Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(tetraphenylphosphonium) bis[*N*-(trifluoromethylsulfonyl)dithiocarbimato(2−)-$\kappa^2 S,S'$]zincate(II)

Paula S. Pinto,[a] Mayura M. M. Rubinger,[a] Silvana Guilardi,[b]* Drielly A. Paixão[b] and Marcelo R. L. Oliveira[a]

[a]Departamento de Química – UFV, Viçosa MG, Brazil, and [b]Instituto de Química – UFU, Uberlândia, MG, Brazil
Correspondence e-mail: silvana@ufu.br

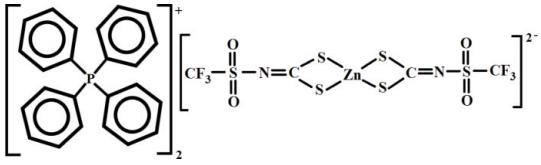
Received 23 November 2011; accepted 2 December 2011

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.058; wR factor = 0.169; data-to-parameter ratio = 18.5.

The title salt, $(C_{24}H_{20}P)_2[Zn(C_2F_3NO_2S_3)_2]$, consists of a complex dianion and two tetraphenylphosphonium cations. The Zn^{II} ion displays a distorted tetrahedral coordination environment with four S atoms from two *S*,*S*′-chelated *N*-(trifluoromethylsulfonyl)dithiocarbimate anions. In the crystal, besides the ionic interaction of the oppositely charged ions, intermolecular C—H···O interactions between cations and anions are observed. One of the cations interacts with an inversion-related equivalent by π–π stacking between phenyl rings, with a centroid–centroid distance of 3.932 (4) Å.

Related literature

For the antifungal and vulcanization activities and crystal structures of dithiocarbimato complexes, see: Amim *et al.* (2011); Alves *et al.* (2009); Mariano *et al.* (2007); Oliveira *et al.* (2007); Perpétuo *et al.* (2003). For further synthetic details, see: Franca *et al.* (2006). For other literature related to fungicides, see: Hogarth (2005).



Experimental

Crystal data

$(C_{24}H_{20}P)_2[Zn(C_2F_3NO_2S_3)_2]$
M_r = 1190.53
Monoclinic, $P2_1/c$
a = 8.8461 (1) Å
b = 29.1869 (5) Å
c = 20.6963 (3) Å
β = 93.578 (1)°
V = 5333.17 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.82 mm^{-1}
T = 295 K
0.42 × 0.18 × 0.12 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.758, T_{max} = 0.950
57739 measured reflections
11977 independent reflections
8307 reflections with $I > 2\sigma(I)$
R_{int} = 0.082

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.169
S = 1.05
11977 reflections
646 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.18 e Å^{-3}
$\Delta\rho_{min}$ = −1.66 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn—S1	2.3346 (10)	Zn—S4	2.3376 (9)
Zn—S2	2.3340 (10)	Zn—S5	2.3566 (10)
S2—Zn—S1	77.84 (3)	S4—Zn—S5	77.63 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O1	0.93	2.68	3.424 (4)	138
C31—H31···O4	0.93	2.62	3.470 (4)	153
C33—H33···O2^{i}	0.93	2.47	3.283 (4)	145

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

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank Professor Dr Javier Ellena of the IFSC, USP, Brazil, for the X-ray data collection. This work was supported financially by FAPEMIG and CAPES.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2371).

References

Alves, L. C., Rubinger, M. M. M., Lindemann, R. H., Perpétuo, G. J., Janczak, J., Miranda, L. D. L., Zambolim, L. & Oliveira, M. R. L. (2009). *J. Inorg. Biochem.* **103**, 1045–1053.
Amim, R. S., Oliveira, M. R. L., Janczak, J., Rubinger, M. M. M., Vieira, L. M. M., Alves, L. C. & Zambolim, L. (2011). *Polyhedron*, **30**, 683–689.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Franca, E. F., Oliveira, M. R. L., Guilardi, S., Andrade, R. P., Lindemann, R. H., Amim, J. Jr, Ellena, J., De Bellis, V. M. & Rubinger, M. M. M. (2006). *Polyhedron*, **25**, 2119–2126.
Hogarth, G. A. (2005). *Prog. Inorg. Chem.* **53**, 71–561.
Mariano, R. M., Oliveira, M. R. L., Rubinger, M. M. M. & Visconte, L. L. Y. (2007). *Eur. Polym. J.* **43**, 4706–4711.
Nonius (2000). *COLLECT*. Nonius BV, Delft, The Netherlands.

Oliveira, M. R. L., Perpétuo, G. J., Janczak, J. & Rubinger, M. M. M. (2007). *Polyhedron*, **26**, 163–168.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Perpétuo, G. J., Oliveira, M. R. L., Janczak, J., Vieira, H. P., Amaral, F. F. & De Bellis, V. M. (2003). *Polyhedron*, **22**, 3355–3362.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2012). E**68**, m33-m34 [**doi:10.1107/S160053681105207X**]

Bis(tetraphenylphosphonium) bis[*N*-(trifluoromethylsulfonyl)dithiocarbimato(2-)-$\kappa^2 S,S'$]zincate(II)

P. S. Pinto, M. M. M. Rubinger, S. Guilardi, D. A. Paixão and M. R. L. Oliveira

Comment

We became interested in the syntheses and characterization of dithiocarbimato-metal complexes due to their similarities with dithiocarbamato complexes, which are important fungicides (Hogarth, 2005). While the dithiocarbamato- metal(II) are neutral substances, the analogous dithiocarbimato-complexes are necessarily anionic species. Thus, the choice of metallic ion, active counter ions or the use of different *R* groups on the dithiocarbimate structures could improve and/or modulate the antifungal activity.

The title complex is a new member of the class of Zn complexes with general formula $[Zn(RSO_2N{=}CS_2)_2]^{2-}$ (Amim *et al.*, 2011; Alves *et al.*, 2009; Mariano *et al.*, 2007; Perpétuo *et al.*, 2003). The literature describes only one complex of this class having an alkyl group (methyl) attached to the SO_2 moiety (Oliveira *et al.*, 2007). The asymmetric unit of the title compound is shown in Fig. 1, and consists of one $[Zn(CF_3SO_2N{=}CS_2)_2]^{2-}$ anion and two Ph_4P^+ cations. The Zn^{II} ion is coordinated by two *S*,*S*'-chelated *N*-trifluoromethylsulfonyldithiocarbimate ligands, resulting in a slightly distorted ZnS_4 tetrahedral geometry. Due to the formation of the two ZnS_2C four membered rings, the two S—Zn—S angles containing both sulfur atoms of the same ligand are significantly smaller than those containing the sulfur atoms from two ligands (Table 1). The dihedral angle between the two ZnS_2C four membered rings [87.40 (4)°] is greater than that found in the salt $(Ph_4P)_2[Zn(CH_3SO_2N{=}CS_2)_2]$ of 79.1 (1)° (Oliveira *et al.*, 2007). The C—S [average value of 1.731 Å] and C=N bond distances [1.315 (4) and 1.314 (4) Å] have double bond character. This behavior indicates that the electron density is delocalized over the entire NCS_2 moiety. The S1–C1–N1 and S5–C3–N2 angles are significantly greater than S2–C1–N1 and S4–C3–N2 due to the repulsive interactions between the two SO_2CF_3 groups and the S1 and S5 atoms, respectively, which are *cis* in relation to the C1–N1 and C3–N2 bonds. Similar behavior is observed for other zinc complexes with dithiocarbimato ligands (Amim *et al.*, 2011; Alves *et al.*, 2009; Oliveira *et al.*, 2007; Perpétuo *et al.*, 2003). The torsion angles of C1–N1–S3–C2 and C3–N2–S6–C4 describing the conformation of the dithiocarbimato ligands are -175.9 (3)° and 180.0 (3)°, respectively. These angles are -67.1 (2)° and 159.6 (2)° in the compound $(Ph_4P)_2[Zn(CH_3SO_2N{=}CS_2)_2]$ (Oliveira *et al.*, 2007), probably due to the larger size of the CF_3 group and the intermolecular interaction present in the title compound.

