



## Synthetic, structural and biological studies of organosilicon(IV) complexes of Schiff bases derived from pyrrole-2-carboxaldehyde

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**Abstract:** Selected new organosilicon(IV) complexes having the general formula  $R_2SiCl[L]$  and  $R_2Si[L]_2$  were synthesized by the reactions of  $Me_2SiCl_2$  with Schiff bases (5-mercaptopro-4-[(1*H*-pyrrol-2ylmethylene)amino]-*s*-triazole, 5-mercaptopro-3-methyl-4-[(1*H*-pyrrol-2ylmethylene)amino]-*s*-triazole and 3-ethyl-5-mercaptopro-4-[(1*H*-pyrrol-2ylmethylene)amino]-*s*-triazole) in 1:1 and 1:2 molar ratios. All of the compounds were characterized by elemental analysis, molar conductance, and IR, UV, <sup>1</sup>H-, <sup>13</sup>C- and <sup>29</sup>Si-NMR spectral studies. All the spectral data suggest an involvement with an azomethine nitrogen in coordination to the central silicon atom. With the help of above-mentioned spectral studies, penta and hexacoordinated environments around the central silicon atoms in the 1:1 and 1:2 complexes, respectively, are proposed. Finally, the free ligands and their metal complexes were tested *in vitro* against some pathogenic bacteria and fungi to assess their antimicrobial properties.

**Keywords:** antifungal; antibacterial; silicon complexes; *s*-triazole; Schiff bases.

### INTRODUCTION

The current research dealing with metal complexes of heteronuclear Schiff bases has expanded enormously and includes diversified subjects comprising their various aspects in bio-coordination and bio-inorganic chemistry. It is known that the presence of metal ions bonded to biologically active compounds may enhance their activity.<sup>1–6</sup> Heteronuclear Schiff base complexes have found applications as magnetic materials, catalysts and in the field of bio-engineering.<sup>7–10</sup> Organosilicon compounds of nitrogen- and sulphur-containing ligands are well known for their anticarcinogenic, antibacterial, tuberculostatic, antifungal, insecticidal and acaricidal activities.<sup>11–16</sup>

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The interest in organosilicon(IV)<sup>16–18</sup> compounds is due to their versatile applicability in the pharmaceutical industries. Generally, organosilicon compounds seem to owe their antitumour properties to the immuno-defensive system of the organism.<sup>19–22</sup> The medical applications and effectiveness of the silatranes in the treatment of wounds and tumours are thought to be related to the role of silicon in the growth of epithelial and connective tissues and hair, where their function is to impart strength, elasticity, and impermeability to water.<sup>23</sup> In view of this, the synthesis of organosilicon(IV) metal complexes of Schiff bases derived from the condensation of pyrrole-2-carboxaldehyde with different triazole derivatives is reported herein. The characterization of the complexes was realised by elemental analysis and spectroscopic (UV, IR, <sup>1</sup>H-, <sup>13</sup>C- and <sup>29</sup>Si-NMR) studies. Their antibacterial and antifungal activities were screened against various fungi and bacteria.

## EXPERIMENTAL

### Materials and methods

Analytical grade organosilicon chlorides, pyrrole-2-carboxaldehyde, hydrazine hydrate, carbon disulphide, methanol, dimethyl sulphoxide and cyclohexane were purchased from Acros and HiMedia. All the apparatus used during the experimental work were fitted with quick fit interchangeable standard ground joints. Strictly anhydrous conditions were maintained during the synthesis of the metal complexes, since the dichlorodimethylsilane and the product complexes are highly moisture-sensitive.

Silicon was determined gravimetrically as silicon dioxide. Melting points were measured using a capillary melting point apparatus. The molar conductance was measured with a Systronic type 305 conductivity bridge. The electronic spectra of ligands and their metal complexes were recorded in the region 1100–200 nm on a Hitachi U-2000 spectrophotometer, in dry methanol. The IR spectra were recorded on Buck scientific M500 grating spectrophotometer in nujol mulls in the range of 4000–250 cm<sup>-1</sup>. Multinuclear magnetic resonance spectra (<sup>1</sup>H, <sup>13</sup>C, and <sup>29</sup>Si) were recorded on a Bruker 400ACF spectrometer.

