of the complexes [29].

C-Electronic Spectroscopic Study :

The electronic spectra of the metal complexes were recorded for their solution in chloroform in the range (200-1100) nm.

F1: The electronic spectral bands of the prepared complex in the present work are presented in Table (3), along with their assigned transitions and the calculated values of 10 Dq, B’ and β. Low spin Co(III) has the electronic configuration d⁶, the ground term for which in Oh stereochemistry is ¹A₁g, two bands are expected to appear in the visible region due to the transition to the ¹T₁g and ⁵T₂g states.

These transition correspond to the electronic promotion t₂g⁶ → t₂g⁵eg¹ with the promoted electron maintaining its spin unaltered. The orbital multiplicity of t₂g⁵ → eg¹ is 6 and so corresponds to two orbital triplet terms ¹T₁g and ¹T₂g[30,31]. In the spectrum of our complex , a weak band was observed at 12315 cm⁻¹, this band was attributed to the spin-forbidden ¹A₁g → ³T₁g transition which may occur when the promoted electron changes its spin and the two T terms be ³T₁g and ³T₂g. The assignments are made by fitting the ratio of ν₁/ν₂ to Tanaba- sugano diagram, which produces the values of B’, β as well as 10 Dq. The magnetic susceptibility and molar conductivity measurements indicated that the complex to be diamagnetic (0.5 BM), and non conducting.

F2: The present green CuL complex had shown a limited solubility in some solvents, this suggests, to some extent, a polymerization of the product. The electronic spectrum of this complex showed a broad band at 12610 cm⁻¹; in addition, other bands appear at higher than 23200 cm⁻¹. The position of the bands as well as their intensities were not consistent with tetrahedral, distorted octahedral Cu(II) complexes . The band observed, i.e. 12610 cm⁻¹ in the visible region, for the present complex was attributed to the transition ²Eg → ²T₂g, the other bands can be assigned as charg transfer. The value of magnetic moment was found to be (1.32 BM), which agreed well with square planar geometry around Cu (II) ion, and the conductivity measurement showed that the complex was non ionic, Table (3).

F3: The olive colour of spectrum vanadyl (IV) complex, show three main absorption bands, Table (3), which are assigned to the ³B₂ → ³Eg , ²B₂→ ²B₁g and ²B₂→²A₁ respectively in a squar pyramidal geometry [30]. The magnetic moment (2.03) is higher than spin value of vanadium metal only; this result indicates a higher orbital contribution [32]. Conductivity measurement in DMF showed that the complex was non ionic.

F4: The brown palladium complex, show three absorption bands which were observed at (23529, 27173, and 30030) cm⁻¹. The spectrum was typical of squar planer Pd (II) complexes [33,34]. The measured magnetic moment (0.87) BM showed that the complex to be low-spin, and conductivity measurement showed that the complex was non electrolyte, Table (3).

F5: The prepared orang Pt(IV) complex showed three bands at (23255, 27397, and 31125)cm⁻¹, which indicate an octahedral geometry [35,36]. Magnetic moment of solid complex, was found to be (0.52) BM showed a higher orbital contribution [32]. Conductivity in DMF showed that the complex was non ionic, Table (3).
D-Solution Study:
Molar ratio method was followed to determine the M:L ratio. The results of complexes in ethanol solution, suggest that the metal to ligand ratio was (2:1) for all prepared compounds, which were comparable to these obtained from isolated solid state study Table (1).

E- Theoretical Study:
(i) The program hyperchem6 was used for the semi-empirical and molecular mechanic calculations, at optimized geometries energies, the result on PM3, ZINDO/1 and AMBER methods of calculation in gas phase for the heat of formation ($\Delta H^\circ$) and binding energy ($\Delta E_b$) for the ligands and their complexes were calculated and tabulated in Table (4). Also PM3 was used for evaluation the vibrational spectra of the BTOM and Mannich base to compare the theoretically calculated wave numbers with the experimental values. Theoretically calculated wave numbers for these ligands showed that some deviations from the experimental values, these deviations are generally acceptable in theoretical calculations and are described in Table (5) and (2), and the Figs. (1,2).

