Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Di-μ-chlorido-bis({2-[(triisopropylsilyl)-aminomethyl]pyridine-κN}lithium(I))

Christian Koch, Helmar Görls and Matthias Westerhausen*

Institute of Inorganic and Analytical Chemistry, Friedrich-Schiller-Universität Jena, August-Bebel-Strasse 2, D-07743 Jena, Germany
Correspondence e-mail: m.we@uni-jena.de

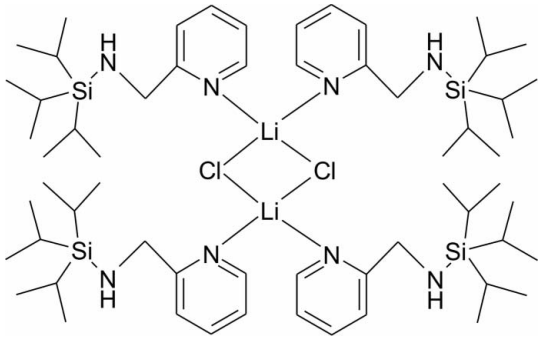
Received 20 September 2007; accepted 21 September 2007

Key indicators: single-crystal X-ray study; T = 183 K; mean σ(C–C) = 0.007 Å; R factor = 0.076; wR factor = 0.215; data-to-parameter ratio = 19.3.

The title compound, $[Li_2Cl_2(C_{15}H_{38}N_2Si)_4]$, is a centrosymmetric dimer. Each Li atom is coordinated in a distorted tetrahedral manner by two pyridyl rings and two chloride anions. Only one of the two symmetry-independent NH groups is involved in hydrogen bonding.

Related literature

For related literature, see: Baker *et al.* (2005); Bickley *et al.* (2004); Buttery *et al.* (2006); Chen *et al.* (2002); DeAngelis *et al.* (1992); Engelhardt *et al.* (1988, 1990); Hahn & Rupprecht (1991); Ho *et al.* (1993); Pratt *et al.* (2006); Solari *et al.* (1992); Tayebani *et al.* (1998); Westerhausen *et al.* (2002, 2004, 2006).



Experimental

Crystal data

$[Li_2Cl_2(C_{15}H_{38}N_2Si)_4]$
M_r = 1142.72
Triclinic, $P\overline{1}$
a = 9.6312 (19) Å
b = 13.806 (3) Å
c = 14.802 (3) Å
α = 113.036 (10)°
β = 95.653 (17)°
γ = 102.388 (12)°
V = 1732.2 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 183 (2) K
0.05 × 0.05 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
10497 measured reflections
6997 independent reflections
4247 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.215
S = 1.05
6997 reflections
363 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2A—H1NA···Cl1	0.81 (5)	2.73 (6)	3.430 (5)	146 (4)

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Siemens, 1990); software used to prepare material for publication: *SHELXL97*.

The authors thank the Deutsche Forschungsgemeinschaft (DFG, Bonn–Bad Godesberg, Germany) and the Fonds der Chemischen Industrie (Frankfurt/Main, Germany) for generous financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2518).

References

Baker, R. J., Jones, C., Mills, D. P., Murphey, D. M., Hey-Hawkins, E. & Wolf, R. (2005). *Dalton Trans.* pp. 64–72.
Bickley, J. F., Copsey, M. C., Jeffery, J. C., Leedham, A. P., Russell, C. A., Stalke, D., Steiner, A., Stey, T. & Zacchini, S. (2004). *Dalton Trans.* pp. 989–995.
Buttery, J. H. N., Effendy, H. P., Mutrofin, S., Plackett, N. C., Skelton, B. W., Somers, N., Whitaker, C. R. & White, A. H. (2006). *Z. Anorg. Allg. Chem.* **632**, 1839–1850.
Chen, X., Du, C., Guo, J.-P., Wei, X.-H. & Liu, D.-S. (2002). *J. Organomet. Chem.* **655**, 89–95.
DeAngelis, S., Solari, E., Gallo, E., Floriani, C., Chiesi-Willa, A. & Rizzoli, C. (1992). *Inorg. Chem.* **31**, 2520–2527.
Engelhardt, L. M., Jacobsen, G. E., Junk, P. C., Raston, C. L. & White, A. H. (1990). *J. Chem. Soc. Chem. Commun.* pp. 89–91.
Engelhardt, L. M. G. E., Junk, P. C., Raston, C. L., Skelton, B. W. & White, A. H. (1988). *J. Chem. Soc. Dalton Trans.* pp. 1011–1020.
Hahn, F. E. & Rupprecht, S. (1991). *Z. Naturforsch.* **46b**, 143–146.
Ho, J., Hou, Z., Drake, R. J. & Stephan, D. W. (1993). *Organometallics*, **12**, 3145–3157.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
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.
Pratt, L. M., Merry, S., Nguyen, S. C., Quan, P. & Thanh, P. T. (2006). *Tetrahedron*, **62**, 10821–10828.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1990). *XP* in *SHELXTL*. Version 4.2. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Solari, E., DeAngelis, S., Floriani, C., Chiesi-Willa, A. & Rizzoli, C. (1992). *Inorg. Chem.* **31**, 96–101.

