IUCrData

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Bis[2,6-bis(trimethylsilylamino)pyridine-κN^1]-{[6-bis(trimethylsilylamino)pyridin-2-yl-κN^1]-(trimethylsilyl)azanido-κN}lithium

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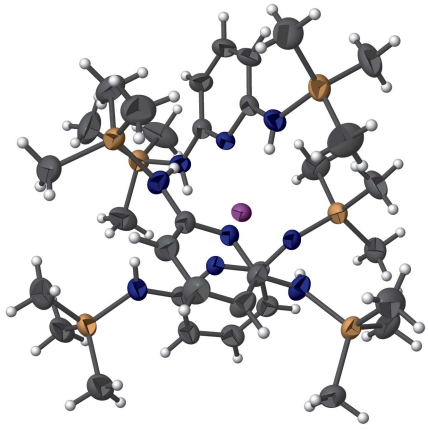
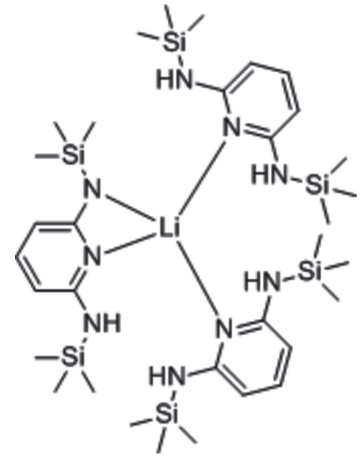
Structural data: full structural data are available from iucrdata.iucr.org

The title complex, $[Li(C_{11}H_{22}N_3Si_2)(C_{11}H_{23}N_3Si_2)_2]$, contains a single lithium cation coordinated to three ligands. This is the first reported example of the ligand 2,6-bis(trimethylsilylamino)pyridine supporting a monometallic complex. One ligand is mono-anionic and forms a four-membered chelate ring with the lithium cation *via* the pyridine and silylamido N atoms. The other two ligands are neutral and bind *via* the pyridine nitrogen. The lithium cation is coordinated in a tetrahedral environment. No intra- or intermolecular hydrogen bonding is observed in the crystal structure, likely indicating that weak electrostatic interactions are the dominant feature of the crystal packing.

3D view



Chemical scheme



Structure description

The title complex (Fig. 1) contrasts two previously reported lithium complexes that utilize the same 2,6-bis(trimethylsilylamino)pyridine ligand in that the complex reported herein is monometallic and excludes solvent coordination. Other examples include a tetranuclear complex bearing tetrahydrofuran ligands (Glatz & Kempe, 2008*a*) and a hexanuclear complex bearing benzonitrile ligands (Skvortsov *et al.*, 2013). The coordination environment is distorted tetrahedral with one anionic ligand occupying two coordination sites in a bidentate fashion and neutral ligands occupying the other two coordination sites. The bidentate ligand binds *via* the pyridyl nitrogen (N1) and the silylamido nitrogen (N2) with bond lengths of 2.006 (6) Å and 1.996 (6) Å, respectively. A four-membered chelate ring is formed between pyridyl N atom, Li^+, and silyl-amido N atom, with a bond angle N1—Li01—N2 = 69.6 (2)° indicative of ring strain. This four-membered chelate ring is observed in these other two lithium structures with similar bond angles. The bond

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Li(C_{11}H_{22}N_3Si_2)(C_{11}H_{23}N_3Si_2)_2]$
M_r	766.44
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, b, c (Å)	23.077 (11), 18.798 (9), 11.169 (6)
β (°)	98.744 (7)
V (Å^3)	4789 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.21
Crystal size (mm)	0.27 × 0.24 × 0.21
Data collection	
Diffractometer	Rigaku XtaLAB mini
Absorption correction	Multi-scan (*REQAB*; Rigaku, 1998)
T_{min}, T_{max}	0.868, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	41940, 10960, 6216
R_{int}	0.098
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.068, 0.175, 1.03
No. of reflections	10960
No. of parameters	462
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.38

Computer programs: *CrystalClear* (Rigaku, 2009), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009).

