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# 11-[Bis(trimethylsilyl)amino]-2,4-bis(trimethylsilyl)-7,8,9,10-tetrahydro-6*H*-cyclohepta[1,2-*b*]quinoline

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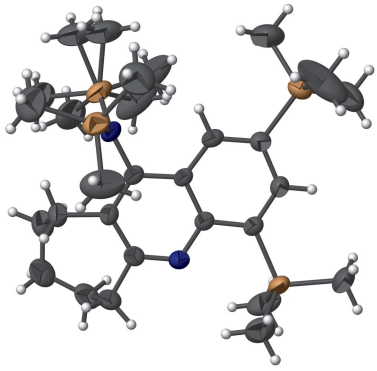
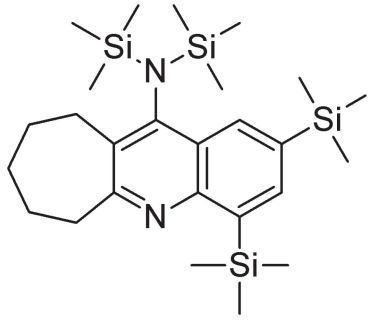
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{26}H_{48}N_2Si_4$, the cycloheptane ring adopts a chair conformation, while the quinolinyl ring system is almost planar [maximum deviation = 0.040 (3) Å for one of the C atoms carrying a $Me_3Si$ group]. In the crystal, in the absence of classical hydrogen bonding, the packing is dominated by van der Waals forces. One of the N-bound trimethylsilyl groups is disordered by rotation about the C—$SiMe_3$ bond, and was modelled over two sets of sites in the ratio 0.873 (8):0.127 (8).

**3D view**



**Chemical scheme**




## Structure description

Tacrine (9-amino-1,2,3,4-tetrahydroacridine) inhibits acetylcholinesterase, and has been used as a drug for treating Alzheimer's disease (Recanatini *et al.*, 2000; Peçanha *et al.*, 2001; Katzman, 1986; Shutske *et al.*, 1988) since 1993. However, serious side-effects have restricted its use against this disease (McKenna *et al.*, 1997; da Costa *et al.*, 2009). In recent years, several groups have focused upon synthesizing new tacrine derivatives and exploring their inhibitory effects on cancer cell lines and acetylcholinesterase in the desire to minimize side effects.

The Friedländer reaction is a well known method for synthesizing quinolines and hetero bicyclic aromatics with *N*-functionality (Peçanha *et al.*, 2001; Zong *et al.*, 2006). 9-Amino-1,2,3,4-tetrahydroacridine-1-ol, an effective anti-Alzheimer's agent, has been prepared by a copper-assisted Friedländer method (Shutske *et al.*, 1989). A recent study (Ekiz *et al.*, 2016) demonstrated a novel and convenient approach to prepare tacrine

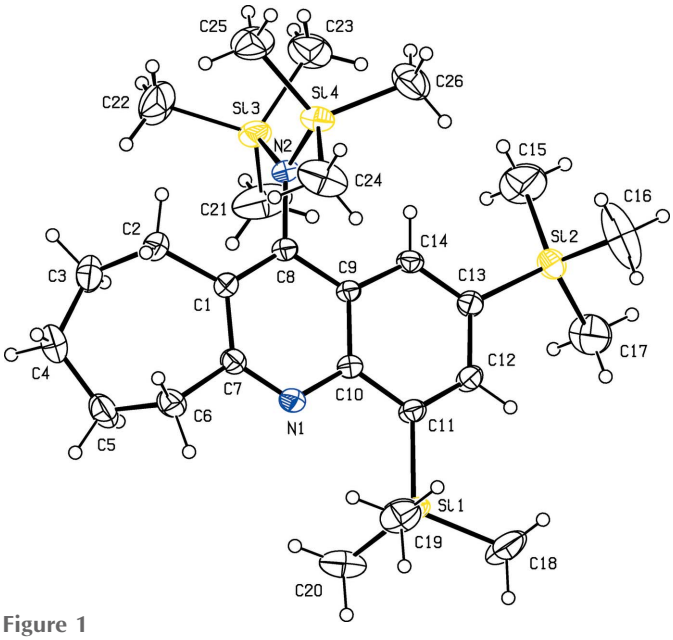



**Figure 1**
View of the title compound, showing the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. The minor component of the disordered $Me_3Si$ group has been omitted.

derivatives expanding on the restricted studies in the literature. In this study we present the structure of 11-[bis(trimethylsilyl)amino]-2,4-bis(trimethylsilyl)-7,8,9,10-tetrahydro-6*H*-cyclohepta[1,2-*b*] quinoline.

As shown in Fig. 1, the cycloheptane ring of the title molecule adopts a chair conformation with puckering parameters