In both tetraphenylphosphonium cations, the P–C bond lengths range from 1.785 (3) to 1.803 (3) Å, the C–P–C angles range from 106.6 (2) to 112.1 (1)°, and the P atoms display slightly distorted tetrahedral geometry. The arrangement of molecules is mainly determined by the electrostatic interactions between oppositely charged units. Moreover, there are intermolecular C—H···O interactions between cations and anions (Table 2) and π-π stacking between phenyl rings on inversion related (1-x, -y, 2-z) cations.

Experimental

The potassium trifluoromethylsulfonyldithiocarbimate dihydrate was prepared in dimethylformamide from trifluoromethanesulfonamide as described in the literature (Franca *et al.*, 2006). The title compound was prepared in 1:1 (10 ml) methanol:water by the reaction of zinc acetate dihydrate (1.0 mmol) with trifluoromethylsulfonyldithiocarbimate dihydrate (2.0 mmol) and tetraphenylphosphanium chloride (2.0 mmol). The reaction mixture was stirred for 1 h at room temperature. The white solid obtained was filtered, washed with distilled water and dried under reduced pressure. The title compound is insoluble in water but soluble in chloroform, methanol and dichloromethane. Suitable crystals were obtained after slow evaporation of the solution in dichloromethene:ethanol 2:1 mixture. *M*.p. 161.5–163.3 °C. IR (selected bands, cm^{-1}): 1395, 1378 *v*(C═N); 1315, 1183 (*v*CF_3), 1298 $v_{as}(SO_2)$; 1110 $v_{sym}(SO_2)$; 951 $v_{as}(CS_2)$ and 323 *v*(ZnS). ^{13}C NMR (dithiocarbimate anion signals) (δ): 119.3 (q, CF_3, *J* = 317,2 Hz), 226.3 (s, C═N). All spectra (IR, ^{1}H NMR and ^{13}C NMR) showed the expected signals for the tetraphenylphosphonium cation.

Refinement

H atoms were geometrically positioned (C–H 0.93 Å) and refined as riding, with $U_{iso}(H) = 1.2\ U_{eq}$ of the parent atom. Anisotropic displacement parameters were made equal for the S3, O2 and O1 atoms, using the SHELXL-97 EADP constraint. Reflections (-1 1 2) and (0 4 2) were omitted because they were partially obscured by the beamstop.

Figures

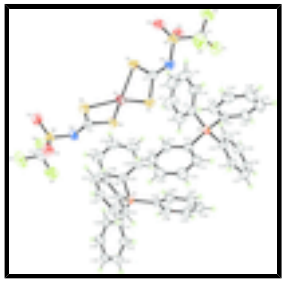


Fig. 1. Representation of the title compound, with displacement ellipsoids drawn at the 30% probability level.

Bis(tetraphenylphosphonium) bis[*N*-(trifluoromethylsulfonyl)dithiocarbimato(2-)- $\kappa^2 S,S'$]zincate(II)

Crystal data

$(C_{24}H_{20}P)_2[Zn(C_2F_3NO_2S_3)_2]$	*F*(000) = 2432
M_r = 1190.53	D_x = 1.483 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo *K*α radiation, λ = 0.71073 Å
a = 8.8461 (1) Å	Cell parameters from 80040 reflections
b = 29.1869 (5) Å	θ = 2.9–27.5°
c = 20.6963 (3) Å	μ = 0.82 mm^{-1}
β = 93.578 (1)°	*T* = 295 K
V = 5333.17 (13) $Å^3$	Prism, colourless
Z = 4	0.42 × 0.18 × 0.12 mm

Data collection

Nonius KappaCCD diffractometer	11977 independent reflections
Radiation source: Enraf Nonius FR590	8307 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.082$
Detector resolution: 9 pixels mm^{-1}	$\theta_{max} = 27.5°$, $\theta_{min} = 2.9°$
CCD rotation images, thick slices scans	$h = -11 \rightarrow 7$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	$k = -37 \rightarrow 37$
$T_{min} = 0.758$, $T_{max} = 0.950$	$l = -26 \rightarrow 26$
57739 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.058$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.169$	H-atom parameters constrained
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0872P)^2 + 2.420P]$ where $P = (F_o^2 + 2F_c^2)/3$
11977 reflections	$(\Delta/\sigma)_{max} = 0.003$
646 parameters	$\Delta\rho_{max} = 1.18$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -1.66$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn	0.76875 (4)	0.258126 (13)	1.300410 (19)	0.05905 (14)
S1	0.76765 (13)	0.32502 (3)	1.36222 (5)	0.0744 (3)
S2	0.89252 (11)	0.30995 (3)	1.23596 (4)	0.0636 (2)
S3	0.88481 (12)	0.42771 (3)	1.34592 (5)	0.0706 (2)
S4	0.57897 (9)	0.20559 (3)	1.26862 (5)	0.0615 (2)

