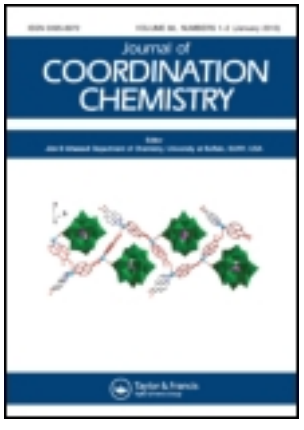

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Synthesis, characterization, semi-empirical study and biological activities of homobimetallic complexes of tranexamic acid with organotin(IV)

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The Schiff base has been synthesized by reacting tranexamic acid with indol-3-carboxyaldehyde in the first step and then with carbon disulfide at room temperature in the second step. The homobimetallic complexes have been synthesized by reaction of Schiff base with R_2SnCl_2 and R_3SnCl in 1 : 2 M ratio under stirring, where R = methyl, *n*-butyl and phenyl. The ligand and complexes have been characterized by elemental analysis, FT-IR, multinuclear NMR (^1H, ^{13}C and ^{119}Sn) and semi-empirical study. IR data reveal the bidentate nature of the ligand. Five- or six-coordinate geometry was confirmed in solution by NMR spectroscopy. The homobimetallic complexes and ligand were tested *in vitro* against some pathogenic bacteria and fungi to assess their antimicrobial properties. The complexes show biological activities with few exceptions.

Keywords: Tranexamic acid; Indol-3-carboxyaldehyde; Organotin(IV); FT-IR; NMR; Semi-empirical study; Biological activity

1. Introduction

Organotin(IV) complexes of Schiff bases have been studied because they have interesting structures, thermal stability, biological properties, high synthesis flexibility and medicinal utility [1]. Schiff bases have wide applications in food industry, dye industry, analytical chemistry, catalysis, fungicidal, agrochemical, and biological activities [2]. Schiff base complexes are important models in main group and transition metal coordination chemistry due to their preparative accessibility and structural variety [3]. Attention has been devoted to Schiff base complexes of organotin(IV) moieties for potential applications in medicinal chemistry and biotechnology [4–6].

Studies of Schiff base organotin complexes containing carboxylates with additional donors (e.g. O or S), available for coordinating to tin, reveal that new structural types may

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lead to different activities. In continuation of our previous work [7–12], we report synthesis, characterization, semi-empirical study and biological activities of homobimetallic complexes containing organotin(IV) with Schiff base ligand.

2. Experimental

2.1. *Chemicals and instrumentation*

Indol-3-carboxaldehyde, ethanol, carbon disulfide, and organotin chlorides were purchased from Aldrich Chemical Company (USA). Tranexamic acid was purchased from the market. Nutrient agar, nutrient broth, and potato dextrose agar (PDA) were purchased from Oxoid Company (UK). All reagents were of analytical grade.

The melting points were determined in capillary tubes on an electrothermal melting point apparatus, model Stuart (SMP3) (UK) and are uncorrected. Infrared spectra were recorded using a Perkin-Elmer 1000 FT-IR spectrophotometer as KBr disks from 4000 to 250 cm^{-1}. NMR spectra were recorded on a Bruker AM-250 MHz FT-NMR spectrometer (Germany) using deuterated $CDCl_3$ as internal reference. ^{119}Sn NMR spectra were recorded on a Bruker AM 250 spectrometer (Germany) using $CDCl_3$ as an internal reference and Me_4Sn as external reference [δ(Sn) = 37.290665]. The percentage compositions of C, H, N, and S were determined by using a CHNS-932 Leco (USA). The antimicrobial activities of the ligand and organotin(IV) complexes were performed in an Incubator (Sanyo, Germany) and sterilized in an autoclave (Omron, Japan). The minimum inhibitory concentration and antioxidant activities were determined in a Micro Quant apparatus (BioTek, USA).

