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IR spectroscopic study and DFT calculations on dibenzyltin dichloride

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ABSTRACT

Benzyl chloride and tin powder were used to prepare dibenzyltin dichloride according to a literature procedure. In this study, IR spectroscopy, HOMO-LUMO energy gap, NBO analysis, polarizability, some geometrical parameters, natural charge and electrical potential of atoms, global hardness, electronic chemical potential, global electrophilicity index, and molar volume of dibenzyltin dichloride were calculated. DFT calculations were performed at the B3LYP and B3PW91 methods with LanL2DZ basis set on the title compound. The title compound presents a total dipole moment of 4.2996 and 4.3235 Debye at the B3LYP and B3PW91 methods, respectively. Moreover, the HOMO–LUMO energy gap of 0.16988 and 0.17155 a.u. were obtained for the title compound using B3LYP and B3PW91 methods, respectively. The infrared spectrum of (C6H5CH2)2SnCl2 was studied and analyzed. A good correlation was found between calculated and experimental data. Characteristic vibrational bands of the dibenzyltin dichloride associated with the Sn-C and Sn-Cl stretching vibrations were also identified.

Keywords: IR spectroscopy; HOMO-LUMO energy gap; Dibenzyltin dichloride; DFT

INTRODUCTION

In recent years, considerable progress has been made in the synthesis, characterization, and applications of organotin compounds [1]. Organotin compounds are classified as mono-, di-, tri- and tetraorganotins. In compounds of industrial interests, methyl, butyl, octyl, and phenyl groups form the organic substituents, while the anion is usually chloride, fluoride, oxide, hydroxide, carboxylate or thiolate [2]. Organotin (IV) complexes show a large spectrum of biological activities. In recent years, several investigations to test their antitumour activities have been carried out and much attention has been paid to on their antitumour properties and applications in antioncogenesis [3]. Also, they are commercially used as bactericides, fungicides, acaricides as well as agricultural biocides [4, 5]. Dibenzyltin dichloride is extensively used as a starting material in organotin chemistry.

The aim of this paper is to study the molecular structure, molar volume, polarizability, natural charge and electrical potential of atoms, the energies of highest occupied molecular orbital (E_{HOMO}) and the lowest unoccupied molecular orbital (E_{LUMO}), the energy difference (ΔE)

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between E_{HOMO} and E_{LUMO}, global hardness (η) and softness (s), the global electrophilicity (ω), electronic chemical potential (μ), and infrared spectroscopic of dibenzyltin dichloride. In order to reach to the aforementioned purpose, DFT calculations of the title compound are calculated by B3LYP and B3PW91 methods using LanL2DZ basis set.

EXPERIMENTAL

Instrumentation

As a part of this study for vibrational spectra of dibenzyltin dichloride, we have analyzed the infrared spectra recorded on a FT Bruker Vector 22 infrared spectrophotometer using pressed KBr disk. The melting point was determined using a BarnStead (BI 9300) Electrothermal apparatus.

Synthesis of the complex

Organotin (IV) compound with the general formula of $(C_6H_5CH_2)_2SnCl_2$ are synthesized by the reaction of benzyl chloride with tin powder prepared in toluene; the reaction was carried out in dry toluene [6], refluxed for 3 h and the final product was purified with 1-Butanol. The synthesized compound was characterized by IR spectroscopy (m.p. 160-160.5ºC). The synthesis reaction, in the presence of toluene, can simply be shown as follows:

$2C_6H_5CH_2Cl + Sn \rightarrow (C_6H_5CH_2)_2SnCl_2$

COMPUTATIONAL DETAILS

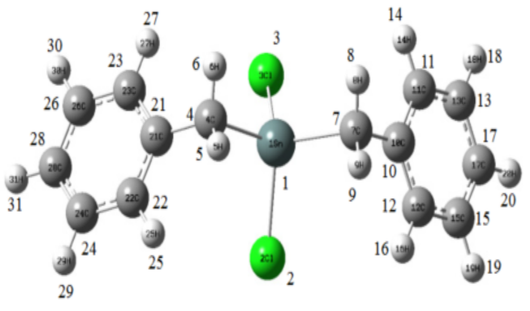
The molecular structure of dibenzyltin dichloride was optimized at the B3LYP [7] and B3PW91 [8] methods with LanL2DZ basis set using Gaussian 09 software [9]. The widely used LanL2DZ basis set with quasi-relativistic effective core potentials (LanL2) and double-zeta quality (DZ) [10] was used to include the atomic cores potential, effectively.

