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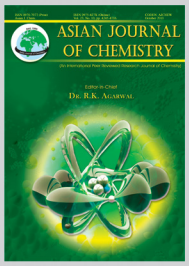

Ternary Zinc(II) Complex with 2-Amino Benzothiazole and Phenoxyacetic Acid: Synthesis, Crystal Structure and Antimicrobial Activity

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A novel ternary complex of $Zn(pa)_2(aben)_2$ (pa = phenoxyacetic acid anion, aben = 2-amino benzothiazole) was synthesized by the reaction of zinc chloride, 2-amino benzothiazole and phenoxyacetic acid. Elemental analysis, IR, ^1H NMR, ^{13}C NMR and X-ray single-crystal diffraction were carried out to determine the composition and crystal structure. The complex crystallizes in the monoclinic system, space group C2/c with a = 26.8731(5), b = 30.1325(8), c = 14.9696(4) Å, β = 91.045(2)°, $C_{30}H_{26}O_6N_4S_2Zn$, M_r = 668.04, V = 12119.7(5) Å^3, T = 296(2), Z = 16, D_c = 1.464 mg/mm^3, μ(Mo Ka) = 0.998 mm^{-1}, F(000) = 5504, 26154 reflections measured, 12378 unique (R_{int} = 0.0196) which were used in all calculations. The final w$R(F_2)$ was 0.0869 (all data). The Zn(II) atom is four-coordinated with two carboxylate oxygen atoms of the two phenoxyacetic acid and two nitrogen atoms in thiazole rings of the two 2-amino benzothiazole. The analysis of crystal structure shows that there are intermolecular and intramolecular hydrogen bonding between amino-nitrogen atoms of the two 2-amino benzothiazole and carboxylate-oxygen and ether-oxygen atoms of the two phenoxyacetic acid. The antimicrobial properties of the title complex and the ligands i.e., phenoxyacetic acid and 2-amino benzothiazole were tested against representative bacterial and fungal strains. Results show that it exhibits excellent inhibitory effect against the tested bacteria, yeasts and moulds, which is better than that of its two free ligands.

Key Words: Benzothiazole, Phenoxyacetic acid, Ternary zinc complex, Crystal structure, Antimicrobial activity.

INTRODUCTION

Due to the increasing microbial resistance, the development of novel and powerful antimicrobial compounds is strongly required in many fields such as medicine, agricultural chemicals, cosmetic, paint, leather, textile, *etc.* The purpose of present research program is to synthesize new compounds bearing different active structures, evaluate *in vitro* their antimicrobial activities and estimate their potential as a leather antimicrobial agent.

In general, benzothiazole derivatives have diverse biological activities such as antimicrobial, antiviral, anticancer and other different inhibitory activities[1-8]. They are widely used in medical and industrial fields. For example, in leather industry, 2-(thiocyanomethylthio)benzothiazole (TCMTB) is the commonest fungicide used to inhibit the growth of moulds on tanned leather [9,10]. Similarly, phenoxyacetic acid derivatives were reported to possess a number of biological activities and they are often used to produce bactericides, insecticides, herbicides, plant growth regulator, *etc.*[11-15]. So, compounds with these two active structures may improved antimicrobial activities. In this study, considering the antimicrobial property and coordinate action with carboxyl and benzothiazole[4,6,14,16-18], zinc chloride was chosen to react with 2-amino benzothiazole and phenoxyacetic acid for the preparation of a novel compound with the above two active moieties. Elemental analysis, IR, ^1H NMR, ^{13}C NMR and X-ray single-crystal diffraction were used to characterize its structure, furthermore, the antimicrobial activities of the ternary zinc complex and its original compounds were compared by determining the minimum inhibitory concentrations.