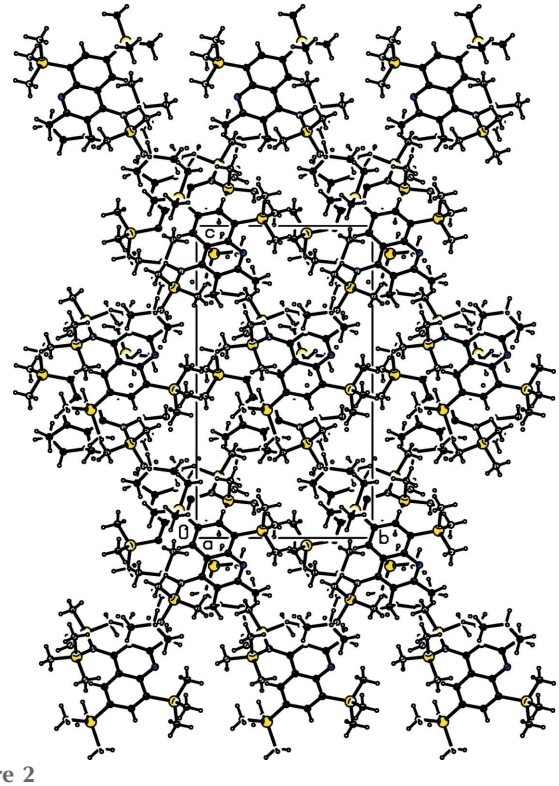



**Figure 2**
View of the packing of the title compound down the *a* axis.

**Table 1**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{26}H_{48}N_2Si_4$ |
| $M_r$ | 501.02 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 296 |
| $a, b, c$ (Å) | 13.4760 (14), 11.5597 (11), 20.883 (2) |
| $\beta$ (°) | 100.614 (5) |
| $V$ (Å$^3$) | 3197.5 (5) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.20 |
| Crystal size (mm) | 0.15 × 0.12 × 0.11 |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Sheldrick, 2003) |
| $T_{min}$, $T_{max}$ | 0.678, 0.740 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 56997, 6468, 4643 |
| $R_{int}$ | 0.068 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.630 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.078, 0.166, 1.19 |
| No. of reflections | 6468 |
| No. of parameters | 299 |
| No. of restraints | 15 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.27, −0.34 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *PLATON* (Spek, 2009) and *PARST* (Nardelli, 1995).

$Q_T$ = 0.781 (4) Å, $\varphi$(2) 51.3 (5)° and $\varphi$(3) = 77.1 (3)°, while the quinoline ring system is almost planar with maximum deviations of 0.040 (3) Å for atom C13 and −0.037 (3) Å for atom C8. The Si3—N2—Si4 angle in the amino-di(trimethylsilyl) group is wide at 124.33 (15)°. Generally, the observed bond lengths are comparable to those reported for the similar compounds (Glöcklhofer *et al.*, 2014; Sparrow *et al.*, 2012; Akkurt *et al.*, 2010).

In the crystal, in the absence of classical hydrogen bonds, the packing of the molecules is controlled by van der Waals forces (Fig. 2).

## Synthesis and crystallization

The title compound was prepared according to a reported procedure (Ekiz *et al.*, 2016). Colourless crystals suitable for X-ray diffraction were obtained by slow evaporation from its hexane/chloroform (50:50) solution.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. In the title molecule, each methyl group of one the N2-bound trimethylsilyl groups is disordered over two sites, in a 0.873 (8): 0.127 (8) ratio. The Si3—methyl bond lengths were restrained to be equal with a standard uncertainty value = 0.02 Å.

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## References

Akkurt, M., Çelik, Í., Küçükbay, H., Sireci, N. & Büyükgüngör, O. (2010). *Acta Cryst.* E**66**, o1770–o1771.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Costa, J. S. da, Pisoni, D. S., da Silva, C. B., Petzhold, C. L., Russowsky, D. & Ceschi, M. A. (2009). *J. Braz. Chem. Soc.* **20**, 1448–1454.
Ekiz, M., Tutar, A. & Ökten, S. (2016). *Tetrahedron*, **72**, 5323–5330.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Glöcklhofer, F., Fröhlich, J., Stöger, B. & Weil, M. (2014). *Acta Cryst.* E**70**, 77–79.
Katzman, R. N. (1986). *N. Engl. J. Med.* **314**, 964–973.
McKenna, M. T., Proctor, G. R., Young, L. C. & Harvey, A. L. (1997). *J. Med. Chem.* **40**, 3516–3523.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Peçanha, E. P., Fraga, C. A. M., Barreiro, E. J., Braga, M. F. M., Pereira, E. F. R. & Albuquerque, E. X. (2001). *J. Braz. Chem. Soc.* **12**, 408–412.
Recanatini, M., Cavalli, A., Belluti, F., Piazzi, L., Rampa, A., Bisi, A., Gobbi, S., Valenti, P., Andrisano, V., Bartolini, M. & Cavrini, V. (2000). *J. Med. Chem.* **43**, 2007–2018.
Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Shutske, G. M., Pierrat, F. A., Cornfeldt, M. L., Szewczak, M. R., Huger, F. P., Bores, G. M., Haroutunian, V. & Davis, K. L. (1988). *J. Med. Chem.* **31**, 1278–1279.
Shutske, G. M., Pierrat, F. A., Kapples, K. J., Cornfeldt, M. L., Szewczak, M. R., Huger, F. P., Bores, G. M., Haroutunian, V. & Davis, K. L. (1989). *J. Med. Chem.* **32**, 1805–1813.
Sparrow, C. R., Fronczek, F. R. & Watkins, S. F. (2012). *Acta Cryst.* E**68**, o2809.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Zong, R., Wang, D., Hammitt, R. & Thummel, R. P. (2006). *J. Org. Chem.* **71**, 167–175.