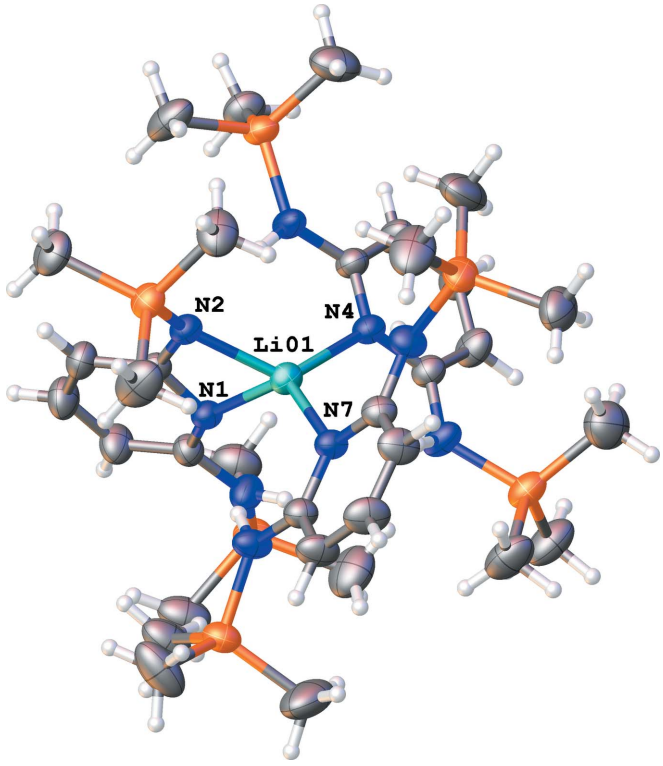


Figure 1
A view of the molecular structure of the title compound, with the Li and coordinating N atoms labeled. Displacement ellipsoids are drawn at the 50% probability level.

angle with the pyridyl N atoms of the two neutral ligands with the central Li^+ cation, N4—Li01—N7, is 112.9 (3)°.

While the title complex is monometallic, the ligand family is known to support a variety of metal nuclearities as exhibited by a dinuclear Co^{II} (Glatz & Kempe, 2008*b*), octanuclear Cu^{I} (Glatz & Kempe, 2008*c*), and a mixed-valent, dinuclear chromium complex (Huang *et al.*, 2012).

Synthesis and crystallization

2,6-Bis(trimethylsilylamino)pyridine was synthesized according to a previous report (Danièle *et al.*, 2001). The title complex was synthesized under an inert atmosphere by the addition of 4.27 ml of a 2.45 *M* solution of *n*-BuLi in cyclohexanes (10.5 mmol) to 0.513 g of 2,6-diaminopyridine (4.70 mmol) in tetrahydrofuran at −30°C. The reaction was stirred overnight at room temperature. The following day the tetrahydrofuran was removed under vacuum to yield a yellow oil. X-ray quality crystals of the title complex formed upon sitting over approximately two days.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

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full crystallographic data

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Crystal data

$[Li(C_{11}H_{22}N_3Si_2)(C_{11}H_{23}N_3Si_2)_2]$
M_r = 766.44
Monoclinic, $P2_1/c$
a = 23.077 (11) Å
b = 18.798 (9) Å
c = 11.169 (6) Å
β = 98.744 (7)°
V = 4789 (4) Å^3
Z = 4
$F(000)$ = 1664
D_x = 1.063 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7935 reflections
θ = 1.8–27.5°
μ = 0.21 mm^{-1}
T = 173 K
Prism, colourless
0.27 × 0.24 × 0.21 mm

Data collection

Rigaku XtaLAB mini diffractometer
Radiation source: Sealed Tube
Graphite Monochromator monochromator
Detector resolution: 13.6612 pixels mm^{-1}
profile data from ω–scans
Absorption correction: multi-scan (*REQAB*; Rigaku, 1998)
T_{min} = 0.868, T_{max} = 1.000
41940 measured reflections
10960 independent reflections
6216 reflections with $I > 2\sigma(I)$
R_{int} = 0.098
θ_{max} = 27.5°, θ_{min} = 2.1°
h = −29→29
k = −24→22
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.175
S = 1.03
10960 reflections
462 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2 + 2.1629P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Special details

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Si1	0.86556 (4)	0.47055 (5)	0.99863 (9)	0.0393 (2)
Si2	0.57717 (4)	0.67305 (6)	0.73332 (10)	0.0427 (3)
Si3	0.91106 (4)	0.68732 (5)	0.76465 (9)	0.0381 (2)
Si4	0.66066 (4)	0.47004 (6)	0.36428 (9)	0.0434 (3)
Si5	0.88418 (4)	0.38257 (6)	0.52716 (9)	0.0467 (3)
Si6	0.60570 (4)	0.38794 (6)	0.86619 (9)	0.0419 (3)
N1	0.72413 (10)	0.56916 (14)	0.8570 (2)	0.0313 (6)
N2	0.81604 (11)	0.52450 (14)	0.9160 (2)	0.0333 (6)
N3	0.63576 (11)	0.61564 (16)	0.7679 (2)	0.0424 (7)
H3	0.6383	0.5827	0.7168	0.064*
N4	0.77536 (11)	0.57212 (14)	0.6050 (2)	0.0322 (6)
N5	0.85024 (11)	0.63256 (15)	0.7260 (2)	0.0395 (7)
H5	0.8442	0.6030	0.7804	0.059*
N6	0.69833 (12)	0.50962 (15)	0.4947 (3)	0.0428 (8)
H6	0.7090 (5)	0.4791 (15)	0.544 (2)	0.064*
N7	0.74797 (10)	0.40533 (14)	0.7074 (2)	0.0313 (6)
N8	0.82413 (11)	0.40797 (16)	0.5957 (3)	0.0402 (7)
H8	0.8194	0.4501	0.5978	0.060*
N9	0.67205 (11)	0.40971 (16)	0.8212 (3)	0.0392 (7)
H9	0.6828 (5)	0.451 (2)	0.8335 (6)	0.059*
C1	0.77227 (13)	0.56443 (17)	0.9461 (3)	0.0311 (7)
C2	0.77178 (16)	0.60351 (19)	1.0540 (3)	0.0426 (9)
H2	0.8027	0.5997	1.1176	0.051*
C3	0.72523 (16)	0.6471 (2)	1.0639 (3)	0.0486 (9)
H3A	0.7252	0.6733	1.1345	0.058*
C4	0.67796 (16)	0.6532 (2)	0.9708 (3)	0.0481 (9)
H4	0.6465	0.6830	0.9777	0.058*
C5	0.67966 (14)	0.61301 (18)	0.8677 (3)	0.0347 (7)
C6	0.8304 (2)	0.3852 (2)	1.0311 (4)	0.0696 (13)
H6A	0.7996	0.3943	1.0782	0.104*
H6B	0.8591	0.3544	1.0756	0.104*
H6C	0.8142	0.3627	0.9562	0.104*
C7	0.92218 (17)	0.4501 (2)	0.9014 (4)	0.0613 (12)
H7A	0.9034	0.4359	0.8225	0.092*
H7B	0.9468	0.4123	0.9373	0.092*
H7C	0.9456	0.4917	0.8943	0.092*
C8	0.90367 (17)	0.5056 (2)	1.1466 (3)	0.0553 (11)
H8A	0.9211	0.5508	1.1340	0.083*
H8B	0.9336	0.4727	1.1802	0.083*
H8C	0.8758	0.5112	1.2016	0.083*
C9	0.52294 (16)	0.6624 (2)	0.8383 (4)	0.0622 (12)
H9A	0.5063	0.6155	0.8295	0.093*
H9B	0.4924	0.6971	0.8196	0.093*
H9C	0.5420	0.6689	0.9201	0.093*
C10	0.60288 (17)	0.7663 (2)	0.7371 (4)	0.0617 (11)

