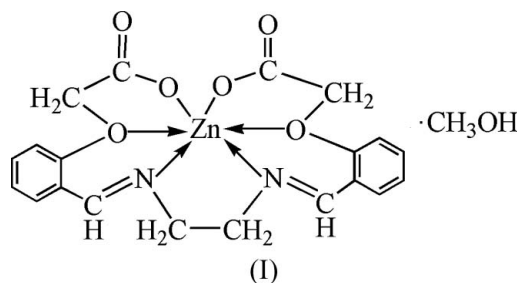


{2,2'-[Ethane-1,2-diylbis(nitrilomethylidyne)]-diphenoxyacetato}zinc(II) methanol solvate**Jing Wang, Dong-Sheng Zhu,*
Kui-Zhan Shao and Lin Xu**Department of Chemistry, Northeast Normal
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Republic of ChinaCorrespondence e-mail:
zhuds206@nenu.edu.cn**Key indicators**Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
 R factor = 0.048
 wR factor = 0.070
Data-to-parameter ratio = 13.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The title compound, $[\text{Zn}(\text{C}_{20}\text{H}_{18}\text{N}_2\text{O}_6)] \cdot \text{CH}_3\text{OH}$, has been synthesized through a one-step procedure in a methanol solvent. The Zn atom exhibits a distorted trigonal prismatic geometry consisting of two imine N-atom donors, two O-atom donors of the phenoxy groups and two O-atom donors of the deprotonated carboxyl groups. C—H \cdots O interactions stabilize the structure.

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Zinc(II) complexes with polydentate salicylaldehyde Schiff bases have been synthesized and reported extensively as these complexes have important properties and potential applications in different areas (Xiong *et al.*, 1996; Mizukami *et al.*, 2003). Tridentate and tetradentate ligands have been reported by Thompson *et al.* (2000) and Sekerci & Sonmez (2002), while pentadentate and hexadentate ligands have been synthesized by Marvel *et al.* (1956) and Chantarasiri *et al.* (2000, 2004) using triethylenetetramine. However, to our knowledge, six-coordinated zinc(II)–Schiff base complexes prepared without using triethylenetetramine have not been reported. We have introduced a carboxyl substituent to replace the phenolic H atom, to give O donor atoms instead of the usual methods which add N-donor atoms of amine, and obtained the title compound, (I).



The structure determination indicates that the Zn^{II} ion is coordinated by two imine N atoms, two O atoms of the phenoxy groups and two O atoms of the deprotonated carboxyl groups from the same ligand (Fig. 1). The metal ion shows a slightly distorted trigonal prismatic geometry. The Zn—O(carboxylate), Zn—O(phenoxy) and Zn—N distances (Table 1) are near to the values in other related zinc compounds (Lin *et al.*, 2004). The complex molecule is connected to the methanol molecule through an O—H \cdots O hydrogen bond (Yohannan *et al.*, 2004; Gilli *et al.*, 2005), with an O \cdots O distance of 2.764 (4) Å.

Fig. 2 shows that the crystal packing in (I) is mainly dominated by C—H \cdots O interactions involving atoms O2 and

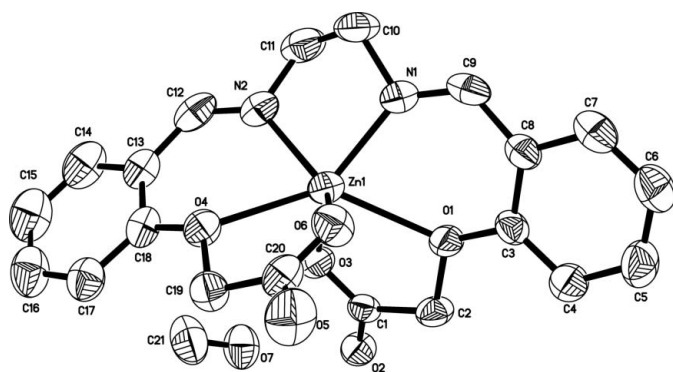


Figure 1
View of the molecular structure of (I). H atoms have been omitted.