### Synthesis

4-Amino-5-mercaptop-s-triazole (AMT), 4-amino-5-mercaptop-3-methyl-s-triazole (AMMT) and 4-amino-3-ethyl-5-mercaptop-s-triazole (AEMT) were synthesized by a reported method.<sup>24</sup> The ligands, 5-mercaptop-4-[(1*H*-pyrrol-2-ylmethylene)amino]-s-triazole (HL<sup>1</sup>), 5-mercaptop-3-methyl-4-[(1*H*-pyrrol-2-ylmethylene)amino]-s-triazole (HL<sup>2</sup>), 3-ethyl-5-mercaptop-4-[(1*H*-pyrrol-2-ylmethylene)amino]-s-triazole (HL<sup>3</sup>) were synthesized by the condensation in ethanol of pyrrole-2-carboxaldehyde with AMT, AMMT and AEMT, respectively. The reaction mixture was refluxed for 3–4 h and allowed to cool. The products were filtered, washed and recrystallized from the same solvent and dried. The yields of the ligands HL<sup>1</sup>, HL<sup>2</sup> and HL<sup>3</sup> were 80, 77 and 72 %, respectively. The structure of the prepared ligands are given in Fig. 1.

### Synthesis of silicon complexes

To a weighed amount of Me<sub>2</sub>SiCl<sub>2</sub> in dry methanol was added the required amount of the sodium salt of the ligand HL<sup>1</sup>, HL<sup>2</sup> or HL<sup>3</sup> in 1:1 or 1:2 molar ratio. The reaction mixture was refluxed for about 12 h on a fractionating column. The sodium chloride formed during the reaction was removed by filtration. The excess of solvent was removed under reduced pressure

and the complexes were dried *in vacuo* at 35±5 °C after repeated washing with dry cyclohexane. The yields of the newly synthesized silicon complexes ranged from 67–70 %.

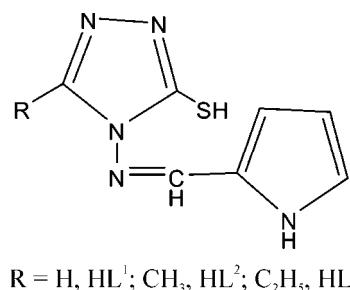


Fig. 1. 5-Mercapto-4-[(1*H*-pyrrol-2ylmethylene)amino]-*s*-triazole ( $\text{HL}^1$ ), 3-methyl-5-mercaptop-4-[1*H*-pyrrol-2ylmethylene)amino]-*s*-triazole ( $\text{HL}^2$ ) and 3-ethyl-5-mercaptop-4-[1*H*-pyrrol-2ylmethylene)amino]-*s*-triazole ( $\text{HL}^3$ ).

#### In vitro antifungal activity<sup>25</sup>

Potato dextrose agar medium (PDA) was prepared in flasks and sterilized before being poured into petri plates. The requisite quantity (100 µg/ml) of the standard antibiotic (ampicilline) was added to the medium just before pouring to check the growth of bacteria. Test samples were prepared in different concentrations (10 µg, 50 µg and 100 µg per ml) in dimethyl sulphoxide (DMSO) and 200 µl of each sample was added to PDA plates containing mycelial discs taken from 5–7-day-old cultures of fungi (*Aspergillus flavus* or *A. niger*). These plates were incubated for 5–7 days at 28±1 °C. Control plates underwent the same treatment except for the addition of the test samples. The efficacy of each sample was determined by measuring the radial mycelial growth. The radial growth of the colony was measured in two directions at right angle to each other and the average of two replicates was recorded in each case. Data were expressed as percent inhibition over control calculated from the size of colonies, and subjected to two-way analysis of variance. The percent inhibition was calculated using the formula:

$$\% \text{Inhibition} = (C-T) \times 100/C$$

where  $C$  is the diameter of the fungus colony in the control plate after 96 h incubation and  $T$  is the diameter of the fungus colony in the tested plate after same incubation period.

