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(2-Ethylimidazole-κN)bis(tri-*tert*-butoxysilanethiolato-$\kappa^2 O,S$)zinc(II) propan-2-ol solvate

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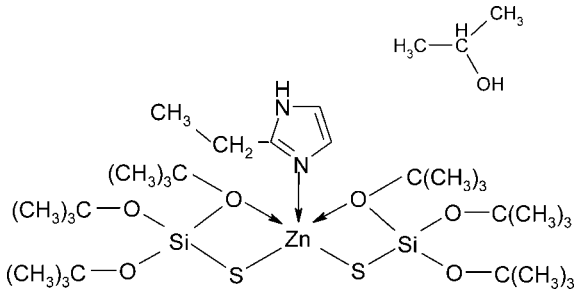
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.096; data-to-parameter ratio = 17.7.

In the title compound, $[Zn(C_{12}H_{27}O_3SSi)_2(C_5H_8N_2)]\cdot C_3H_8O$, the Zn^{II} centre is coordinated by the N atom of the 2-ethylimidazole ligand and two S and two O atoms of the two thiolate ligands in a trigonal–bipyramidal geometry. The hydroxyl group of the propan-2-ol solvent molecule forms N—H···O and O—H···S hydrogen bonds with adjacent molecules, linking them into chains.

Related literature

For an analogous compound with 1-methylimidazole, see Dołęga *et al.* (2004).



Experimental

Crystal data

$[Zn(C_{12}H_{27}O_3SSi)_2(C_5H_8N_2)]\cdot C_3H_8O$
M_r = 780.57
Monoclinic, $P2_1/c$
a = 9.8958 (2) Å
b = 25.3673 (6) Å
c = 19.8040 (5) Å
β = 116.064 (2)°
V = 4465.82 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.74 mm^{-1}
T = 120 (2) K
0.32 × 0.16 × 0.09 mm

Data collection

Oxford Diffraction KM-4-CCD κ-geometry diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.769, T_{max} = 0.885
25240 measured reflections
7709 independent reflections
6892 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.096
S = 1.13
7709 reflections
436 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.0134 (17)	Zn1—O1	2.5436 (14)
Zn1—S2	2.2749 (6)	S1—Si1	2.0897 (7)
Zn1—S1	2.2878 (5)	S2—Si2	2.0818 (7)
Zn1—O4	2.4039 (12)		
N1—Zn1—S2	120.90 (5)	S2—Zn1—S1	128.70 (2)
N1—Zn1—S1	110.16 (5)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O7^{i}	0.88	1.89	2.774 (2)	179
O7—H7···S1^{ii}	0.84	2.37	3.1976 (16)	168

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $x+1, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2271).

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supplementary materials

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(2-Ethylimidazole-κN)bis(tri-*tert*-butoxysilanethiolato-$\kappa^2 O,S$)zinc(II) propan-2-ol solvate

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Comment

The geometry of coordinating atoms in the molecule of the title complex, (I) (Fig. 1), may be approximated to distorted trigonal bipyramidal·The central atom of zinc is coordinated by five atoms; two sulfur S1, S2, one nitrogen N1 and two oxygen atoms O1 and O4 (Fig. 1). The basal trigonal plane is formed by atoms Zn1, S1, S2 and N1; Zn1 deviates from the plane at the O4 side by 0.0460 (5) Å and it is the most deviating atom. The O1 and O4 atoms occupy two apical positions. The perpendicular distances between O1, O4 and plane Zn1—S1—S2—N1 are 2.4134 (14) Å and 2.3701 (13) Å respectively. Complexation of O1 and O4 with zinc is reflected in the respective Si—O bond lengths: Si1—O1 and Si2—O4 are definitely longer then the rest of Si—O bonds.

Molecules of zinc thiolate and 2-propanol are linked *via* N—H···O and O—H···S hydrogen bonds to generate antiparallel chains along the *c* axis, as shown in Fig. 2. The *tert*-butyl groups on both sides of each chain prevent other interactions than hydrophobic between the chains.

The analogous penta-coordinated complex with 1-methylimidazole (which has a blocked N—H function) also has a tbp geometry (Dołęga Anna *et al.*, 2004) but the molecules pack in crystal as discrete units.

Experimental

The title compound crystallized from acetonitrile and 2-propanol solution of equimolar quantities of zinc acetyloacetonate, tri-*tert*-butoxysilanethiol and 2-ethylimidazole at 255 K.

Refinement

All H atoms were positioned geometrically and refined using riding model with C—H distances of 0.93 and with isotropic temperature factors U_{iso} 1.2 times the equivalent isotropic temperature factors U_{eq} of their attached atoms.

