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catena-Poly[[bis(*O*,*O*′-diisopropyl dithiophosphato-κ^2S,S')zinc(II)]-μ-1,2-bis(3-pyridylmethylene)hydrazine-$\kappa^2N:N'$]

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.006 Å
R factor = 0.044
wR factor = 0.109
Data-to-parameter ratio = 16.1

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

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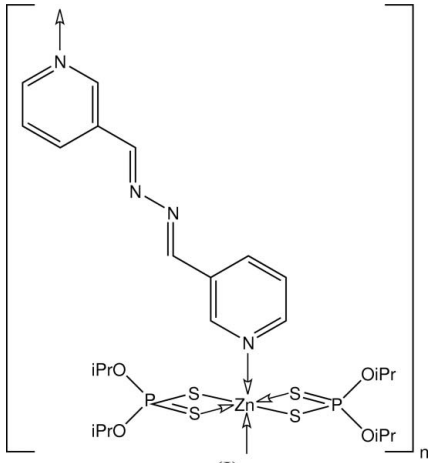
In the polymeric title compound, $[Zn(C_6H_{14}O_2PS_2)_2(C_{12}H_{10}N_4)]_n$, the Zn atom lies on a centre of inversion and the bridging diimine ligand is disposed about another centre of inversion. The Zn atom is in an octahedral geometry defined by a *trans*-N_2S_4 donor set. The polymer topology is that of a step-ladder.

Comment

Structures (Chen *et al.*, 2005; Lai & Tiekink, 2006) related to the title compound, (I), have been investigated as a part of an ongoing study of the nature of polymer formation in zinc and cadmium dithiophosphates [$^-S_2P(OR)_2$; Lai *et al.*, 2004; Lai & Tiekink, 2004; Chen *et al.*, 2006]. In (I), the Zn atom exists within a *trans*-N_2S_4 donor set that defines an approximately octahedral geometry. The Zn atom is situated on a centre of inversion and the bis(4-pyridylmethylene)hydrazine is disposed about another inversion centre. The coordination geometry is distorted octahedral defined by a *trans*-N_2S_4 donor set (Fig. 1).



(I)

The dithiophosphate ligand coordinates in a symmetric fashion and this coordination mode is reflected in the near equivalence of P—S bond distances and of the Zn—S—P bond angles (Table 1). A view of the polymer in (I) is shown in Fig. 2. The polymer topology, consistent with that found for the isomorphous Cd analogue (Lai & Tiekink, 2006), is that of a step-ladder.

Experimental

Compound (I) was prepared by refluxing the parent $Zn[S_2P(OiPr)_2]_2$ compound with bis(3-pyridylmethylene)hydrazine (Aldrich)

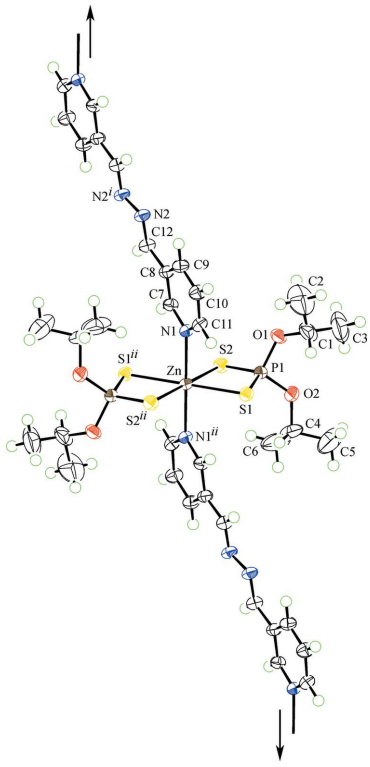


Figure 1
Part of the polymeric structure of (I), showing the crystallographic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $1-x, -y, 2-z$; (ii) $-x, -y, 1-z$.]

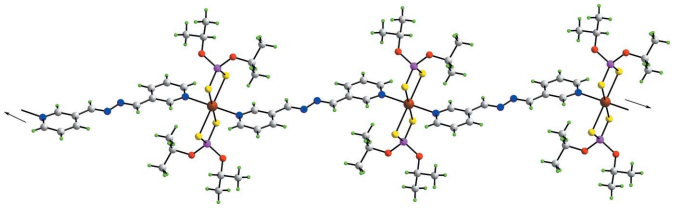


Figure 2
Polymer topology in (I). Colour code: Zn brown, S yellow, P pink, O red, N blue, C grey and H green.

according to a literature procedure (Lai & Tiekink, 2004). Yellow crystals were isolated by the slow evaporation of an 2-propanol solution of the compound (m.p. 381–384 K). IR (KBr disk): ν(C═N) 1464 (*w*), ν(C—O) 1101 (*w*), ν(P—O) 960 (*s*), ν(P—S)$_{asymm}$ 646 (*s*) cm^{-1}.

Crystal data

$[Zn(C_6H_{14}O_2PS_2)_2(C_{12}H_{10}N_4)]$
M_r = 702.13
Monoclinic, $P2_1/n$
a = 11.809 (3) Å
b = 11.243 (3) Å
c = 12.933 (3) Å
β = 108.712 (5)°
V = 1626.3 (7) Å^3
Z = 2
D_x = 1.434 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.15 mm^{-1}
T = 150 (2) K
Plate, yellow
0.30 × 0.25 × 0.08 mm

Data collection

AFC12K/SATURN724 diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.722, T_{max} = 1
(expected range = 0.659–0.912)
34154 measured reflections
2864 independent reflections
2793 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.109
S = 1.08
2864 reflections
178 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2 + 4.0311P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn—S1	2.5420 (9)	S2—P1	1.9792 (11)
Zn—S2	2.5540 (9)	N2—N2^{i}	1.412 (5)
Zn—N1	2.228 (2)	N2—C12	1.268 (4)
S1—P1	2.0013 (11)		
S1—Zn—S2	81.23 (3)	S2—Zn—N1	92.20 (7)
S1—Zn—N1	89.65 (7)	S2—Zn—N1^{ii}	87.80 (7)
S1—Zn—S2^{ii}	98.77 (3)	Zn—S1—P1	82.50 (3)
S1^{ii}—Zn—N1	90.35 (7)	Zn—S2—P1	82.61 (4)

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

H atoms were included in the riding-model approximation, with C—H = 0.95–1.00 Å and U_{iso}(H) = 1.5U_{eq}(methyl C) or 1.2U_{eq}(C). The highest peak is located 1.36 Å from atom C4.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *PATTY* in *DIRDIF92* (Beurskens *et al.*, 1992); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

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