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Synthesis and structure of ethyl 2,2-dimethyl-3-(naphthalen-1-yl)-1,2-dihydrobenzo[*c*]siline-4-carboxylate

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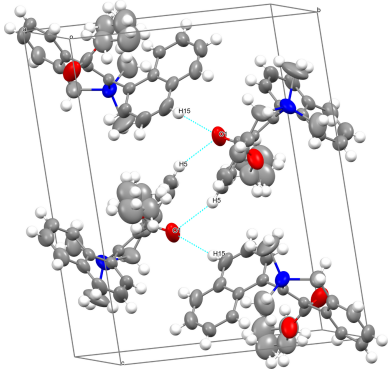
In the title compound, $C_{24}H_{24}O_2Si$, the six-membered silacyclic ring adopts a twisted boat conformation and the naphthyl substituent is nearly orthogonal to the plane of the benzo[*c*]siline fused framework. The terminal ethyl ester fragment displays two-site static disorder. In the extended structure, weak C—H···O hydrogen bonds link adjacent molecules into infinite zigzag ribbons propagating parallel to the [010] direction.

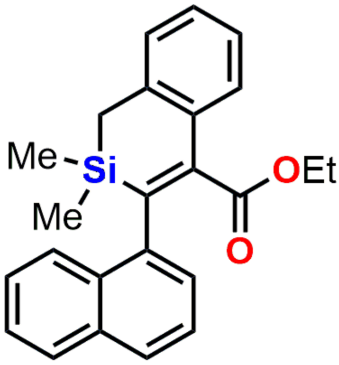
1. Chemical context

Silacyclic fused skeletons represent appealing building blocks for synthetic chemistry, optoelectronic materials and medicinal chemistry (Bains *et al.*, 2003; Ikeno *et al.*, 2017; Fujii *et al.*, 2017). Silicon possesses a larger covalent radius, elongated Si—C bonds and accessible σ^*–π^* conjugation, which enables precise modulation of electronic and biological properties (Franz *et al.*, 2013; Gately *et al.*, 2007; Meanwell *et al.*, 2011). Silicon isosteres can simultaneously enhance molecular lipophilicity and chemical stability (Min *et al.*, 2013; Rémond *et al.*, 2016). Conjugated six-membered benzo[*c*]silines feature rigid and readily tunable almost planar backbones, yet synthetic and crystallographic investigations of functionalized derivatives lag significantly behind those of five-membered silole analogues (Santra, 2020).

The parent 1,2-dihydrobenzo[*c*]siline framework features an sp^3-hybridized tetrahedral silicon atom. Endocyclic alkene, aryl and ester substituents can establish multiple intramolecular conjugation pathways. Functionalization with *gem*-dimethyl, 1-naphthyl and ethyl carboxylate groups extends the effective π-conjugation length; steric hindrance originating from the *gem*-dimethyl substituents modulates ring geometry, and the naphthalene moiety provides abundant sites for intermolecular π-related interactions. To date, no single-crystal X-ray diffraction data have been documented for this triple-substituted scaffold, leaving its solid-state molecular conformation and supramolecular packing unexplored. Ring expansion of benzosilacyclobutene provides a facile, atom-economic synthetic route to functionalized benzo[*c*]silines (Wang *et al.*, 2020; Wang *et al.*, 2025).

As part of our studies in this area, we now describe the synthesis and structure of the title compound, $C_{24}H_{24}O_2Si$ (**3**) (Fig. 1).





2. Structural commentary

The tetrahedral silicon atom Si1 has four distinct Si—C single bonds ranging from 1.847 (3) to 1.879 (2) Å; the longest Si1—C1 bond corresponds to the olefin-linked carbon atom, which leads to a narrow C9—Si1—C1 angle of 100.76 (11)°, producing obvious puckering of the silacyclic ring. The C1═C2 double bond at 1.340 (3) Å is the shortest carbon–carbon linkage within the whole skeleton, consistent with the characteristic length of C═C olefin bonds. The six-membered silacyclic ring adopts a twisted boat conformation with C2/C3/C8/C9 almost coplanar (r.m.s. deviation = 0.010 Å) and Si1 and C1 displaced from their mean plane by 0.947 (1) and 0.437 (2) Å, respectively. The torsion angle Si1—C1—C2—C3 of −5.4 (3)° confirms minor deviation of the unsaturated segment from the ring mean plane. The fused benzene moiety on the silacycle remains nearly planar, with the C3—C8—C9 bond angle of 121.5 (2)° matching standard aromatic C—C—C angles. The torsion angle C3—C8—C9—Si1 = −36.2 (3)° quantifies the out-of-plane displacement of the Si atom relative to the benzo-fused plane.

