

Poly[[μ -3,3'-(dimethylsilanediyl)-dibenzoato][μ -1,1'-(1,4-phenylene)-di-1*H*-imidazole]zinc] monohydrate]

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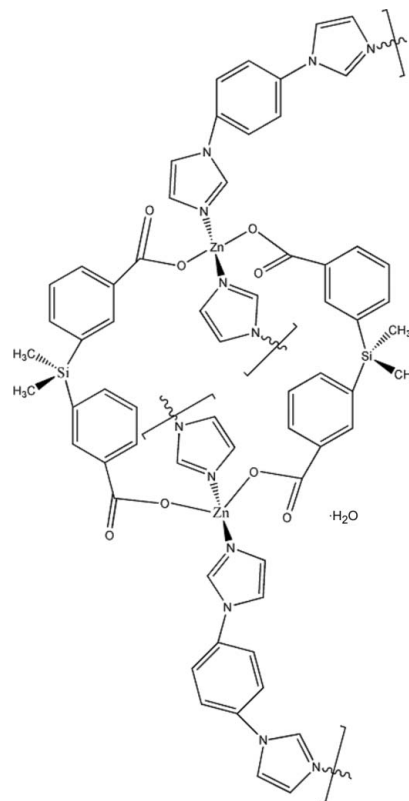
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.055; wR factor = 0.161; data-to-parameter ratio = 14.3.

The asymmetric unit of the title compound, $\{[\text{Zn}(\text{C}_{16}\text{H}_{16}\text{O}_4\text{Si})(\text{C}_{12}\text{H}_{10}\text{N}_4)] \cdot \text{H}_2\text{O}\}_n$, consists of one Zn^{II} ion, two half 3,3'-(dimethylsilanediyl)dibenzoate ligands and two half 1,1'-(1,4-phenylene)di-1*H*-imidazole ligands. The Zn^{II} ion is four-coordinated by two O atoms from two carboxylate ligands, two N atoms from two imidazole ligands. Two Zn^{II} ions are bridged by two carboxylate groups in chelating mode, generating a binuclear secondary building unit (SBU), which is further coordinated by two N atoms from two imidazole ligands in monodentate mode. Thus, the binuclear SBUs are further bridged by imidazole ligands in two different directions, giving rise to a chain. The water solvent molecules are hydrogen bonded within the chain along the c axis.

Related literature

For a similar presentation where the binuclear SBUs are further bridged by phenylenedicarboxylate ligands in different directions to give a three-dimensional porous framework containing three-dimensional channels, see: He *et al.* (2010).



Experimental

Crystal data

$[\text{Zn}(\text{C}_{16}\text{H}_{14}\text{O}_4\text{Si})(\text{C}_{12}\text{H}_{10}\text{N}_4)] \cdot \text{H}_2\text{O}$
 $M_r = 591.99$
 Monoclinic, $P2_1/c$
 $a = 9.4480$ (11) Å
 $b = 23.959$ (3) Å
 $c = 12.3083$ (13) Å
 $\beta = 110.029$ (2)°

$V = 2617.7$ (5) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.03$ mm⁻¹
 $T = 298$ K
 0.15 × 0.10 × 0.05 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.861$, $T_{\text{max}} = 0.950$

15353 measured reflections
 5881 independent reflections
 3694 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.054$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.153$
 $S = 1.02$
 5881 reflections

352 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.69$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.74$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O1W}-\text{H1WB} \cdots \text{O2}^i$	0.79	1.90	2.696 (8)	178
$\text{O1W}-\text{H1WA} \cdots \text{O2}$	0.78	2.08	2.852 (8)	171

Symmetry code: (i) $-x + 1, -y, -z + 1$.

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve

structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DS2187).

References

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supplementary materials

Acta Cryst. (2012). E68, m865–m866 [doi:10.1107/S1600536812019642]

Poly[[μ -3,3'-(dimethylsilanediyl)dibenzoato][μ -1,1'-(1,4-phenylene)di-1*H*-imidazole]zinc] monohydrate]

