

Syntheses, characterization and crystal structures of Schiff base zinc(II) complexes with antimicrobial activity

Yi-Xin Chen, Shu-Juan Liu,* Xin-Ran Chen, Bin-Hao Ye, Xiao-Yang Qiu*

College of Science and Technology, Ningbo University, Ningbo 315315, P. R. China

* Corresponding author: E-mail: lsj_578@126.com (Shu-Juan Liu),
xiaoyang_qiu@126.com (Xiao-Yang Qiu)

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Abstract

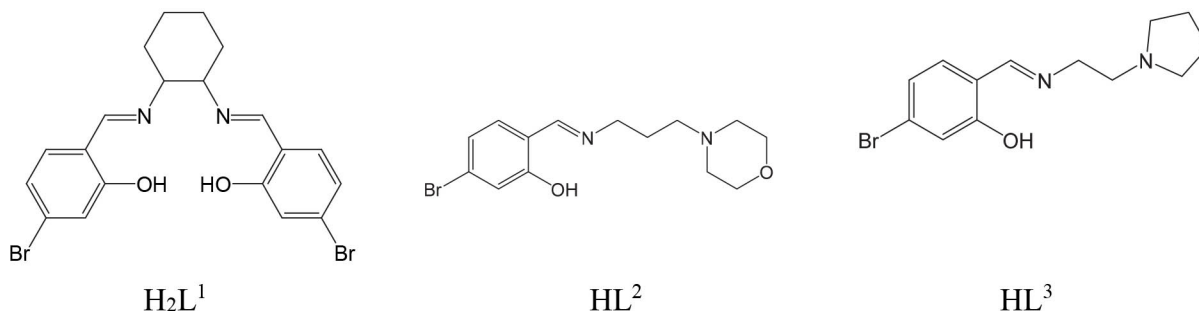
Three new zinc(II) complexes, $[\text{ZnL}^1(\text{CH}_3\text{OH})]$ (**1**), $[\text{ZnBrL}^2]$ (**2**), and $[\text{ZnBr}_2(\text{HL}^3)] \cdot \text{CH}_3\text{OH}$ (**3**· CH_3OH), where L^1 is the dianionic form of N,N' -bis(4-bromosalicylidene)cyclohexane-1,2-diamine (H_2L^1), L^2 is the monoanionic form of 5-bromo-2-(((3-morpholinopropyl)imino)methyl)phenol (HL^2), and HL^3 is the zwitterionic form of 5-bromo-2-(((2-pyrrolidin-1-yl)ethyl)imino)methyl)phenol (HL^3), were facile prepared by reaction of 1:1 molar ratio of the Schiff bases with zinc bromide in methanol. The complexes were characterized by IR and UV-Vis spectroscopy. Detailed structures of the three complexes were confirmed by single crystal X-ray determination. The Zn(II) atom in complex **1** has a square pyramidal coordination, with the Schiff base ligand L^1 coordinated to the Zn(II) atom through phenolate oxygen and imino nitrogen atoms. The Zn(II) atom in complex **2** has a tetrahedral coordination, with the Schiff base ligand L^2 coordinated to the Zn(II) atom through phenolate oxygen, imino nitrogen and morpholine nitrogen atoms. The Zn(II) atom in complex **3**· CH_3OH has a tetrahedral coordination, with the Schiff base ligand L^3 coordinated to the Zn(II) atom through phenolate oxygen and imino nitrogen atoms. The remaining sites are occupied by one methanol oxygen atom for **1**, one Br ligand for **2**, and two Br ligands for **3**· CH_3OH . The compounds show significant antimicrobial activities.

Keywords: Schiff base, zinc(II) complex, crystal structure, antimicrobial activity

1. Introduction

The design and synthesis of metal complexes with biological activities have received great attention in coordination chemistry. Schiff bases are the best choice for their facile synthesis and widely biological activities, as well as in the construction of metal complexes with versatile structures.¹ Zinc complexes with Schiff base ligands are reported to have various biological activities, and are used as excellent alternatives for classic organic type anti-fungal, antibacterial and antitumor agents.² Despite the

large number of metal complexes with antibacterial activities, it is necessary to prepare new zinc complexes with high activity. It has been reported that compounds with electron-withdrawing groups can improve their antimicrobial ability.³ The compounds with chloro, fluoro, iodo and bromo groups have shown remarkable antimicrobial activities.⁴ Recently, we have reported some Schiff base complexes with interesting biological activities.⁵ In pursuit of new Schiff base complexes with potential antimicrobial activity, three new zinc(II) complexes $[\text{ZnL}^1(\text{CH}_3\text{OH})]$ (**1**), $[\text{ZnBrL}^2]$ (**2**), and $[\text{ZnBr}_2(\text{HL}^3)] \cdot \text{CH}_3\text{OH}$ (**3**· CH_3OH),



Scheme 1. The Schiff bases.

where L^1 is the dianionic form of *N,N'*-bis(4-bromosalicylidene)cyclohexane-1,2-diamine (H_2L^1), L^2 is the mono-anionic form of 5-bromo-2-(((3-morpholinopropyl)imino)methyl)phenol (HL^2), and L^3H is the zwitterionic form of 5-bromo-2-(((2-(pyrrolidin-1-yl)ethyl)imino)methyl)phenol (HL^3) (Scheme 1), and their antimicrobial activities are present. The compounds show significant antimicrobial activities.