EXPERIMENTAL

All the reagents used in this experimental were research grade. Elemental analyses (C, H, N) were performed on a Carlo-Erba 1106 analyser and zinc ion content was determined at a ICP-AES (Optima 2100DV, PERKIN ELMER, USA). Infrared spectra were obtained on a FT-IR spectrophotometer (MAGNA.IR506, Nicolet Ltd., USA) by using KBr disk in the range 4000-400 cm^{-1}. Measurement of the crystal was carried out on a CCD X-ray single crystal diffractometer (Xcalibur, Eos, Britain). ^1H NMR and ^{13}C NMR spectra were recorded on a Bruker Avance 600 instrument in deuterated dimethyl sulfoxide solutions. Chemical shifts were reported as δ (ppm) relative to TMS as internal standard.

Synthesis of the title complex: Phenoxyacetic acid (0.152 g, 0.001 mol) and 2-amino benzothiazole (0.150 g, 0.001 mol)

TABLE-1
CRYSTAL DATA AND STRUCTURE REFINEMENT FOR THE Zn(II) COMPLEX

Empirical formula	$C_{30}H_{26}O_6N_4S_2Zn$	Crystal size (mm^3)	0.36 × 0.28 × 0.21
Formula weight	668.04	θ range for data collection (º)	3.03–26.37
Temperature (K)	296(2)	Index ranges	$-31 \le h \le 33$, $-37 \le k \le 35$, $-12 \le l \le 18$
Wavelength (Å)	0.7107	Reflections collected	26154
Crystal system	Monoclinic	Independent reflections (R_{int})	12378 (0.0196)
Space group	C2/c	Observed reflections	7161
a (Å)	26.8731(5)	Absorption correction	multi-scan
b (Å)	30.1325(8)	Max. and min. transmission	1.0 and 0.93622
c (Å)	14.9696(4)	Refinement method	Full-matrix least-squares on F^2
β (º)	91.045(2)	Data/restraints/parameters	12378/0/775
Volume ($Å^3$)	12119.7(5)	Goodness-of-fit on F^2	1.010
Z	16	Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0376$, $wR_2 = 0.0806$
D_c (mg mm^{-3})	1.464	R indices (all data)	$R_1 = 0.0783$, $wR_2 = 0.0869$
F (000)	5504	Largest diff. peak and hole (e $Å^{-3}$)	0.496 and -0.203
μ (mm^{-1})	0.998		

were dissolved in 40 mL distilled water at 50 ºC and the pH value was adjusted to about 6 using 0.5 mol/L NaOH solution. Then, 15 mL water solution of zinc chloride (0.0682g, 0.0005 mol) was slowly added to the above stirred solution within 10 minutes. The solution was stirred at 50 ºC for 1 h and a white powdered solid was obtained after cooling. After filtration, the filtered solution was placed at room temperature and white crystals were obtained over several weeks. The total yield is 68.3 %. Anal. calcd. (%) for $C_{30}H_{26}O_6N_4S_2Zn$: C, 53.93; H, 3.92; N, 8.39; Zn, 9.79. Found (%): C, 53.83; H, 3.98; N, 8.44; Zn, 9.86. Slected IR data (KBr, ν_{max}, cm^{-1}): 3396.91, 3344.52 (m, H-NH), 3065.65, 2917.82(s, H-CH), 1623.40 (s, thiazole C=N), 1654.39, 1591.13, 1530.02, 1511.51, 1453.43 (m, benzene C=C), 1235.61, 1067.51 (m, Ar-O-C), 817.64 (vs, Ar-H (*para*)) and 753.17 (vs, Ar-H (*ortho*)). ^{1}H NMR (DMSO-d_6, 292.2 K, ppm): 7.658, 7.645 (d, 1H,), 7.557 (s, 2H,), 7.351, 7.338 (d, 1H), 7.254, 7.240, 7.227 (t, 2H), 7.218, 7.205, 7.192 (t, 1H), 7.022, 7.010, 6.997 (t, 1H), 6.906, 6.894, 6.882 (t, 1H), 6.859, 6.846 (d, 2H), 4.438 (s, 2H, -OCH_2-). ^{13}C NMR (DMSO-d_6, 295.7 K, ppm): 173.56, 168.05, 158.71, 152.07, 130.50, 129.71, 126.08, 121.65, 121.51, 120.81, 118.02, 114.90, 66.46 (-OCH_2-).

