Synthesis, spectroscopic characterization, and 3D molecular modeling of lead(II) complexes of unsymmetrical tetradentate Schiff-base ligands

Har Lal Singh

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Abstract Solid complexes of Pb(II) with unsymmetrical Schiff-base ligands (H₂L) derived from 2-aminobenzophenone, thiosemicarbazide, semicarbazide, salicylaldehyde, 2-hydroxynaphthaldehyde, and *o*-hydroxyacetophenone have been synthesized and characterized by elemental analysis, conductance measurements, molecular weight measurement, and UV–Vis, FTIR, ¹H NMR, and ¹³C NMR spectroscopy. The spectral studies suggest the ligands behave as dibasic tetradentate ligands with ONNO/ONNS donor atom sequences toward the central metal ion. From the microanalytical data, the stoichiometry of the complexes was found to be 1:1 (metal:ligand). The physicochemical data suggest a tetracoordinated environment around the metal ion. Three-dimensional molecular modeling and analysis of bond lengths and bond angles have also been conducted for a representative compound, [PbL¹], to substantiate the proposed structures.

Keywords Unsymmetrical tetradentate Schiff base · Pb(II) complexes · 2-Aminobenzophenone · Thiosemicarbazide · Semicarbazide · Aldehyde/ketone · Spectral studies

Introduction

The coordination chemistry of Schiff bases has been widely explored, though its use in supramolecular coordination chemistry remains largely unexplored. The Schiff base moiety is potentially ambidenate and can coordinate through nitrogen with either oxygen or sulfur atoms. The vast literature on structural studies of Schiff-base complexes reveals some interesting features of their coordination behavior [1–8].

H. L. Singh (🖂)

Department of Chemistry, Faculty of Engineering & Technology, Mody Institute of Technology and Science, Lakshmangarh, Sikar, Rajasthan, India

e-mail: hlsingh9@rediffmail.com

Thiosemicarbazones and semicarbazones are now well established as important classes of sulfur and oxygen donor ligands, particularly for transition metal ions [9-12]. This is because of the remarkable biological activity observed for these compounds, which has since been shown to be related to their metal-complexing ability. These compounds have a great variety of biological activity ranging from antimicrobial, antineoplastic, antimalarial, antiviral, and antitumor [13-17].

Schiff bases with N_2O_2 donor atoms are well known to co-ordinate with a variety of metal ions and have attracted much interest in recent years because of their rich co-ordination chemistry [18–20]. Tetradentate Schiff bases are reported to have a variety of biological, clinical, and analytical applications [21–24]. Many symmetrical tetradentate Schiff bases of diamines with aldehydes and ketones have been prepared and studied intensively. However, less attention has been focused on unsymmetrical tetradentate Schiff bases derived from diamines with different aldehydes and ketones [25–27].

For this reason, this paper reports the results of an investigation of unsymmetrical Schiff-base complexes. Schiff bases $(L^1H_2-L^6H_2)$ were obtained by means of the condensation reaction among 2-aminobenzophenone, thiosemicarbazide, semicarbazide, salicylaldehyde, 2-hydroxynaphthaldehyde, and *o*-hydroxyacetophenone in the hope they might provide us with valuable theoretical information for exploring metal-based bacteriostatic and carcinostatic pharmaceuticals with high efficacy and low toxicity. In this effort, we also introduced the azomethine (-C=N-) linkage in the hope it would result in notable variety in the chemistry and other behavior of such compounds. The synthesized compounds $(L^1H_2-L^6H_2)$ were used as tetradentate ligands toward divalent metal atom solely through the azomethine nitrogen and phenolic oxygen, forming a stable chelate ring.

Experimental

Chemicals used in this work, viz, 2-aminobenzophenone, thiosemicarbazide, semicarbazide, salicylaldehyde, 2-hydroxynaphthaldehyde, *o*-hydroxyacetophenone, and lead(II) acetate were of analytical grade. Solvents used were dried and purified by standard methods and moisture was excluded from the glass apparatus by use of CaCl₂ drying tubes. Melting points are determined in open capillaries and are uncorrected.

General procedure for synthesis of the ligands

The ligands were prepared by a reported method [28]. A typical procedure for synthesis of Schiff bases is as follows. A 50-mL solution of 0.001 mol (0.197 g) 2-aminobenzophenone, 0.001 mol thiosemicarbazide (0.0911 g)/semicarbazide (0.0751 g), and 0.001 mol salicylaldehyde (0.122 g)/2-hydroxynaphthaldehyde (0.172 g)/o-hydroxyacetophenone (0.137 g), in absolute ethanol was heated under reflux for approximately 4 h. The precipitate thus formed was cooled to room temperature and collected by filtration, followed by recrystallization from ethanol (Scheme 1).



Scheme 1 Synthesis of ligands

L¹**H**₂ is prepared by reacting 2-aminobenzophenone with salicylaldehyde and semicarbazone (H₂L¹); colour, yellow; yield, 72%; mp, 162 °C (dec.) and elemental analysis (%), calcd. for C₂₁H₁₈N₄O₂: C, 70.40; H, 5.06; N, 15.63; found: C: 70.52; H, 5.02; N, 15.56; molecular weight: found, 343.63, calcd. 358.39. Infrared (KBr, cm⁻¹): v(C=N), 1655 (1648); v(OH/NH), 3300–3070; v(C=O), 1705; v(C–O) 1220; v(C–N) 1352; v(N–N) 1040. UV–Vis (λmax, nm): 390, 214, 265. ¹H NMR (DMSO-d₆, δ ppm): 12.97(s, 1H, Ph-OH), 9.12 (s, 1H, –CH=N–), 8.09 (s, 1H, NH), 6.96–7.69 (m, 13H, aromatic), 4.67 (s, 2H, NH₂); ¹³C NMR (DMSO, δ ppm): 172.5 (–C=O), 167.9 (C–OH), 162.2 (158.6) (C=N), 164.1, 137.2, 128.4, 128.1, 121.8, 119.9 (aromatic carbons).

L²**H**₂ is prepared by reacting 2-aminobenzophenone with o-hydroxyacetophenone and semicarbazone; colour, brownish yellow; yield, 68%; mp, 180–182 °C (d) and elemental analysis (%), calcd. for C₂₂H₂₀N₄O₂: C, 70.95; H, 5.41; N, 15.04; found: C: 70.84; H, 5.47; N, 14.93; molecular weight: found, 381.58, calcd. 372.43. Infrared (KBr, cm⁻¹): *v*(C=N), 1660 (1658); *v*(OH/NH), 3300–3070; *v*(C=O),1710; *v*(C–O) 1220; *v*(C–N) 1355; *v*(N–N) 1037. UV–Vis (λ max, nm): 390, 214, 265. ¹H NMR (DMSO-d₆, δ ppm): 12.94 (s, 1H, Ph-OH), 8.10 (s, 1H, NH), 6.90–7.65 (m, 13H, aromatic), 4.45 (s, 2H, NH₂), 2.18 (s, 3H, –C(CH₃)=N–); ¹³C NMR (DMSO, δ ppm): 172.5 (–C=O), 168.5 (C–OH), 162.2 (158.6) (C=N), 164.1, 137.2, 128.4, 121.8, 128.1, 119.9 (aromatic carbons).

L³**H**₂ is prepared by reacting 2-aminobenzophenone with salicylaldehyde and thiosemicarbazone; colour, brownish yellow; yield, 75%; and elemental analysis (%), calcd. for C₂₁H₁₈N₄OS: C, 67.36; H, 4.85; N, 14.96; S, 8.56; found: C: 67.26; H, 4.87; N, 14.90; S, 8.60; molecular weight: found, 382.88, calcd. 374.45. Infrared (KBr, cm⁻¹): v(C=N), 1650 (1648); v(OH/NH), 3300–3070; v(C=S), 1325; v(C–O) 1218; v(C–N) 1352; v(C–) 860; v(N–N) 1034. UV–Vis (λ max, nm): 390, 214, 265. ¹H NMR (DMSO-d₆, δ ppm): 12.40 (s, 1H, Ph-OH), 9.09 (s, 1H, –CH=N–), 8.02 (s, 1H, NH), 6.95–7.55 (m, 13H, aromatic), 4.50 (s, 2H, NH₂); ¹³C NMR (DMSO, δ ppm): 172.5 (–C=O), 169.8 (C–OH), 162.2 (158.6) (C=N), 164.1, 137.2, 128.4, 128.1, 121.8, 119.9 (aromatic carbons).

