Asian Journal of Chemistry; Vol. 34, No. 2 (2022), 311-318

ASIAN JOURNAL OF CHEMISTRY

https://doi.org/10.14233/ajchem.2022.23508

Bonding Ability of Isopthalic Acid-*bis*(thiosemicarbozone) to Manganese and Cobalt Metal Ions: Preparation, Spectral Investigation, Computational and *in vitro* Antipathogenic Screening

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Received: 31 August 2021; *Accepted*: 11 October 2021; *Published online*: 11 January 2022; AJC-20653

Manganese and cobalt complexes have been designed and prepared with a tetradentate ligand *i.e*. isopthalic acid-*bis*(thiosemicarbozone) (IPBT), which bind to metal ions *via* donor atoms present in ligand. Different spectroscopic techniques *viz*. nuclear magnetic resonance, infrared, mass, electronic spin resonance and analytical studies have been used to determine the chemical composition of synthesized IPBT and its Mn(II) and Co(II) complexes. The spectroscopic data exposed that IPBT behaves in a tetradentate (N_2S_2) mode by having ability to bind with metal ions through N_2S_2 atoms. An octahedral structure for manganese and cobalt complexes has been suggested on the basis of spectroscopic as well as analytical studies. The ligand (IPBT) and its metal(II) complexes have been screened to determine their antipathogenic activity against some selective microorganisms *S. aureus*, *P. aeruginosa*, *E. coli*, *A. niger*, *M. phasolina* and *P. glomerata*. In this experimental work, well diffusion and poisoned food techniques have been introduced for screening purpose and as standard drugs neomycin and chlorothalonil have been used. Data for antipathogenic screening exposed that metal complexes exerted higher activity towards all examined microbes (bacteria and fungi) even than ligand.

Keywords: Tetradentate ligand, Isopthalic acid, Metal complexes, Antimicrobial screening, Poisoned food method.

INTRODUCTION

Over the last decade, in the field of coordination chemistry, there has been rising alertness and attention to study the role of a broad range of inorganic elements such as transition metal ions and organic ligands, which contain donor atoms *i.e*. nitrogen, oxygen and sulphur [1]. Metal ions are vital factor in the structural association with biomolecules and operating functional processes in the genetic and metabolic system [2]. Transition metal complexes with ligands play an important role in biological systems [3]. Ligands which contain thiosemicarbazide moiety have emerged as the most preferred compounds [4-6]. Thiosemicarbazide is a privileged moiety with significant biological properties such as antimicrobial [7-11], anticancer [12, 13], anti-tumor [14] DNA binding and DNA cleavage [15], *etc*.

Moreover, tetradentate ligands, which have thiosemicarbazide in their structure and self possessed of nitrogen and sulphur donor atom framework have been acknowledged as important chelates, which have significance applications in various fields such as biological, polymer, sensor, dyes, catalytic, *etc*. [16-18]. Form the literature survey, it has been also resulted out that not only these free ligands but also their manganese and cobalt complexes also exhibited an essential role in the field of biological activities [19,20]. It has been observed that metal complexes of ligands exhibited higher activity or more inhibition against the growth of microorganism comparatively free ligands [21,22]. From a long time, the organic frame work for nitrogen and sulphur donor atoms containing ligands had been prepared by use of thiosemicarbozide as an amine moiety [23]. Keeping in mind these significance applications of these type of comp-

ounds, we have designed, synthesized, characterized and evaluated for antipathogenic screening to isopthalic acid-*bis*(thiosemicarbozone) (IPBT) and its manganese and cobalt complexes.

EXPERIMENTAL

AR grade chemicals and solvents were used in the present work. Elemental analysis (CHN) was done on Carlo-Erba 1106 instrument. In the region of 4000-400 cm^{-1} IR spectra were recorded in KBr pellet and Shimardzu UV-Vis. mini-1240 spectrophotometer has been used to record electronic spectra. By using Gouy balance with $CuSO_4 \cdot 5H_2O$ magnetic moment was calculated for complexes. Electron spin resonance spectral study has been done by using E4-electron spin spectrometer at SAIF, IIT Bombay and Bruker Advanced DPX-300 spectrometer is used for proton nuclear magnetic resonance of IPBT its complexes. Hyperchem. 7.51 verion is applied for the computational study. JMS-DX-303 mass spectrometer has been used for recording mass spectrum.

Synthesis of ligand [Isopthalicacid-*bis*(thiosemicarbazone) (IPBT)]: The ligand has been synthesized by mixing isopthalic acid (1 mol) and thiosemicarbazide (2 mol) as reactants in ethanolic medium. This reaction content was refluxed for 5 h at about 80-82 ºC with continuous stirring on a magnetic stirrer. Now the reaction solution is cooled at room temperature and then allowed to cool overnight at 0 ºC. After cooling, white precipitate obtained which was filtered and by using cold distilled water and ethanol washing procedure had been performed. After washing, product was dried under vacuum over P_4O_{10}. The general route for the synthesis of IPBT is shown in **Scheme-I**.