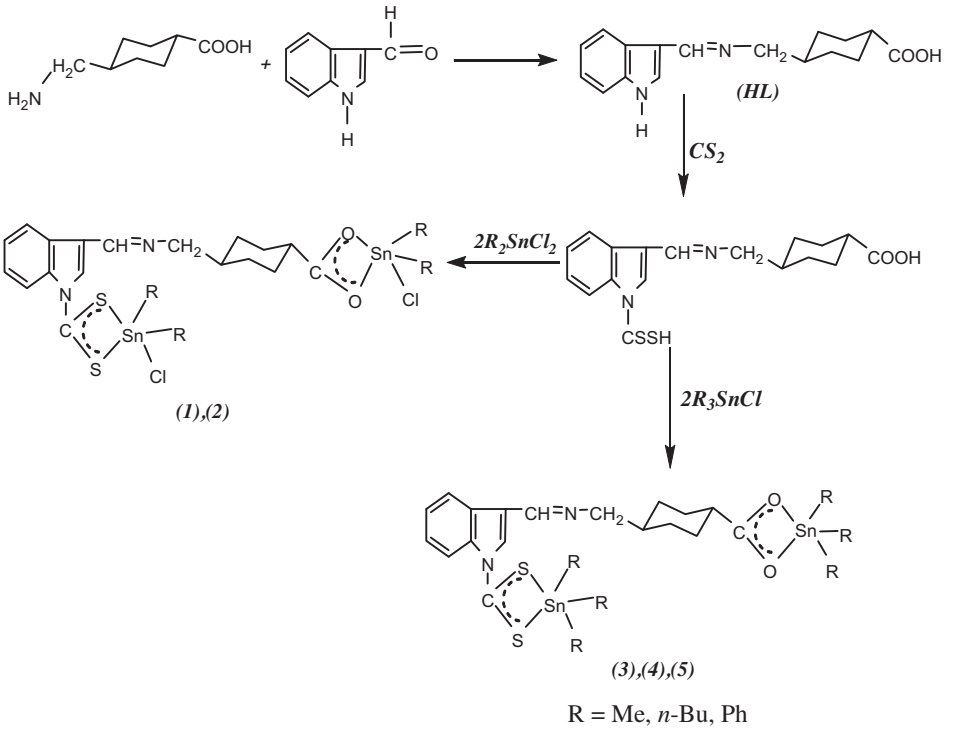
The molecules were modeled by MOPAC 2007 [13] program in the gas phase using the PM3 method [14, 15]. Selected parts of the complexes not containing the metal ion were pre-optimized using the molecular mechanics method. Several cycles of energy minimization had to be carried out for each of the molecules. Geometry was optimized using the Eigen Vector. The root mean square gradient for molecules was less than one. Self-consistent field was achieved in each case.

2.2. *Synthesis of HL*

Tranexamic acid (0.755 g, 5 mM) was dissolved in distilled water (15 mL) in a round bottom two necked flask with continuous stirring. To this solution, indol-3-carboxaldehyde (0.725 g, 5 mM) in ethanol (15 mL) was added drop wise and the reaction mixture was refluxed for 4–5 h with continuous stirring. Precipitates were filtered off and dried in air (scheme 1).

2.3. *General procedure for synthesis of homobimetallic chlorodi-/triorganotin complexes*

HL was dissolved in methanol (15 mL) in a round bottom two necked flask with stirring. To the above solution, CS_2 (3 mL, 5 mM) was added dropwise at room temperature and the reaction mixture was stirred for half an hour. Then, to the reaction mixture, R_2SnCl_2/R_3SnCl (R = methyl, butyl) was added in 1 : 2 M ratio and the resulting mixture was refluxed for 6–7 h with stirring. Solvent was evaporated slowly at room temperature and the product obtained was dried in air (scheme 1).



Scheme 1. Synthesis of ligand and organotin(IV) derivatives.

2.4. *Antibacterial assay*

2.4.1. Bacterial growth medium, cultures, and inoculum preparation. Pure cultures were maintained on nutrient agar medium in the petri plates. For inoculum preparation, 13 g L^{-1} of nutrient broth was suspended in distilled water, mixed well and distributed homogeneously. Then, 10 µL of pure autoclaved culture of a bacterial strain was mixed in medium and placed in a shaker for 24 h at 37 °C. The inocula were stored at 4 °C. Inocula with 1×10^8 spores mL^{-1} were used for further analysis.