# full crystallographic data

*IUCrData* (2017). **2**, x170888 [https://doi.org/10.1107/S2414314617008884]

## 11-[Bis(trimethylsilyl)amino]-2,4-bis(trimethylsilyl)-7,8,9,10-tetrahydro-6*H*-cyclohepta[1,2-*b*]quinoline

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**11-[Bis(trimethylsilyl)amino]-2,4-bis(trimethylsilyl)-7,8,9,10-tetrahydro-6*H*-cyclohepta[1,2-*b*]quinoline**

*Crystal data*

$C_{26}H_{48}N_2Si_4$
$M_r$ = 501.02
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a$ = 13.4760 (14) Å
$b$ = 11.5597 (11) Å
$c$ = 20.883 (2) Å
$\beta$ = 100.614 (5)°
$V$ = 3197.5 (5) Å$^3$
$Z$ = 4
$F(000)$ = 1096
$D_x$ = 1.041 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9086 reflections
$\theta$ = 2.9–26.5°
$\mu$ = 0.20 mm$^{-1}$
$T$ = 296 K
Prism, colourless
0.15 × 0.12 × 0.11 mm

*Data collection*

Bruker APEXII CCD diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min}$ = 0.678, $T_{max}$ = 0.740
56997 measured reflections
6468 independent reflections
4643 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.068
$\theta_{max}$ = 26.6°, $\theta_{min}$ = 2.9°
$h$ = −16→16
$k$ = −14→14
$l$ = −26→26

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.078
$wR(F^2)$ = 0.166
$S$ = 1.19
6468 reflections
299 parameters
15 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0279P)^2 + 4.8053P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.34 e Å$^{-3}$

*Special details*

**Geometry**. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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.
All H atoms were placed in idealized positions and refined as riding atoms with C—H bond lengths fixed to 0.93–0.97 Å, and with $U_{iso}(H) = 1.2–1.5U_{eq}(C)$.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Si1 | 0.20359 (9) | 0.87480 (8) | 0.47603 (5) | 0.0498 (3) | |
| Si2 | 0.11596 (8) | 0.40010 (9) | 0.41068 (5) | 0.0504 (3) | |
| Si3 | 0.46955 (9) | 0.31878 (9) | 0.62008 (6) | 0.0565 (4) | |
| Si4 | 0.29921 (9) | 0.37413 (9) | 0.69699 (5) | 0.0537 (3) | |
| N1 | 0.3448 (2) | 0.7656 (2) | 0.58641 (13) | 0.0403 (9) | |
| N2 | 0.3825 (2) | 0.4130 (2) | 0.64494 (13) | 0.0411 (9) | |
| C1 | 0.4295 (2) | 0.6191 (3) | 0.65948 (15) | 0.0383 (10) | |
| C2 | 0.5063 (3) | 0.5961 (3) | 0.72000 (18) | 0.0540 (12) | |
| C3 | 0.6139 (3) | 0.6285 (4) | 0.7141 (2) | 0.0681 (16) | |
| C4 | 0.6403 (3) | 0.7561 (4) | 0.7239 (2) | 0.0750 (17) | |
| C5 | 0.5779 (3) | 0.8377 (4) | 0.6755 (2) | 0.0677 (17) | |
| C6 | 0.4654 (3) | 0.8352 (3) | 0.67596 (19) | 0.0535 (14) | |
| C7 | 0.4103 (3) | 0.7357 (3) | 0.63832 (16) | 0.0394 (10) | |
| C8 | 0.3757 (2) | 0.5318 (3) | 0.62370 (15) | 0.0365 (10) | |
| C9 | 0.3072 (2) | 0.5611 (2) | 0.56529 (15) | 0.0323 (9) | |
| C10 | 0.2934 (2) | 0.6801 (3) | 0.54910 (15) | 0.0344 (9) | |
| C11 | 0.2246 (3) | 0.7158 (3) | 0.49251 (16) | 0.0390 (10) | |
| C12 | 0.1755 (3) | 0.6304 (3) | 0.45336 (16) | 0.0427 (11) | |
| C13 | 0.1882 (3) | 0.5101 (3) | 0.46656 (16) | 0.0398 (10) | |
| C14 | 0.2526 (2) | 0.4788 (3) | 0.52293 (15) | 0.0375 (10) | |
| C15 | 0.1850 (5) | 0.2602 (4) | 0.4183 (3) | 0.118 (3) | |
| C16 | −0.0093 (4) | 0.3801 (6) | 0.4302 (3) | 0.140 (3) | |
| C17 | 0.1043 (5) | 0.4514 (5) | 0.3253 (2) | 0.102 (2) | |
| C18 | 0.1013 (4) | 0.8889 (4) | 0.4031 (2) | 0.097 (2) | |
| C19 | 0.1606 (4) | 0.9486 (4) | 0.5449 (2) | 0.0740 (17) | |
| C20 | 0.3197 (4) | 0.9444 (4) | 0.4585 (3) | 0.086 (2) | |
| C21 | 0.5034 (6) | 0.3687 (7) | 0.5443 (4) | 0.121 (4) | 0.873 (8) |
| C21A | 0.450 (4) | 0.307 (5) | 0.5296 (8) | 0.121 (4) | 0.127 (8) |
| C22 | 0.5879 (4) | 0.3074 (6) | 0.6830 (4) | 0.106 (3) | 0.873 (8) |
| C22A | 0.6023 (15) | 0.371 (4) | 0.631 (3) | 0.106 (3) | 0.127 (8) |
| C23 | 0.4138 (5) | 0.1719 (4) | 0.6112 (4) | 0.088 (3) | 0.873 (8) |
| C23A | 0.465 (4) | 0.1645 (18) | 0.642 (3) | 0.088 (3) | 0.127 (8) |
| C24 | 0.2436 (4) | 0.5072 (4) | 0.7259 (3) | 0.094 (2) | |
| C25 | 0.3684 (4) | 0.2976 (5) | 0.7697 (2) | 0.093 (2) | |
| C26 | 0.1928 (4) | 0.2838 (4) | 0.6554 (3) | 0.0852 (19) | |
| H2A | 0.50450 | 0.51450 | 0.73060 | 0.0650* | |
| H2B | 0.48760 | 0.63910 | 0.75580 | 0.0650* | |

