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Synthesis, spectral and structural investigations, theoretical studies, and antibacterial activity of 4-(2-hydroxynaphthalen-3-ylamino)pent-3-en-2-one and its diphenyltin(IV) complex

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The Schiff base, 4-(2-hydroxynaphthalen-3-ylamino)pent-3-en-2-one (H_2L) and its diphenyltin complex have been synthesized and characterized by elemental analysis and FT-IR, ^1H, or ^{119}Sn NMR spectroscopy. The structures of free ligand and complex have been confirmed by single-crystal X-ray diffraction. In the structure of H_2L, enolic proton is transferred to imine nitrogen and there is an intramolecular hydrogen bond between amine and carbonyl group. There are also 1-D intermolecular hydrogen-bonded chains with π–π stacking between chains. $SnPh_2L$ is crystallized in the *Pca*2(1) orthorhombic space group with four molecules in an asymmetric unit cell. The geometry around tin is a highly distorted trigonal bipyramid with Schiff base completely deprotonated and coordinated tridentate to tin *via* phenolic and enolic oxygen atoms in axial and imine nitrogen in equatorial positions. The results of X-ray diffraction were also compared with density functional theory calculations. These calculations also confirm the keto-amine tautomeric form for Schiff base in solid phase. The *in vitro* antibacterial activities of ligand and complex have been evaluated against Gram-positive (*Bacillus cereus* and *Staphylococcus aureus*) and Gram-negative (*Escherichia coli* and *Pseudomonas aeruginosa*) bacteria. H_2L showed no activity but the diphenyltin(IV) complex exhibited good activities along with the standard antibacterial drugs.

Keywords: Diorganotin(IV); Schiff base; X-ray crystallography; DFT calculations; Antibacterial activity

1. Introduction

Tin has played a considerable role in organometallic chemistry, stimulated by a variety of applications. The most significant developments have been increasing use of organotin compounds in industry, agriculture, and medicine, though in recent years these have been circumscribed by environmental considerations [1–7]. Structural studies have always been prominent in organotin chemistry. The organotin(IV) halides have a

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marked tendency to increase their coordination number and are convenient systems for investigation of Lewis acid–base interactions. Organotin(IV) complexes have demonstrated various coordination geometries in coordination numbers three through seven. They present a variety of structural possibilities, so that remarkable diversity in structure may be observed even when only a small change occurs [8, 9]. Considerable efforts have been made to synthesize and characterize organotin compounds having heterodonors (O, N, and S), which have different applications and stabilities depending on the number, type, and arrangement of ligands about tin; many studies have been focused on their structure-activity correlations [10–15]. In general, the biochemical activity of organotin compounds is influenced by the structure and coordination number of tin.

Organotin(IV) complexes with Schiff bases have potential applications in medicinal chemistry and biotechnology and structural variety due to the multidenticity of these ligands [3, 16–20]. Both aliphatic and aromatic Schiff bases in their neutral and deprotonated forms react with organotin(IV) halides; the complexes formed exhibit variable stoichiometry in the metal to ligand ratio and different modes of coordination [21–30]. As an extension of this research and since little attention has been paid to systems in which the Schiff base is derived from a β-diketone, we synthesize a Schiff base (figure 1) derived from condensation of 3-amino-2-naphthol and acetylacetone and its organotin(IV) complex. The structures of Schiff base and organotin complex have been investigated by spectroscopic methods as well as X-ray crystallography and theoretical calculations. The *in vitro* antibacterial activities of ligand and its complex have also been evaluated.

2. Experimental

2.1. *Materials and methods*

All starting materials were purchased from Merck except diphenyltin dichloride from Acros Company and were all used as received. All solvents were reagent grade and used without purification. Infrared (IR) spectra were obtained using a FT BOMEM MB102 spectrophotometer. ^{1}H and ^{119}Sn NMR spectra were recorded with a Bruker 400 MHz Avance Ultrashield spectrometer. The C, H, and N analyses were performed by the microanalytical service of the N.I.O.C. Research Institute of Petroleum Industry.

