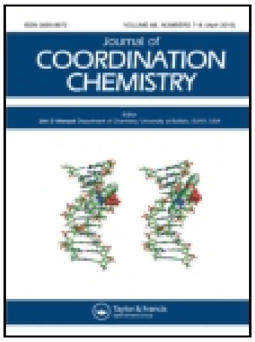

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Synthesis and characterization of a thioether Schiff base ligand and its metal complexes and crystal structure determination of the nickel(II) complex

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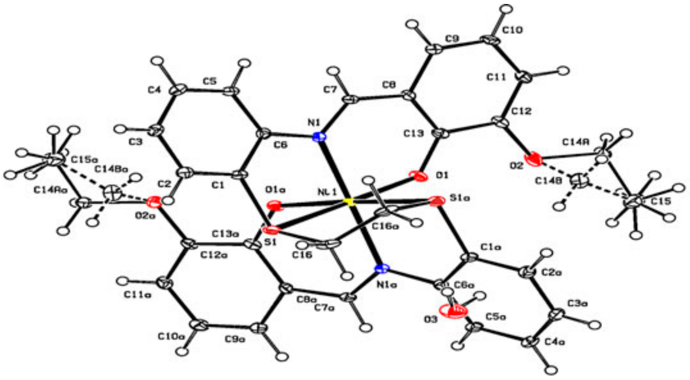

Reactions of 1,2-di(o-aminophenylthio)ethane with 3-ethoxy-2-hydroxybenzaldehyde yield the new hexadentate $N_2S_2O_2$ donor thioether Schiff base 1,2-bis(2-((2-(thio)phenylimino)methyl)-6-ethoxyphenol)ethane (H_2L). Ni(II), Zn(II), Cd(II), and Hg(II) complexes of this ligand were prepared. Of these complexes, $[NiL]\cdot 2H_2O$ has been structurally characterized by X-ray crystallography. The coordination geometry around Ni(II) was described as octahedral. Zn(II), Cd(II), and Hg(II) complexes and the Schiff base ligand have been characterized by CHN analyses, molar conductivity, UV–vis, FT-IR, ^{1}H, and ^{13}C NMR spectroscopy.

Keywords: Schiff base complex; Hexadentate ligand; Nickel(II) complex; Thioether ligand; $N_2S_2O_2$ donor

1. Introduction

The complexation properties of thioether donor ligands have been studied [1–3]. Such ligands usually form strong bonds with soft metals and more rarely with hard ones. They

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*Corresponding author. Email: aadehghani@yazd.ac.ir are considered both poor σ-donor and poor π-acceptor ligands. This π-acceptor character can contribute to the M–S bond strength. In addition, their *trans* influence is lower than that of phosphines and higher than that of primary amines [4, 5]. One of the synthetic methods for the preparation of thioethers derivatives has been reported by the reaction of thiols with organic halides [6–8]; di-, tri-, and poly-thioether ligands have been obtained by this method [3, 9–13]. Thioether ligands with other donors such as nitrogen and oxygen, due to the presence of hard and soft donors, are of special interest to chemists and bioinorganic chemists. These ligands have structural similarities with natural biological systems and readily coordinate with a range of transition metal ions [14, 15].

Some thioether donor ligands are Schiff bases obtained by condensation of different types of thioether amines with various ketones and aldehydes [8, 9, 16–18], and many of these are hexadentate ligands [3, 19, 20]. $N_2S_2O_2$ donor Schiff base ligands are hexadentate ligands that have hard and soft donors in its structure. These ligands are promising from the viewpoint of coordination chemistry because of their ability toward complexation and involvement in a wide range of biological and non-biological processes [21–23]. The presence of both hard and soft donors in $N_2S_2O_2$ donor Schiff base ligands allow coordination with a wide range of transition metal ions and several metal complexes with $N_2S_2O_2$ donor Schiff base ligands have been reported [23–27].

