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catena-Poly[[[aquazinc(II)]-μ-*N*-(3-carboxy-2-oxidobenzylidene)glycinato-$\kappa^4O,N,O':O''$] monohydrate]

Zhi-Hong Wu,[a] Ying-Hua Zhou[b]* and Jin-Hua Cai[a]

[a]Department of Chemistry and Life Science, Hechi University, Yizhou 546300, Guangxi, People's Republic of China, and [b]School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, Guangdong, People's Republic of China
Correspondence e-mail: cjhzse@163.com

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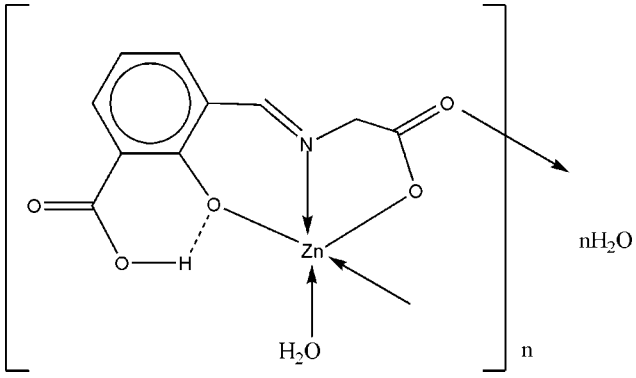
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.026; wR factor = 0.078; data-to-parameter ratio = 14.8.

The title polymeric compound, $\{[Zn(C_{10}H_7NO_5)(H_2O)]\cdot H_2O\}_n$, consists of a one-dimensional chain, in which the Zn^{2+} centre is coordinated by two O atoms and one N atom from the tridentate dianionic *N*-(3-carboxy-2-oxidobenzylidene)glycinate ligand, one water molecule and a bridging carboxylate O atom from an adjacent ligand. This results in a square-based pyramidal coordination.

Related literature

For biological activity, see: Yang *et al.* (2000); May *et al.* (2004). For flexible coordination modes, see: Ranford *et al.* (1999); Erxleben (2001). For synthesis of related compounds, see: Cai *et al.* (2006, 2007).



Experimental

Crystal data

$[Zn(C_{10}H_7NO_5)(H_2O)]\cdot H_2O$
M_r = 322.59
Monoclinic, $P2_1/c$
a = 8.3985 (9) Å
b = 6.8730 (7) Å
c = 19.637 (2) Å
β = 90.781 (2)°
V = 1133.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.20 mm^{-1}
T = 173 (2) K
0.49 × 0.41 × 0.22 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.354, T_{max} = 0.617
5599 measured reflections
2479 independent reflections
2171 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.078
S = 1.06
2479 reflections
166 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −0.87 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O5^{i}	1.9951 (15)	Zn1—O3	2.0234 (15)
Zn1—O6	2.0065 (16)	Zn1—O4	2.1211 (15)
Zn1—N1	2.0161 (18)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6A···O1^{ii}	0.837 (10)	1.94 (3)	2.768 (2)	172 (3)
O6—H6B···O7^{iii}	0.843 (10)	1.798 (11)	2.637 (2)	173 (4)
O7—H7A···O1^{iv}	0.85 (3)	1.96 (3)	2.806 (2)	175 (3)
O7—H7B···O5	0.85 (3)	1.923 (10)	2.763 (2)	176 (3)
O2—H2···O3	0.97 (3)	1.52 (3)	2.450 (2)	158 (3)

Symmetry codes: (ii) $-x, -y, -z$; (iii) $x-1, y, z$; (iv) $x+1, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2099).

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supplementary materials

Acta Cryst. (2007). E**63**, m2223-m2224 [**doi:10.1107/S1600536807035647**]

catena-Poly[[[aquazinc(II)]-μ-*N*-(3-carboxy-2-oxidobenzylidene)glycinato-κ^4*O*,*N*,*O*':*O*''] monohydrate]

Z.-H. Wu, Y.-H. Zhou and J.-H. Cai

Comment

Schiff bases have been intensively investigated recently owing to their strong coordination capability and diverse biological activities, such as antibacterial, antitumor activities *etc* (Yang *et al.*, 2000; May *et al.*, 2004). Among these Schiff bases, aminophenol-containing Schiff base have received extraordinatry attention for its' flexible coordination codes. some unusual structures have been synthesized through these ligands, such as helical structures (Ranford *et al.*,1999;Erxleben,2001).