A single C1—C12 σ-bond links the silacyclic core and pendant naphthalene ring. The large torsion angle Si1—C1—C12—C13 = −93.6 (2)° reveals that the naphthalene plane is nearly perpendicular to the benzosiline plane, a result of steric repulsion from the *gem*-dimethyl substituents on silicon, which restricts intramolecular π-conjugation between the two aromatic systems. The naphthalene fragment maintains ideal aromatic geometry, exemplified by the C16—C21—C12 bond angle of 119.7 (2)°.

At the C2 position of the silacycle lies an ethyl carboxylate group. The carbonyl bond C22═O1 [1.195 (3) Å] and ester single bond C22—O2 [1.320 (3) Å] show typical carbonyl/ether bond lengths for carboxylate esters. The bond angle O1—C22—O2 reaches 124.8 (3)°, while O2—C22—C2 is 111.2 (2)°, reflecting the sp^2 hybridization state of carbonyl carbon atom C22. The terminal ethyl group on O2 suffers two-site static disorder, as demonstrated by the torsion angle C22—O2—C23—C24 of 101.7 (10)° for one disordered alkyl conformation; the other disordered ethyl chain adopts a separate rotational orientation with different torsion value. Apart from the disordered ethoxy alkyl chain, all rigid aromatic and silacyclic fragments display normal bond lengths and angles without significant structural distortion.

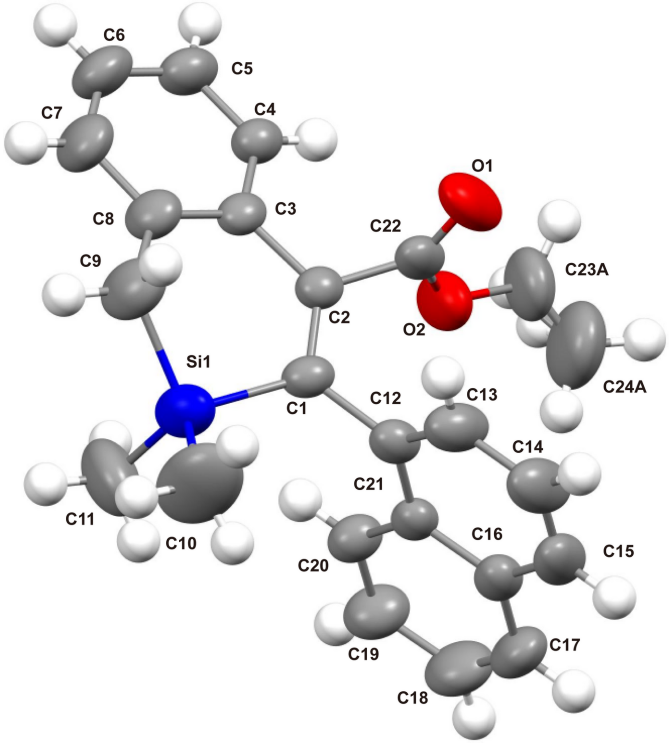


Figure 1
The molecular structure of **3** with displacement ellipsoids drawn at the 50% probability level. Only the major disorder component of the ester side chain is shown; hydrogen atoms are omitted for clarity.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15···O1^{i}	0.93	2.49	3.359 (4)	156

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

3. Supramolecular features

In the extended structure of **3**, weak C15—H15···O1 hydrogen bonds link the molecules into infinite zigzag ribbons propagating parallel to the [010] crystallographic direction (Fig. 2). Geometric parameters for this interaction are listed in Table 1.

4. Database survey

Searches were carried out with the Cambridge Structural Database(CSD, Version 6.01, update November 2025; Groom *et al.*, 2016) together with the *ConQuest* search program (Version 2025.3.1; Bruno *et al.*, 2002).

An unrestricted search for the parent 1,2-dihydrobenzo[*c*]-siline fused silacyclic core without extra fused aromatic rings returned a moderate number of hits, most of which carry simple alkyl or phenyl substituents only (Wang *et al.*, 2026).