| | | | | | |
|---|---|---|---|---|---|
| H3A | 0.66020 | 0.58420 | 0.74600 | 0.0810* | |
| H3B | 0.62490 | 0.60570 | 0.67130 | 0.0810* | |
| H4A | 0.63230 | 0.77820 | 0.76750 | 0.0900* | |
| H4B | 0.71090 | 0.76620 | 0.72130 | 0.0900* | |
| H5A | 0.60230 | 0.91600 | 0.68480 | 0.0820* | |
| H5B | 0.58840 | 0.81820 | 0.63210 | 0.0820* | |
| H6A | 0.45560 | 0.83090 | 0.72070 | 0.0640* | |
| H6B | 0.43570 | 0.90720 | 0.65770 | 0.0640* | |
| H12 | 0.13110 | 0.65260 | 0.41580 | 0.0510* | |
| H14 | 0.26030 | 0.40070 | 0.53350 | 0.0450* | |
| H15A | 0.25080 | 0.27130 | 0.40800 | 0.1760* | |
| H15B | 0.19150 | 0.23210 | 0.46220 | 0.1760* | |
| H15C | 0.14820 | 0.20490 | 0.38880 | 0.1760* | |
| H16A | −0.00300 | 0.35360 | 0.47430 | 0.2100* | |
| H16B | −0.04500 | 0.45240 | 0.42530 | 0.2100* | |
| H16C | −0.04580 | 0.32390 | 0.40120 | 0.2100* | |
| H17A | 0.17040 | 0.46190 | 0.31520 | 0.1530* | |
| H17B | 0.06780 | 0.39530 | 0.29630 | 0.1530* | |
| H17C | 0.06860 | 0.52370 | 0.32040 | 0.1530* | |
| H18A | 0.12160 | 0.85130 | 0.36660 | 0.1460* | |
| H18B | 0.04080 | 0.85330 | 0.41180 | 0.1460* | |
| H18C | 0.08880 | 0.96930 | 0.39330 | 0.1460* | |
| H19A | 0.10060 | 0.91170 | 0.55340 | 0.1110* | |
| H19B | 0.21260 | 0.94410 | 0.58300 | 0.1110* | |
| H19C | 0.14650 | 1.02830 | 0.53390 | 0.1110* | |
| H20A | 0.34110 | 0.90530 | 0.42280 | 0.1280* | |
| H20B | 0.30610 | 1.02410 | 0.44720 | 0.1280* | |
| H20C | 0.37220 | 0.93980 | 0.49630 | 0.1280* | |
| H21A | 0.55120 | 0.31620 | 0.53130 | 0.1810* | 0.873 (8) |
| H21B | 0.44400 | 0.37200 | 0.51100 | 0.1810* | 0.873 (8) |
| H21C | 0.53290 | 0.44440 | 0.55070 | 0.1810* | 0.873 (8) |
| H21D | 0.49840 | 0.25460 | 0.51760 | 0.1810* | 0.127 (8) |
| H21E | 0.38280 | 0.27810 | 0.51350 | 0.1810* | 0.127 (8) |
| H21F | 0.45710 | 0.38170 | 0.51120 | 0.1810* | 0.127 (8) |
| H22A | 0.63400 | 0.25520 | 0.66790 | 0.1590* | 0.873 (8) |
| H22B | 0.61860 | 0.38240 | 0.69020 | 0.1590* | 0.873 (8) |
| H22C | 0.57170 | 0.27890 | 0.72300 | 0.1590* | 0.873 (8) |
| H22D | 0.64340 | 0.31240 | 0.61610 | 0.1590* | 0.127 (8) |
| H22E | 0.60500 | 0.44040 | 0.60680 | 0.1590* | 0.127 (8) |
| H22F | 0.62710 | 0.38540 | 0.67660 | 0.1590* | 0.127 (8) |
| H23A | 0.46090 | 0.11920 | 0.59760 | 0.1320* | 0.873 (8) |
| H23B | 0.39890 | 0.14710 | 0.65230 | 0.1320* | 0.873 (8) |
| H23C | 0.35270 | 0.17340 | 0.57920 | 0.1320* | 0.873 (8) |
| H23D | 0.51700 | 0.12310 | 0.62570 | 0.1320* | 0.127 (8) |
| H23E | 0.47670 | 0.15720 | 0.68890 | 0.1320* | 0.127 (8) |
| H23F | 0.40060 | 0.13300 | 0.62400 | 0.1320* | 0.127 (8) |
| H24A | 0.19810 | 0.48620 | 0.75430 | 0.1420* | |
| H24B | 0.29660 | 0.55500 | 0.74910 | 0.1420* | |

