Anisotropic Temperature Factor Coefficients - U's

for $C_{63}H_{50}AlNO_2Si_2, C_7H_8$

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Si(1)	0.0292(3)	0.0284(2)	0.0259(2)	-0.0019(2)	0.0007(2)	-0.0006(2)
Si(2)	0.0263(2)	0.0295(2)	0.0300(3)	0.0013(2)	0.0020(2)	0.0019(2)
Al	0.0273(3)	0.0303(2)	0.0281(3)	-0.0001(2)	-0.0016(2)	0.0005(2)
O(1)	0.0280(6)	0.0314(6)	0.0294(6)	0.0029(5)	0.0005(5)	0.0034(5)
O(2)	0.0288(6)	0.0310(6)	0.0255(6)	-0.0037(5)	-0.0013(5)	-0.0012(5)
N(31)	0.0260(8)	0.0324(7)	0.0315(8)	0.0006(6)	0.0009(7)	0.0019(6)
C(1)	0.0378(11)	0.0379(10)	0.0311(10)	-0.0006(9)	-0.0061(8)	-0.0018(8)
C(2)	0.0531(14)	0.0811(17)	0.0389(12)	-0.0172(13)	-0.0047(11)	0.0065(12)
C(11)	0.0245(9)	0.0247(8)	0.0280(9)	-0.0022(7)	-0.0014(7)	0.0003(7)
C(12)	0.0257(9)	0.0271(8)	0.0306(9)	-0.0044(7)	0.0009(8)	-0.0026(7)
C(13)	0.0247(9)	0.0322(9)	0.0315(10)	-0.0002(7)	0.0027(8)	-0.0016(8)
C(14)	0.0242(9)	0.0287(8)	0.0329(10)	-0.0023(7)	-0.0011(8)	-0.0001(8)
C(15)	0.0261(9)	0.0380(10)	0.0387(11)	0.0021(8)	-0.0017(8)	0.0004(8)
C(16)	0.0323(10)	0.0433(10)	0.0374(11)	0.0051(9)	-0.0055(9)	0.0055(9)
C(17)	0.0374(11)	0.0434(10)	0.0299(10)	-0.0004(9)	-0.0028(9)	0.0068(9)
C(18)	0.0292(10)	0.0363(9)	0.0295(9)	-0.0011(8)	0.0009(8)	0.0024(7)
C(19)	0.0268(9)	0.0272(8)	0.0279(9)	-0.0045(7)	-0.0010(7)	-0.0002(7)
C(1A)	0.0236(8)	0.0247(8)	0.0305(9)	-0.0011(7)	-0.0004(7)	-0.0018(7)
C(21)	0.0299(9)	0.0231(8)	0.0274(9)	0.0010(7)	-0.0029(8)	0.0016(7)
C(22)	0.0263(9)	0.0265(8)	0.0288(9)	0.0022(7)	0.0009(8)	0.0020(8)
C(23)	0.0327(10)	0.0283(8)	0.0270(9)	0.0047(7)	0.0045(8)	0.0019(7)
C(24)	0.0342(10)	0.0232(8)	0.0299(10)	0.0004(8)	-0.0001(8)	0.0034(7)
C(25)	0.0482(13)	0.0276(9)	0.0305(10)	-0.0018(9)	0.0021(9)	-0.0013(8)
C(26)	0.0513(13)	0.0313(9)	0.0334(10)	-0.0088(9)	-0.0031(10)	-0.0040(8)
C(27)	0.0403(11)	0.0351(9)	0.0378(11)	-0.0109(9)	-0.0058(9)	0.0010(8)
C(28)	0.0328(10)	0.0328(9)	0.0330(10)	-0.0042(8)	0.0003(8)	0.0034(8)
C(29)	0.0321(10)	0.0262(8)	0.0254(9)	0.0001(7)	-0.0026(8)	0.0023(7)
C(2A)	0.0274(9)	0.0258(8)	0.0239(9)	0.0006(7)	0.0001(7)	0.0033(7)
C(32)	0.0310(11)	0.0422(10)	0.0486(12)	0.0011(9)	-0.0041(9)	-0.0020(9)
C(33)	0.0389(12)	0.0523(12)	0.0518(13)	0.0148(11)	-0.0052(10)	-0.0056(10)
C(34)	0.0546(14)	0.0348(10)	0.0517(14)	0.0094(10)	-0.0014(11)	-0.0022(9)
C(35)	0.0460(13)	0.0330(10)	0.0640(14)	-0.0001(10)	-0.0098(12)	-0.0036(10)
C(36)	0.0308(11)	0.0326(9)	0.0545(13)	-0.0013(8)	-0.0068(9)	0.0007(9)
C(111)	0.0335(10)	0.0296(9)	0.0332(10)	0.0008(8)	-0.0010(8)	-0.0038(7)
C(112)	0.0427(11)	0.0379(10)	0.0356(11)	-0.0090(9)	-0.0004(9)	-0.0014(9)
C(113)	0.0502(13)	0.0422(11)	0.0471(13)	-0.0155(10)	0.0016(11)	-0.0019(10)
C(114)	0.0480(13)	0.0373(10)	0.0588(14)	-0.0066(10)	-0.0163(11)	-0.0082(10)
C(115)	0.0674(15)	0.0406(11)	0.0469(13)	-0.0091(11)	-0.0253(12)	0.0026(10)
C(116)	0.0500(12)	0.0337(9)	0.0392(11)	-0.0085(9)	-0.0124(9)	0.0057(9)
C(121)	0.0408(11)	0.0290(8)	0.0245(9)	-0.0025(8)	0.0037(8)	-0.0036(7)
C(122)	0.0457(12)	0.0337(9)	0.0359(11)	-0.0005(9)	-0.0032(9)	-0.0010(8)
C(123)	0.0665(15)	0.0348(10)	0.0386(12)	0.0062(11)	-0.0073(11)	-0.0014(9)
C(124)	0.0899(19)	0.0315(9)	0.0343(11)	-0.0021(13)	0.0118(12)	-0.0011(9)
C(125)	0.0678(16)	0.0363(11)	0.0476(13)	-0.0151(11)	0.0200(12)	-0.0060(10)

Anisotropic Temperature Factor Coefficients - U's (Continued)

