Crystal structure and Hirshfeld surface analysis of
$N$-[[Diphenyl(vinyl)silyl]methyl]-2-methylpropan-2-amine chloride

Christoph Schwab, Andreas Voss and Carsten Strohmann*

TU Dortmund University, Faculty of Chemistry and Chemical Biology, Otto-Hahn-Str. 6, 44227 Dortmund, Germany.

*Correspondence e-mail: carsten.strohmann@tu-dortmund.de

$N$-[[Diphenyl(vinyl)silyl]methyl]-2-methylpropan-2-amine, $C_{19}H_{25}NSi$, is a newly synthesized secondary aminomethylsilane that can be used, for example, to study carbolithiation reactions of vinylsilanes. Because the neutral compound did not crystallize well, the hydrochloride salt, $C_{19}H_{26}NSi^+\cdot Cl^-$, was formed, in which the two chloride ions in the asymmetric unit have crystallographic $1$ site symmetry. An unusually long Si—C bond of 1.9117 (10) Å is observed in the cation, which may be ascribed to electronic effects due to the $N^+$ species. In the crystal, the cations and anions are linked by $N$—H/Cl hydrogen bonds to generate [001] chains. To further investigate the intermolecular interactions, a Hirshfeld surface analysis was performed, which showed that $H$—$H$, $C$—$H$ and $H$—$Cl$ contacts contribute 70.4, 20.0 and 8.3%, respectively.

1. Chemical context

There are only a few secondary (aminomethyl)silanes known to date because the synthesis is not feasible due to the high energy requirement and reaction time. With the assistance of a Finkelstein reaction, the iodomethylsilane can be synthesized to enhance the reactivity and shorten the reaction time (Finkelstein et al., 1910; Abele & Strohmann, 1997). However, it was possible to synthesize the (aminomethyl)diphenylvinylsilane 1 in an efficient way, starting from a (chloro-methyl)silane. Because the (aminomethyl)silane 1 did not crystallize well, the hydrochloride salt 2 was formed to characterize the compound via X-ray diffraction. For example, the newly synthesized (aminomethyl)vinylsilane 1, $C_{19}H_{25}NSi$, can be used for investigations of a carbolithiation reaction of the silane’s vinyl group via lithiumalkyls. The received product can be used for the synthesis of functionalized alcohols by a Tamao oxidation (Tamao et al., 1983). The molecular structure is defined by an unusually long Si—C bond, which thus favors the cleavage of this bond. Usually, the aminomethyl sidearm contains two or three nitrogen centers and is essential for the feasibility of the reaction. It helps to break down the lithiumalkyl aggregates by forming a dative bond and also precoordinates the lithium ions, so they are in proximity to the vinyl group of the silane. Our own studies have shown that this stabilizes the transition state of the reaction, hence the activation energy of the deprotonation of the vinyl group is minimized and the reaction can be done under low temperatures and kinetic control, to prevent side reactions such as the $\alpha$-deprotonation or polymerization (Unkelbach & Strohmann, 2009). This new (aminomethyl)silane 1 contains only one nitrogen center in the sidearm and undergoes the carbolit-
thiation by a new mechanism for vinylsilanes. This mechanism is known from stilbenes, where two lithium cations stabilize the negative charge at the anionic carbon atom. With the use of chiral ligands, the reaction can be performed under stereogenic control (Tricotet et al., 2009). This opens a new field for interesting research in organosilicon chemistry.

2. Structural commentary

Compound 2 crystallized in a few minutes from an aqueous 1 M HCl solution of 1 at room temperature as a hydrochloride salt, C_{19}H_{26}NSi+Cl−, in the form of colorless needles in the centrosymmetric space group P2_1/n. The molecular structure is illustrated in Fig. 1. Both chloride ions are located on special positions with 1 site symmetry.