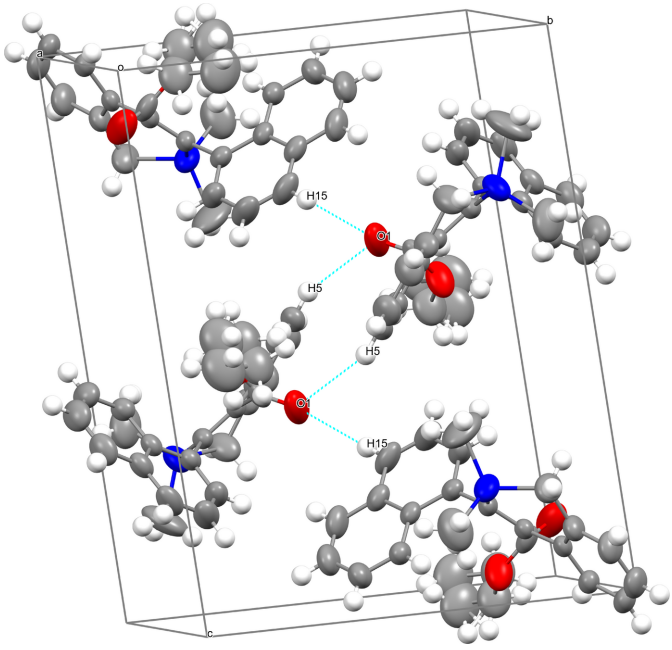


Figure 2
Crystal packing diagram for **3** with hydrogen bonds represented by dashed lines.

Limiting the query to 2,2-dimethyl-substituted 1,2-dihydrobenzo[*c*]siline skeletons yielded far fewer recorded structures, indicating this dimethylsilacyclic scaffold remains underexplored in single-crystal crystallography.

Further constraints were applied to narrow the screening: the silacycle bears an ethyl carboxylate group at the C2 position and a pendant naphthalen-1-yl group attached to the ring olefinic carbon atom. After applying this triple substitution filter (*gem*-dimethyl silicon, 4-carboxylate ester, 3-naphthyl), zero matching crystal structures were retrieved from the CSD.

The few reported analogues of 1,2-dihydrobenzo[*c*]siline only incorporate small monocyclic aryl groups such as phenyl, rather than extended polycyclic naphthalene fragments. A supplementary restricted search was performed for carboxylate-functionalized benzosilacyclic molecules without naphthyl substitution. Only a few simple phenyl-substituted ethyl benzo[*c*]siline carboxylate entries were found (Tang *et al.*, 2022; Tang *et al.*, 2024), none of which feature the bulky naphthalene π-extended moiety on the silacyclic backbone.

5. Synthesis and crystallization

The synthetic route for the title compound is shown in Fig. 3. A solution of $Pd(OAc)_2$ (2.2 mg, 0.01 mmol, 5 mol %) and [(2,2-dimethyl-1,3-dioxolane-4,5-diyl)dimethanediyl]bis(diphenylphosphane (DIOP) (10.0 mg, 0.02 mmol, 10 mol %) in EtOAc (0.5 ml) was stirred at 298 K for 3 min. Alkyne **2** (44.8 mg, 0.2 mmol, 1.0 equiv.), benzosilacyclobutene **1** (59.3 mg, 0.4 mmol, 2.0 equiv.) and additional EtOAc (1.5 ml) were added sequentially. The mixture was kept at 298 K for 12 h. The solvent was removed under reduced pressure, and the residue was purified by silica gel column chromatography with gradient elution (petroleum ether, then petroleum ether/ethyl acetate = 50:1) to furnish the target product **3** (yield: 30 mg, 40%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88–7.82 (*m*, 2H), 7.71 (*d*, *J* = 8.3 Hz, 1H), 7.47–7.39 (*m*, 4H), 7.21–7.12 (*m*, 4H), 3.71 (*q*, *J* = 7.1, 2H), 2.36 (*s*, 2H), 0.45 (*t*, *J* = 7.1 Hz, 3H), 0.03 (*s*, 3H), −0.01 (*s*, 3H). A solution of **3** (20 mg) in 2.0 ml mixed solvent of CH_2Cl_2/*n*-hexane (CH_2Cl_2:*n*-hexane = 1:3) was transferred to a test tube and sealed with plastic film. Suitable single crystals of **3** were obtained by slow solvent evaporation over 3 days at room temperature.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{24}O_2Si$
M_r	372.52
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, *b*, *c* (Å)	9.8031 (5), 13.0620 (6), 17.1604 (10)
β (°)	105.412 (6)
V (Å^3)	2118.3 (2)
Z	4
D_x (Mg m^{-3})	1.168
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.13
Crystal size (mm)	0.35 × 0.30 × 0.25
Data collection	
Diffractometer	Xcalibur, Eos
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.977, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9418, 4331, 2739
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.144, 1.02
No. of reflections	4331
No. of parameters	255
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.22

Computer programs: *CrysAlis PRO* (Agilent, 2014), *OLEX2.solve* (Bourhis *et al.*, 2015), *SHELXL* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

6. Refinement

Details of data collection and structure refinement are summarized in Table 2. The terminal ethyl group of the ester moiety exhibits two-site static positional disorder. Two sets of

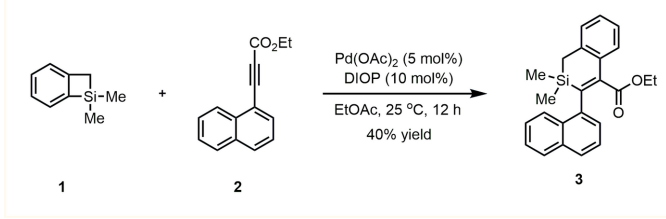


Figure 3
The synthesis of compound **3**.