for $C_{63}H_{50}AlNO_2Si_2, C_7H_8$

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C(126)	0.0439(12)	0.0337(10)	0.0438(12)	-0.0059(9)	0.0089(10)	-0.0049(9)
C(131)	0.0350(10)	0.0320(9)	0.0257(9)	0.0006(8)	0.0029(8)	0.0041(7)
C(132)	0.0394(11)	0.0362(10)	0.0385(11)	-0.0005(9)	0.0062(9)	-0.0018(9)
C(133)	0.0577(15)	0.0357(10)	0.0502(13)	0.0074(10)	0.0125(11)	-0.0037(10)
C(134)	0.0455(13)	0.0418(11)	0.0504(13)	0.0137(10)	0.0145(11)	0.0091(10)
C(135)	0.0317(11)	0.0633(14)	0.0475(13)	0.0013(10)	0.0000(10)	0.0151(11)
C(136)	0.0357(11)	0.0509(11)	0.0328(10)	-0.0013(9)	0.0014(8)	0.0003(9)
C(211)	0.0220(9)	0.0369(9)	0.0323(10)	0.0006(7)	0.0013(8)	0.0002(8)
C(212)	0.0309(10)	0.0422(10)	0.0324(10)	-0.0034(8)	0.0004(8)	0.0032(9)
C(213)	0.0323(11)	0.0551(12)	0.0326(10)	-0.0029(9)	-0.0010(9)	-0.0069(9)
C(214)	0.0294(10)	0.0397(10)	0.0469(12)	-0.0013(8)	-0.0023(9)	-0.0094(9)
C(215)	0.0346(11)	0.0331(9)	0.0443(12)	-0.0005(8)	-0.0007(9)	-0.0016(9)
C(216)	0.0302(10)	0.0320(9)	0.0349(11)	0.0016(8)	0.0004(8)	0.0007(8)
C(221)	0.0364(10)	0.0275(9)	0.0355(10)	-0.0005(8)	0.0050(8)	-0.0004(8)
C(222)	0.0427(11)	0.0441(10)	0.0351(10)	-0.0063(10)	0.0012(9)	0.0040(9)
C(223)	0.0657(15)	0.0463(11)	0.0363(11)	-0.0125(11)	-0.0028(11)	0.0077(9)
C(224)	0.0709(16)	0.0400(11)	0.0343(11)	-0.0124(11)	0.0167(11)	-0.0013(9)
C(225)	0.0504(13)	0.0460(11)	0.0548(14)	-0.0015(11)	0.0218(11)	0.0002(11)
C(226)	0.0393(11)	0.0419(11)	0.0420(11)	0.0008(9)	0.0098(9)	0.0012(9)
C(231)	0.0254(10)	0.0378(9)	0.0416(11)	0.0032(8)	0.0049(9)	0.0084(8)
C(232)	0.0317(11)	0.0450(11)	0.0575(14)	-0.0007(9)	-0.0032(10)	0.0117(10)
C(233)	0.0340(12)	0.0602(14)	0.0872(19)	-0.0003(11)	-0.0105(12)	0.0241(13)
C(234)	0.0372(13)	0.0497(13)	0.112(2)	0.0112(11)	-0.0030(14)	0.0300(14)
C(235)	0.0509(15)	0.0386(11)	0.095(2)	0.0089(11)	0.0000(14)	0.0102(12)
C(236)	0.0392(12)	0.0364(10)	0.0617(14)	0.0038(9)	-0.0006(11)	0.0047(10)
C(911)	0.0691(19)	0.0639(16)	0.075(2)	-0.0160(14)	-0.0129(16)	0.0124(15)
C(912)	0.093(2)	0.087(2)	0.077(2)	-0.026(2)	0.0128(19)	0.0059(17)
C(913)	0.077(2)	0.0774(19)	0.108(3)	-0.0144(16)	0.002(2)	0.0175(19)
C(914)	0.100(3)	0.0679(18)	0.095(3)	-0.0212(19)	-0.018(2)	0.0187(18)
C(915)	0.111(3)	0.0628(17)	0.079(2)	-0.0031(18)	-0.005(2)	-0.0058(16)
C(916)	0.099(2)	0.0578(15)	0.085(2)	-0.0054(15)	-0.017(2)	-0.0041(15)
C(917)	0.102(3)	0.128(3)	0.100(3)	-0.022(2)	0.005(2)	0.018(2)

The form of the anisotropic temperature factor is:

$\exp[-2\pi \{h^2a^{*2}U(1,1) + k^2b^{*2}U(2,2) + l^2c^{*2}U(3,3) + 2hka^*b^*U(1,2) + 2hla^*c^*U(1,3)$

$+ 2klb^*c^*U(2,3)\}]$ where a^*, b^*, and c^* are reciprocal lattice constants.

Table of Bond Distances in Angstroms

for $C_{63}H_{50}AlNO_2Si_2, C_7H_8$

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
Si(1)	C(111)	1.8736(19)	C(34)	C(35)	1.361(3)
Si(1)	C(12)	1.8801(18)	C(35)	C(36)	1.384(3)
Si(1)	C(131)	1.8863(19)	C(111)	C(116)	1.392(3)
Si(1)	C(121)	1.8870(18)	C(111)	C(112)	1.396(3)
Si(2)	C(231)	1.8831(18)	C(112)	C(113)	1.385(3)
Si(2)	C(22)	1.8843(18)	C(113)	C(114)	1.392(3)
Si(2)	C(211)	1.8852(18)	C(114)	C(115)	1.379(3)
Si(2)	C(221)	1.8889(19)	C(115)	C(116)	1.381(3)
Al	O(1)	1.7539(13)	C(121)	C(122)	1.388(3)
Al	O(2)	1.7621(12)	C(121)	C(126)	1.395(3)
Al	C(1)	1.9441(19)	C(122)	C(123)	1.393(3)
Al	N(31)	1.9869(15)	C(123)	C(124)	1.377(3)
O(1)	C(11)	1.360(2)	C(124)	C(125)	1.376(4)
O(2)	C(21)	1.361(2)	C(125)	C(126)	1.395(3)
N(31)	C(36)	1.340(2)	C(131)	C(136)	1.393(3)
N(31)	C(32)	1.353(2)	C(131)	C(132)	1.394(3)
C(1)	C(2)	1.507(3)	C(132)	C(133)	1.390(3)
C(11)	C(1A)	1.380(2)	C(133)	C(134)	1.370(3)
C(11)	C(12)	1.441(2)	C(134)	C(135)	1.377(3)
C(12)	C(13)	1.375(2)	C(135)	C(136)	1.389(3)
C(13)	C(14)	1.412(2)	C(211)	C(216)	1.395(2)
C(14)	C(15)	1.416(3)	C(211)	C(212)	1.402(3)
C(14)	C(19)	1.420(2)	C(212)	C(213)	1.391(3)
C(15)	C(16)	1.369(3)	C(213)	C(214)	1.387(3)
C(16)	C(17)	1.397(3)	C(214)	C(215)	1.385(3)
C(17)	C(18)	1.374(3)	C(215)	C(216)	1.387(3)
C(18)	C(19)	1.417(2)	C(221)	C(222)	1.389(3)
C(19)	C(1A)	1.446(2)	C(221)	C(226)	1.400(3)
C(1A)	C(2A)	1.495(2)	C(222)	C(223)	1.390(3)
C(21)	C(2A)	1.393(2)	C(223)	C(224)	1.370(3)
C(21)	C(22)	1.427(2)	C(224)	C(225)	1.369(3)
C(22)	C(23)	1.382(2)	C(225)	C(226)	1.391(3)
C(23)	C(24)	1.419(3)	C(231)	C(232)	1.387(3)
C(24)	C(25)	1.414(3)	C(231)	C(236)	1.402(3)
C(24)	C(29)	1.415(3)	C(232)	C(233)	1.387(3)
C(25)	C(26)	1.352(3)	C(233)	C(234)	1.381(4)
C(26)	C(27)	1.403(3)	C(234)	C(235)	1.372(4)
C(27)	C(28)	1.367(3)	C(235)	C(236)	1.380(3)
C(28)	C(29)	1.424(3)	C(911)	C(912)	1.379(4)
C(29)	C(2A)	1.438(2)	C(911)	C(916)	1.392(4)
C(32)	C(33)	1.376(3)	C(911)	C(917)	1.495(4)
C(33)	C(34)	1.380(3)	C(912)	C(913)	1.382(4)

Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C(913)	C(914)	1.381(4)	C(915)	C(916)	1.373(4)
C(914)	C(915)	1.364(4)			