The Si1—C15 bond length in the cation is 1.9117 (10) Å, which is slightly longer than the average for an Si—C bond and the Si1—C15—N1 bond angle is 116.21 (7)°. The Si—C bond lengths are normally in the range of 1.857 to 1.905 Å for Csp^3—SiX$_3$ compounds (Allen et al., 1987). The extended bond length may be ascribed to the cationic nitrogen atom in the β-position to the silicon atom. It increases the electronegativity, which enhances the electron-withdrawing effect of the substituted α-aminofunctionality. This enhances the p-character of the Si1—C15 bond, which leads to an elongated bond (Bent, 1961). The extended Si1—C15—N1 bond angle is due to the steric demand of the tert-butyl group. Some further examples are given in the Database survey section (Kirchoff et al., 2022). The angle between the C3–C8 and C9–C14 phenyl groups in 2 is 89.63 (2)°, which is caused by the steric repulsion of the aromatic hydrogen atoms. The Si1—C1 bond length is 1.8577 (11) Å and C1—C2 is 1.3293 (16) Å; the latter is positioned at the end of the default range of Csp^3—Csp^2 bonds, which lie between 1.299 and 1.328 Å.

The cationic nitrogen center features a slightly disordered tetrahedral geometry. The angle between the hydrogen atoms is 107.2 (13)° (H1A—N1—H1B), the angles between the C atoms and the H atoms are 107.8 (10)° (H1B—N1—C15) and 109.6 (9)° (H1A—N1—C15). Between the carbon atoms, the angle is 117.10 (7)° (C15—N1—C16). All angles vary slightly from the ideal tetrahedron angles of 109.5°: the large C—N—C angle results from the bigger space requirement of the carbon atoms in comparison to the H atoms. The sum of angles around the nitrogen atom is 441.7°, so the overall structure is distorted tetrahedral. The bond length between N1 and C15 is 1.4928 (12) Å and it is 1.5330 (13) Å between N1 and C16. In the literature, Csp^3—N bond lengths are in the range of 1.4816 to 1.5034 Å, so the N1—C16 bond is slightly extended.

3. Supramolecular features

In the extended structure of 2 (Fig. 2), the cations and anions are linked by N···H···Cl hydrogen bonds (Table 1) to generate chains propagating in the [001] direction. The N···Cl
separation of 3.1184 (8) Å for the N1—H1B···Cl2 hydrogen bond is slightly longer than that for N1—H1A···Cl1 at 3.0968 (8) Å. This may be due to the different surroundings of the Cl1 and Cl2 ions in the crystal. As shown in Fig. 3, Cl1 accepts two weak, near linear hydrogen-bond contacts [C6—H6···Cl1: 165.82 (7)°] from the aromatic para-hydrogen atoms H6 with a C6···Cl1 distance of 4.0013 (11) Å while Cl2 accepts two weak, near linear hydrogen-bond contacts [C7—H7···Cl2: 165.74 (7)°] from the aromatic meta-hydrogen atoms H7 with a C7···Cl2 distance of 3.9419 (12) Å. Both contacts are formed by the same aromatic ring. The bond angle for N1—H1B···Cl2 is 164.0 (13)°, compared to 172.8 (13)° for N1—H1A···Cl1. They differ from the optimal angle of 180° because of the different surroundings in the crystal packing.

To further analyze the supramolecular packing interactions, a Hirshfeld surface analysis was performed (Spackman & Jayatilaka, 2009). The Hirshfeld surface of the cation mapped over \( d_{	ext{norm}} \) in the range from 0.54 to 1.49 arbitrary units, generated by CrystalExplorer2021 (Spackman et al., 2021; Turner et al., 2017), is shown in Fig. 4. The fingerprint plots are illustrated in Fig. 5 and were also generated by CrystalExplorer2021. Particularly noticeable on the Hirshfeld surface are the short N—H···Cl contacts, which are shown in red on the potential surface, see Fig. 4. Although they represent the smallest fraction of interactions (8.3%), they presumably have the greatest effect on the crystal structure. The H···H contacts (70.4%) are the biggest fraction, but play a minor role in terms of the crystal packing. Analysis of the hydrogen-bonding network leads to the result that H1 can be assigned the graph-set symbols \( D_1^1(2) \) and \( D_1^2(3) \), which means that the hydrogen bond extends from N1—H1A···Cl1 to another H1A···N1 grouping of a neighboring molecule. H2 can also be assigned \( D_1^1(2) \) and \( D_1^2(3) \) (Etter et al., 1990). Here, the hydrogen bond extends from N1—H1B···Cl2 to another H1B···N1 group of a neighboring molecule. These hydrogen bonds may be the reason why 2 crystallizes well compared to the neutral molecule 1.