atomic coordinates (C23/C24 and C23*A*/C24*A*) were modelled for the disordered alkyl fragment sharing the ether oxygen atom O2. Suitable distance restraints and anisotropic displacement parameter constraints were adopted to achieve stable refinement of the disordered part. All H atoms were included using a riding model starting from calculated positions. Methyl groups were refined as idealized rigid groups, with C—H = 0.96 Å and H—C—H = 109.5°, allowed to rotate but not tip (AFIX 137 card in *SHELXL*). Methylene and aromatic H atoms were constrained with C—H = 0.97 Å and 0.93 Å, respectively. The U_{iso}(H) values were fixed at 1.5U_{eq} of the parent C atoms for methyl groups and at 1.2U_{eq} for the remaining H atoms.

Funding information

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References

Agilent (2014). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Bains, W. & Tacke, R. (2003). *Curr. Opin. Drug Discov. Dev.* **6**, 526–543.
Bourhis, L. J., Dolomanov, O. V., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2015). *Acta Cryst.* A**71**, 59–75.
Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Franz, A. K. & Wilson, S. O. (2013). *J. Med. Chem.* **56**, 388–405.
Fujii, S. & Hashimoto, Y. (2017). *Future Med. Chem.* **9**, 485–505.
Gately, S. & West, R. (2007). *Drug Dev. Res.* **68**, 156–163.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Ikeno, T., Nagano, T. & Hanaoka, K. (2017). *Chem. Asian J.* **12**, 1435–1446.
Meanwell, N. A. (2011). *J. Med. Chem.* **54**, 2529–2591.
Min, G. K., Hernández, D. & Skrydstrup, T. (2013). *Acc. Chem. Res.* **46**, 457–470.
Rémond, E., Martin, C., Martinez, J. & Cavelier, F. (2016). *Chem. Rev.* **116**, 11654–11684.
Santra, S. (2020). *ChemistrySelect* **5**, 9034–9058.
Sheldrick, G. M. (2015). *J. Appl. Cryst*. 48, 3–10.
Tang, X.-X., Tang, Y., Peng, J., Du, H., Huang, L., Gao, J., Liu, S., Wang, D., Wang, W., Gao, L., Lan, Y. & Song, Z.-L. (2024). *J. Am. Chem. Soc.* **146**, 26639–26648.
Tang, X.-X., Zhang, Y., Tang, Y.-L., Li, Y., Zhou, J., Wang, D., Gao, L., Su, Z.-S. & Song, Z.-L. (2022). *ACS Catal.* **12**, 5185–5196.
Wang, X.-B., Guo, J.-J., Chen, C., Si, J.-W., Xu, Z., Zhao, Z.-Y., Shi, Z., Kwong, F. Y. & Xu, L.-W. (2025). *ACS Catal.* **15**, 20594–20604.
Wang, X.-B., Guo, J.-J., Shen, M.-H., Li, L., Shi, Z. & Xu, L.-W. (2026). *Org. Lett.* **28**, 2050–2055.
Wang, X.-B., Zheng, Z., Xie, J., Gu, X., Mu, Q., Yin, G., Ye, F., Xu, Z. & Xu, L. (2020). *Angew. Chem. Int. Ed.* **59**, 790–797.

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Synthesis and structure of ethyl 2,2-dimethyl-3-(naphthalen-1-yl)-1,2-dihydrobenzo[*c*]siline-4-carboxylate

Xiaoxiao Tang and Liyun Zhang

Computing details

Ethyl 2,2-dimethyl-3-(naphthalen-1-yl)-1,2-dihydrobenzo[*c*]siline-4-carboxylate

Crystal data

$C_{24}H_{24}O_2Si$
$M_r = 372.52$
Monoclinic, $P2_1/n$
$a = 9.8031$ (5) Å
$b = 13.0620$ (6) Å
$c = 17.1604$ (10) Å
$\beta = 105.412$ (6)°
$V = 2118.3$ (2) Å^3
$Z = 4$
$F(000) = 792$
$D_x = 1.168$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2164 reflections
$\theta = 3.8$–24.9°
$\mu = 0.13$ mm^{-1}
$T = 293$ K
Block, colourless
0.35 × 0.30 × 0.25 mm