It is well known that global reactivity indices defined within conceptual DFT is a powerful tool to explain reactivity and the molecular properties [11]. Consequently, we have calculated global hardness, defined as $\eta = (I-A)/2$ [12] and electronic chemical potential, defined as $\mu = -(I+A)/2$ [13], where I and A denote ionization potential and electron affinity, respectively. In addition, global softness, defined as $S = 1/2\eta$ [14], and global electrophilicity index, defined as $\omega = \mu^2/2\eta$ [15], were also calculated. Following Koopman's theorem [16] allows to evaluate μ as $(\varepsilon_H + \varepsilon_L)/2$ and η as $(\varepsilon_L - \varepsilon_H)/2$ where ε_H and ε_L indicate the energy of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), respectively [13, 17]. Detection of the calculated wavenumbers was performed using the animation option of the GaussView 5.0 software to present the shape of the vibrational modes [18].

RESULTS AND DISCUSSION

Molecular structure and DFT calculations

All calculations support tetrahedral geometry of the studied compound. The geometry of dibenzyltin dichloride optimized by B3LYP and B3PW91 with basis set of LanL2DZ is shown in Fig. 1.



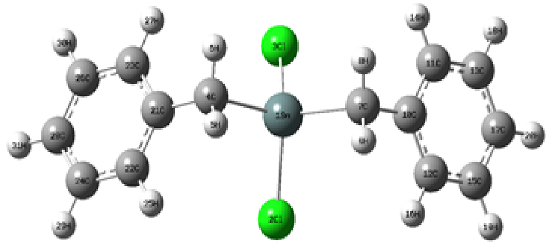


Fig.1. The optimized geometry of dibenzyltin dichloride at the B3LYP (Up) and B3PW91 (Down) methods using LanL2Dz basis set.

Stoichiometry, optimized energy, molar volume, dipole moment, and polarizability of dibenzyltin dichloride are given in Table 1. The dipole moment of dibenzyltin dichloride at B3LYP and B3PW91 methods are 4.2996 and 4.3235 Debye, respectively.

Dipole moment can be considered as a direct consequence of the electron distribution in a given molecule of known geometry. It is a physical constant which can experimentally be obtained and/or theoretically evaluated [19].

Crystallographic and theoretical structures of diorganotin dichlorides of dibenzyltin dichloride have previously been reported in the literature [20, 21]. Bond lengths and bond angles of dibenzyltin dichloride calculated through B3LYP and B3PW91 using LanL2DZ basis set are given in Table 2.

In Table 2, the bond lengths of Sn-Cl and Sn-C as well as the bond angles of C-Sn-Cl are shown as R1-R4 and A1-A4, respectively.

Electrical potential and natural charge of atoms

The electrostatic potential has primarily been used for predicting reactive sites and relative reactivities toward electrophilic attack, and also in the studies of biological recognition and hydrogen bonding interactions [22, 23]. In Table 3, there are several possible sites for the electrophilic attacks over the C4, C7 and atoms connected to the ring system of benzene (C10-C13, C15, C17, C21-C24, C26, and C28). The average of the maximum negative electrostatic potential values for these electrophilic sites calculated at the B3LYP/LANL2DZ and B3PW91/LANL2DZ are about -14.7 a.u.

Natural bond orbital (NBO) analysis is an effective method to study the existence of internal and external molecular bonding and also confirm the intramolecular charge transfer [24, 25]. The natural charges corresponding to those electrostatic potentials are given in Table 3.

