



Received: 10-12-2013  
Accepted: 02-01-2014

ISSN: 2321-4902  
Volume 1 Issue 4



Online Available at [www.chemijournal.com](http://www.chemijournal.com)

## International Journal of Chemical Studies

# Synthesis, Structural Characterization And Biological Activity Of Transition Metal Complexes Of Schiff Base Ligand – Furan Derivatives

Mohd. Asif Khan<sup>1\*</sup>, Ruchi Agarwal<sup>1</sup>, Shamim Ahmad<sup>1</sup>

1. Department of Chemistry, Bareilly College, Bareilly U.P.-243005,(India)

\*[Email: [asif\\_sw07@yahoo.com](mailto:asif_sw07@yahoo.com)]

A series of Ti (III), Mn (III), V (III), Fe (III), Co (III), Ru (III), Ru (II), V (IV) and Cu (II) complexes have been synthesized from the Schiff base ligand. The Schiff base ligand is derived from 2-furancarboxaldehyde and O-phenylenediamine. The resulting complexes were characterized by elemental analyses, magnetic moment measurement, molar conductance, thermal analyses (TGA), IR, <sup>1</sup>H-NMR and solid reflectance. The ligand dissociation, as well as metal ligand stability constants were calculated, pH-metrically at 25 °C and ionic strength  $m = 0.1$  (IM NaCl). IR spectra show that ligand is coordinated to the metal ions in a tetradentate manner, with ONNO donor sites of azomethine N and furan O. The molar conductance data reveals that all metal chelates are electrolytes. The electronic spectral data of the complexes displayed the proper transitions and octahedral geometry. The synthesized ligands in comparison to their metal complexes, were also screened for their antibacterial activity against bacterial species, *Escherichia coli*, *Pseudomonas aeruginosa* and *Staphylococcus pyogenes*. The activity data show the metal complexes to be more potent antibacterials than Schiff base ligand against one or more bacterial species.

**Keyword:** Transition metal complexes, 2-furan castoxaldehyde, O-phenylenediamine, Biological activity.

### 1. Introduction

The chemistry of the carbon-nitrogen double bond plays a vital role in the progress of chemical science<sup>[1]</sup>. Schiff base compounds have been used as five chemicals and medical substrates. In the field of coordination chemistry, Schiff base metal complexes have a curious history<sup>[2,3]</sup>. Metal ion play vital roles in the vast number of biological processes. Metal complexes with Schiff base ligand have been studied for their application in biological, clinical, analytical and pharmacological areas<sup>[4]</sup>. The importance of furan derivatives is quite evident from a number of papers, patents etc. published every year. Furan derivatives exhibiting anti-inflammatory<sup>[5]</sup>, antituberculosis<sup>[6]</sup>, anticancer<sup>[7]</sup>, antimicrobial<sup>[8]</sup>,

antifungal<sup>[9]</sup> activity have been reported in literature. Many potent antibacterial and antifungal compounds synthesized by condensation of aldehydes with various heterocyclic have been reported<sup>[10-12]</sup>. Manganese, Vanadium and Ruthenium Possess as number of oxidation states and have excellent complexing property. The last two metals and their complexes exhibits biological properties<sup>[13-14]</sup>. Keeping in view these facts we have synthesized ligand having oxygen, nitrogen, donor atoms and study their complexation behaviour and biological activity.

### 2. Material and Reagents

All chemicals used were of analytical reagent

grade (AR) and of the highest purity available. They included 2-furan carboxaldehyde (sigma), O-phenylenediamine (Aldrich), Titanium (III), chloride (merck p.a.), manganese (III), chloride (Aldrich p.a.), Vanadium (III) chloride (Aldrich p.a.), Iron (III) chloride (B.D.H.), Cobalt (III) chloride (Merck p.a.). The organic solvents used included absolute ethyl alcohol, diethylether and dimethylformamide (DMF). These solvents were either spectroscopically pure from BDH or purified by the recommended method<sup>[15]</sup> and tested for their spectral purity. De-ionized water collected from all-glass equipments was normally used in all preparations. Fresh stock solutions of  $1 \times 10^{-3}$  M ligand, were prepared by dissolving the accurately weighed amount of Schiff base ligand (0.264 gm/L) in the appropriate volume of absolute ethanol. The  $1 \times 10^{-3}$  M stock solutions of metal salts Fe (III), Ti (III), V (III), Mn (III), Co (III), Ru (III), Cu (II) were prepared by dissolving accurately weighed amounts of the metal salts in appropriate volume of de-ionized water.

### 3. Instrumentation

Melting points were determined on a JSGW apparatus and are uncorrected. I.R. spectra were recorded using a Perkin Elmer 1600 FT spectrometer <sup>1</sup>H-NMR spectra were measured on a Bruker WH-500 MHz spectrometer at Ca 5-15% solution in DMSO – d<sup>6</sup> (T.M.S. as internal standard). Elemental analyses was carried out on vitro EL III elementor. Thin layer chromatography (TLC) was performed on Silica gel G for TLC (merck) and spots were visualized by Iodine vapours.