| | | | | |
|---|---|---|---|---|
| H24C | 0.20750 | 0.54900 | 0.68910 | 0.1420* |
| H25A | 0.32220 | 0.27690 | 0.79770 | 0.1380* |
| H25B | 0.39900 | 0.22900 | 0.75630 | 0.1380* |
| H25C | 0.41990 | 0.34750 | 0.79280 | 0.1380* |
| H26A | 0.14950 | 0.26470 | 0.68560 | 0.1280* |
| H26B | 0.15510 | 0.32590 | 0.61930 | 0.1280* |
| H26C | 0.21880 | 0.21400 | 0.63980 | 0.1280* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Si1 | 0.0707 (7) | 0.0310 (5) | 0.0446 (6) | 0.0121 (5) | 0.0024 (5) | 0.0032 (4) |
| Si2 | 0.0573 (7) | 0.0422 (5) | 0.0494 (6) | −0.0058 (5) | 0.0038 (5) | −0.0107 (5) |
| Si3 | 0.0516 (6) | 0.0393 (5) | 0.0780 (8) | 0.0119 (5) | 0.0106 (6) | 0.0113 (5) |
| Si4 | 0.0669 (7) | 0.0403 (5) | 0.0559 (6) | −0.0046 (5) | 0.0169 (5) | 0.0087 (5) |
| N1 | 0.0456 (17) | 0.0303 (13) | 0.0430 (16) | −0.0026 (12) | 0.0031 (13) | 0.0007 (12) |
| N2 | 0.0441 (16) | 0.0314 (14) | 0.0453 (16) | 0.0024 (12) | 0.0016 (13) | 0.0099 (12) |
| C1 | 0.0363 (18) | 0.0391 (17) | 0.0376 (17) | −0.0008 (14) | 0.0018 (14) | 0.0055 (14) |
| C2 | 0.054 (2) | 0.050 (2) | 0.050 (2) | −0.0032 (18) | −0.0110 (18) | 0.0057 (17) |
| C3 | 0.050 (2) | 0.076 (3) | 0.070 (3) | −0.003 (2) | −0.011 (2) | −0.003 (2) |
| C4 | 0.054 (3) | 0.080 (3) | 0.084 (3) | −0.023 (2) | −0.006 (2) | −0.006 (3) |
| C5 | 0.067 (3) | 0.065 (3) | 0.066 (3) | −0.029 (2) | −0.001 (2) | −0.005 (2) |
| C6 | 0.064 (3) | 0.0396 (19) | 0.053 (2) | −0.0100 (18) | 0.0003 (19) | −0.0045 (17) |
| C7 | 0.0415 (19) | 0.0363 (17) | 0.0397 (18) | −0.0044 (15) | 0.0056 (15) | −0.0006 (14) |
| C8 | 0.0376 (18) | 0.0309 (16) | 0.0403 (17) | 0.0018 (14) | 0.0057 (14) | 0.0051 (14) |
| C9 | 0.0332 (17) | 0.0271 (15) | 0.0363 (16) | 0.0021 (13) | 0.0053 (13) | 0.0045 (12) |
| C10 | 0.0370 (17) | 0.0307 (15) | 0.0356 (16) | 0.0019 (13) | 0.0072 (14) | 0.0018 (13) |
| C11 | 0.0457 (19) | 0.0315 (16) | 0.0384 (18) | 0.0050 (14) | 0.0041 (15) | 0.0031 (14) |
| C12 | 0.047 (2) | 0.0390 (18) | 0.0384 (18) | 0.0078 (16) | −0.0017 (15) | 0.0013 (15) |
| C13 | 0.0410 (19) | 0.0351 (17) | 0.0419 (18) | 0.0013 (14) | 0.0043 (15) | −0.0022 (14) |
| C14 | 0.0397 (18) | 0.0269 (15) | 0.0465 (19) | 0.0019 (13) | 0.0093 (15) | 0.0034 (14) |
| C15 | 0.167 (6) | 0.056 (3) | 0.115 (5) | 0.020 (3) | −0.014 (4) | −0.025 (3) |
| C16 | 0.092 (4) | 0.198 (7) | 0.142 (6) | −0.075 (5) | 0.055 (4) | −0.099 (5) |
| C17 | 0.151 (5) | 0.090 (4) | 0.056 (3) | −0.024 (4) | −0.004 (3) | −0.013 (3) |
| C18 | 0.136 (5) | 0.058 (3) | 0.077 (3) | 0.034 (3) | −0.034 (3) | 0.005 (2) |
| C19 | 0.093 (3) | 0.057 (3) | 0.073 (3) | 0.023 (2) | 0.018 (3) | −0.006 (2) |
| C20 | 0.116 (4) | 0.047 (2) | 0.102 (4) | 0.003 (3) | 0.041 (3) | 0.018 (2) |
| C21 | 0.128 (7) | 0.114 (6) | 0.148 (6) | 0.064 (5) | 0.099 (6) | 0.067 (5) |
| C21A | 0.128 (7) | 0.114 (6) | 0.148 (6) | 0.064 (5) | 0.099 (6) | 0.067 (5) |
| C22 | 0.072 (4) | 0.088 (5) | 0.145 (7) | 0.035 (4) | −0.015 (4) | −0.005 (4) |
| C22A | 0.072 (4) | 0.088 (5) | 0.145 (7) | 0.035 (4) | −0.015 (4) | −0.005 (4) |
| C23 | 0.095 (5) | 0.048 (3) | 0.126 (6) | 0.012 (3) | 0.034 (4) | −0.008 (3) |
| C23A | 0.095 (5) | 0.048 (3) | 0.126 (6) | 0.012 (3) | 0.034 (4) | −0.008 (3) |
| C24 | 0.112 (4) | 0.066 (3) | 0.124 (5) | −0.002 (3) | 0.071 (4) | −0.006 (3) |
| C25 | 0.123 (5) | 0.092 (4) | 0.062 (3) | −0.011 (3) | 0.016 (3) | 0.029 (3) |
| C26 | 0.081 (3) | 0.081 (3) | 0.097 (4) | −0.028 (3) | 0.025 (3) | 0.005 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Si1—C11 | 1.882 (4) | C12—H12 | 0.9300 |
| Si1—C18 | 1.864 (5) | C14—H14 | 0.9300 |
| Si1—C19 | 1.854 (5) | C15—H15A | 0.9600 |
| Si1—C20 | 1.855 (6) | C15—H15B | 0.9600 |
| Si2—C13 | 1.873 (4) | C15—H15C | 0.9600 |
| Si2—C15 | 1.858 (5) | C16—H16A | 0.9600 |
| Si2—C16 | 1.823 (6) | C16—H16B | 0.9600 |
| Si2—C17 | 1.858 (4) | C16—H16C | 0.9600 |
| Si3—N2 | 1.748 (3) | C17—H17A | 0.9600 |
| Si3—C21 | 1.820 (8) | C17—H17B | 0.9600 |
| Si3—C22 | 1.875 (7) | C17—H17C | 0.9600 |
| Si3—C23 | 1.852 (5) | C18—H18A | 0.9600 |
| Si3—C21A | 1.864 (17) | C18—H18B | 0.9600 |
| Si3—C22A | 1.86 (3) | C18—H18C | 0.9600 |
| Si3—C23A | 1.85 (3) | C19—H19A | 0.9600 |
| Si4—N2 | 1.759 (3) | C19—H19B | 0.9600 |
| Si4—C24 | 1.860 (5) | C19—H19C | 0.9600 |
| Si4—C25 | 1.854 (5) | C20—H20A | 0.9600 |
| Si4—C26 | 1.855 (6) | C20—H20B | 0.9600 |
| N1—C7 | 1.312 (4) | C20—H20C | 0.9600 |
| N1—C10 | 1.366 (4) | C21—H21A | 0.9600 |
| N2—C8 | 1.441 (4) | C21—H21B | 0.9600 |
| C1—C2 | 1.502 (5) | C21—H21C | 0.9600 |
| C1—C7 | 1.427 (5) | C21A—H21D | 0.9600 |
| C1—C8 | 1.379 (5) | C21A—H21E | 0.9700 |
| C2—C3 | 1.524 (6) | C21A—H21F | 0.9600 |
| C3—C4 | 1.522 (6) | C22—H22C | 0.9600 |
| C4—C5 | 1.518 (6) | C22—H22A | 0.9600 |
| C5—C6 | 1.518 (6) | C22—H22B | 0.9600 |
| C6—C7 | 1.509 (5) | C22A—H22E | 0.9500 |
| C8—C9 | 1.428 (4) | C22A—H22D | 0.9600 |
| C9—C10 | 1.421 (4) | C22A—H22F | 0.9600 |
| C9—C14 | 1.410 (4) | C23—H23C | 0.9600 |
| C10—C11 | 1.422 (5) | C23—H23A | 0.9600 |
| C11—C12 | 1.372 (5) | C23—H23B | 0.9600 |
| C12—C13 | 1.422 (5) | C23A—H23E | 0.9700 |
| C13—C14 | 1.376 (5) | C23A—H23D | 0.9600 |
| C2—H2A | 0.9700 | C23A—H23F | 0.9500 |
| C2—H2B | 0.9700 | C24—H24A | 0.9600 |
| C3—H3A | 0.9700 | C24—H24C | 0.9600 |
| C3—H3B | 0.9700 | C24—H24B | 0.9600 |
| C4—H4A | 0.9700 | C25—H25B | 0.9600 |
| C4—H4B | 0.9700 | C25—H25C | 0.9600 |
| C5—H5A | 0.9700 | C25—H25A | 0.9600 |
| C5—H5B | 0.9700 | C26—H26C | 0.9600 |
| C6—H6A | 0.9700 | C26—H26A | 0.9600 |

