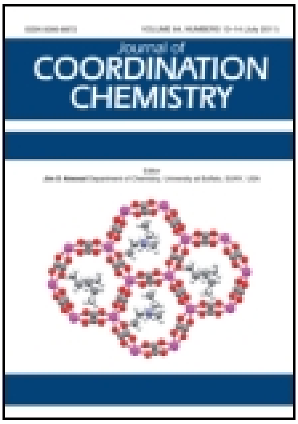
This article was downloaded by: [Renmin University of China]
On: 13 October 2013, At: 10:28
Publisher: Taylor & Francis
Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



Journal of Coordination Chemistry
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gcoo20

Synthesis, spectroscopic, thermal, and biological activities of mixed ligand complexes containing E-N′-(3,4,5-trimethoxybenzylidene)benzofuran-2-carbohydrazide and 2-aminothiophenol

M.B. Halli [a] & Vijayalaxmi B. Patil [a]

[a] Department of Chemistry , Gulbarga University , Gulbarga-585106, Karnataka, India

Published online: 28 Oct 2011.

To cite this article: M.B. Halli & Vijayalaxmi B. Patil (2011) Synthesis, spectroscopic, thermal, and biological activities of mixed ligand complexes containing E-N′-(3,4,5-trimethoxybenzylidene)benzofuran-2-carbohydrazide and 2-aminothiophenol, Journal of Coordination Chemistry, 64:21, 3740-3750, DOI: 10.1080/00958972.2011.630730

To link to this article: http://dx.doi.org/10.1080/00958972.2011.630730

PLEASE SCROLL DOWN FOR ARTICLE

Taylor & Francis makes every effort to ensure the accuracy of all the information (the "Content") contained in the publications on our platform. However, Taylor & Francis, our agents, and our licensors make no representations or warranties whatsoever as to the accuracy, completeness, or suitability for any purpose of the Content. Any opinions and views expressed in this publication are the opinions and views of the authors, and are not the views of or endorsed by Taylor & Francis. The accuracy of the Content should not be relied upon and should be independently verified with primary sources of information. Taylor and Francis shall not be liable for any losses, actions, claims, proceedings, demands, costs, expenses, damages, and other liabilities whatsoever or howsoever caused arising directly or indirectly in connection with, in relation to or arising out of the use of the Content.

This article may be used for research, teaching, and private study purposes. Any substantial or systematic reproduction, redistribution, reselling, loan, sub-licensing, systematic supply, or distribution in any form to anyone is expressly forbidden. Terms &

Journal of Coordination Chemistry
Vol. 64, No. 21, 10 November 2011, 3740–3750

Synthesis, spectroscopic, thermal, and biological activities of mixed ligand complexes containing E-N′-(3,4,5-trimethoxybenzylidene)benzofuran-2-carbohydrazide and 2-aminothiophenol

M.B. HALLI* and VIJAYALAXMI B. PATIL

Department of Chemistry, Gulbarga University, Gulbarga-585106, Karnataka, India

(*Received 8 August 2011; in final form 22 September 2011*)

Complexes [M(L)(L′)Cl · H_2O], where M = Co(II), Ni(II), Cu(II), Zn(II), Cd(II), and Hg(II), L = ligand derived from reaction between benzofuran-2-carbohydrazide and 3,4,5-trimethoxybenzaldehyde (TMeOBFC) and L′ = 2-aminothiophenol (2-atp), have been synthesized. The structures of the complexes have been proposed from analytical data, IR, UV-Vis, ^{1}H NMR, direct analysis in real time-mass spectra, ESR spectral data, magnetic, and thermal studies. The complexes are soluble in DMF and DMSO. Molar conductance values indicate that the complexes are non-electrolytes. Antibacterial and antifungal activities of the ligands and their metal complexes have been obtained against bacteria *Escherichia coli* and *Staphylococcus aureus* and against fungi *Aspergillus niger* and *Aspergillus flavus*.

Keywords: Benzofuran Schiff base; Mixed ligand complexes; Spectral studies; Thermal studies; Biological activity

1. Introduction

Schiff bases are an important class of ligands due to their synthetic flexibility, sensitivity toward the central metal, structural similarities with natural biological substances, and the presence of imine (–N=CH–) which assists in elucidating the mechanism of transformation and racemization in biological systems [1]. Schiff bases and their metal complexes have biological, clinical, analytical, and industrial applications, in addition to their important roles in catalysis and organic synthesis [2–9]. Nitrogen and sulfur donors play key roles in coordination at the active sites of numerous metallobiomolecules [10]. Transition metal complexes are of current interest because they can provide new materials with useful properties, such as magnetic exchange [11, 12], electrical conductivity [13], photoluminescence [14], nonlinear optical property [15], and antimicrobial activity [16].

