

3-Nitro-1-(triisopropylsilyl)-1H-pyrrole

Alan R. Kennedy,^{a*} Abedawn I. Khalaf,^a Colin J. Suckling^a and Roger D. Waigh^b^aWestCHEM, Department of Pure & Applied Chemistry, University of Strathclyde, 295 Cathedral Street, Glasgow G1 1XL, Scotland, and ^bDepartment of Pharmaceutical Sciences, University of Strathclyde, 27 Taylor Street, Glasgow G4 0NR, ScotlandCorrespondence e-mail:
a.r.kennedy@strath.ac.uk

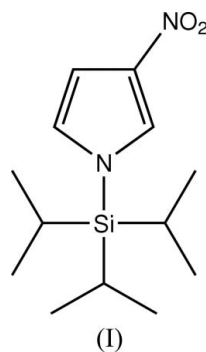
Key indicators

Single-crystal X-ray study
 $T = 123$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.059
 wR factor = 0.123
Data-to-parameter ratio = 18.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The nitration of 1-(triisopropylsilyl)-1H-pyrrole leads to a mixture of products following partial acid cleavage of the triisopropylsilyl protecting group. Structural determination showed the isolated products to be the title compound, $\text{C}_{13}\text{H}_{24}\text{N}_2\text{O}_2\text{Si}$, and 2,4-dinitropyrrole. In the solid state, the title compound exists as discrete molecules with only weak $\text{C}-\text{H} \cdots \text{nitro}$ hydrogen bonds between them.

Comment

The quest for *N*-alkyl-substituted pyrroles bearing a nitro group at position three has led us to the use of the cleavable and bulky triisopropylsilyl (TIPS) group. This work is in connection with our research into minor-groove binding compounds (Khalaf *et al.*, 2004). These compounds are analogues of naturally occurring distamycin and netropsin, which bind primarily to the adenine-thymine-rich minor groove of DNA. 3-Nitropyrrole (Bray *et al.*, 1990) was required as a precursor; however, the straightforward nitration of pyrrole favours position two. To prevent the nitration from occurring at position two of the pyrrole, a TIPS protecting group was first attached to the nitrogen of the pyrrole ring. This led to the nitro group being directed to position three (as anticipated), giving rise to the desired product (I) (Fig. 1) in 32% yield. However, during the course of the reaction, and due to the presence of acetic acid, the TIPS group cleaved. The removal of the TIPS group allowed the nitration reaction to occur once again. However, this time it occurred at position two, leading to the formation of the undesired product, 2,4-dinitropyrrole (II), in 19% yield.



Despite the large number of substituted pyrroles reported in the Cambridge Structural Database (Version 5.27 with updates to May 2006; Allen, 2002), a search found only nine relevant 3-nitro derivatives. All of the ring bond lengths and angles (Table 1) of (I) fall within the ranges found for these nine structures, with the exception that in (I) the $\text{C}2-\text{N}1-\text{C}5$

Received 29 June 2006

Accepted 5 July 2006

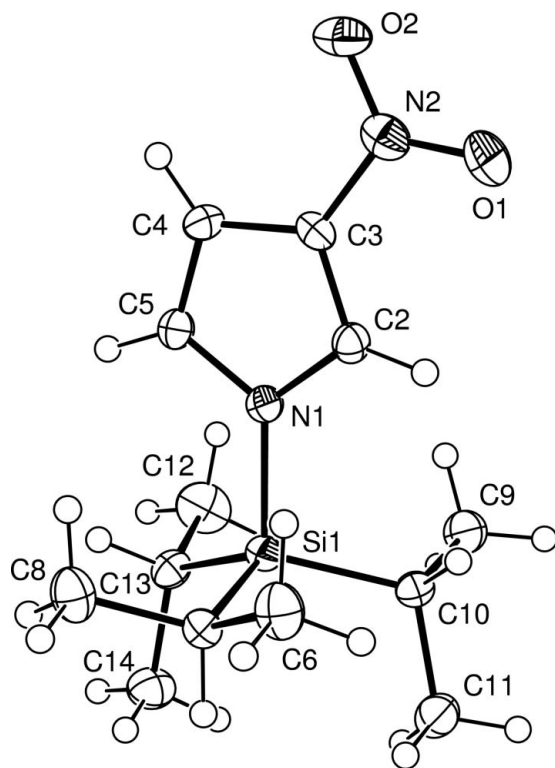


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

angle is slightly below the literature range [106.8 (2)° *cf.* 107.7–110.2°]. This is presumably due to the bulk and inductive effects of the attached TIPS group as no such relevant *N*-silyl substituent was found in the database. All of the literature nitro groups are approximately coplanar with their pyrrole rings; it can be seen from Table 1 that this is also the case for (I).

