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Hexaethylguanidinium tetrakis(trimethylsilylethynyl)borate diethyl ether monosolvate

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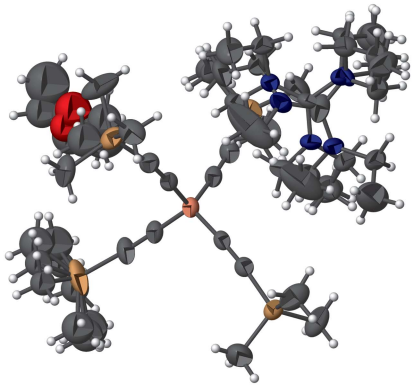
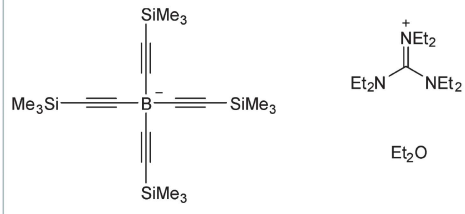
The solvated molecular salt, $C_{13}H_{30}N_3^+\cdot C_{20}H_{36}BSi_4^-\cdot C_4H_{10}O$, was obtained by the reaction of trimethylsilylethyne with boron trichloride in the presence of *tert*-butyllithium, followed by ion metathesis. The cation exhibits positional disorder and one of the Me_3Si groups shows rotational disorder. No significant directional intermolecular interactions are observed.

3D view



Chemical scheme



Structure description

Hexaethylguanidinium salts have been described and used principally as phase transfer catalysts (Kantlehner *et al.*, 1984; Caringi *et al.*, 1999). The conformations of these cations have been studied recently (Salchner *et al.*, 2014). Large anions in which bulky groups at the end of a rigid rod assembly shield the charge were synthesized not long ago (Vitze, 2008). It was intended to combine these non-coordinating ions in order to benefit from their respective advantageous properties. The resulting salt or even more bulky analogues may be of interest as potential supporting electrolytes for lithium–air batteries (Luntz & McCloskey, 2014).

The molecular structure of the title compound is shown in Fig. 1. The complete cation is disordered (Fig. 2*a*) with an occupancy ratio of the two components of 0.65:0.35. In the anion, one Me_3Si group is disordered over three orientations (0.40:0.33:0.27; Fig. 2*b*) related by a rotation about the Si4—C30 bond. The complete solvent molecule is disordered over two positions (0.6:0.4; Fig. 2*c*).

The central C1 atom does not deviate significantly from the N1/N2/N3 plane [by 0.01 (1) Å; the analogous value in the minor disorder component is 0.02 (2) Å]. The central C—N bond lengths lie between 1.336 (6) and 1.350 (6) Å [in the minor component between 1.341 (7) and 1.348 (7) Å]. The pertinent N—C—N angles are close to the ideal value of 120° and range from 119.0 (5) to 120.5 (6)° [from 118.8 (8) to 120.6 (8)° in

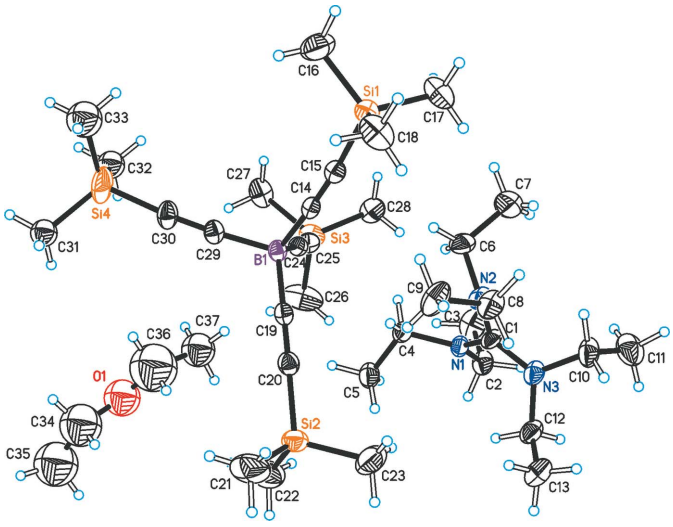


Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids for non-H atoms and the atom-labelling scheme. Minor-disorder components have been omitted for clarity.

the minor component]. The conformations of the six ethyl groups can be described by the corresponding torsion angles C1—N—C—C [−120.6 (7), −131.3 (8), −96.0 (8), −119.0 (9), −106.5 (13) and −115.5 (12)°], which are similar to those found in the related tetrachlorocuprate(II) (Salchner *et al.*, 2014).

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{30}N_3^+\cdot C_{20}H_{36}BSi_4^-\cdot C_4H_{10}O$
M_r	702.17
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	193
a, b, c (Å)	12.9107 (7), 17.8720 (8), 21.6094 (11)
β (°)	95.0374 (16)
V (Å^3)	4966.9 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.15
Crystal size (mm)	0.19 × 0.15 × 0.11
Data collection	
Diffractometer	Bruker D8 QUEST PHOTON 100
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.922, 0.971
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	82487, 8834, 5918
R_{int}	0.079
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.597
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.068, 0.193, 1.00
No. of reflections	8834
No. of parameters	597
No. of restraints	458
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.34, −0.35

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXTL2013* and *XP*/*SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008).

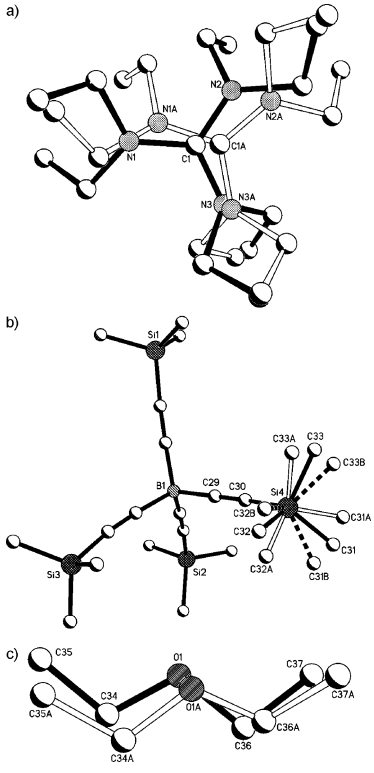


Figure 2
Disorder models for (*a*) the cation, (*b*) the anion and (*c*) the solvent molecule. Minor-disorder components are drawn as having open [in (*a*), (*b*) and (*c*)] or dashed [in (*b*)] bonds.

In the tetrahedral anion, the C—B—C angles range from 105.5 (2)° to 111.5 (2)°. The B—C—C angles deviate only marginally from linearity with values between 174.5 (3) and 176.9 (3)°, whereas the deformation of the C—C—Si angles [170.0 (3) to 175.0 (2)°] is more pronounced. The arrangement of the ions in the unit cell is shown in Fig. 3. The crystal

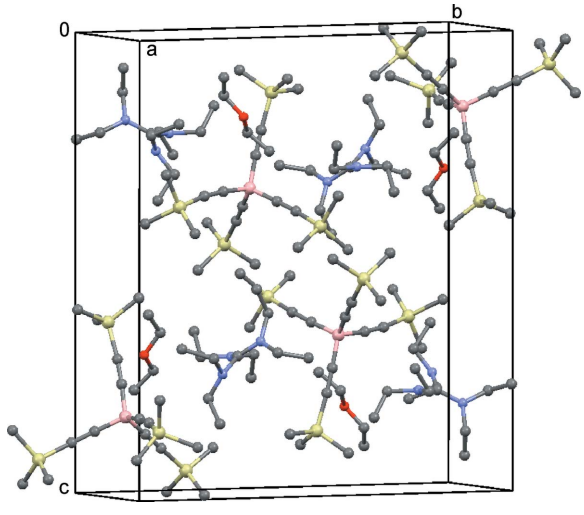


Figure 3
Unit cell of the title compound, viewed perpendicular to the *bc* plane.

structure does not exhibit any significant directed intermolecular interactions.

