Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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Received 8 February 2007
Accepted 13 February 2007

Key indicators

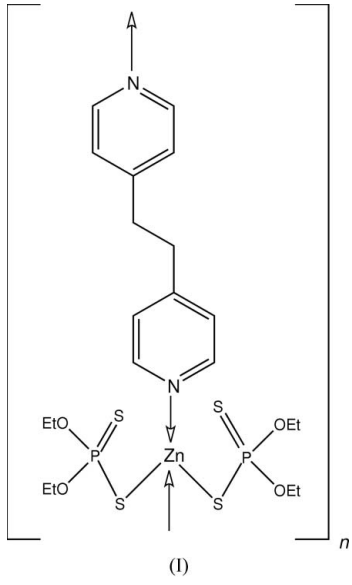
Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.042
wR factor = 0.142
Data-to-parameter ratio = 20.1

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.

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 = ^{i}Pr and Cy (Lai *et al.*, 2004*a*), zigzag polymeric chains are found. By contrast, increasing the bulk of R to ^{i}Bu, results in the formation of a straight chain (Lai *et al.*, 2004*b*).



(I)

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···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

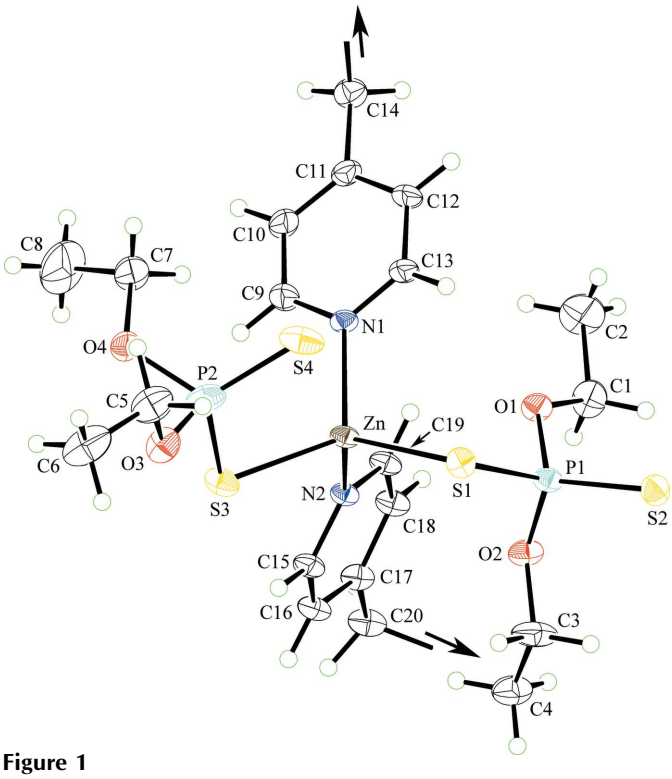


Figure 1
The asymmetric unit of (I), showing the atom-labelling scheme. Only the major component of the disorder is shown. Displacement ellipsoids are drawn at the 35% probability level (arbitrary spheres for the H atoms).

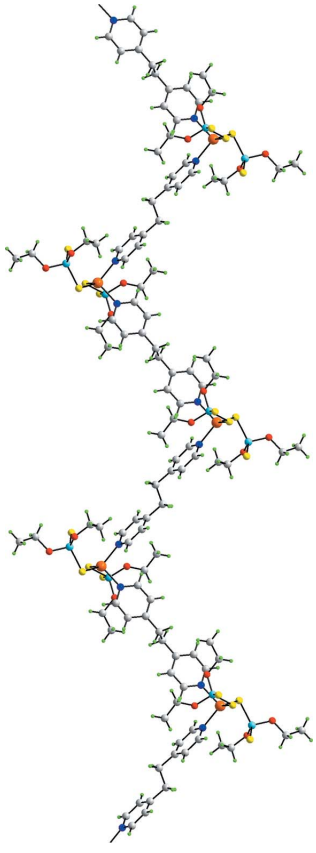


Figure 2
View of the linear polymer in (I). Colour code: Zn brown, S yellow, P pink, O red, N blue, C grey and H green.

procedure (Lai *et al.*, 2004*a*). Colourless crystals of (I) were isolated by the slow evaporation of an acetonitrile/$CHCl_3$ (1:3) solution (m.p. 389–391 K).

