IUCrData

ISSN 2414-3146

Bis[μ-*N*,*N*′-(pyridine-2,6-diyl)bis(trimethylsilylamido)-1κ^2N^1,N^2;2:3κ^2N^6:N^6]bis(tetrahydrofuran)-2:3κ^2O-1-nickel(II)-2,3-lithium(I)

Alan M. Boltin and Gary L. Guillet*

Department of Chemistry and Biochemistry, Georgia Southern University, Savannah, GA 31419, USA. *Correspondence e-mail: gary.guillet@armstrong.edu

Received 13 December 2017
Accepted 9 January 2018

Edited by S. Bernès, Benemérita Universidad Autónoma de Puebla, México

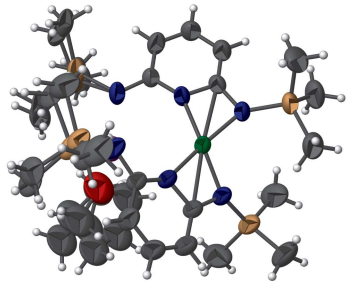
Keywords: crystal structure; lithium complex; nickel(II) complex; heteromultimetallic; 2,6-bis(trimethylsilylamino)pyridine.

CCDC reference: 1815878

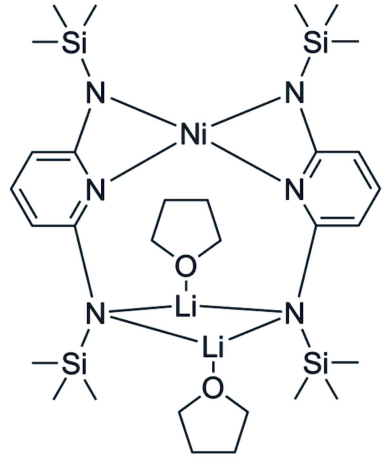
Structural data: full structural data are available from iucrdata.iucr.org

The title complex, $[Li_2Ni(C_{11}H_{21}N_3Si_2)_2(C_4H_8O)_2]$, is a trimetallic complex of two Li^I cations and a Ni^{II} cation bridged by two *N*,*N*′-(pyridine-2,6-diyl)bis(trimethylsilylamide) ligands that crystallizes in the *Fdd*2 space group. The molecule has C_2 rotational symmetry, with the Ni^{II} cation located on the twofold axis. The coordination sphere of the Ni^{II} cation is composed of two amido N and two pyridyl N-atom donors in a distorted square-planar geometry. The Li^I cations are coordinated by two amido N-atom donors and a tetrahydrofuran molecule with a long interaction with a pyridyl N-atom donor. The coordinating tetrahydrofuran ligand and a trimethylsilyl group are disordered. Intra- or intermolecular hydrogen bonding, as well as π–π stacking, are not observed between the molecules, likely indicating that weak electrostatic interactions are the dominant feature leading to the crystal structure.

3D view



Chemical scheme



Structure description

The title complex (Fig. 1) represents a unique mixed trimetallic complex of Li^I and Ni^{II}. There are a number of multimetallic complexes supported by 2,6-bis(trialkylsilylamido)pyridines (see: Glatz & Kempe, 2008*a*,*b*,*c*; Huang *et al.*, 2012), but to the best of the authors' knowledge this is the first with Ni^{II} and the first with an alkali metal and a transition metal cation. Although there are multiple metals in close proximity, there is no indication of a metal-to-metal interaction with an Li1···Ni1 distance of 3.20 (2) Å.

The Ni1 dication is in a special position on a twofold rotation axis. The coordination geometry about Ni1 is best described as distorted square planar. Ni1 is coordinated by pyridyl atoms N1 and N1^i with bond distances of 1.952 (6) Å and to the amido atoms N2 and N2^i with bond distances of 1.911 (6) Å [symmetry code: (i) $\frac{3}{2}-x,\frac{1}{2}-y,z$]. The extent