Synthesis of manganese and cobalt complexes: Cobalt and manganese complexes were synthesized by following condensation reactions *i.e*. synthesized IPBT (0.001 mol) dissolved in ethanol and refluxed with alcoholic solution of corresponding metal salts (0.001 mol) *i.e.* $Co(CH_3COO)_2 \cdot H_2O$, $CoCl_2 \cdot 6H_2O$, $MnCl_2 \cdot 4H_2O$ and $Mn(CH_3COO)_2 \cdot 4H_2O$ with constant stirring. Progress of the reaction *i.e*. conversion of reactants into product was confirmed by TLC method. On cooling the coloured to colourless complexes have been obtained and filtered off, washed with absolute ethanol and dried.

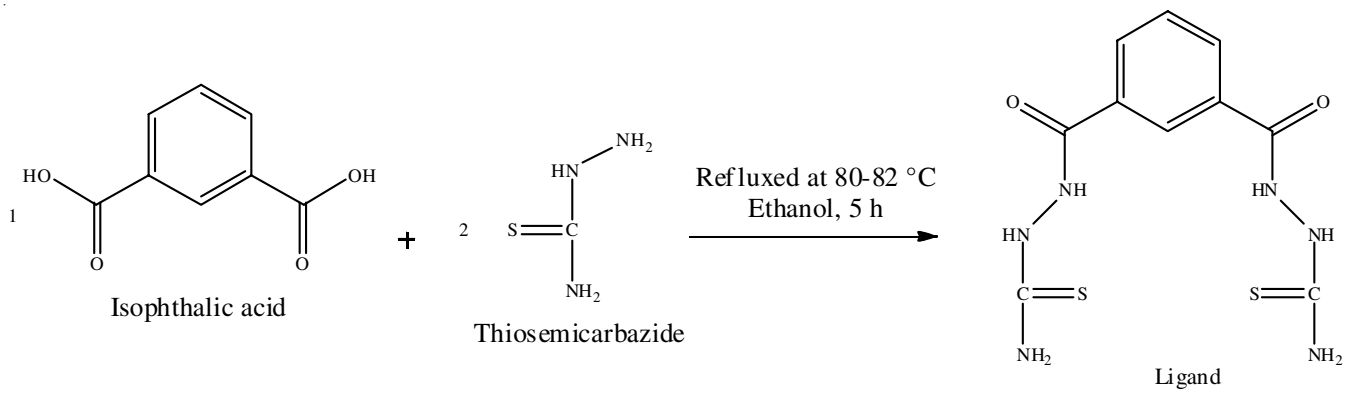
Computational study: The computational study of the synthesized ligand (IPBT) and its manganese and cobalt complexes with different anions was performed by implementation of semiempirical (PM6) method of the Gaussian 09W package, in the gas phase. For clarity purpose hydrogen atoms were omitted from all compounds structure. Fully computational optimization study suggested the six coordinated geometry. The correct geometry optimization has been secure by following some modification in coordinates to obtain reasonable low energy molecular geometries. For each compound numerous cycles of energy minimization have been conducted.

Antipathogenic screening: Well diffusion and poison food techniques have been followed for antipathogenic screening (to examine growth of bacteria and fungi, respectively) [24,25]. In well-diffusion techniques, after transferring autoclaved nutrient agar in disposable petri plates, agar is allowed to solidify and then well have been made in it. Synthesized ligand (IPBT) and its complexes have been examined against three tested bacteria *i.e*. *S. aureus*, *P. aeruginosa* and *E. coli*. The prohibition of the bacterial growth has been expressed in (%) and determined by comparison by test plate with control plate (DMSO). In poisoned food technique procedure, synthesized compounds have been mixed at two concentrations *i.e*. 1000 ppm and 500 ppm in autoclaved sabaround dextrose agar medium and mixed well by using glass rod. Then, the medium was transferred in petri plates. After mixing procedure, tested fungi (*A. niger*, *M. phasolina* and *P. glomerata*) have been put in the center of plates. After incubation period, growth of microorganism in tested plate as well as in control plate has been exactly measured carefully.

RESULTS AND DISCUSSION

All data obtained after spectroscopic as well as analytical studies for tetradentate (IPBT) molecule and its complexes is reported in Table-1. Isopthalicacid-*bis*(thiosemicarbozone) formed thermally stable complexes with different metal salts. The elemental analyses of complexes revealed that all the complexes have formula MLX_2 where M = taken metal ions L = IPBT and X = CH_3COO^- and Cl^- ions The molar conductance values (15-22 Ω^{-1} cm^{-1} mol^{-1}) represent that complexes not behave as electrolyte means counter ions are present inside the coordination sphere and formulate as $[MLX_2]$ (Fig. 1) [26,27]. Ligand was found insoluble in water but soluble in ethanol and all the metal(II) complexes were insoluble in water as well as in all organic solvents but soluble in DMSO and DMF solvents.