Structures of related tetraethynylborates (Gusev *et al.*, 1977 and 1978) are known. The structures of silylated tetraethynylborates were described more recently, and the angles of their anions were similar to those observed in the present structure (Vitze, 2008).

Synthesis and crystallization

To a cooled solution (190 K) of trimethylsilylethyne (2.20 ml, 16 mmol) in toluene (20 ml) *tert*-BuLi (10 ml 1.7 *M*, 17 mmol) was added and stirred at room temperature for 1 h. The mixture was cooled again at 190 K, and BCl_3 (4.0 ml 1*M* in toluene, 4 mmol) was added. Stirring was continued for 36 h at room temperature. After addition of Aliquat HTA-1 (3.0 ml, *ca* 4.2 mmol; Aldrich) and saturated NH_4Cl solution (3 ml), the phases were separated. Colourless crystals grew in the aqueous phase and were collected by filtration. Washing with Et_2O and drying under reduced pressure resulted in 1.10 g of the product (44%); m.p. 449 K. ^{1}H NMR (300 MHz, DMSO-d_6): δ 0.04 (*s*, 36H), 1.12 (*t*, J = 7.5 Hz, 18H), 3.11 and 3.27 (*m*, 24H) p.p.m. ^{13}C NMR (75 MHz, DMSO-d_6): δ 0.8 (12 C), 12.6 (6 C), 43.0 (6 C), 94.3 (*q*, J = 12 Hz, 4 C), 128.0 (*q*, J = 66 Hz, 4 C), 162.7 p.p.m. IR (neat): ν 2958, 2100, 1534, 1241, 955, 831, 754 cm^{-1}.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The complete solvent molecule is disordered over two positions (0.6:0.4; Fig. 2*c*). Distance restraints (SAME/SADI) were applied for all chemically equivalent 1,2- and 1,3-distances. All 1,2- and 1,3-distances in the disordered solvent molecule were restrained to target values (DFIX). All non-H atomic positions involved in a disorder were refined isotropically, except for the major component of the cation, which was refined anisotropically.

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full crystallographic data

IUCrData (2017). **2**, x170724 [https://doi.org/10.1107/S2414314617007246]

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Crystal data

$C_{13}H_{30}N_3^+·C_{20}H_{36}BSi_4^-·C_4H_{10}O$
M_r = 702.17
Monoclinic, $P2_1/n$
a = 12.9107 (7) Å
b = 17.8720 (8) Å
c = 21.6094 (11) Å
β = 95.0374 (16)°
V = 4966.9 (4) Å^3
Z = 4
$F(000)$ = 1552
D_x = 0.939 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9883 reflections
θ = 2.2–24.3°
μ = 0.15 mm^{-1}
T = 193 K
Prism, colourless
0.19 × 0.15 × 0.11 mm

Data collection

Bruker D8 QUEST PHOTON 100 diffractometer
Radiation source: Incoatec Microfocus
Multi layered optics monochromator
Detector resolution: 10.4 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2012)
T_{min} = 0.922, T_{max} = 0.971
82487 measured reflections
8834 independent reflections
5918 reflections with $I > 2\sigma(I)$
R_{int} = 0.079
θ_{max} = 25.1°, θ_{min} = 2.1°
h = −15→15
k = −21→21
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.193
S = 1.00
8834 reflections
597 parameters
458 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
$w = 1/[\sigma^2(F_o^2) + (0.095P)^2 + 3.190P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 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	0.82059 (6)	0.25828 (4)	0.45129 (4)	0.0474 (2)	
Si2	0.57950 (8)	0.42589 (5)	0.12930 (4)	0.0611 (3)	
Si3	0.41942 (7)	0.58398 (5)	0.42690 (4)	0.0576 (3)	
Si4	0.26088 (9)	0.23439 (7)	0.37953 (6)	0.0930 (4)	
B1	0.5461 (2)	0.37341 (16)	0.33687 (14)	0.0383 (7)	
C14	0.6465 (2)	0.33713 (13)	0.37359 (12)	0.0368 (6)	
C15	0.7195 (2)	0.30760 (14)	0.40350 (12)	0.0427 (6)	
C16	0.7580 (3)	0.1983 (2)	0.5072 (2)	0.0984 (14)	
H16A	0.8117	0.1728	0.5344	0.148*	
H16B	0.7140	0.1610	0.4844	0.148*	
H16C	0.7153	0.2293	0.5324	0.148*	
C17	0.9099 (3)	0.32537 (19)	0.49402 (18)	0.0815 (11)	
H17A	0.9683	0.2981	0.5156	0.122*	
H17B	0.8724	0.3526	0.5245	0.122*	
H17C	0.9363	0.3609	0.4646	0.122*	
C18	0.8968 (3)	0.1994 (2)	0.40136 (17)	0.0813 (11)	
H18A	0.9537	0.1752	0.4269	0.122*	
H18B	0.9254	0.2307	0.3698	0.122*	
H18C	0.8515	0.1610	0.3810	0.122*	
C19	0.56311 (19)	0.38643 (14)	0.26528 (13)	0.0409 (6)	
C20	0.5730 (2)	0.39932 (16)	0.21087 (13)	0.0486 (7)	
C21	0.5703 (4)	0.3415 (2)	0.07899 (18)	0.1155 (17)	
H21A	0.5691	0.3567	0.0354	0.173*	
H21B	0.5064	0.3141	0.0855	0.173*	
H21C	0.6306	0.3092	0.0896	0.173*	
C22	0.4679 (3)	0.4880 (3)	0.1030 (2)	0.1015 (14)	
H22A	0.4695	0.4988	0.0586	0.152*	
H22B	0.4733	0.5349	0.1266	0.152*	
H22C	0.4025	0.4630	0.1100	0.152*	
C23	0.7039 (3)	0.4753 (2)	0.1207 (2)	0.0965 (13)	
H23A	0.7086	0.4879	0.0769	0.145*	
H23B	0.7622	0.4429	0.1352	0.145*	
H23C	0.7065	0.5213	0.1455	0.145*	
C24	0.5167 (2)	0.45080 (14)	0.36753 (12)	0.0395 (6)	
C25	0.4864 (2)	0.50746 (15)	0.39096 (13)	0.0472 (7)	
C26	0.3561 (4)	0.6432 (2)	0.36347 (18)	0.1148 (18)	
H26A	0.3189	0.6844	0.3815	0.172*	
H26B	0.3068	0.6127	0.3371	0.172*	
H26C	0.4092	0.6634	0.3384	0.172*	