Crystal structure determination: A single crystal of the title compound with dimensions of 0.36 mm × 0.28 mm × 0.21 mm was mounted on a glass fiber. X-ray diffraction intensity data were collected on a Xcalibur, Eos diffractometer equipped with a graphite-monochromated MoKa (λ = 0.7107 Å) radiation by using the ω-2θ scan technique at 296(2) K. In the range of $3.03º \le \theta \le 26.37º$ ($-31 \le h \le 33$, $-37 \le k \le 35$, $-12 \le l \le 18$), a total of 26154 reflections were collected, of which 12378 are independent ($R_{int} = 0.0196$) and 7161 were observed with [$I > 2\sigma(I)$] and used in the succeeding structure calculations. The Multi-scan/CrysAlisPro, Oxford Diffraction Ltd., was used for the data reduction and absorption correction[19]. The structure was solved by direct methods using SHELXS-97 and refined by full matrix least squares methods for all the non-hydrogen atoms[20]. The hydrogen atoms of amino groups that were located in a difference Fourier map were limitedly refined with isotropic temperature factors and the other hydrogen atoms that were added in their calculated position were refined using a riding model[20]. The final cycle of refinement gave R = 0.0376, wR = 0.0806 ($\omega = 1/[s^2(Fo)^2 + (0.0402 P)^2 + 0.0000 P]$, where $P = (Fo^2 + 2Fc^2)/3$), S = 1.010, $(\Delta/\sigma)_{max} = 0.001$, $(\Delta\rho)_{max} = 0.496$ and $(\Delta\rho)_{min} = -0.203$ e/$Å^3$. A summary of the crystal data and structure refinement parameters for the Zn(II) complex are given in Table-1.

Antimicrobial activity determination: The evaluation of the inhibitory effect of the Zn(II) complex and its two free ligands (phenoxyacetic acid and 2-amino benzothiazole) on the bacterial and fungal growth was carried out by the two-fold serial dilution method[21]. The following test microorganisms were used: *Escherichia coli, Staphylococcus aureus, Bacillus subtilis, Stenotrophomonas maltophilia, Bacillus cereus strain* G8639, *Enterobacter hormaechei, Acinetobacter sp*. ANT9054, *Bacillus fusiformis strain* SW-B9, *Klebsiella sp. strain zlmy* and *Bacillus sphaericus* (bacteria), *Candida albicans, Rhodotorula mucilaginosa* and *Cryptococcus albidosimilis* (yeasts), *Penicillium citrinum, Aspergillus niger*, *Aspergillus flavus*, *Trichoderma viride*, *Chaetomium globasum* and *Rhizopus stolonifer* (moulds). Nutrient Agar and potato medium (PDA) were employed as culture media for bacteria and fungi, respectively. The compounds were dissolved in dimethyl sulfoxide and tested at concentrations ranging from 0.01 to 100 μg/mL. Test inoculum of 5×10^4 bacteria/ mL and 10^3 yeasts or spores/mL was applied. The criterion of effectiveness was taken in the absence of microbial growth after an incubation period of 24 h at 37 ºC for bacteria or of 48 h at 30 ºC for fungi. In every case, the lowest concentration (μg/mL) of compound, which inhibits the growth of bacteria after 24 h incubation at 37 ºC and of fungi after 48 h incubation at 30 ºC was taken as the minimum inhibitory concentration (MIC). The concentration of DMSO in the medium did not affect the growth of any of the microorganisms tested. All experiments were made in duplicate and the results were confirmed in three independent experiments.

