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Bis(thiocyanato-κN)bis(triphenylphosphine oxide-κO)zinc(II)

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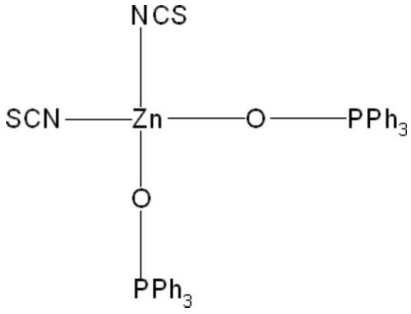
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.032; wR factor = 0.090; data-to-parameter ratio = 14.8.

The title compound, $[Zn(NCS)_2\{(C_6H_5)_3PO\}_2]$, crystallizes with two molecules in the asymmetric unit. The coordination environment of the Zn atom is distorted tetrahedral.

Related literature

The corresponding four-coordinate complex dichlorobis(triphenylphosphine oxide)zinc(II) has been reported by Zeller *et al.* (2001).

For related literature, see: Cotton & Goodgame (1960). For synthesis, see: Pinkas *et al.* (1998).



Experimental

Crystal data

$[Zn(NCS)_2(C_{18}H_{15}OP)_2]$
M_r = 738.07
Triclinic, $P\overline{1}$
a = 9.9695 (6) Å
b = 19.6036 (12) Å
c = 21.2407 (12) Å
α = 116.799 (3)°
β = 98.316 (3)°
γ = 95.098 (3)°
V = 3610.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.92 mm^{-1}
T = 298 (2) K
0.20 × 0.15 × 0.12 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.837, T_{max} = 0.898
37146 measured reflections
12513 independent reflections
10612 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.091
S = 1.07
12513 reflections
847 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *XPREP* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2473).

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Pinkas, J., Wessel, H., Yang, Y., Monter, M. L., Noltermeye, M., Frolba, M. & Roesky, H. W. (1998). *Inorg. Chem.* **37**, 2450–2457.
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supplementary materials

Acta Cryst. (2007). E**63**, m2359 [**doi:10.1107/S1600536807039700**]

Bis(thiocyanato-κ*N*)bis(triphenylphosphine oxide-κ*O*)zinc(II)

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Comment

Some $[(C_6H_5)_3PO]_2NiX_2$ complexes (X = Cl, Br, I) were prepared (Cotton & Goodgame, 1960) and their electronic spectra, IR spectra and magnetic moments were recorded and analyzed in order to demonstrate that the Ni ion, in each case, was tetrahedrally coordinated. Recently, the structure of $[(C_6H_5)_3PO]_2ZnCl_2$ had been reported (Zeller *et al.*, 2001). Here we report the structure of $[(C_6H_5)_3PO]_2Zn(SCN)_2$ as shown in Fig. 1.

The Zn atom is tetrahedrally coordinated. The analogous dichlorobis(triphenylphosphine oxide)zinc(II) compound (Zeller *et al.*, 2001) has comparable geometric parameters.

Experimental

The title compound was synthesized according to a method described previously (Pinkas *et al.*, 1998). The product of this synthesis was recrystallized by slow evaporation of an acetone solution at room temperature to give yellow block shaped crystals. Analysis calculated for $C_{38}H_{30}N_2O_2P_2S_2Zn$: C 61.83, H 4.10, N 3.80%; foud (%): C 61.48, H 4.49, N 3.67%.

Refinement

All H atoms were placed at geometrically idealized positions and were treated as riding, with C—H = 0.93Å and U_{iso}(H) = 1.2U_{eq}(partent atom).

Figures

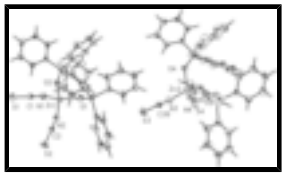

Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

Bis(thiocyanato-κ*N*)bis(triphenylphosphine oxide-κ*O*)zinc(II)

Crystal data

$[Zn_1(N_1C_1S_1)_2(C_{18}H_{15}O_1P_1)_2]$	Z = 4
M_r = 738.07	F_{000} = 1520
Triclinic, $P\overline{1}$	D_x = 1.358 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 9.9695 (6) Å	Cell parameters from 22725 reflections

b = 19.6036 (12) Å	θ = 2.2–28.2º
c = 21.2407 (12) Å	μ = 0.92 mm^{-1}
α = 116.799 (3)º	T = 298 (2) K
β = 98.316 (3)º	Block, yellow
γ = 95.098 (3)º	0.20 × 0.15 × 0.12 mm
V = 3610.2 (4) Å^3	