2. Experimental

2.1. Materials and methods

4-Bromosalicylaldehyde, 1,2-diaminocyclohexane, 4-(3-aminopropyl)morpholine, *N*-(2-aminoethyl)pyrrolidine, and zinc bromide were obtained from Sigma-Aldrich. All other chemicals were commercial obtained from Xiya Chemical Co. Ltd. The Schiff bases were prepared according to the literature method.⁶ Elemental analyses of C, H and N were carried out in a Perkin-Elmer automated model 2400 Series II CHNS/O analyzer. FT-IR spectra were obtained on a Perkin-Elmer 377 FT-IR spectrometer with samples prepared as KBr pellets. UV-Vis spectra were obtained on a Lambda 35 spectrometer. Molar conductivities of the complexes in DMSO solutions (10^{-3} mol L^{-1}) at room temperature were measured using a Systronic model 303 direct reading conductivity meter.

2.2. Synthesis of the complexes

2.2.1. $[ZnL^1(CH_3OH)]$ (1)

H_2L^1 (0.10 mmol, 48 mg) and zinc bromide (0.10 mmol, 23 mg) were mixed in methanol (20 mL). The mixture was stirred at 25 °C for 30 min to give a colorless solution. Block single crystals were formed upon slow evaporation. The crystals were obtained by filtration. Yield: 36 mg (63%). Anal. calc. for $C_{21}H_{22}Br_2N_2O_3Zn$: C, 43.82; H, 3.85; N, 4.87; found: C, 43.63; H, 3.91; N, 4.80%. IR data (cm^{-1}): 1634 ($\nu_{C=N}$), 1586, 1522, 1472, 1449, 1422, 1392, 1352, 1305, 1282, 1245, 1182, 1135, 1068, 1018, 918, 853, 781, 729, 596, 499, 475, 425. UV-Vis data (MeOH, λ_{max} (nm), ϵ ($L\ mol^{-1}\ cm^{-1}$)): 229, 3.13×10^3 ; 246, 3.05×10^3 ; 267, 1.56×10^3 ; 350, 8.91×10^2 . Molar conductance (10^{-3} mol L^{-1} in DMSO): $25\ \Omega^{-1}\ cm^2\ mol^{-1}$.

2.2.2. $[ZnBrL^2]$ (2)

HL^2 (0.10 mmol, 33 mg) and zinc bromide (0.10 mmol, 23 mg) were mixed in methanol (20 mL). The mixture was stirred at 25 °C for 30 min to give a colorless solution. Block single crystals were formed upon slow evaporation. The crystals were obtained by filtration. Yield: 27 mg (57%). Anal. calc. for $C_{14}H_{18}Br_2N_2O_2Zn$: C, 35.66; H, 3.85; N, 5.94; found: C, 35.81; H, 3.93; N, 5.86%. IR data (cm^{-1}): 1639 ($\nu_{C=N}$), 1586, 1519, 1462, 1425, 1392, 1337, 1310, 1287, 1267, 1210, 1177, 1138, 1115, 1095, 1060, 1038,

990, 971, 923, 886, 866, 836, 791, 604, 459. UV-Vis data (MeOH, λ_{max} (nm), ϵ ($L\ mol^{-1}\ cm^{-1}$)): 245, 2.87×10^3 ; 278, 1.33×10^3 ; 365, 6.62×10^2 . Molar conductance (10^{-3} mol L^{-1} in DMSO): $31\ \Omega^{-1}\ cm^2\ mol^{-1}$.