#### In vitro antibacterial assay

The newly synthesized ligands and their corresponding metal complexes were screened for their antibacterial activity against test bacteria, namely *Escherichia coli* (MTCC 51) and *Bacillus stearothermophilus*. Their antibacterial activities were determined by reported methods.<sup>26</sup> Turbidity of the control was adjusted to 0.5 McFarland standards.<sup>27</sup> All the test cultures were streaked on nutrient agar medium (peptone, 10 g l<sup>-1</sup>; yeast extract, 3.0 g l<sup>-1</sup>; NaCl, 5.0 g l<sup>-1</sup>; agar, 2 %) (NAM) and incubated overnight at 37 °C. By preparing bacterial suspension of 3–5 well-isolated colonies of the same morphological type selected from a NAM plate, the cultures were further diluted 10-fold to obtain an inoculum size of 1.2 CFU ml<sup>-1</sup>. A stock solution of 500 µg ml<sup>-1</sup> of each compound were prepared in DMSO and appropriately diluted to obtain final concentrations of 100 and 50 µg ml<sup>-1</sup>. The requisite quantity of antifungal compound (cyclohexamide) was added to the medium to obtain its desirable final concentration of 100 µg ml<sup>-1</sup>. Each appropriately diluted 100 µl test sample was spread over the solidified NAM. Separate flasks were taken for each test dilution. The test bacterial culture were spotted in a predefined pattern by aseptically transferring 5 µl of each bacterial culture onto the surface of solidified agar-agar plates and incubated at 35 °C for 24 h.

## RESULTS AND DISCUSSION

All the newly synthesized complexes were coloured solids soluble in DMSO, DMF and methanol. The conductivity values measured for 10<sup>-3</sup> M solutions in anhydrous DMF were in the range 10–15 Ω<sup>-1</sup> cm<sup>2</sup> mol<sup>-1</sup>, which indicates their non-electrolytic nature. The analytical data were in good agreement with the proposed stoichiometry of the complexes. The colour, physical and analytical data of the ligands and their silicon complexes are presented in Table I.

TABLE I. Physical characteristics and analytical data of the ligands and their silicon complexes