Data collection

Siemens SMART CCD diffractometer	12513 independent reflections
Radiation source: fine-focus sealed tube	10612 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.057
T = 298(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 1.1º
Absorption correction: empirical (using intensity measurements) (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 11$
T_{min} = 0.837, T_{max} = 0.898	$k = -23 \rightarrow 16$
37146 measured reflections	$l = -23 \rightarrow 25$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.032	H-atom parameters constrained
$wR(F^2)$ = 0.091	$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 0.9616P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001
12513 reflections	$\Delta\rho_{max}$ = 0.45 e Å^{-3}
847 parameters	$\Delta\rho_{min}$ = −0.48 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Zn1	0.13192 (2)	1.052920 (13)	0.847081 (13)	0.04077 (7)
Zn2	0.56423 (2)	0.630566 (14)	0.368980 (13)	0.04653 (8)
S1	−0.08062 (8)	1.26379 (4)	0.88646 (4)	0.0737 (2)
S2	0.45853 (9)	1.23027 (5)	1.04395 (5)	0.0906 (3)
S3	0.53990 (8)	0.89535 (4)	0.48324 (4)	0.0757 (2)
S4	0.75445 (13)	0.51796 (5)	0.50542 (5)	0.1086 (4)
P1	0.25043 (5)	0.96611 (3)	0.69865 (3)	0.04347 (13)
P2	−0.10195 (5)	0.91425 (3)	0.83896 (3)	0.04148 (13)
P3	0.74093 (5)	0.62405 (3)	0.24295 (3)	0.04247 (13)
P4	0.31137 (5)	0.49654 (3)	0.26626 (3)	0.04336 (13)
O1	0.21036 (16)	0.98176 (9)	0.76912 (8)	0.0544 (4)
O2	−0.00785 (17)	0.98849 (9)	0.86071 (9)	0.0616 (4)
O3	0.65577 (16)	0.60806 (10)	0.28875 (9)	0.0599 (4)
O4	0.37749 (14)	0.57989 (8)	0.31675 (9)	0.0551 (4)
N1	0.0359 (2)	1.13118 (12)	0.83707 (12)	0.0614 (5)
N2	0.2797 (2)	1.10586 (12)	0.93108 (11)	0.0611 (5)
N3	0.5642 (2)	0.74096 (13)	0.41903 (12)	0.0692 (6)
N4	0.6444 (3)	0.58588 (14)	0.42612 (13)	0.0782 (7)
C1	−0.0123 (2)	1.18685 (14)	0.85828 (12)	0.0490 (5)
C2	0.3557 (2)	1.15767 (13)	0.97794 (12)	0.0495 (5)
C3	0.1311 (2)	0.99525 (13)	0.64781 (12)	0.0489 (5)
C4	0.1331 (3)	1.07421 (16)	0.67189 (17)	0.0763 (8)
H4	0.2023	1.1103	0.7099	0.092*
C5	0.0335 (4)	1.0991 (2)	0.6398 (2)	0.0942 (10)
H5	0.0361	1.1520	0.6561	0.113*
C6	−0.0686 (3)	1.0476 (2)	0.5848 (2)	0.0893 (10)
H6	−0.1367	1.0653	0.5642	0.107*
C7	−0.0719 (3)	0.9698 (2)	0.55953 (19)	0.0881 (10)
H7	−0.1414	0.9345	0.5212	0.106*
C8	0.0285 (2)	0.94324 (17)	0.59094 (15)	0.0673 (7)
H8	0.0264	0.8902	0.5735	0.081*
C9	0.4192 (2)	1.01616 (12)	0.71102 (11)	0.0460 (5)
C10	0.5157 (2)	1.03588 (13)	0.77341 (13)	0.0532 (5)
H10	0.4900	1.0277	0.8102	0.064*
C11	0.6501 (2)	1.06763 (14)	0.78059 (15)	0.0617 (6)
H11	0.7143	1.0812	0.8225	0.074*
C12	0.6893 (2)	1.07927 (15)	0.72641 (15)	0.0632 (7)
H12	0.7804	1.0996	0.7312	0.076*
C13	0.5940 (3)	1.06093 (16)	0.66515 (14)	0.0666 (7)
H13	0.6204	1.0696	0.6287	0.080*
C14	0.4593 (2)	1.02972 (15)	0.65734 (13)	0.0588 (6)
H14	0.3951	1.0177	0.6158	0.071*
C15	0.2511 (2)	0.86410 (12)	0.64717 (12)	0.0454 (5)
C16	0.3470 (2)	0.83581 (14)	0.60491 (14)	0.0632 (7)
H16	0.4141	0.8703	0.6028	0.076*

C17	0.3439 (3)	0.75717 (16)	0.56604 (16)	0.0752 (8)
H17	0.4090	0.7391	0.5380	0.090*
C18	0.2457 (3)	0.70546 (15)	0.56835 (16)	0.0699 (7)
H18	0.2440	0.6524	0.5421	0.084*
C19	0.1498 (3)	0.73258 (15)	0.60967 (17)	0.0749 (8)
H19	0.0822	0.6976	0.6110	0.090*
C20	0.1525 (3)	0.81102 (14)	0.64913 (15)	0.0640 (7)
H20	0.0875	0.8286	0.6774	0.077*
C21	−0.1479 (2)	0.85453 (12)	0.74305 (11)	0.0441 (5)
C22	−0.1879 (2)	0.88990 (16)	0.70127 (14)	0.0608 (6)
H22	−0.1818	0.9435	0.7227	0.073*
C23	−0.2365 (3)	0.8456 (2)	0.62824 (16)	0.0796 (9)
H23	−0.2648	0.8692	0.6004	0.096*
C24	−0.2433 (3)	0.7667 (2)	0.59641 (16)	0.0851 (10)
H24	−0.2756	0.7371	0.5469	0.102*
C25	−0.2033 (3)	0.73135 (17)	0.63665 (15)	0.0759 (8)
H25	−0.2076	0.6778	0.6144	0.091*
C26	−0.1563 (2)	0.77469 (13)	0.71037 (13)	0.0559 (6)
H26	−0.1303	0.7504	0.7379	0.067*
C27	−0.0242 (2)	0.85997 (12)	0.87847 (11)	0.0457 (5)
C28	0.1077 (2)	0.84514 (16)	0.86907 (14)	0.0638 (7)
H28	0.1508	0.8608	0.8405	0.077*
C29	0.1739 (3)	0.80750 (18)	0.90191 (17)	0.0814 (9)
H29	0.2618	0.7976	0.8955	0.098*
C30	0.1110 (4)	0.78457 (17)	0.94402 (17)	0.0841 (9)
H30	0.1567	0.7595	0.9665	0.101*
C31	−0.0192 (4)	0.79833 (18)	0.95330 (17)	0.0808 (8)
H31	−0.0614	0.7824	0.9819	0.097*
C32	−0.0876 (3)	0.83564 (15)	0.92060 (14)	0.0635 (6)
H32	−0.1761	0.8445	0.9267	0.076*
C33	−0.2620 (2)	0.93378 (12)	0.86656 (12)	0.0441 (5)
C34	−0.3809 (2)	0.87841 (14)	0.83064 (15)	0.0653 (7)
H34	−0.3774	0.8302	0.7932	0.078*
C35	−0.5050 (3)	0.89542 (16)	0.85093 (17)	0.0702 (7)
H35	−0.5845	0.8581	0.8274	0.084*
C36	−0.5110 (3)	0.96633 (17)	0.90499 (14)	0.0627 (7)
H36	−0.5947	0.9775	0.9180	0.075*
C37	−0.3951 (3)	1.02105 (16)	0.94019 (14)	0.0663 (7)
H37	−0.4003	1.0694	0.9770	0.080*
C38	−0.2685 (2)	1.00533 (14)	0.92164 (12)	0.0552 (6)
H38	−0.1894	1.0427	0.9462	0.066*
C39	0.5547 (2)	0.80563 (14)	0.44501 (12)	0.0509 (5)
C40	0.6879 (3)	0.55690 (16)	0.45897 (14)	0.0682 (7)
C41	0.6649 (2)	0.68279 (12)	0.20796 (12)	0.0454 (5)
C42	0.5521 (3)	0.71419 (17)	0.23084 (16)	0.0727 (8)
H42	0.5198	0.7085	0.2675	0.087*
C43	0.4862 (3)	0.7542 (2)	0.19961 (19)	0.0940 (10)
H43	0.4094	0.7748	0.2151	0.113*
C44	0.5331 (3)	0.76350 (16)	0.14668 (16)	0.0737 (8)

