

Bis{ μ -1,3-bis(dimethyl(pyridin-3-yl)silyl)propane- $\kappa^2N:N'$ }bis[diiodidozinc(II)] from synchrotron data

Jiyeong Song,^a Dongwon Kim^{b*} and Young-A Lee^{a*}

^aDepartment of Chemistry, Jeonbuk National University, Jeonju 54896, Republic of Korea, and ^bBeamline Department, Pohang Acceleratory Laboratory, Pohang 37673, Republic of Korea. *Correspondence e-mail: dwkim7459@postech.ac.kr, ylee@jbnu.ac.kr

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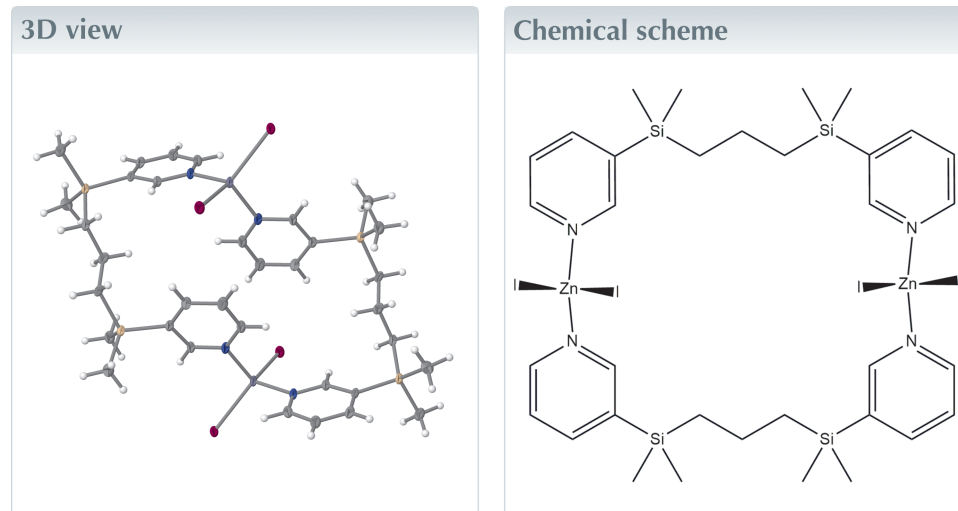
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Keywords: crystal structure; metallamacrocyclic complex; 1,3-bis(dimethylsilyl-3-pyridine)propane ligand; zinc(II) complexes; Synchrotron data.

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Structural data: full structural data are available from iucrdata.iucr.org

The structure of the title compound, $[Zn_2I_4(C_{34}H_{52}N_4Si_4)_2]$, has been determined from synchrotron data, $\lambda = 0.70000$ Å. The complete metallacyclic molecule is generated by crystallographic inversion symmetry, with the Zn^{II} ion located in a general position. The 1,3-bis(dimethylsilyl-3-pyridine)propane ligand binds to two zinc(II) ions in a horse-shoe fashion, resulting in formation of a dimeric 24-membered macrocycle. The Zn^{II} ion has a typical tetrahedral geometry *via* two iodide ions and two N donor atoms of the 1,3-bis(dimethylsilyl-3-pyridine)propane ligand. The macrocyclic dimers interact *via* weak interactions [$I \cdots H(H_3CSi^-) = 3.08, 3.27$ Å].