L⁴**H**₂ is prepared by reacting 2-aminobenzophenone with *o*-hydroxyacetophenone and thiosemicarbazide; colour, brown; yield, 77%; and elemental analysis (%), calcd. for C₂₂H₂₀N₄OS: C, 68.02; H, 5.12; N, 14.42; S, 8.25; found: C: 67.84; H, 5.10; N, 14.35; S, 8.30; molecular weight: found, 397.65, calcd. 388.49. Infrared (KBr, cm⁻¹): v(C=N), 1660 (1656); v(OH/NH), 3300–3070; v(C=S), 1320; v(C–O) 1225; v(C–S) 840; v(N–N) 1032; UV–Vis (λ max, nm): 390, 214, 265. ¹H NMR (DMSO-d₆, δ ppm): 12.18 (s, 1H, Ph-OH), 8.15 (s, 1H, NH), 6.92–7.62 (m, 13H, aromatic), 4.45 (s, 2H, NH₂), 2.15 (s, 3H, –CH=N–); ¹³C NMR (DMSO, δ ppm): 172.5 (–C=O), 167.8 (C–OH), 162.2 (158.6) (C=N), 164.1, 137.2, 128.4, 128.1, 121.8, 119.9 (aromatic carbons);

L⁵**H**₂ is prepared by reacting 2-aminobenzophenone with 2-hydroxynaphthaldehyde and semicarbazone; colour, orange; yield, 78%; mp, 204 °C (d) and elemental analysis (%), calcd. for C₂₅H₂₀N₄O₂: C, 73.51; H, 4.94; N, 13.72; found: C: 73.36; H, 4.90; N, 13.76; molecular weight: found, 401.25, calcd. 408.46. Infrared (KBr, cm⁻¹): v(C=N), 1658 (1652); v(OH/NH), 3300–3070; v(C=O), 1702; v(C–O) 1222; v(C–N) 1350; v(v–v) 1035. UV–Vis (λmax, nm): 390, 214, 265. ¹H NMR (DMSOd₆, δ ppm): 13.12 (s, 1H, Ph-OH), 9.86 (s, 1H, –CH=N–), 8.12 (s, 1H, NH), 6.78–7.92 (m, 15H, aromatic), 4.38 (s, 2H, NH₂); ¹³C NMR (DMSO, δ ppm): 172.5 (–C=O), 170.1 (C–OH), 162.2 (158.6) (C=N), 164.1, 137.2, 128.4, 128.1, 121.8, 119.9 (aromatic carbons).

L⁶**H**₂ is prepared by reacting 2-aminobenzophenone with 2-hydroxynaphthaldehyde and thiosemicarbazide; colour, dark brown; yield, 70%; and elemental analysis (%), calcd. for C₂₅H₂₀N₄OS: C, 70.73; H, 4.75; N, 13.20; S, 7.55; found: C: 70.65; H, 4.83; N, 13.06; S, 7.60; molecular weight: found, 415.21, calcd. 424.52. Infrared (KBr, cm⁻¹): v(C=N), 1655 (1650); v(OH/NH), 3300–3070; v(C=S), 1322; v(C–O) 1220; v(C–N) 1350; v(C–S) 835; v(N–N) 1038; UV–Vis (λ max, nm): 390, 214, 265; ¹H NMR (DMSO-d₆, δ ppm): 11.90 (s, 1H, Ph-OH), 9.95 (s, 1H, –CH=N–), 8.06 (s, 1H, NH), 7.02–7.92 (m, 15H, aromatic), 4.60 (s, 2H, NH₂); ¹³C NMR (DMSO, δ ppm): 172.5 (–C=O), 168.4 (C–OH), 162.2 (158.6) (C=N), 164.1, 137.2, 128.4, 128.1, 121.8, 119.9 (aromatic carbons).

Synthesis of lead(II) complexes

The complexes were prepared under anhydrous conditions by slow addition of a dry, hot methanol solution of lead(II) acetate in 1:1 molar ratio to a solution of the Schiff base in hot absolute methanol. The mixture was heated under reflux with constant

stirring for 30 min, giving a clear solution; heating under reflux was then continued for 5–7 h. The acetic acid liberated in the reaction was removed azeotropically with solvent. Excess solvent was removed under reduced pressure and the compound was dried under vacuum at 45 \pm 5 °C after repeated washing with dry cyclohexane. The compounds were purified by recrystallization from methanol. The purity of the compounds was checked by TLC using silica gel G as adsorbent.

Analytical methods and spectral measurements

Lead was determined gravimetrically as lead sulfate. Nitrogen and sulfur were determined by the Kjeldahl and Messenger methods, respectively. Molar conductance measurements were made in anhydrous dimethylformamide at 45 ± 5 °C using a Systronics model 305 conductivity bridge. Molecular weight determinations were carried out by the Rast camphor method. Electronic spectra were recorded in DMSO on a Thermo Scientific UV1 spectrophotometer. Infrared spectra in the region 4,000–400 cm⁻¹ were recorded on a Perkin–Elmer RX1 FTIR spectrometer. ¹H NMR spectra were recorded on a Jeol (model FX 90Q) using DMSO-d₆ as solvent at 89.55 MHz. ¹³C NMR spectra were recorded on a 90 MHz Jeol (FX 90Q) NMR spectrometer using dry DMSO as solvent at 84.25 MHz. TMS was used as internal reference for ¹H NMR and ¹³C NMR.

Three-dimensional molecular modeling studies

Three-dimensional molecular modeling was performed for a representative compound by use of CS Chem 3D Ultra Molecular Modeling and Analysis software [29], interactive graphics software that enables rapid structure building and geometry optimization with minimum energy and molecular display.

Results and discussion

New lead–Schiff-base complexes were synthesized by reaction of lead(II) acetate with the ligands in 1:1 molar ratios using anhydrous methanol as solvent. These reactions proceed with the liberation of acetic acid, which was removed azeotropically, as indicated below (Scheme 2).

The reactions were found to be quite facile and were complete after heating under reflux for 5–7 h. Physical characteristics, and micro analytical and molar conductance data for the metal–ligand complexes are given in Table 1. The analytical data for the complexes are indicative of a 1:1 molar ratio (metal:ligand) and correspond well with the general formula [Pb(ONNX)]. All the complexes are intensely coloured

Pb(OOCCH₃)₂ + HONN XH
$$\longrightarrow$$
 Pb(ONN X) + 2CH₃COOH
where HONN XH represents the donor system of the Schiff bases

Scheme 2 Representative equation illustrating the formation of Pb(II) complexes

Table 1 Results Irol	m pnysic	al characterization	, and analytical and m	iolar conduc	stance data to	r the metal com	plexes			
Complex		Mol. wt. found	Molar conductance	M.P. (°C)	Yield (%)	% Elemental a	nalysis, found (ca	alcd.)		
Formula and colour	Abbr.	(calca.)	(7 - CM - MOI -)			Pb	С	Н	N	S
PbC ₂₁ H ₁₆ N ₄ O ₂ Licht vellow	PbL^{1}	578.1 (563.6)	18.05	147	69	36.72 (36.77)	44.84 (44.76)	2.91 (2.86)	9.88 (9.94)	1
$PbC_{22}H_{18}N_4O_2$	PbL^2	557.8 (577.6)	19.15	125	72	35.83 (35.87)	45.61 (45.75)	3.02 (3.14)	9.78 (9.70)	I
Light yellow PbC ₂₁ H ₁₆ N ₄ OS	PbL^3	565.3 (579.6)	22.15	72	78	35.70 (35.75)	43.65 (43.52)	2.74 (2.78)	9.61 (9.67)	5.66 (5.53)
Brown PbC ₂₂ H ₁₈ N ₄ OS	PbL^4	584.6 (593.7)	25.02	62	75	34.78 (34.90)	44.44 (44.51)	3.15 (3.06)	9.52 (9.44)	5.45 (5.40)
Dark brown PbC ₂₅ H ₁₈ N ₄ O ₂	PbL^{5}	623.2 (613.6)	20.65	182	73	33.82 (33.77)	48.98 (48.93)	2.93 (2.96)	9.06 (9.13)	I
Dark yellow PbC ₂₅ H ₁₈ N ₄ OS Brown	PbL ⁶	643.5 (629.7)	23.10	142	70	32.98 (32.90)	47.80 (47.69)	2.69 (2.88)	8.70 (8.90)	5.01 (5.09)