| | | | |
|---|---|---|---|
| C6—H6B | 0.9700 | C26—H26B | 0.9600 |
| | | | |
| C11—Si1—C18 | 107.38 (19) | Si2—C15—H15A | 109.00 |
| C11—Si1—C19 | 111.44 (18) | Si2—C15—H15B | 109.00 |
| C11—Si1—C20 | 110.8 (2) | Si2—C15—H15C | 109.00 |
| C18—Si1—C19 | 107.7 (2) | H15A—C15—H15B | 109.00 |
| C18—Si1—C20 | 108.9 (2) | H15A—C15—H15C | 110.00 |
| C19—Si1—C20 | 110.4 (2) | H15B—C15—H15C | 109.00 |
| C13—Si2—C15 | 110.1 (2) | Si2—C16—H16A | 109.00 |
| C13—Si2—C16 | 110.1 (2) | Si2—C16—H16B | 109.00 |
| C13—Si2—C17 | 108.9 (2) | Si2—C16—H16C | 109.00 |
| C15—Si2—C16 | 109.9 (3) | H16A—C16—H16B | 110.00 |
| C15—Si2—C17 | 108.2 (3) | H16A—C16—H16C | 110.00 |
| C16—Si2—C17 | 109.7 (3) | H16B—C16—H16C | 109.00 |
| N2—Si3—C21 | 110.5 (3) | Si2—C17—H17A | 109.00 |
| N2—Si3—C22 | 111.5 (2) | Si2—C17—H17B | 109.00 |
| N2—Si3—C23 | 108.6 (2) | Si2—C17—H17C | 109.00 |
| N2—Si3—C21A | 111.7 (17) | H17A—C17—H17B | 110.00 |
| N2—Si3—C22A | 116.4 (14) | H17A—C17—H17C | 109.00 |
| N2—Si3—C23A | 118.3 (17) | H17B—C17—H17C | 109.00 |
| C21—Si3—C22 | 108.3 (3) | Si1—C18—H18A | 109.00 |
| C21—Si3—C23 | 111.5 (4) | Si1—C18—H18B | 110.00 |
| C22—Si3—C23 | 106.4 (3) | Si1—C18—H18C | 109.00 |
| C21A—Si3—C22A | 96 (3) | H18A—C18—H18B | 109.00 |
| C21A—Si3—C23A | 100 (3) | H18A—C18—H18C | 109.00 |
| C22A—Si3—C23A | 111 (2) | H18B—C18—H18C | 109.00 |
| N2—Si4—C24 | 109.30 (19) | Si1—C19—H19A | 109.00 |
| N2—Si4—C25 | 110.3 (2) | Si1—C19—H19B | 109.00 |
| N2—Si4—C26 | 112.4 (2) | Si1—C19—H19C | 109.00 |
| C24—Si4—C25 | 107.5 (3) | H19A—C19—H19B | 110.00 |
| C24—Si4—C26 | 107.1 (2) | H19A—C19—H19C | 110.00 |
| C25—Si4—C26 | 110.1 (2) | H19B—C19—H19C | 109.00 |
| C7—N1—C10 | 118.3 (3) | Si1—C20—H20A | 110.00 |
| Si3—N2—Si4 | 124.33 (15) | Si1—C20—H20B | 110.00 |
| Si3—N2—C8 | 120.7 (2) | Si1—C20—H20C | 110.00 |
| Si4—N2—C8 | 115.0 (2) | H20A—C20—H20B | 109.00 |
| C2—C1—C7 | 119.0 (3) | H20A—C20—H20C | 109.00 |
| C2—C1—C8 | 122.6 (3) | H20B—C20—H20C | 109.00 |
| C7—C1—C8 | 118.4 (3) | Si3—C21—H21A | 110.00 |
| C1—C2—C3 | 114.0 (3) | Si3—C21—H21B | 109.00 |
| C2—C3—C4 | 115.4 (3) | Si3—C21—H21C | 109.00 |
| C3—C4—C5 | 115.2 (4) | H21A—C21—H21B | 110.00 |
| C4—C5—C6 | 114.5 (3) | H21A—C21—H21C | 109.00 |
| C5—C6—C7 | 114.0 (3) | H21B—C21—H21C | 109.00 |
| N1—C7—C1 | 124.1 (3) | Si3—C21A—H21E | 109.00 |
| N1—C7—C6 | 114.9 (3) | Si3—C21A—H21F | 110.00 |
| C1—C7—C6 | 121.0 (3) | H21D—C21A—H21E | 109.00 |
| N2—C8—C1 | 122.2 (3) | H21D—C21A—H21F | 110.00 |