S5	0.87243 (10)	0.18826 (3)	1.33924 (5)	0.0658 (2)
S6	0.77346 (10)	0.08409 (3)	1.33543 (4)	0.0600 (2)
P1	0.58019 (9)	0.36494 (3)	1.07700 (4)	0.0529 (2)
P2	0.41864 (8)	0.12861 (3)	1.04277 (4)	0.04373 (18)
F1	0.8570 (4)	0.48605 (10)	1.25094 (14)	0.1171 (10)
F2	1.0842 (3)	0.47099 (9)	1.28085 (14)	0.1085 (9)
F3	0.9532 (4)	0.51320 (8)	1.33994 (13)	0.1030 (9)
F4	0.6206 (4)	0.03089 (10)	1.25260 (17)	0.1194 (10)
F5	0.7129 (4)	−0.00242 (9)	1.33781 (18)	0.1227 (11)
F6	0.5171 (3)	0.03994 (10)	1.34194 (19)	0.1285 (11)
N1	0.9004 (3)	0.39051 (10)	1.29069 (13)	0.0605 (7)
N2	0.6657 (3)	0.12278 (9)	1.30365 (13)	0.0559 (6)
O1	0.7346 (3)	0.43889 (9)	1.36095 (12)	0.0706 (2)
O2	0.9950 (3)	0.42280 (8)	1.39932 (12)	0.0706 (2)
O3	0.7885 (4)	0.08521 (10)	1.40437 (13)	0.0839 (8)
O4	0.9063 (3)	0.07468 (9)	1.30165 (13)	0.0758 (7)
C1	0.8577 (3)	0.34775 (11)	1.29750 (15)	0.0537 (7)
C2	0.9492 (5)	0.47687 (14)	1.3012 (2)	0.0765 (11)
C3	0.7047 (3)	0.16624 (11)	1.30466 (14)	0.0503 (7)
C4	0.6486 (5)	0.03583 (14)	1.3155 (3)	0.0853 (12)
C5	0.4940 (4)	0.36160 (13)	1.15287 (17)	0.0638 (9)
C6	0.3858 (6)	0.32851 (19)	1.1625 (2)	0.0986 (15)
H6	0.3616	0.3069	1.1305	0.118*
C7	0.3137 (7)	0.3277 (3)	1.2198 (3)	0.128 (2)
H7	0.2419	0.3052	1.2268	0.153*
C8	0.3489 (7)	0.3605 (3)	1.2668 (3)	0.125 (2)
H8	0.2972	0.3608	1.3046	0.151*
C9	0.4583 (6)	0.3920 (2)	1.2581 (2)	0.1071 (17)
H9	0.4846	0.413	1.2908	0.129*
C10	0.5303 (4)	0.39325 (15)	1.20132 (18)	0.0744 (10)
H10	0.6037	0.4154	1.1953	0.089*
C11	0.6968 (4)	0.31543 (11)	1.06493 (16)	0.0558 (8)
C12	0.6925 (4)	0.27720 (12)	1.10471 (17)	0.0664 (9)
H12	0.6242	0.2759	1.1371	0.08*
C13	0.7902 (6)	0.24120 (13)	1.0960 (2)	0.0816 (13)
H13	0.7874	0.2157	1.1228	0.098*
C14	0.8906 (6)	0.24230 (15)	1.0487 (3)	0.0889 (14)
H14	0.9562	0.2178	1.0436	0.107*
C15	0.8946 (5)	0.27990 (17)	1.0084 (2)	0.0878 (12)
H15	0.9617	0.2805	0.9755	0.105*
C16	0.7991 (4)	0.31657 (14)	1.01673 (18)	0.0693 (9)
H16	0.8034	0.3421	0.99	0.083*
C17	0.7020 (4)	0.41366 (11)	1.07582 (15)	0.0537 (7)
C18	0.8430 (4)	0.41156 (14)	1.11035 (18)	0.0672 (9)
H18	0.8731	0.3851	1.1326	0.081*
C19	0.9370 (5)	0.44945 (15)	1.1109 (2)	0.0793 (11)
H19	1.0305	0.4485	1.1341	0.095*
C20	0.8941 (6)	0.48820 (16)	1.0781 (2)	0.0939 (14)
H20	0.9586	0.5134	1.0787	0.113*

C21	0.7568 (6)	0.49019 (16)	1.0441 (3)	0.1064 (17)
H21	0.7281	0.5167	1.0216	0.128*
C22	0.6601 (5)	0.45280 (13)	1.0432 (2)	0.0794 (11)
H22	0.5664	0.4543	1.0203	0.095*
C23	0.4320 (3)	0.37039 (11)	1.01393 (16)	0.0536 (7)
C24	0.2849 (4)	0.38278 (15)	1.0277 (2)	0.0750 (10)
H24	0.2615	0.3879	1.0703	0.09*
C25	0.1748 (4)	0.38742 (15)	0.9783 (2)	0.0790 (11)
H25	0.0768	0.3953	0.9879	0.095*
C26	0.2071 (4)	0.38068 (13)	0.9152 (2)	0.0698 (10)
H26	0.1316	0.3839	0.8822	0.084*
C27	0.3520 (4)	0.36912 (14)	0.90089 (19)	0.0698 (9)
H27	0.3748	0.3649	0.858	0.084*
C28	0.4642 (4)	0.36372 (12)	0.95011 (16)	0.0616 (8)
H28	0.5617	0.3556	0.9401	0.074*
C29	0.6183 (3)	0.12592 (9)	1.06577 (13)	0.0418 (6)
C30	0.6682 (3)	0.12508 (10)	1.13043 (14)	0.0475 (6)
H30	0.5996	0.129	1.1623	0.057*
C31	0.8211 (3)	0.11840 (11)	1.14776 (15)	0.0525 (7)
H31	0.8553	0.1173	1.1911	0.063*
C32	0.9212 (3)	0.11350 (11)	1.09979 (16)	0.0527 (7)
H32	1.0234	0.1087	1.1112	0.063*
C33	0.8732 (3)	0.11551 (11)	1.03584 (16)	0.0528 (7)
H33	0.9427	0.1127	1.0042	0.063*
C34	0.7213 (3)	0.12172 (11)	1.01815 (15)	0.0507 (7)
H34	0.6883	0.1231	0.9746	0.061*
C35	0.3211 (3)	0.13903 (11)	1.11472 (15)	0.0510 (7)
C36	0.2516 (4)	0.18093 (13)	1.12335 (18)	0.0625 (8)
H36	0.2526	0.2033	1.0914	0.075*
C37	0.1799 (4)	0.18924 (16)	1.1806 (2)	0.0781 (12)
H37	0.1345	0.2175	1.1871	0.094*
C38	0.1766 (4)	0.15591 (19)	1.22685 (19)	0.0811 (13)
H38	0.126	0.1614	1.2642	0.097*
C39	0.2459 (4)	0.11501 (17)	1.21909 (17)	0.0741 (11)
H39	0.2439	0.0929	1.2514	0.089*
C40	0.3192 (3)	0.10597 (13)	1.16364 (15)	0.0588 (8)
H40	0.3673	0.078	1.1588	0.071*
C41	0.3778 (3)	0.17355 (10)	0.98562 (14)	0.0489 (7)
C42	0.4799 (4)	0.20877 (11)	0.97580 (18)	0.0634 (9)
H42	0.5729	0.2095	0.9994	0.076*
C43	0.4427 (5)	0.24267 (13)	0.9309 (2)	0.0813 (12)
H43	0.5116	0.2659	0.9238	0.098*
C44	0.3046 (5)	0.24214 (14)	0.8969 (2)	0.0821 (12)
H44	0.2797	0.2652	0.8672	0.099*
C45	0.2028 (5)	0.20768 (15)	0.90656 (19)	0.0764 (11)
H45	0.1087	0.2079	0.8838	0.092*
C46	0.2388 (4)	0.17285 (13)	0.94965 (17)	0.0637 (9)
H46	0.171	0.149	0.9548	0.076*
C47	0.3599 (3)	0.07588 (10)	1.00384 (14)	0.0472 (6)

