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catena-Poly[bis(4-pyridylthioacetato)zinc(II)]

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.046
wR factor = 0.109
Data-to-parameter ratio = 16.4

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

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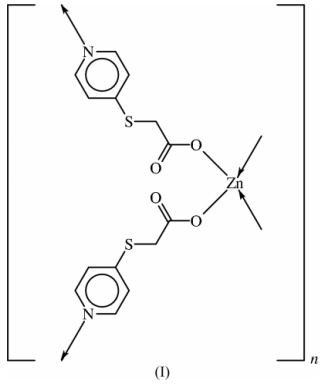
The Zn atom in the polymeric $[Zn(C_7H_6NO_2S)_2]_n$ chain of the title compound lies on a twofold axis. It is covalently bonded to the carboxyl O atoms of two ligands and datively bonded to the pyridyl N atoms of two other ligands in a tetrahedral environment.

Comment

The reaction (Kondo *et al.*, 2002) of zinc nitrate and 4-pyridylthioacetic acid in water in the presence of triethylamine as the H-atom abstractor yields $[Zn(OH)(C_7N_6NO_2S)]$, which adopts a helical chain structure [$Zn-O_{carboxyl}$ 1.966 (5) and $Zn-N_{pyridyl}$ 2.063 (5) Å]. The compound crystallizes in a chiral space group, a property that the authors suggest would be useful if the crystals are to be used as functional materials (Kondo *et al.*, 2002).

A modification of the synthesis with copper nitrate in place of zinc nitrate led to a centrosymmetric compound in which the metal atom is coordinated by two water molecules and also by a molecule of the ammonia that was used as the base (Huang *et al.*, 2003). Curiously, the title compound, (I), was obtained free of water, probably because the hydrothermal conditions employed involved a different reaction mechanism.



(I)

Compound (I) (Fig. 1) exists as a polymeric chain. The Zn atom in the chain lies on a twofold axis and is covalently bonded to the carboxyl O atoms of two ligands [Zn—O 1.942 (2) Å] and datively bonded to the pyridyl N atoms of two other ligands [Zn—N 2.040 (3) Å], so that a tetrahedral environment results.

Experimental

A mixture of zinc acetate dihydrate (0.27 g, 1 mmol), 4-pyridylthioacetic acid (0.13 g, 0.8 mmol) and water (7 ml) was treated with 2 *M* sodium hydroxide to a pH of about 6. The mixture was transferred into a 15 ml Teflon-lined stainless steel reactor and heated at 443 K

for 120 h. Colourless crystals of (I) were obtained from the cooled solution in about 50% yield. Analysis found: C 41.82, H 3.06, N 6.91, S 15.94%; calculated for $C_{14}H_{12}N_2O_4S_2Zn$: C 41.85, H 3.01, N 6.97, S 15.96%.

Crystal data

$[Zn(C_7H_6NO_2S)_2]$	D_x = 1.655 Mg m^{-3}
M_r = 401.75	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 2658 reflections
a = 14.968 (1) Å	θ = 3.4–27.0°
b = 8.450 (1) Å	μ = 1.80 mm^{-1}
c = 14.084 (1) Å	T = 298 (2) K
β = 115.19 (5)°	Prism, colourless
V = 1612.0 (2) Å^3	0.32 × 0.26 × 0.18 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	1726 independent reflections
	1126 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.069
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 27.0°
	$h = -11 \rightarrow 18$
T_{min} = 0.059, T_{max} = 0.816	$k = -10 \rightarrow 9$
4426 measured reflections	$l = -17 \rightarrow 16$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.046	$w = 1/[\sigma^2(F_o^2) + (0.052P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.109	
S = 0.83	$(\Delta/\sigma)_{max}$ = 0.001
1726 reflections	$\Delta\rho_{max}$ = 0.89 e Å^{-3}
105 parameters	$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.942 (2)	Zn1—N1^{i}	2.040 (3)
O1—Zn1—O1^{ii}	137.2 (2)	O1—Zn1—N1^{iii}	103.9 (1)
O1—Zn1—N1^{i}	101.9 (1)	N1^{i}—Zn1—N1^{iii}	104.6 (2)

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

H atoms were placed at calculated positions (C—H = 0.93 Å for aromatic H atoms and 0.97 Å for methylene H atoms) and their displacement factors were set to $1.2U_{eq}$(C). The final difference map had a peak of 0.9 e Å^{-3} near Zn1.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

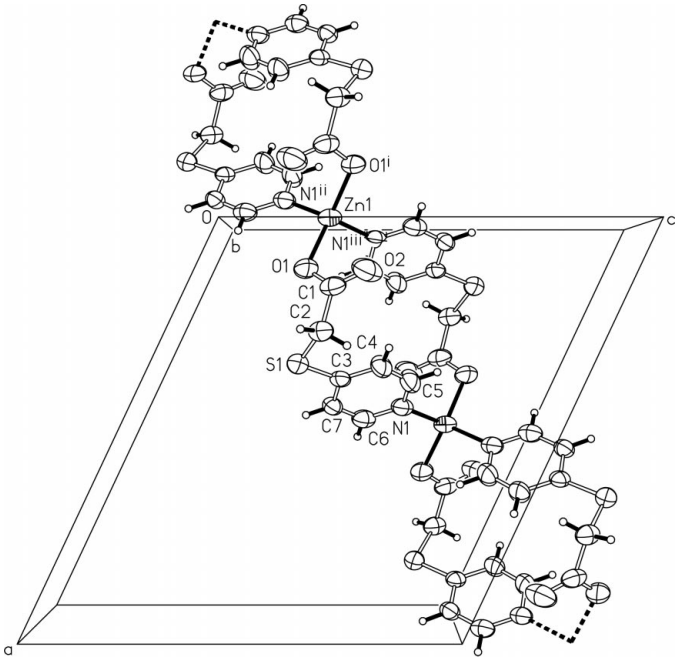


Figure 1
A view of the polymeric $[Zn(C_7H_6NO_2S)_2]_n$ chain of (I), with displacement ellipsoids drawn at the 50% probability level. Symmetry codes: (i) $-x, y, \frac{1}{2}-z$; (ii) $x-\frac{1}{2}, \frac{1}{2}-y, z-\frac{1}{2}$; (iii) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$.

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