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Bond Angles in Degrees

for $C_{63}H_{50}AlNO_2Si_2, C_7H_8$

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C(111)	Si(1)	C(12)	108.57(8)	C(11)	C(1A)	C(2A)	123.21(15)
C(111)	Si(1)	C(131)	107.72(8)	C(19)	C(1A)	C(2A)	117.36(15)
C(12)	Si(1)	C(131)	108.83(8)	O(2)	C(21)	C(2A)	120.24(15)
C(111)	Si(1)	C(121)	109.73(8)	O(2)	C(21)	C(22)	117.85(15)
C(12)	Si(1)	C(121)	114.66(7)	C(2A)	C(21)	C(22)	121.90(15)
C(131)	Si(1)	C(121)	107.10(8)	C(23)	C(22)	C(21)	117.58(16)
C(231)	Si(2)	C(22)	109.00(8)	C(23)	C(22)	Si(2)	119.83(13)
C(231)	Si(2)	C(211)	110.25(8)	C(21)	C(22)	Si(2)	122.58(13)
C(22)	Si(2)	C(211)	116.78(7)	C(22)	C(23)	C(24)	122.39(17)
C(231)	Si(2)	C(221)	106.38(8)	C(25)	C(24)	C(29)	118.89(17)
C(22)	Si(2)	C(221)	107.90(8)	C(25)	C(24)	C(23)	122.15(18)
C(211)	Si(2)	C(221)	105.98(8)	C(29)	C(24)	C(23)	118.91(16)
O(1)	Al	O(2)	106.65(6)	C(26)	C(25)	C(24)	121.48(19)
O(1)	Al	C(1)	122.36(8)	C(25)	C(26)	C(27)	120.06(18)
O(2)	Al	C(1)	113.28(7)	C(28)	C(27)	C(26)	120.61(19)
O(1)	Al	N(31)	101.66(6)	C(27)	C(28)	C(29)	120.51(18)
O(2)	Al	N(31)	106.43(6)	C(24)	C(29)	C(28)	118.43(16)
C(1)	Al	N(31)	104.76(7)	C(24)	C(29)	C(2A)	119.56(16)
C(11)	O(1)	Al	124.24(10)	C(28)	C(29)	C(2A)	121.99(16)
C(21)	O(2)	Al	114.17(10)	C(21)	C(2A)	C(29)	118.45(15)
C(36)	N(31)	C(32)	117.18(16)	C(21)	C(2A)	C(1A)	121.96(15)
C(36)	N(31)	Al	121.60(12)	C(29)	C(2A)	C(1A)	119.44(15)
C(32)	N(31)	Al	121.21(13)	N(31)	C(32)	C(33)	122.68(19)
C(2)	C(1)	Al	120.90(14)	C(32)	C(33)	C(34)	118.8(2)
O(1)	C(11)	C(1A)	122.07(15)	C(35)	C(34)	C(33)	119.39(19)
O(1)	C(11)	C(12)	116.59(15)	C(34)	C(35)	C(36)	118.98(19)
C(1A)	C(11)	C(12)	121.34(15)	N(31)	C(36)	C(35)	122.93(18)
C(13)	C(12)	C(11)	118.27(16)	C(116)	C(111)	C(112)	117.14(17)
C(13)	C(12)	Si(1)	120.25(13)	C(116)	C(111)	Si(1)	121.21(14)
C(11)	C(12)	Si(1)	121.31(13)	C(112)	C(111)	Si(1)	121.56(14)
C(12)	C(13)	C(14)	122.61(16)	C(113)	C(112)	C(111)	121.45(19)
C(13)	C(14)	C(15)	121.54(16)	C(112)	C(113)	C(114)	120.0(2)
C(13)	C(14)	C(19)	118.93(16)	C(115)	C(114)	C(113)	119.38(19)
C(15)	C(14)	C(19)	119.52(17)	C(114)	C(115)	C(116)	120.1(2)
C(16)	C(15)	C(14)	121.17(18)	C(115)	C(116)	C(111)	121.94(19)
C(15)	C(16)	C(17)	119.34(17)	C(122)	C(121)	C(126)	116.92(16)
C(18)	C(17)	C(16)	121.24(18)	C(122)	C(121)	Si(1)	121.52(14)
C(17)	C(18)	C(19)	120.85(17)	C(126)	C(121)	Si(1)	121.51(15)
C(18)	C(19)	C(14)	117.84(15)	C(121)	C(122)	C(123)	122.0(2)
C(18)	C(19)	C(1A)	122.89(16)	C(124)	C(123)	C(122)	119.7(2)
C(14)	C(19)	C(1A)	119.25(15)	C(125)	C(124)	C(123)	119.90(18)
C(11)	C(1A)	C(19)	119.40(15)	C(124)	C(125)	C(126)	119.9(2)

Bond Angles (cont.)

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C(121)	C(126)	C(125)	121.6(2)	C(224)	C(223)	C(222)	119.9(2)
C(136)	C(131)	C(132)	116.71(17)	C(225)	C(224)	C(223)	120.3(2)
C(136)	C(131)	Si(1)	123.28(14)	C(224)	C(225)	C(226)	119.9(2)
C(132)	C(131)	Si(1)	119.93(14)	C(225)	C(226)	C(221)	121.3(2)
C(133)	C(132)	C(131)	121.76(19)	C(232)	C(231)	C(236)	117.26(18)
C(134)	C(133)	C(132)	120.2(2)	C(232)	C(231)	Si(2)	123.73(15)
C(133)	C(134)	C(135)	119.46(19)	C(236)	C(231)	Si(2)	118.60(15)
C(134)	C(135)	C(136)	120.4(2)	C(231)	C(232)	C(233)	121.2(2)
C(135)	C(136)	C(131)	121.49(19)	C(234)	C(233)	C(232)	120.2(2)
C(216)	C(211)	C(212)	116.99(17)	C(235)	C(234)	C(233)	119.6(2)
C(216)	C(211)	Si(2)	119.92(14)	C(234)	C(235)	C(236)	120.2(2)
C(212)	C(211)	Si(2)	123.02(14)	C(235)	C(236)	C(231)	121.5(2)
C(213)	C(212)	C(211)	121.15(18)	C(912)	C(911)	C(916)	118.5(3)
C(214)	C(213)	C(212)	120.30(19)	C(912)	C(911)	C(917)	121.9(3)
C(215)	C(214)	C(213)	119.66(18)	C(916)	C(911)	C(917)	119.6(3)
C(214)	C(215)	C(216)	119.56(18)	C(911)	C(912)	C(913)	121.7(3)
C(215)	C(216)	C(211)	122.34(18)	C(914)	C(913)	C(912)	118.4(3)
C(222)	C(221)	C(226)	116.97(18)	C(915)	C(914)	C(913)	120.9(3)
C(222)	C(221)	Si(2)	125.25(15)	C(914)	C(915)	C(916)	120.5(3)
C(226)	C(221)	Si(2)	117.62(15)	C(915)	C(916)	C(911)	120.0(3)
C(221)	C(222)	C(223)	121.6(2)				

Numbers in parentheses are estimated standard deviations in the least significant digits.

$[LiAl(O_2C_{20}H_{10}\{SiPh_3\}_2\text{-}3,3')(NHMe_2)(NMe_2)_2]$ (*S*)-6.