C48	0.2587 (4)	0.04559 (11)	1.02871 (16)	0.0559 (7)
H48	0.2166	0.0519	1.0678	0.067*
C49	0.2205 (4)	0.00612 (12)	0.99541 (19)	0.0668 (9)
H49	0.1515	−0.0141	1.012	0.08*
C50	0.2826 (4)	−0.00369 (12)	0.93823 (19)	0.0652 (9)
H50	0.257	−0.0307	0.9164	0.078*
C51	0.3832 (4)	0.02640 (14)	0.91288 (19)	0.0718 (10)
H51	0.4256	0.0197	0.874	0.086*
C52	0.4205 (4)	0.06620 (13)	0.94506 (17)	0.0670 (9)
H52	0.4868	0.0868	0.9275	0.08*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.0568 (2)	0.0545 (2)	0.0660 (3)	−0.00555 (17)	0.00531 (18)	−0.00531 (17)
S1	0.0976 (7)	0.0628 (5)	0.0662 (6)	−0.0187 (5)	0.0324 (5)	−0.0122 (4)
S2	0.0715 (6)	0.0615 (5)	0.0595 (5)	−0.0087 (4)	0.0170 (4)	−0.0105 (4)
S3	0.0793 (5)	0.0670 (5)	0.0670 (5)	−0.0189 (4)	0.0169 (4)	−0.0131 (4)
S4	0.0452 (4)	0.0540 (5)	0.0840 (6)	0.0023 (3)	−0.0067 (4)	−0.0026 (4)
S5	0.0505 (5)	0.0657 (5)	0.0792 (6)	−0.0007 (4)	−0.0113 (4)	0.0004 (4)
S6	0.0575 (5)	0.0567 (5)	0.0661 (5)	0.0069 (4)	0.0063 (4)	0.0033 (4)
P1	0.0490 (4)	0.0558 (5)	0.0538 (5)	−0.0078 (4)	0.0028 (3)	−0.0004 (4)
P2	0.0310 (3)	0.0516 (4)	0.0485 (4)	−0.0019 (3)	0.0015 (3)	−0.0016 (3)
F1	0.167 (3)	0.0894 (18)	0.0918 (18)	0.0078 (18)	−0.0169 (19)	0.0137 (14)
F2	0.114 (2)	0.0865 (17)	0.131 (2)	−0.0304 (16)	0.0558 (18)	−0.0042 (16)
F3	0.149 (3)	0.0613 (13)	0.0995 (18)	−0.0193 (15)	0.0172 (17)	−0.0187 (12)
F4	0.129 (2)	0.0855 (18)	0.139 (3)	−0.0078 (17)	−0.028 (2)	−0.0277 (17)
F5	0.119 (2)	0.0566 (14)	0.191 (3)	0.0091 (14)	0.003 (2)	0.0182 (17)
F6	0.0822 (18)	0.0841 (18)	0.223 (4)	−0.0127 (15)	0.042 (2)	0.006 (2)
N1	0.0680 (17)	0.0590 (16)	0.0557 (15)	−0.0102 (13)	0.0132 (13)	−0.0067 (12)
N2	0.0491 (14)	0.0513 (15)	0.0670 (17)	0.0027 (11)	0.0029 (12)	−0.0022 (12)
O1	0.0793 (5)	0.0670 (5)	0.0670 (5)	−0.0189 (4)	0.0169 (4)	−0.0131 (4)
O2	0.0793 (5)	0.0670 (5)	0.0670 (5)	−0.0189 (4)	0.0169 (4)	−0.0131 (4)
O3	0.102 (2)	0.0844 (18)	0.0650 (16)	0.0128 (16)	0.0061 (14)	0.0117 (13)
O4	0.0603 (14)	0.0793 (17)	0.0889 (18)	0.0176 (13)	0.0128 (13)	0.0008 (14)
C1	0.0469 (16)	0.0598 (19)	0.0545 (18)	−0.0038 (14)	0.0030 (14)	−0.0058 (14)
C2	0.097 (3)	0.062 (2)	0.072 (2)	−0.013 (2)	0.008 (2)	−0.0079 (19)
C3	0.0435 (15)	0.0583 (18)	0.0501 (16)	0.0029 (13)	0.0112 (13)	−0.0027 (13)
C4	0.076 (3)	0.060 (2)	0.121 (4)	0.006 (2)	0.009 (3)	0.003 (2)
C5	0.0565 (19)	0.073 (2)	0.062 (2)	−0.0092 (17)	0.0054 (16)	0.0066 (17)
C6	0.090 (3)	0.122 (4)	0.087 (3)	−0.046 (3)	0.023 (2)	−0.005 (3)
C7	0.105 (4)	0.172 (6)	0.110 (4)	−0.057 (4)	0.043 (3)	0.012 (4)
C8	0.110 (4)	0.183 (6)	0.088 (4)	−0.026 (4)	0.045 (3)	0.007 (4)
C9	0.111 (4)	0.142 (5)	0.071 (3)	−0.010 (4)	0.028 (3)	−0.014 (3)
C10	0.067 (2)	0.096 (3)	0.061 (2)	−0.006 (2)	0.0141 (18)	−0.010 (2)
C11	0.0572 (18)	0.0539 (17)	0.0546 (18)	−0.0058 (14)	−0.0099 (15)	−0.0023 (14)
C12	0.077 (2)	0.057 (2)	0.062 (2)	−0.0165 (18)	−0.0148 (18)	0.0035 (16)
C13	0.096 (3)	0.052 (2)	0.092 (3)	−0.008 (2)	−0.035 (3)	0.0041 (19)