The molar conductance of solid complexes in DMF was measured using OK – 102 (Hungary) conductivity-meter. Magnetic susceptibility was measured with a faraday balance at room temperature. pH measurements were performed using a metrohm 716 DMS titrino connected to metrohm 728 stirrer. C, H, and N were analyzed using M.L.W. micro-elementary CHN analyses. Thermogravimetric analyses was performed with a DU-Pont 2000 thermal analyses.

### 4. Synthesis of Ligand

A hot solution (60 °C) of o-phenylenediamine (1.08 g, 10 mmol) was mixed with a hot solution (60 °C) of 2-furancarboxaldehyde (1.92 g, 20 mmol) in 50 mL of ethanol. The resulting mixture was left under reflux for 2 hr and the solid product formed was separated by filtration, purified by crystallization from ethanol, washed with diethyl ether and then dried in a vacuum over anhydrous calcium chloride. The yellow product is produced in 80% yield<sup>[16]</sup>.

### 5. Synthesis Of Metal Complexes

The metal complexes of the Schiff bases, ligand were prepared by the addition of a hot solution (60 °C) of the appropriate metal chloride, (1 mmol) in an ethanol-water mixture (1:1, 25 mL) to the hot solution (60 °C) of the Schiff bases (0.264 g 2 mmol) in the same solvent (25 mL). The resulting mixture was stirred under reflux for 1 hr whereupon the complexes precipitated. They were collected by filtration, washed with a 1:1 ethanol water mixture and diethyl ether. The analytical data for C, H, N, and S were repeated twice.

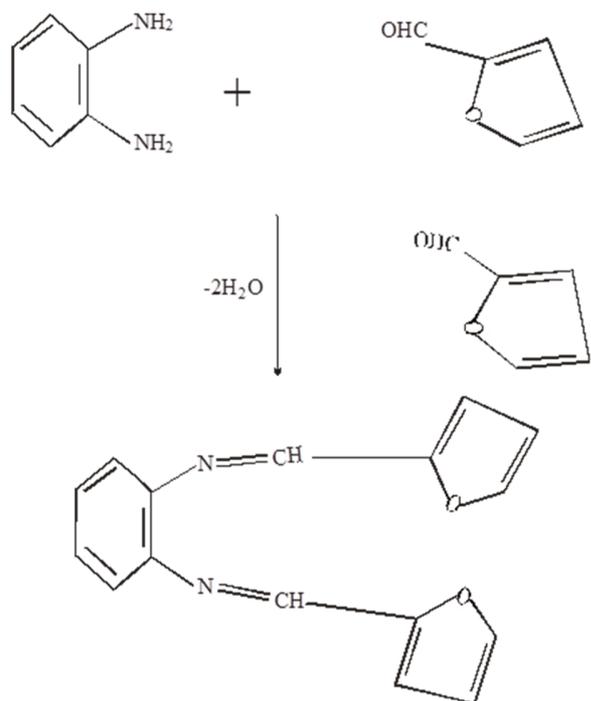
### 6. Biological Activity

A 0.5 mL spore suspension ( $10^{-6}$  –  $10^{-7}$  spore/mL) of each of the investigated organisms was added to a sterile agar medium just before solidification, then poured into sterile Petri dishes (9 cm in diameter) and left to solidify. Using a sterile cork borer (6 mm in diameter), 3 holes (wells) were made in each dish and then 0.1 mL of the tested compounds, dissolved in DMF (100 mg/mL), was poured into these holes. Finally, the dishes were incubated at 37 °C for 48 hr. Then clear or inhibition zones were detected around each hole. DMF alone (0.1 mL) was used as a control under the same condition for each organism, and by substrating the diameter of inhibition zone resulting with DMF from that obtained in each case, both antibacterial activities were calculated as a mean of 3 replicates<sup>[17-18]</sup>.

## 7. Result And Discussion

The ligand and its transition metal complexes with Ti (III), V (III), Mn (III), Co (III), VO (IV), Fe (III), Ru (III), Cu (II) & Ru (II) were subjected to elemental analyses where as metal and complexes were estimated gravimetrically in the lab, validated by jobs method. All this analytical data suggested 1:1 M:L stoichiometry for all the complexes.

The M.P. of the ligand and its metal complexes were determined and compared in order to find out the possibilities of formation of complexes. The M.Pt. are given in Table (1). The observed value of magnetic susceptibility was used to calculate to magnetic moment of the complexes. These values suggested paramagnetic nature for Ti (III), Mn (III), V (III), Cr (III), Fe (III) complexes as expected for octahedral  $d^1$ ,  $d^4$ ,  $d^2$   $d^3$  and  $d^5$  complexes. The Co (III) complex is diamagnetic in nature as expected for low spin  $d^6$  ion. The value of magnetic moments of complexes are given in Table (1).