C27	0.3206 (2)	0.5415 (2)	0.47330 (17)	0.0764 (10)	
H27A	0.2867	0.5809	0.4958	0.115*	
H27B	0.3544	0.5059	0.5031	0.115*	
H27C	0.2685	0.5154	0.4456	0.115*	
C28	0.5103 (3)	0.64243 (18)	0.47729 (16)	0.0732 (10)	
H28A	0.4722	0.6840	0.4942	0.110*	
H28B	0.5646	0.6622	0.4529	0.110*	
H28C	0.5423	0.6120	0.5115	0.110*	
C29	0.4495 (2)	0.31905 (15)	0.34457 (13)	0.0455 (7)	
C30	0.3757 (2)	0.28119 (18)	0.35500 (15)	0.0593 (8)	
C31	0.1720 (7)	0.2040 (6)	0.3136 (3)	0.073 (2)*	0.4
H31A	0.1465	0.2477	0.2896	0.109*	0.4
H31B	0.1132	0.1772	0.3289	0.109*	0.4
H31C	0.2089	0.1706	0.2870	0.109*	0.4
C32	0.1952 (8)	0.2995 (5)	0.4306 (5)	0.082 (3)*	0.4
H32A	0.2444	0.3150	0.4654	0.124*	0.4
H32B	0.1359	0.2741	0.4467	0.124*	0.4
H32C	0.1707	0.3436	0.4067	0.124*	0.4
C33	0.3008 (11)	0.1483 (6)	0.4271 (6)	0.123 (5)*	0.4
H33A	0.3345	0.1124	0.4011	0.185*	0.4
H33B	0.2390	0.1252	0.4423	0.185*	0.4
H33C	0.3494	0.1627	0.4625	0.185*	0.4
C31A	0.2094 (10)	0.1641 (6)	0.3244 (5)	0.088 (4)*	0.33
H31D	0.2001	0.1861	0.2827	0.132*	0.33
H31E	0.1422	0.1462	0.3363	0.132*	0.33
H31F	0.2581	0.1221	0.3243	0.132*	0.33
C32A	0.1680 (11)	0.3112 (7)	0.3936 (8)	0.130 (6)*	0.33
H32D	0.1983	0.3435	0.4271	0.195*	0.33
H32E	0.1028	0.2897	0.4055	0.195*	0.33
H32F	0.1541	0.3408	0.3556	0.195*	0.33
C33A	0.2990 (12)	0.1844 (9)	0.4535 (5)	0.117 (5)*	0.33
H33D	0.2370	0.1628	0.4696	0.175*	0.33
H33E	0.3317	0.2197	0.4839	0.175*	0.33
H33F	0.3482	0.1444	0.4459	0.175*	0.33
C31B	0.1604 (14)	0.2484 (12)	0.3122 (6)	0.136 (8)*	0.27
H31G	0.1466	0.3020	0.3066	0.203*	0.27
H31H	0.0961	0.2227	0.3206	0.203*	0.27
H31I	0.1862	0.2279	0.2744	0.203*	0.27
C32B	0.2154 (11)	0.2732 (8)	0.4503 (4)	0.070 (4)*	0.27
H32G	0.2678	0.2645	0.4852	0.105*	0.27
H32H	0.1501	0.2489	0.4587	0.105*	0.27
H32I	0.2039	0.3271	0.4450	0.105*	0.27
C33B	0.2817 (18)	0.1314 (5)	0.3878 (9)	0.151 (9)*	0.27
H33G	0.3099	0.1119	0.3504	0.226*	0.27
H33H	0.2153	0.1068	0.3933	0.226*	0.27
H33I	0.3308	0.1214	0.4240	0.226*	0.27
N1	0.7562 (4)	0.6243 (3)	0.2917 (3)	0.0445 (13)	0.65
N2	0.8692 (4)	0.5254 (3)	0.3205 (2)	0.0521 (12)	0.65

N3	0.9219 (5)	0.6227 (3)	0.2587 (3)	0.055 (3)	0.65
C1	0.8496 (5)	0.5907 (4)	0.2905 (4)	0.0443 (16)	0.65
C2	0.7477 (4)	0.7067 (3)	0.2937 (2)	0.0574 (12)	0.65
H2A	0.7057	0.7242	0.2560	0.069*	0.65
H2B	0.8180	0.7288	0.2936	0.069*	0.65
C3	0.6985 (5)	0.7335 (3)	0.3501 (3)	0.0844 (18)	0.65
H3A	0.6260	0.7167	0.3479	0.127*	0.65
H3B	0.7007	0.7883	0.3517	0.127*	0.65
H3C	0.7365	0.7130	0.3875	0.127*	0.65
C4	0.6610 (3)	0.5796 (3)	0.2977 (2)	0.0487 (11)	0.65
H4A	0.6381	0.5867	0.3398	0.058*	0.65
H4B	0.6772	0.5259	0.2927	0.058*	0.65
C5	0.5742 (6)	0.6015 (5)	0.2502 (4)	0.0625 (18)	0.65
H5A	0.5539	0.6534	0.2573	0.094*	0.65
H5B	0.5144	0.5685	0.2539	0.094*	0.65
H5C	0.5977	0.5969	0.2085	0.094*	0.65
C6	0.8332 (4)	0.5123 (3)	0.38250 (19)	0.0632 (13)	0.65
H6A	0.8110	0.4595	0.3855	0.076*	0.65
H6B	0.7720	0.5444	0.3876	0.076*	0.65
C7	0.9148 (7)	0.5284 (6)	0.4332 (3)	0.156 (4)	0.65
H7A	0.9812	0.5078	0.4226	0.234*	0.65
H7B	0.8957	0.5054	0.4718	0.234*	0.65
H7C	0.9214	0.5826	0.4389	0.234*	0.65
C8	0.9355 (6)	0.4680 (3)	0.2950 (4)	0.066 (2)	0.65
H8A	0.9962	0.4582	0.3252	0.079*	0.65
H8B	0.9618	0.4871	0.2563	0.079*	0.65
C9	0.8775 (10)	0.3965 (5)	0.2814 (6)	0.080 (3)	0.65
H9A	0.8563	0.3754	0.3202	0.120*	0.65
H9B	0.9225	0.3608	0.2622	0.120*	0.65
H9C	0.8157	0.4065	0.2530	0.120*	0.65
C10	1.0327 (3)	0.6228 (3)	0.2827 (3)	0.0693 (15)	0.65
H10A	1.0752	0.6068	0.2491	0.083*	0.65
H10B	1.0431	0.5859	0.3168	0.083*	0.65
C11	1.0698 (11)	0.6975 (6)	0.3061 (11)	0.095 (5)	0.65
H11A	1.0689	0.7328	0.2713	0.142*	0.65
H11B	1.1409	0.6929	0.3257	0.142*	0.65
H11C	1.0240	0.7159	0.3366	0.142*	0.65
C12	0.8956 (4)	0.6614 (3)	0.1990 (2)	0.0612 (13)	0.65
H12A	0.9214	0.7135	0.2028	0.073*	0.65
H12B	0.8190	0.6635	0.1911	0.073*	0.65
C13	0.9390 (13)	0.6260 (10)	0.1444 (3)	0.075 (4)	0.65
H13A	1.0151	0.6270	0.1502	0.112*	0.65
H13B	0.9152	0.6536	0.1066	0.112*	0.65
H13C	0.9151	0.5740	0.1406	0.112*	0.65
N1A	0.7941 (8)	0.5997 (6)	0.3122 (3)	0.052 (2)	0.35
N2A	0.9133 (6)	0.5034 (5)	0.2994 (6)	0.059 (3)	0.35
N3A	0.9307 (10)	0.6193 (5)	0.2516 (5)	0.055 (7)	0.35
C1A	0.8786 (11)	0.5734 (5)	0.2869 (8)	0.063 (5)	0.35