### Table 1: Hydrogen-bond geometry (Å, °)

|      | D—H ·· A | D—H | H ·· A | D···A | D—H ·· A |
|------|----------|------|--------|-------|----------|
| N1—H1A···Cl1 | 0.923 (15) | 2.179 (15) | 3.0968 (8) | 172.8 (13) | 164.0 (13) |
| N1—H1B···Cl2 | 0.912 (15) | 2.231 (15) | 3.1184 (8) | 164.0 (13) | 172.8 (13) |

Figure 3
The crystal packing of compound 2 showing the C—H···Cl contacts.

Figure 4
The Hirshfeld surface of compound 2 generated by CrystalExplorer21.

Figure 5
Two-dimensional fingerprint plots of compound 2 showing (a) all contributions in the crystal and those delineated into (b) H···H, (c) C···H/H···C (d) Cl···H/H···Cl interactions.
4. Database survey

There are examples of crystallographically characterized structures with motifs like those in compound 2. The following examples were found in the Cambridge Structural Database (WebCSD, May 2022; Groom et al., 2016): 3,3-dimethyl-1-(4-methylbenzene-1-sulfonfyl)-5-phenyl-1,2,3,6-tetrahydro-1,3-azasiline, C_{19}H_{20}NO_{3}Si (CSD refcode AZAFOZ; Wang et al., 2021), (S,S)-2-methoxyethyl-1-[1-phenylethyl(dimethyl)silylmethyl]pyrrolidinium iodide, C_{17}H_{30}NOSi+ (DAFKUT; Otte et al., 2020), iron(II) tetrafluoroborate, C_{40}H_{37}FeNOPSi+. (AGILLIL; Strohmann et al., 2002), [3-(diphenylphosphino)amino(triphenylsilylmethylidene)carbonyl(η⁵-cyclopentadienyl)-iron(II) tetrafluoroborate, C_{40}H_{37}FeNOPSi+. (BF4-) (AMINO; Yu et al., 2010), 2-(triphenylsilyl)pyrrolidin-1-ium chloride methanol solvate, C_{12}H_{24}NSi+·CH_{3}O·Cl- (LAGLUE; Bauer & Strohmann, 2017), 1-[(benzyldimethylsilyl)methyl]-1-ethylpyrroliperidin-1-ium ethansulfonate, C_{17}H_{20}NSi-·C_{2}H_{4}O_{3}S- (WAVXAW; Kirchhoff et al., 2022), 2-[ethenyl(dimethyl)silyl]-1-[(4-nitrophenyl)sulfonyl]aziridine, C_{13}H_{10}N_{2}O_{3}S_{2} (WOLSEY; Astakhova et al., 2019) and 1-[(benzyldimethylsilyl)methyl]-1-methylpyrroliperidin-1-ium iodide, C_{16}H_{24}NSi (DAFKUT; Otte et al., 2017).

In LAGLUE, the N–H...Cl hydrogen bond has a slightly longer N...Cl separation (3.124 Å) than compound 2. The Si–C bond is shorter [1.907 (5) Å] and the Si–C–N bond angle is marginally shorter [114.9 (7)°] than in compound 2, which is caused by the cyclic structure of the aziridine ring and the electron-withdrawing effect of the (nitrophenyl)sulfonyl group located at the nitrogen center. In addition, the Si–C bond lengths are 1.9074 (11) and the Si–C–N bond angle is slightly shorter [114.9 (7)°] than in compound 2, which is caused by the cyclic structure of the aziridine ring and the electron-withdrawing effect of the (nitrophenyl)sulfonyl group located at the nitrogen center.
Etter, M. C., MacDonald, J. C. & Bernstein, J. (1990). *Acta Cryst.* **B46**, 256–262.

Finkelstein, H. (1910). *Ber. Dtsch. Chem. Ges.* **43**, 1528–1532.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.