Schiff base Ligand - 2-furancarboxaldehyde-o-phenylene diamine

Figure 1

Ti (III), Mn (III), V (III), Ru (III), Fe (III) complexes as expected for octahedral  $d^1$ ,  $d^4$ ,  $d^2$

and  $d^5$  complexes. The Co (III) complex is diamagnetic in nature as expected for low spin  $d^6$  ion. The value of magnetic moments of complexes are given in Table (1).

By using the relation  $\mu_m = K/C$ , the molar conductance of the complexes ( $\mu_m$ ) can be calculated, where C is the molar concentration of the metal complex solutions. The chelates were dissolved in DMF and the molar conductivities of  $10^{-3}$  M of their solutions at  $25 \pm 2$  °C were measured. Tables-1 show the molar conductance values of the complexes. The value of molar conductance indication the 1:3 and 1:2 electrolytic nature of synthesized complexes.

## 8. Electronic Spectra

The electronic spectrum of the complex of Ti (III) exhibits a single broad band at  $19250 \text{ cm}^{-1}$  assignable to  ${}^2t_{2g} \longrightarrow {}^2E_g$  transition for  $O_h$  symmetry<sup>[19]</sup>. The electronic spectrum of complex V (III) exhibits band at  $16100 \text{ cm}^{-1}$  with a shoulder at  $20,400 \text{ cm}^{-1}$ . The low energy band has been assigned to  ${}^2A_{1g} \longrightarrow {}^3A_{2g}$  while the high energy band may be due to  ${}^2A_{1g} \longrightarrow {}^3T_{2g}(P)$  transition. These bands are characteristic of Octahedral geometry<sup>[20]</sup>.

The electronic spectrum of Mn (III) complex showed an intense and sharp charge transfer band at  $19800 \text{ cm}^{-1}$  and a spin allowed d-d transition band  ${}^5E_g \longrightarrow {}^5T_{2g}$  at  $18230 \text{ cm}^{-1}$ . This broad band occurring at lower frequency with increased intensity indicates the lowering of symmetry from Octahedral Configuration<sup>[21]</sup>.

The electronic spectrum of the complex of Fe (III) exhibited these bands at  $11300$ ,  $21600$  and  $27880 \text{ cm}^{-1}$  assignable to  ${}^6A_{1g} \longrightarrow {}^4T_{1g}$ ,  ${}^6A_{1g} \longrightarrow {}^4T_{2g}$  and  ${}^6A_{1g} \longrightarrow {}^4E_g$  transitions respectively. These transitions are characteristics of Octahedral Fe (III) complexes<sup>[22]</sup>.

The electronic spectrum of Co (III) complex displays bands at  $15110$ ,  $21000$  and  $23300 \text{ cm}^{-1}$  assignable to  ${}^3A_{1g} \longrightarrow {}^3T_{2g}$ ,  ${}^1A_{1g} \longrightarrow {}^1T_{1g}$  and  ${}^1A_{1g} \longrightarrow {}^1T_{2g}$  transitions respectively. These are similar to those reported for other six coordinated Co(III) complexes<sup>[23]</sup>.

The electronic spectrum of complex of Ru (III) shows three bands at  $13700$ ,  $17650$  and  $22500 \text{ cm}^{-1}$ . These bands are assigned to  ${}^4T_g \longrightarrow {}^4T_{1g}$ ,

${}^2T_{2g} \longrightarrow {}^4T_{2g}$  and  ${}^2T_{2g} \longrightarrow {}^2A_{2g}, {}^2T_{1g}$  respectively. These are similar to those reported for other Ru (III) octahedral complexes<sup>[24]</sup>. The electronic spectrum of Ru (II) complex shows a band at  $22000\text{ cm}^{-1}$ , this band has been assigned to charge transfer transition arising from excitation of an electron from metal  $t_{2g}$  level to unfilled molecular orbitals derived from  $p^*$  level

of the ligands in accordance with the assignment made for similar octahedral Ru (II) complexes<sup>[25]</sup>. The electronic spectrum of oxovanadium (IV) complex exhibited three bands at 11870, 19425 and  $26120\text{ cm}^{-1}$  assignable to  $dxy(b_2) \longrightarrow dxy$ ,  $dyz(e^*, dxy(b_2) \longrightarrow dx^2-y^2(b_1))$  and  $dxy(b_2) \longrightarrow dz^2(a_1)$  transitions respectively for octahedral stereochemistry<sup>[26]</sup>.