In the absence of obvious hydrogen-bonding groups, nitro aromatics often display nitro-to-nitro interactions of the type described by Wozniak *et al.* (1994); however, none is found in (I). The only intermolecular interactions of any note are weak C–H···O contacts utilizing both *sp*² and *sp*³ CH groups (see Table 2). This can be rationalized as a consequence of the bulky triisopropylsilyl group, which ensures that the ring systems are widely separated from each other.

Experimental

A solution of cupric nitrate trihydrate (2.70 g, 11.2 mmol) in acetic anhydride (20 ml) was cooled to 273 K and 1-(triisopropylsilyl)-1*H*-pyrrole (2.50 g, 11.2 mmol) was added dropwise with stirring. The ice bath was removed and stirring was continued for 1 h at room temperature. The reaction mixture was poured slowly over a saturated sodium hydrogen carbonate solution with stirring. After extraction with diethyl ether the organic layer was collected, dried (MgSO₄) and the solvent was removed under reduced pressure. The residue was subjected to flash chromatography on silica gel, using ethyl acetate/hexane (1:12) to elute (I). The solvents were removed under reduced pressure and a slow stream of air was passed over the

residue to remove any volatile material. The product was obtained as colourless crystals [0.947 g, 32%; m.p. 325–327 K, literature m.p. 325–327 K (Bray *et al.*, 1990)]. Compound (II) was eluted using ethyl acetate–hexane (1:4). This material was obtained, after the removal of the solvents, as pale-yellow crystals [0.338 g, 19%; m.p. 422–423 K, literature m.p. 423–424 K (Sharnin *et al.*, 1975)].

Crystal data

C ₁₃ H ₂₄ N ₂ O ₂ Si	Z = 4
<i>M_r</i> = 268.43	<i>D_x</i> = 1.144 Mg m ⁻³
Monoclinic, <i>P</i> 2 ₁ / <i>n</i>	Mo <i>K</i> α radiation
<i>a</i> = 9.6924 (5) Å	<i>μ</i> = 0.15 mm ⁻¹
<i>b</i> = 15.9437 (10) Å	<i>T</i> = 123 (2) K
<i>c</i> = 10.1267 (6) Å	Cut fragment, colourless
<i>β</i> = 95.089 (4)°	0.30 × 0.12 × 0.08 mm
<i>V</i> = 1558.74 (16) Å ³	

Data collection

Nonius KappaCCD diffractometer	3060 independent reflections
<i>ω</i> and <i>φ</i> scans	1685 reflections with <i>I</i> > 2σ(<i>I</i>)
Absorption correction: none	<i>R</i> _{int} = 0.108
13088 measured reflections	<i>θ</i> _{max} = 26.0°

Refinement

Refinement on <i>F</i> ²	<i>w</i> = 1/[σ ² (<i>F_o</i> ²) + (0.0471 <i>P</i>) ²
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)] = 0.059	+ 0.0035 <i>P</i>]
<i>wR</i> (<i>F</i> ²) = 0.123	where <i>P</i> = (<i>F_o</i> ² + 2 <i>F_c</i> ²)/3
<i>S</i> = 1.01	(Δ/ <i>σ</i>) _{max} = 0.001
3060 reflections	Δ <i>ρ</i> _{max} = 0.34 e Å ⁻³
169 parameters	Δ <i>ρ</i> _{min} = -0.36 e Å ⁻³
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

Si1–N1	1.805 (2)	C2–C3	1.365 (3)
N1–C2	1.365 (3)	C3–C4	1.410 (4)
N1–C5	1.395 (3)	C4–C5	1.358 (4)
C2–N1–C5	106.8 (2)	C5–C4–C3	105.3 (2)
C3–C2–N1	108.4 (2)	C4–C5–N1	110.3 (2)
C2–C3–C4	109.1 (2)		
O1–N2–C3–C2	-0.5 (4)	O2–N2–C3–C2	178.9 (2)

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>
C5–H5···O2 ⁱ	0.95	2.47	3.403 (4)	166
C10–H10···O1 ⁱⁱ	1.00	2.55	3.245 (4)	126

Symmetry codes: (i) *x* + ½, -*y* + ½, *z* + ½; (ii) -*x* + 1, -*y*, -*z*.