RESULTS AND DISCUSSION

IR spectrum: For the sake of comparison, the IR spectra of the both ligands were also recorded with KBr pellets in the 4000-400 cm^{-1} region. The main IR data of phenoxyacetic acid is 3446 (m, O-H), 3037, 2919, (s, HC-H), 1734, 1702 (s, C=O), 1597, 1584, 1499, 1487, 1439 (m, benzene C=C), 1234, 1095 (m, Ar-O-C), 755 (vs) and 689 (s, mono substituted Ar-H). The main IR data of 2-amino benzothiazole is 3396, 3273 (m,

TABLE-2
SELECTED BOND LENGTHS (Å) AND ANGLES (º) FOR THE TITLE COMPLEX

Bond	Dist.	Bond	Dist.	Bond	Dist.
Zn1-O1	1.9281(17)	Zn2-N5	2.016(2)	O5-C9	1.225(3)
Zn1-O4	1.9222(18)	Zn2-N7	2.0172(18)	O7-C31	1.268(3)
Zn1-N1	2.0409(18)	O1-C1	1.255(3)	O8-C31	1.226(3)
Zn1-N3	2.0320(18)	O2-C1	1.222(3)	O10-C39	1.268(3)
Zn2-O7	1.9230(18)	O4-C9	1.267(3)	O11-C39	1.215(3)
Zn2-O10	1.9228(16)				
Angle	(°)	Angle	(°)	Angle	(°)
O1-Zn1-N1	96.59(7)	O7-Zn2-O10	118.26(8)	C24-N3-Zn1	126.35(17)
O1-Zn1-N3	113.94(8)	O10-Zn2-N5	113.60(8)	C25-N3-Zn1	122.44(15)
O1-Zn1-O4	121.96(9)	O10-Zn2-N7	100.63(7)	C31-O7-Zn2	124.99(16)
O4-Zn1-N1	116.22(8)	N5-Zn2-N7	108.74(8)	C39-O10-Zn2	127.98(15)
O4-Zn1-N3	96.66(7)	C1-O1-Zn1	125.46(17)	C33-N5-Zn2	125.3(2)
N1-Zn1-N3	112.45(8)	C9-O4-Zn1	129.78(16)	C56-N5-Zn2	123.21(16)
O7-Zn2-N5	100.64(8)	C17-N1-Zn1	126.45(17)	C47-N7-Zn2	126.61(17)
O7-Zn2-N7	115.20(8)	C23-N1-Zn1	121.92(14)	C49-N7-Zn2	122.47(15)

Symmetry transformations used to generate equivalent atoms: #1 –x + 1, -y, -z + 1

TABLE-3
SELECTED TORSION LENGTHS (Å) FOR THE TITLE COMPLEX

Angle	(°)	Angle	(°)	Angle	(°)
Zn1-O1-C1-O2	-1.5(4)	Zn2-N5-C56-C55	-179.08(18)	N1-Zn1-O1-C1	-172.7(2)
Zn1-O1-C1-C2	179.87(17)	Zn2-N5-C56-C57	-0.5(4)	N1-Zn1-O4-C9	73.7(2)
Zn1-O4-C9-O5	-7.9(4)	Zn2-N7-C47-S4	177.99(12)	N1-Zn1-N3-C24	145.19(19)
Zn1-O4-C9-C10	172.34(15)	Zn2-N7-C47-N8	-3.4(4)	N3-Zn1-O1-C1	69.2(2)
Zn1-N1-C17-S1	172.93(11)	Zn2-N7-C49-C48	179.84(18)	N3-Zn1-O4-C9	-167.2(2)
Zn1-N1-C17-N2	-9.1(4)	Zn2-N7-C49-C50	1.8(4)	N3-Zn1-N1-C17	134.3(2)
Zn1-N1-C23-C18	-172.71(17)	O1-Zn1-O4-C9	-43.6(2)	N5-Zn2-O7-C31	-162.7(2)
Zn1-N1-C23-C22	6.2(3)	O1-Zn1-N1-C17	15.0(2)	N5-Zn2-O10-C39	76.5(2)
Zn1-N3-C24-S2	170.91(11)	O1-Zn1-N3-C24	-106.2(2)	N5-Zn2-N7-C47	127.9(2)
Zn1-N3-C24-N4	-8.9(4)	O4-Zn1-O1-C1	-46.1(2)	N7-Zn2-O7-C31	80.6(2)
Zn1-N3-C25-C26	-171.43(16)	O4-Zn1-N1-C17	-115.6(2)	N7-Zn2-O10-C39	-167.5(2)
Zn1-N3-C25-C30	9.7(3)	O4-Zn1-N3-C24	23.2(2)	N7-Zn2-N5-C33	124.9(2)
Zn2-O7-C31-O8	-9.9(4)	O7-Zn2-O10-C39	-41.2(2)	S3-C55-C56-N5	1.2(3)
Zn2-O7-C31-C32	171.93(15)	O7-Zn2-N5-C33	3.5(2)	C33-S3-C55-C56	-1.2(2)
Zn2-O10-C39-O11	-6.7(4)	O7-Zn2-N7-C47	-120.1(2)	S4-C48-C49-N7	2.4(3)
Zn2-O1-C39-C40	172.16(18)	O10-Zn2-O7-C31	-38.4(2)	C47-S4-C48-C49	-2.7(2)
Zn2-N5-C33-S3	178.11(12)	O10-Zn2-N5-C33	-124.0(2)		
Zn2-N5-C33-N6	-3.4(4)	O10-Zn2-N7-C47	8.3(2)		