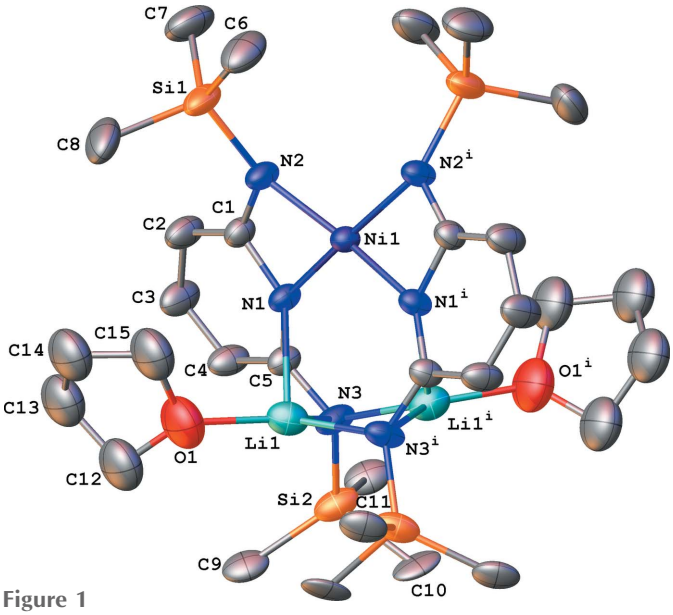


Figure 1
Structure of the title complex. H atoms and the minor disorder components of the disordered $SiMe_3$ group and THF molecule were omitted for clarity. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} - y, z$].

of distortion from planarity about Ni1 can be described by the distance of N1^{i} or N2^{i} from the plane defined by Ni1, N1, C1, and N2. For N1^{i} this distance is 0.38 (1) Å and for N2^{i} it is 0.52 (1) Å. The angle N1—Ni1—N2 is 69.6 (3)°, a typical value for a bidentate 2-silylamidopyridine. The angles N1—Ni—N1^{i} and N2—Ni—N2^{i} are 115.3 (4)° and 109.0 (4)°, respectively.

The coordination about Li1 is best described as distorted tetrahedral with one bond significantly longer than the other three. Li1 has typical bond lengths to amido atoms N3 and N3^{i}, N3—Li1 = 2.085 (17) Å and N3^{i}—Li1 = 2.031 (18) Å, and ethereal O1—Li1 = 1.854 (19) Å. On the other hand, the bond length to the pyridyl atom N1, N1—Li1 = 2.473 (17) Å, is significantly longer. Li1 is lifted only slightly out of the trigonal plane O1, N3, and N3^{i} by 0.12 (2) Å towards N1. The three bond angles in the trigonal plane about Li1 sum to 358.9°. The behaviour of Li1 could be described as a trigonal plane that is capped by N1. It is hoped that the title complex could be a useful synthon for heterometallic transition metal complexes.

Synthesis and crystallization

For this synthesis, bis-2,6-(trimethylsilylamino)pyridine (H_2L) is lithiated with *n*-butyllithium in tetrahydrofuran (THF) prior to reaction with transition metals. The lithiated starting material (Li_4L_2·4THF, 0.151 g, 0.184 mmol) was dissolved in 5 ml of THF and $NiCl_2$ (0.048 g, 0.368 mmol) was added directly to the reaction mixture. The reaction proceeded overnight and in that time the solution turned from pale yellow to black with concomitant LiCl precipitation. The solvent was removed under vacuum, the residue taken up in 5 ml of diethyl ether, and then filtered through celite. The resulting solution was allowed to evaporate slowly until crystal formation began, at which point the reaction was cooled to −30°C to induce further crystallization. The title complex was isolated as dark-purple block-shaped crystals.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Li_2Ni(C_{11}H_{21}N_3Si_2)_2(C_4H_8O)_2]$
M_r	719.77
Crystal system, space group	Orthorhombic, *Fdd*2
Temperature (K)	170
a, *b*, *c* (Å)	21.023 (7), 28.508 (9), 13.566 (4)
V (Å^3)	8129 (4)
Z	8
Radiation type	Mo *Kα*
μ (mm^{-1})	0.63
Crystal size (mm)	0.4 × 0.29 × 0.18
Data collection	
Diffractometer	Rigaku XtaLAB mini
Absorption correction	Multi-scan (*REQAB*; Rigaku, 1998)
T_{min}, T_{max}	0.733, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17664, 3717, 3041
R_{int}	0.075
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.060, 0.156, 1.05
No. of reflections	3717
No. of parameters	239
No. of restraints	207
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.34
Absolute structure	Flack *x* determined using 1094 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.022 (14)

Computer programs: *CrystalClear* (Rigaku, 2009), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. One $SiMe_3$ group is disordered over two positions, Si2/C9/C10/C11 and Si2*A*/C9*A*/C10*A*/C11*A*, with site occupancies converging to 0.70 (7) and 0.30 (7). The solvated THF molecule is disordered over two positions, C12/C13/C14/C15 and C12*A*/C13*A*/C14*A*/C15*A*, with site occupancies converging to 0.70 (1) and 0.30 (1). The thermal displacement parameters for O1/C12/C13/C14/C15/C12*A*/C13*A*/C14*A*/C15*A* were constrained.