(ii) Electrostatic potential (E.P):- Electron distribution governs the electrostatic potential of molecules and describes the interaction of energy of the molecular system with a positive point charge, so it is useful for finding sites of reaction in a molecule positive charged species tend to attack a molecule where the E.P is strongly negative electrophilic attack [37,38]. (E.P) of free ligand was calculated and plotted as 2D contour to investigate the reactive sites of the molecules Fig. (3), and one can interpret the stereochemistry and rates of many reactions involving soft electrophiles and nucleophiles in terms of the properties of frontier orbitals (HOMO and LUMO). Overlap between the HOMO and LUMO is a governing factor in many reactions. The HOMO and LUMO values were plotted as 2D contour to get more information about these molecules. The results of calculation showed that the LUMO of transition metal ion prefer to react with the HOMO of sulfur and nitrogen atoms of Mannich bases ligand.

(iii) Optimized Geometries Energy of Metal Complexes for Mannih Base: - All theoretically probable structures of metal complexes with Mannich base have been calculated to search for the most probable model building stable structure, these shapes Fig. (4), show the calculated optima geometries for (L) and their metal complexes. The results of PM3 and ZINDO/1 methods of calculation in gas phase for the binding energies and heat of formation of Co (III), Cu (II), Pd (II) and V(IV), while AMBER method was used to calculate the binding energies which is equal to heat formation of Pt (IV) complex, and are described in Table (4).

F- Biological Activity:-
As a result from the study of antimicrobial of prepared compounds and their metal complexes Fig(5,6), the following points were concluded:-

1) The results of antibacterial activity study for the Mannich base indicated that the new compounds exhibited antibacterial activity against the studied bacteria at low and high concentrations.

2) The inhibition which is exhibited from L toward the bacteria used in this study, at higher and lower concentrations, is similar to the inhibition of Ampicilin compound at the same species of bacteria and concentration.

3) The results reflected that the starting material BTOM exhibited more inhibition than the prepared new donor bases toward Bacillus Subtilis, at higher and lower concentrations.

4) The study of antibacterial activities revealed that the(L), exhibited a greater activity against the studied bacteria Pseudomonas aeruginosa, compared to that (BTOM), when we use low concentration. This indicates that introductions of the aminomethyl group on the oxadiazole derivatives ring raised the killing zone.

5) Generally, the result of the prepared complexes exhibited antibacterial activity toward Pseudomonas aeruginosa bacteria
was more than the complexes inhibition on Bacillus Subtilis bacteria.

6) The study of the antibacterial activities revealed that the complexes of (L) toward G+ve bacteria showed a high activity at 10 mmole (except vanadium and platinum complex).

7) The results of the antibacterial activities of the new complexes of donor base, showed that there is no effect toward G−ve bacteria when we use the two concentration, except copper and plutin complexes which they exhibit at the same bacteria only when we use high and low concentration respectively.

Table (1)

<table>
<thead>
<tr>
<th>Symb.</th>
<th>Color</th>
<th>Crystallization solvent</th>
<th>M.P. °C or decomp.</th>
<th>Yield %</th>
<th>Metal analyses</th>
<th>Metal to ligand ratio</th>
<th>Suggest Molecular formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>L</td>
<td>Pale yellow</td>
<td>hot ethanol</td>
<td>132 - 134</td>
<td>52%</td>
<td>_</td>
<td>_</td>
<td>C₂₃H₄₂N₆S₂O₂</td>
</tr>
<tr>
<td>F₁</td>
<td>Brick-red</td>
<td>Washing with hot ethanol and cold water</td>
<td>270 D</td>
<td>66%</td>
<td>11.04 (11.99)</td>
<td>2:1</td>
<td>[Co₂LCl₄(OH)₂(Η₂O)]₂. 4H₂O</td>
</tr>
<tr>
<td>F₂</td>
<td>Green</td>
<td>Washing with hot ethanol and cold water</td>
<td>200 D</td>
<td>83%</td>
<td>13.51 (13.78)</td>
<td>2:1</td>
<td>[Cu₂LCl₄]. 4EtOH</td>
</tr>
<tr>
<td>F₃</td>
<td>Olive</td>
<td>Washing with hot ethanol and cold water</td>
<td>119 D</td>
<td>56%</td>
<td>(13.74)</td>
<td>2:1</td>
<td>[(VO)₂ L(SO₄)₂]. H₂O</td>
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<tr>
<td>F₄</td>
<td>Brown</td>
<td>Washing with hot ethanol and cold water</td>
<td>218 D</td>
<td>64%</td>
<td>18.98 (18.88)</td>
<td>2:1</td>
<td>[Pd₂LCl₄]. 4EtOH</td>
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<tr>
<td>F₅</td>
<td>Light Orange</td>
<td>Washing with hot ethanol and cold water</td>
<td>189 D</td>
<td>70%</td>
<td>26.88 (26.13)</td>
<td>2:1</td>
<td>[Pt₂LCl₄]. 5EtOH</td>
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Table (2)