---

*Corresponding author. Email: mbhalli@rediffmail.com

Journal of Coordination Chemistry
ISSN 0095-8972 print/ISSN 1029-0389 online © 2011 Taylor & Francis
http://dx.doi.org/10.1080/00958972.2011.630730

This study synthesizes Co(II), Ni(II), Cu(II), Zn(II), Cd(II), and Hg(II) complexes with ligand derived from benzofuran-2-carbohydrazide and 3,4,5-trimethoxybenzaldehyde (TMeOBFC) and 2-aminothiophenol (2-atp). The structures are proposed from analytical data, IR, UV-Vis, ^{1}H NMR, direct analysis in real time-mass spectra (DART-MS), ESR spectral data, magnetic, and thermal studies. The Schiff base and complexes were screened for antibacterial and antifungal activities.

2. Experimental

All chemicals used were of analytical reagent grade (AR) and of highest purity available. Benzofuran-2-carbohydrazide was synthesized according to the literature procedure [17]. Metal and chloride contents were determined as per Vogel's procedure [18].

2.1. *Synthesis of (E)-N′-(3,4,5-trimethoxybenzylidene)benzofuran-2-carbohydrazide [TMeOBFC]*

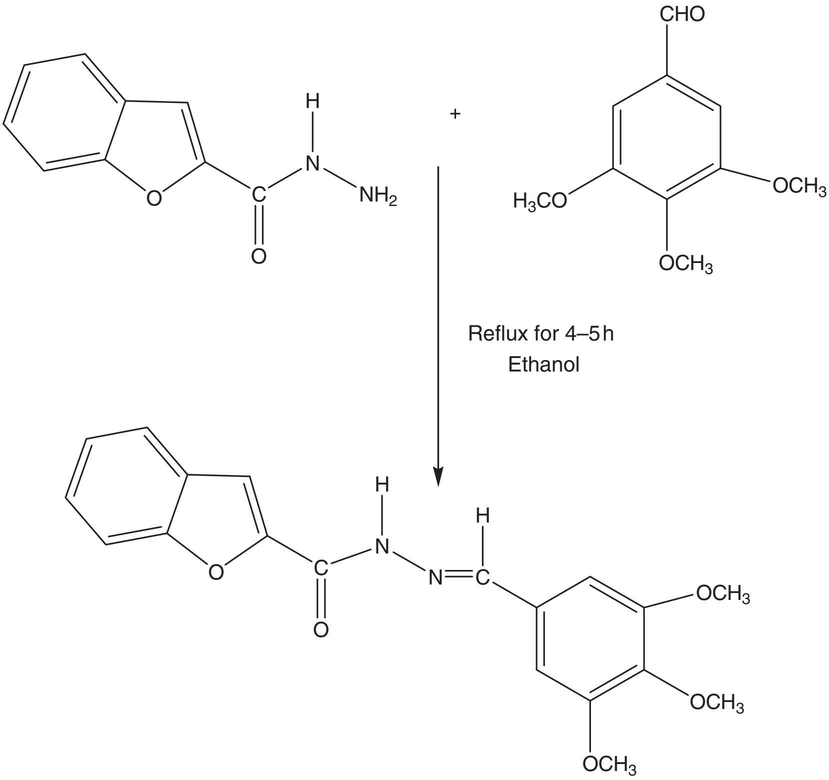
A solution of benzofuran-2-carbohydrazide (1.76 g, 0.01 mol) in ethanol (25 mL) was added to 3,4,5-trimethoxybenzaldehyde (1.96 g, 0.01 mol) in ethanol (20 mL) and refluxed on a water bath for 4–5 h. On partial removal of solvent and cooling to room temperature, the Schiff base was separated as yellowish crystalline solid, which was then filtered, washed with ethanol, and recrystallized from ethanol. The synthesis of the Schiff base is shown in scheme 1. $C_{19}H_{18}O_5N_2$ [TMeOBFC]: Mol. wt = 354, m.p. = 233°C, yield = 72%.

2.2. *Synthesis of metal(II) mixed ligand complexes*

An ethanolic solution (20 mL, 0.01 mol) of the appropriate metal chloride, MCl_2 (M = Co, 2.378 g; M = Ni, 2.377 g; M = Cu, 1.705 g; M = Zn, 1.363 g; M = Cd, 2.013 g; M = Hg, 2.715 g), was added to an ethanolic solution (30 mL) of TMeOBFC (3.54 g, 0.01 mol). An ethanolic solution (20 mL, 0.01 mol) of the 2-aminothiophenol (1.25 g) was added to the previous solution and the reaction mixture was refluxed for 3 h on a water bath and then aqueous alcoholic solution of sodium acetate was added to the mixture to adjust pH to 6–7 and further refluxed for an hour. The precipitated complexes were filtered and washed with distilled water, then with alcohol and finally dried in vacuum over fused calcium chloride (yield = 56–62%).