Crystal data

$[Zn(C_4H_{10}O_2PS_2)_2(C_{12}H_{12}N_2)]$
M_r = 620.03
Monoclinic, $P2_1/c$
a = 11.6895 (2) Å
b = 16.9503 (4) Å
c = 14.6979 (3) Å
β = 103.599 (1)°
V = 2830.6 (1) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.30 mm^{-1}
T = 120 (2) K
0.25 × 0.25 × 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_{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
$\Delta\rho_{max}$ = 1.00 e Å^{-3}
$\Delta\rho_{min}$ = −1.27 e Å^{-3}

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···A	D—H	H···A	D···A	D—H···A
C5—H5a···S4^{i}	0.99	2.80	3.770 (5)	165
C18—H18···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_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). Disorder was modelled for the O4 ethyl group in that two positions were resolved 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: *PATTY* in *DIRDIF92* (Beurskens *et al.*, 1992); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006) and *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

This work was supported by the departmental research grant AX-0026 from The Robert A. Welch Foundation. Cheminova is thanked for the gift of the dithiophosphate ligand used in this study. The authors also thank the EPSRC X-ray Crystallographic Service, University of Southampton for the data collection.

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supporting information

Acta Cryst. (2007). E**63**, m818–m820 [https://doi.org/10.1107/S1600536807007544]

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$c = 14.6979$ (3) Å
$\beta = 103.599$ (1)°
$V = 2830.6$ (1) Å^3
$Z = 4$
$F(000) = 1288$
$D_x = 1.455$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 6612 reflections
$\theta = 1.0$–$27.5°$
$\mu = 1.30$ mm^{-1}
$T = 120$ K
Block, colourless
0.25 × 0.25 × 0.20 mm

Data collection

Bruker-Nonius 95mm CCD camera on κ-goniostat diffractometer
Radiation source: Bruker-Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.829$, $T_{max} = 1$
41164 measured reflections
6173 independent reflections
4828 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 27.0°$, $\theta_{min} = 1.9°$
$h = -14\rightarrow13$
$k = -20\rightarrow21$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.142$
$S = 1.10$
6173 reflections
307 parameters
9 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0866P)^2 + 1.3066P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.00$ e Å^{-3}
$\Delta\rho_{min} = -1.27$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn	0.20747 (3)	0.19424 (2)	0.27185 (2)	0.02651 (13)	
S1	0.03650 (7)	0.12678 (5)	0.27755 (5)	0.0330 (2)	
S2	−0.22485 (8)	0.09117 (5)	0.13540 (6)	0.0393 (2)	
S3	0.32373 (9)	0.24764 (5)	0.40808 (6)	0.0388 (2)	
S4	0.32107 (11)	0.05103 (6)	0.41255 (7)	0.0522 (3)	
P1	−0.07909 (7)	0.15089 (5)	0.15571 (6)	0.0293 (2)	
O1	−0.0056 (2)	0.13769 (14)	0.07833 (15)	0.0347 (5)	
O2	−0.1019 (2)	0.24322 (13)	0.14423 (17)	0.0362 (5)	
O3	0.4127 (2)	0.15756 (17)	0.57328 (18)	0.0466 (6)	
N1	0.2989 (2)	0.13575 (15)	0.18959 (17)	0.0268 (5)	
N2	0.1731 (2)	0.29633 (14)	0.19270 (17)	0.0263 (5)	
C1	−0.0597 (4)	0.1493 (3)	−0.0199 (3)	0.0517 (10)	
H1A	−0.0652	0.2063	−0.0349	0.062*	
H1B	−0.1401	0.1268	−0.0353	0.062*	
C2	0.0156 (5)	0.1085 (4)	−0.0748 (3)	0.0812 (17)	
H2A	−0.0188	0.1154	−0.1419	0.122*	
H2B	0.0200	0.0521	−0.0596	0.122*	
H2C	0.0949	0.1312	−0.0590	0.122*	
C3	−0.1762 (4)	0.2814 (2)	0.1971 (4)	0.0571 (12)	
H3A	−0.1419	0.2753	0.2650	0.069*	
H3B	−0.2554	0.2569	0.1822	0.069*	
C4	−0.1854 (4)	0.3668 (2)	0.1715 (3)	0.0528 (10)	
H4A	−0.2354	0.3937	0.2067	0.079*	
H4B	−0.2200	0.3723	0.1043	0.079*	
H4C	−0.1068	0.3906	0.1866	0.079*	
C5	0.4511 (4)	0.0905 (3)	0.6350 (3)	0.0589 (11)	
H5A	0.5131	0.0610	0.6137	0.071*	
H5B	0.3840	0.0545	0.6332	0.071*	
C6	0.4982 (4)	0.1195 (3)	0.7326 (3)	0.0708 (15)	
H6A	0.5244	0.0745	0.7742	0.106*	
H6B	0.4362	0.1481	0.7537	0.106*	
H6C	0.5648	0.1549	0.7341	0.106*	
P2	0.39999 (9)	0.14657 (6)	0.46451 (7)	0.0436 (3)	0.662 (9)
O4	0.5421 (3)	0.1528 (2)	0.4746 (3)	0.0408 (13)	0.662 (9)
C7	0.5930 (5)	0.1253 (4)	0.3991 (4)	0.057 (2)	0.662 (9)

