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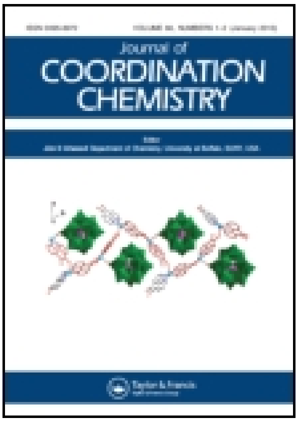

Journal of Coordination Chemistry
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gcoo20

Synthesis, characterization, and crystal structure of two zinc(II) complexes with a Schiff base derived from amantadine

Xu-Dong Jin[a], Chong Xu[a], Xiao-Chen Liu[a], Xue-Yue Yin[a], Yu-Chen Gang[b], Qi Yang[a] & Yue-Hong Jin[c]

[a] College of Chemistry, Liaoning University, Shenyang, P.R. China

[b] College of Agriculture and Biotechnology, China Agricultural University, Beijing, P.R. China

[c] Liaoning Provincial Institute of Measurement, Shenyang, P.R. China

Accepted author version posted online: 18 Oct 2013.Published online: 26 Nov 2013.

To cite this article: Xu-Dong Jin, Chong Xu, Xiao-Chen Liu, Xue-Yue Yin, Yu-Chen Gang, Qi Yang & Yue-Hong Jin (2013) Synthesis, characterization, and crystal structure of two zinc(II) complexes with a Schiff base derived from amantadine, Journal of Coordination Chemistry, 66:22, 3970-3978, DOI: 10.1080/00958972.2013.855732

To link to this article: http://dx.doi.org/10.1080/00958972.2013.855732

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Journal of Coordination Chemistry, 2013
Vol. 66, No. 22, 3970–3978, http://dx.doi.org/10.1080/00958972.2013.855732

Synthesis, characterization, and crystal structure of two zinc (II) complexes with a Schiff base derived from amantadine

XU-DONG JIN*†, CHONG XU†, XIAO-CHEN LIU†, XUE-YUE YIN†,
YU-CHEN GANG‡, QI YANG† and YUE-HONG JIN§

†College of Chemistry, Liaoning University, Shenyang, P.R. China
‡College of Agriculture and Biotechnology, China Agricultural University, Beijing, P.R. China
§Liaoning Provincial Institute of Measurement, Shenyang, P.R. China

(*Received 3 September 2013; accepted 4 October 2013*)

By condensation of amantadine and 4-methoxysalicylaldehyde a new Schiff base **HL** was synthesized. A mixture of **HL** and zinc(II) chloride in an alcoholic medium leads to $[Zn(HL)_2Cl_2]$ (**1**). However, the same reactants gave another different complex (ZnL_2) (**2**) in the presence of NaOH. The two complexes were characterized by IR, ^{1}H NMR, elemental analysis, molar conductance, and single-crystal X-ray diffraction. X-ray diffraction analysis reveals that complex **1** crystallizes in the triclinic system, $P\bar{1}$ space group; each asymmetric unit consists of one zinc(II), two **HL**, and two chlorides. The tetra coordination of central zinc is attained by two chlorides and two oxygens from the Schiff base, forming a distorted tetrahedral geometry. Complex **2** crystallizes in the monoclinic system, $P2_1/c$ space group; each asymmetric unit consists of one zinc(II) and two **L**. The tetra coordination of central zinc is attained by two nitrogens and two oxygens from the Schiff base, forming a distorted tetrahedral geometry.

Keywords: Zinc(II) complexes; Amantadine; Schiff base; Synthesis; Crystal structures

1. Introduction

Condensation of primary amines with carbonyl compounds yields Schiff bases [1]. In the past few years, transition metal complexes of Schiff bases have been one of the most widely studied coordination compounds, particularly as biochemical, analytical, and antimicrobial reagents [2, 3]. Zinc is a vital biological element and an important enzyme-active site [4, 5]. Zinc(II) complexes of Schiff bases are also biologically active and exhibit enhanced activities compared with the free Schiff bases [6]. Tricyclo [3.3.1.1(3,7)] decane-1-amine (amantadine) is an antivirotic drug that has been used to treat influenza and Parkinson's disease [7–9]. Salicylaldehyde and its derivatives were used to produce efficient herbicides, insecticides, and fungicides [10], due to their antibacterial and antiviral activities. In this study, we designed and synthesized two zinc(II) complexes with the same Schiff base derived from amantadine and a salicylaldehyde derivative. The coordination behavior of the ligand toward zinc(II) was investigated, and the absolute structures of two zinc complexes were determined by single-crystal X-ray diffraction analysis.

