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Electronic Supplementary Information for:

A Heterocyclic Organogallium Peroxide Possessing Two Alkylgallium Groups Bridged by a Peroxide Dianion

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Single-Crystal X-ray Structure Determinations: Crystals were mounted on a glass fibre in paraffin oil and cooled with a flow of cold nitrogen gas. Data was collected on a Bruker APEX II diffractometer at 153 K (Mo-Kα, 0.71073). The structures were solved by direct methods using *SHELXTL*. Non-hydrogen atoms were first refined isotropically followed by anisotropic refinement by full matrix least-squares calculations based on F^2 using *SHELXTL*. Hydrogen atoms except the hydroxo hydrogen atom H03 of compound **2** were positioned geometrically and allowed to ride on their respective parent atoms. The position of H03 was taken from the electron density map and its parameters (x, y, z, U) were kept fixed during refinement. Compound **2** has three disordered $SiMe_3$ groups. The methyl groups on Si31 and Si42 are both disordered over two positions that were refined to occupation factors of 0.5 and 0.42 : 0.58, respectively. The $SiMe_3$ group at Si32 is disordered as a whole over two positions, which were refined to occupations factors of 0.42 and 0.58. For these groups the following restraints were used. Thermal expansion parameters (SIMU, DELU) were refined using the default values and bond distances and angles were restricted (SAME) based on the values of $SiMe_3$ group Si21. No restraints were necessary for compound **3**.

References

SHELXTL-Plus, REL. 4.1; Siemens Analytical X-RAY Instruments Inc.: Madison, WI, 1990; G. M. Sheldrick, *SHELXL-97*, Program for the Refinement of Structures; Universität Göttingen, 1997.

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Crystallographic data for compound 2

Empirical formula	C34 H89 Ga2 Li N2 O3 Si8
Formula weight	945.17
Temperature	153(2) K
Wavelength	71.073 pm
Crystal system	monoclinic
Space group	Cc (TWIN; BASF 0.29)
Unit cell dimensions	a = 2253.7(5) pm alpha = 90 deg b = 1160.2(2) pm beta = 116.71(3) deg c = 2258.6(5) pm gamma = 90 deg
Volume, Z	5.2755(18) nm^3, 4
Density (calculated)	1.190 Mg/m^3
Absorption coefficient	1.233 mm^-1
F(000)	2032
Crystal size	0.13 x 0.11 x 0.04 mm
Theta range for data collection	2.02 to 31.40 deg
Limiting indices	-32 < h < 31, -16 < k < 16, -32 < l < 32
Reflections collected	30166
Independent reflections	15235 (R(int) = 0.0546)
Completeness to theta =	31.40 deg 92.9 %
Max. and min. transmission	0.9523 and 0.8561
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15235 / 333 / 553
Goodness-of-fit on F^2	1.069
Final R indices [I>2Sigma(I)] =	0.0797, wR2 = 0.1786
R indices (all data) =	0.1305, wR2 = 0.2039
Absolute structure parameter	0.00(3)
Largest diff. peak and hole	1373 and -829 e.nm^-3

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2 x 10^-1) for compound 2. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ga(1)	1416(1)	5145(1)	9804(1)	33(1)
C(1)	1791(3)	6422(6)	9486(3)	37(2)
Si(11)	1645(1)	7932(2)	9674(1)	61(1)
C(111)	1529(5)	8087(8)	10454(5)	69(3)
C(112)	2378(7)	8793(9)	9792(8)	120(5)
C(113)	844(6)	8541(10)	9010(5)	89(4)
Si(12)	1659(1)	6212(2)	8616(1)	59(1)
C(121)	2051(6)	7347(11)	8344(7)	101(4)
C(122)	769(6)	6265(14)	7994(5)	109(5)
C(123)	2108(8)	4813(11)	8571(7)	102(5)
C(2)	1953(3)	4120(5)	10564(3)	31(1)
Si(21)	2361(1)	2858(2)	10395(1)	39(1)
C(211)	3190(4)	3214(8)	10466(5)	65(3)
C(212)	2459(5)	1628(6)	10975(4)	59(2)
C(213)	1852(4)	2207(7)	9550(3)	51(2)
Si(22)	2497(1)	4920(2)	11353(1)	32(1)
C(221)	3073(4)	5934(7)	11222(5)	57(2)
C(222)	3038(4)	3941(7)	12049(4)	49(2)
C(223)	1987(4)	5765(8)	11668(4)	55(2)
Ga(2)	-128(1)	4563(1)	9382(1)	37(1)
C(3)	-475(4)	3486(6)	9831(3)	45(2)
Si(31)	-424(1)	1918(2)	9663(1)	58(1)
C(311)	-440(20)	1710(20)	8835(9)	123(16)
C(312)	382(8)	1290(20)	10260(10)	85(9)
C(313)	-1096(11)	990(20)	9670(20)	190(30)
C(31A)	-785(15)	1630(20)	8762(7)	74(9)
C(31B)	401(8)	1250(20)	10042(15)	77(9)
C(31C)	-936(14)	1025(19)	9980(15)	91(11)
Si(32)	-112(4)	3629(6)	10800(4)	38(2)
C(321)	-669(12)	3060(30)	11130(11)	91(10)
C(322)	-12(12)	5193(12)	11031(9)	67(6)
C(323)	722(7)	2960(18)	11289(9)	63(6)
Si(3A)	-382(3)	3905(7)	10645(3)	57(2)
C(3A1)	-676(13)	2776(19)	11048(13)	124(10)
C(3A2)	-808(9)	5233(11)	10662(9)	75(5)
C(3A3)	539(6)	4140(20)	11211(7)	110(8)
C(4)	-661(3)	5687(5)	8654(3)	30(1)
Si(41)	-1220(1)	5032(2)	7861(1)	29(1)
C(411)	-752(4)	4066(7)	7559(4)	44(2)
C(412)	-1631(7)	6082(9)	7158(4)	106(5)
C(413)	-1862(4)	4135(8)	7941(5)	66(3)
Si(42)	-1038(1)	6929(3)	8905(1)	77(1)
C(421)	-485(10)	7530(20)	9734(9)	32(4)
C(422)	-1874(6)	6706(15)	8825(9)	32(4)
C(423)	-1121(8)	8232(11)	8323(8)	40(6)
C(42A)	-438(10)	7650(20)	9679(9)	64(7)
C(42B)	-1692(12)	6280(20)	9112(16)	186(19)
C(42C)	-1459(19)	8050(20)	8269(9)	260(30)
O(1)	852(2)	4334(5)	8992(2)	49(1)
O(2)	425(2)	3544(4)	9146(2)	43(1)
O(3)	645(2)	5451(4)	9941(2)	39(1)
N(1)	635(4)	1900(6)	7746(4)	57(2)
N(2)	549(4)	537(8)	6799(4)	81(3)
CN1	464(8)	2509(12)	7111(7)	121(6)
CN2	408(9)	1754(12)	6570(5)	142(7)

CN3	1258(6)	1246(13)	7922(6)	109(5)
CN4	1178(7)	497(15)	7336(8)	159(9)
CN5	125(6)	1035(10)	7605(7)	100(4)
CN6	78(7)	288(12)	7014(7)	115(5)
Li	648(9)	2996(16)	8513(10)	86(6)

Table 2. Bond lengths [pm] and angles [deg] for compound 2.

Ga(1)-O(3)	193.2(4)
Ga(1)-O(1)	194.1(5)
Ga(1)-C(2)	199.0(6)
Ga(1)-C(1)	199.2(7)
C(1)-Si(11)	186.5(7)
C(1)-Si(12)	186.8(7)
C(1)-H(1)	100.00
Si(11)-C(112)	184.5(12)
Si(11)-C(113)	189.1(11)
Si(11)-C(111)	190.4(10)
C(111)-H(11A)	98.00
C(111)-H(11B)	98.00
C(111)-H(11C)	98.00
C(112)-H(11D)	98.00
C(112)-H(11E)	98.00
C(112)-H(11F)	98.00
C(113)-H(11G)	98.00
C(113)-H(11H)	98.00
C(113)-H(11I)	98.00
Si(12)-C(121)	183.7(10)
Si(12)-C(122)	186.2(12)
Si(12)-C(123)	193.8(13)
C(121)-H(12A)	98.00
C(121)-H(12B)	98.00
C(121)-H(12C)	98.00
C(122)-H(12D)	98.00
C(122)-H(12E)	98.00
C(122)-H(12F)	98.00
C(123)-H(12G)	98.00
C(123)-H(12H)	98.00
C(123)-H(12I)	98.00
C(2)-Si(21)	185.8(6)
C(2)-Si(22)	189.1(6)
C(2)-H(2)	100.00
Si(21)-C(211)	184.9(8)
Si(21)-C(212)	188.3(7)
Si(21)-C(213)	188.7(7)
C(211)-H(21A)	98.00
C(211)-H(21B)	98.00
C(211)-H(21C)	98.00
C(212)-H(21D)	98.00
C(212)-H(21E)	98.00
C(212)-H(21F)	98.00
C(213)-H(21G)	98.00
C(213)-H(21H)	98.00
C(213)-H(21I)	98.00
Si(22)-C(221)	187.0(9)
Si(22)-C(222)	187.8(8)
Si(22)-C(223)	187.8(8)
C(221)-H(22A)	98.00
C(221)-H(22B)	98.00
C(221)-H(22C)	98.00