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Experimental

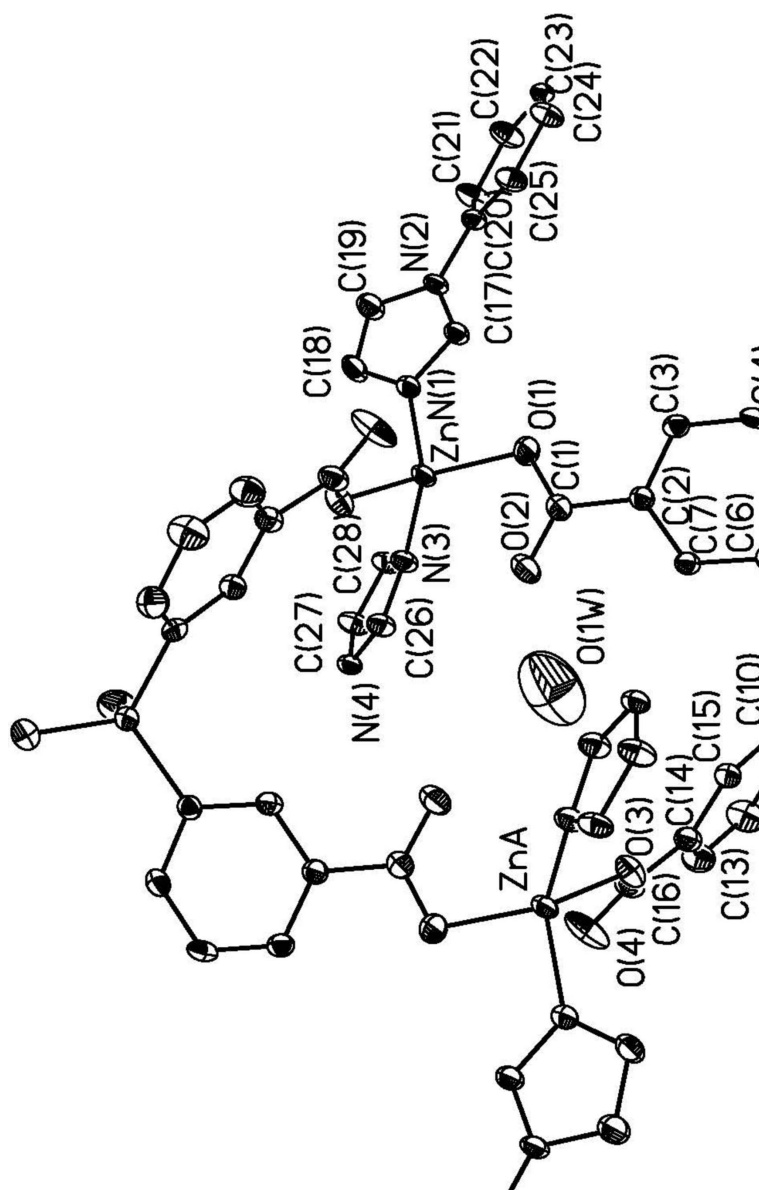
4,4'-(Dimethylsilanediyl)dibenzoate (1 mg, 0.0033 mmol), 1,4-bis(1-imidazolyl)benzene (10.8, 0.0038 mmol) and $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (4 mg, 0.0159 mmol) were dissolved into 1 ml a mixed solution (DMF–EtOH–H₂O = 1:1:1). The mixed solution was sealed into a Pyrex glass tube. The mixed solution was heated to 75 centigrade degree in 10 h, and kept the temperature at 75 centigrade degree for 72 h, and then was cooled down to room temperature in 10 h. colourless rod crystals were obtained. The crystals were filtered, washed with water and dried in air.

Refinement

Water H atoms were located in a difference Fourier map and refined with distance restraints of O—H = 0.78 (2) Å and H···H = 1.37 (2) Å, and with $\text{Uiso}(\text{H}) = 1.2\text{Ueq}(\text{O})$. The carbon H-atoms were placed in calculated positions [C—H (aromatic) = 0.93 Å and C—H (methyl) = 0.96 Å] and were included in the refinement in the riding model approximation, with $\text{Uiso}(\text{H}) = 1.2\text{Ueq}(\text{C})$ and $1.5\text{Ueq}(\text{C})$ for methylene C—H.

Computing details

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINTE* (Bruker, 2005); data reduction: *SAINTE* (Bruker, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

**Figure 1**

The asymmetric unit of the title compound.