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*Corresponding author. Email: jinxudong@lnu.edu.cn

2. Experimental

2.1. *Materials and methods*

All chemicals and solvents were of analytical grade and used as received. Elemental analysis was carried out on a Perkin Elmer Flash EA 1112. Chemical shifts (δ) for ^{1}H NMR spectra were recorded at 300 MHz on a Varian Mercury-Vx300 spectrometer in $CDCl_3$ solvent containing TMS as an internal standard. Infrared spectra (IR) were scanned from 4000 to 400 cm^{-1} with KBr pellets on a Nicolet NEXUS FT-IR 5700 spectrophotometer. Melting points were measured on a WRS-1B micro melting point apparatus and were not corrected. The molar conductances of the complexes in DMF (1.0×10^{-3} mo1 L^{-1}) were measured using DDS-11A conductometer.

2.2. *Synthesis of HL*

HL (figure 1) was prepared by an improved method based on the literature [11]. Amantadine hydrochloride (563 mg, 3.0 mmol) and KOH (168 mg, 3.0 mmol) in 50 mL anhydrous ethanol were stirred for 24 h. The white precipitates (KCl) were filtered out, and the transparent liquid was added dropwise to a solution of 4-methoxysalicylaldehyde (457 mg, 3.0 mmol) in 30 mL anhydrous ethanol. The resulted solution was refluxed for 2 h at 60 °C and cooled to room temperature. A colored crysta1 was filtered and evaporated under reduced pressure.

HL: 190 mg, yield 65%. Yellow powder. M.p. 106.7~107.7 °C. IR (KBr): 3586(m), 3434(m), 2907(s), 2848(s), 1625(s), 1531(m), 1452(m), 1412(w), 1366(m), 1342(m), 1309 (m), 1227(s), 1210(m), 1187(m), 1169(m), 1116(m), 1088(m), 1032(m), 967(m), 939(w), 922(w), 831(m), 815(w), 787(w), 645(w), 585(w), 528(w), 502(w), 456(w), 424(w). ^{1}H NMR ($CDCl_3$, 300 MHz): δ 11.50 (*s*, 1H, Ar-OH); 8.24 (*s*, 1H, CH=N); 7.02-6.21 (*m*, 3H, Ar–H); 3.79 (*s*, 3H, Ar–OCH_3); 2.19 (*s*, 3H, CH, adam.H); 1.89-1.71 (*m*, 12H, CH_2, adam.H). Anal. Calcd for $C_{18}H_{23}NO_2$ (285.38): C, 75.76; H, 8.12; N, 4.91.

2.3. *Synthesis of the complexes*

2.3.1. Synthesis of complex 1. Zinc(II) chloride (136 mg, 1.0 mmol) in 20 mL anhydrous ethanol was added dropwise to a hot solution of **HL** (571 mg, 2.0 mmol) in 20 mL anhydrous ethanol. Thereafter, the mixture was refluxed for 2 h at 60 °C and then kept at room temperature overnight; complex precipitates were filtered off and dried.

Complex **1**: 540 mg, yield 76%. White powder. M.p. 264.5~265.5 °C. IR (KBr): 3428 (w), 2910(s), 2853(m), 1641(s), 1612(s), 1537(s), 1490(s), 1456(m), 1358(m), 1302(s), 1230(s), 1275(m), 1215(s), 1189(m), 1174(m), 1142(w), 1118(m), 1084(m), 1025(m), 975 (m), 937(w), 840(w), 814(w), 791(m), 746(w), 662(w), 611(m), 565(w), 536(m), 496(w),

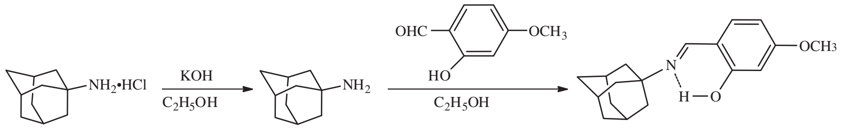


Figure 1. The formation of the Schiff base.