H10A	0.6171	0.7797	0.8192	0.093*
H10B	0.5710	0.7968	0.7048	0.093*
H10C	0.6339	0.7707	0.6892	0.093*
C11	0.54388 (19)	0.6480 (3)	0.5779 (4)	0.0764 (14)
H11A	0.5720	0.6546	0.5238	0.115*
H11B	0.5102	0.6773	0.5525	0.115*
H11C	0.5322	0.5989	0.5768	0.115*
C12	0.73411 (14)	0.56889 (18)	0.5048 (3)	0.0359 (8)
C13	0.72796 (16)	0.6213 (2)	0.4174 (3)	0.0462 (9)
H13	0.6997	0.6175	0.3489	0.055*
C14	0.76453 (16)	0.6793 (2)	0.4335 (3)	0.0479 (9)
H14	0.7610	0.7153	0.3758	0.057*
C15	0.80653 (16)	0.68420 (19)	0.5352 (3)	0.0451 (9)
H15	0.8316	0.7231	0.5465	0.054*
C16	0.81064 (14)	0.62973 (18)	0.6208 (3)	0.0355 (8)
C17	0.59410 (17)	0.5208 (2)	0.3040 (4)	0.0679 (13)
H17A	0.5716	0.5299	0.3680	0.102*
H17B	0.5709	0.4938	0.2412	0.102*
H17C	0.6052	0.5652	0.2714	0.102*
C18	0.7089 (2)	0.4616 (3)	0.2472 (4)	0.0751 (14)
H18A	0.7177	0.5081	0.2191	0.113*
H18B	0.6894	0.4341	0.1805	0.113*
H18C	0.7446	0.4383	0.2811	0.113*
C19	0.6407 (2)	0.3813 (2)	0.4143 (4)	0.0705 (13)
H19A	0.6757	0.3546	0.4413	0.106*
H19B	0.6176	0.3570	0.3480	0.106*
H19C	0.6184	0.3862	0.4797	0.106*
C20	0.94094 (18)	0.6612 (2)	0.9210 (4)	0.0639 (12)
H20A	0.9119	0.6691	0.9727	0.096*
H20B	0.9751	0.6892	0.9490	0.096*
H20C	0.9514	0.6118	0.9228	0.096*
C21	0.89256 (16)	0.78330 (19)	0.7621 (4)	0.0503 (10)
H21A	0.8808	0.7984	0.6799	0.075*
H21B	0.9263	0.8101	0.7975	0.075*
H21C	0.8610	0.7912	0.8076	0.075*
C22	0.96453 (17)	0.6708 (2)	0.6595 (4)	0.0665 (12)
H22A	0.9794	0.6232	0.6706	0.100*
H22B	0.9964	0.7040	0.6759	0.100*
H22C	0.9455	0.6766	0.5775	0.100*
C23	0.70768 (14)	0.36972 (18)	0.7600 (3)	0.0359 (8)
C24	0.70295 (16)	0.29586 (19)	0.7529 (4)	0.0465 (9)
H24	0.6753	0.2717	0.7899	0.056*
C25	0.74028 (16)	0.2599 (2)	0.6897 (4)	0.0507 (10)
H25	0.7376	0.2106	0.6837	0.061*
C26	0.78129 (15)	0.29480 (18)	0.6353 (3)	0.0451 (9)
H26	0.8063	0.2701	0.5923	0.054*
C27	0.78429 (13)	0.36808 (18)	0.6464 (3)	0.0354 (8)
C28	0.9198 (2)	0.4682 (3)	0.5049 (4)	0.0785 (15)