Structure description

Designed horse-shoe bidentate N-donors provide, *via* the introduction of appropriate metal cations, wider opportunities for task-specific metallacycles as receptors (Na *et al.*, 2008). Specifically, Zn^{II} complexes of functional N-donor ligands have been extensively examined for metallo-enzymes, zinc finger proteins, transmetallation, recognition, photoluminescence (PL), and catalysts (Porchia *et al.*, 2020). In particular, arrays of macrocyclic molecular units, especially after the emergence of additional functionalities, have attracted crystal engineers for the past decade (Lindoy *et al.*, 2013) in the fields of molecular adsorption, recognition, ion exchange, confinement catalysis, and luminescent chemosensing. Here, we report the crystal structure of a Zn^{II} 24-membered macrocycle, $[ZnI_2(L)]_2$, *via* self-assembly of ZnI_2 with 1,3-bis(dimethylsilyl-*m*-pyridine)propane (*L*) as a hemi-circular bidentate ligand. The incorporation of the flexible dimethylsilyl spacers in *L* plays a crucial role in the assembly process. This moiety provides the necessary conformational freedom and specific curvature to accommodate the tetrahedral coordination geometry of the Zn^{II} ions, thereby facilitating the formation of a discrete, strain-free macrocyclic architecture without significant steric hindrance.

Table 1
Selected geometric parameters (Å, °).

Zn1–I1	2.5680 (7)	Zn1–N1	2.051 (3)
Zn1–I2	2.5688 (9)	Zn1–N2 ⁱ	2.058 (3)
N1–Zn1–N2 ⁱ	101.75 (11)	N1–Zn1–I2	103.93 (8)
N1–Zn1–I1	112.18 (9)	N2 ⁱ –Zn1–I2	110.36 (8)
N2 ⁱ –Zn1–I1	105.99 (8)	I1–Zn1–I2	121.03 (2)

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

The defining structural feature of the title complex is the formation of a 24-membered centrosymmetric macrocyclo-dimer. The relevant bond lengths and angles are listed in Table 1. The local geometry around the Zn^{II} cation approximates to a typical tetrahedral arrangement with two N donors from two ligands [N–Zn–N = 101.75 (11)°] and two iodide ions [I–Zn–I = 121.03 (2)°]. For the 24-membered macrocycle, the intramolecular Zn···Zn separation distance is 8.118 (2) Å, and the shortest distance [C1···C2ⁱⁱⁱ or C2···C1ⁱⁱⁱ; symmetry code: (iii) $1 - x, 1 - y, 1 - z$] between two pyridyl moieties is 3.404 (7) Å. Fig. 1 illustrates the molecular structure of the centrosymmetric dimer. The propyl linkers adopt an extended all-anti conformation with close to 180° torsion angles, effectively minimizing intramolecular steric strain within the macrocycle. The flexible silicon bridges accommodate a slightly distorted tetrahedral geometry around the Zn^{II} center, allowing the formation of a discrete, strain-free assembly. This arrangement is further stabilized by the specific intermolecular interactions described below.

The crystal packing of the title complex is primarily consolidated by a network of weak intermolecular C–H···I hydrogen bonds involving the pyridyl ligands (Table 2 and Fig. 2). Specifically, the pyridyl ring hydrogen atom H1 forms a hydrogen bond with the iodide atom I1 of an adjacent mol-

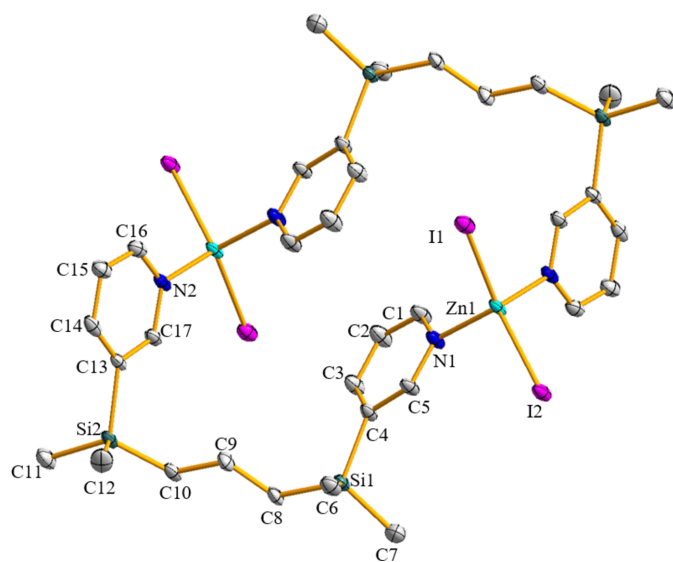


Figure 1
A view of the molecular structure of the title compound, showing the macrocyclic dimers with displacement ellipsoids drawn at the 30% probability level. For clarity, H atoms have been omitted. Symmetry operation used to generate equivalent atoms: $1 - x, 1 - y, 1 - z$.

