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Synthesis, structure, and theoretical studies of bis(fivecoordinate) μ -O-[CuL₂]₂: predicting distortion toward trigonality

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ABSTRACT

An oxo-bridged binuclear Cu(II) complex, $[CuL_2]_2$, has been synthesized and characterized by microanalysis, spectra (infrared and electronic), and X-ray diffraction crystallography. The theoretical properties of the complex were studied using the semi-empirical PM3 method. The optimized geometries, dipole moment, thermodynamic parameters, and vibrational frequencies were investigated. The crystal structure revealed that each Cu(II) was five-coordinate with a distorted square pyramidal geometry (τ =0.324 and 0.307). The two units of the complex were bridged by phenolic oxygens to give a binuclear Cu(II) complex with the average bridging angle and Cu⁻⁻⁻Cu distance being 98.49° and 3.413 Å, respectively. Theoretical studies revealed that the geometric parameters are in agreement with the experimental data. The compound was stable and has good non-linear optical properties.

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KEYWORDS

Bridging ligands; trigonality; metal complexes; semiempirical calculations; nonlinear properties



1. Introduction

Polydentate ligands, especially N_2O_2 Schiff base ligands form stable five- or six-membered chelates with transition metal ions [1–5]. Many salicylaldimine-based metal complexes have been evaluated for applications in organic synthesis [6, 7], catalytic activity [8, 9], electrochemistry [10, 11], corrosion inhibition [12], and medicinal uses [13–15]. Complexes of copper(II) ions are known with coordination numbers of four, five, or six. In the five-coordinate CuL_s chromophore, few regular trigonal bipyramidal and regular

square pyramidal complexes are known because the vast majority of five-coordinate complexes involve distorted stereochemistry [16], generally through the presence of non-equivalent ligands [17]. Thus, there is a need to determine the degree of distortion from the regular geometry of the complexes. The degree of distortion toward trigonality has been defined by Addison *et al.* geometric parameter [18]. Addison *et al.* introduced geometric parameter (τ) for distinguishing between square pyramidal and trigonal bipyramidal geometries in five-coordinate metal complexes $\tau = (\beta - \alpha)/60$, where α and β are the two largest basal *trans* angles [18].

Polynuclear Cu(II) complexes [4, 19–23] are of special interest because the magnetic spin interaction between the metal centers provides information required for the fabrication of ferromagnetic materials. In this article, we report the synthesis and structural characterization of an oxo-bridged binuclear Cu(II) complex of LH, N-[(2-methylphenyl)-4-methoxysalicylaldimine, derived from condensation of 5-methoxyl-2-hydroxylbenzaldehyde (*p*-vanillin) with 2-methylaniline (*o*-toludine). The compound has been characterized with a combination of analytical, spectral, and X-ray diffraction crystallography data. The degree of distortion of the complex toward trigonality has been determined using τ [18]. Geometric properties (bond distances, bond angles, and dihedral), vibrational frequencies, thermodynamic properties, heat of formation, and electronic properties of the molecule have been calculated using the Spartan10 program package [24] with the semi-empirical PM3 (Parameterization Method 3). The semi-empirical method (PM3) has been best in predicting the geometric properties and vibrational frequencies of transition metal and organometallic complexes [25]. Several studies have shown that the PM3 method gives data that agree with the experimental values [26–31].

2. Experimental

2.1. Materials and methods

All chemicals and reagents used were of analytical grade and used without purification. The ¹H- and ¹³C-NMR spectra were recorded in CDCl₃ with SiMe₄ (TMS) as internal standard on a Bruker Avance NMR operating at 400 MHz. The mid-infrared absorption frequencies (4000–700 cm⁻¹) were recorded on a Perkin-Elmer Spectrum 100 FT-IR equipped with universal attenuated total reflectance (ATR) accessory, while the far-infrared (700–30 cm⁻¹) spectra were recorded in Nujol mull on a Perkin-Elmer Spectrum 400 FT-IR. UV–vis spectra were obtained from a Perkin-Elmer Lambda 25 spectrophotometer. The C, H, N elemental analysis was done on a Vario MICRO V1.6.2 elemental analysen systeme GmbH, while the percentage metal content was determined on a Perkin-Elmer A Analyst atomic absorption spectrometer. Molar conductivity measurement for the complex was done in DMF using Az^{*} 86,555 pH/mV/Cond./ TDS/Temp. Melting points (uncorrected) of compounds were determined using a Galenkemp melting point apparatus.