Funding information

The authors would like to thank Armstrong State University for funding.

References

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Glatz, G. & Kempe, R. (2008*a*). *Z. Kristallogr. New Cryst. Struct.* **223**, 307–308.
Glatz, G. & Kempe, R. (2008*b*). *Z. Kristallogr. New Cryst. Struct.* **223**, 313–315.

Glatz, G. & Kempe, R. (2008*c*). *Z. Kristallogr. New Cryst. Struct.* **223**, 309–310.
Huang, Y.-L., Lu, D.-Y., Yu, H.-C., Yu, J. K., Hsu, C.-W., Kuo, T.-S., Lee, G.-H., Wang, Y. & Tsai, Y.-C. (2012). *Angew. Chem. Int. Ed.* **51**, 7781–7785.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Rigaku (1998). *REQAB*. Rigaku Corporation, Tokyo, Japan.
Rigaku (2009). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2018). **3**, x180058 [https://doi.org/10.1107/S2414314618000585]

Bis[μ-*N*,*N*′-(pyridine-2,6-diyl)bis(trimethylsilylamido)-1κ^2N^1,*N*^{2};2:3κ^2N^6:*N*^{6}]bis-(tetrahydrofuran)-2:3κ^2O-1-nickel(II)-2,3-lithium(I)

Alan M. Boltin and Gary L. Guillet

Bis[μ-*N*,*N*′-(pyridine-2,6-diyl)bis(trimethylsilylamido)-1κ^2N^1,*N*^{2};2:3κ^2N^6:*N*^{6}]bis(tetrahydrofuran)-2:3κ^2O-1-nickel(II)-2,3-lithium(I)

Crystal data

$[Li_2Ni(C_{11}H_{21}N_3Si_2)_2(C_4H_8O)_2]$
M_r = 719.77
Orthorhombic, *Fdd*2
a = 21.023 (7) Å
b = 28.508 (9) Å
c = 13.566 (4) Å
V = 8129 (4) Å^3
Z = 8
F(000) = 3088
D_x = 1.176 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 3922 reflections
θ = 1.9–25.4°
μ = 0.63 mm^{-1}
T = 170 K
Block, clear dark violet
0.4 × 0.29 × 0.18 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} = 0.733, T_{max} = 1.000
17664 measured reflections
3717 independent reflections
3041 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 25.4°, θ_{min} = 2.4°
h = −25→25
k = −34→34
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.156
S = 1.05
3717 reflections
239 parameters
207 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0788P)^2 + 9.9425P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack *x* determined using 1094 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.022 (14)