442(w). ^{1}H NMR ($CDCl_3$, 300 MHz): δ 13.05 (*d*, ^3J = 10.8, 1H, Ar-OH); 7.85 (*d*, ^3J = 14.1, 1H, CH=N); 7.05 (*d*, ^3J = 9.0, 1H, Ar-H); 6.81 (*s*, 1H, Ar-H): 6.23 (dd, ^3J = 9.0/2.1, 1H, Ar-H); 3.76 (*s*, 3H, Ar-OCH_3); 2.17 (*s*, 3H, CH, adam.H); 1.91 (*s*, 6H, CH_2, adam.H); 1.68 (*q*, ^3J = 12.6, 6H, CH_2, adam.H). Anal. Calcd for $C_{36}H_{46}Cl_2N_2O_4Zn$ (707.05): C, 61.15; H, 6.56; N, 3.96. Found: C, 60.79; H, 6.72; N, 3.69.

2.3.2. Synthesis of 2. About 20 mL ethanolic NaOH (80 mg, 2.0 mmol) was added to a solution of **HL** (571 mg, 2.0 mmol) in 20 mL anhydrous ethanol. After the solution was stirred for ten minutes, zinc(II) chloride (136 mg, 1.0 mmol) in 20 ml anhydrous ethanol was added and the mixture was refluxed for another 2 h at 60 °C. Then, the solution was kept at room temperature overnight and complex precipitates were filtered off and dried.

Complex **2**: 390 mg, yield 61%. Yellowish powder. M.p. > 280 °C. IR (KBr): 2909(s), 2849(m), 1609(s), 1526(s), 1409(s), 1357(m), 1306(m), 1216(s), 1117(s), 1081(m), 1033 (m), 978(m), 932(m), 886(w), 838(m), 782(m), 734(w), 655(w), 611(m), 526(m), 488(w). ^{1}H NMR ($CDCl_3$, 300 MHz): 8.15 (*s*, 1H, CH=N); 6.97 (*d*, ^3J = 8.4, 1H, Ar-H); 6.30 (*s*, 1H, Ar-H); 6.18 (*d*, 3*J* = 8.7, 1H, Ar-H); 3.17 (*s*, 3H, Ar-OCH3); 2.08 (*s*, 3H, CH, adam.H); 1.93 (*d*, ^3J = 12.0, 3H, CH_2, adam.H); 1.64 (*d*, ^3J = 12.3, 3H, CH_2, adam.H); 1.55 (*d*, ^3J = 12.3, 3H, CH_2, adam.H). Anal. Calcd for $C_{36}H_{44}N_2O_4Zn$ (634.13): C, 68.19; H, 6.99; N, 4.42. Found: C, 68.12; H, 7.10; N, 4.57.

2.4. *X-ray crystallography*

The complexes were dissolved in C_2H_5OH/CH_2Cl_2 (2:1 v/v) solution. The solvent was slowly evaporated in air affording white crystals for complex **1** and light yellow crystals for complex **2** for X-ray analysis. The crystallographic data collections were conducted on a Bruker Smart Apex II CCD with graphite monochromated Mo K_α radiation (λ = 0.71073 Å) at 296(2) K for complex **1** and 153(2) for complex **2** using the ω-scan technique. The data were integrated by using SAINT, which also corrected the intensities for Lorentz and polarization effects [12]. An empirical absorption correction was applied using SADABS [13]. The structures were solved by direct methods using SHELXS-97, and all nonhydrogen atoms were refined anisotropically on F^2 by full-matrix least-squares using the SHELXL-97 crystallographic software package [14]. Hydrogens were generated geometrically. All calculations were performed on a personal computer with the SHELXL-97 crystallographic software package. The details of the crystal parameters, data collection, and refinement are summarized in table 1. Selected bond lengths and angles with their estimated standard deviations are given in table 2. Hydrogen-bond geometry of complex **1** is listed in table 3. The molecular structures of complexes **1** and **2** are shown in figures 1 and 2, were visualized by diamond [15].

3. Results and discussion

3.1. *Elemental analysis and molar conductance*

From the analysis, it was observed that the presence of C, H, and N contents suggest that complex **1** consists of one zinc(II), two **HL,** and two chlorides, while **2** consists of one zinc (II) and two **L** (figure 2). Although both compounds are soluble in dichloromethane and chloroform, the complexes are less soluble than the ligand in other solvents such as alcohol,

Table 1. Crystallographic data for **1** and **2**.

