Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

A one-dimensional helical chain polymer: *catena*-poly[[[bis(1*H*-imidazole)zinc(II)]-μ-3-carboxylatophenoxyacetato] trihydrate]

Xian-Fa Zhang, Shan Gao,* Li-Hua Huo and Jing-Gui Zhao

Laboratory of Functional Materials, School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China

Correspondence e-mail: shangao67@yahoo.com

Received 7 October 2005
Accepted 10 October 2005
Online 15 October 2005

Key indicators

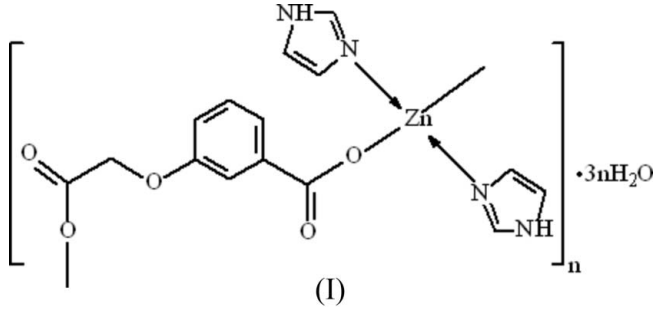
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.110
Data-to-parameter ratio = 16.3

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

In the title one-dimensional polymer, $\{[Zn(3\text{-}CPOA)(C_3H_4N_2)_2]\cdot 3H_2O\}_n$ (3-CPOA^{2-} is the 3-carboxylatophenoxyacetate dianion, $C_9H_6O_5$), the Zn atom shows tetrahedral coordination, as it is linked to two N atoms from two imidazole molecules and two carboxylate O atoms from two different 3-CPOA^{2-} groups. Adjacent Zn atoms are linked by 3-CPOA^{2-} ligands into a helical chain. The chains are linked into a three-dimensional network by hydrogen bonds.

Comment

3-Carboxyphenoxyacetic acid (3-CPOAH_2) is a dicarboxylic acid that is capable of complex formation. Recently, we reported two Zn^{II} polymers of the dianion, namely $\{[Zn(4,4'\text{-bipyridine})(H_2O)_4](3\text{-CPOA})\}_n$ (in which the 3-CPOA^{2-} ligands exist as free counterions) (Zhao *et al.*, 2005) and $[Zn(3\text{-CPOA})(1H\text{-benzimidazole})_2]_n$ (in which the 3-CPOA^{2-} ligand acts in a bis-monodentate mode to connect two adjacent tetrahedrally coordinated Zn^{II} atoms to form a linear chain; Gao *et al.*, 2005). In our investigations on the bonding nature of carboxylato-bridged zinc complexes, we now report the structure of the title helical chain polymer, $\{[Zn(3\text{-CPOA})(C_3H_4N_2)_2]\cdot 3H_2O\}_n$, (I).



(I)

As depicted in Fig. 1, the asymmetric unit consists of the $[Zn(3\text{-CPOA})(C_3H_4N_2)_2]$ molecule and three uncoordinated water molecules. The water molecules form hydrogen bonds with the uncoordinated imidazole N2 atom and the carboxyl O atoms (O2 and O4) (Table 2). The Zn^{II} centre exhibits a deformed tetrahedral coordination geometry defined by two N atoms from two imidazole molecules and two carboxyl O atoms from two different 3-CPOA^{2-} groups. The Zn–O and Zn–N lengths are similar to the corresponding distances in the reported complexes. The oxyacetate group is twisted out of the benzene plane, the C12—O3—C14—C15 torsion angle being −71.5 (2)°. On the other hand, in the 4,4′-bipyridine adduct, the oxyacetate group is coplanar with the ring, the C13—O3—C12—C11 torsion angle being 6.0 (2)° (Zhao *et al.*, 2005).

