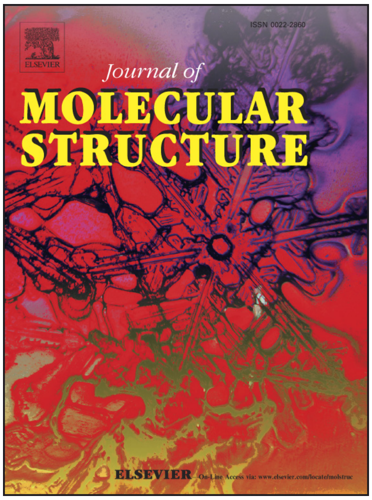


Crystal structure, spectroscopic properties and DFT studies on copper(II) complex of bis{(*E*)-1-[(2-phenoxyphenylimino)methyl]naphthalene-2-ol}chloroform solvate

Mustafa Macit, Gökhan Alpaslan

PII: S0022-2860(14)00511-0
DOI: http://dx.doi.org/10.1016/j.molstruc.2014.05.025
Reference: MOLSTR 20624

To appear in: *Journal of Molecular Structure*

Received Date: 31 January 2014
Revised Date: 6 March 2014
Accepted Date: 12 May 2014

Please cite this article as: M. Macit, G. Alpaslan, Crystal structure, spectroscopic properties and DFT studies on copper(II) complex of bis{(*E*)-1-[(2-phenoxyphenylimino)methyl]naphthalene-2-ol}chloroform solvate, *Journal of Molecular Structure* (2014), doi: http://dx.doi.org/10.1016/j.molstruc.2014.05.025

Crystal structure, spectroscopic properties and DFT studies on copper(II) complex of bis{(*E*)-1-[(2-phenoxyphenylimino)methyl]naphthalene-2-ol}chloroform solvate

Mustafa Macit[a], **Gökhan Alpaslan**[b*]

[a]*Department of Chemistry, Faculty of Arts & Science, Ondokuz Mayıs University, 55139, Samsun, Turkey*

[b]*Department of Medical Services and Techniques, Vocational High School of Health Services, Giresun University, 28200, Giresun, Turkey*

Abstract

Copper (II) complex of the title Schiff base compound was synthesized from the reaction of 2-hydroxy-1-naphthaldehyde with 2-phenoxyaniline. The complex has been characterized by FT-IR, and X-ray single-crystal techniques. The molecular geometry, vibrational frequencies values of the compound in the ground state have been calculated using the density functional theory (DFT/B3LYP) method with the LANL2DZ basis set and compared with the experimental data. The calculated results show that the optimized geometry is compatible with the crystal structure and the theoretical vibrational frequencies are in good agreement with the experimental values. The energetic behavior of the compound in solvent media has been examined using B3LYP method with the LANL2DZ basis set by applying the polarizable continuum model (PCM). In addition, frontier molecular orbital analysis (HOMO-LUMO), natural bond orbital analysis (NBO) and non-linear optical (NLO) properties of the compound were investigated using same theoretical calculations.

Keywords: Schiff base complex · X-ray · FT-IR · DFT · Non-linear optic

---

***Corresponding author. Tel : +904543101000**

E-mail : gokhan.alpaslan@giresun.edu.tr

1. Introduction

Schiff bases compounds have been widely used due to their potential applications in many fields, such as photochromic and thermochromic properties [1], proton transfer tautomeric equilibria [2], biological and pharmacological activities [3–6]. They may have interesting chemical properties, depending on the substituents with different electron-donating or electron-withdrawing groups [7]. This cause their non-linear properties have an importance for the design of various molecular electronic devices such as optical switches and optical data storage devices [8,9]. Schiff base compounds have often been used as chelating ligands in the field coordination chemistry [10]. These properties have resulted in wide applications in the biological field [10,11]. Copper (II) complexes are known to be effective against *rheumatoid arthritis* and they also show anti-ulcer activity [12]. In additional, some copper (II) complexes with Schiff base possess antifungal, antibacterial, and anticancer properties [13–15].

In recently years, theoretical calculation methods are used to describe the molecular structures and spectroscopic properties as well as experimental studies. Density functional theory (DFT) which is one of these methods have been widely used in literature because of its great accuracy in reproducing the experimental values in molecule geometry, vibrational frequencies, atomic charges, dipole moment, electronic properties etc [16-19].

In previous work ligand (E)-1-((2-phenoxyphenylimino)methyl)naphthalen-2-ol molecule was synthesized and characterized by X-ray single diffraction [20]. In this study, we present the synthesis and structural behavior of bis{(E)-1-[(2-phenoxyphenylimino)methyl]naphthalene-2-ol}Cu(II) chloroform solvate obtained by reaction of (E)-1-((2-phenoxyphenylimino)methyl)naphthalen-2-ol with $Cu(CO_2CH_3)_2.H_2O$. The aim of this study is to investigate molecular structure and vibrational frequencies of the title compound, both experimentally and theoretically. The properties of the structural geometry, natural bond orbital (NBO) analysis, frontier molecular orbitals (FMOs), and nonlinear optical (NLO) properties for the compound at the DFT/B3LYP/LANL2DZ level were studied.