However, in those reported literatures, Seldom helical structures with the ligand of 3-Carboxysalicylaldehyde have been generated. We have reported two structures derived from the ligand 3-Carboxysalicylideneglycinate(Cai *et al.*,2006; Cai *et al.*,2007). As an extension of the work, We report here the preparations and crystal structure characterizations of the title helical coordination polymer(I).

The crystal structure of the title complex(I) is very similar to the former reported structure (Cai *et al.*,2007).there is one Zn^{II}atom,one 3-Carboxysalicylideneglycinate anion, one coordinated water molecule and one lattice water molecule in each independent crystallographic unit, Each Zn^{II} atom adapts a square-based pyramidal geometry·It is worthy of mention that the remaining protonated carboxylate group does not participate in coordination, but involve in hydrogen bonding·In the title complex,each pair of adjacent Zn^{II} atom are bridged by a carboxy group of the ligand to form a chiral helical chain running along a crystallographic 2_1 axis in the b direction with a pitch of 6.873 Å. There are two kinds of hydrogen bonding interactions in the title complex·The acidic H atom forms a strong intramolecular O—H···O hydrogen bond to the phenoxy O atom [O···O = 2.450 (2) Å]. The other hydrogen bonding interactions are involving the carboxylate O atoms and coordinated/uncoordinated water molecules. By which the chains are connected to form a three-dimensional network.

Experimental

Glycine (2 mmol, 0.150 g), 3-carboxysalicylaldehyde (2 mmol, 0.336 g) and sodium hydroxide (2 mmol, 0.08 g) were dissolved in 80% aqueous methanol (25 ml). To the clear yellow solution was added an aqueous solution (15 ml) of Zinc(II) nitrate (2 mmol, 0.376 g). The solution was filtered after keeping at 323 K for 6 h. Yellow crystals separated from the solution after two weeks in about 46% yield (according to Zinc).

Refinement

The C-bound H atoms were placed at calculated positions (C—H = 0.95 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C). The other H atoms were located in a difference Fourier map and refined with O—H distance restraints of 0.85–0.97 Å, and with U_{iso}(H) values of 1.5U_{eq}(O).

Figures

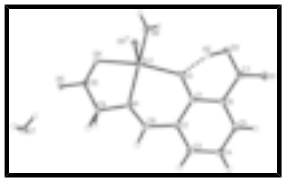

Fig. 1. Asymmetric unit of (I) showing 30% probability displacement ellipsoids. Hydrogen bonds are indicated by dashed lines.[(i) −*x* + 1,*y* + 1/2,-*z* + 1/2)]

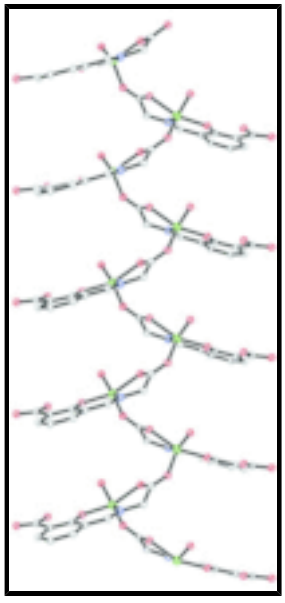

Fig. 2. The one-dimensional helical chains in (I)·The hydrogen atoms are omitted for clarity.the water molecules are not shown

catena-Poly[[[aquazinc(II)]-μ-_N_-(3-carboxy-2- oxidobenzylidene)glycinato-κ^4_O,N,O'_:_O''_] monohydrate]