2.3. *Physical measurements*

Carbon, hydrogen, and nitrogen analysis were carried out microanalytically on a Perkin Elmer 240C at the Central Drug Research Institute (CDRI) Lucknow. IR spectra of the Schiff base and complexes were recorded in KBr pellets from 4000 to 350 cm^{-1} on a Perkin Elmer 783 FT-IR spectrophotometer. Electronic spectra of Co(II), Ni(II), and Cu(II) complexes were recorded on an Elico-SL-164 double beam UV-Vis



Scheme 1. Synthesis of TMeOBFC.

spectrophotometer from 200 to 1100 nm in DMF (10^{-3} mol L^{-1}). ^{1}H NMR spectra were recorded in DMSO-d_6 on a Bruker 300 MHz spectrophotometer using TMS as an internal standard. The ESR spectrum of the Cu(II) complex in polycrystalline state was recorded on a Varian-E-4X band EPR spectrophotometer using TCNE as "*g*" marker ($g = 2.00277$) at room temperature. DART-MS were recorded on a JEOL-AccuTOF JMS-T100LC Mass Spectrometer having a DART source. Dry helium was used with 4 LPM flow rate for ionization at 350°C, the orifice 1 set at 28 V. Thermal analyses were measured from room temperature to 1000°C in N_2 on a Perkin Elmer, Diamond TG/DTA model thermal analyzer at STIC, Cochin, with a heating rate of 10°C min^{-1}. Molar conductivity measurements were recorded on an Elico CM-180 conductivity bridge in DMF (10^{-3} mol L^{-1}) using a dip-type conductivity cell fitted with a platinum electrode and the magnetic susceptibility measurements were made at room temperature on a Gouy balance using $Hg[Co(NCS)_4]$ as the calibrant.

2.4. *Biological activities*

The Schiff base and Co(II), Ni(II), Cu(II), Zn(II), Cd(II), and Hg(II) complexes have been studied for their antibacterial and antifungal activities by the agar diffusion method in DMF against *Escherichia coli* and *Staphylococcus aureus* bacteria and *Aspergillus niger* and *Aspergillus flavus* fungi [19, 20].

2.5. *Antibacterial screening*

Media used: Peptone 10 g, NaCl 10 g and yeast extract 5 g, Agar 20 g in 1000 mL of distilled water.

Initially, stock cultures of *E. coli* and *S. aureus* were revived by inoculating in broth media and grown at 37°C for 18 h. The agar plates of the above media were prepared and wells were made in the plate. Each plate was inoculated with 18 h old cultures and spread evenly on the plate. After 20 min, the wells were filled with test solutions. Gentamycin was used as the standard antibacterial drug. All the plates were incubated at 37°C for 24 h and the diameters of inhibition zones were noted.

2.6. *Antifungal screening*

Media used: Potato Dextrose Agar (PDA). 250 g of peeled potato were boiled for 20 min and squeezed and filtered. To this filtrate 20 g of dextrose was added and the volume was made up to 1000 mL by distilled water.

Initially, stock cultures of *A. flavus* and *A. niger* were revived by inoculating in broth media and grown at 37°C for 48 h. The agar plates of the above media were prepared and wells were made in the plate. Each plate was inoculated with 18 h old cultures and spread evenly on the plate. After 20 min, the wells were filled with test solutions. Fluconazole was used as the standard antifungal drug. All the plates were incubated at 37°C for 48 h and the diameters of inhibition zones were noted.

3. Results and discussion

Analytical data show that all of the complexes have 1 : 1 : 1 (metal : ligand : ligand) stoichiometry (table 1). The molar conductance values (9.23–14.16 $\Omega^{-1}\,cm^2\,mol^{-1}$) are too low to account for dissociation of the complexes in DMF, indicating non-electrolytes [21]. All the complexes are light in color, stable, non-hygroscopic and possess high melting points. The complexes are insoluble in common organic solvents but soluble in DMF and DMSO.

3.1. *Magnetic properties*

Magnetic susceptibility measurements at room temperature show paramagnetism for Co(II), Ni(II), and Cu(II) complexes and μ_{eff} values are listed in table 1. The Co(II) complex is 4.86 BM, suggesting octahedral geometry [22, 23]. The Ni(II) complex is 2.94 BM, indicating octahedral Ni(II) [24, 25]. The observed magnetic moment for the Cu(II) complex is 1.76 BM, suggesting a distorted octahedral geometry [26].

