ORGANOMETALLICS
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Table 1. Crystal data and structure refinement for 1.

| | |
|---|---|
| Identification code | bg08 |
| Empirical formula | C6 H16 Li N Si |
| Formula weight | 137.23 |
| Temperature | 193(2) K |
| Wavelength | 0.71073 A |
| Crystal system | Monoclinic |
| Space group | C2/c |
| Unit cell dimensions | a = 17.910(3) A alpha = 90 deg.<br>b = 10.410(2) A beta = 102.08(2) deg.<br>c = 15.829(2) A gamma = 90 deg. |
| Volume | 2885.9(7) A^3 |
| Z | 12 |
| Density (calculated) | 0.948 Mg/m^3 |
| Absorption coefficient | 0.171 mm^-1 |
| F(000) | 912 |
| Crystal size | 0.20 x 0.20 x 0.20 mm |
| Theta range for data collection | 2.28 to 27.01 deg. |
| Index ranges | 0<=h<=22, 0<=k<=13, -20<=l<=19 |
| Reflections collected | 3232 |
| Independent reflections | 3134 [R(int) = 0.0186] |
| Reflections [I>2sigma(I)] | 1127 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 3134 / 3 / 171 |
| Goodness-of-fit on F^2 | 1.008 |
| Final R indices [I>2sigma(I)] | R1 = 0.0839, wR2 = 0.2261 |
| R indices (all data) | R1 = 0.2240, wR2 = 0.3151 |
| Largest diff. peak and hole | 0.286 and -0.293 e.A^-3 |

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

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Li(1) | 5000 | 9063(12) | 2500 | 76(4) |
| N(1) | 3934(2) | 9584(3) | 2267(2) | 55(1) |
| C(1) | 3550(3) | 9077(5) | 2948(4) | 66(1) |
| C(2) | 3018(6) | 10076(10) | 3167(7) | 99(3) |
| C(2') | 3893(11) | 7704(21) | 3182(12) | 99(3) |
| C(3) | 3032(7) | 7923(12) | 2646(6) | 111(3) |
| C(3') | 3748(13) | 9906(22) | 3723(14) | 111(3) |
| C(4) | 4117(5) | 8671(12) | 3726(6) | 90(3) |
| C(4') | 2656(9) | 8997(21) | 2698(11) | 90(3) |
| Si(1) | 3580(1) | 9417(2) | 1198(1) | 71(1) |
| C(5) | 3536(4) | 7787(7) | 735(4) | 130(3) |
| C(6) | 2643(4) | 10149(7) | 725(4) | 103(2) |
| Li(2) | 4206(5) | 11394(8) | 2466(6) | 74(2) |
| N(2) | 5000 | 12696(5) | 2500 | 58(2) |
| Si(2) | 5052(3) | 13214(5) | 3487(4) | 68(1) |
| C(8) | 4360(10) | 14311(16) | 3755(12) | 114(5) |
| C(9) | 5906(12) | 13705(16) | 4023(17) | 127(9) |
| C(10) | 4895(11) | 13694(16) | 1755(13) | 73(6) |
| C(11) | 4087(15) | 13798(31) | 1178(18) | 301(30) |
| C(12) | 5379(10) | 14888(13) | 1913(14) | 134(6) |
| C(13) | 5376(13) | 12961(25) | 1117(10) | 184(11) |

Table 3. Bond lengths [A] and angles [deg] for 1.