2.2.3. $[ZnBr_2(HL^3)] \cdot CH_3OH$ (3- CH_3OH)

HL^3 (0.10 mmol, 30 mg) and zinc bromide (0.10 mmol, 23 mg) were mixed in methanol (20 mL). The mixture was stirred at 25 °C for 30 min to give a colorless solution. Block single crystals were formed upon slow evaporation. The crystals were obtained by filtration. Yield: 25 mg (45%). Anal. calc. for $C_{14}H_{21}Br_3N_2O_2Zn$: C, 30.33; H, 3.82; N, 5.05; found: C, 30.45; H, 3.76; N, 4.98%. IR data (cm^{-1}): 3440, 1629 ($\nu_{C=N}$), 1585, 1527, 1475, 1460, 1392, 1275, 1192, 1143, 1043, 921, 849, 806, 594, 574, 457. UV-Vis data (MeOH, λ_{max} (nm), ϵ ($L\ mol^{-1}\ cm^{-1}$)): 226, 3.02×10^3 ; 245, 2.98×10^3 ; 276, 1.67×10^3 ; 370, 8.87×10^2 . Molar conductance (10^{-3} mol L^{-1} in DMSO): $36\ \Omega^{-1}\ cm^2\ mol^{-1}$.

2.3. X-ray crystallography

X-ray diffraction was done with a Bruker APEX II CCD area diffractometer equipped with Mo-K α radiation ($\lambda = 0.71073\ \text{\AA}$). The collected data were reduced with SAINT.⁷ Multi-scan absorption correction was performed with SADABS.⁸ Structures of the three zinc complexes were solved by direct method, and refined against F^2 by full-matrix least-squares method with SHELXTL.⁹ All non-hydrogen atoms were refined anisotropically. H3, H6 atoms in complex 1, and H2 and H2A atoms in complex 3- CH_3OH were located from difference Fourier maps and refined isotropically, with O–H and N–H distances restrained to 0.85(1) and 0.90(1) $\text{\AA}$, respectively. The remaining hydrogen atoms were placed in calculated positions and constrained to ride on their parent atoms. The crystallographic data and refinement parameters for the complexes are listed in Table 1.

2.4. Antimicrobial assay

The three zinc(II) complexes were assayed against bacteria strains *Bacillus subtilis*, *Staphylococcus aureus*, *Escherichia coli*, and *Pseudomonas fluorescense* using MH (Mueller-Hinton) medium. The compounds were also assayed against fungi *Candida albicans* and *Aspergillus niger* using RPMI-1640 medium. The MIC values were determined by a colorimetric method using MTT.¹⁰ A stock solution of the compound at concentration of $150\ \mu g\ mL^{-1}$ in DMSO was prepared and graded quantities (75, 37.5, 18.8, 9.4, 4.7, 2.3, 1.2, and $0.59\ \mu g\ mL^{-1}$), which were incorporated in specified quantity of the corresponding sterilized liquid medium. A specified quantity of the medium containing the compound was poured into micro-titration plates. Suspension of the microorganism was prepared to contain 1.0×10^5 cfu mL^{-1} and applied to micro-titration

Table 1. Crystallographic and refinement data for the complexes

Complex	1	2	3-CH ₃ OH
Formula	C ₂₁ H ₂₂ Br ₂ N ₂ O ₃ Zn	C ₁₄ H ₁₈ Br ₂ N ₂ O ₂ Zn	C ₁₄ H ₂₁ Br ₃ N ₂ O ₂ Zn
Formula weight	575.59	471.49	554.43
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> (Å)	10.7614(15)	14.8984(12)	14.9780(13)
<i>b</i> (Å)	14.9279(16)	8.6343(10)	10.4811(9)
<i>c</i> (Å)	15.9556(17)	13.0209(12)	12.5581(11)
α (°)	103.6030(10)	90	90
β (°)	108.4640(10)	100.5950(10)	97.1700(10)
γ (°)	104.5300(10)	90	90
<i>V</i> (Å ³)	2211.0(5)	1646.4(3)	1956.0(3)
<i>Z</i>	4	4	4
<i>D</i> _{calc} (g cm ⁻³)	1.729	1.902	1.883
μ (Mo K α) (mm ⁻¹)	4.749	6.350	7.390
<i>F</i> (000)	1144	928	1080
Measured reflections	11272	8498	9910
Unique reflections	7460	3059	3631
Observed reflections (<i>I</i> ≥ 2 σ (<i>I</i>))	4384	2197	2407
Parameters	531	190	206
Restraints	2	0	2
GOOF	0.980	1.040	0.945
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> ≥ 2 σ (<i>I</i>)] ^a	0.0451, 0.0884	0.0391, 0.0978	0.0396, 0.1000
<i>R</i> ₁ , <i>wR</i> ₂ (all data) ^a	0.0987, 0.1049	0.0643, 0.1111	0.0726, 0.1188

$$^a R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|, wR_2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$$

plates with serially diluted compounds in DMSO to be tested and incubated at 37 °C for 24 h and 48 h for bacteria and fungi, respectively. Then the MIC values were visually determined on each of the microtitration plates, 50 μ L of PBS (phosphate buffered saline 0.01 mol L⁻¹, pH = 7.4) containing 2 mg of MTT mL⁻¹ was added to each well. Incubation was continued at room temperature for 4–5 h. The content of each well was removed and 100 μ L solution of 95% isopropanol and 1 mol L⁻¹ 5% HCl was added to extract the dye. After 12 h of incubation at room temperature, the optical density was measured with a microplate reader at 550 nm.

