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# A polymeric mixed-metal hexamethyldisilazide

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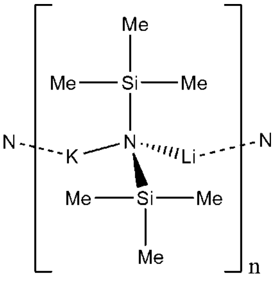
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(N–Li) = 0.001 Å; disorder in main residue; $R$ factor = 0.029; $wR$ factor = 0.083; data-to-parameter ratio = 14.1.

The title compound, *catena*-poly[[$\mu_2$-bis(trimethylsilyl)amido-$\kappa^2N$:$N$]-lithium(I)-[$\mu_2$-bis(trimethylsilyl)amido-$\kappa^2N$:$N$]potassium], $[LiK(C_6H_{18}NSi_2)_2]_n$ or $[\{(Me_3Si)_2NLi\}\{(Me_3Si)_2NK\}]_\infty$, is a polymeric one-dimensional chain composed of alternating lithium and potassium centers bridged through the amide N atoms of the hexamethyldisilazide anions. The repeat unit is centrosymmetric, with K on a center of symmetry, Li on a twofold rotation axis, and the complete hexamethydisilazide anion in the asymmetric unit. All of the methyl C atoms in the hexamethyldisilazide anion are disordered over two sites, with the site occupancies refined to 0.63 (2) for the major component of one trimethylsilyl group and 0.54 (3) for the major component of the second trimethylsilyl group.

## Related literature

The isostructural one-dimensional chain polymer sodium hexamethyldisilazide (Grüning & Atwood, 1977), the dimeric mixed lithium–potassium hexamethyldisilazide solvated by THF (Williard & Nichols, 1991), and the related homometallic ferrocene solvates (Morris *et al.*, 2007) have been reported.



## Experimental

### Crystal data

$[LiK(C_6H_{18}NSi_2)_2]$
$M_r$ = 366.83
Monoclinic, $C2/c$
$a$ = 11.3154 (3) Å
$b$ = 17.5465 (5) Å
$c$ = 12.6528 (5) Å
$\beta$ = 109.657 (1)°
$V$ = 2365.76 (13) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.42 mm$^{-1}$
$T$ = 100 (2) K
0.32 × 0.30 × 0.24 mm

### Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{\min}$ = 0.86, $T_{\max}$ = 0.90
24282 measured reflections
2265 independent reflections
1943 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.029

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.083
$S$ = 1.08
2265 reflections
161 parameters
30 restraints
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{\min}$ = −0.23 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Li1—N1 | 1.9348 (11) | N1—Si2 | 1.6738 (12) |
| K1—N1 | 2.8612 (11) | N1—Si1 | 1.6798 (12) |
| | | | |
| N1—Li1—N1$^{\rm i}$ | 176.4 (3) | Si2—N1—Si1 | 132.29 (7) |
| N1—K1—N1$^{\rm ii}$ | 180.0 | Li1—N1—K1 | 107.80 (9) |

Symmetry codes: (i) $-x, y, -z + \frac{1}{2}$; (ii) $-x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2* and *SAINT* (Bruker, 2006); data reduction: *SAINT* and *XPREP* (Sheldrick, 2003); program(s) used to solve structure: *XS* in *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *XL* in *SHELXTL*; molecular graphics: *XP* in *SHELXTL*; software used to prepare material for publication: *XCIF* in *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2045).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m2477 [ **doi:10.1107/S1600536807033922** ]