C14	0.089 (3)	0.067 (3)	0.106 (3)	0.018 (2)	−0.030 (3)	−0.014 (2)
C15	0.083 (3)	0.093 (3)	0.086 (3)	0.030 (2)	0.000 (2)	0.002 (2)
C16	0.072 (2)	0.074 (2)	0.062 (2)	0.0119 (19)	0.0010 (18)	0.0075 (17)
C17	0.0503 (17)	0.0574 (18)	0.0541 (17)	−0.0048 (14)	0.0080 (14)	−0.0067 (14)
C18	0.0544 (19)	0.076 (2)	0.071 (2)	−0.0137 (17)	0.0012 (16)	0.0005 (18)
C19	0.063 (2)	0.090 (3)	0.085 (3)	−0.026 (2)	0.004 (2)	−0.012 (2)
C20	0.101 (3)	0.076 (3)	0.105 (3)	−0.038 (3)	0.012 (3)	−0.008 (3)
C21	0.109 (4)	0.063 (2)	0.143 (5)	−0.025 (3)	−0.024 (3)	0.016 (3)
C22	0.079 (3)	0.061 (2)	0.096 (3)	−0.0155 (19)	−0.011 (2)	0.005 (2)
C23	0.0469 (16)	0.0531 (17)	0.0607 (19)	−0.0063 (13)	0.0032 (14)	−0.0014 (14)
C24	0.0534 (19)	0.095 (3)	0.077 (2)	0.0010 (19)	0.0082 (18)	−0.008 (2)
C25	0.0465 (19)	0.094 (3)	0.096 (3)	−0.0001 (19)	0.0016 (19)	−0.004 (2)
C26	0.056 (2)	0.065 (2)	0.085 (3)	−0.0047 (16)	−0.0183 (18)	−0.0004 (19)
C27	0.063 (2)	0.079 (2)	0.065 (2)	0.0018 (18)	−0.0080 (17)	−0.0002 (18)
C28	0.0518 (18)	0.071 (2)	0.062 (2)	0.0013 (16)	0.0013 (15)	0.0037 (16)
C29	0.0331 (12)	0.0454 (14)	0.0469 (15)	−0.0032 (11)	0.0020 (11)	−0.0006 (12)
C30	0.0348 (13)	0.0587 (17)	0.0494 (16)	−0.0034 (12)	0.0041 (12)	−0.0051 (13)
C31	0.0399 (14)	0.0650 (19)	0.0520 (17)	−0.0042 (13)	−0.0019 (13)	0.0009 (14)
C32	0.0306 (13)	0.0585 (18)	0.069 (2)	−0.0038 (12)	0.0005 (13)	−0.0011 (15)
C33	0.0365 (14)	0.0634 (19)	0.0599 (19)	−0.0062 (13)	0.0134 (13)	−0.0071 (14)
C34	0.0394 (14)	0.0643 (18)	0.0487 (16)	−0.0062 (13)	0.0043 (12)	−0.0005 (14)
C35	0.0295 (12)	0.071 (2)	0.0521 (17)	−0.0027 (13)	0.0025 (12)	−0.0085 (15)
C36	0.0449 (16)	0.072 (2)	0.071 (2)	−0.0025 (15)	0.0037 (15)	−0.0159 (17)
C37	0.0470 (19)	0.104 (3)	0.083 (3)	0.0028 (19)	0.0070 (18)	−0.037 (2)
C38	0.0469 (19)	0.140 (4)	0.058 (2)	−0.009 (2)	0.0088 (16)	−0.025 (3)
C39	0.0489 (18)	0.122 (3)	0.0514 (19)	−0.011 (2)	0.0017 (15)	−0.002 (2)
C40	0.0377 (15)	0.085 (2)	0.0541 (18)	−0.0022 (15)	0.0026 (13)	0.0011 (16)
C41	0.0399 (14)	0.0518 (16)	0.0545 (17)	0.0022 (12)	−0.0009 (12)	−0.0022 (13)
C42	0.0588 (19)	0.0536 (18)	0.076 (2)	−0.0053 (15)	−0.0123 (17)	0.0027 (16)
C43	0.086 (3)	0.056 (2)	0.100 (3)	−0.0090 (19)	−0.011 (2)	0.019 (2)
C44	0.091 (3)	0.070 (2)	0.083 (3)	0.012 (2)	−0.014 (2)	0.014 (2)
C45	0.064 (2)	0.086 (3)	0.077 (3)	0.012 (2)	−0.0208 (19)	0.006 (2)
C46	0.0435 (16)	0.071 (2)	0.075 (2)	−0.0003 (15)	−0.0071 (16)	0.0052 (18)
C47	0.0342 (13)	0.0515 (16)	0.0554 (17)	−0.0028 (12)	−0.0011 (12)	−0.0014 (13)
C48	0.0513 (17)	0.0577 (18)	0.0594 (18)	−0.0017 (14)	0.0090 (14)	0.0051 (15)
C49	0.067 (2)	0.0517 (18)	0.082 (2)	−0.0154 (16)	0.0069 (19)	0.0053 (17)
C50	0.068 (2)	0.0477 (17)	0.079 (2)	−0.0017 (15)	−0.0035 (19)	−0.0047 (16)
C51	0.067 (2)	0.076 (2)	0.073 (2)	−0.0100 (19)	0.0159 (18)	−0.0179 (19)
C52	0.0578 (19)	0.076 (2)	0.068 (2)	−0.0235 (17)	0.0161 (16)	−0.0166 (18)

Geometric parameters (Å, °)

Zn—S1	2.3346 (10)	C20—C21	1.366 (7)
Zn—S2	2.3340 (10)	C20—H20	0.93
Zn—S4	2.3376 (9)	C21—C22	1.386 (6)
Zn—S5	2.3566 (10)	C21—H21	0.93
S1—C1	1.733 (3)	C22—H22	0.93
S2—C1	1.727 (3)	C23—C28	1.382 (5)
S3—O1	1.421 (3)	C23—C24	1.397 (5)

S3—O2	1.435 (3)	C24—C25	1.375 (5)
S3—N1	1.589 (3)	C24—H24	0.93
S3—C2	1.818 (4)	C25—C26	1.369 (6)
S4—C3	1.735 (3)	C25—H25	0.93
S5—C3	1.730 (3)	C26—C27	1.375 (5)
S6—O3	1.425 (3)	C26—H26	0.93
S6—O4	1.431 (3)	C27—C28	1.386 (5)
S6—N2	1.593 (3)	C27—H27	0.93
S6—C4	1.821 (5)	C28—H28	0.93
P1—C17	1.785 (3)	C29—C30	1.383 (4)
P1—C5	1.790 (4)	C29—C34	1.389 (4)
P1—C23	1.798 (3)	C30—C31	1.391 (4)
P1—C11	1.802 (3)	C30—H30	0.93
P2—C41	1.788 (3)	C31—C32	1.379 (4)
P2—C35	1.793 (3)	C31—H31	0.93
P2—C47	1.799 (3)	C32—C33	1.366 (4)
P2—C29	1.802 (3)	C32—H32	0.93
F1—C2	1.309 (5)	C33—C34	1.383 (4)
F2—C2	1.303 (5)	C33—H33	0.93
F3—C2	1.328 (4)	C34—H34	0.93
F4—C4	1.319 (6)	C35—C36	1.385 (5)
F5—C4	1.323 (5)	C35—C40	1.400 (5)
F6—C4	1.321 (5)	C36—C37	1.399 (5)
N1—C1	1.314 (4)	C36—H36	0.93
N2—C3	1.314 (4)	C37—C38	1.367 (7)
C5—C6	1.383 (5)	C37—H37	0.93
C5—C10	1.386 (5)	C38—C39	1.356 (6)
C6—C7	1.381 (7)	C38—H38	0.93
C6—H6	0.93	C39—C40	1.379 (5)
C7—C8	1.387 (8)	C39—H39	0.93
C7—H7	0.93	C40—H40	0.93
C8—C9	1.356 (8)	C41—C42	1.391 (4)
C8—H8	0.93	C41—C46	1.397 (4)
C9—C10	1.372 (6)	C42—C43	1.382 (5)
C9—H9	0.93	C42—H42	0.93
C10—H10	0.93	C43—C44	1.372 (6)
C11—C12	1.389 (5)	C43—H43	0.93
C11—C16	1.389 (5)	C44—C45	1.373 (6)
C12—C13	1.380 (6)	C44—H44	0.93
C12—H12	0.93	C45—C46	1.377 (5)
C13—C14	1.362 (7)	C45—H45	0.93
C13—H13	0.93	C46—H46	0.93
C14—C15	1.381 (7)	C47—C48	1.381 (4)
C14—H14	0.93	C47—C52	1.389 (4)
C15—C16	1.381 (6)	C48—C49	1.374 (5)
C15—H15	0.93	C48—H48	0.93
C16—H16	0.93	C49—C50	1.366 (5)
C17—C22	1.366 (5)	C49—H49	0.93
C17—C18	1.400 (5)	C50—C51	1.377 (5)