2.2. General procedure

The binuclear complex was prepared from copper(II) acetate monohydrate and LH in a ratio 1:2. LH was synthesized by condensing equimolar mixture of 5-methoxyl-2-hydroxylbenzaldehyde (*p*-vanillin) and 2-methylaniline (*o*-toluidine) in absolute ethanol.

2.2.1. Synthesis of LH

The Schiff base was synthesized according to the general synthetic procedure in the literature [32]. A hot 5 mmol solution (0.76 g) of 5-methoxyl-2-hydroxylbenzaldehyde (*p*-vanillin) in 5 mL ethanol was mixed with 5 mmol (0.55 mL) of 2-methylaniline in 5 mL ethanol. The resulting yellow solution was refluxed for 2 h in a 50-mL round bottom flask equipped with an air-cooled condenser to obtain a yellow precipitate. The precipitate was filtered under suction, washed with ethanol, and recryztallized from ethanol. It was dried over silica gel. Yield: 1.51 g (62.6%); m.p.: 92–94 °C; ¹H-NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 14.04(s, 1H, –OH); 8.52(s, 1H, HC = N); 7.22(s, 1H); 7.18(d, 2H, NMR (400 MHz, CDCl₃, 25 °C, TMS): δ

Empirical formula			
Empirica formula Formula weight	1088 17		
Tomporaturo (V)	200(2)		
Weyeles eth (Å)	200(2)		
wavelength (A)	0.71073		
Crystal system	Iriclinic		
Space group	P-1		
a (A)	11.4233 (2)		
b (Å)	14.6534 (3)		
<i>c</i> (Å)	16.6189 (3)		
a (°)	68.5070 (10)		
β(°)	86.0340 (10)		
γ (°)	81.5850 (10)		
V (Å ³)	2560.17 (8)		
Ζ	2		
<i>D</i> (gcm ⁻³)	1.412		
$\mu ({\rm mm^{-1}})$	0.892		
F (000)	1132		
Θ range for data collection (°)	1.80-28.00		
No. reflections/observed	12,301/9743		
R _{int}	0.0208		
Data/restraints/parameters	12,301/0/707		
Goodness of fit	1.016		
Refinement method	Full-matrix least-squares of F ²		
Final <i>R</i> indices [$F > 4\sigma$ (<i>F</i>)]	$R_1 = 0.0299, wR_2 = 0.0720$		
R indices (all data)	$R_1 = 0.0463, WR_2 = 0.0792$		

Table 1. Crystal data and structure refinements for [CuL₂]₂.

Table 2. Selected calculated and experimental bond lengths and angles for [CuL₂]₂.

Bond distance	Calculated (Å)	Experimental	Bond angle	Calculated (°)	Experimental
Cu ₂ -O ₂₁	1.84	1.88	0 ₁₁ -Cu ₁ -N ₁₁	93.06	93.11
0,1-Cu,	2.11	2.55	0,,-Cu,-N,,	105.88	113.91
Cu,-0,	1.87	1.90	0,1-Cu,-N,1	112.07	115.45
Cu ₁ -O ₁₂	1.90	1.89	0,1-Cu2-N2	85.13	90.23
Cu1-0,2	1.95	2.59	0,1-Cu,-0,2	73.04	77.57
Cu,-N,1	1.93	2.01	0,,-Cu,-0,,	88.52	87.64
Cu ₁ -N ₁₂	1.91	2.00	Cu,-0,-Cu,	114.36	97.89
Cu ₂ -N ₂₁	1.91	2.00	Cu, -0, -Cu,	119.17	99.09
Cu ₂ -N ₂₂	1.90	2.01	N ₂₁ -Cu ₂ -N ₂₂	143.67	145.18
Cu ₁ -Cu ₂	3.37	3.41	N ₁₁ ² -Cu ₁ ² -N ₁₂ ²²	166.91	146.49

d, J = 7.8); 7.14(t, 2H, J = 8.2); 6.54(t, 2H, J = 7.5); 3.86(s, 3H, $-OCH_3$) and 2.42(s, 3H, $-CH_3$); ¹³C-NMR (400 MHz, CDCl₃, 25 °C, TMS): $\delta = 164.74(Ar-OCH_3)$; 164.49(Ar-OH); 161.43(HC = N); 147.63(Ar-N = C); 132.46(ArCH_3); 133.88, 131.10, 127.42, 126.79, 118.06, 113.68, 107.53, 101.56(Ar-C); 55.90($-OCH_3$); 18.64($-CH_3$). IR (ATR): 3109–2339 cm⁻¹ v(O-H); 1610 cm⁻¹ v(C = N); 1292 cm⁻¹ v(C-O). UV-vis (DMF): 285; 340; 420 nm. Elemental Anal. Calcd (%) for C₁₅H₁₅NO₂: %C: 74.60, %H: 6.27, %N: 5.80; found: %C: 74.55, %H: 6.9, %N: 5.78.