Empirical formula	$C_{36}H_{46}Cl_2N_2O_4Zn$ (**1**)	$C_{36}H_{44}N_2O_4Zn$ (**2**)
Formula weight (g mol^{-1})	705.00	634.13
Crystal size (mm)	0.30 × 0.28 × 0.21	0.41 × 0.33 × 0.23
Crystal system	Triclinic	Monoclinic
Color	White	Light yellow
Space group	$P\bar{1}$	$P2_1/c$
a (Å)	13.0940(13)	16.0086(5)
b (Å)	13.5529(13)	11.0097(3)
c (Å)	22.508(2)	22.7874(8)
α (°)	86.930(2)	90.00
β (°)	76.107(2)	129.863(2)
γ (°)	66.905(2)	90.00
V (Å^3)	3563.0(6)	3082.81(17)
Z	4	4
θ Range (°)	0.93–27.57	2.48–25.00
Index ranges	$-16 \le h \le 10$, $-17 \le k \le 17$, $-29 \le l \le 29$	$-13 \le h \le 19$, $-13 \le k \le 12$, $-27 \le l \le 27$
ρ (g cm^{-3})	1.314	1.366
μ (mm^{-1})	0.879	0.840
Reflections collected/unique	44,245/16,287 [R(int) = 0.0606]	11,886/5414 [R(int) = 0.0240]
Data/restraints/parameters	16,287/54 /843	5414/0/472
Goodness-of-fit (GoF)	1.000	1.035
F (0 0 0)	1480	1344
T/K	296(2)	153 (2)
$R_1{}^a/wR_2{}^b$ ($I > 2\sigma(I)$)	0.0613/0.1652	0.0341/0.0769
R_1/wR_2 (all data)	0.1343/0.2270	0.0538/0.0865

Notes: $^aR_1 = \Sigma||Fo|-|Fc||/|Fo|$.
$^bwR_2 = [\Sigma w(Fo^2-Fc^2)^2/\Sigma w(Fo^2)^2]^{1/2}$.

tetrahydrofuran, benzene, and ethyl acetate. The molar conductance values (Λ_M) for complexes **1** and **2** are 9.23 and 2.30 S cm^2 mol^{-1}, which should belong to nonelectrolyte complexes [16].

3.2. *IR spectra*

In table 4, the important IR data for the complexes are listed, in which several main data for **HL** are also provided for comparison. Broad and intense absorptions at 3434 and 3428 cm^{-1} for **HL** and complex **1** can be identified as OH stretches, indicating phenolic hydroxyl is not eliminated as complex **1** is formed. These bands are absent in complex **2**, illustrating coordination through deprotonated phenolic OH. A band assigned to C=N stretch (1625 cm^{-1}) in **HL** moves to higher wavenumber 1641 cm^{-1} in complex **1**, but lower wavenumber 1609 cm^{-1} in complex **2**, implying coordination of azomethine nitrogen to Zn(II) in **2** instead of **1**. The spectra of **HL** display a strong band at 1227 cm^{-1} from C–O stretch; this band occurs in **1** at higher frequency, 1230 cm^{-1}, while it occurs at lower frequency, 1216 cm^{-1}, in complex **2**. In the low-frequency regions, the presence of absorptions at 496 and 488 cm^{-1} for complexes **1** and **2** reveals Zn–O, indicating that oxygen of the Schiff base is coordinated to Zn(II).

3.3. *^{1}H NMR analysis*

^{1}H NMR data for complexes in $CDCl_3$ are shown in table 5, in which all data for **HL** are also provided for comparison. Single peaks at 15.19 and 13.05 for **HL** and complex **1** are

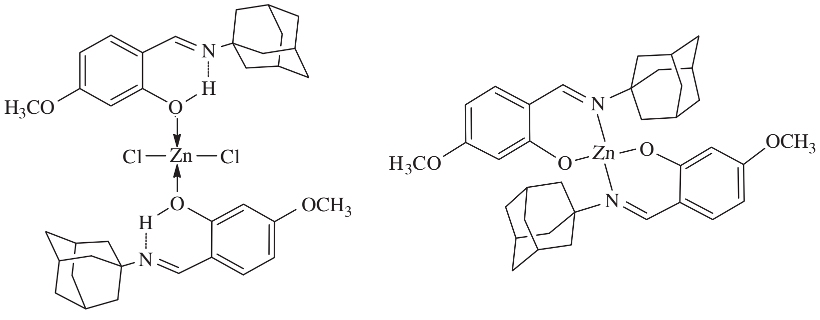
Table 2. Selected bond lengths (Å) and angles (°) in **1** and **2**.