C18—C19	1.383 (5)	C50—H50	0.93
C18—H18	0.93	C51—C52	1.369 (5)
C19—C20	1.362 (7)	C51—H51	0.93
C19—H19	0.93	C52—H52	0.93
S2—Zn—S1	77.84 (3)	C19—C20—C21	120.2 (4)
S2—Zn—S4	128.21 (4)	C19—C20—H20	119.9
S1—Zn—S4	132.48 (4)	C21—C20—H20	119.9
S2—Zn—S5	124.69 (4)	C20—C21—C22	120.1 (4)
S1—Zn—S5	123.49 (4)	C20—C21—H21	119.9
S4—Zn—S5	77.63 (3)	C22—C21—H21	119.9
C1—S1—Zn	83.04 (11)	C17—C22—C21	120.2 (4)
C1—S2—Zn	83.17 (11)	C17—C22—H22	119.9
O1—S3—O2	117.00 (15)	C21—C22—H22	119.9
O1—S3—N1	116.02 (16)	C28—C23—C24	118.8 (3)
O2—S3—N1	113.61 (16)	C28—C23—P1	119.8 (2)
O1—S3—C2	104.9 (2)	C24—C23—P1	121.4 (3)
O2—S3—C2	104.58 (19)	C25—C24—C23	120.0 (4)
N1—S3—C2	97.43 (17)	C25—C24—H24	120
C3—S4—Zn	83.31 (11)	C23—C24—H24	120
C3—S5—Zn	82.82 (11)	C26—C25—C24	121.0 (4)
O3—S6—O4	117.73 (18)	C26—C25—H25	119.5
O3—S6—N2	114.39 (16)	C24—C25—H25	119.5
O4—S6—N2	115.02 (15)	C25—C26—C27	119.6 (3)
O3—S6—C4	105.2 (2)	C25—C26—H26	120.2
O4—S6—C4	104.2 (2)	C27—C26—H26	120.2
N2—S6—C4	96.67 (18)	C26—C27—C28	120.3 (4)
C17—P1—C5	110.23 (16)	C26—C27—H27	119.9
C17—P1—C23	109.44 (15)	C28—C27—H27	119.9
C5—P1—C23	108.09 (16)	C23—C28—C27	120.3 (3)
C17—P1—C11	106.60 (15)	C23—C28—H28	119.8
C5—P1—C11	110.89 (17)	C27—C28—H28	119.8
C23—P1—C11	111.59 (15)	C30—C29—C34	120.1 (3)
C41—P2—C35	109.70 (15)	C30—C29—P2	120.3 (2)
C41—P2—C47	106.90 (14)	C34—C29—P2	119.5 (2)
C35—P2—C47	112.13 (14)	C29—C30—C31	119.9 (3)
C41—P2—C29	111.16 (13)	C29—C30—H30	120.1
C35—P2—C29	107.61 (13)	C31—C30—H30	120.1
C47—P2—C29	109.39 (13)	C32—C31—C30	119.2 (3)
C1—N1—S3	122.3 (2)	C32—C31—H31	120.4
C3—N2—S6	121.9 (2)	C30—C31—H31	120.4
N1—C1—S2	117.5 (2)	C33—C32—C31	121.2 (3)
N1—C1—S1	126.6 (3)	C33—C32—H32	119.4
S2—C1—S1	115.92 (19)	C31—C32—H32	119.4
F2—C2—F1	108.0 (4)	C32—C33—C34	120.1 (3)
F2—C2—F3	108.0 (4)	C32—C33—H33	120
F1—C2—F3	108.0 (4)	C34—C33—H33	120
F2—C2—S3	112.5 (3)	C33—C34—C29	119.6 (3)
F1—C2—S3	111.5 (3)	C33—C34—H34	120.2
F3—C2—S3	108.7 (3)	C29—C34—H34	120.2

N2—C3—S5	125.6 (2)	C36—C35—C40	119.3 (3)
N2—C3—S4	118.1 (2)	C36—C35—P2	119.8 (3)
S5—C3—S4	116.24 (18)	C40—C35—P2	120.8 (2)
F4—C4—F6	107.6 (4)	C35—C36—C37	119.4 (4)
F4—C4—F5	107.6 (4)	C35—C36—H36	120.3
F6—C4—F5	107.6 (4)	C37—C36—H36	120.3
F4—C4—S6	112.5 (3)	C38—C37—C36	120.1 (4)
F6—C4—S6	111.9 (3)	C38—C37—H37	120
F5—C4—S6	109.4 (3)	C36—C37—H37	120
C6—C5—C10	119.5 (4)	C39—C38—C37	120.9 (4)
C6—C5—P1	120.1 (3)	C39—C38—H38	119.5
C10—C5—P1	120.4 (3)	C37—C38—H38	119.5
C7—C6—C5	119.8 (5)	C38—C39—C40	120.5 (4)
C7—C6—H6	120.1	C38—C39—H39	119.8
C5—C6—H6	120.1	C40—C39—H39	119.8
C6—C7—C8	119.7 (5)	C39—C40—C35	119.8 (4)
C6—C7—H7	120.2	C39—C40—H40	120.1
C8—C7—H7	120.2	C35—C40—H40	120.1
C9—C8—C7	120.5 (5)	C42—C41—C46	119.4 (3)
C9—C8—H8	119.8	C42—C41—P2	122.2 (2)
C7—C8—H8	119.8	C46—C41—P2	118.5 (2)
C8—C9—C10	120.3 (5)	C43—C42—C41	119.8 (3)
C8—C9—H9	119.9	C43—C42—H42	120.1
C10—C9—H9	119.9	C41—C42—H42	120.1
C9—C10—C5	120.3 (4)	C44—C43—C42	120.2 (4)
C9—C10—H10	119.9	C44—C43—H43	119.9
C5—C10—H10	119.9	C42—C43—H43	119.9
C12—C11—C16	119.2 (3)	C43—C44—C45	120.3 (4)
C12—C11—P1	121.7 (3)	C43—C44—H44	119.8
C16—C11—P1	119.0 (3)	C45—C44—H44	119.8
C13—C12—C11	119.6 (4)	C44—C45—C46	120.5 (4)
C13—C12—H12	120.2	C44—C45—H45	119.8
C11—C12—H12	120.2	C46—C45—H45	119.8
C14—C13—C12	121.2 (4)	C45—C46—C41	119.7 (3)
C14—C13—H13	119.4	C45—C46—H46	120.2
C12—C13—H13	119.4	C41—C46—H46	120.2
C13—C14—C15	119.7 (4)	C48—C47—C52	119.4 (3)
C13—C14—H14	120.2	C48—C47—P2	123.8 (2)
C15—C14—H14	120.2	C52—C47—P2	116.7 (2)
C14—C15—C16	120.1 (4)	C49—C48—C47	119.7 (3)
C14—C15—H15	119.9	C49—C48—H48	120.2
C16—C15—H15	119.9	C47—C48—H48	120.2
C15—C16—C11	120.2 (4)	C50—C49—C48	120.7 (3)
C15—C16—H16	119.9	C50—C49—H49	119.7
C11—C16—H16	119.9	C48—C49—H49	119.7
C22—C17—C18	119.6 (3)	C49—C50—C51	120.1 (3)
C22—C17—P1	121.8 (3)	C49—C50—H50	120
C18—C17—P1	118.5 (3)	C51—C50—H50	120
C19—C18—C17	119.1 (4)	C52—C51—C50	119.8 (3)