H7A	0.5317	0.1241	0.3398	0.069*	0.662 (9)
H7B	0.6237	0.0710	0.4127	0.069*	0.662 (9)
C8	0.6886 (5)	0.1779 (4)	0.3894 (5)	0.109 (2)	0.662 (9)
H8A	0.7223	0.1594	0.3382	0.163*	0.662 (9)
H8B	0.7496	0.1783	0.4479	0.163*	0.662 (9)
H8C	0.6577	0.2315	0.3755	0.163*	0.662 (9)
P22	0.39999 (9)	0.14657 (6)	0.46451 (7)	0.0436 (3)	0.338 (9)
O24	0.5095 (6)	0.1304 (5)	0.4224 (6)	0.047 (3)*	0.338 (9)
C27	0.5977 (9)	0.1927 (7)	0.4438 (9)	0.067 (4)*	0.338 (9)
H27A	0.5603	0.2448	0.4268	0.081*	0.338 (9)
H27B	0.6349	0.1930	0.5117	0.081*	0.338 (9)
C28	0.6886 (5)	0.1779 (4)	0.3894 (5)	0.109 (2)	0.338 (9)
H28A	0.7504	0.2181	0.4052	0.163*	0.338 (9)
H28B	0.6518	0.1805	0.3222	0.163*	0.338 (9)
H28C	0.7231	0.1255	0.4049	0.163*	0.338 (9)
C9	0.3959 (3)	0.1690 (2)	0.1721 (3)	0.0395 (8)	
H9	0.4247	0.2165	0.2038	0.047*	
C10	0.4552 (3)	0.1374 (2)	0.1106 (3)	0.0412 (8)	
H10	0.5258	0.1615	0.1031	0.049*	
C11	0.4139 (3)	0.0725 (2)	0.0606 (2)	0.0369 (8)	
C12	0.3157 (3)	0.0362 (2)	0.0806 (3)	0.0478 (10)	
H12	0.2863	−0.0115	0.0500	0.057*	
C13	0.2607 (3)	0.0698 (2)	0.1452 (2)	0.0377 (8)	
H13	0.1936	0.0445	0.1578	0.045*	
C14	0.4725 (3)	0.0394 (2)	−0.0142 (2)	0.0407 (8)	
H14A	0.4129	0.0341	−0.0741	0.049*	
H14B	0.5336	0.0767	−0.0241	0.049*	
C15	0.1647 (3)	0.36711 (19)	0.2319 (2)	0.0324 (7)	
H15	0.1827	0.3707	0.2983	0.039*	
C16	0.1316 (3)	0.43427 (19)	0.1806 (2)	0.0361 (7)	
H16	0.1261	0.4829	0.2113	0.043*	
C17	0.1059 (3)	0.43093 (19)	0.0834 (2)	0.0333 (7)	
C18	0.1170 (3)	0.35852 (19)	0.0433 (2)	0.0338 (7)	
H18	0.1017	0.3538	−0.0229	0.041*	
C19	0.1501 (3)	0.29310 (18)	0.0989 (2)	0.0302 (7)	
H19	0.1569	0.2439	0.0698	0.036*	
C20	0.0656 (3)	0.50259 (19)	0.0234 (3)	0.0399 (8)	
H20A	0.1112	0.5068	−0.0253	0.048*	
H20B	0.0808	0.5507	0.0627	0.048*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.0355 (2)	0.0271 (2)	0.0220 (2)	0.00067 (14)	0.01688 (15)	−0.00188 (13)
S1	0.0391 (4)	0.0375 (4)	0.0258 (4)	−0.0057 (3)	0.0145 (3)	0.0035 (3)
S2	0.0375 (5)	0.0428 (5)	0.0396 (5)	−0.0072 (4)	0.0135 (4)	−0.0051 (4)
S3	0.0566 (6)	0.0371 (5)	0.0222 (4)	0.0061 (4)	0.0082 (4)	−0.0010 (3)
S4	0.0826 (8)	0.0403 (5)	0.0395 (5)	0.0165 (5)	0.0262 (5)	0.0029 (4)