CRYSTALLOGRAPHIC DATA FOR

$C_{62}H_{59}AlLiN_3O_2Si_2$

$C_{62}H_{59}AlLiN_3O_2Si_2$	formula weight 968.27
a = 12.9970(3)Å	space group $P2_12_12_1$ (No. 19)
b = 18.2917(5)Å	T = 150. K
c = 22.4617(7)Å	λ = 0.71073Å
V = 5340.0(4)Å^3	ρ_{calc} = 1.204g cm^{-3}
Z = 4	μ = 0.124mm^{-1}
	transmission coeff = 0.788-0.967
	$R(F_o)^a$ = 0.053
	$R_w(F_o^2)^b$ = 0.131

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[a] $R = \Sigma \; ||F_o| - |F_c|| / \Sigma \; |F_o|$ for $F_o^2 > 2\sigma(F_o^2)$

[b] $R_w = [\Sigma \; w \; (|F_o^2| - |F_c^2|)^2 / \Sigma \; w \; |F_o^2|^2]^{1/2}$

CRYSTAL DATA AND DATA COLLECTION PARAMETERS for

$C_{62}H_{59}AlLiN_3O_2Si_2$

formula	$C_{62}H_{59}AlLiN_3O_2Si_2$
formula weight	968.27
space group	$P2_12_12_1$ (No. 19)
a, Å	12.9970(3)
b, Å	18.2917(5)
c, Å	22.4617(7)
V, Å^3	5340.0(4)
Z	4
d_{calc}, g cm^{-3}	1.204
crystal dimensions, mm	0.43x0.35x0.28
temperature, K	150.
radiation (wavelength)	MO K_α(0.71073Å)
monochromator	graphite
linear abs coef, mm^{-1}	0.124
absorption correction applied	empirical[a]
transmission factors: min, max	0.79, 0.97
diffractometer	Nonius KappaCCD
h, k, l range	-14 to 14 -20 to 20 -24 to 24
2θ range, deg	3.62-45.94
mosaicity, deg	0.41
programs used	SHELXL-97
F_{000}	2048.0
weighting	$1/[\sigma^2(Fo^2)+(0.0786P)^2+1.8437P]$ where $P=(Fo^2+2Fc^2)/3$
data collected	18706
unique data	7311
R_{int}	0.061
data used in refinement	7307
cutoff used in R-factor calculations	$F_o^2>2.0\sigma(F_o^2)$
data with $I>2.0\sigma(I)$	6035
number of variables	646
largest shift/esd in final cycle	0.00
$R(F_o)$	0.053
$R_w(F_o^2)$	0.131
goodness of fit	1.028
absolute structure determination	Flack parameter[b] (-0.1(1))

[a] Otwinowski Z. & Minor, W. Methods Enzymol.,**1996**, 276, 307.
[b] Flack, H. D. Acta Cryst., Sect. A **1983**, A39, 876.

Positional Parameters and Their Estimated Standard Deviations

for $C_{62}H_{59}AlLiN_3O_2Si_2$

Atom	x	y	z	U(Å²)
Si(1)	0.68509(8)	-0.20026(6)	0.41123(5)	0.0335(3)
Si(2)	0.60572(9)	0.20316(6)	0.60819(5)	0.0381(3)
Al	0.61662(12)	0.03761(7)	0.46410(6)	0.0469(4)
O(1)	0.6975(2)	-0.04221(14)	0.46875(12)	0.0412(8)
O(2)	0.6008(2)	0.06450(15)	0.53895(12)	0.0406(8)
N(3)	0.7143(4)	0.0888(2)	0.41993(19)	0.0767(18)
N(4)	0.4905(4)	0.0281(3)	0.43313(19)	0.0740(17)
N(9)	0.9383(5)	-0.0122(4)	0.4704(4)	0.132(3)
C(11)	0.6844(3)	-0.0954(2)	0.51096(17)	0.0337(10)
C(12)	0.6710(3)	-0.1687(2)	0.49034(17)	0.0330(10)
C(13)	0.6479(3)	-0.2206(2)	0.53265(17)	0.0347(10)
C(14)	0.6342(3)	-0.2027(2)	0.59355(17)	0.0350(10)
C(15)	0.6028(3)	-0.2568(2)	0.63558(18)	0.0420(14)
C(16)	0.5887(3)	-0.2389(3)	0.69420(19)	0.0477(15)
C(17)	0.6066(3)	-0.1671(3)	0.71256(19)	0.0477(14)
C(18)	0.6407(3)	-0.1150(3)	0.67442(18)	0.0400(12)
C(19)	0.6551(3)	-0.1314(2)	0.61288(18)	0.0360(10)
C(1A)	0.6878(3)	-0.0770(2)	0.57062(16)	0.0330(10)
C(21)	0.6780(3)	0.0603(2)	0.57927(17)	0.0380(12)
C(22)	0.7019(3)	0.1264(2)	0.61021(17)	0.0347(10)
C(23)	0.7846(3)	0.1273(2)	0.64767(17)	0.0357(10)
C(24)	0.8455(3)	0.0640(2)	0.65764(17)	0.0360(10)
C(25)	0.9334(3)	0.0660(3)	0.69542(18)	0.0410(12)
C(26)	0.9878(3)	0.0044(3)	0.70772(19)	0.0463(14)
C(27)	0.9583(3)	-0.0613(2)	0.68216(19)	0.0433(14)
C(28)	0.8753(3)	-0.0660(2)	0.64515(18)	0.0407(10)
C(29)	0.8151(3)	-0.0034(2)	0.63142(16)	0.0347(10)
C(2A)	0.7265(3)	-0.0047(2)	0.59260(16)	0.0333(10)
C(31)	0.7926(6)	0.1327(4)	0.4505(4)	0.114(3)
C(32)	0.6809(9)	0.1274(4)	0.3645(3)	0.157(4)
C(41)	0.3979(5)	0.0554(4)	0.4616(3)	0.095(2)
C(42)	0.4634(7)	0.0039(6)	0.3753(4)	0.184(5)
C(91)	0.9636(6)	-0.0832(7)	0.4951(4)	0.133(4)
C(92)	1.0292(8)	0.0256(7)	0.4459(8)	0.252(9)
C(111)	0.7665(3)	-0.1388(2)	0.36324(17)	0.0363(10)
C(112)	0.8721(3)	-0.1443(3)	0.3580(2)	0.0533(15)
C(113)	0.9300(4)	-0.0953(3)	0.3245(3)	0.0637(17)
C(114)	0.8822(4)	-0.0408(3)	0.2934(2)	0.0507(15)
C(115)	0.7775(3)	-0.0343(3)	0.2952(2)	0.0473(15)
C(116)	0.7201(3)	-0.0834(3)	0.32907(19)	0.0463(14)
C(121)	0.5574(3)	-0.2084(2)	0.37336(18)	0.0417(12)
C(122)	0.4666(4)	-0.1978(4)	0.4032(2)	0.0720(19)
C(123)	0.3730(4)	-0.2061(5)	0.3748(3)	0.103(3)
C(124)	0.3699(5)	-0.2252(4)	0.3154(3)	0.084(2)

Positional Parameters and Their Estimated Standard Deviations (cont.)