H44	0.4873	0.7895	0.1253	0.088*
C45	0.6471 (3)	0.73484 (18)	0.12472 (18)	0.0776 (8)
H45	0.6807	0.7425	0.0894	0.093*
C46	0.7125 (3)	0.69439 (18)	0.15505 (17)	0.0735 (8)
H46	0.7899	0.6746	0.1396	0.088*
C47	0.9126 (2)	0.67214 (13)	0.29397 (13)	0.0491 (5)
C48	0.9381 (3)	0.69812 (17)	0.36752 (15)	0.0719 (7)
H48	0.8688	0.6883	0.3889	0.086*
C49	1.0668 (3)	0.7388 (2)	0.40967 (19)	0.0947 (10)
H49	1.0834	0.7565	0.4592	0.114*
C50	1.1686 (3)	0.75293 (18)	0.3787 (2)	0.0931 (11)
H50	1.2549	0.7799	0.4071	0.112*
C51	1.1447 (3)	0.72767 (18)	0.3063 (2)	0.0865 (10)
H51	1.2150	0.7376	0.2856	0.104*
C52	1.0162 (2)	0.68712 (15)	0.26282 (16)	0.0686 (7)
H52	1.0003	0.6703	0.2134	0.082*
C53	0.7476 (2)	0.53510 (12)	0.16532 (12)	0.0432 (5)
C54	0.8561 (3)	0.49588 (15)	0.16201 (16)	0.0683 (7)
H54	0.9330	0.5171	0.1996	0.082*
C55	0.8510 (3)	0.42478 (16)	0.10277 (19)	0.0873 (10)
H55	0.9255	0.3989	0.1003	0.105*
C56	0.7372 (3)	0.39215 (15)	0.04772 (16)	0.0739 (8)
H56	0.7343	0.3443	0.0081	0.089*
C57	0.6274 (3)	0.43035 (16)	0.05126 (15)	0.0728 (7)
H57	0.5492	0.4079	0.0144	0.087*
C58	0.6327 (2)	0.50157 (15)	0.10901 (14)	0.0619 (6)
H58	0.5588	0.5277	0.1106	0.074*
C59	0.2675 (2)	0.48219 (14)	0.17566 (13)	0.0502 (5)
C60	0.2558 (3)	0.54711 (18)	0.16597 (17)	0.0772 (8)
H60	0.2744	0.5963	0.2057	0.093*
C61	0.2165 (4)	0.5387 (2)	0.0977 (2)	0.1054 (12)
H61	0.2075	0.5823	0.0915	0.126*
C62	0.1910 (4)	0.4678 (3)	0.0395 (2)	0.0995 (11)
H62	0.1653	0.4630	−0.0064	0.119*
C63	0.2026 (3)	0.4026 (2)	0.04727 (16)	0.0835 (9)
H63	0.1845	0.3539	0.0069	0.100*
C64	0.2415 (3)	0.40969 (16)	0.11559 (14)	0.0647 (7)
H64	0.2501	0.3657	0.1211	0.078*
C65	0.4176 (2)	0.42756 (12)	0.26716 (12)	0.0455 (5)
C66	0.5101 (2)	0.40487 (15)	0.22166 (14)	0.0626 (6)
H66	0.5143	0.4234	0.1885	0.075*
C67	0.5954 (3)	0.35495 (18)	0.22573 (16)	0.0778 (9)
H67	0.6570	0.3393	0.1951	0.093*
C68	0.5896 (3)	0.32809 (15)	0.27513 (18)	0.0768 (9)
H68	0.6457	0.2933	0.2769	0.092*
C69	0.5016 (3)	0.35221 (18)	0.32184 (19)	0.0788 (9)
H69	0.5005	0.3353	0.3563	0.095*
C70	0.4145 (2)	0.40171 (16)	0.31761 (16)	0.0646 (7)
H70	0.3537	0.4176	0.3488	0.077*