P1	0.0357 (4)	0.0305 (4)	0.0262 (4)	−0.0003 (3)	0.0163 (3)	−0.0015 (3)
O1	0.0380 (12)	0.0469 (14)	0.0230 (11)	0.0018 (10)	0.0147 (9)	−0.0022 (10)
O2	0.0428 (13)	0.0325 (12)	0.0406 (13)	0.0044 (10)	0.0243 (11)	0.0069 (10)
O3	0.0436 (14)	0.0600 (17)	0.0353 (14)	0.0048 (12)	0.0074 (11)	0.0085 (12)
N1	0.0291 (13)	0.0338 (14)	0.0204 (12)	0.0043 (11)	0.0117 (10)	−0.0019 (11)
N2	0.0338 (14)	0.0257 (13)	0.0238 (13)	−0.0004 (10)	0.0153 (11)	−0.0012 (10)
C1	0.050 (2)	0.082 (3)	0.0254 (18)	−0.003 (2)	0.0140 (16)	−0.0022 (18)
C2	0.081 (3)	0.134 (5)	0.034 (2)	0.010 (3)	0.026 (2)	−0.024 (3)
C3	0.074 (3)	0.0337 (19)	0.083 (3)	0.004 (2)	0.057 (3)	−0.002 (2)
C4	0.059 (2)	0.038 (2)	0.067 (3)	0.0092 (18)	0.027 (2)	0.0043 (19)
C5	0.057 (3)	0.063 (3)	0.057 (3)	0.017 (2)	0.015 (2)	0.019 (2)
C6	0.066 (3)	0.104 (4)	0.045 (2)	0.034 (3)	0.019 (2)	0.030 (3)
P2	0.0482 (6)	0.0490 (6)	0.0410 (5)	0.0148 (4)	0.0257 (4)	0.0104 (4)
O4	0.034 (2)	0.057 (3)	0.035 (2)	−0.0022 (17)	0.0145 (17)	−0.0093 (19)
C7	0.045 (4)	0.081 (5)	0.054 (4)	−0.010 (3)	0.030 (3)	−0.020 (3)
C8	0.068 (4)	0.164 (7)	0.111 (5)	−0.029 (4)	0.055 (4)	−0.015 (5)
P22	0.0482 (6)	0.0490 (6)	0.0410 (5)	0.0148 (4)	0.0257 (4)	0.0104 (4)
C28	0.068 (4)	0.164 (7)	0.111 (5)	−0.029 (4)	0.055 (4)	−0.015 (5)
C9	0.0382 (19)	0.0454 (19)	0.0382 (19)	−0.0023 (16)	0.0157 (15)	−0.0122 (16)
C10	0.0310 (17)	0.058 (2)	0.039 (2)	−0.0016 (16)	0.0167 (15)	−0.0103 (17)
C11	0.0301 (16)	0.049 (2)	0.0333 (17)	0.0065 (15)	0.0121 (13)	−0.0052 (15)
C12	0.0390 (19)	0.050 (2)	0.060 (2)	−0.0027 (17)	0.0230 (17)	−0.0300 (19)
C13	0.0323 (17)	0.0388 (18)	0.047 (2)	−0.0004 (14)	0.0199 (15)	−0.0124 (16)
C14	0.043 (2)	0.047 (2)	0.0345 (18)	0.0038 (16)	0.0134 (15)	0.0007 (15)
C15	0.0429 (18)	0.0309 (16)	0.0283 (16)	0.0003 (14)	0.0183 (14)	−0.0055 (13)
C16	0.048 (2)	0.0256 (16)	0.0391 (18)	0.0011 (14)	0.0205 (15)	−0.0053 (14)
C17	0.0430 (18)	0.0261 (15)	0.0379 (18)	−0.0003 (14)	0.0237 (15)	0.0047 (14)
C18	0.049 (2)	0.0311 (16)	0.0271 (16)	0.0013 (14)	0.0210 (15)	0.0019 (13)
C19	0.0447 (18)	0.0249 (15)	0.0261 (16)	0.0005 (13)	0.0185 (14)	−0.0013 (12)
C20	0.059 (2)	0.0260 (16)	0.043 (2)	0.0023 (16)	0.0290 (17)	0.0068 (14)