H28A	0.8921	0.4993	0.4579	0.118*
H28B	0.9526	0.4603	0.4629	0.118*
H28C	0.9332	0.4895	0.5822	0.118*
C29	0.86057 (18)	0.3373 (3)	0.3808 (4)	0.0672 (13)
H29A	0.8385	0.2954	0.3940	0.101*
H29B	0.8944	0.3240	0.3455	0.101*
H29C	0.8365	0.3689	0.3270	0.101*
C30	0.93327 (18)	0.3224 (3)	0.6274 (4)	0.0770 (15)
H30A	0.9481	0.3467	0.7013	0.115*
H30B	0.9654	0.3082	0.5874	0.115*
H30C	0.9118	0.2810	0.6455	0.115*
C31	0.55496 (19)	0.3578 (3)	0.7314 (5)	0.0914 (18)
H31A	0.5492	0.3954	0.6728	0.137*
H31B	0.5180	0.3450	0.7548	0.137*
H31C	0.5714	0.3171	0.6966	0.137*
C32	0.6134 (2)	0.3186 (2)	0.9855 (4)	0.0798 (15)
H32A	0.6389	0.2817	0.9652	0.120*
H32B	0.5756	0.2988	0.9914	0.120*
H32C	0.6296	0.3394	1.0618	0.120*
C33	0.57894 (18)	0.4703 (2)	0.9278 (4)	0.0623 (12)
H33A	0.6073	0.4870	0.9937	0.093*
H33B	0.5425	0.4610	0.9566	0.093*
H33C	0.5730	0.5058	0.8655	0.093*
Li01	0.7685 (2)	0.5091 (3)	0.7532 (5)	0.0333 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0402 (5)	0.0385 (6)	0.0367 (5)	0.0034 (4)	−0.0023 (4)	0.0037 (4)
Si2	0.0319 (5)	0.0435 (6)	0.0523 (6)	0.0052 (4)	0.0056 (4)	0.0015 (5)
Si3	0.0327 (5)	0.0378 (6)	0.0421 (5)	−0.0072 (4)	0.0006 (4)	0.0017 (4)
Si4	0.0415 (5)	0.0367 (6)	0.0474 (6)	−0.0002 (4)	−0.0079 (4)	−0.0027 (4)
Si5	0.0333 (5)	0.0620 (8)	0.0459 (6)	0.0055 (5)	0.0098 (4)	−0.0105 (5)
Si6	0.0351 (5)	0.0420 (6)	0.0508 (6)	−0.0025 (4)	0.0139 (4)	0.0021 (5)
N1	0.0279 (13)	0.0319 (15)	0.0337 (14)	−0.0011 (11)	0.0035 (11)	−0.0014 (11)
N2	0.0298 (14)	0.0339 (16)	0.0347 (14)	−0.0003 (12)	0.0004 (11)	0.0011 (12)
N3	0.0355 (15)	0.0501 (19)	0.0405 (16)	0.0087 (14)	0.0015 (12)	−0.0080 (14)
N4	0.0278 (13)	0.0313 (15)	0.0364 (15)	0.0000 (11)	0.0011 (11)	0.0003 (12)
N5	0.0393 (15)	0.0420 (18)	0.0348 (15)	−0.0142 (13)	−0.0016 (12)	0.0067 (13)
N6	0.0431 (17)	0.0342 (17)	0.0460 (17)	−0.0053 (13)	−0.0098 (13)	0.0061 (13)
N7	0.0293 (13)	0.0264 (15)	0.0384 (15)	0.0011 (11)	0.0060 (11)	−0.0011 (11)
N8	0.0347 (15)	0.0375 (17)	0.0505 (18)	0.0043 (13)	0.0128 (13)	−0.0011 (14)
N9	0.0339 (15)	0.0295 (16)	0.0567 (19)	−0.0028 (12)	0.0148 (13)	−0.0046 (13)
C1	0.0332 (16)	0.0273 (17)	0.0328 (17)	−0.0046 (14)	0.0052 (13)	0.0005 (13)
C2	0.048 (2)	0.045 (2)	0.0335 (18)	−0.0005 (17)	0.0010 (15)	−0.0049 (16)
C3	0.055 (2)	0.055 (3)	0.037 (2)	0.0086 (19)	0.0075 (17)	−0.0097 (17)
C4	0.043 (2)	0.059 (3)	0.042 (2)	0.0126 (18)	0.0080 (16)	−0.0080 (18)
C5	0.0346 (17)	0.037 (2)	0.0330 (17)	0.0016 (15)	0.0068 (13)	−0.0013 (14)