1			
Zn1–Cl1	2.221(15)	Zn2–Cl3	2.220(15)
Zn1–Cl2	2.218(15)	Zn2–Cl4	2.222(17)
Zn1–O2	1.959(3)	Zn2–O6	1.967(3)
Zn1–O4	1.975(3)	Zn2–O7	1.978(3)
N1–C8	1.293(6)	N3–C44	1.314(6)
N1–C9	1.483(6)	N3–C45	1.471(6)
N2–C26	1.300(6)	N4–C62	1.312(6)
N2–C27	1.481(6)	N4–C63	1.480(6)
O4–C19	1.309(5)	O5–C43	1.415(7)
O2–C1	1.304(5)	O6–C37	1.303(5)
Cl1–Zn1–Cl2	116.58(8)	Cl3–Zn2–Cl4	119.62(7)
C1–Zn1–O4	115.05(12)	Cl3–Zn2–O6	111.78(12)
C1–Zn1–O2	110.51(12)	Cl3–Zn2–O7	110.29(12)
O2–Zn1–Cl2	112.67(13)	O6–Zn2–Cl4	110.99(13)
O2–Zn1–O4	98.88(14)	O6–Zn2–O7	97.60(14)
Cl2–Zn1–O4	101.56(10)	Cl4–Zn2–O7	103.97(11)
C8–N1–C9	127.8(4)	C44–N3–C45	128.5(4)
C26–N2–C27	126.5(4)	C62–N4–C63	127.3(4)
2			
Zn1–O1	1.930(16)	Zn1–N1	2.013(18)
Zn1–O3	1.938(15)	Zn1–N2	2.018(19)
N1–C9	1.495(3)	N2–C27	1.495(3)
N1–C7	1.293(3)	N2–C26	1.289(3)
O1–C1	1.301(3)	O3–C19	1.305(3)
O1–C1–C2	118.2(2)	N1–C7–C6	129.0(2)
O1–C1–C6	123.7(2)	C7–N1–C9	117.11(19)
N1–C9–C15	107.80(18)	C26–N2–Zn1	118.01(16)
N1–C9–Cl0	111.01(19)	C27–N2–Zn1	123.42(14)
N1–C9–Cl4	111.74(19)	C1–O1–Zn1	125.33(15)
N2–C26–C24	129.5(2)	C19–O3–Zn1	124.36(15)
N2–C27–C28	106.9(2)	O1–Zn1–O3	112.81(7)
N2–C27–C29	107.1(2)	O1–Zn1–N1	96.88(7)
N2–C27–C30	115.5(2)	O3–Zn1–N1	115.13(7)
C7–N1–Zn1	118.38(16)	O1–Zn1–N2	113.57(7)
C9–N1–Zn1	124.46(14)	O3–Zn1–N2	97.19(7)
C26–N2–C27	118.5(2)	N1–Zn1–N2	122.19(7)

Table 3. Hydrogen-bond geometry (Å, °) in **1**.

D-H···*A*	*D*-H	H···*A*	*D*···*A*	*D*-H···*A*
N1–H1···O2	0.86	1.89	2.587(5)	136.9
N2–H2···O4	0.86	1.88	2.576(5)	136.4
N3–H3···O6	0.86	1.90	2.602(5)	137.5
N4–H4···O7	0.86	1.89	2.586(5)	137.0

assigned to phenolic hydroxyl protons. Owing of intramolecular hydrogen bonds of −CH = N···HO−, they are observed at lower field. The presence of integrated 1H for complex **1** illustrates that phenolic hydroxyl proton of the ligand is not eliminated when complex **1** is formed, and the preservation of phenolic hydroxyl proton is confirmed. In complex **2**, the phenolic hydroxyl proton of **HL** is eliminated, resulting in disappearance of the single peak to the phenolic hydroxyl proton as well as the intramolecular hydrogen bond. In **HL,** a signal at 8.24 ppm is assigned to HC=N [17]. However, in spectra of complexes, this signal is observed at 7.85 and 8.15 ppm for complexes **1** and **2**, respectively.



1 **2**

Figure 2. Proposed structures of complexes.

