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catena-Poly[[zinc(II)-μ-[2-(2-carboxylatophenyliminomethyl)phenolato-1κ^3O,N,O':1'$\kappa O''$]] methanol solvate]

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Key indicators

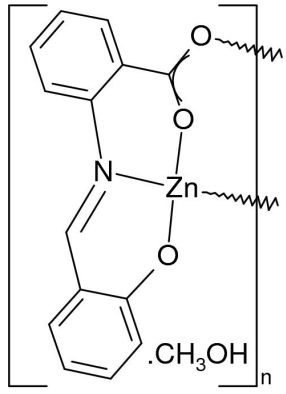
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.031
wR factor = 0.086
Data-to-parameter ratio = 14.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $\{[Zn(C_{14}H_9NO_3)]\cdot CH_3OH\}_n$, is a polynuclear zinc(II) complex. Each Zn^{II} atom is coordinated by one N and two O atoms of a Schiff base ligand, and another O atom of another Schiff base ligand, forming a severely distorted square-planar geometry.

Comment

Zinc(II) complexes are of great interest in coordination chemistry (Vallee & Auld, 1993; Lipscomb & Sträter, 1996; Hou, 2005). As an extension of work on the structural characterization of zinc compounds, the title polymeric zinc(II) compound, (I), is reported.



(I)

Compound (I) is a polynuclear zinc(II) complex (Fig. 1). Each Zn^{II} ion is coordinated by one N and two O atoms of a Schiff base ligand, and another O atom of another Schiff base ligand, forming a severely distorted square-planar geometry; the *trans* angles in the ZnO_3N square plane are 153.10 (11) and 162.82 (10)° (Table 1). The Zn—N and Zn—O bond lengths are comparable to the values observed in other zinc(II) complexes (Chisholm *et al.*, 2001). There are no short contacts between the molecules in the crystal structure (Fig. 2).

Experimental

o-Aminobenzoic acid (0.1 mmol, 13.7 mg), salicylaldehyde (0.1 mmol, 12.2 mg) and $Zn(CH_3COO)_2\cdot 2H_2O$ (0.1 mmol, 22.0 mg) were dissolved in methanol (10 ml). The mixture was stirred for 1 h and filtered. After leaving the filtrate to stand in air for 20 d, colorless block-shaped crystals were formed.

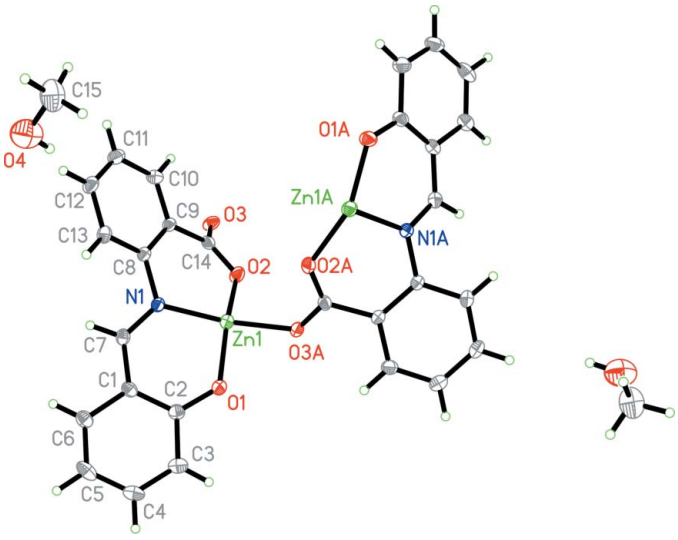


Figure 1
Two repeat units of the polymeric structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Atoms labelled with the suffix A and unlabelled atoms are at the symmetry position $(2 - x, \frac{1}{2} + y, 1 - z)$.

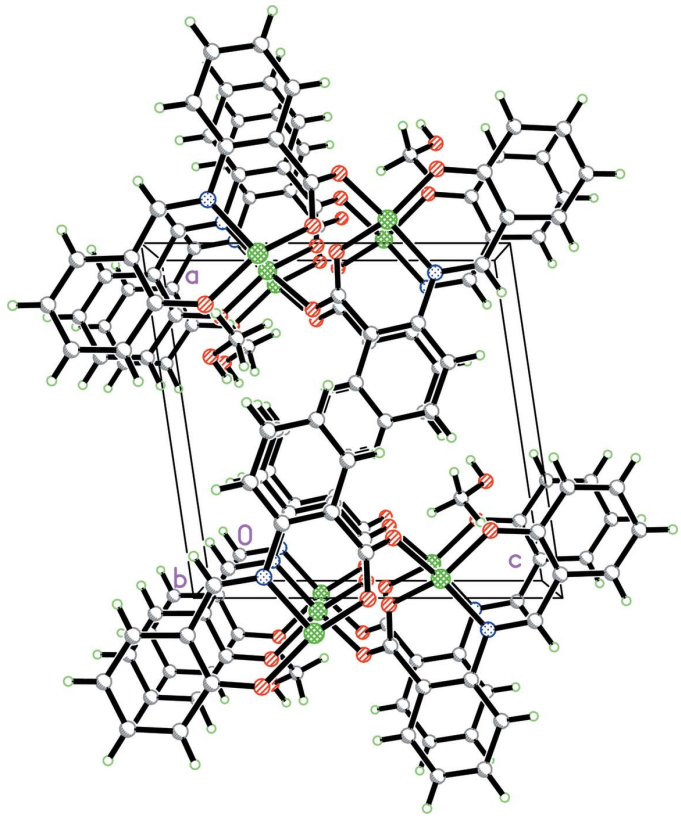


Figure 2
The crystal packing of (I), viewed along the *b* axis.

Crystal data

$[Zn(C_{14}H_9NO_3)]\cdot CH_4O$	D_x = 1.654 Mg m^{-3}
M_r = 336.63	Mo $K\alpha$ radiation
Monoclinic, $P2_1$	Cell parameters from 3124 reflections
a = 9.663 (2) Å	θ = 2.7–28.2°
b = 7.128 (2) Å	μ = 1.83 mm^{-1}
c = 9.922 (2) Å	T = 298 (2) K
β = 98.42 (3)°	Block, colorless
V = 676.0 (3) Å^3	0.33 × 0.28 × 0.22 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	2753 independent reflections
ω scans	2667 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.016
T_{min} = 0.583, T_{max} = 0.689	θ_{max} = 27.5°
3989 measured reflections	$h = -12 \rightarrow 12$
	$k = -8 \rightarrow 9$
	$l = -12 \rightarrow 7$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 0.0457P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.031	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.086	$\Delta\rho_{max}$ = 0.58 e Å^{-3}
S = 1.05	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
2753 reflections	Absolute structure: Flack (1983), 1076 Friedel pairs
191 parameters	Flack parameter: 0.076 (15)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.889 (2)	Zn1—O2	1.936 (2)
Zn1—N1	1.935 (2)	Zn1—O3^{i}	1.944 (2)
O1—Zn1—N1	94.95 (10)	O1—Zn1—O3^{i}	86.80 (9)
O1—Zn1—O2	153.10 (11)	N1—Zn1—O3^{i}	162.82 (10)
N1—Zn1—O2	92.84 (10)	O2—Zn1—O3^{i}	93.23 (10)

Symmetry code: (i) $-x+2, y+\frac{1}{2}, -z+1$.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances in the range 0.93–0.96 Å and an O—H distance of 0.82 Å, and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C,O).

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

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