Data collection

Xcalibur, Eos diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.0874 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysalisPro; Agilent, 2014)
$T_{min} = 0.977$, $T_{max} = 1.000$
9418 measured reflections
4331 independent reflections
2739 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 26.4°$, $\theta_{min} = 3.1°$
$h = -12\rightarrow11$
$k = -10\rightarrow16$
$l = -21\rightarrow21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.144$
$S = 1.02$
4331 reflections
255 parameters
2 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.4704P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.005$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Si1	0.19934 (7)	0.86055 (6)	0.28273 (5)	0.0677 (3)	
O1	0.6312 (2)	0.64582 (15)	0.36738 (13)	0.0948 (7)	
O2	0.65900 (17)	0.78080 (15)	0.44955 (13)	0.0849 (6)	
C1	0.3927 (2)	0.82910 (15)	0.32118 (12)	0.0451 (5)	
C2	0.4304 (2)	0.74794 (15)	0.36995 (12)	0.0414 (5)	
C3	0.3349 (2)	0.68302 (15)	0.40340 (12)	0.0432 (5)	
C4	0.3930 (2)	0.62571 (15)	0.47252 (13)	0.0496 (6)	
H4	0.490195	0.628386	0.495618	0.060*	
C5	0.3114 (3)	0.56525 (18)	0.50777 (16)	0.0618 (7)	
H5	0.352714	0.528183	0.554331	0.074*	
C6	0.1692 (3)	0.5602 (2)	0.47376 (19)	0.0760 (8)	
H6	0.113043	0.519214	0.496946	0.091*	
C7	0.1087 (3)	0.6156 (2)	0.40530 (19)	0.0766 (8)	
H7	0.011395	0.611590	0.382979	0.092*	
C8	0.1887 (2)	0.67750 (18)	0.36838 (15)	0.0585 (6)	
C9	0.1192 (3)	0.7340 (2)	0.29122 (18)	0.0804 (8)	
H9A	0.019767	0.743510	0.288184	0.096*	
H9B	0.125079	0.692078	0.245566	0.096*	
C10	0.1588 (4)	0.9036 (3)	0.1761 (2)	0.1390 (16)	
H10A	0.209245	0.965751	0.172977	0.208*	
H10B	0.058954	0.915557	0.156109	0.208*	
H10C	0.187152	0.851655	0.144024	0.208*	
C11	0.1435 (3)	0.9572 (3)	0.3466 (2)	0.1177 (13)	
H11A	0.174468	0.936650	0.402202	0.177*	
H11B	0.042264	0.963050	0.330741	0.177*	
H11C	0.184829	1.022193	0.339953	0.177*	
C12	0.5024 (2)	0.88483 (16)	0.29121 (13)	0.0480 (5)	
C13	0.5465 (3)	0.84581 (19)	0.22820 (15)	0.0684 (7)	
H13	0.506983	0.785008	0.204275	0.082*	
C14	0.6496 (3)	0.8948 (2)	0.19860 (18)	0.0820 (9)	
H14	0.677997	0.866046	0.155836	0.098*	
C15	0.7083 (3)	0.9840 (2)	0.23209 (18)	0.0741 (8)	
H15	0.776477	1.016121	0.211939	0.089*	
C16	0.6667 (2)	1.02835 (18)	0.29737 (15)	0.0556 (6)	
C17	0.7270 (3)	1.1201 (2)	0.3343 (2)	0.0747 (8)	
H17	0.796146	1.152936	0.315451	0.090*	
C18	0.6855 (3)	1.1609 (2)	0.3966 (2)	0.0817 (8)	
H18	0.726806	1.221327	0.420416	0.098*	
C19	0.5817 (3)	1.11345 (19)	0.42555 (16)	0.0702 (7)	