The stability of metal complexes with polydentate ligands depends on factors such as the number and type of donors present, their relative positions within the ligand, the nature of the ligand backbone, and the number and size of chelate rings formed on complexation. Herein, we present the synthesis and characterization of a $N_2S_2O_2$ donor Schiff base derived from 1,2-di(o-aminophenylthio)ethane and 3-ethoxy-2-hydroxybenzaldehyde (scheme 1). This ligand shows all of the previously mentioned properties and Ni(II), Zn(II), Cd(II), Hg (II) complexes of this $N_2S_2O_2$ donor thioether Schiff base ligand have been synthesized. ^1H NMR data for Zn(II) and ^1H and ^{13}C NMR data for Cd(II) and Hg(II) complexes are presented with correlations to their structures and the X-ray structural analysis of Ni(II) complex displayed thioether coordination. On the basis of X-ray crystallography we conclude that the ligand is hexadentate and nickel(II) complex is assigned distorted octahedral structure.

2. Experimental

2.1. *Chemical and starting materials*

2-Aminothiophenol, 1,2-dibromoethane, 3-ethoxy-2-hydroxybenzaldehyde, $Ni(CH_3COO)_2\cdot 4H_2O$, $Zn(CH_3COO)_2\cdot 2H_2O$, $Cd(CH_3COO)_2\cdot 2H_2O$, and $Hg(CH_3COO)_2$ were commercial products (from Merck, Aldrich, and Fluka) and used without purification. Other reagents and solvents were of analytical grade and purchased commercially.

2.2. *Instrumentation*

The elemental analyses were performed in a CHNS-O-2400 II Perkin-Elmer. Conductivity measurements were carried out in 10^{-3} mol dm^{-3} CH_3CN or DMF solutions at 25 °C using a Metrohm 660 conductometer. The electronic spectra were taken in a GBC UV-Visible Cintra 101 spectrophotometer with 1-cm quartz cell in the range of 200–1100 nm at 25 °C.

Infrared spectra were recorded in ATR using a Bruker FT-IR Equinax-55 spectrophotometer (4000–400 cm^{-1}). ^1H and ^{13}C NMR spectra were taken in $CDCl_3$ on Bruker NMR 500 and 400 MHz spectrometers using $Si(CH_3)_4$ as an internal standard.

2.3. *X-ray crystal structure determination*

Single crystal of Ni(II) complex suitable for X-ray analyses was selected from those obtained by open evaporation of ethanolic solution of the reaction mixture at 298 K. The details of the X-ray crystal data and of the structure solution and refinement are given in table 1. The X-ray diffraction measurements were made on a STOE IPDS-G diffractometer with graphite-monochromated Mo Kα radiation ($\lambda = 0.71073$ Å). Cell constants and an orientation matrix for data collection were obtained by least-squares refinement of diffraction data from 3871 unique reflections. The structure was solved by direct methods and refined on F^2 by a full-matrix least-squares procedure using anisotropic displacement parameters for all non-hydrogen atoms. Hydrogens were located in their calculated positions and refined using a riding model.

2.4. *Synthesis of the 1,2-di(o-aminophenylthio)ethane*

The 1,2-di(o-aminophenylthio)ethane was prepared by reaction of 2-aminothiophenol and sodium with 1,2-dibromoethane according to the procedure of Cannon et al. [28]. 2-Aminothiophenol (12.5 g, 0.1 mol) was added to ethanol (40 mL) containing sodium (2.31 g, 0.1 mol). 1,2-Dibromoethane (4.27 g, 0.05 mol) in ethanol (40 mL) was added

Table 1. Crystal data and structure refinement for $[NiL]\cdot 2H_2O$.