 doi:10.1107/S1600536807046442

Tayebani, M., Gambarotta, S. & Yap, G. (1998). *Organometallics*, **17**, 3639–3641.
Westerhausen, M., Bollwein, T., Makropoulos, N., Schneiderbauer, S., Suter, M., Nöth, H., Mayer, P., Piotrowski, H., Polborn, K. & Pfitzner, A. (2002). *Eur. J. Inorg. Chem.* pp. 389–404.
Westerhausen, M., Kneifel, A. N. & Makropoulos, N. (2004). *Inorg. Chem. Commun.* **7**, 990–993.
Westerhausen, M., Kneifel, A. N. & Mayer, P. (2006). *Z. Anorg. Allg. Chem.* **632**, 634–638.

supplementary materials

Acta Cryst. (2007). E**63**, m2633-m2634 [**doi:10.1107/S1600536807046442**]

Di-μ-chlorido-bis({2-[(triisopropylsilyl)aminomethyl]pyridine-κN}lithium(I))

C. Koch, H. Görls and M. Westerhausen

Comment

In the past, metallated (2-pyridylmethyl)(trialkysilyl)amines were used for C–C coupling reactions in order to prepare tetradentate ligands. The zincation of (2-pyridylmethyl)(triisopropylsilyl)amine (**A**) gives dimeric methylzinc-(2-pyridylmethyl)(triisopropylsilyl)-amide. Further addition of dimethylzinc to a toluene solution to **A** at raised temperatures yields the C–C coupling product bis(methylzinc)[1,2-dipyridyl-1,2-bis(triisopropylsilylamido)ethane]. The synthesis of compound **A** is described but no structural data have been published (Westerhausen *et al.* 2002). An excess of LiCl led to the formation of single crystals of is[lithiumchloride-bis{(κN 2-pyridylmethyl)(triisopropylsilyl)amine}] (**(A)**$_2$LiCl]$_2$, **1**) at ambient temperature. In **1**, the (2-pyridylmethyl)(triisopropylsily)amines bond *via* the pyridyl-nitrogen atoms to the Li atoms forming a centosymmetric four-membered LiClLi^{i}Cl^i ring [symmetry code:(i) $1-x$, $1-y$, $2-z$]. The amine reacts as a monodentate ligand. The lithium atoms in the central fragment Li_2Cl_2 have a transannular Li···Li^i distance of 292.5 (15) pm. The lithium atoms are distorted tetrahedral coordinated by two chloride atoms and two nitrogen atoms with LiCl bond lengths of 234.6 (7) pm and 235.5 (7) pm. These data are similar to those in [(THF)$_2$LiCl]$_2$ (Hahn & Rupprecht 1991, Hahn & Rupprecht 1991, Baker *et al.* 2005, Bickley *et al.* 2004, DeAngelis *et al.* 1992, Ho *et al.* 1993, Pratt *et al.* 2006, Solari *et al.* 1992, Tayebani *et al.* 1998). Due to this fact the bulkiness of the amines **A** is compareable of the THF molecules. The average Li···N distance of 210.0 pm in bis[lithiumchloride-bis{(κN2-pyridylmethyl) (di-*tert*-butylsilyl)amine}] (**2**, Westerhausen *et al.* 2004) is very similar to the values of **1** (209.8 (8) pm and 209.0 (8) pm) (Buttery *et al.* 2006; Chen *et al.* 2002; Engelhardt *et al.* 1988). In contrast to these LiCl adducts **1** and **2**, dimeric LiI forms a 1/1 complex of bis[lithiumiodide-bis(2-pyridylmethyl)(*tert*-butyldimethylsilyl)amine] (Westerhausen *et al.* 2006). The lithiation of (2-pyridylmethyl)(*tert*-butyldimethylsilyl)amine in THF yields semi(tetrahydrofuran)lithium-(2-pyridylmethyl) (*tert*-butyldimethylsilyl)amide and the reaction with an other equivalent of methyllithium yields octameric dilithium (2-pyridylmethylido)(*tert*-butyldimethylsilyl)amide (Westerhausen *et al.* 2004). Reactions of halogenboranes with silylamines yield aminoboranes *via* elimination of chlorosilanes (Engelhardt *et al.*, 1990).

Experimental

All manipulations were carried out in an atmosphere of argon using standard Schlenk techniques. THF and pentane were dried (Na/benzophenone) and distilled prior to use. 2-pyridylmethylamine and butyllithium were purchased form Aldrich. Tert-butyldimethylchlorosilane was purchased from Merck. ^{1}H NMR and ^{13}C NMR spectra were recorded at[D_6]benzene solution at ambient temperature on a Bruker AC 400 MHz s pectrometer and were referenced to deuterated benzene as an internal standard.

Bis[lithiumchloride-bis{(κN 2-pyridylmethyl)(triisopropylsilyl)amine}] was prepared according to a literature procedure (Westerhausen *et al.* 2002) and recrystallized from pentane. Reduction of the volume to 1/3 of the original volume, single crystals precipitated at ambient temperature within five days.

Physical data:

Mp: 52 °C (decomposition).