Molecular orbitals

Energies of the HOMO and LUMO are important parameters in quantum chemical calculations [26]. While the energy of the HOMO is directly related to the ionization potential, LUMO energy is directly related to the electron affinity. Energy difference between HOMO and LUMO orbital is called "energy gap" that is an important parameter for structural stability [27]. Higher HOMO energy corresponds to the more reactive molecule in the reactions with electrophiles, while lower LUMO energy is essential for molecular reactions with nucleophiles [28].

Moreover, 3-dimensional representation of the HOMO and the LUMO of dibenzyltin dichloride are shown on the left and right sides, respectively, of figures 2 and 3. According to the calculations of B3LYP and B3PW91 methods with LanL2DZ basis set, the energy gap (transferring from HOMO to LUMO) of dibenzyltin dichloride were 0.16988 and 0.17155 a.u., respectively. Energy difference (gap) of dibenzyltin dichloride is given in Table 4.

Table 1. Stoichiometry, optimized energy, molar volume, dipole moment, and polarizability for the dibenzyltin dichloride at two different methods using LanL2Dz basis set

Method	**Stoichiometry**	**E(RB3LYP) (a.u.)**	**Molar volume (cm^3/mol)**	**Dipole Moment (Debye)**	**Polarizability (a.u.)**
B3LYP	$C_{14}H_{14}Cl_2Sn$	-575.21874	201.333	4.2996	197.63634
B3PW91	$C_{14}H_{14}Cl_2Sn$	-575.07712	210.770	4.3235	196.90499

Table 2. Optimized geometrical parameters of dibenzyltin dichloride. Bond lengths and bond angles are given in angstrom (Å) and degree (º), respectively