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## Comment

The title complex was synthesized during the attempted synthesis of mixed alkali metal hexamethyldisilazide complexes coordinated by ferrocene (Morris *et al.*, 2007). The asymmetric unit contains a hexamethyldisilazide (HMDS) anion that coordinates to both a lithium and potassium through the nitrogen center (Fig. 1). The nitrogen has an approximately tetrahedral coordination geometry, bonding to two silicons, a potassium and a lithium. Symmetry expansion gives a polymeric one-dimensional chain composed of alternating lithium and potassium cations, each coordinated to two bridging HMDS anions (Fig. 2). The one-dimensional chain polymer adopts a zigzag conformation with a K—N—Li angle of 107.80 (9)°, which is slightly larger than the Na—N—Na angle of 102.0° seen in the isostructural sodium hexamethyldisilazide complex (Grüning & Atwood, 1977). The potassium has a crystallographically required linear N—K—N coordination environment with a K—N distance of 2.861 (1) Å, while the lithium has a near linear N—Li—N angle of 176.4 (2)° and a Li—N distance of 1.935 (1). In addition, the potassium has short K—C agostic interactions of 3.136 (13) Å for K1—C4 and 3.336 (13) Å for K1—C2. The structure is notable in forming a chain polymer rather than a $LiN_2K$ heterodimeric ring, as found for the THF solvate $[\{(Me_3Si)_2N\}_2LiK\}(THF)_3]$ (Williard & Nichols, 1991).

## Experimental

All experimental manipulations were performed under a purified nitrogen atmosphere using standard Schlenk techniques. n-Butyllithium was purchased from Aldrich and standardized prior to use. KHMDS was purchased from Aldrich and used as received. Toluene was dried immediately before use by passage through columns of copper-based catalyst and alumina and stored over 4 Å molecular sieves. Ferrocene was purchased from Aldrich and dried by sublimation. Hexamethyldisilazane was purchased from Fluka and distilled over $CaH_2$ prior to use. NMR spectroscopy data were recorded on a Varian Unity Plus 300 spectrometer at 298 K. For the synthesis of the title compound, n-BuLi (2.5 mmol of a 1.6 *M* solution in hexane) was added to a stirred solution of hexamethyldisilazane (2.5 mmol) in toluene (6.0 ml) at 273 K. KHMDS (2.5 mmol) and ferrocene (2.5 mmol) were added to give an orange solution. The solution was then cooled to 263 K, which gave colourless crystals within 24 h. $^1$H NMR (300 MHz, Toluene-$d_8$, 298 K): δ 0.15 (s, $Si(CH_3)_3$).

## Refinement

H atoms were placed in calculated positions and allowed to ride on their respective parent atom. The isotropic methyl hydrogen thermal parameters were set to $1.5U_{eq}$(C). All of the methyl carbons in the hexamethyldisilazide anion are disordered over two sites, with the site occupancy refined to 0.63 (2) for the major component of the first trimethylsilyl group (C1—C3) and 0.54 (3) for the major component of the second trimethylsilyl group (C4—C6). In addition, all Si—C bonds were restrained to be equal using the SADI restraint (30 total restraints).

## Figures

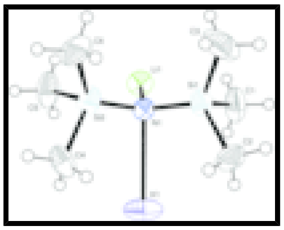

Fig. 1. Asymmetric unit showing 50% probability displacement ellipsoids. Only the the methyl groups of the major component of the disordered hexamethyldisilazide anion are shown for clarity.

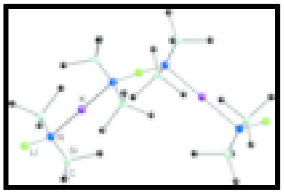

Fig. 2. Section of the polymeric zigzag chain of the title compound highlighting the alternating lithium and potassium metal sites.