Crystal data

$[Zn(C_{10}H_7NO_5)(H_2O)]\cdot H_2O$	F_{000} = 656
M_r = 322.59	D_x = 1.890 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 978 reflections
a = 8.3985 (9) Å	θ = 3.1–27.0º
b = 6.8730 (7) Å	μ = 2.20 mm^{-1}
c = 19.637 (2) Å	T = 173 (2) K
β = 90.781 (2)º	Block, yellow
V = 1133.4 (2) Å^3	0.49 × 0.41 × 0.22 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2479 independent reflections
Radiation source: fine-focus sealed tube	2171 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.017

Detector resolution: 0 pixels mm^{-1}

T = 173(2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

T_{min} = 0.354, T_{max} = 0.617

5599 measured reflections

θ_{max} = 27.0º

θ_{min} = 2.4º

h = −10→5

k = −7→8

l = −24→25

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.026

$wR(F^2)$ = 0.078

S = 1.06

2479 reflections

166 parameters

6 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0474P)^2 + 0.7019P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.84 e $Å^{-3}$

$\Delta\rho_{min}$ = −0.87 e $Å^{-3}$

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.35846 (3)	0.11867 (3)	0.168087 (11)	0.01598 (10)
N1	0.5830 (2)	0.1334 (2)	0.13345 (9)	0.0168 (4)
O1	0.01579 (19)	0.2942 (3)	−0.09655 (8)	0.0276 (4)
O2	0.0220 (2)	0.2399 (3)	0.01427 (8)	0.0299 (4)
H2	0.108 (4)	0.227 (5)	0.0478 (16)	0.045*
O3	0.27673 (17)	0.1979 (2)	0.07472 (7)	0.0215 (3)
O4	0.47631 (17)	−0.0620 (2)	0.24040 (7)	0.0194 (3)
O5	0.71706 (17)	−0.1686 (2)	0.27122 (7)	0.0193 (3)
O6	0.1646 (2)	−0.0488 (3)	0.17852 (9)	0.0327 (4)