for $C_{62}H_{59}AlLiN_3O_2Si_2$

Atom	x	y	z	U(Å²)
C(125)	0.4573(4)	-0.2357(3)	0.2850(2)	0.0623(17)
C(126)	0.5521(4)	-0.2268(3)	0.3129(2)	0.0527(15)
C(131)	0.7431(3)	-0.2942(2)	0.41631(17)	0.0373(10)
C(132)	0.6889(4)	-0.3558(2)	0.3980(2)	0.0557(15)
C(133)	0.7317(5)	-0.4254(3)	0.4005(3)	0.073(2)
C(134)	0.8293(5)	-0.4343(3)	0.4216(3)	0.074(2)
C(135)	0.8832(4)	-0.3755(3)	0.4413(2)	0.0630(15)
C(136)	0.8415(3)	-0.3058(3)	0.43951(19)	0.0460(15)
C(211)	0.6492(3)	0.2756(2)	0.6617(2)	0.0443(14)
C(212)	0.6470(4)	0.2636(3)	0.7208(2)	0.0627(17)
C(213)	0.6765(4)	0.3155(4)	0.7624(2)	0.0700(19)
C(214)	0.7093(5)	0.3801(3)	0.7462(3)	0.079(2)
C(215)	0.7023(7)	0.3990(4)	0.6874(3)	0.111(3)
C(216)	0.6740(6)	0.3477(3)	0.6451(3)	0.094(2)
C(221)	0.5878(3)	0.2479(2)	0.53362(19)	0.0440(14)
C(222)	0.6646(4)	0.2913(3)	0.5096(2)	0.0663(18)
C(223)	0.6549(6)	0.3301(4)	0.4567(3)	0.090(2)
C(224)	0.5627(6)	0.3244(4)	0.4271(3)	0.097(3)
C(225)	0.4869(6)	0.2842(5)	0.4484(3)	0.112(3)
C(226)	0.4970(5)	0.2440(4)	0.5020(2)	0.083(2)
C(231)	0.4817(3)	0.1670(2)	0.63907(17)	0.0403(14)
C(232)	0.3972(4)	0.2113(3)	0.64583(19)	0.0523(15)
C(233)	0.3054(4)	0.1870(3)	0.6727(2)	0.0620(17)
C(234)	0.3004(4)	0.1172(3)	0.6938(2)	0.0613(17)
C(235)	0.3839(4)	0.0713(3)	0.6891(3)	0.0657(18)
C(236)	0.4717(4)	0.0962(3)	0.6613(2)	0.0540(15)
Li	0.8038(7)	-0.0084(4)	0.4181(4)	0.061(3)

$U_{eq} = (1/3)\Sigma_i\Sigma_j\ U_{ij}a^*_i a^*_j \mathbf{a}_i \cdot \mathbf{a}_j$

Positional Parameters and Their Estimated Standard Deviations

for $C_{62}H_{59}AlLiN_3O_2Si_2$

Atom	x	y	z	U(Å²)
H(9)	0.921	0.016	0.504	0.159
H(13)	0.641	-0.270	0.521	0.042
H(15)	0.591	-0.306	0.623	0.050
H(16)	0.567	-0.275	0.722	0.057
H(17)	0.595	-0.154	0.753	0.057
H(18)	0.655	-0.067	0.689	0.048
H(23)	0.802	0.171	0.668	0.043
H(25)	0.954	0.111	0.712	0.049
H(26)	1.046	0.006	0.734	0.055
H(27)	0.997	-0.104	0.691	0.052
H(28)	0.857	-0.112	0.628	0.049
H(112)	0.906	-0.183	0.378	0.064
H(113)	1.003	-0.100	0.323	0.077
H(114)	0.922	-0.007	0.270	0.061
H(115)	0.744	0.003	0.273	0.057
H(116)	0.647	-0.079	0.329	0.056
H(122)	0.468	-0.185	0.444	0.086
H(123)	0.311	-0.199	0.396	0.124
H(124)	0.305	-0.231	0.296	0.101
H(125)	0.455	-0.249	0.244	0.075
H(126)	0.614	-0.233	0.291	0.063
H(132)	0.621	-0.350	0.383	0.067
H(133)	0.693	-0.467	0.387	0.087
H(134)	0.859	-0.481	0.423	0.088
H(135)	0.951	-0.382	0.456	0.076
H(136)	0.880	-0.266	0.454	0.055
H(212)	0.624	0.217	0.735	0.075
H(213)	0.673	0.304	0.803	0.084
H(214)	0.737	0.413	0.775	0.095
H(215)	0.717	0.448	0.675	0.133
H(216)	0.671	0.361	0.604	0.113
H(222)	0.728	0.295	0.531	0.080
H(223)	0.709	0.359	0.442	0.107
H(224)	0.553	0.350	0.391	0.117
H(225)	0.424	0.282	0.427	0.135
H(226)	0.442	0.215	0.516	0.099
H(232)	0.401	0.260	0.632	0.063
H(233)	0.248	0.219	0.676	0.074
H(234)	0.239	0.100	0.712	0.074
H(235)	0.381	0.023	0.705	0.079
H(236)	0.528	0.064	0.657	0.064
H(31A)	0.849	0.143	0.423	0.170
H(31B)	0.819	0.106	0.485	0.170
H(31C)	0.762	0.179	0.464	0.170

Positional Parameters and Their Estimated Standard Deviations (cont.)

for $C_{62}H_{59}AlLiN_3O_2Si_2$

Atom	x	y	z	U(Å²)
H(32A)	0.647	0.174	0.375	0.236
H(32B)	0.632	0.096	0.343	0.236
H(32C)	0.741	0.138	0.340	0.236
H(41A)	0.370	0.096	0.438	0.142
H(41B)	0.414	0.072	0.502	0.142
H(41C)	0.347	0.016	0.464	0.142
H(42A)	0.432	-0.045	0.378	0.276
H(42B)	0.525	0.002	0.350	0.276
H(42C)	0.414	0.038	0.358	0.276
H(91A)	0.999	-0.113	0.465	0.199
H(91B)	0.900	-0.108	0.507	0.199
H(91C)	1.008	-0.077	0.530	0.199
H(92A)	1.075	0.040	0.479	0.379
H(92B)	1.007	0.069	0.424	0.379
H(92C)	1.066	-0.007	0.419	0.379