Table 1. Elemental analysis, molar conductance, and magnetic susceptibility data for TMeOBFC complexes.

Molecular formula of Schiff base/ Complexes	Mol. weight	C%		H%		N%		M%		Cl%		Λ_M[a]	μ_{eff} (BM)
		Found	Calcd	Found	Calcd	Found	Calcd	Found	Calcd	Found	Calcd		
$C_{19}H_{18}O_5N_2$ TMeOBFC (L)	354	64.21	64.41	4.82	5.08	7.76	7.91	–	–	–	–	–	–
$[Co(L)(L')Cl\cdot H_2O]$	590.94	50.68	50.81	4.23	4.43	6.94	7.11	9.85	9.97	5.82	6.00	11.45	4.86
$[Ni(L)(L')Cl\cdot H_2O]$	590.70	50.66	50.83	4.21	4.44	6.92	7.11	9.81	9.94	5.78	6.00	12.14	2.94
$[Cu(L)(L')Cl\cdot H_2O]$	595.55	50.23	50.42	4.18	4.40	6.89	7.06	10.49	10.67	5.76	5.95	11.33	1.76
$[Zn(L)(L')Cl\cdot H_2O]$	597.40	50.09	50.26	4.16	4.39	6.86	7.03	10.78	10.95	5.72	5.93	10.21	–
$[Cd(L)(L')Cl\cdot H_2O]$	644.42	46.47	46.60	3.92	4.07	6.40	6.52	17.23	17.44	5.23	5.50	14.16	–
$[Hg(L)(L')Cl\cdot H_2O]$	732.60	40.78	40.99	3.40	3.58	5.62	5.74	27.21	27.38	4.61	4.84	9.23	–

[a] Molar conductance values in $\Omega^{-1}\,cm^2\,mol^{-1}$.

Table 2. Electronic spectral bands and ligand field parameters of the Co(II), Ni(II), and Cu(II) complexes in DMF (10^{-3} mol L^{-1}).

Complexes	Transitions (cm^{-1}) ν_1[a]	ν_2	ν_3	Dq (cm^{-1})	B′ (cm^{-1})	β	β%	ν_2/ν_1	LFSE (k.cal)
$[Co(L)(L')Cl \cdot H_2O]$	7441	16021	20641	858	955	0.983	1.648	2.153	14.708
$[Ni(L)(L')Cl \cdot H_2O]$	9610	15621	26123	961	861	0.828	17.212	1.625	32.948
$[Cu(L)(L')Cl \cdot H_2O]$	12630–17084			1486	–	–	–	–	25.474

[a]Calculated values.

3.2. *Electronic spectral studies*

Electronic spectra of the Co(II), Ni(II), and Cu(II) complexes were recorded for freshly prepared solution in DMF (10^{-3} mol L^{-1}) at room temperature and their spectral data are presented in table 2. The Co(II) complex shows two bands at 16021 and 20641 cm^{-1}, assignable to ${}^4T_{1g}$ (F) → ${}^4A_{2g}$ (F) (ν_2) and ${}^4T_{1g}$ (F) → ${}^4T_{1g}$ (P) (ν_3) transitions, respectively, in an octahedral environment [27]. The ν_1 band could not be observed; however, it was calculated using an equation suggested by Underhill and Billing [28].

The Ni(II) complex exhibits two bands at 15,621 and 26,123 cm^{-1} assignable to ${}^3A_{2g}$ (F) → ${}^3T_{1g}$ (F) (ν_2) and ${}^3A_{2g}$ (F) → ${}^3T_{1g}$ (P) (ν_3), respectively. The ν_1 could not be observed due to limited range of the instrument, but was calculated by using a band fitting procedure [28].

The Cu(II) complex exhibits a single broad asymmetric band at 12,630–17,084 cm^{-1}. The broadness indicates that the three expected transitions ${}^2B_{1g} \rightarrow {}^2A_{1g}$ (ν_1), ${}^2B_{1g} \rightarrow {}^2B_{2g}$ (ν_2), and ${}^2B_{1g} \rightarrow {}^2E_g$ (ν_3) are similar in energy and give one broad band. The broadness may be due to dynamic Jahn–Teller distortion. All of these data suggest a distorted octahedral geometry around Cu(II).

The octahedral geometry [29] is further supported by the values of ligand field parameters such as Racah inter-electronic repulsion parameter (B′), covalency factor (β), and ligand field stabilization energy (LFSE) [30]. The B′ values for the complexes were lower than free ion values, an indication of orbital overlap and delocalization of d-orbitals. The β values obtained are less than unity suggesting considerable covalent character for the metal–ligand bonds. The β value for Ni(II) complex is less than the Co(II) complex, indicating more covalency of the M–L bond [31].