H6A	0.109 (3)	−0.113 (4)	0.1510 (11)	0.049*
H6B	0.117 (3)	−0.049 (5)	0.2159 (8)	0.049*
O7	1.0306 (2)	−0.0718 (3)	0.29892 (9)	0.0307 (4)
H7A	1.024 (3)	0.017 (4)	0.3286 (13)	0.046*
H7B	0.9363 (17)	−0.107 (4)	0.2905 (16)	0.046*
C1	0.3562 (2)	0.2400 (3)	0.01927 (10)	0.0166 (4)
C2	0.5254 (2)	0.2373 (3)	0.01671 (10)	0.0165 (4)
C3	0.60165 (9)	0.28856 (11)	−0.04338 (4)	0.0191 (4)
H3	0.7147	0.2866	−0.0446	0.023*
C4	0.51580 (9)	0.34244 (11)	−0.10149 (4)	0.0202 (4)
H4	0.5698	0.3798	−0.1416	0.024*
C5	0.35162 (9)	0.34113 (11)	−0.10031 (4)	0.0199 (4)
H5	0.2928	0.3768	−0.1401	0.024*
C6	0.27022 (9)	0.28780 (11)	−0.04124 (4)	0.0173 (4)
C7	0.09381 (9)	0.27567 (11)	−0.04348 (4)	0.0214 (4)
C8	0.62914 (9)	0.18023 (11)	0.07343 (4)	0.0178 (4)
H8	0.7404	0.1774	0.0654	0.021*
C9	0.70227 (9)	0.06991 (11)	0.18359 (4)	0.0181 (4)
H9A	0.8115	0.1060	0.1840	0.022*
H9B	0.7886	0.0065	0.1631	0.022*
C10	0.62358 (9)	−0.06344 (11)	0.23515 (4)	0.0166 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01372 (14)	0.02076 (15)	0.01347 (14)	−0.00010 (8)	0.00097 (9)	−0.00047 (8)
N1	0.0156 (8)	0.0178 (9)	0.0172 (9)	0.0001 (6)	0.0002 (7)	0.0015 (7)
O1	0.0243 (8)	0.0353 (10)	0.0231 (8)	−0.0049 (7)	−0.0080 (6)	0.0029 (7)
O2	0.0173 (8)	0.0503 (11)	0.0221 (8)	−0.0012 (7)	−0.0011 (6)	0.0050 (8)
O3	0.0150 (7)	0.0335 (9)	0.0160 (7)	−0.0007 (6)	0.0009 (6)	0.0043 (6)
O4	0.0160 (7)	0.0244 (8)	0.0178 (7)	−0.0003 (6)	0.0018 (5)	0.0028 (6)
O5	0.0155 (7)	0.0242 (8)	0.0183 (7)	−0.0016 (6)	−0.0014 (5)	0.0058 (6)
O6	0.0295 (9)	0.0483 (11)	0.0203 (8)	−0.0212 (8)	0.0036 (7)	−0.0062 (8)
O7	0.0183 (8)	0.0427 (10)	0.0312 (10)	−0.0054 (7)	0.0042 (7)	−0.0095 (8)
C1	0.0187 (10)	0.0152 (9)	0.0159 (9)	−0.0004 (8)	0.0003 (8)	−0.0012 (7)
C2	0.0177 (10)	0.0155 (9)	0.0163 (10)	0.0002 (8)	0.0010 (8)	−0.0008 (7)
C3	0.0184 (10)	0.0174 (10)	0.0217 (10)	−0.0005 (8)	0.0032 (8)	−0.0022 (8)
C4	0.0272 (11)	0.0205 (10)	0.0130 (9)	−0.0024 (9)	0.0042 (8)	−0.0001 (8)
C5	0.0263 (11)	0.0180 (10)	0.0154 (10)	0.0009 (9)	−0.0021 (8)	−0.0015 (8)
C6	0.0202 (10)	0.0163 (10)	0.0154 (9)	−0.0007 (8)	−0.0015 (8)	−0.0028 (8)
C7	0.0222 (11)	0.0210 (11)	0.0211 (10)	−0.0016 (8)	−0.0035 (8)	−0.0006 (8)
C8	0.0160 (10)	0.0176 (10)	0.0197 (10)	−0.0005 (8)	0.0012 (8)	−0.0005 (8)
C9	0.0124 (9)	0.0247 (10)	0.0172 (10)	−0.0003 (8)	0.0002 (7)	0.0038 (8)
C10	0.0200 (10)	0.0172 (10)	0.0126 (9)	−0.0018 (8)	−0.0002 (7)	−0.0022 (7)

Geometric parameters (Å, °)

Zn1—O5^{i}	1.9951 (15)	O7—H7B	0.85 (3)