Empirical formula	$C_{32}H_{34}N_2NiO_6S$
Formula weight	665.44
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*C2/c*
Unit cell dimensions	$a = 20.855(4)$ Å
	$b = 8.0536(16)$ Å $\beta = 94.17(3)°$
	$c = 17.285(3)$ Å
Volume	2895.5(10) $Å^3$
Z	4
Density (calculated)	1.526 Mg/m^3
Absorption coefficient	0.864 mm^{-1}
$F(0\,0\,0)$	1392
Crystal size	0.20 × 0.15 × 0.08 mm^3
θ range for data collection	2.71–29.21°
Limiting indices	$-24 \le h \le 28$, $-11 \le k \le 10$, $-23 \le l \le 23$
Reflections collected/unique	11,465/3871 [$R_{(int)} = 0.1114$]
Completeness to θ =	29.21, 98.8%
Absorption correction	Numerical
Max. and min. transmission	0.9341 and 0.8461
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3871/2/211
Goodness-of-fit on F^2	1.055
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0719$, $wR_2 = 0.1226$
R indices (all data)	$R_1 = 0.1197$, $wR_2 = 0.1370$
Largest diff. peak and hole	0.479 and −0.503 e.$Å^{-3}$

during 30 min to the refluxing solution. The mixture was cooled, poured into water (100 mL), filtered off, washed well with water, and dried in vacuo. Recrystallization from ethanol yielded 9.8 g (71%). IR (ATR, cm^{-1}) 3387, 3291, 1616 $\nu(NH_2)$; 749 ν(C–S); ^{1}H NMR ($CDCl_3$, ppm): δH 2.83 (4H, s), 4.0–4.5 (4H, br), 6.68 (1H, t), 6.73 (1H, d), 7.12 (1H, t), 7.28 (1H, d); ^{13}C NMR ($CDCl_3$, ppm): δC 34.6, 115.1, 118.7, 130.0, 136.2, 148.6, 154.7.

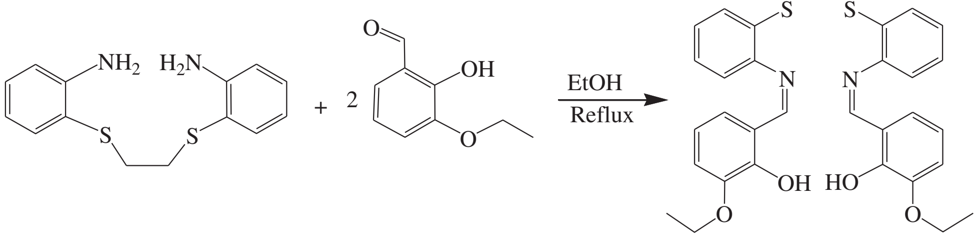
2.5. *Synthesis of 1,2-bis(2-((2-(thio)phenylimino)methyl)-6-ethoxyphenol)ethane (H_2L)*

A solution of 1,2-di(o-aminophenylthio)ethane (1.38 g, 5 mmol) in ethanol (30 mL) was added dropwise to a refluxing solution of 3-ethoxy-2-hydroxybenzaldehyde (1.66 g, 10 mmol) in ethanol (20 mL). After refluxing for 8 h the solution was vacuum evaporated to yield the crude product as a yellow precipitate (scheme 1). Yield: 2.4 g (84%). Anal. Calcd for $C_{32}H_{32}N_2O_4S_2$: C, 67.11; H, 5.63; N, 4.89%. Found: C, 66.97; H, 5.53; N, 5.02%; IR (ATR, cm^{-1}) 1608 ν(C=N); 735 ν(C–S); ^{1}H NMR ($CDCl_3$, ppm): δH 1.53 (6H, $J = 6.8$ Hz, t), 3.14 (4H, s), 4.18 (4H, $J = 6.8$ Hz, q), 6.87 (2H, t), 7.03 (4H, d), 7.20–7.33 (8H, m), 8.62 (2H, s), 13.45 (2H, s); ^{13}C NMR ($CDCl_3$, ppm): δC 14.92, 31.54, 64.59, 116.32, 117.91, 118.57, 119.32, 123.94, 126.88, 127.56, 128.40, 131.60, 146.96, 147.80, 156.55, 162.23; UV-vis in CH_3CN (λ, nm) 308 ($\log\varepsilon = 3.32$), 362 ($\log\varepsilon = 3.12$); Λ_m (CH_3CN) 3.42 Ω^{-1} cm^2 mol^{-1}.