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

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C1–H1···I1 ⁱⁱ	0.95	3.08	3.805 (4)	135
C15–H15···I2 ⁱⁱⁱ	0.95	3.27	3.756 (3)	114

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

ecule. In addition, the other pyridyl hydrogen atom H15 also participates in a significant interaction with the iodide ligand. Although classical π – π stacking interactions are not prominent, these multiple weak C–H···I interactions serve as the principal forces that connect the layers and enhance the overall stability of the molecular arrangement in the solid state.

A search of the Cambridge Structural Database (CSD, version 6.00 with updates through April 2025; Groom *et al.*, 2016) indicated that Hg^{II} complexes with the 1,3-bis(dimethylsilyl-3-pyridine)propane ligand had been reported previously. These complexes have been studied for straightforward formation of dianionic acetonates (Hong *et al.*, 2021). Furthermore, including the work by Na *et al.* (2008), a total of 14 complexes involving a cognate ligand, 1,3-bis-[dimethyl(pyridin-3-yl)silyl]ethane, have been reported in the CSD. However, no corresponding Zn^{II} complex with the ligand has been reported and the title compound was newly synthesized for this research.

Synthesis and crystallization

The title Zn^{II} complex was prepared as follows. A solution was prepared by dissolving ZnI₂ (0.02 mmol) in ethanol, and another by dissolving 1,3-bis(dimethylsilyl-3-pyridine)propane (0.02 mmol) in ethanol. Slow diffusion of the two solutions over several days afforded colorless needle-shaped crystals suitable for X-ray diffraction. Yield: 91.4%. FT-IR

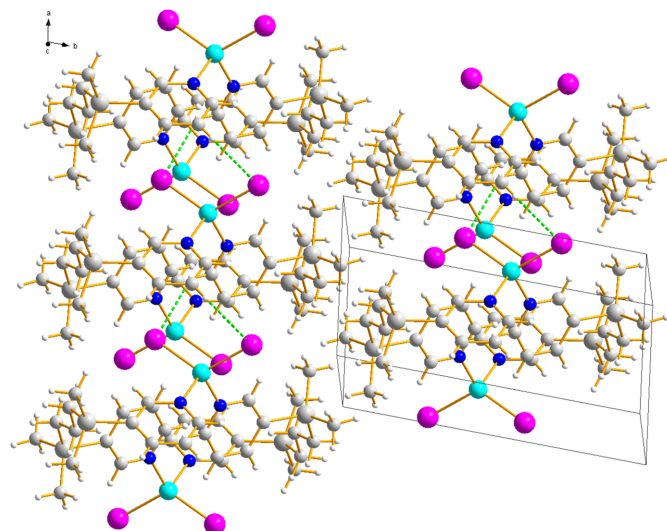


Figure 2
The crystal packing in title compound. Dashed lines represent C–H···I interactions.

(KBr pellet, cm^{-1}): 3436 (*s*), 2903 (*m*), 1589 (*m*), 1399 (*m*), 1255 (*m*), 1133 (*m*), 907 (*m*), 842 (*m*), 818 (*m*), 801 (*m*), 703 (*m*). ^1H NMR (400 MHz, $\text{Me}_2\text{SO}-d_6$, ppm): 8.59 (*d*, $J = 1.4$ Hz, 2H), 8.54 (*dd*, $J = 4.9, 1.9$ Hz, 2H), 7.82 (*dt*, $J = 7.5, 1.9$ Hz, 2H), 7.35 (*dd*, $J = 7.5, 4.9$ Hz, 2H), 1.50–1.20 (*m*, 2H), 0.81 (*dd*, $J = 6.9, 3.8$ Hz, 4H), 0.23 (*s*, 12H). Analysis calculated for $\text{Zn}_2\text{Si}_4\text{N}_4\text{I}_4\text{C}_{34}\text{H}_{52}\cdot 2.5\text{H}_2\text{O}$ (reflecting hygroscopic moisture) ($M = 1312.57$): C = 31.11%; H = 4.38%; N = 4.27%. Found: C = 31.10%; H = 4.11%; N = 4.38%.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