| | |
|---|---|
| Li(1)-N(1)#1 | 1.945(5) |
| Li(1)-N(1) | 1.945(5) |
| Li(1)-C(4) | 2.778(10) |
| Li(1)-C(4)#1 | 2.778(10) |
| Li(1)-Li(2)#1 | 2.807(14) |
| Li(1)-Li(2) | 2.807(14) |
| Li(1)-Si(1)#1 | 2.943(2) |
| Li(1)-Si(1) | 2.943(2) |
| N(1)-C(1) | 1.492(6) |
| N(1)-Si(1) | 1.687(4) |
| N(1)-Li(2) | 1.955(9) |
| C(1)-C(3') | 1.48(2) |
| C(1)-C(4) | 1.483(10) |
| C(1)-C(2) | 1.500(11) |
| C(1)-C(4') | 1.57(2) |
| C(1)-C(3) | 1.532(11) |
| C(1)-C(2') | 1.57(2) |
| C(2)-C(3') | 1.43(2) |
| C(2)-C(4') | 1.42(2) |
| C(2')-C(4) | 1.33(2) |
| C(2')-C(3) | 1.61(2) |
| C(3)-C(4') | 1.32(2) |
| C(3')-C(4) | 1.44(2) |
| Si(1)-C(5) | 1.844(7) |
| Si(1)-C(6) | 1.851(6) |
| Si(1)-Li(2) | 2.929(9) |
| Li(2)-N(2) | 1.957(9) |
| Li(2)-Si(2) | 2.734(10) |
| Li(2)-C(13)#1 | 2.75(2) |
| Li(2)-Li(2)#1 | 2.82(2) |
| Li(2)-Si(2)#1 | 2.909(11) |
| N(2)-C(10) | 1.55(2) |
| N(2)-C(10)#1 | 1.55(2) |
| N(2)-Si(2)#1 | 1.636(7) |
| N(2)-Si(2) | 1.636(7) |
| N(2)-Li(2)#1 | 1.957(9) |
| Si(2)-C(10)#1 | 0.648(13) |
| Si(2)-C(13)#1 | 1.12(2) |
| Si(2)-C(11)#1 | 1.64(3) |
| Si(2)-C(9) | 1.67(2) |
| Si(2)-C(8) | 1.80(2) |
| Si(2)-C(12)#1 | 1.96(2) |
| Si(2)-Li(2)#1 | 2.909(11) |
| C(8)-C(12)#1 | 1.38(2) |
| C(8)-C(13)#1 | 1.48(3) |
| C(8)-C(10)#1 | 1.82(3) |
| C(9)-C(11)#1 | 0.34(5) |
| C(9)-C(10)#1 | 1.68(3) |
| C(10)-Si(2)#1 | 0.648(13) |
| C(10)-C(12) | 1.51(2) |
| C(10)-C(11) | 1.55(2) |
| C(10)-C(13) | 1.65(2) |
| C(10)-C(9)#1 | 1.68(3) |
| C(10)-C(8)#1 | 1.82(3) |
| C(11)-C(9)#1 | 0.34(5) |
| C(11)-Si(2)#1 | 1.64(3) |

| | |
|---|---|
| C(12)-C(8)#1 | 1.38(2) |
| C(12)-Si(2)#1 | 1.96(2) |
| C(13)-Si(2)#1 | 1.12(2) |
| C(13)-C(8)#1 | 1.48(3) |
| C(13)-Li(2)#1 | 2.75(2) |

| | |
|---|---|
| N(1)#1-Li(1)-N(1) | 147.6(7) |
| N(1)#1-Li(1)-C(4) | 126.0(2) |
| N(1)-Li(1)-C(4) | 59.6(2) |
| N(1)#1-Li(1)-C(4)#1 | 59.6(2) |
| N(1)-Li(1)-C(4)#1 | 126.0(2) |
| C(4)-Li(1)-C(4)#1 | 163.1(7) |
| N(1)#1-Li(1)-Li(2)#1 | 44.1(3) |
| N(1)-Li(1)-Li(2)#1 | 103.6(5) |
| C(4)-Li(1)-Li(2)#1 | 118.3(5) |
| C(4)#1-Li(1)-Li(2)#1 | 77.3(3) |
| N(1)#1-Li(1)-Li(2) | 103.6(5) |
| N(1)-Li(1)-Li(2) | 44.1(3) |
| C(4)-Li(1)-Li(2) | 77.3(3) |
| C(4)#1-Li(1)-Li(2) | 118.3(5) |
| Li(2)#1-Li(1)-Li(2) | 60.4(4) |
| N(1)#1-Li(1)-Si(1)#1 | 33.03(12) |
| N(1)-Li(1)-Si(1)#1 | 140.2(4) |
| C(4)-Li(1)-Si(1)#1 | 93.7(2) |
| C(4)#1-Li(1)-Si(1)#1 | 88.4(2) |
| Li(2)#1-Li(1)-Si(1)#1 | 61.2(2) |
| Li(2)-Li(1)-Si(1)#1 | 105.4(4) |
| N(1)#1-Li(1)-Si(1) | 140.2(4) |
| N(1)-Li(1)-Si(1) | 33.03(12) |
| C(4)-Li(1)-Si(1) | 88.4(2) |
| C(4)#1-Li(1)-Si(1) | 93.7(2) |
| Li(2)#1-Li(1)-Si(1) | 105.4(4) |
| Li(2)-Li(1)-Si(1) | 61.2(2) |
| Si(1)#1-Li(1)-Si(1) | 165.6(5) |
| C(1)-N(1)-Si(1) | 123.7(3) |
| C(1)-N(1)-Li(1) | 110.3(3) |
| Si(1)-N(1)-Li(1) | 108.0(2) |
| C(1)-N(1)-Li(2) | 111.2(4) |
| Si(1)-N(1)-Li(2) | 106.8(4) |
| Li(1)-N(1)-Li(2) | 92.1(5) |
| C(3')-C(1)-N(1) | 109.0(8) |
| C(3')-C(1)-C(4) | 58.3(10) |
| N(1)-C(1)-C(4) | 111.2(5) |
| C(3')-C(1)-C(2) | 57.2(10) |
| N(1)-C(1)-C(2) | 109.4(5) |
| C(4)-C(1)-C(2) | 111.3(7) |
| C(3')-C(1)-C(4') | 107.2(12) |
| N(1)-C(1)-C(4') | 115.9(7) |
| C(4)-C(1)-C(4') | 132.8(8) |
| C(2)-C(1)-C(4') | 55.3(9) |
| C(3')-C(1)-C(3) | 137.7(8) |
| N(1)-C(1)-C(3) | 113.1(5) |
| C(4)-C(1)-C(3) | 107.5(7) |
| C(2)-C(1)-C(3) | 104.0(7) |
| C(4')-C(1)-C(3) | 50.2(8) |
| C(3')-C(1)-C(2') | 108.8(12) |
| N(1)-C(1)-C(2') | 106.0(7) |
| C(4)-C(1)-C(2') | 51.6(8) |
| C(2)-C(1)-C(2') | 144.5(8) |
| C(4')-C(1)-C(2') | 109.9(11) |