## *catena*-poly[[μ$_2$-bis(trimethylsilyl)amido-κ$^2$*N*:*N*]-lithium(I)-\ [μ$_2$-bis(trimethylsilyl)amido-κ$^2$*N*:*N*]-potassium]

### *Crystal data*

$[LiK(C_6H_{18}N_1Si_2)_2]$

$M_r = 366.83$

Monoclinic, *C*2/*c*

Hall symbol: -C 2yc

$a = 11.3154\ (3)$ Å

$b = 17.5465\ (5)$ Å

$c = 12.6528\ (5)$ Å

$\beta = 109.6570\ (10)^\circ$

$V = 2365.76\ (13)$ Å$^3$

$Z = 4$

$F_{000} = 800$

$D_x = 1.030$ Mg m$^{-3}$

Mo *K*α radiation
λ = 0.71073 Å

Cell parameters from 5346 reflections

θ = 2.4–25.6°

$\mu = 0.42$ mm$^{-1}$

$T = 100\ (2)$ K

Parallelepiped, colourless

0.32 × 0.30 × 0.24 mm

### *Data collection*

Bruker SMART APEX II CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 8.33 pixels mm$^{-1}$

$T = 100(2)$ K

ω and φ scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2004)

$T_{min} = 0.86$, $T_{max} = 0.90$

24282 measured reflections

2265 independent reflections

1943 reflections with $I > 2\sigma(I)$

$R_{int} = 0.029$

$\theta_{max} = 25.8^\circ$

$\theta_{min} = 2.2^\circ$

$h = -13 \rightarrow 13$

$k = -21 \rightarrow 16$

$l = -15 \rightarrow 15$

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.029$ | H-atom parameters constrained |
| $wR(F^2) = 0.083$ | $w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 0.9001P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.08$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 2265 reflections | $\Delta\rho_{max} = 0.23$ e Å$^{-3}$ |
| 161 parameters | $\Delta\rho_{min} = -0.23$ e Å$^{-3}$ |
| 30 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Li1 | 0.0000 | 0.1461 (2) | 0.2500 | 0.0508 (9) | |
| K1 | 0.2500 | 0.2500 | 0.5000 | 0.0795 (2) | |
| N1 | 0.18132 (10) | 0.14957 (6) | 0.31084 (9) | 0.0352 (3) | |
| Si1 | 0.23253 (4) | 0.06732 (2) | 0.37876 (4) | 0.04687 (15) | |
| Si2 | 0.22947 (4) | 0.20084 (3) | 0.22140 (4) | 0.04769 (15) | |
| C1 | 0.1043 (5) | 0.0361 (7) | 0.4356 (9) | 0.075 (2) | 0.64 (2) |
| H1A | 0.0875 | 0.0772 | 0.4811 | 0.112* | 0.64 (2) |
| H1B | 0.1319 | −0.0095 | 0.4822 | 0.112* | 0.64 (2) |
| H1C | 0.0277 | 0.0246 | 0.3729 | 0.112* | 0.64 (2) |
| C1' | 0.1023 (8) | 0.0058 (10) | 0.3916 (18) | 0.077 (4) | 0.36 (2) |
| H1D | 0.0514 | 0.0351 | 0.4264 | 0.115* | 0.36 (2) |
| H1E | 0.1380 | −0.0387 | 0.4384 | 0.115* | 0.36 (2) |
| H1F | 0.0495 | −0.0113 | 0.3169 | 0.115* | 0.36 (2) |
| C2 | 0.3699 (8) | 0.0751 (7) | 0.5133 (5) | 0.061 (2) | 0.64 (2) |
| H2A | 0.4364 | 0.1054 | 0.5001 | 0.092* | 0.64 (2) |
| H2B | 0.4019 | 0.0240 | 0.5389 | 0.092* | 0.64 (2) |
| H2C | 0.3428 | 0.0999 | 0.5707 | 0.092* | 0.64 (2) |