^{1}H NMR studies: In the NMR spectrum of the synthesized ligand (IPBT), signals at δ 7.2-8.2 ppm, which was attributed



Scheme-I: Preparation route for IPBT ligand

TABLE-1
PHYSICO-ANALYTICAL DATA OF THE SYNTHESIZED LIGAND IPBT AND ITS METAL COMPLEXES

Compounds	m.w. (g/mol)	Yield (%)	Reflux time (h)	Colour	Elemental analyses (%): Found (calcd.)			
					C	H	N	Mn/Co
(IPBT) $C_{10}H_{12}N_6S_2O_2$	312	52	5	White	38.46 (38.44)	3.84 (3.85)	26.92 (26.91)	–
IPBT-C1 $MnC_{10}H_8N_6S_2O_2Cl_2$	437.9	50	12	White	27.40 (27.40)	2.74 (2.75)	19.18 (19.18)	12.53 (12.54)
IPBT-C2 $MnC_{14}H_8N_6S_2O_6$	484.9	54	15	Pink	34.64 (64.65)	3.71 (3.70)	17.32 (17.30)	11.32 (11.35)
IPBT-C3 $CoC_{10}H_{12}N_6S_2O_2Cl_2$	441.9	57	7	Pink	27.15 (27.12)	2.71 (2.70)	19.00 (19.00)	13.21 (13.20)
IPBT-C4 $CoC_{14}H_{18}N_6S_2O_6$	488.9	54	24	Light Pink	34.36 (34.35)	3.68 (3.65)	17.18 (17.20)	12.04 (12.04)

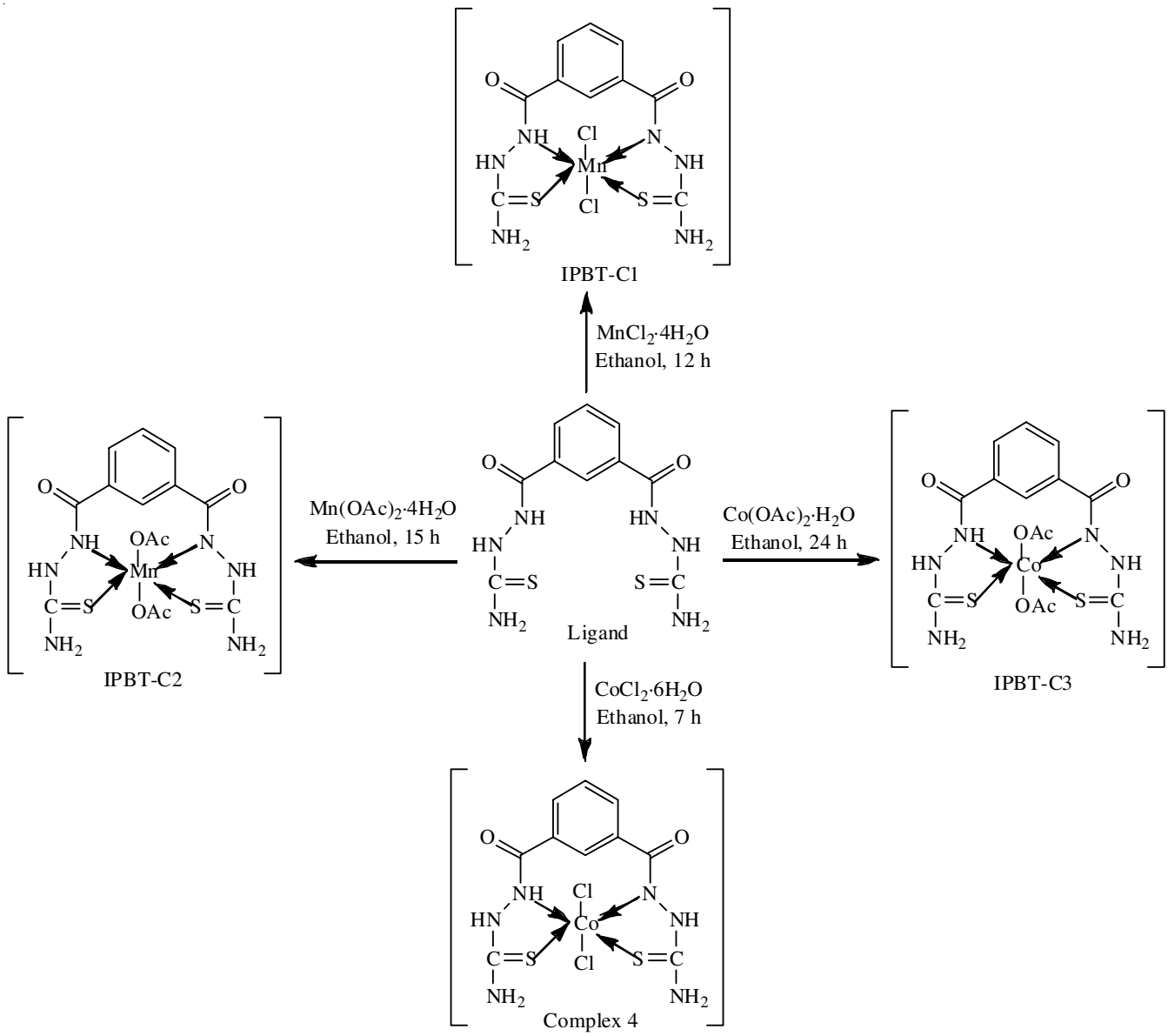


Fig. 1. Representation of preparation of metal complexes of IPBT

to the presence of aromatic proton [6H, Ar-H], δ 11.9-12.2 ppm corresponded to proton of [4H, NH] group and δ 5.1 ppm indicated to the presence of proton of [4H, NH_2] group in the chemical structure of (IPBT) (Fig. 2) [28,29].