B3LYP/LanL2DZ						B3PW91/ LanL2DZ					
Bond length (Rn) and bond angle (Am)						Bond length (Rn) and bond angle (Am)					
Parameters	Bond length (Å)		Parameters	Bond angle (◦)		Parameters	Bond length (Å)		Parameters	Bond angle (◦)	
R1	R(1,2)	2.416	A1	A(2,1,3)	108.5	R1	R(1,2)	2.410	A1	A(2,1,3)	108.4
R2	R(1,3)	2.416	A2	A(2,1,4)	107.8	R2	R(1,3)	2.410	A2	A(2,1,4)	107.7
R3	R(1,4)	2.159	A3	A(2,1,7)	106.7	R3	R(1,4)	2.159	A3	A(2,1,7)	106.7
R4	R(1,7)	2.159	A4	A(3,1,4)	106.7	R4	R(1,7)	2.159	A4	A(3,1,4)	106.7
R5	R(4,5)	1.097	A5	A(3,1,7)	107.8	R5	R(4,5)	1.097	A5	A(3,1,7)	107.7
R6	R(4,6)	1.098	A6	A(4,1,7)	119.0	R6	R(4,6)	1.097	A6	A(4,1,7)	119.3
R7	R(4,21)	1.514	A7	A(1,4,5)	105.7	R7	R(4,21)	1.508	A7	A(1,4,5)	105.7
R8	R(7,8)	1.097	A8	A(1,4,6)	105.2	R8	R(7,8)	1.097	A8	A(1,4,6)	105.2
R9	R(7,9)	1.098	A9	A(1,4,21)	114.5	R9	R(7,9)	1.097	A9	A(1,4,21)	114.1
R10	R(7,10)	1.514	A10	A(5,4,6)	107.9	R10	R(7,10)	1.508	A10	A(5,4,6)	108.0
R11	R(10,11)	1.414	A11	A(5,4,21)	111.5	R11	R(10,11)	1.411	A11	A(5,4,21)	111.6
R12	R(10,12)	1.414	A12	A(6,4,21)	111.6	R12	R(10,12)	1.411	A12	A(6,4,21)	111.7
R13	R(11,13)	1.406	A13	A(1,7,8)	105.7	R13	R(11,13)	1.403	A13	A(1,7,8)	105.7
R14	R(11,14)	1.088	A14	A(1,7,9)	105.2	R14	R(11,14)	1.088	A14	A(1,7,9)	105.2
R15	R(12,15)	1.406	A15	A(1,7,10)	114.5	R15	R(12,15)	1.403	A15	A(1,7,10)	114.1
R16	R(12,16)	1.088	A16	A(8,7,9)	107.9	R16	R(12,16)	1.088	A16	A(8,7,9)	108.0
R17	R(13,17)	1.408	A17	A(8,7,10)	111.5	R17	R(13,17)	1.405	A17	A(8,7,10)	111.6
R18	R(13,18)	1.087	A18	A(9,7,10)	111.6	R18	R(13,18)	1.087	A18	A(9,7,10)	111.7
R19	R(15,17)	1.408	A19	A(7,10,11)	120.6	R19	R(15,17)	1.405	A19	A(7,10,11)	120.6
R20	R(15,19)	1.087	A20	A(7,10,12)	120.8	R20	R(15,19)	1.087	A20	A(7,10,12)	120.7
R21	R(17,20)	1.087	A21	A(11,10,12)	118.6	R21	R(17,20)	1.088	A21	A(11,10,12)	118.6
R22	R(21,22)	1.414	A22	A(10,11,13)	120.7	R22	R(21,22)	1.411	A22	A(10,11,13)	120.7
R23	R(21,23)	1.414	A23	A(10,11,14)	119.7	R23	R(21,23)	1.411	A23	A(10,11,14)	119.7
R24	R(22,24)	1.406	A24	A(13,11,14)	119.6	R24	R(22,24)	1.403	A24	A(13,11,14)	119.6
R25	R(22,25)	1.088	A25	A(10,12,15)	120.7	R25	R(22,25)	1.089	A25	A(10,12,15)	120.7
R26	R(23,26)	1.406	A26	A(10,12,16)	119.8	R26	R(23,26)	1.403	A26	A(10,12,16)	119.7
R27	R(23,27)	1.088	A27	A(15,12,16)	119.6	R27	R(23,27)	1.087	A27	A(15,12,16)	119.6
R28	R(24,28)	1.408	A28	A(11,13,17)	120.2	R28	R(24,28)	1.405	A28	A(11,13,17)	120.2
R29	R(24,29)	1.087	A29	A(11,13,18)	119.7	R29	R(24,29)	1.087	A29	A(11,13,18)	119.7
R30	R(26,28)	1.408	A30	A(17,13,18)	120.0	R30	R(26,28)	1.405	A30	A(17,13,18)	120.1
R31	R(26,30)	1.087	A31	A(12,15,17)	120.3	R31	R(26,30)	1.087	A31	A(12,15,17)	120.3
R32	R(28,31)	1.087	A32	A(12,15,19)	119.7	R32	R(28,31)	1.087	A32	A(12,15,19)	119.7
			A33	A(17,15,19)	120.0				A33	A(17,15,19)	120.1
			A34	A(13,17,15)	119.5				A34	A(13,17,15)	119.5
			A35	A(13,17,20)	120.3				A35	A(13,17,20)	120.2
			A36	A(15,17,20)	120.3				A36	A(15,17,20)	120.3
			A37	A(4,21,22)	120.6				A37	A(4,21,22)	120.6

	A38	A(4,21,23)	120.8		A38	A(4,21,23)	120.7
	A39	A(22,21,23)	118.6		A39	A(22,21,23)	118.6
	A40	A(21,22,24)	120.7		A40	A(21,22,24)	120.7
	A41	A(21,22,25)	119.7		A41	A(21,22,25)	119.7
	A42	A(24,22,25)	119.6		A42	A(24,22,25)	119.6
	A43	A(21,23,26)	120.7		A43	A(21,23,26)	120.7
	A44	A(21,23,27)	119.8		A44	A(21,23,27)	119.7
	A45	A(26,23,27)	119.6		A45	A(26,23,27)	119.6
	A46	A(22,24,28)	120.2		A46	A(22,24,28)	120.2
	A47	A(22,24,29)	119.7		A47	A(22,24,29)	119.7
	A48	A(28,24,29)	120.0		A48	A(28,24,29)	120.1
	A49	A(23,26,28)	120.3		A49	A(23,26,28)	120.3
	A50	A(23,26,30)	119.7		A50	A(23,26,30)	119.7
	A51	A(28,26,30)	120.0		A51	A(28,26,30)	120.1
	A52	A(24,28,26)	119.5		A52	A(24,28,26)	119.5
	A53	A(24,28,31)	120.3		A53	A(24,28,31)	120.2
	A54	A(26,28,31)	120.3		A54	A(26,28,31)	120.3

