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Crystal Structure of a Chiral Schiff Base Zinc (II) Complex, [Zn ($C_{15}H_{12}Br_2NO_2)_2$]

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Abstract

The crystal of the title compound, [Zn ($C_{15}H_{12}Br_2NO_2)_2$], bis [2,4-dibromo-6-[[(1-phenylethyl)imino-κN]2-hydroxymethyl]phenolato-κO]-zinc (II) is reported. A coordination compound was synthesized from (*R*)-(−)-2-phenylglycinol, 3, 5-dibromosalicylaldehyde, and zinc (II) acetate dihydrate. Central Zn (II) ion on a symmetry center affords a four-coordinated tetrahedral coordination geometry, Zn-N and Zn-O bond distances being 2.034(5) and 1.940(4) Å, respectively. Benzene rings of ligands formed intramolecular π−π stacking not indicating flexible feature of the rings of (*R*)-(−)-2-phenylglycinol moiety.

Keywords: Chirality; Schiff base; Zinc (II) complex; Molecular structure

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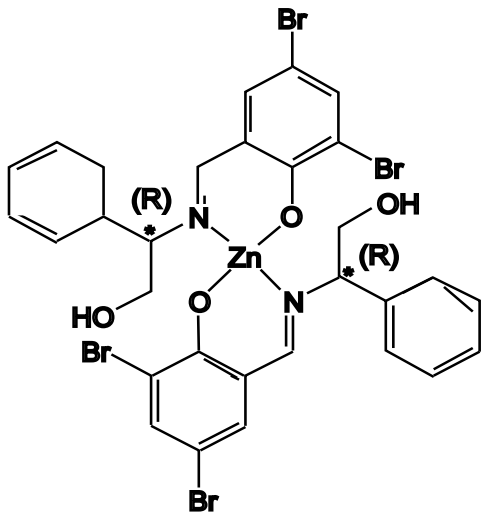
Introduction

We have studied on organic/inorganic hybrid materials of chiral Schiff base metal complexes and photochromic dyes such as azobenzene in polymer films to investigate molecular orientation control by irradiation of polarized UV light [1-3]. In this kind of materials, not only molecular structures of metal complexes but also intra- or inter-molecular interaction are important. Since crystal structure of the title compound (**Scheme 1**), which may be expected π-π stacking and hydrogen bonds, has not been determined yet [4], we report it herein.



Scheme 1 The molecular structure of the title compound.

Experimental

Synthesis

Synthesis of the title compound was published in our previous paper [4]. Yellow prismatic crystals of (I) were obtained from reaction solution by solvent diffusion method with water in sample tube at 278 K over 7 days.

Data collection

X-ray diffraction intensity data were collected on Bruker Kappa Apex II single crystal X-ray diffractometer equipped with graphite monochromated MoKα (λ=0.71073 Å) radiation and CCD detector. Crystal of suitable size was mounted on a glass fiber after determination of the unit cell parameters, the intensity data were collected with an average fourfold redundancy per reflection and optimum resolution. The intensity data collection, frames integration, Lorentz and polarization correction and decay correction were done using SAINT software [5]. Empirical absorption correction (multi-scan) was performed using SADABS program [5].

Results and Discussion

Structure solving and refinement

Crystal structure was solved by direct methods using SHELXS-97 [6]. All the non-hydrogen atoms were located automatically. The structure was then refined by full-matrix least-squares method using SHELXL- 97 [6]. The model of non-hydrogen atoms was refined using by anisotropic thermal parameters. Hydrogen atoms were positioned geometrically C–H=0.93–0.98 Å and allowed to ride on their parent atoms, with *U*iso(H)=1.5 *U*eq(C) for methyl H 1.2 *U*eq(C) for other H atoms mainly. The relevant crystallographic data are listed in **Table 1**.

The molecular structure (ORTEP diagram) of the title compound is shown in **Figure 1**. Selected bond lengths and angles are listed in **Table 2**. The title zinc(II) complex affords a four-coordinated tetrahedral coordination geometry and umbrella conformation affected in which both ligands bend towards the same side, with Zn_1-N_1 and Zn_1-O_1 bond distances being 2.034(5) and 1.940(4) Å, respectively. Because of symmetric center, coordination bond angles are O_1-Zn_1-N_1=94.00(19)°, O_1-Zn_1-N_1'=109.07(19)°, O_1-Zn_1-O_1'=131.1(3)°, and N_1-Zn_1-N_1'=122.8(3)° ('denotes symmetry code: 1-x, y, 1-z). The values are within common range of the related complexes [7-11]. Benzene rings of ligands, parts of (*R*)-(−)-2-phenylglycinol and 3, 5-dibromosalicylaldehyde, formed weak intramolecular π-π stacking structure, affecting its umbrella conformation. Contrary to our expectation, there are no relevant hydrogen bonds within 3.3 Å.

Additional Information

Crystallographic data for the structures reported here have been deposited with CCDC Deposition No CCDC 1482903. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK, Fax: +441223336033; E-mail: deposit@ccdc.cam.ac.uk.