Figures

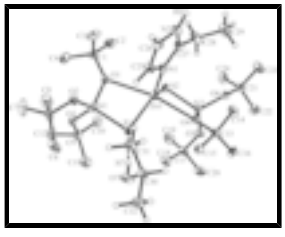

Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms. H-atoms of *tert*-butyl groups have been omitted.

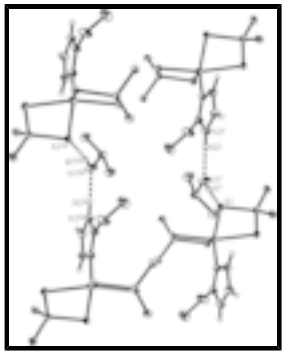

Fig. 2. The packing of (I) viewed approximately down the *c* axis. The antiparallel chains connected by O—H···S and N—H···O hydrogen bonds (dashed lines) are shown. All *tert*-butyl groups have been omitted as are most H-atoms. Symmetry codes: i: *x* − 1,*y*,*z*; ii: −*x*,-*y* + 2,-*z*; iii: −*x* − 1,-*y* + 2,-*z*

(2-Ethylimidazole-κ*N*)bis(tri-*tert*-butoxysilanethiolato-κ^2*O*,*S*)zinc(II) propan-2-ol solvate

Crystal data

$[Zn(C_{12}H_{27}O_3SSi)_2(C_5H_8N_2)]\cdot C_3H_8O$	F_{000} = 1688
M_r = 780.57	D_x = 1.161 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 26429 reflections
a = 9.8958 (2) Å	θ = 2.2–32.3º
b = 25.3673 (6) Å	μ = 0.74 mm^{-1}
c = 19.8040 (5) Å	*T* = 120 (2) K
β = 116.064 (2)º	Prism, colourless
V = 4465.82 (18) Å^3	0.32 × 0.16 × 0.09 mm
Z = 4	

Data collection

Oxford Diffraction KM-4-CCD κ-geometry diffractometer	7709 independent reflections
Monochromator: graphite	6892 reflections with $I > 2\sigma(I)$
Detector resolution: 8.1883 pixels mm^{-1}	R_{int} = 0.018
T = 120(2) K	θ_{max} = 25.1º
ω scans, 0.75° width	θ_{min} = 2.2º
Absorption correction: analytical (CrysAlis RED; Oxford Diffraction, 2006)	*h* = −11→11
T_{min} = 0.769, T_{max} = 0.885	*k* = −29→30
25240 measured reflections	*l* = −23→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.034	H-atom parameters constrained
$wR(F^2)$ = 0.096	$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 1.9663P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{max} = 0.002$
7709 reflections	$\Delta\rho_{max} = 0.43$ e Å^{-3}
436 parameters	$\Delta\rho_{min} = -0.32$ 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	0.11065 (2)	0.858298 (9)	0.168011 (12)	0.02689 (9)
S1	−0.14032 (5)	0.838733 (18)	0.11807 (3)	0.02538 (12)
S2	0.27814 (6)	0.866765 (19)	0.29095 (3)	0.02821 (12)
Si1	−0.09197 (6)	0.75822 (2)	0.12344 (3)	0.02343 (13)
Si2	0.22006 (6)	0.94624 (2)	0.28076 (3)	0.02166 (12)
O1	0.09257 (15)	0.75833 (5)	0.15834 (8)	0.0287 (3)
O2	−0.15485 (17)	0.72856 (5)	0.04283 (8)	0.0306 (3)
O3	−0.15266 (17)	0.72450 (5)	0.17437 (8)	0.0303 (3)
O4	0.09130 (14)	0.95017 (5)	0.19224 (7)	0.0226 (3)
O5	0.16053 (15)	0.96744 (5)	0.34042 (8)	0.0283 (3)
O6	0.35044 (15)	0.98787 (5)	0.28657 (7)	0.0247 (3)
N1	0.17911 (19)	0.86101 (6)	0.08619 (10)	0.0274 (4)
N2	0.3103 (2)	0.86372 (7)	0.02171 (10)	0.0350 (4)
H2	0.3855	0.869	0.0102	0.042*
C1	0.1993 (3)	0.71605 (9)	0.16691 (14)	0.0388 (5)
C2	0.3435 (3)	0.73192 (11)	0.23355 (16)	0.0534 (7)
H2A	0.3738	0.7671	0.2248	0.064*
H2B	0.4228	0.7065	0.24	0.064*
H2C	0.3275	0.7325	0.279	0.064*
C3	0.2208 (4)	0.71335 (12)	0.09567 (16)	0.0575 (7)
H3A	0.1239	0.7062	0.0526	0.069*
H3B	0.2919	0.6851	0.1003	0.069*
H3C	0.2605	0.7471	0.088	0.069*
C4	0.1415 (3)	0.66356 (10)	0.18129 (17)	0.0538 (7)
H4A	0.1212	0.6668	0.2253	0.065*
H4B	0.2176	0.6362	0.1906	0.065*