Table 4. Main IR data for ligands and complexes (cm^{-1}).

Compound	$\upsilon_{C=N}$	$\upsilon_{C–O}$	υ_{CH2}	$\upsilon_{O–H}$	$\upsilon_{M–O}$
L	1625(s)	1227(s)	2848(s)	3434(w)	
1	1641(s)	1230(s)	2853(m)	3428(w)	496(w)
2	1609(s)	1216(s)	2848(m)		488(w)

Notes: s: strong; m: medium; w: weak.

Table 5. ^{1}H NMR data for ligand and complexes (δ in ppm, J in Hz).

Compound	Ar–OH	CH=N	Ar–H	Ar–OCH$_3$	Adamantane ring-H
L	15.19 (*s*, 1H)	8.24 (*s*, 1H)	6.86–6.82 (*m*, 2H); 6.68 (*t*-like, ^3J = 8.1/7.8, 1H)	3.88 (*s*, 3H)	2.18 (*s*, 3H, CH); 1.85–1.78 (*m*, 12H, CH$_2$)
1	13.05 (*d*, ^3J=10.8, 1H)	7.85 (*d*, ^3J=14.1, 1H)	7.05 (*d*, ^3J = 9.0, 1H); 6.81 (*s*, 1H); 6.23 (dd, ^3J= 9.0, ^4J=2.1, 1H)	3.76 (*s*, 3H)	2.17 (*s*, 3H, CH); 1.91 (*s*, 6H, CH$_2$); 1.68 (*q*, ^3J=12.6, 6H, CH$_2$)
2		8.15 (*s*, 1H)	6.97 (*d*, ^3J=8.4, 1H); 6.30 (*s*, 1H); 6.18 (*d*, ^3J=8.7, 1H)	3.17 (*s*, 3H)	2.08 (*s*, 3H, CH); 1.93 (*d*, ^3J=12.0, 3H, CH$_2$); 1.64 (*d*, ^3J=12.3, 3H, CH$_2$); 1.55 (*d*, ^3J=12.3, 3H, CH$_2$)

Multiplet at 6.18–7.05 ppm can be assigned to aromatic protons in **HL** and complexes. The CH and CH$_2$ groups from adamantane are identified from 2.18 to 1.55.

3.4. *Crystal structures of complexes 1 and 2*

From the crystallographic analysis, it was revealed that complex **1** crystallizes in the triclinic system, $P\bar{1}$ space group. In each asymmetric unit, there are two independent molecules. Zinc (II) is coordinated with two chlorides and two oxygens from two monodentate ligands. The geometry around Zn(II) in complex **1** is intermediate between square planar and tetrahedral, where the dihedral angle between the two coordination planes defined by Cl1−Zn1−Cl2 and O2−Zn1−O4 is 83.97°. Bond angles also show that the coordination geometry about the zinc in complex **1** is distorted tetrahedral (τ_4 = [360-(α + β)]/141° = 0.91) [18], with Cl1−Zn1−Cl2 (α) and Cl1−Zn1−O4 (β) angles of 116.58(8)° and 115.05(12)°, respectively.

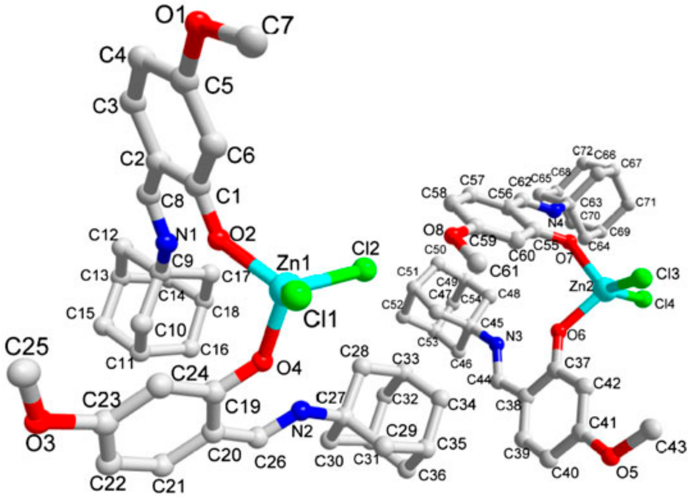


Figure 3. Molecular structure of **1** (two independent molecules in each asymmetric unit). Hydrogens have been omitted for clarity.