C(222)-H(22D)	98.00
C(222)-H(22E)	98.00
C(222)-H(22F)	98.00
C(223)-H(22G)	98.00
C(223)-H(22H)	98.00
C(223)-H(22I)	98.00
Ga(2)-O(3)	192.7(4)
Ga(2)-O(2)	195.6(5)
Ga(2)-C(3)	198.0(7)
Ga(2)-C(4)	201.7(6)
C(3)-Si(3A)	182.0(8)
C(3)-Si(31)	187.3(6)
C(3)-Si(32)	197.0(9)
C(3)-H(3)	100.00
Si(31)-C(31B)	183.5(12)
Si(31)-C(31A)	185.2(12)
Si(31)-C(312)	185.5(12)
Si(31)-C(313)	186.8(14)
Si(31)-C(311)	186.8(13)
Si(31)-C(31C)	191.2(12)
C(311)-H(31A)	96.00
C(311)-H(31B)	96.00
C(311)-H(31C)	96.00
C(312)-H(31D)	96.00
C(312)-H(31E)	96.00
C(312)-H(31F)	96.00
C(313)-H(31G)	96.00
C(313)-H(31H)	96.00
C(313)-H(31I)	96.00
C(31A)-H(31J)	96.00
C(31A)-H(31K)	96.00
C(31A)-H(31L)	96.00
C(31B)-H(31M)	96.00
C(31B)-H(31N)	96.00
C(31B)-H(31O)	96.00
C(31C)-H(31P)	96.00
C(31C)-H(31Q)	96.00
C(31C)-H(31R)	96.00
Si(32)-C(321)	184.6(12)
Si(32)-C(323)	186.8(13)
Si(32)-C(322)	187.3(12)
C(321)-H(32A)	96.00
C(321)-H(32B)	96.00
C(321)-H(32C)	96.00
C(322)-H(32D)	96.00
C(322)-H(32E)	96.00
C(322)-H(32F)	96.00
C(323)-H(32G)	96.00
C(323)-H(32H)	96.00
C(323)-H(32I)	96.00
Si(3A)-C(3A2)	182.5(12)
Si(3A)-C(3A1)	187.8(11)
Si(3A)-C(3A3)	190.5(12)
C(3A1)-H(3A1)	96.00
C(3A1)-H(3A2)	96.00
C(3A1)-H(3A3)	96.00
C(3A2)-H(3A4)	96.00
C(3A2)-H(3A5)	96.00
C(3A2)-H(3A6)	96.00
C(3A3)-H(3A7)	96.00
C(3A3)-H(3A8)	96.00
C(3A3)-H(3A9)	96.00
C(4)-Si(41)	182.9(6)

C(4)-Si(42)	188.5(6)
C(4)-H(4)	100.00
Si(41)-C(413)	185.7(8)
Si(41)-C(411)	186.5(7)
Si(41)-C(412)	188.2(9)
C(411)-H(41A)	98.00
C(411)-H(41B)	98.00
C(411)-H(41C)	98.00
C(412)-H(41D)	98.00
C(412)-H(41E)	98.00
C(412)-H(41F)	98.00
C(413)-H(41G)	98.00
C(413)-H(41H)	98.00
C(413)-H(41I)	98.00
Si(42)-C(422)	182.9(11)
Si(42)-C(42C)	185.0(13)
Si(42)-C(421)	185.7(11)
Si(42)-C(42A)	185.8(11)
Si(42)-C(42B)	189.2(14)
Si(42)-C(423)	195.6(11)
C(421)-H(42A)	96.00
C(421)-H(42B)	96.00
C(421)-H(42C)	96.00
C(422)-H(42D)	96.00
C(422)-H(42E)	96.00
C(422)-H(42F)	96.00
C(423)-H(42G)	96.00
C(423)-H(42H)	96.00
C(423)-H(42I)	96.00
C(42A)-H(42J)	96.00
C(42A)-H(42K)	96.00
C(42A)-H(42L)	96.00
C(42B)-H(42M)	96.00
C(42B)-H(42N)	96.00
C(42B)-H(42O)	96.00
C(42C)-H(42P)	96.00
C(42C)-H(42Q)	96.00
C(42C)-H(42R)	96.00
O(1)-O(2)	148.1(7)
O(1)-Li	182.9(15)
O(2)-Li	183.0(15)
O(3)-H(03)	81.62
N(1)-CN5	144.8(12)
N(1)-CN3	148.5(13)
N(1)-CN1	148.6(13)
N(1)-Li	214.0(15)
N(2)-CN6	138.2(16)
N(2)-CN4	139.2(14)
N(2)-CN2	148.8(16)
CN1-CN2	146.1(17)
CN1-HN1A	99.00
CN1-HN1B	99.00
CN2-HN2A	99.00
CN2-HN2B	99.00
CN3-CN4	152.4(17)
CN3-HN3A	99.00
CN3-HN3B	99.00
CN4-HN4A	99.00
CN4-HN4B	99.00
CN5-CN6	155.6(15)
CN5-HN5A	99.00
CN5-HN5B	99.00
CN6-HN6A	99.00

CN6-HN6B 99.00

O(3)-Ga(1)-O(1)	89.2(2)
O(3)-Ga(1)-C(2)	102.3(2)
O(1)-Ga(1)-C(2)	114.3(2)
O(3)-Ga(1)-C(1)	118.7(3)
O(1)-Ga(1)-C(1)	103.0(3)
C(2)-Ga(1)-C(1)	124.3(3)
Si(11)-C(1)-Si(12)	113.6(4)
Si(11)-C(1)-Ga(1)	118.0(4)
Si(12)-C(1)-Ga(1)	112.9(3)
Si(11)-C(1)-H(1)	103.3
Si(12)-C(1)-H(1)	103.3
Ga(1)-C(1)-H(1)	103.3
C(112)-Si(11)-C(1)	107.7(5)
C(112)-Si(11)-C(113)	112.7(6)
C(1)-Si(11)-C(113)	112.0(4)
C(112)-Si(11)-C(111)	107.6(6)
C(1)-Si(11)-C(111)	114.3(4)
C(113)-Si(11)-C(111)	102.6(5)
Si(11)-C(111)-H(11A)	109.5
Si(11)-C(111)-H(11B)	109.5
H(11A)-C(111)-H(11B)	109.5
Si(11)-C(111)-H(11C)	109.5
H(11A)-C(111)-H(11C)	109.5
H(11B)-C(111)-H(11C)	109.5
Si(11)-C(112)-H(11D)	109.5
Si(11)-C(112)-H(11E)	109.5
H(11D)-C(112)-H(11E)	109.5
Si(11)-C(112)-H(11F)	109.5
H(11D)-C(112)-H(11F)	109.5
H(11E)-C(112)-H(11F)	109.5
Si(11)-C(113)-H(11G)	109.5
Si(11)-C(113)-H(11H)	109.5
H(11G)-C(113)-H(11H)	109.5
Si(11)-C(113)-H(11I)	109.5
H(11G)-C(113)-H(11I)	109.5
H(11H)-C(113)-H(11I)	109.5
C(121)-Si(12)-C(122)	103.9(6)
C(121)-Si(12)-C(1)	112.6(5)
C(122)-Si(12)-C(1)	113.4(5)
C(121)-Si(12)-C(123)	104.1(5)
C(122)-Si(12)-C(123)	113.5(7)
C(1)-Si(12)-C(123)	108.9(5)
Si(12)-C(121)-H(12A)	109.5
Si(12)-C(121)-H(12B)	109.5
H(12A)-C(121)-H(12B)	109.5
Si(12)-C(121)-H(12C)	109.5
H(12A)-C(121)-H(12C)	109.5
H(12B)-C(121)-H(12C)	109.5
Si(12)-C(122)-H(12D)	109.5
Si(12)-C(122)-H(12E)	109.5
H(12D)-C(122)-H(12E)	109.5
Si(12)-C(122)-H(12F)	109.5
H(12D)-C(122)-H(12F)	109.5
H(12E)-C(122)-H(12F)	109.5
Si(12)-C(123)-H(12G)	109.5
Si(12)-C(123)-H(12H)	109.5
H(12G)-C(123)-H(12H)	109.5
Si(12)-C(123)-H(12I)	109.5
H(12G)-C(123)-H(12I)	109.5
H(12H)-C(123)-H(12I)	109.5