H4C	0.0486	0.6539	0.1373	0.065*
C5	−0.2955 (3)	0.70240 (9)	−0.00344 (12)	0.0383 (5)
C6	−0.4276 (3)	0.73258 (12)	−0.00333 (16)	0.0556 (7)
H6A	−0.4215	0.7323	0.0474	0.067*
H6B	−0.5218	0.7159	−0.0383	0.067*
H6C	−0.4249	0.7691	−0.019	0.067*
C7	−0.2893 (4)	0.64690 (10)	0.02595 (17)	0.0646 (9)
H7A	−0.2012	0.6286	0.0269	0.078*
H7B	−0.3808	0.6278	−0.007	0.078*
H7C	−0.2817	0.6483	0.0769	0.078*
C8	−0.3043 (3)	0.70145 (11)	−0.08191 (13)	0.0487 (6)
H8A	−0.3056	0.7377	−0.0994	0.058*
H8B	−0.3964	0.6833	−0.1162	0.058*
H8C	−0.2166	0.6828	−0.0808	0.058*
C9	−0.1582 (3)	0.73539 (9)	0.24493 (12)	0.0355 (5)
C10	−0.0101 (3)	0.75815 (10)	0.30176 (13)	0.0428 (6)
H10A	0.0715	0.7334	0.3094	0.051*
H10B	−0.0149	0.764	0.3496	0.051*
H10C	0.0088	0.7917	0.283	0.051*
C11	−0.2876 (3)	0.77313 (11)	0.23045 (15)	0.0494 (6)
H11A	−0.2652	0.8075	0.2152	0.059*
H11B	−0.3005	0.7772	0.2765	0.059*
H11C	−0.3803	0.759	0.1904	0.059*
C12	−0.1868 (4)	0.68200 (11)	0.27136 (15)	0.0555 (7)
H12A	−0.2846	0.6684	0.2351	0.067*
H12B	−0.1869	0.6859	0.3206	0.067*
H12C	−0.1075	0.6573	0.2754	0.067*
C13	0.0247 (2)	0.99659 (7)	0.14529 (11)	0.0264 (4)
C14	0.1271 (3)	1.01286 (10)	0.10996 (13)	0.0399 (5)
H14A	0.2263	1.0223	0.1496	0.048*
H14B	0.0836	1.0433	0.0771	0.048*
H14C	0.1374	0.9835	0.0804	0.048*
C15	−0.1274 (2)	0.97845 (8)	0.08538 (11)	0.0302 (4)
H15A	−0.113	0.9493	0.0568	0.036*
H15B	−0.1773	1.0078	0.0513	0.036*
H15C	−0.19	0.9666	0.1095	0.036*
C16	0.0056 (3)	1.04084 (8)	0.19196 (13)	0.0374 (5)
H16A	−0.058	1.0287	0.2153	0.045*
H16B	−0.0419	1.0712	0.1595	0.045*
H16C	0.1043	1.0512	0.2312	0.045*
C17	0.0593 (3)	0.94675 (10)	0.36897 (12)	0.0361 (5)
C18	−0.0770 (3)	0.92107 (11)	0.30563 (13)	0.0432 (6)
H18A	−0.1272	0.9468	0.2653	0.052*
H18B	−0.1474	0.9091	0.3251	0.052*
H18C	−0.0441	0.8908	0.2858	0.052*
C19	0.1431 (3)	0.90773 (12)	0.43099 (14)	0.0530 (7)
H19A	0.175	0.8777	0.4104	0.064*
H19B	0.077	0.8954	0.4528	0.064*
H19C	0.2318	0.9248	0.4701	0.064*