Funding information

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Table 3

Experimental details.

Crystal data	
Chemical formula	$[\text{Zn}_2\text{I}_4(\text{C}_{34}\text{H}_{52}\text{N}_4\text{Si}_4)_2]$
M_r	1267.49
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, b, c (Å)	6.6360 (13), 13.531 (3), 14.416 (3)
α, β, γ (°)	107.03 (3), 91.52 (3), 100.29 (3)
V (Å ³)	1213.5 (5)
Z	1
Radiation type	Synchrotron, $\lambda = 0.700$ Å
μ (mm ⁻¹)	3.48
Crystal size (mm)	0.15 × 0.11 × 0.07
Data collection	
Diffractometer	Rayonix MX225HS CCD area detector
Absorption correction	Empirical (using intensity measurements) (<i>HKL3000sm SCALEPACK</i> ; Otwinowski <i>et al.</i> , 2003)
T_{\min}, T_{\max}	0.942, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13971, 7000, 6774
R_{int}	0.020
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.704
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.042, 0.126, 1.15
No. of reflections	7000
No. of parameters	222
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.75, -1.60

Computer programs: *PAL BL2D-SMDC Program* (Shin *et al.*, 2025), *HKL3000sm* (Otwinowski *et al.*, 2003), *SHELXT2018* (Sheldrick, 2015a), *SHELXL2025* (Sheldrick, 2015b), *DIAMOND 4* (Putz & Brandenburg, 2014) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2026). **11**, x260183 [https://doi.org/10.1107/S2414314626001835]

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Bis{ μ -1,3-bis[dimethyl(pyridin-3-yl)silyl]propane- κ^2 N:N'}bis[diiodidozinc(II)]

Crystal data

[Zn₂I₄(C₃₄H₅₂N₄Si₄)₂]

$M_r = 1267.49$

Triclinic, $P\bar{1}$

$a = 6.6360$ (13) Å

$b = 13.531$ (3) Å

$c = 14.416$ (3) Å

$\alpha = 107.03$ (3)°

$\beta = 91.52$ (3)°

$\gamma = 100.29$ (3)°

$V = 1213.5$ (5) Å³

$Z = 1$

$F(000) = 612$

$D_x = 1.734$ Mg m⁻³

Synchrotron radiation, $\lambda = 0.700$ Å

Cell parameters from 25750 reflections

$\theta = 0.4$ – 29.5 °

$\mu = 3.48$ mm⁻¹

$T = 100$ K

Block, colorless

$0.15 \times 0.11 \times 0.07$ mm

Data collection

Rayonix MX225HS CCD area detector
diffractometer

Radiation source: PLSII 2D bending magnet

ω scan

Absorption correction: empirical (using
intensity measurements)

(*HKL3000sm Scalepack*; Otwinowski *et al.*,
2003)

$T_{\min} = 0.942$, $T_{\max} = 1.000$

13971 measured reflections

7000 independent reflections

6774 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$

$\theta_{\max} = 29.6$ °, $\theta_{\min} = 1.5$ °

$h = -9 \rightarrow 9$

$k = -19 \rightarrow 19$

$l = -20 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.126$

$S = 1.15$

7000 reflections

222 parameters

0 restraints

Primary atom site location: dual

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0818P)^2 + 1.9207P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.75$ e Å⁻³