Kirchhoff, J.-L., Koller, S. G., Louven, K. & Strohmann, C. (2022). *Acta Cryst.* **E78**, 135–139.

Otte, F., Koller, S. G., Cuellar, E., Golz, C. & Strohmann, C. (2017). *Inorg. Chem. Acta*. **456**, 44–48.

Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.

Spackman, M. A. & Jayatilaka, D. (2009). *CrystEngComm*. **11**, 19–32.

Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.

Strohmann, C., Lehmen, K., Wild, K. & Schildbach, D. (2002). *Organometallics*. **21**, 3079–3081.

Tamao, K., Ishida, N., Tanaka, T. & Kumada, M. (1983). *Organometallics*. **2**, 1694–1696.

Tricotet, T., Fleming, P., Cotter, J., Hogan, A. L., Strohmann, C., Gessner, V. H. & O’Shea, D. F. (2009). *J. Am. Chem. Soc.* **131**, 3142–3143.

Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Spackmann, P. R., Jayatilaka, D. & Spackman, M. A. (2017). *CrystalExplorer17*, University of Western Australia.

Unkelbach, C. & Strohmann, C. (2009). *J. Am. Chem. Soc.* **131**, 17044–17045.

Wang, W., Zhou, S., Li, L., He, Y., Dong, X., Gao, L., Wang, Q. & Song, Z. (2021). *J. Am. Chem. Soc.* **143**, 11141–11151.

Yu, I., Wallis, C. J., Patrick, B. O., Diaconescu, P. L. & Mehrkhodavandi, P. (2010). *Organometallics*. **29**, 6065–6076.
supporting information

*Acta Cryst.* (2022). E78, 1039-1043  
[https://doi.org/10.1107/S2056989022009112](https://doi.org/10.1107/S2056989022009112)

Crystal structure and Hirshfeld surface analysis of \(N\)-[[diphenyl(vinyl)-silyl]methyl]-2-methylpropan-2-ammonium chloride

Christoph Schwab, Andreas Voss and Carsten Strohmann

Computing details

Data collection: *APEX2* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: *olex2.solve* (Bourhis et al., 2015); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov et al., 2009); software used to prepare material for publication: *OLEX2* (Dolomanov et al., 2009).

tert-Butyl[[ethenyldiphenylsilyl]methyl]azanium chloride

Crystal data

\[
\begin{align*}
C_{19}H_{26}NSi^+ \cdot Cl^- & \quad F(000) = 712 \\
M_r & = 331.95 \\
Monoclinic, P2_1/n & \quad D_x = 1.162 \text{ Mg m}^{-3} \\
a = 9.7320 (11) \AA & \quad \text{Mo } K\alpha \text{ radiation, } \lambda = 0.71073 \text{ Å} \\
b = 19.0598 (15) \AA & \quad \text{Cell parameters from 1675 reflections} \\
c = 10.9186 (10) \AA & \quad \theta = 2.3 - 26.3^\circ \\
\beta = 110.526 (4)^\circ & \quad \mu = 0.26 \text{ mm}^{-1} \\
V = 1896.7 (3) \text{ Å}^3 & \quad T = 100 \text{ K} \\
Z = 4 & \quad \text{Block, colourless} \\
\end{align*}
\]

Data collection

| 7200 independent reflections |
|-----------------------------|
| 5850 reflections with \( I > 2\sigma(I) \) |
| \( \theta_{\text{min}} = 0.045 \) |
| \( \theta_{\text{max}} = 33.1^\circ \) |
| \( h = -14 \rightarrow 13 \) |
| \( k = -29 \rightarrow 29 \) |
| \( l = -16 \rightarrow 16 \) |
| 58662 measured reflections |