All H atoms were positioned geometrically, C–H = 0.95 (*Csp*²), 0.98 (CH₃) or 1.00 Å (*Csp*³), and refined using a riding model [*U*_{iso}(H) = 1.5*U*_{eq}(C) for CH₃ and 1.2*U*_{eq}(C) for all others].

Data collection: *COLLECT* (Hooft, 1988) and *DENZO* (Otwinowski & Minor, 1997); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

References

- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.
- Bray, B. L., Mathies, P. H., Naef, R., Solas, D. R., Tidwell, T. T., Artis, D. R. & Muchowski, J. M. (1990). *J. Org. Chem.* **55**, 6317–6328.
- Hoof, R. (1988). *COLLECT*. Nonius BV, Delft, The Netherlands.
- Johnson, C. K. (1976). *ORTEP II*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Khalaf, A. I., Ebrahimabadi, A. H., Drummond, A. J., Anthony, N. G., Mackay, S. P., Suckling, C. J. & Waigh, R. D. (2004). *Org. Biomol. Chem.* **2**, 3119–3127.
- Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography, Part A*, edited by C. W. Carter Jr & R. M. Sweet, pp 307–326. New York: Academic Press.
- Sharnin, G. P., Falyakhov, I. F. & Butovetskii, D. N. (1975). *Khim. Geterotsikl. Soedin.* **5**, 655–658. *Chem. Heterocycl. Compd (Engl. Transl.)*, **11**, 571–573.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Wozniak, K., He, H., Klinowski, J., Jones, W. & Grech, E. (1994). *J. Phys. Chem.* **98**, 13755–13765.

supporting information

Acta Cryst. (2006). E62, o3282–o3284 [https://doi.org/10.1107/S1600536806025943]

3-Nitro-1-(triisopropylsilyl)-1*H*-pyrrole

Alan R. Kennedy, Abedawn I. Khalaf, Colin J. Suckling and Roger D. Waigh

3-Nitro-1-(triisopropylsilyl)-1*H*-pyrrole*Crystal data*

$C_{13}H_{24}N_2O_2Si$

$M_r = 268.43$

Monoclinic, $P2_1/n$

$a = 9.6924$ (5) Å

$b = 15.9437$ (10) Å

$c = 10.1267$ (6) Å

$\beta = 95.089$ (4)°

$V = 1558.74$ (16) Å³

$Z = 4$

$F(000) = 584$

$D_x = 1.144$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3020 reflections

$\theta = 1.0$ – 26.1 °

$\mu = 0.15$ mm⁻¹

$T = 123$ K

Cut fragment, colourless

$0.30 \times 0.12 \times 0.08$ mm

Data collection

Nonius KappaCCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω and ϕ scans

13088 measured reflections

3060 independent reflections

1685 reflections with $I > 2\sigma(I)$

$R_{int} = 0.108$

$\theta_{max} = 26.0$ °, $\theta_{min} = 2.4$ °

$h = -11 \rightarrow 11$

$k = -19 \rightarrow 19$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.059$