2.2.2. Synthesis of [CuL₂]_{2.}

A hot ethanolic solution of copper(II) acetate monohydrate, $Cu(OAc)_2 \cdot H_2O$ (0.624 mmol, 0.124 g), was gradually mixed with hot ethanolic solution of the ligand (1.243 mmol, 0.30 g) in a 50-mL round bottom flask. The resulting solution was refluxed overnight to obtain a green precipitate. The precipitate was filtered under suction, washed with ethanol, and dried in a vacuum desiccator over silica gel. Yield: 0.27 g (78%); m.p.:196–198 °C; IR (ATR): 1605 cm⁻¹ v(C = N), 1310 cm⁻¹ v(C–O); IR(Nujol): 522 cm⁻¹ v(Cu–O), 465 v(Cu–N); UV-vis (DMF): 286, 351, 472, 548 nm. Conductivity (DMF): 2.6 Ω^{-1} cm² mol⁻¹. Elemental Anal. Calcd (%) for Cu₂C₆₀H₅₆N₄O₈: %C: 66.22, %H: 5.19, %N: 5.15, %Cu: 12.04; found: %C: 65.55, %H: 5.40, %N: 4.96, %Cu: 11.85.

2.3. Crystallographic studies

Single crystals suitable for X-ray diffraction were obtained via slow evaporation of the saturated DMF solution of the complex. A suitable single crystal of the complex was diffracted using a Bruker KAPPA APEX II single-crystal X-ray diffractometer, with a four-circle Kappa goniometer.

Crystallographic data were collected at 200 K and 0.71073 nm (λ) on a sensitive CCD detector with graphite-monochromated MoK α radiation; a total of 12,301 reflections were collected of which 9743 were considered observed [$I > 2\sigma$ (I)]. The structure was solved by direct methods using SHELXS-97 and refined anisotropically by full-matrix least-squares on F^2 using SHELXL-97 [33]. Details of crystallographic parameters, data collection, and refinements are listed in Table 1 with selected bond lengths and angles presented in Table 2.

2.4. Computational details

Conformational search was conducted on the modeled structure using the molecular mechanic force field calculation in aqueous medium which makes use of the systematic algorithm to obtain the structure with the lowest energy; this is to establish the most stable structure [29]. The best conformer has energy of 2843.00 kJ mol⁻¹. Quantum mechanical calculations on ground-state molecular geometry, dipole moment, polarizability, energy, and frontier orbital energies (E_{HOMO} and E_{LUMO}) of the complex were carried out using the PM3 semi-empirical method with SPARTAN10 software package [24] on a 1.70-GHz personal computer. PM3 has been proven to be the best method to account for the properties of transition metal complexes [23, 24, 26, 27, 29].

3. Results and discussion

3.1. Elemental analysis and conductivity measurement

Elemental analysis results for the complex suggested that the complex was of the form $[CuL_2]_2$, with the Cu^{2+} coordinating to the Schiff base ligand in a ratio 1:2. The low conductivity value for the complex (Table 1) implies that the Schiff base ligand is coordinated [34] via the deprotonated phenolic oxygens and the imine nitrogens.

3.2. Spectroscopic characterization of compounds

3.2.1. ¹H- and ¹³C-NMR

Assignments of the main NMR signals are given in the Experimental section. Evidence for the formation of the Schiff base was indicated by the azomethine signal (HC = N) as one proton singlet at 8.52 ppm in the ¹H-NMR spectrum of the ligand. This was further confirmed by the appearance of the azomethine carbon at 161.43 ppm. The phenolic hydroxyl proton absorbed far downfield as a broad signal at 14.04 ppm, due to a strong intramolecular hydrogen bonding between the imine nitrogen and the hydroxyl proton. Strong signals at 3.86 and 2.42 ppm were assigned to the methoxy and methyl protons of the *p*-vanillin and the *o*-toluidine, respectively. The purity of the ligands was, however, indicated by the disappearance of the amino and aldehyde protons at 3–4 and 9–10 ppm, respectively.