C2A	0.7201 (8)	0.6502 (8)	0.2778 (6)	0.064 (4)	0.35
H2A1	0.7459	0.6624	0.2372	0.077*	0.35
H2A2	0.7155	0.6974	0.3014	0.077*	0.35
C3A	0.6138 (9)	0.6161 (11)	0.2673 (9)	0.083 (5)	0.35
H3A1	0.6167	0.5721	0.2404	0.124*	0.35
H3A2	0.5654	0.6529	0.2474	0.124*	0.35
H3A3	0.5900	0.6009	0.3073	0.124*	0.35
C4A	0.7689 (8)	0.5733 (5)	0.3744 (4)	0.071 (3)	0.35
H4A1	0.8129	0.5295	0.3867	0.086*	0.35
H4A2	0.6954	0.5570	0.3719	0.086*	0.35
C5A	0.7858 (18)	0.6326 (10)	0.4225 (6)	0.182 (10)	0.35
H5A1	0.8592	0.6331	0.4386	0.273*	0.35
H5A2	0.7425	0.6223	0.4566	0.273*	0.35
H5A3	0.7669	0.6813	0.4041	0.273*	0.35
C6A	1.0259 (6)	0.4875 (5)	0.3076 (5)	0.071 (3)	0.35
H6A1	1.0655	0.5338	0.3008	0.085*	0.35
H6A2	1.0440	0.4499	0.2767	0.085*	0.35
C7A	1.0544 (10)	0.4587 (10)	0.3718 (6)	0.131 (6)	0.35
H7A1	1.0305	0.4939	0.4022	0.196*	0.35
H7A2	1.1301	0.4532	0.3785	0.196*	0.35
H7A3	1.0214	0.4099	0.3767	0.196*	0.35
C8A	0.8406 (8)	0.4406 (5)	0.3044 (5)	0.070 (3)	0.35
H8A1	0.7689	0.4584	0.2931	0.084*	0.35
H8A2	0.8447	0.4234	0.3481	0.084*	0.35
C9A	0.862 (2)	0.3760 (10)	0.2637 (12)	0.090 (6)	0.35
H9A1	0.8601	0.3928	0.2205	0.135*	0.35
H9A2	0.8098	0.3371	0.2675	0.135*	0.35
H9A3	0.9315	0.3557	0.2765	0.135*	0.35
C10A	0.9484 (7)	0.6985 (4)	0.2688 (4)	0.066 (3)	0.35
H10C	0.8947	0.7146	0.2960	0.079*	0.35
H10D	0.9405	0.7295	0.2307	0.079*	0.35
C11A	1.0533 (14)	0.7121 (12)	0.3015 (14)	0.059 (4)	0.35
H11D	1.0578	0.6879	0.3423	0.088*	0.35
H11E	1.0645	0.7661	0.3068	0.088*	0.35
H11F	1.1067	0.6913	0.2768	0.088*	0.35
C12A	0.9810 (8)	0.5916 (5)	0.1971 (4)	0.069 (3)	0.35
H12C	0.9832	0.5363	0.1984	0.083*	0.35
H12D	1.0536	0.6100	0.1997	0.083*	0.35
C13A	0.927 (3)	0.616 (2)	0.1365 (6)	0.104 (12)	0.35
H13D	0.8518	0.6072	0.1370	0.156*	0.35
H13E	0.9531	0.5867	0.1027	0.156*	0.35
H13F	0.9397	0.6690	0.1300	0.156*	0.35
O1	0.1463 (6)	0.4353 (4)	0.1788 (4)	0.147 (3)*	0.6
C34	0.1105 (10)	0.3852 (7)	0.1326 (6)	0.194 (7)*	0.6
H34A	0.0874	0.3387	0.1522	0.233*	0.6
H34B	0.1683	0.3721	0.1073	0.233*	0.6
C35	0.0232 (11)	0.4162 (9)	0.0915 (7)	0.220 (7)*	0.6
H35A	−0.0257	0.4416	0.1167	0.330*	0.6

H35B	−0.0128	0.3755	0.0680	0.330*	0.6
H35C	0.0501	0.4520	0.0625	0.330*	0.6
C36	0.2428 (11)	0.4114 (8)	0.2096 (9)	0.248 (10)*	0.6
H36A	0.2939	0.4001	0.1794	0.297*	0.6
H36B	0.2333	0.3664	0.2352	0.297*	0.6
C37	0.2769 (7)	0.4762 (5)	0.2491 (5)	0.126 (3)*	0.6
H37A	0.2787	0.5211	0.2232	0.190*	0.6
H37B	0.3465	0.4664	0.2693	0.190*	0.6
H37C	0.2280	0.4838	0.2807	0.190*	0.6
O1A	0.1379 (6)	0.4166 (5)	0.2028 (4)	0.099 (3)*	0.4
C34A	0.1185 (11)	0.3614 (9)	0.1574 (8)	0.159 (7)*	0.4
H34C	0.1141	0.3120	0.1778	0.191*	0.4
H34D	0.1770	0.3597	0.1307	0.191*	0.4
C35A	0.0201 (9)	0.3758 (8)	0.1180 (6)	0.118 (4)*	0.4
H35D	−0.0365	0.3839	0.1447	0.177*	0.4
H35E	0.0037	0.3326	0.0910	0.177*	0.4
H35F	0.0283	0.4204	0.0925	0.177*	0.4
C36A	0.2432 (7)	0.4180 (7)	0.2287 (6)	0.091 (4)*	0.4
H36C	0.2878	0.4424	0.1996	0.109*	0.4
H36D	0.2689	0.3664	0.2368	0.109*	0.4
C37A	0.2458 (11)	0.4606 (8)	0.2872 (6)	0.131 (5)*	0.4
H37D	0.2385	0.5141	0.2779	0.196*	0.4
H37E	0.3122	0.4517	0.3117	0.196*	0.4
H37F	0.1886	0.4443	0.3109	0.196*	0.4

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0463 (5)	0.0464 (4)	0.0495 (5)	0.0090 (3)	0.0040 (3)	−0.0019 (3)
Si2	0.0728 (6)	0.0665 (6)	0.0444 (5)	−0.0028 (5)	0.0072 (4)	−0.0009 (4)
Si3	0.0677 (6)	0.0524 (5)	0.0527 (5)	0.0206 (4)	0.0061 (4)	−0.0110 (4)
Si4	0.0585 (6)	0.1111 (9)	0.1153 (10)	−0.0377 (6)	0.0403 (6)	−0.0278 (7)
B1	0.0333 (15)	0.0407 (16)	0.0411 (16)	−0.0013 (12)	0.0056 (12)	−0.0061 (13)
C14	0.0382 (15)	0.0333 (13)	0.0405 (14)	−0.0050 (11)	0.0120 (12)	−0.0075 (11)
C15	0.0447 (16)	0.0387 (14)	0.0454 (15)	−0.0012 (12)	0.0080 (13)	−0.0042 (12)
C16	0.087 (3)	0.108 (3)	0.101 (3)	0.010 (3)	0.019 (2)	0.049 (3)
C17	0.080 (3)	0.069 (2)	0.089 (3)	0.0127 (19)	−0.027 (2)	−0.016 (2)
C18	0.069 (2)	0.089 (3)	0.085 (3)	0.031 (2)	0.0010 (19)	−0.025 (2)
C19	0.0337 (14)	0.0431 (15)	0.0460 (16)	−0.0020 (11)	0.0038 (12)	−0.0090 (12)
C20	0.0457 (17)	0.0517 (16)	0.0485 (17)	−0.0031 (13)	0.0051 (13)	−0.0090 (13)
C21	0.179 (5)	0.106 (3)	0.062 (2)	−0.004 (3)	0.016 (3)	−0.024 (2)
C22	0.096 (3)	0.120 (4)	0.086 (3)	0.011 (3)	−0.007 (2)	0.026 (3)
C23	0.090 (3)	0.110 (3)	0.094 (3)	−0.010 (3)	0.030 (2)	0.026 (3)
C24	0.0372 (14)	0.0430 (15)	0.0384 (14)	0.0014 (12)	0.0049 (11)	0.0002 (12)
C25	0.0504 (17)	0.0480 (16)	0.0440 (15)	0.0058 (13)	0.0087 (13)	−0.0011 (13)
C26	0.167 (5)	0.091 (3)	0.083 (3)	0.077 (3)	−0.008 (3)	−0.005 (2)
C27	0.054 (2)	0.093 (3)	0.083 (2)	0.0084 (19)	0.0153 (18)	−0.033 (2)
C28	0.095 (3)	0.058 (2)	0.068 (2)	−0.0071 (18)	0.020 (2)	−0.0140 (17)