$wR(F^2) = 0.123$

$S = 1.01$

3060 reflections

169 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 0.0035P]$

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

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

$\Delta\rho_{max} = 0.34$ e Å⁻³

$\Delta\rho_{min} = -0.36$ e Å⁻³

Special details

Experimental. A solution of cupric nitrate trihydrate (2.70 g, 11.2 mmol) in acetic anhydride (20 ml) was cooled to 273 K and 1-(triisopropylsilyl)-1H-pyrrole (2.50 g, 11.2 mmol) was added dropwise with stirring. The ice bath was removed and stirring was continued for 1 h at room temperature. The reaction mixture was poured slowly over a saturated sodium hydrogen carbonate solution with stirring. After extraction with ether the organic layer was collected, dried (MgSO₄) and the solvent was removed under reduced pressure. The residue was subjected to flash chromatography on silica gel, using ethyl acetate/hexane (1:12) to elute (I). The solvents were removed under reduced pressure and a slow stream of air was passed over it to remove any volatile material. The product was obtained as colourless crystals [0.947 g, 32%; m.p. 325–327 K, literature m.p. 325–327 K (Bray *et al.*, 1990)]. ¹H NMR (DMSO-*d*₆): δ 7.88 (1H, *dd*, *J* = 2.6, 5.4 Hz), 6.88 (1H, *dd*, *J* = 3.9, 7.8 Hz), 6.67 (1H, *dd*, *J* = 3.9, 6.4 Hz), 1.05–0.86 (21H, *m*). IR (KBr): 1550, 1330, 1240 cm⁻¹. Compound (II) was eluted using ethyl acetate–hexane (1:4). This material was obtained, after the removal of the solvents, as pale-yellow crystals [0.338 g, 19%; m.p. 422–423 K, literature m.p. 423–424 K (Sharnin *et al.*, 1975)]. ¹H NMR (DMSO-*d*₆): δ 14.4 (1H, *br*), 8.26 (1H, *d*, *J* = 2.9 Hz), 7.71 (1H, *d*, *J* = 2.9 Hz). IR (KBr): 3195, 3153, 1554, 1488, 1347, 1239, 1124, 1080, 957, 846, 815, 751 cm⁻¹.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Si1	0.84500 (8)	0.11350 (5)	0.27816 (7)	0.0205 (2)
O1	0.5558 (2)	0.07380 (14)	−0.21907 (19)	0.0418 (6)
O2	0.6482 (2)	0.17835 (13)	−0.31778 (19)	0.0346 (6)
N1	0.8022 (2)	0.15042 (14)	0.1111 (2)	0.0215 (6)
N2	0.6353 (2)	0.13427 (17)	−0.2192 (2)	0.0287 (6)
C2	0.7113 (3)	0.11329 (18)	0.0182 (3)	0.0217 (7)
H2	0.6543	0.0662	0.0326	0.026*
C3	0.7160 (3)	0.15521 (17)	−0.0989 (3)	0.0211 (7)
C4	0.8127 (3)	0.22120 (18)	−0.0811 (3)	0.0252 (7)
H4	0.8369	0.2605	−0.1456	0.030*
C5	0.8639 (3)	0.21657 (18)	0.0480 (3)	0.0249 (7)
H5	0.9321	0.2531	0.0893	0.030*
C6	0.9494 (3)	−0.03860 (18)	0.1823 (3)	0.0342 (8)
H6A	0.9218	−0.0196	0.0917	0.051*
H6B	0.8714	−0.0675	0.2177	0.051*
H6C	1.0280	−0.0772	0.1814	0.051*
C7	0.9916 (3)	0.03755 (17)	0.2703 (3)	0.0220 (7)
H7	1.0150	0.0159	0.3622	0.026*
C8	1.1233 (3)	0.07824 (19)	0.2257 (3)	0.0327 (8)
H8A	1.1960	0.0357	0.2233	0.049*
H8B	1.1547	0.1226	0.2883	0.049*
H8C	1.1033	0.1024	0.1371	0.049*
C9	0.5574 (3)	0.11509 (19)	0.3264 (3)	0.0314 (8)
H9A	0.4739	0.0804	0.3265	0.047*