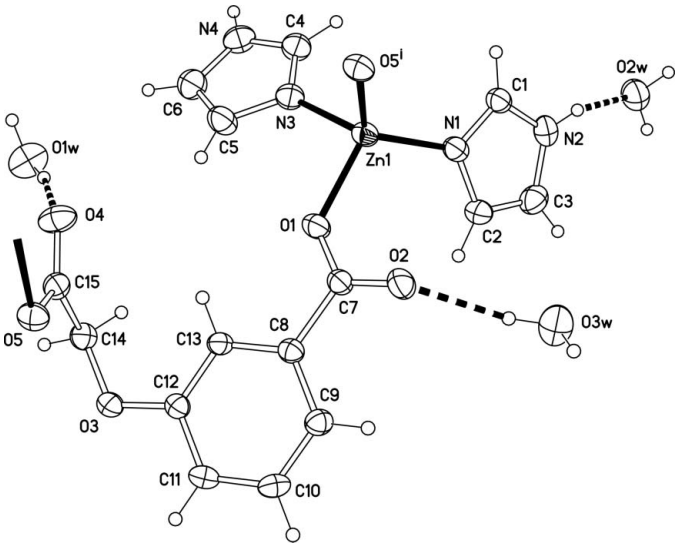


Figure 1
A plot of the title complex, with displacement ellipsoids drawn at the 30% probability level and H atoms shown as small spheres of arbitrary radii. Hydrogen bonds are shown as dashed lines. [Symmetry code: (i) $\frac{3}{2} - x$, $1 + y$, $\frac{3}{2} - z$.]

The chain in (I) is helical and is parallel to the crystallographic *b* axis (Fig. 2). The chains are connected through extensive intermolecular hydrogen bonds involving the water molecules, the imidazole N atom and the carboxyl O atom, to yield a three-dimensional supramolecular network (Table 2 and Fig. 3).

Experimental

The title complex was synthesized by the addition of zinc diacetate dihydrate (2.20 g, 10 mmol) and imidazole (0.68 g, 10 mmol) to a hot aqueous solution of 3-carboxyphenoxyacetic acid (1.96 g, 10 mmol). The pH was adjusted to 6 with 0.2*M* NaOH. The solution was allowed to evaporate at room temperature, and colourless prismatic crystals were obtained after several days. CHN analysis, calculated for $C_{15}H_{20}N_4O_8Zn$: C 40.06, H 4.48, N 12.46%; found: C 40.02, H 4.45, N 12.48%.

Crystal data

$[Zn(C_9H_6O_5)(C_3H_4N_2)_2]\cdot 3H_2O$	$D_x = 1.552$ Mg m^{-3}
$M_r = 449.74$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 17845 reflections
$a = 11.320$ (2) Å	$\theta = 3.2$–$27.5°$
$b = 10.122$ (2) Å	$\mu = 1.33$ mm^{-1}
$c = 17.690$ (4) Å	$T = 295$ (2) K
$\beta = 108.28$ (3)°	Prism, colourless
$V = 1924.7$ (7) Å^3	0.38 × 0.26 × 0.19 mm
$Z = 4$	

Data collection

Rigaku R-AXIS RAPID diffractometer	4408 independent reflections
ω scans	3606 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$R_{int} = 0.047$
$T_{min} = 0.633$, $T_{max} = 0.787$	$\theta_{max} = 27.5°$
18076 measured reflections	$h = -14 \rightarrow 14$
	$k = -12 \rightarrow 13$
	$l = -22 \rightarrow 22$