^{1}H NMR (400 MHz, Benzene [D6]) δ = 8.48 (d, $^3J(H^1,H^2)$ = 4.4, 1H, Pyr1); 7.61 (dt, $^5J(H^3,H^1)$ = 2.0, $^3J(H^3,H^{2/4})$ = 7.4, 1H, Pyr3); 7.06 (d, $^3J(H^4,H^3)$ = 7.6, 1H, Pyr4); 6.63 (t, $^3J(H^1,H^3)$ = 5.6, 1H, Pyr2); 4.15 (d, $^3J(H^6,NH)$ = 8.0, 2H, CH_2); 1.29 (s, br, 1H, NH); 1.07 (s, 21H, $SiCH(CH_3)_2$/ $SiCH(CH_3)_2$).

^{13}C NMR (100 MHz, Benzene [D6]) δ = 163.25 (Pyr5); 149.28 (Pyr1); 135.80 (Pyr3); 121.29 (Pyr2); 120.68 (Pyr4); 48.62 (^2J, CH2); 18.49 (CH_3); 13.91 ($CH(CH_3)_2$)

MS (EI, *m/z* [%]): 265 (*M*, 11), 264 (M^+, 46), 263 (M^+—H, 100), 223 (5), 222 (19), 221 ($M^+C_3H_7$, 70), 220 (11), 219 (10), 136 (5), 135 (29), 134 (9), 87 (5), 73 (6), 59 (10).

IR (cm^{-1}): 3373, 3091, 3011, 2942, 2892, 2863, 2758, 2722, 1700, 1646, 1592, 1571, 1464, 1434, 1407, 1387, 1382, 1366, 1342, 1319, 1294, 1255, 1249, 1213, 1145, 1125, 1094, 1084, 1070, 1047, 1013, 994, 952, 918, 883, 841, 799, 752, 728, 680, 639, 602, 553, 502, 462, 402.

Refinement

The hydrogen atoms bound to the amine N atoms were located in a difference Fourier synthesis and freely refined. All other hydrogen atoms were set to idealized positions and were refined with 1.2 times (1.5 for methyl groups) the isotropic displacement parameter of the corresponding carbon atom. The methyl groups were allowed to rotate but not to tip.

Figures

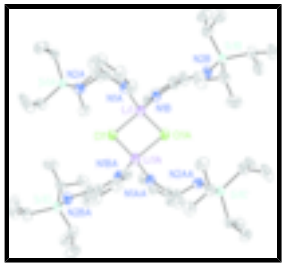


Fig. 1.n a i
The molecular structure of the title compound, showing 40% prabability displacement ellipsoides and the numbering scheme for the non-carbon atoms. H atoms have been omitted for clarity.

Di-μ-chlorido-bis({2-[(triisopropylsilyl)aminomethyl]pyridine-κ*N*}lithium(I))

Crystal data

$[Li_2Cl_2(C_{15}H_{38}N_2Si)_4]$	Z = 1
M_r = 1142.72	F_{000} = 624
Triclinic, $P\bar{1}$	D_x = 1.095 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 9.6312 (19) Å	Cell parameters from 10497 reflections
b = 13.806 (3) Å	θ = 1.7–27.6°
c = 14.802 (3) Å	μ = 0.20 mm^{-1}

α = 113.036 (10)º	T = 183 (2) K
β = 95.653 (17)º	Prism, colourless
γ = 102.388 (12)º	0.05 × 0.05 × 0.05 mm
V = 1732.2 (6) Å^3	

Data collection

Nonius KappaCCD diffractometer	4247 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.039
Monochromator: graphite	θ_{max} = 27.6º
T = 183(2) K	θ_{min} = 1.7º
φ and ω scans	h = −12→12
Absorption correction: none	k = −17→15
10497 measured reflections	l = −16→19
6997 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.076	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.215	$w = 1/[\sigma^2(F_o^2) + (0.0735P)^2 + 2.7204P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
6997 reflections	$\Delta\rho_{max}$ = 0.52 e Å^{-3}
363 parameters	$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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.

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Li1	0.5468 (8)	0.4002 (6)	0.9583 (5)	0.0482 (17)