Si(21)-C(2)-Si(22)	114.1(3)
Si(21)-C(2)-Ga(1)	117.3(4)
Si(22)-C(2)-Ga(1)	113.9(3)
Si(21)-C(2)-H(2)	103.0
Si(22)-C(2)-H(2)	103.0
Ga(1)-C(2)-H(2)	103.0
C(211)-Si(21)-C(2)	112.4(4)
C(211)-Si(21)-C(212)	108.1(4)
C(2)-Si(21)-C(212)	111.6(4)
C(211)-Si(21)-C(213)	108.0(4)
C(2)-Si(21)-C(213)	113.0(3)
C(212)-Si(21)-C(213)	103.2(4)
Si(21)-C(211)-H(21A)	109.5
Si(21)-C(211)-H(21B)	109.5
H(21A)-C(211)-H(21B)	109.5
Si(21)-C(211)-H(21C)	109.5
H(21A)-C(211)-H(21C)	109.5
H(21B)-C(211)-H(21C)	109.5
Si(21)-C(212)-H(21D)	109.5
Si(21)-C(212)-H(21E)	109.5
H(21D)-C(212)-H(21E)	109.5
Si(21)-C(212)-H(21F)	109.5
H(21D)-C(212)-H(21F)	109.5
H(21E)-C(212)-H(21F)	109.5
Si(21)-C(213)-H(21G)	109.5
Si(21)-C(213)-H(21H)	109.5
H(21G)-C(213)-H(21H)	109.5
Si(21)-C(213)-H(21I)	109.5
H(21G)-C(213)-H(21I)	109.5
H(21H)-C(213)-H(21I)	109.5
C(221)-Si(22)-C(222)	106.1(4)
C(221)-Si(22)-C(223)	108.5(4)
C(222)-Si(22)-C(223)	106.1(4)
C(221)-Si(22)-C(2)	111.2(4)
C(222)-Si(22)-C(2)	113.2(3)
C(223)-Si(22)-C(2)	111.4(4)
Si(22)-C(221)-H(22A)	109.5
Si(22)-C(221)-H(22B)	109.5
H(22A)-C(221)-H(22B)	109.5
Si(22)-C(221)-H(22C)	109.5
H(22A)-C(221)-H(22C)	109.5
H(22B)-C(221)-H(22C)	109.5
Si(22)-C(222)-H(22D)	109.5
Si(22)-C(222)-H(22E)	109.5
H(22D)-C(222)-H(22E)	109.5
Si(22)-C(222)-H(22F)	109.5
H(22D)-C(222)-H(22F)	109.5
H(22E)-C(222)-H(22F)	109.5
Si(22)-C(223)-H(22G)	109.5
Si(22)-C(223)-H(22H)	109.5
H(22G)-C(223)-H(22H)	109.5
Si(22)-C(223)-H(22I)	109.5
H(22G)-C(223)-H(22I)	109.5
H(22H)-C(223)-H(22I)	109.5
O(3)-Ga(2)-O(2)	90.2(2)
O(3)-Ga(2)-C(3)	116.8(2)
O(2)-Ga(2)-C(3)	101.8(2)
O(3)-Ga(2)-C(4)	102.7(2)
O(2)-Ga(2)-C(4)	112.8(2)
C(3)-Ga(2)-C(4)	126.7(3)
Si(3A)-C(3)-Si(31)	118.3(5)
Si(3A)-C(3)-Si(32)	18.8(2)
Si(31)-C(3)-Si(32)	105.9(4)

Si(3A)-C(3)-Ga(2)	117.1(4)
Si(31)-C(3)-Ga(2)	115.8(3)
Si(32)-C(3)-Ga(2)	117.0(4)
Si(3A)-C(3)-H(3)	88.2
Si(31)-C(3)-H(3)	105.7
Si(32)-C(3)-H(3)	105.7
Ga(2)-C(3)-H(3)	105.7
C(31B)-Si(31)-C(31A)	106.7(10)
C(31B)-Si(31)-C(312)	16.1(8)
C(31A)-Si(31)-C(312)	122.0(12)
C(31B)-Si(31)-C(313)	114.1(12)
C(31A)-Si(31)-C(313)	87.2(15)
C(312)-Si(31)-C(313)	107.5(11)
C(31B)-Si(31)-C(311)	88.5(11)
C(31A)-Si(31)-C(311)	22.3(12)
C(312)-Si(31)-C(311)	104.6(10)
C(313)-Si(31)-C(311)	106.5(12)
C(31B)-Si(31)-C(3)	117.3(10)
C(31A)-Si(31)-C(3)	111.2(9)
C(312)-Si(31)-C(3)	111.2(10)
C(313)-Si(31)-C(3)	115.8(10)
C(311)-Si(31)-C(3)	110.6(7)
C(31B)-Si(31)-C(31C)	104.6(10)
C(31A)-Si(31)-C(31C)	105.8(9)
C(312)-Si(31)-C(31C)	94.4(12)
C(313)-Si(31)-C(31C)	18.9(14)
C(311)-Si(31)-C(31C)	124.0(13)
C(3)-Si(31)-C(31C)	110.4(8)
Si(31)-C(311)-H(31A)	109.5
Si(31)-C(311)-H(31B)	109.5
H(31A)-C(311)-H(31B)	109.5
Si(31)-C(311)-H(31C)	109.5
H(31A)-C(311)-H(31C)	109.5
H(31B)-C(311)-H(31C)	109.5
Si(31)-C(312)-H(31D)	109.5
Si(31)-C(312)-H(31E)	109.5
H(31D)-C(312)-H(31E)	109.5
Si(31)-C(312)-H(31F)	109.5
H(31D)-C(312)-H(31F)	109.5
H(31E)-C(312)-H(31F)	109.5
Si(31)-C(313)-H(31G)	109.5
Si(31)-C(313)-H(31H)	109.5
H(31G)-C(313)-H(31H)	109.5
Si(31)-C(313)-H(31I)	109.5
H(31G)-C(313)-H(31I)	109.5
H(31H)-C(313)-H(31I)	109.5
Si(31)-C(31A)-H(31J)	109.5
Si(31)-C(31A)-H(31K)	109.5
H(31J)-C(31A)-H(31K)	109.5
Si(31)-C(31A)-H(31L)	109.5
H(31J)-C(31A)-H(31L)	109.5
H(31K)-C(31A)-H(31L)	109.5
Si(31)-C(31B)-H(31M)	109.5
Si(31)-C(31B)-H(31N)	109.5
H(31M)-C(31B)-H(31N)	109.5
Si(31)-C(31B)-H(31O)	109.5
H(31M)-C(31B)-H(31O)	109.5
H(31N)-C(31B)-H(31O)	109.5
Si(31)-C(31C)-H(31P)	109.5
Si(31)-C(31C)-H(31Q)	109.5
H(31P)-C(31C)-H(31Q)	109.5
Si(31)-C(31C)-H(31R)	109.5
H(31P)-C(31C)-H(31R)	109.5