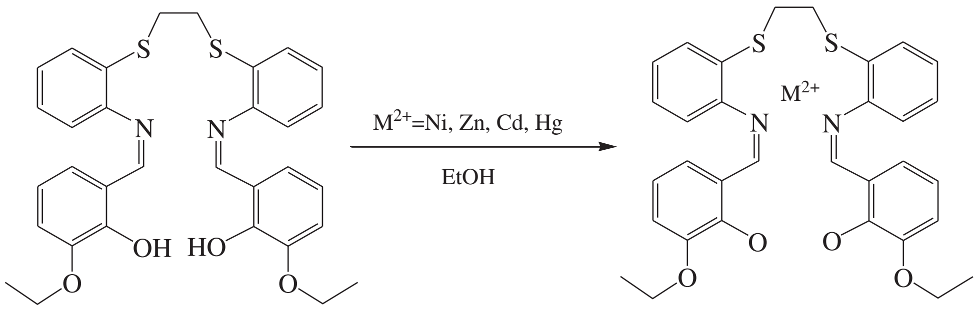
2.6. *General synthesis of the complexes*

A solution of the corresponding metal salt (1 mmol) in ethanol (30 mL) was added dropwise to the solution of $N_2S_2O_2$ ligand (H_2L) (0.573 g, 1 mmol) in ethanol (20 mL) and the reaction mixture was stirred for 5 h. The solution was then concentrated in a rotary evaporator to *ca.* 5–10 mL. The complexes were filtered off, washed with cold ethanol, and air dried (scheme 2). Crystal of [NiL]·$2H_2O$ suitable for X-ray work was obtained by slow evaporation of ethanolic solution of the complex.

2.6.1. [Zn(L)]·2H$_2$O. Yield: 407 mg (61%). Anal. Calcd for $C_{32}H_{34}N_2O_6S_2Zn$: C, 57.18; H, 5.10; N, 4.17%. Found: C, 56.48; H, 4.94; N, 3.80%; IR (ATR, cm^{-1}) 1608 ν(C=N); 752 ν(C–S); ^{1}H NMR ($CDCl_3$, ppm): δH 1.53 (6H, $J = 8$ Hz, t), 3.14 (4H, s), 4.16 (4H, $J = 8$ Hz, q), 6.86–7.37 (12H, m), 8.58 (2H, s); ^{13}C NMR ($CDCl_3$, ppm): δC 14.8, 31.5,



Scheme 1. Synthesis of H_2L.



Scheme 2. Synthesis of the complexes.

64.7, 116.3, 117.9, 118.6, 119.4, 124.0, 126.9, 127.6, 128.4, 131.6, 147.0, 147.9, 151.5, 162.2; UV–vis in CH_3CN (λ, nm) 310 ($\log\varepsilon = 3.47$), 422 ($\log\varepsilon = 3.18$); Λ_m (CH_3CN) 3.95 Ω^{-1} cm^2 mol^{-1}.

2.6.2. [Cd(L)]·4H$_2$O. Yield: 581 mg (77%). Anal. Calcd for $C_{32}H_{38}CdN_2O_8S_2$: C, 50.89; H, 5.07; N, 3.71%. Found: C, 50.15; H, 4.72; N, 3.23%; IR (ATR, cm^{-1}) 1609 ν(C=N); 751 ν(C–S); ^{1}H NMR ($CDCl_3$, ppm): δH 1.53 (3H, J = 9 Hz, t), 1.54 (3H, J = 9 Hz, t), 3.15 (4H, s), 4.17 (2H, J = 9 Hz, q), 4.18 (2H, J = 9 Hz, q), 6.87 (2H, J = 7 Hz, t), 7.03 (4H, J = 8 Hz, t), 7.20–7.30 (6H, m), 7.32 (2H, J = 9 Hz, d), 8.62 (2H, s); ^{13}C NMR ($CDCl_3$, ppm): δC 14.9, 31.5, 64.6, 116.3, 117.9, 118.6, 119.3, 123.9, 126.9, 127.6, 128.4, 131.6, 146.9, 147.8, 151.4, 162.2; UV–vis in CH_3CN (λ, nm) 309 ($\log\varepsilon = 3.40$), 427 ($\log\varepsilon = 3.01$); Λ_m (CH_3CN) 4.83 Ω^{-1} cm^2 mol^{-1}.