3. Results and Discussion

3.1. Synthesis and characterization

The three zinc(II) complexes were facile prepared by reaction of the Schiff base ligands with zinc bromide in 1:1 molar ratio in methanol (Scheme 2). Single crystals of the three complexes were obtained from their methanolic solution. Elemental analyses of the complexes are in accordance with their molecular structures determined by single crystal X-ray analysis.

3.2. Spectroscopic studies

The intense absorptions at 1629–1639 cm⁻¹ for the complexes are generated by the vibrations of the C=N

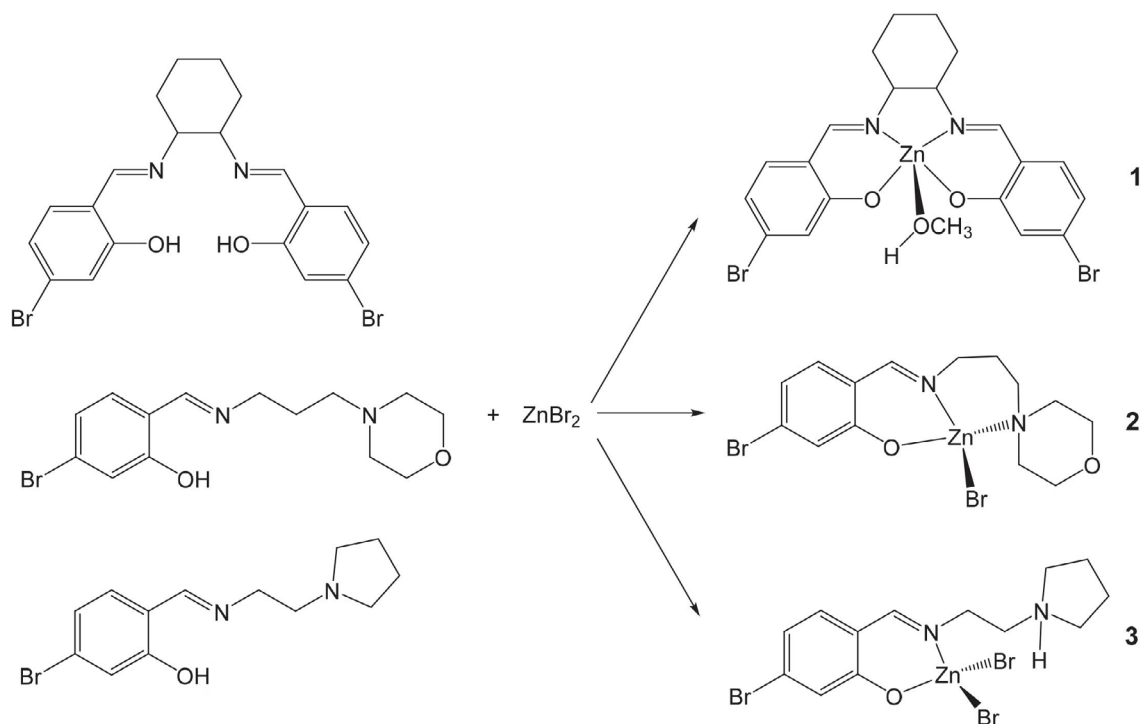
bonds of the Schiff base ligands which are formed from the condensation reaction of 4-bromosalicylaldehyde with 1,2-diaminocyclohexane, 4-(3-aminopropyl)morpholine, and *N*-(2-aminoethyl)pyrrolidine, respectively.¹¹

In the electronic spectra of the three complexes, the bands at 350–370 nm are attributed to azomethine chromophore $\pi \rightarrow \pi^*$ transition.¹² The bands at higher energies (220–230 and 240–280 nm) are associated with benzene $\pi \rightarrow \pi^*$ transition.¹²

3.3. Structure description of the complexes

3.3.1. [ZnL¹(CH₃OH)] (1)

The bond lengths and angles related to the Zn(II) atoms for the compound are listed in Table 2. Molecular structure of the compound is shown in Figure 1. There are two independent molecules which are linked by hydrogen bonds (Table 3) in the compound. The Zn(II) atom in each molecule is in square pyramidal coordination, with the basal plane defined by the two phenolate oxygens and two imino nitrogens of the Schiff base ligand, and with the apical position occupied by the methanol oxygen. The definition of the square pyramidal coordination is based on index factor τ of 0.25 for Zn1 and 0.38 for Zn2.¹³ The Schiff base ligand L¹ acts as a tetradentate ligand, chelating the Zn(II) atom by generating one five and two six-membered rings with bite angles of 79.65(16)°, 89.80(16)° and 88.93(14)° for Zn1 molecule, and 79.77(18)°, 89.96(16)° and 88.89(16)° for Zn2 molecule. The *cis* and *trans* bond