H(31Q)-C(31C)-H(31R)	109.5
C(321)-Si(32)-C(323)	107.5(11)
C(321)-Si(32)-C(322)	104.6(11)
C(323)-Si(32)-C(322)	106.0(10)
C(321)-Si(32)-C(3)	113.5(8)
C(323)-Si(32)-C(3)	115.3(7)
C(322)-Si(32)-C(3)	109.2(7)
Si(32)-C(321)-H(32A)	109.5
Si(32)-C(321)-H(32B)	109.5
H(32A)-C(321)-H(32B)	109.5
Si(32)-C(321)-H(32C)	109.5
H(32A)-C(321)-H(32C)	109.5
H(32B)-C(321)-H(32C)	109.5
Si(32)-C(322)-H(32D)	109.5
Si(32)-C(322)-H(32E)	109.5
H(32D)-C(322)-H(32E)	109.5
Si(32)-C(322)-H(32F)	109.5
H(32D)-C(322)-H(32F)	109.5
H(32E)-C(322)-H(32F)	109.5
Si(32)-C(323)-H(32G)	109.5
Si(32)-C(323)-H(32H)	109.5
H(32G)-C(323)-H(32H)	109.5
Si(32)-C(323)-H(32I)	109.5
H(32G)-C(323)-H(32I)	109.5
H(32H)-C(323)-H(32I)	109.5
C(3)-Si(3A)-C(3A2)	115.1(7)
C(3)-Si(3A)-C(3A1)	113.4(9)
C(3A2)-Si(3A)-C(3A1)	106.0(10)
C(3)-Si(3A)-C(3A3)	108.2(6)
C(3A2)-Si(3A)-C(3A3)	107.0(9)
C(3A1)-Si(3A)-C(3A3)	106.8(10)
Si(3A)-C(3A1)-H(3A1)	109.5
Si(3A)-C(3A1)-H(3A2)	109.5
H(3A1)-C(3A1)-H(3A2)	109.5
Si(3A)-C(3A1)-H(3A3)	109.5
H(3A1)-C(3A1)-H(3A3)	109.5
H(3A2)-C(3A1)-H(3A3)	109.5
Si(3A)-C(3A2)-H(3A4)	109.5
Si(3A)-C(3A2)-H(3A5)	109.5
H(3A4)-C(3A2)-H(3A5)	109.5
Si(3A)-C(3A2)-H(3A6)	109.5
H(3A4)-C(3A2)-H(3A6)	109.5
H(3A5)-C(3A2)-H(3A6)	109.5
Si(3A)-C(3A3)-H(3A7)	109.5
Si(3A)-C(3A3)-H(3A8)	109.5
H(3A7)-C(3A3)-H(3A8)	109.5
Si(3A)-C(3A3)-H(3A9)	109.5
H(3A7)-C(3A3)-H(3A9)	109.5
H(3A8)-C(3A3)-H(3A9)	109.5
Si(41)-C(4)-Si(42)	114.0(3)
Si(41)-C(4)-Ga(2)	115.2(3)
Si(42)-C(4)-Ga(2)	115.7(3)
Si(41)-C(4)-H(4)	103.2
Si(42)-C(4)-H(4)	103.2
Ga(2)-C(4)-H(4)	103.2
C(4)-Si(41)-C(413)	111.2(4)
C(4)-Si(41)-C(411)	110.7(3)
C(413)-Si(41)-C(411)	107.0(4)
C(4)-Si(41)-C(412)	114.7(4)
C(413)-Si(41)-C(412)	109.6(6)
C(411)-Si(41)-C(412)	103.1(5)
Si(41)-C(411)-H(41A)	109.5
Si(41)-C(411)-H(41B)	109.5

H(41A)-C(411)-H(41B)	109.5
Si(41)-C(411)-H(41C)	109.5
H(41A)-C(411)-H(41C)	109.5
H(41B)-C(411)-H(41C)	109.5
Si(41)-C(412)-H(41D)	109.5
Si(41)-C(412)-H(41E)	109.5
H(41D)-C(412)-H(41E)	109.5
Si(41)-C(412)-H(41F)	109.5
H(41D)-C(412)-H(41F)	109.5
H(41E)-C(412)-H(41F)	109.5
Si(41)-C(413)-H(41G)	109.5
Si(41)-C(413)-H(41H)	109.5
H(41G)-C(413)-H(41H)	109.5
Si(41)-C(413)-H(41I)	109.5
H(41G)-C(413)-H(41I)	109.5
H(41H)-C(413)-H(41I)	109.5
C(422)-Si(42)-C(42C)	82.9(14)
C(422)-Si(42)-C(421)	110.2(9)
C(42C)-Si(42)-C(421)	113.4(14)
C(422)-Si(42)-C(42A)	115.9(11)
C(42C)-Si(42)-C(42A)	108.6(11)
C(421)-Si(42)-C(42A)	7.3(17)
C(422)-Si(42)-C(4)	116.5(6)
C(42C)-Si(42)-C(4)	116.5(8)
C(421)-Si(42)-C(4)	113.7(7)
C(42A)-Si(42)-C(4)	113.0(8)
C(422)-Si(42)-C(42B)	23.8(11)
C(42C)-Si(42)-C(42B)	106.6(11)
C(421)-Si(42)-C(42B)	98.2(14)
C(42A)-Si(42)-C(42B)	105.2(9)
C(4)-Si(42)-C(42B)	106.0(9)
C(422)-Si(42)-C(423)	105.1(7)
C(42C)-Si(42)-C(423)	22.4(13)
C(421)-Si(42)-C(423)	101.9(10)
C(42A)-Si(42)-C(423)	95.6(11)
C(4)-Si(42)-C(423)	108.0(6)
C(42B)-Si(42)-C(423)	128.6(11)
Si(42)-C(421)-H(42A)	109.5
Si(42)-C(421)-H(42B)	109.5
H(42A)-C(421)-H(42B)	109.5
Si(42)-C(421)-H(42C)	109.5
H(42A)-C(421)-H(42C)	109.5
H(42B)-C(421)-H(42C)	109.5
Si(42)-C(422)-H(42D)	109.5
Si(42)-C(422)-H(42E)	109.5
H(42D)-C(422)-H(42E)	109.5
Si(42)-C(422)-H(42F)	109.5
H(42D)-C(422)-H(42F)	109.5
H(42E)-C(422)-H(42F)	109.5
Si(42)-C(423)-H(42G)	109.5
Si(42)-C(423)-H(42H)	109.5
H(42G)-C(423)-H(42H)	109.5
Si(42)-C(423)-H(42I)	109.5
H(42G)-C(423)-H(42I)	109.5
H(42H)-C(423)-H(42I)	109.5
Si(42)-C(42A)-H(42J)	109.5
Si(42)-C(42A)-H(42K)	109.5
H(42J)-C(42A)-H(42K)	109.5
Si(42)-C(42A)-H(42L)	109.5
H(42J)-C(42A)-H(42L)	109.5
H(42K)-C(42A)-H(42L)	109.5
Si(42)-C(42B)-H(42M)	109.5
Si(42)-C(42B)-H(42N)	109.5

H(42M)-C(42B)-H(42N)	109.5
Si(42)-C(42B)-H(42O)	109.5
H(42M)-C(42B)-H(42O)	109.5
H(42N)-C(42B)-H(42O)	109.5
Si(42)-C(42C)-H(42P)	109.5
Si(42)-C(42C)-H(42Q)	109.5
H(42P)-C(42C)-H(42Q)	109.5
Si(42)-C(42C)-H(42R)	109.5
H(42P)-C(42C)-H(42R)	109.5
H(42Q)-C(42C)-H(42R)	109.5
O(2)-O(1)-Li	66.2(6)
O(2)-O(1)-Ga(1)	107.3(3)
Li-O(1)-Ga(1)	148.7(8)
O(1)-O(2)-Li	66.1(6)
O(1)-O(2)-Ga(2)	104.5(3)
Li-O(2)-Ga(2)	148.7(8)
Ga(2)-O(3)-Ga(1)	114.2(2)
Ga(2)-O(3)-H(03)	106.9
Ga(1)-O(3)-H(03)	113.6
CN5-N(1)-CN3	105.4(9)
CN5-N(1)-CN1	106.4(10)
CN3-N(1)-CN1	107.8(9)
CN5-N(1)-Li	108.0(8)
CN3-N(1)-Li	114.8(8)
CN1-N(1)-Li	113.7(9)
CN6-N(2)-CN4	109.2(13)
CN6-N(2)-CN2	104.0(11)
CN4-N(2)-CN2	108.0(13)
CN2-CN1-N(1)	114.1(10)
CN2-CN1-HN1A	108.7
N(1)-CN1-HN1A	108.7
CN2-CN1-HN1B	108.7
N(1)-CN1-HN1B	108.7
HN1A-CN1-HN1B	107.6
CN1-CN2-N(2)	110.7(9)
CN1-CN2-HN2A	109.5
N(2)-CN2-HN2A	109.5
CN1-CN2-HN2B	109.5
N(2)-CN2-HN2B	109.5
HN2A-CN2-HN2B	108.1
N(1)-CN3-CN4	109.2(9)
N(1)-CN3-HN3A	109.8
CN4-CN3-HN3A	109.8
N(1)-CN3-HN3B	109.8
CN4-CN3-HN3B	109.8
HN3A-CN3-HN3B	108.3
N(2)-CN4-CN3	114.5(10)
N(2)-CN4-HN4A	108.6
CN3-CN4-HN4A	108.6
N(2)-CN4-HN4B	108.6
CN3-CN4-HN4B	108.6
HN4A-CN4-HN4B	107.6
N(1)-CN5-CN6	108.4(10)
N(1)-CN5-HN5A	110.0
CN6-CN5-HN5A	110.0
N(1)-CN5-HN5B	110.0
CN6-CN5-HN5B	110.0
HN5A-CN5-HN5B	108.4
N(2)-CN6-CN5	114.6(10)
N(2)-CN6-HN6A	108.6
CN5-CN6-HN6A	108.6
N(2)-CN6-HN6B	108.6
CN5-CN6-HN6B	108.6