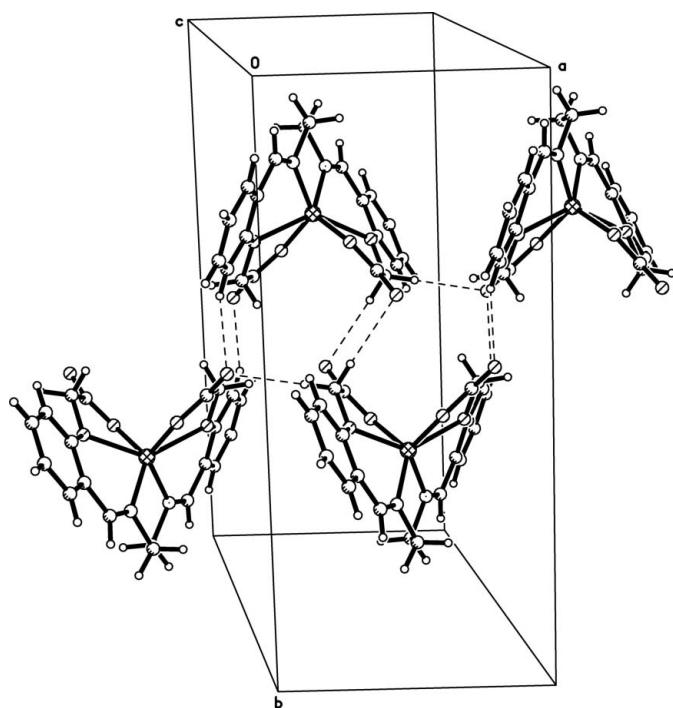


Figure 2
The crystal packing in (I), showing the C—H...O interactions (dashed lines).

O5, with the C—H...O angles ranging from 156 to 172° and H...O distances ranging from 2.49 to 2.58 Å. These angles and distances are similar to those in related compounds (Desiraju *et al.*, 1990; Guru Row *et al.*, 2004).

Experimental

To a mixture of zinc(II) dichloride (0.136 g, 1 mmol) and *o*-formylphenoxyacetic acid (0.36 g, 2 mmol) in absolute methanol (20 ml) was added ethylenediamine (0.066 g, 1.1 mmol) and triethylamine (0.212 g, 2.1 mmol). After stirring at 333 K for 0.5 h, the solution was filtered. Colourless cubic crystals were obtained by evaporation of methanol at room temperature over a period of 2 d (yield 61%). Analysis calculated for C₂₁H₂₂N₂O₇Zn: C 57.62, H 2.98, N 15.51%; found: C 57.79, H 2.86, N 15.62%.

Crystal data

[Zn(C₂₀H₁₈N₂O₆)]·CH₂O
M_r = 479.78
 Monoclinic, *P*₂₁/*c*
a = 8.200 (2) Å
b = 18.274 (5) Å
c = 14.191 (4) Å
 β = 101.974 (5)°
V = 2080.1 (10) Å³

Z = 4
D_x = 1.532 Mg m⁻³
 Mo *K*α radiation
 μ = 1.23 mm⁻¹
T = 293 (2) K
 Block, colourless
 0.45 × 0.33 × 0.26 mm

Data collection

Bruker SMART area-detector
 diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
T_{min} = 0.268, *T_{max}* = 0.304
 (expected range = 0.641–0.727)

11533 measured reflections
 4073 independent reflections
 2426 reflections with *I* > 2σ(*I*)
R_{int} = 0.065
 θ_{\max} = 26.1°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.048
wR (*F*²) = 0.070
S = 0.94
 4073 reflections
 296 parameters

H atoms treated by a mixture of
 independent and constrained
 refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0113P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} = 0.001
 Δρ_{max} = 0.61 e Å⁻³
 Δρ_{min} = -0.36 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

N1—Zn1	2.075 (3)	O3—Zn1	1.961 (2)
N2—Zn1	2.074 (3)	O4—Zn1	2.353 (2)
O1—Zn1	2.389 (2)	O6—Zn1	1.947 (3)
O6—Zn1—O3	115.86 (9)	N1—Zn1—O4	141.94 (10)
O6—Zn1—N1	98.17 (11)	N2—Zn1—O4	77.09 (10)
O3—Zn1—N1	130.87 (11)	O6—Zn1—O1	86.29 (9)
O6—Zn1—N2	130.56 (11)	O3—Zn1—O1	72.55 (9)
O3—Zn1—N2	99.06 (11)	N1—Zn1—O1	75.70 (9)
N1—Zn1—N2	81.87 (12)	N2—Zn1—O1	139.46 (10)
O6—Zn1—O4	73.30 (9)	O4—Zn1—O1	138.21 (7)
O3—Zn1—O4	83.98 (9)		

The H atoms of the ligand were positioned geometrically and refined as riding atoms, with C—H = 0.93 (CH) and 0.97 Å (CH₂), and *U*_{iso}(H) = 1.2*U*_{eq}(C). The H atoms of the methanol molecule were found in difference maps and refined isotropically.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

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