Compd.	Empirical formula/FW	Colour	M.p. °C	Calcd. (Found), %				
				C	N	H	S	Si
HL <sup>1</sup>	C <sub>7</sub> H <sub>7</sub> N <sub>5</sub> S/193	Grey	168–170	43.09 (43.52)	35.57 (36.26)	3.17 (3.62)	15.91 (16.58)	—
Me <sub>2</sub> SiCl(L <sup>1</sup> )	C <sub>9</sub> H <sub>12</sub> N <sub>5</sub> SiClS/285	Bluish	196–198	37.44 (37.89)	24.33 (24.56)	3.98 (4.21)	11.06 (11.22)	9.10 (9.82)
Me <sub>2</sub> Si(L <sup>1</sup> ) <sub>2</sub>	C <sub>16</sub> H <sub>18</sub> N <sub>10</sub> S <sub>2</sub> Si/442	Dark bluish	183–185	43.79 (42.43)	31.18 (31.67)	3.85 (4.07)	14.35 (14.47)	5.99 (6.33)
HL <sup>2</sup>	C <sub>8</sub> H <sub>9</sub> N <sub>5</sub> S/207	Light violet	165–168	46.87 (45.37)	33.26 (33.81)	4.05 (4.34)	15.30 (15.45)	—
Me <sub>2</sub> SiCl(L <sup>2</sup> )	C <sub>10</sub> H <sub>14</sub> N <sub>5</sub> SiClS/299	Light grey	210–212	39.78 (40.13)	23.13 (23.41)	4.22 (4.68)	10.03 (10.70)	9.12 (9.36)
Me <sub>2</sub> Si(L <sup>2</sup> ) <sub>2</sub>	C <sub>18</sub> H <sub>22</sub> N <sub>10</sub> SiS <sub>2</sub> /470	Dark grey	194–195	45.64 (45.95)	29.41 (29.78)	4.00 (4.68)	13.25 (13.61)	5.04 (5.95)
HL <sup>3</sup>	C <sub>9</sub> H <sub>11</sub> N <sub>5</sub> S/221	Grey	218–220	48.52 (48.86)	31.09 (31.67)	4.62 (4.97)	14.00 (14.47)	—
Me <sub>2</sub> SiCl(L <sup>3</sup> )	C <sub>11</sub> H <sub>16</sub> N <sub>5</sub> SiClS/313	Blackish	176–178	42.12 (42.17)	22.30 (22.36)	4.87 (5.11)	10.18 (10.22)	8.27 (8.94)
Me <sub>2</sub> Si(L <sup>3</sup> ) <sub>2</sub>	C <sub>20</sub> H <sub>26</sub> N <sub>10</sub> SiS <sub>2</sub> /498	Blackish	197–199	48.86 (47.19)	27.99 (28.11)	5.18 (5.22)	12.76 (12.85)	5.06 (5.62)

*Electronic spectra*

The electronic spectra of the ligands (HL<sup>1</sup> and HL<sup>2</sup>) and their silicon complexes of Si(IV) were studied by dissolving the ligands and their complexes in dry methanol. The electronic spectra of the ligands HL<sup>1</sup> and HL<sup>2</sup> exhibited maxima at 387 and 358 nm, respectively, which can be assigned to the n–π\* transition of the azomethine group. These bands showed a blue shift in the Si (1:1 and 1:2) complexes and appeared at 370 (Me<sub>2</sub>SiL<sup>1</sup>Cl), 341 (Me<sub>2</sub>Si{L<sup>1</sup>}<sub>2</sub>), 340 (Me<sub>2</sub>SiL<sup>2</sup>Cl) and 321 nm (Me<sub>2</sub>Si{L<sup>2</sup>}<sub>2</sub>), respectively. This clearly indicates the coordination of the azomethine nitrogen atom to the silicon atom. Furthermore, two medium intensity bands at 294 and 223 nm due to π–π\* transitions in the ligands remained unchanged in the spectra of the silicon complexes.



### *IR Spectra*

The ligands exhibited a broad band at  $\approx 2750 \text{ cm}^{-1}$  due to  $\nu(\text{S}-\text{H})$ ,<sup>28</sup> which disappeared in the spectra of silicon complexes, indicating deprotonation and complexation through the sulphur atom. A new band appears at  $\approx 750 \text{ cm}^{-1}$ , which was assigned to  $\nu(\text{C}-\text{S})$  and which further confirms the coordination of the ligand through the sulphur atom. Silicon–sulphur bond formation was further supported by a band at  $\approx 450 \text{ cm}^{-1}$  of  $\nu(\text{Si}-\text{S})$ .<sup>29</sup> The sharp and strong band at  $\approx 1597 \pm 5 \text{ cm}^{-1}$ , assignable to  $\nu(-\text{N}=\text{CH}<)$ ,<sup>30</sup> was shifted to higher wavelength numbers  $\approx 1605 \pm 5 \text{ cm}^{-1}$  in the spectra of the metal complexes, indicating coordination through the azomethine nitrogen to the silicon atom. This shift can be explained by a reduction of the carbon–nitrogen double bond character in the azomethine group. Formation of a silicon–nitrogen bond was further confirmed by the presence of a band at  $\approx 575 \text{ cm}^{-1}$  of  $\nu(\text{Si}-\text{N})$ .<sup>31</sup> A strong band in the region of  $485$ – $431 \text{ cm}^{-1}$  was assigned to  $\nu(\text{M}-\text{Cl})$ <sup>32</sup> in the 1:1 metal complexes. A characteristic band at  $\approx 3250 \text{ cm}^{-1}$ , due to  $\nu(\text{N}-\text{H})$  of pyrrole, was observed in the spectra of the ligands and their silicon complexes. The infrared spectral data of the ligands and their silicon complexes are listed in Table II.