$\Delta\rho_{\min} = -1.60$ e Å⁻³

Extinction correction: SHELXL2025/1

(Sheldrick 2015b),

$F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0393 (15)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
I1	0.02739 (3)	0.60462 (2)	0.71151 (2)	0.02188 (9)
I2	−0.04076 (3)	0.28606 (2)	0.75347 (2)	0.02388 (9)
Zn1	0.18295 (5)	0.44768 (3)	0.72356 (2)	0.01825 (11)
Si1	0.20755 (13)	0.11080 (7)	0.36959 (6)	0.01815 (17)
Si2	0.29081 (13)	0.19038 (7)	0.00126 (6)	0.01876 (17)
N1	0.3265 (4)	0.3852 (2)	0.6019 (2)	0.0211 (5)
N2	0.5728 (4)	0.4903 (2)	0.17215 (19)	0.0188 (5)
C1	0.5162 (5)	0.4319 (3)	0.5905 (2)	0.0251 (6)
H1	0.579527	0.495898	0.638031	0.030*
C9	0.2785 (5)	0.1499 (3)	0.1859 (2)	0.0221 (6)
H9A	0.319184	0.225709	0.222588	0.027*
H9B	0.127944	0.134290	0.169839	0.027*
C10	0.3857 (5)	0.1284 (2)	0.0903 (2)	0.0206 (6)
H10A	0.364468	0.051314	0.059107	0.025*
H10B	0.535313	0.155339	0.105999	0.025*
C11	0.4132 (6)	0.1526 (3)	−0.1155 (3)	0.0291 (7)
H11A	0.348469	0.178332	−0.163340	0.044*
H11B	0.395268	0.075655	−0.140057	0.044*
H11C	0.560138	0.183835	−0.104471	0.044*
C12	0.0055 (5)	0.1505 (3)	−0.0225 (3)	0.0300 (7)
H12A	−0.041008	0.178965	−0.072628	0.045*
H12B	−0.058849	0.178144	0.037643	0.045*
H12C	−0.033317	0.073428	−0.044895	0.045*
C13	0.3555 (4)	0.3384 (2)	0.0570 (2)	0.0177 (5)
C14	0.2430 (5)	0.4065 (3)	0.0321 (2)	0.0214 (6)
H14	0.130060	0.378651	−0.016029	0.026*
C15	0.2954 (5)	0.5143 (3)	0.0771 (2)	0.0233 (6)
H15	0.219466	0.560577	0.060122	0.028*
C16	0.4601 (5)	0.5533 (2)	0.1470 (2)	0.0210 (6)
H16	0.494752	0.627136	0.178439	0.025*
C17	0.5198 (5)	0.3852 (2)	0.1279 (2)	0.0193 (5)
H17	0.598922	0.340795	0.146053	0.023*
C2	0.6227 (5)	0.3902 (3)	0.5118 (3)	0.0284 (7)
H2	0.757203	0.424652	0.505495	0.034*
C3	0.5296 (5)	0.2971 (3)	0.4423 (2)	0.0239 (6)
H3	0.600523	0.267856	0.387566	0.029*
C4	0.3325 (5)	0.2458 (2)	0.4519 (2)	0.0192 (5)
C5	0.2384 (5)	0.2944 (2)	0.5337 (2)	0.0196 (6)
H5	0.103813	0.261679	0.541876	0.024*