| | |
|---|---|
| C(3)-C(1)-C(2') | 62.7(9) |
| C(3')-C(2)-C(4') | 118.8(14) |
| C(3')-C(2)-C(1) | 60.7(10) |
| C(4')-C(2)-C(1) | 64.8(9) |
| C(4)-C(2')-C(1) | 60.9(10) |
| C(4)-C(2')-C(3) | 111(2) |
| C(1)-C(2')-C(3) | 57.5(8) |
| C(4')-C(3)-C(1) | 66.3(9) |
| C(4')-C(3)-C(2') | 122.1(13) |
| C(1)-C(3)-C(2') | 59.7(9) |
| C(2)-C(3')-C(4) | 118(2) |
| C(2)-C(3')-C(1) | 62.1(10) |
| C(4)-C(3')-C(1) | 60.9(10) |
| C(2')-C(4)-C(3') | 126.6(13) |
| C(2')-C(4)-C(1) | 67.5(9) |
| C(3')-C(4)-C(1) | 60.8(9) |
| C(2')-C(4)-Li(1) | 78.3(9) |
| C(3')-C(4)-Li(1) | 101.2(9) |
| C(1)-C(4)-Li(1) | 76.7(4) |
| C(3)-C(4')-C(2) | 121.3(14) |
| C(3)-C(4')-C(1) | 63.5(9) |
| C(2)-C(4')-C(1) | 59.9(8) |
| N(1)-Si(1)-C(5) | 118.0(3) |
| N(1)-Si(1)-C(6) | 118.8(3) |
| C(5)-Si(1)-C(6) | 105.0(3) |
| N(1)-Si(1)-Li(2) | 39.7(2) |
| C(5)-Si(1)-Li(2) | 153.8(3) |
| C(6)-Si(1)-Li(2) | 99.9(3) |
| N(1)-Si(1)-Li(1) | 38.9(2) |
| C(5)-Si(1)-Li(1) | 97.0(3) |
| C(6)-Si(1)-Li(1) | 155.7(3) |
| Li(2)-Si(1)-Li(1) | 57.1(3) |
| N(2)-Li(2)-N(1) | 145.8(5) |
| N(2)-Li(2)-Si(2) | 36.3(2) |
| N(1)-Li(2)-Si(2) | 148.4(5) |
| N(2)-Li(2)-C(13)#1 | 59.6(5) |
| N(1)-Li(2)-C(13)#1 | 136.0(7) |
| Si(2)-Li(2)-C(13)#1 | 23.6(4) |
| N(2)-Li(2)-Li(1) | 103.7(4) |
| N(1)-Li(2)-Li(1) | 43.8(2) |
| Si(2)-Li(2)-Li(1) | 111.8(3) |
| C(13)#1-Li(2)-Li(1) | 116.5(6) |
| N(2)-Li(2)-Li(2)#1 | 43.8(3) |
| N(1)-Li(2)-Li(2)#1 | 102.8(3) |
| Si(2)-Li(2)-Li(2)#1 | 63.1(3) |
| C(13)#1-Li(2)-Li(2)#1 | 82.4(6) |
| Li(1)-Li(2)-Li(2)#1 | 59.8(2) |
| N(2)-Li(2)-Si(2)#1 | 32.4(2) |
| N(1)-Li(2)-Si(2)#1 | 132.0(5) |
| Si(2)-Li(2)-Si(2)#1 | 66.3(3) |
| C(13)#1-Li(2)-Si(2)#1 | 87.7(6) |
| Li(1)-Li(2)-Si(2)#1 | 106.8(3) |
| Li(2)#1-Li(2)-Si(2)#1 | 56.9(3) |
| N(2)-Li(2)-Si(1) | 132.7(4) |
| N(1)-Li(2)-Si(1) | 33.5(2) |
| Si(2)-Li(2)-Si(1) | 167.8(4) |
| C(13)#1-Li(2)-Si(1) | 167.5(6) |
| Li(1)-Li(2)-Si(1) | 61.7(2) |
| Li(2)#1-Li(2)-Si(1) | 105.4(4) |
| Si(2)#1-Li(2)-Si(1) | 104.7(3) |