C6	0.086 (3)	0.049 (3)	0.068 (3)	−0.010 (2)	−0.008 (2)	0.019 (2)
C7	0.050 (2)	0.074 (3)	0.058 (3)	0.026 (2)	0.0031 (19)	−0.002 (2)
C8	0.056 (2)	0.059 (3)	0.044 (2)	0.009 (2)	−0.0112 (18)	0.0037 (19)
C9	0.044 (2)	0.051 (3)	0.097 (3)	0.0056 (19)	0.028 (2)	0.005 (2)
C10	0.054 (2)	0.050 (3)	0.082 (3)	0.001 (2)	0.017 (2)	0.008 (2)
C11	0.063 (3)	0.089 (4)	0.069 (3)	0.020 (3)	−0.016 (2)	−0.006 (3)
C12	0.0327 (17)	0.036 (2)	0.0378 (18)	0.0009 (15)	0.0004 (14)	0.0011 (15)
C13	0.050 (2)	0.042 (2)	0.042 (2)	−0.0002 (17)	−0.0087 (16)	0.0063 (16)
C14	0.058 (2)	0.044 (2)	0.039 (2)	−0.0017 (18)	−0.0023 (17)	0.0114 (17)
C15	0.052 (2)	0.041 (2)	0.039 (2)	−0.0161 (17)	−0.0026 (16)	0.0077 (16)
C16	0.0330 (17)	0.036 (2)	0.0359 (18)	−0.0050 (14)	0.0011 (14)	0.0012 (14)
C17	0.057 (3)	0.061 (3)	0.076 (3)	0.007 (2)	−0.022 (2)	−0.013 (2)
C18	0.080 (3)	0.072 (3)	0.075 (3)	−0.001 (3)	0.019 (3)	−0.015 (3)
C19	0.075 (3)	0.051 (3)	0.077 (3)	−0.017 (2)	−0.015 (2)	0.000 (2)
C20	0.066 (3)	0.052 (3)	0.064 (3)	−0.015 (2)	−0.022 (2)	0.006 (2)
C21	0.053 (2)	0.037 (2)	0.060 (2)	−0.0039 (18)	0.0019 (18)	−0.0035 (18)
C22	0.048 (2)	0.065 (3)	0.092 (3)	−0.006 (2)	0.029 (2)	−0.009 (3)
C23	0.0312 (17)	0.036 (2)	0.0409 (19)	−0.0013 (14)	0.0067 (14)	−0.0011 (15)
C24	0.044 (2)	0.030 (2)	0.067 (3)	−0.0069 (16)	0.0155 (18)	−0.0029 (18)
C25	0.049 (2)	0.027 (2)	0.076 (3)	0.0007 (17)	0.010 (2)	−0.0030 (18)
C26	0.045 (2)	0.029 (2)	0.063 (2)	0.0072 (16)	0.0151 (17)	−0.0058 (17)
C27	0.0302 (17)	0.0333 (19)	0.0423 (19)	0.0042 (14)	0.0037 (14)	0.0016 (15)
C28	0.069 (3)	0.091 (4)	0.086 (3)	−0.024 (3)	0.046 (3)	−0.019 (3)
C29	0.061 (3)	0.086 (4)	0.056 (3)	0.005 (2)	0.013 (2)	−0.021 (2)
C30	0.050 (3)	0.102 (4)	0.076 (3)	0.033 (3)	−0.001 (2)	−0.015 (3)
C31	0.047 (3)	0.118 (5)	0.105 (4)	−0.016 (3)	0.000 (3)	−0.033 (4)
C32	0.111 (4)	0.058 (3)	0.084 (3)	0.020 (3)	0.057 (3)	0.020 (3)
C33	0.063 (3)	0.050 (3)	0.082 (3)	0.005 (2)	0.039 (2)	0.004 (2)
Li01	0.034 (3)	0.029 (3)	0.037 (3)	0.002 (2)	0.004 (2)	−0.002 (2)

Geometric parameters (Å, º)

Si1—N2	1.693 (3)	C8—H8C	0.9600
Si1—C6	1.859 (4)	C9—H9A	0.9600
Si1—C7	1.861 (4)	C9—H9B	0.9600
Si1—C8	1.870 (4)	C9—H9C	0.9600
Si2—N3	1.727 (3)	C10—H10A	0.9600
Si2—C9	1.851 (4)	C10—H10B	0.9600
Si2—C10	1.848 (4)	C10—H10C	0.9600
Si2—C11	1.850 (4)	C11—H11A	0.9600
Si3—N5	1.741 (3)	C11—H11B	0.9600
Si3—C20	1.844 (4)	C11—H11C	0.9600
Si3—C21	1.853 (4)	C12—C13	1.380 (5)
Si3—C22	1.855 (4)	C13—H13	0.9300
Si4—N6	1.745 (3)	C13—C14	1.374 (5)
Si4—C17	1.847 (4)	C14—H14	0.9300
Si4—C18	1.849 (5)	C14—C15	1.379 (5)
Si4—C19	1.839 (4)	C15—H15	0.9300