2. Experimental and computational method

2.1. Physical measurement

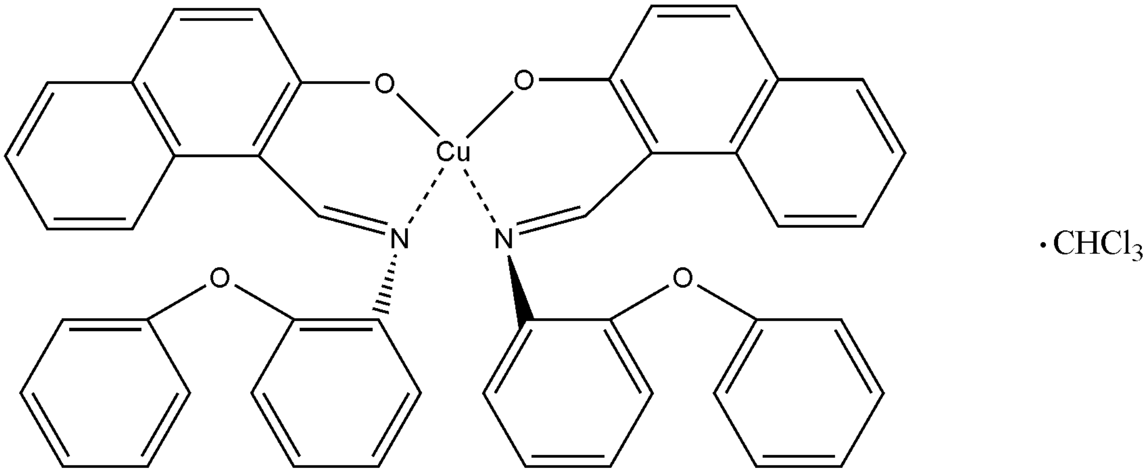
The FT- IR spectrum of the title compound was recorded in the 4000- 400 cm^{-1} region with a Shimadzu FTIR-8900 spectrophotometer using KBr pellet. X-ray single crystal structure was determined on a STOE IPDS II diffractometer.

2.2. Synthesis of (E)-1-[(2-phenoxyphenylimino)methyl]naphthalen-2-ol

(E)-1-((2-phenoxyphenylimino)methyl)naphthalen-2-ol was synthesized according to the literature method [20]. (E)-1-((2-phenoxyphenylimino)methyl)naphthalen-2-ol was prepared by refluxing a mixture of a solution containing 2-hydroxy-1-naphthaldehyde (17,2 mg, 0,1 mmol) in ethanol (30 ml) and a solution containing 2-phenoxyaniline (18,5 mg, 0,1 mmol) in ethanol (20 ml). The reaction mixture was stirred for 2 hour under reflux. Crystals of the title compound were obtained by slow evaporation of an ethanol solution (Yield 68%; m.p. 411-413 K).

2.3. Synthesis of bis{(E)-1-[(2-phenoxyphenylimino)methyl]naphthalene-2-ol}Cu(II)

Cu(II) complex was prepared by refluxing a mixture of a solution containing (E)-1-((2 phenoxyphenylimino)methyl)naphthalen-2-ol (67,8 mg, 0,2 mmol) in ethanol (30 ml) and a solution containing $Cu(CO_2CH_3)_2.H_2O$ (19,9 mg, 0,1 mmol) in ethanol (20 ml). The reaction mixture was stirred for 4 hour under reflux. Single crystals of the title compound for X-ray analysis were obtained by slow evaporation of an chloroform-propanol mixture solution (64%, mp:470-473 K, Scheme 1).



Scheme 1. The chemical diagram of bis{(E)-1-[(2-phenoxyphenylimino)methyl]naphthalene-2-ol}Cu(II) chloroform solvate.

2.3. X-ray crystallography

Data collection was done at 298 K on a STOE IPDS II diffractometer by the w scan technique using graphite monochromated MoK_α radiation (λ=0.71073 Å). Cell refinement was performed using X-AREA software [21]. Absorption correction (μ = 0.79 mm^{-1}) was obtained by the integration method via X-RED32 software [21]. The crystal structure was solved by direct methods using SHELXS–97 [22]. The scattering factors were taken from SHELXL-97 [22]. The molecular graphics were done using Ortep-3 for Windows [23]. The data collection conditions and parameters of refinement process are listed in Table 1.

2.4. Theoretical methods

All theoretical computations were done by using Gaussian 03 W program package [24]. For calculation of molecule geometry was created using the atomic coordinates obtained from X-ray geometry. Geometry optimization of the molecule was performed by using DFT method with Becke's three parameters hybrid exchange-correlation functional (B3LYP) [25] at LANL2DZ basis set [26-28]. The harmonic vibrational frequencies were calculated at the same level of theory for the optimized structure and the obtained frequencies were scaled by

0.9611 [29]. The assignments of vibrational bands have been made by using Gauss-View molecular visualization program [30]. The energetic and dipole moments behavior in solvent media of the title compound were carried out by using PCM method [31–34]. The linear polarizability and first hyperpolarizability properties of the compound were obtained from molecular polarizabilities based on theoretical calculations. In addition, NBO analysis was performed at B3LYP/LANL2DZ level by means of the NBO 3.1 program within the Gaussian 03 W package [35].

Table 1

Crystal data and refinement for the title compound.

Chemical formula	$C_{46}H_{32}CuN_2O_4{\cdot}CHCl_3$
Crystal shape/color	Prism/Black
Formula weight	859.64
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell parameters	a = 13.7884(5) Å b = 16.1674(8) Å c = 20.9582(8) Å β= 120.812(2)°
Volume	4012.6(3) Å^3
Z	4
D_x (Mg cm^{-3})	1.423
μ(mm^{-1})	0.79
F_{000}	1764
Crystal size (mm^3)	0.78×0.61×0.33
Data collection	
Diffractometer/meas.meth	STOE IPDS II/*w*-scan
Absorption correction	Integration
T_{min}	0.632
T_{max}	0.804
No. of measured, independent and observed reflections	18071, 7808, 5040
Criterion for observed reflections	$I > 2\sigma(I)$
R_{int}	0.043
θ_{max}	26.0
Refinement	
Refinement on	F^2
$R[F^2 > 2\sigma (F^2)], wR, S$	0.046, 0.125, 0.92
No. of reflection	7808
No. of parameters	546
Weighting scheme	$w=1/[\sigma^2(F_0^2)+(0.074P)^2 + 0.2501\,P]$ $P=(F_0^2+2F_c^2)/3$
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å^{-3})	0.59, -0.40