Scheme 2. The synthetic procedure for the complexes.

angles in the basal planes are 79.65(16)–96.24(14)° and 150.51(18)–165.80(16)° for Zn1 molecule, and 79.77(18)–95.33(15)° and 143.93(18)–166.75(16)° for Zn2 molecule. The bond angles among the apical and basal donor atoms are 93.59(14)–108.81(17)° for Zn1 molecule, and 93.06(15)–113.30(16)° for Zn2 molecule. Thus, the coordination geometries of both molecules are deviated from ideal square pyramid. The coordinate bond lengths and

Table 2. Selected bond distances (Å) and angles (°) for the complexes

1			
Zn1–O1	1.960(4)	Zn1–O2	1.995(3)
Zn1–N1	2.078(4)	Zn1–O3	2.079(4)
Zn1–N2	2.088(4)	Zn2–O4	1.958(4)
Zn2–O5	1.981(3)	Zn2–N3	2.053(4)
Zn2–O6	2.064(4)	Zn2–N4	2.102(4)
O1–Zn1–O2	96.24(14)	O1–Zn1–N1	89.80(16)
O2–Zn1–N1	165.80(16)	O1–Zn1–O3	99.85(17)
O2–Zn1–O3	93.59(14)	N1–Zn1–O3	98.03(16)
O1–Zn1–N2	150.51(18)	O2–Zn1–N2	88.93(14)
N1–Zn1–N2	79.65(16)	O3–Zn1–N2	108.81(17)
O4–Zn2–O5	95.33(15)	O4–Zn2–N3	89.96(16)
O5–Zn2–N3	166.75(16)	O4–Zn2–O6	102.25(16)
O5–Zn2–O6	93.06(15)	N3–Zn2–O6	97.69(16)
O4–Zn2–N4	143.93(18)	O5–Zn2–N4	88.89(16)
N3–Zn2–N4	79.77(18)	O6–Zn2–N4	113.30(16)
2			
Zn1–O1	1.905(3)	Zn1–N1	1.983(4)
Zn1–N2	2.103(4)	Zn1–Br2	2.3512(9)
O1–Zn1–N1	96.49(16)	O1–Zn1–N2	122.74(16)
N1–Zn1–N2	94.52(17)	O1–Zn1–Br2	114.39(12)
N1–Zn1–Br2	119.54(12)	N2–Zn1–Br2	107.85(11)
3·CH₃OH			
Zn1–O1	1.935(3)	Zn1–N1	2.014(4)
Zn1–Br2	2.3605(8)	Zn1–Br3	2.3436(8)
O1–Zn1–N1	94.24(16)	O1–Zn1–Br3	113.67(11)
N1–Zn1–Br3	108.28(12)	O1–Zn1–Br2	109.35(12)
N1–Zn1–Br2	114.92(12)	Br3–Zn1–Br2	114.73(3)

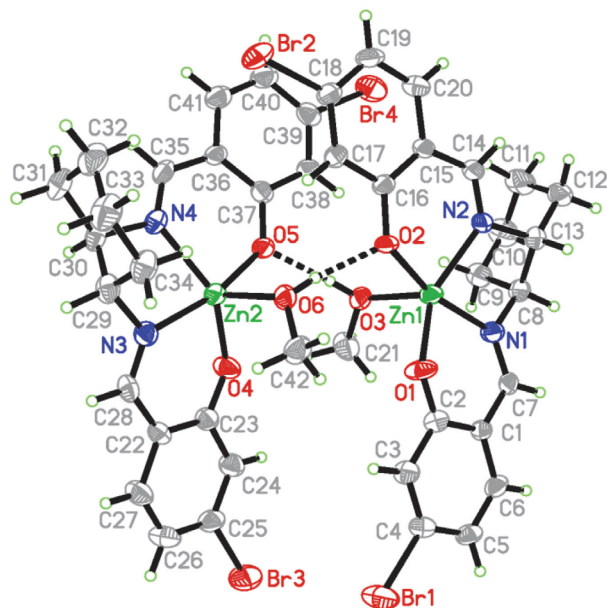


Figure 1. A perspective view of complex 1 with the atom labeling scheme. Thermal ellipsoids are drawn at the 30% probability level. Hydrogen bonds are drawn as dashed lines.