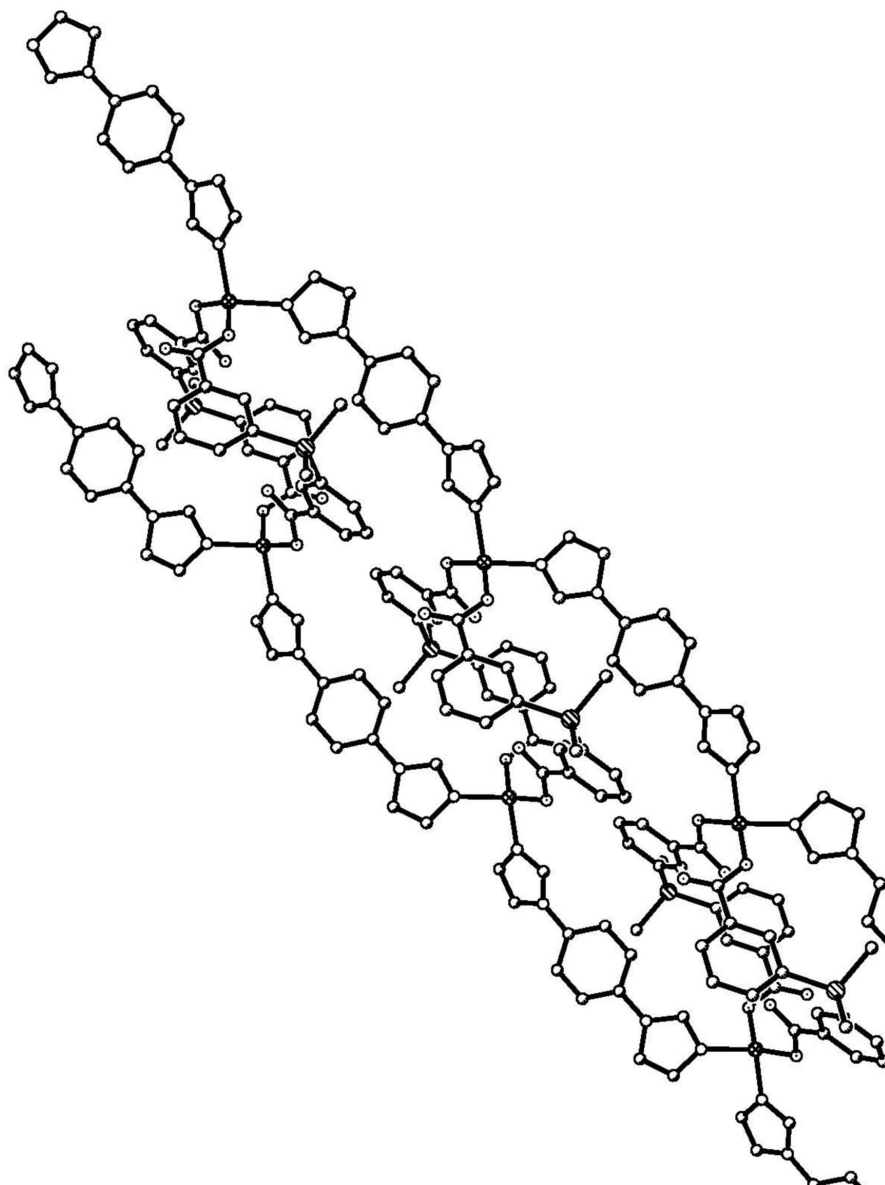


Figure 2

The one-dimensional chain of the title compound viewed by *a* axis.

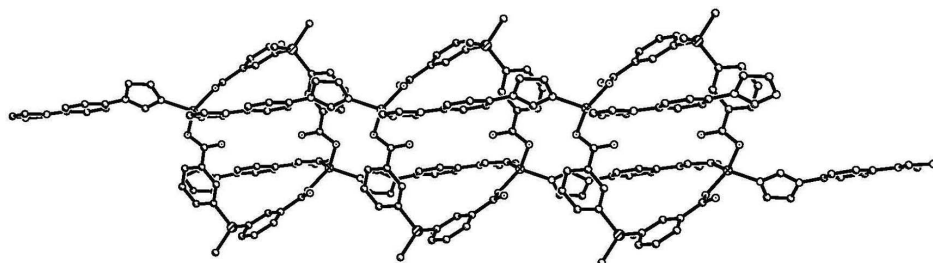
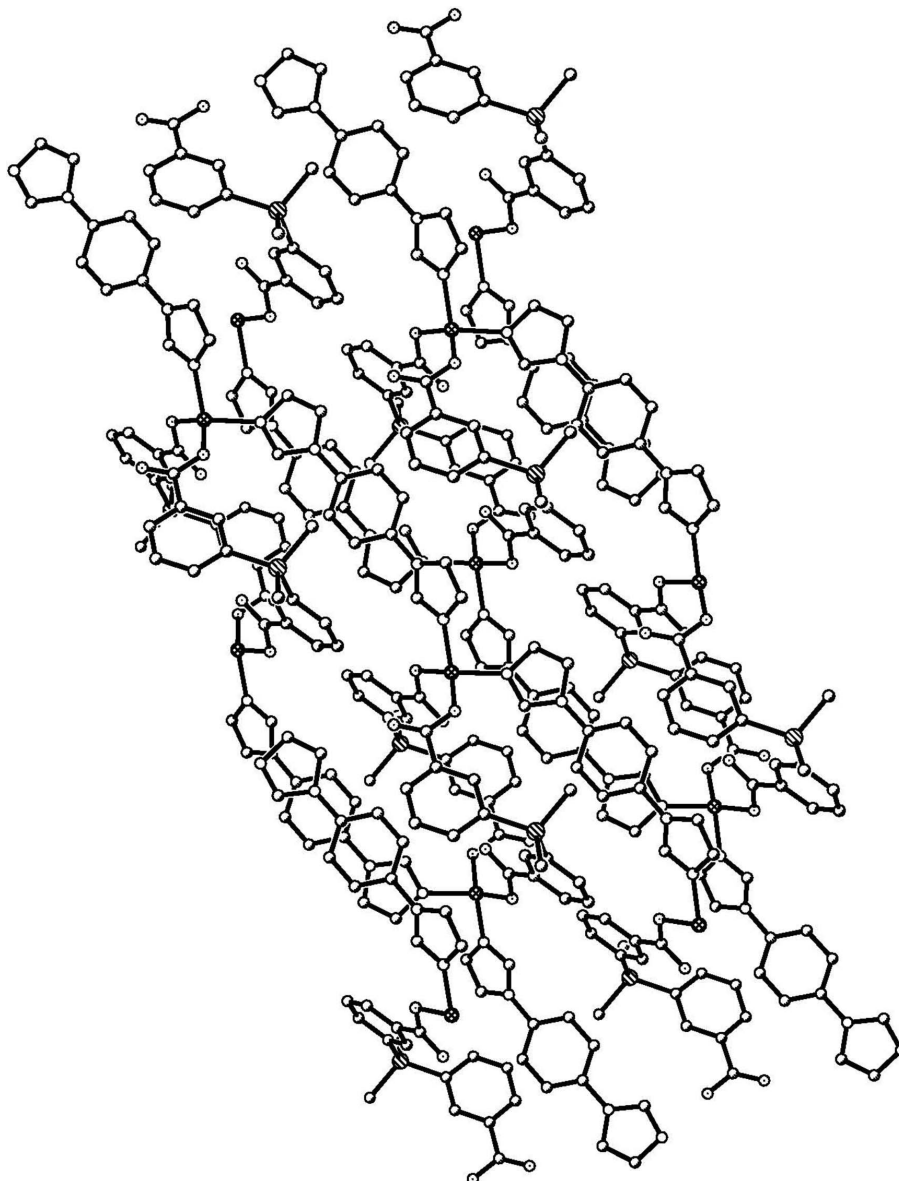