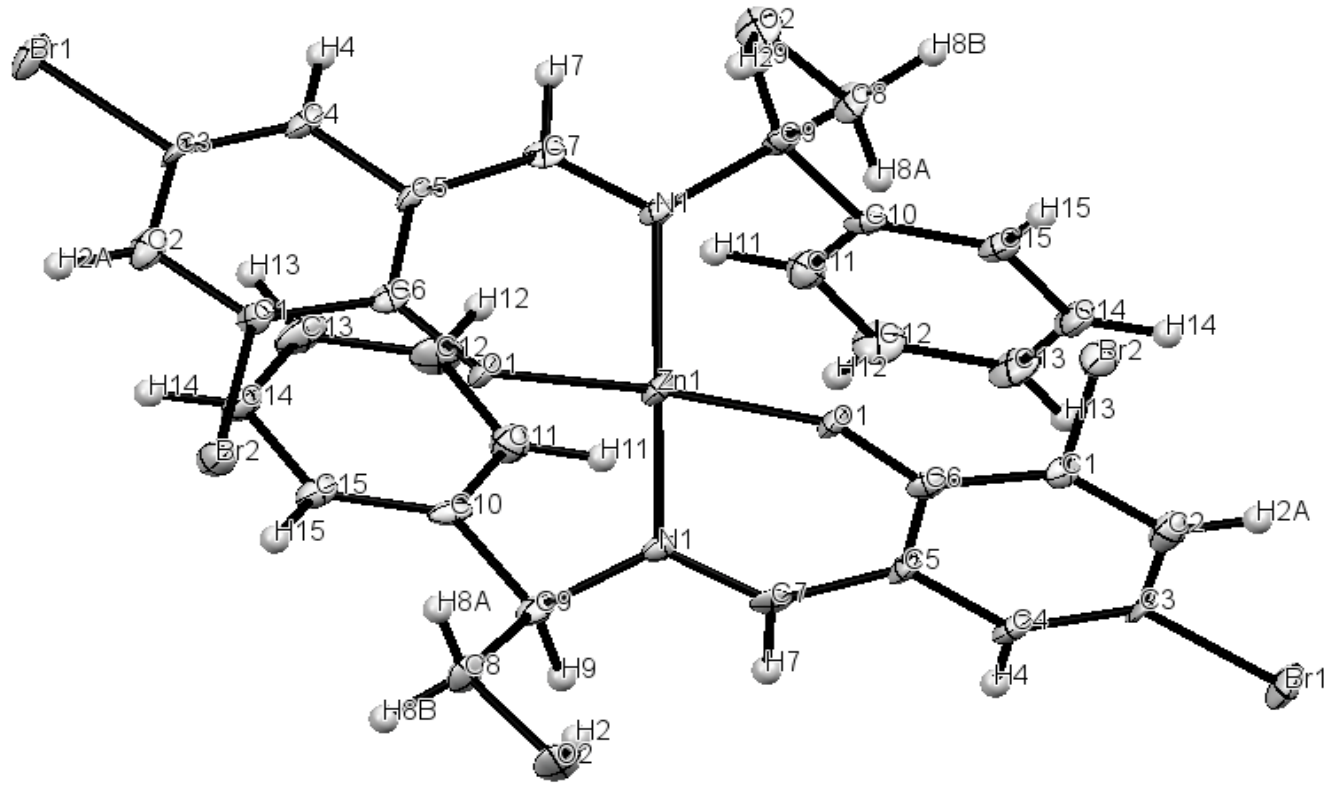


Figure 1 The molecular structure of the title compound, showing the atomic numbering and displacement ellipsoids drawn at the 30% probability level.

Table 1 Crystal data for the title compound.

Parameters	Values
Empirical formula	$C_{30}H_{24}Br_4N_2O_4Zn$
Formula weight	861.50
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, *C2*
Unit cell dimensions	a=10.782(4) Å
	b=10.380(2) Å, β=106.664(4)°
	c=13.169(3) Å
Volume	1434.8(7) $Å^3$
Z, Calculated density	2, 1.994 Mg/m^3
Absorption coefficient	6.466 mm^{-1}
F (000)	840
Crystal size	0.151 × 0.128 × 0.108 mm^3
Theta range for data collection	2.21 to 27.35°
Limiting indices	-13 ≦ h ≦ 7, -11 ≦ k ≦13, -17 ≦ l ≦15
Reflections collected/unique	3749/2 2369 [R(int)=0.0578]
Completeness to theta=27.35	86.7%
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3285 / 1 / 187
Goodness-of-fit on F^2	0.780
Final R indices [I>2sigma(I)]	R1=0.0345, wR2=0.0955
R indices (all data)	R1=0.0354, wR2=0.0963
Largest diff. peak and hole	1.559 and -0.975 e. $Å^{-3}$
Flack Parameter	0.061(11)

Table 2 Selected bond lengths (Å) and angles (°) (‘denotes symmetry code: 1-x, y, 1-z).

Zn_1-N_1	2.034(5)	O_1-Zn_1-N_1	94.00(19)
Zn_1-O_1	1.940(4)	O_1-Zn_1-N ’	109.07(19)
N_1-C_7	1.287(8)	O1-Zn_1-O_1’	131.1(3)
O_1-C_6	1.308(8)	N_1-Zn_1-N_1’	122.8(3)
C_6-C_5	1.421(9)	N_1-C_7-C_5	127.4(6)
Br_1-C_3	1.915(6)	C_7-N_1-Zn_1	119.8(4)
Br_2 C_1	1.903(6)	C_6-O_1-Zn_1	122.5(4)

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