Special details

Refinement. H atoms bonded to C atoms were included at calculated positions using a riding model, with aromatic, methylene, and methyl C—H bond lengths of 0.93, 0.97 and 0.96 Å, respectively, and U_{iso}(H) set to 1.2U_{equiv}(C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ni1	0.7500	0.2500	0.42790 (10)	0.0421 (3)	
Si1	0.67645 (12)	0.30931 (11)	0.24185 (18)	0.0736 (8)	
O1	0.7103 (5)	0.3553 (3)	0.6360 (8)	0.131 (3)	
N1	0.6730 (3)	0.2608 (2)	0.5049 (5)	0.0469 (14)	
N2	0.6842 (3)	0.2750 (2)	0.3461 (5)	0.0545 (16)	
N3	0.6770 (3)	0.2341 (3)	0.6654 (5)	0.0603 (17)	
C1	0.6418 (3)	0.2746 (3)	0.4207 (6)	0.0508 (16)	
C2	0.5769 (4)	0.2841 (4)	0.4233 (7)	0.074 (2)	
H2	0.5557	0.2952	0.3679	0.089*	
C3	0.5451 (4)	0.2765 (4)	0.5106 (7)	0.077 (3)	
H3	0.5019	0.2833	0.5141	0.092*	
C4	0.5749 (4)	0.2593 (3)	0.5915 (6)	0.067 (2)	
H4	0.5518	0.2532	0.6486	0.080*	
C5	0.6415 (3)	0.2504 (3)	0.5892 (6)	0.0485 (17)	
C6	0.7539 (5)	0.3125 (5)	0.1748 (9)	0.109 (4)	
H6A	0.7753	0.3412	0.1916	0.163*	
H6B	0.7463	0.3116	0.1050	0.163*	
H6C	0.7800	0.2863	0.1933	0.163*	
C7	0.6143 (6)	0.2860 (5)	0.1556 (8)	0.114 (4)	
H7A	0.6173	0.2525	0.1527	0.170*	
H7B	0.6209	0.2989	0.0910	0.170*	
H7C	0.5729	0.2948	0.1790	0.170*	
C8	0.6535 (7)	0.3702 (4)	0.2800 (10)	0.115 (4)	
H8A	0.6129	0.3694	0.3124	0.173*	
H8B	0.6508	0.3899	0.2228	0.173*	
H8C	0.6849	0.3825	0.3244	0.173*	
Li1	0.7346 (7)	0.2929 (6)	0.6448 (12)	0.069 (4)	
Si2	0.6452 (16)	0.2234 (19)	0.778 (3)	0.068 (6)	0.30 (7)
C9	0.603 (2)	0.271 (2)	0.847 (3)	0.074 (10)	0.30 (7)
H9A	0.6318	0.2860	0.8922	0.112*	0.30 (7)
H9B	0.5678	0.2582	0.8832	0.112*	0.30 (7)
H9C	0.5872	0.2943	0.8013	0.112*	0.30 (7)
C10	0.7127 (19)	0.201 (3)	0.856 (3)	0.075 (11)	0.30 (7)
H10A	0.7241	0.1702	0.8346	0.112*	0.30 (7)
H10B	0.6999	0.2005	0.9235	0.112*	0.30 (7)
H10C	0.7487	0.2217	0.8484	0.112*	0.30 (7)
C11	0.587 (2)	0.174 (2)	0.760 (4)	0.075 (11)	0.30 (7)
H11A	0.5500	0.1857	0.7273	0.113*	0.30 (7)
H11B	0.5755	0.1615	0.8232	0.113*	0.30 (7)
H11C	0.6066	0.1500	0.7210	0.113*	0.30 (7)
C12	0.6601 (11)	0.3780 (7)	0.6872 (16)	0.131 (3)	0.701 (12)