Mass studies: By showing a peak at 312 amu in mass spectrum, which confirm formula corresponding to the moiety $[(C_{10}H_{12}N_6S_2O_2)^+$ (Fig. 3). Presence of other peaks in spectrum *i.e.* 297, 253, 238, 195, 179, 135, 120 and 77, which are corres-

TABLE-2
CHARACTERISTIC INFRARED SPECTRAL BANDS OF SYNTHESIZED LIGAND AND ITS MANGANESE AND COBALT COMPLEXES

Compounds	Characteristic IR bands (cm^{-1})					Characteristic bands (cm^{-1})
	ν(C=O)	ν(N-H)	ν(C=S)	ν(M–N)	ν(M–S)	
IPBT	1694	1581	728	–	–	–
IPBT-C1	1696	1508	711	482	530	Peak at 345 refers to Mn-Cl bonding
IPBT-C2	1690	1506	705	479	545	ν_{as}(OAc) = 1436, ν_s(OAc) = 1338, Δν = 94 refers to bonding of acetato group to Mn(II) ion
IPBT-C3	1606	1508	711	480	529	Peak at 339 refers to Co-Cl bonding
IPBT-C4	1609	1506	705	486	538	Peaks at ν_{as}(OAc) = 1450, ν_s(OAc) = 1281, Δν = 169 refers to bonding of acetato group to Co(II) ion

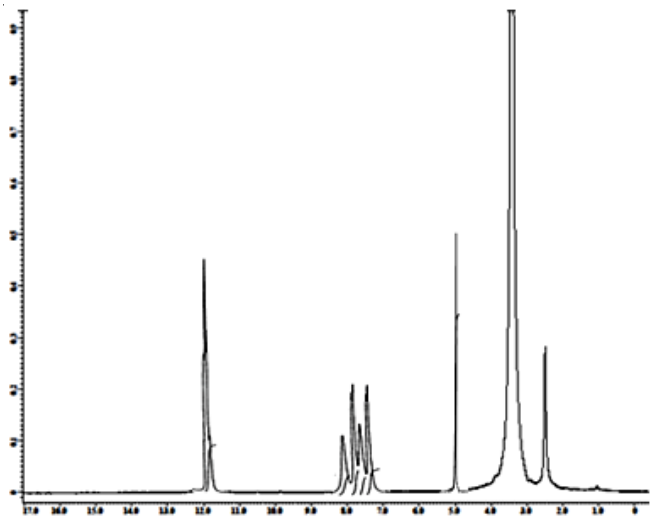


Fig. 2. ^{1}H NMR spectrum of ligand

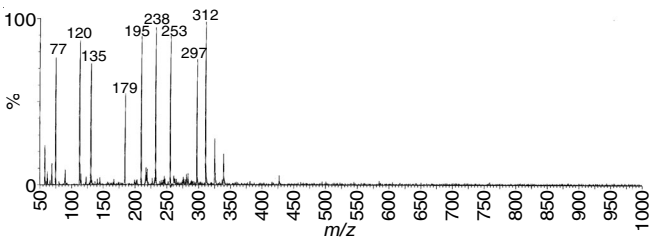


Fig. 3. Mass spectrum of of ligand

pond to the presence of following fragments *i.e.* $C_{10}H_{11}N_5S_2O_2$, $C_9H_{11}N_5SO_2$, $C_9H_{10}N_4SO_2$, $C_8H_9N_3SO$, $C_8H_7N_2SO$, $C_7H_7N_2O$, C_7H_6NO and C_6H_6, respectively (Fig. 4).

IR studies: The infrared spectrum of tetradentate ligand not exhibited any characteristic bands which demonstrate the presence of free amino and acid groups. The characteristics IR bands corresponding to the presence of ν(C=O) and ν(N-H) of amide group, appeared at 1694 cm^{-1} and 1581 cm^{-1} [30]. Due to the presence of ν(N-H) group and ν(C=S) group IR bands are present at positions 2999 cm^{-1} and 728 cm^{-1} [31,32]. IR spectra of metal complexes show shifting in above bands which indicated that the ligand (IPBT) has been bound to metal ions through amide groups and thiosemicarbazone group [33]. The data revealed that the ligand IPBT has the binding ability to coordinate with metal ions through N_2S_2 donor atoms (Table-2). This binding behaviour of IPBT to metal ions is also confirmed by appearance of some exacting peaks *i.e.* 449-426 cm^{-1} and 545-529 cm^{-1} which refers coordination of metal ions through nitrogen and sulphur atoms, respectively [34]. In chloride complexes, band present at position 328 cm^{-1} refers coordination of Co(II) and Mn(II) metal with chloride ions [35]. Binding with acetate group is confirmed by presence of specific bands positions 1443-1441 and 1344-1277 cm^{-1} due to ν_{as}(OAc), ν_s(OAc) stretching vibration [36]. By the presence of these bands, unidentate manner has been assigned for acetate group coordinated to the metal ions [37].