C20	0.0106 (3)	0.99499 (12)	0.39924 (15)	0.0511 (7)
H20A	0.0994	1.0119	0.4386	0.061*
H20B	−0.0579	0.9839	0.4203	0.061*
H20C	−0.0409	1.0201	0.3582	0.061*
C21	0.4762 (2)	1.01019 (8)	0.35030 (11)	0.0266 (4)
C22	0.4187 (3)	1.05600 (10)	0.38037 (15)	0.0447 (6)
H22A	0.3676	1.0816	0.34	0.054*
H22B	0.5036	1.0731	0.4217	0.054*
H22C	0.3479	1.0427	0.3987	0.054*
C23	0.5826 (3)	1.03099 (12)	0.32033 (15)	0.0506 (6)
H23A	0.6187	1.0017	0.3004	0.061*
H23B	0.6684	1.0482	0.361	0.061*
H23C	0.5298	1.0565	0.2802	0.061*
C24	0.5511 (3)	0.96889 (10)	0.40965 (14)	0.0490 (6)
H24A	0.4788	0.9552	0.4267	0.059*
H24B	0.6368	0.9846	0.4523	0.059*
H24C	0.5865	0.94	0.3886	0.059*
C25	0.0917 (2)	0.84240 (9)	0.01462 (12)	0.0343 (5)
H25	−0.0091	0.8304	−0.0035	0.041*
C26	0.1718 (3)	0.84400 (9)	−0.02545 (13)	0.0378 (5)
H26	0.1388	0.8335	−0.0763	0.045*
C27	0.3117 (2)	0.87356 (8)	0.08902 (12)	0.0318 (5)
C28	0.4440 (3)	0.89577 (12)	0.15449 (14)	0.0539 (7)
H28A	0.4124	0.9055	0.1938	0.065*
H28B	0.5215	0.8679	0.1755	0.065*
C29	0.5123 (4)	0.94198 (12)	0.13745 (17)	0.0628 (8)
H29A	0.5409	0.9333	0.0973	0.075*
H29B	0.602	0.9525	0.1826	0.075*
H29C	0.4398	0.9711	0.1211	0.075*
O7	0.54940 (18)	0.62127 (8)	0.48632 (9)	0.0447 (4)
H7	0.6368	0.6308	0.5162	0.054*
C30	0.5533 (2)	0.59525 (9)	0.42315 (12)	0.0328 (5)
H30	0.6121	0.5618	0.4405	0.039*
C31	0.6262 (3)	0.62962 (10)	0.38684 (14)	0.0424 (6)
H31A	0.729	0.6381	0.4235	0.051*
H31B	0.5682	0.6623	0.3692	0.051*
H31C	0.6288	0.6109	0.3441	0.051*
C32	0.3924 (3)	0.58204 (11)	0.37114 (14)	0.0456 (6)
H32A	0.3343	0.6147	0.3538	0.055*
H32B	0.3495	0.5605	0.398	0.055*
H32C	0.3888	0.5623	0.3278	0.055*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02290 (14)	0.03310 (15)	0.02241 (14)	−0.00520 (9)	0.00787 (11)	−0.00236 (9)
S1	0.0221 (2)	0.0231 (2)	0.0275 (3)	−0.00115 (18)	0.0077 (2)	−0.00005 (18)
S2	0.0275 (3)	0.0241 (2)	0.0242 (3)	0.00294 (19)	0.0032 (2)	0.00118 (18)