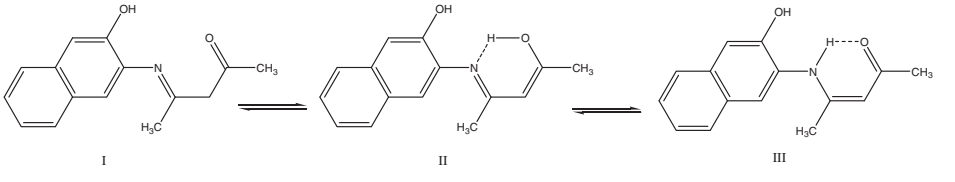

Figure 1. Tautomeric forms for 4-(2-hydroxynaphthalen-3-ylamino)pent-3-en-2-one (H_2L); I: keto-imine, II: enol-imine, and III: keto-amine.

2.2. *Synthesis of 4-(2-hydroxynaphthalen-3-ylamino)pent-3-en-2-one (H_2L)*

The Schiff base was synthesized by refluxing a mixture of 3-amino-2-naphthol (0.397 g, 2.5 mmol) and acetylacetone (0.207 g, 2.5 mmol) in ethanol (35 mL) for 4 h. The resulting product was filtered, washed with ethanol, and dried. Hexagonal pale yellow single crystals suitable for X-ray crystallography were collected by slow evaporation of dilute ethanolic solution of the compound after 20 days. Yield: 0.506 g (84%); m.p. 162–164°C; Anal. Calcd for $C_{15}H_{15}NO_2$ (%): C, 74.67; H, 6.27; N, 5.81. Found (%): C, 74.61; H, 6.48; N, 5.48: FT-IR (KBr, cm^{-1}): 3051, ν(OH); 1633, ν(C=N); 1595, ν(C=C). ^{1}H NMR (DMSO-d_6): $\delta = 2.00$ (s, 3H, C(5)H_3), 2.17 (s, 3H, C(1)H_3), 5.28 (s, 1H, H_3), 7.22–7.33 (m, 3H, $H_{8,12,15}$), 7.63–7.74 (m, 3H, $H_{10,11,13}$), 10.42 (s, 1H, OH_{enolic}), 12.42 (s, 1H, $OH_{phenolic}$).

2.3. *Synthesis of $SnPh_2L$*

KOH (0.056 g, 1 mmol) was added to a methanolic (20 mL) solution of H_2L (0.121 g, 0.5 mmol) and yellow anionic solution was obtained. A solution of $SnPh_2Cl_2$ (0.172 g, 0.5 mmol) in methanol (5 mL) was added dropwise to this anionic solution with stirring at room temperature. A yellow precipitate formed after 15 min, was filtered, washed with methanol, and dissolved in chloroform to eliminate KCl precipitate. Recrystallization in methanol gave yellow needle single crystals suitable for X-ray crystallography by slow evaporation after 12 days. Yield: 0.181 g (71%); m.p. 131–133°C; Anal. Calcd for $C_{27}H_{23}NO_2Sn$ (%): C, 63.31; H, 4.53; N, 2.73. Found (%): C, 63.49; H, 4.31; N, 3.06. FT-IR (KBr, cm^{-1}): 1593, ν(C=O); 1620, ν(C=N)/ν(C=C); 506, ν(Sn–O); 446, ν(Sn–N). ^{1}H NMR (DMSO-d_6): $\delta = 2.17$ (s, 3H, C(24)H_3), 2.45 (s, 3H, C(27)H_3), 5.51 (s, 1H, H_{25}), 7.13–7.31 (m, 3H, $H_{14,17,21}$), 7.33–7.44 (m, 6H, $H_{m,p}$ in Sn–Ph), 7.59–7.74 (m, 7H, H_o in Sn–Ph and $H_{16,18,19}$). ^{119}Sn NMR ($CDCl_3$): $\delta = -306.69$ ppm.

2.4. *X-ray structure determination*

Data were collected at room temperature with a Bruker APEX II CCD area-detector diffractometer using Mo-Kα radiation ($\lambda = 0.71073$ Å). Data collection, cell refinement, data reduction, and absorption correction were performed using multiscan methods with Bruker software [31]. The structures were solved by direct methods using SIR2004 [32].