HN6A-CN6-HN6B	107.6
O(1)-Li-O(2)	47.7(4)
O(1)-Li-N(1)	153.1(11)
O(2)-Li-N(1)	158.6(10)

Symmetry transformations used to generate equivalent atoms:

Table 3. Anisotropic displacement parameters [pm^2 x 10^-1] for compound 2. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ga(1)	21(1)	42(1)	30(1)	12(1)	8(1)	0(1)
C(1)	28(3)	39(3)	30(3)	1(3)	1(3)	-9(3)
Si(11)	65(2)	32(1)	65(2)	8(1)	11(1)	4(1)
C(111)	84(7)	48(5)	72(6)	3(4)	33(5)	15(4)
C(112)	130(11)	49(6)	154(13)	-10(7)	40(10)	-32(7)
C(113)	113(10)	86(7)	74(8)	32(6)	47(7)	47(7)
Si(12)	65(2)	76(2)	47(1)	4(1)	36(1)	-18(1)
C(121)	108(9)	110(9)	112(9)	60(8)	74(8)	6(7)
C(122)	92(9)	177(14)	42(6)	17(7)	14(6)	-38(9)
C(123)	151(13)	112(10)	88(9)	-29(7)	95(9)	-32(8)
C(2)	28(3)	28(3)	26(3)	-2(3)	2(2)	2(3)
Si(21)	31(1)	40(1)	34(1)	-5(1)	4(1)	2(1)
C(211)	45(5)	70(6)	77(7)	-23(5)	25(5)	8(4)
C(212)	76(6)	36(4)	44(5)	15(3)	7(4)	7(4)
C(213)	52(5)	49(4)	32(4)	-10(3)	0(3)	6(3)
Si(22)	28(1)	31(1)	29(1)	0(1)	7(1)	3(1)
C(221)	55(5)	46(4)	62(5)	-15(4)	20(4)	-15(4)
C(222)	41(4)	56(4)	33(4)	-5(3)	2(3)	3(3)
C(223)	53(5)	70(5)	44(5)	-10(4)	22(4)	4(4)
Ga(2)	21(1)	57(1)	31(1)	4(1)	10(1)	0(1)
C(3)	45(4)	47(4)	50(5)	-11(3)	27(4)	-6(3)
Si(31)	54(1)	43(1)	53(1)	-1(1)	3(1)	6(1)
C(311)	190(40)	38(13)	47(13)	-29(10)	-33(17)	39(17)
C(312)	47(10)	190(30)	32(11)	64(13)	33(9)	51(12)
C(313)	39(12)	39(14)	370(60)	0(20)	-20(20)	-11(10)
C(31A)	100(20)	63(13)	57(14)	-28(11)	36(15)	-43(14)
C(31B)	57(12)	130(19)	53(15)	67(14)	34(11)	38(11)
C(31C)	90(20)	67(15)	140(20)	-52(16)	80(20)	-50(14)
Si(32)	39(4)	46(3)	40(4)	-7(3)	27(3)	-17(3)
C(321)	62(12)	170(20)	54(15)	-55(16)	43(12)	-78(16)
C(322)	108(18)	67(8)	32(10)	-19(8)	36(11)	0(9)
C(323)	46(8)	76(13)	60(13)	-20(11)	18(9)	-15(8)
Si(3A)	40(3)	105(5)	32(3)	-1(3)	22(2)	-24(3)
C(3A1)	160(20)	130(15)	140(20)	68(17)	116(18)	14(15)
C(3A2)	92(12)	79(9)	69(12)	-26(8)	50(10)	-29(7)
C(3A3)	50(8)	230(30)	28(8)	-40(12)	-5(7)	-22(10)
C(4)	18(3)	44(4)	33(3)	-4(3)	17(3)	-2(2)
Si(41)	30(1)	27(1)	28(1)	1(1)	10(1)	4(1)
C(411)	36(4)	68(5)	32(4)	-7(3)	20(3)	5(3)
C(412)	199(14)	59(6)	32(5)	12(4)	27(7)	51(7)
C(413)	45(5)	82(6)	79(6)	-43(5)	35(5)	-31(4)
Si(42)	36(1)	98(2)	60(2)	-48(2)	-10(1)	29(1)
C(421)	16(6)	41(8)	33(8)	-11(6)	6(5)	10(5)
C(422)	16(6)	41(8)	33(8)	-11(6)	6(5)	10(5)
C(423)	20(7)	12(7)	48(11)	2(6)	-20(7)	3(6)

C(42A)	79(15)	57(12)	64(13)	-17(10)	38(11)	-2(9)
C(42B)	42(12)	270(40)	230(40)	-190(30)	49(19)	-21(18)
C(42C)	230(40)	270(40)	96(18)	-110(20)	-80(20)	210(30)
O(1)	34(3)	54(3)	41(3)	1(2)	1(2)	-1(2)
O(2)	31(2)	60(3)	38(3)	2(2)	18(2)	3(2)
O(3)	23(2)	53(3)	38(2)	3(2)	11(2)	-2(2)
N(1)	57(4)	48(4)	64(5)	0(3)	26(4)	7(3)
N(2)	74(5)	108(7)	50(4)	-18(5)	17(4)	28(5)
CN1	180(16)	114(10)	82(8)	34(8)	69(10)	58(10)
CN2	238(19)	129(11)	40(6)	19(7)	45(9)	109(12)
CN3	91(8)	133(11)	68(7)	-28(7)	5(6)	28(7)
CN4	85(9)	205(17)	108(11)	-68(11)	-25(8)	88(10)
CN5	85(8)	79(8)	145(11)	-48(8)	59(8)	-26(6)
CN6	107(11)	120(10)	121(11)	-76(9)	53(9)	-15(8)
Li	93(12)	86(11)	101(13)	-64(10)	62(11)	-34(9)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2 x 10^-1) for compound 2.

	x	y	z	U(eq)
H(1)	2282	6323	9754	44
H(11A)	1369	8865	10473	104
H(11B)	1954	7955	10845	104
H(11C)	1203	7520	10446	104
H(11D)	2373	8931	9361	180
H(11E)	2783	8374	10080	180
H(11F)	2368	9533	9997	180
H(11G)	902	8730	8616	134
H(11H)	725	9241	9176	134
H(11I)	489	7970	8893	134
H(12A)	2478	7561	8713	152
H(12B)	1760	8024	8202	152
H(12C)	2123	7063	7973	152
H(12D)	706	5816	7602	164
H(12E)	639	7068	7865	164
H(12F)	494	5941	8188	164
H(12G)	2431	4587	9019	152
H(12H)	2338	4949	8299	152
H(12I)	1781	4196	8373	152
H(2)	1610	3756	10670	37
H(21A)	3491	3408	10928	97
H(21B)	3153	3875	10181	97
H(21C)	3366	2549	10328	97
H(21D)	2019	1347	10897	89
H(21E)	2701	1894	11435	89
H(21F)	2707	1002	10897	89
H(21G)	1816	2760	9207	77
H(21H)	1407	2020	9498	77
H(21I)	2068	1502	9506	77
H(22A)	3382	6269	11648	85
H(22B)	2815	6550	10919	85
H(22C)	3323	5513	11031	85
H(22D)	2760	3475	12188	73
H(22E)	3346	4404	12424	73
H(22F)	3290	3432	11899	73
H(22G)	1644	6199	11301	83
H(22H)	2275	6302	12012	83
H(22I)	1776	5236	11854	83