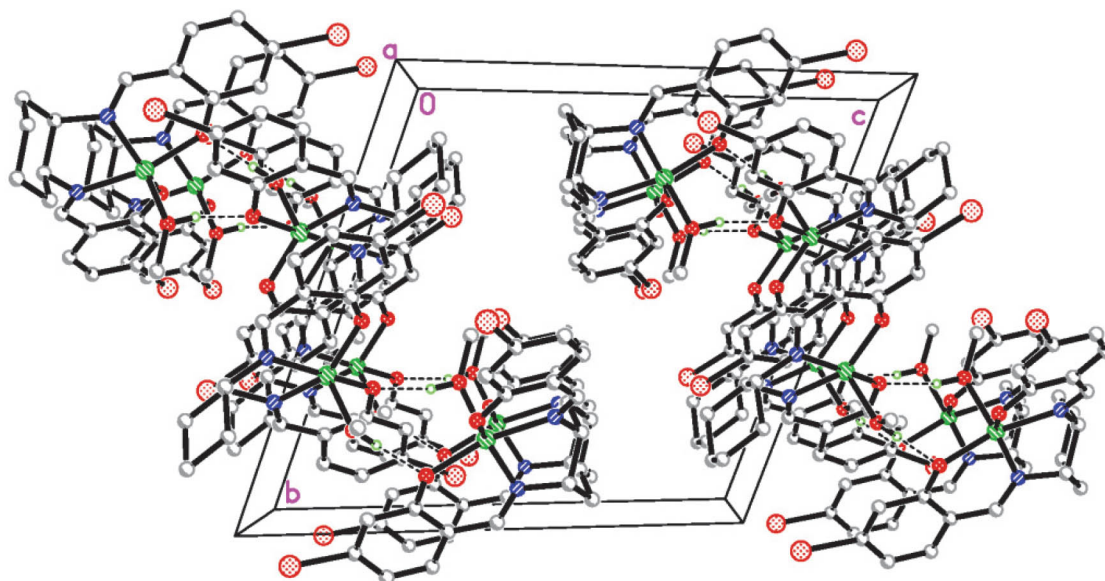


Figure 2. The crystal structure of complex 1, viewed along the *a* axis. Hydrogen bonds are drawn as dashed lines.

angles in both molecules are similar to each other, and are comparable to those in reported Schiff base zinc(II) complexes.¹⁴

In the crystal structure of the complex, two adjacent molecules are linked by two O–H...O hydrogen bonds (Table 3) to form a dimer. The dimers are stack along *a* axis with no obvious short contact (Figure 2).

Table 3. Hydrogen bond distances (Å) and angles (°) for complexes 1 and 3·CH₃OH

<i>D</i> –H... <i>A</i>	<i>d</i> (D–H)	<i>d</i> (H... <i>A</i>)	<i>d</i> (D... <i>A</i>)	Angle (D–H... <i>A</i>)
1				
O3–H3...O5	0.85(1)	1.774(12)	2.622(4)	177(7)
O6–H6...O2	0.85(1)	1.767(19)	2.600(4)	166(7)
3·CH₃OH				
N2–H2A...N1	0.90(1)	2.59(7)	3.013(6)	110(6)
N2–H2A...O2	0.90(1)	1.93(3)	2.767(6)	154(7)
O2–H2...O1 ⁱ	0.85(1)	1.83(2)	2.668(5)	166(9)

Symmetry code for *i*: *x*, ½ – *y*, –½ + *z*.

3.3.2. [ZnBrL²] (2)

The bond lengths and angles related to the Zn(II) atom for the compound are listed in Table 2. Molecular structure of the compound is shown in Figure 3. The Zn(II) atom is coordinated by one phenolate oxygen, one imino nitrogen and one morpholine nitrogen atoms of the Schiff base ligand L², and one Br ligand, forming a tetrahedral coordination. The Schiff base ligand L² acts as a tri-

dentate ligand, chelating the Zn(II) atom by generating one two six-membered rings with bite angles of 96.49(16)° and 94.52(17)°. The bond angles are 94.52(17)–122.74(16)°, indicating the tetrahedral coordination is slightly distorted from ideal model. The τ_4 value is 0.83, which proves the tetrahedral coordination.¹⁵ The coordinate bond lengths and angles in the complex are comparable to those in reported Schiff base zinc(II) complexes.¹⁶

In the crystal structure of the complex, the complex molecules are stack along *b* axis with no obvious short contact (Figure 4).