2.4.2. Antibacterial assay by disk diffusion method. Antibacterial activities of samples were determined by using the disk diffusion method [16]. Nutrient agar 28 g L^{-1} was suspended in distilled water, mixed well and distributed homogeneously. The medium was sterilized by autoclaving at 121 °C for 15 min. Before the medium was transferred to petri plates, inoculum (100 µL/100 mL) was added to the medium and poured in sterilized petri plates.

After this, small filter paper disks were laid flat on growth medium containing 100 µL of sample solution. The petri plates were then incubated at 37 °C for 24 h for the growth of bacteria. Sample having antibacterial activity inhibited the bacterial growth and clear zones were formed. The zones of inhibition were measured in millimeters using a zone reader [17].

2.5. *Antifungal assay*

2.5.1. Growth medium, cultures, and inoculum preparation. Pure culture of the fungi were maintained on PDA medium in slant or petri plates that were pre-sterilized in a hot air oven at 180 °C for 3 h. These culture slants were incubated at 28 °C for 3–4 days for multiplication of fungal strains.

2.5.2. Antifungal assay by disk diffusion method. The prepared sterilized growth medium was transferred to the sterilized petri plates. The petri plates were then incubated at 28 °C for 48 h for growth of fungus. Small filter paper disks were laid flat on growth medium having fungal growth and 100 µL of each sample was applied on each disk. The petri plates were again incubated. The sample having antifungal activity exhibit clear zones around the disks. The zones of inhibition were measured in millimeters using a zone reader [17].

3. Results and discussion

The ligand and complexes are solids, stable in air, have sharp melting points and are soluble in common organic solvents. Elemental analyzes were performed of carbon, hydrogen, nitrogen and sulfur and found to be in agreement. The physical data of homobimetallic complexes are summarized in table 1.

3.1. *Infrared spectroscopy*

Infrared spectra of **1–5** and ligand were recorded from 4000 to 250 cm^{-1} to study the binding behavior of Schiff base to organotin(IV). Important absorptions are listed in table 2.

The IR spectra of ligand and **1–5** show strong absorptions at 1648–1640 cm^{-1}, assigned to ν(C=N). The IR stretching frequencies of carboxylic group [(ν(COOasym) and ν(COOsym)] in organotin(IV) complexes support elucidation of the structure and bonding of the ligand [18]. In all complexes, the difference $\Delta\nu$ is less than 200 cm^{-1} which shows bidentate ligand. A band due to ν(C–S) is used to distinguish between mono and bidentate ligand [19]. The presence of single ν(C–S) from 982 to 920 cm^{-1} confirms that the ligand is bidentate [20]. Medium to sharp bands are observed in the far IR for **1** and **2** at 358–368 cm^{-1} due to ν(Sn–Cl). Medium to sharp bands are observed in the range of 550–558 cm^{-1} and 440–453 cm^{-1} assigned to ν(Sn–C) and ν(Sn–O), respectively, except **5**, which gives ν(Sn–C) band at 342 cm^{-1} due to phenyl.

3.2. *^{1}H NMR*

^{1}H NMR spectral data of ligand and complexes are given in table 3. All protons have been identified at position and number with protons calculated from the incremental method [21]. The OH and SH groups which appear as singlets at 11.2 and 10.9 ppm, respectively, in **HL** are absent in complexes, confirming deprotonation of the ligand during complexation. Multiplets at 1.21–1.87 ppm do not show any significant shift upon complexation. The CH_3 in **1** is a singlet at 1.27 ppm with tin satellites having ^2J [119Sn–1H] = 96 Hz. In **2**, the protons of butyl are multiplets at 0.88–0.93 ppm. The terminal CH_3

Table 1. Physical data of homobimetallic complexes.

