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catena-Poly[[(1,10-phenanthroline-κ^2N,N')-zinc(II)]-μ-3-carboxylatophenoxyacetato-$\kappa^2O,O':\kappa^2O'',O'''$]

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.088
Data-to-parameter ratio = 15.6

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

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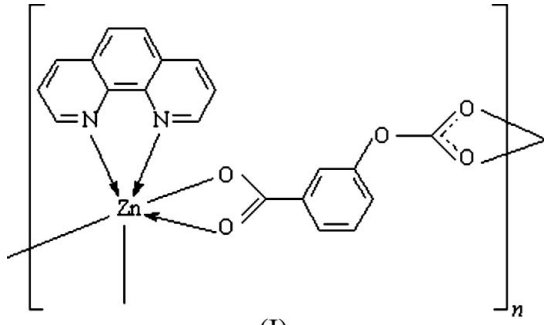
In the title coordination polymer, $[Zn(C_9H_6O_5)(C_8H_{12}N_2)]_n$, the Zn^{II} atom is surrounded by two chelating 3-carboxylatophenoxyacetate (3-CPOA) dianions and one 1,10-phenanthroline (phen) ligand. Adjacent Zn^{II} atoms are bridged by 3-CPOA to form a zigzag chain structure. The polymeric chains are connected *via* π–π stacking interactions.

Comment

3-Carboxyphenoxyacetic acid (3-CPOAH_2) can be regarded as an excellent bridging ligand with both rigid and flexible parts. We have recently reported the structures of three Zn^{II} complexes of 3-CPOA, with different aromatic ligands, namely benzimidazole, imidazole and 4,4′-bipyridine (Zhao *et al.*, 2005; Gao *et al.*, 2005; Zhang *et al.*, 2005). We report here the title Zn^{II} complex, (I), in which the aromatic ligand is phenanthroline.



(I)

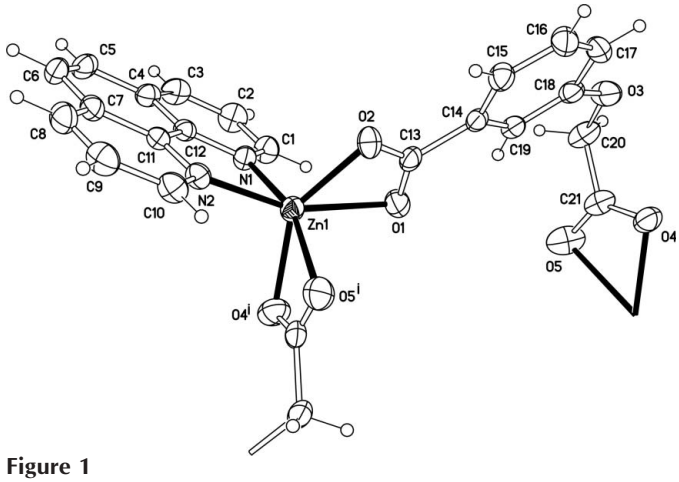


Figure 1
ORTEPII plot (Johnson, 1976) of (I), with displacement ellipsoids drawn at the 30% probability level [symmetry code: (i) $-x+\frac{3}{2}$, $y-\frac{1}{2}$, $-z+\frac{3}{2}$].

As illustrated in Fig. 1, the six-coordinated Zn^{II} atom is surrounded by two chelating 3-CPOA and one 1,10-phenanthroline (phen) ligand. The Zn—N and Zn—O bond distances (Table 1) are somewhat longer than the corresponding distances found for tetrahedrally coordinated Zn^{II} atoms (Gao *et al.*, 2005; Zhang *et al.*, 2005). The oxyacetate group is twisted out of the benzene plane, with a C18—O3—C20—C21 torsion angle of −76.4 (3)°.

Adjacent Zn^{II} atoms are linked by the 3-CPOA to form a one-dimensional zigzag chain, with a Zn1···Zn1*A* distance of 8.230 (3) Å and a Zn1···Zn1*A*···Zn1*B* angle of 141.5 (3)° [symmetry codes: (*A*) $-x+3/2, y+1/2, -z+3/2$; (*B*) $x, y+1, z$] (Fig. 2). The centroid-to-centroid separation of 3.451 (2) Å between parallel benzene rings of neighboring phen ligands suggests π–π stacking interaction. With the help of such interactions, the polymeric chains are assembled to form a two-dimensional supramolecular network (Fig. 3).