TABLE II. IR Spectroscopic data ( $\text{cm}^{-1}$ ) of the ligands and their silicon complexes

Compd.	$\nu(\text{S}-\text{H})$	$\nu(\text{N}-\text{H})$	$\nu(-\text{C}=\text{N})$	$\nu(-\text{C}-\text{S})$	$\nu_{\text{Si}-\text{S}}$	$\nu_{\text{Si}-\text{N}}$
$\text{HL}^1$	2760	3238	1597	—	—	—
$\text{Me}_2\text{SiCl}(\text{L}^1)$	—	3240	1603	746	443	555
$\text{Me}_2\text{Si}(\text{L}^1)_2$	—	3240	1607	749	448	578
$\text{HL}^2$	2744	3251	1611	734	—	—
$\text{Me}_2\text{SiCl}(\text{L}^2)$	—	3255	1620	745	451	545
$\text{Me}_2\text{Si}(\text{L}^2)_2$	—	3254	1613	—	455	571
$\text{HL}^3$	2768	3256	1593	—	—	—
$\text{Me}_2\text{SiCl}(\text{L}^3)$	—	3260	1597	752	450	535
$\text{Me}_2\text{Si}(\text{L}^3)_2$	—	3260	1603	757	455	567

### *<sup>1</sup>H-NMR Spectra*

To confirm further the bonding pattern in these complexes, the  $^1\text{H-NMR}$  spectra of the ligands and their silicon complexes were recorded in  $\text{DMSO}-d_6$  using TMS as the internal standard. The  $^1\text{H-NMR}$  spectroscopic data of the ligands and their silicon complexes are given in Table III. The  $^1\text{H-NMR}$  spectra of the ligands showed  $-\text{SH}$  proton signal at  $\delta 13.70 \pm 0.15 \text{ ppm}$ . The disappearance of this signal due to  $-\text{SH}$  protons in the spectra of the silicon complexes indicates deprotonation of the thiol group, which supported the coordination of silicon through the sulphur atom of the ligand. A signal at  $\delta 9.40 \pm 0.10 \text{ ppm}$  was observed in the spectra of the silicon complexes due to the azomethine protons, which moved downfield in comparison to their original position in the free ligands, thereby indicating the coordination through the azomethine nitrogen to the

silicon atom. A sharp singlet due to  $-\text{NH}$  proton (pyrrole) was also observed at  $\delta$  11.5–12.0 ppm in the spectra of ligands. Some additional signals at  $\delta$  3.5–4.0 ppm (*s*,  $-\text{H}$ , triazole),  $\delta$  2.0–3.5 ppm (*s*,  $-\text{CH}_3$ , triazole),  $\delta$  2.0–3.0 ppm (*q*,  $-\text{CH}_2\text{CH}_3$ , triazole) and  $\delta$  1.0–2.0 ppm (*t*,  $-\text{CH}_2\text{CH}_3$ , triazole) were observed in the ligands and their silicon complexes. Furthermore, the additional signals in the region  $\delta$  0.5–1.0 ppm were due to  $\text{Me}_2\text{Si}$  groups of the complexes.<sup>33,34</sup>

TABLE III.  $^1\text{H-NMR}$  Chemical shifts of the ligands and their silicon complexes