**Table 1:** Characterization of Ligand and its Metal Complexes Prepared

S. No	Formula of the Ligand and Complex and Molecular Weight	Colour	M.P. °C	Elemental analyses					Molar Conductance ohm-1 cm <sup>2</sup> mole <sup>-1</sup>	Magnetic Moments in (B.M.)
				% of C	% of H	% of N	% of M	% of Cl		
1	C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> Mol. Wt. = 264	Yellow	122	72.73 (72.70)	4.54 (4.45)	10.61 (10.50)	-	-	-	-
2	[Ti(C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub> Cl <sub>3</sub> ] Mol. Wt. = 454.5	Yellow	197	42.24 (42.20)	3.52 (3.48)	6.16 (6.12)	10.56 (10.52)	23.43 (23.40)	125	1.77
3	[Mn(C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub> Cl <sub>3</sub> ] Mol. Wt. = 461.5	Dark Brown	202	41.60 (41.56)	3.47 (3.41)	6.07 (6.02)	11.92 (11.88)	23.08 (23.03)	135	5.40
4	[V(C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub> Cl <sub>3</sub> ] Mol. Wt. = 457.5	Light Yellow	199	41.97 (41.90)	3.50 (3.46)	6.12 (6.09)	11.15 (11.10)	23.28 (23.23)	130	2.90
5	[Fe(C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub> Cl <sub>3</sub> ] Mol. Wt. = 462.5	Brown	208	41.51 (41.46)	3.46 (3.40)	6.05 (6.02)	12.11 (12.07)	23.03 (23.00)	140	5.90
6	[Co(C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub> Cl <sub>3</sub> ] Mol. Wt. = 465.5	Dark Brown	212	41.24 (41.20)	3.44 (3.40)	6.01 (6.00)	12.67 (12.61)	22.88 (22.82)	138	Diamagnetic
7	[Ru(C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub> Cl <sub>3</sub> ] Mol. Wt. = 507.5	Green	245	37.83 (37.81)	3.15 (3.11)	5.52 (5.50)	19.90 (19.86)	20.98 (20.94)	142	1.80
8	[Ru(C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub> Cl <sub>2</sub> ] Mol. Wt. = 472.0	Dull White	239	40.68 (40.61)	3.39 (3.35)	5.93 (5.90)	21.40 (21.38)	15.04 (15.01)	80	Diamagnetic
9	[VO(C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> )(H <sub>2</sub> O)]Cl <sub>2</sub> Mol. Wt. = 420.0	Yellowish Orange	190	45.71 (45.62)	3.33 (3.25)	6.66 (6.60)	12.14 (12.10)	16.90 (16.82)	85	1.71
10	[Cu(C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> )(H <sub>2</sub> O) <sub>2</sub> Cl <sub>2</sub> ] Mol. Wt. = 434.5	Greenish Yellow	195	44.18 (44.11)	3.68 (3.62)	6.44 (6.38)	14.61 (14.56)	16.34 (16.29)	90	1.88

Figures in parenthesis are observed values.

## 9. I.R. Spectra

The IR data of the spectra of Schiff base ligand and its complexes are presented in Table-2. The IR spectra of the complexes were compared with those of the free ligands in order to determine the coordination sites that may be involved in chelation. There were some guide peaks in the spectra of the ligands, which were helpful in achieving this goal. The position and/or the intensities of these peaks are expected to change upon chelation. New peaks are also guide peaks, as is water, in chelation. Upon comparison, it was determined that the  $n(C=N)$  stretching vibration is

found in the free ligand at  $1615\text{ cm}^{-1}$ . This band was shifted to higher wavenumbers in the complex indicating the participation of the azomethine nitrogen in coordination (M-N)<sup>[27]</sup>. Medium to sharp bands, due to  $n(C-O-C)$  stretching vibration of furan, appeared at  $1229\text{ cm}^{-1}$  in the ligand<sup>[28]</sup>. This band shifted to  $1274\text{ cm}^{-1}$  in metal complex<sup>[29]</sup>. These shifts refer to the coordination through a furan O atom. New bands are found in the spectra of the complexes in the region  $552$  (furan O), which are assigned to  $n(M-O)$  stretching vibration for metal complexes. The band at  $420-453\text{ cm}^{-1}$  metal complex

have been assigned to n(M-N) mode. Therefore, from the IR spectra, it is concluded that the ligand

behaves as a neutral tetradentate ligand coordinated to the metal ions via azomethine N and furan O.

**Table 2:** IR data (4000-400  $\text{cm}^{-1}$ ) of Ligand and its metal complexes

Compound (C=N)	$\nu(\text{C-O-C})$	$\nu(\text{Water})$	$\nu(\text{OH (Hydrated water)})$	$\delta(\text{H}_2\text{O (coordinated (M-O)})$	$\nu(\text{M-N})$	$\nu$
Ligand-L	1614sh	1229m	3349br	-	-	-
$[\text{Fe}(\text{L})(\text{H}_2\text{O})_2]\text{Cl}_3 \cdot 3\text{H}_2\text{O}$	1628sh	1237m	3320sh	928m, 884m	552s	432m
$[\text{Co}(\text{L})(\text{H}_2\text{O})_2]\text{Cl}_3$	1626s	1232m	3401sh	931m, 884m	557s	452m
$[\text{Ru}(\text{L})(\text{H}_2\text{O})_2]\text{Cl}_3$	1611sh	1274m	3394br	928m, 883m	595m	420s
$[\text{Cu}(\text{L})(\text{H}_2\text{O})_2]\text{Cl}_3 \cdot 2\text{H}_2\text{O}$	1617sh	1231sh	3381br	912m, 883m	657s	445m

Sh=sharp, m=medium, br=broad, s=small, w=weak.