Compound	ν(OH)	v(C=N-)	v(C–N)	v(C=O/C=S)	v(C-O/C-S)	v(N-N)	$v(\text{Pb} \leftarrow \text{N})$	v(Pb–O)
L^1H_2	3300-3070	1655	1352	1705	1220	1040	_	-
PbL^1	_	1625	1385	1685	1252	1072	535	466
L^2H_2	3300-3070	1660	1355	1710	1220	1037	_	_
PbL^2	_	1635	1386	1696	1254	1070	538	470
$L^{3}H_{2}$	3300-3070	1650	1352	1325	1218/860	1034	_	_
PbL ³	-	1622	1380	1290	1248/780	1066	530	462
L^4H_2	3300-3070	1660	1354	1320	1225/840	1032	_	_
PbL^4	_	1632	1385	1292	1252/790	1061	540	460
L^5H_2	3300-3070	1658	1350	1702	1222	1035	-	_
PbL ⁵	_	1630	1380	1688	1256	1070	540	460
$L^{6}H_{2}$	3300-3070	1655	1350	1322	1220/835	1038	_	_
PbL ⁶	-	1626	1382	1285	1245/790	1065	542	455

Table 2 Important IR spectral data (cm⁻¹) of Schiff bases and their corresponding lead(II) complexes

solids. They are partly soluble in common organic solvents and only soluble in DMF and DMSO. The chelates were dissolved in DMF and the molar conductance of 10^{-3} M solution at 45 °C was measured. The molar conductance valves of the complexes fall in the range 18–25 Ω^{-1} cm² mol⁻¹ indicating that these chelates are non-electrolytes. The elemental analysis results agree with the formulae proposed for the ligands and also confirmed the Pb(ONNX) (Fig. 2) composition of the Pb(II) chelates.

Infrared spectra

The IR spectra of the free ligands (Table 2) show characteristic bands at 3070–3300, 1703, 1657 (1650), 1354 and 1219 cm⁻¹ assignable to intramolecular hydrogen bonded hydroxyl v(OH), carbonyl v(C=O), azomethine v(C=N), aryl azomethine v(C-N), and phenolic v(C-O) stretching modes [30, 31], respectively, (Table 2). The absence of a weak broad band in the 3070–3300 cm⁻¹ region, noted in the spectra of the metal complexes, indicates deprotonation of the intramolecular hydrogen bonded OH group on complexation and subsequent coordination of phenolic v(C-O) [32] to the extent of 25–40 cm⁻¹. On complexation, the v(C=N) band is shifted to lower wave number relative to the free ligand, indicating that the nitrogen of the azomethine group is coordinated to the metal ion, which may be attributed to lowering of the v(C=N) bond order as a result of Pb \leftarrow N bond formation [33]. This is supported by upward shift in v(C-N) to the extent of 10–30 cm⁻¹. The FTIR spectra of metal chelates contained new bands in the 530–542 cm⁻¹ range, assigned to (Pb \leftarrow N), and in the 455–470 cm⁻¹ range, assigned to (Pb–O) [34, 35].

The disappearance of a band due to v(C=O) and appearance of new bands at 1550–1570 and 1365–1370 cm⁻¹ assignable to $v(NCO^{-})$ [36] are indicative of deprotonation of the NH proton and bonding through the imidolate oxygen. The IR

spectra of the thiosemicarbazones do not show any absorption band at $\sim 2570 \text{ cm}^{-1}$, indicating that in the solid state the thione form is present. Further, for the ligands a strong band at $\sim 1322 \text{ cm}^{-1}$ is indicative of v(C=S). The lowering of this band in the form of v(C=S) can be attributed to coordination of the ligands through the thiolo sulfur atom. For the ligands, the bands observed at 3450–3370 cm⁻¹ are because of the symmetric and asymmetric modes of the amino (NH₂) group. These bands are observed at almost the same position in the spectra of the lead complexes suggesting the non-involvement of this amino group in chelation.

Electronic spectra

In the electronic spectra of the ligands a band at 220 nm is observed which may be assigned to the IB band of the phenyl ring. This shifts to longer wavelength on complexation and is observed at 232 nm in the complexes. Also, the ligands' chromophore >C=N, which is observed at 280 nm, shifts to higher wavelength and is observed at 295 nm in the complexes. In the spectra of ligands, a band observed at 345 nm, because of the secondary band of benzene, which is red shifted because of the presence of >C=N–. However, this appears at 372 nm in the complexes, possibly because of polarization of the C=N bond by the metal–ligand electron interaction. Three sharp bands are observed in the region 240–262 nm and are assigned as charge-transfer bands, indicating the formation of σ bond and $(d\pi-p\pi)$ bonds between the p-orbitals of sulfur and the vacant d orbitals of the metal atom. Complexes are then expected to show long-wavelength metal to ligand charge transfer (MLCT) bands if the ligands provide empty orbitals at low energies. Accordingly, compounds are coloured owing to the presence of such MLCT bands in the visible region.

¹H NMR spectra

All the protons were found in their expected regions. The conclusions drawn from these studies lend further support to the mode of bonding discussed in their IR spectra. In the spectra of lead(II) complexes, coordination of the ligands via azomethine nitrogen, phenolic and ketonic oxygen, and thiolic sulfur was established by the downfield shifting of these signals in the lead(II) complexes, because of the increased conjugation and coordination [37]. The number of protons calculated from the integration curves and those obtained from the values of the expected CHN analyses agree with each other. It was observed that DMSO had no coordinating effect either on the spectra of the ligands or on its metal complexes. In the proton magnetic resonance spectra of the ligands, sharp signals at δ 2.18 ppm and δ 9.09–9.95 ppm are observed, because of -C(CH₃)=N- and -CH=N-, respectively. These move downfield (δ 0.10 ppm) in the complexes in comparison with the original position in the ligands, because of coordination of azomethine nitrogen with the metal atom. This is probably because of the donation of a lone pair of electrons by the nitrogen to the central metal atom resulting in the formation of a coordinate linkage (Pb \leftarrow N). The ligands also give OH proton signals at δ

12.50 \pm 0.50 ppm (s) which is absent from the spectra of the corresponding lead complexes, showing, thereby, chelation of the ligand moiety through the deprotonated phenolic oxygen. The broad signal exhibited by the ligand because of the NH proton at δ 8.08 \pm 0.07 ppm disappears in the lead complexes, indicating coordination of the nitrogen by covalent bond formation by the sulfur/oxygen with the metal because of tautomerisation of the ligand in the enol-keto form. The ligands give a complex multiplet signal in the region δ 6.78–7.92 ppm (m) for the aromatic protons and these remain at almost the same position in the spectra of the metal complexes. The appearance of signals from NH₂ protons at the same positions in the ligand and its complexes show the non-involvement of this group in coordination.