The non hydrogen atoms were refined anisotropically by full-matrix least-squares on F^2 using SHELXL-97 [33]. All hydrogen atoms were placed at calculated positions and constrained to ride on their parent atoms. Details concerning collection and analysis are reported in table 1.

2.5. *Antibacterial tests*

The *in vitro* antibacterial activities of ligand and its corresponding organotin(IV) complex were investigated against the standard strains of two Gram-positive (*Bacillus cereus* and *Staphylococcus aureus* ATCC 6538) and two Gram-negative (*Escherichia coli* ATCC 11303 and *Pseudomonas aeruginosa* ATCC 27853) bacteria. In order to compare

Table 1. Crystallographic and structure refinement data for H_2L and $SnPh_2L$.

	H_2L	$SnPh_2L$
Empirical formula	$C_{15}H_{15}NO_2$	$C_{27}H_{23}NO_2Sn$
Formula weight	241.28	512.15
Temperature (K)	296(2)	293(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Orthorhombic
Space group	$P2_1/c$	$Pca2(1)$
Unit cell dimensions (Å, °)		
a	11.3450(3)	13.712(5)
b	11.4614(3)	12.949(5)
c	10.4112(3)	12.796(4)
β	113.9780(10)	90.00
Volume (Å^3), Z	1236.94(6), 4	2272.0(14), 4
Calculated density (g cm^{-3})	1.296	1.497
Absorption coefficient (mm^{-1})	0.086	1.148
$F(000)$	512	1032
Crystal size (mm^3)	$0.17 \times 0.23 \times 0.92$	$0.20 \times 0.29 \times 0.31$
θ range for data collection (°)	2.65–29.94	2.16–23.94
Limiting indices	$-14 \le h \le 14$; $-14 \le k \le 14$; $-13 \le l \le 13$	$-16 \le h \le 16$; $-15 \le k \le 15$; $-15 \le l \le 15$
Reflections collected	2707	4225
Independent reflection	1774 [R(int) = 0.0330]	3127 [R(int) = 0.0494]
Parameters/restraints	164/0	281/1
Goodness-of-fit on F^2	1.027	0.926
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0509$, $wR_2 = 0.1579$	$R_1 = 0.0362$, $wR_2 = 0.0900$
R indices (all data)	$R_1 = 0.0755$, $wR_2 = 0.1714$	$R_1 = 0.0654$, $wR_2 = 0.1142$
Extinction coefficient	Not measured	0.00070(17)
Flack parameter	–	0.08(2)
Largest difference peak and hole (e Å^{-3})	0.342 and −0.266	0.855 and −0.777

the results, Vancomycin (30 mg disc^{-1}), Streptomycin (10 mg disc^{-1}), penicillin (10 mg disc^{-1}), Nalidixic acid (30 mg disc^{-1}), and Gentamicin (10 mg disc^{-1}) were used as standard antibacterial drugs. Determination of the antibacterial activity was carried out by paper-disc diffusion method. The compounds were dissolved in DMSO at 5 mg mL^{-1}. Mueller–Hinton broth was used for preparing basal media for the bioassay of the organisms. A lawn culture from 0.5 MacFarland suspension of each strain was prepared on Mueller–Hinton agar. Blank paper discs (6.4 mm diameter) were saturated with a solution of test compound (40 µL) and placed on the surface of the agar plates. On one paper disc only DMSO was poured as a control. The plates were incubated at 37°C for 24 h. The inhibition zone diameters around each disc were measured in mm.

3. Results and discussions

3.1. *Synthesis*

H_2L was synthesized by reaction of acetylacetone with 3-amino-2-naphthol in ethanol. This Schiff base, similar to other Schiff bases derived from β-diketones [18, 28, 34–36], can exist as three tautomeric forms (figure 1). The diphenyltin(IV) complex has been

Table 2. Selected bond lengths (Å) and angles (°) for H_2L, calculated values *vs.* experimental X-ray data.

