Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[bis[(pyridine-κN)zinc(II)](*Zn*—*Zn*)-μ_4-carboxylatophenoxyacetato]

Li-Hua Huo,[a] Shan Gao[a] and Seik Weng Ng[b]*

[a]College of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and [b]Department of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.032
wR factor = 0.080
Data-to-parameter ratio = 16.2

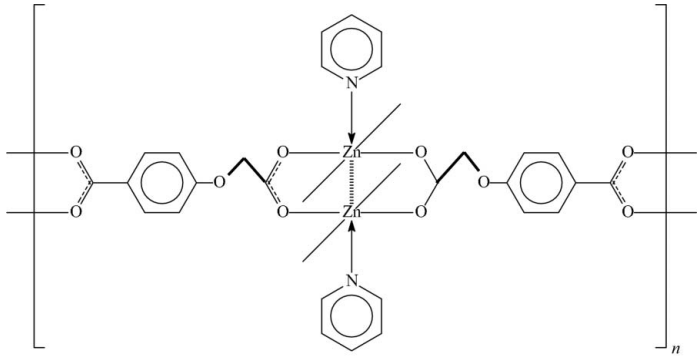
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 28 September 2005
Accepted 5 October 2005
Online 12 October 2005

The title compound, $[Zn_2(C_9H_6O_5)_2(C_5H_5N)_2]$, contains pairs of pyridine-coordinated Zn^{2+} ions [Zn···Zn = 2.987 (1) Å] which are bridged by two carboxylate fragments and two –O–CH_2–CO_2 fragments of four 4-carboxylatophenoxyacetate dianions to give rise to ZnO_4N square-based pyramids. The extended connectivity results in a layered structure.

Comment

The 4-carboxylatophenoxyacetate dianion chelates to zinc(II) through its two carboxylate ends to form a polymeric compound in its diaqua derivative (Zhao *et al.*, 2005). Assuming that the same species exists in solution, the addition of pyridine readily displaces the water molecules to afford the bis-pyridine adduct which was crystallized as the title compound, (I).



(I)

Compound (I) can be described as a polymer of dinuclear units (Fig. 1). Two adjacent zinc cations are linked by a pair of 4-carboxy–CO_2 units and also by a pair of oxyacetate —O–CH_2–CO_2 units of four different dianions to furnish two intersecting centrosymmetric $C_2O_4Zn_2$ rings. Around each Zn atom, the four O atoms constitute an approximate ZnO_4 square plane, above which lies the N atom of the pyridine molecule. The Zn atom is displaced from its O-atom neighbours, in the direction of the N atom, by 0.378 (1) Å, probably due to the presence of the second Zn atom opposite the axial site at a distance of 2.987 (1) Å. The bridging mode of the —CO_2 and —O—CH_2–CO_2 units leads to a tightly held layer structure.

Experimental

An aqueous solution of zinc(II) acetate dihydrate (1.10 g, 5 mmol) was added to an aqueous solution of 4-carboxyphenoxyacetic acid (0.98 g, 5 mmol). An excess (1 ml) of pyridine was then added,

followed by drops of aqueous sodium hydroxide (0.1 *M*) until the pH of the mixture was 6. Colorless crystals of (I) were isolated from the filtered solution after several days. Analysis calculated for $C_{14}H_{11}NO_5Zn$: C 49.66, H 3.27, N 4.14%; found: C 49.62, H 3.25, N 4.11%.

Crystal data

$[Zn_2(C_9H_6O_5)_2(C_5H_5N)_2]$	D_x = 1.677 Mg m^{-3}
M_r = 677.22	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 12595 reflections
a = 9.354 (2) Å	θ = 3.5–27.5°
b = 14.876 (3) Å	μ = 1.85 mm^{-1}
c = 10.231 (2) Å	T = 295 (2) K
β = 109.58 (3)°	Block, colorless
V = 1341.3 (5) Å^3	0.34 × 0.25 × 0.16 mm
Z = 2	