<table>
<thead>
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<th>Symb.</th>
<th>ʋ_C=S</th>
<th>ʋ_NCS</th>
<th>ʋ_N-N</th>
<th>ʋ_CH₂-N</th>
<th>ʋ_NCN</th>
<th>ʋ_M-S</th>
<th>ʋ_M-N</th>
<th>ʋ_M-O</th>
<th>ʋ_M-X</th>
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<tr>
<td>L</td>
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<td>1049</td>
<td>1141</td>
<td>1450</td>
<td>2846</td>
<td>2923</td>
<td>1380</td>
<td>_</td>
<td>_</td>
</tr>
<tr>
<td>F₁</td>
<td>1280</td>
<td>1072</td>
<td>1126</td>
<td>1455</td>
<td>2869</td>
<td>2931</td>
<td>1378</td>
<td>471</td>
<td>525</td>
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<tr>
<td>F₂</td>
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<td>1126</td>
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<td>2854</td>
<td>2931</td>
<td>1378</td>
<td>478</td>
<td>530</td>
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<tr>
<td>F₃</td>
<td>1250</td>
<td>1064</td>
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<td>2931</td>
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<td>520</td>
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<td>1064</td>
<td>1126</td>
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<td>2854</td>
<td>2923</td>
<td>1380</td>
<td>470</td>
<td>515</td>
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Table (3)
Electronic spectra, conductance and magnetic moment, for metal complexes of (L).

<table>
<thead>
<tr>
<th>Symb.</th>
<th>Absorption Bands, cm(^{-1})</th>
<th>Transitions</th>
<th>B</th>
<th>B'</th>
<th>β</th>
<th>10Dq</th>
<th>Dq/B'</th>
<th>15B'</th>
<th>μ eff BM</th>
<th>Molar conductivity μs/cm(^{-1})</th>
<th>Suggested structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>F(_1)</td>
<td>12315 16393 22831 27922 28985</td>
<td>(^{1})A(_g) → (^{3})T(_g)(f) (^{1})A(_g) → (^{1})T(_g)(f) (^{1})A(_g) → (^{3})T(_g)(p)</td>
<td>1400</td>
<td>472</td>
<td>0.337</td>
<td>160047</td>
<td>3.4</td>
<td>106200</td>
<td>0.5</td>
<td>37</td>
<td>Octahedral</td>
</tr>
<tr>
<td>F(_2)</td>
<td>12610 23809 28985</td>
<td>(^{2})E(_g) → (^{2})T(_g)</td>
<td>C.T</td>
<td>C.T</td>
<td></td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>F(_3)</td>
<td>12330 23148 27777</td>
<td>(^{2})B(_g) → (^{2})E(_g) (^{2})B(_g) → (^{2})B(_g) (^{2})B(_g) → (^{2})A(_g)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>2.03</td>
<td>75</td>
</tr>
<tr>
<td>F(_4)</td>
<td>23529 27173 30030</td>
<td>(^{1})A(_g) → (^{1})B(_g) (^{1})A(_g) → (^{1})E(_g) L → Pd(C.T)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.87</td>
<td>32</td>
</tr>
<tr>
<td>F(_5)</td>
<td>23255 27397 31125</td>
<td>(^{1})A(_g) → (^{1})T(_g) (^{1})A(_g) → (^{1})T(_2) g L → Pt (C.T)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.52</td>
<td>41</td>
<td>Octahedral</td>
</tr>
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### Table (4)

Comparison of experimental and theoretical vibrational frequencies.