3. Results and discussion

3.1. Crystal description

The title complex, an Ortep-3 view of which is shown in Fig.1, crystallizes in the monoclinic space group $P2_1/c$ with Z = 4 in the unit cell. The complex contains two (E)-1-[(2-phenoxyphenylimino)methyl]naphthalen-2-ol ligands with a Cu(II) metal atom and a solvate chloroform molecule. The metal center is distorted square-planar which is supported by the *cis*-N_2O_2 donor atoms of the coordinated Schiff base ligands. The N-Cu-O *trans* angles are 155.04(10)° and 152.53(10)°, indicating a distortion of the square-planar coordination. However, the O–Cu–O and N–Cu–N *cis* angle are 88.95(8)° and 98.89(10)°, respectively. The maximum deviation is 0.4599 (14) Å for atom O3 in the square-planar coordination (Cu1, N1, N2, O1, O3). In addition, the deviations for Cu1, N1, N2 and O1 atoms in the square-planar coordination are -0.0162 (9), 0.4034 (11), -0.3938 (11), and -0.4532 (14) Å, respectively, from the mean plane through these five atoms. The dihedral angle between coordination plane with six-membered chelating plane A[O1,N1,C1,C2,C11] is 21.70°, while the dihedral angle between the one and the other chelating plane B[O3,N2,C24,C25,C34] is 24.88°. Just as the Cu–O1 and Cu–O3 bond lengths are 1.905 (2) and 1.904 (2) Å, the Cu–N1 and Cu–N2 bond lengths are 1.962 (3) and 1.961 (2) Å, respectively. The Cu–N and Cu–O values in the title compound agree with those in other naphthalene complexes. In the literature, the Cu–N have values between 1.870 and 1.920 Å, while the Cu–O bond lengths are range from 1.970 to 2.010 Å [36-40]. The Cl atoms of chloroform molecule are disordered over two positions with site occupancies of 0.684(7) and 0.316(7). The complex molecules are linked via solvent chloroform molecules by C–H···O hydrogen bonds. In addition, there is a C–H···πinteraction of C45–H45 and the phenyl ring.

Perpendicular distance between atom H45 and the plane of the phenyl ring is 2.88 Å (Fig. 2). The details of the hydrogen bonds are summarized in Table 2.

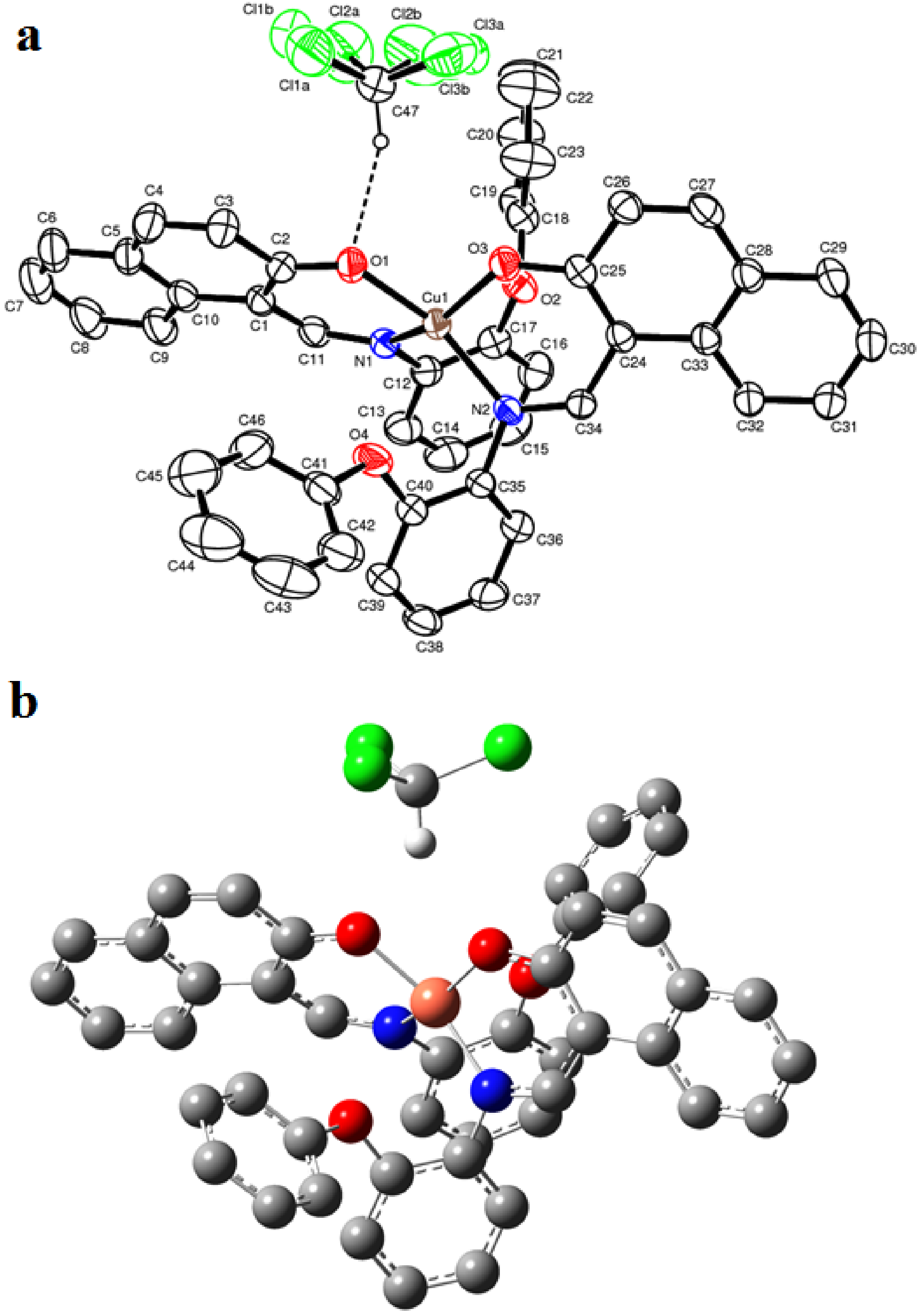


Fig. 1. a) Ortep-3 diagram of the title compound. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular hydrogen bond is shown as a dashed line. b) The

theoretical geometric structure of the title compound (at B3LYP/LANL2DZ level). H atoms are omitted for the sake of clarity.