¹³C NMR spectra

¹³C NMR spectra of the ligands and their corresponding lead complexes were recorded in dry DMSO. The signals from the carbon atoms attached to the ketonic/ thiolic and azomethine groups in the ligands appear at $\sim \delta$ 167.6 ppm and $\sim \delta$ 160.1 (158.9) ppm, respectively. However, in the spectra of the corresponding lead complexes, these signals appear at δ 161.5 ppm (because of the ketone/thiol group) and δ 152.4 (149.7) ppm (because of the azomethine groups), respectively. The substantial shifts in the positions of these signals clearly indicate the involvement of these functional groups in bond formation with the metal. Although it is also possible that the shifting of the azomethine carbon signal is because of a change in hybridization of the nitrogen attached to the ketone/thiol group, in the light of IR, UV, and ¹H NMR spectral studies it seems more plausible that the shifting of the signals for these carbons is because of the involvement of ketonic oxygen/sulfur and azomethine nitrogen in bonding.

Thus, on the basis of above discussion, it is evident that the ligands coordinate through the phenolic/ketonic oxygen, thiolic sulfur, and azomethine nitrogen to the lead atom and thus the ligand behaves as a bifunctional tetradentate species. The Pb(II) complexes can possibly be represented by the structure in Fig. 1, with the central lead atom being in the tetra-coordinate environment. The structures proposed for all the Pb(II) complexes are shown in Fig. 1.



 $X = S \text{ or } O; R = H \text{ or } CH_3$







3D molecular modeling and analysis

Because of the tetra-coordination of these complexes and taking into account of the irregular tetrahedral geometry, 3D molecular modeling was performed for compound $[PbL^{1}]$ (1), as representative compound, on the basis of the irregular tetrahedral structure. Details of the bond lengths and bond angles as per the 3D structure (Fig. 2) are given in Tables 3 and Table 4, respectively. For convenient study of the different bond lengths and bond angles, the various atoms of the compound in question are numbered in Arabic numerals. In all, 130 measurements of the bond lengths (49 in numbers), plus the bond angles (81 in numbers) are listed. Except for a few cases, optimum values of both the bond lengths and the bond angles are given in the tables, with the actual values. The actual bond lengths/bond angles given in Tables 3 and 4 are calculated values as a result of energy optimization in CHEM 3D Ultra, and the optimum bond length/bond angle values are the standard bond lengths/bond angles established by the builder unit of CHEM 3D. Some values of standard bond lengths/bond angles are missing, possibly because of limitations of the software; we have already noticed this when modeling other systems. In most cases, the actual bond lengths and bond angles are close to the optimum values, confirming the proposed structure of the compound $[Pb(II)L^1]$.

Conclusion

Complexes L^1-L^6 , derivatives of Schiff bases, have been successfully synthesized and characterized. Elemental analysis C, H, N, and Pb results were in agreement with predicted formulae. Results from infrared and NMR spectroscopy of the ligands and complexes showed that coordination takes place via the oxygen atom from the ketone group and the nitrogen atom from the azomethine groups. As a result, in the solid and liquid states the lead(II) atoms are in a four coordinated environment.