Refinement

| Hydrogen site location: mixed |
|-----------------------------|
| H atoms treated by a mixture of independent and constrained refinement |
| \( w = 1/\left[ \sigma^2(F^2) + (0.0302P)^2 + 0.8457P \right] \) |
| where \( P = (F^2 + 2F_c^2)/3 \) |
| \( (\Delta/\sigma)_{\text{max}} = 0.001 \) |
| \( \Delta P_{\text{max}} = 0.38 \text{ e Å}^{-3} \) |
| \( \Delta P_{\text{min}} = -0.25 \text{ e Å}^{-3} \) |
**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     | Uiso*/Ueq |
|----|-------|-------|-------|-----------|
| Cl1| 0.500 | 0.500 | 0.500 | 0.02034 (7) |
| Cl2| 0.500 | 0.500 | 0.000 | 0.03673 (12) |
| Si1| 0.7004 (3) | 0.35895 (2) | 0.32477 (3) | 0.01456 (6) |
| N1 | 0.42114 (9) | 0.43180 (4) | 0.22648 (7) | 0.01257 (14) |
| H1A| 0.4520 (16) | 0.4537 (8) | 0.3070 (14) | 0.023 (4)* |
| H1B| 0.4530 (17) | 0.4584 (8) | 0.1722 (15) | 0.027 (4)* |
| C1 | 0.78182 (12) | 0.44067 (6) | 0.28760 (11) | 0.0215 (2) |
| H1 | 0.7881 | 0.4451 | 0.2031 | 0.026* |
| C2 | 0.83213 (14) | 0.49340 (6) | 0.37106 (14) | 0.0298 (3) |
| H2A| 0.8276 | 0.4908 | 0.4564 | 0.036* |
| H2B| 0.8726 | 0.5337 | 0.3453 | 0.036* |
| C3 | 0.75986 (11) | 0.28120 (5) | 0.25064 (10) | 0.01589 (17) |
| C4 | 0.72391 (13) | 0.27683 (6) | 0.11477 (11) | 0.0212 (2) |
| H4 | 0.6756 | 0.3151 | 0.0612 | 0.025* |
| C5 | 0.75786 (14) | 0.21724 (6) | 0.05711 (11) | 0.0249 (2) |
| H5 | 0.7325 | 0.2152 | −0.0351 | 0.030* |
| C6 | 0.82860 (13) | 0.16072 (6) | 0.13383 (12) | 0.0237 (2) |
| H6 | 0.8505 | 0.1199 | 0.0941 | 0.028* |
| C7 | 0.86709 (13) | 0.16410 (6) | 0.26881 (12) | 0.0225 (2) |
| H7 | 0.9162 | 0.1258 | 0.3218 | 0.027* |
| C8 | 0.83342 (12) | 0.22401 (5) | 0.32627 (10) | 0.01833 (18) |
| H8 | 0.8609 | 0.2261 | 0.4187 | 0.022* |
| C9 | 0.75476 (11) | 0.34357 (5) | 0.50486 (10) | 0.01573 (17) |
| C10| 0.90359 (11) | 0.34952 (5) | 0.58312 (10) | 0.01859 (18) |
| H10| 0.9723 | 0.3637 | 0.5441 | 0.022* |
| C11| 0.95274 (12) | 0.33515 (6) | 0.71661 (11) | 0.0212 (2) |
| H11| 1.0538 | 0.3399 | 0.7678 | 0.025* |
| C12| 0.85334 (13) | 0.31377 (6) | 0.77462 (11) | 0.0222 (2) |
| H12| 0.8863 | 0.3038 | 0.8656 | 0.027* |
| C13| 0.70528 (13) | 0.30706 (6) | 0.69892 (11) | 0.0221 (2) |
| H13| 0.6372 | 0.2924 | 0.7383 | 0.027* |
| C14| 0.65699 (12) | 0.32180 (5) | 0.56568 (11) | 0.01951 (19) |
| H14| 0.5558 | 0.3170 | 0.5150 | 0.023* |
| C15| 0.49188 (11) | 0.36139 (5) | 0.23862 (10) | 0.01691 (17) |
| H15A| 0.4685 | 0.3417 | 0.1497 | 0.020* |
| H15B| 0.4470 | 0.3301 | 0.2866 | 0.020* |
| C16| 0.25301 (11) | 0.43398 (5) | 0.17306 (9) | 0.01689 (17) |
| C17| 0.19498 (13) | 0.39711 (7) | 0.26910 (11) | 0.0244 (2) |
| H17A| 0.2192 | 0.3471 | 0.2726 | 0.037* |
### Atomic displacement parameters (Å²)