3.3. *IR spectral studies*

IR spectra of the ligand and complexes are complex. It is not possible to assign all the bands, however, some of the important vibrational stretching bands are assigned on the basis of the reports available in the literature.

TMeOBFC shows medium broad bands at 3448 and 3216 cm^{-1} due to ν_{asym} and ν_{sym} of secondary amide of hydrazine. These bands shift to higher wavenumber by 6–15 cm^{-1} in the complexes, showing non-involvement of "N" of NH in bonding with metal [32]. Strong bands at 1695 cm^{-1} and 1626 cm^{-1} are assigned to ν(C=O) and ν(C=N), respectively, in free ligand. These bands shift to lower wavenumber by 23–51 cm^{-1} in spectra of complexes indicating coordination through oxygen of C=O and nitrogen of –N=CH– [33, 34]. The band at 1031 cm^{-1} is assigned to ν(N–N) of hydrazine which shifts to higher wavenumber by 10–17 cm^{-1} in the metal complexes, confirming bonding through one nitrogen of hydrazine [35].

2-Aminothiophenol shows a broad band at 3372 cm^{-1} due to ν(NH) of the primary amine. In all metal complexes the band shifts to lower wavenumber, indicating nitrogen of amine coordination with metal. The strong band at 2560 cm^{-1} is assigned to –SH stretch. The disappearance of this band on complexation indicates deprotonation of the thiol upon coordination [36].

The metal-ligand vibrations are difficult to assign since they are sensitive to both the ligand and the metal. However, non-ligand new bands appear at 532–521 cm^{-1} and 465–402 cm^{-1}, assigned to ν(M–O) and ν(M–N) [37, 38]. Weak bands at 395–366 cm^{-1} are assigned to ν(M–Cl). Bands at 375–330 cm^{-1} are due to metal–sulfur bond formation. Coordinated water was suggested by the broad band at 3450–3550 cm^{-1} in IR spectra of all complexes.

3.4. ^{1}H NMR spectral studies

^{1}H NMR spectra of TMeOBFC and Zn(II) and Cd(II) complexes were recorded in DMSO-d_6. The signal at δ (12.13) (s, 1H) is assigned to amide proton (–CONH–) and the signal at δ (8.44) (s, 1H) is assigned to azomethine proton (–N=CH–). Signals due to (–CONH–) are shifted downfield in the spectra of Zn(II) δ (12.54) (s, 1H) and Cd(II) δ (12.48) (s, 1H) complexes, indicating coordination of oxygen of –CONH–. The azomethine protons shift downfield δ (8.69, 8.74) (s, 1H) supporting coordination of the –N=CH- with metal. Aromatic protons at δ (6.94 – 7.83) shift downfield in the complexes. Signals at δ (3.29) (s, 3H, $-OCH_3$), δ (3.67) (s, 3H, $-OCH_3$) and δ (3.91) (s, 3H, $-OCH_3$) are due to protons of three $-OCH_3$ groups present on the phenyl. Thus ^{1}H NMR spectral observations supplement the assigned geometry.

2-Aminothiophenol signals at δ (3.00) (s, 1H) and δ (4.00) (s, 2H) were assigned to thiol and primary amine. The signal due to thiol disappears in complexes indicating deprotonation of the thiol upon coordination. The signal due to protons of primary amine shift downfield in the spectra of Zn(II) and Cd(II) complexes δ (6.48–6.65) (s, 2H) indicating the involvement of nitrogen of amino group in bonding with metal. Signals at δ (3.95) (s, 2H), and δ (3.98) (s, 2H) are due to coordinated water in the complexes [39].

3.5. Mass spectral studies

The DART-mass spectrum of TMeOBFC shows a molecular ion peak at m/z 355, one mass unit more than the molecular weight of the Schiff base. The DART-mass spectrum of the $[Ni(L)(L')Cl \cdot H_2O]$ showed a molecular ion peak at m/z 591, which is same as that of the molecular weight of the complex. Thus mass spectral studies support the proposed composition.