	Experimental	B3LYP/6-31G*	B3LYP/6-311 + G**
C(1)–C(2)	1.504(2)	1.522	1.518
C(2)–C(3)	1.404(3)	1.445	1.441
C(3)–C(4)	1.352(3)	1.379	1.380
C(4)–N(1)	1.377(2)	1.363	1.359
N(1)–C(6)	1.415(2)	1.400	1.402
C(6)–C(7)	1.422(2)	1.436	1.433
C(2)–O(1)	1.254(2)	1.244	1.242
C(7)–O(2)	1.356(3)	1.365	1.365
O(1)–C(2)–C(1)	119.01(19)	119.45	119.00
O(1)–C(2)–C(3)	123.22(16)	123.35	123.06
C(2)–C(3)–C(4)	125.62(16)	124.34	124.29
C(3)–C(4)–C(5)	119.00(15)	119.57	119.49
N(1)–C(4)–C(3)	120.97(15)	120.12	120.23
N(1)–C(4)–C(5)	120.00(16)	120.27	120.24
N(1)–C(6)–C(7)	117.31(15)	116.03	116.62
O(2)–C(7)–C(6)	116.18(14)	115.22	115.39

synthesized from $SnPh_2Cl_2$ and H_2L in methanol at room temperature in the presence of KOH in a 1 : 1 : 2 ratio with a slight excess of KOH.

3.2. *X-ray structures*

Selected bond angles and distances for H_2L are listed in table 2. The molecular structure with atom numbering scheme of H_2L is given in figure 2. H_2L is crystallized in the $P2_1/c$ monoclinic space group and four molecules are present in an asymmetric unit cell. In the structure of H_2L, there are a strong intramolecular hydrogen bond (N1–H1$\cdots$O1) between amine and carbonyl and a weak hydrogen bond (N1–H1$\cdots$O2) between amine and hydroxyl, with amine participating in two intramolecular hydrogen bonds. The C3–C4 bond length, 1.377(3), is close to C=C distance of 1.34 [37] and C2–O1 bond length, 1.254(2), is similar to the value observed for conjugated C=O bonds [38], confirming that enolic proton is transferred to imine nitrogen and H_2L is in keto-amine form III. In this compound, there are also 1-D intermolecular hydrogen-bonded chains (O2–H2$\cdots$O1) with π–π stacking interactions between planes of parallel rings providing additional stabilization (figure 3). Therefore, O1 participates in both intermolecular and intramolecular hydrogen bonding. Hydrogen bond distances and angles are listed in table 3.

Selected bond angles and distances for $SnPh_2L$ are listed in table 4. The molecular structure with atom numbering scheme is given in figure 4. $SnPh_2L$ crystallizes in the *Pca*2(1) orthorhombic space group and four molecules are present in the asymmetric unit cell. The Schiff base is bonded to the $SnPh_2$ as an ONO dianionic tridentate ligand *via* phenolic and enolic oxygen atoms and imine nitrogen. Therefore, the tin is five coordinate with an O_2NC_2 core. To quantify the extent of distortion from either ideal square pyramid (SP) or trigonal bipyramid (TBP), the index of trigonality, τ, has been found from $\tau = (\alpha - \beta)/60$ defined by Reedijk and coworkers [39], α and β are two

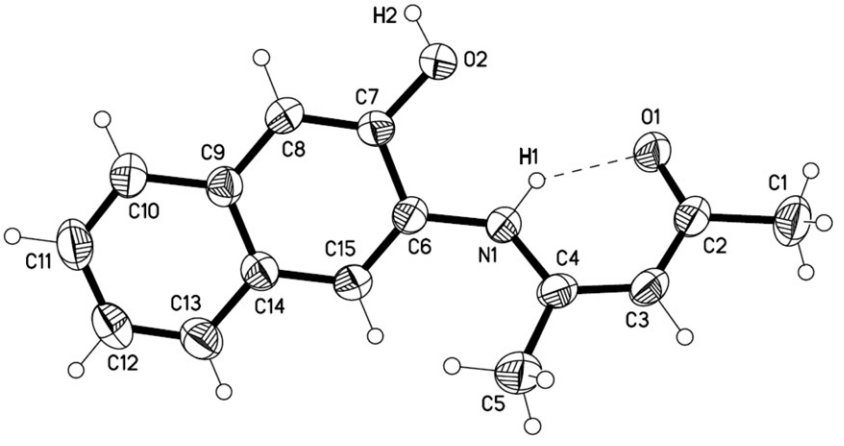

Figure 2. Crystal structure of H_2L.