3.2.2. Infrared study

The strong band at 1610 cm⁻¹ was assigned to the imine (C = N) functional group of the free ligand. As expected, the imine band was red-shifted ($\Delta v = -5$ cm⁻¹) in the spectrum of the complex, indicating coordination of the Schiff base via the azomethine nitrogen [35, 36]. The phenolic stretching vibration v(C–O) of the free ligand appeared as a strong band at 1292 cm⁻¹ and consequently blue-shifted to 1310 cm⁻¹ upon complexation [35, 36], suggesting the involvement of the phenolic oxygen in coordination. Likewise, the O–H stretching vibration of the free Schiff base was observed as a broad band at 3109–2339 cm⁻¹, due to strong intramolecular hydrogen bonding [35, 37]. This band, however,



Figure 1. Labeled ORTEP diagram for [CuL₂]₂, showing 50% probability ellipsoids.

Table 3. Summary of τ values for various five-coordinate Cu(II) complexes.

Complex ^a	β (°)	a (°)	τ	Geometry	Refs.
ⁱ [Cu(salgly)(urea)]	176.06	163.93	0.2	SPY	[22]
"[Cu,LCl,(H,O)]	174.7	158.0	0.278	SPY	[21]
"[Cu͡,CoĹ,Cĺ _s]	176.4	156.64	0.33	*SPY/TBPY	[18]
^{iv} [LCu(NCS)] ⁴	167.16	138.41	0.479	SPY/TBY	[43]
[CuL,],	164.91	146.49	0.307	SPY	This work
22	164.59	145.18	0.324	SPY	

^a(i) salgly: N-salicylideneglycinato-; (ii) [Cu₂LCl₂(H₂O)]: L = N,N-o-phenylenebis(salicylideneimine); (iii) [Cu₂CoL₂Cl₆]: L = 1,3,5-tris(pyrazol-l-ylmethyl)benzene (L); (iv) [LCu(NCS)]⁺: L = NC₅H₄C(CH₃)=N(CH₂)₃ N = C(CH₃)C₅H₄ N.

*SPY/TBPY: intermediate geometry between square pyramidal and trigonal bipyramidal.

disappeared in the spectrum of the complex due to deprotonation and involvement of oxygen in the coordination sphere. The coordination mode was further substantiated by the appearance of two new bands in the far-infrared spectra of the complexes at 490–465 and 522 cm⁻¹. These bands were assigned to the v(Cu-O) and v(Cu-N) stretching vibrations, respectively [5, 38].

3.2.3. UV-vis study

The electronic transition study of the compounds was carried out in DMF. Three absorption maxima were observed in spectra of the Schiff base ligand. The high-energy band at 285 nm was assigned to the $\pi \rightarrow \pi^*$ transition of the benzene ring, and the azomethine chromophore of the Schiff base ligand [39], while the band at 340 nm was assigned to $n \rightarrow \pi^*$ transition of the imine functional group [40]. The band at 420 nm implies existence of the Schiff base ligand in keto-imine form [41, 42] due to tautomerism of

the orthohydroxyl Schiff base ligand. The $\pi \rightarrow \pi^*$ absorption did not shift upon complexation, but rather a shift to lower energy was observed for the $n \rightarrow \pi^*$ band, thus indicating coordination via the imine nitrogen. The spectrum of $[CuL_2]_2$ has a band at 472 nm corresponding to ligand-to-metal charge-transfer transition [19]. The broad asymmetrical band centered at 621 nm was tentatively assigned to the d–d transition of the Cu(II) complex.