C71	0.15697 (19)	0.47608 (12)	0.29288 (12)	0.0435 (5)
C72	0.0756 (2)	0.40260 (14)	0.25765 (14)	0.0582 (6)
H72	0.0988	0.3630	0.2180	0.070*
C73	−0.0393 (2)	0.38894 (16)	0.28186 (16)	0.0701 (7)
H73	−0.0933	0.3397	0.2587	0.084*
C74	−0.0753 (2)	0.44714 (17)	0.33991 (16)	0.0696 (7)
H74	−0.1531	0.4373	0.3559	0.084*
C75	0.0033 (3)	0.51953 (16)	0.37412 (15)	0.0697 (7)
H75	−0.0217	0.5590	0.4132	0.084*
C76	0.1194 (2)	0.53448 (14)	0.35106 (13)	0.0584 (6)
H76	0.1725	0.5839	0.3746	0.070*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.03915 (12)	0.03626 (13)	0.04320 (14)	0.00350 (9)	0.00903 (10)	0.01595 (11)
Zn2	0.04996 (14)	0.04471 (15)	0.04040 (14)	0.00410 (11)	0.00907 (10)	0.01699 (12)
S1	0.0772 (4)	0.0592 (4)	0.0834 (5)	0.0265 (3)	0.0200 (4)	0.0290 (4)
S2	0.0891 (5)	0.0618 (4)	0.0803 (5)	−0.0048 (4)	−0.0310 (4)	0.0161 (4)
S3	0.0885 (5)	0.0505 (4)	0.0766 (5)	0.0154 (3)	0.0079 (4)	0.0225 (4)
S4	0.1950 (11)	0.0843 (6)	0.0607 (5)	0.0675 (6)	0.0265 (6)	0.0385 (4)
P1	0.0471 (3)	0.0440 (3)	0.0416 (3)	0.0107 (2)	0.0150 (2)	0.0198 (3)
P2	0.0433 (3)	0.0378 (3)	0.0433 (3)	0.0040 (2)	0.0161 (2)	0.0175 (2)
P3	0.0393 (3)	0.0442 (3)	0.0480 (3)	0.0103 (2)	0.0128 (2)	0.0237 (3)
P4	0.0381 (3)	0.0402 (3)	0.0513 (3)	0.0066 (2)	0.0111 (2)	0.0206 (3)
O1	0.0659 (9)	0.0591 (9)	0.0481 (9)	0.0216 (8)	0.0273 (7)	0.0272 (8)
O2	0.0674 (10)	0.0462 (9)	0.0632 (10)	−0.0080 (7)	0.0266 (8)	0.0184 (8)
O3	0.0622 (9)	0.0656 (10)	0.0632 (10)	0.0136 (8)	0.0291 (8)	0.0350 (9)
O4	0.0464 (8)	0.0405 (8)	0.0686 (11)	0.0032 (6)	0.0113 (7)	0.0183 (8)
N1	0.0599 (12)	0.0569 (13)	0.0732 (14)	0.0161 (10)	0.0121 (10)	0.0349 (11)
N2	0.0515 (11)	0.0559 (12)	0.0576 (13)	0.0042 (9)	−0.0009 (9)	0.0155 (11)
N3	0.0771 (14)	0.0505 (13)	0.0616 (14)	0.0067 (11)	0.0115 (11)	0.0123 (11)
N4	0.1013 (18)	0.0761 (16)	0.0599 (14)	0.0168 (13)	0.0049 (12)	0.0375 (13)
C1	0.0462 (11)	0.0522 (14)	0.0499 (13)	0.0048 (10)	0.0054 (9)	0.0272 (11)
C2	0.0481 (12)	0.0517 (13)	0.0497 (13)	0.0144 (10)	0.0058 (10)	0.0250 (12)
C3	0.0500 (12)	0.0564 (14)	0.0470 (13)	0.0125 (10)	0.0166 (10)	0.0277 (11)
C4	0.093 (2)	0.0579 (16)	0.0744 (19)	0.0222 (14)	0.0061 (15)	0.0295 (15)
C5	0.119 (3)	0.085 (2)	0.098 (3)	0.050 (2)	0.025 (2)	0.054 (2)
C6	0.0753 (19)	0.126 (3)	0.108 (3)	0.041 (2)	0.0258 (19)	0.084 (3)
C7	0.0593 (16)	0.121 (3)	0.092 (2)	−0.0030 (17)	−0.0059 (15)	0.067 (2)
C8	0.0576 (14)	0.0720 (17)	0.0752 (18)	0.0029 (12)	0.0040 (13)	0.0415 (15)
C9	0.0497 (11)	0.0436 (12)	0.0422 (12)	0.0079 (9)	0.0107 (9)	0.0177 (10)
C10	0.0613 (13)	0.0512 (13)	0.0517 (14)	0.0093 (11)	0.0074 (10)	0.0294 (11)
C11	0.0562 (13)	0.0604 (15)	0.0651 (16)	0.0057 (11)	−0.0060 (11)	0.0328 (13)
C12	0.0491 (13)	0.0596 (15)	0.0751 (18)	0.0017 (11)	0.0074 (12)	0.0298 (14)
C13	0.0651 (15)	0.0759 (18)	0.0568 (15)	−0.0043 (13)	0.0156 (12)	0.0317 (14)
C14	0.0559 (13)	0.0706 (16)	0.0431 (13)	−0.0036 (11)	0.0051 (10)	0.0249 (12)
C15	0.0461 (11)	0.0447 (12)	0.0470 (12)	0.0109 (9)	0.0134 (9)	0.0215 (10)