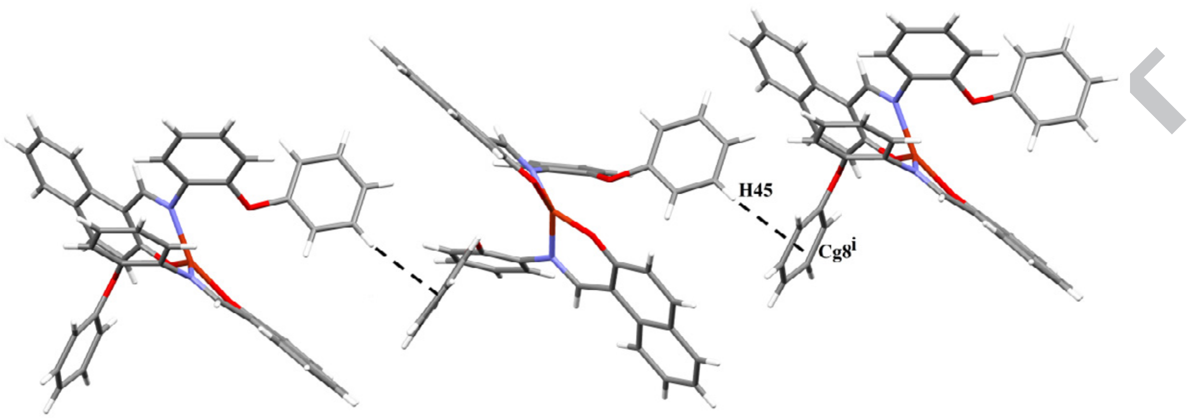


Fig. 2. A partial packing diagram for the title compound, with C–H···π interactions.

Table 2

Hydrogen-bond geometry (Å, °).

D–H···A	**D–H**	**H···A**	**D···A**	**D–H···A**
C47–H47···O1	0.97 (5)	2.26 (5)	3.174 (5)	156 (4)
C45–H45···*Cg*8^{i}	0.93	2.88	3.786 (6)	164

Symmetry code (i) : *x-1, 1/2-y, z-1/2*.
(Cg8 is the centroids of the C18-C23 ring).

3.2. Theoretical structure

Geometric optimization of investigated compound was performed by using DFT/B3LYP method with LANL2DZ basis set (Fig. 1b). The some bond lengths, bond angles and torsion angles of the optimized structure are listed in Table S1 (Supplementary Information) and compared with the experimental data of the compound. As can be seen from Table S1 (Supplementary Information), most of molecular geometric parameters are slightly different from the experimental ones. According to crystallographic studies, the dihedral angle between the coordination plane and chelating plane [A] is 21.70°, while this angle has been calculated at 37.42° for optimized structure. In additional, the N–Cu–O *trans* angles are calculated 155.04(10)° and 152.53(10)°, as well as the O–Cu–O and N–Cu–N *cis* angle are found 88.95(8)° and 98.89(10)°, respectively. The Cu–O1, Cu–O3, Cu–N1 and Cu–N2 bond lengths obtained by B3LYP differ by 0.047, 0.045, 0.048 and 0.046 Å, respectively, from the experimental results. The biggest differences between experimental and calculated bond lengths and angles as 0.068 Å in C20–C21 bond and are 5.47° in O3–Cu1–N1 angle, respectively. In order to compare the theoretical results with the experimental values, root mean square error (RMSE) is used. The calculated RMSE for bond lengths and bond angles are 0.032 Å and 1.21°, respectively. It is well known that the experimental results in the solid state are related to molecular packing, but the theoretical results are related to the gas phase of the isolated molecules. According to these results, it is seen that the B3LYP calculation well reproduce the geometry of the compound.

3.3. Vibrational analysis

FT-IR spectrum of the investigated compound was measured in the 4000-400 cm^{-1} region using KBr pellet on a Shimadzu FT-IR 8900 spectrophotometer (Fig. 3). FT-IR spectra of compounds derived from 2-hydroxy-1-naphthaldehyde Schiff bases have some characteristic stretching bands (CH, CN, CO). The vibrational frequencies of the compound were calculated by using B3LYP/LANL2DZ method. Determinations of the calculated vibrational bands have been made by using Gauss-View molecular visualization program. The assignments of the observed vibration bands have been performed and compared with the calculated frequencies. The experimental and calculated vibrational frequencies, and their assignments are given in Table S2 (Supplementary Information). Because of the states such as negligence of anharmonicity, incomplete inclusion of electron correlation effects and basis set deficiencies, the calculated harmonic vibrational frequencies become bigger than the observed ones [41, 42]. For this reason, the calculated wavenumbers are usually scaled by scaling factor to compare with observed wavenumbers and at the present work, the scaling factor are taken as 0.9611 for B3LYP/LANL2DZ level [29].

The aromatic C–H stretching, C–H in-plane bending and C–H out-of-plane bending vibrations appear in 2900–3100 cm^{-1}, 1000–1500 cm^{-1} and 700–1000 cm^{-1} frequency ranges, respectively [43]. The C–H stretching bands for phenyl rings have been observed at 3056 cm^{-1}, while ones for naphthalene rings are found 2964, 3010 and 3032 cm^{-1}. The C–H in-plane bending vibrations are observed at the interval 1037–1578 cm^{-1} as the combined with other bands. Similarly, the C–H out-of-plane bending vibrations are found between 691–983 cm^{-1} and they are usually observed as strong bands. The CC stretching modes in aromatic rings can occur between 1600–1400 cm^{-1} in fingerprint region [44]. The observed bands at 1603, 1578, 1536, 1508, 1484, 1453, 1429, 1396, 1363, 1309, 1275, 1242, 1211 and 1037 cm^{-1} as combined with other vibrations modes can attribute to CC stretching modes of phenyl and naphthalene rings. Additionally, the CCC in-plane bending modes of phenyl rings are observed at 562 and 853 cm^{-1}. The observed bands at 416, 460 and 477 cm^{-1} can be assigned to CCCC out of plane bending modes of aromatic rings. The CO stretching bands are observed at 1242 and 1396 cm^{-1}, while NC ones are found at 1179 and 1536 cm^{-1}. The Cu–N and Cu–O stretching modes for copper (Cu) atom the coordinated with nitrogen (N) and oxygen (O) atoms are observed at 536 and 501 cm^{-1}, respectively. These results are in agreement with the literature [40, 45].