C6	-0.0741 (5)	0.1046 (3)	0.3501 (3)	0.0253 (6)
H6A	-0.139978	0.033687	0.309674	0.038*
H6B	-0.096958	0.156130	0.317310	0.038*
H6C	-0.133232	0.120667	0.413133	0.038*
C7	0.2577 (6)	0.0153 (3)	0.4333 (3)	0.0296 (7)
H7A	0.177913	-0.054853	0.398498	0.044*
H7B	0.217186	0.037456	0.499969	0.044*
H7C	0.404478	0.012956	0.434917	0.044*
C8	0.3300 (5)	0.0847 (2)	0.2514 (2)	0.0202 (5)
H8A	0.480997	0.098998	0.265646	0.024*
H8B	0.286597	0.008978	0.214817	0.024*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01598 (12)	0.02058 (13)	0.02297 (13)	-0.00243 (8)	0.00322 (8)	0.00066 (8)
I2	0.02429 (13)	0.01873 (13)	0.01943 (13)	-0.00750 (8)	0.00749 (8)	-0.00180 (8)
Zn1	0.01568 (17)	0.01609 (17)	0.01450 (17)	-0.00495 (12)	0.00393 (12)	-0.00377 (12)
Si1	0.0185 (4)	0.0162 (4)	0.0140 (3)	-0.0020 (3)	0.0017 (3)	-0.0012 (3)
Si2	0.0167 (4)	0.0176 (4)	0.0140 (3)	-0.0055 (3)	0.0015 (3)	-0.0023 (3)
N1	0.0173 (11)	0.0201 (12)	0.0165 (11)	-0.0059 (9)	0.0047 (9)	-0.0032 (9)
N2	0.0165 (11)	0.0169 (11)	0.0152 (10)	-0.0042 (9)	0.0034 (8)	-0.0030 (9)
C1	0.0202 (14)	0.0231 (14)	0.0214 (14)	-0.0087 (12)	0.0063 (11)	-0.0025 (12)
C9	0.0244 (14)	0.0237 (14)	0.0159 (12)	0.0058 (12)	0.0057 (11)	0.0013 (11)
C10	0.0185 (13)	0.0191 (13)	0.0161 (12)	-0.0039 (10)	0.0029 (10)	-0.0027 (10)
C11	0.0325 (17)	0.0271 (16)	0.0197 (14)	0.0001 (14)	0.0069 (13)	-0.0020 (12)
C12	0.0187 (14)	0.0339 (18)	0.0303 (17)	-0.0111 (13)	-0.0030 (12)	0.0089 (15)
C13	0.0156 (12)	0.0173 (12)	0.0133 (11)	-0.0034 (10)	0.0042 (9)	-0.0025 (9)
C14	0.0155 (12)	0.0250 (14)	0.0161 (12)	-0.0026 (11)	0.0026 (10)	-0.0017 (11)
C15	0.0223 (14)	0.0208 (14)	0.0220 (14)	0.0012 (11)	0.0055 (11)	0.0006 (11)
C16	0.0206 (13)	0.0166 (13)	0.0208 (13)	-0.0008 (11)	0.0051 (11)	0.0004 (10)
C17	0.0194 (13)	0.0162 (12)	0.0166 (12)	-0.0030 (10)	0.0024 (10)	0.0000 (10)
C2	0.0204 (14)	0.0298 (17)	0.0235 (15)	-0.0070 (13)	0.0076 (12)	-0.0028 (13)
C3	0.0183 (13)	0.0245 (15)	0.0203 (14)	-0.0038 (12)	0.0071 (11)	-0.0024 (12)
C4	0.0169 (12)	0.0191 (13)	0.0152 (12)	-0.0036 (10)	0.0020 (10)	-0.0006 (10)
C5	0.0158 (12)	0.0169 (13)	0.0184 (13)	-0.0053 (10)	0.0043 (10)	-0.0019 (10)
C6	0.0204 (14)	0.0238 (15)	0.0252 (15)	-0.0029 (12)	0.0025 (11)	0.0016 (12)
C7	0.0381 (19)	0.0221 (15)	0.0244 (15)	0.0004 (14)	-0.0008 (13)	0.0044 (12)
C8	0.0214 (13)	0.0211 (13)	0.0127 (12)	0.0014 (11)	0.0029 (10)	-0.0017 (10)

Geometric parameters (Å, °)

I1—Zn1	2.5680 (7)	C11—H11C	0.9800
I2—Zn1	2.5688 (9)	C12—H12A	0.9800
Zn1—N1	2.051 (3)	C12—H12B	0.9800
Zn1—N2 ⁱ	2.058 (3)	C12—H12C	0.9800
Si1—C7	1.859 (4)	C13—C17	1.396 (4)
Si1—C6	1.866 (4)	C13—C14	1.401 (5)