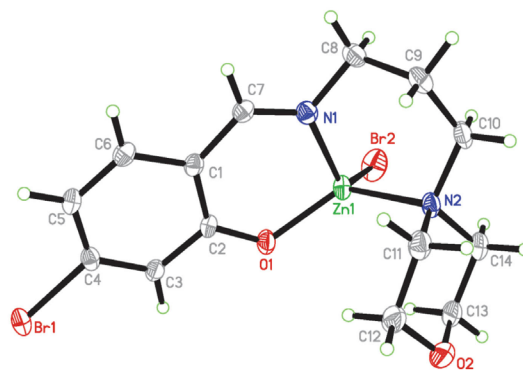


Figure 3. A perspective view of complex 2 with the atom labeling scheme. Thermal ellipsoids are drawn at the 30% probability level.

3.3.3. [ZnBr₂(L³H)]·CH₃OH (3·CH₃OH)

The bond lengths and angles related to the Zn(II) atom for the compound are listed in Table 2. Molecular structure of the compound is shown in Figure 5. The compound contains a [ZnBr₂(L³H)] molecule and a methanol

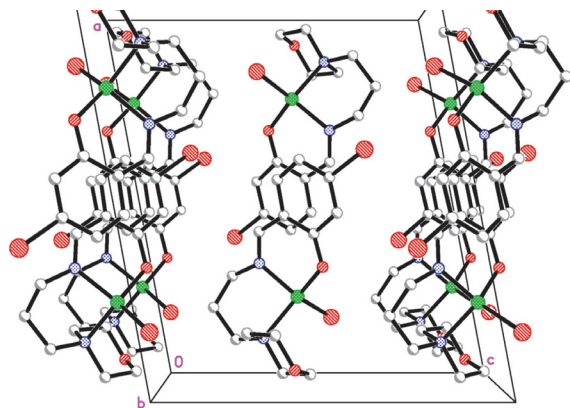


Figure 4. The crystal structure of complex 2, viewed along the *b* axis.

molecule of crystallization. The Zn(II) atom is coordinated by one phenolate oxygen and one imino nitrogen of the Schiff base ligand L^3H , and two Br ligands, forming a tetrahedral coordination. The Schiff base ligand, in a zwitterionic form, acts as a bidentate ligand, chelating the Zn(II) atom by generating one five-membered ring with bite angle of $94.24(16)^\circ$. The bond angles are $94.24(16)$ – $114.92(12)^\circ$, indicating slight distortion of the coordination from ideal tetrahedral geometry. The τ_4 value is 0.92, which proves the tetrahedral coordination.¹⁵ The coordinate bond lengths and angles are comparable to those in reported Schiff base zinc(II) complexes.¹⁷

In the crystal structure of the compound, the complex molecules are linked by methanol molecules through O–H...O and N–H...O hydrogen bonds (Table 3), to form chains running along *a* axis (Figure 6).

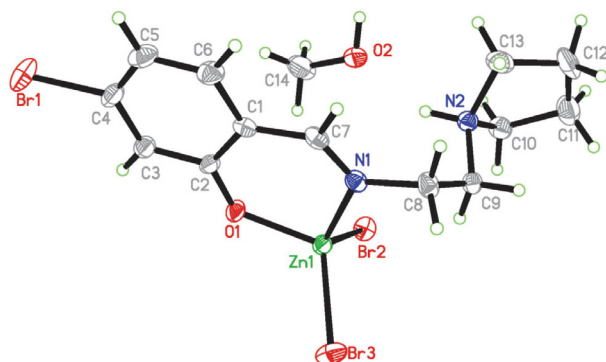


Figure 5. A perspective view of complex 3-CH₃OH with the atom labeling scheme. Thermal ellipsoids are drawn at the 30% probability level.

3.4. Antimicrobial activity

The compounds and related starting materials were assayed for antibacterial activities against Gram-positive bacterial strains *Bacillus subtilis* and *Staphylococcus aureus*, and Gram-negative bacterial strains *Escherichia coli* and *Pseudomonas fluorescens* by MTT method. The MIC

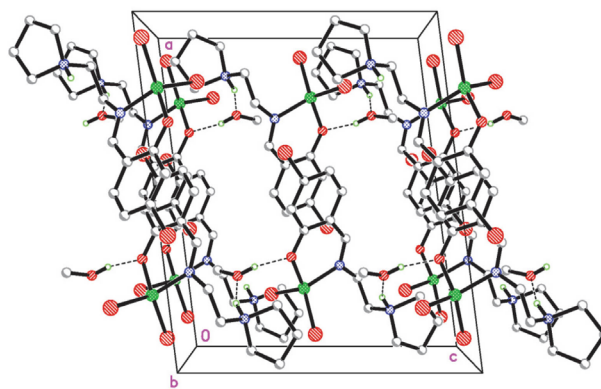


Figure 6. The crystal structure of complex 3-CH₃OH, viewed along the *b* axis. Hydrogen bonds are drawn as dashed lines.