Comp. no.	Molecular formula	MW	MP (°C)	Yield (%)	Elemental analysis			
					%C Calcd (found)	%H Calcd (found)	%N Calcd (found)	%S Calcd (found)
HL	$C_{17}H_{20}N_2O_2$	284.35	181–183	64	71.74 (71.79)	7.03 (7.00)	9.84 (9.89)	–
1	$C_{22}H_{30}N_2S_2O_2Sn_2Cl_2$	726.94	155–156	96	36.31 (36.36)	4.12 (4.16)	3.85 (3.82)	8.80 (8.77)
2	$C_{34}H_{54}N_2S_2O_2Sn_2Cl_2$	895.26	201–203	104	45.57 (45.54)	6.03 (6.06)	3.12 (3.16)	7.14 (7.11)
3	$C_{24}H_{36}N_2O_2S_2Sn_2$	686.10	130–135	54	41.97 (41.94)	5.24 (5.29)	4.08 (4.02)	9.32 (9.28)
4	$C_{42}H_{72}N_2O_2S_2Sn_2$	938.58	202–203	55	53.69 (53.69)	7.67 (7.63)	2.98 (2.95)	6.81 (6.86)
5	$C_{54}H_{48}N_2O_2S_2Sn_2$	1058.52	209–211	64	61.21 (61.29)	4.53 (4.50)	2.64 (2.60)	6.04 (6.09)

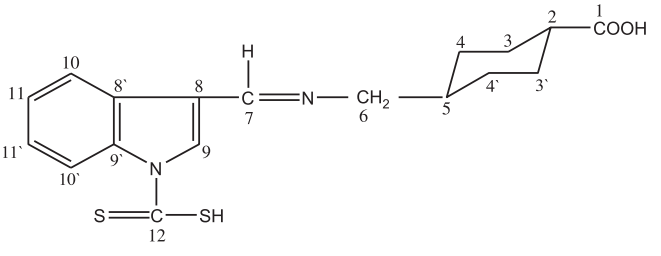
Table 2. Characteristic IR bands (cm^{-1}) of homobimetallic complexes.

Comp. no.	ν(N–H)	ν(C=N)	ν(C=S)	ν(C–S)	ν(COO) asym	ν(COO) sym	$\Delta\nu$	ν(Sn–C)	ν(Sn–O)	ν(Sn–S)	ν(Sn–Cl)
HL	3463	1640	1087	943	1555	1320	235	–	–	–	–
1	–	1642	1082	982	1548	1459	189	558	444	453	368
2	–	1641	1078	960	1585	1422	163	551	432	449	358
3	–	1646	1079	982	1535	1410	125	550	421	450	–
4	–	1648	1073	954	1572	1380	192	551	454	440	–
5	–	1644	1072	920	1567	1381	186	342	432	440	–

Table 3. ^{1}H NMR data[a–c] of homobimetallic complexes.

	Chemical shift (ppm)					
Proton	**HL**	**1**	**2**	**3**	**4**	**5**
2	1.81–1.87 m	1.81–1.86 m	1.82–1.87 m	1.81–1.87 m	1.82–1.86 m	1.82–1.87 m
3,3′	1.73–1.76 m	1.72–1.76 m	1.73–1.75 m	1.72–1.76 m	1.72–1.76 m	1.73–1.75 m
4,4′	1.63–1.66 m	1.63–1.65 m	1.62–1.66 m	1.63–1.65 m	1.63–1.66 m	1.63–1.66 m
5	1.21–1.24 m	1.22–1.24 m	1.21–1.23 m	1.21–1.24 m	1.21–1.24 m	1.21–1.23 m
6	1.58s	1.57s	1.58s	1.58s	1.57s	1.58s
7	5.21s	5.22s	5.21s	5.23s	5.21s	5.21s
9	6.35s	6.35s	6.34s	6.35s	6.34s	6.34s
10,10′	6.92d (8.1)	6.93d (8.1)	6.92d (8.1)	6.91d (8.1)	6.92d (8.1)	6.92d (8.1)
11,11′	6.87d,d (8.0)	6.86d,d (8.0)	6.87d,d (8.0)	6.86d,d (8.0)	6.86d,d (8.0)	6.87d,d (8.0)

[a]Compound **1** Sn–CH_3, 1.27s ^{2}J[96]; Compound **2** Sn–$CH_2CH_2CH_2CH_3$, 0.88–0.93 m, 0.23t (7.2); Compound **3** Sn–CH_3, 0.51s ^{2}J[82]; Compound **4** Sn–$CH_2CH_2CH_2CH_3$, 0.64–1.1 m, 0.23t (7.2); Compound **5** Sn–C_6H_5, 7.91d ^{2}J[57], 7.50–7.53 m, 7.42–7.50 m.
[b]Chemical shifts (δ) in ppm. ^{2}J[^{119}Sn,^{1}H] and ^{n}J(^{1}H,^{1}H) in Hz are listed in square brackets and parenthesis, respectively.
[c]



of butyl is a triplet at 0.23 ppm with ^{3}J[^{1}H–^{1}H] coupling of 7.2 Hz. The methyl in **3**, attached to Sn, gives a singlet at 0.51 ppm with ^{2}J[^{119}Sn–^{1}H] coupling constant of 82 Hz, in the range expected for five-coordinate tin and consistent with C–Sn–C angle of 126.5°.