Cl1	0.47045 (13)	0.47397 (9)	1.11048 (8)	0.0521 (3)
Si1A	0.37243 (13)	0.16461 (10)	1.16902 (9)	0.0434 (3)
N1A	0.3840 (4)	0.2556 (3)	0.8693 (2)	0.0452 (8)
N2A	0.3501 (4)	0.2063 (3)	1.0739 (3)	0.0478 (9)
C1A	0.3073 (5)	0.2509 (4)	0.7861 (3)	0.0568 (12)
H1AA	0.3394	0.3083	0.7663	0.068*
C2A	0.1865 (5)	0.1689 (5)	0.7284 (4)	0.0651 (14)
H2AA	0.1373	0.1687	0.6694	0.078*
C3A	0.1368 (6)	0.0865 (4)	0.7568 (4)	0.0668 (14)
H3AA	0.0521	0.0285	0.7184	0.080*
C4A	0.2131 (5)	0.0899 (4)	0.8425 (4)	0.0591 (12)
H4AA	0.1808	0.0341	0.8641	0.071*
C5A	0.3355 (4)	0.1743 (3)	0.8965 (3)	0.0443 (10)
C6A	0.4233 (5)	0.1793 (4)	0.9897 (3)	0.0489 (10)
H6AA	0.4428	0.1075	0.9745	0.059*
H6AB	0.5179	0.2350	1.0087	0.059*
C7A	0.2504 (5)	0.2223 (4)	1.2538 (3)	0.0560 (12)
H7AA	0.2918	0.3036	1.2833	0.067*
C8A	0.2544 (7)	0.1923 (6)	1.3429 (4)	0.0862 (19)
H8AA	0.1994	0.2323	1.3894	0.129*
H8AB	0.3553	0.2119	1.3774	0.129*
H8AC	0.2111	0.1134	1.3189	0.129*
C9A	0.0954 (5)	0.2001 (5)	1.2028 (4)	0.0686 (14)
H9AA	0.0476	0.2483	1.2490	0.103*
H9AB	0.0430	0.1236	1.1835	0.103*
H9AC	0.0954	0.2142	1.1428	0.103*
C10A	0.3299 (5)	0.0107 (3)	1.1087 (3)	0.0457 (10)
H10A	0.3907	−0.0074	1.0566	0.055*
C11A	0.1722 (5)	−0.0475 (4)	1.0525 (4)	0.0671 (13)
H11A	0.1629	−0.1248	1.0110	0.101*
H11B	0.1442	−0.0130	1.0097	0.101*
H11C	0.1085	−0.0419	1.1010	0.101*
C12A	0.3745 (6)	−0.0382 (4)	1.1805 (4)	0.0612 (13)
H12A	0.3572	−0.1175	1.1430	0.092*
H12B	0.3169	−0.0239	1.2329	0.092*
H12C	0.4778	−0.0045	1.2113	0.092*
C13A	0.5639 (5)	0.2228 (4)	1.2452 (3)	0.0482 (10)
H13A	0.5671	0.1962	1.2990	0.058*
C14A	0.6065 (5)	0.3484 (4)	1.2971 (4)	0.0622 (13)
H14A	0.7085	0.3760	1.3317	0.093*
H14B	0.5452	0.3723	1.3459	0.093*
H14C	0.5930	0.3771	1.2469	0.093*
C15A	0.6740 (5)	0.1829 (4)	1.1828 (4)	0.0611 (13)
H15A	0.7703	0.2100	1.2264	0.092*
H15B	0.6769	0.2105	1.1311	0.092*
H15C	0.6456	0.1027	1.1510	0.092*
Si1B	0.79713 (13)	0.28106 (10)	0.60696 (8)	0.0474 (3)
N1B	0.7537 (4)	0.3767 (3)	0.9785 (2)	0.0433 (8)
N2B	0.8546 (5)	0.3306 (4)	0.7349 (3)	0.0536 (10)

C1B	0.8156 (5)	0.3954 (3)	1.0715 (3)	0.0479 (10)
H1BA	0.7613	0.4149	1.1229	0.057*
C2B	0.9527 (5)	0.3878 (4)	1.0962 (3)	0.0530 (11)
H2BA	0.9916	0.4010	1.1628	0.064*
C3B	1.0328 (5)	0.3606 (4)	1.0225 (4)	0.0564 (12)
H3BA	1.1284	0.3554	1.0373	0.068*
C4B	0.9709 (5)	0.3411 (4)	0.9262 (3)	0.0508 (11)
H4BA	1.0241	0.3220	0.8742	0.061*
C5B	0.8324 (4)	0.3493 (3)	0.9062 (3)	0.0434 (9)
C6B	0.7567 (5)	0.3295 (4)	0.8040 (3)	0.0519 (11)
H6BA	0.6824	0.2577	0.7746	0.062*
H6BB	0.7058	0.3866	0.8115	0.062*
C7B	0.6639 (5)	0.3478 (4)	0.5710 (3)	0.0573 (12)
H7BA	0.6485	0.3220	0.4966	0.069*
C8B	0.7227 (8)	0.4725 (5)	0.6175 (5)	0.0914 (19)
H8BA	0.6538	0.5035	0.5924	0.137*
H8BB	0.8162	0.4927	0.5994	0.137*
H8BC	0.7357	0.5012	0.6906	0.137*
C9B	0.5148 (6)	0.3168 (6)	0.5962 (4)	0.0822 (18)
H9BA	0.4484	0.3487	0.5701	0.123*
H9BB	0.5248	0.3448	0.6691	0.123*
H9BC	0.4761	0.2368	0.5656	0.123*
C10B	0.9672 (5)	0.3055 (4)	0.5550 (3)	0.0609 (13)
H10B	0.9979	0.2366	0.5362	0.073*
C11B	1.0943 (6)	0.3945 (5)	0.6265 (4)	0.0847 (18)
H11D	1.1781	0.3963	0.5941	0.127*
H11E	1.1171	0.3810	0.6857	0.127*
H11F	1.0714	0.4650	0.6468	0.127*
C12B	0.9371 (6)	0.3185 (5)	0.4578 (4)	0.0725 (15)
H12D	1.0268	0.3275	0.4322	0.109*
H12E	0.9015	0.3831	0.4707	0.109*
H12F	0.8635	0.2532	0.4080	0.109*
C13B	0.7081 (5)	0.1308 (4)	0.5560 (3)	0.0580 (12)
H13B	0.6231	0.1229	0.5888	0.070*
C14B	0.8030 (7)	0.0662 (5)	0.5822 (5)	0.0814 (17)
H14D	0.7452	−0.0095	0.5610	0.122*
H14E	0.8401	0.1000	0.6547	0.122*
H14F	0.8846	0.0667	0.5475	0.122*
C15B	0.6462 (7)	0.0775 (4)	0.4429 (4)	0.0735 (15)
H15D	0.5995	−0.0006	0.4211	0.110*
H15E	0.7250	0.0862	0.4071	0.110*
H15F	0.5745	0.1129	0.4282	0.110*
H1NB	0.925 (6)	0.391 (4)	0.764 (4)	0.067 (16)*
H1NA	0.347 (4)	0.269 (4)	1.095 (3)	0.038 (12)*