2.6.3. [Hg(L)]·H$_2$O. Yield: 602 mg (76%). Anal. Calcd for $C_{32}H_{32}HgN_2O_5S_2$: C, 48.69; H, 4.09; N, 3.55%. Found: C, 48.41; H, 4.10; N, 3.47%; IR (ATR, cm^{-1}) 1608 ν(C=N); 751 ν(C–S); ^{1}H NMR ($CDCl_3$, ppm): δH 1.53 (6H, J = 9 Hz, t), 3.14 (4H, s), 4.18 (4H, J = 9 Hz, q), 6.89 (2H, J = 7 Hz, t), 7.03 (4H, J = 7 Hz, t), 7.20–7.35 (8H, m), 8.62 (2H, s); ^{13}C NMR ($CDCl_3$, ppm): δC 14.9, 31.6, 64.6, 116.3, 117.9, 118.6, 119.3, 124.0, 126.9, 127.6, 128.4, 131.6, 147.0, 147.8, 151.6, 162.2; UV–vis in DMF (λ, nm) 308 ($\log\varepsilon = 3.32$), 383 ($\log\varepsilon = 3.14$); Λ_m (DMF) 60.94 Ω^{-1} cm^2 mol^{-1}.

2.6.4. [Ni(L)]·2H$_2$O. Yield: 498 mg (75%). Anal. Calcd for $C_{32}H_{34}N_2O_6S_2Ni$: C, 57.76; H, 5.15; N, 4.21%. Found: C, 58.46; H, 4.79; N, 4.33%; IR (ATR, cm^{-1}) 3383 ν(O–H); 1598 ν(C=N); 766 ν(C–S); UV-vis in DMF (λ, nm) 307 ($\log\varepsilon = 3.35$), 455 ($\log\varepsilon = 3.22$), 562 ($\log\varepsilon = 2.31$), 754 ($\log\varepsilon = 2.06$); Λ_m (DMF) 12.96 Ω^{-1} cm^2 mol^{-1}.

3. Results and discussion

The IR spectrum for 1,2-di(o-aminophenylthio)ethane shows bands at 3387, 3291, and 1616 cm^{-1} assignable to the aromatic primary amine vibrations and a band at 749 cm^{-1} due to the thioether stretch. The IR spectrum for H_2L confirms the presence of imine

(1608 cm^{-1}) and the absence of carbonyl and amine functional groups of the starting materials. The vibration peak of C–S is observed at 735 cm^{-1}. In IR spectra of Cd(II), Zn (II), and Hg(II) complexes, the band at 1608 cm^{-1} or 1609 cm^{-1} is associated with *ν*(C=N) vibration, and the vibrations of C–S are at 751 cm^{-1} or 752 cm^{-1}. In the IR spectrum for Ni(II) complex, the band at 1598 cm^{-1} is associated with *ν*(C=N) vibration and the vibration of C–S at 766 cm^{-1}. The vibration of C–S is shifted relative to the similar band of the ligand that shows the thioether sulfur coordinated to the metal ion. Also there is an intense broad band centered at ~3383 cm^{-1} consistent with the presence of water as observed from the X-ray data.