3.3. Molecular structure of $[CuL_2]_2$

Selected bond angles and bond lengths of the compound are presented in Table 2, while the labeled ORTEP diagram is presented in Figure 1. The complex crystallized in the triclinic system with a space group of *P*-1 having a = 11.4233(2) Å, b = 14.6534(3) Å, c = 16.6189(3) Å, $\alpha = 68.5070(10)^\circ$, $\beta = 86.0340(10)^\circ$, and $\gamma = 81.5850(10)^\circ$. Two symmetric units of the Schiff base ligand coordinated to Cu(II) as monobasic bidentate via the imine N and the phenolic oxygen. Two of the phenolic oxygens (O22 and O11) were tridentate, bridging between the two Cu(II) centers, resulting in a binuclear complex. The crystal structure of the complex indicates a distorted square pyramidal geometry around copper(II). The basal plane consisted of the imine nitrogens (N11, N12; N21 N22) and the deprotonated phenolic oxygens (O11, O12; O21, O211), while the apex was occupied by the bridging phenolic oxygens (O11; O22). The axial Cu–O bond lengths were equivalent; Cu1–O22 (2.591 Å) and Cu2–O11 (2.549 Å) and longer than the other Cu–O bonds; Cu1–O11 (1.903 Å), Cu1–O12 (1.889 Å), Cu2–O21 (1.880 Å), and 94.47(12)° for equatorial plane. Valent *et al.* [23] reported values of 1.915(3), 2.406(3) Å, and 94.47(12)° for equatorial Cu–O, and Cu–O1–Cu of a similar oxo-bridged binuclear Cu(II) complex. The bridging Cu₂O₂ unit was constrained to be planar by the presence of the crystallographic center with the Cu1…Cu2 distance of 3.413 Å while the bridging angles are 97.89(5)°–99.09(5)°.

The degree of distortion toward trigonality has been defined by Addison *et al.* [18] geometric parameter (τ) for distinguishing between square pyramidal and trigonal bipyramidal geometries in five-coordinate complexes; $\tau = (\beta - \alpha)/60$, where α and β are the two largest basal *trans* angles. Generally, $\tau = 0$ for an ideal square-based pyramid (since $\alpha = \beta = 180^\circ$) and $\tau = 1$ for an ideal trigonal bipyramidal geometry (for $\alpha = 120^\circ$; $\beta = 180^\circ$). Maity *et al.* [22] and Chang *et al.* [19] assigned square pyramidal ($\tau = 0.28$) and square pyramidal/trigonal bipyramidal ($\tau = 0.33$) geometries for the five-coordinate Cu(II) complex. A summary of assigned geometries for some five-coordinate Cu(II) complexes with varying τ values is given in Table 3.

In this complex, the values of τ were large (0.324 and 0.307) for the two copper(II) centers, indicating distortion from square-based pyramidal geometry toward trigonal bipyramidal geometry. The deviation from an ideal square pyramidal geometry was further observed from the basal *trans* angles: N11-Cu1–N12 (146.49°); O11–Cu1–O12 (164.91°); N21–Cu2–N22 (145.18°); and O21–Cu2–O22 (164.59°), which differed markedly from the ideal angle of 180° for a true square pyramidal geometry. In addition, the values of α [146.49° (N11–Cu1–N12) and 145.18° (N21–Cu2–N22)] were between 180° (ideal square pyramidal geometry) and 120° (ideal trigonal bipyramidal geometry) which shows that the geometry was intermediate between the two extremes [19].

3.4. Theoretical calculations on the complex

3.4.1. Geometric properties

The optimized structure for the Cu(II) complex is presented in Figure 2. In order to study the theoretical properties, geometric parameters were taken into consideration. Bond lengths and bond angles are recorded in Table 2. Both the bond distances and bond angles were compared with the experimental results.

Bond lengths Cu_1-O_1 (1.84 Å), Cu_1-O_3 (2.11 Å), Cu_2-O_2 (1.87 Å), Cu_2-O_3 (1.90 Å), Cu_2-O_8 (1.95 Å), Cu_1-N_1 (1.93 Å), Cu_1-N_2 (1.91 Å), Cu_2-N_3 (1.91 Å), and Cu_2-N_4 (1.90 Å) in the calculated data compared with the bond lengths in the experimental data Cu_1-O_1 (1.88 Å), Cu_1-O_3 (2.55 Å), Cu_2-O_2 (1.90 Å), Cu_2-O_3 (1.89 Å), Cu_2-O_8 (2.59 Å), Cu_1-N_1 (2.01 Å), Cu_1-N_2 (2.00 Å), Cu_2-N_3 (2.00 Å), and Cu_2-N_4 (2.01 Å) were in



Figure 2. The structure of the Cu(II) complex after optimization using the ball and wire model.

Property	[CuL ₂]
LUMO energy (eV)	-13.94
HOMO energy (eV)	-17.16
ΔE (eV)	3.22
$H = \Delta E/2$ (eV)	1.61
μ (debye)	13.71
Polarizability	40.61

Table 5. Vibrational frequencies with their corresponding vibrations.