C29	0.0367 (15)	0.0507 (16)	0.0500 (16)	−0.0005 (13)	0.0095 (12)	−0.0102 (13)
C30	0.0430 (17)	0.067 (2)	0.070 (2)	−0.0102 (15)	0.0173 (15)	−0.0162 (16)
N1	0.036 (3)	0.043 (4)	0.054 (4)	−0.005 (2)	0.000 (3)	0.010 (3)
N2	0.053 (3)	0.038 (2)	0.065 (3)	0.001 (2)	0.006 (2)	0.020 (2)
N3	0.043 (5)	0.045 (6)	0.077 (5)	−0.001 (4)	0.001 (4)	0.024 (4)
C1	0.049 (5)	0.036 (3)	0.049 (4)	−0.005 (3)	0.009 (3)	0.014 (3)
C2	0.056 (3)	0.036 (2)	0.079 (3)	−0.002 (2)	0.000 (3)	0.008 (2)
C3	0.095 (4)	0.052 (3)	0.110 (5)	−0.001 (3)	0.024 (4)	−0.019 (3)
C4	0.044 (3)	0.046 (3)	0.056 (3)	−0.003 (2)	0.005 (2)	0.011 (2)
C5	0.047 (5)	0.059 (4)	0.080 (4)	−0.006 (3)	−0.002 (4)	0.008 (3)
C6	0.080 (4)	0.054 (3)	0.055 (3)	−0.005 (3)	−0.001 (3)	0.018 (2)
C7	0.169 (9)	0.210 (10)	0.081 (5)	−0.113 (8)	−0.038 (5)	0.039 (6)
C8	0.058 (4)	0.046 (4)	0.095 (5)	0.012 (3)	0.014 (3)	0.017 (4)
C9	0.089 (8)	0.047 (6)	0.111 (7)	−0.005 (4)	0.044 (7)	−0.003 (4)
C10	0.040 (3)	0.061 (3)	0.106 (4)	−0.003 (2)	0.000 (3)	0.020 (3)
C11	0.076 (7)	0.082 (7)	0.121 (10)	0.006 (6)	−0.021 (6)	0.015 (8)
C12	0.055 (3)	0.059 (3)	0.071 (3)	−0.003 (2)	0.012 (2)	0.024 (3)
C13	0.083 (7)	0.064 (5)	0.082 (7)	−0.010 (6)	0.030 (6)	0.006 (5)
N1A	0.054 (7)	0.064 (7)	0.038 (6)	−0.009 (5)	0.001 (5)	0.010 (4)
N2A	0.039 (7)	0.053 (9)	0.084 (8)	0.001 (5)	−0.002 (5)	0.033 (7)
N3A	0.056 (11)	0.047 (11)	0.068 (10)	0.000 (8)	0.037 (9)	0.013 (7)
C1A	0.039 (7)	0.066 (11)	0.081 (10)	0.001 (7)	0.001 (6)	−0.025 (9)
C2A	0.051 (8)	0.080 (11)	0.061 (7)	0.014 (7)	0.005 (6)	0.020 (7)
C3A	0.047 (10)	0.103 (12)	0.100 (14)	−0.012 (8)	0.022 (9)	0.023 (11)
C4A	0.062 (6)	0.082 (7)	0.070 (6)	−0.008 (5)	0.009 (5)	0.021 (5)
C5A	0.26 (2)	0.22 (2)	0.071 (9)	−0.147 (19)	0.048 (12)	−0.037 (11)
C6A	0.040 (5)	0.059 (6)	0.113 (9)	0.002 (4)	0.000 (5)	0.026 (6)
C7A	0.088 (10)	0.165 (15)	0.133 (13)	−0.015 (10)	−0.025 (9)	0.058 (11)
C8A	0.065 (7)	0.061 (6)	0.083 (7)	−0.012 (5)	0.000 (6)	0.023 (6)
C9A	0.078 (9)	0.043 (9)	0.145 (18)	−0.007 (8)	−0.013 (11)	0.005 (8)
C10A	0.068 (6)	0.053 (5)	0.079 (7)	0.006 (5)	0.014 (5)	0.013 (5)
C11A	0.042 (8)	0.064 (9)	0.066 (9)	−0.006 (7)	−0.012 (7)	0.008 (8)
C12A	0.067 (6)	0.063 (6)	0.082 (7)	0.009 (5)	0.025 (5)	0.008 (5)
C13A	0.094 (16)	0.10 (2)	0.111 (18)	−0.011 (15)	−0.009 (12)	0.010 (14)

Geometric parameters (Å, º)

Si1—C15	1.820 (3)	C4—H4B	0.9900
Si1—C18	1.851 (3)	C5—H5A	0.9800
Si1—C17	1.853 (3)	C5—H5B	0.9800
Si1—C16	1.853 (3)	C5—H5C	0.9800
Si2—C20	1.835 (3)	C6—C7	1.480 (6)
Si2—C23	1.856 (4)	C6—H6A	0.9900
Si2—C21	1.857 (4)	C6—H6B	0.9900
Si2—C22	1.868 (4)	C7—H7A	0.9800
Si3—C25	1.827 (3)	C7—H7B	0.9800
Si3—C28	1.852 (3)	C7—H7C	0.9800
Si3—C27	1.853 (3)	C8—C9	1.498 (7)