| | | | |
|---|---|---|---|
| N2—C8—C9 | 118.9 (3) | H21E—C21A—H21F | 109.00 |
| C1—C8—C9 | 118.8 (3) | Si3—C21A—H21D | 110.00 |
| C8—C9—C10 | 117.9 (3) | H22A—C22—H22C | 110.00 |
| C8—C9—C14 | 123.8 (3) | Si3—C22—H22B | 109.00 |
| C10—C9—C14 | 118.3 (3) | H22B—C22—H22C | 110.00 |
| N1—C10—C9 | 122.3 (3) | Si3—C22—H22A | 109.00 |
| N1—C10—C11 | 116.7 (3) | Si3—C22—H22C | 109.00 |
| C9—C10—C11 | 121.0 (3) | H22A—C22—H22B | 109.00 |
| Si1—C11—C10 | 119.2 (3) | Si3—C22A—H22F | 109.00 |
| Si1—C11—C12 | 123.7 (3) | Si3—C22A—H22E | 110.00 |
| C10—C11—C12 | 117.1 (3) | Si3—C22A—H22D | 109.00 |
| C11—C12—C13 | 124.1 (3) | H22D—C22A—H22E | 110.00 |
| Si2—C13—C12 | 120.9 (3) | H22D—C22A—H22F | 109.00 |
| Si2—C13—C14 | 121.9 (3) | H22E—C22A—H22F | 110.00 |
| C12—C13—C14 | 117.2 (3) | H23B—C23—H23C | 109.00 |
| C9—C14—C13 | 122.2 (3) | H23A—C23—H23C | 110.00 |
| C1—C2—H2A | 109.00 | Si3—C23—H23B | 109.00 |
| C1—C2—H2B | 109.00 | Si3—C23—H23C | 109.00 |
| C3—C2—H2A | 109.00 | Si3—C23—H23A | 109.00 |
| C3—C2—H2B | 109.00 | H23A—C23—H23B | 109.00 |
| H2A—C2—H2B | 108.00 | Si3—C23A—H23F | 110.00 |
| C2—C3—H3A | 108.00 | H23D—C23A—H23E | 109.00 |
| C2—C3—H3B | 108.00 | Si3—C23A—H23E | 109.00 |
| C4—C3—H3A | 108.00 | Si3—C23A—H23D | 109.00 |
| C4—C3—H3B | 108.00 | H23E—C23A—H23F | 109.00 |
| H3A—C3—H3B | 108.00 | H23D—C23A—H23F | 110.00 |
| C3—C4—H4A | 109.00 | Si4—C24—H24B | 109.00 |
| C3—C4—H4B | 108.00 | Si4—C24—H24A | 109.00 |
| C5—C4—H4A | 109.00 | H24B—C24—H24C | 110.00 |
| C5—C4—H4B | 108.00 | H24A—C24—H24C | 110.00 |
| H4A—C4—H4B | 107.00 | Si4—C24—H24C | 109.00 |
| C4—C5—H5A | 109.00 | H24A—C24—H24B | 110.00 |
| C4—C5—H5B | 109.00 | Si4—C25—H25B | 110.00 |
| C6—C5—H5A | 109.00 | H25A—C25—H25C | 109.00 |
| C6—C5—H5B | 109.00 | Si4—C25—H25C | 109.00 |
| H5A—C5—H5B | 108.00 | H25A—C25—H25B | 109.00 |
| C5—C6—H6A | 109.00 | Si4—C25—H25A | 109.00 |
| C5—C6—H6B | 109.00 | H25B—C25—H25C | 109.00 |
| C7—C6—H6A | 109.00 | Si4—C26—H26C | 109.00 |
| C7—C6—H6B | 109.00 | H26A—C26—H26C | 109.00 |
| H6A—C6—H6B | 108.00 | H26B—C26—H26C | 109.00 |
| C11—C12—H12 | 118.00 | H26A—C26—H26B | 110.00 |
| C13—C12—H12 | 118.00 | Si4—C26—H26A | 109.00 |
| C9—C14—H14 | 119.00 | Si4—C26—H26B | 109.00 |
| C13—C14—H14 | 119.00 | | |