Table 3. Natural charge and electrical potential of atoms of dibenzyltin dichloride calculated at the B3LYPand B3PW91 methods using LanL2DZ basis set

Natural charge (e)				Electrical potential (a.u.)			
B3LYP/LanL2DZ		B3PW91/LanL2DZ		B3LYP/LanL2DZ		B3PW91/LanL2DZ	
Atom No.	Natural charge	Atom No.	Natural charge	No.	Electrical potential	No.	Electrical potential
Sn 1	1.890	Sn 1	1.860	1 Atom	-1.540	1 Atom	-1.547
Cl 2	-0.508	Cl 2	-0.503	2 Atom	-4.776	2 Atom	-4.776
Cl 3	-0.508	Cl 3	-0.503	3 Atom	-4.776	3 Atom	-4.776
C 4	-0.944	C 4	-0.944	4 Atom	-14.730	4 Atom	-14.729
H 5	0.251	H 5	0.257	5 Atom	-1.067	5 Atom	-1.064
H 6	0.253	H 6	0.259	6 Atom	-1.067	6 Atom	-1.064
C 7	-0.944	C 7	-0.944	7 Atom	-14.730	7 Atom	-14.729
H 8	0.251	H 8	0.257	8 Atom	-1.067	8 Atom	-1.064
H 9	0.253	H 9	0.259	9 Atom	-1.067	9 Atom	-1.064
C 10	-0.040	C 10	-0.044	10 Atom	-14.726	10 Atom	-14.727
C 11	-0.219	C 11	-0.222	11 Atom	-14.749	11 Atom	-14.751
C 12	-0.220	C 12	-0.224	12 Atom	-14.749	12 Atom	-14.751
C 13	-0.202	C 13	-0.206	13 Atom	-14.748	13 Atom	-14.751
H 14	0.218	H 14	0.222	14 Atom	-1.094	14 Atom	-1.093
C 15	-0.202	C 15	-0.206	15 Atom	-14.748	15 Atom	-14.751
H 16	0.221	H 16	0.226	16 Atom	-1.095	16 Atom	-1.094
C 17	-0.217	C 17	-0.220	17 Atom	-14.750	17 Atom	-14.752
H 18	0.221	H 18	0.225	18 Atom	-1.098	18 Atom	-1.097
H 19	0.221	H 19	0.226	19 Atom	-1.098	19 Atom	-1.097
H 20	0.220	H 20	0.224	20 Atom	-1.099	20 Atom	-1.097
C 21	-0.040	C 21	-0.044	21 Atom	-14.726	21 Atom	-14.727
C 22	-0.219	C 22	-0.222	22 Atom	-14.749	22 Atom	-14.751
C 23	-0.220	C 23	-0.224	23 Atom	-14.749	23 Atom	-14.751
C 24	-0.202	C 24	-0.206	24 Atom	-14.748	24 Atom	-14.751
H 25	0.218	H 25	0.222	25 Atom	-1.094	25 Atom	-1.093
C 26	-0.202	C 26	-0.206	26 Atom	-14.748	26 Atom	-14.751
H 27	0.221	H 27	0.226	27 Atom	-1.095	27 Atom	-1.094
C 28	-0.217	C 28	-0.220	28 Atom	-14.750	28 Atom	-14.752
H 29	0.221	H 29	0.225	29 Atom	-1.098	29 Atom	-1.097
H 30	0.221	H 30	0.226	30 Atom	-1.098	30 Atom	-1.097
H 31	0.220	H 31	0.224	31 Atom	-1.099	31 Atom	-1.097

