

# catena-Poly[[bis(*O,O'*-diethyl dithiophosphato- $\kappa^2S,S'$ )zinc(II)]- $\mu$ -1,2-di-4-pyridylethane- $\kappa^2N:N'$ ]

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### Key indicators

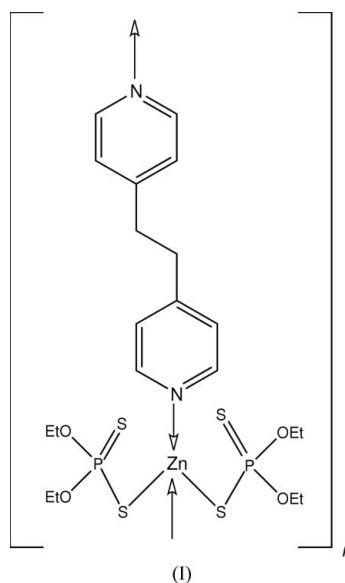
 Single-crystal X-ray study  
 $T = 120$  K  
 Mean  $\sigma(C-C) = 0.005$  Å  
 Disorder in main residue  
 $R$  factor = 0.042  
 $wR$  factor = 0.142  
 Data-to-parameter ratio = 20.1

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

 In the zigzag polymeric title compound,  $[Zn(S_2P(OEt)_2)_2(NC_5H_4CH)_2CH_2C_5H_4N]_n$  or  $[Zn(C_4H_{10}O_2PS_2)_2(C_{12}H_{12}N_2)]_n$ , the Zn atom adopts a distorted tetrahedral  $ZnN_2S_2$  geometry; the bridging di-4-pyridylethane molecules are each disposed about a centre of inversion.

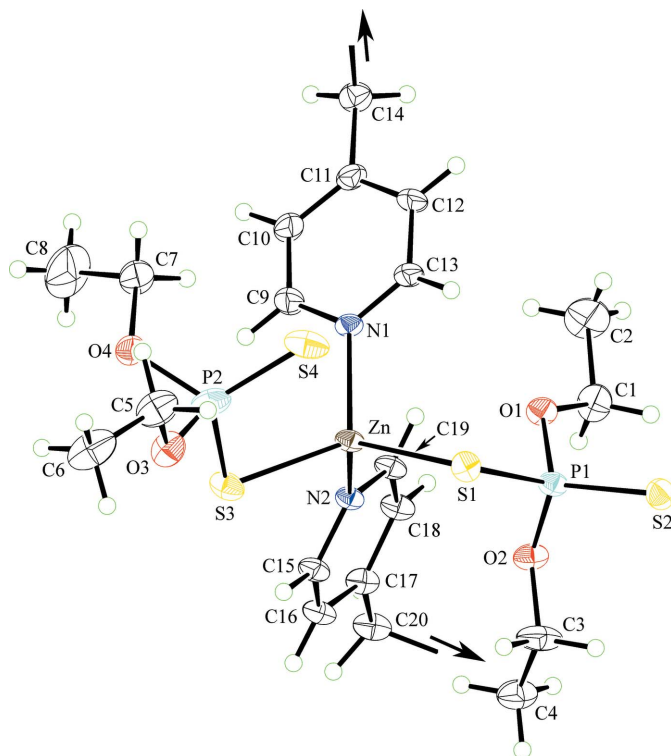
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### Comment

 Previous work on structures related to the title compound,  $[Zn(S_2P(OR)_2)_2(NC_5H_4CH_2CH_2C_5H_4N)]_n$ , (I), has shown that when  $R = ^iPr$  and  $Cy$  (Lai *et al.*, 2004a), zigzag polymeric chains are found. By contrast, increasing the bulk of  $R$  to  $^tBu$ , results in the formation of a straight chain (Lai *et al.*, 2004b).

 The asymmetric unit in (I) comprises  $Zn[S_2P(OEt)_2]_2$  and half each of two 1,2-di-4-pyridylethane ligands, as each of these is disposed about an inversion centre. The coordination geometry (Fig. 1) is distorted tetrahedral, with both dithiophosphate ligands coordinating in the monodentate mode. This is substantiated by the relatively narrow range of tetrahedral angles and the disparity in the P–S bond distances (Table 1). In keeping with expectation (Chen *et al.*, 2006), the topology of the polymeric chain formed in (I) is zigzag (Fig. 2). Chains are linked *via* C–H $\cdots$ S interactions (details in Table 2).