H-N-H), 1644 (s, thiazole C=N), 1589, 1528, 1446 (m, benzene C=C) and 741 (vs, Ar-H (*ortho*)) cm^{-1}. IR spectrum of the zinc complex shows characteristic absorption peaks of amino group ($-NH_2$) at 3396 and 3344 cm^{-1}, similar to those of 2-amino benzothiazole. Therefore, it can be inferred that there is no coordination between the zinc ion and nitrogen atom of amino group in the molecule of the zinc complex. But, for the characteristic absorption peaks of ν(C=N) in the benzothiazole ring, the complex and 2-amino benzothiazole have different wave numbers of 1623 and 1644 cm^{-1}, respectively. The shift should be attributed to the coordination between the zinc ion and the nitrogen atom of thiazole ring. The characteristic absorption peaks of carboxyl group (-COOH) in phenoxyacetic acid at 3446, 1734 and 1702 cm^{-1} are disappeared in the IR spectrum of the Zn(II) complex, indicating that the zinc ion coordinates to carboxyl anion ($-COO^-$) of phenoxyacetic acid. And for the antisymmetric and symmetric vibration absorption of (C-O-C) bands, there is no obvious shift in the spectra of the complex and phenoxyacetic acid, so, no coordination exists between the oxygen atom of (C-O-C) group and Zn(II) atom.

Crystal structure: The crystal structure and crystal group accumulate chart of the complex are shown in Figs. 1 and 2, respectively. The selected bond lengths and bond angles are listed in Table-2. The data in Table-3 are selected torsion angles for the complex. The intermolecular and intramolecular hydrogen bonds are listed in Table-4.