3.3. *^{13}C and ^{119}Sn NMR*

^{13}C and ^{119}Sn NMR spectral data of the complexes are listed in table 4. The ^{13}C signals are assigned by comparison with the values calculated from the incremental method [21]. ^{13}C NMR chemical shifts due to phenyl attached to Sn were observed at positions comparable with related compounds [22].

The carbon positions of C=S and –COO of ligand shift upfield and downfield, respectively, upon complexation. The upfield shift is attributed to lowering of C=S bond order upon coordination and a shift of N→C electron density producing a partial double bond character in the C–N bond.

The coupling constants ^{n}J[^{119}Sn, ^{13}C] are important parameters for characterization of organotin(IV) compounds. For triorganotin(IV) derivatives, the magnitude of ^{1}J[^{119}Sn, ^{13}C] coupling suggested tetrahedral tin in solution [23]. Geometry of chlorodiorganotin carboxylates in noncoordinating solvents could not be defined due to fluxional behavior of the carboxylate oxygens in coordination with tin [24]. The C–Sn–C angle (°) based on NMR parameters for the complexes are given in table 5. The geometric data are consistent with five and six coordination [20, 25–28].

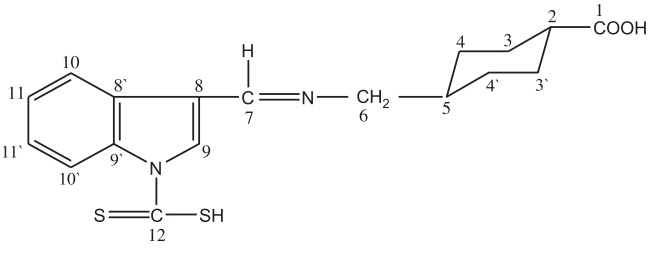
Table 4. ^{13}C and ^{119}Sn NMR data[a–c] of homobimetallic complexes.

	Chemical shift (ppm)					
Carbon	**HL**	**1**	**2**	**3**	**4**	**5**
1	169.2	172.4	172.7	172.5	172.5	172.8
2	51.4	51.2	51.5	51.6	51.2	51.1
3,3′	59.7	59.7	59.8	59.6	59.7	59.6
4,4′	24.7	24.6	24.2	24.8	24.3	24.9
5	32.2	32.2	32.1	32.7	32.5	32.8
6	47.2	47.3	47.3	47.2	47.2	47.2
7	32.0	32.0	32.2	32.0	32.0	32.0
8,8′	136.5	136.5	136.4	136.5	136.5	136.4
9	139.2	139.3	139.2	139.2	139.3	139.2
9′	126.2	126.1	126.2	126.2	126.2	126.1
10,10′	131.8	131.8	131.8	131.9	131.9	131.8
11,11′	134.5	134.4	134.4	134.5	134.5	134.5
12	211.7	197.6	195.8	195.7	195.5	198.9

[a]Compound **1** Sn–CH_3, (C–α) 10.5 ^{1}J[641]; δ $^{119}Sn = -336.2$; Compound **2** Sn–$CH_2CH_2CH_2CH_3$, (C–α) 22.78 ^{1}J[341.0], (C–β) 28.69 ^{2}J[22]; (C–γ) 27.08 ^{3}J[63]; (C–δ) 13.70; δ $^{119}Sn = -129.4$; Compound **3** Sn–CH_3, −2.0 ^{1}J[571.0]; Compound **4** Sn–$CH_2CH_2CH_2CH_3$, (C–α) 22.6 ^{1}J[578.0], (C–β) 28.7 ^{2}J[34.29], (C–γ) 27.6 ^{3}J[87.2], (C–δ) 14.2; Compound **5** Sn–C_6H_5, (C–α) 136.75, (C–β) 129.11 ^{2}J[47]; (C–γ) 128.52, (C–δ) 128.11; δ $^{119}Sn = -80.0$.