3.6. ESR spectrum of Cu(II) complex

The ESR spectrum of the copper(II) complex in a polycrystalline state has been recorded at room temperature. The $g_{\parallel}$ and $g_{\perp}$ values are 2.267 and 2.059, respectively; g_{av} was calculated to be 2.131. The spectra have asymmetric bands with

$g_{\|} > g_{\perp} > 2.00277$ (TCNE), indicating that the unpaired electrons lie predominantly in the $d_{x^2-y^2}$ orbital with possibly mixing of d_{z^2} because of low symmetry [40]. The axial symmetry parameter "G" is determined as $G = (g_{\|} - 2.00277)/(g_{\perp} - 2.00277) = 4.693$, which is more than 4 suggesting the absence of exchange coupling between Cu(II) centers in the solid state [41]. The molecular-orbital coefficient parameters, α^2, a measure of the covalency of the in-plane σ-bonding between the 3d and ligand orbitals and β^2, the covalency of the in-plane π-bonding, were calculated employing the equations,

$$\alpha^2 = (A_{\|}/0.036) + (g_{\|} - 2.00277) + 3/7(g_{\perp} - 2.00277) + 0.04,$$
$$\beta^2 = (g_{\|} - 2.00277)E/ - 8\lambda\alpha^2,$$

where $\lambda = -828\,\mathrm{cm}^{-1}$ for free Cu(II) and E is the electronic transition energy. The α^2 and β^2 values are 0.889 and 0.945, respectively. The lower value of α^2 compared to β^2 indicates σ-bonding in plane is more covalent than in-plane π-bonding. These data are in agreement with the proposed geometry [42, 43].

3.7. *Thermal studies*

The thermal behavior of the complexes are all the same; $[Zn(L)(L')Cl \cdot H_2O]$ is used as a representative example (Supplementary material). The thermal decomposition takes place in three steps as indicated by DTG peaks around 240–270°C, 300–380°C, and 450–880°C, corresponding to mass loss of coordinated water and chloride in the first step, 2-atp and TMeOBFC in the second and third steps, respectively, leaving metal oxide residue [44–46]. The proposed chemical changes with temperature range and percentage of metal oxide obtained are given in table 3.

3.8. *Antibacterial and antifungal activities*

The compounds were tested for their activity against two bacteria *E. coli* and *S. aureus* and against two fungi *A. niger* and *A. flavus* by the agar diffusion method. The results are summarized in table 4 along with standards. Comparative study of the ligands and their complexes indicates complexes have higher antimicrobial activity than the free ligands [47, 48]. From table 4 Cu(II), Zn(II), and Cd(II) complexes are more potent than other complexes. Results described by Nishat *et al.* [49] show comparatively high activities, while the microbial action of Kumarguru and Santha kumar [50] correlates with our results. Antimicrobial activity of all the compounds was increased on coordination [42].

4. Conclusion

We report complexes $[M(L)(L')Cl \cdot H_2O]$, where M = Co(II), Ni(II), Cu(II), Zn(II), Cd(II), and Hg(II), L = TMeOBFC, and L′ = 2-atp. The Schiff base TMeOBFC is a neutral bidentate ligand coordinating through azomethine nitrogen and oxygen of –CONH–; 2-atp is bidentate coordinating through "N" of primary amine and "S"

Table 3. Thermogravimetric data of the complexes.

Complexes	Decomposition temperature (°C)	Mass loss (%) Found	Mass loss (%) Calcd	Metal oxide (%) Found	Metal oxide (%) Calcd	Assignment
[Co(L)(L′)Cl · H_2O]	240–265	8.76	9.05	12.23	12.68	Loss of coordinated water molecule and chloride ion
	310–380	20.45	20.98			Loss of secondary ligand
	480–820	59.52	59.90			Loss of TMeOBFC
[Ni(L)(L′)Cl · H_2O]	245–270	8.79	9.05	12.21	12.64	Loss of coordinated water molecule and chloride ion
	315–375	20.58	20.99			Loss of secondary ligand
	460–840	59.65	59.93			Loss of TMeOBFC
[Cu(L)(L′)Cl · H_2O]	250–270	8.64	8.98	12.99	13.36	Loss of coordinated water molecule and chloride ion
	300–370	20.69	20.82			Loss of secondary ligand
	465–790	59.21	59.44			Loss of TMeOBFC
[Zn(L)(L′)Cl · H_2O]	240–270	8.60	8.96	13.21	13.62	Loss of coordinated water molecule and chloride ion
	300–360	20.42	20.75			Loss of secondary ligand
	450–880	58.84	59.25			Loss of TMeOBFC
[Cd(L)(L′)Cl · H_2O]	240–265	7.96	8.30	19.58	19.92	Loss of coordinated water molecule and chloride ion
	320–380	18.89	19.24			Loss of secondary ligand
	470–860	54.65	54.93			Loss of TMeOBFC
[Hg(L)(L′)Cl · H_2O]	245–265	6.92	7.30	29.23	29.60	Loss of coordinated water molecule and chloride ion
	310–365	16.58	16.93			Loss of secondary ligand
	460–800	48.05	48.32			Loss of TMeOBFC

Table 4. Antimicrobial activities of the ligands and their complexes.