Vibration	Experimental (cm ⁻¹)	Calculated (cm ⁻¹)
$v(C=N)_{str}$	1605	1610–1601
$v(C-O)_{str}^{Str}$	1310	1354–1294
$v(O-H)_{str}^{Str}$	3109–2339	3030-2898
v(Cu–O)	490–465	-
v(Cu–N) _{str}	522	543

agreement as shown in Table 2. Bond angles were also close except for the bond angles of $Cu_1-O_3-Cu_2$ (114.36°), $Cu_1-O_2-Cu_2$ (124.02°), $N_{21}-Cu_2-N_2$ (98.99°), and $N_1-Cu_1-N_2$ (92.11°) which gave $Cu_1-O_3-Cu_2$ (97.37°), $Cu_1-O_2-Cu_2$ (99.09°), $N_{21}-Cu_2-N_2$ (145.18°), and $N_1-Cu_1-N_2$ (146.49°), respectively. The $Cu_1\cdots Cu_2$ interaction distance was 3.37 Å which agreed with 3.41 Å in the experiment.

However, there are significant differences between the found and calculated values of some bond distances and angles (Table 2). This is owing to the fact that the interatomic potentials are based on approximations and derived from different types of experimental data. Some existing energy functions do not account for electronic polarization of the environment, an effect that can significantly reduce electrostatic interactions of partial atomic charges, and the nature of the dielectric depends on the model used. All types of van der Waals forces are also strongly environment-dependent because these forces originate from interactions of induced and "instantaneous" dipoles [44].

3.4.2. Electronic properties and stability

Energy levels of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) were determined. A band gap was obtained, indicating the complex has a good non-linear optical property. The calculated E_{HOMO} and $E_{LUMO'}$, ΔE (band gap), hardness (H), and dipole moment (μ) are recorded in Table 4. The molecule was stable as shown by low energy gap and high polarizability. Energy band gaps obtained from band structure calculations for solids are analogous to HOMO–LUMO energy differences in molecules [45].

Dipole moment is used to study molecular interactions involving the non-bonded-type dipoledipole interactions, which increase with low/decrease in band gap of molecules [46–48]. Polarizability increases with the size of a molecule and/or low band gap. A molecule with a low band gap is polarizable and is generally said to be chemically reactive. In addition, such molecules possess high non-linear optical property and are said to be soft [42]. Non-linear optical properties are of interest due to their potential usefulness for unique optical devices such as frequency-doubling devices, optical signal processing, and optical computers [49]. The thermodynamic properties for the complex were: heat of formation = 2903.62 kJ mol⁻¹, free energy = 5433.75 kJ mol⁻¹, enthalpy = 5775.00 kJ mol⁻¹, and entropy = 1130.43 J mol⁻¹ K⁻¹.

3.4.3. Vibrational frequencies

Vibrational frequencies given in Table 5 are in agreement with the experimental values. The $v(C = N)_{str}$ and $v(C-O)_{str}$ absorptions are at 1610–1601 and 1354–1294 cm⁻¹, respectively. No absorption was observed for $v(Cu-O)_{str}$ although $v(Cu-N)_{str}$ appeared at 543 cm⁻¹. The calculated IR spectrum for the complex is presented in the Supplementary Data.

4. Conclusion

A new oxo-bridged binuclear Cu(II) complex, μ -O-[CuL₂]₂, was synthesized from *p*-vanillin Schiff base ligand. The ligand was coordinated to the Cu(II) via the imine nitrogen and the phenolic oxygen. The deprotonated phenolic oxygen bridged two units of the resulting complex to give a bis(five-coordinate) binuclear Cu(II) complex. The binuclear Cu(II) complex has a low band gap which accounted for its high dipole moment and polarizability. The complex is a probable non-linear optical material and can be exploited for future research.

Supplementary material

X-ray crystallography data of the binuclear complex, μ -O-[CuL₂]₂, have been deposited with the Cambridge Crystallographic Data Center (CCDC number 888458) and can be obtained free of charge on request at http://www.ccdc.cam.ac.uk/conts/retrieving.html or from the Cambridge Crystallographic Data Center (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; Fax:+44(0)1223 336033; E-mail: deposit@ccdc.cam.ac.uk.

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Disclosure statement

No potential conflict of interest was reported by the authors.

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