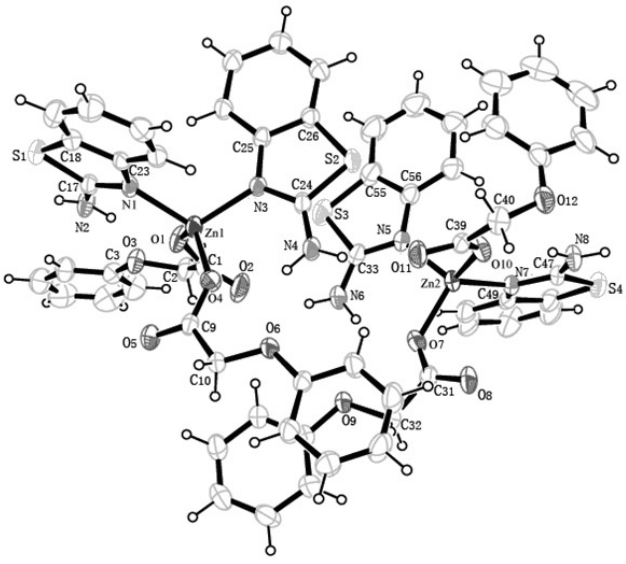

Fig. 1. Molecular structure of the Zn(II) complex

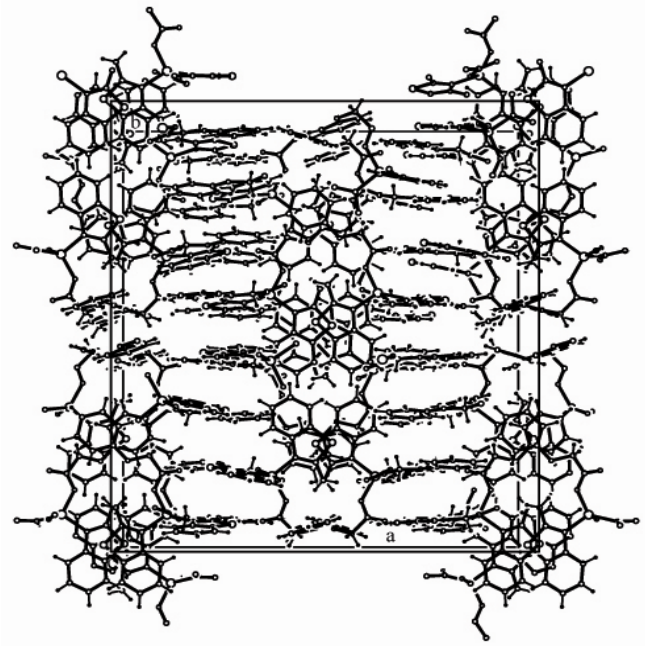

Fig. 2. Crystal packing diagram of the Zn(II) complex

TABLE-4
HYDROGEN BONDS FOR THE Zn(II) COMPLEX

D – H···A	D-H (Å)	H···A (Å)	D···A (Å)	< (DHA) (º)
N2- H2A···O1	0.86	1.96	2.730(3)	148.6
N2- H2A···O3	0.86	2.55	3.267(3)	142.0
N2- H2B···O5[1]	0.86	1.95	2.777(2)	161.1
N4- H4A···O4	0.86	2.01	2.773(3)	146.6
N4- H4A···O6	0.86	2.38	3.071(3)	137.2
N4- H4B···O11	0.86	2.01	2.848(2)	162.8
N6- H6B···O7	0.86	1.95	2.738(3)	151.5
N6- H6B···O9	0.86	2.65	3.344(3)	139.1
N6- H6A···O2	0.86	1.97	2.742(3)	148.5
N8- H8A···O10	0.86	2.01	2.792(3)	150.9
N8- H8B···O8[2]	0.86	1.93	2.775(2)	166.1

Symmetry code: [1]-X, +Y, 3/2-Z; [2]1-X, +Y, 3/2-Z

As shown in Fig.1, both of the two central Zn(II) ions (Zn1 and Zn2) in the complex are four-coordinated with two oxygen atoms (O1 and O4, or O7 and O10) of carboxyl anion (-COO^-) in the two phenoxyacetic acid ligands and two nitrogen atoms (N1and N3, or N5 and N7) of thiazole rings in the two 2-amino benzothiazole ligands. The nitrogen atom of amino group and sulfur atom of thiazole rings in 2-amino benzothiazole ligand do not take part in the coordination.