The correlation graphics between the calculated and experimental IR vibrational frequencies of the compound is presented in Fig. 4 and correlation coefficient is obtained as 0.9997. As we can see from the correlation graph in Fig. 4, the experimental values are in a good agreement with the calculation ones.

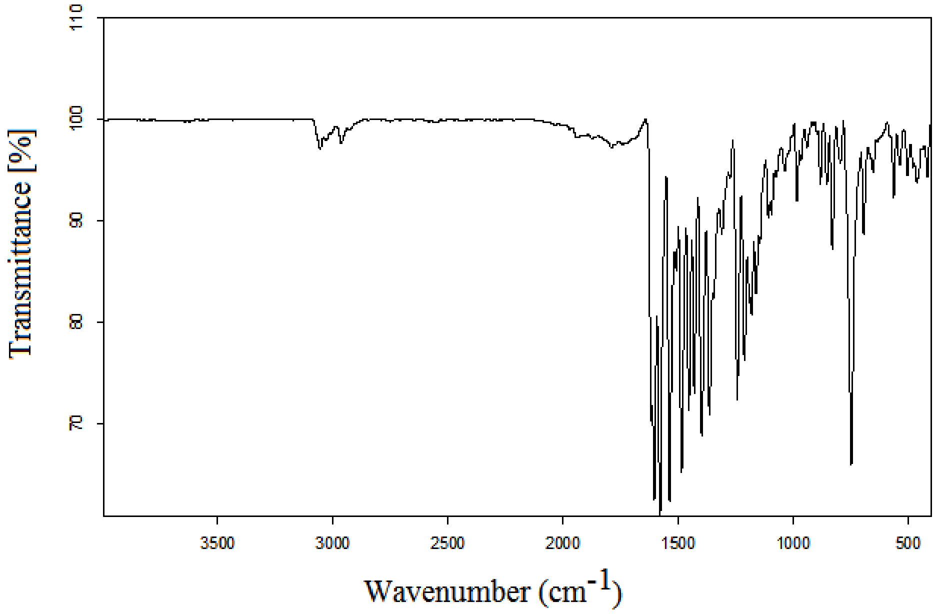


Fig. 3. FT-IR spectrum of the title complex.

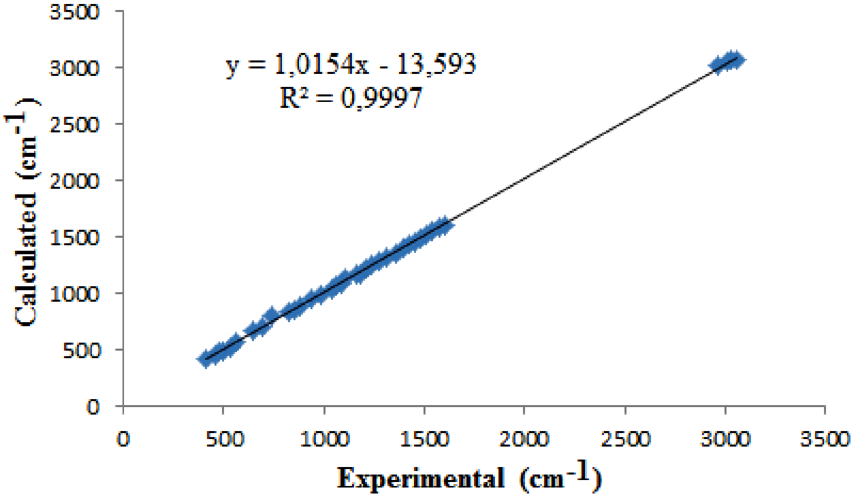


Fig. 4. Correlation graph of calculated and experimental frequencies of the title compound

3.4. Frontier molecular orbitals (FMOs)

The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are named as frontier molecular orbitals (FMOs). The FMO are very important in determining molecular properties such as electric, optic, and chemical reactions [46]. The distributions and energy levels of the α (spin-up) and β (spin-down) frontier molecular orbitals (FMOs) were computed at B3LYP/LANL2DZ level for the compound and are shown in Fig. 5. The value of the energy gap of the compound between the HOMO and LUMO is 3.249 eV for α(spin-up) orbitals and 2.645 eV for β(spin-down) orbitals. These energy gaps are in agreement with the value of 2-3 eV often encountered for stable transition metal complexes [47, 48].

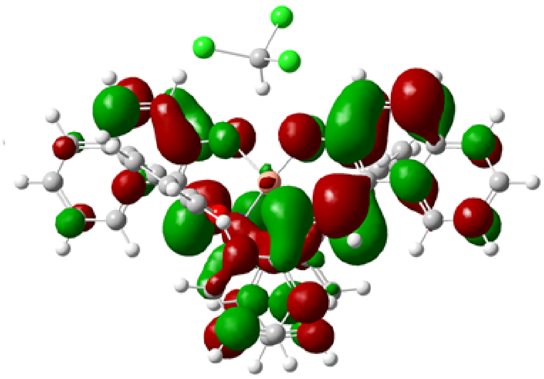
3.5. Total energies in solvent media

In order to evaluate the energetic behavior of the compound in solvent media, we carried out calculations in gas phase and three kinds of solvent (= 4.9, chloroform; = 24.55, ethanol; = 78.39, water). The calculated total and dipole moment using the PCM by B3LYP/LANL2DZ are listed in Table 3. From Table 3, we can conclude that the total molecular energies obtained by PCM method decrease with the increasing polarity of the solvent, while the dipole moments will increase with the increase of the polarity of the solvent. According to these results, the stability of the title compound increases in going from the gas phase to the solution phase.