Si5—N8	1.748 (3)	C15—C16	1.394 (4)
Si5—C28	1.840 (5)	C17—H17A	0.9600
Si5—C29	1.850 (4)	C17—H17B	0.9600
Si5—C30	1.853 (4)	C17—H17C	0.9600
Si6—N9	1.731 (3)	C18—H18A	0.9600
Si6—C31	1.851 (4)	C18—H18B	0.9600
Si6—C32	1.853 (4)	C18—H18C	0.9600
Si6—C33	1.839 (4)	C19—H19A	0.9600
N1—C1	1.377 (4)	C19—H19B	0.9600
N1—C5	1.336 (4)	C19—H19C	0.9600
N1—Li01	2.006 (6)	C20—H20A	0.9600
N2—C1	1.342 (4)	C20—H20B	0.9600
N2—Li01	1.996 (6)	C20—H20C	0.9600
N3—H3	0.8500	C21—H21A	0.9600
N3—C5	1.389 (4)	C21—H21B	0.9600
N4—C12	1.356 (4)	C21—H21C	0.9600
N4—C16	1.350 (4)	C22—H22A	0.9600
N4—Li01	2.061 (6)	C22—H22B	0.9600
N5—H5	0.8500	C22—H22C	0.9600
N5—C16	1.376 (4)	C23—C24	1.394 (5)
N6—H6	0.81 (4)	C24—H24	0.9300
N6—C12	1.381 (4)	C24—C25	1.372 (5)
N7—C23	1.351 (4)	C25—H25	0.9300
N7—C27	1.353 (4)	C25—C26	1.367 (5)
N7—Li01	2.054 (6)	C26—H26	0.9300
N8—H8	0.8001	C26—C27	1.384 (5)
N8—C27	1.373 (4)	C28—H28A	0.9600
N9—H9	0.82 (4)	C28—H28B	0.9600
N9—C23	1.371 (4)	C28—H28C	0.9600
C1—C2	1.413 (4)	C29—H29A	0.9600
C2—H2	0.9300	C29—H29B	0.9600
C2—C3	1.369 (5)	C29—H29C	0.9600
C3—H3A	0.9300	C30—H30A	0.9600
C3—C4	1.392 (5)	C30—H30B	0.9600
C4—H4	0.9300	C30—H30C	0.9600
C4—C5	1.383 (5)	C31—H31A	0.9600
C6—H6A	0.9600	C31—H31B	0.9600
C6—H6B	0.9600	C31—H31C	0.9600
C6—H6C	0.9600	C32—H32A	0.9600
C7—H7A	0.9600	C32—H32B	0.9600
C7—H7B	0.9600	C32—H32C	0.9600
C7—H7C	0.9600	C33—H33A	0.9600
C8—H8A	0.9600	C33—H33B	0.9600
C8—H8B	0.9600	C33—H33C	0.9600

N2—Si1—C6	110.16 (17)	H11A—C11—H11B	109.5
N2—Si1—C7	106.31 (16)	H11A—C11—H11C	109.5
N2—Si1—C8	117.32 (16)	H11B—C11—H11C	109.5

C6—Si1—C7	107.6 (2)	N4—C12—N6	116.1 (3)
C6—Si1—C8	107.00 (19)	N4—C12—C13	122.4 (3)
C7—Si1—C8	108.10 (19)	C13—C12—N6	121.5 (3)
N3—Si2—C9	111.87 (17)	C12—C13—H13	120.7
N3—Si2—C10	110.47 (17)	C14—C13—C12	118.6 (3)
N3—Si2—C11	104.45 (18)	C14—C13—H13	120.7
C10—Si2—C9	109.5 (2)	C13—C14—H14	119.9
C10—Si2—C11	110.4 (2)	C13—C14—C15	120.1 (3)
C11—Si2—C9	110.0 (2)	C15—C14—H14	119.9
N5—Si3—C20	104.40 (16)	C14—C15—H15	120.6
N5—Si3—C21	113.37 (16)	C14—C15—C16	118.8 (3)
N5—Si3—C22	109.44 (17)	C16—C15—H15	120.6
C20—Si3—C21	109.00 (19)	N4—C16—N5	116.8 (3)
C20—Si3—C22	111.5 (2)	N4—C16—C15	121.5 (3)
C21—Si3—C22	109.1 (2)	N5—C16—C15	121.6 (3)
N6—Si4—C17	111.42 (17)	Si4—C17—H17A	109.5
N6—Si4—C18	110.48 (19)	Si4—C17—H17B	109.5
N6—Si4—C19	104.41 (17)	Si4—C17—H17C	109.5
C17—Si4—C18	110.1 (2)	H17A—C17—H17B	109.5
C19—Si4—C17	110.3 (2)	H17A—C17—H17C	109.5
C19—Si4—C18	110.1 (2)	H17B—C17—H17C	109.5
N8—Si5—C28	102.72 (18)	Si4—C18—H18A	109.5
N8—Si5—C29	111.47 (17)	Si4—C18—H18B	109.5
N8—Si5—C30	110.78 (18)	Si4—C18—H18C	109.5
C28—Si5—C29	111.1 (2)	H18A—C18—H18B	109.5
C28—Si5—C30	111.8 (2)	H18A—C18—H18C	109.5
C29—Si5—C30	108.9 (2)	H18B—C18—H18C	109.5
N9—Si6—C31	108.3 (2)	Si4—C19—H19A	109.5
N9—Si6—C32	112.51 (19)	Si4—C19—H19B	109.5
N9—Si6—C33	105.77 (17)	Si4—C19—H19C	109.5
C31—Si6—C32	110.4 (3)	H19A—C19—H19B	109.5
C33—Si6—C31	110.8 (2)	H19A—C19—H19C	109.5
C33—Si6—C32	108.9 (2)	H19B—C19—H19C	109.5
C1—N1—Li01	87.4 (2)	Si3—C20—H20A	109.5
C5—N1—C1	121.4 (3)	Si3—C20—H20B	109.5
C5—N1—Li01	149.9 (3)	Si3—C20—H20C	109.5
Si1—N2—Li01	129.9 (2)	H20A—C20—H20B	109.5
C1—N2—Si1	132.1 (2)	H20A—C20—H20C	109.5
C1—N2—Li01	88.8 (2)	H20B—C20—H20C	109.5
Si2—N3—H3	115.9	Si3—C21—H21A	109.5
C5—N3—Si2	130.7 (2)	Si3—C21—H21B	109.5
C5—N3—H3	113.3	Si3—C21—H21C	109.5
C12—N4—Li01	120.5 (3)	H21A—C21—H21B	109.5
C16—N4—C12	118.5 (3)	H21A—C21—H21C	109.5
C16—N4—Li01	118.3 (3)	H21B—C21—H21C	109.5
Si3—N5—H5	115.0	Si3—C22—H22A	109.5
C16—N5—Si3	129.8 (2)	Si3—C22—H22B	109.5
C16—N5—H5	115.2	Si3—C22—H22C	109.5