H9B	0.5495	0.1518	0.2485	0.047*
H9C	0.5673	0.1493	0.4070	0.047*
C10	0.6848 (3)	0.05834 (17)	0.3218 (3)	0.0216 (7)
H10	0.6610	0.0173	0.2487	0.026*
C11	0.7071 (3)	0.00593 (18)	0.4497 (3)	0.0309 (8)
H11A	0.7244	0.0434	0.5260	0.046*
H11B	0.7869	-0.0313	0.4442	0.046*
H11C	0.6242	-0.0277	0.4602	0.046*
C12	0.7990 (3)	0.28032 (18)	0.3786 (3)	0.0412 (9)
H12A	0.7233	0.2635	0.4309	0.062*
H12B	0.7618	0.2932	0.2878	0.062*
H12C	0.8448	0.3301	0.4186	0.062*
C13	0.9040 (3)	0.20860 (17)	0.3765 (3)	0.0239 (7)
H13	0.9839	0.2318	0.3322	0.029*
C14	0.9625 (3)	0.18556 (18)	0.5188 (3)	0.0323 (8)
H14A	1.0043	0.2354	0.5627	0.049*
H14B	1.0330	0.1417	0.5152	0.049*
H14C	0.8873	0.1650	0.5688	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0208 (4)	0.0213 (5)	0.0190 (4)	-0.0002 (4)	0.0003 (3)	0.0005 (4)
O1	0.0396 (14)	0.0471 (15)	0.0365 (13)	-0.0144 (12)	-0.0085 (10)	-0.0055 (12)
O2	0.0399 (13)	0.0426 (14)	0.0211 (12)	0.0074 (11)	0.0013 (10)	0.0046 (11)
N1	0.0226 (14)	0.0214 (14)	0.0201 (13)	-0.0030 (11)	0.0001 (11)	0.0005 (11)
N2	0.0252 (15)	0.0341 (17)	0.0266 (16)	0.0064 (13)	0.0012 (12)	-0.0037 (14)
C2	0.0213 (15)	0.0185 (16)	0.0252 (17)	-0.0006 (13)	0.0016 (13)	0.0001 (14)
C3	0.0181 (15)	0.0250 (17)	0.0196 (16)	0.0021 (14)	-0.0016 (13)	-0.0022 (14)
C4	0.0249 (17)	0.0266 (18)	0.0240 (17)	-0.0008 (14)	0.0016 (13)	0.0089 (14)
C5	0.0255 (17)	0.0221 (17)	0.0265 (18)	-0.0072 (14)	-0.0013 (13)	0.0022 (14)
C6	0.0292 (18)	0.032 (2)	0.0413 (19)	0.0012 (15)	0.0048 (15)	-0.0053 (16)
C7	0.0214 (16)	0.0232 (18)	0.0212 (16)	-0.0009 (13)	0.0003 (13)	-0.0001 (13)
C8	0.0249 (18)	0.0315 (18)	0.042 (2)	0.0011 (15)	0.0029 (15)	-0.0052 (16)
C9	0.0233 (17)	0.037 (2)	0.0343 (18)	0.0037 (15)	0.0059 (13)	0.0060 (16)
C10	0.0232 (16)	0.0233 (17)	0.0185 (16)	-0.0003 (14)	0.0026 (12)	0.0014 (13)
C11	0.0304 (17)	0.0294 (19)	0.0334 (18)	-0.0001 (15)	0.0063 (14)	0.0045 (15)
C12	0.051 (2)	0.0266 (19)	0.045 (2)	0.0056 (17)	-0.0019 (17)	-0.0090 (17)
C13	0.0276 (17)	0.0208 (17)	0.0238 (16)	-0.0011 (14)	0.0046 (13)	0.0000 (14)
C14	0.0415 (19)	0.0307 (19)	0.0240 (17)	-0.0020 (15)	-0.0016 (15)	-0.0024 (15)

Geometric parameters (Å, °)

Si1—N1	1.805 (2)	C8—H8A	0.9800
Si1—C10	1.871 (3)	C8—H8B	0.9800
Si1—C7	1.874 (3)	C8—H8C	0.9800
Si1—C13	1.876 (3)	C9—C10	1.535 (4)
O1—N2	1.234 (3)	C9—H9A	0.9800

O2—N2	1.237 (3)	C9—H9B	0.9800
N1—C2	1.365 (3)	C9—H9C	0.9800
N1—C5	1.395 (3)	C10—C11	1.540 (4)
N2—C3	1.428 (3)	C10—H10	1.0000
C2—C3	1.365 (3)	C11—H11A	0.9800
C2—H2	0.9500	C11—H11B	0.9800
C3—C4	1.410 (4)	C11—H11C	0.9800
C4—C5	1.358 (4)	C12—C13	1.532 (4)
C4—H4	0.9500	C12—H12A	0.9800
C5—H5	0.9500	C12—H12B	0.9800
C6—C7	1.540 (4)	C12—H12C	0.9800
C6—H6A	0.9800	C13—C14	1.545 (4)
C6—H6B	0.9800	C13—H13	1.0000
C6—H6C	0.9800	C14—H14A	0.9800
C7—C8	1.535 (3)	C14—H14B	0.9800
C7—H7	1.0000	C14—H14C	0.9800
N1—Si1—C10	104.37 (11)	C7—C8—H8C	109.5
N1—Si1—C7	106.44 (11)	H8A—C8—H8C	109.5
C10—Si1—C7	110.77 (12)	H8B—C8—H8C	109.5
N1—Si1—C13	105.56 (11)	C10—C9—H9A	109.5
C10—Si1—C13	118.35 (12)	C10—C9—H9B	109.5
C7—Si1—C13	110.39 (12)	H9A—C9—H9B	109.5
C2—N1—C5	106.8 (2)	C10—C9—H9C	109.5
C2—N1—Si1	125.80 (18)	H9A—C9—H9C	109.5
C5—N1—Si1	127.14 (18)	H9B—C9—H9C	109.5
O1—N2—O2	123.5 (2)	C9—C10—C11	110.4 (2)
O1—N2—C3	118.5 (2)	C9—C10—Si1	114.63 (19)
O2—N2—C3	118.0 (3)	C11—C10—Si1	113.34 (18)
C3—C2—N1	108.4 (2)	C9—C10—H10	105.9
C3—C2—H2	125.8	C11—C10—H10	105.9
N1—C2—H2	125.8	Si1—C10—H10	105.9
C2—C3—C4	109.1 (2)	C10—C11—H11A	109.5
C2—C3—N2	124.6 (3)	C10—C11—H11B	109.5
C4—C3—N2	126.3 (3)	H11A—C11—H11B	109.5
C5—C4—C3	105.3 (2)	C10—C11—H11C	109.5
C5—C4—H4	127.3	H11A—C11—H11C	109.5
C3—C4—H4	127.3	H11B—C11—H11C	109.5
C4—C5—N1	110.3 (2)	C13—C12—H12A	109.5
C4—C5—H5	124.9	C13—C12—H12B	109.5
N1—C5—H5	124.9	H12A—C12—H12B	109.5
C7—C6—H6A	109.5	C13—C12—H12C	109.5
C7—C6—H6B	109.5	H12A—C12—H12C	109.5
H6A—C6—H6B	109.5	H12B—C12—H12C	109.5
C7—C6—H6C	109.5	C12—C13—C14	110.7 (2)
H6A—C6—H6C	109.5	C12—C13—Si1	116.03 (19)
H6B—C6—H6C	109.5	C14—C13—Si1	111.87 (19)
C8—C7—C6	110.4 (2)	C12—C13—H13	105.8