Geometric parameters (Å, º)

Zn—S1	2.3211 (9)	C7—C8	1.463 (4)
Zn—S3	2.3228 (9)	C7—H7A	0.9900
Zn—N1	2.048 (2)	C7—H7B	0.9900
Zn—N2	2.071 (3)	C8—H8A	0.9800
S1—P1	2.0153 (12)	C8—H8B	0.9800
S2—P1	1.9437 (12)	C8—H8C	0.9800
S3—P2	2.0174 (13)	P22—O24	1.571 (3)
S4—P2	1.9303 (16)	O24—C27	1.458 (4)
P1—O1	1.594 (2)	C27—C28	1.493 (4)
P1—O2	1.590 (2)	C27—H27A	0.9900
O1—C1	1.447 (4)	C27—H27B	0.9900
O2—C3	1.447 (4)	C28—H28A	0.9800
O3—C5	1.457 (5)	C28—H28B	0.9800
O3—P22	1.581 (3)	C28—H28C	0.9800
O3—P2	1.581 (3)	C9—C10	1.371 (5)

N1—C13	1.318 (4)	C9—H9	0.9500
N1—C9	1.345 (4)	C10—C11	1.348 (5)
N2—C19	1.342 (4)	C10—H10	0.9500
N2—C15	1.344 (4)	C11—C12	1.393 (5)
C1—C2	1.497 (6)	C11—C14	1.532 (5)
C1—H1A	0.9900	C12—C13	1.387 (5)
C1—H1B	0.9900	C12—H12	0.9500
C2—H2A	0.9800	C13—H13	0.9500
C2—H2B	0.9800	C14—C14^{i}	1.498 (7)
C2—H2C	0.9800	C14—H14A	0.9900
C3—C4	1.494 (5)	C14—H14B	0.9900
C3—H3A	0.9900	C15—C16	1.370 (5)
C3—H3B	0.9900	C15—H15	0.9500
C4—H4A	0.9800	C16—C17	1.390 (5)
C4—H4B	0.9800	C16—H16	0.9500
C4—H4C	0.9800	C17—C18	1.381 (4)
C5—C6	1.494 (6)	C17—C20	1.510 (5)
C5—H5A	0.9900	C18—C19	1.378 (4)
C5—H5B	0.9900	C18—H18	0.9500
C6—H6A	0.9800	C19—H19	0.9500
C6—H6B	0.9800	C20—C20^{ii}	1.529 (8)
C6—H6C	0.9800	C20—H20A	0.9900
P2—O4	1.636 (3)	C20—H20B	0.9900
O4—C7	1.454 (4)		

S1—Zn—S3	119.67 (3)	O4—C7—H7B	109.7
S1—Zn—N1	110.85 (8)	C8—C7—H7B	109.7
S1—Zn—N2	112.14 (8)	H7A—C7—H7B	108.2
S3—Zn—N1	114.64 (8)	C7—C8—H8A	109.5
S3—Zn—N2	98.95 (7)	C7—C8—H8B	109.5
N1—Zn—N2	97.59 (10)	H8A—C8—H8B	109.5
Zn—S1—P1	105.73 (4)	C7—C8—H8C	109.5
P2—S3—Zn	97.81 (5)	H8A—C8—H8C	109.5
O1—P1—O2	99.63 (12)	H8B—C8—H8C	109.5
O1—P1—S2	114.67 (10)	O24—P22—O3	121.8 (4)
O2—P1—S2	112.18 (10)	O24—P22—S4	93.2 (3)
O1—P1—S1	104.14 (10)	O3—P22—S4	114.93 (12)
O2—P1—S1	110.76 (10)	O24—P22—S3	107.9 (3)
S2—P1—S1	114.28 (5)	O3—P22—S3	104.07 (11)
C1—O1—P1	120.7 (2)	S4—P22—S3	115.21 (7)
C3—O2—P1	119.3 (2)	P22—O24—C27	112.9 (5)
C5—O3—P22	118.7 (3)	C28—C27—O24	108.6 (5)
C5—O3—P2	118.7 (3)	C28—C27—H27A	110.0
C13—N1—C9	117.6 (3)	O24—C27—H27A	110.0
C13—N1—Zn	122.7 (2)	C28—C27—H27B	110.0
C9—N1—Zn	119.4 (2)	O24—C27—H27B	110.0
C19—N2—C15	117.4 (3)	H27A—C27—H27B	108.4
C19—N2—Zn	120.6 (2)	C27—C28—H28A	109.5