Si1—C8	1.874 (3)	C14—C15	1.386 (4)
Si1—C4	1.889 (3)	C14—H14	0.9500
Si2—C11	1.863 (4)	C15—C16	1.383 (5)
Si2—C12	1.867 (4)	C15—H15	0.9500
Si2—C10	1.877 (4)	C16—H16	0.9500
Si2—C13	1.890 (3)	C17—H17	0.9500
N1—C1	1.342 (4)	C2—C3	1.386 (5)
N1—C5	1.350 (4)	C2—H2	0.9500
N2—C16	1.346 (4)	C3—C4	1.398 (4)
N2—C17	1.353 (4)	C3—H3	0.9500
C1—C2	1.385 (5)	C4—C5	1.395 (4)
C1—H1	0.9500	C5—H5	0.9500
C9—C8	1.539 (5)	C6—H6A	0.9800
C9—C10	1.543 (4)	C6—H6B	0.9800
C9—H9A	0.9900	C6—H6C	0.9800
C9—H9B	0.9900	C7—H7A	0.9800
C10—H10A	0.9900	C7—H7B	0.9800
C10—H10B	0.9900	C7—H7C	0.9800
C11—H11A	0.9800	C8—H8A	0.9900
C11—H11B	0.9800	C8—H8B	0.9900
N1—Zn1—N2 ⁱ	101.75 (11)	Si2—C12—H12C	109.5
N1—Zn1—I1	112.18 (9)	H12A—C12—H12C	109.5
N2 ⁱ —Zn1—I1	105.99 (8)	H12B—C12—H12C	109.5
N1—Zn1—I2	103.93 (8)	C17—C13—C14	116.5 (3)
N2 ⁱ —Zn1—I2	110.36 (8)	C17—C13—Si2	120.4 (2)
I1—Zn1—I2	121.03 (2)	C14—C13—Si2	123.1 (2)
C7—Si1—C6	110.83 (18)	C15—C14—C13	120.4 (3)
C7—Si1—C8	109.85 (17)	C15—C14—H14	119.8
C6—Si1—C8	111.23 (15)	C13—C14—H14	119.8
C7—Si1—C4	106.29 (16)	C16—C15—C14	119.0 (3)
C6—Si1—C4	109.39 (16)	C16—C15—H15	120.5
C8—Si1—C4	109.12 (14)	C14—C15—H15	120.5
C11—Si2—C12	109.74 (18)	N2—C16—C15	122.2 (3)
C11—Si2—C10	111.15 (17)	N2—C16—H16	118.9
C12—Si2—C10	110.25 (16)	C15—C16—H16	118.9
C11—Si2—C13	109.42 (16)	N2—C17—C13	123.7 (3)
C12—Si2—C13	107.79 (17)	N2—C17—H17	118.2
C10—Si2—C13	108.42 (14)	C13—C17—H17	118.2
C1—N1—C5	118.2 (3)	C1—C2—C3	118.8 (3)
C1—N1—Zn1	120.1 (2)	C1—C2—H2	120.6
C5—N1—Zn1	121.6 (2)	C3—C2—H2	120.6
C16—N2—C17	118.3 (3)	C2—C3—C4	120.6 (3)
C16—N2—Zn1 ⁱ	120.8 (2)	C2—C3—H3	119.7
C17—N2—Zn1 ⁱ	121.0 (2)	C4—C3—H3	119.7
N1—C1—C2	122.2 (3)	C5—C4—C3	116.1 (3)
N1—C1—H1	118.9	C5—C4—Si1	120.1 (2)
C2—C1—H1	118.9	C3—C4—Si1	123.4 (2)