Atomic displacement parameters (Å^2)

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Li1	0.048 (4)	0.057 (5)	0.046 (4)	0.013 (3)	0.010 (3)	0.028 (4)
Cl1	0.0677 (7)	0.0551 (7)	0.0490 (6)	0.0241 (5)	0.0230 (5)	0.0317 (5)
Si1A	0.0457 (6)	0.0484 (7)	0.0429 (6)	0.0169 (5)	0.0108 (5)	0.0240 (5)
N1A	0.0460 (19)	0.053 (2)	0.0428 (19)	0.0142 (16)	0.0096 (16)	0.0265 (17)
N2A	0.057 (2)	0.050 (2)	0.048 (2)	0.0246 (19)	0.0137 (18)	0.0262 (19)
C1A	0.059 (3)	0.070 (3)	0.049 (3)	0.010 (2)	0.006 (2)	0.038 (2)
C2A	0.059 (3)	0.088 (4)	0.051 (3)	0.011 (3)	0.004 (2)	0.039 (3)
C3A	0.058 (3)	0.064 (3)	0.066 (3)	−0.001 (2)	−0.001 (3)	0.026 (3)
C4A	0.055 (3)	0.061 (3)	0.066 (3)	0.009 (2)	0.006 (2)	0.037 (3)
C5A	0.043 (2)	0.051 (3)	0.049 (2)	0.019 (2)	0.014 (2)	0.026 (2)
C6A	0.048 (2)	0.061 (3)	0.050 (2)	0.017 (2)	0.013 (2)	0.035 (2)
C7A	0.058 (3)	0.065 (3)	0.051 (3)	0.027 (2)	0.013 (2)	0.025 (2)
C8A	0.084 (4)	0.155 (6)	0.055 (3)	0.069 (4)	0.036 (3)	0.058 (4)
C9A	0.058 (3)	0.102 (4)	0.060 (3)	0.038 (3)	0.019 (3)	0.038 (3)
C10A	0.050 (2)	0.051 (3)	0.043 (2)	0.016 (2)	0.015 (2)	0.025 (2)
C11A	0.061 (3)	0.059 (3)	0.070 (3)	0.008 (2)	0.009 (3)	0.022 (3)
C12A	0.083 (3)	0.058 (3)	0.059 (3)	0.024 (3)	0.023 (3)	0.038 (2)
C13A	0.050 (2)	0.056 (3)	0.046 (2)	0.015 (2)	0.007 (2)	0.030 (2)
C14A	0.062 (3)	0.059 (3)	0.064 (3)	0.010 (2)	−0.001 (2)	0.031 (3)
C15A	0.046 (3)	0.080 (4)	0.064 (3)	0.017 (2)	0.005 (2)	0.038 (3)
Si1B	0.0501 (7)	0.0587 (8)	0.0385 (6)	0.0154 (6)	0.0138 (5)	0.0246 (6)
N1B	0.0459 (19)	0.049 (2)	0.0409 (18)	0.0117 (16)	0.0099 (16)	0.0253 (16)
N2B	0.057 (2)	0.065 (3)	0.040 (2)	0.010 (2)	0.0155 (19)	0.025 (2)
C1B	0.054 (3)	0.052 (3)	0.040 (2)	0.010 (2)	0.010 (2)	0.023 (2)
C2B	0.054 (3)	0.061 (3)	0.047 (2)	0.014 (2)	0.003 (2)	0.028 (2)
C3B	0.049 (3)	0.063 (3)	0.062 (3)	0.018 (2)	0.004 (2)	0.033 (3)
C4B	0.051 (3)	0.061 (3)	0.048 (2)	0.019 (2)	0.018 (2)	0.027 (2)
C5B	0.046 (2)	0.046 (2)	0.045 (2)	0.0135 (19)	0.013 (2)	0.024 (2)
C6B	0.055 (3)	0.067 (3)	0.041 (2)	0.021 (2)	0.013 (2)	0.028 (2)
C7B	0.065 (3)	0.069 (3)	0.047 (2)	0.029 (3)	0.018 (2)	0.027 (2)
C8B	0.127 (5)	0.075 (4)	0.087 (4)	0.053 (4)	0.029 (4)	0.035 (3)
C9B	0.066 (3)	0.136 (6)	0.056 (3)	0.046 (4)	0.015 (3)	0.043 (3)
C10B	0.058 (3)	0.080 (4)	0.050 (3)	0.017 (3)	0.017 (2)	0.033 (3)
C11B	0.070 (4)	0.102 (5)	0.078 (4)	0.001 (3)	0.030 (3)	0.041 (4)
C12B	0.078 (4)	0.103 (4)	0.060 (3)	0.031 (3)	0.031 (3)	0.050 (3)
C13B	0.062 (3)	0.063 (3)	0.049 (3)	0.011 (2)	0.005 (2)	0.028 (2)
C14B	0.091 (4)	0.068 (4)	0.088 (4)	0.020 (3)	−0.002 (3)	0.041 (3)
C15B	0.092 (4)	0.061 (3)	0.054 (3)	0.007 (3)	−0.001 (3)	0.021 (3)