Zn1—O6	2.0065 (16)	C1—C6	1.42052
Zn1—N1	2.0161 (18)	C1—C2	1.423 (3)
Zn1—O3	2.0234 (15)	C2—C3	1.395 (2)
Zn1—O4	2.1211 (15)	C2—C8	1.45845
N1—C8	1.28660	C3—C4	1.3916
N1—C9	1.46162	C3—H3	0.9500
O1—C7	1.23004	C4—C5	1.3794
O2—C7	1.31486	C4—H4	0.9500
O2—H2	0.97 (3)	C5—C6	1.4031
O3—C1	1.317 (2)	C5—H5	0.9500
O4—C10	1.24258	C6—C7	1.4840
O5—C10	1.27487	C8—H8	0.9500
O5—Zn1^{ii}	1.9951 (15)	C9—C10	1.5233
O6—H6A	0.837 (10)	C9—H9A	0.9500
O6—H6B	0.843 (10)	C9—H9B	0.9415
O7—H7A	0.85 (3)		
O5^{i}—Zn1—O6	95.42 (7)	C4—C3—C2	121.46
O5^{i}—Zn1—N1	118.12 (7)	C4—C3—H3	119.3
O6—Zn1—N1	145.80 (7)	C2—C3—H3	119.3
O5^{i}—Zn1—O3	103.74 (6)	C5—C4—C3	119.4
O6—Zn1—O3	88.92 (7)	C5—C4—H4	120.3
N1—Zn1—O3	89.32 (7)	C3—C4—H4	120.3
O5^{i}—Zn1—O4	100.26 (6)	C4—C5—C6	120.9
O6—Zn1—O4	88.14 (7)	C4—C5—H5	119.5
N1—Zn1—O4	79.92 (6)	C6—C5—H5	119.5
O3—Zn1—O4	155.98 (6)	C5—C6—C1	120.27
C8—N1—C9	118.66	C5—C6—C7	119.2
C8—N1—Zn1	128.06	C1—C6—C7	120.51
C9—N1—Zn1	113.16	O1—C7—O2	120.32
C7—O2—H2	105.00	O1—C7—C6	122.64
C1—O3—Zn1	129.71 (13)	O2—C7—C6	117.03
C10—O4—Zn1	113.89	N1—C8—C2	125.64
C10—O5—Zn1^{ii}	123.30 (10)	N1—C8—H8	117.2
Zn1—O6—H6A	133 (2)	C2—C8—H8	117.2
Zn1—O6—H6B	119 (2)	N1—C9—C10	109.14
H6A—O6—H6B	107.1 (16)	N1—C9—H9A	125.4
H7A—O7—H7B	105.9 (15)	C10—C9—H9A	125.4
O3—C1—C6	119.00	N1—C9—H9B	112.0
O3—C1—C2	122.95 (18)	C10—C9—H9B	110.5
C6—C1—C2	118.04	H9A—C9—H9B	51.3
C3—C2—C1	119.79 (16)	O4—C10—O5	124.37
C3—C2—C8	115.94	O4—C10—C9	119.46
C1—C2—C8	124.27	O5—C10—C9	116.16

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2; (ii) −*x*+1, *y*−1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

O6—H6A···O1^{iii}	0.837 (10)	1.94 (3)	2.768 (2)	172 (3)
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O7—H7B···O5	0.85 (3)	1.923 (10)	2.763 (2)	176 (3)
O2—H2···O3	0.97 (3)	1.52 (3)	2.450 (2)	158 (3)

Symmetry codes: (iii) −*x*, −*y*, −*z*; (iv) *x*−1, *y*, *z*; (v) *x*+1, −*y*+1/2, *z*+1/2.

Fig. 1

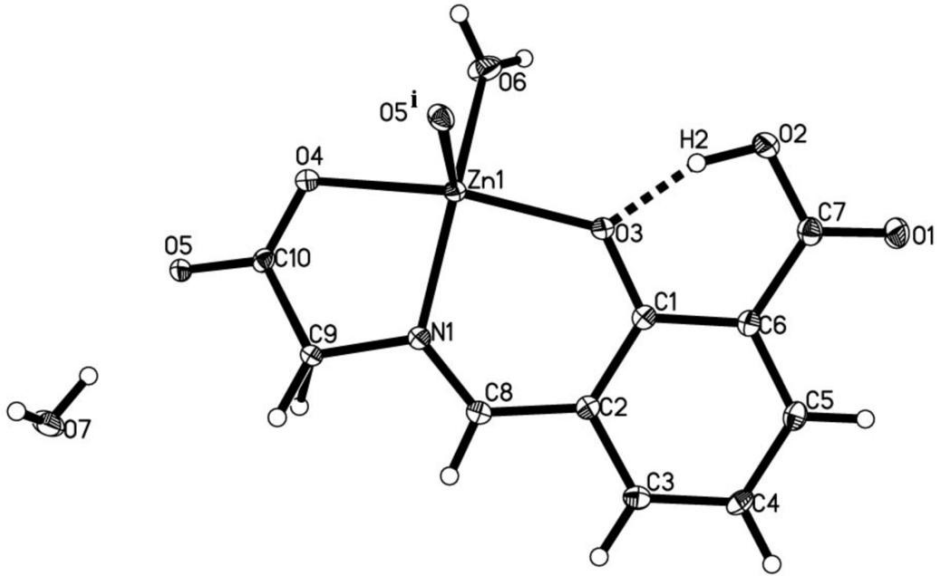

Fig. 2