Si3—C26	1.862 (3)	C8—H8A	0.9900
Si4—C31A	1.817 (6)	C8—H8B	0.9900
Si4—C30	1.821 (3)	C9—H9A	0.9800
Si4—C32B	1.822 (6)	C9—H9B	0.9800
Si4—C31	1.831 (6)	C9—H9C	0.9800
Si4—C33A	1.859 (7)	C10—C11	1.491 (7)
Si4—C32	1.859 (6)	C10—H10A	0.9900
Si4—C32A	1.865 (7)	C10—H10B	0.9900
Si4—C33B	1.867 (7)	C11—H11A	0.9800
Si4—C31B	1.878 (7)	C11—H11B	0.9800
Si4—C33	1.897 (6)	C11—H11C	0.9800
B1—C24	1.594 (4)	C12—C13	1.490 (7)
B1—C14	1.596 (4)	C12—H12A	0.9900
B1—C19	1.599 (4)	C12—H12B	0.9900
B1—C29	1.601 (4)	C13—H13A	0.9800
C14—C15	1.216 (4)	C13—H13B	0.9800
C16—H16A	0.9800	C13—H13C	0.9800
C16—H16B	0.9800	N1A—C1A	1.347 (7)
C16—H16C	0.9800	N1A—C2A	1.468 (7)
C17—H17A	0.9800	N1A—C4A	1.486 (6)
C17—H17B	0.9800	N2A—C1A	1.348 (7)
C17—H17C	0.9800	N2A—C8A	1.473 (6)
C18—H18A	0.9800	N2A—C6A	1.476 (6)
C18—H18B	0.9800	N3A—C1A	1.341 (7)
C18—H18C	0.9800	N3A—C10A	1.477 (7)
C19—C20	1.216 (4)	N3A—C12A	1.480 (7)
C21—H21A	0.9800	C2A—C3A	1.500 (8)
C21—H21B	0.9800	C2A—H2A1	0.9900
C21—H21C	0.9800	C2A—H2A2	0.9900
C22—H22A	0.9800	C3A—H3A1	0.9800
C22—H22B	0.9800	C3A—H3A2	0.9800
C22—H22C	0.9800	C3A—H3A3	0.9800
C23—H23A	0.9800	C4A—C5A	1.487 (8)
C23—H23B	0.9800	C4A—H4A1	0.9900
C23—H23C	0.9800	C4A—H4A2	0.9900
C24—C25	1.213 (4)	C5A—H5A1	0.9800
C26—H26A	0.9800	C5A—H5A2	0.9800
C26—H26B	0.9800	C5A—H5A3	0.9800
C26—H26C	0.9800	C6A—C7A	1.494 (8)
C27—H27A	0.9800	C6A—H6A1	0.9900
C27—H27B	0.9800	C6A—H6A2	0.9900
C27—H27C	0.9800	C7A—H7A1	0.9800
C28—H28A	0.9800	C7A—H7A2	0.9800
C28—H28B	0.9800	C7A—H7A3	0.9800
C28—H28C	0.9800	C8A—C9A	1.491 (8)
C29—C30	1.206 (4)	C8A—H8A1	0.9900
C31—H31A	0.9800	C8A—H8A2	0.9900
C31—H31B	0.9800	C9A—H9A1	0.9800

C31—H31C	0.9800	C9A—H9A2	0.9800
C32—H32A	0.9800	C9A—H9A3	0.9800
C32—H32B	0.9800	C10A—C11A	1.492 (8)
C32—H32C	0.9800	C10A—H10C	0.9900
C33—H33A	0.9800	C10A—H10D	0.9900
C33—H33B	0.9800	C11A—H11D	0.9800
C33—H33C	0.9800	C11A—H11E	0.9800
C31A—H31D	0.9800	C11A—H11F	0.9800
C31A—H31E	0.9800	C12A—C13A	1.494 (8)
C31A—H31F	0.9800	C12A—H12C	0.9900
C32A—H32D	0.9800	C12A—H12D	0.9900
C32A—H32E	0.9800	C13A—H13D	0.9800
C32A—H32F	0.9800	C13A—H13E	0.9800
C33A—H33D	0.9800	C13A—H13F	0.9800
C33A—H33E	0.9800	O1—C34	1.389 (7)
C33A—H33F	0.9800	O1—C36	1.425 (7)
C31B—H31G	0.9800	C34—C35	1.481 (7)
C31B—H31H	0.9800	C34—H34A	0.9900
C31B—H31I	0.9800	C34—H34B	0.9900
C32B—H32G	0.9800	C35—H35A	0.9800
C32B—H32H	0.9800	C35—H35B	0.9800
C32B—H32I	0.9800	C35—H35C	0.9800
C33B—H33G	0.9800	C36—C37	1.481 (7)
C33B—H33H	0.9800	C36—H36A	0.9900
C33B—H33I	0.9800	C36—H36B	0.9900
N1—C1	1.350 (6)	C37—H37A	0.9800
N1—C2	1.477 (5)	C37—H37B	0.9800
N1—C4	1.481 (5)	C37—H37C	0.9800
N2—C1	1.349 (5)	O1A—C34A	1.399 (7)
N2—C8	1.473 (5)	O1A—C36A	1.424 (7)
N2—C6	1.474 (5)	C34A—C35A	1.487 (8)
N3—C1	1.336 (6)	C34A—H34C	0.9900
N3—C12	1.477 (5)	C34A—H34D	0.9900
N3—C10	1.478 (6)	C35A—H35D	0.9800
C2—C3	1.501 (6)	C35A—H35E	0.9800
C2—H2A	0.9900	C35A—H35F	0.9800
C2—H2B	0.9900	C36A—C37A	1.474 (7)
C3—H3A	0.9800	C36A—H36C	0.9900
C3—H3B	0.9800	C36A—H36D	0.9900
C3—H3C	0.9800	C37A—H37D	0.9800
C4—C5	1.503 (6)	C37A—H37E	0.9800
C4—H4A	0.9900	C37A—H37F	0.9800

C15—Si1—C18	109.65 (15)	C4—C5—H5A	109.5
C15—Si1—C17	110.70 (14)	C4—C5—H5B	109.5
C18—Si1—C17	108.61 (18)	H5A—C5—H5B	109.5
C15—Si1—C16	108.57 (16)	C4—C5—H5C	109.5
C18—Si1—C16	109.6 (2)	H5A—C5—H5C	109.5

C17—Si1—C16	109.7 (2)	H5B—C5—H5C	109.5
C20—Si2—C23	109.41 (17)	N2—C6—C7	112.4 (5)
C20—Si2—C21	110.26 (17)	N2—C6—H6A	109.1
C23—Si2—C21	109.8 (2)	C7—C6—H6A	109.1
C20—Si2—C22	110.32 (17)	N2—C6—H6B	109.1
C23—Si2—C22	109.7 (2)	C7—C6—H6B	109.1
C21—Si2—C22	107.3 (2)	H6A—C6—H6B	107.8
C25—Si3—C28	111.91 (15)	C6—C7—H7A	109.5
C25—Si3—C27	107.29 (15)	C6—C7—H7B	109.5
C28—Si3—C27	110.10 (16)	H7A—C7—H7B	109.5
C25—Si3—C26	107.79 (16)	C6—C7—H7C	109.5
C28—Si3—C26	109.1 (2)	H7A—C7—H7C	109.5
C27—Si3—C26	110.6 (2)	H7B—C7—H7C	109.5
C31A—Si4—C30	112.8 (4)	N2—C8—C9	111.7 (7)
C30—Si4—C32B	113.6 (5)	N2—C8—H8A	109.3
C30—Si4—C31	112.3 (3)	C9—C8—H8A	109.3
C31A—Si4—C33A	106.6 (7)	N2—C8—H8B	109.3
C30—Si4—C33A	108.1 (5)	C9—C8—H8B	109.3
C30—Si4—C32	108.1 (4)	H8A—C8—H8B	107.9
C31—Si4—C32	111.1 (4)	C8—C9—H9A	109.5
C31A—Si4—C32A	114.3 (6)	C8—C9—H9B	109.5
C30—Si4—C32A	105.1 (6)	H9A—C9—H9B	109.5
C33A—Si4—C32A	109.8 (6)	C8—C9—H9C	109.5
C30—Si4—C33B	111.5 (7)	H9A—C9—H9C	109.5
C32B—Si4—C33B	110.5 (6)	H9B—C9—H9C	109.5
C30—Si4—C31B	103.8 (7)	N3—C10—C11	113.1 (6)
C32B—Si4—C31B	110.3 (6)	N3—C10—H10A	109.0
C33B—Si4—C31B	106.8 (7)	C11—C10—H10A	109.0
C30—Si4—C33	110.0 (5)	N3—C10—H10B	109.0
C31—Si4—C33	107.6 (5)	C11—C10—H10B	109.0
C32—Si4—C33	107.6 (5)	H10A—C10—H10B	107.8
C24—B1—C14	111.0 (2)	C10—C11—H11A	109.5
C24—B1—C19	109.5 (2)	C10—C11—H11B	109.5
C14—B1—C19	111.5 (2)	H11A—C11—H11B	109.5
C24—B1—C29	105.5 (2)	C10—C11—H11C	109.5
C14—B1—C29	107.9 (2)	H11A—C11—H11C	109.5
C19—B1—C29	111.3 (2)	H11B—C11—H11C	109.5
C15—C14—B1	176.6 (3)	N3—C12—C13	114.8 (6)
C14—C15—Si1	175.0 (2)	N3—C12—H12A	108.6
Si1—C16—H16A	109.5	C13—C12—H12A	108.6
Si1—C16—H16B	109.5	N3—C12—H12B	108.6
H16A—C16—H16B	109.5	C13—C12—H12B	108.6
Si1—C16—H16C	109.5	H12A—C12—H12B	107.6
H16A—C16—H16C	109.5	C12—C13—H13A	109.5
H16B—C16—H16C	109.5	C12—C13—H13B	109.5
Si1—C17—H17A	109.5	H13A—C13—H13B	109.5
Si1—C17—H17B	109.5	C12—C13—H13C	109.5
H17A—C17—H17B	109.5	H13A—C13—H13C	109.5