C16	0.0613 (14)	0.0537 (15)	0.0708 (17)	0.0101 (12)	0.0286 (13)	0.0219 (13)
C17	0.0787 (18)	0.0626 (17)	0.0791 (19)	0.0256 (14)	0.0353 (15)	0.0212 (15)
C18	0.0850 (18)	0.0477 (14)	0.0730 (18)	0.0210 (13)	0.0141 (14)	0.0239 (13)
C19	0.0836 (18)	0.0506 (15)	0.099 (2)	0.0116 (13)	0.0307 (16)	0.0390 (16)
C20	0.0694 (15)	0.0546 (15)	0.0822 (18)	0.0164 (12)	0.0359 (13)	0.0374 (14)
C21	0.0405 (10)	0.0466 (12)	0.0464 (12)	0.0056 (9)	0.0152 (9)	0.0216 (10)
C22	0.0639 (14)	0.0674 (16)	0.0608 (16)	0.0182 (12)	0.0163 (12)	0.0363 (14)
C23	0.0683 (17)	0.119 (3)	0.0653 (19)	0.0128 (17)	0.0055 (14)	0.058 (2)
C24	0.0741 (18)	0.110 (3)	0.0479 (16)	−0.0131 (17)	0.0020 (13)	0.0252 (18)
C25	0.0833 (18)	0.0594 (16)	0.0557 (17)	−0.0147 (14)	0.0171 (14)	0.0061 (14)
C26	0.0641 (14)	0.0476 (13)	0.0499 (14)	−0.0003 (11)	0.0159 (11)	0.0183 (11)
C27	0.0459 (11)	0.0450 (12)	0.0401 (11)	0.0056 (9)	0.0074 (9)	0.0156 (10)
C28	0.0525 (13)	0.0711 (17)	0.0632 (16)	0.0162 (12)	0.0123 (11)	0.0267 (14)
C29	0.0705 (17)	0.079 (2)	0.077 (2)	0.0308 (15)	0.0024 (15)	0.0216 (17)
C30	0.109 (2)	0.0595 (17)	0.071 (2)	0.0254 (17)	−0.0117 (17)	0.0260 (15)
C31	0.105 (2)	0.0759 (19)	0.074 (2)	0.0131 (17)	0.0124 (16)	0.0486 (17)
C32	0.0694 (15)	0.0672 (16)	0.0666 (17)	0.0150 (13)	0.0196 (13)	0.0403 (14)
C33	0.0491 (11)	0.0446 (12)	0.0480 (12)	0.0134 (9)	0.0204 (9)	0.0259 (10)
C34	0.0571 (14)	0.0488 (14)	0.0828 (18)	0.0070 (11)	0.0305 (13)	0.0205 (13)
C35	0.0520 (13)	0.0699 (17)	0.093 (2)	0.0097 (12)	0.0308 (13)	0.0371 (16)
C36	0.0594 (14)	0.0856 (19)	0.0661 (16)	0.0326 (14)	0.0321 (13)	0.0462 (15)
C37	0.0808 (18)	0.0714 (17)	0.0512 (15)	0.0370 (15)	0.0280 (13)	0.0243 (13)
C38	0.0621 (13)	0.0567 (14)	0.0431 (13)	0.0164 (11)	0.0125 (10)	0.0187 (11)
C39	0.0501 (12)	0.0543 (15)	0.0390 (12)	0.0027 (10)	0.0028 (9)	0.0171 (11)
C40	0.096 (2)	0.0609 (16)	0.0435 (14)	0.0212 (14)	0.0151 (13)	0.0196 (13)
C41	0.0416 (10)	0.0417 (11)	0.0508 (13)	0.0068 (9)	0.0069 (9)	0.0208 (10)
C42	0.0778 (17)	0.089 (2)	0.0745 (18)	0.0469 (15)	0.0340 (14)	0.0474 (17)
C43	0.097 (2)	0.113 (3)	0.100 (3)	0.071 (2)	0.0377 (19)	0.060 (2)
C44	0.0880 (19)	0.0561 (16)	0.0742 (19)	0.0235 (14)	−0.0021 (15)	0.0317 (14)
C45	0.0848 (19)	0.083 (2)	0.095 (2)	0.0217 (16)	0.0236 (16)	0.0648 (19)
C46	0.0600 (15)	0.094 (2)	0.104 (2)	0.0303 (14)	0.0314 (14)	0.0713 (19)
C47	0.0438 (11)	0.0442 (12)	0.0569 (14)	0.0115 (9)	0.0054 (10)	0.0225 (11)
C48	0.0633 (15)	0.0818 (19)	0.0647 (18)	0.0117 (14)	−0.0010 (13)	0.0338 (16)
C49	0.078 (2)	0.100 (3)	0.077 (2)	0.0189 (18)	−0.0169 (17)	0.0258 (19)
C50	0.0553 (17)	0.0660 (19)	0.118 (3)	0.0117 (14)	−0.0196 (18)	0.020 (2)
C51	0.0489 (14)	0.0704 (19)	0.122 (3)	0.0043 (13)	0.0158 (16)	0.031 (2)
C52	0.0488 (13)	0.0664 (16)	0.0800 (19)	0.0044 (12)	0.0148 (12)	0.0261 (15)
C53	0.0430 (10)	0.0407 (11)	0.0502 (12)	0.0076 (9)	0.0137 (9)	0.0240 (10)
C54	0.0527 (13)	0.0528 (14)	0.0847 (19)	0.0175 (11)	0.0038 (12)	0.0214 (14)
C55	0.0745 (18)	0.0554 (16)	0.112 (3)	0.0314 (14)	0.0181 (17)	0.0197 (17)
C56	0.093 (2)	0.0468 (14)	0.0705 (18)	0.0160 (14)	0.0227 (15)	0.0154 (13)
C57	0.0779 (17)	0.0609 (16)	0.0580 (16)	0.0058 (14)	0.0012 (13)	0.0146 (14)
C58	0.0554 (13)	0.0632 (16)	0.0614 (16)	0.0173 (12)	0.0089 (11)	0.0243 (13)
C59	0.0450 (11)	0.0573 (14)	0.0575 (14)	0.0143 (10)	0.0170 (10)	0.0320 (12)
C60	0.107 (2)	0.0699 (18)	0.080 (2)	0.0374 (16)	0.0399 (17)	0.0475 (16)
C61	0.158 (4)	0.112 (3)	0.099 (3)	0.065 (3)	0.055 (3)	0.079 (3)
C62	0.115 (3)	0.142 (3)	0.077 (2)	0.049 (2)	0.0295 (19)	0.074 (3)
C63	0.087 (2)	0.100 (2)	0.0570 (18)	0.0140 (17)	0.0092 (14)	0.0334 (17)
C64	0.0663 (15)	0.0667 (17)	0.0602 (16)	0.0082 (12)	0.0073 (12)	0.0315 (14)