(minimum inhibitory concentration, $\mu\text{g mL}^{-1}$) values against the bacteria are summarized in Table 4. Penicillin G was used as a reference. The three zinc(II) complexes have better activities against all the bacteria strains than the free Schiff bases and zinc bromide. Complexes 1 and 2 show strong activity against *B. subtilis*, *S. aureus* and *E. coli*, while medium activity against *P. fluorescens*. Complex 3 shows strong activities against all the bacteria strains. The three complexes have similar or stronger activity against all the bacteria than Penicillin G. Complex 3 has the most effective activity against *B. subtilis*, *S. aureus*, *E. coli* and *P. fluorescens*, with MICs of 1.2, 0.59, 1.2 and 4.7 $\mu\text{g mL}^{-1}$. However, the three complexes have no activity on the fungal strains *Candida albicans* and *Aspergillus niger*. The complexes have similar antimicrobial activities with the zinc complexes derived from 5-bromo-2-(((2-piperazin-1-yl)ethyl)imino)methyl)phenol,¹⁸ and higher activities than the nickel complexes with Schiff base ligands.¹⁹

Table 4. Antibacterial activities of the assayed compounds (MIC, $\mu\text{g mL}^{-1}$)

Tested material	<i>B. subtilis</i>	<i>S. aureus</i>	<i>E. coli</i>	<i>P. fluorescens</i>
1	4.7	4.7	9.4	18.8
2	2.3	2.3	4.7	18.8
3	.2	0.59	1.2	4.7
H ₂ L ¹	18.8	37.5	75	> 150
HL ²	9.4	18.8	37.5	> 150
HL ³	9.4	37.5	37.5	> 150
ZnBr ₂	18.8	18.8	75	> 150
Penicillin G	2.3	4.7	>150	> 150

4. Conclusion

In this paper, three new zinc(II) complexes were synthesized from the Schiff bases *N,N'*-bis(4-bromosalicylidene)cyclohexane-1,2-diamine, 5-bromo-2-(((3-morpholinopropyl)imino)methyl)phenol and 5-bromo-2-(((2-

(pyrrolidin-1-yl)ethyl)imino)methyl)phenol with zinc bromide in methanol. The complexes were characterized by physico-chemical methods. X-ray single crystal structure determination indicates that the Zn(II) atoms in the complexes are in square pyramidal and tetrahedral coordination. The complexes have potential activities against bacteria *B. subtilis*, *S. aureus*, *E. coli* and *P. fluorescens*, which deserves further study.

Acknowledgments

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Supplementary Data

CCDC 2519457 (1), 2519458 (2) and 2519459 (3) contain the supplementary crystallographic data for the compounds. 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 e-mail: deposit@ccdc.cam.ac.uk.

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Povzetek

Tri nove cinkove(II) komplekse $[\text{ZnL}^1(\text{CH}_3\text{OH})]$ (**1**), $[\text{ZnBrL}^2]$ (**2**), and $[\text{ZnBr}_2(\text{HL}^3)] \cdot \text{CH}_3\text{OH}$ (**3**· CH_3OH), kjer je L^1 dianionska oblika N,N' -bis(4-bromosaliciliden)cikloheksan-1,2-diamina (H_2L^1), L^2 je monoanionska oblika 5-bromo-2-(((3-morfolinopropil)imino)metil)fenola (HL^2), in HL^3 je zwitterionska oblika 5-bromo-2-(((2-(pirolidin-1-il)etil)imino)metil)fenola (HL^3), smo sintetizirali z reakcijo Schiffovih baz z bromidom cinka v metanolu v molskem razmerju 1:1. Kompleksi so bili okarakterizirani z IR in UV-Vis spektroskopijo. Strukture treh kompleksov so bile potrjene z rentgensko monokristalno analizo. Atom Zn(II) v kompleksu **1** ima kvadratno piramidalno koordinacijo, pri čemer se ligand Schiffove baze L^1 koordinira na Zn(II) preko fenolatnih kisikovih in imino dušikovih atomov. Atom Zn(II) v kompleksu **2** ima tetraedrično koordinacijo, pri čemer se ligand Schiffove baze L^2 koordinira na Zn(II) preko fenolatnega kisikovega, imino dušikovega in morfolinskega dušikovega atoma. Atom Zn(II) v kompleksu **3**· CH_3OH ima tetraedrično koordinacijo, pri čemer se ligand Schiffove baze HL^3 koordinira na Zn(II) preko fenolatnega kisikovega in imino dušikovega atoma. Preostala mesta zasedajo en metanolov kisikov atom pri **1**, en Br ligand pri **2** in dva Br liganda pri **3**· CH_3OH . Spojine kažejo znatno protimikrobno delovanje.



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