1 N(7)-Pb(27) 2.1460 2 Pb(27)-O(28) 2.1100 3 C(17)-O(28) 4.0620 1.4210 4 N(9)-Pb(27) 2.1460 5 5 C(19)-H(40) 1.1000 1.0500 6 N(18)-H(39) 1.0500 1.0500 7 N(18)-H(38) 1.0500 1.0500 8 C(15)-H(37) 1.1000 1.1000 9 C(14)-H(36) 1.1000 1.1000 10 C(13)-H(35) 1.1000 1.1000 11 C(12)-H(34) 1.1000 1.1000 12 C(11)-H(33) 1.1000 1.1000 13 C(6)-H(32) 1.1000 1.1000 14 C(3)-H(41) 1.1000 1.1000 15 C(2)-H(30) 1.1000 1.1000 16 C(1)-H(29) 1.1000 1.1000 17 C(23)-H(42) 1.1000 1.1000 18 Pb(27)-O(26) 2.1100 1.2000 <t< th=""><th>No.</th><th>Atoms</th><th>Actual (Å)</th><th>Optimum (Å)</th></t<>	No.	Atoms	Actual (Å)	Optimum (Å)
2 $Pb(27)-O(28)$ 2.11003 $C(17)-O(28)$ 4.06201.42104 $N(9)-Pb(27)$ 2.14605 $C(19)-H(40)$ 1.10001.10006 $N(18)-H(39)$ 1.05001.05007 $N(18)-H(38)$ 1.05001.05008 $C(15)-H(37)$ 1.10001.10009 $C(14)-H(36)$ 1.10001.100010 $C(13)-H(35)$ 1.10001.100011 $C(12)-H(34)$ 1.10001.100012 $C(11)-H(33)$ 1.10001.100013 $C(6)-H(32)$ 1.10001.100014 $C(3)-H(31)$ 1.10001.100015 $C(2)-H(30)$ 1.10001.100016 $C(1)-H(29)$ 1.10001.100017 $C(23)-H(42)$ 1.10001.100018 $Pb(27)-O(26)$ 2.3701.420020 $C(23)-C(24)$ 1.51691.420021 $C(22)-C(23)$ 1.33701.420022 $C(21)-O(26)$ 2.79451.355023 $C(21)-C(20)$ 1.33701.420024 $C(25)-C(20)$ 1.33701.420025 $C(20)-C(21)$ 1.33701.420026 $C(19)-C(20)$ 1.33701.420027 $C(24)-H(43)$ 1.10001.100028 $C(17)-N(18)$ 1.26601.462029 $N(16)-C(17)$ 1.26001.2600		N(7)–Pb(27)	2.1460	
3 $C(17)-O(28)$ 4.0620 1.4210 4 $N(9)-Pb(27)$ 2.1460 5 $C(19)-H(40)$ 1.1000 1.0000 6 $N(18)-H(39)$ 1.0500 1.0500 7 $N(18)-H(38)$ 1.0500 1.0500 8 $C(15)-H(37)$ 1.1000 1.1000 9 $C(14)-H(36)$ 1.1000 1.1000 10 $C(13)-H(35)$ 1.1000 1.1000 11 $C(12)-H(34)$ 1.1000 1.1000 12 $C(11)-H(33)$ 1.1000 1.1000 13 $C(6)-H(32)$ 1.1000 1.1000 14 $C(3)-H(31)$ 1.1000 1.1000 15 $C(2)-H(30)$ 1.1000 1.1000 16 $C(1)-H(29)$ 1.1000 1.1000 17 $C(23)-H(42)$ 1.1000 1.1000 18 $Pb(27)-O(26)$ 2.1100 1.4200 20 $C(23)-C(24)$ 1.5169 1.4200 21 $C(22)-C(23)$ 1.3370 1.4200 22 $C(21)-O(26)$ 2.7945 1.3550 23 $C(21)-C(20)$ 1.3370 1.4200 24 $C(25)-C(20)$ 1.3370 1.4200 25 $C(20)-C(21)$ 1.3370 1.4200 26 $C(19)-C(20)$ 1.3370 1.4200 27 $C(24)-H(43)$ 1.1000 1.1000 28 $C(17)-N(18)$ 1.2660 1.4620 29 $N(16)-C(17)$ 1.2600 1.2600	2	Pb(27)-O(28)	2.1100	
4 $N(9)-Pb(27)$ 2.1460 5 $C(19)-H(40)$ 1.1000 1.0000 6 $N(18)-H(39)$ 1.0500 1.0500 7 $N(18)-H(38)$ 1.0500 1.0500 8 $C(15)-H(37)$ 1.1000 1.1000 9 $C(14)-H(36)$ 1.1000 1.1000 10 $C(13)-H(35)$ 1.1000 1.1000 11 $C(12)-H(34)$ 1.1000 1.1000 12 $C(11)-H(33)$ 1.1000 1.1000 13 $C(6)-H(32)$ 1.1000 1.1000 14 $C(3)-H(31)$ 1.1000 1.1000 15 $C(2)-H(30)$ 1.1000 1.1000 16 $C(1)-H(29)$ 1.1000 1.1000 17 $C(23)-H(42)$ 1.1000 1.1000 18 $Pb(27)-O(26)$ 2.1100 1.4200 20 $C(23)-C(24)$ 1.5169 1.4200 21 $C(22)-C(23)$ 1.3370 1.4200 22 $C(21)-O(26)$ 2.7945 1.3550 23 $C(21)-C(22)$ 1.3370 1.4200 24 $C(25)-C(20)$ 1.3370 1.4200 25 $C(20)-C(21)$ 1.3370 1.4200 26 $C(19)-C(20)$ 1.3370 1.4200 27 $C(24)-H(43)$ 1.1000 1.1000 28 $C(17)-N(18)$ 1.2600 1.4620 29 $N(16)-C(17)$ 1.2600 1.2600	3	C(17)-O(28)	4.0620	1.4210
5 $C(19)-H(40)$ 1.1000 1.1000 6 $N(18)-H(39)$ 1.0500 1.0500 7 $N(18)-H(38)$ 1.0500 1.0500 8 $C(15)-H(37)$ 1.1000 1.1000 9 $C(14)-H(36)$ 1.1000 1.1000 10 $C(13)-H(35)$ 1.1000 1.1000 11 $C(12)-H(34)$ 1.1000 1.1000 12 $C(11)-H(33)$ 1.1000 1.1000 13 $C(6)-H(32)$ 1.1000 1.1000 14 $C(3)-H(31)$ 1.1000 1.1000 15 $C(2)-H(30)$ 1.1000 1.1000 16 $C(1)-H(29)$ 1.1000 1.1000 17 $C(23)-H(42)$ 1.1000 1.1000 18 $Pb(27)-O(26)$ 2.1100 1.4200 20 $C(23)-C(24)$ 1.5169 1.4200 21 $C(22)-C(23)$ 1.3370 1.4200 22 $C(21)-O(26)$ 2.7945 1.3550 23 $C(21)-C(22)$ 1.3370 1.4200 24 $C(25)-C(20)$ 1.3370 1.4200 25 $C(20)-C(21)$ 1.3370 1.4200 26 $C(19)-C(20)$ 1.3370 1.4200 27 $C(24)-H(43)$ 1.1000 1.1000 28 $C(17)-N(18)$ 1.2660 1.4620 29 $N(16)-C(17)$ 1.2600 1.2600	Ļ	N(9)-Pb(27)	2.1460	
6 $N(18)-H(39)$ 1.0500 1.0500 7 $N(18)-H(38)$ 1.0500 1.0500 8 $C(15)-H(37)$ 1.1000 1.1000 9 $C(14)-H(36)$ 1.1000 1.1000 10 $C(13)-H(35)$ 1.1000 1.1000 11 $C(12)-H(34)$ 1.1000 1.1000 12 $C(11)-H(33)$ 1.1000 1.1000 13 $C(6)-H(32)$ 1.1000 1.1000 14 $C(3)-H(31)$ 1.1000 1.1000 15 $C(2)-H(30)$ 1.1000 1.1000 16 $C(1)-H(29)$ 1.1000 1.1000 17 $C(23)-H(42)$ 1.1000 1.1000 18 $Pb(27)-O(26)$ 2.1100 1.4200 20 $C(23)-C(24)$ 1.5169 1.4200 21 $C(22)-C(23)$ 1.3370 1.4200 22 $C(21)-O(26)$ 2.7945 1.3550 23 $C(21)-C(22)$ 1.3370 1.4200 24 $C(25)-C(20)$ 1.3370 1.4200 25 $C(20)-C(21)$ 1.3370 1.4200 26 $C(19)-C(20)$ 1.3370 1.4200 27 $C(24)-H(43)$ 1.1000 1.1000 28 $C(17)-N(18)$ 1.2660 1.4620 29 $N(16)-C(17)$ 1.2600 1.2600	i	C(19)-H(40)	1.1000	1.1000
7 $N(18)-H(38)$ 1.0500 1.0500 8 $C(15)-H(37)$ 1.1000 1.1000 9 $C(14)-H(36)$ 1.1000 1.1000 10 $C(13)-H(35)$ 1.1000 1.1000 11 $C(12)-H(34)$ 1.1000 1.1000 12 $C(11)-H(33)$ 1.1000 1.1000 13 $C(6)-H(32)$ 1.1000 1.1000 14 $C(3)-H(31)$ 1.1000 1.1000 15 $C(2)-H(30)$ 1.1000 1.1000 16 $C(1)-H(29)$ 1.1000 1.1000 17 $C(23)-H(42)$ 1.1000 1.1000 18Pb(27)-O(26) 2.1100 1.4200 20 $C(23)-C(24)$ 1.5169 1.4200 21 $C(22)-C(23)$ 1.3370 1.4200 22 $C(21)-O(26)$ 2.7945 1.3550 23 $C(21)-C(22)$ 1.3370 1.4200 24 $C(25)-C(20)$ 1.3370 1.4200 25 $C(20)-C(21)$ 1.3370 1.4200 26 $C(19)-C(20)$ 1.3370 1.4200 27 $C(24)-H(43)$ 1.1000 1.1000 28 $C(17)-N(18)$ 1.2600 1.4600 29 $N(16)-C(17)$ 1.2600 1.2600	j.	N(18)-H(39)	1.0500	1.0500
8 C(15)-H(37) 1.1000 1.1000 9 C(14)-H(36) 1.1000 1.1000 10 C(13)-H(35) 1.1000 1.1000 11 C(12)-H(34) 1.1000 1.1000 12 C(11)-H(33) 1.1000 1.1000 13 C(6)-H(32) 1.1000 1.1000 14 C(3)-H(31) 1.1000 1.1000 15 C(2)-H(30) 1.1000 1.1000 16 C(1)-H(29) 1.1000 1.1000 17 C(23)-H(42) 1.1000 1.1000 18 Pb(27)-O(26) 2.1100 1.4200 20 C(24)-C(25) 1.3370 1.4200 21 C(22)-C(23) 1.3370 1.4200 22 C(21)-O(26) 2.7945 1.3550 23 C(21)-C(22) 1.3370 1.4200 24 C(25)-C(20) 1.3370 1.4200 25 C(20)-C(21) 1.3370 1.4200 26 C(19)-C(20) 1.3370<	,	N(18)-H(38)	1.0500	1.0500
9 C(14)-H(36) 1.1000 1.1000 10 C(13)-H(35) 1.1000 1.1000 11 C(12)-H(34) 1.1000 1.1000 12 C(11)-H(33) 1.1000 1.1000 13 C(6)-H(32) 1.1000 1.1000 14 C(3)-H(31) 1.1000 1.1000 15 C(2)-H(30) 1.1000 1.1000 16 C(1)-H(29) 1.1000 1.1000 17 C(23)-H(42) 1.1000 1.1000 18 Pb(27)-O(26) 2.1100 1.1000 20 C(24)-C(25) 1.3370 1.4200 21 C(22)-C(23) 1.3370 1.4200 22 C(1)-O(26) 2.7945 1.3550 23 C(21)-C(22) 1.3370 1.4200 24 C(25)-C(20) 1.3370 1.4200 25 C(20)-C(21) 1.3370 1.4200 26 C(19)-C(20) 1.3370 1.4200 27 C(24)-H(43) 1.1000 1.1000 28 C(17)-N(18) 1.2660 1.4620 <td>3</td> <td>C(15)-H(37)</td> <td>1.1000</td> <td>1.1000</td>	3	C(15)-H(37)	1.1000	1.1000