Cmpd.	Aromatic- <b>H</b>	-NH (pyrrole)	-SH	Azomethine- <b>H</b>	-H,-CH <sub>3</sub> , -C <sub>2</sub> H <sub>5</sub>
HL <sup>1</sup>	6.2–7.1	11.4	13.7	9.5	3.5 ( <i>s</i> )
$\text{Me}_2\text{SiCl(L}^1\text{)}$	6.1–7.1	11.2	—	9.4	3.4 ( <i>s</i> ), 0.74 ( <i>s</i> )
$\text{Me}_2\text{Si(L}^1\text{)}_2$	6.0–7.2	11.2	—	9.4	3.4 ( <i>s</i> ), 0.52 ( <i>s</i> )
HL <sup>2</sup>	6.2–7.1	11.5	13.6	9.4	2.2 ( <i>s</i> )
$\text{Me}_2\text{SiCl(L}^2\text{)}$	6.0–7.1	11.4	—	8.4	2.1 ( <i>s</i> ), 0.86 ( <i>s</i> )
$\text{Me}_2\text{Si(L}^2\text{)}_2$	6.1–7.2	11.3	—	8.4	2.1 ( <i>s</i> ), 0.56 ( <i>s</i> )
HL <sup>3</sup>	6.0–6.8	11.9	13.3	9.3	2.3 ( <i>q</i> ), 1.9 ( <i>t</i> )
$\text{Me}_2\text{SiCl(L}^3\text{)}$	6.6–7.2	11.6	—	9.1	2.1 ( <i>q</i> ), 1.7 ( <i>t</i> ), 0.89 ( <i>s</i> )
$\text{Me}_2\text{Si(L}^3\text{)}_2$	6.2–7.1	11.7	—	9.1	2.1 ( <i>q</i> ), 1.8 ( <i>t</i> ), 0.50 ( <i>s</i> )

### *<sup>13</sup>C-NMR Spectra*

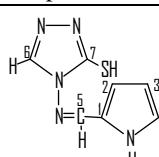
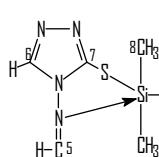
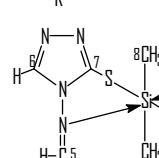
The  $^{13}\text{C-NMR}$  spectra of the ligand HL<sup>1</sup> and its corresponding 1:1 and 1:2 silicon complexes were recorded and the data are given in Table IV. The signal due to the azomethine carbon atom of the ligand appears at  $\delta$  151.61 ppm. However, in the spectra of the corresponding silicon complexes, the signal appeared at higher  $\delta$  values. The considerable shifting in the carbon atom attached to the azomethine nitrogen indicates coordination of nitrogen to the central metal atom in the 1:1 and 1:2 metal complexes. Furthermore, the shifting of the  $^{13}\text{C}$  resonance that is attached to the sulphur atom in the spectra of the 1:1 and 1:2 silicon complexes, compared to the free ligands, indicates coordination through sulphur to the silicon atom. Additional signals in the  $^{13}\text{C-NMR}$  spectra of the silicon complexes were observed at  $\delta$  10.32 ppm and  $\delta$  8.57 ppm (Si–C) in the 1:1 and 1:2 silicon complexes, respectively.

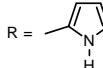
### *<sup>29</sup>Si-NMR Spectra*

In order to confirm the geometry of the complexes,  $^{29}\text{Si-NMR}$  spectra of the complexes were recorded. The value of  $\delta^{29}\text{Si}$  in the spectra reflects the coordination number of the nucleus in the corresponding silicon complex.<sup>35,36</sup> In general,  $^{29}\text{Si}$  chemical shifts move to lower frequency with increasing coordination number of the nuclei. The spectra show in each case only one sharp singlet indicating the formation of a single species. The  $^{29}\text{Si-NMR}$  spectra of the 1:1 and 1:2 silicon complexes exhibited sharp signals at  $\delta$  –97.38 ppm and  $\delta$  –107.78 ppm,

which is indicative of a penta- and a hexa-coordinated environment around the silicon atom, respectively.