Table 4. HOMO and LUMO energies and corresponding HOMO-LUMO energy gap of dibenzyltin dichloride calculated at the B3LYP and B3PW91 methods using LanL2DZ basis set

Method	HOMO (a.u.)	LUMO (a.u.)	HOMO-LUMO energy gap (a.u.)
B3LYP	-0.23726	-0.06738	0.16988
B3PW91	-0.24024	-0.06873	0.17151

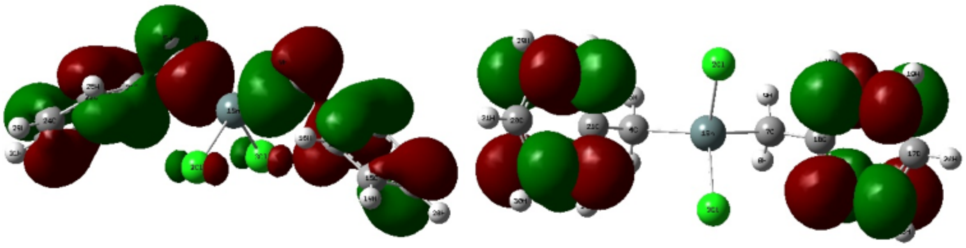


Fig. 2. Schematic representation of HOMO, left and LUMO, right, of dibenzyltin dichloride with B3LYP/LanL2DZ.

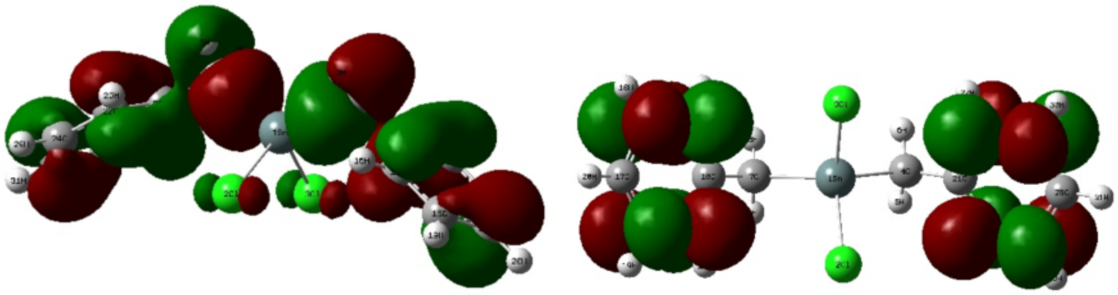


Fig. 3. Schematic representation of HOMO, left, LUMO, right, of dibenzyltin dichloride with B3PW91/LanL2DZ.

Table 5. Global hardness, electronic chemical potential, global electrophilicity and global softness of the dibenzyltin dichloride calculated at the B3LYP/LANL2DZ and B3PW91/LANL2DZ levels

Method	**Global hardness η(ev)**	**electronic chemical potential μ(ev)**	**Global electrophilicity ω(ev)**	**Global softness $S(ev)^{-1}$**
B3LYP	2.31	-4.14	3.72	0.22
B3PW91	2.33	-4.20	3.79	0.21

In the dibenzyltin dichloride molecule, the HOMO and the LUMO are mainly delocalized throughout the system with the HOMO having the maximum amplitude coefficients on C4, C7, C17 and C28 atoms while the LUMO has the maximum amplitude coefficient on C11, C12, C13, C15, C22, C23, C24 and C26 atoms.

The HOMO is the orbital that donates electrons to the electron deficient species and the LUMO is the orbital that accepts electrons from electron rich species. A hard acid and/or base is associated with the large difference between ionization energy and electron affinity.