<table>
<thead>
<tr>
<th>Symb.</th>
<th>( v_{NH} )</th>
<th>( \delta_{NH} + v_{C=N + C=S} )</th>
<th>( v_{C=N + C=S} )</th>
<th>( v_{NCS} )</th>
<th>( v_{N-N} )</th>
<th>( v_{C=S} )</th>
<th>( v_{NCN} )</th>
<th>( v_{CH2-alph.} )</th>
<th>( v_{CH2-N} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>BTOM</td>
<td>(3285)(^<em>) (3403)(^<strong>) (-3.5)(^</strong></em>)</td>
<td>(1643,1620)(^<em>) (1445.9)(^<strong>) (11.9,10.8)(^</strong></em>)</td>
<td>(1396.3)(^<em>) (1381)(^<strong>) (1.1)(^</strong></em>)</td>
<td>(985,998)(^<em>) (979.9)(^<strong>) (0.51,1.81)(^</strong></em>)</td>
<td>(1056)(^<em>) (1021)(^<strong>) (3.31)(^</strong></em>)</td>
<td>(1272)(^<em>) (1233.2)(^<strong>) (3.05)(^</strong></em>)</td>
<td>-</td>
<td>(2916,2839)(^<em>) (2998,2938)(^<strong>) (-2.81, -3.49)(^</strong></em>)</td>
<td>-</td>
</tr>
<tr>
<td>L</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>(1049,1141)(^<em>) (1049,1039)(^<strong>) (3.3,8.9)(^</strong></em>)</td>
<td>(1450)(^<em>) (1386.9)(^<strong>) (4.3)(^</strong></em>)</td>
<td>(1288)(^<em>) (1234)(^<strong>) (4.2)(^</strong></em>)</td>
<td>(1380)(^<em>) (1347)(^<strong>) (2.4)(^</strong></em>)</td>
</tr>
</tbody>
</table>

Where:

* : Experimental frequency

**: Theoretical frequency

***: Error % due to main difference in the experimental measurements and theoretical treatment of vibrational spectrum.

### Table (5)

Comparison of experimental and theoretical vibrational frequencies.

<table>
<thead>
<tr>
<th>Symb.</th>
<th>( \chi^1 )</th>
<th>( \tilde{\chi}^1 )</th>
<th>( \chi^2 )</th>
<th>( \tilde{\chi}^2 )</th>
<th>( \chi^3 )</th>
<th>( \tilde{\chi}^3 )</th>
<th>( \chi^4 )</th>
<th>( \tilde{\chi}^4 )</th>
<th>( \chi^5 )</th>
<th>( \tilde{\chi}^5 )</th>
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<td>BTOM</td>
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<td>-89.7602</td>
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<td>-1671.057</td>
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<td>-74472.027</td>
<td>-967738.00</td>
<td>-9551.728</td>
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Fig. (1) : The Calculated vibrational frequencies of BTOM.
Fig. (2) : The Calculated vibrational frequencies of Mannich base L.
Fig. (3) : HOMO and Electrostatic Potential as 2D Contours for Starting material and L.

Fig. (4) : Conformational Structure of L and their metal Complex (F₁-F₅).
Fig. (5) : Shows the effect of Pseudomonas aeruginosa bacterial toward complexes of L.

References


الخلاصة

تم تحضير قياس مانع الجديده (N-4) ثنائي

(II) والحساس (VI) والفلازيم (II) والبلاديوم (VI) والبلاديوم (II) والفلازيم (VI)

وتوزع العناصر الجديدة وتشخيص طيف

الإشعاع تحت الحمراء وطبقة الأمين (L) من المكانيك الجزيئي وشبه التجريبي في الحساب باستخدام الدوال لحساب حرارة التكوين AMBER,ZINDO/1,PM3 وطلاقة التركيب (ΔHf) ودرجة حرارة 298 كلفن لليكين ومعدن محببة، لأننا نحسب الجهد الالكترونيكي لبيان المواقع المعامة لقاعدة مانح وحري حساب التردود الالزمري نظريًا و باستخدام الدالة لقاعدة مانح ومقامتهاtp بالقيم المعامه عمليًا باستخدام ثاني

(5-ثائيون-3,1-أوكساسيدازول-2) ميثان كمركب قياسي ووجد بأن هناك تفاوتًا كبيرًا بين القيم المعالم والمحسوب نظريًا مع زيادة امكانيه تشخيص الحزم بشكل

 wholesale