H19	0.553016	1.142822	0.467961	0.084*	
C20	0.5221 (2)	1.02434 (17)	0.39214 (13)	0.0536 (6)	
H20	0.454311	0.992613	0.412859	0.064*	
C21	0.5612 (2)	0.97902 (16)	0.32639 (13)	0.0454 (5)	
C22	0.5840 (3)	0.7176 (2)	0.39466 (16)	0.0576 (6)	
C23	0.8087 (12)	0.7740 (13)	0.4996 (10)	0.101 (3)	0.445 (11)
H23A	0.844249	0.704576	0.500442	0.121*	0.445 (11)
H23B	0.817204	0.796147	0.554594	0.121*	0.445 (11)
C24	0.8871 (15)	0.8457 (13)	0.4572 (10)	0.143 (4)	0.555 (11)
H24A	0.862779	0.830092	0.400473	0.214*	0.555 (11)
H24B	0.987223	0.837422	0.479513	0.214*	0.555 (11)
H24C	0.861109	0.915184	0.464637	0.214*	0.555 (11)
C23A	0.8130 (9)	0.7548 (10)	0.4550 (9)	0.101 (3)	0.555 (11)
H23C	0.839613	0.688670	0.480229	0.121*	0.555 (11)
H23D	0.831899	0.755889	0.402343	0.121*	0.555 (11)
C24A	0.8855 (19)	0.8400 (16)	0.5071 (12)	0.143 (4)	0.445 (11)
H24D	0.855128	0.904124	0.480903	0.214*	0.445 (11)
H24E	0.986018	0.833151	0.515975	0.214*	0.445 (11)
H24F	0.862360	0.837720	0.557994	0.214*	0.445 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0569 (4)	0.0664 (5)	0.0688 (5)	−0.0029 (4)	−0.0025 (3)	0.0175 (4)
O1	0.1178 (17)	0.0744 (13)	0.1161 (17)	0.0434 (12)	0.0727 (14)	0.0215 (12)
O2	0.0432 (9)	0.0742 (13)	0.1242 (17)	0.0014 (9)	−0.0006 (10)	0.0113 (13)
C1	0.0577 (12)	0.0368 (11)	0.0410 (12)	−0.0052 (10)	0.0137 (10)	0.0001 (10)
C2	0.0500 (12)	0.0357 (11)	0.0403 (11)	−0.0018 (10)	0.0150 (9)	−0.0035 (10)
C3	0.0527 (12)	0.0345 (10)	0.0450 (12)	−0.0055 (10)	0.0172 (10)	−0.0056 (10)
C4	0.0584 (13)	0.0425 (12)	0.0517 (14)	−0.0019 (11)	0.0211 (11)	0.0013 (11)
C5	0.0782 (17)	0.0507 (14)	0.0620 (16)	−0.0047 (13)	0.0282 (14)	0.0082 (12)
C6	0.0823 (19)	0.0629 (17)	0.092 (2)	−0.0192 (15)	0.0395 (17)	0.0083 (16)
C7	0.0566 (15)	0.0706 (17)	0.100 (2)	−0.0222 (14)	0.0162 (15)	0.0036 (17)
C8	0.0569 (13)	0.0512 (13)	0.0629 (16)	−0.0152 (12)	0.0080 (12)	−0.0026 (12)
C9	0.0619 (15)	0.085 (2)	0.0791 (19)	−0.0241 (15)	−0.0075 (13)	0.0090 (17)
C10	0.115 (3)	0.174 (4)	0.101 (3)	−0.007 (3)	−0.017 (2)	0.077 (3)
C11	0.0648 (19)	0.107 (3)	0.177 (4)	0.0185 (19)	0.023 (2)	−0.015 (3)
C12	0.0583 (13)	0.0437 (12)	0.0452 (13)	0.0066 (11)	0.0193 (10)	0.0080 (11)
C13	0.102 (2)	0.0504 (14)	0.0643 (16)	0.0039 (14)	0.0426 (16)	0.0048 (13)
C14	0.117 (2)	0.0681 (18)	0.084 (2)	0.0192 (18)	0.0670 (19)	0.0151 (16)
C15	0.0771 (18)	0.0685 (18)	0.094 (2)	0.0139 (15)	0.0525 (17)	0.0324 (17)
C16	0.0522 (13)	0.0528 (14)	0.0653 (16)	0.0071 (12)	0.0216 (12)	0.0199 (13)
C17	0.0608 (16)	0.0620 (17)	0.102 (2)	−0.0156 (14)	0.0221 (16)	0.0156 (17)
C18	0.085 (2)	0.0609 (17)	0.093 (2)	−0.0248 (16)	0.0127 (17)	−0.0042 (17)
C19	0.0853 (18)	0.0589 (16)	0.0651 (17)	−0.0166 (15)	0.0175 (14)	−0.0089 (14)
C20	0.0617 (13)	0.0500 (13)	0.0501 (13)	−0.0084 (12)	0.0168 (11)	0.0024 (12)
C21	0.0453 (11)	0.0420 (12)	0.0490 (13)	0.0035 (10)	0.0126 (10)	0.0117 (10)
C22	0.0649 (15)	0.0490 (14)	0.0698 (17)	0.0099 (13)	0.0369 (14)	0.0225 (13)

C23	0.0436 (18)	0.111 (5)	0.143 (9)	0.006 (3)	0.016 (5)	0.006 (7)
C24	0.063 (2)	0.168 (5)	0.196 (14)	−0.014 (3)	0.032 (9)	0.021 (11)
C23A	0.0436 (18)	0.111 (5)	0.143 (9)	0.006 (3)	0.016 (5)	0.006 (7)
C24A	0.063 (2)	0.168 (5)	0.196 (14)	−0.014 (3)	0.032 (9)	0.021 (11)

Geometric parameters (Å, º)