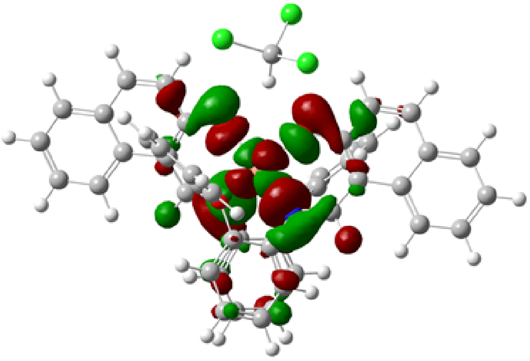
Table 3

Total energies and dipole moments of the title compound in different solvents.

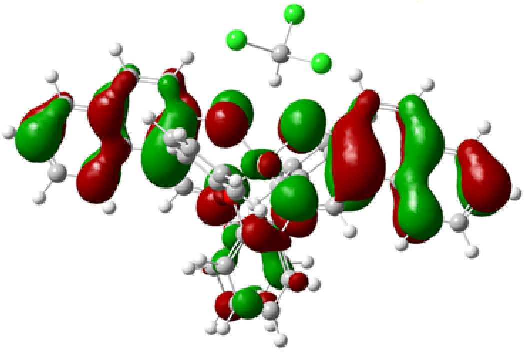
Method	ε	Energy (a.u)	ΔE (kcal/mol)	μ(Debye)
LANL2DZ	1	-2461.98070571		7.9073
PCM	4.9	-2462.00379379	-14.4877	10.0484
	24.55	-2462.01498787	-21.5120	11.1274
	78.39	-2462.01979672	-24.5296	11.6104



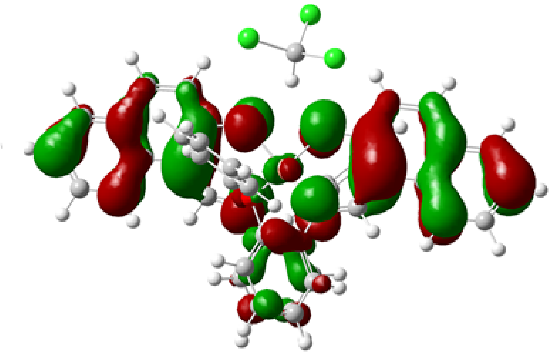
α LUMO (-2.043 eV)



β LUMO (-2.599 eV)



β HOMO (-5.379 eV)



α HOMO (-5.433 eV)

Fig. 5. Molecular orbital surfaces and energy levels given in parantheses for the α(spin-up) and β(spin-down) HOMO–LUMO of the title compound computed at B3LYP/LANL2DZ level.

3.6. NBO analysis

Natural bond orbital analysis method provides important information about the electronic structure of the metal complexes [49]. The NBO analysis of the compound was calculated by using B3LYP/LANL2DZ method (Table 4). According to the NBO analysis, the electron number of 3d, 4s and 4p orbits of Cu are 9.31, 0.27 and 0.35, respectively as well as the electron number of 2s and 2p orbits of N1 are 1.34 and 4.24 and the electron number of 2s and 2p orbits of N2 are 1.35 and 4.25, respectively. Similarly, the electron number of 2s of the O1 and O3 atoms are 1.69 while one of 2p of the O1 and O3 atoms are 5.04 and 5.02, respectively. According to these results, we can deduced that 3d, 4s and 4p orbits of the Cu atom coordinate with N1, N2, O1 and O3 atoms. Similarly, coordination with copper atom of nitrogen and oxygen atoms are formed by using their 2s and 2p orbits. In additional, the Natural Population Analysis (NPA) atomic charge distributions on the atoms of the title complex were calculated by B3LYP method using the LANL2DZ basis set. The calculated natural charge on the Cu atom in the title complex is + 1.06. The obtained result show that charge transfer realized from the ligands to the Cu (II) ion. The largest negative charges are located on the oxygen atoms O1 (-0.73) and O3 (-0.72) for copper (II) complex.

Table 4

Selected natural atomic charges and electronic configurations for title complex.

Atoms	Net Charge	Electronic Configuration
Cu	1.06	[core]4s(0.27)3d(9.31)4p(0.35)5p(0.01)
N2	-0.60	[core]2s(1.34)2p(4.24)3p(0.02)
N1	-0.61	[core]2s(1.35)2p(4.25)3p(0.02)
O1	-0.73	[core]2s(1.69)2p(5.04)3p(0.01)
O3	-0.72	[core]2s(1.69)2p(5.02)3p(0.01)

3.7. Non-linear optical effects

Non-linear optical (NLO) effects arise from the interactions of electromagnetic fields in various media to produce new fields altered in phase, frequency, amplitude or other propagation characteristics from the incident fields [50]. NLO is at the forefront of current research because of its importance in providing the key functions of frequency shifting, optical modulation, optical switching, optical logic, and optical memory for the emerging technologies in areas such as telecommunications, signal processing, and optical interconnections [51-54]. The total static dipole moment (μ), the linear polarizability (α) and the first hyperpolarizability (β) using the x, y, z components are defined as [55, 56]:

$$\mu = \sqrt{\mu_x^2 + \mu_y^2 + \mu_z^2} \tag{2}$$

$$\alpha = \frac{\alpha_{xx} + \alpha_{yy} + \alpha_{zz}}{3} \tag{3}$$

$$\beta = \sqrt{(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{xxy} + \beta_{yzz})^2 + (\beta_{zzz} + \beta_{xxz} + \beta_{yyz})^2} \tag{4}$$

It is well known that the higher values of molecular polarizability and hyperpolarizability are important for more active NLO properties. The polarizabilities and hyperpolarizability are reported in terms of atomic units (a.u) and the calculated values have been converted by using 1 a.u^3 = $(0.529)^3$ Å^3 for α and 1 a.u = $8.641\text{x}10^{-33}$ cm^5/esu for β [57]. The Schiff base compounds have been under investigation for several years because of their potential application to optical communications and because many of them have NLO behavior [43, 58,59]. The effect of electron donor–acceptor substituents on the first hyperpolarizability of conjugated systems has received a great deal attention in recent years [60]. To understand the NLO properties of the title compound, the linear polarizability (α) and the first hyperpolarizability (β) were calculated at the B3LYP/LANL2DZ level using Gaussian 03W program package and the results obtained from calculation were given in Table 5. The calculated polarizability (α) and first hyperpolarizability (β) for the compound are 67.504 $Å^3$ and 12.051 x 10^{-30} cm^5/esu, respectively. Urea is one of the essential molecules used for determition of the NLO properties of molecular systems. Therefore, it is used as reference molecule in NLO studies. The calculated α and β values with B3LYP/LANL2DZ method of urea are 3.882 $Å^3$ and 0.409 x 10^{-30} cm^5/esu. The polarizability and first hyperpolarizability for title molecule is approximately 17.3 and 29.4 times than those of urea. When it is compared to the related Schiff base metal complex in the literature, the calculated value of β of the compound is bigger than that of bis[2-hydroxy-κO-*N*-(2-pyridyl)-1-naphthaldiminato-κ*N*]zinc(II) (β = 11.387 x 10^{-30} cm^5/esu) [43]. These results indicate that title compound is a good candidate of nonlinear optical material.