Hydrogens included in calculation of structure factors but not refined

Anisotropic Temperature Factor Coefficients - U's

for $C_{62}H_{59}AlLiN_3O_2Si_2$

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Si(1)	0.0388(6)	0.0323(6)	0.0294(6)	-0.0027(5)	-0.0032(5)	-0.0020(5)
Si(2)	0.0510(7)	0.0334(6)	0.0299(6)	0.0038(6)	0.0051(5)	0.0002(5)
Al	0.0741(9)	0.0361(7)	0.0305(7)	0.0090(7)	-0.0037(7)	-0.0006(6)
O(1)	0.0616(18)	0.0309(15)	0.0311(15)	0.0015(14)	0.0040(14)	-0.0018(13)
O(2)	0.0483(17)	0.0420(16)	0.0314(15)	0.0088(14)	-0.0083(13)	-0.0094(13)
N(3)	0.142(5)	0.037(2)	0.051(3)	0.001(3)	0.029(3)	0.006(2)
N(4)	0.104(4)	0.065(3)	0.053(3)	0.032(3)	-0.040(3)	-0.016(2)
N(9)	0.092(5)	0.128(6)	0.177(8)	-0.021(4)	0.011(5)	-0.058(6)
C(11)	0.038(2)	0.032(2)	0.031(2)	0.0026(19)	-0.0004(18)	-0.0009(18)
C(12)	0.032(2)	0.034(2)	0.033(2)	0.0054(18)	-0.0007(17)	-0.0017(19)
C(13)	0.034(2)	0.036(2)	0.034(2)	-0.0025(17)	-0.0038(17)	-0.001(2)
C(14)	0.033(2)	0.040(2)	0.032(2)	-0.0056(18)	0.0005(16)	0.005(2)
C(15)	0.039(2)	0.044(3)	0.043(3)	-0.010(2)	0.000(2)	0.000(2)
C(16)	0.053(3)	0.053(3)	0.037(3)	-0.009(2)	0.003(2)	0.008(2)
C(17)	0.053(3)	0.058(3)	0.032(2)	-0.003(2)	-0.001(2)	-0.001(2)
C(18)	0.046(2)	0.047(3)	0.027(2)	-0.006(2)	0.0020(18)	-0.003(2)
C(19)	0.032(2)	0.037(2)	0.039(2)	0.0033(18)	-0.0008(17)	-0.004(2)
C(1A)	0.034(2)	0.034(2)	0.031(2)	0.0051(18)	0.0005(17)	-0.0039(18)
C(21)	0.044(2)	0.043(3)	0.027(2)	0.002(2)	0.0054(19)	-0.0052(19)
C(22)	0.046(2)	0.032(2)	0.026(2)	0.0009(19)	0.0031(18)	0.0019(18)
C(23)	0.048(2)	0.031(2)	0.028(2)	-0.0014(19)	0.0104(18)	-0.0048(18)
C(24)	0.039(2)	0.040(2)	0.029(2)	-0.0033(19)	0.0079(17)	0.0018(19)
C(25)	0.041(2)	0.051(3)	0.031(2)	-0.006(2)	0.0025(19)	-0.005(2)
C(26)	0.044(3)	0.057(3)	0.038(2)	-0.002(2)	-0.001(2)	-0.002(2)
C(27)	0.043(2)	0.045(3)	0.042(3)	0.008(2)	-0.001(2)	0.001(2)
C(28)	0.048(2)	0.040(2)	0.034(2)	0.001(2)	0.0026(19)	-0.006(2)
C(29)	0.041(2)	0.036(2)	0.027(2)	0.0000(19)	0.0058(19)	-0.0028(18)
C(2A)	0.043(2)	0.033(2)	0.024(2)	-0.0006(18)	0.0017(18)	-0.0034(18)
C(31)	0.154(7)	0.063(4)	0.124(6)	-0.035(5)	0.083(5)	-0.021(4)
C(32)	0.308(13)	0.085(5)	0.079(5)	0.067(7)	0.071(7)	0.047(4)
C(41)	0.076(4)	0.149(6)	0.060(4)	-0.025(4)	0.001(3)	-0.010(4)
C(42)	0.141(7)	0.270(13)	0.141(7)	0.129(8)	-0.096(6)	-0.144(8)
C(91)	0.098(6)	0.211(12)	0.090(6)	0.012(7)	0.005(4)	-0.043(7)
C(92)	0.106(7)	0.190(11)	0.46(3)	-0.082(8)	-0.005(11)	-0.087(15)
C(111)	0.042(2)	0.037(2)	0.030(2)	-0.0037(19)	-0.0032(18)	-0.0058(19)
C(112)	0.042(3)	0.043(3)	0.075(3)	0.004(2)	-0.002(2)	0.015(3)
C(113)	0.040(3)	0.063(3)	0.088(4)	0.000(2)	0.010(3)	0.029(3)
C(114)	0.054(3)	0.048(3)	0.050(3)	-0.006(2)	0.009(2)	0.006(2)
C(115)	0.052(3)	0.050(3)	0.040(3)	-0.001(2)	-0.001(2)	0.011(2)
C(116)	0.042(2)	0.055(3)	0.042(3)	-0.001(2)	-0.005(2)	0.007(2)
C(121)	0.048(2)	0.041(3)	0.036(2)	-0.012(2)	-0.0093(19)	0.009(2)
C(122)	0.043(3)	0.123(5)	0.050(3)	-0.015(3)	-0.006(2)	0.008(3)
C(123)	0.043(3)	0.195(8)	0.071(4)	-0.019(4)	-0.008(3)	0.015(5)
C(124)	0.063(4)	0.108(5)	0.082(4)	-0.027(4)	-0.026(3)	0.030(4)

Anisotropic Temperature Factor Coefficients - U's (Continued)

for $C_{62}H_{59}AlLiN_3O_2Si_2$

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C(125)	0.075(4)	0.061(3)	0.051(3)	-0.023(3)	-0.026(3)	0.010(3)
C(126)	0.061(3)	0.052(3)	0.045(3)	-0.010(2)	-0.015(2)	0.005(2)
C(131)	0.051(2)	0.035(2)	0.026(2)	0.003(2)	0.0036(18)	-0.001(2)
C(132)	0.071(3)	0.044(3)	0.052(3)	-0.002(3)	-0.007(3)	-0.004(2)
C(133)	0.111(5)	0.037(3)	0.071(4)	-0.001(3)	-0.007(3)	-0.014(3)
C(134)	0.104(5)	0.046(3)	0.071(4)	0.026(3)	0.005(4)	-0.004(3)
C(135)	0.065(3)	0.058(3)	0.066(3)	0.020(3)	0.009(3)	0.011(3)
C(136)	0.049(3)	0.038(3)	0.051(3)	0.001(2)	0.000(2)	0.004(2)
C(211)	0.063(3)	0.028(2)	0.042(3)	-0.003(2)	0.005(2)	-0.001(2)
C(212)	0.065(3)	0.082(4)	0.041(3)	-0.022(3)	0.010(2)	-0.003(3)
C(213)	0.073(3)	0.099(5)	0.038(3)	-0.011(3)	0.005(3)	-0.024(3)
C(214)	0.135(6)	0.052(4)	0.051(4)	0.005(4)	-0.008(3)	-0.014(3)
C(215)	0.183(8)	0.062(4)	0.088(5)	-0.045(5)	0.015(5)	-0.018(4)
C(216)	0.149(6)	0.071(4)	0.062(4)	-0.022(4)	0.011(4)	0.002(3)
C(221)	0.054(3)	0.046(3)	0.032(2)	0.011(2)	0.006(2)	0.005(2)
C(222)	0.080(4)	0.072(4)	0.047(3)	-0.004(3)	0.002(3)	0.020(3)
C(223)	0.114(5)	0.092(5)	0.063(4)	0.011(4)	0.021(4)	0.031(4)
C(224)	0.102(5)	0.133(6)	0.057(4)	0.041(5)	0.017(4)	0.043(4)
C(225)	0.088(5)	0.195(9)	0.054(4)	0.026(6)	-0.018(4)	0.036(5)
C(226)	0.079(4)	0.126(6)	0.043(3)	-0.006(4)	0.003(3)	0.018(3)
C(231)	0.051(3)	0.041(3)	0.029(2)	0.006(2)	0.0008(19)	-0.003(2)
C(232)	0.059(3)	0.054(3)	0.044(3)	0.008(3)	0.009(2)	0.011(2)
C(233)	0.049(3)	0.081(4)	0.056(3)	0.007(3)	0.002(2)	0.009(3)
C(234)	0.051(3)	0.073(4)	0.060(3)	-0.020(3)	0.008(2)	-0.010(3)
C(235)	0.075(4)	0.041(3)	0.081(4)	-0.015(3)	0.018(3)	-0.004(3)
C(236)	0.059(3)	0.041(3)	0.062(3)	0.000(2)	0.015(2)	0.000(2)
Li	0.083(6)	0.052(5)	0.048(4)	0.001(4)	0.011(4)	-0.003(4)

The form of the anisotropic temperature factor is:

$\exp[-2\pi (h^2a^{*2}U(1,1) + k^2b^{*2}U(2,2) + l^2c^{*2}U(3,3) + 2hka^*b^*U(1,2) + 2hla^*c^*U(1,3) + 2klb^*c^*U(2,3))]$ where a^*, b^*, and c^* are reciprocal lattice constants.