| | | | | | |
|---|---|---|---|---|---|
| C2' | 0.3637 (17) | 0.0856 (15) | 0.5143 (13) | 0.092 (7) | 0.36 (2) |
| H2D | 0.4361 | 0.1067 | 0.4982 | 0.138* | 0.36 (2) |
| H2E | 0.3878 | 0.0376 | 0.5557 | 0.138* | 0.36 (2) |
| H2F | 0.3357 | 0.1220 | 0.5597 | 0.138* | 0.36 (2) |
| C3 | 0.2750 (14) | −0.0137 (6) | 0.3029 (11) | 0.098 (3) | 0.64 (2) |
| H3A | 0.2043 | −0.0251 | 0.2347 | 0.147* | 0.64 (2) |
| H3B | 0.2945 | −0.0587 | 0.3516 | 0.147* | 0.64 (2) |
| H3C | 0.3485 | 0.0002 | 0.2826 | 0.147* | 0.64 (2) |
| C3' | 0.303 (2) | 0.0040 (10) | 0.2957 (15) | 0.082 (4) | 0.36 (2) |
| H3D | 0.2457 | 0.0006 | 0.2181 | 0.124* | 0.36 (2) |
| H3E | 0.3168 | −0.0470 | 0.3293 | 0.124* | 0.36 (2) |
| H3F | 0.3833 | 0.0254 | 0.2966 | 0.124* | 0.36 (2) |
| C4 | 0.3468 (10) | 0.2758 (6) | 0.2978 (11) | 0.059 (2) | 0.54 (3) |
| H4A | 0.3065 | 0.3121 | 0.3338 | 0.088* | 0.54 (3) |
| H4B | 0.3772 | 0.3029 | 0.2442 | 0.088* | 0.54 (3) |
| H4C | 0.4177 | 0.2514 | 0.3550 | 0.088* | 0.54 (3) |
| C4' | 0.3276 (17) | 0.2872 (8) | 0.2749 (16) | 0.089 (5) | 0.46 (3) |
| H4D | 0.2808 | 0.3234 | 0.3047 | 0.133* | 0.46 (3) |
| H4E | 0.3486 | 0.3111 | 0.2135 | 0.133* | 0.46 (3) |
| H4F | 0.4050 | 0.2724 | 0.3347 | 0.133* | 0.46 (3) |
| C5 | 0.0906 (7) | 0.2606 (5) | 0.1331 (9) | 0.071 (2) | 0.54 (3) |
| H5A | 0.0527 | 0.2865 | 0.1824 | 0.107* | 0.54 (3) |
| H5B | 0.0282 | 0.2274 | 0.0809 | 0.107* | 0.54 (3) |
| H5C | 0.1196 | 0.2985 | 0.0905 | 0.107* | 0.54 (3) |
| C5' | 0.0863 (8) | 0.2267 (16) | 0.0976 (14) | 0.111 (6) | 0.46 (3) |
| H5D | 0.0403 | 0.1802 | 0.0653 | 0.167* | 0.46 (3) |
| H5E | 0.1126 | 0.2528 | 0.0408 | 0.167* | 0.46 (3) |
| H5F | 0.0319 | 0.2603 | 0.1226 | 0.167* | 0.46 (3) |
| C6 | 0.3043 (16) | 0.1554 (8) | 0.1259 (12) | 0.078 (3) | 0.54 (3) |
| H6A | 0.3830 | 0.1309 | 0.1708 | 0.117* | 0.54 (3) |
| H6B | 0.3217 | 0.1944 | 0.0777 | 0.117* | 0.54 (3) |
| H6C | 0.2474 | 0.1170 | 0.0792 | 0.117* | 0.54 (3) |
| C6' | 0.3196 (17) | 0.1392 (10) | 0.1535 (16) | 0.092 (4) | 0.46 (3) |
| H6D | 0.4002 | 0.1250 | 0.2094 | 0.138* | 0.46 (3) |
| H6E | 0.3344 | 0.1674 | 0.0923 | 0.138* | 0.46 (3) |
| H6F | 0.2711 | 0.0930 | 0.1235 | 0.138* | 0.46 (3) |