Figure 3

The one-dimensional chain of the title compound viewed by *b* axis.

**Figure 4**

The packed structure of the title compound viewed by *b* axis.

Poly[[[μ -4,4'-(dimethylsilanediyl)dibenzoato][μ -1,1'-(1,4-phenylene)di-1*H*-imidazole]zinc] monohydrate]

Crystal data

[Zn(C₁₆H₁₄O₄Si)(C₁₂H₁₀N₄)]·H₂O

M_r = 591.99

Monoclinic, *P*2₁/*c*

Hall symbol: -P 2ybc

a = 9.4480 (11) Å

b = 23.959 (3) Å

c = 12.3083 (13) Å

β = 110.029 (2)°

V = 2617.7 (5) Å³

Z = 4

F(000) = 1224

D_x = 1.502 Mg m⁻³

Mo *K* α radiation, λ = 0.71073 Å

Cell parameters from 2106 reflections

θ = 2.3–23.3°

μ = 1.03 mm⁻¹

T = 298 K

Rod, colourless

0.15 × 0.10 × 0.05 mm

Data collection

Bruker APEXII CCD area-detector diffractometer	15353 measured reflections
Radiation source: fine-focus sealed tube	5881 independent reflections
Graphite monochromator	3694 reflections with $I > 2\sigma(I)$
phi and ω scans	$R_{\text{int}} = 0.054$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 1.7^\circ$
$T_{\text{min}} = 0.861$, $T_{\text{max}} = 0.950$	$h = -11 \rightarrow 12$
	$k = -29 \rightarrow 30$
	$l = -15 \rightarrow 9$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.153$	$w = 1/[\sigma^2(F_o^2) + (0.0685P)^2 + 1.2685P]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
5881 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
352 parameters	$\Delta\rho_{\text{max}} = 0.69 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.74 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn	0.55041 (5)	-0.072654 (19)	0.85116 (4)	0.03338 (16)
Si	0.77758 (13)	0.22634 (5)	0.67361 (9)	0.0332 (3)
O1	0.6985 (3)	-0.01204 (12)	0.8930 (2)	0.0470 (8)
O2	0.5877 (4)	0.01169 (15)	0.7116 (3)	0.0737 (12)
O3	0.4631 (3)	0.13056 (12)	0.2612 (2)	0.0443 (7)
O4	0.2206 (4)	0.13460 (18)	0.2361 (3)	0.0769 (12)
N2	0.6888 (3)	-0.10157 (14)	1.2029 (2)	0.0316 (7)
N1	0.5830 (4)	-0.09931 (13)	1.0146 (3)	0.0324 (7)
N3	0.3262 (4)	-0.05579 (14)	0.7877 (3)	0.0355 (8)
C1	0.6826 (5)	0.02014 (18)	0.8076 (4)	0.0406 (10)
C2	0.7819 (4)	0.07052 (16)	0.8297 (3)	0.0309 (8)
C3	0.9083 (4)	0.07470 (16)	0.9284 (3)	0.0322 (9)
H3	0.9347	0.0450	0.9802	0.039*
C4	0.9954 (4)	0.12246 (17)	0.9508 (3)	0.0359 (9)
H4	1.0812	0.1247	1.0166	0.043*
C5	0.9539 (4)	0.16695 (17)	0.8745 (3)	0.0369 (9)
H5	1.0122	0.1992	0.8908	0.044*