The chemical hardness of a molecule is a good indicator of the chemical stability. From the HOMO–LUMO energy gap, one can find whether the molecule is hard or soft. The molecules having large energy gap are known as hard and molecules having a small energy gap are known as soft. The soft molecules are more polarizable than the hard ones because they need small energy to excitation [29]. Global electrophilicity index (ω) is estimated by using the electronegativity and chemical hardness parameters. A high value of electrophilicity describes a good electrophile while a small value describes a good nucleophile [30]. Table 5 gives the global hardness, electronic chemical potential, global electrophilicity and global softness values obtained from B3LYP/LANL2DZ and B3PW91/LANL2DZ levels for dibenzyltin dichloride.

IR Spectroscopy

Infrared spectroscopic studies are usually carried out in order to assign absorption bands to a particular vibrational mode, or to investigate the variation of the vibrational frequencies with structure [31]. The dibenzyltin dichloride molecule has 31 atoms, which possess 87 normal modes of vibrations. The IR vibrations of dibenzyltin dichloride with B3LYP/LanL2DZ and with B3PW91/LanL2DZ and their wavenumbers are given in Table 6. Positive values of all the calculated vibrational wavenumbers confirmed the optimized structure of the title molecule is stable.

Both experimental and calculated FT-IR spectra are shown in Fig. 4. As can be seen, the theoretically predicted infrared data of the dibenzyltin dichloride shows a good agreement with the experimental ones. It is worth to note that the signal observed in 3421 cm^{-1} is corresponded to the water in KBr.

The low frequency region of the vibrational spectra of organormetallic compounds is of particular interest. The important absorption frequencies are (Sn-C) stretching, (Sn-Cl) stretching, and (C-H) stretching in ring and H-C-H stretching in CH$_2$ group. The characteristic metal-halide stretching and bending vibrations are found at the wavenumbers below 350 cm^{-1}.

The tin-carbon stretching frequencies are observed at 524 cm^{-1} and 563 cm^{-1} in (CH$_3$)$_2$SnCl$_2$ and at 548 cm^{-1} in CH$_3$SnCl$_3$ [32]. In the title compound, the Sn-C asymmetric stretching frequencies are easily assigned at 579 cm^{-1} (B3LYP/LANL2DZ) and 581 cm^{-1} (B3PW91/LANL2DZ).

In the B3LYP predicted spectrum of the dibenzyltin dichloride, the ν_{asy} (342 cm^{-1}) and ν_{sym} (320 cm^{-1}) can be related to the strong bands of Sn-Cl.

In the 3100-3250 cm^{-1} region, the dibenzyltin dichloride exhibits typical bands of C-H stretching due to the aromatic ring.

We noted some bands at 3058-3146 cm^{-1}. These absorptions are antisymmetric and symmetric H-C-H stretching vibrations due to methylene groups.

Table 6. Experimental and calculated vibrational wavenumbers and assignments of dibenzyltin dichloride with B3LYP/LanL2DZ and B3PW91/LanL2DZ