Geometric parameters (Å, °)

Li1—N1A	2.090 (8)	C15A—H15A	0.9800
Li1—N1B	2.098 (8)	C15A—H15B	0.9800
Li1—Cl1	2.346 (7)	C15A—H15C	0.9800
Li1—Cl1^{i}	2.357 (7)	Si1B—N2B	1.726 (4)
Li1—Li1^{i}	2.925 (15)	Si1B—C13B	1.869 (5)
Cl1—Li1^{i}	2.357 (7)	Si1B—C7B	1.881 (5)
Si1A—N2A	1.728 (4)	Si1B—C10B	1.898 (5)

Si1A—C7A	1.871 (5)	N1B—C1B	1.346 (5)
Si1A—C10A	1.885 (4)	N1B—C5B	1.353 (5)
Si1A—C13A	1.888 (4)	N2B—C6B	1.460 (5)
N1A—C1A	1.343 (5)	N2B—H1NB	0.87 (5)
N1A—C5A	1.345 (5)	C1B—C2B	1.372 (6)
N2A—C6A	1.454 (5)	C1B—H1BA	0.9500
N2A—H1NA	0.81 (4)	C2B—C3B	1.376 (6)
C1A—C2A	1.359 (7)	C2B—H2BA	0.9500
C1A—H1AA	0.9500	C3B—C4B	1.386 (6)
C2A—C3A	1.371 (7)	C3B—H3BA	0.9500
C2A—H2AA	0.9500	C4B—C5B	1.376 (6)
C3A—C4A	1.381 (7)	C4B—H4BA	0.9500
C3A—H3AA	0.9500	C5B—C6B	1.506 (6)
C4A—C5A	1.372 (6)	C6B—H6BA	0.9900
C4A—H4AA	0.9500	C6B—H6BB	0.9900
C5A—C6A	1.514 (6)	C7B—C8B	1.528 (8)
C6A—H6AA	0.9900	C7B—C9B	1.533 (7)
C6A—H6AB	0.9900	C7B—H7BA	1.0000
C7A—C9A	1.514 (6)	C8B—H8BA	0.9800
C7A—C8A	1.529 (6)	C8B—H8BB	0.9800
C7A—H7AA	1.0000	C8B—H8BC	0.9800
C8A—H8AA	0.9800	C9B—H9BA	0.9800
C8A—H8AB	0.9800	C9B—H9BB	0.9800
C8A—H8AC	0.9800	C9B—H9BC	0.9800
C9A—H9AA	0.9800	C10B—C11B	1.487 (7)
C9A—H9AB	0.9800	C10B—C12B	1.526 (6)
C9A—H9AC	0.9800	C10B—H10B	1.0000
C10A—C11A	1.533 (6)	C11B—H11D	0.9800
C10A—C12A	1.538 (6)	C11B—H11E	0.9800
C10A—H10A	1.0000	C11B—H11F	0.9800
C11A—H11A	0.9800	C12B—H12D	0.9800
C11A—H11B	0.9800	C12B—H12E	0.9800
C11A—H11C	0.9800	C12B—H12F	0.9800
C12A—H12A	0.9800	C13B—C14B	1.526 (7)
C12A—H12B	0.9800	C13B—C15B	1.533 (6)
C12A—H12C	0.9800	C13B—H13B	1.0000
C13A—C15A	1.525 (6)	C14B—H14D	0.9800
C13A—C14A	1.534 (6)	C14B—H14E	0.9800
C13A—H13A	1.0000	C14B—H14F	0.9800
C14A—H14A	0.9800	C15B—H15D	0.9800
C14A—H14B	0.9800	C15B—H15E	0.9800
C14A—H14C	0.9800	C15B—H15F	0.9800
N1A—Li1—N1B	113.6 (4)	C13A—C15A—H15B	109.5
N1A—Li1—Cl1	105.2 (3)	H15A—C15A—H15B	109.5
N1B—Li1—Cl1	112.2 (3)	C13A—C15A—H15C	109.5
N1A—Li1—Cl1^{i}	106.9 (3)	H15A—C15A—H15C	109.5
N1B—Li1—Cl1^{i}	114.9 (3)	H15B—C15A—H15C	109.5
Cl1—Li1—Cl1^{i}	103.1 (3)	N2B—Si1B—C13B	108.2 (2)