C6	0.8268 (4)	0.16490 (15)	0.7735 (3)	0.0285 (8)
C7	0.7439 (4)	0.11537 (16)	0.7529 (3)	0.0306 (9)
H7	0.6606	0.1122	0.6857	0.037*
C8	0.9110 (5)	0.2296 (2)	0.5922 (4)	0.0617 (14)
H8A	0.9026	0.1961	0.5476	0.093*
H8B	1.0121	0.2332	0.6456	0.093*
H8C	0.8871	0.2613	0.5413	0.093*
C9	0.7933 (6)	0.29139 (19)	0.7606 (4)	0.0599 (14)
H9A	0.7244	0.2895	0.8026	0.090*
H9B	0.7692	0.3231	0.7100	0.090*
H9C	0.8943	0.2950	0.8141	0.090*
C10	0.5782 (4)	0.21887 (15)	0.5732 (3)	0.0328 (9)
C11	0.4595 (5)	0.24408 (19)	0.5982 (4)	0.0447 (11)
H11	0.4807	0.2645	0.6662	0.054*
C13	0.2791 (5)	0.2091 (2)	0.4252 (4)	0.0489 (11)
H13	0.1797	0.2062	0.3759	0.059*
C14	0.3906 (4)	0.18279 (17)	0.3963 (3)	0.0352 (9)
C15	0.5394 (4)	0.18807 (16)	0.4710 (3)	0.0323 (9)
H15	0.6153	0.1704	0.4519	0.039*
C16	0.3508 (5)	0.14646 (18)	0.2886 (3)	0.0400 (10)
C18	0.5100 (5)	-0.13739 (19)	1.0587 (3)	0.0452 (11)
H18	0.4282	-0.1588	1.0149	0.054*
C19	0.5730 (5)	-0.13969 (19)	1.1743 (4)	0.0466 (11)
H19	0.5444	-0.1623	1.2246	0.056*
C17	0.6897 (4)	-0.07880 (16)	1.1052 (3)	0.0333 (9)
H17	0.7576	-0.0515	1.1011	0.040*
C20	0.7923 (4)	-0.08999 (16)	1.3165 (3)	0.0320 (9)
C25	0.9402 (4)	-0.08007 (18)	1.3314 (3)	0.0393 (10)
H25	0.9718	-0.0797	1.2676	0.047*
C21	0.7454 (5)	-0.0894 (2)	1.4111 (4)	0.0515 (13)
H21	0.6444	-0.0950	1.4012	0.062*
C22	0.8485 (5)	-0.0804 (2)	1.5203 (3)	0.0482 (12)
H22	0.8169	-0.0801	1.5840	0.058*
C23	0.9971 (4)	-0.07189 (16)	1.5350 (3)	0.0308 (8)
C24	1.0435 (5)	-0.07055 (19)	1.4409 (3)	0.0431 (11)
H24	1.1437	-0.0633	1.4506	0.052*
C27	0.0798 (5)	-0.06543 (18)	0.7533 (3)	0.0413 (10)
H27	-0.0125	-0.0691	0.7640	0.050*
C26	0.2541 (4)	-0.05871 (17)	0.6749 (3)	0.0375 (10)
H26	0.3011	-0.0569	0.6198	0.045*
C28	0.2151 (5)	-0.05982 (18)	0.8359 (3)	0.0401 (10)
H28	0.2315	-0.0588	0.9148	0.048*
N4	0.1048 (3)	-0.06458 (13)	0.6492 (2)	0.0309 (7)
O1W	0.4293 (9)	-0.0453 (4)	0.5016 (6)	0.227 (4)
H1WA	0.4808	-0.0308	0.5580	0.272*
H1WB	0.4248	-0.0348	0.4393	0.272*
C12	0.3113 (5)	0.2396 (2)	0.5253 (4)	0.0567 (13)
H12	0.2346	0.2571	0.5438	0.068*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.0337 (3)	0.0394 (3)	0.0205 (2)	-0.0083 (2)	0.00091 (18)	-0.00123 (19)
Si	0.0376 (6)	0.0302 (6)	0.0275 (6)	-0.0039 (5)	0.0057 (5)	0.0010 (4)
O1	0.0557 (19)	0.0427 (18)	0.0385 (17)	-0.0169 (15)	0.0109 (14)	0.0076 (14)
O2	0.080 (3)	0.069 (2)	0.0442 (19)	-0.038 (2)	-0.0149 (18)	0.0108 (17)
O3	0.0414 (17)	0.0526 (19)	0.0376 (16)	-0.0095 (14)	0.0118 (14)	-0.0159 (14)