| | | | |
|---|---|---|---|
| C18—Si1—C11—C12 | 3.9 (4) | C2—C1—C8—N2 | 5.8 (5) |
| C19—Si1—C11—C12 | 121.6 (4) | C8—C1—C7—N1 | −0.5 (5) |

| | | | |
|---|---|---|---|
| C20—Si1—C11—C12 | −115.0 (4) | C7—C1—C8—N2 | −173.5 (3) |
| C20—Si1—C11—C10 | 66.3 (4) | C7—C1—C8—C9 | 3.3 (4) |
| C18—Si1—C11—C10 | −174.9 (3) | C2—C1—C7—C6 | −0.3 (5) |
| C19—Si1—C11—C10 | −57.2 (4) | C2—C1—C7—N1 | −179.8 (3) |
| C17—Si2—C13—C14 | −145.5 (3) | C8—C1—C2—C3 | 115.4 (4) |
| C15—Si2—C13—C14 | −27.1 (4) | C2—C1—C8—C9 | −177.4 (3) |
| C16—Si2—C13—C14 | 94.2 (4) | C1—C2—C3—C4 | 81.3 (4) |
| C16—Si2—C13—C12 | −83.4 (4) | C2—C3—C4—C5 | −61.1 (5) |
| C17—Si2—C13—C12 | 36.8 (4) | C3—C4—C5—C6 | 60.7 (5) |
| C15—Si2—C13—C12 | 155.3 (4) | C4—C5—C6—C7 | −80.5 (4) |
| C21—Si3—N2—C8 | −23.8 (4) | C5—C6—C7—C1 | 66.4 (5) |
| C21—Si3—N2—Si4 | 157.0 (3) | C5—C6—C7—N1 | −114.2 (4) |
| C22—Si3—N2—Si4 | −82.5 (3) | N2—C8—C9—C14 | −6.8 (4) |
| C22—Si3—N2—C8 | 96.7 (3) | C1—C8—C9—C10 | −3.8 (4) |
| C23—Si3—N2—C8 | −146.4 (3) | C1—C8—C9—C14 | 176.3 (3) |
| C23—Si3—N2—Si4 | 34.5 (3) | N2—C8—C9—C10 | 173.1 (3) |
| C26—Si4—N2—C8 | 106.1 (3) | C14—C9—C10—C11 | 1.5 (4) |
| C25—Si4—N2—Si3 | 48.5 (3) | C10—C9—C14—C13 | 0.9 (4) |
| C25—Si4—N2—C8 | −130.7 (3) | C8—C9—C10—C11 | −178.5 (3) |
| C24—Si4—N2—Si3 | 166.5 (2) | C8—C9—C14—C13 | −179.1 (3) |
| C26—Si4—N2—Si3 | −74.7 (3) | C8—C9—C10—N1 | 1.6 (4) |
| C24—Si4—N2—C8 | −12.8 (3) | C14—C9—C10—N1 | −178.5 (3) |
| C10—N1—C7—C1 | −1.8 (5) | C9—C10—C11—Si1 | 176.4 (2) |
| C7—N1—C10—C11 | −178.7 (3) | N1—C10—C11—C12 | 177.6 (3) |
| C7—N1—C10—C9 | 1.2 (5) | C9—C10—C11—C12 | −2.4 (5) |
| C10—N1—C7—C6 | 178.7 (3) | N1—C10—C11—Si1 | −3.7 (4) |
| Si3—N2—C8—C9 | 90.8 (3) | Si1—C11—C12—C13 | −177.7 (3) |
| Si4—N2—C8—C1 | 86.9 (3) | C10—C11—C12—C13 | 1.0 (6) |
| Si4—N2—C8—C9 | −89.9 (3) | C11—C12—C13—C14 | 1.3 (6) |
| Si3—N2—C8—C1 | −92.4 (3) | C11—C12—C13—Si2 | 179.0 (3) |
| C7—C1—C2—C3 | −65.3 (4) | Si2—C13—C14—C9 | −180.0 (2) |
| C8—C1—C7—C6 | 179.0 (3) | C12—C13—C14—C9 | −2.2 (5) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2*A*···N2 | 0.97 | 2.49 | 2.959 (4) | 110 |
| C14—H14···N2 | 0.93 | 2.60 | 2.914 (4) | 101 |