It can be seen from Table-2 that, in the complex, there is a little difference for the coordination environment between the two zinc ions, although they have the same coordination mode. For example, Zn1-N1 and Zn1-N3 bonds are 2.0409(18) and 2.0320(18) Å, respectively. Their bond lengths show a little difference, although the two nitrogen atoms are from two same ligands of 2-amino benzothiazole. Similar situation can be found in the bond lengths of Zn1-O1 and Zn1-O4. However, for the Zn2, the coordinated atoms from the same ligands have the same bond lengths to it. Namely, the bond lengths of Zn2-O7 and Zn2-O10 are equal, 1.9230(18) and 1.9228(16) Å, respectively, the bond length of Zn2-N5 (2.016(2) Å) is equal to that of Zn2-N7 (2.0172(18) Å). The bond angles formed by the two central zinc ions and coordinated atoms are also different. The bond angles of O1-Zn1-N1 and O4-Zn1-N3 are equal to about 96.60º, but, at the corresponding locations, the bond angles of O7-Zn2-N5 and O10-Zn2-N7 are equal to 100.64º or so. Similarly, the bond angles of O1-Zn1-N3 and O4-Zn1-N1 are 113.94(8)º and 116.22(8)º, respectively, but the O7-Zn2-N7 and O10-Zn2-N5 are 115.20(8)º and 113.60(8)º, respectively; the O1-Zn1-O4 of 121.96(9)º is not equal to the O7-Zn2-O10 of 118.26(8)º; and the N1-Zn1-N3 of 112.45(8)º is not equal to the N5-Zn2-N7 of 108.74(8)º.

From the torsion angles listed in Table-3, the different coordination environments also can be seen between Zn1 and Zn2. In the situation of the former, the torsion angels of Zn1-O1-C1-O2 and Zn1-O1-C1-C2 are close to 0º and 180º , respectively, which shows that the Zn1, C2 and carboxyl anion (COO^-) from one ligand of phenoxyacetic acid almost locate in one plane. And for the other phenoxyacetic acid ligand, its carboxyl anion is not coplanar with the central zinc ion because the torsion angle of Zn1-O4-C9-O5 (-7.9(4)º) is not close to 0º. The torsion angels of Zn1-N1-C17-S1 and Zn1-N3-C24-S2 are 172.93(11)º and 170.91(11)º, which are nearly identical but not equal to 180º, so, the Zn1 and two thiazole rings in 2-amino benzothiazole ligands are not coplanar, too. Furthermore, the atoms of a thiazole ring don't locate in a plane either, because the torsion angle of Zn1-N1-C17-S1 (172.93(11)º) is not equal that of Zn1-N1-C23-C18 (-172.71(17)º) and similar situation can be found in the other ligand of 2-amino benzothiazole. For the latter, the torsion angles of Zn2-O7-C31-O8 and Zn2-O10-C39-O11 are -9.9(4)º and -6.7(4)º, respectively, which are distinctly not close to 0°, so, the central Zn2 and carboxyl anion (COO^-) from phenoxyacetic acid ligands are not in a plane. However, the Zn2 and two thiazole rings of 2-amino benzothiazole ligands are nearly coplanar as all the torsion angels of Zn2-N5-C33-S3, Zn2-N5-C56-C55, Zn2-N7-C47-S4 and Zn2-N7-C49-C48 are fairly near 180º. In addition, the atoms of every thiazole ring locate in a plane, too, because all the torsion angels of S3-C55-C56-N5, C33-S3-C55-C56, S4-C48-C49-N7 and C47-S4-C48-C49 are close to 0º.

The crystal structure analysis (Table-4) shows intramolecular and intermolecular hydrogen bonds in the unit cell. There is intramolecular hydrogen bonding between the amino-nitrogen atoms (N2, N4, N5 and N8) of 2-amino benzothiazole ligands and carboxyl oxygen atoms (O1, O4, O7 and O10, which are coordinated to central zinc ions at the same time) and ether-oxygen atoms (O3, O6 and O9, except for O12) of phenoxyacetic acid ligands. Therefore, the hydrogen bond lengths of H2A···O1, H4A···O4, H6B···O7 and H8A···O10 are 1.96, 2.01, 1.95 and 2.01 Å, respectively and the bond angles of N2-H2A···O1, N4-H4A···O4, N6-H6B···O7 and N8-H8A···O10 are 148.6º, 146.6º, 151.5º and 150.9º, respectively; the hydrogen bond lengths of H2A···O3, H4A···O6 and H6B···O9 are 2.55, 2.38 and 2.65 Å, respectively and the bond angles of N2- H2A···O3, N4- H4A···O6 and N6- H6B···O9 are 142.0º, 137.2º and 139.1º, respectively. Besides, there exist intermolecular bonding between the amino-nitrogen atoms (N2, N4, N5 and N8) of 2-amino benzothiazole ligands and oxygen atoms (O51, O11, O2 and O82, which are not coordinated to central zinc ions) of carboxyl groups in phenoxyacetic acid ligands. The bond lengths of H2B···O51, H4B···O11,