^{1}H NMR and ^{13}C NMR results, obtained for prepared compounds at ambient temperature in $CDCl_3$, are presented in section 2. ^{1}H and ^{13}C NMR spectra of the amine indicate that this compound were synthesized. The slightly broad signal at *δ*H 13.45 ppm in the ^{1}H NMR spectrum of ligand is assigned to OH, and CH=N protons of ligand exhibit a singlet at *δ*H 8.62 ppm. The ^{1}H NMR spectrum of ligand shows the aromatic ring protons from *δ*H 6.87–7.33 ppm and the aliphatic protons at *δ*H 1.53–4.18 ppm. The ^{13}C NMR spectrum of ligand features 16 signals, as expected for the symmetry of the ligand. In this spectrum, azomethine carbon resonance is at 162.23 ppm and carbon resonances for CH_3, SCH_2, and OCH_2 are at 14.92, 31.54, and 64.59 ppm, respectively. The resonances for the aromatic ring carbons are from 116.32 to 156.55 ppm. The ^{1}H NMR spectra of Zn(II), Cd(II), and Hg(II) complexes exhibit a singlet at *δ*H 8.58–8.62 ppm, which has been assigned to the azomethine proton (CH=N) and these spectra exhibit the aromatic ring protons at *δ*H 6.86–7.37 ppm and the aliphatic protons from *δ*H 1.53–4.18 ppm. Cd(II) complex exhibits two triplets at 1.53 ppm and 1.54 ppm, corresponding to methyl protons and two quartets at 4.17 ppm and 4.18 ppm, corresponding to methylene protons (figure 1). This indicates that

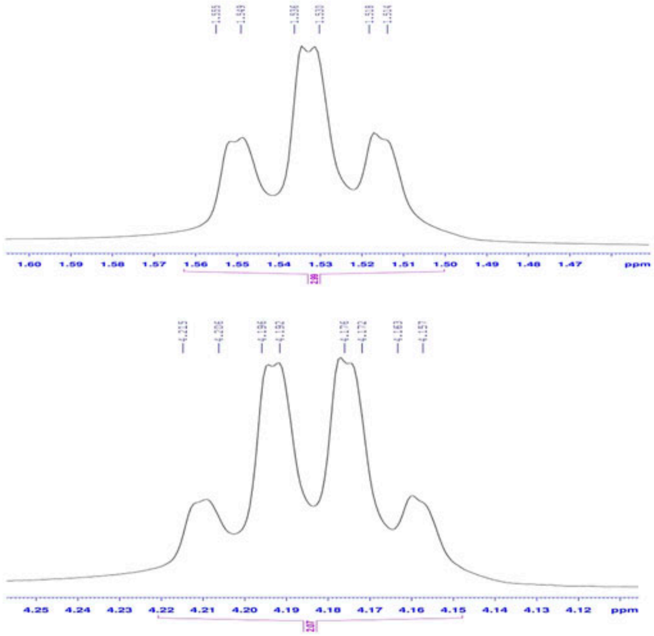


Figure 1. Methyl and methylene protons of ethyl groups in Cd(II) complex.

the two ethyl protons are in different magnetic environments. In the ^{13}C NMR spectra of Zn(II), Cd(II), and Hg(II) complexes, azomethine carbon resonances are at 162.2 ppm and the carbon resonances for CH_3, SCH_2, and OCH_2 are from 14.9 to 64.7 ppm. The resonances for the aromatic ring carbons are from 116.3 to 151.6 ppm.

The electronic spectrum of H_2L shows two absorptions at 308 nm ($\log\varepsilon = 3.32$) and 362 nm ($\log\varepsilon = 3.12$); the band at 362 nm is the $n \rightarrow \pi^*$ transition, while the 280 nm band involves a $\pi \rightarrow \pi^*$ transition. The electronic spectrum in solution agrees well with the pseudo-octahedral geometry for the nickel(II) complex. This complex shows a band at 307 nm ($\log\varepsilon = 3.35$, $\pi \rightarrow \pi^*$) and three bands at 455 nm ($\log\varepsilon = 3.32$) assigned as a metal→ligand charge transfer band, 562 nm ($\log\varepsilon = 2.31$) and 754 nm ($\log\varepsilon = 2.06$) assigned as $d \rightarrow d$ transitions. The electronic spectra of the Zn(II), Cd(II), and Hg(II) complexes show absorptions at 308–310 nm ($\log\varepsilon = 3.32$–3.47) and 383–427 nm ($\log\varepsilon = 3.01$–3.18). The band at higher energy is attributable to $\pi \rightarrow \pi^*$ transition and the band at low energy arises from metal→ligand charge transfer band [3].