C65	0.0373 (10)	0.0402 (11)	0.0520 (13)	0.0034 (8)	0.0054 (9)	0.0175 (10)
C66	0.0537 (13)	0.0730 (17)	0.0541 (15)	0.0207 (12)	0.0099 (11)	0.0226 (13)
C67	0.0581 (15)	0.086 (2)	0.0677 (18)	0.0342 (14)	0.0072 (13)	0.0158 (16)
C68	0.0541 (15)	0.0528 (15)	0.104 (2)	0.0150 (12)	−0.0092 (15)	0.0267 (16)
C69	0.0578 (15)	0.084 (2)	0.121 (3)	0.0120 (14)	0.0068 (16)	0.074 (2)
C70	0.0509 (13)	0.0769 (18)	0.0868 (19)	0.0169 (12)	0.0212 (12)	0.0533 (16)
C71	0.0379 (10)	0.0458 (12)	0.0489 (12)	0.0094 (9)	0.0093 (9)	0.0236 (10)
C72	0.0481 (12)	0.0481 (13)	0.0688 (16)	0.0060 (10)	0.0183 (11)	0.0181 (12)
C73	0.0513 (13)	0.0574 (15)	0.093 (2)	−0.0023 (11)	0.0189 (13)	0.0294 (15)
C74	0.0483 (13)	0.0816 (19)	0.0813 (19)	0.0057 (13)	0.0248 (13)	0.0382 (17)
C75	0.0633 (15)	0.0737 (18)	0.0640 (16)	0.0120 (13)	0.0295 (13)	0.0206 (14)
C76	0.0526 (13)	0.0536 (14)	0.0569 (15)	0.0033 (11)	0.0135 (11)	0.0162 (12)

Geometric parameters (Å, °)

Zn1—N2	1.931 (2)	C30—C31	1.373 (5)
Zn1—O2	1.9376 (15)	C30—H30	0.9300
Zn1—O1	1.9454 (15)	C31—C32	1.375 (4)
Zn1—N1	1.952 (2)	C31—H31	0.9300
Zn2—N4	1.919 (2)	C32—H32	0.9300
Zn2—N3	1.934 (2)	C33—C38	1.378 (3)
Zn2—O4	1.9400 (14)	C33—C34	1.388 (3)
Zn2—O3	1.9429 (15)	C34—C35	1.388 (3)
S1—C1	1.607 (3)	C34—H34	0.9300
S2—C2	1.603 (2)	C35—C36	1.360 (4)
S3—C39	1.602 (3)	C35—H35	0.9300
S4—C40	1.605 (3)	C36—C37	1.360 (4)
P1—O1	1.5084 (15)	C36—H36	0.9300
P1—C9	1.792 (2)	C37—C38	1.395 (3)
P1—C3	1.792 (2)	C37—H37	0.9300
P1—C15	1.797 (2)	C38—H38	0.9300
P2—O2	1.4959 (15)	C41—C42	1.375 (3)
P2—C27	1.789 (2)	C41—C46	1.380 (3)
P2—C33	1.793 (2)	C42—C43	1.386 (4)
P2—C21	1.793 (2)	C42—H42	0.9300
P3—O3	1.4939 (16)	C43—C44	1.355 (4)
P3—C41	1.793 (2)	C43—H43	0.9300
P3—C53	1.795 (2)	C44—C45	1.362 (4)
P3—C47	1.802 (2)	C44—H44	0.9300
P4—O4	1.5095 (15)	C45—C46	1.378 (4)
P4—C71	1.788 (2)	C45—H45	0.9300
P4—C59	1.795 (2)	C46—H46	0.9300
P4—C65	1.795 (2)	C47—C48	1.382 (4)
N1—C1	1.157 (3)	C47—C52	1.382 (3)
N2—C2	1.153 (3)	C48—C49	1.388 (4)
N3—C39	1.152 (3)	C48—H48	0.9300
N4—C40	1.145 (3)	C49—C50	1.359 (5)
C3—C8	1.375 (3)	C49—H49	0.9300
C3—C4	1.391 (3)	C50—C51	1.362 (5)