	Zone of inhibition in mm			
	Bacteria		Fungi	
Schiff base/Complexes	*E. coli*	*S. aureus*	*A. niger*	*A. flavus*
TMeOBFC (L)	11	12	14	16
2-atp (L′)	12	14	13	18
[Co(L)(L′)Cl · H_2O]	16	15	16	18
[Ni(L)(L′)Cl · H_2O]	15	14	17	17
[Cu(L)(L′)Cl · H_2O]	18	19	17	20
[Zn(L)(L′)Cl · H_2O]	17	19	19	19
[Cd(L)(L′)Cl · H_2O]	18	20	20	21
[Hg(L)(L′)Cl · H_2O]	17	16	18	17
Gentamycin	20	22	–	–
Fluconazole	–	–	22	23

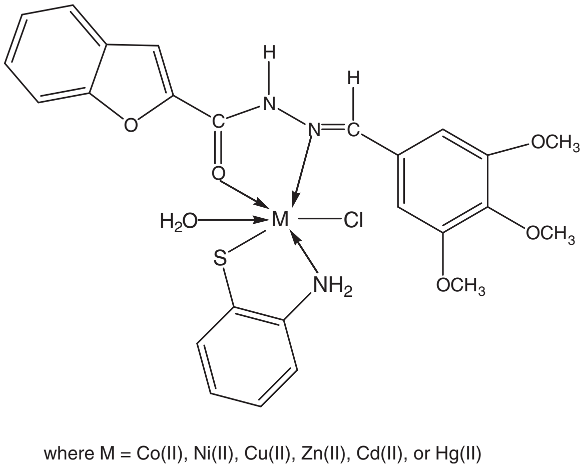


Figure 1. Suggested structures of metal complexes of TMeOBFC and 2-atp.

of –SH. Based on analytical data, spectral, and thermal studies we propose octahedral structures to all complexes (figure 1). Biological activity results show that metal complexes are more active than ligands.

Acknowledgments

The authors are grateful to the Chairman, Department of Chemistry, Gulbarga University, Gulbarga for encouragement and facilities. One of the authors (VBP) thanks UGC New Delhi for UGC Research Fellowship for meritorious students under RFSMS Scheme.

References

[1] N. Nahid, A.K. Shamim, P. Shadma, R. Raza. *J. Coord. Chem.*, **63**, 3944 (2010).
[2] E. Ispir. *Phosphorus, Sulfur, Silicon*, **184**, 3160 (2009).
[3] P.M. Alex, K.K. Aravindakshan. *Synth. React. Inorg. Met.-Org. Chem.*, **39**, 718 (2009).
[4] N.S. Youssef, E.A. El-Zahany, N. Barsoum, M.A. El-Seidy. *Transition Met. Chem.*, **34**, 905 (2009).
[5] P. Ramakanth, P. Ali, J.S. Meshram. *J. Coord. Chem.*, **62**, 4009 (2009).
[6] A.M. Amado, P.J. Ribeiro-Claro. *Inorg. Biochem.*, **98**, 561 (2004).
[7] J. Park, Y. Chung, Y. Suh, H. Rhee. *Catal. Today*, **93–95**, 445 (2004).
[8] M. Asadi, S. Esmaielzadeh, K. Mohammadi. *Phosphorus, Sulfur, Silicon*, **185**, 1445 (2010).
[9] A.S. Ramasubramanian, B.R. Bhat, R. Dileep. *J. Coord. Chem.*, **63**, 3108 (2010).
[10] A.A. Nejo, G.A. Kolawole, M.C. Dumbeley, A.R. Opoku. *J. Coord. Chem.*, **63**, 4367 (2010).
[11] R.C. Maurya, P. Sharma, D. Sutradhar. *Synth. React. Inorg. Met.-Org. Chem.*, **33**, 669 (2003).
[12] Y.T. Li, C.W. Yan, C.Y. Zhu, H.S. Guan. *Synth. React. Inorg. Met.-Org. Chem.*, **34**, 1165 (2005).
[13] Y. Aydogdu, F. Yakuphanoglu, A. Aydogdu, E. Cukurovah. *Mater. Lett.*, **57**, 3755 (2003).
[14] S.H. Ramadan, H.K. Fun, B.K. Ghosh. *Polyhedron*, **24**, 3091 (2005).
[15] H.Y. Bie, J.H. Yu, Q.J. Xu, Y. Li, Y.B. Cui, Y. Zhang, Y.H. Sun, L.Y. Pan. *J. Mol. Struct.*, **660**, 107 (2003).

[16] X. Xu, T. Xu, J. Gao, M. Wang, S. Niu, S. Ni, G. Xu. *Synth. React. Inorg. Met.-Org. Chem.*, **36**, 681 (2006).