Data collection

Rigaku RAXIS-RAPID diffractometer	3069 independent reflections
ω scan	2553 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	R_{int} = 0.026
T_{min} = 0.459, T_{max} = 0.756	θ_{max} = 27.5°
12817 measured reflections	$h = -12 \rightarrow 12$
	$k = -19 \rightarrow 19$
	$l = -12 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0461P)^2 + 0.5185P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.032	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.080	$\Delta\rho_{max}$ = 0.64 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
3069 reflections	
190 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.051 (2)	Zn1—O5^{iii}	2.087 (2)
Zn1—O2^{i}	2.011 (2)	Zn1—N1	2.032 (2)
Zn1—O4^{ii}	2.059 (2)	Zn1—Zn1^{i}	2.987 (1)
O1—Zn1—O2^{i}	158.45 (7)	O2^{i}—Zn1—O5^{iii}	87.03 (7)
O1—Zn1—O4^{ii}	89.76 (7)	O2^{i}—Zn1—N1	107.22 (8)
O1—Zn1—O5^{iii}	86.35 (7)	O4^{ii}—Zn1—O5^{iii}	158.88 (7)
O1—Zn1—N1	94.17 (7)	O4^{ii}—Zn1—N1	100.16 (7)
O2^{i}—Zn1—O4^{ii}	89.07 (7)	O5^{iii}—Zn1—N1	100.82 (7)

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

H atoms were positioned geometrically (C—H = 0.93 Å for the aromatic H atoms and 0.97 Å for the aliphatic H atoms) and were included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$. The displacement factors of atoms C1, C2, and C3 perhaps suggest some static or dynamic disorder of the pyridine ring, but no attempt was made to model this further.

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 (No. 20101003), the Scientific Fund for Remarkable Teachers of Heilongjiang Province (No. 1054 G036) and the University of Malaya for supporting this study.

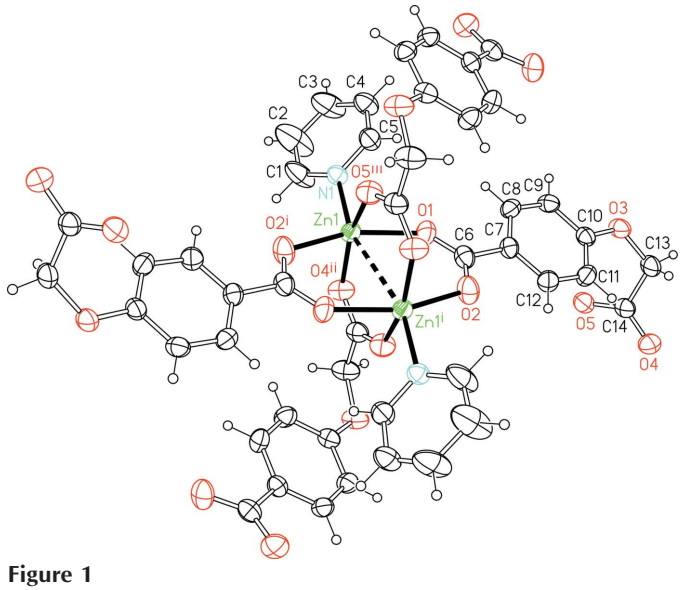


Figure 1
View of a fragment of (I), showing the close association of two zinc cations. Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii. Symmetry codes are as given in Table 1.

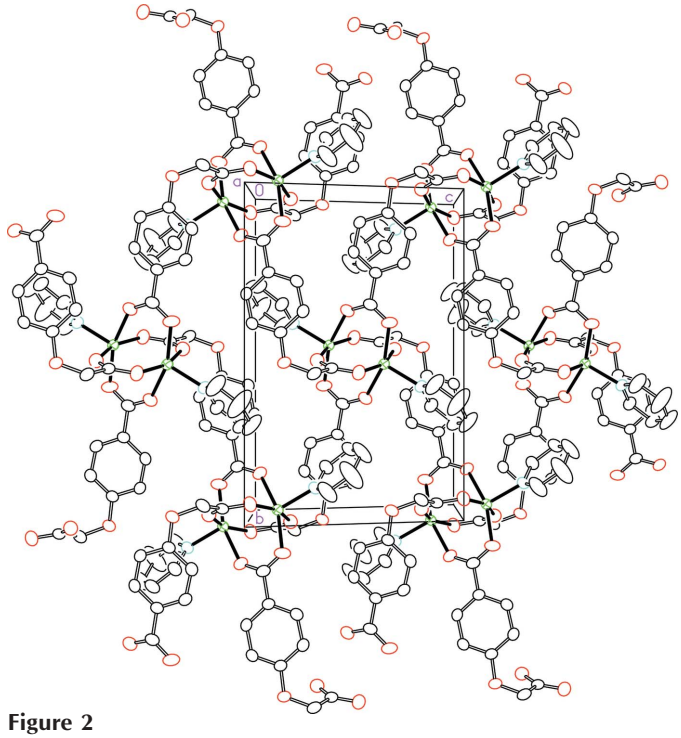


Figure 2
View of the layered structure of (I).

References

Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC Inc., 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Zhao, J. G., Gao, S., Huo, L. H. & Ng, S. W. (2005). *Acta Cryst.* E**61**, m115–m116.