O4	0.0359 (19)	0.131 (4)	0.053 (2)	-0.016 (2)	0.0016 (16)	-0.033 (2)
N2	0.0305 (18)	0.0401 (19)	0.0190 (16)	-0.0025 (14)	0.0016 (13)	-0.0018 (13)
N1	0.0345 (18)	0.0347 (18)	0.0237 (16)	-0.0047 (15)	0.0045 (14)	0.0007 (14)
N3	0.0342 (19)	0.045 (2)	0.0221 (17)	-0.0042 (15)	0.0037 (14)	0.0011 (14)
C1	0.042 (3)	0.040 (2)	0.034 (2)	-0.0089 (19)	0.0054 (19)	0.0005 (19)
C2	0.031 (2)	0.033 (2)	0.0274 (19)	-0.0024 (17)	0.0079 (16)	0.0009 (16)
C3	0.036 (2)	0.035 (2)	0.0247 (19)	0.0021 (18)	0.0091 (16)	0.0038 (16)
C4	0.027 (2)	0.048 (3)	0.025 (2)	0.0016 (18)	-0.0008 (16)	0.0034 (18)
C5	0.036 (2)	0.035 (2)	0.036 (2)	-0.0087 (18)	0.0074 (18)	-0.0048 (18)
C6	0.030 (2)	0.029 (2)	0.0262 (19)	0.0001 (16)	0.0088 (16)	-0.0032 (15)
C7	0.028 (2)	0.037 (2)	0.0257 (19)	-0.0011 (17)	0.0069 (16)	0.0021 (16)
C8	0.058 (3)	0.081 (4)	0.047 (3)	-0.010 (3)	0.019 (2)	0.014 (3)
C9	0.068 (3)	0.041 (3)	0.051 (3)	-0.003 (2)	-0.004 (2)	-0.007 (2)
C10	0.041 (2)	0.027 (2)	0.026 (2)	0.0022 (17)	0.0070 (17)	0.0051 (16)
C11	0.050 (3)	0.046 (3)	0.040 (2)	0.006 (2)	0.017 (2)	-0.005 (2)
C13	0.035 (2)	0.063 (3)	0.045 (3)	0.004 (2)	0.008 (2)	-0.002 (2)
C14	0.034 (2)	0.040 (2)	0.030 (2)	-0.0005 (18)	0.0079 (17)	0.0005 (17)
C15	0.032 (2)	0.035 (2)	0.029 (2)	0.0008 (17)	0.0090 (17)	0.0001 (16)
C16	0.039 (3)	0.051 (3)	0.026 (2)	-0.006 (2)	0.0060 (19)	0.0020 (18)
C18	0.045 (3)	0.053 (3)	0.030 (2)	-0.022 (2)	0.0032 (19)	-0.0019 (19)
C19	0.047 (3)	0.056 (3)	0.032 (2)	-0.017 (2)	0.008 (2)	0.003 (2)
C17	0.032 (2)	0.041 (2)	0.0226 (19)	-0.0068 (17)	0.0039 (16)	0.0017 (17)
C20	0.032 (2)	0.037 (2)	0.0217 (19)	0.0009 (17)	0.0030 (16)	0.0003 (16)
C25	0.034 (2)	0.059 (3)	0.025 (2)	0.005 (2)	0.0097 (17)	-0.0044 (18)
C21	0.032 (2)	0.091 (4)	0.029 (2)	-0.012 (2)	0.0069 (19)	0.002 (2)
C22	0.039 (3)	0.083 (4)	0.021 (2)	-0.011 (2)	0.0096 (18)	0.001 (2)
C23	0.031 (2)	0.034 (2)	0.0217 (18)	0.0015 (17)	0.0008 (15)	0.0006 (16)
C24	0.030 (2)	0.068 (3)	0.028 (2)	0.000 (2)	0.0059 (17)	-0.007 (2)
C27	0.035 (2)	0.063 (3)	0.024 (2)	0.003 (2)	0.0081 (17)	-0.0039 (19)
C26	0.036 (2)	0.050 (3)	0.025 (2)	-0.0019 (19)	0.0077 (17)	0.0018 (17)
C28	0.043 (3)	0.052 (3)	0.020 (2)	0.002 (2)	0.0039 (18)	-0.0032 (17)
N4	0.0306 (18)	0.0365 (19)	0.0209 (15)	0.0005 (14)	0.0029 (13)	-0.0005 (13)
O1W	0.238 (9)	0.309 (11)	0.153 (6)	-0.097 (8)	0.092 (6)	-0.052 (7)
C12	0.042 (3)	0.075 (4)	0.054 (3)	0.017 (3)	0.017 (2)	-0.010 (3)