C8—C7—Si1	113.14 (19)	C14—C13—H13	105.8
C6—C7—Si1	111.76 (18)	Si1—C13—H13	105.8
C8—C7—H7	107.1	C13—C14—H14A	109.5
C6—C7—H7	107.1	C13—C14—H14B	109.5
Si1—C7—H7	107.1	H14A—C14—H14B	109.5
C7—C8—H8A	109.5	C13—C14—H14C	109.5
C7—C8—H8B	109.5	H14A—C14—H14C	109.5
H8A—C8—H8B	109.5	H14B—C14—H14C	109.5
C10—Si1—N1—C2	-29.4 (2)	N1—Si1—C7—C8	63.3 (2)
C7—Si1—N1—C2	87.8 (2)	C10—Si1—C7—C8	176.16 (18)
C13—Si1—N1—C2	-154.9 (2)	C13—Si1—C7—C8	-50.8 (2)
C10—Si1—N1—C5	157.3 (2)	N1—Si1—C7—C6	-62.1 (2)
C7—Si1—N1—C5	-85.5 (2)	C10—Si1—C7—C6	50.8 (2)
C13—Si1—N1—C5	31.8 (2)	C13—Si1—C7—C6	-176.13 (18)
C5—N1—C2—C3	-0.2 (3)	N1—Si1—C10—C9	-64.0 (2)
Si1—N1—C2—C3	-174.65 (18)	C7—Si1—C10—C9	-178.14 (19)
N1—C2—C3—C4	0.0 (3)	C13—Si1—C10—C9	53.0 (2)
N1—C2—C3—N2	179.8 (2)	N1—Si1—C10—C11	168.10 (19)
O1—N2—C3—C2	-0.5 (4)	C7—Si1—C10—C11	53.9 (2)
O2—N2—C3—C2	178.9 (2)	C13—Si1—C10—C11	-75.0 (2)
O1—N2—C3—C4	179.3 (3)	N1—Si1—C13—C12	59.0 (2)
O2—N2—C3—C4	-1.3 (4)	C10—Si1—C13—C12	-57.3 (2)
C2—C3—C4—C5	0.2 (3)	C7—Si1—C13—C12	173.6 (2)
N2—C3—C4—C5	-179.6 (2)	N1—Si1—C13—C14	-172.69 (18)
C3—C4—C5—N1	-0.3 (3)	C10—Si1—C13—C14	71.0 (2)
C2—N1—C5—C4	0.3 (3)	C7—Si1—C13—C14	-58.1 (2)
Si1—N1—C5—C4	174.66 (19)		

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>
C5—H5...O2 ⁱ	0.95	2.47	3.403 (4)	166
C10—H10...O1 ⁱⁱ	1.00	2.55	3.245 (4)	126

Symmetry codes: (i) $x+1/2, -y+1/2, z+1/2$; (ii) $-x+1, -y, -z$.