TABLE IV.  $^{13}\text{C}$ -NMR Chemical shifts of the ligands and their silicon complexes

Compd.	C <sub>1</sub>	C <sub>2</sub>	C <sub>3</sub>	C <sub>4</sub>	C <sub>5</sub>	C <sub>6</sub>	C <sub>7</sub>	M-CH <sub>3</sub>
	125.52	124.45	110.37	118.10	151.61	161.26	155.82	—
	125.35	124.21	110.32	118.02	155.99	161.30	152.37	10.32
	125.40	124.11	110.33	118.12	156.12	161.45	152.36	8.57



Based on the above evidences, it is suggested that the geometries around the silicon atom in the complexes investigated were trigonal bipyramidal and octahedral in the 1:1 and 1:2 ratios, respectively, as shown in Fig. 2.

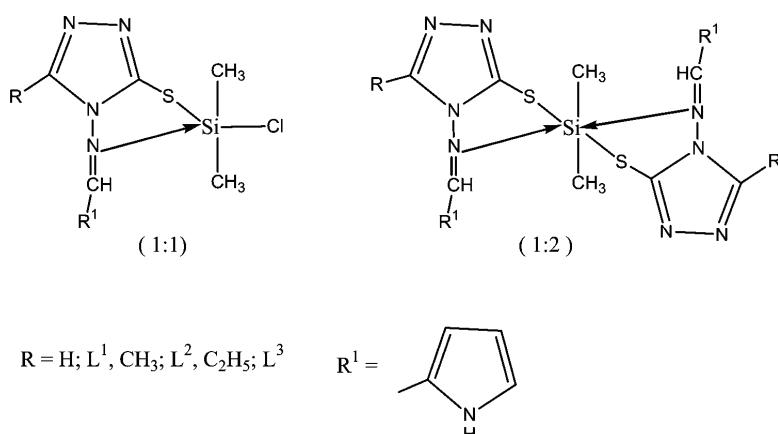


Fig. 2. Proposed structures of the 1:1 and 1:2 complexes.

### *Biological aspects*

The free ligands and their silicon complexes were screened against various fungi and bacteria to assess their potential as antimicrobial agents. The fungicidal and bactericidal activities of free ligands HL<sup>1</sup>, HL<sup>2</sup> and HL<sup>3</sup> and their organo-silicon(IV) complexes against various fungi and bacteria are given in Tables V and VI, respectively.

TABLE V. Antifungal screening (average percentage inhibition after 96 h)

Compd.	Concentration, $\mu\text{g ml}^{-1}$	<i>A. flavus</i>	<i>A. niger</i>
$\text{C}_7\text{H}_7\text{N}_5\text{S}$	Control	Nil	Nil
	50	Nil	Nil
	100	Nil	Nil
	500	Nil	Nil
$\text{C}_9\text{H}_{12}\text{N}_5\text{SiCl}_3$	Control	0.00	0.00
	10	9.20	7.31
	50	29.31	13.55
	100	52.11	37.69
$\text{C}_{16}\text{H}_{18}\text{N}_{10}\text{S}_2\text{Si}$	Control	0.00	0.00
	10	32.71	19.73
	50	48.14	79.43
	100	84.12	94.71
$\text{C}_8\text{H}_9\text{N}_5\text{S}$	Control	Nil	Nil
	10	Nil	Nil
	50	0.01	0.00
	100	11.10	13.05
$\text{C}_{10}\text{H}_{14}\text{N}_5\text{SiCl}_3$	Control	0.00	0.00
	10	45.54	35.12
	50	64.72	78.64
	100	89.47	89.41
$\text{C}_{18}\text{H}_{22}\text{N}_{10}\text{SiS}_2$	Control	0.00	0.00
	10	45.79	35.13
	50	57.89	68.32
	100	84.41	78.62
$\text{C}_9\text{H}_{11}\text{N}_5\text{S}$	Control	0.00	0.00
	10	Nil	Nil
	50	Nil	Nil
	100	Nil	Nil
$\text{C}_{11}\text{H}_{16}\text{N}_5\text{SiCl}_3$	Control	0.00	0.00
	10	10.87	9.30
	50	26.33	20.55
	100	62.58	47.90
$\text{C}_{20}\text{H}_{26}\text{N}_{10}\text{SiS}_2$	Control	0.00	0.00
	10	35.40	40.21
	50	62.25	71.43
	100	88.27	90.23