| | |
|---|---|
| C(10)-N(2)-C(10)#1 | 96.0(11) |
| C(10)-N(2)-Si(2)#1 | 23.3(5) |
| C(10)#1-N(2)-Si(2)#1 | 118.5(7) |
| C(10)-N(2)-Si(2) | 118.5(7) |
| C(10)#1-N(2)-Si(2) | 23.3(5) |
| Si(2)#1-N(2)-Si(2) | 141.5(5) |
| C(10)-N(2)-Li(2)#1 | 117.1(8) |
| C(10)#1-N(2)-Li(2)#1 | 118.1(7) |
| Si(2)#1-N(2)-Li(2)#1 | 98.7(4) |
| Si(2)-N(2)-Li(2)#1 | 107.8(4) |
| C(10)-N(2)-Li(2) | 118.1(7) |
| C(10)#1-N(2)-Li(2) | 117.1(8) |
| Si(2)#1-N(2)-Li(2) | 107.8(4) |
| Si(2)-N(2)-Li(2) | 98.7(4) |
| Li(2)#1-N(2)-Li(2) | 92.3(6) |
| C(10)#1-Si(2)-C(13)#1 | 136(3) |
| C(10)#1-Si(2)-C(11)#1 | 70(2) |
| C(13)#1-Si(2)-C(11)#1 | 128.0(14) |
| C(10)#1-Si(2)-N(2) | 71(2) |
| C(13)#1-Si(2)-N(2) | 123.2(10) |
| C(11)#1-Si(2)-N(2) | 107.0(10) |
| C(10)#1-Si(2)-C(9) | 80(2) |
| C(13)#1-Si(2)-C(9) | 116.8(14) |
| C(11)#1-Si(2)-C(9) | 12(2) |
| N(2)-Si(2)-C(9) | 116.8(9) |
| C(10)#1-Si(2)-C(8) | 81(2) |
| C(13)#1-Si(2)-C(8) | 55.3(14) |
| C(11)#1-Si(2)-C(8) | 109.6(12) |
| N(2)-Si(2)-C(8) | 121.9(7) |
| C(9)-Si(2)-C(8) | 106.8(9) |
| C(10)#1-Si(2)-C(12)#1 | 39(2) |
| C(13)#1-Si(2)-C(12)#1 | 97(2) |
| C(11)#1-Si(2)-C(12)#1 | 93.1(13) |
| N(2)-Si(2)-C(12)#1 | 92.6(7) |
| C(9)-Si(2)-C(12)#1 | 98.6(8) |
| C(8)-Si(2)-C(12)#1 | 42.9(7) |
| C(10)#1-Si(2)-Li(2) | 108(2) |
| C(13)#1-Si(2)-Li(2) | 78.9(10) |
| C(11)#1-Si(2)-Li(2) | 144.7(11) |
| N(2)-Si(2)-Li(2) | 45.0(3) |
| C(9)-Si(2)-Li(2) | 148.2(7) |
| C(8)-Si(2)-Li(2) | 104.8(6) |
| C(12)#1-Si(2)-Li(2) | 107.1(6) |
| C(10)#1-Si(2)-Li(2)#1 | 93(2) |
| C(13)#1-Si(2)-Li(2)#1 | 125.3(14) |
| C(11)#1-Si(2)-Li(2)#1 | 84.8(11) |
| N(2)-Si(2)-Li(2)#1 | 39.8(3) |
| C(9)-Si(2)-Li(2)#1 | 89.6(7) |
| C(8)-Si(2)-Li(2)#1 | 161.2(7) |
| C(12)#1-Si(2)-Li(2)#1 | 127.2(7) |
| Li(2)-Si(2)-Li(2)#1 | 59.9(4) |
| C(12)#1-C(8)-C(13)#1 | 112(2) |
| C(12)#1-C(8)-C(10)#1 | 54.2(9) |
| C(13)#1-C(8)-C(10)#1 | 58.8(9) |
| C(12)#1-C(8)-Si(2) | 74.6(10) |
| C(13)#1-C(8)-Si(2) | 38.3(9) |
| C(10)#1-C(8)-Si(2) | 20.6(4) |
| C(11)#1-C(9)-Si(2) | 80(8) |
| C(11)#1-C(9)-C(10)#1 | 60(7) |
| Si(2)-C(9)-C(10)#1 | 22.3(6) |