| Atom | U¹¹ | U²² | U³³ | U¹² | U¹³ | U²³ |
|------|-----|-----|-----|-----|-----|-----|
| Cl1  | 0.02810 (18) | 0.01878 (15) | 0.01229 (13) | −0.00014 (13) | 0.00477 (12) | −0.00446 (11) |
| Cl2  | 0.0490 (3) | 0.0444 (3) | 0.01419 (15) | −0.0234 (2) | 0.00777 (16) | 0.00500 (15) |
| Si1  | 0.01262 (12) | 0.01221 (11) | 0.01785 (12) | −0.00029 (9) | 0.00410 (9) | −0.00132 (9) |
| N1   | 0.01950 (4) | 0.00115 (3) | 0.00101 (3) | 0.00129 (3) | 0.0030 (3) | 0.00096 (2) |
| C1   | 0.0188 (5) | 0.00170 (4) | 0.0285 (5) | −0.0015 (4) | 0.0080 (4) | 0.0023 (4) |
| C2   | 0.0261 (6) | 0.00172 (5) | 0.00144 (7) | −0.00045 (4) | 0.0058 (5) | −0.0013 (5) |
| C3   | 0.0149 (4) | 0.00143 (4) | 0.00196 (4) | −0.00002 (3) | 0.0074 (3) | −0.0010 (3) |
| C4   | 0.0247 (5) | 0.00187 (4) | 0.00214 (5) | 0.0008 (4) | 0.0096 (4) | 0.0005 (4) |
| C5   | 0.0305 (6) | 0.00249 (5) | 0.00231 (5) | −0.0014 (4) | 0.0143 (5) | −0.0046 (4) |
| C6   | 0.0249 (5) | 0.00189 (5) | 0.0326 (6) | −0.0011 (4) | 0.0168 (5) | −0.0067 (4) |
| C7   | 0.0215 (5) | 0.00171 (4) | 0.0312 (5) | 0.0039 (4) | 0.0121 (4) | 0.0006 (4) |
| C8   | 0.0173 (5) | 0.00171 (4) | 0.0212 (4) | 0.0021 (3) | 0.0075 (4) | 0.0002 (3) |
| C9   | 0.0136 (4) | 0.00136 (4) | 0.00191 (4) | 0.0010 (3) | 0.0046 (3) | −0.0027 (3) |
| C10  | 0.0147 (4) | 0.00181 (4) | 0.0221 (5) | 0.0003 (4) | 0.0012 (4) | −0.0030 (4) |
| C11  | 0.0184 (5) | 0.00183 (4) | 0.0222 (5) | 0.0003 (4) | 0.0012 (4) | −0.0030 (4) |
| C12  | 0.0276 (6) | 0.00163 (4) | 0.0201 (5) | 0.0059 (4) | 0.0052 (4) | 0.0005 (4) |
| C13  | 0.0233 (5) | 0.00193 (5) | 0.0255 (5) | 0.0031 (4) | 0.0107 (4) | 0.0040 (4) |
| C14  | 0.0161 (5) | 0.00182 (4) | 0.0240 (5) | 0.0010 (3) | 0.0067 (4) | 0.0009 (4) |
| C15  | 0.0142 (4) | 0.00114 (4) | 0.0221 (4) | 0.0009 (3) | 0.0026 (3) | −0.0024 (3) |
| C16  | 0.0148 (4) | 0.00166 (4) | 0.0155 (4) | 0.0040 (3) | 0.0006 (3) | −0.0014 (3) |
| C17  | 0.0187 (5) | 0.00310 (6) | 0.0255 (5) | −0.0009 (4) | 0.0100 (4) | −0.0024 (4) |
| C18  | 0.0294 (6) | 0.00188 (5) | 0.0300 (6) | 0.0112 (4) | −0.0015 (5) | −0.0022 (4) |
| C19  | 0.0223 (5) | 0.0231 (5) | 0.0164 (4) | 0.0014 (4) | −0.0024 (4) | −0.0034 (4) |