*Atomic displacement parameters ($Å^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Li1 | 0.0303 (17) | 0.063 (2) | 0.057 (2) | 0.000 | 0.0117 (15) | 0.000 |
| K1 | 0.0700 (4) | 0.0934 (5) | 0.0703 (4) | −0.0042 (3) | 0.0174 (3) | −0.0453 (4) |
| N1 | 0.0298 (6) | 0.0391 (6) | 0.0357 (6) | 0.0020 (5) | 0.0099 (5) | 0.0012 (5) |
| Si1 | 0.0353 (2) | 0.0437 (3) | 0.0515 (3) | 0.00070 (17) | 0.00125 (18) | 0.01018 (18) |
| Si2 | 0.0339 (2) | 0.0634 (3) | 0.0458 (3) | −0.00183 (18) | 0.01350 (18) | 0.0130 (2) |
| C1 | 0.057 (2) | 0.066 (4) | 0.092 (4) | −0.008 (2) | 0.012 (2) | 0.037 (3) |
| C1' | 0.060 (4) | 0.051 (6) | 0.106 (8) | −0.014 (4) | 0.011 (4) | 0.028 (5) |
| C2 | 0.053 (3) | 0.070 (4) | 0.041 (3) | 0.010 (3) | −0.010 (2) | −0.001 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2' | 0.080 (9) | 0.085 (9) | 0.095 (11) | 0.045 (7) | 0.009 (7) | 0.042 (7) |
| C3 | 0.103 (5) | 0.045 (5) | 0.114 (5) | 0.018 (4) | −0.006 (3) | −0.022 (4) |
| C3' | 0.107 (10) | 0.030 (6) | 0.077 (5) | 0.022 (6) | −0.013 (5) | −0.007 (4) |
| C4 | 0.052 (3) | 0.044 (3) | 0.085 (4) | −0.014 (3) | 0.030 (2) | 0.005 (3) |
| C4' | 0.107 (9) | 0.056 (5) | 0.124 (9) | 0.008 (4) | 0.068 (8) | 0.025 (5) |
| C5 | 0.046 (2) | 0.082 (4) | 0.076 (4) | 0.001 (2) | 0.006 (2) | 0.043 (3) |
| C5' | 0.068 (4) | 0.170 (13) | 0.089 (7) | −0.001 (6) | 0.017 (4) | 0.085 (8) |
| C6 | 0.106 (5) | 0.095 (5) | 0.052 (5) | −0.018 (4) | 0.053 (4) | −0.009 (4) |
| C6' | 0.101 (7) | 0.134 (9) | 0.065 (7) | −0.046 (6) | 0.060 (6) | −0.021 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Li1—N1 | 1.9348 (11) | C1'—H1E | 0.9800 |
| Li1—N1$^{\rm i}$ | 1.9348 (11) | C1'—H1F | 0.9800 |
| Li1—Si2$^{\rm i}$ | 2.9032 (14) | C2—H2A | 0.9800 |
| Li1—Si1$^{\rm i}$ | 2.933 (2) | C2—H2B | 0.9800 |
| Li1—K1$^{\rm i}$ | 3.9133 (19) | C2—H2C | 0.9800 |
| K1—N1 | 2.8612 (11) | C2'—H2D | 0.9800 |
| K1—N1$^{\rm ii}$ | 2.8612 (11) | C2'—H2E | 0.9800 |
| K1—C4$^{\rm ii}$ | 3.136 (13) | C2'—H2F | 0.9800 |
| K1—C2'$^{\rm ii}$ | 3.14 (3) | C3—H3A | 0.9800 |
| K1—C4'$^{\rm ii}$ | 3.315 (19) | C3—H3B | 0.9800 |
| K1—C2$^{\rm ii}$ | 3.336 (13) | C3—H3C | 0.9800 |
| K1—Si1$^{\rm ii}$ | 3.5303 (5) | C3'—H3D | 0.9800 |
| K1—Si2$^{\rm ii}$ | 3.5599 (5) | C3'—H3E | 0.9800 |
| K1—Li1$^{\rm ii}$ | 3.9133 (19) | C3'—H3F | 0.9800 |
| N1—Si2 | 1.6738 (12) | C4—H4A | 0.9800 |
| N1—Si1 | 1.6798 (12) | C4—H4B | 0.9800 |
| Si1—C3 | 1.866 (5) | C4—H4C | 0.9800 |
| Si1—C1' | 1.878 (6) | C4'—H4D | 0.9800 |
| Si1—C2' | 1.880 (7) | C4'—H4E | 0.9800 |
| Si1—C3' | 1.881 (7) | C4'—H4F | 0.9800 |
| Si1—C2 | 1.884 (3) | C5—H5A | 0.9800 |
| Si1—C1 | 1.904 (4) | C5—H5B | 0.9800 |
| Si2—C4' | 1.866 (7) | C5—H5C | 0.9800 |
| Si2—C6 | 1.872 (5) | C5'—H5D | 0.9800 |
| Si2—C6' | 1.881 (6) | C5'—H5E | 0.9800 |
| Si2—C4 | 1.888 (5) | C5'—H5F | 0.9800 |
| Si2—C5' | 1.891 (6) | C6—H6A | 0.9800 |
| Si2—C5 | 1.907 (5) | C6—H6B | 0.9800 |
| C1—H1A | 0.9800 | C6—H6C | 0.9800 |
| C1—H1B | 0.9800 | C6'—H6D | 0.9800 |
| C1—H1C | 0.9800 | C6'—H6E | 0.9800 |
| C1'—H1D | 0.9800 | C6'—H6F | 0.9800 |
| N1—Li1—N1$^{\rm i}$ | 176.4 (3) | N1—Si2—C4 | 111.2 (4) |
| N1—Li1—Si2$^{\rm i}$ | 144.40 (12) | C6—Si2—C4 | 103.6 (7) |