| | |
|---|---|
| Si(2)#1-C(10)-C(12) | 126(3) |
| Si(2)#1-C(10)-C(11) | 87(2) |
| C(12)-C(10)-C(11) | 118(2) |
| Si(2)#1-C(10)-N(2) | 86(2) |
| C(12)-C(10)-N(2) | 116.9(14) |
| C(11)-C(10)-N(2) | 116(2) |
| Si(2)#1-C(10)-C(13) | 28(2) |
| C(12)-C(10)-C(13) | 97(2) |
| C(11)-C(10)-C(13) | 103(2) |
| N(2)-C(10)-C(13) | 99.2(13) |
| Si(2)#1-C(10)-C(9)#1 | 77(2) |
| C(12)-C(10)-C(9)#1 | 119(2) |
| C(11)-C(10)-C(9)#1 | 11(2) |
| N(2)-C(10)-C(9)#1 | 120.6(13) |
| C(13)-C(10)-C(9)#1 | 92(2) |
| Si(2)#1-C(10)-C(8)#1 | 78(2) |
| C(12)-C(10)-C(8)#1 | 48.0(10) |
| C(11)-C(10)-C(8)#1 | 113(2) |
| N(2)-C(10)-C(8)#1 | 126.2(14) |
| C(13)-C(10)-C(8)#1 | 50.5(11) |
| C(9)#1-C(10)-C(8)#1 | 105(2) |
| C(9)#1-C(11)-C(10) | 109(8) |
| C(9)#1-C(11)-Si(2)#1 | 89(8) |
| C(10)-C(11)-Si(2)#1 | 23.2(6) |
| C(8)#1-C(12)-C(10) | 77.8(13) |
| C(8)#1-C(12)-Si(2)#1 | 62.6(9) |
| C(10)-C(12)-Si(2)#1 | 15.6(8) |
| Si(2)#1-C(13)-C(8)#1 | 86(2) |
| Si(2)#1-C(13)-C(10) | 16.0(9) |
| C(8)#1-C(13)-C(10) | 70.7(14) |
| Si(2)#1-C(13)-Li(2)#1 | 77.5(10) |
| C(8)#1-C(13)-Li(2)#1 | 115.2(12) |
| C(10)-C(13)-Li(2)#1 | 82.1(11) |

---

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

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1.
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 |
|---|---|---|---|---|---|---|
| Li(1) | 69(8) | 57(7) | 94(10) | 0 | 0(7) | 0 |
| N(1) | 50(2) | 58(2) | 54(2) | -2(2) | 4(2) | -11(2) |
| C(1) | 57(3) | 69(3) | 72(3) | 8(3) | 15(3) | -6(3) |
| C(2) | 93(6) | 116(8) | 89(6) | 17(6) | 22(5) | -4(6) |
| C(2') | 93(6) | 116(8) | 89(6) | 17(6) | 22(5) | -4(6) |
| C(3) | 99(7) | 136(9) | 105(8) | 17(7) | 35(6) | -39(7) |
| C(3') | 99(7) | 136(9) | 105(8) | 17(7) | 35(6) | -39(7) |
| C(4) | 75(6) | 114(8) | 79(6) | 22(6) | 15(5) | 0(6) |
| C(4') | 75(6) | 114(8) | 79(6) | 22(6) | 15(5) | 0(6) |
| Si(1) | 59(1) | 81(1) | 66(1) | -13(1) | 1(1) | -8(1) |
| C(5) | 118(6) | 128(6) | 130(6) | -54(5) | -8(5) | 25(5) |
| C(6) | 94(5) | 126(5) | 78(4) | -11(4) | -7(4) | 6(4) |
| Li(2) | 65(5) | 64(5) | 92(7) | -9(5) | 16(5) | -13(5) |
| N(2) | 52(3) | 48(3) | 69(4) | 0 | -2(3) | 0 |
| Si(2) | 64(2) | 62(3) | 80(4) | -18(2) | 16(2) | -9(2) |
| C(8) | 124(14) | 74(10) | 151(16) | -12(10) | 43(11) | 14(9) |
| C(9) | 94(16) | 84(11) | 202(23) | -26(13) | 24(14) | 27(12) |
| C(10) | 108(13) | 51(11) | 63(10) | -7(7) | 24(8) | -11(9) |
| C(11) | 164(29) | 519(64) | 271(35) | 282(40) | 160(27) | 171(31) |
| C(12) | 118(13) | 72(10) | 193(19) | 45(10) | -10(12) | -6(10) |
| C(13) | 139(18) | 291(34) | 117(15) | 102(19) | 17(14) | 47(21) |

