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catena-Poly[[bis(1*H*-benzimidazole-κN^3)zinc(II)]-μ-3-carboxyphenoxyacetato-$\kappa^2 O:O'$]

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.008 Å
R factor = 0.060
wR factor = 0.151
Data-to-parameter ratio = 17.0

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

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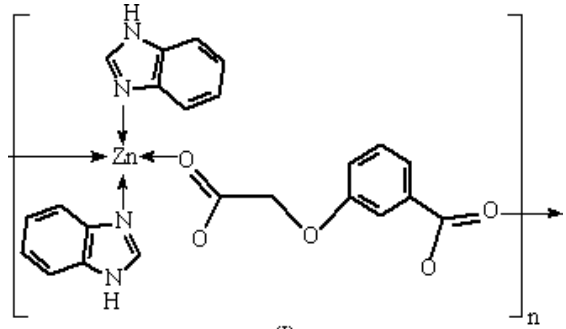
In the title one-dimensional polymer, $[Zn(C_9H_6O_5)(C_7H_6N_2)_2]_n$, the Zn^{II} center exhibits a deformed tetrahedral coordination geometry defined by two N atoms from two benzimidazole molecules and two carboxyl O atoms from two different 4-carboxyphenoxyacetate groups. Each 4-carboxyphenoxyacetate ligand acts in a bis-monodentate mode to connect two adjacent Zn^{II} ions, forming a chain structure. Hydrogen bonds serve to connect the chains into a two-dimensional supramolecular network.

Comment

Carboxyphenoxyacetic acids ($CPOAH_2$) can be regarded as a family of excellent bridging ligands with both rigid and flexible parts, and hence they can be used to form coordination polymers because of their versatile coordination modes and high structural stability. Recently, we have reported the structures of three zinc^{II} polymers constructed by 3- or 4-$CPOA^{2-}$ ligands (3- and 4-carboxyphenoxyacetate, respectively), namely $[Zn(4\text{-}CPOA)(2,2'\text{-bipy})(H_2O)]_n$, (II) (Gao *et al.*, 2004), $[Zn(4\text{-}CPOA)(H_2O)_2]_n$, (III) (Zhao, Gao *et al.*, 2005), in which the octahedrally coordinated Zn^{II} atoms are bridged by 4-$CPOA^{2-}$ ligands, forming a chain structure, as well as $\{[Zn(4,4'\text{-bipy})(H_2O)_4](3\text{-}CPOA)\}_n$ (4,4′-bipy is 4,4′-bipyridine), (IV), in which the octahedrally coordinated Zn^{II} atoms are linked by 4,4′-bipy ligands into infinite cationic polymeric chains (Zhao, Gu *et al.*, 2005). In our efforts to investigate the bonding nature of carboxylate-bridged Zn^{II} polymers, we have now synthesized $[Zn(3\text{-}CPOA)(1H\text{-benzimidazole})_2]_n$, (I).



(I)

As depicted in Fig. 1, the Zn^{II} atom exists in a distorted tetrahedral coordination that is defined by two N atoms from two benzimidazole molecules and two carboxyl O atoms from two different 3-$CPOA^{2-}$ groups. The oxyacetate group is twisted out of the benzene ring plane. Each 3-$CPOA^{2-}$ ligand links two adjacent Zn^{II} atoms, utilizing its two monodentate

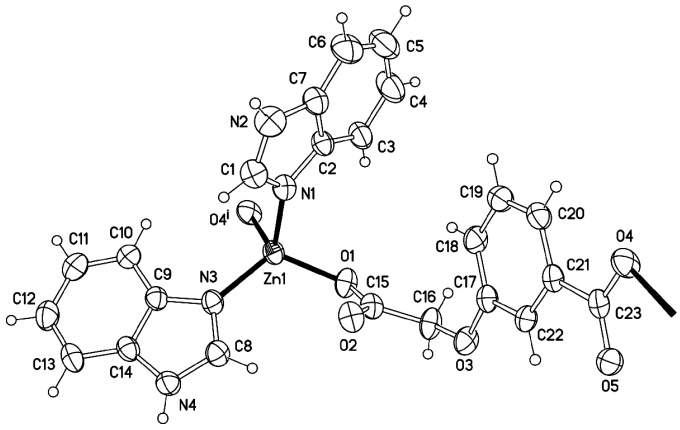


Figure 1
ORTEPII plot (Johnson, 1976) of the title complex, with displacement ellipsoids drawn at the 30% probability level. See Table 1 for symmetry codes.

carboxyl groups to form a one-dimensional infinite chain structure (Fig. 2). The chains are connected through intermolecular hydrogen bonds, forming a two-dimensional supramolecular network (Table 2).