| | | | |
|---|---|---|---|
| N1$^{i}$—Li1—Si2$^{i}$ | 33.48 (5) | N1—Si2—C5' | 107.8 (3) |
| N1—Li1—Si1$^{i}$ | 150.35 (18) | C4'—Si2—C5' | 110.2 (7) |
| N1$^{i}$—Li1—Si1$^{i}$ | 32.95 (6) | C6'—Si2—C5' | 101.8 (8) |
| Si2$^{i}$—Li1—Si1$^{i}$ | 63.407 (14) | N1—Si2—C5 | 107.5 (3) |
| N1—Li1—K1$^{i}$ | 133.50 (12) | C6—Si2—C5 | 108.6 (5) |
| N1$^{i}$—Li1—K1$^{i}$ | 44.12 (6) | C4—Si2—C5 | 102.5 (5) |
| Si2$^{i}$—Li1—K1$^{i}$ | 60.84 (4) | Si1—C1—H1A | 109.5 |
| Si1$^{i}$—Li1—K1$^{i}$ | 60.069 (19) | Si1—C1—H1B | 109.5 |
| N1—K1—N1$^{ii}$ | 180.0 | Si1—C1—H1C | 109.5 |
| N1—K1—C4$^{ii}$ | 121.49 (9) | Si1—C1'—H1D | 109.5 |
| N1$^{ii}$—K1—C4$^{ii}$ | 58.51 (9) | Si1—C1'—H1E | 109.5 |
| N1—K1—C2'$^{ii}$ | 121.81 (18) | H1D—C1'—H1E | 109.5 |
| N1$^{ii}$—K1—C2'$^{ii}$ | 58.19 (18) | Si1—C1'—H1F | 109.5 |
| N1—K1—C4'$^{ii}$ | 121.43 (13) | H1D—C1'—H1F | 109.5 |
| N1$^{ii}$—K1—C4'$^{ii}$ | 58.57 (13) | H1E—C1'—H1F | 109.5 |
| N1—K1—C2$^{ii}$ | 122.21 (8) | Si1—C2—H2A | 109.5 |
| N1$^{ii}$—K1—C2$^{ii}$ | 57.79 (8) | Si1—C2—H2B | 109.5 |
| C4$^{ii}$—K1—C2$^{ii}$ | 85.8 (3) | Si1—C2—H2C | 109.5 |
| N1—K1—Si1$^{ii}$ | 151.94 (2) | Si1—C2'—H2D | 109.5 |
| N1$^{ii}$—K1—Si1$^{ii}$ | 28.06 (2) | Si1—C2'—H2E | 109.5 |
| C4$^{ii}$—K1—Si1$^{ii}$ | 76.14 (15) | H2D—C2'—H2E | 109.5 |
| C2'$^{ii}$—K1—Si1$^{ii}$ | 32.07 (14) | Si1—C2'—H2F | 109.5 |
| C4'$^{ii}$—K1—Si1$^{ii}$ | 78.3 (2) | H2D—C2'—H2F | 109.5 |
| C2$^{ii}$—K1—Si1$^{ii}$ | 31.69 (6) | H2E—C2'—H2F | 109.5 |
| N1—K1—Si2$^{ii}$ | 152.43 (2) | Si1—C3—H3A | 109.5 |
| N1$^{ii}$—K1—Si2$^{ii}$ | 27.57 (2) | Si1—C3—H3B | 109.5 |
| C4$^{ii}$—K1—Si2$^{ii}$ | 31.96 (9) | Si1—C3—H3C | 109.5 |
| C2'$^{ii}$—K1—Si2$^{ii}$ | 73.9 (3) | Si1—C3'—H3D | 109.5 |
| C4'$^{ii}$—K1—Si2$^{ii}$ | 31.23 (12) | Si1—C3'—H3E | 109.5 |
| C2$^{ii}$—K1—Si2$^{ii}$ | 73.56 (13) | H3D—C3'—H3E | 109.5 |
| Si1$^{ii}$—K1—Si2$^{ii}$ | 51.263 (10) | Si1—C3'—H3F | 109.5 |
| N1—K1—Li1$^{ii}$ | 151.92 (3) | H3D—C3'—H3F | 109.5 |
| N1$^{ii}$—K1—Li1$^{ii}$ | 28.08 (3) | H3E—C3'—H3F | 109.5 |
| C4$^{ii}$—K1—Li1$^{ii}$ | 76.34 (11) | Si2—C4—H4A | 109.5 |
| C2'$^{ii}$—K1—Li1$^{ii}$ | 77.83 (16) | Si2—C4—H4B | 109.5 |
| C4'$^{ii}$—K1—Li1$^{ii}$ | 74.08 (18) | Si2—C4—H4C | 109.5 |
| C2$^{ii}$—K1—Li1$^{ii}$ | 77.48 (8) | Si2—C4'—H4D | 109.5 |
| Si1$^{ii}$—K1—Li1$^{ii}$ | 46.06 (5) | Si2—C4'—H4E | 109.5 |
| Si2$^{ii}$—K1—Li1$^{ii}$ | 45.415 (10) | H4D—C4'—H4E | 109.5 |
| Si2—N1—Si1 | 132.29 (7) | Si2—C4'—H4F | 109.5 |
| Si2—N1—Li1 | 106.91 (9) | H4D—C4'—H4F | 109.5 |