H(3)	-960	3662	9649	54
H(31A)	-845	2035	8498	147
H(31B)	-426	903	8753	147
H(31C)	-67	2091	8829	147
H(31D)	394	490	10164	102
H(31E)	432	1380	10702	102
H(31F)	737	1688	10221	102
H(31G)	-1521	1304	9378	230
H(31H)	-1056	959	10115	230
H(31I)	-1057	224	9532	230
H(31J)	-1219	1966	8544	89
H(31K)	-817	811	8688	89
H(31L)	-505	1958	8588	89
H(31M)	362	447	9922	92
H(31N)	591	1316	10515	92
H(31O)	683	1628	9886	92
H(31P)	-1380	1325	9799	109
H(31Q)	-737	1064	10455	109
H(31R)	-949	237	9844	109
H(32A)	-749	2256	11025	109
H(32B)	-1083	3471	10934	109
H(32C)	-466	3160	11602	109
H(32D)	300	5538	10904	80
H(32E)	147	5268	11501	80
H(32F)	-434	5575	10806	80
H(32G)	1034	3287	11154	76
H(32H)	693	2143	11211	76
H(32I)	869	3105	11752	76
H(3A1)	-624	3053	11469	149
H(3A2)	-418	2087	11113	149
H(3A3)	-1136	2609	10769	149
H(3A4)	-734	5386	11108	90
H(3A5)	-1275	5151	10381	90
H(3A6)	-638	5861	10507	90
H(3A7)	599	4368	11642	132
H(3A8)	707	4728	11028	132
H(3A9)	776	3432	11247	132
H(4)	-317	6067	8556	35
H(41A)	-601	3382	7843	65
H(41B)	-367	4479	7573	65
H(41C)	-1042	3829	7102	65
H(41D)	-1291	6539	7108	159
H(41E)	-1923	6596	7253	159
H(41F)	-1894	5659	6747	159
H(41G)	-2014	4522	8233	99
H(41H)	-1673	3383	8128	99
H(41I)	-2239	4026	7502	99
H(42A)	-48	7641	9770	38
H(42B)	-464	7004	10071	38
H(42C)	-659	8256	9790	38
H(42D)	-2160	6436	8387	38
H(42E)	-2041	7421	8903	38
H(42F)	-1858	6145	9145	38
H(42G)	-695	8399	8342	48
H(42H)	-1277	8895	8464	48
H(42I)	-1430	8041	7876	48
H(42J)	-655	8270	9783	77
H(42K)	-71	7938	9619	77
H(42L)	-280	7098	10036	77
H(42M)	-2009	5864	8735	223
H(42N)	-1914	6884	9225	223
H(42O)	-1484	5764	9481	223
H(42P)	-1765	7687	7863	308

H(42Q)	-1134	8475	8194	308
H(42R)	-1696	8561	8420	308
HN1A	37	2918	6975	145
HN1B	809	3097	7185	145
HN2A	726	2006	6404	171
HN2B	-46	1810	6201	171
HN3A	1356	754	8314	131
HN3B	1633	1788	8035	131
HN4A	1509	744	7186	190
HN4B	1279	-311	7489	190
HN5A	-307	1412	7491	121
HN5B	239	544	8000	121
HN6A	121	-534	7146	139
HN6B	-369	393	6638	139
H(03)	532	6127	9891	80

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Crystallographic data for compound 3

Empirical formula	C80 H200 Ga4 Li4 N8 O12 Si16
Formula weight	2222.56
Temperature	153(2) K
Wavelength	154.184 pm
Crystal system	tetragonal
Space group	P4(2)/n
Unit cell dimensions	a = 2005.65(3) pm alpha = 90 deg b = 2005.65(3) pm beta = 90 deg c = 1508.69(5) pm gamma = 90 deg
Volume, Z	6.0689(2) nm^3, 2
Density (calculated)	1.216 Mg/m^3
Absorption coefficient	2.922 mm^-1
F(000)	2384
Crystal size	0.42 x 0.15 x 0.13 mm
Theta range for data collection	3.12 to 72.50 deg
Limiting indices	-24 < h < 21, -24 < k < 24, -16 < l < 18
Reflections collected	35368
Independent reflections	5941 (R(int) = 0.0630)
Completeness to theta =	72.50 deg 98.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5941 / 0 / 292
Goodness-of-fit on F^2	1.062
Final R indices [I>2Sigma(I)] =	0.0463, wR2 = 0.1261
R indices (all data) =	0.0518, wR2 = 0.1334
Largest diff. peak and hole	993 and -349 e.nm^-3

Table 5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2 x 10^-1) for compound 3. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ga(1)	2730(1)	215(1)	9372(1)	23(1)
C(1)	2577(1)	-516(1)	8511(2)	29(1)
Si(11)	3329(1)	-1048(1)	8336(1)	36(1)
C(111)	3302(2)	-1503(2)	7242(2)	49(1)
C(112)	4090(1)	-504(2)	8299(2)	43(1)
C(113)	3418(2)	-1681(1)	9241(2)	50(1)
Si(12)	1750(1)	-934(1)	8655(1)	37(1)
C(121)	1620(2)	-1633(1)	7855(2)	55(1)
C(122)	1649(2)	-1295(2)	9780(2)	50(1)
C(123)	1078(2)	-303(2)	8451(2)	47(1)
C(2)	2858(1)	95(1)	10671(1)	26(1)
Si(21)	2214(1)	590(1)	11291(1)	29(1)
C(211)	2110(2)	284(2)	12452(2)	45(1)
C(212)	1371(1)	507(2)	10760(2)	38(1)
C(213)	2438(2)	1496(1)	11324(2)	40(1)
Si(22)	3735(1)	203(1)	11071(1)	28(1)
C(221)	4147(1)	922(1)	10495(2)	41(1)
C(222)	4244(1)	-562(1)	10884(2)	40(1)
C(223)	3806(1)	370(1)	12291(2)	38(1)
O(1)	3086(1)	996(1)	8829(1)	29(1)
O(2)	2311(1)	1027(1)	8998(1)	29(1)
O(3)	2574(1)	1792(1)	6855(1)	22(1)
N(1)	2666(1)	1214(1)	6359(1)	22(1)
C(3)	3324(1)	903(1)	6596(2)	25(1)
C(4)	3418(1)	270(1)	6017(2)	33(1)
C(5)	2116(1)	728(1)	6556(2)	26(1)
C(6)	2241(1)	87(1)	5999(2)	32(1)
C(7)	2657(1)	1381(1)	5390(1)	27(1)
C(8)	2753(1)	726(1)	4858(2)	32(1)
N(2)	2838(1)	149(1)	5445(2)	31(1)
Li(1)	2597(2)	1764(2)	8203(2)	24(1)

Table 6. Bond lengths [pm] and angles [deg] for compound 3.

Ga(1)-O(1)	190.55(16)
Ga(1)-O(2)	191.71(15)
Ga(1)-C(1)	198.3(2)
Ga(1)-C(2)	199.1(2)
C(1)-Si(11)	186.7(2)
C(1)-Si(12)	187.1(3)
C(1)-H(1)	96.00
Si(11)-C(113)	187.3(3)
Si(11)-C(112)	187.6(3)
Si(11)-C(111)	188.7(3)
C(111)-H(11A)	95.99
C(111)-H(11B)	95.99
C(111)-H(11C)	95.99
C(112)-H(11D)	95.99
C(112)-H(11E)	95.99
C(112)-H(11F)	95.99
C(113)-H(11G)	95.99
C(113)-H(11H)	95.99

C(113)-H(11I)	95.99
Si(12)-C(122)	185.6(3)
Si(12)-C(121)	186.9(3)
Si(12)-C(123)	187.3(3)
C(121)-H(12A)	95.99
C(121)-H(12B)	95.99
C(121)-H(12C)	95.99
C(122)-H(12D)	95.99
C(122)-H(12E)	95.99
C(122)-H(12F)	95.99
C(123)-H(12G)	95.99
C(123)-H(12H)	95.99
C(123)-H(12I)	95.99
C(2)-Si(22)	187.1(2)
C(2)-Si(21)	187.8(3)
C(2)-H(2)	96.00
Si(21)-C(211)	186.9(3)
Si(21)-C(213)	187.3(3)
Si(21)-C(212)	187.8(3)
C(211)-H(21A)	95.99
C(211)-H(21B)	95.99
C(211)-H(21C)	95.99
C(212)-H(21D)	95.99
C(212)-H(21E)	95.99
C(212)-H(21F)	95.99
C(213)-H(21G)	95.99
C(213)-H(21H)	95.99
C(213)-H(21I)	95.99
Si(22)-C(222)	186.5(3)
Si(22)-C(221)	187.6(3)
Si(22)-C(223)	187.8(3)
C(221)-H(22A)	95.99
C(221)-H(22B)	95.99
C(221)-H(22C)	95.99
C(222)-H(22D)	95.99
C(222)-H(22E)	95.99
C(222)-H(22F)	95.99
C(223)-H(22G)	95.99
C(223)-H(22H)	95.99
C(223)-H(22I)	95.99
O(1)-O(2)	157.5(2)
O(1)-Li(1)	205.6(4)
O(2)-Li(1)	198.8(4)
O(3)-N(1)	139.4(2)
O(3)-Li(1)	203.5(4)
O(3)-Li(1)#1	203.5(4)
O(3)-Li(1)#2	209.3(4)
N(1)-C(7)	150.0(3)
N(1)-C(5)	150.2(3)
N(1)-C(3)	150.2(3)
C(3)-C(4)	155.3(3)
C(3)-H(3A)	96.00
C(3)-H(3B)	96.00
C(4)-N(2)	146.8(3)
C(4)-H(4A)	96.00
C(4)-H(4B)	96.00
C(5)-C(6)	155.7(3)
C(5)-H(5A)	96.00
C(5)-H(5B)	96.00
C(6)-N(2)	146.5(3)
C(6)-H(6A)	96.00
C(6)-H(6B)	96.00
C(7)-C(8)	155.0(3)