Table 5. Hydrogen coordinates ( x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2A) | 3309(6) | 10833(10) | 3364(7) | 80 |
| H(2B) | 2640(6) | 10276(10) | 2659(7) | 80 |
| H(2C) | 2770(6) | 9773(10) | 3612(7) | 80 |
| H(3A) | 3353(7) | 7251(12) | 2508(6) | 80 |
| H(3B) | 2784(7) | 7636(12) | 3094(6) | 80 |
| H(3C) | 2653(7) | 8138(12) | 2141(6) | 80 |
| H(4A) | 4433(5) | 9394(12) | 3940(6) | 80 |
| H(4B) | 3853(5) | 8384(12) | 4160(6) | 80 |
| H(4C) | 4430(5) | 7987(12) | 3586(6) | 80 |
| H(1) | 4139(32) | 10029(49) | 796(35) | 101(18) |
| H(5A) | 3091(4) | 7706(7) | 278(4) | 80 |
| H(5B) | 3985(4) | 7628(7) | 510(4) | 80 |
| H(5C) | 3509(4) | 7175(7) | 1181(4) | 80 |
| H(6A) | 2426(4) | 9749(7) | 183(4) | 80 |
| H(6B) | 2304(4) | 10042(7) | 1116(4) | 80 |
| H(6C) | 2717(4) | 11048(7) | 636(4) | 80 |
| H(2) | 4680(3) | 12828(5) | 4027(4) | 80 |
| H(8A) | 4619(10) | 14987(16) | 4113(12) | 80 |
| H(8B) | 4086(10) | 14667(16) | 3219(12) | 80 |
| H(8C) | 4007(10) | 13894(16) | 4046(12) | 80 |
| H(9A) | 5937(12) | 14564(16) | 4249(17) | 80 |
| H(9B) | 5977(12) | 13101(16) | 4491(17) | 80 |
| H(9C) | 6297(12) | 13582(16) | 3697(17) | 80 |
| H(11A) | 3784(15) | 14280(31) | 1501(18) | 80 |
| H(11B) | 4098(15) | 14238(31) | 648(18) | 80 |
| H(11C) | 3867(15) | 12961(31) | 1052(18) | 80 |
| H(12A) | 5170(10) | 15440(13) | 2291(14) | 80 |
| H(12B) | 5884(10) | 14629(13) | 2194(14) | 80 |
| H(12C) | 5399(10) | 15340(13) | 1390(14) | 80 |
| H(13A) | 5369(13) | 13437(25) | 596(10) | 80 |
| H(13B) | 5895(13) | 12798(25) | 1403(10) | 80 |
| H(13C) | 5114(13) | 12159(25) | 978(10) | 80 |

Table 1. Crystal data and structure refinement

| | |
|---|---|
| Identification code | BG13 |
| Empirical formula | C12 H32 Mg N2 Si2 |
| Formula weight | 284.89 |
| Temperature | 173(2) K |
| Wavelength | 0.71073 A |
| Crystal system | Monoclinic |
| Space group | P2(1)/c |
| Unit cell dimensions | a = 11.371(2) A alpha = 90 deg.<br>b = 13.497(2) A beta = 106.58(2) deg.<br>c = 12.168(3) A gamma = 90 deg. |
| Volume | 1789.8(5) A^3 |
| Z | 4 |
| Density (calculated) | 1.057 Mg/m^3 |
| Absorption coefficient | 0.220 mm^-1 |
| F(000) | 632 |
| Crystal size | 0.40 x 0.40 x 0.30 mm |
| Theta range for data collection | 2.31 to 26.28 deg. |
| Index ranges | 0<=h<=14, 0<=k<=16, -15<=l<=14 |
| Reflections collected | 3662 |
| Independent reflections | 3623 [R(int) = 0.0294] |
| Reflections [I>2sig.(I)] | 2866 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 3623 / 0 / 282 |
| Goodness-of-fit on F^2 | 1.023 |
| Final R indices [I>2sigma(I)] | R1 = 0.0319, wR2 = 0.0814 |
| R indices (all data) | R1 = 0.0495, wR2 = 0.0922 |
| Largest diff. peak and hole | 0.364 and -0.206 e.A^-3 |

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

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Si(1) | 6637(1) | 149(1) | 8729(1) | 23(1) |
| Mg(1) | 3923(1) | 348(1) | 9138(1) | 17(1) |
| N(1) | 5814(1) | 745(1) | 9540(1) | 18(1) |
| C(1) | 6051(2) | 195(2) | 7133(2) | 39(1) |
| Si(2) | 2401(1) | -11(1) | 6930(1) | 22(1) |
| N(2) | 2432(1) | 823(1) | 7966(1) | 20(1) |
| C(2) | 8319(2) | 399(2) | 9093(2) | 42(1) |
| C(3) | 5970(2) | 1854(1) | 9703(2) | 23(1) |
| C(4) | 1140(2) | -952(2) | 6540(2) | 40(1) |
| C(5) | 2624(2) | 414(2) | 5541(2) | 41(1) |
| C(6) | 1554(2) | 1654(1) | 7845(2) | 26(1) |
| C(31) | 4992(2) | 2259(2) | 10201(2) | 32(1) |
| C(32) | 7220(2) | 2123(2) | 10529(2) | 35(1) |
| C(33) | 5832(2) | 2363(2) | 8543(2) | 35(1) |
| C(61) | 2049(2) | 2577(2) | 7400(2) | 47(1) |
| C(62) | 1355(2) | 1890(2) | 9005(2) | 34(1) |
| C(63) | 299(2) | 1394(2) | 7020(2) | 46(1) |