10 $C(13)-H(35)$ 1.1000 1.1000 11 $C(12)-H(34)$ 1.1000 1.1000 12 $C(11)-H(33)$ 1.1000 1.1000 13 $C(6)-H(32)$ 1.1000 1.1000 14 $C(3)-H(31)$ 1.1000 1.1000 15 $C(2)-H(30)$ 1.1000 1.1000 16 $C(1)-H(29)$ 1.1000 1.1000 17 $C(23)-H(42)$ 1.1000 1.1000 18 $Pb(27)-O(26)$ 2.1100 1.4200 20 $C(24)-C(25)$ 1.3370 1.4200 21 $C(22)-C(23)$ 1.3370 1.4200 22 $C(21)-O(26)$ 2.7945 1.3550 23 $C(21)-C(22)$ 1.3370 1.4200 24 $C(25)-C(20)$ 1.3370 1.4200 25 $C(20)-C(21)$ 1.3370 1.4200 26 $C(19)-C(20)$ 1.3370 1.4200 27 $C(24)-H(43)$ 1.1000 1.1000 28 $C(17)-N(18)$ 1.2660 1.4620 29 $N(16)-C(17)$ 1.2600 1.2600)	C(14)-H(36)	1.1000	1.1000
11 $C(12)-H(34)$ 1.1000 1.1000 12 $C(11)-H(33)$ 1.1000 1.1000 13 $C(6)-H(32)$ 1.1000 1.1000 14 $C(3)-H(31)$ 1.1000 1.1000 15 $C(2)-H(30)$ 1.1000 1.1000 16 $C(1)-H(29)$ 1.1000 1.1000 17 $C(23)-H(42)$ 1.1000 1.1000 18 $Pb(27)-O(26)$ 2.1100 1.4200 20 $C(24)-C(25)$ 1.3370 1.4200 21 $C(22)-C(23)$ 1.3370 1.4200 22 $C(21)-O(26)$ 2.7945 1.3550 23 $C(21)-C(22)$ 1.3370 1.4200 24 $C(25)-C(20)$ 1.3370 1.4200 25 $C(20)-C(21)$ 1.3370 1.4200 26 $C(19)-C(20)$ 1.3370 1.4200 27 $C(24)-H(43)$ 1.1000 1.1000 28 $C(17)-N(18)$ 1.2660 1.4620 29 $N(16)-C(17)$ 1.2600 1.2600	0	C(13)-H(35)	1.1000	1.1000
12 $C(11)-H(33)$ 1.1000 1.1000 13 $C(6)-H(32)$ 1.1000 1.1000 14 $C(3)-H(31)$ 1.1000 1.1000 15 $C(2)-H(30)$ 1.1000 1.1000 16 $C(1)-H(29)$ 1.1000 1.1000 17 $C(23)-H(42)$ 1.1000 1.1000 18Pb(27)-O(26) 2.1100 1.4200 20 $C(24)-C(25)$ 1.3370 1.4200 21 $C(22)-C(23)$ 1.3370 1.4200 22 $C(21)-O(26)$ 2.7945 1.3550 23 $C(21)-C(22)$ 1.3370 1.4200 24 $C(25)-C(20)$ 1.3370 1.4200 25 $C(20)-C(21)$ 1.3370 1.4200 26 $C(19)-C(20)$ 1.3370 1.4200 27 $C(24)-H(43)$ 1.1000 1.1000 28 $C(17)-N(18)$ 1.2600 1.4620 29 $N(16)-C(17)$ 1.2600 1.2600	1	C(12)-H(34)	1.1000	1.1000
13 $C(6)-H(32)$ 1.10001.100014 $C(3)-H(31)$ 1.10001.100015 $C(2)-H(30)$ 1.10001.100016 $C(1)-H(29)$ 1.10001.100017 $C(23)-H(42)$ 1.10001.100018Pb(27)-O(26)2.11001.420020 $C(24)-C(25)$ 1.33701.420021 $C(22)-C(23)$ 1.33701.420022 $C(21)-O(26)$ 2.79451.355023 $C(21)-C(22)$ 1.33701.420024 $C(25)-C(20)$ 1.33701.420025 $C(20)-C(21)$ 1.33701.420026 $C(19)-C(20)$ 1.33701.503027 $C(24)-H(43)$ 1.10001.100028 $C(17)-N(18)$ 1.26001.462029 $N(16)-C(17)$ 1.26001.2600	2	C(11)-H(33)	1.1000	1.1000
14 $C(3)-H(31)$ 1.1001.100015 $C(2)-H(30)$ 1.10001.100016 $C(1)-H(29)$ 1.10001.100017 $C(23)-H(42)$ 1.10001.100018Pb(27)-O(26)2.11001.420020 $C(23)-C(24)$ 1.51691.420021 $C(22)-C(23)$ 1.33701.420022 $C(21)-O(26)$ 2.79451.355023 $C(21)-C(22)$ 1.33701.420024 $C(25)-C(20)$ 1.33701.420025 $C(20)-C(21)$ 1.33701.420026 $C(19)-C(20)$ 1.33701.503027 $C(24)-H(43)$ 1.10001.100028 $C(17)-N(18)$ 1.26601.462029 $N(16)-C(17)$ 1.26001.2600	.3	C(6)–H(32)	1.1000	1.1000
15 $C(2)$ -H(3)1.1001.10016 $C(1)$ -H(29)1.10001.100017 $C(23)$ -H(42)1.10001.100018Pb(27)-O(26)2.1100119 $C(24)$ - $C(25)$ 1.33701.420020 $C(23)$ - $C(24)$ 1.51691.420021 $C(22)$ - $C(23)$ 1.33701.420022 $C(21)$ - $O(26)$ 2.79451.355023 $C(21)$ - $C(22)$ 1.33701.420024 $C(25)$ - $C(20)$ 1.33701.420025 $C(20)$ - $C(21)$ 1.33701.420026 $C(19)$ - $C(20)$ 1.33701.503027 $C(24)$ -H(43)1.10001.100028 $C(17)$ - $N(18)$ 1.26601.462029 $N(16)$ - $C(17)$ 1.26001.2600	4	C(3)–H(31)	1.1000	1.1000
16 $C(1)-H(29)$ 1.1000 1.1000 17 $C(23)-H(42)$ 1.1000 1.1000 18 $Pb(27)-O(26)$ 2.1100 19 $C(24)-C(25)$ 1.3370 1.4200 20 $C(23)-C(24)$ 1.5169 1.4200 21 $C(22)-C(23)$ 1.3370 1.4200 22 $C(21)-O(26)$ 2.7945 1.3550 23 $C(21)-C(22)$ 1.3370 1.4200 24 $C(25)-C(20)$ 1.3370 1.4200 25 $C(20)-C(21)$ 1.3370 1.4200 26 $C(19)-C(20)$ 1.3370 1.5030 27 $C(24)-H(43)$ 1.1000 1.1000 28 $C(17)-N(18)$ 1.2660 1.4620 29 $N(16)-C(17)$ 1.2600 1.2600	.5	C(2)-H(30)	1.1000	1.1000
17 $C(23)$ -H(42) 1.100 1.100 18 Pb(27)-O(26) 2.1100 19 $C(24)$ -C(25) 1.3370 1.4200 20 $C(23)$ -C(24) 1.5169 1.4200 21 $C(22)$ -C(23) 1.3370 1.4200 22 $C(21)$ -O(26) 2.7945 1.3550 23 $C(21)$ -C(22) 1.3370 1.4200 24 $C(25)$ -C(20) 1.3370 1.4200 25 $C(20)$ -C(21) 1.3370 1.4200 26 $C(19)$ -C(20) 1.3370 1.5030 27 $C(24)$ -H(43) 1.1000 1.1000 28 $C(17)$ -N(18) 1.2660 1.4620 29 N(16)-C(17) 1.2600 1.2600	.6	C(1)–H(29)	1.1000	1.1000
18Pb(27)-O(26)2.110019 $C(24)-C(25)$ 1.3370 1.4200 20 $C(23)-C(24)$ 1.5169 1.4200 21 $C(22)-C(23)$ 1.3370 1.4200 22 $C(21)-O(26)$ 2.7945 1.3550 23 $C(21)-C(22)$ 1.3370 1.4200 24 $C(25)-C(20)$ 1.3370 1.4200 25 $C(20)-C(21)$ 1.3370 1.4200 26 $C(19)-C(20)$ 1.3370 1.5030 27 $C(24)-H(43)$ 1.1000 1.1000 28 $C(17)-N(18)$ 1.2660 1.4620 29 $N(16)-C(17)$ 1.2600 1.2600	.7	C(23)-H(42)	1.1000	1.1000
19 $C(24)-C(25)$ 1.33701.420020 $C(23)-C(24)$ 1.51691.420021 $C(22)-C(23)$ 1.33701.420022 $C(21)-O(26)$ 2.79451.355023 $C(21)-C(22)$ 1.33701.420024 $C(25)-C(20)$ 1.33701.420025 $C(20)-C(21)$ 1.33701.420026 $C(19)-C(20)$ 1.33701.503027 $C(24)-H(43)$ 1.10001.100028 $C(17)-N(18)$ 1.26601.462029 $N(16)-C(17)$ 1.26001.2600	8	Pb(27)–O(26)	2.1100	
20 $C(23)-C(24)$ 1.5169 1.4200 21 $C(22)-C(23)$ 1.3370 1.4200 22 $C(21)-O(26)$ 2.7945 1.3550 23 $C(21)-C(22)$ 1.3370 1.4200 24 $C(25)-C(20)$ 1.3370 1.4200 25 $C(20)-C(21)$ 1.3370 1.4200 26 $C(19)-C(20)$ 1.3370 1.5030 27 $C(24)-H(43)$ 1.1000 1.1000 28 $C(17)-N(18)$ 1.2660 1.4620 29 $N(16)-C(17)$ 1.2600 1.2600	9	C(24)–C(25)	1.3370	1.4200
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20	C(23)–C(24)	1.5169	1.4200
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	21	C(22)–C(23)	1.3370	1.4200
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	22	C(21)–O(26)	2.7945	1.3550
24 C(25)-C(20) 1.3370 1.4200 25 C(20)-C(21) 1.3370 1.4200 26 C(19)-C(20) 1.3370 1.5030 27 C(24)-H(43) 1.1000 1.1000 28 C(17)-N(18) 1.2660 1.4620 29 N(16)-C(17) 1.2600 1.2600	23	C(21)–C(22)	1.3370	1.4200
25 C(20)-C(21) 1.3370 1.4200 26 C(19)-C(20) 1.3370 1.5030 27 C(24)-H(43) 1.1000 1.1000 28 C(17)-N(18) 1.2660 1.4620 29 N(16)-C(17) 1.2600 1.2600	24	C(25)–C(20)	1.3370	1.4200
26 C(19)-C(20) 1.3370 1.5030 27 C(24)-H(43) 1.1000 1.1000 28 C(17)-N(18) 1.2660 1.4620 29 N(16)-C(17) 1.2600 1.2600	25	C(20)–C(21)	1.3370	1.4200
27 C(24)-H(43) 1.1000 1.1000 28 C(17)-N(18) 1.2660 1.4620 29 N(16)-C(17) 1.2600 1.2600	26	C(19)–C(20)	1.3370	1.5030
28 C(17)–N(18) 1.2660 1.4620 29 N(16)–C(17) 1.2600 1.2600	27	C(24)–H(43)	1.1000	1.1000
29 N(16)-C(17) 1.2600 1.2600	28	C(17)–N(18)	1.2660	1.4620
	29	N(16)-C(17)	1.2600	1.2600
30 C(14)–C(15) 1.3949 1.4200	80	C(14)-C(15)	1.3949	1.4200
31 C(13)-C(14) 1.3948 1.4200	51	C(13)–C(14)	1.3948	1.4200
32 C(12)–C(13) 1.3948 1.4200	32	C(12)–C(13)	1.3948	1.4200
33 C(11)–C(12) 1.3949 1.4200	33	C(11)–C(12)	1.3949	1.4200
34 C(15)-C(10) 1.3948 1.4200	34	C(15)-C(10)	1.3948	1.4200
35 C(10)-C(11) 1.3948 1.4200	5	C(10)–C(11)	1.3948	1.4200
36 C(25)-H(44) 1.1000 1.1000	6	C(25)-H(44)	1.1000	1.1000
37 N(9)–N(16) 1.2480 1.4180	37	N(9)–N(16)	1.2480	1.4180
38 C(8)–C(10) 1.3370 1.5030	8	C(8)–C(10)	1.3370	1.5030
39 C(8)–N(9) 1.6579 1.2600	9	C(8)–N(9)	1.6579	1.2600
40 C(22)-H(41) 1.1000 1.1000	0	C(22)–H(41)	1.1000	1.1000
41 N(7)–C(19) 1.2600 1.2600	1	N(7)–C(19)	1.2600	1.2600
42 C(5)–N(7) 1.2600 1.4560	2	C(5)–N(7)	1.2600	1.4560