C15—N2—Zn	121.9 (2)	C27—C28—H28B	109.5
O1—C1—C2	107.5 (4)	H28A—C28—H28B	109.5
O1—C1—H1A	110.2	C27—C28—H28C	109.5
C2—C1—H1A	110.2	H28A—C28—H28C	109.5
O1—C1—H1B	110.2	H28B—C28—H28C	109.5
C2—C1—H1B	110.2	N1—C9—C10	122.8 (3)
H1A—C1—H1B	108.5	N1—C9—H9	118.6
C1—C2—H2A	109.5	C10—C9—H9	118.6
C1—C2—H2B	109.5	C11—C10—C9	120.4 (3)
H2A—C2—H2B	109.5	C11—C10—H10	119.8
C1—C2—H2C	109.5	C9—C10—H10	119.8
H2A—C2—H2C	109.5	C10—C11—C12	116.9 (3)
H2B—C2—H2C	109.5	C10—C11—C14	121.8 (3)
O2—C3—C4	108.3 (3)	C12—C11—C14	121.3 (3)
O2—C3—H3A	110.0	C13—C12—C11	120.1 (3)
C4—C3—H3A	110.0	C13—C12—H12	120.0
O2—C3—H3B	110.0	C11—C12—H12	120.0
C4—C3—H3B	110.0	N1—C13—C12	122.0 (3)
H3A—C3—H3B	108.4	N1—C13—H13	119.0
C3—C4—H4A	109.5	C12—C13—H13	119.0
C3—C4—H4B	109.5	C14^{i}—C14—C11	111.2 (4)
H4A—C4—H4B	109.5	C14^{i}—C14—H14A	109.4
C3—C4—H4C	109.5	C11—C14—H14A	109.4
H4A—C4—H4C	109.5	C14^{i}—C14—H14B	109.4
H4B—C4—H4C	109.5	C11—C14—H14B	109.4
O3—C5—C6	109.4 (4)	H14A—C14—H14B	108.0
O3—C5—H5A	109.8	N2—C15—C16	123.0 (3)
C6—C5—H5A	109.8	N2—C15—H15	118.5
O3—C5—H5B	109.8	C16—C15—H15	118.5
C6—C5—H5B	109.8	C15—C16—C17	119.8 (3)
H5A—C5—H5B	108.2	C15—C16—H16	120.1
C5—C6—H6A	109.5	C17—C16—H16	120.1
C5—C6—H6B	109.5	C18—C17—C16	117.1 (3)
H6A—C6—H6B	109.5	C18—C17—C20	120.9 (3)
C5—C6—H6C	109.5	C16—C17—C20	122.0 (3)
H6A—C6—H6C	109.5	C19—C18—C17	120.2 (3)
H6B—C6—H6C	109.5	C19—C18—H18	119.9
O3—P2—O4	92.76 (17)	C17—C18—H18	119.9
O3—P2—S4	114.93 (12)	N2—C19—C18	122.5 (3)
O4—P2—S4	118.09 (15)	N2—C19—H19	118.8
O3—P2—S3	104.07 (11)	C18—C19—H19	118.8
O4—P2—S3	108.87 (16)	C17—C20—C20^{ii}	111.0 (3)
S4—P2—S3	115.21 (7)	C17—C20—H20A	109.4
C7—O4—P2	119.9 (3)	C20^{ii}—C20—H20A	109.4
O4—C7—C8	109.7 (4)	C17—C20—H20B	109.4
O4—C7—H7A	109.7	C20^{ii}—C20—H20B	109.4
C8—C7—H7A	109.7	H20A—C20—H20B	108.0