largest bond angles around the metal atom. For a perfect SP geometry, the trigonality index is equal to zero, while it becomes unity for ideal TBP. The τ value is 0.531 and indicates the geometry of the complex is between square-pyramidal and trigonal-bipyramidal. Therefore, the geometry around the tin is a highly distorted TBP with phenolic and enolic oxygen atoms in axial and azomethine nitrogen and two *ipso*-carbon atoms from phenyl groups in equatorial positions. This distortion from trigonal-bipyramidal geometry is confirmed by the bond angles O(1)–Sn(1)–N(1) 77.10(18)°, O(2)–Sn(1)–N(1) 83.0(2)°, O(1)–Sn(1)–C(7) 98.5(2)°, O(2)–Sn(1)–C(7) 94.5(2)°, O(2)–Sn(1)–C(1) 89.2(3)°, and O(1)–Sn(1)–C(1) 96.1(2)° deviating from the 90° expected for a perfect structure. The angle subtended at tin(IV) by two oxygen atoms is compressed to 158.9(2)°. The C(1)–Sn–C(7) 126.9(3)°, C(7)–Sn–N1 109.5(2)°, and C(1)–Sn–N(1) 123.6(3)° angles also deviate from the exact trigonal angle of 120°. These distortions are mainly due to the rigidity of chelate rings and large covalent radius of tin(IV) [24, 40]. The sum of the equatorial angles is 360°; therefore, the Sn is completely in the plane defined by N(1), C(1), and C(7). The Sn–N2, Sn–O1, and Sn–O2 bond lengths are very similar to the sum of the covalent radii of Sn–N (2.15 Å) and Sn–O (2.10 Å) [41–43], indicating very strong tin–nitrogen and tin–oxygen interactions.

3.3. *Spectroscopic studies*

In the IR spectrum of H_2L, there is no band in the free C=O stretching region, ruling out the keto-imine form I. A band at 1633 cm^{-1} has been assigned as a perturbed carbonyl stretch with the frequency lowered from a free carbonyl due to conjugation and hydrogen bonding in keto-amine form III [18, 28, 44]. In the IR spectrum of complex, this band shifts to lower frequency, indicating participation of oxygen in bonding with tin. A broad band at 3000–3100 cm^{-1} assigned to NH or OH in the spectrum of free ligand is absent in the complex due to deprotonation of the ligand during coordination. New bands in the IR spectrum of the complex assigned to ν(Sn–N) and ν(Sn–O) confirm the bonding of nitrogen and oxygen to tin [27, 28, 30, 45].