TABLE VI. Antibacterial screening data of the ligands and their metal complexes

Cmpd.	Concentration, $\mu\text{g ml}^{-1}$	Inhibition, %	
		<i>E. coli</i>	<i>B. stearothermophilus</i>
$\text{C}_7\text{H}_7\text{N}_5\text{S}$	50	Nil	Nil
	100	Nil	Nil
	500	14	20
$\text{C}_9\text{H}_{12}\text{N}_5\text{SiClS}$	50	16	31
	100	37	58
	500	63	73
$\text{C}_{16}\text{H}_{18}\text{N}_{10}\text{S}_2\text{Si}$	50	21	29
	100	32	47
	500	56	61
$\text{C}_8\text{H}_9\text{N}_5\text{S}$	50	Nil	Nil
	100	Nil	Nil
	500	17	21
$\text{C}_{10}\text{H}_{14}\text{N}_5\text{SiClS}$	50	45	29
	100	83	60
	500	91	83
$\text{C}_{18}\text{H}_{22}\text{N}_{10}\text{SiS}_2$	50	22	19
	100	38	42
	500	55	72
$\text{C}_9\text{H}_{11}\text{N}_5\text{S}$	50	Nil	Nil
	100	11	14
	500	31	38
$\text{C}_{11}\text{H}_{16}\text{N}_5\text{SiClS}$	50	20	13
	100	43	32
	500	68	43
$\text{C}_{20}\text{H}_{26}\text{N}_{10}\text{SiS}_2$	50	24	30
	100	49	40
	500	72	51

The antimicrobial data revealed that the complexes were superior to the free ligands. The activity increased as the concentration increased. These complexes were found to be more potent inhibitor for the growth of *E. coli* among test bacterial cultures and nearly equally sensitive for test fungal cultures. Thus, it can be postulated that further studies of these complexes in this direction could lead to interesting results.

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## ИЗВОД

## СИНТЕЗА И СТРУКТУРНО И БИОЛОШКО ИСПИТИВАЊЕ ОРГАНОСИЛИЦИЈУМ(IV)-КОМПЛЕКСА ШИФОВИХ БАЗА ДОБИЈЕНИХ ИЗ ПИРОЛ-2-КАРБОАЛДЕХИДА

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Одабрани нови органосилицијум(IV)-комплекси, опште формуле  $R_2SiCl[L]$  и  $R_2Si[L]_2$  синтетизовани су у реакцијама  $Me_2SiCl_2$  са Schiff-овим базама (5-меркапто-4-[(1Н-пирол-2-илметилен)амино]-s-триазолом, 5-меркапто-3-метил-4-[(1Н-пирол-2-илметилен)амино]-s-триазолом и 3-етил-5-меркапто-4-[(1Н-пирол-2-илметилен)амино]-s-триазолом) у 1:1 и 1:2 моларним односима. Сва једињења окарактерисана су помоћу елементалне анализе, моларне проводљивости, IR, UV, <sup>1</sup>H-, <sup>13</sup>C- и <sup>29</sup>Si-NMR спектралним проучавањем. Спектроскопски подаци сугеришу да је азометински азот укључен у координацију са централним силицијумовим атомом. На основу поменутих спектралних података предложена је пента- и хексакоординација око централних силицијумових атома у 1:1, односно 1:2 комплексима. Коначно, слободни лиганди и њихови силицијумови комплекси тестирани су *in vitro* на неке патогене бактерије и гљивице у циљу процене њихових антимикробних особина.

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