Si1—C1	1.879 (2)	C12—C13	1.365 (3)
Si1—C9	1.853 (3)	C12—C21	1.423 (3)
Si1—C10	1.853 (3)	C13—H13	0.9300
Si1—C11	1.847 (3)	C13—C14	1.401 (3)
O1—C22	1.195 (3)	C14—H14	0.9300
O2—C22	1.320 (3)	C14—C15	1.358 (4)
O2—C23	1.493 (12)	C15—H15	0.9300
O2—C23A	1.526 (9)	C15—C16	1.414 (3)
C1—C2	1.340 (3)	C16—C17	1.409 (4)
C1—C12	1.498 (3)	C16—C21	1.416 (3)
C2—C3	1.487 (3)	C17—H17	0.9300
C2—C22	1.505 (3)	C17—C18	1.351 (4)
C3—C4	1.390 (3)	C18—H18	0.9300
C3—C8	1.401 (3)	C18—C19	1.391 (4)
C4—H4	0.9300	C19—H19	0.9300
C4—C5	1.374 (3)	C19—C20	1.359 (3)
C5—H5	0.9300	C20—H20	0.9300
C5—C6	1.362 (4)	C20—C21	1.415 (3)
C6—H6	0.9300	C23—H23A	0.9700
C6—C7	1.373 (4)	C23—H23B	0.9700
C7—H7	0.9300	C23—C24	1.516 (17)
C7—C8	1.391 (3)	C24—H24A	0.9600
C8—C9	1.511 (3)	C24—H24B	0.9600
C9—H9A	0.9700	C24—H24C	0.9600
C9—H9B	0.9700	C23A—H23C	0.9700
C10—H10A	0.9600	C23A—H23D	0.9700
C10—H10B	0.9600	C23A—C24A	1.484 (16)
C10—H10C	0.9600	C24A—H24D	0.9600
C11—H11A	0.9600	C24A—H24E	0.9600
C11—H11B	0.9600	C24A—H24F	0.9600
C11—H11C	0.9600		

C9—Si1—C1	100.76 (11)	C12—C13—C14	121.9 (3)
C9—Si1—C10	111.35 (17)	C14—C13—H13	119.1
C10—Si1—C1	110.16 (15)	C13—C14—H14	119.9
C11—Si1—C1	111.79 (12)	C15—C14—C13	120.3 (2)
C11—Si1—C9	111.38 (16)	C15—C14—H14	119.9
C11—Si1—C10	111.0 (2)	C14—C15—H15	119.7
C22—O2—C23	130.5 (7)	C14—C15—C16	120.5 (2)
C22—O2—C23A	105.0 (5)	C16—C15—H15	119.7
C2—C1—Si1	118.51 (15)	C15—C16—C21	118.9 (2)

C2—C1—C12	119.63 (19)	C17—C16—C15	122.0 (2)
C12—C1—Si1	121.48 (15)	C17—C16—C21	119.1 (2)
C1—C2—C3	126.47 (19)	C16—C17—H17	119.6
C1—C2—C22	118.28 (18)	C18—C17—C16	120.9 (2)
C3—C2—C22	115.25 (18)	C18—C17—H17	119.6
C4—C3—C2	118.63 (19)	C17—C18—H18	119.7
C4—C3—C8	118.6 (2)	C17—C18—C19	120.6 (3)
C8—C3—C2	122.8 (2)	C19—C18—H18	119.7
C3—C4—H4	119.0	C18—C19—H19	119.8
C5—C4—C3	122.0 (2)	C20—C19—C18	120.3 (3)
C5—C4—H4	119.0	C20—C19—H19	119.8
C4—C5—H5	120.4	C19—C20—H20	119.4
C6—C5—C4	119.2 (2)	C19—C20—C21	121.1 (2)
C6—C5—H5	120.4	C21—C20—H20	119.4
C5—C6—H6	119.9	C16—C21—C12	119.7 (2)
C5—C6—C7	120.1 (2)	C20—C21—C12	122.32 (19)
C7—C6—H6	119.9	C20—C21—C16	117.9 (2)
C6—C7—H7	119.1	O1—C22—O2	124.8 (3)
C6—C7—C8	121.9 (2)	O1—C22—C2	124.0 (3)
C8—C7—H7	119.1	O2—C22—C2	111.2 (2)
C3—C8—C9	121.5 (2)	O2—C23—H23A	111.1
C7—C8—C3	118.1 (2)	O2—C23—H23B	111.1
C7—C8—C9	120.4 (2)	O2—C23—C24	103.5 (10)
Si1—C9—H9A	108.8	H23A—C23—H23B	109.0
Si1—C9—H9B	108.8	C24—C23—H23A	111.1
C8—C9—Si1	113.76 (17)	C24—C23—H23B	111.1
C8—C9—H9A	108.8	C23—C24—H24A	109.5
C8—C9—H9B	108.8	C23—C24—H24B	109.5
H9A—C9—H9B	107.7	C23—C24—H24C	109.5
Si1—C10—H10A	109.5	H24A—C24—H24B	109.5
Si1—C10—H10B	109.5	H24A—C24—H24C	109.5
Si1—C10—H10C	109.5	H24B—C24—H24C	109.5
H10A—C10—H10B	109.5	O2—C23A—H23C	111.7
H10A—C10—H10C	109.5	O2—C23A—H23D	111.7
H10B—C10—H10C	109.5	H23C—C23A—H23D	109.5
Si1—C11—H11A	109.5	C24A—C23A—O2	100.3 (10)
Si1—C11—H11B	109.5	C24A—C23A—H23C	111.7
Si1—C11—H11C	109.5	C24A—C23A—H23D	111.7
H11A—C11—H11B	109.5	C23A—C24A—H24D	109.5
H11A—C11—H11C	109.5	C23A—C24A—H24E	109.5
H11B—C11—H11C	109.5	C23A—C24A—H24F	109.5
C13—C12—C1	119.8 (2)	H24D—C24A—H24E	109.5
C13—C12—C21	118.7 (2)	H24D—C24A—H24F	109.5
C21—C12—C1	121.43 (18)	H24E—C24A—H24F	109.5
C12—C13—H13	119.1		