Si1	0.0273 (3)	0.0212 (3)	0.0222 (3)	−0.0029 (2)	0.0113 (2)	−0.0008 (2)
Si2	0.0200 (3)	0.0229 (3)	0.0185 (3)	0.0002 (2)	0.0052 (2)	−0.00069 (19)
O1	0.0280 (8)	0.0257 (7)	0.0315 (8)	0.0033 (6)	0.0122 (7)	0.0012 (6)
O2	0.0374 (8)	0.0301 (7)	0.0256 (8)	−0.0085 (6)	0.0149 (7)	−0.0053 (6)
O3	0.0419 (9)	0.0269 (7)	0.0258 (7)	−0.0070 (6)	0.0182 (7)	−0.0018 (6)
O4	0.0201 (7)	0.0216 (6)	0.0203 (7)	0.0012 (5)	0.0036 (6)	0.0016 (5)
O5	0.0269 (7)	0.0346 (8)	0.0237 (7)	−0.0022 (6)	0.0113 (6)	−0.0037 (6)
O6	0.0219 (7)	0.0277 (7)	0.0198 (7)	−0.0025 (5)	0.0048 (6)	−0.0009 (5)
N1	0.0251 (9)	0.0285 (9)	0.0267 (9)	−0.0032 (7)	0.0096 (8)	−0.0008 (7)
N2	0.0300 (10)	0.0440 (11)	0.0345 (10)	−0.0017 (8)	0.0174 (9)	0.0028 (8)
C1	0.0382 (13)	0.0324 (11)	0.0470 (14)	0.0135 (10)	0.0198 (11)	0.0051 (10)
C2	0.0346 (14)	0.0544 (16)	0.0619 (18)	0.0154 (12)	0.0127 (13)	0.0028 (13)
C3	0.0698 (19)	0.0546 (16)	0.0609 (18)	0.0253 (14)	0.0404 (16)	0.0045 (13)
C4	0.0567 (16)	0.0319 (13)	0.0716 (19)	0.0143 (12)	0.0271 (15)	0.0093 (12)
C5	0.0481 (14)	0.0354 (12)	0.0281 (12)	−0.0207 (10)	0.0138 (11)	−0.0098 (9)
C6	0.0407 (15)	0.0767 (19)	0.0458 (16)	−0.0236 (13)	0.0158 (13)	−0.0202 (14)
C7	0.102 (3)	0.0393 (14)	0.0476 (16)	−0.0335 (15)	0.0280 (17)	−0.0087 (12)
C8	0.0609 (17)	0.0530 (15)	0.0287 (13)	−0.0182 (13)	0.0166 (12)	−0.0106 (11)
C9	0.0498 (14)	0.0361 (12)	0.0263 (11)	−0.0087 (10)	0.0219 (11)	−0.0010 (9)
C10	0.0582 (16)	0.0429 (13)	0.0277 (12)	−0.0087 (11)	0.0192 (12)	0.0001 (10)
C11	0.0584 (16)	0.0609 (16)	0.0430 (15)	−0.0023 (13)	0.0353 (14)	−0.0032 (12)
C12	0.088 (2)	0.0476 (15)	0.0413 (15)	−0.0232 (14)	0.0375 (16)	0.0003 (11)
C13	0.0240 (10)	0.0236 (9)	0.0233 (10)	0.0010 (8)	0.0028 (9)	0.0049 (8)
C14	0.0322 (12)	0.0464 (13)	0.0349 (12)	−0.0047 (10)	0.0091 (10)	0.0122 (10)
C15	0.0246 (10)	0.0315 (10)	0.0256 (11)	0.0011 (8)	0.0029 (9)	0.0031 (8)
C16	0.0350 (12)	0.0267 (10)	0.0339 (12)	0.0061 (9)	0.0001 (10)	−0.0008 (9)
C17	0.0325 (12)	0.0525 (14)	0.0268 (11)	−0.0091 (10)	0.0161 (10)	−0.0055 (9)
C18	0.0343 (13)	0.0610 (15)	0.0361 (13)	−0.0151 (11)	0.0172 (11)	−0.0092 (11)
C19	0.0545 (16)	0.0713 (18)	0.0346 (14)	−0.0109 (14)	0.0208 (13)	0.0078 (12)
C20	0.0425 (14)	0.0752 (18)	0.0424 (14)	−0.0064 (13)	0.0248 (12)	−0.0205 (13)
C21	0.0221 (10)	0.0290 (10)	0.0215 (10)	−0.0041 (8)	0.0031 (8)	−0.0027 (8)
C22	0.0401 (14)	0.0395 (13)	0.0439 (14)	−0.0024 (10)	0.0088 (12)	−0.0116 (10)
C23	0.0394 (14)	0.0657 (17)	0.0432 (15)	−0.0195 (12)	0.0148 (12)	−0.0081 (12)
C24	0.0393 (14)	0.0429 (14)	0.0390 (14)	−0.0043 (11)	−0.0065 (12)	0.0052 (11)
C25	0.0290 (11)	0.0437 (12)	0.0281 (11)	−0.0096 (9)	0.0106 (10)	−0.0062 (9)
C26	0.0410 (13)	0.0439 (13)	0.0290 (12)	−0.0072 (10)	0.0158 (11)	−0.0053 (9)
C27	0.0292 (11)	0.0351 (11)	0.0300 (11)	−0.0025 (9)	0.0120 (10)	0.0053 (9)
C28	0.0367 (14)	0.0796 (19)	0.0365 (14)	−0.0215 (13)	0.0079 (12)	0.0050 (13)
C29	0.0608 (18)	0.0635 (18)	0.0585 (18)	−0.0278 (15)	0.0209 (15)	−0.0179 (14)
O7	0.0265 (8)	0.0795 (12)	0.0296 (9)	−0.0119 (8)	0.0137 (7)	−0.0124 (8)
C30	0.0286 (11)	0.0398 (12)	0.0293 (11)	0.0002 (9)	0.0121 (10)	0.0012 (9)
C31	0.0415 (14)	0.0523 (14)	0.0394 (13)	−0.0064 (11)	0.0233 (12)	−0.0001 (11)
C32	0.0376 (13)	0.0612 (16)	0.0373 (13)	−0.0107 (11)	0.0158 (11)	−0.0080 (11)

Geometric parameters (Å, °)

Zn1—N1	2.0134 (17)	C12—H12C	0.98
Zn1—S2	2.2749 (6)	C13—C16	1.518 (3)
Zn1—S1	2.2878 (5)	C13—C14	1.519 (3)