Other angles show expected values. The shortest distances between two adamantane carbons of two ligands are, respectively, 4.934 Å for C16−C30 and 4.446 Å for C48−C64 (figure 3), they are structurally very similar to another zinc(II) complex reported by Zhao *et al.* [19]. The crystal structure involves strong O–H···N intramolecular hydrogen bonds between the imino N and phenol O forming an additional six-membered ring. Complex **2** crystallizes in

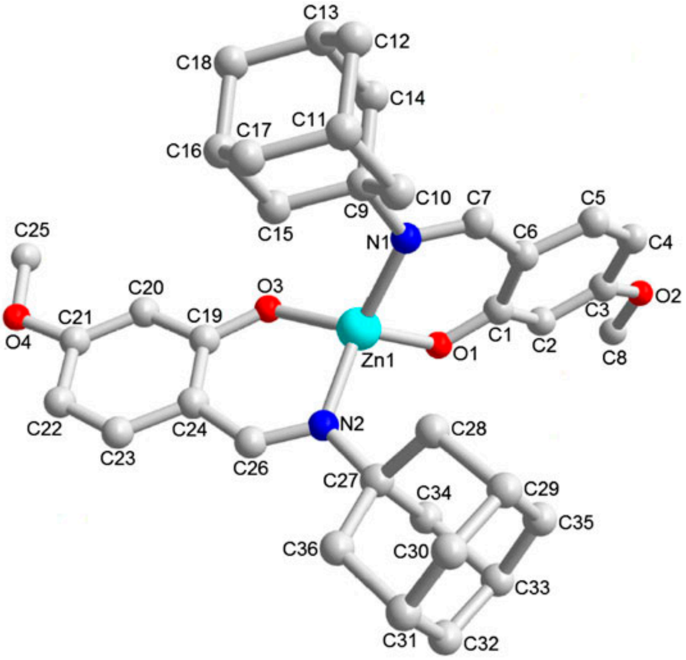


Figure 4. Molecular structure of **2**. Hydrogens have been omitted for clarity.

the monoclinic system, $P2_1/c$ space group. In each asymmetric unit there is one independent molecule. The central Zn(II) is bonded to an oxygen and a nitrogen of two bidentate ligands. The geometry around Zn(II) in complex **2** is intermediate between square planar and tetrahedral, where the dihedral angle between the two coordination planes defined by O1−Zn1−N1 and O3−Zn1−N2 is 87.87°. Bond angles also show that the coordination geometry about the zinc in complex **2** is distorted tetrahedral (τ_4 = [360-(α + β)]/141° = 0.87) [18], with N1−Zn1−N2 (α) and O3−Zn1−N1 (β) angles of 122.19(7)° and 115.13(7)°, respectively. Other angles show expected values. The shortest distance between two adamantane carbons from two ligands is 3.933 Å for C10−C28 (figure 4). The bidentate coordination mode of the complex does not involve intramolecular hydrogen bonds because the ligand has been deprotonated, but there also exist two six-membered rings through a zinc ion, two oxygens and two nitrogens.

Two complexes possess neither intermolecular hydrogen bonding nor π–π interactions in stacking. The complex molecules are regularly arranged by weak van der Waals forces to construct a net structure containing adamantine cages.

4. Conclusions

A new Schiff base **HL** has been synthesized by the reaction of amantadine hydrochloride and 4-methoxysalicylaldehyde. Then by using **HL** as ligand, two new zinc(II) complexes have been obtained in the absence or presence of NaOH. Their single-crystal structural analysis reveals that in complex **1** each Schiff base is monodentate coordinating through an oxygen. However, in complex **2,** each deprotonated Schiff base is bidentate coordinating through an oxygen and a nitrogen. Both complexes have distorted tetrahedral structures.

Funding

This study was financially supported by the Foundation of Liaoning Provincial Department of Education Innovation Team Projects [LT2012001]; the Cause of Public Welfare Scientific Research Fund [2012004001]; Shenyang Science and Technology Plan Project [130496]; Liaoning University Foundation of 211 Project for Innovative Talents Training and the Technology Major Projects Research Foundation [2011ZX09102–007-02], China.

Supplementary material

Supplementary X-ray crystallographic data for **1** (CCDC 853,685) and **2** (CCDC 937,463) can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Center, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: (+44) 1223–336-033; or deposit@ccdc.cam.ac.uk).

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