Experimental

Zinc diacetate dihydrate (0.88 g, 10 mmol) and phen (1.99 g, 10 mmol) were dissolved in a hot aqueous solution (20 ml) of 3-CPOAH_2 (1.96 g, 10 mmol). The pH value of the solution was adjusted to 7 with 0.1 *M* sodium hydroxide solution. Colorless crystals of (I) were obtained from the solution after several days. Analysis calculated for $C_{21}H_{14}N_2O_5Zn$: C 57.36, H 3.21, N 6.37%; found: C 57.32, H 3.22, N 6.39%.

Crystal data

$[Zn(C_9H_6O_5)(C_8H_{12}N_2)]$	D_x = 1.630 Mg m^{-3}
M_r = 439.73	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 15325 reflections
a = 7.6164 (15) Å	θ = 3.0–27.5°
b = 15.542 (3) Å	μ = 1.41 mm^{-1}
c = 15.186 (3) Å	T = 295 (2) K
β = 94.60 (3)°	Prism, colorless
V = 1791.8 (6) Å^3	0.37 × 0.24 × 0.19 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	4085 independent reflections
ω scans	3241 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	R_{int} = 0.030
T_{min} = 0.624, T_{max} = 0.775	θ_{max} = 27.5°
17147 measured reflections	$h = -9 \rightarrow 9$
	$k = -20 \rightarrow 20$
	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 0.3474P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.088	$\Delta\rho_{max}$ = 0.33 e Å^{-3}
S = 1.03	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
4085 reflections	
262 parameters	
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

Zn1—O1	2.4622 (17)	Zn1—O5^{i}	2.298 (2)
Zn1—O2	2.0053 (16)	Zn1—N1	2.0962 (18)
Zn1—O4^{i}	2.0745 (19)	Zn1—N2	2.1093 (17)

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

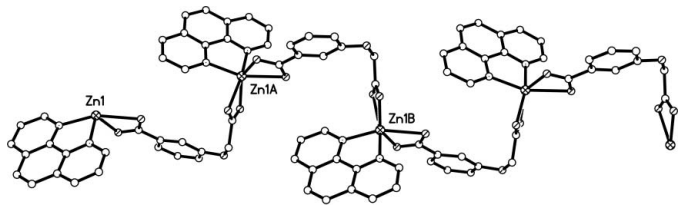


Figure 2
The zigzag chain structure of (I). The H atoms have been omitted. [Symmetry codes: (A) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (B) $x, y+1, z$.]

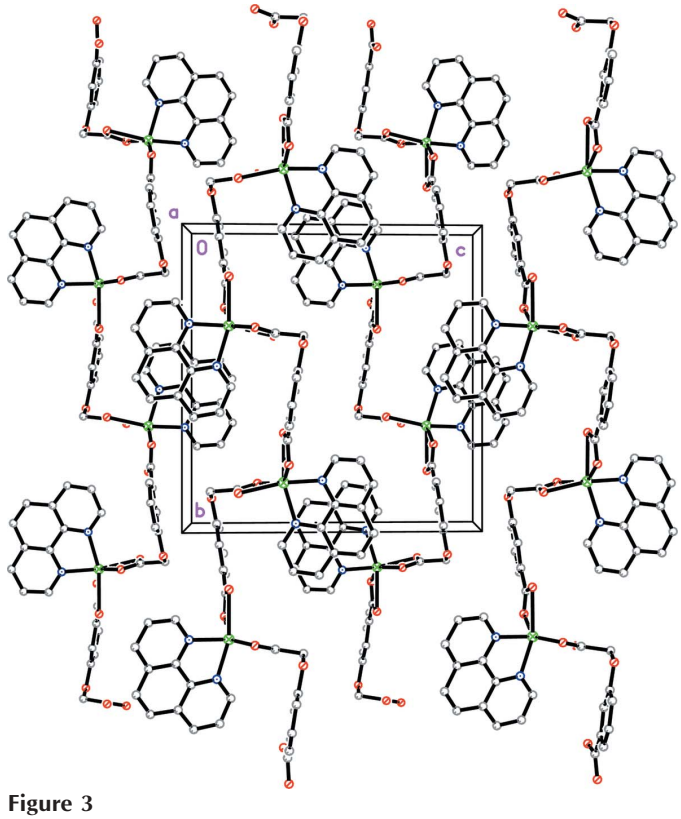


Figure 3
Packing diagram of (I), viewed along the *a* axis. All H atoms have been omitted.

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

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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