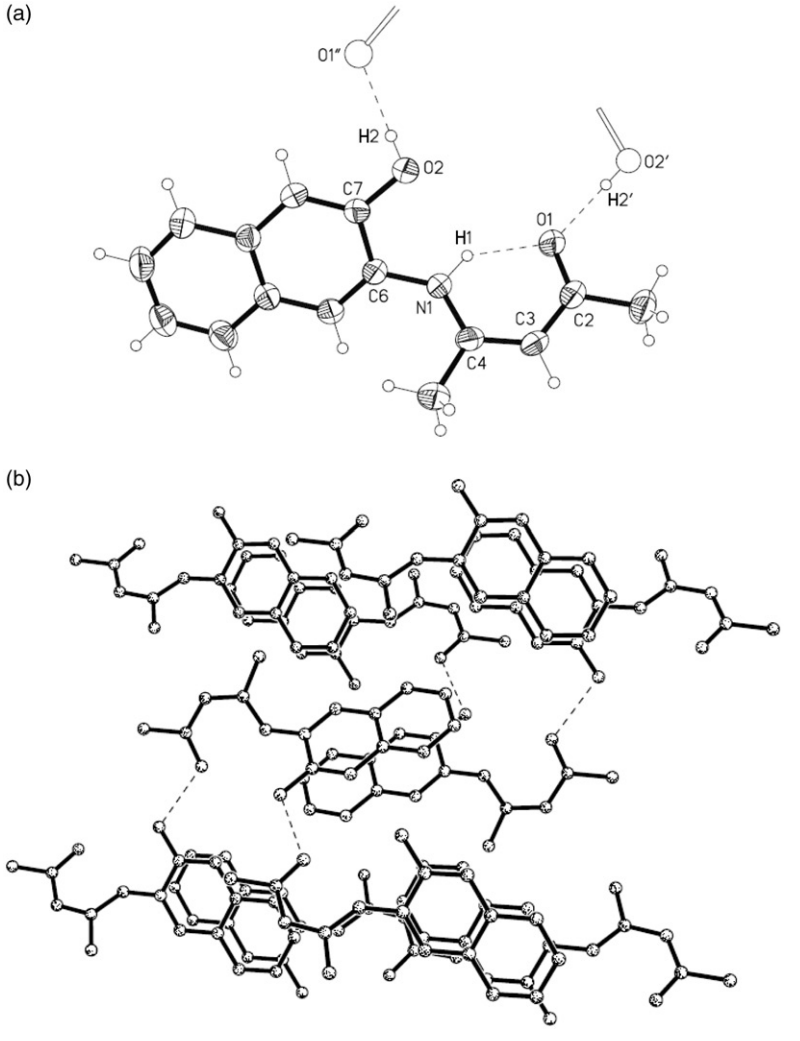

Figure 3. A representation of (a) intermolecular and intramolecular hydrogen bonds and (b) π–π interactions of H_2L. All dashed lines are for hydrogen bonding.

Table 3. Hydrogen bond lengths (Å) and angles (°) in H_2L.

D–H···A	*d*(H···A)	*d*(D···A)	∠(DHA)
N1–H1···O1	2.008	2.695	136.19
N1–H1···O2	2.469	2.671	94.01
O2–H2···O1[a]	1.819	2.63	169.72

[a]Symmetry transformations used to generate equivalent atoms: $x, -y-1/2, z-1/2$.

The NMR data for ligand and complex are presented in Section 2 according to the X-ray atom numbering. In the ^{1}H NMR spectrum of H_2L, a signal at 5.2 ppm (1H) corresponds to the vinylic hydrogen and absence of a methylene signal near 3 ppm (2H) confirms no participation of keto-imine form I in solution. No broadening of the signal

Table 4. Selected bond lengths (Å) and angles (°) for $SnPh_2L$, calculated values *vs.* experimental X-ray data.

	Experimental	B3LYP/SDD/6-31G*
Sn(1)–O(1)	2.081(5)	2.099
Sn(1)–O(2)	2.139(5)	2.178
Sn(1)–C(1)	2.107(5)	2.144
Sn(1)–C(7)	2.121(7)	2.141
Sn(1)–N(1)	2.131(5)	2.216
C(23)–C(25)	1.355(11)	1.417
C(25)–C(26)	1.392(11)	1.391
C(26)–C(27)	1.494(9)	1.510
C(26)–O(2)	1.272(9)	1.291
C(22)–O(1)	1.313(10)	1.334
N(1)–C(23)	1.342(9)	1.335
N(1)–C(13)	1.407(8)	1.417
O(1)–Sn(1)–C(7)	98.5(2)	97.50
O(2)–Sn(1)–C(7)	94.5(2)	92.10
O(1)–Sn(1)–C(1)	96.1(2)	95.69
O(2)–Sn(1)–C(1)	89.2(3)	93.36
C(1)–Sn(1)–C(7)	126.9(3)	125.78
C(23)–C(25)–C(26)	127.0(7)	127.78
C(26)–O(2)–Sn(1)	123.0(5)	125.66
C(23)–N(1)–Sn(1)	120.5(5)	123.43
O(1)–Sn(1)–O(2)	158.9(2)	159.37
O(1)–Sn(1)–N(1)	77.10(18)	76.60
O(2)–Sn(1)–N(1)	83.0(2)	82.76
C(7)–Sn(1)–N(1)	109.5(2)	117.85
C(1)–Sn(1)–N(1)	123.6(3)	116.35
C(25)–C(23)–N(1)	123.5(7)	123.38
O(2)–C(26)–C(25)	125.0(6)	125.32
C(22)–O(1)–Sn(1)	115.5(5)	114.28