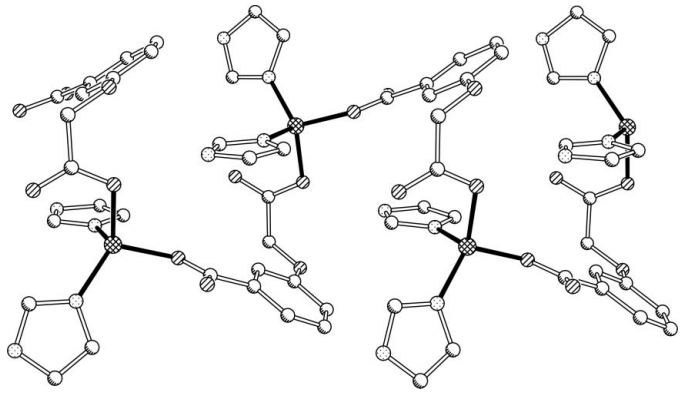


Figure 2
The helical chain structure of the title complex. The water molecules and H atoms are not shown.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.5348P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.041$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.110$	$\Delta\rho_{max} = 0.51$ e Å^{-3}
$S = 1.04$	$\Delta\rho_{min} = -0.41$ e Å^{-3}
4408 reflections	
271 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	1.9776 (19)	O1—C7	1.270 (3)
Zn1—N3	2.000 (2)	O2—C7	1.237 (3)
Zn1—O1	1.9507 (16)	O4—C15	1.232 (3)
Zn1—O5^{i}	1.9782 (19)	O5—C15	1.274 (3)
N1—Zn1—N3	111.80 (8)	O1—Zn1—N3	97.90 (8)
N1—Zn1—O5^{i}	121.55 (8)	O1—Zn1—O5^{i}	105.38 (7)
O1—Zn1—N1	113.12 (8)	O5^{i}—Zn1—N3	104.18 (8)

Symmetry code: (i) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H16···O2W	0.86	1.96	2.770 (3)	156
N4—H17···O5^{ii}	0.86	1.99	2.814 (3)	160
O1W—H1W1···O4	0.85 (4)	2.03 (4)	2.864 (3)	166 (4)
O1W—H1W2···O3W^{iii}	0.85 (3)	2.04 (3)	2.874 (3)	166 (4)
O2W—H2W1···O2^{iv}	0.84 (3)	2.01 (3)	2.825 (3)	163 (3)
O2W—H2W2···O1W^{v}	0.84 (3)	2.11 (3)	2.854 (4)	148 (3)
O3W—H3W1···O2^{vi}	0.85 (3)	2.05 (3)	2.906 (3)	178 (4)
O3W—H3W2···O2	0.86 (4)	2.17 (2)	2.983 (3)	158 (4)

Symmetry codes: (ii) $x, y + 1, z$; (iii) $x - \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$; (iv) $-x + 2, -y + 2, -z + 1$; (v) $-x + 1, -y + 2, -z + 1$; (vi) $-x + 2, -y + 1, -z + 1$.

H atoms on C and N atoms were placed in calculated positions [C—H = 0.93 Å (aromatic) or 0.97 Å (aliphatic), and N—H = 0.86 Å (imidazole)] and refined using the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C,N)$]. The H atoms of the water molecules were located in a difference Fourier map and refined with O—H distance restraints of 0.85 (1) and with $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: *RAPID AUTO* (Rigaku, 1998); cell refinement: *RAPID AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

The authors thank the National Natural Science Foundation of China (grant No. 20101003), the Scientific Fund of Remarkable Teachers of Heilongjiang Province (grant No. 1054 G036) and Heilongjiang University for supporting this work.

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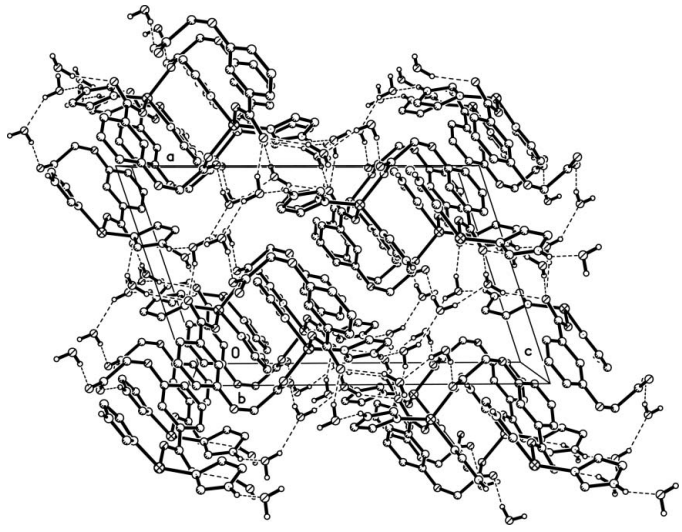

Figure 3
A packing diagram for the title complex. Hydrogen bonds are shown as dashed lines.

Zhao, J.-G., Gu, C.-S., Huo, L.-H., Liu, J.-W. & Gao, S. (2005). *Acta Cryst.* E**61**, m76–m78.