H12A	0.6760	0.4017	0.7322	0.157*	0.701 (12)
H12B	0.6339	0.3558	0.7231	0.157*	0.701 (12)
C13	0.6251 (10)	0.3992 (6)	0.6035 (17)	0.131 (3)	0.701 (12)
H13A	0.5978	0.4246	0.6250	0.157*	0.701 (12)
H13B	0.5999	0.3761	0.5685	0.157*	0.701 (12)
C14	0.6842 (10)	0.4183 (6)	0.5366 (18)	0.131 (3)	0.701 (12)
H14A	0.6707	0.4234	0.4691	0.157*	0.701 (12)
H14B	0.7006	0.4475	0.5629	0.157*	0.701 (12)
C15	0.7315 (10)	0.3823 (6)	0.5413 (19)	0.131 (3)	0.701 (12)
H15A	0.7738	0.3954	0.5485	0.157*	0.701 (12)
H15B	0.7303	0.3623	0.4834	0.157*	0.701 (12)
Si2A	0.6446 (6)	0.2070 (8)	0.7699 (10)	0.062 (3)	0.70 (7)
C9A	0.6048 (10)	0.2500 (13)	0.8547 (15)	0.084 (6)	0.70 (7)
H9AA	0.6348	0.2736	0.8741	0.126*	0.70 (7)
H9AB	0.5895	0.2339	0.9121	0.126*	0.70 (7)
H9AC	0.5697	0.2645	0.8212	0.126*	0.70 (7)
C10A	0.7124 (10)	0.1789 (14)	0.837 (2)	0.092 (7)	0.70 (7)
H10D	0.7197	0.1481	0.8113	0.138*	0.70 (7)
H10E	0.7022	0.1767	0.9061	0.138*	0.70 (7)
H10F	0.7500	0.1976	0.8291	0.138*	0.70 (7)
C11A	0.5866 (11)	0.1586 (10)	0.739 (2)	0.091 (6)	0.70 (7)
H11D	0.5653	0.1658	0.6785	0.136*	0.70 (7)
H11E	0.5558	0.1559	0.7912	0.136*	0.70 (7)
H11F	0.6091	0.1295	0.7326	0.136*	0.70 (7)
C12A	0.638 (2)	0.3589 (11)	0.672 (5)	0.131 (3)	0.299 (12)
H12C	0.6085	0.3493	0.6204	0.157*	0.299 (12)
H12D	0.6303	0.3409	0.7309	0.157*	0.299 (12)
C13A	0.635 (2)	0.4091 (11)	0.690 (4)	0.131 (3)	0.299 (12)
H13C	0.6445	0.4165	0.7580	0.157*	0.299 (12)
H13D	0.5942	0.4221	0.6720	0.157*	0.299 (12)
C14A	0.6915 (19)	0.4276 (11)	0.616 (4)	0.131 (3)	0.299 (12)
H14C	0.6755	0.4305	0.5491	0.157*	0.299 (12)
H14D	0.7071	0.4580	0.6372	0.157*	0.299 (12)
C15A	0.7421 (18)	0.3929 (14)	0.620 (5)	0.131 (3)	0.299 (12)
H15C	0.7654	0.3912	0.5587	0.157*	0.299 (12)
H15D	0.7715	0.3993	0.6738	0.157*	0.299 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0426 (6)	0.0483 (6)	0.0355 (6)	−0.0009 (6)	0.000	0.000
Si1	0.0678 (15)	0.107 (2)	0.0465 (13)	0.0204 (14)	0.0037 (11)	0.0264 (13)
O1	0.165 (7)	0.080 (4)	0.148 (7)	0.008 (4)	0.003 (6)	−0.025 (4)
N1	0.041 (3)	0.060 (3)	0.040 (3)	−0.002 (3)	−0.004 (3)	0.010 (3)
N2	0.048 (4)	0.076 (5)	0.039 (3)	0.007 (3)	0.000 (3)	0.012 (3)
N3	0.047 (3)	0.090 (4)	0.043 (4)	−0.006 (3)	−0.001 (3)	0.021 (3)
C1	0.046 (4)	0.060 (4)	0.047 (4)	0.004 (3)	−0.005 (4)	0.007 (4)
C2	0.056 (5)	0.112 (7)	0.054 (5)	0.017 (4)	−0.003 (5)	0.016 (5)

C3	0.045 (4)	0.122 (8)	0.063 (6)	0.017 (5)	0.005 (4)	0.018 (6)
C4	0.050 (5)	0.104 (7)	0.047 (4)	−0.004 (4)	0.005 (4)	0.013 (5)
C5	0.037 (4)	0.063 (4)	0.045 (4)	−0.004 (3)	−0.001 (3)	0.009 (4)
C6	0.097 (7)	0.151 (11)	0.078 (7)	0.026 (6)	0.024 (6)	0.052 (8)
C7	0.106 (8)	0.171 (11)	0.064 (7)	0.023 (7)	−0.022 (6)	0.021 (7)
C8	0.144 (10)	0.101 (7)	0.100 (8)	0.050 (7)	0.024 (7)	0.047 (6)
Li1	0.062 (8)	0.083 (10)	0.062 (9)	−0.015 (7)	0.003 (7)	−0.008 (8)
Si2	0.059 (6)	0.092 (17)	0.054 (8)	−0.026 (10)	−0.008 (5)	0.025 (10)
C9	0.076 (17)	0.10 (2)	0.047 (16)	−0.026 (15)	0.012 (13)	0.027 (15)
C10	0.066 (12)	0.12 (3)	0.036 (16)	−0.022 (15)	0.008 (10)	0.045 (17)
C11	0.065 (15)	0.10 (2)	0.06 (2)	−0.030 (14)	0.010 (13)	0.026 (16)
C12	0.165 (7)	0.080 (4)	0.148 (7)	0.008 (4)	0.003 (6)	−0.025 (4)
C13	0.165 (7)	0.080 (4)	0.148 (7)	0.008 (4)	0.003 (6)	−0.025 (4)
C14	0.165 (7)	0.080 (4)	0.148 (7)	0.008 (4)	0.003 (6)	−0.025 (4)
C15	0.165 (7)	0.080 (4)	0.148 (7)	0.008 (4)	0.003 (6)	−0.025 (4)
Si2A	0.051 (3)	0.089 (7)	0.046 (3)	−0.015 (4)	0.001 (2)	0.026 (4)
C9A	0.078 (10)	0.116 (14)	0.056 (8)	−0.010 (9)	0.025 (7)	0.024 (9)
C10A	0.065 (8)	0.128 (17)	0.084 (14)	−0.007 (9)	0.002 (7)	0.044 (12)
C11A	0.087 (10)	0.103 (12)	0.082 (14)	−0.036 (9)	−0.005 (10)	0.033 (10)
C12A	0.165 (7)	0.080 (4)	0.148 (7)	0.008 (4)	0.003 (6)	−0.025 (4)
C13A	0.165 (7)	0.080 (4)	0.148 (7)	0.008 (4)	0.003 (6)	−0.025 (4)
C14A	0.165 (7)	0.080 (4)	0.148 (7)	0.008 (4)	0.003 (6)	−0.025 (4)
C15A	0.165 (7)	0.080 (4)	0.148 (7)	0.008 (4)	0.003 (6)	−0.025 (4)