Wavenumber (cm^{-1})		Band assignment	Exp. (cm^{-1})	Wavenumber (cm^{-1})		Band assignment	Exp. (cm^{-1})	Wavenumber (cm^{-1})		Band assignment	Exp. (cm^{-1})
B3LYP	B3PW91			B3LYP	B3PW91			B3LYP	B3PW91		
12	12	R, ClSnCl		761	762	T, CH_2		1236	1249	R, CH_2	
22	22			790	791	T, CH_2		1372	1375		
27	27			795	796	W, CH_2		1373	1375		
40	43			796	796	T, CH_2	754	1378	1399		
52	54			812	818			1378	1399		
63	61	W, ClSnCl		817	823	S, CSnC	799	1477	1476	S, CH_2	1408
87	86			883	884			1481	1481	S, CH_2	
94	93			884	885			1483	1490	T, CH_2	1451
105	104	R, CH_2		957	958			1483	1490	S, CH_2	1493
114	113	S, ClSnCl		959	959		904	1524	1533		
129	129	W, ClSnCl		1015	1018			1524	1533		
198	198			1015	1018			1631	1648	υC=C	
232	231			1018	1019			1632	1648		
320	325	υ_sClSnCl		1018	1019			1651	1668		
328	329	R, CH_2		1040	1039			1652	1668	υC=C	1598
331	331	R, CH_2		1040	1040			3059	3073	$\upsilon_s CH_2$	2925
342	346	υ_{as}ClSnCl		1051	1058		1030	3061	3075	$\upsilon_s CH_2$	
418	418			1051	1058			3124	3145	$\upsilon_{as} CH_2$	
418	418			1083	1088	T, CH_2		3125	3146	$\upsilon_{as} CH_2$	3059
448	449	W, CSnC		1090	1095	T, CH_2	1055	3187	3206	υC-H (ph)	3080
450	452	T, CSnC		1144	1148	T, CH_2		3187	3206	υC-H (ph)	
558	557	R, CSnC	435	1153	1156	T, CH_2		3190	3209	υC-H (ph)	
559	559	S, CSnC		1191	1189	W, CH_2	1114	3191	3209	υC-H (ph)	
579	581	υ_{as} CSnC		1199	1197	W, CH_2		3203	3221	υC-H (ph)	
585	586	W, CSnC	547	1206	1210			3203	3222	υC-H (ph)	
636	636		579	1206	1210			3215	3233	υC-H (ph)	
636	636			1224	1230			3215	3233	υC-H (ph)	
725	726			1225	1230			3231	3249	υC-H (ph)	
725	727		690	1236	1249	W, CH_2	1208	3231	3249	υC-H (ph)	

υ (stretching), υ_s (symmetric stretching), υ_{as} (asymmetric stretching), W (wagging), T (twisting), S (scissoring), R (rocking), Exp. (experimental) and ph (phenyl).

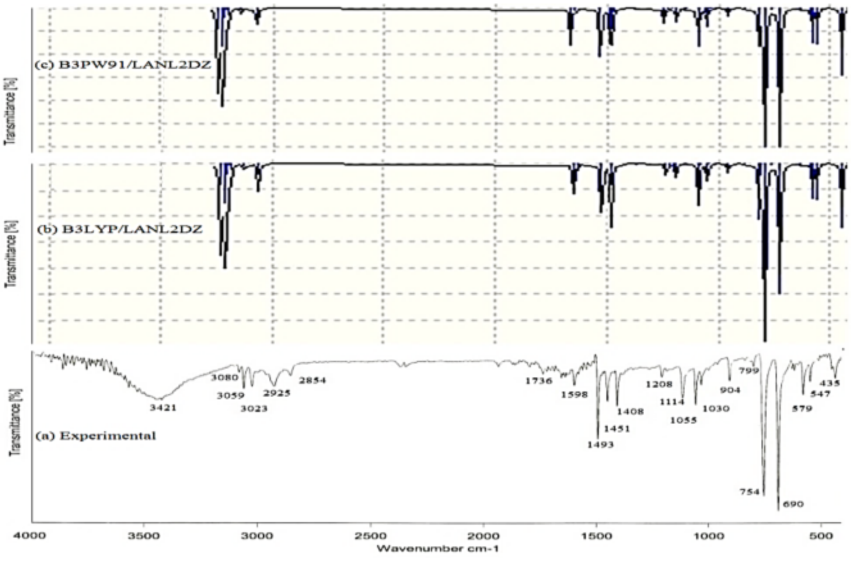


Fig. 4. Theoretical and experimental IR Spectra of the title compound.

CONCLUSION

In this investigation, molecular structure, vibrational frequencies, global hardness, global electronegativity index, polarizability analysis, HOMO-LUMO and NBO analysis of dibenzyltin dichloride were studied using DFT (B3LYP/LANL2DZ and B3PW91/LANL2DZ) calculation for the first time. HOMO, LUMO and corresponding energy gap values along with their 3D plot were also studied. The reactivity can be related to the hardness and HOMO-LUMO energy gap. There are no significant differences in the spectroscopic parameters obtained from experimental data and DFT calculations.

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