The molar conductance values for H_2L, Zn(II) and Cd(II) complexes measured in CH_3CN solution (1×10^{-3} mol dm^{-3}) are 3.42–4.83 Ω^{-1} cm^2 mol^{-1} and Hg(II) and Ni(II) complexes measured in DMF solution (1×10^{-3} mol dm^{-3}) are 12.97–60.94 Ω^{-1} cm^2 mol^{-1}. These observed values of the molar conductance are well within the expected range for non-electrolytes [29]. Also, the elemental analyses of the complex indicated the absence of counter ions in the formula.

3.1. *Description of the crystal structure*

The structure of [NiL], determined by single-crystal X-ray diffraction, is shown in figure 2. Selected bond lengths, bond angles, and hydrogen bonds are given in tables 2 and 3. The molecular structure of the complex has a distorted octahedral geometry around the Ni(II) center, as can be judged from spread in its observed angles [84.89(10)–95.25(18)°] and the *trans* angles [173.5(2)–176,015(9)°]. The Schiff base ligand is a hexadentate ligand through both thioether sulfurs (*cis* coordinated with a bond angle of 88.52(6)°), both imine N (*trans* coordinated with a bond angle of 173.5(2)°) and both phenolic O (*cis* coordinated with a

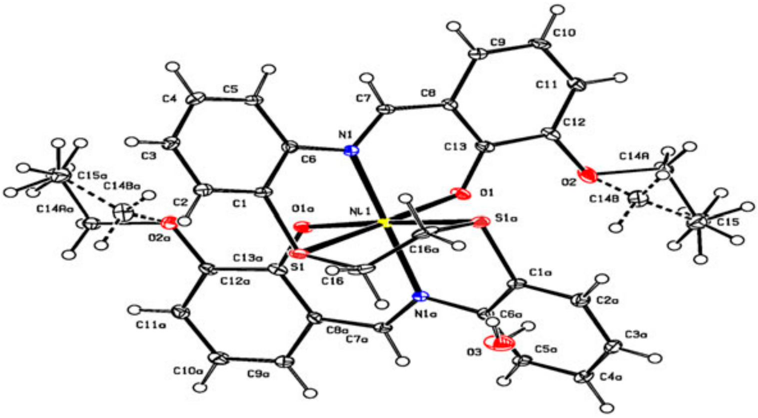


Figure 2. Crystal structure of $[NiL]\cdot 2H_2O$ showing 50% displacement ellipsoids.

Table 2. Selected bond lengths (Å) and angles (°) for [NiL]·$2H_2O$.

Bond lengths	*d* (Å)	Bond angles	*a* (°)
Ni(1)–O(1)	2.000(3)	O(1)–Ni(1)–O(1a)	95.25(18)
Ni(1)–O(1a)	2.000(3)	O(1)–Ni(1)–N(1)	93.20(12)
Ni(1)–N(1)	2.045(3)	O(1a)–Ni(1)–N(1)	91.19(12)
Ni(1)–N(1a)	2.045(3)	O(1)–Ni(1)–N(1a)	91.19(12)
Ni(1)–S(1)	2.4067(12)	O(1a)–Ni(1)–N(1a)	93.20(12)
Ni(1)–S(1a)	2.4066(12)	N(1)–Ni(1)–N(1a)	173.5(12)
S(1)–C(1)	1.770(4)	O(1)–Ni(1)–S(1)	176.15(9)
S(1)–C(16)	1.827(5)	O(1a)–Ni(1)–S(1)	88.14(9)
O(1)–C(13)	1.305(4)	N(1)–Ni(1)–S(1)	84.89(10)
N(1)–C(7)	1.295(5)	N(1a)–Ni(1)–S(1)	90.44(10)
N(1)–C(6)	1.417(5)	O(1)–Ni(1)–S(1a)	88.15(9)
O(2)–C(12)	1.380(4)	O(1a)–Ni(1)–S(1a)	176.15(9)
C(16)–C(16a)	1.509(9)	N(1)–Ni(1)–S(1a)	90.44(10)
O(12)–C(13)	1.437(5)	N(1a)–Ni(1)–S(1a)	84.89(10)
C(7)–C(8)	1.438(5)	S(1)–Ni(1)–S(1a)	88.52(6)