N1A—Li1—Li1^{i}	116.4 (4)	N2B—Si1B—C7B	113.3 (2)
N1B—Li1—Li1^{i}	130.0 (5)	C13B—Si1B—C7B	108.4 (2)
Cl1—Li1—Li1^{i}	51.7 (2)	N2B—Si1B—C10B	106.1 (2)
Cl1^{i}—Li1—Li1^{i}	51.4 (2)	C13B—Si1B—C10B	109.8 (2)
Li1—Cl1—Li1^{i}	76.9 (3)	C7B—Si1B—C10B	110.9 (2)
N2A—Si1A—C7A	105.29 (19)	C1B—N1B—C5B	117.5 (4)
N2A—Si1A—C10A	107.33 (19)	C1B—N1B—Li1	117.5 (3)
C7A—Si1A—C10A	115.7 (2)	C5B—N1B—Li1	124.9 (3)
N2A—Si1A—C13A	112.41 (19)	C6B—N2B—Si1B	123.8 (3)
C7A—Si1A—C13A	107.6 (2)	C6B—N2B—H1NB	108 (3)
C10A—Si1A—C13A	108.56 (19)	Si1B—N2B—H1NB	117 (3)
C1A—N1A—C5A	117.0 (4)	N1B—C1B—C2B	123.6 (4)
C1A—N1A—Li1	117.4 (3)	N1B—C1B—H1BA	118.2
C5A—N1A—Li1	124.8 (3)	C2B—C1B—H1BA	118.2
C6A—N2A—Si1A	124.7 (3)	C1B—C2B—C3B	118.7 (4)
C6A—N2A—H1NA	111 (3)	C1B—C2B—H2BA	120.7
Si1A—N2A—H1NA	112 (3)	C3B—C2B—H2BA	120.7
N1A—C1A—C2A	124.0 (4)	C2B—C3B—C4B	118.6 (4)
N1A—C1A—H1AA	118.0	C2B—C3B—H3BA	120.7
C2A—C1A—H1AA	118.0	C4B—C3B—H3BA	120.7
C1A—C2A—C3A	118.8 (4)	C5B—C4B—C3B	119.9 (4)
C1A—C2A—H2AA	120.6	C5B—C4B—H4BA	120.0
C3A—C2A—H2AA	120.6	C3B—C4B—H4BA	120.0
C2A—C3A—C4A	118.3 (5)	N1B—C5B—C4B	121.7 (4)
C2A—C3A—H3AA	120.8	N1B—C5B—C6B	114.7 (4)
C4A—C3A—H3AA	120.8	C4B—C5B—C6B	123.6 (4)
C5A—C4A—C3A	119.8 (4)	N2B—C6B—C5B	113.5 (4)
C5A—C4A—H4AA	120.1	N2B—C6B—H6BA	108.9
C3A—C4A—H4AA	120.1	C5B—C6B—H6BA	108.9
N1A—C5A—C4A	122.0 (4)	N2B—C6B—H6BB	108.9
N1A—C5A—C6A	116.8 (4)	C5B—C6B—H6BB	108.9
C4A—C5A—C6A	121.2 (4)	H6BA—C6B—H6BB	107.7
N2A—C6A—C5A	112.7 (3)	C8B—C7B—C9B	109.2 (5)
N2A—C6A—H6AA	109.1	C8B—C7B—Si1B	112.1 (4)
C5A—C6A—H6AA	109.1	C9B—C7B—Si1B	113.8 (4)
N2A—C6A—H6AB	109.1	C8B—C7B—H7BA	107.1
C5A—C6A—H6AB	109.1	C9B—C7B—H7BA	107.1
H6AA—C6A—H6AB	107.8	Si1B—C7B—H7BA	107.1
C9A—C7A—C8A	110.9 (4)	C7B—C8B—H8BA	109.5
C9A—C7A—Si1A	115.6 (3)	C7B—C8B—H8BB	109.5
C8A—C7A—Si1A	112.8 (3)	H8BA—C8B—H8BB	109.5
C9A—C7A—H7AA	105.5	C7B—C8B—H8BC	109.5
C8A—C7A—H7AA	105.5	H8BA—C8B—H8BC	109.5
Si1A—C7A—H7AA	105.5	H8BB—C8B—H8BC	109.5
C7A—C8A—H8AA	109.5	C7B—C9B—H9BA	109.5
C7A—C8A—H8AB	109.5	C7B—C9B—H9BB	109.5
H8AA—C8A—H8AB	109.5	H9BA—C9B—H9BB	109.5
C7A—C8A—H8AC	109.5	C7B—C9B—H9BC	109.5