Zn1—O4	2.4039 (12)	C13—C15	1.522 (3)
Zn1—O1	2.5436 (14)	C14—H14A	0.98
S1—Si1	2.0897 (7)	C14—H14B	0.98
S2—Si2	2.0818 (7)	C14—H14C	0.98
Si1—O1	1.6442 (15)	C15—H15A	0.98
Si1—O2	1.6214 (14)	C15—H15B	0.98
Si1—O3	1.6253 (14)	C15—H15C	0.98
Si2—O4	1.6563 (13)	C16—H16A	0.98
Si2—O5	1.6261 (14)	C16—H16B	0.98
Si2—O6	1.6317 (14)	C16—H16C	0.98
O1—C1	1.462 (2)	C17—C19	1.510 (4)
O2—C5	1.448 (3)	C17—C18	1.527 (3)
O3—C9	1.449 (2)	C17—C20	1.531 (3)
O4—C13	1.465 (2)	C18—H18A	0.98
O5—C17	1.448 (2)	C18—H18B	0.98
O6—C21	1.443 (2)	C18—H18C	0.98
N1—C27	1.327 (3)	C19—H19A	0.98
N1—C25	1.379 (3)	C19—H19B	0.98
N2—C27	1.350 (3)	C19—H19C	0.98
N2—C26	1.370 (3)	C20—H20A	0.98
N2—H2	0.88	C20—H20B	0.98
C1—C2	1.512 (4)	C20—H20C	0.98
C1—C3	1.518 (3)	C21—C24	1.504 (3)
C1—C4	1.524 (3)	C21—C23	1.513 (3)
C2—H2A	0.98	C21—C22	1.525 (3)
C2—H2B	0.98	C22—H22A	0.98
C2—H2C	0.98	C22—H22B	0.98
C3—H3A	0.98	C22—H22C	0.98
C3—H3B	0.98	C23—H23A	0.98
C3—H3C	0.98	C23—H23B	0.98
C4—H4A	0.98	C23—H23C	0.98
C4—H4B	0.98	C24—H24A	0.98
C4—H4C	0.98	C24—H24B	0.98
C5—C7	1.514 (3)	C24—H24C	0.98
C5—C6	1.515 (4)	C25—C26	1.346 (3)
C5—C8	1.518 (3)	C25—H25	0.95
C6—H6A	0.98	C26—H26	0.95
C6—H6B	0.98	C27—C28	1.490 (3)
C6—H6C	0.98	C28—C29	1.464 (4)
C7—H7A	0.98	C28—H28A	0.99
C7—H7B	0.98	C28—H28B	0.99
C7—H7C	0.98	C29—H29A	0.98
C8—H8A	0.98	C29—H29B	0.98
C8—H8B	0.98	C29—H29C	0.98
C8—H8C	0.98	O7—C30	1.430 (3)
C9—C10	1.516 (3)	O7—H7	0.8401
C9—C11	1.521 (4)	C30—C31	1.501 (3)
C9—C12	1.523 (3)	C30—C32	1.506 (3)
C10—H10A	0.98	C30—H30	1

C10—H10B	0.98	C31—H31A	0.98
C10—H10C	0.98	C31—H31B	0.98
C11—H11A	0.98	C31—H31C	0.98
C11—H11B	0.98	C32—H32A	0.98
C11—H11C	0.98	C32—H32B	0.98
C12—H12A	0.98	C32—H32C	0.98
C12—H12B	0.98		
N1—Zn1—S2	120.90 (5)	O4—C13—C16	110.46 (16)
N1—Zn1—S1	110.16 (5)	O4—C13—C14	107.82 (16)
S2—Zn1—S1	128.70 (2)	C16—C13—C14	111.48 (18)
N1—Zn1—O4	102.24 (6)	O4—C13—C15	105.46 (15)
S2—Zn1—O4	77.25 (3)	C16—C13—C15	110.65 (17)
S1—Zn1—O4	97.47 (3)	C14—C13—C15	110.76 (17)
N1—Zn1—O1	90.62 (6)	C13—C14—H14A	109.5
S2—Zn1—O1	99.72 (3)	C13—C14—H14B	109.5
S1—Zn1—O1	73.98 (3)	H14A—C14—H14B	109.5
O4—Zn1—O1	166.52 (4)	C13—C14—H14C	109.5
Si1—S1—Zn1	90.53 (2)	H14A—C14—H14C	109.5
Si2—S2—Zn1	86.98 (2)	H14B—C14—H14C	109.5
O2—Si1—O3	106.26 (7)	C13—C15—H15A	109.5
O2—Si1—O1	106.83 (8)	C13—C15—H15B	109.5
O3—Si1—O1	112.64 (8)	H15A—C15—H15B	109.5
O2—Si1—S1	115.04 (6)	C13—C15—H15C	109.5
O3—Si1—S1	114.04 (6)	H15A—C15—H15C	109.5
O1—Si1—S1	101.94 (6)	H15B—C15—H15C	109.5
O5—Si2—O6	105.21 (7)	C13—C16—H16A	109.5
O5—Si2—O4	113.16 (7)	C13—C16—H16B	109.5
O6—Si2—O4	104.62 (7)	H16A—C16—H16B	109.5
O5—Si2—S2	114.99 (6)	C13—C16—H16C	109.5
O6—Si2—S2	116.35 (6)	H16A—C16—H16C	109.5
O4—Si2—S2	102.24 (5)	H16B—C16—H16C	109.5
C1—O1—Si1	131.29 (14)	O5—C17—C19	109.18 (19)
C1—O1—Zn1	134.39 (12)	O5—C17—C18	110.31 (17)
Si1—O1—Zn1	93.54 (6)	C19—C17—C18	111.1 (2)
C5—O2—Si1	133.00 (13)	O5—C17—C20	104.71 (18)
C9—O3—Si1	132.76 (13)	C19—C17—C20	111.1 (2)
C13—O4—Si2	129.96 (12)	C18—C17—C20	110.2 (2)
C13—O4—Zn1	134.86 (11)	C17—C18—H18A	109.5
Si2—O4—Zn1	93.52 (6)	C17—C18—H18B	109.5
C17—O5—Si2	134.23 (13)	H18A—C18—H18B	109.5
C21—O6—Si2	131.84 (12)	C17—C18—H18C	109.5
C27—N1—C25	106.70 (17)	H18A—C18—H18C	109.5
C27—N1—Zn1	130.56 (15)	H18B—C18—H18C	109.5
C25—N1—Zn1	122.31 (14)	C17—C19—H19A	109.5
C27—N2—C26	108.30 (18)	C17—C19—H19B	109.5
C27—N2—H2	125.8	H19A—C19—H19B	109.5
C26—N2—H2	125.9	C17—C19—H19C	109.5
O1—C1—C2	105.24 (18)	H19A—C19—H19C	109.5
O1—C1—C3	108.31 (18)	H19B—C19—H19C	109.5