Table of Bond Distances in Angstroms

for $C_{62}H_{59}AlLiN_3O_2Si_2$

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
Si(1)	C(121)	1.871(4)	C(25)	C(26)	1.360(6)
Si(1)	C(12)	1.877(4)	C(26)	C(27)	1.386(6)
Si(1)	C(131)	1.880(4)	C(27)	C(28)	1.364(6)
Si(1)	C(111)	1.883(4)	C(28)	C(29)	1.421(6)
Si(2)	C(231)	1.876(4)	C(29)	C(2A)	1.445(6)
Si(2)	C(211)	1.877(4)	C(111)	C(112)	1.381(6)
Si(2)	C(221)	1.878(4)	C(111)	C(116)	1.407(6)
Si(2)	C(22)	1.881(4)	C(111)	Li	2.727(9)
Al	O(2)	1.764(3)	C(112)	C(113)	1.391(6)
Al	N(4)	1.790(5)	C(113)	C(114)	1.368(6)
Al	O(1)	1.802(3)	C(114)	C(115)	1.366(6)
Al	N(3)	1.864(5)	C(115)	C(116)	1.394(6)
Al	Li	2.774(9)	C(116)	Li	2.657(10)
O(1)	C(11)	1.369(5)	C(121)	C(122)	1.371(6)
O(1)	Li	1.893(9)	C(121)	C(126)	1.400(6)
O(2)	C(21)	1.354(5)	C(122)	C(123)	1.382(7)
N(3)	C(31)	1.467(9)	C(123)	C(124)	1.381(9)
N(3)	C(32)	1.496(8)	C(124)	C(125)	1.340(8)
N(3)	Li	2.126(10)	C(125)	C(126)	1.391(7)
N(4)	C(42)	1.416(7)	C(131)	C(132)	1.392(6)
N(4)	C(41)	1.452(8)	C(131)	C(136)	1.397(6)
N(9)	C(91)	1.449(11)	C(132)	C(133)	1.391(7)
N(9)	C(92)	1.475(13)	C(133)	C(134)	1.364(8)
N(9)	Li	2.108(12)	C(134)	C(135)	1.357(8)
C(11)	C(1A)	1.383(5)	C(135)	C(136)	1.386(7)
C(11)	C(12)	1.429(6)	C(211)	C(212)	1.346(6)
C(12)	C(13)	1.377(5)	C(211)	C(216)	1.407(7)
C(13)	C(14)	1.418(6)	C(212)	C(213)	1.385(7)
C(14)	C(19)	1.400(6)	C(213)	C(214)	1.308(8)
C(14)	C(15)	1.428(6)	C(214)	C(215)	1.369(9)
C(15)	C(16)	1.369(6)	C(215)	C(216)	1.385(9)
C(16)	C(17)	1.397(7)	C(221)	C(226)	1.378(7)
C(17)	C(18)	1.356(6)	C(221)	C(222)	1.386(7)
C(18)	C(19)	1.427(6)	C(222)	C(223)	1.390(8)
C(19)	C(1A)	1.440(6)	C(223)	C(224)	1.374(10)
C(1A)	C(2A)	1.498(5)	C(224)	C(225)	1.318(10)
C(21)	C(2A)	1.378(6)	C(225)	C(226)	1.418(8)
C(21)	C(22)	1.428(6)	C(231)	C(232)	1.374(6)
C(22)	C(23)	1.364(6)	C(231)	C(236)	1.393(6)
C(23)	C(24)	1.420(6)	C(232)	C(233)	1.410(7)
C(24)	C(29)	1.421(6)	C(233)	C(234)	1.363(7)
C(24)	C(25)	1.424(6)	C(234)	C(235)	1.376(7)

Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C(235)	C(236)	1.378(7)	Li	N(9)	2.108(12)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Bond Angles in Degrees

for $C_{62}H_{59}AlLiN_3O_2Si_2$

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C(121)	Si(1)	C(12)	111.62(18)	C(13)	C(12)	Si(1)	117.5(3)
C(121)	Si(1)	C(131)	108.10(19)	C(11)	C(12)	Si(1)	125.7(3)
C(12)	Si(1)	C(131)	105.24(17)	C(12)	C(13)	C(14)	122.2(4)
C(121)	Si(1)	C(111)	106.61(18)	C(19)	C(14)	C(13)	119.4(4)
C(12)	Si(1)	C(111)	114.40(18)	C(19)	C(14)	C(15)	119.7(4)
C(131)	Si(1)	C(111)	110.78(18)	C(13)	C(14)	C(15)	120.9(4)
C(231)	Si(2)	C(211)	105.75(19)	C(16)	C(15)	C(14)	120.6(4)
C(231)	Si(2)	C(221)	112.14(19)	C(15)	C(16)	C(17)	119.1(4)
C(211)	Si(2)	C(221)	107.5(2)	C(18)	C(17)	C(16)	121.9(4)
C(231)	Si(2)	C(22)	107.38(18)	C(17)	C(18)	C(19)	120.5(4)
C(211)	Si(2)	C(22)	108.15(19)	C(14)	C(19)	C(18)	118.1(4)
C(221)	Si(2)	C(22)	115.40(18)	C(14)	C(19)	C(1A)	119.8(4)
O(2)	Al	N(4)	106.90(19)	C(18)	C(19)	C(1A)	122.1(4)
O(2)	Al	O(1)	103.82(14)	C(11)	C(1A)	C(19)	117.4(4)
N(4)	Al	O(1)	118.57(19)	C(11)	C(1A)	C(2A)	123.1(4)
O(2)	Al	N(3)	116.53(19)	C(19)	C(1A)	C(2A)	119.5(3)
N(4)	Al	N(3)	117.8(2)	O(2)	C(21)	C(2A)	122.3(4)
O(1)	Al	N(3)	92.32(18)	O(2)	C(21)	C(22)	116.0(4)
O(2)	Al	Li	122.8(2)	C(2A)	C(21)	C(22)	121.6(4)
N(4)	Al	Li	129.0(2)	C(23)	C(22)	C(21)	118.8(4)
O(1)	Al	Li	42.6(2)	C(23)	C(22)	Si(2)	121.9(3)
N(3)	Al	Li	50.0(2)	C(21)	C(22)	Si(2)	118.4(3)
C(11)	O(1)	Al	122.9(2)	C(22)	C(23)	C(24)	121.8(4)
C(11)	O(1)	Li	137.7(4)	C(23)	C(24)	C(29)	119.1(4)
Al	O(1)	Li	97.3(3)	C(23)	C(24)	C(25)	121.4(4)
C(21)	O(2)	Al	122.3(2)	C(29)	C(24)	C(25)	119.5(4)
C(31)	N(3)	C(32)	109.5(6)	C(26)	C(25)	C(24)	121.2(4)
C(31)	N(3)	Al	119.8(4)	C(25)	C(26)	C(27)	119.4(4)
C(32)	N(3)	Al	118.8(6)	C(28)	C(27)	C(26)	121.7(4)
C(31)	N(3)	Li	95.0(5)	C(27)	C(28)	C(29)	121.1(4)
C(32)	N(3)	Li	122.5(4)	C(28)	C(29)	C(24)	117.2(4)
Al	N(3)	Li	87.8(3)	C(28)	C(29)	C(2A)	123.8(4)
C(42)	N(4)	C(41)	107.8(5)	C(24)	C(29)	C(2A)	119.0(3)
C(42)	N(4)	Al	127.9(5)	C(21)	C(2A)	C(29)	118.8(3)
C(41)	N(4)	Al	123.7(3)	C(21)	C(2A)	C(1A)	122.4(3)
C(91)	N(9)	C(92)	112.4(9)	C(29)	C(2A)	C(1A)	118.7(3)
C(91)	N(9)	Li	115.5(6)	C(112)	C(111)	C(116)	115.6(4)
C(92)	N(9)	Li	116.2(9)	C(112)	C(111)	Si(1)	124.3(3)
O(1)	C(11)	C(1A)	119.6(3)	C(116)	C(111)	Si(1)	120.1(3)
O(1)	C(11)	C(12)	117.2(3)	C(112)	C(111)	Li	85.7(3)
C(1A)	C(11)	C(12)	123.2(4)	C(116)	C(111)	Li	72.1(3)
C(13)	C(12)	C(11)	116.8(3)	Si(1)	C(111)	Li	111.3(2)