**Table 3:** Proton NMR spectral data of Ligand

Compound	Chemical shift, (d) ppm	Assignment
$\text{C}_{16}\text{H}_{12}\text{N}_2\text{O}_2$	8.102 5.83–7.84 3.7 2.5	(s, 2H, azomethine H) (m, 10H, 4ArH and 6 furan H) (br, 2H, $\text{H}_2\text{O}$ ) $\text{CH}_3$ of solvent)

### 10. Thermal Analysis (TGA And Dr TG)

Thermogravimetric analysis (TGA and DrTA) of the Schiff base ligand and its chelates are used to : (i) get information about the thermal stability of these new complexes, (ii) decide whether the water molecules (if present) are inside or outside the inner coordination sphere of the central metal ion, and (iii) suggest a general scheme for thermal decomposition of these chelates. In the present investigation, heating rates were suitably controlled at  $10\text{ }^\circ\text{C min}^{-1}$  under nitrogen atmosphere, and the weight loss was measured from the ambient temperature up to @  $1000\text{ }^\circ\text{C}$ . The data are provided in Table-4. The weight loss for each chelate was calculated within the corresponding temperature ranges. The TGA curve of Schiff base ligand exhibits a first estimated mass loss of 49.93% (calcd: 50.76%) at  $30 - 400\text{ }^\circ\text{C}$ , which may be attributed to the liberation of  $\text{C}_8\text{H}_6\text{O}_2$  as gases. In the 3<sup>rd</sup> and 4<sup>th</sup> stages within the temperature range  $400-900\text{ }^\circ\text{C}$ , ligand loses the remaining part with an estimated

mass loss of 50.07% (calcd: 49.24%) with a complete decomposition as  $\text{CO}$ ,  $\text{CO}_2$ ,  $\text{NO}$ ,  $\text{NO}_2$ , etc. gases. The Fe (III) L. chelate shows 5 decomposition steps within the temperature range  $30-1000\text{ }^\circ\text{C}$ . The first 2 steps of decomposition within the temperature range  $25-5000\text{ }^\circ\text{C}$  correspond to the loss of water molecules of hydration and  $\text{HCl}$ ,  $\text{H}_2$ , and  $\text{O}_2$  gases, with a mass loss of 28.13% (calcd: 27.59%) for the Fe (III) L. chelate. The overall weight loss amounts to 86.01% (calcd: 84.52%) for the Fe(III) chelates with ligand (L).  $[\text{Cu}(\text{L})(\text{H}_2\text{O})_2]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$  chelate exhibit 1 to 4 decomposition steps. For the Cu(II)-L chelate, the first step is in the temperature range  $30-120\text{ }^\circ\text{C}$  (mass loss = 7.96%; calcd for  $2\text{H}_2\text{O}$ : 7.65%), which may account for the loss of water molecules of hydration. As shown in Table-4 the mass losses of the remaining decomposition steps amount to 22.85% (calcd: 22.74%) and correspond to the removal of  $\text{HCl}$ ,  $\text{H}_2\text{O}$ ,  $\frac{1}{2}\text{O}_2$  L molecules, leaving  $\text{CuO}$  as a residue.

**Table 4:** Thermoanalytical results (TG, DrTG) of L and its metal complexes

Compound	TG range (°C)	DrTG <sup>max</sup> (°C)	n*	Mass loss Estim	Total mass loss (Calcd.) %	Assignment	Metallic residue
L	30-400	70, 267	2	49.93(50.76)	100.(100.0)	-Loss of C <sub>8</sub> H <sub>6</sub> O <sub>2</sub> -Loss of C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> -Loss of 3H <sub>2</sub> O	-
	400-900	570, 758	2	50.07(49.24)			
	30-130	63	1	10.83(10.46)			
(1)	130-500	182, 320	2	28.13(27.59)	86.01(84.52)	-Loss of 3HCl, ½ H <sub>2</sub> and O <sub>2</sub> -Loss of C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> -Loss of 3H <sub>2</sub> O	½ Fe <sub>2</sub> O <sub>3</sub>
	500-1000	620, 880	2	47.05(46.47)			
	30-100	79	1	14.89(14.34)			
(2)	120-470	195, 280	2	22.83(22.74)	83.90(83.10)	-Loss of 2HCl, ½ O <sub>2</sub> and H <sub>2</sub> O -Loss of C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O -Loss of 3H <sub>2</sub> O	CuO
	470-850	740	1	53.11(52.71)			
	30-100	79	2	7.58(7.20)			