TABLE-5
MICS OF THE TITLE COMPLEX AND ITS TWO FREE LIGANDS (μg/mL)

Microoganisms	Compounds			Microoganisms	Compounds		
	1	2	3		1	2	3
Bacteria				Yeasts			
Escherichia coli	75	5.0	1.0	*Candida albicans*	> 100	25	1.0
Staphylococcus aureus	50	1.0	0.5	*Rhodotorula mucilaginosa*	> 100	20	0.5
Bacillus subtilis	75	10	0.5	*Cryptococcus albidosimilis*	75	20	0.1
Stenotrophomonas maltophilia	> 100	10	0.5	Moulds			
Bacillus cereus strain G8639	50	5.0	1.0	*Penicillium citrinum*	100	25	0.5
Enterobacter hormaechei	100	10	5.0	*Aspergillus niger*	> 100	50	1.0
Acinetobacter sp. ANT9054	> 100	25	10	*Aspergillus flavus*	> 100	25	0.1
Bacillus fusiformis strain SW-B9	100	50	10	*Trichoderma viride*	100	25	0.5
Klebsiella sp. strain zlmy	50	10	5.0	*Chaetomium globasum*	> 100	75	0.5
Bacillus sphaericus	> 100	20	5.0	*Rhizopus stolonifer*	> 100	50	0.1

Note: 1 — phenoxyacetic acid; 2 —2-amino benzothiazo5le; 2 — the zinc complex

H6A···O2 and H8B···O82 are 1.95 Å, 2.01 Å, 1.97 Å and 1.93 Å, respectively and the bond angles of N2-H2B···O5[1], N4-H4B···O11, N6-H6A···O2 and N8-H8B···O8[2] are 161.1º, 162.8º, 148.5º and 166.1º.

Antimicrobial activity: The *in vitro* antimicrobial properties of the zinc(II) complex and phenoxy acetic acid and 2-amino benzothiazole were evaluated against bacteria, yeasts and moulds and the obtained results are reported in Table-5. For the tested bacteria, the complex shows a moderate inhibitory effect and its minimum inhibitory concentrations (MICs) are between 0.5 to 10 μg/mL and for the tested fungi, a significant inhibitory activity is exhibited by the zinc complex, the MICs are 0.1-1.0 μg/mL. Noticeably, for all the tested strains, the values of MICs for the present complex are lower than those of the phenoxy acetic acid and 2-amino benzothiazole. Evidently, the complexation with zinc ion can enhance the antimicrobial activity. After complexation, the corresponding two active structures (benzothiazole ring and phenoxyacetic acid structure) in the title complex may play a synergistic inhibitory effect against the bacteria, yeasts and moulds or the antimicrobial mechanism of the complex probably is changed because of the introduction of Zn(II) with antimicrobial property. Howsoever, these results should be useful in the development of new compounds with good antimicrobial activities.

Conclusion

In summary, a novel ternary zinc(II) complex has been successfully designed and synthesized using 2-amino benzothiazole and phenoxyacetic acid as ligands. In this complex, each zinc(II) ion is four coordinated, but there is a little difference for the coordination environment, including bond lengths, bond angles and torsion angles, between the two zinc ions. Antimicrobial tests show that the title complex display good antimicrobial activity which is stronger than that of its free ligands.

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