Experimental

The title complex was prepared by the addition of stoichiometric amounts of zinc diacetate dihydrate (0.44 g, 5 mmol) and benzimidazole (0.68 g, 10 mmol) to an aqueous solution of 3-$CPOAH_2$ (0.39 g, 5 mmol), and adjusting the pH to 7 with 0.1 *M* NaOH. The mixture was sealed in a 50 ml Teflon-lined stainless steel bomb and held at 423 K for 3 d. The bomb was cooled slowly to room temperature and colorless prismatic crystals were obtained over several days. Analysis calculated for $C_{23}H_{18}N_4O_5Zn$: C 55.72, H 3.66, N 11.30%; found: C 55.86, H 3.62, N 11.33%.

Crystal data

$[Zn(C_9H_6O_5)(C_7H_6N_2)_2]$	$Z = 2$
$M_r = 495.80$	$D_x = 1.459$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 10.580$ (3) Å	Cell parameters from 8851 reflections
$b = 11.356$ (3) Å	$\theta = 3.4$–$27.5°$
$c = 11.492$ (3) Å	$\mu = 1.13$ mm^{-1}
$\alpha = 116.06$ (2)°	$T = 295$ (2) K
$\beta = 100.32$ (2)°	Prism, colorless
$\gamma = 104.936$ (14)°	0.37 × 0.26 × 0.18 mm
$V = 1128.4$ (6) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	5055 independent reflections
ω scans	3129 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$R_{int} = 0.045$
$T_{min} = 0.679$, $T_{max} = 0.822$	$\theta_{max} = 27.5°$
10127 measured reflections	$h = -13 \rightarrow 13$
	$k = -14 \rightarrow 14$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0715P)^2 + 0.3509P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.060$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.151$	$\Delta\rho_{max} = 0.43$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.26$ e Å^{-3}
5055 reflections	
298 parameters	
H-atom parameters constrained	

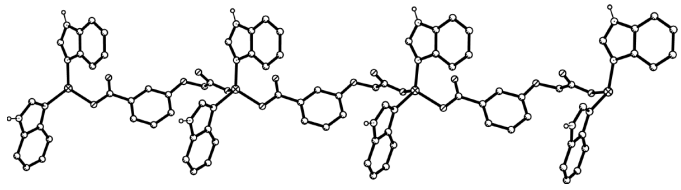


Figure 2
The one-dimensional chain structure of the title complex. H atoms have been omitted for clarity.

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.942 (3)	O1—C15	1.266 (4)
Zn1—O4^{i}	1.986 (3)	O2—C15	1.231 (5)
Zn1—N1	2.027 (3)	O4—C23	1.277 (5)
Zn1—N3	2.011 (3)	O5—C23	1.232 (5)
O1—Zn1—O4^{i}	110.49 (12)	O4^{i}—Zn1—N1	100.62 (12)
O1—Zn1—N1	105.98 (13)	O4^{i}—Zn1—N3	111.56 (12)
O1—Zn1—N3	119.11 (13)	N3—Zn1—N1	107.20 (14)

Symmetry code: (i) $x, 1 + y, z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H24···O2^{ii}	0.86	1.93	2.747 (5)	158
N4—H25···O5^{iii}	0.86	1.93	2.688 (4)	146

Symmetry codes: (ii) $1 - x, 1 - y, 1 - z$; (iii) $2 - x, 1 - y, 1 - z$.

H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å, N—H = 0.86 Å and $U_{iso}(H) = 1.2U_{eq}$(C,N), and were refined in the riding-model approximation.

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*.

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