N\* = number of decomposition steps (1) [Fe(L)(H<sub>2</sub>O)<sub>2</sub>]Cl<sub>3</sub>.3H<sub>2</sub>O (2) [Cu(L)(H<sub>2</sub>O)<sub>2</sub>]Cl<sub>2</sub>.2H<sub>2</sub>O

### 11. Calculation of activation thermodynamic parameters

The thermodynamic activation parameters of decomposition processes of dehydrated complexes, namely activation energy (E\*),

enthalpy (ΔH\*), and Gibbs free energy changes of the decomposition (ΔG\*), were evaluated graphically by employing the Coats-Redfern relation<sup>[30]</sup>.

$$\log \left[ \frac{\log(W_f/W_f - W)}{T^2} \right] = \log \left[ \left( \frac{AR}{E^*} \right) \left( 1 - \frac{2RT}{E^*} \right) \right] - \frac{E^*}{2.303RT} \quad (1)$$

where  $W_f$  is the mass loss at the completion of the reaction,  $W$  is the mass loss up to temperature  $T$ ,  $R$  is the gas constant,  $E^*$  is the activation energy in  $\text{kJ}\cdot\text{mol}^{-1}$ ,  $q$  is the heating rate, and  $(1 - (2RT/E^*)) @ 1$ . A plot of the left-hand side of equation (1) against  $1/T$  gave a slope from which  $E^*$  was calculated and  $A$  (Arrhenius factor) was determined from the intercept. The entropy of

activation ( $\Delta S^*$ ), enthalpy of activation ( $\Delta H^*$ ), and the free energy change of activation ( $\Delta G^*$ ) were calculated using the following equations:

$$\Delta S^* = 2.30 [\log(Ah/kT)]R \quad (2)$$

$$\Delta H^* = E^* - RT \quad (3)$$

$$\Delta G^* = \Delta H^* - T\Delta S^* \quad (4)$$

**Table 5:** Thermodynamic data of the thermal decomposition of metal complexes of L

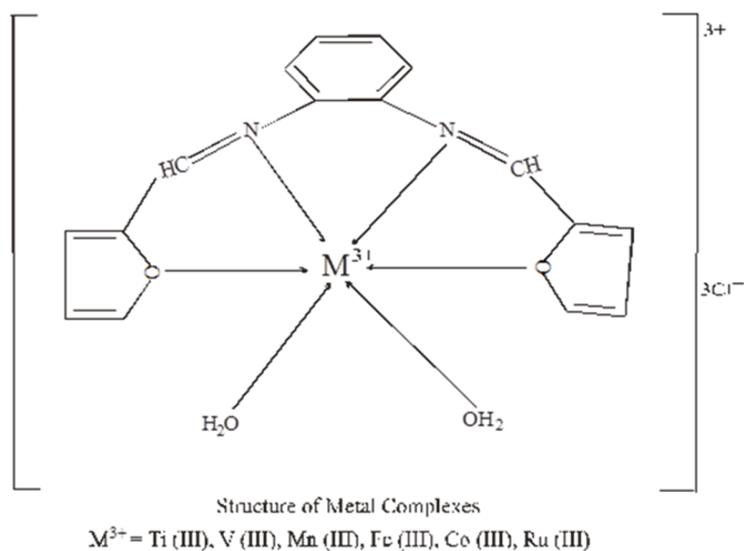
Compound	Decomp.	E*	A	DS*	DH*	DG*
	Temp.(C)	kJ mol <sup>-1</sup>	s <sup>-1</sup>	KJ mol <sup>-1</sup>	kJ mol <sup>-1</sup>	kJ mol <sup>-1</sup>
[Fe(L)(H <sub>2</sub> O) <sub>2</sub> ]Cl <sub>3</sub> .3H <sub>2</sub> O	30-130	35.73	1.23x10 <sup>5</sup>	-108	73.48	72.65
	130-220	49.14	4.05x10 <sup>7</sup>	-136	61.49	96.2
	220-430	93.34	4.51x10 <sup>10</sup>	-224	98.39	48.68
	570-700	119.54	6.23x10 <sup>9</sup>	-104.6	101.6	66.5
	820-960	135	5.01x10 <sup>10</sup>	-202.6	96.43	88.08
[Cu(L)(H <sub>2</sub> O) <sub>2</sub> ]Cl <sub>2</sub> .2H <sub>2</sub> O	30-120	80.8	4.21x10 <sup>10</sup>	-35.69	73.12	87.32
	120-210	145.7	8.69x10 <sup>14</sup>	-109.8	194.5	156
	210-450	223.7	5.89x10 <sup>14</sup>	-184.9	262.3	201.3
	500-800	267.2	4.01x10 <sup>10</sup>	-65.78	218.4	284.2

The data are summarized in Table-5. The activation energies of decomposition were in the range 55.42 – 350.6 kJ mol<sup>-1</sup>. The high values of the activation energies reflect the thermal stability of the complexes. The entropy of activation had negative values in all the complexes, which indicates that the decomposition reactions proceed with a lower rate than the normal ones.