Table 3. Bond lengths [A] and angles [deg] for 1.

| | |
|---|---|
| Si(1)-N(1) | 1.7394(14) |
| Si(1)-C(1) | 1.865(2) |
| Si(1)-C(2) | 1.867(2) |
| Si(1)-Mg(1)#1 | 2.9217(9) |
| Mg(1)-N(2) | 1.984(2) |
| Mg(1)-N(1) | 2.1328(14) |
| Mg(1)-N(1)#1 | 2.1394(14) |
| Mg(1)-Si(2) | 2.7915(10) |
| Mg(1)-Mg(1)#1 | 2.8906(12) |
| Mg(1)-Si(1)#1 | 2.9217(9) |
| N(1)-C(3) | 1.514(2) |
| N(1)-Mg(1)#1 | 2.1394(14) |
| Si(2)-N(2) | 1.6823(14) |
| Si(2)-C(5) | 1.869(2) |
| Si(2)-C(4) | 1.872(2) |
| N(2)-C(6) | 1.481(2) |
| C(3)-C(31) | 1.513(3) |
| C(3)-C(32) | 1.533(2) |
| C(3)-C(33) | 1.536(3) |
| C(6)-C(62) | 1.526(3) |
| C(6)-C(61) | 1.528(3) |
| C(6)-C(63) | 1.533(3) |
| | |
| N(1)-Si(1)-C(1) | 119.03(9) |
| N(1)-Si(1)-C(2) | 117.54(10) |
| C(1)-Si(1)-C(2) | 106.18(12) |
| N(1)-Si(1)-Mg(1)#1 | 46.59(5) |
| C(1)-Si(1)-Mg(1)#1 | 145.98(8) |
| C(2)-Si(1)-Mg(1)#1 | 107.37(9) |
| N(2)-Mg(1)-N(1) | 133.05(6) |
| N(2)-Mg(1)-N(1)#1 | 132.11(6) |
| N(1)-Mg(1)-N(1)#1 | 94.84(5) |
| N(2)-Mg(1)-Si(2) | 36.55(4) |
| N(1)-Mg(1)-Si(2) | 124.90(5) |
| N(1)#1-Mg(1)-Si(2) | 121.27(4) |
| N(2)-Mg(1)-Mg(1)#1 | 179.35(5) |
| N(1)-Mg(1)-Mg(1)#1 | 47.52(4) |
| N(1)#1-Mg(1)-Mg(1)#1 | 47.33(4) |
| Si(2)-Mg(1)-Mg(1)#1 | 143.75(3) |
| N(2)-Mg(1)-Si(1)#1 | 110.78(5) |
| N(1)-Mg(1)-Si(1)#1 | 108.32(5) |
| N(1)#1-Mg(1)-Si(1)#1 | 36.20(4) |
| Si(2)-Mg(1)-Si(1)#1 | 125.64(3) |
| Mg(1)#1-Mg(1)-Si(1)#1 | 68.57(3) |
| C(3)-N(1)-Si(1) | 117.97(10) |
| C(3)-N(1)-Mg(1) | 110.57(10) |
| Si(1)-N(1)-Mg(1) | 115.10(7) |
| C(3)-N(1)-Mg(1)#1 | 126.69(10) |
| Si(1)-N(1)-Mg(1)#1 | 97.21(6) |
| Mg(1)-N(1)-Mg(1)#1 | 85.16(5) |
| N(2)-Si(2)-C(5) | 119.49(10) |
| N(2)-Si(2)-C(4) | 119.68(10) |
| C(5)-Si(2)-C(4) | 105.71(12) |
| N(2)-Si(2)-Mg(1) | 44.62(5) |
| C(5)-Si(2)-Mg(1) | 127.55(8) |
| C(4)-Si(2)-Mg(1) | 125.56(8) |

| | |
|---|---|
| C(6)-N(2)-Si(2) | 124.27(11) |
| C(6)-N(2)-Mg(1) | 136.81(11) |
| Si(2)-N(2)-Mg(1) | 98.83(7) |
| N(1)-C(3)-C(31) | 109.73(14) |
| N(1)-C(3)-C(32) | 111.91(14) |
| C(31)-C(3)-C(32) | 107.5(2) |
| N(1)-C(3)-C(33) | 110.22(14) |
| C(31)-C(3)-C(33) | 108.2(2) |
| C(32)-C(3)-C(33) | 109.2(2) |
| N(2)-C(6)-C(62) | 109.92(14) |
| N(2)-C(6)-C(61) | 110.3(2) |
| C(62)-C(6)-C(61) | 108.9(2) |
| N(2)-C(6)-C(63) | 111.5(2) |
| C(62)-C(6)-C(63) | 107.3(2) |
| C(61)-C(6)-C(63) | 108.8(2) |