Table 5

Calculated polarizability and first hyperpolarizability components (a.u.) for the title compound.

Parameters	Value (a.u)	Parameters	Value (a.u)
α_{xx}	825.4394472	β_{xxx}	341.063192
α_{xy}	27.7710207	β_{xxy}	-775.8296823
α_{xz}	516.410009	β_{xyy}	-156.7744231
α_{yy}	19.9040715	β_{yyy}	-100.2058864
α_{yz}	-70.3999642	β_{xxz}	619.3965722
α_{zz}	522.9993496	β_{xyz}	149.922692
α_{total}	1368.342868	β_{xzz}	-54.973419
$\Delta\alpha$	456.1142894	β_{yzz}	-248.0151873
		β_{zzz}	92.9380384
		β_0	-10.4047554

4. Conclusion

In this study, $C_{46}H_{32}CuN_2O_4{\cdot}CHCl_3$ complex has been synthesized and characterized by IR and X-ray single-crystal diffraction. The crystal structure of the complex is stabilized by C–H···O hydrogen bond and C–H···πinteraction. In addition to the X-ray crystal structure, the molecular geometry and vibrational frequencies of the title compound were calculated using the density functional method (B3LYP) with the LANL2DZ basis set. The calculated results show that the optimized geometries can well reproduce the crystal structure, and the theoretical vibrational frequencies show good agreement with experimental values. The total energy of the title compound decreases with increasing polarity of the solvent. The Natural Population Analysis show that charge transfer occurred from the ligands to the Cu (II) ion. This study also demonstrates that the title compound can be used as a good nonlinear optical material.

Acknowledgment

We sincerely thank to Professor Dr Orhan Büyükgüngör for his help with the data collection.

Supplementary data

Crystallographic data for the structure reported in this article have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication number CCDC 951665. Copies of the data can be obtained free of charge on application to CCDC 12 Union Road, Cambridge CB21 EZ, UK

(Fax: (+44) 1223 336-033; e-mail: data_request@ccdc.cam. ac.uk).

References

[1] E. Hadjoudis, I.M. Mavridis, Chem. Soc. Rev. 33 (2004) 579–588.

[2] A. Filarowski, J. Phys. Org. Chem. 18 (2005) 686–698.

[3] D. Sinha, A.K. Tiwari, S. Singh, G. Shukla, P. Mishra, H. Chandra, A.K. Mishra, Eur. J. Med. Chem. 43 (2008) 160–165.

[4] M.S. Karthikeyan, D.J. Prasad, B. Poojary, K.S. Bhat, B.S. Holla, N.S.Kumari, Bioorg. Med. Chem. 14 (2006) 7482–7489.

[5] P. Panneerselvam, R.R. Nair, G. Vijayalakshmi, E.H. Subramanian, S.K. Sridhar, Eur. J. Med. Chem. 40 (2005) 225–229.

[6] R.K. Parashar, R.C. Sharma, A. Kumar, G. Mohan, Inorg. Chim. Acta 151 (1988) 201–210.

[7] A. Blagus, D. Cinčić , T. Friščić , B. Kaitner, V. Stilinović, Maced, J. Chem. Eng. 29 (2010) 117–138.

[8] A.P. Alivisatos, P.F. Barbara, A.W. Castleman, J. Chang, D.A. Dixon, M.L. Klein, G.L. McLendon, J.S. Miller, M.A. Ratner, P.J. Rossky, S.I. Stupp, M.E. Thompson, Adv. Mater. 10 (1998) 1297–1336.

[9] L. Dalton, Adv. Polym. Sci. 158 (2002) 1–86.

[10] A.D. Garnovski, A.L. Nivorozhkin, V.I. Minkin, Coord. Chem. Rev. 126 (1993) 1–69.

[11] W.M.I. Hassan, E.M. Zayed, A.K. Elkholy, H. Moustafa, G.G. Mohamed, Spectrochim. Acta Part A 103 (2013) 378–387.

[12] S.B. Desai, P.B. Desai, K.R. Desai, Hetrocycl. Commun. 7 (2001) 83–90.

[13] P. Lumme, H. Elo, Inorg. Chim. Acta 94 (1984) 241–251.

[14] F.M. Antony, R.S. Mahony, M.W. Joyce, Croat. Chem. Acta 72 (1999) 685–703.

[15] Y. Xiao, C.F. Bi, Y.H Fan, Q.Z. Cui, X. Zhang, Q.P. Dou, Int. J. Oncol. 33 (2008) 1073–1079.

[16] P.M.W. Gill, B.G. Johnson, J.A. Pople, M.J. Frisch, Chem. Phys. Lett. 197 (1992) 499–505.

[17] H. Tanak, A. Ağar, M. Yavuz, J. Mol. Mod. 16 (2010) 577–587.

[18] H. Gökçe, S. Bahçeli, Spectrochim. Acta Part A 78 (2011) 803–808.

[19] B. Koşar, Ç. Albayrak, C. C. Ersanlı, M. Odabaşoğlu, O. Büyükgüngör, Spectrochim. Acta Part A 93 (2012) 1–9.

[20] E. Temel, E. Ağar, O. Büyükgüngör, Acta Crystallogr. E66 (2010) o1131.