Geometric parameters (Å, º)

Ni1—N1^{i}	1.952 (6)	Si2—C11	1.88 (2)
Ni1—N1	1.952 (6)	C9—H9A	0.9600
Ni1—N2	1.911 (6)	C9—H9B	0.9600
Ni1—N2^{i}	1.911 (6)	C9—H9C	0.9600
Ni1—C1^{i}	2.382 (7)	C10—H10A	0.9600
Ni1—C1	2.382 (7)	C10—H10B	0.9600
Ni1—Li1^{i}	3.202 (16)	C10—H10C	0.9600
Ni1—Li1	3.202 (16)	C11—H11A	0.9600
Si1—N2	1.727 (7)	C11—H11B	0.9600
Si1—C6	1.868 (10)	C11—H11C	0.9600
Si1—C7	1.875 (11)	C12—H12A	0.9700
Si1—C8	1.875 (12)	C12—H12B	0.9700
O1—Li1	1.854 (19)	C12—C13	1.48 (2)
O1—C12	1.42 (2)	C13—H13A	0.9700
O1—C15	1.56 (2)	C13—H13B	0.9700
O1—C12A	1.60 (4)	C13—C14	1.63 (3)
O1—C15A	1.28 (4)	C14—H14A	0.9700
N1—C1	1.374 (10)	C14—H14B	0.9700
N1—C5	1.353 (10)	C14—C15	1.43 (2)
N1—Li1	2.473 (17)	C15—H15A	0.9700
N2—C1	1.349 (10)	C15—H15B	0.9700
N3—C5	1.356 (10)	Si2A—Li1^{i}	3.05 (2)

N3—Li1^{i}	2.031 (18)	Si2A—C9A	1.880 (15)
N3—Li1	2.085 (17)	Si2A—C10A	1.872 (13)
N3—Si2	1.70 (3)	Si2A—C11A	1.887 (14)
N3—Si2A	1.753 (14)	C9A—H9AA	0.9600
C1—C2	1.391 (10)	C9A—H9AB	0.9600
C2—H2	0.9300	C9A—H9AC	0.9600
C2—C3	1.378 (13)	C10A—H10D	0.9600
C3—H3	0.9300	C10A—H10E	0.9600
C3—C4	1.355 (12)	C10A—H10F	0.9600
C4—H4	0.9300	C11A—H11D	0.9600
C4—C5	1.424 (11)	C11A—H11E	0.9600
C6—H6A	0.9600	C11A—H11F	0.9600
C6—H6B	0.9600	C12A—H12C	0.9700
C6—H6C	0.9600	C12A—H12D	0.9700
C7—H7A	0.9600	C12A—C13A	1.45 (3)
C7—H7B	0.9600	C13A—H13C	0.9700
C7—H7C	0.9600	C13A—H13D	0.9700
C8—H8A	0.9600	C13A—C14A	1.64 (3)
C8—H8B	0.9600	C14A—H14C	0.9700
C8—H8C	0.9600	C14A—H14D	0.9700
Li1—N3^{i}	2.031 (17)	C14A—C15A	1.46 (3)
Si2—Li1^{i}	3.14 (4)	C15A—H15C	0.9700
Si2—C9	1.88 (2)	C15A—H15D	0.9700
Si2—C10	1.88 (2)		