 Table 3 Bond lengths of the compound [PbL¹]

No.	Atoms	Actual (Å)	Optimum (Å)
43	C(5)–C(6)	1.3370	1.4200
44	C(4)–C(8)	1.3370	1.5030
45	C(4)–C(5)	1.3370	1.4200
46	C(3)–C(4)	1.3370	1.4200
47	C(2)–C(3)	1.3370	1.4200
48	C(6)–C(1)	1.3370	1.4200
49	C(1)–C(2)	1.5259	1.4200

Table 3 continued

 Table 4 Bond angles of the compound [Pb(II)L¹]

No.	Atoms	Actual (°)	Optimum (°)
1	Pb(27)–O(28)–C(17)	53.1730	
2	O(28)-Pb(27)-O(26)	114.6507	
3	O(28)-Pb(27)-N(9)	104.0000	
4	O(28)-Pb(27)-N(7)	109.5000	
5	O(26)-Pb(27)-N(9)	109.5000	
6	O(26)-Pb(27)-N(7)	109.5000	
7	N(9)-Pb(27)-N(7)	109.5000	
8	Pb(27)-O(26)-C(21)	60.5255	
9	H(44)-C(25)-C(24)	120.0000	120.0000
10	H(44)-C(25)-C(20)	120.0000	120.0000
11	C(24)-C(25)-C(20)	120.0000	
12	H(43)-C(24)-C(25)	122.9658	120.0000
13	H(43)-C(24)-C(23)	122.9658	120.0000
14	C(25)-C(24)-C(23)	114.0685	
15	H(42)-C(23)-C(24)	123.6612	120.0000
16	H(42)-C(23)-C(22)	123.6612	120.0000
17	C(24)-C(23)-C(22)	112.6776	
18	H(41)-C(22)-C(23)	120.0000	120.0000
19	H(41)-C(22)-C(21)	120.0000	120.0000
20	C(23)-C(22)-C(21)	120.0000	
21	O(26)-C(21)-C(22)	104.4290	124.3000
22	O(26)-C(21)-C(20)	135.5707	124.3000
23	C(22)-C(21)-C(20)	119.9992	120.0000
24	C(25)–C(20)–C(21)	119.9988	120.0000
25	C(25)-C(20)-C(19)	119.9988	120.0000
26	C(21)-C(20)-C(19)	120.0000	120.0000
27	H(40)-C(19)-C(20)	120.0000	120.0000
28	H(40)-C(19)-N(7)	120.0000	116.5000
29	C(20)-C(19)-N(7)	120.0000	123.5000