C4—C5	1.370 (4)	C50—H50	0.9300
C4—H4	0.9300	C51—C52	1.393 (4)
C5—C6	1.352 (5)	C51—H51	0.9300
C5—H5	0.9300	C52—H52	0.9300
C6—C7	1.366 (5)	C53—C54	1.374 (3)
C6—H6	0.9300	C53—C58	1.391 (3)
C7—C8	1.389 (4)	C54—C55	1.384 (4)
C7—H7	0.9300	C54—H54	0.9300
C8—H8	0.9300	C55—C56	1.370 (4)
C9—C14	1.384 (3)	C55—H55	0.9300
C9—C10	1.391 (3)	C56—C57	1.372 (4)
C10—C11	1.383 (3)	C56—H56	0.9300
C10—H10	0.9300	C57—C58	1.371 (4)
C11—C12	1.372 (4)	C57—H57	0.9300
C11—H11	0.9300	C58—H58	0.9300
C12—C13	1.373 (4)	C59—C64	1.385 (3)
C12—H12	0.9300	C59—C60	1.390 (3)
C13—C14	1.380 (3)	C60—C61	1.377 (5)
C13—H13	0.9300	C60—H60	0.9300
C14—H14	0.9300	C61—C62	1.350 (5)
C15—C16	1.385 (3)	C61—H61	0.9300
C15—C20	1.386 (3)	C62—C63	1.372 (5)
C16—C17	1.377 (3)	C62—H62	0.9300
C16—H16	0.9300	C63—C64	1.386 (4)
C17—C18	1.367 (4)	C63—H63	0.9300
C17—H17	0.9300	C64—H64	0.9300
C18—C19	1.371 (4)	C65—C70	1.379 (3)
C18—H18	0.9300	C65—C66	1.387 (3)
C19—C20	1.375 (4)	C66—C67	1.375 (4)
C19—H19	0.9300	C66—H66	0.9300
C20—H20	0.9300	C67—C68	1.376 (4)
C21—C26	1.385 (3)	C67—H67	0.9300
C21—C22	1.389 (3)	C68—C69	1.371 (4)
C22—C23	1.374 (4)	C68—H68	0.9300
C22—H22	0.9300	C69—C70	1.382 (4)
C23—C24	1.371 (4)	C69—H69	0.9300
C23—H23	0.9300	C70—H70	0.9300
C24—C25	1.362 (4)	C71—C76	1.383 (3)
C24—H24	0.9300	C71—C72	1.392 (3)
C25—C26	1.382 (4)	C72—C73	1.374 (3)
C25—H25	0.9300	C72—H72	0.9300
C26—H26	0.9300	C73—C74	1.372 (4)
C27—C32	1.387 (3)	C73—H73	0.9300
C27—C28	1.394 (3)	C74—C75	1.365 (4)
C28—C29	1.373 (4)	C74—H74	0.9300
C28—H28	0.9300	C75—C76	1.378 (3)
C29—C30	1.368 (5)	C75—H75	0.9300
C29—H29	0.9300	C76—H76	0.9300
N2—Zn1—O2	111.57 (9)	C32—C31—H31	119.8

N2—Zn1—O1	106.88 (8)	C31—C32—C27	119.8 (3)
O2—Zn1—O1	105.69 (7)	C31—C32—H32	120.1
N2—Zn1—N1	107.80 (9)	C27—C32—H32	120.1
O2—Zn1—N1	103.88 (8)	C38—C33—C34	119.7 (2)
O1—Zn1—N1	120.98 (8)	C38—C33—P2	119.87 (17)
N4—Zn2—N3	116.34 (10)	C34—C33—P2	120.35 (17)
N4—Zn2—O4	113.40 (9)	C35—C34—C33	119.7 (2)
N3—Zn2—O4	107.47 (8)	C35—C34—H34	120.2
N4—Zn2—O3	109.50 (9)	C33—C34—H34	120.2
N3—Zn2—O3	108.76 (9)	C36—C35—C34	120.3 (2)
O4—Zn2—O3	100.07 (7)	C36—C35—H35	119.8
O1—P1—C9	112.56 (10)	C34—C35—H35	119.8
O1—P1—C3	110.67 (9)	C35—C36—C37	120.3 (2)
C9—P1—C3	107.94 (10)	C35—C36—H36	119.8
O1—P1—C15	109.13 (10)	C37—C36—H36	119.8
C9—P1—C15	107.21 (10)	C36—C37—C38	120.6 (2)
C3—P1—C15	109.24 (11)	C36—C37—H37	119.7
O2—P2—C27	110.57 (10)	C38—C37—H37	119.7
O2—P2—C33	110.33 (10)	C33—C38—C37	119.3 (2)
C27—P2—C33	109.39 (10)	C33—C38—H38	120.4
O2—P2—C21	112.59 (10)	C37—C38—H38	120.4
C27—P2—C21	108.77 (10)	N3—C39—S3	178.2 (2)
C33—P2—C21	105.01 (10)	N4—C40—S4	177.9 (3)
O3—P3—C41	111.22 (10)	C42—C41—C46	118.2 (2)
O3—P3—C53	110.14 (10)	C42—C41—P3	120.25 (19)
C41—P3—C53	105.46 (10)	C46—C41—P3	121.46 (17)
O3—P3—C47	110.51 (11)	C41—C42—C43	120.4 (3)
C41—P3—C47	109.37 (10)	C41—C42—H42	119.8
C53—P3—C47	110.01 (10)	C43—C42—H42	119.8
O4—P4—C71	108.46 (9)	C44—C43—C42	120.4 (3)
O4—P4—C59	110.00 (10)	C44—C43—H43	119.8
C71—P4—C59	108.65 (10)	C42—C43—H43	119.8
O4—P4—C65	113.75 (9)	C43—C44—C45	120.2 (3)
C71—P4—C65	107.38 (10)	C43—C44—H44	119.9
C59—P4—C65	108.46 (11)	C45—C44—H44	119.9
P1—O1—Zn1	144.35 (10)	C44—C45—C46	119.8 (3)
P2—O2—Zn1	153.74 (11)	C44—C45—H45	120.1
P3—O3—Zn2	157.78 (11)	C46—C45—H45	120.1
P4—O4—Zn2	133.60 (9)	C45—C46—C41	121.0 (2)
C1—N1—Zn1	154.5 (2)	C45—C46—H46	119.5
C2—N2—Zn1	157.2 (2)	C41—C46—H46	119.5
C39—N3—Zn2	174.6 (2)	C48—C47—C52	119.4 (2)
C40—N4—Zn2	177.3 (3)	C48—C47—P3	118.05 (19)
N1—C1—S1	179.1 (2)	C52—C47—P3	122.4 (2)
N2—C2—S2	178.8 (2)	C47—C48—C49	120.2 (3)
C8—C3—C4	118.6 (2)	C47—C48—H48	119.9
C8—C3—P1	122.65 (19)	C49—C48—H48	119.9
C4—C3—P1	118.35 (19)	C50—C49—C48	120.1 (3)
C5—C4—C3	120.3 (3)	C50—C49—H49	119.9