[b]Chemical shifts (δ) in ppm. $^{n}J[^{119}Sn,^{13}C]$ in Hz is listed in parenthesis.

[c]



3.4. *Antibacterial activity*

The ligand and complexes were screened for antibacterial activity using the disk diffusion method [16] against *Bacillus subtilis*, *Escherichia coli*, *Pasturella multocida,* and *Staphylococcus aureus*. The standard drug rifampicine was used as a positive control. Complex **2** showed lower activity and **5** was most active. While the compounds are active, their activity is less than that of the standard drug (rifampicin) [29] (table 6).

Table 5. C–Sn–C angles (°) calculated from NMR.

			C–Sn–C angles (°)	
Compound no.	$^{1}J[^{119}Sn–^{13}C]$ (Hz)	$^{2}J[^{119}Sn–^{1}H]$ (Hz)	^{1}J	^{2}J
2	341.0	–	–	106.6
3	571.0	82.0	126.8	126.5
4	578.0	–	127.5	–

Table 6. Antibacterial activity of homobimetallic complexes of Schiff base[a–d].

	Bacteria zone size (mm)			
Complex no.	*B. subtilus*	*P. multocida*	*S. aureus*	*E. coli*
HL	0^{c}	0^{c}	0^{c}	0^{c}
1	$22^{a,b} \pm 1$	$23^{b} \pm 1$	$23^{a,b} \pm 1$	$23^{a,b} \pm 1$
2	$20^{b,c} \pm 1$	$18^{b,c} \pm 1$	$16^{b,c} \pm 1$	$16^{b,c} \pm 1$
3	$20^{b,c} \pm 1$	$24^{a,b} \pm 1$	$19^{b,c} \pm 1$	$20^{b} \pm 1$
4	$21^{b} \pm 1$	$17^{b,c} \pm 1$	$20^{b} \pm 1$	$17^{b,c} \pm 1$
5	$24^{a,b} \pm 1$	$23^{b} \pm 1$	$22^{a,b} \pm 1$	$20^{b} \pm 1$
Standard	$28^{a} \pm 1$	$26^{a} \pm 1$	$26^{a} \pm 2$	$27^{a} \pm 1$

[a]Concentration.
[b]Standard drug (Rifampicine).
[c]Values are mean ± SD of three samples analyzed individually in triplicate at $p < 0.1$.
[d]Different letters in superscript indicate significant and non-significant differences with sample.

3.5. *Antifungal activity*

The antifungal activities of ligand and **1–5** were checked by using the disk diffusion method [16] against *Aspergillus niger*, *Aspergillus flavus*, *Ganoderma lucidum*, and *Alternaria alternata*. The results show that within a given series the triorganotin(IV) compounds are more active than diorganotin(IV) against fungal strains [12]. The results are shown in table 7.

3.6. *Structure activity relationship*

The results show that activity increases on chelation of ligand with metal with a direct relation between the activity and the coordination environment. All complexes show tetrahedral geometry in solution, consistent with species generating tetrahedral geometry in solution being more active [7, 9]. The activity of the ligand is affected by the nature of the substituent related to lipophilicity of the ligand. This could be attributed to the difference in structures of cell walls. The walls of Gram (−) cells are more complex than those of Gram (+) cells. The lipopolysaccharide forms an outer-lipid membrane and contributes to the complex antigenic specificity for the Gram (−) cells.

Table 7. Antifungal activity of homobimetallic complexes of Schiff base[a–d].