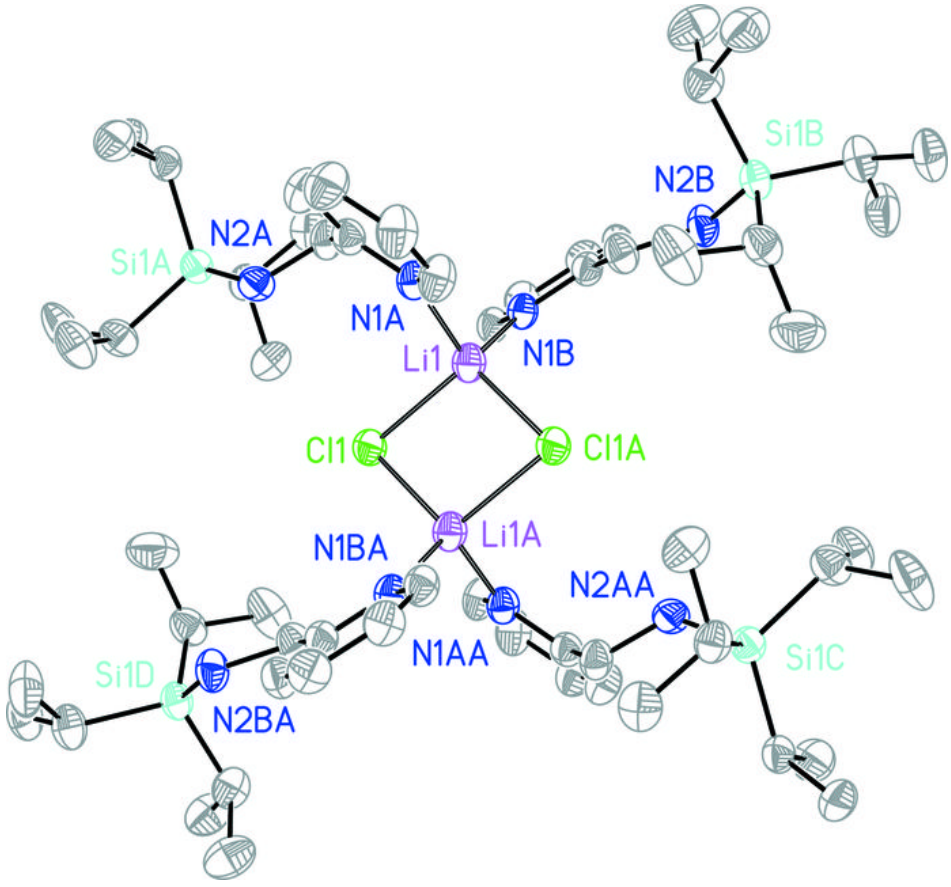
H8AA—C8A—H8AC	109.5	H9BA—C9B—H9BC	109.5
H8AB—C8A—H8AC	109.5	H9BB—C9B—H9BC	109.5
C7A—C9A—H9AA	109.5	C11B—C10B—C12B	110.8 (4)
C7A—C9A—H9AB	109.5	C11B—C10B—Si1B	116.0 (3)
H9AA—C9A—H9AB	109.5	C12B—C10B—Si1B	112.4 (3)
C7A—C9A—H9AC	109.5	C11B—C10B—H10B	105.5
H9AA—C9A—H9AC	109.5	C12B—C10B—H10B	105.5
H9AB—C9A—H9AC	109.5	Si1B—C10B—H10B	105.5
C11A—C10A—C12A	110.6 (4)	C10B—C11B—H11D	109.5
C11A—C10A—Si1A	113.9 (3)	C10B—C11B—H11E	109.5
C12A—C10A—Si1A	113.9 (3)	H11D—C11B—H11E	109.5
C11A—C10A—H10A	105.9	C10B—C11B—H11F	109.5
C12A—C10A—H10A	105.9	H11D—C11B—H11F	109.5
Si1A—C10A—H10A	105.9	H11E—C11B—H11F	109.5
C10A—C11A—H11A	109.5	C10B—C12B—H12D	109.5
C10A—C11A—H11B	109.5	C10B—C12B—H12E	109.5
H11A—C11A—H11B	109.5	H12D—C12B—H12E	109.5
C10A—C11A—H11C	109.5	C10B—C12B—H12F	109.5
H11A—C11A—H11C	109.5	H12D—C12B—H12F	109.5
H11B—C11A—H11C	109.5	H12E—C12B—H12F	109.5
C10A—C12A—H12A	109.5	C14B—C13B—C15B	110.2 (4)
C10A—C12A—H12B	109.5	C14B—C13B—Si1B	114.1 (4)
H12A—C12A—H12B	109.5	C15B—C13B—Si1B	113.4 (3)
C10A—C12A—H12C	109.5	C14B—C13B—H13B	106.1
H12A—C12A—H12C	109.5	C15B—C13B—H13B	106.1
H12B—C12A—H12C	109.5	Si1B—C13B—H13B	106.1
C15A—C13A—C14A	110.7 (4)	C13B—C14B—H14D	109.5
C15A—C13A—Si1A	112.3 (3)	C13B—C14B—H14E	109.5
C14A—C13A—Si1A	111.6 (3)	H14D—C14B—H14E	109.5
C15A—C13A—H13A	107.3	C13B—C14B—H14F	109.5
C14A—C13A—H13A	107.3	H14D—C14B—H14F	109.5
Si1A—C13A—H13A	107.3	H14E—C14B—H14F	109.5
C13A—C14A—H14A	109.5	C13B—C15B—H15D	109.5
C13A—C14A—H14B	109.5	C13B—C15B—H15E	109.5
H14A—C14A—H14B	109.5	H15D—C15B—H15E	109.5
C13A—C14A—H14C	109.5	C13B—C15B—H15F	109.5
H14A—C14A—H14C	109.5	H15D—C15B—H15F	109.5
H14B—C14A—H14C	109.5	H15E—C15B—H15F	109.5
C13A—C15A—H15A	109.5		

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2A—H1NA···Cl1	0.81 (5)	2.73 (6)	3.430 (5)	146 (4)

Fig. 1


Si1B
N2B
N2A
Si1A
N1A
Li1
N1B
Cl1
Cl1A
N1BA
Li1A
N2AA
N1AA
Si1C
Si1D
N2BA