Si1—C1—C2—C3	−5.4 (3)	C10—Si1—C9—C8	158.9 (2)
Si1—C1—C2—C22	174.72 (17)	C11—Si1—C1—C2	94.9 (2)

Si1—C1—C12—C13	−93.6 (2)	C11—Si1—C1—C12	−92.2 (2)
Si1—C1—C12—C21	85.7 (2)	C11—Si1—C9—C8	−76.6 (2)
C1—Si1—C9—C8	42.1 (2)	C12—C1—C2—C3	−178.53 (19)
C1—C2—C3—C4	−158.4 (2)	C12—C1—C2—C22	1.6 (3)
C1—C2—C3—C8	21.3 (3)	C12—C13—C14—C15	−0.4 (4)
C1—C2—C22—O1	−104.5 (3)	C13—C12—C21—C16	−2.0 (3)
C1—C2—C22—O2	75.1 (3)	C13—C12—C21—C20	−179.6 (2)
C1—C12—C13—C14	−179.5 (2)	C13—C14—C15—C16	0.3 (4)
C1—C12—C21—C16	178.78 (19)	C14—C15—C16—C17	179.1 (3)
C1—C12—C21—C20	1.2 (3)	C14—C15—C16—C21	−1.0 (4)
C2—C1—C12—C13	79.3 (3)	C15—C16—C17—C18	−179.9 (3)
C2—C1—C12—C21	−101.5 (2)	C15—C16—C21—C12	1.8 (3)
C2—C3—C4—C5	178.90 (19)	C15—C16—C21—C20	179.5 (2)
C2—C3—C8—C7	−179.0 (2)	C16—C17—C18—C19	−0.3 (4)
C2—C3—C8—C9	3.0 (4)	C17—C16—C21—C12	−178.2 (2)
C3—C2—C22—O1	75.7 (3)	C17—C16—C21—C20	−0.5 (3)
C3—C2—C22—O2	−104.8 (2)	C17—C18—C19—C20	1.0 (4)
C3—C4—C5—C6	0.7 (4)	C18—C19—C20—C21	−1.4 (4)
C3—C8—C9—Si1	−36.2 (3)	C19—C20—C21—C12	178.8 (2)
C4—C3—C8—C7	0.7 (3)	C19—C20—C21—C16	1.2 (3)
C4—C3—C8—C9	−177.3 (2)	C21—C12—C13—C14	1.3 (4)
C4—C5—C6—C7	−0.4 (4)	C21—C16—C17—C18	0.1 (4)
C5—C6—C7—C8	0.3 (4)	C22—O2—C23—C24	101.7 (10)
C6—C7—C8—C3	−0.5 (4)	C22—O2—C23A—C24A	171.2 (8)
C6—C7—C8—C9	177.5 (3)	C22—C2—C3—C4	21.4 (3)
C7—C8—C9—Si1	145.8 (2)	C22—C2—C3—C8	−158.9 (2)
C8—C3—C4—C5	−0.8 (3)	C23—O2—C22—O1	−9.8 (9)
C9—Si1—C1—C2	−23.5 (2)	C23—O2—C22—C2	170.7 (8)
C9—Si1—C1—C12	149.41 (18)	C23A—O2—C22—O1	11.2 (6)
C10—Si1—C1—C2	−141.2 (2)	C23A—O2—C22—C2	−168.3 (6)
C10—Si1—C1—C12	31.7 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···O1^{i}	0.93	2.49	3.359 (4)	156

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