	Fungal zone size (mm)			
Complex no.	*A. niger*	*A. flavus*	*A. alternata*	*G. lucidum*
HL	0^{c}	0^{c}	0^{c}	0^{c}
1	$18^{b} \pm 1$	$18^{b} \pm 1$	$16^{b,c} \pm 1$	$15^{b,c} \pm 1$
2	0^{c}	0^{c}	0^{c}	0^{c}
3	0^{c}	0^{c}	0^{c}	0^{c}
4	$15^{b,c} \pm 1$	$14^{b,c} \pm 1$	$17^{b} \pm 1$	$17^{b} \pm 1$
5	$20^{a,b} \pm 1$	$21^{a,b} \pm 1$	$22^{a,b} \pm 1$	$20^{a,b} \pm 1$
Standard	$25^{a} \pm 1$	$23^{a} \pm 1$	$23^{a} \pm 2$	$23^{a} \pm 1$

[a]Concentration.
[b]Standard drug (Fluconazol).
[c]Values are mean ± SD of three samples analyzed individually in triplicate at $p < 0.1$.
[d]Different letters in superscript indicate significant and non-significant differences with sample.

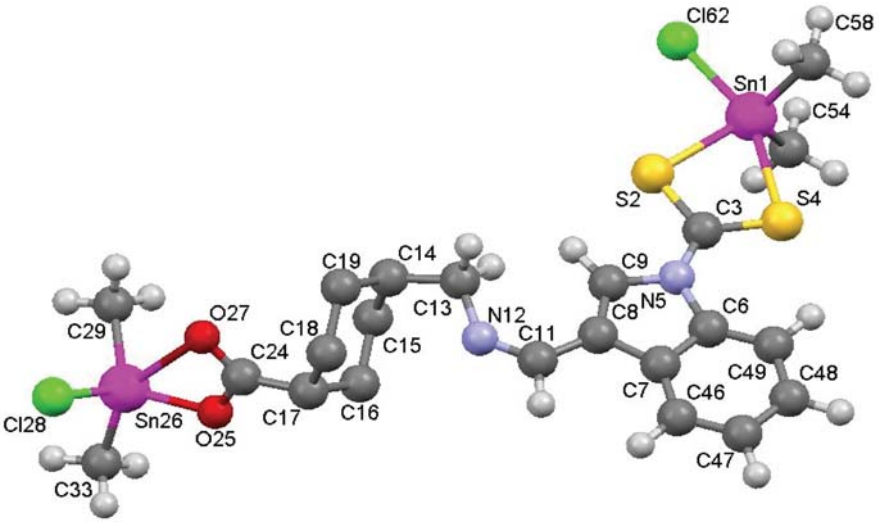


Figure 1. Geometry optimized structure of **1**. Complexes **2–5** are provided in Supplementary Material.

3.7. *Mechanism of action*

The mechanism of action is not fully understood, but it is assumed that the organic ligand supports the transport of organotin moiety to the site of action where it is released by hydrolysis. The anionic ligand also plays an important role in determining the degree of activity of organotin compounds [30, 31].

3.8. *Semi-empirical study*

In **1** and **2**, the ligand is bidentate to two Sn(IV). The two-methyl/butyl groups, Cl, dithio, and carboxylato are distorted trigonal bipyramidal. The Sn–S bond distances are 2.63 and 2.75 Å, respectively. The Sn–C bond lengths are 2.12 and 2.16 Å and Sn–Cl distances are 2.40 and 2.41 Å. The Sn–S–C bond angles are 93.1° and 91.9° and S–C–S bond angles are 114.3° and 114.3°, while the Cl–Sn–S angles are 153.8° and 154.3°.

In **3–5**, the ligand binds bidentate to two Sn(IV). The three-methyl/butyl/phenyl groups, dithio, and carboxylato are distorted trigonal bipyramidal. The Sn–S bond distances are 2.67 and 2.76 Å. The Sn–C bond lengths are 2.13, 2.18 and 2.08 Å. The Sn–S–C bond angles are 152.1°, 155.2° and 151.6° and S–C–S bond angles are 113.9°, 114.1° and 113.7°.

All bond lengths and angles are comparable to literature values [32]. The selected bond lengths and angles of the optimized structures are provided in Supplementary material. The optimized structure of **1** as a sample is given in figure 1.

4. Conclusion

IR spectroscopy indicated bidentate carboxylate and dithioic groups and suggests five-coordinate tin, which was also confirmed by the semi-empirical study. NMR data show five- or six-coordinate geometry in solution. These complexes were also checked for their

antimicrobial activity and the screening results showed that the reported compounds exhibit high antimicrobial activity as compared with free ligand.

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