C8—C9—C10	113.7 (3)	N1—C5—C4	124.1 (3)
C8—C9—H9A	108.8	N1—C5—H5	118.0
C10—C9—H9A	108.8	C4—C5—H5	118.0
C8—C9—H9B	108.8	Si1—C6—H6A	109.5
C10—C9—H9B	108.8	Si1—C6—H6B	109.5
H9A—C9—H9B	107.7	H6A—C6—H6B	109.5
C9—C10—Si2	113.8 (2)	Si1—C6—H6C	109.5
C9—C10—H10A	108.8	H6A—C6—H6C	109.5
Si2—C10—H10A	108.8	H6B—C6—H6C	109.5
C9—C10—H10B	108.8	Si1—C7—H7A	109.5
Si2—C10—H10B	108.8	Si1—C7—H7B	109.5
H10A—C10—H10B	107.7	H7A—C7—H7B	109.5
Si2—C11—H11A	109.5	Si1—C7—H7C	109.5
Si2—C11—H11B	109.5	H7A—C7—H7C	109.5
H11A—C11—H11B	109.5	H7B—C7—H7C	109.5
Si2—C11—H11C	109.5	C9—C8—Si1	115.0 (2)
H11A—C11—H11C	109.5	C9—C8—H8A	108.5
H11B—C11—H11C	109.5	Si1—C8—H8A	108.5
Si2—C12—H12A	109.5	C9—C8—H8B	108.5
Si2—C12—H12B	109.5	Si1—C8—H8B	108.5
H12A—C12—H12B	109.5	H8A—C8—H8B	107.5
C5—N1—C1—C2	-0.1 (6)	C14—C13—C17—N2	0.2 (4)
Zn1—N1—C1—C2	177.1 (3)	Si2—C13—C17—N2	-178.8 (2)
C8—C9—C10—Si2	170.5 (2)	N1—C1—C2—C3	0.3 (6)
C11—Si2—C10—C9	-175.7 (2)	C1—C2—C3—C4	-0.6 (6)
C12—Si2—C10—C9	-53.8 (3)	C2—C3—C4—C5	0.7 (5)
C13—Si2—C10—C9	64.0 (2)	C2—C3—C4—Si1	-172.2 (3)
C11—Si2—C13—C17	-96.0 (3)	C7—Si1—C4—C5	-77.1 (3)
C12—Si2—C13—C17	144.7 (2)	C6—Si1—C4—C5	42.6 (3)
C10—Si2—C13—C17	25.4 (3)	C8—Si1—C4—C5	164.5 (3)
C11—Si2—C13—C14	85.1 (3)	C7—Si1—C4—C3	95.4 (3)
C12—Si2—C13—C14	-34.2 (3)	C6—Si1—C4—C3	-144.9 (3)
C10—Si2—C13—C14	-153.5 (2)	C8—Si1—C4—C3	-23.0 (3)
C17—C13—C14—C15	-0.3 (4)	C1—N1—C5—C4	0.2 (5)
Si2—C13—C14—C15	178.6 (2)	Zn1—N1—C5—C4	-176.9 (3)
C13—C14—C15—C16	-0.1 (5)	C3—C4—C5—N1	-0.5 (5)
C17—N2—C16—C15	-1.0 (5)	Si1—C4—C5—N1	172.6 (3)
Zn1 ⁱ —N2—C16—C15	179.8 (2)	C10—C9—C8—Si1	178.6 (2)
C14—C15—C16—N2	0.8 (5)	C7—Si1—C8—C9	173.1 (2)
C16—N2—C17—C13	0.5 (4)	C6—Si1—C8—C9	50.0 (3)
Zn1 ⁱ —N2—C17—C13	179.7 (2)	C4—Si1—C8—C9	-70.7 (3)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1—H1 ⁱ —H1 ⁱⁱ	0.95	3.08	3.805 (4)	135

C15—H15···I2 ⁱⁱⁱ	0.95	3.27	3.756 (3)	114
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Symmetry codes: (ii) $x+1, y, z$; (iii) $-x, -y+1, -z+1$.