C(7)-H(7A)	96.00
C(7)-H(7B)	96.00
C(8)-N(2)	146.7(3)
C(8)-H(8A)	96.00
C(8)-H(8B)	96.00
Li(1)-O(3)#2	203.5(4)
Li(1)-O(3)#1	209.3(4)
Li(1)-Li(1)#3	297.8(7)
Li(1)-Li(1)#1	298.8(6)
Li(1)-Li(1)#2	298.8(6)

O(1)-Ga(1)-O(2)	48.67(7)
O(1)-Ga(1)-C(1)	112.56(9)
O(2)-Ga(1)-C(1)	111.52(9)
O(1)-Ga(1)-C(2)	118.32(8)
O(2)-Ga(1)-C(2)	116.69(9)
C(1)-Ga(1)-C(2)	125.14(9)
Si(11)-C(1)-Si(12)	118.46(12)
Si(11)-C(1)-Ga(1)	112.94(12)
Si(12)-C(1)-Ga(1)	113.12(12)
Si(11)-C(1)-H(1)	103.3
Si(12)-C(1)-H(1)	103.3
Ga(1)-C(1)-H(1)	103.3
C(1)-Si(11)-C(113)	111.18(14)
C(1)-Si(11)-C(112)	109.23(12)
C(113)-Si(11)-C(112)	109.75(14)
C(1)-Si(11)-C(111)	112.14(13)
C(113)-Si(11)-C(111)	108.23(14)
C(112)-Si(11)-C(111)	106.18(14)
Si(11)-C(111)-H(11A)	109.5
Si(11)-C(111)-H(11B)	109.5
H(11A)-C(111)-H(11B)	109.5
Si(11)-C(111)-H(11C)	109.5
H(11A)-C(111)-H(11C)	109.5
H(11B)-C(111)-H(11C)	109.5
Si(11)-C(112)-H(11D)	109.5
Si(11)-C(112)-H(11E)	109.5
H(11D)-C(112)-H(11E)	109.5
Si(11)-C(112)-H(11F)	109.5
H(11D)-C(112)-H(11F)	109.5
H(11E)-C(112)-H(11F)	109.5
Si(11)-C(113)-H(11G)	109.5
Si(11)-C(113)-H(11H)	109.5
H(11G)-C(113)-H(11H)	109.5
Si(11)-C(113)-H(11I)	109.5
H(11G)-C(113)-H(11I)	109.5
H(11H)-C(113)-H(11I)	109.5
C(122)-Si(12)-C(121)	106.39(15)
C(122)-Si(12)-C(1)	112.22(13)
C(121)-Si(12)-C(1)	112.63(14)
C(122)-Si(12)-C(123)	109.63(16)
C(121)-Si(12)-C(123)	107.43(14)
C(1)-Si(12)-C(123)	108.42(12)
Si(12)-C(121)-H(12A)	109.5
Si(12)-C(121)-H(12B)	109.5
H(12A)-C(121)-H(12B)	109.5
Si(12)-C(121)-H(12C)	109.5
H(12A)-C(121)-H(12C)	109.5
H(12B)-C(121)-H(12C)	109.5
Si(12)-C(122)-H(12D)	109.5
Si(12)-C(122)-H(12E)	109.5
H(12D)-C(122)-H(12E)	109.5

Si(12)-C(122)-H(12F)	109.5
H(12D)-C(122)-H(12F)	109.5
H(12E)-C(122)-H(12F)	109.5
Si(12)-C(123)-H(12G)	109.5
Si(12)-C(123)-H(12H)	109.5
H(12G)-C(123)-H(12H)	109.5
Si(12)-C(123)-H(12I)	109.5
H(12G)-C(123)-H(12I)	109.5
H(12H)-C(123)-H(12I)	109.5
Si(22)-C(2)-Si(21)	115.15(12)
Si(22)-C(2)-Ga(1)	115.11(11)
Si(21)-C(2)-Ga(1)	109.72(12)
Si(22)-C(2)-H(2)	105.3
Si(21)-C(2)-H(2)	105.3
Ga(1)-C(2)-H(2)	105.3
C(211)-Si(21)-C(213)	108.72(14)
C(211)-Si(21)-C(2)	111.73(12)
C(213)-Si(21)-C(2)	111.12(12)
C(211)-Si(21)-C(212)	105.70(13)
C(213)-Si(21)-C(212)	108.28(13)
C(2)-Si(21)-C(212)	111.09(11)
Si(21)-C(211)-H(21A)	109.5
Si(21)-C(211)-H(21B)	109.5
H(21A)-C(211)-H(21B)	109.5
Si(21)-C(211)-H(21C)	109.5
H(21A)-C(211)-H(21C)	109.5
H(21B)-C(211)-H(21C)	109.5
Si(21)-C(212)-H(21D)	109.5
Si(21)-C(212)-H(21E)	109.5
H(21D)-C(212)-H(21E)	109.5
Si(21)-C(212)-H(21F)	109.5
H(21D)-C(212)-H(21F)	109.5
H(21E)-C(212)-H(21F)	109.5
Si(21)-C(213)-H(21G)	109.5
Si(21)-C(213)-H(21H)	109.5
H(21G)-C(213)-H(21H)	109.5
Si(21)-C(213)-H(21I)	109.5
H(21G)-C(213)-H(21I)	109.5
H(21H)-C(213)-H(21I)	109.5
C(222)-Si(22)-C(2)	111.79(12)
C(222)-Si(22)-C(221)	108.75(14)
C(2)-Si(22)-C(221)	110.70(11)
C(222)-Si(22)-C(223)	104.69(12)
C(2)-Si(22)-C(223)	114.10(11)
C(221)-Si(22)-C(223)	106.45(13)
Si(22)-C(221)-H(22A)	109.5
Si(22)-C(221)-H(22B)	109.5
H(22A)-C(221)-H(22B)	109.5
Si(22)-C(221)-H(22C)	109.5
H(22A)-C(221)-H(22C)	109.5
H(22B)-C(221)-H(22C)	109.5
Si(22)-C(222)-H(22D)	109.5
Si(22)-C(222)-H(22E)	109.5
H(22D)-C(222)-H(22E)	109.5
Si(22)-C(222)-H(22F)	109.5
H(22D)-C(222)-H(22F)	109.5
H(22E)-C(222)-H(22F)	109.5
Si(22)-C(223)-H(22G)	109.5
Si(22)-C(223)-H(22H)	109.5
H(22G)-C(223)-H(22H)	109.5
Si(22)-C(223)-H(22I)	109.5
H(22G)-C(223)-H(22I)	109.5
H(22H)-C(223)-H(22I)	109.5