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

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1. 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 |
|---|---|---|---|---|---|---|
| Si(1) | 19(1) | 26(1) | 26(1) | 5(1) | 9(1) | 1(1) |
| Mg(1) | 14(1) | 18(1) | 17(1) | 2(1) | 1(1) | 0(1) |
| N(1) | 15(1) | 18(1) | 19(1) | 3(1) | 3(1) | -2(1) |
| C(1) | 43(1) | 49(1) | 29(1) | 1(1) | 16(1) | 4(1) |
| Si(2) | 20(1) | 27(1) | 17(1) | -1(1) | 1(1) | 0(1) |
| N(2) | 16(1) | 22(1) | 19(1) | 1(1) | 0(1) | 3(1) |
| C(2) | 24(1) | 46(1) | 60(2) | 2(1) | 17(1) | 0(1) |
| C(3) | 21(1) | 17(1) | 29(1) | 3(1) | 3(1) | -5(1) |
| C(4) | 32(1) | 38(1) | 40(1) | -7(1) | -5(1) | -8(1) |
| C(5) | 42(1) | 60(2) | 22(1) | 5(1) | 8(1) | 8(1) |
| C(6) | 22(1) | 28(1) | 25(1) | 3(1) | -1(1) | 9(1) |
| C(31) | 32(1) | 24(1) | 38(1) | -5(1) | 10(1) | -4(1) |
| C(32) | 28(1) | 30(1) | 43(1) | -2(1) | 2(1) | -11(1) |
| C(33) | 43(1) | 25(1) | 38(1) | 9(1) | 13(1) | -1(1) |
| C(61) | 55(2) | 33(1) | 52(1) | 16(1) | 16(1) | 14(1) |
| C(62) | 30(1) | 35(1) | 36(1) | -3(1) | 7(1) | 14(1) |
| C(63) | 26(1) | 61(2) | 40(1) | -8(1) | -8(1) | 19(1) |

Table 5. Hydrogen coordinates ( x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1) | 6510(18) | -821(15) | 9034(16) | 31(5) |
| H(1C) | 6257(28) | 765(24) | 6848(26) | 79(10) |
| H(1B) | 6440(27) | -295(21) | 6788(24) | 70(9) |
| H(1A) | 5264(33) | 166(24) | 6897(26) | 84(11) |
| H(2) | 3511(17) | -558(14) | 7543(15) | 24(5) |
| H(2C) | 8446(22) | 1050(19) | 8804(20) | 49(7) |
| H(2B) | 8708(24) | 345(19) | 9907(24) | 57(7) |
| H(2A) | 8649(24) | -114(19) | 8762(22) | 53(7) |
| H(4C) | 903(24) | -1134(19) | 7206(23) | 58(8) |
| H(4B) | 489(27) | -668(22) | 6056(25) | 68(8) |
| H(4A) | 1388(28) | -1517(24) | 6227(24) | 80(10) |
| H(5C) | 3293(28) | 886(22) | 5612(23) | 68(8) |
| H(5B) | 1897(26) | 696(20) | 5053(23) | 61(8) |
| H(5A) | 2850(30) | -94(24) | 5168(28) | 83(11) |
| H(31C) | 5072(20) | 2976(19) | 10278(19) | 45(6) |
| H(31B) | 4198(21) | 2149(16) | 9715(18) | 36(6) |
| H(31A) | 5032(19) | 2001(16) | 10906(18) | 33(6) |
| H(32C) | 7910(21) | 1926(16) | 10282(18) | 38(6) |
| H(32B) | 7281(20) | 2809(19) | 10642(19) | 45(6) |
| H(32A) | 7328(21) | 1850(18) | 11291(21) | 49(7) |
| H(33C) | 6485(22) | 2188(17) | 8227(19) | 45(6) |
| H(33B) | 5849(18) | 3093(17) | 8651(17) | 34(5) |
| H(33A) | 5045(21) | 2200(17) | 7998(18) | 40(6) |
| H(61C) | 2141(26) | 2444(20) | 6671(25) | 67(8) |
| H(61B) | 1482(24) | 3124(20) | 7344(21) | 58(7) |
| H(61A) | 2834(26) | 2815(19) | 7967(23) | 62(8) |
| H(62C) | 2149(21) | 2075(16) | 9568(18) | 38(6) |
| H(62B) | 1017(20) | 1317(18) | 9281(18) | 40(6) |
| H(62A) | 777(22) | 2432(18) | 8950(19) | 49(6) |
| H(63C) | -53(23) | 777(21) | 7299(21) | 54(7) |
| H(63A) | 377(21) | 1269(17) | 6264(21) | 48(7) |
| H(63B) | -219(24) | 1938(21) | 6969(20) | 57(7) |