Magnetic moment: The experimental magnetic moment values for of manganese and cobalt complexes are 5.99-5.87 B.M. and 4.79-4.73-B.M., respectively (Table-3). The values 5.87 B.M. and 4.79-4.73-B.M. correspond to paramagnetic the behaviour of synthesized complexes *i.e.* presence of five and three unpaired electrons for manganese and cobalt, respectively. These values are well closed and agreed with the theoretically calculated values [38].

TABLE-3
MOLAR CONDUCTANCE AND ELECTRONIC DATA OF METAL COMPLEXES OF IPBT

Complexes	Molar conductors (Ω^{-1} cm^{-1} mol^{-1})	λ_{max} (cm^{-1})
IPBT-C1	17	17954, 23135, 34843
IPBT-C2	20	17094, 24360, 35730
IPBT-C3	15	9766, 17002, 20315, 36783
IPBT-C4	22	9882, 17725, 19988, 38634

Electronic spectra: This electronic study for manganese and cobalt complexes has been done by dissolving complexes in DMSO. All the characteristic bands are summarized in Table-3. Bands of absorption for manganese complexes present in the range of 17954-17094 cm^{-1}, 24360-23135 cm^{-1} and 35730-34843 cm^{-1}. Following transitions are caused due to these obtained bands at $^6A_{1g} \rightarrow {}^4T_{1g}$ (4G), $^6A_{1g} \rightarrow {}^4E_g$, $^6A_{1g} \rightarrow {}^4E_g$ (4D) and $^6A_{1g} \rightarrow {}^4T_{1g}$ (P), respectively. Due to these transitions an octahedral geometry is assigned for IPBT-C1 and IPBT-C2 complexes [39]. In case of cobalt complexes absorption bands are presented as 9882-9766, 17725-17002, 20315-19988 and 38634-36783 cm^{-1} (Fig. 5) [40]. Appearance of these bands corresponded to the following transitions $^4T_{1g}(F) \rightarrow {}^4T_{2g}(\nu_1)$, $^4T_{1g}(F) \rightarrow {}^4A_{2g}(\nu_2)$, $^4T_{1g}(F) \rightarrow {}^4T_{1g}(P)$ (ν_3). On the basis of aforesaid transitions, it has been concluded that IPBT-C3 and IPBT-C4 complexes possessed six coordinated geometry [41].

Ligand field parameters (LFP): Different LFP *i.e.* nephelauxetic parameter (β), ligand field splitting stabilization energy (D_q), Racah inter-electronic repulsion parameters