N1—Zn—S1—P1	−77.86 (9)	Zn—S3—P2—S4	−17.64 (7)
N2—Zn—S1—P1	30.06 (9)	O3—P2—O4—C7	162.9 (4)
S3—Zn—S1—P1	145.21 (4)	S4—P2—O4—C7	42.6 (5)
N1—Zn—S3—P22	−58.80 (9)	S3—P2—O4—C7	−91.3 (4)
N2—Zn—S3—P22	−161.47 (8)	P2—O4—C7—C8	142.2 (5)
S1—Zn—S3—P22	76.60 (5)	C5—O3—P22—O24	−66.0 (5)
N1—Zn—S3—P2	−58.80 (9)	P2—O3—P22—O24	0 (100)
N2—Zn—S3—P2	−161.47 (8)	C5—O3—P22—S4	45.1 (3)
S1—Zn—S3—P2	76.60 (5)	P2—O3—P22—S4	0 (28)
Zn—S1—P1—O1	47.05 (10)	C5—O3—P22—S3	172.1 (3)
Zn—S1—P1—O2	−59.21 (10)	P2—O3—P22—S3	0 (100)
Zn—S1—P1—S2	172.92 (5)	P2—S4—P22—O24	0 (100)
O2—P1—O1—C1	−65.8 (3)	P2—S4—P22—O3	0 (29)
S2—P1—O1—C1	54.2 (3)	P2—S4—P22—S3	0 (45)
S1—P1—O1—C1	179.8 (3)	P2—S3—P22—O24	0 (68)
O1—P1—O2—C3	174.8 (3)	Zn—S3—P22—O24	84.9 (4)
S2—P1—O2—C3	53.0 (3)	P2—S3—P22—O3	0 (43)
S1—P1—O2—C3	−76.0 (3)	Zn—S3—P22—O3	−144.39 (11)
N2—Zn—N1—C13	−115.6 (3)	P2—S3—P22—S4	0 (14)
S3—Zn—N1—C13	140.9 (2)	Zn—S3—P22—S4	−17.64 (7)
S1—Zn—N1—C13	1.6 (3)	O3—P22—O24—C27	−59.0 (9)
N2—Zn—N1—C9	57.7 (3)	S4—P22—O24—C27	178.9 (8)
S3—Zn—N1—C9	−45.8 (3)	S3—P22—O24—C27	61.1 (9)
S1—Zn—N1—C9	175.0 (2)	P22—O24—C27—C28	−171.7 (8)
N1—Zn—N2—C19	36.4 (3)	C13—N1—C9—C10	0.3 (5)
S3—Zn—N2—C19	152.9 (2)	Zn—N1—C9—C10	−173.4 (3)
S1—Zn—N2—C19	−79.8 (2)	N1—C9—C10—C11	3.4 (6)