Geometric parameters (\AA , $^\circ$)

Zn—O3 ⁱ	1.932 (3)	C9—H9C	0.9600
Zn—O1	1.959 (3)	C10—C15	1.395 (5)
Zn—N1	2.031 (3)	C10—C11	1.398 (6)
Zn—N3	2.032 (3)	C11—C12	1.384 (6)
Si—C8	1.862 (5)	C11—H11	0.9300

Si—C9	1.868 (5)	C13—C12	1.374 (6)
Si—C6	1.872 (4)	C13—C14	1.375 (6)
Si—C10	1.875 (4)	C13—H13	0.9300
O1—C1	1.271 (5)	C14—C15	1.397 (5)
O2—C1	1.231 (5)	C14—C16	1.522 (6)
O3—C16	1.276 (5)	C15—H15	0.9300
O3—Zn ⁱ	1.932 (3)	C18—C19	1.342 (5)
O4—C16	1.212 (5)	C18—H18	0.9300
N2—C17	1.324 (5)	C19—H19	0.9300
N2—C19	1.375 (5)	C17—H17	0.9300
N2—C20	1.432 (4)	C20—C25	1.367 (5)
N1—C17	1.316 (5)	C20—C21	1.380 (5)
N1—C18	1.363 (5)	C25—C24	1.386 (5)
N3—C26	1.322 (5)	C25—H25	0.9300
N3—C28	1.375 (5)	C21—C22	1.380 (6)
C1—C2	1.495 (5)	C21—H21	0.9300
C2—C3	1.385 (5)	C22—C23	1.368 (6)
C2—C7	1.394 (5)	C22—H22	0.9300
C3—C4	1.381 (5)	C23—C24	1.372 (5)
C3—H3	0.9300	C23—N4 ⁱⁱ	1.436 (4)
C4—C5	1.386 (5)	C24—H24	0.9300
C4—H4	0.9300	C27—C28	1.339 (5)
C5—C6	1.403 (5)	C27—N4	1.380 (5)
C5—H5	0.9300	C27—H27	0.9300
C6—C7	1.396 (5)	C26—N4	1.343 (5)
C7—H7	0.9300	C26—H26	0.9300
C8—H8A	0.9600	C28—H28	0.9300
C8—H8B	0.9600	N4—C23 ⁱⁱⁱ	1.436 (4)
C8—H8C	0.9600	O1W—H1WA	0.7791
C9—H9A	0.9600	O1W—H1WB	0.7946
C9—H9B	0.9600	C12—H12	0.9300
O3 ⁱ —Zn—O1	125.92 (13)	C12—C11—C10	122.2 (4)
O3 ⁱ —Zn—N1	115.69 (13)	C12—C11—H11	118.9
O1—Zn—N1	96.91 (12)	C10—C11—H11	118.9
O3 ⁱ —Zn—N3	93.61 (13)	C12—C13—C14	121.5 (4)
O1—Zn—N3	120.70 (13)	C12—C13—H13	119.3
N1—Zn—N3	103.17 (13)	C14—C13—H13	119.3
C8—Si—C9	109.8 (3)	C13—C14—C15	118.4 (4)
C8—Si—C6	109.0 (2)	C13—C14—C16	120.4 (4)
C9—Si—C6	109.04 (19)	C15—C14—C16	121.2 (4)
C8—Si—C10	111.2 (2)	C10—C15—C14	122.4 (4)
C9—Si—C10	108.8 (2)	C10—C15—H15	118.8
C6—Si—C10	108.99 (17)	C14—C15—H15	118.8
C1—O1—Zn	111.1 (3)	O4—C16—O3	125.0 (4)
C16—O3—Zn ⁱ	123.1 (3)	O4—C16—C14	120.1 (4)
C17—N2—C19	107.0 (3)	O3—C16—C14	114.9 (4)
C17—N2—C20	126.3 (3)	C19—C18—N1	110.4 (4)
C19—N2—C20	126.6 (3)	C19—C18—H18	124.8

C17—N1—C18	104.9 (3)	N1—C18—H18	124.8
C17—N1—Zn	122.3 (3)	C18—C19—N2	105.6 (4)
C18—N1—Zn	132.8 (3)	C18—C19—H19	127.2
C26—N3—C28	104.7 (3)	N2—C19—H19	127.2
C26—N3—Zn	119.2 (3)	N1—C17—N2	112.0 (3)
C28—N3—Zn	132.0 (3)	N1—C17—H17	124.0
O2—C1—O1	122.4 (4)	N2—C17—H17	124.0
O2—C1—C2	120.8 (4)	C25—C20—C21	119.6 (4)
O1—C1—C2	116.7 (3)	C25—C20—N2	119.3 (3)
C3—C2—C7	118.9 (3)	C21—C20—N2	121.1 (4)
C3—C2—C1	121.1 (3)	C20—C25—C24	120.4 (4)
C7—C2—C1	120.0 (3)	C20—C25—H25	119.8
C4—C3—C2	120.7 (4)	C24—C25—H25	119.8
C4—C3—H3	119.6	C22—C21—C20	120.0 (4)
C2—C3—H3	119.6	C22—C21—H21	120.0
C3—C4—C5	119.4 (4)	C20—C21—H21	120.0
C3—C4—H4	120.3	C23—C22—C21	120.1 (4)
C5—C4—H4	120.3	C23—C22—H22	119.9
C4—C5—C6	122.1 (4)	C21—C22—H22	119.9
C4—C5—H5	118.9	C24—C23—C22	120.1 (3)
C6—C5—H5	118.9	C24—C23—N4 ⁱⁱ	120.0 (3)
C7—C6—C5	116.6 (3)	C22—C23—N4 ⁱⁱ	119.9 (3)
C7—C6—Si	123.5 (3)	C23—C24—C25	119.7 (4)
C5—C6—Si	120.0 (3)	C23—C24—H24	120.1
C2—C7—C6	122.3 (3)	C25—C24—H24	120.1
C2—C7—H7	118.9	C28—C27—N4	106.3 (4)
C6—C7—H7	118.9	C28—C27—H27	126.8
Si—C8—H8A	109.5	N4—C27—H27	126.8
Si—C8—H8B	109.5	N3—C26—N4	112.0 (4)
H8A—C8—H8B	109.5	N3—C26—H26	124.0
Si—C8—H8C	109.5	N4—C26—H26	124.0
H8A—C8—H8C	109.5	C27—C28—N3	110.5 (4)
H8B—C8—H8C	109.5	C27—C28—H28	124.7
Si—C9—H9A	109.5	N3—C28—H28	124.7
Si—C9—H9B	109.5	C26—N4—C27	106.4 (3)
H9A—C9—H9B	109.5	C26—N4—C23 ⁱⁱⁱ	125.3 (3)
Si—C9—H9C	109.5	C27—N4—C23 ⁱⁱⁱ	128.1 (3)
H9A—C9—H9C	109.5	H1WA—O1W—H1WB	122.0
H9B—C9—H9C	109.5	C13—C12—C11	119.2 (4)
C15—C10—C11	116.4 (4)	C13—C12—H12	120.4
C15—C10—Si	122.7 (3)	C11—C12—H12	120.4
C11—C10—Si	121.0 (3)		
O3 ⁱ —Zn—O1—C1	64.2 (3)	C12—C13—C14—C16	176.4 (4)
N1—Zn—O1—C1	-166.9 (3)	C11—C10—C15—C14	0.6 (6)
N3—Zn—O1—C1	-57.1 (3)	Si—C10—C15—C14	-179.8 (3)
O3 ⁱ —Zn—N1—C17	129.7 (3)	C13—C14—C15—C10	0.1 (6)
O1—Zn—N1—C17	-5.8 (3)	C16—C14—C15—C10	-176.8 (4)
N3—Zn—N1—C17	-129.6 (3)	Zn ⁱ —O3—C16—O4	-12.7 (6)