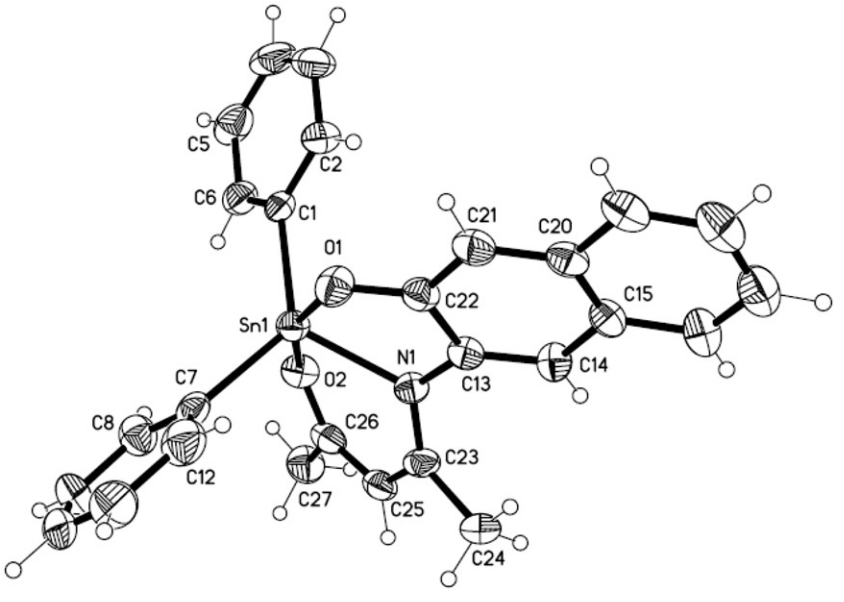

Figure 4. Crystal structure of $SnPh_2L$.

Table 5. Relative energies of H_2L tautomers at two different basis sets.[a]

	B3LYP/6-31G*			B3LYP/6-311 + G**		
Molecule	Relative *E*	Relative *H*	Relative *G*	Relative *E*	Relative *H*	Relative *G*
keto-imine (I)	8.92	8.05	6.96	10.02	9.09	7.83
enol-imine (II)	6.52	5.91	6.64	5.19	4.67	5.12
keto-amine (III)	0	0	0	0	0	0

[a]All energies reported in kcal mol^{-1}.

at 10.42 ppm, attributable to OH, rules out proton transfer to imine nitrogen in keto-amine form III [46, 47]. Therefore in DMSO, enol-imine form II is preferred. In the complex, absence of both phenolic and enolic signals supports coordination of dianionic ligand to tin.

The ^{119}Sn NMR spectrum of complex in $CDCl_3$ shows one sharp singlet at lower frequency than the original $SnPh_2Cl_2$ (−32 ppm) [8]. According to empirical chemical shift ranges reported for five-coordinate organotin(IV) derivatives [3, 29, 48–51], the coordination number of complex is five in solution.

3.4. *Theoretical calculations*

In order to verify the most stable tautomeric form of H_2L (figure 1) and to compare the structural features obtained by X-ray data with theoretical calculations, an investigation was undertaken at density functional theory (DFT) level with the hybrid B3LYP functional [52]. For geometry optimization of H_2L, two basis sets (6–31G* and 6–311 + G**) have been used and for complex SDD basis set was used for tin and 6–31G* basis set for C, H, N, and O atoms. All the stationary points are positively identified as local minima or as the transition state. These calculations were performed with Gaussian−98 program [53] package.