| | | | |
|---|---|---|---|
| Si1—N1—Li1 | 108.27 (13) | H4E—C4'—H4F | 109.5 |
| Si2—N1—K1 | 100.13 (5) | Si2—C5—H5A | 109.5 |
| Si1—N1—K1 | 98.70 (5) | Si2—C5—H5B | 109.5 |
| Li1—N1—K1 | 107.80 (9) | Si2—C5—H5C | 109.5 |
| N1—Si1—C3 | 119.7 (5) | Si2—C5'—H5D | 109.5 |
| N1—Si1—C1' | 113.1 (4) | Si2—C5'—H5E | 109.5 |
| N1—Si1—C2' | 110.5 (8) | H5D—C5'—H5E | 109.5 |
| C1'—Si1—C2' | 114.9 (10) | Si2—C5'—H5F | 109.5 |
| N1—Si1—C3' | 111.1 (7) | H5D—C5'—H5F | 109.5 |
| C1'—Si1—C3' | 101.6 (8) | H5E—C5'—H5F | 109.5 |
| C2'—Si1—C3' | 104.9 (10) | Si2—C6—H6A | 109.5 |
| N1—Si1—C2 | 115.9 (4) | Si2—C6—H6B | 109.5 |
| C3—Si1—C2 | 104.1 (6) | Si2—C6—H6C | 109.5 |
| N1—Si1—C1 | 105.4 (2) | Si2—C6'—H6D | 109.5 |
| C3—Si1—C1 | 109.6 (4) | Si2—C6'—H6E | 109.5 |
| C2—Si1—C1 | 100.4 (5) | H6D—C6'—H6E | 109.5 |
| N1—Si2—C4' | 118.7 (6) | Si2—C6'—H6F | 109.5 |
| N1—Si2—C6 | 121.9 (5) | H6D—C6'—H6F | 109.5 |
| N1—Si2—C6' | 110.4 (6) | H6E—C6'—H6F | 109.5 |
| C4'—Si2—C6' | 106.6 (9) | | |