Table 3. Hydrogen bonds (Å and deg) for [NiL]·$2H_2O$.

(D–H…A)	*d* (D–H)	*d* (H…A)	*d* (D…A)	< (DHA)
O(3)–H(3A)…O(1)#2	0.855(19)	1.96(2)	2.807(4)	171(5)
C(7)–H(7)…O(3)#3	0.95	2.55	3.460(5)	159.8

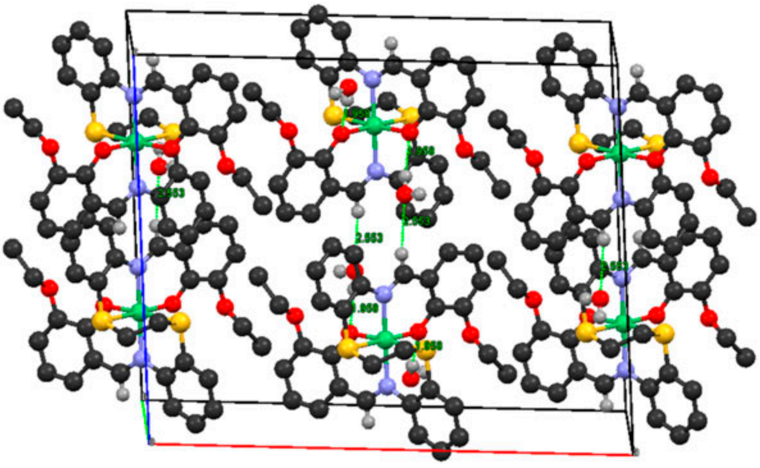


Figure 3. Crystal packing of [NiL]·$2H_2O$ showing the hydrogen bonds (Å).

bond angle of 95.25(18)°). Thus, the Ni(II) is bound through $N_2O_2S_2$ donors. The bond lengths found in the structure are within the normal ranges for this geometry (Ni–S 2.4067 (12) Å, Ni–N 2.045(3) Å and Ni–O 2.000(3) Å). Nickel is in the plane formed by the two oxygens and two sulfurs, and the sum of four angles in this plane is 360.06°. The angle between this plane and the plane including the metal and the two axial nitrogens, N1 and

N1a, is 87.16°. In each molecular unit of the complex, two waters have hydrogen bond interactions with the Schiff base ligand through O(3)–H(3)….O(1) and C(7)–H(7)…O(3). The phenolic oxygens have strong hydrogen bond interactions with hydrogen from water, and four units of [NiL]·$2H_2O$ are present in its unit cell (figure 3).

4. Conclusion

We report the synthesis of a new hexadentate $N_2S_2O_2$ donor thioether Schiff base (H_2L) and prepared Ni(II), Zn(II), Cd(II), and Hg(II) complexes of this ligand. The complexes have been characterized by spectroscopic methods. In addition, the solid state structure of [NiL]·$2H_2O$ shows that the ligand is hexadentate with a distorted octahedral geometry around the Ni(II) center.

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Disclosure statement

No potential conflict of interest was reported by the authors.

Supplementary data

CCDC 1042129 contains the supplementary crystallographic data for [NiL]·$2H_2O$. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: (+44) 1223-336-033; or Email: deposit@ccdc.cam.ac.uk.

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