[21] Stoe & Cie, X-AREA (Version 1.18) and X-RED32 (Version 1.04), Darmstadt, Germany, 2002.

[22] G.M. Sheldrick, Acta Crystallogr. A64 (2008) 112–122.

[23] L.J. Farrugia, ORTEPIII for Windows J. Appl. Crystallogr. 30 (1997) 565.

[24] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery Jr., T. Vreven, K.N. Kudin, J.C. Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G.A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.E. Knox, H.P. Hratchian, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich, A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S. Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez, J.A. Pople, Gaussian 03, Revision E.01, Gaussian, Inc., Wallingford, CT, 2004.

[25] A.D. Becke, J. Chem. Phys. 98 (1993) 5648–5652.

[26] P.J. Hay, W.R. Wadt, J. Chem. Phys. 82 (1985) 270–283.

[27] W.R. Wadt, P.J. Hay, J. Chem. Phys. 82 (1985) 284–298.

[28] P.J. Hay, W.R. Wadt, J. Chem. Phys. 82 (1985) 299–310.

[29] K.K. Irikura, R.D. Johnson III, R.N. Kacker, J. Phys. Chem. A 109 (2005) 8430–8437.

[30] R. Dennington II, T. Keith, J. Millam, GaussView, Version 4.1.2, Semichem, Inc., Shawnee Mission, KS, 2007.

[31] S. Miertus, E. Scrocco, J. Tomasi, Chem. Phys. 55 (1981) 117–129.

[32] V. Barone, M. Cossi, J. Phys. Chem. A 102 (1998) 1995–2001.

[33] M. Cossi, N. Rega, G. Scalmani, V. Barone, J. Comput. Chem. 24 (2003) 669–681.

[34] J. Tomasi, B. Mennucci, R. Cammi, Chem. Rev. 105 (2005) 2999–3093.

[35] E.D. Glendening, J.K. Badenhoop, A.E. Reed, J.E. Carpenter, F. Weinhold, NBO Version 3.1, Theoretical Chemistry Institute, University of Wisconsin, Madison, 1995.

[36] G.R. Clark, J.M. Waters, G.J. J. Williams, Inorg. Nucl. Chem. 39 (1977) 1971–1975.

[37] Acevedo-Arauz, E.; Fernandez, G.J.M.; Rosales-Hoz, M.; Toscano, R.A. Acta Crystallogr. C 48 (1992) 115–120.

[38] Y. Elerman, A. Elmali, S. Özbey, Acta Crystallogr. C 54 (1998) 1072–1074.

[39] H. Ünver, and T. Nuri Durlu, J. Chem. Crystallogr. 31 (2001) 479–483.

[40] H. Ünver, J. Mol. Struct. 641 (2002) 35–40.

[41] A.E. Özel, S. Çelik, S. Akyüz, S. Keçel, Vib. Spectrosc. 53 (2010) 151.

[42] H. Gökçe, S. Bahçeli, Spectrochim. Acta Part A 116 (2013) 242–250.

[43] H. Tanak, M. Toy, Spectrochim. Acta Part A 115 (2013) 145–153.

[44] R.M. Silverstein, F.X. Webster, D.J. Kiemle, Spectrometric Identification of Organic Compounds, seventh ed., John Wiley & Sons, New York, 2005.

[45] O.Z. Yeşilel, I. İlker, M. S. Soylu, C. Darcan, Y. Süzen, Polyhedron 39 (2012) 14–24.

[46] I. Fleming, Frontier orbitals and organic chemical reactions, Wiley, London, 1976.

[47] P.J. Blower, J.R. Dilworth, R. I. Maurer, G.D. Mullen, C.A. Reynolds, Y. Zheng, J. Inorg. Biochem. 85 (2001) 15–22.

[48] N. Özdemir, O. Dayan, M. Dinçer, B. Çetinkaya, J. Struct. Chem. 53, (2012) 251–252.

[49] H. Vural, İ. Uçar, M.S. Soylu, Spectrochim. Acta Part A (2014),http://dx.doi.org/10.1016/j.saa.2013.12.027.

[50] Y.X. Sun, Q.L. Hao,W.X. Wei, Z.X. Yu, L.D. Lu, X. Wang, Y.S. Wang, J. Mol. Struct.: Theochem. 904 (2009)74–82.

[51] C. Andraud, T. Brotin, C. Garcia, F. Pelle, P. Goldner, B. Bigot, A. Collet, J. Am. Chem. Soc. 116 (1994) 2094–2102.

[52] M. Nakano, H. Fujita, M. Takahata, K. Yamaguchi, J. Am. Chem. Soc. 124 (2002) 9648–9655.

[53] V. M. Geskin, C. Lambert, J. L. Bredas, J. Am. Chem. Soc. 125 (2003) 15651–15658.

[54] D. Sajan, H. Joe, V. S. Jayakumar, J. Zaleski, J. Mol. Struct. 785 (2006) 43–53.

[55] R. Zhang, B. Du, G. Sun, Y. Sun, Spectrochim. Acta A 75 (2010) 1115–1124.

[56] H. Tanak, J. Mol. Struct.:Theochem. 950 (2010) 5–12.

[57] D.R. Kanis, M.A. Ratner, T.J. Marks, Chem. Rev. 94 (1994) 195–242.

[58] M. Jalali-Heravi, A.A. Khandar, I. Sheikshoaie, Spectrochim. Acta A 55 (1999) 2537–2544.

[59] J.F. Nicoud, R.J. Twieg, in: D.S. Chemla, J. Zyss (Eds.), Nonlinear Optical Properties of Organic Molecules and Crystals, vol. 1, Academic Press, New York, 1987, p. 277 (Chapter II).

[60] M. Blanchard-Desce, C. Runser, A. Fort, M. Barzoukas, J.M. Lehn, V. Bloy, V. Alain, Chem. Phys. 199 (1995) 253–261.

Highlights

► The compound was characterized by IR and X-ray crystallography.

► Molecular geometry was determined by DFT method.

► The calculated results were compared with experimental results.

► NLO and NBO analysis of the compound were studied.