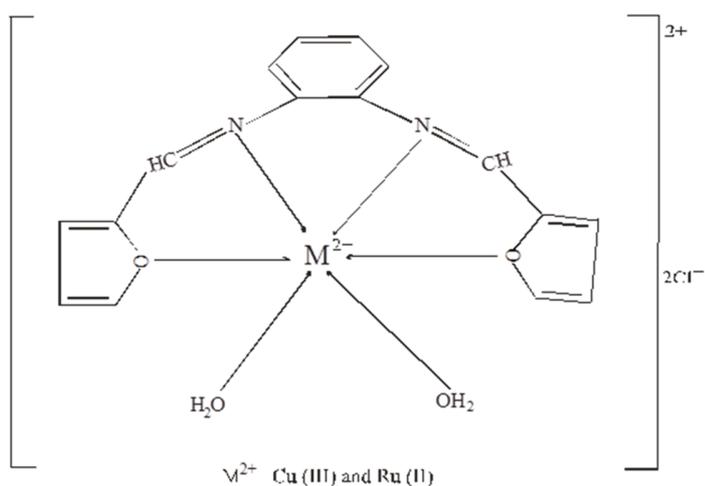
## 12. Conclusion

The structures of the complexes of Schiff bases L and complexes of Fe(III), Co (III), V (III), Cu

(II), Ru (III), Mn (III) and Vo (IV) ions were confirmed by elemental analyses, IR, NMR, molar conductance, magnetic, solid reflectance, UV-Vis, mass and thermal analysis data. Therefore, from the IR spectra, it is concluded that L behaves as a neutral tetradentate ligand, coordinated to the metal ions via azomethine N and furan O. On the basis of above observations and magnetic and solid reflectance measurements, an octahedral geometry may be proposed for all the synthesized complexes.



**Figure 2**



**Figure 3**

### 13. Biological Activity

In testing the antibacterial activity of these compounds we used more than one test organism to increase the chance of detecting the antibiotic potential of the tested materials. The sensitivity of a microorganism to antibiotics and other antimicrobial agents was determined by the assay plates, which were incubated at 28 °C for 2 days (for yeasts) and at 37 °C for 1 day (for bacteria). All of the tested compounds showed a remarkable biological activity against different types of Gram-positive and Gram-negative bacteria. The data are listed in Table-6. Upon comparison of the biological activity of the Schiff base and its metal complexes with the standard (Traivid and Tavinic), it is seen that the biological activity of L

are less than that of Tavinic, but higher than that of Traivid. For Schiff base (L) complexes, the biological activity of Fe (III), Co (III), Cu (II) and Ru (III) complexes is higher than that of the ligand and Traivid, while their activity is Fe(III), Co (III), Cu (II) and Ru (III) complexes is higher than that of the ligand and Traivid, while their activity is comparable with that of standard Travinic. The biological activity of the complexes follow the order Fe (III) = Co (III) = Cu (II) = Ru (III) > Mn (III) > Vo (IV) > Ni (II).

The importance of this lies in the fact that these complexes could reasonably be used for the treatment of some common diseases caused by E. coli, e.g., septicemia, gastroenteritis, urinary tract infections, and hospital-acquired infections<sup>[31]</sup>.

Table 6: Biological activity of L and its metal complexes

Sample	<i>Staphylococcus pyogenes</i>			<i>Pseudomonas aeruginosa</i>			Fungus ( <i>Candida</i> ) ( <i>Candida</i> )			Escherichia		
	5	2.5	1	5	2.5	1	5	2.5	1	5	2.5	1
L	++	++	+	++	+	+	+	-	-	++	+	-
[Fe(L)(H <sub>2</sub> O) <sub>2</sub> ]Cl <sub>3</sub> .3H <sub>2</sub> O	+++	++	+	++	++	+	+	+	-	++	++	+
[Co(L)]Cl <sub>3</sub> .H <sub>2</sub> O	+++	++	+	++	++	+	+	-	-	++	+	+
[VO(L)(H <sub>2</sub> O) <sub>2</sub> ]Cl <sub>2</sub> .4H <sub>2</sub> O	++	+	-	++	+	+	+	-	-	+++	++	+
[Cu(L)(H <sub>2</sub> O) <sub>2</sub> ]Cl <sub>2</sub> .2H <sub>2</sub> O	+++	++	++	+++	++	+	+	-	-	++	++	+
[Mn(L)(H <sub>2</sub> O) <sub>2</sub> ] Cl <sub>3</sub>	++	+	+	++	+	-	+	-	-	+++	++	+
[Ru(L)(H <sub>2</sub> O) <sub>2</sub> ]Cl <sub>3</sub>	+++	++	+	++	++	+	+	+	-	+++	++	+
Traivid	++	+	-	++	+	-	-	-	-	++	+	-
Tavinic	+++	++	+	+++	++	+	-	-	-	+++	++	+

The test was performed using the diffusion agar technique, Inhibition values = 0.1 – 0.5 cm beyond control = + Inhibition values = 0.6 – 1.0 cm beyond control = ++ Inhibition values = 1.1 – 1.5 cm beyond control = +++.