### Geometric parameters (Å, °)

| Bond                  | Length (Å) | Angle (°)  |
|----------------------|------------|------------|
| Si1—C1               | 1.8577 (11) | C9—C14     | 1.4006 (14) |
| Si1—C3               | 1.8763 (10) | C10—H10    | 0.9500     |
| Si1—C9               | 1.8713 (10) | C10—C11    | 1.3926 (15) |
| Si1—C15              | 1.9117 (10) | C11—H11    | 0.9500     |
| N1—H1A               | 0.923 (15)  | C11—C12    | 1.3902 (17) |
| N1—H1B               | 0.912 (15)  | C12—H12    | 0.9500     |
| N1—C15               | 1.4928 (12) | C12—C13    | 1.3931 (17) |
| N1—C16               | 1.5330 (13) | C13—H13    | 0.9500     |
| Bond          | Distance (A) | Bond          | Distance (A) |
|---------------|--------------|---------------|--------------|
| C1—H1         | 0.9500       | C13—C14       | 1.3917 (15)  |
| C1—C2         | 1.3293 (16)  | C14—H14       | 0.9500       |
| C2—H2A        | 0.9500       | C15—H15A      | 0.9900       |
| C2—H2B        | 0.9500       | C15—H15B      | 0.9900       |
| C3—C4         | 1.4022 (15)  | C16—C17       | 1.5256 (15)  |
| C3—C8         | 1.4028 (14)  | C16—C18       | 1.5281 (15)  |
| C4—H4         | 0.9500       | C16—C19       | 1.5260 (14)  |
| C4—C5         | 1.3933 (15)  | C17—H17A      | 0.9800       |
| C5—H5         | 0.9500       | C17—H17B      | 0.9800       |
| C5—C6         | 1.3899 (17)  | C17—H17C      | 0.9800       |
| C6—H6         | 0.9500       | C18—H18A      | 0.9800       |
| C6—C7         | 1.3890 (17)  | C18—H18B      | 0.9800       |
| C7—H7         | 0.9500       | C18—H18C      | 0.9800       |
| C7—C8         | 1.3961 (14)  | C19—H19A      | 0.9800       |
| C8—H8         | 0.9500       | C19—H19B      | 0.9800       |
| C9—C10        | 1.4047 (14)  | C19—H19C      | 0.9800       |