Relative electronic energies, enthalpies, and Gibbs free energies of three tautomers of H_2L in 1 atm pressure at 298.15 K are given in table 5. These data indicate that the stability of three tautomeric forms is III > II > I, therefore, the keto-amine form (III) is the most stable tautomer, consistent with X-ray data. Two main classes of tautomerism (keto-enol and imine-amine) can be observed in these three tautomers. Energy difference between these two types of tautomerism can be obtained from table 5. For example, keto-enol tautomerism can be observed between I and II with ΔG of 2.71 kcal mol^{-1}. Imine-amine tautomerism can be observed between I and III with ΔG of 7.83 kcal mol^{-1}. These data were extracted from B3LYP/6–311 + G** calculations. These theoretical calculations show that energy difference between imine-amine tautomers is higher than energy difference between keto-enol tautomers, suggesting that keto-enol tautomerism is more important than imine-amine tautomerism. For H_2L, selected bond distances and angles extracted from theoretical calculation are compared with X-ray data in table 2.

The geometry of $SnPh_2L$ was optimized by DFT/B3LYP method and relativistic effective core potential was employed for Sn (SDD basis set) [54]. The B3LYP/SDD/6–31 G* optimized and experimental values of selected geometrical parameters for

Table 6. Antibacterial activity data of ligands and their organotin(IV) complexes.

Compound	Inhibition zone (mm)			
	E. coli	*P. aeruginosa*	*S. aureus*	*B. cereus*
H_2L	n.a.	n.a.	n.a.	n.a.
$SnPh_2L$	17	13*	18	14
Vancomycin	22	8	16	15
Streptomycin	11	11	11	18
penicillin	16	n.a.	17	n.a.
Nalidixic acid	28	10	11	17
Gentamicin	21	19	17	20

*Pigment production inhibition; n.a. = no activity.

complex are compared in table 4. In general, the predicted bond lengths and angles are in agreement with the values based upon the X-ray crystal structure data.

3.5. *Antibacterial studies*

The *in vitro* antibacterial activities of H_2L and its organotin(IV) complex were studied with five standard antibacterial drugs, *viz*., Vancomycin, Streptomycin, penicillin, Nalidixic acid, and Gentamycin. The microorganisms used in this work include *B. cereus* and *S. aureus* (as Gram-positive bacteria) and *E. coli* and *P. aeruginosa* (as Gram-negative bacteria). The results are presented in table 6. Comparing the biological activity of the ligand, organotin(IV) complex and standard drugs show that H_2L has no activity while the complex exhibits good inhibitory effect towards all bacterial strains. The enhancement in activity of the ligand on complexation may be due to electron delocalization and therefore increasing the lipophilic character and efficient diffusion of the metal complexes into bacterial cell (chelation theory) [55–57], and also because of the intrinsic biological activity effects of organotin moieties. The complex shows only pigment production inhibition against *P. aeruginosa*; it may be postulated that this compound inhibits a part of metabolic pathways of this organism.

4. Conclusions

New Schiff base, H_2L, and its diphenyltin(IV) complex were synthesized and characterized by elemental analysis, IR spectroscopy, ^1H NMR, ^{119}Sn NMR, and X-ray single-crystal diffraction. These experimental methods as well as DFT calculations indicate that the Schiff base exists as keto-amine tautomeric form in solid phase and is coordinated to tin as dibasic tridentate *via* imine nitrogen and phenolic and enolic oxygen atoms. Geometry of the complex is a highly distorted TBP. The synthesized organotin complex shows activities against both Gram-positive (*B. cereus* and *S. aureus*) and Gram-negative (*E. coli* and *P. aeruginosa*) bacteria. According to earlier reports [58, 59], diphenyltin(IV) complexes exhibit less toxicity than other

diorganotin(IV) derivatives. Therefore, the new diphenyltin(IV) complex may be a good candidate for cytotoxicity studies and has potential to be used as a drug.

Supplementary material

Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Center, CCDC Nos. 837233 (H_2L) and 837232 ($SnPh_2L$). Copies of this information may be obtained free of charge *via* http://www.ccdc.cam.ac.uk or from the Cambridge Crystallographic Data Center, 12 Union Road, Cambridge, CB2 1EZ, UK (Fax: +44−1223−336033; E-mail: deposit@ccdc.cam.ac.uk).

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