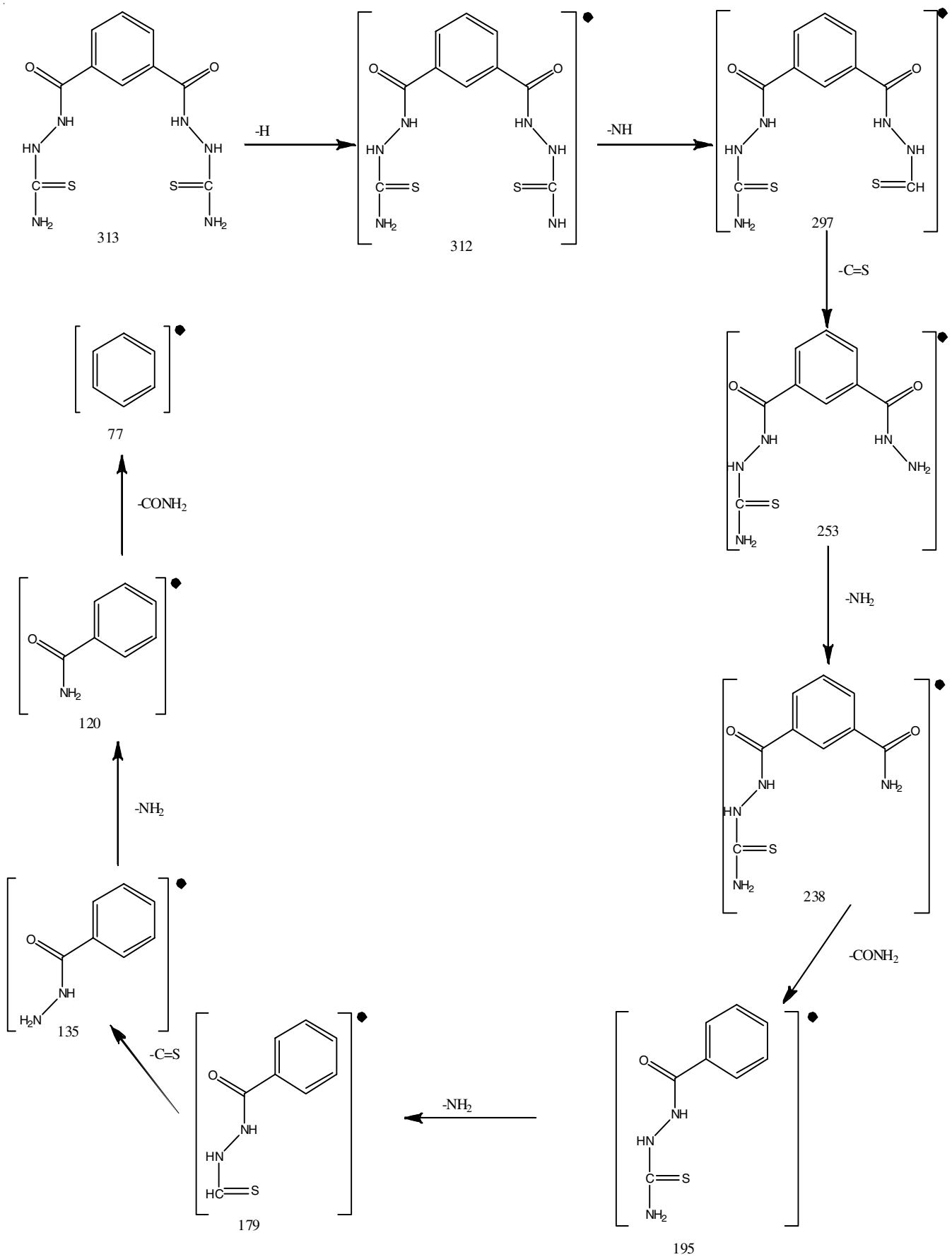


Fig. 4. Mass fragmentation of IPBT

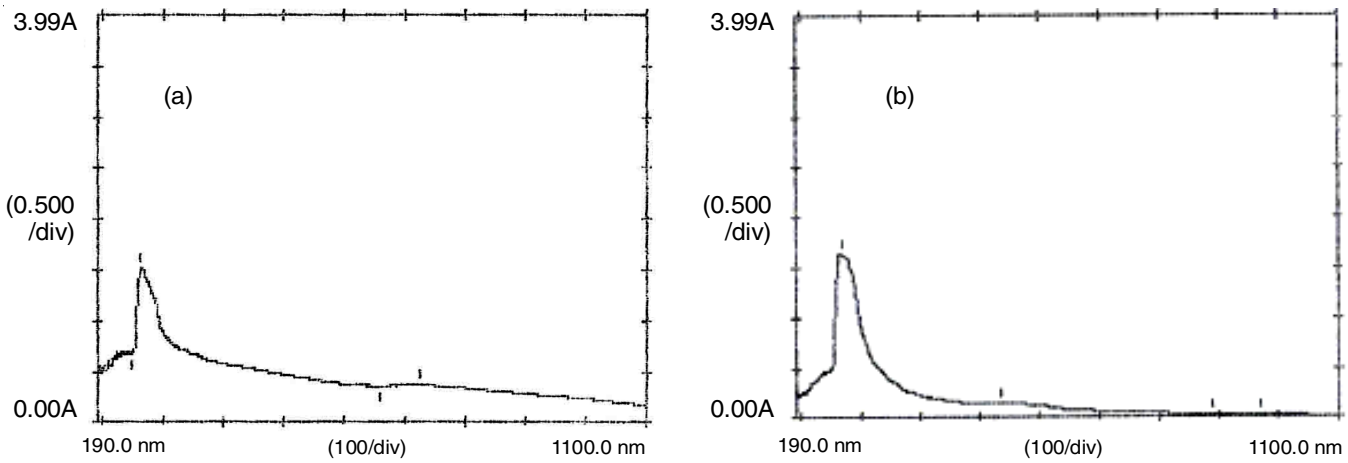


Fig. 5. Electronic spectra of complexes (a) IPBT-C2 (b) IPBT-C3

(B and C), slator condon parameters (F_2 and F_4) have been deliberated for complexes by following specific equations. The values of parameter β have been found in the range of 0.29-0.94 which states covalancy factor is present in complexes [42,43]. With the help of first transition, values of stabilization energy have been calculated [44]. Values of F_2 and F_4 parameters have been calculated by using Racah parameters *i.e.* $C = 35F_4$ and $B = F_2 - 5F_4$. All the calculated parameters are summarized in Table-4.