However, Fe (III), Cu (II), Ru (III), Co (III), VO (IV) and Cu (II) complexes of L ligand were specialized in inhibiting Gram positive bacterial strains (*Staphylococcus pyogenes* and *Pseudomonas aeruginosa*). The importance of this unique property of the investigated Schiff base complexes is that they could be administered safely for the treatment of infections caused by any of these particular strains. In addition, all metal complexes of L inhibit fungi at high concentration (5 mg/L), more so than the parent ligands and standards. Therefore, it is claimed here that such compounds might have a possible antitumor effect since Gram-negative bacteria are considered a quantitative microbiological method for testing beneficial and important drugs.

### 14. References

1. Patai S. The chemistry of Carbon Nitrogen double bond. John Wiley & Sons Ltd., London, 1970.
2. Yamada S, Coord Chem Rev 1999; 537:190 - 192.
3. Singh S, Das S, Dhakarey R. E-J Chem 2009; 6(1):99 - 105.
4. Raman N, Syed Ali, Fathima S, Dhaveethu RJ. Serbian Chem Soc 2008; 73(2):1063-1071.
5. Joshi N, Balasubramanian G, Gharat LA, PCT Int Appl WO 2006051390; Chem Abstr 2006; 144:488509.
6. Tangallaply RP, Lee REB, Lenaerts AJM, Lee RE. Bioorg Med Chem Litt 2006; 16:2584.

7. Srivastava V, Negi AS, Kumar JK, Faridi U, Sisodia BS, Darokar MP, Luqman S, Khaunja SPS. *Bioorg Med Chem Litt* 2006; 16:911.
8. Nagaraja GK, Kumaraswaney MN, Vaidya VP, Mahadevan KM. *ARKIVOC* (Geinesville, FL, united states) 2006; 10:1.
9. Shehata IA, *Saudi pharmaceutical journal* 2003, 11, 87; *Chem. Abstr.* 2004; 140, 357263.
10. Singh RV, *Synth. React. Inorg. Met-org Chem* 1986; 16:21-27.
11. Mohammad MA, El-Enamy MM, Basies EL. *Egypt J Pharm Sci* 1981; 22:9-15.
12. Scozzafava A, Menabuoni L, Mincione G, Supuran CT. *Bioorg. Med Chem Litt* 2001; 11:578-588.
13. Sondhi SM, Dinodia M, Kumar A. *Bioorg Med Chem* 2006; 14:4657.
14. Sondhi SM, Dinodia M, Singh J, Rani R. *Current bioactive compounds* 2007; 3:91.
15. Vogel AI. "Practical organic chemistry including quantitative organic analysis". Edn 3, Longmans, London, 1956, 854.
16. Feng D, Wang B. *Transition Met. Chem.* 18, 101 (13), (1993), M. Kumar, *Asian J Chem* 1994; 6:576 - 80.
17. Ibrahim ME, Ali AAH, Maher FMM. *J Chem Tech Biotechnol* 1992; 55, 217.
18. Sari N, Arsalan S, Logoglu E, Sakiyan Z. *J of Sci* 2003; 16:283.
19. Mohammad A, Shamim A. *oriental J C* 2011; 27(2):673-677.
20. Rahul KR, Poonam G, Shamim A. *Asian Journal of Chem* 2009; 21(8):6144-6148.
21. Bhadange GS, Mohod RB, Aswar AS. *Indian Journal of Chem* 2001; 40A:1110-1113.
22. Patel MM, Patel MR, Patel MN, Patel RP. *Indian J Chem Soc* 1981; 20A:6623.
23. Chaudhary CK, Chaudhary RK, Mishra LK. *J Indian Chem Soc* 2003; 80:693-695.
24. Mahesh K. Singh AK, Singh PK, Gupta J, Sharma LKI. *J Chem* 2002; 41:1385.
25. Karvembu R, Natrajan K. *Polyhedron* 2002; 21:219.
26. Pancholi HB, Patel MM. *J Polym Moter* 1996; 13:261.
27. Soliman AA, Linert W. *Thermochimica Acta* 1999; 333:67-75.
28. Kriza A, Voiculescu M, Nicolae A. *Analele Universitatii Bucurestii Chemie* 2002; 11:197-201.
29. Nag JK, Das D, De BB, Sinha C. *J Indian Chem Soc* 1998; 75:496-498.
30. El-sharief AMS, Ammar MS, Ammar YA, Zak ME. *Ind J Chem* 1983; 22B:700 - 704.
31. El-Sharief AMS, Ammar MS, Mohammad YA, *Egypt J Chem* 1984; 27:535-546.