C2—C1—C3	111.0 (2)	C17—C20—H20A	109.5
O1—C1—C4	110.58 (19)	C17—C20—H20B	109.5
C2—C1—C4	110.9 (2)	H20A—C20—H20B	109.5
C3—C1—C4	110.6 (2)	C17—C20—H20C	109.5
C1—C2—H2A	109.5	H20A—C20—H20C	109.5
C1—C2—H2B	109.5	H20B—C20—H20C	109.5
H2A—C2—H2B	109.5	O6—C21—C24	110.46 (17)
C1—C2—H2C	109.5	O6—C21—C23	105.98 (16)
H2A—C2—H2C	109.5	C24—C21—C23	111.1 (2)
H2B—C2—H2C	109.5	O6—C21—C22	108.30 (16)
C1—C3—H3A	109.5	C24—C21—C22	111.5 (2)
C1—C3—H3B	109.5	C23—C21—C22	109.33 (19)
H3A—C3—H3B	109.5	C21—C22—H22A	109.5
C1—C3—H3C	109.5	C21—C22—H22B	109.5
H3A—C3—H3C	109.5	H22A—C22—H22B	109.5
H3B—C3—H3C	109.5	C21—C22—H22C	109.5
C1—C4—H4A	109.5	H22A—C22—H22C	109.5
C1—C4—H4B	109.5	H22B—C22—H22C	109.5
H4A—C4—H4B	109.5	C21—C23—H23A	109.5
C1—C4—H4C	109.5	C21—C23—H23B	109.5
H4A—C4—H4C	109.5	H23A—C23—H23B	109.5
H4B—C4—H4C	109.5	C21—C23—H23C	109.5
O2—C5—C7	108.5 (2)	H23A—C23—H23C	109.5
O2—C5—C6	110.94 (18)	H23B—C23—H23C	109.5
C7—C5—C6	111.0 (2)	C21—C24—H24A	109.5
O2—C5—C8	105.17 (18)	C21—C24—H24B	109.5
C7—C5—C8	110.7 (2)	H24A—C24—H24B	109.5
C6—C5—C8	110.4 (2)	C21—C24—H24C	109.5
C5—C6—H6A	109.5	H24A—C24—H24C	109.5
C5—C6—H6B	109.5	H24B—C24—H24C	109.5
H6A—C6—H6B	109.5	C26—C25—N1	109.25 (19)
C5—C6—H6C	109.5	C26—C25—H25	125.4
H6A—C6—H6C	109.5	N1—C25—H25	125.4
H6B—C6—H6C	109.5	C25—C26—N2	106.31 (19)
C5—C7—H7A	109.5	C25—C26—H26	126.8
C5—C7—H7B	109.5	N2—C26—H26	126.8
H7A—C7—H7B	109.5	N1—C27—N2	109.44 (19)
C5—C7—H7C	109.5	N1—C27—C28	127.0 (2)
H7A—C7—H7C	109.5	N2—C27—C28	123.6 (2)
H7B—C7—H7C	109.5	C29—C28—C27	114.8 (2)
C5—C8—H8A	109.5	C29—C28—H28A	108.6
C5—C8—H8B	109.5	C27—C28—H28A	108.6
H8A—C8—H8B	109.5	C29—C28—H28B	108.6
C5—C8—H8C	109.5	C27—C28—H28B	108.6
H8A—C8—H8C	109.5	H28A—C28—H28B	107.5
H8B—C8—H8C	109.5	C28—C29—H29A	109.5
O3—C9—C10	110.77 (18)	C28—C29—H29B	109.5
O3—C9—C11	108.88 (18)	H29A—C29—H29B	109.5
C10—C9—C11	111.0 (2)	C28—C29—H29C	109.5