N1—Ni1—N1^{i}	115.3 (4)	C9—Si2—Li1^{i}	140.8 (16)
N1—Ni1—C1^{i}	149.4 (3)	C10—Si2—Li1^{i}	70.4 (15)
N1^{i}—Ni1—C1^{i}	35.2 (3)	C10—Si2—C9	108.9 (18)
N1^{i}—Ni1—C1	149.4 (3)	C11—Si2—Li1^{i}	109.7 (18)
N1—Ni1—C1	35.2 (3)	C11—Si2—C9	107.5 (17)
N1—Ni1—Li1	50.5 (3)	C11—Si2—C10	108.1 (18)
N1^{i}—Ni1—Li1^{i}	50.5 (3)	Si2—C9—H9A	109.5
N1—Ni1—Li1^{i}	69.7 (3)	Si2—C9—H9B	109.5
N1^{i}—Ni1—Li1	69.7 (3)	Si2—C9—H9C	109.5
N2^{i}—Ni1—N1	166.0 (3)	H9A—C9—H9B	109.5
N2^{i}—Ni1—N1^{i}	69.6 (3)	H9A—C9—H9C	109.5
N2—Ni1—N1^{i}	166.0 (3)	H9B—C9—H9C	109.5
N2—Ni1—N1	69.6 (3)	Si2—C10—H10A	109.5
N2^{i}—Ni1—N2	109.0 (4)	Si2—C10—H10B	109.5
N2—Ni1—C1	34.5 (3)	Si2—C10—H10C	109.5
N2—Ni1—C1^{i}	141.0 (3)	H10A—C10—H10B	109.5
N2^{i}—Ni1—C1	141.0 (3)	H10A—C10—H10C	109.5
N2^{i}—Ni1—C1^{i}	34.5 (3)	H10B—C10—H10C	109.5
N2^{i}—Ni1—Li1	138.5 (3)	Si2—C11—H11A	109.5
N2—Ni1—Li1^{i}	138.5 (3)	Si2—C11—H11B	109.5
N2^{i}—Ni1—Li1^{i}	108.5 (4)	Si2—C11—H11C	109.5
N2—Ni1—Li1	108.5 (4)	H11A—C11—H11B	109.5
C1—Ni1—C1^{i}	175.3 (4)	H11A—C11—H11C	109.5

C1—Ni1—Li1^{i}	104.3 (3)	H11B—C11—H11C	109.5
C1^{i}—Ni1—Li1	104.3 (3)	O1—C12—H12A	111.7
C1^{i}—Ni1—Li1^{i}	80.2 (3)	O1—C12—H12B	111.7
C1—Ni1—Li1	80.2 (3)	O1—C12—C13	100.4 (16)
Li1^{i}—Ni1—Li1	46.5 (6)	H12A—C12—H12B	109.5
N2—Si1—C6	110.1 (4)	C13—C12—H12A	111.7
N2—Si1—C7	112.1 (5)	C13—C12—H12B	111.7
N2—Si1—C8	108.8 (5)	C12—C13—H13A	111.6
C6—Si1—C7	108.7 (6)	C12—C13—H13B	111.6
C6—Si1—C8	108.3 (6)	C12—C13—C14	100.6 (15)
C7—Si1—C8	108.7 (6)	H13A—C13—H13B	109.4
C12—O1—Li1	127.6 (12)	C14—C13—H13A	111.6
C12—O1—C15	112.8 (13)	C14—C13—H13B	111.6
C15—O1—Li1	116.7 (10)	C13—C14—H14A	110.7
C12A—O1—Li1	107.8 (14)	C13—C14—H14B	110.7
C15A—O1—Li1	132.1 (18)	H14A—C14—H14B	108.8
C15A—O1—C12A	119 (2)	C15—C14—C13	105.4 (15)
Ni1—N1—Li1	92.0 (4)	C15—C14—H14A	110.7
C1—N1—Ni1	89.7 (5)	C15—C14—H14B	110.7
C1—N1—Li1	141.5 (6)	O1—C15—H15A	111.5
C5—N1—Ni1	145.4 (5)	O1—C15—H15B	111.5
C5—N1—C1	122.2 (6)	C14—C15—O1	101.1 (15)
C5—N1—Li1	71.8 (5)	C14—C15—H15A	111.5
Si1—N2—Ni1	139.1 (4)	C14—C15—H15B	111.5
C1—N2—Ni1	92.2 (4)	H15A—C15—H15B	109.4
C1—N2—Si1	123.8 (5)	N3—Si2A—Li1^{i}	39.4 (5)
C5—N3—Li1^{i}	121.9 (7)	N3—Si2A—C9A	112.3 (8)
C5—N3—Li1	86.7 (6)	N3—Si2A—C10A	106.7 (10)
C5—N3—Si2	122.2 (14)	N3—Si2A—C11A	113.3 (10)
C5—N3—Si2A	123.7 (7)	C9A—Si2A—Li1^{i}	135.2 (7)
Li1^{i}—N3—Li1	75.8 (8)	C9A—Si2A—C11A	108.9 (9)
Si2—N3—Li1	119.6 (18)	C10A—Si2A—Li1^{i}	68.9 (9)
Si2—N3—Li1^{i}	114.6 (15)	C10A—Si2A—C9A	108.6 (10)
Si2A—N3—Li1	133.5 (9)	C10A—Si2A—C11A	106.7 (10)
Si2A—N3—Li1^{i}	107.4 (7)	C11A—Si2A—Li1^{i}	114.6 (9)
N1—C1—C2	120.1 (8)	Si2A—C9A—H9AA	109.5
N2—C1—N1	108.1 (6)	Si2A—C9A—H9AB	109.5
N2—C1—C2	131.7 (8)	Si2A—C9A—H9AC	109.5
C1—C2—H2	121.1	H9AA—C9A—H9AB	109.5
C3—C2—C1	117.8 (8)	H9AA—C9A—H9AC	109.5
C3—C2—H2	121.1	H9AB—C9A—H9AC	109.5
C2—C3—H3	119.0	Si2A—C10A—H10D	109.5
C4—C3—C2	122.0 (8)	Si2A—C10A—H10E	109.5
C4—C3—H3	119.0	Si2A—C10A—H10F	109.5
C3—C4—H4	120.0	H10D—C10A—H10E	109.5
C3—C4—C5	120.0 (8)	H10D—C10A—H10F	109.5
C5—C4—H4	120.0	H10E—C10A—H10F	109.5
N1—C5—N3	116.8 (6)	Si2A—C11A—H11D	109.5