C19—C18—H18	120.5	C52—C51—H51	120.1
C17—C18—H18	120.5	C50—C51—H51	120.1
C20—C19—C18	120.7 (4)	C51—C52—C47	120.3 (3)
C20—C19—H19	119.6	C51—C52—H52	119.9
C18—C19—H19	119.6	C47—C52—H52	119.9
S2—Zn—S1—C1	1.16 (11)	C23—P1—C17—C18	−165.3 (3)
S4—Zn—S1—C1	−130.18 (11)	C11—P1—C17—C18	−44.5 (3)
S5—Zn—S1—C1	124.91 (11)	C22—C17—C18—C19	0.3 (6)
S1—Zn—S2—C1	−1.17 (11)	P1—C17—C18—C19	−178.6 (3)
S4—Zn—S2—C1	134.03 (11)	C17—C18—C19—C20	−0.5 (6)
S5—Zn—S2—C1	−123.66 (11)	C18—C19—C20—C21	0.3 (7)
S2—Zn—S4—C3	123.96 (10)	C19—C20—C21—C22	0.2 (8)
S1—Zn—S4—C3	−125.12 (10)	C18—C17—C22—C21	0.2 (6)
S5—Zn—S4—C3	−0.72 (10)	P1—C17—C22—C21	179.1 (4)
S2—Zn—S5—C3	−127.47 (10)	C20—C21—C22—C17	−0.4 (8)
S1—Zn—S5—C3	133.86 (10)	C17—P1—C23—C28	73.9 (3)
S4—Zn—S5—C3	0.72 (10)	C5—P1—C23—C28	−166.0 (3)
O1—S3—N1—C1	−65.2 (3)	C11—P1—C23—C28	−43.8 (3)
O2—S3—N1—C1	74.6 (3)	C17—P1—C23—C24	−103.9 (3)
C2—S3—N1—C1	−175.9 (3)	C5—P1—C23—C24	16.1 (3)
O3—S6—N2—C3	70.0 (3)	C11—P1—C23—C24	138.3 (3)
O4—S6—N2—C3	−70.8 (3)	C28—C23—C24—C25	1.0 (6)
C4—S6—N2—C3	−180.0 (3)	P1—C23—C24—C25	178.9 (3)
S3—N1—C1—S2	−175.78 (19)	C23—C24—C25—C26	−0.9 (7)
S3—N1—C1—S1	4.8 (5)	C24—C25—C26—C27	−0.1 (6)
Zn—S2—C1—N1	−177.8 (3)	C25—C26—C27—C28	0.9 (6)
Zn—S2—C1—S1	1.71 (16)	C24—C23—C28—C27	−0.2 (5)
Zn—S1—C1—N1	177.7 (3)	P1—C23—C28—C27	−178.1 (3)
Zn—S1—C1—S2	−1.71 (16)	C26—C27—C28—C23	−0.7 (6)
O1—S3—C2—F2	−176.8 (3)	C41—P2—C29—C30	129.3 (2)
O2—S3—C2—F2	59.5 (3)	C35—P2—C29—C30	9.2 (3)
N1—S3—C2—F2	−57.3 (3)	C47—P2—C29—C30	−112.9 (2)
O1—S3—C2—F1	−55.3 (3)	C41—P2—C29—C34	−54.8 (3)
O2—S3—C2—F1	−179.0 (3)	C35—P2—C29—C34	−175.0 (2)
N1—S3—C2—F1	64.2 (3)	C47—P2—C29—C34	63.0 (3)
O1—S3—C2—F3	63.6 (4)	C34—C29—C30—C31	−2.3 (4)
O2—S3—C2—F3	−60.1 (4)	P2—C29—C30—C31	173.6 (2)
N1—S3—C2—F3	−176.9 (3)	C29—C30—C31—C32	1.1 (5)
S6—N2—C3—S5	−0.1 (4)	C30—C31—C32—C33	0.6 (5)
S6—N2—C3—S4	179.99 (16)	C31—C32—C33—C34	−1.2 (5)
Zn—S5—C3—N2	179.0 (3)	C32—C33—C34—C29	0.0 (5)
Zn—S5—C3—S4	−1.06 (15)	C30—C29—C34—C33	1.7 (5)
Zn—S4—C3—N2	−179.0 (2)	P2—C29—C34—C33	−174.2 (2)
Zn—S4—C3—S5	1.07 (15)	C41—P2—C35—C36	−10.6 (3)
O3—S6—C4—F4	178.5 (3)	C47—P2—C35—C36	−129.2 (2)
O4—S6—C4—F4	−57.0 (3)	C29—P2—C35—C36	110.5 (3)
N2—S6—C4—F4	61.0 (3)	C41—P2—C35—C40	172.0 (2)
O3—S6—C4—F6	57.3 (4)	C47—P2—C35—C40	53.3 (3)
O4—S6—C4—F6	−178.3 (3)	C29—P2—C35—C40	−67.0 (3)