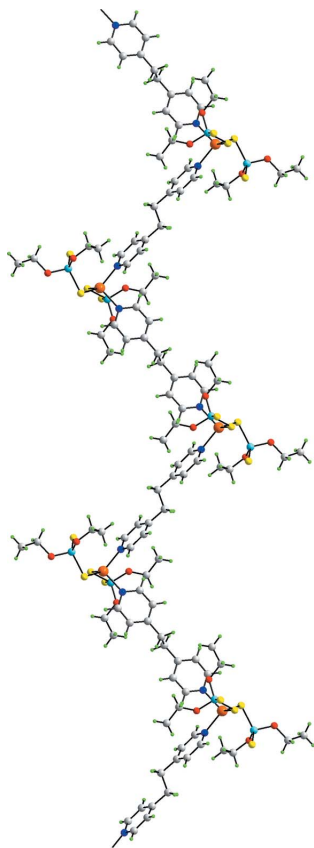
### Experimental

The title compound was prepared by refluxing the parent zinc dithiophosphate with 1,2-di-4-pyridylethane according to a literature



**Figure 1**

The asymmetric unit of (I), showing the atom-labelling scheme. Only the major component of the disorder is shown. Displacement ellipsoids are drawn at the 35% probability level (arbitrary spheres for the H atoms).



**Figure 2**

View of the linear polymer in (I). Colour code: Zn brown, S yellow, P pink, O red, N blue, C grey and H green.

procedure (Lai *et al.*, 2004a). Colourless crystals of (I) were isolated by the slow evaporation of an acetonitrile/ $\text{CHCl}_3$  (1:3) solution (m.p. 389–391 K).

#### Crystal data

$[\text{Zn}(\text{C}_4\text{H}_{10}\text{O}_2\text{PS}_2)_2(\text{C}_{12}\text{H}_{12}\text{N}_2)]$   
 $M_r = 620.03$   
 Monoclinic,  $P2_1/c$   
 $a = 11.6895$  (2) Å  
 $b = 16.9503$  (4) Å  
 $c = 14.6979$  (3) Å  
 $\beta = 103.599$  (1)°

$V = 2830.6$  (1) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.30$  mm<sup>-1</sup>  
 $T = 120$  (2) K  
 $0.25 \times 0.25 \times 0.20$  mm

#### Data collection

Bruker–Nonius 95mm KappaCCD diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)  
 $T_{\min} = 0.829$ ,  $T_{\max} = 1$   
 (expected range = 0.639–0.770)

41164 measured reflections  
 6173 independent reflections  
 4828 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.043$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.142$   
 $S = 1.10$   
 6173 reflections

307 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 1.00$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -1.27$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Zn–S1	2.3211 (9)	S1–P1	2.0153 (12)
Zn–S3	2.3228 (9)	S2–P1	1.9437 (12)
Zn–N1	2.048 (2)	S3–P2	2.0174 (13)
Zn–N2	2.071 (3)	S4–P2	1.9303 (16)
S1–Zn–S3	119.67 (3)	S3–Zn–N1	114.64 (8)
S1–Zn–N1	110.85 (8)	S3–Zn–N2	98.95 (7)
S1–Zn–N2	112.14 (8)	N1–Zn–N2	97.59 (10)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C5-H5a\cdots S4^i$	0.99	2.80	3.770 (5)	165
$C18-H18\cdots S1^{ii}$	0.95	2.87	3.805 (3)	168

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

H atoms were positioned geometrically ( $C-H = 0.95-0.99$  Å) and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ . Disorder was modelled for the atoms O4 and C7 [occupancy of the major component = 0.662 (9)] but not for the other atoms of this group. The atoms of the minor component were refined isotropically. The maximum and minimum residual electron-density peaks are located 0.96 and 0.78 Å, respectively, from atoms C14 and S4.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *PATY* in *DIRDIF92* (Beurskens *et al.*, 1992); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006) and *ORTEPIII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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