Si4—N6—H6	109.3	H22A—C22—H22B	109.5
C12—N6—Si4	128.9 (2)	H22A—C22—H22C	109.5
C12—N6—H6	113.6	H22B—C22—H22C	109.5
C23—N7—C27	118.9 (3)	N7—C23—N9	116.7 (3)
C23—N7—Li01	120.7 (3)	N7—C23—C24	121.4 (3)
C27—N7—Li01	118.7 (3)	N9—C23—C24	121.8 (3)
Si5—N8—H8	113.8	C23—C24—H24	121.0
C27—N8—Si5	131.0 (2)	C25—C24—C23	118.1 (3)
C27—N8—H8	115.2	C25—C24—H24	121.0
Si6—N9—H9	115.7	C24—C25—H25	119.2
C23—N9—Si6	129.7 (2)	C26—C25—C24	121.5 (4)
C23—N9—H9	114.4	C26—C25—H25	119.2
N1—C1—C2	118.2 (3)	C25—C26—H26	121.1
N2—C1—N1	114.2 (3)	C25—C26—C27	117.8 (3)
N2—C1—C2	127.5 (3)	C27—C26—H26	121.1
C1—C2—H2	120.4	N7—C27—N8	115.4 (3)
C3—C2—C1	119.2 (3)	N7—C27—C26	122.3 (3)
C3—C2—H2	120.4	N8—C27—C26	122.3 (3)
C2—C3—H3A	119.2	Si5—C28—H28A	109.5
C2—C3—C4	121.6 (3)	Si5—C28—H28B	109.5
C4—C3—H3A	119.2	Si5—C28—H28C	109.5
C3—C4—H4	121.3	H28A—C28—H28B	109.5
C5—C4—C3	117.3 (3)	H28A—C28—H28C	109.5
C5—C4—H4	121.3	H28B—C28—H28C	109.5
N1—C5—N3	115.3 (3)	Si5—C29—H29A	109.5
N1—C5—C4	122.1 (3)	Si5—C29—H29B	109.5
C4—C5—N3	122.7 (3)	Si5—C29—H29C	109.5
Si1—C6—H6A	109.5	H29A—C29—H29B	109.5
Si1—C6—H6B	109.5	H29A—C29—H29C	109.5
Si1—C6—H6C	109.5	H29B—C29—H29C	109.5
H6A—C6—H6B	109.5	Si5—C30—H30A	109.5
H6A—C6—H6C	109.5	Si5—C30—H30B	109.5
H6B—C6—H6C	109.5	Si5—C30—H30C	109.5
Si1—C7—H7A	109.5	H30A—C30—H30B	109.5
Si1—C7—H7B	109.5	H30A—C30—H30C	109.5
Si1—C7—H7C	109.5	H30B—C30—H30C	109.5
H7A—C7—H7B	109.5	Si6—C31—H31A	109.5
H7A—C7—H7C	109.5	Si6—C31—H31B	109.5
H7B—C7—H7C	109.5	Si6—C31—H31C	109.5
Si1—C8—H8A	109.5	H31A—C31—H31B	109.5
Si1—C8—H8B	109.5	H31A—C31—H31C	109.5
Si1—C8—H8C	109.5	H31B—C31—H31C	109.5
H8A—C8—H8B	109.5	Si6—C32—H32A	109.5
H8A—C8—H8C	109.5	Si6—C32—H32B	109.5
H8B—C8—H8C	109.5	Si6—C32—H32C	109.5
Si2—C9—H9A	109.5	H32A—C32—H32B	109.5
Si2—C9—H9B	109.5	H32A—C32—H32C	109.5
Si2—C9—H9C	109.5	H32B—C32—H32C	109.5