C5—C4—H4	119.9	C48—C49—H49	119.9
C3—C4—H4	119.9	C49—C50—C51	120.2 (3)
C6—C5—C4	120.8 (3)	C49—C50—H50	119.9
C6—C5—H5	119.6	C51—C50—H50	119.9
C4—C5—H5	119.6	C50—C51—C52	120.8 (3)
C5—C6—C7	120.1 (3)	C50—C51—H51	119.6
C5—C6—H6	119.9	C52—C51—H51	119.6
C7—C6—H6	119.9	C47—C52—C51	119.2 (3)
C6—C7—C8	120.1 (3)	C47—C52—H52	120.4
C6—C7—H7	120.0	C51—C52—H52	120.4
C8—C7—H7	120.0	C54—C53—C58	118.9 (2)
C3—C8—C7	120.1 (3)	C54—C53—P3	122.70 (18)
C3—C8—H8	119.9	C58—C53—P3	118.14 (16)
C7—C8—H8	119.9	C53—C54—C55	120.0 (2)
C14—C9—C10	119.2 (2)	C53—C54—H54	120.0
C14—C9—P1	121.45 (17)	C55—C54—H54	120.0
C10—C9—P1	119.15 (17)	C56—C55—C54	120.6 (2)
C11—C10—C9	119.8 (2)	C56—C55—H55	119.7
C11—C10—H10	120.1	C54—C55—H55	119.7
C9—C10—H10	120.1	C55—C56—C57	119.7 (3)
C12—C11—C10	120.5 (2)	C55—C56—H56	120.1
C12—C11—H11	119.7	C57—C56—H56	120.1
C10—C11—H11	119.7	C58—C57—C56	120.1 (3)
C11—C12—C13	119.9 (2)	C58—C57—H57	119.9
C11—C12—H12	120.1	C56—C57—H57	119.9
C13—C12—H12	120.1	C57—C58—C53	120.6 (2)
C12—C13—C14	120.3 (2)	C57—C58—H58	119.7
C12—C13—H13	119.8	C53—C58—H58	119.7
C14—C13—H13	119.8	C64—C59—C60	118.9 (2)
C13—C14—C9	120.3 (2)	C64—C59—P4	123.14 (18)
C13—C14—H14	119.9	C60—C59—P4	117.9 (2)
C9—C14—H14	119.9	C61—C60—C59	120.1 (3)
C16—C15—C20	118.1 (2)	C61—C60—H60	120.0
C16—C15—P1	122.48 (17)	C59—C60—H60	120.0
C20—C15—P1	119.43 (17)	C62—C61—C60	120.5 (3)
C17—C16—C15	120.8 (2)	C62—C61—H61	119.8
C17—C16—H16	119.6	C60—C61—H61	119.8
C15—C16—H16	119.6	C61—C62—C63	120.8 (3)
C18—C17—C16	120.5 (2)	C61—C62—H62	119.6
C18—C17—H17	119.7	C63—C62—H62	119.6
C16—C17—H17	119.7	C62—C63—C64	119.7 (3)
C17—C18—C19	119.4 (3)	C62—C63—H63	120.2
C17—C18—H18	120.3	C64—C63—H63	120.2
C19—C18—H18	120.3	C59—C64—C63	120.0 (3)
C18—C19—C20	120.6 (3)	C59—C64—H64	120.0
C18—C19—H19	119.7	C63—C64—H64	120.0
C20—C19—H19	119.7	C70—C65—C66	119.8 (2)
C19—C20—C15	120.7 (2)	C70—C65—P4	119.25 (18)
C19—C20—H20	119.7	C66—C65—P4	120.71 (19)

C15—C20—H20	119.7	C67—C66—C65	119.8 (3)
C26—C21—C22	119.5 (2)	C67—C66—H66	120.1
C26—C21—P2	122.59 (18)	C65—C66—H66	120.1
C22—C21—P2	117.70 (17)	C66—C67—C68	120.0 (3)
C23—C22—C21	120.0 (3)	C66—C67—H67	120.0
C23—C22—H22	120.0	C68—C67—H67	120.0
C21—C22—H22	120.0	C69—C68—C67	120.5 (3)
C24—C23—C22	120.0 (3)	C69—C68—H68	119.7
C24—C23—H23	120.0	C67—C68—H68	119.7
C22—C23—H23	120.0	C68—C69—C70	119.8 (3)
C25—C24—C23	120.6 (3)	C68—C69—H69	120.1
C25—C24—H24	119.7	C70—C69—H69	120.1
C23—C24—H24	119.7	C65—C70—C69	120.0 (3)
C24—C25—C26	120.3 (3)	C65—C70—H70	120.0
C24—C25—H25	119.9	C69—C70—H70	120.0
C26—C25—H25	119.9	C76—C71—C72	119.3 (2)
C25—C26—C21	119.7 (3)	C76—C71—P4	118.95 (16)
C25—C26—H26	120.2	C72—C71—P4	121.74 (17)
C21—C26—H26	120.2	C73—C72—C71	119.6 (2)
C32—C27—C28	119.3 (2)	C73—C72—H72	120.2
C32—C27—P2	122.37 (17)	C71—C72—H72	120.2
C28—C27—P2	118.28 (18)	C74—C73—C72	120.7 (2)
C29—C28—C27	120.0 (3)	C74—C73—H73	119.7
C29—C28—H28	120.0	C72—C73—H73	119.7
C27—C28—H28	120.0	C75—C74—C73	120.0 (2)
C30—C29—C28	120.2 (3)	C75—C74—H74	120.0
C30—C29—H29	119.9	C73—C74—H74	120.0
C28—C29—H29	119.9	C74—C75—C76	120.4 (2)
C29—C30—C31	120.4 (3)	C74—C75—H75	119.8
C29—C30—H30	119.8	C76—C75—H75	119.8
C31—C30—H30	119.8	C75—C76—C71	120.1 (2)
C30—C31—C32	120.4 (3)	C75—C76—H76	120.0
C30—C31—H31	119.8	C71—C76—H76	120.0

Fig. 1