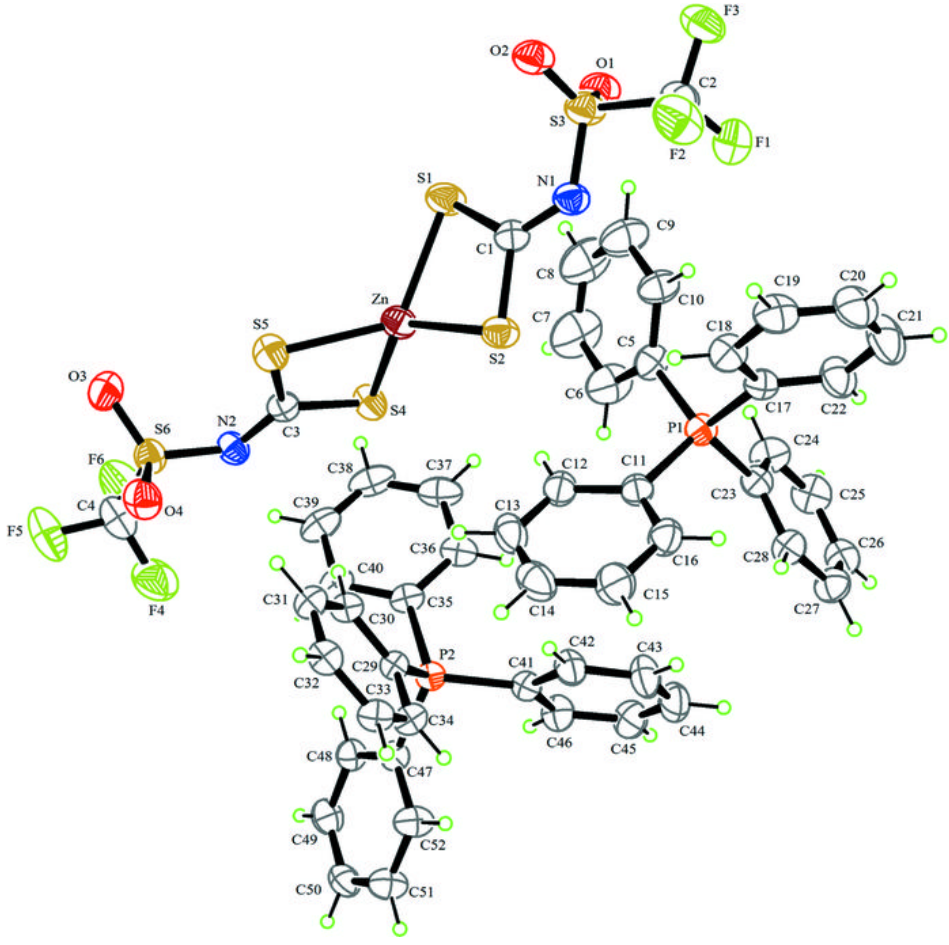
N2—S6—C4—F6	−60.3 (4)	C40—C35—C36—C37	−0.5 (5)
O3—S6—C4—F5	−62.0 (4)	P2—C35—C36—C37	−178.0 (3)
O4—S6—C4—F5	62.5 (4)	C35—C36—C37—C38	−1.1 (5)
N2—S6—C4—F5	−179.5 (3)	C36—C37—C38—C39	1.9 (6)
C17—P1—C5—C6	174.8 (4)	C37—C38—C39—C40	−1.1 (6)
C23—P1—C5—C6	55.3 (4)	C38—C39—C40—C35	−0.6 (5)
C11—P1—C5—C6	−67.4 (4)	C36—C35—C40—C39	1.3 (5)
C17—P1—C5—C10	−2.4 (4)	P2—C35—C40—C39	178.8 (2)
C23—P1—C5—C10	−122.0 (3)	C35—P2—C41—C42	102.1 (3)
C11—P1—C5—C10	115.4 (3)	C47—P2—C41—C42	−136.1 (3)
C10—C5—C6—C7	0.8 (8)	C29—P2—C41—C42	−16.8 (3)
P1—C5—C6—C7	−176.5 (5)	C35—P2—C41—C46	−78.2 (3)
C5—C6—C7—C8	0.9 (10)	C47—P2—C41—C46	43.6 (3)
C6—C7—C8—C9	−2.9 (11)	C29—P2—C41—C46	162.9 (3)
C7—C8—C9—C10	3.1 (10)	C46—C41—C42—C43	0.2 (5)
C8—C9—C10—C5	−1.3 (8)	P2—C41—C42—C43	179.9 (3)
C6—C5—C10—C9	−0.7 (7)	C41—C42—C43—C44	1.1 (6)
P1—C5—C10—C9	176.6 (4)	C42—C43—C44—C45	−0.7 (7)
C17—P1—C11—C12	131.2 (3)	C43—C44—C45—C46	−1.1 (7)
C5—P1—C11—C12	11.2 (3)	C44—C45—C46—C41	2.5 (6)
C23—P1—C11—C12	−109.4 (3)	C42—C41—C46—C45	−2.0 (5)
C17—P1—C11—C16	−45.4 (3)	P2—C41—C46—C45	178.3 (3)
C5—P1—C11—C16	−165.4 (3)	C41—P2—C47—C48	−124.1 (3)
C23—P1—C11—C16	74.1 (3)	C35—P2—C47—C48	−3.9 (3)
C16—C11—C12—C13	0.3 (5)	C29—P2—C47—C48	115.4 (3)
P1—C11—C12—C13	−176.2 (3)	C41—P2—C47—C52	55.2 (3)
C11—C12—C13—C14	−0.3 (6)	C35—P2—C47—C52	175.4 (3)
C12—C13—C14—C15	−0.4 (6)	C29—P2—C47—C52	−65.3 (3)
C13—C14—C15—C16	1.2 (7)	C52—C47—C48—C49	0.7 (5)
C14—C15—C16—C11	−1.2 (7)	P2—C47—C48—C49	179.9 (3)
C12—C11—C16—C15	0.4 (5)	C47—C48—C49—C50	0.6 (5)
P1—C11—C16—C15	177.1 (3)	C48—C49—C50—C51	−0.9 (6)
C5—P1—C17—C22	−103.0 (3)	C49—C50—C51—C52	−0.1 (6)
C23—P1—C17—C22	15.8 (4)	C50—C51—C52—C47	1.4 (6)
C11—P1—C17—C22	136.6 (3)	C48—C47—C52—C51	−1.7 (5)
C5—P1—C17—C18	75.9 (3)	P2—C47—C52—C51	179.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O1	0.93	2.68	3.424 (4)	138.
C31—H31···O4	0.93	2.62	3.470 (4)	153.
C33—H33···O2^{i}	0.93	2.47	3.283 (4)	145.

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

Fig. 1


F3
O2
O1
C2
S3
F2
F1
S1
N1
C1
C9
C8
C10
C19
C20
Zn
C7
C18
C21
S5
S2
C5
O3
C6
C17
C22
S6
N2
C3
S4
P1
C24
F6
C38
C37
C12
C11
C23
C25
C4
O4
C39
C13
C36
C16
C28
C26
F5
C40
C31
C35
C14
C15
C27
C30
F4
C42
C43
C29
P2
C41
C32
C33
C34
C46
C45
C44
C48
C47
C49
C52
C50
C51