Si1—C17—H17C	109.5	H13B—C13—H13C	109.5
H17A—C17—H17C	109.5	C1A—N1A—C2A	121.6 (9)
H17B—C17—H17C	109.5	C1A—N1A—C4A	120.3 (9)
Si1—C18—H18A	109.5	C2A—N1A—C4A	117.9 (9)
Si1—C18—H18B	109.5	C1A—N2A—C8A	121.3 (8)
H18A—C18—H18B	109.5	C1A—N2A—C6A	120.6 (8)
Si1—C18—H18C	109.5	C8A—N2A—C6A	118.2 (8)
H18A—C18—H18C	109.5	C1A—N3A—C10A	121.2 (8)
H18B—C18—H18C	109.5	C1A—N3A—C12A	121.8 (8)
C20—C19—B1	176.9 (3)	C10A—N3A—C12A	116.8 (7)
C19—C20—Si2	174.7 (3)	N3A—C1A—N1A	118.8 (8)
Si2—C21—H21A	109.5	N3A—C1A—N2A	120.4 (8)
Si2—C21—H21B	109.5	N1A—C1A—N2A	120.6 (8)
H21A—C21—H21B	109.5	N1A—C2A—C3A	111.8 (11)
Si2—C21—H21C	109.5	N1A—C2A—H2A1	109.2
H21A—C21—H21C	109.5	C3A—C2A—H2A1	109.2
H21B—C21—H21C	109.5	N1A—C2A—H2A2	109.2
Si2—C22—H22A	109.5	C3A—C2A—H2A2	109.2
Si2—C22—H22B	109.5	H2A1—C2A—H2A2	107.9
H22A—C22—H22B	109.5	C2A—C3A—H3A1	109.5
Si2—C22—H22C	109.5	C2A—C3A—H3A2	109.5
H22A—C22—H22C	109.5	H3A1—C3A—H3A2	109.5
H22B—C22—H22C	109.5	C2A—C3A—H3A3	109.5
Si2—C23—H23A	109.5	H3A1—C3A—H3A3	109.5
Si2—C23—H23B	109.5	H3A2—C3A—H3A3	109.5
H23A—C23—H23B	109.5	N1A—C4A—C5A	112.1 (8)
Si2—C23—H23C	109.5	N1A—C4A—H4A1	109.2
H23A—C23—H23C	109.5	C5A—C4A—H4A1	109.2
H23B—C23—H23C	109.5	N1A—C4A—H4A2	109.2
C25—C24—B1	174.8 (3)	C5A—C4A—H4A2	109.2
C24—C25—Si3	170.0 (3)	H4A1—C4A—H4A2	107.9
Si3—C26—H26A	109.5	C4A—C5A—H5A1	109.5
Si3—C26—H26B	109.5	C4A—C5A—H5A2	109.5
H26A—C26—H26B	109.5	H5A1—C5A—H5A2	109.5
Si3—C26—H26C	109.5	C4A—C5A—H5A3	109.5
H26A—C26—H26C	109.5	H5A1—C5A—H5A3	109.5
H26B—C26—H26C	109.5	H5A2—C5A—H5A3	109.5
Si3—C27—H27A	109.5	N2A—C6A—C7A	109.7 (8)
Si3—C27—H27B	109.5	N2A—C6A—H6A1	109.7
H27A—C27—H27B	109.5	C7A—C6A—H6A1	109.7
Si3—C27—H27C	109.5	N2A—C6A—H6A2	109.7
H27A—C27—H27C	109.5	C7A—C6A—H6A2	109.7
H27B—C27—H27C	109.5	H6A1—C6A—H6A2	108.2
Si3—C28—H28A	109.5	C6A—C7A—H7A1	109.5
Si3—C28—H28B	109.5	C6A—C7A—H7A2	109.5
H28A—C28—H28B	109.5	H7A1—C7A—H7A2	109.5
Si3—C28—H28C	109.5	C6A—C7A—H7A3	109.5
H28A—C28—H28C	109.5	H7A1—C7A—H7A3	109.5

H28B—C28—H28C	109.5	H7A2—C7A—H7A3	109.5
C30—C29—B1	174.5 (3)	N2A—C8A—C9A	113.1 (10)
C29—C30—Si4	171.5 (3)	N2A—C8A—H8A1	109.0
Si4—C31—H31A	109.5	C9A—C8A—H8A1	109.0
Si4—C31—H31B	109.5	N2A—C8A—H8A2	109.0
H31A—C31—H31B	109.5	C9A—C8A—H8A2	109.0
Si4—C31—H31C	109.5	H8A1—C8A—H8A2	107.8
H31A—C31—H31C	109.5	C8A—C9A—H9A1	109.5
H31B—C31—H31C	109.5	C8A—C9A—H9A2	109.5
Si4—C32—H32A	109.5	H9A1—C9A—H9A2	109.5
Si4—C32—H32B	109.5	C8A—C9A—H9A3	109.5
H32A—C32—H32B	109.5	H9A1—C9A—H9A3	109.5
Si4—C32—H32C	109.5	H9A2—C9A—H9A3	109.5
H32A—C32—H32C	109.5	N3A—C10A—C11A	112.9 (9)
H32B—C32—H32C	109.5	N3A—C10A—H10C	109.0
Si4—C33—H33A	109.5	C11A—C10A—H10C	109.0
Si4—C33—H33B	109.5	N3A—C10A—H10D	109.0
H33A—C33—H33B	109.5	C11A—C10A—H10D	109.0
Si4—C33—H33C	109.5	H10C—C10A—H10D	107.8
H33A—C33—H33C	109.5	C10A—C11A—H11D	109.5
H33B—C33—H33C	109.5	C10A—C11A—H11E	109.5
Si4—C31A—H31D	109.5	H11D—C11A—H11E	109.5
Si4—C31A—H31E	109.5	C10A—C11A—H11F	109.5
H31D—C31A—H31E	109.5	H11D—C11A—H11F	109.5
Si4—C31A—H31F	109.5	H11E—C11A—H11F	109.5
H31D—C31A—H31F	109.5	N3A—C12A—C13A	113.4 (11)
H31E—C31A—H31F	109.5	N3A—C12A—H12C	108.9
Si4—C32A—H32D	109.5	C13A—C12A—H12C	108.9
Si4—C32A—H32E	109.5	N3A—C12A—H12D	108.9
H32D—C32A—H32E	109.5	C13A—C12A—H12D	108.9
Si4—C32A—H32F	109.5	H12C—C12A—H12D	107.7
H32D—C32A—H32F	109.5	C12A—C13A—H13D	109.5
H32E—C32A—H32F	109.5	C12A—C13A—H13E	109.5
Si4—C33A—H33D	109.5	H13D—C13A—H13E	109.5
Si4—C33A—H33E	109.5	C12A—C13A—H13F	109.5
H33D—C33A—H33E	109.5	H13D—C13A—H13F	109.5
Si4—C33A—H33F	109.5	H13E—C13A—H13F	109.5
H33D—C33A—H33F	109.5	C34—O1—C36	111.4 (7)
H33E—C33A—H33F	109.5	O1—C34—C35	112.2 (9)
Si4—C31B—H31G	109.5	O1—C34—H34A	109.2
Si4—C31B—H31H	109.5	C35—C34—H34A	109.2
H31G—C31B—H31H	109.5	O1—C34—H34B	109.2
Si4—C31B—H31I	109.5	C35—C34—H34B	109.2
H31G—C31B—H31I	109.5	H34A—C34—H34B	107.9
H31H—C31B—H31I	109.5	C34—C35—H35A	109.5
Si4—C32B—H32G	109.5	C34—C35—H35B	109.5
Si4—C32B—H32H	109.5	H35A—C35—H35B	109.5
H32G—C32B—H32H	109.5	C34—C35—H35C	109.5