O(2)-O(1)-Ga(1)	66.05(8)
O(2)-O(1)-Li(1)	64.83(13)
Ga(1)-O(1)-Li(1)	129.43(13)
O(1)-O(2)-Ga(1)	65.28(8)
O(1)-O(2)-Li(1)	69.36(13)
Ga(1)-O(2)-Li(1)	133.06(13)
N(1)-O(3)-Li(1)	120.69(15)
N(1)-O(3)-Li(1)#1	125.77(15)
Li(1)-O(3)-Li(1)#1	94.49(15)
N(1)-O(3)-Li(1)#2	122.37(15)
Li(1)-O(3)-Li(1)#2	92.76(15)
Li(1)#1-O(3)-Li(1)#2	92.33(15)
O(3)-N(1)-C(7)	109.62(16)
O(3)-N(1)-C(5)	109.61(16)
C(7)-N(1)-C(5)	109.14(17)
O(3)-N(1)-C(3)	109.59(15)
C(7)-N(1)-C(3)	109.63(17)
C(5)-N(1)-C(3)	109.23(17)
N(1)-C(3)-C(4)	108.19(17)
N(1)-C(3)-H(3A)	110.1
C(4)-C(3)-H(3A)	110.1
N(1)-C(3)-H(3B)	110.1
C(4)-C(3)-H(3B)	110.1
H(3A)-C(3)-H(3B)	108.4
N(2)-C(4)-C(3)	111.65(19)
N(2)-C(4)-H(4A)	109.3
C(3)-C(4)-H(4A)	109.3
N(2)-C(4)-H(4B)	109.3
C(3)-C(4)-H(4B)	109.3
H(4A)-C(4)-H(4B)	108.0
N(1)-C(5)-C(6)	108.08(18)
N(1)-C(5)-H(5A)	110.1
C(6)-C(5)-H(5A)	110.1
N(1)-C(5)-H(5B)	110.1
C(6)-C(5)-H(5B)	110.1
H(5A)-C(5)-H(5B)	108.4
N(2)-C(6)-C(5)	111.66(18)
N(2)-C(6)-H(6A)	109.3
C(5)-C(6)-H(6A)	109.3
N(2)-C(6)-H(6B)	109.3
C(5)-C(6)-H(6B)	109.3
H(6A)-C(6)-H(6B)	107.9
N(1)-C(7)-C(8)	108.26(18)
N(1)-C(7)-H(7A)	110.0
C(8)-C(7)-H(7A)	110.0
N(1)-C(7)-H(7B)	110.0
C(8)-C(7)-H(7B)	110.0
H(7A)-C(7)-H(7B)	108.4
N(2)-C(8)-C(7)	111.76(19)
N(2)-C(8)-H(8A)	109.3
C(7)-C(8)-H(8A)	109.3
N(2)-C(8)-H(8B)	109.3
C(7)-C(8)-H(8B)	109.3
H(8A)-C(8)-H(8B)	107.9
C(6)-N(2)-C(8)	108.5(2)
C(6)-N(2)-C(4)	109.0(2)
C(8)-N(2)-C(4)	108.45(19)
O(2)-Li(1)-O(3)	128.08(19)
O(2)-Li(1)-O(3)#2	142.4(2)
O(3)-Li(1)-O(3)#2	87.08(15)
O(2)-Li(1)-O(1)	45.81(10)
O(3)-Li(1)-O(1)	119.42(19)
O(3)#2-Li(1)-O(1)	109.34(17)

O(2)-Li(1)-O(3)#1	105.93(18)
O(3)-Li(1)-O(3)#1	85.56(15)
O(3)#2-Li(1)-O(3)#1	87.47(15)
O(1)-Li(1)-O(3)#1	149.6(2)
O(2)-Li(1)-Li(1)#3	134.37(16)
O(3)-Li(1)-Li(1)#3	88.24(11)
O(3)#2-Li(1)-Li(1)#3	44.61(10)
O(1)-Li(1)-Li(1)#3	143.67(17)
O(3)#1-Li(1)-Li(1)#3	43.07(10)
O(2)-Li(1)-Li(1)#1	125.82(19)
O(3)-Li(1)-Li(1)#1	42.76(12)
O(3)#2-Li(1)-Li(1)#1	87.94(11)
O(1)-Li(1)-Li(1)#1	156.0(2)
O(3)#1-Li(1)-Li(1)#1	42.85(7)
Li(1)#3-Li(1)-Li(1)#1	60.12(7)
O(2)-Li(1)-Li(1)#2	165.4(2)
O(3)-Li(1)-Li(1)#2	44.38(13)
O(3)#2-Li(1)-Li(1)#2	42.75(8)
O(1)-Li(1)-Li(1)#2	122.76(19)
O(3)#1-Li(1)-Li(1)#2	86.91(10)
Li(1)#3-Li(1)-Li(1)#2	60.12(7)
Li(1)#1-Li(1)-Li(1)#2	59.76(14)

Symmetry transformations used to generate equivalent atoms:
#1 y,-x+1/2,-z+3/2 #2 -y+1/2,x,-z+3/2
#3 -x+1/2,-y+1/2,z

Table 7. Anisotropic displacement parameters [pm^2 x 10^-1] for compound 3. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ga(1)	27(1)	19(1)	23(1)	1(1)	-1(1)	1(1)
C(1)	39(1)	21(1)	26(1)	-1(1)	-5(1)	1(1)
Si(11)	48(1)	27(1)	32(1)	-4(1)	-3(1)	9(1)
C(111)	68(2)	37(1)	41(2)	-11(1)	2(1)	11(1)
C(112)	41(2)	47(2)	42(2)	-1(1)	0(1)	10(1)
C(113)	73(2)	31(1)	47(2)	4(1)	-11(1)	10(1)
Si(12)	44(1)	25(1)	41(1)	-3(1)	-7(1)	-6(1)
C(121)	69(2)	31(1)	67(2)	-13(1)	-21(2)	-7(1)
C(122)	60(2)	39(2)	52(2)	6(1)	2(1)	-14(1)
C(123)	41(2)	39(2)	62(2)	-8(1)	-12(1)	-4(1)
C(2)	32(1)	23(1)	22(1)	4(1)	-1(1)	0(1)
Si(21)	33(1)	30(1)	25(1)	1(1)	2(1)	2(1)
C(211)	49(2)	56(2)	30(1)	9(1)	8(1)	4(1)
C(212)	31(1)	45(2)	39(1)	-3(1)	3(1)	4(1)
C(213)	47(2)	32(1)	41(2)	-5(1)	-5(1)	5(1)
Si(22)	31(1)	28(1)	27(1)	3(1)	-4(1)	0(1)
C(221)	34(1)	42(2)	47(2)	12(1)	-8(1)	-8(1)
C(222)	39(1)	43(2)	38(1)	1(1)	-5(1)	11(1)
C(223)	41(1)	41(1)	32(1)	-1(1)	-10(1)	2(1)
O(1)	25(1)	25(1)	36(1)	6(1)	1(1)	-2(1)
O(2)	28(1)	25(1)	34(1)	6(1)	4(1)	6(1)
O(3)	23(1)	18(1)	23(1)	-4(1)	-1(1)	1(1)
N(1)	22(1)	20(1)	23(1)	-2(1)	-1(1)	0(1)
C(3)	24(1)	25(1)	27(1)	-2(1)	-3(1)	2(1)
C(4)	33(1)	28(1)	39(1)	-7(1)	-4(1)	6(1)
C(5)	24(1)	22(1)	31(1)	1(1)	1(1)	-5(1)

C(6)	36(1)	23(1)	35(1)	-3(1)	0(1)	-6(1)
C(7)	33(1)	28(1)	22(1)	1(1)	-1(1)	-1(1)
C(8)	34(1)	36(1)	25(1)	-7(1)	1(1)	0(1)
N(2)	33(1)	26(1)	34(1)	-8(1)	-2(1)	1(1)
Li(1)	25(2)	20(2)	27(2)	1(1)	-2(1)	-1(1)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2 x 10^-1) for compound 3.

	x	y	z	U(eq)
H(1)	2530	-285	7956	34
H(11A)	2936	-1812	7242	58
H(11B)	3712	-1741	7156	58
H(11C)	3243	-1187	6770	58
H(11D)	4060	-206	7803	52
H(11E)	4480	-778	8239	52
H(11F)	4119	-251	8838	52
H(11G)	3362	-1467	9806	60
H(11H)	3852	-1880	9211	60
H(11I)	3084	-2020	9171	60
H(12A)	1916	-1993	7998	66
H(12B)	1709	-1479	7264	66
H(12C)	1167	-1785	7892	66
H(12D)	1997	-1614	9885	60
H(12E)	1223	-1512	9821	60
H(12F)	1674	-946	10214	60
H(12G)	652	-494	8594	57
H(12H)	1083	-174	7838	57
H(12I)	1154	82	8815	57
H(2)	2751	-363	10785	31
H(21A)	2515	357	12777	54
H(21B)	2010	-184	12445	54
H(21C)	1752	521	12732	54
H(21D)	1047	744	11106	46
H(21E)	1250	44	10730	46
H(21F)	1386	689	10172	46
H(21G)	2833	1556	11674	48
H(21H)	2078	1744	11581	48
H(21I)	2519	1653	10732	48
H(22A)	4180	829	9872	49
H(22B)	4585	988	10735	49
H(22C)	3886	1318	10582	49
H(22D)	4046	-931	11193	48
H(22E)	4688	-491	11101	48
H(22F)	4260	-659	10261	48
H(22G)	3588	783	12430	46
H(22H)	4268	399	12453	46
H(22I)	3599	14	12615	46
H(3A)	3330	785	7212	30
H(3B)	3680	1213	6487	30
H(4A)	3808	321	5655	40
H(4B)	3485	-110	6395	40
H(5A)	1692	919	6402	31
H(5B)	2112	622	7176	31
H(6A)	2293	-287	6390	38
H(6B)	1861	3	5627	38
H(7A)	3008	1689	5254	33
H(7B)	2239	1584	5235	33

H(8A)	2372	655	4485	38
H(8B)	3138	768	4484	38