| Bond          | Angle (deg)  | Bond          | Angle (deg)  |
|---------------|--------------|---------------|--------------|
| C1—Si1—C3    | 110.28 (5)   | C10—C11—H11  | 120.1        |
| C1—Si1—C9    | 112.03 (5)   | C12—C11—C10  | 119.74 (10)  |
| C1—Si1—C15   | 109.47 (5)   | C12—C11—H11  | 120.1        |
| C3—Si1—C15   | 104.04 (4)   | C11—C12—H12  | 120.1        |
| C9—Si1—C3    | 108.21 (4)   | C11—C12—C13  | 119.79 (10)  |
| C9—Si1—C15   | 112.51 (5)   | C13—C12—H12  | 120.1        |
| H1A—N1—H1B   | 107.2 (13)   | C12—C13—H13  | 119.9        |
| C15—N1—H1A   | 109.6 (9)    | C14—C13—C12  | 120.10 (10)  |
| C15—N1—H1B   | 107.8 (10)   | C14—C13—H13  | 119.9        |
| C15—N1—C16   | 117.10 (7)   | C9—C14—H14   | 119.4        |
| C16—N1—H1A   | 107.3 (9)    | C13—C14—C9   | 121.26 (10)  |
| C16—N1—H1B   | 107.4 (10)   | C13—C14—H14  | 119.4        |
| Si1—C1—H1    | 117.7        | Si1—C15—H15A | 108.2        |
| C2—C1—Si1    | 124.56 (10)  | Si1—C15—H15B | 108.2        |
| C2—C1—H1     | 117.7        | N1—C15—Si1   | 116.21 (7)   |
| C1—C2—H2A    | 120.0        | N1—C15—H15A  | 108.2        |
| C1—C2—H2B    | 120.0        | N1—C15—H15B  | 108.2        |
| H2A—C2—H2B   | 120.0        | H15A—C15—H15B| 107.4        |
| C4—C3—Si1    | 120.21 (8)   | C17—C16—N1   | 109.21 (8)   |
| C4—C3—C8     | 117.59 (9)   | C17—C16—C18  | 110.46 (10)  |
| C8—C3—Si1    | 122.09 (8)   | C17—C16—C19  | 111.00 (9)   |
| C3—C4—H4     | 119.5        | C18—C16—N1   | 105.20 (9)   |
| C5—C4—C3     | 121.04 (10)  | C19—C16—N1   | 109.50 (8)   |
| C5—C4—H4     | 119.5        | C19—C16—C18  | 111.30 (9)   |
| C4—C5—H5     | 119.8        | C16—C17—H17A | 109.5        |
| C6—C5—C4     | 120.35 (10)  | C16—C17—H17B | 109.5        |
| C6—C5—H5     | 119.8        | C16—C17—H17C | 109.5        |
| C5—C6—H6     | 120.1        | H17A—C17—H17B| 109.5        |
| C7—C6—C5     | 119.72 (10)  | H17A—C17—H17C| 109.5        |
| C7—C6—H6     | 120.1        | H17B—C17—H17C| 109.5        |
| C6—C7—H7     | 120.1        | C16—C18—H18A | 109.5        |
C6—C7—C8 119.76 (10) C16—C18—H18B 109.5
C8—C7—H7 120.1 C16—C18—H18C 109.5
C3—C8—H8 119.2 H18A—C18—H18B 109.5
C7—C8—C3 121.52 (10) H18A—C18—H18C 109.5
C7—C8—H8 119.2 H18B—C18—H18C 109.5
C10—C9—Si1 118.64 (8) C16—C19—H19A 109.5
C14—C9—Si1 123.67 (8) C16—C19—H19B 109.5
C14—C9—C10 117.55 (9) C16—C19—H19C 109.5
C9—C10—H10 119.2 H19A—C19—H19B 109.5
C11—C10—C9 121.55 (10) H19A—C19—H19C 109.5
C11—C10—H10 119.2 H19B—C19—H19C 109.5

Si1—C3—C4—C5 −175.22 (9) C9—Si1—C3—C4 175.80 (8)
Si1—C3—C8—C7 174.88 (8) C9—Si1—C3—C8 −0.37 (10)
Si1—C9—C10—C11 −176.56 (8) C9—C10—C11—C12 0.57 (16)
Si1—C9—C14—C13 176.07 (8) C10—C9—C14—C13 0.42 (15)
C1—Si1—C3—C4 −61.36 (10) C10—C11—C12—C13 −0.17 (16)
C1—Si1—C3—C8 122.47 (9) C11—C12—C13—C14 −0.10 (16)
C1—Si1—C9—C10 −141.05 (11) C12—C13—C14—C9 −0.04 (16)
C1—Si1—C9—C14 136.36 (9) C14—C9—C10—C11 −0.69 (15)
C3—Si1—C1—C2 −141.05 (11) C15—Si1—C1—C2 105.06 (11)
C3—Si1—C9—C10 73.75 (9) C15—Si1—C3—C4 55.95 (9)
C3—Si1—C9—C14 −101.86 (9) C15—Si1—C3—C8 −120.22 (9)
C3—C4—C5—C6 −0.07 (18) C15—Si1—C9—C10 −171.88 (7)
C4—C3—C8—C7 −1.38 (16) C15—Si1—C9—C14 12.52 (10)
C4—C5—C6—C7 −0.76 (18) C15—N1—C16—C17 65.05 (11)
C5—C6—C7—C8 0.50 (17) C15—N1—C16—C18 −176.39 (9)
C6—C7—C8—C3 0.59 (17) C15—N1—C16—C19 −56.69 (11)
C8—C3—C4—C5 1.12 (16) C16—N1—C15—Si1 −172.72 (6)
C9—Si1—C1—C2 −20.47 (12)

Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|-------|-------|---------|
| N1—H1A···Cl1 | 0.923 (15) | 2.179 (15) | 3.0968 (8) | 172.8 (13) |
| N1—H1B···Cl2 | 0.912 (15) | 2.231 (15) | 3.1184 (8) | 164.0 (13) |