[17] Y. Kawas, M. Nakayama, P. Tamatskuri. *Bull. Chem. Soc. Japan*, **35**, 149 (1962); *Chem. Abstr.*, **57**, 2204 (1962).

[18] A.I. Vogel. *A Text Book of Quantitative Inorganic Analysis*, 3rd Edn, Longman ELBS, London (1968).

[19] E.J. Threlfall, I.S.T. Fisher, L. Ward, H. Tschape, P. Gernersmidt. *Microb. Drug Resist.*, **5**, 195 (1999).

[20] J.F. Prescott, J.D. Baggot, R.D. Walker (Eds). In *Antimicrobial Therapy in Veterinary Medicine*, pp. 12–26, Iowa State University Press, Ames, IA (2000).

[21] W.J. Geary. *Coord. Chem. Rev.*, **7**, 81 (1971).

[22] B.N. Figgis, J. Lewis. In *Progress in Inorganic Chemistry*, F.A. Cotton (Ed.), Interscience, New York (1964).

[23] N.N. Greenwood, A. Earnshaw. *Chemistry of the Elements*, 2nd Edn, p. 1132, Butterworth Heimemann, Oxford (1997).

[24] T.A. Khan, S. Naseem, Y. Azim, S. Parveen, M. Shakir. *Transition Met. Chem.*, **32**, 706 (2007).

[25] A. Earnshaw. *Introduction to Magnetochemistry*, Vol. 34, Academic Press, London (1968).

[26] D.W. Smith. *Inorg. Chem.*, **5**, 2236 (1966).

[27] A.B.P. Lever. *Inorganic Electronic Spectroscopy*, Elsevier, New York (1984).

[28] A.E. Underhill, D.E. Billing. *Nature*, **210**, 834 (1966).

[29] C.J. Balhausen. *Introduction of Ligand Field Theory*, McGraw-Hill, New York (1962).

[30] D.N. Satyanarayana. *Electronic Absorption Spectroscopy and Related Techniques*, University Press India Limited, New Delhi (2001).

[31] K. Shivakumar, Shashidhar, P. Vithal Reddy, M.B. Halli. *J. Coord. Chem.*, **61**, 2274 (2008).

[32] K. Nakamoto. *Infrared Spectra of Inorganic and Coordination Compounds*, Wiley, New York (1970).

[33] L.J. Bellamy, *Advances in Infrared Group Frequencies*, Vol. 2, Methuen, London (1961).

[34] J.R. Ferraro. *Low Frequency Vibrations of Inorganic and Coordination Compounds*, Plenum Press, New York (1971).

[35] C.N.R. Rao. *Chemical Applications of Infrared Spectroscopy*, Academic Press, New York (1963).

[36] M.A. Ali, M. Nazimuddin, R. Shaha, J. Ray, J. Butcher, C. Bryan. *Polyhedron*, **17**, 3955 (1998).

[37] N.S. Biradar, V.H. Kulkarni. *J. Inorg. Nucl. Chem.*, **33**, 2451 (1971).

[38] K. Nakamoto. *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, 4th Edn, Wiley & Sons, New York (1986).

[39] K.S. Abou-Melha, H. Faruk. *J. Iran. Chem. Soc.*, **5**, 122 (2008).

[40] D. Kivelson, R. Neiman. *J. Chem. Phys.*, **35**, 149 (1961).

[41] B.J. Hathway. *Struct. Bond.*, **14**, 60 (1973).

[42] N. Raman, A. Sakthivel, R. Jeymurugan. *J. Coord. Chem.*, **63**, 4380 (2010).

[43] P. Bindu, M.R. Prathachandra Kurup, T.R. Stayakerty. *Polyhedron*, **18**, 321 (1999).

[44] A.D. Kulkarni, G.B. Bagihalli, S.A. Patil, P.S. Badami. *J. Coord. Chem.*, **62**, 3060 (2009).

[45] M.P. Sathisha, S. Budagumpi, N.V. Kulkarni, G.S. Kurdekar, V.K. Revankar, K.S.R. Pai. *Eur. J. Med. Chem.*, **45**, 106 (2010).

[46] G.J. Kharadi, K.D. Patel. *J. Therm. Anal. Calorim.*, **96**, 1019 (2009).

[47] Z.H. Chohan, C.T. Supuran, A. Scozzafava. *J. Enzyme Inhib. Med. Chem.*, **19**, 79 (2004).

[48] Z.H. Chohan, M. Praveen. *Appl. Organomet. Chem.*, **15**, 617 (2001).

[49] N. Nishat, S. Parveen, S. Dhyani, Asma. *J. Coord. Chem.*, **62**, 1091 (2009).

[50] N. Kumarguru, K. Santhakumar. *J. Coord. Chem.*, **62**, 3500 (2009).