No.	Atoms	Actual (°)	Optimum (°)
30	H(39)-N(18)-H(38)	120.0000	118.8000
31	H(39)–N(18)–C(17)	120.0000	
32	H(38)–N(18)–C(17)	120.0000	
33	O(28)-C(17)-N(18)	138.4324	
34	O(28)-C(17)-N(16)	83.1352	122.0000
35	N(18)-C(17)-N(16)	138.4324	126.0000
36	C(17)-N(16)-N(9)	104.0000	107.5000
37	H(37)-C(15)-C(14)	120.0002	120.0000
38	H(37)-C(15)-C(10)	120.0002	120.0000
39	C(14)-C(15)-C(10)	119.9996	
40	H(36)-C(14)-C(15)	120.0012	120.0000
41	H(36)-C(14)-C(13)	120.0012	120.0000
42	C(15)-C(14)-C(13)	119.9976	
43	H(35)-C(13)-C(14)	119.9991	120.0000
44	H(35)-C(13)-C(12)	119.9991	120.0000
45	C(14)-C(13)-C(12)	120.0018	
46	H(34)-C(12)-C(13)	119.9994	120.0000
47	H(34)–C(12)–C(11)	119.9994	120.0000
48	C(13)-C(12)-C(11)	120.0013	
49	H(33)-C(11)-C(12)	120.0015	120.0000
50	H(33)-C(11)-C(10)	120.0015	120.0000
51	C(12)-C(11)-C(10)	119.9969	
52	C(15)-C(10)-C(11)	120.0029	120.0000
53	C(15)-C(10)-C(8)	119.9986	120.0000
54	C(11)-C(10)-C(8)	119.9986	120.0000
55	Pb(27)-N(9)-N(16)	104.0000	
56	Pb(27)–N(9)–C(8)	80.0151	
57	N(16)-N(9)-C(8)	107.5000	
58	C(10)-C(8)-N(9)	108.9436	120.0000
59	C(10)-C(8)-C(4)	108.9436	120.0000
60	N(9)-C(8)-C(4)	142.1128	120.0000
61	Pb(27)–N(7)–C(19)	120.0000	
62	Pb(27)–N(7)–C(5)	120.0000	
63	C(19)–N(7)–C(5)	115.0000	
64	H(32)-C(6)-C(5)	120.0000	120.0000
65	H(32)–C(6)–C(1)	120.0000	120.0000
66	C(5)-C(6)-C(1)	120.0000	
67	N(7)-C(5)-C(6)	119.9988	120.0000
68	N(7)-C(5)-C(4)	120.0000	120.0000
69	C(6)-C(5)-C(4)	119.9988	120.0000
70	C(8)–C(4)–C(5)	119.9988	120.0000

Table 4 continued

No.	Atoms	Actual (°)	Optimum (°)
71	C(8)–C(4)–C(3)	119.9988	120.0000
72	C(5)-C(4)-C(3)	120.0000	120.0000
73	H(31)-C(3)-C(4)	120.0000	120.0000
74	H(31)–C(3)–C(2)	120.0000	120.0000
75	C(4)–C(3)–C(2)	120.0000	
76	H(30)–C(2)–C(3)	124.0860	120.0000
77	H(30)-C(2)-C(1)	124.0860	120.0000
78	C(3)–C(2)–C(1)	111.8279	
79	H(29)–C(1)–C(6)	124.0855	120.0000
80	H(29)–C(1)–C(2)	124.0855	120.0000
81	C(6)-C(1)-C(2)	111.8290	

 Table 4 continued

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References

- M.T.H. Tarafder, M.A. Ali, D.J. Wee, K. Azahari, S. Silong, K.A. Crouse, Transit. Met. Chem. 25, 456–460 (2000)
- 2. E. Franco, E. López-Torres, M. Mendiola, M. Sevilla, Polyhedron 19, 441-451 (2000)
- M.A. Ali, A.H. Mirza, R.J. Butcher, M.T.H. Tarafder, A.A. Manaf, Inorg. Chim. Acta 320, 1–6 (2001)
- 4. H.L. Singh, Spectrochim. Acta A 76, 253-258 (2010)
- 5. H.L. Singh, M.K. Gupta, A.K. Varshney, Res. Chem. Intermed. 27, 605–614 (2001)
- 6. D. Zhang, Q. Li, M.-X. Li, D.-Y. Chen, J.-Y. Niu, J. Coord. Chem. 63, 1063–1070 (2010)
- N. Bharti, M.R. Maurya, F. Naqvi, A. Bhattacharya, S. Bhattacharya, A. Azam, Eur. J. Med. Chem. 35, 481–486 (2000)
- M.T.H. Tarafder, A. Asmadi, S.M.S. Talib, A.M. Ali, K.A. Crouse, Transit. Met. Chem. 26, 170–174 (2001)
- 9. H.L. Singh, Phosphorus Sulfur Silicon Relat. Elem. 184, 1768–1778 (2009)
- 10. P. Subhash, K.B. George, Coord. Chem. Rev. 63, 127-160 (1985)
- 11. R.K. Agarwal, S. Prasad, N. Gahlot, Turk. J. Chem. 28, 691-702 (2004)
- M.M. Muthukumar, S. Sivakumar, P. Viswanathamurthi, R. Karvembu, R. Prabhakaran, K. Natarajan, J. Coord. Chem. 63, 296–306 (2010)
- 13. K. Nandi, S. Chaudhuri, S.K. Mazumdar, S. Ghosh, J. Chem. Soc. Perkin Trans. 2, 1729–1734 (1984)
- R. Natarajan, K. Antonysamy, T. Chinnathangavel, J. Kadarkaraithangam, Transit. Met. Chem. 28, 29–36 (2003)
- T. Rosu, M. Negoiu, S. Pasculescu, E. Pahontu, D. Poirier, A. Gulea, Eur. J. Med. Chem. 45, 774–781 (2010)
- 16. L. Latheef, M.R.P. Kurup, Polyhedron 27, 35-43 (2008)
- 17. D.L. Klayman, J.P. Scovill, J.F. Bartosevich, J. Bruce, J. Med. Chem. 26, 35–39 (1983)
- 18. J. Juris, M.T. Gandolti, M.F. Manfrin, V. Balzani, J. Am, J. Am. Chem. Soc. 98, 1047–1048 (1976)
- 19. P.S. Reddy, P.V. Ananthalakshmi, V. Jayatyagaraju, E-J. Chem. 8, 415-420 (2011)
- 20. B.S. Garg, D.N. Kumar, Spectrochim. Acta A 59, 229-234 (2003)
- 21. N.P. Singh, V.P. Tyagi, B. Ratnam, J. Chem. Pharm. Res. 2, 473-477 (2010)

- L.A. Saghatforoush, A. Aminkhani, S. Ershad, G. Karimnezhad, S. Ghammamy, R. Kabiri, Molecules 13, 804–811 (2008)
- 23. A.F. Shabani, L.A. Saghatforoush, S. Ghammamy, Bull. Chem. Soc. Ethiop. 24, 193-199 (2010)
- 24. A. Mohindru, J.M. Fisher, M. Rabinovitz, Nature 303, 64-65 (1983)
- 25. S.M. Abdallah, M.A. Zayed, G.G. Mohamed, Arab. J. Chem. 3, 103-113 (2010)
- 26. A. Biswas, M.G.B. Drew, A. Ghosh, Polyhedron 29, 1029–1034 (2010)
- 27. B. Singh, A.K. Srivastava, Synth. React. Inorg. Met.-Org. Chem. 29, 877-896 (1999)
- 28. S. Munde, A.N. Jagdale, S.M. Jadhav, T.K. Chondhehar, J. Korean Chem. Soc. 53, 407–414 (2009)
- 29. CS Chem. 3D Ultra molecular modeling and analysis, Cambridge. www.cambridgesoft.com.
- 30. S.F. Tan, K.P. Ang, H.L. Jatchandran, Trans. Met. Chem. 9, 390-395 (1984)
- H.L. Singh, A.V. Varshney (2006) Bioinorg. Chem. Appl. Art. no. 23245. doi:10.1155/BCA/2006/ 23245.
- 32. P.V. Rao, A.V. Narasaiah, Indian J. Chem. 42A, 1896–1899 (2003)
- M.K. Gupta, H.L. Singh, U.D. Tripaathi, A.K. Varshney, Synth. React. Inorg. Met.-Org. Chem. 30, 1685–1695 (2000)
- 34. A. Chaudhary, K. Mahajan, R.V. Singh, Appl. Organomet. Chem. 21, 117-127 (2007)
- 35. H.L. Singh, S.S. Chauhan, H. Sachedeva, Res. Chem. Intermed. 36, 1037-1047 (2010)
- 36. A. Braibanti, F. Dallavalle, M.A. Pellinghelli, E. Leporati, Inorg. Chem. 7, 1430-1433 (1968)
- 37. D.J. Pasto, Organic Structure Determination (Prentice Hall, London, 1969)