O3—C9—C12	104.69 (17)	H29A—C29—H29C	109.5
C10—C9—C12	110.4 (2)	H29B—C29—H29C	109.5
C11—C9—C12	110.9 (2)	C30—O7—H7	109.4
C9—C10—H10A	109.5	O7—C30—C31	110.75 (19)
C9—C10—H10B	109.5	O7—C30—C32	105.92 (18)
H10A—C10—H10B	109.5	C31—C30—C32	112.8 (2)
C9—C10—H10C	109.5	O7—C30—H30	109.1
H10A—C10—H10C	109.5	C31—C30—H30	109.1
H10B—C10—H10C	109.5	C32—C30—H30	109.1
C9—C11—H11A	109.5	C30—C31—H31A	109.5
C9—C11—H11B	109.5	C30—C31—H31B	109.5
H11A—C11—H11B	109.5	H31A—C31—H31B	109.5
C9—C11—H11C	109.5	C30—C31—H31C	109.5
H11A—C11—H11C	109.5	H31A—C31—H31C	109.5
H11B—C11—H11C	109.5	H31B—C31—H31C	109.5
C9—C12—H12A	109.5	C30—C32—H32A	109.5
C9—C12—H12B	109.5	C30—C32—H32B	109.5
H12A—C12—H12B	109.5	H32A—C32—H32B	109.5
C9—C12—H12C	109.5	C30—C32—H32C	109.5
H12A—C12—H12C	109.5	H32A—C32—H32C	109.5
H12B—C12—H12C	109.5	H32B—C32—H32C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O7^{i}	0.88	1.89	2.774 (2)	179
O7—H7···S1^{ii}	0.84	2.37	3.1976 (16)	168

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2; (ii) *x*+1, −*y*+3/2, *z*+1/2.

Fig. 1

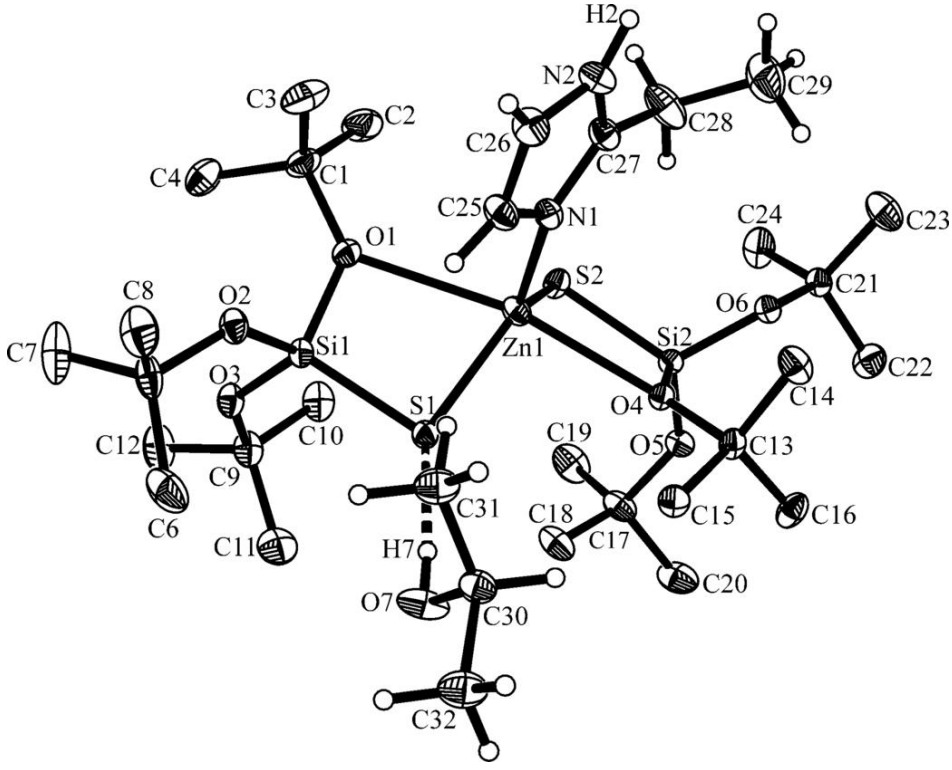
H2
N2
C29
C3
C2
C28
C26
C27
C4
C1
C25
N1
C24
C23
O1
S2
C8
O2
O6
C21
C7
Si1
Zn1
Si2
C22
O3
C14
S1
O4
C19
C10
C12
O5
C13
C9
C31
C15
C16
C6
C18
C17
C11
H7
C20
O7
C30
C32

Fig. 2