Si4—C32B—H32I	109.5	H35A—C35—H35C	109.5
H32G—C32B—H32I	109.5	H35B—C35—H35C	109.5
H32H—C32B—H32I	109.5	O1—C36—C37	103.8 (8)
Si4—C33B—H33G	109.5	O1—C36—H36A	111.0
Si4—C33B—H33H	109.5	C37—C36—H36A	111.0
H33G—C33B—H33H	109.5	O1—C36—H36B	111.0
Si4—C33B—H33I	109.5	C37—C36—H36B	111.0
H33G—C33B—H33I	109.5	H36A—C36—H36B	109.0
H33H—C33B—H33I	109.5	C36—C37—H37A	109.5
C1—N1—C2	120.8 (5)	C36—C37—H37B	109.5
C1—N1—C4	120.8 (5)	H37A—C37—H37B	109.5
C2—N1—C4	118.1 (5)	C36—C37—H37C	109.5
C1—N2—C8	120.9 (5)	H37A—C37—H37C	109.5
C1—N2—C6	120.9 (5)	H37B—C37—H37C	109.5
C8—N2—C6	118.0 (5)	C34A—O1A—C36A	113.2 (7)
C1—N3—C12	122.2 (5)	O1A—C34A—C35A	111.7 (9)
C1—N3—C10	121.2 (5)	O1A—C34A—H34C	109.3
C12—N3—C10	116.5 (5)	C35A—C34A—H34C	109.3
N3—C1—N2	120.5 (6)	O1A—C34A—H34D	109.3
N3—C1—N1	119.0 (5)	C35A—C34A—H34D	109.3
N2—C1—N1	120.4 (5)	H34C—C34A—H34D	107.9
N1—C2—C3	112.4 (4)	C34A—C35A—H35D	109.5
N1—C2—H2A	109.1	C34A—C35A—H35E	109.5
C3—C2—H2A	109.1	H35D—C35A—H35E	109.5
N1—C2—H2B	109.1	C34A—C35A—H35F	109.5
C3—C2—H2B	109.1	H35D—C35A—H35F	109.5
H2A—C2—H2B	107.9	H35E—C35A—H35F	109.5
C2—C3—H3A	109.5	O1A—C36A—C37A	107.2 (8)
C2—C3—H3B	109.5	O1A—C36A—H36C	110.3
H3A—C3—H3B	109.5	C37A—C36A—H36C	110.3
C2—C3—H3C	109.5	O1A—C36A—H36D	110.3
H3A—C3—H3C	109.5	C37A—C36A—H36D	110.3
H3B—C3—H3C	109.5	H36C—C36A—H36D	108.5
N1—C4—C5	112.0 (5)	C36A—C37A—H37D	109.5
N1—C4—H4A	109.2	C36A—C37A—H37E	109.5
C5—C4—H4A	109.2	H37D—C37A—H37E	109.5
N1—C4—H4B	109.2	C36A—C37A—H37F	109.5
C5—C4—H4B	109.2	H37D—C37A—H37F	109.5
H4A—C4—H4B	107.9	H37E—C37A—H37F	109.5

C12—N3—C1—N2	141.9 (7)	C10A—N3A—C1A—N2A	−136.7 (15)
C10—N3—C1—N2	−39.9 (11)	C12A—N3A—C1A—N2A	38 (2)
C12—N3—C1—N1	−37.3 (12)	C2A—N1A—C1A—N3A	39 (2)
C10—N3—C1—N1	140.9 (7)	C4A—N1A—C1A—N3A	−145.8 (12)
C8—N2—C1—N3	−34.2 (11)	C2A—N1A—C1A—N2A	−144.3 (15)
C6—N2—C1—N3	139.9 (7)	C4A—N1A—C1A—N2A	31 (2)
C8—N2—C1—N1	145.0 (8)	C8A—N2A—C1A—N3A	−144.4 (14)
C6—N2—C1—N1	−40.9 (10)	C6A—N2A—C1A—N3A	35 (2)

C2—N1—C1—N3	−36.6 (11)	C8A—N2A—C1A—N1A	39 (2)
C4—N1—C1—N3	150.0 (7)	C6A—N2A—C1A—N1A	−141.9 (14)
C2—N1—C1—N2	144.2 (7)	C1A—N1A—C2A—C3A	117.4 (16)
C4—N1—C1—N2	−29.2 (11)	C4A—N1A—C2A—C3A	−57.9 (17)
C1—N1—C2—C3	−120.6 (7)	C1A—N1A—C4A—C5A	109.6 (16)
C4—N1—C2—C3	52.9 (7)	C2A—N1A—C4A—C5A	−75.0 (16)
C1—N1—C4—C5	−131.3 (8)	C1A—N2A—C6A—C7A	118.3 (15)
C2—N1—C4—C5	55.1 (7)	C8A—N2A—C6A—C7A	−62.5 (15)
C1—N2—C6—C7	−96.0 (8)	C1A—N2A—C8A—C9A	127.0 (18)
C8—N2—C6—C7	78.2 (8)	C6A—N2A—C8A—C9A	−52.2 (17)
C1—N2—C8—C9	−119.0 (9)	C1A—N3A—C10A—C11A	98 (2)
C6—N2—C8—C9	66.8 (10)	C12A—N3A—C10A—C11A	−76.8 (19)
C1—N3—C10—C11	−106.5 (13)	C1A—N3A—C12A—C13A	108 (2)
C12—N3—C10—C11	71.9 (13)	C10A—N3A—C12A—C13A	−77 (2)
C1—N3—C12—C13	−115.5 (12)	C36—O1—C34—C35	−167.9 (16)
C10—N3—C12—C13	66.2 (11)	C34—O1—C36—C37	171.1 (13)
C10A—N3A—C1A—N1A	40 (2)	C36A—O1A—C34A—C35A	−162.3 (13)
C12A—N3A—C1A—N1A	−145.4 (14)	C34A—O1A—C36A—C37A	−162.8 (14)