H9A—C9—H9B	109.5	Si6—C33—H33A	109.5
H9A—C9—H9C	109.5	Si6—C33—H33B	109.5
H9B—C9—H9C	109.5	Si6—C33—H33C	109.5
Si2—C10—H10A	109.5	H33A—C33—H33B	109.5
Si2—C10—H10B	109.5	H33A—C33—H33C	109.5
Si2—C10—H10C	109.5	H33B—C33—H33C	109.5
H10A—C10—H10B	109.5	N1—Li01—N4	104.4 (3)
H10A—C10—H10C	109.5	N1—Li01—N7	124.0 (3)
H10B—C10—H10C	109.5	N2—Li01—N1	69.6 (2)
Si2—C11—H11A	109.5	N2—Li01—N4	123.3 (3)
Si2—C11—H11B	109.5	N2—Li01—N7	116.0 (3)
Si2—C11—H11C	109.5	N7—Li01—N4	112.9 (3)

Si1—N2—C1—N1	−146.0 (2)	C14—C15—C16—N4	1.3 (6)
Si1—N2—C1—C2	37.2 (5)	C14—C15—C16—N5	−177.8 (3)
Si2—N3—C5—N1	−169.2 (3)	C16—N4—C12—N6	−178.5 (3)
Si2—N3—C5—C4	10.4 (5)	C16—N4—C12—C13	1.7 (5)
Si3—N5—C16—N4	165.9 (2)	C17—Si4—N6—C12	−77.0 (4)
Si3—N5—C16—C15	−14.9 (5)	C18—Si4—N6—C12	45.7 (4)
Si4—N6—C12—N4	−154.3 (3)	C19—Si4—N6—C12	164.0 (3)
Si4—N6—C12—C13	25.5 (5)	C20—Si3—N5—C16	178.7 (3)
Si5—N8—C27—N7	170.9 (2)	C21—Si3—N5—C16	60.2 (4)
Si5—N8—C27—C26	−9.4 (5)	C22—Si3—N5—C16	−61.9 (4)
Si6—N9—C23—N7	162.0 (2)	C23—N7—C27—N8	−179.8 (3)
Si6—N9—C23—C24	−18.3 (5)	C23—N7—C27—C26	0.5 (5)
N1—C1—C2—C3	−3.2 (5)	C23—C24—C25—C26	0.3 (6)
N2—C1—C2—C3	173.5 (3)	C24—C25—C26—C27	0.3 (6)
N4—C12—C13—C14	−0.9 (6)	C25—C26—C27—N7	−0.7 (5)
N6—C12—C13—C14	179.3 (3)	C25—C26—C27—N8	179.6 (3)
N7—C23—C24—C25	−0.5 (5)	C27—N7—C23—N9	179.8 (3)
N9—C23—C24—C25	179.9 (3)	C27—N7—C23—C24	0.1 (5)
C1—N1—C5—N3	176.1 (3)	C28—Si5—N8—C27	−172.1 (3)
C1—N1—C5—C4	−3.4 (5)	C29—Si5—N8—C27	68.9 (4)
C1—C2—C3—C4	0.9 (6)	C30—Si5—N8—C27	−52.5 (4)
C2—C3—C4—C5	0.3 (6)	C31—Si6—N9—C23	−54.8 (4)
C3—C4—C5—N1	0.9 (6)	C32—Si6—N9—C23	67.6 (4)
C3—C4—C5—N3	−178.6 (3)	C33—Si6—N9—C23	−173.7 (3)
C5—N1—C1—N2	−172.6 (3)	Li01—N1—C1—N2	−1.7 (3)
C5—N1—C1—C2	4.5 (5)	Li01—N1—C1—C2	175.4 (3)
C6—Si1—N2—C1	76.3 (3)	Li01—N1—C5—N3	14.5 (7)
C6—Si1—N2—Li01	−59.6 (3)	Li01—N1—C5—C4	−165.0 (5)
C7—Si1—N2—C1	−167.4 (3)	Li01—N2—C1—N1	1.7 (3)
C7—Si1—N2—Li01	56.7 (3)	Li01—N2—C1—C2	−175.1 (4)
C8—Si1—N2—C1	−46.4 (4)	Li01—N4—C12—N6	−17.4 (4)
C8—Si1—N2—Li01	177.7 (3)	Li01—N4—C12—C13	162.8 (3)
C9—Si2—N3—C5	−67.0 (4)	Li01—N4—C16—N5	15.7 (4)
C10—Si2—N3—C5	55.2 (4)	Li01—N4—C16—C15	−163.4 (3)
C11—Si2—N3—C5	174.0 (3)	Li01—N7—C23—N9	15.1 (4)

C12—N4—C16—N5	177.3 (3)	Li01—N7—C23—C24	−164.5 (3)
C12—N4—C16—C15	−1.9 (5)	Li01—N7—C27—N8	−14.9 (4)
C12—C13—C14—C15	0.3 (6)	Li01—N7—C27—C26	165.4 (3)
C13—C14—C15—C16	−0.5 (6)		