Electronic spin resonance (ESR) studies: Values for ESR (at liquid nitrogen and room temperature) have been mentioned for all the metal complexes of isopthalic acid-*bis*(thiosemicarbozone) (IPBT) in Table-4. In polycrystalline form, the g_{iso} value for Mn(II) complexes are 2.00-2.04 at room temperature and 2.01-2.04 at liquid nitrogen temperature. These obtained values are nearby to the spin value, which shows that spin orbital coupling is absent in ground state. ESR spectra of cobalt comp-lexes have been done at liquid nitrogen temperature in polycry-stalline state. The values of $g_{||}$, g and g_{iso} are present in the range of 2.02-3.2 1.95-2.45 and 2.14-2.47, respectively. These received values are in support of octahedral geometry for complexes [45].

Computational screening: After performing this study work for IBPT and its manganese complexes, the structural information has been obtained. The optimized structural information *i.e.* bond length and bond angles are summarized in Tables 5 and 6. Structural studies revealed that the ligand IBPT has ability to bind Mn(II) metal ion in a tetradentate mode *via* its donor atoms and counter ions coordinated at vertical place. On the basis of above coordination mode, we

TABLE-4
LFP AND ESR SPECTRAL DATA OF METAL COMPLEXES OF IPBT

Complexes	LFP							ESR dta	
	Dq	B	C	β	F_2	F_4	Hx	g_{iso} (RT)	g_{iso} (LNT)
IPBT-1	1795	480	3667	0.61	1000	104.77	2.57	2.02	2.01
IPBT-2	1709	742	3388	0.94	1222	96.80	1.85	2.03	2.04
IPBT-3	976	534	–	0.47	–	–	–	–	–
IPBT-4	988	537	–	0.48	–	–	–	–	–

TABLE-5
OPTIMIZED BOND LENGTHS (Å) OF IBPT AND ITS MANGANESE COMPLEXES

Bond length	IBPT	IBPT-1	IBPT-2	Bond length	IBPT	IBPT-1	IBPT-2
N_2-C_4	1.43521	1.44442	1.41447	N_{22}-C_{24}	1.42447	1.44267	1.42348
N_2-C_3	1.43708	1.44442	1.42344	N_{18}-C_{20}	1.42562	1.44267	1.41492
C_4-O_5	1.21429	1.21674	1.22053	C_{24}-S_{26}	1.66829	1.65242	1.66453
C_3-O_6	1.21133	1.21674	1.21675	C_{20}-S_{25}	1.66607	1.65242	1.66861
C_3-C_8	1.49329	1.48998	1.49341	N_{30}-H_{31}	1.00684	1.01494	1.00451
C_4-C_{12}	1.49181	1.48998	1.49414	N_{30}-H_{32}	1.01576	1.01827	1.01142
C_8-C_9	1.40129	1.40558	1.40056	N_{27}-H_{28}	1.00676	1.01494	1.00856
C_9-C_{10}	1.39799	1.39870	1.40215	N_{27}-H_{29}	1.01547	1.01827	1.01466
C_{10}-C_{11}	1.39700	1.39870	1.40147	M_{33}-Cl_{34}	–	1.96653	1.99808
C_{11}-C_{12}	1.40397	1.40558	1.40019	M_{33}-Cl_{35}	–	2.22946	1.94709
C_{12}-C_7	1.40000	1.40022	1.40230	M_{33}-N_1	–	2.95197	1.92314
C_8-C_7	1.40051	1.40022	1.40170	M_{33}-N_2	–	2.95197	1.89045
N_2-N_{12}	1.40772	1.42895	1.41244	M_{33}-S_{25}	–	2.19667	2.32551
N_1-N_{18}	1.40815	1.42895	1.41226	M_{33}-S_{26}	–	2.19667	2.29948

TABLE-6
OPTIMIZED BOND ANGLE (°) OF Mn(II) COMPLEXES OF THE SYNTHESIZED LIGAND

Bond angles	IBPT-1	IBPT-2	Bond angles	IBPT-1	IBPT-2	Bond angles	IBPT-1	IBPT-2
C_8-C_7-C_{12}	120.47	117.38	C_{12}-C_4-O_5	124.41	127.68	S_{25}-M_{33}-S_{26}	112.75	56.20
C_7-C_8-C_3	120.46	115.56	O_1-C_4-N_1	120.38	122.83	S_{26}-M_{33}-N_2	71.59	81.03
C_8-C_3-O_6	124.41	128.43	C_1-N_1-N_{18}	116.70	115.91	S_{26}-M_{33}-Cl_{35}*	95.47	124.21
O_6-C_3-N_2	120.38	122.41	N_1-N_{18}-C_{20}	112.07	112.36	S_{25}-M_{33}-Cl_{34}*	105.84	73.97
C_3-N_2-N_{12}	116.70	116.11	N_{18}-C_{20}-S_{25}	129.16	116.10	N_1-M_{33}-Cl_{35}*	74.97	81.34
N_2-N_{22}-C_{24}	112.07	111.24	N_{18}-C_{20}-N_{27}	113.26	119.75	N_2-M_{33}-Cl_{34}*	80.72	105.12
N_{22}-C_{24}-S_{26}	129.16	115.43	C_{20}-N_{27}-H_{28}	116.41	121.09	M_{33}-O_{35}-C_{39}	–	121.79
N_{22}-C_{24}-N_{30}	113.26	120.52	C_{20}-N_{27}-H_{29}	114.34	117.23	M_{33}-O_{34}-C_{38}	–	125.23
C_{24}-N_{30}-H_{31}	116.46	123.54	N_{27}-C_{20}-S_{25}	117.46	123.89	O_{35}-C_{39}-O_{36}	–	121.97
C_{24}-N_{30}-H_{32}	114.34	119.24	Cl_1-M_{33}-Cl_{35}	140.52	159.26	O_{34}-C_{38}-O_{37}	–	122.41
N_{30}-C_{24}-S_{26}	117.46	123.68	N_1-M_{33}-N_2	102.71	142.97	O_{35}-C_{39}-C_{40}	–	112.50
C_7-C_{12}-C_4	120.46	115.32	N_1-M_{33}-S_{26}	71.59	80.37	O_{34}-C_{38}-O_{41}	–	113.67