O3 ⁱ —Zn—N1—C18	-51.9 (4)	Zn ⁱ —O3—C16—C14	167.1 (3)
O1—Zn—N1—C18	172.6 (4)	C13—C14—C16—O4	-9.6 (7)
N3—Zn—N1—C18	48.7 (4)	C15—C14—C16—O4	167.2 (4)
O3 ⁱ —Zn—N3—C26	-36.1 (3)	C13—C14—C16—O3	170.6 (4)
O1—Zn—N3—C26	100.1 (3)	C15—C14—C16—O3	-12.6 (6)
N1—Zn—N3—C26	-153.5 (3)	C17—N1—C18—C19	-0.3 (5)
O3 ⁱ —Zn—N3—C28	117.6 (4)	Zn—N1—C18—C19	-178.9 (3)
O1—Zn—N3—C28	-106.3 (4)	N1—C18—C19—N2	0.2 (5)
N1—Zn—N3—C28	0.2 (4)	C17—N2—C19—C18	-0.1 (5)
Zn—O1—C1—O2	-2.0 (6)	C20—N2—C19—C18	-178.1 (4)
Zn—O1—C1—C2	176.0 (3)	C18—N1—C17—N2	0.2 (5)
O2—C1—C2—C3	-166.5 (4)	Zn—N1—C17—N2	179.0 (3)
O1—C1—C2—C3	15.5 (6)	C19—N2—C17—N1	-0.1 (5)
O2—C1—C2—C7	16.5 (6)	C20—N2—C17—N1	177.9 (4)
O1—C1—C2—C7	-161.5 (4)	C17—N2—C20—C25	-36.5 (6)
C7—C2—C3—C4	0.1 (6)	C19—N2—C20—C25	141.1 (4)
C1—C2—C3—C4	-177.0 (4)	C17—N2—C20—C21	144.3 (4)
C2—C3—C4—C5	1.2 (6)	C19—N2—C20—C21	-38.0 (6)
C3—C4—C5—C6	-1.0 (6)	C21—C20—C25—C24	1.3 (7)
C4—C5—C6—C7	-0.5 (6)	N2—C20—C25—C24	-177.9 (4)
C4—C5—C6—Si	-179.7 (3)	C25—C20—C21—C22	-1.9 (7)
C8—Si—C6—C7	-104.7 (3)	N2—C20—C21—C22	177.3 (4)
C9—Si—C6—C7	135.5 (3)	C20—C21—C22—C23	0.2 (7)
C10—Si—C6—C7	16.9 (4)	C21—C22—C23—C24	2.0 (7)
C8—Si—C6—C5	74.5 (4)	C21—C22—C23—N4 ⁱⁱ	-177.7 (4)
C9—Si—C6—C5	-45.3 (4)	C22—C23—C24—C25	-2.6 (6)
C10—Si—C6—C5	-164.0 (3)	N4 ⁱⁱ —C23—C24—C25	177.2 (4)
C3—C2—C7—C6	-1.6 (6)	C20—C25—C24—C23	0.9 (7)
C1—C2—C7—C6	175.5 (4)	C28—N3—C26—N4	-0.3 (5)
C5—C6—C7—C2	1.8 (5)	Zn—N3—C26—N4	159.8 (3)
Si—C6—C7—C2	-179.0 (3)	N4—C27—C28—N3	-0.4 (5)
C8—Si—C10—C15	35.2 (4)	C26—N3—C28—C27	0.4 (5)
C9—Si—C10—C15	156.2 (3)	Zn—N3—C28—C27	-156.0 (3)
C6—Si—C10—C15	-85.0 (3)	N3—C26—N4—C27	0.1 (5)
C8—Si—C10—C11	-145.2 (4)	N3—C26—N4—C23 ⁱⁱⁱ	-176.5 (3)
C9—Si—C10—C11	-24.2 (4)	C28—C27—N4—C26	0.2 (5)
C6—Si—C10—C11	94.6 (4)	C28—C27—N4—C23 ⁱⁱⁱ	176.7 (4)
C15—C10—C11—C12	-0.9 (6)	C14—C13—C12—C11	0.3 (8)
Si—C10—C11—C12	179.5 (4)	C10—C11—C12—C13	0.5 (7)
C12—C13—C14—C15	-0.5 (7)		

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x+1, y, z+1$; (iii) $x-1, y, z-1$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1WB \cdots O2 ⁱ	0.79	1.90	2.696 (8)	178
O1W—H1WA \cdots O2	0.78	2.08	2.852 (8)	171

Symmetry code: (i) $-x+1, -y, -z+1$.