N1—Zn—N2—C15	−148.3 (2)	C9—C10—C11—C12	−5.3 (6)
S3—Zn—N2—C15	−31.8 (3)	C9—C10—C11—C14	175.2 (3)
S1—Zn—N2—C15	95.5 (2)	C10—C11—C12—C13	3.9 (6)
P1—O1—C1—C2	−162.1 (3)	C14—C11—C12—C13	−176.6 (3)
P1—O2—C3—C4	−178.5 (3)	C9—N1—C13—C12	−1.8 (5)
P22—O3—C5—C6	159.7 (3)	Zn—N1—C13—C12	171.7 (3)
P2—O3—C5—C6	159.7 (3)	C11—C12—C13—N1	−0.3 (6)
C5—O3—P2—O4	−77.7 (3)	C10—C11—C14—C14^{i}	113.1 (5)
P22—O3—P2—O4	0 (100)	C12—C11—C14—C14^{i}	−66.4 (5)
C5—O3—P2—S4	45.1 (3)	C19—N2—C15—C16	1.6 (5)
P22—O3—P2—S4	0 (28)	Zn—N2—C15—C16	−173.8 (3)
C5—O3—P2—S3	172.1 (3)	N2—C15—C16—C17	−0.6 (5)
P22—O3—P2—S3	0 (100)	C15—C16—C17—C18	−0.8 (5)
P22—S4—P2—O3	0 (29)	C15—C16—C17—C20	178.3 (3)
P22—S4—P2—O4	0 (95)	C16—C17—C18—C19	1.2 (5)
P22—S4—P2—S3	0 (45)	C20—C17—C18—C19	−177.9 (3)
P22—S3—P2—O3	0 (43)	C15—N2—C19—C18	−1.2 (5)
Zn—S3—P2—O3	−144.39 (11)	Zn—N2—C19—C18	174.3 (3)
P22—S3—P2—O4	0 (69)	C17—C18—C19—N2	−0.2 (5)

Zn—S3—P2—O4	117.67 (15)	C18—C17—C20—C20^{ii}	72.4 (5)
P22—S3—P2—S4	0 (14)	C16—C17—C20—C20^{ii}	−106.6 (4)

Symmetry codes: (i) −*x*+1, −*y*, −*z*; (ii) −*x*, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5a···S4^{iii}	0.99	2.80	3.770 (5)	165
C18—H18···S1^{iv}	0.95	2.87	3.805 (3)	168

Symmetry codes: (iii) −*x*+1, −*y*, −*z*+1; (iv) *x*, −*y*+1/2, *z*−1/2.