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

**Fig. 1**

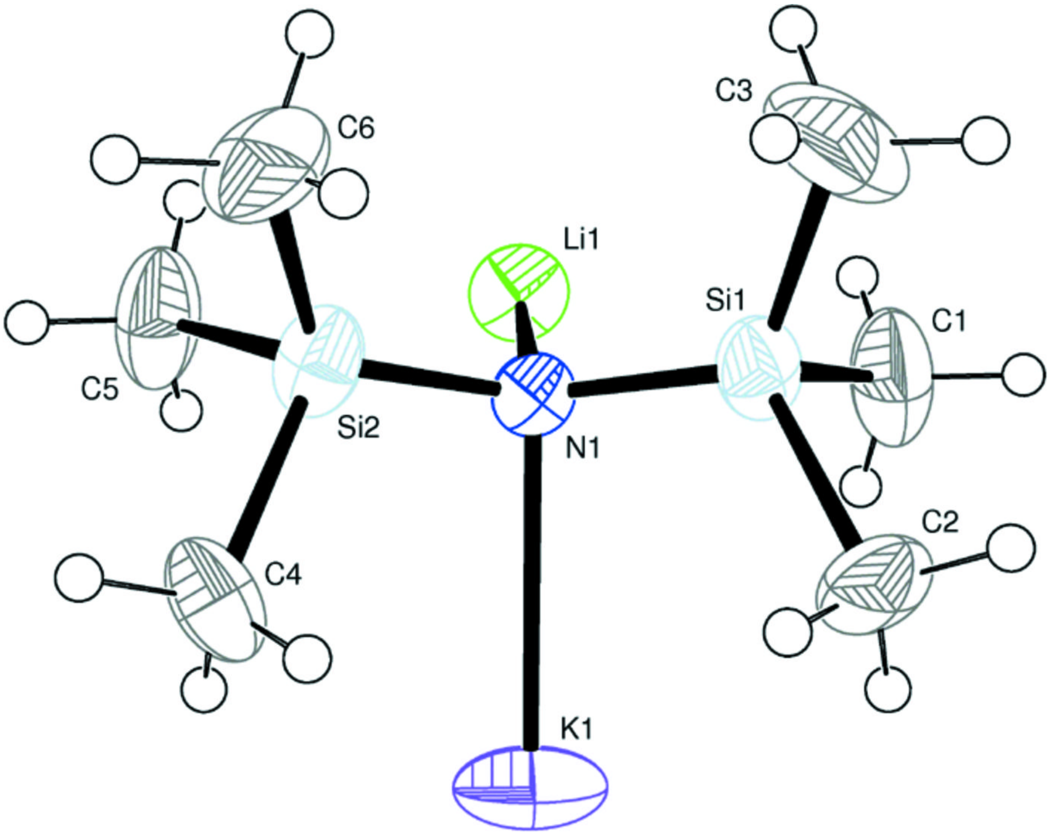

Fig. 2