get six coordinated geometry for IBPT-1 and IBPT-2 complexes. The fully optimized images of complexes are presented in Fig. 6.

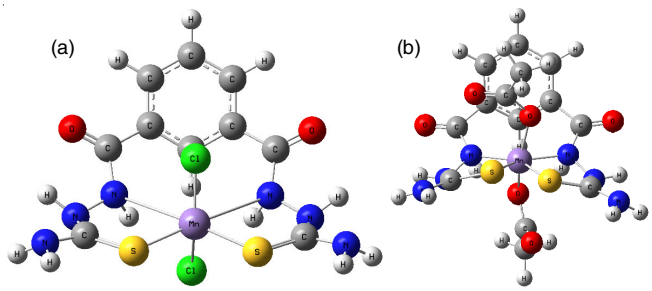


Fig. 6. Optimized structure of complexes with IBPT (a) IBPT-1 (b) IBPT-2 (colour code: purple = manganese, red = oxygen, green = chloride, blue = nitrogen, grey = carbon)

***in vitro* antipathogenic screening:** From Tables 7 and 8, it is resulted out that synthesized ligand (IBPT) and it metal complexes exhibit antibacterial and antifungal activity against the growth of tested pathogen. The results of the growth curve of treated bacteria show that IBPT-2 had bactericidal good effect against bacteria *S. aureus*, *P. aeruginosa* while IBPT-1 and IBPT-3 had only moderate effect against all treated bacteria. All compounds examined for their antibacterial effect against *E. coli* bacteria were found about inactive *i.e.* showing no inhibition zone. On the basis of these studies, it can be acknowledged that metal complexes are more active than free ligand IBPT.

Conclusion

In this work, the interaction between novel synthesized ligand (isopthalic acid-*bis*(thiosemicarbozone), IPBT) and different anions (Cl^-, CH_3COO^-) of taking metal ions *i.e.* cobalt and manganese were investigated. Using analytical and spectral techniques, the synthesized ligand IBPT was found to be bind to manganese and cobalt ions *via* donor atoms and counter ions. Six coordinated geometry has been assigned for the synthesized metal complexes according to spectroscopic as well as by computational data. All the metal complexes have effective and selective antifungal and antibacterial activities than the synthesized ligand IBPT. From the antibacterial biological data, it has been concluded that at concentration 500 ppm, metal complexes IBPT-1 showed maximum inhibitory zone comparatively other tested complexes against bacteria *E. coli* and *S. aureus*.

TABLE-7
ANTIBACTERIAL ACTIVITY OF THE STUDIED SYNTHESIZED COMPOUNDS AT CONCENTRATION 500 ppm EXPRESSED IN DIAMETER OF INHIBITION ZONE (mm)

Compounds	*E. coli*	*S. aureus*	*P. aeruginosa*
IBPT	00	08	03
IBPT-1	02	13	10
IBPT-2	08	22	20
IBPT-3	02	15	10
IBPT-4	06	23	18
Neomycin	14	25	23

TABLE-8
ANTIFUNGAL ACTIVITY OF THE STUDIED SYNTHESIZED COMPOUNDS AT CONCENTRATION 1000 AND 500 ppm EXPRESSED IN DIAMETER OF INHIBITION ZONE (mm)

Compounds	Conc. (ppm)	*A. niger*	*M. phasolina*	*P. glomerata*
IBPT	1000	45	15	35
	500	20	00	10
IBPT-1	1000	65	20	50
	500	40	00	20
IBPT-2	1000	95	45	80
	500	90	20	60
IBPT-3	1000	50	30	45
	500	30	15	20
IBPT-4	1000	97	80	95
	500	95	60	80
Chlorothalonil	1000	100	85	95
	500	90	75	90

ACKNOWLEDGEMENTS

The authors are thankful to University Science Instrumentation Center (USIC), University of Delhi for recording IR, elemental analysis, mass spectra. For recording ESR spectra of complexes and NMR spectrum of ligand, authors acknowledge to IIT Bombay and IIT Delhi, respectively. For financial assistance, the authors are gratefully acknowledge to University Grant Commission, New Delhi, India.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this article.

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