N1—C5—C4	117.4 (7)	Si2A—C11A—H11E	109.5
N3—C5—C4	125.7 (7)	Si2A—C11A—H11F	109.5
Si1—C6—H6A	109.5	H11D—C11A—H11E	109.5
Si1—C6—H6B	109.5	H11D—C11A—H11F	109.5
Si1—C6—H6C	109.5	H11E—C11A—H11F	109.5
H6A—C6—H6B	109.5	O1—C12A—H12C	112.0
H6A—C6—H6C	109.5	O1—C12A—H12D	112.0
H6B—C6—H6C	109.5	H12C—C12A—H12D	109.7
Si1—C7—H7A	109.5	C13A—C12A—O1	99 (2)
Si1—C7—H7B	109.5	C13A—C12A—H12C	112.0
Si1—C7—H7C	109.5	C13A—C12A—H12D	112.0
H7A—C7—H7B	109.5	C12A—C13A—H13C	111.6
H7A—C7—H7C	109.5	C12A—C13A—H13D	111.6
H7B—C7—H7C	109.5	C12A—C13A—C14A	101 (2)
Si1—C8—H8A	109.5	H13C—C13A—H13D	109.4
Si1—C8—H8B	109.5	C14A—C13A—H13C	111.6
Si1—C8—H8C	109.5	C14A—C13A—H13D	111.6
H8A—C8—H8B	109.5	C13A—C14A—H14C	110.4
H8A—C8—H8C	109.5	C13A—C14A—H14D	110.4
H8B—C8—H8C	109.5	H14C—C14A—H14D	108.6
O1—Li1—N3	128.2 (9)	C15A—C14A—C13A	106 (2)
O1—Li1—N3^{i}	128.6 (9)	C15A—C14A—H14C	110.4
O1—Li1—C5	103.7 (8)	C15A—C14A—H14D	110.4
N3^{i}—Li1—N3	102.1 (8)	O1—C15A—C14A	101 (2)
N3—Li1—C5	34.0 (3)	O1—C15A—H15C	111.5
N3^{i}—Li1—C5	126.4 (8)	O1—C15A—H15D	111.5
N3—Si2—Li1^{i}	36.0 (10)	C14A—C15A—H15C	111.5
N3—Si2—C9	120 (2)	C14A—C15A—H15D	111.5
N3—Si2—C10	106 (2)	H15C—C15A—H15D	109.3
N3—Si2—C11	106 (2)		

Symmetry code: (i) $-x+3/2, -y+1/2, z$.