Bond Angles (cont.)

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C(111)	C(112)	C(113)	122.4(4)	C(226)	C(221)	C(222)	116.5(4)
C(114)	C(113)	C(112)	120.1(4)	C(226)	C(221)	Si(2)	122.9(4)
C(115)	C(114)	C(113)	120.0(4)	C(222)	C(221)	Si(2)	120.5(4)
C(114)	C(115)	C(116)	119.5(5)	C(221)	C(222)	C(223)	124.1(6)
C(115)	C(116)	C(111)	122.2(4)	C(224)	C(223)	C(222)	116.9(6)
C(115)	C(116)	Li	81.9(3)	C(225)	C(224)	C(223)	121.3(6)
C(111)	C(116)	Li	77.6(3)	C(224)	C(225)	C(226)	121.8(6)
C(122)	C(121)	C(126)	117.7(4)	C(221)	C(226)	C(225)	119.4(6)
C(122)	C(121)	Si(1)	122.0(3)	C(232)	C(231)	C(236)	115.8(4)
C(126)	C(121)	Si(1)	120.3(3)	C(232)	C(231)	Si(2)	121.3(3)
C(121)	C(122)	C(123)	121.2(5)	C(236)	C(231)	Si(2)	122.7(3)
C(124)	C(123)	C(122)	119.9(6)	C(231)	C(232)	C(233)	122.5(5)
C(125)	C(124)	C(123)	120.3(5)	C(234)	C(233)	C(232)	119.0(5)
C(124)	C(125)	C(126)	120.3(5)	C(233)	C(234)	C(235)	120.5(5)
C(125)	C(126)	C(121)	120.6(5)	C(234)	C(235)	C(236)	119.1(5)
C(132)	C(131)	C(136)	116.8(4)	C(235)	C(236)	C(231)	123.1(5)
C(132)	C(131)	Si(1)	121.2(3)	O(1)	Li	N(9)	105.0(4)
C(136)	C(131)	Si(1)	121.9(3)	O(1)	Li	N(3)	82.1(4)
C(133)	C(132)	C(131)	121.8(5)	N(9)	Li	N(3)	118.0(5)
C(134)	C(133)	C(132)	119.6(5)	O(1)	Li	C(116)	89.2(4)
C(135)	C(134)	C(133)	120.0(5)	N(9)	Li	C(116)	137.9(4)
C(134)	C(135)	C(136)	121.1(5)	N(3)	Li	C(116)	102.9(4)
C(135)	C(136)	C(131)	120.6(5)	O(1)	Li	C(111)	81.8(3)
C(212)	C(211)	C(216)	114.8(5)	N(9)	Li	C(111)	111.8(4)
C(212)	C(211)	Si(2)	120.7(4)	N(3)	Li	C(111)	130.1(4)
C(216)	C(211)	Si(2)	124.1(4)	C(116)	Li	C(111)	30.25(16)
C(211)	C(212)	C(213)	123.1(5)	O(1)	Li	Al	40.14(19)
C(214)	C(213)	C(212)	121.5(5)	N(9)	Li	Al	122.0(4)
C(213)	C(214)	C(215)	118.4(6)	N(3)	Li	Al	42.2(2)
C(214)	C(215)	C(216)	120.5(6)	C(116)	Li	Al	94.5(3)
C(215)	C(216)	C(211)	120.9(6)	C(111)	Li	Al	106.2(3)

Numbers in parentheses are estimated standard deviations in the least significant digits.

$[LiAl(O_2C_{20}H_{10}\{SiPh_3\}_2\text{-}3,3')(NC_5H_5)(NMe_2)_2]$ (*S*)-7.

CRYSTALLOGRAPHIC DATA FOR

$C_{65}H_{57}AlLiN_3O_2Si_2$

$C_{65}H_{57}AlLiN_3O_2Si_2$	formula weight 1002.29
a = 13.3931(4)Å	space group $P2_12_12_1$ (No. 19)
b = 18.2342(6)Å	T = 150. K
c = 22.4204(9)Å	λ = 0.71073Å
V = 5475.3(3)Å^3	ρ_{calc} = 1.216g cm^{-3}
Z = 4	μ = 0.123mm^{-1}
	transmission coeff = 0.888-0.988
	$R(F_o)^a$ = 0.055
	$R_w(F_o^2)^b$ = 0.124

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[a] $R = \Sigma \; ||F_o| - |F_c|| / \Sigma \; |F_o|$ for $F_o^2 > 2\sigma(F_o^2)$

[b] $R_w = [\Sigma \; w \; (|F_o^2| - |F_c^2|)^2 / \Sigma \; w \; |F_o^2|^2]^{1/2}$

CRYSTAL DATA AND DATA COLLECTION PARAMETERS for

$C_{65}H_{57}AlLiN_3O_2Si_2$

formula	$C_{65}H_{57}AlLiN_3O_2Si_2$
formula weight	1002.29
space group	$P2_12_12_1$ (No. 19)
a, Å	13.3931(4)
b, Å	18.2342(6)
c, Å	22.4204(9)
V, Å^3	5475.3(3)
Z	4
d_{calc}, g cm^{-3}	1.216
crystal dimensions, mm	0.25x0.23x0.10
temperature, K	150.
radiation (wavelength)	MO K_α(0.71073Å)
monochromator	graphite
linear abs coef, mm^{-1}	0.123
absorption correction applied	empirical[a]
transmission factors: min, max	0.89, 0.99
diffractometer	Nonius KappaCCD
h, k, l range	-14 to 14 -19 to 19 -24 to 24
2θ range, deg	6.48-44.97
mosaicity, deg	0.67
programs used	SHELXL-97
F_{000}	2112.0
weighting	
$1/[\sigma^2(Fo^2)+(0.0207P)^2+6.2623P]$ where $P=(Fo^2+2Fc^2)/3$	
data collected	13096
unique data	6988
R_{int}	0.072
data used in refinement	6981
cutoff used in R-factor calculations	$F_o^2>2.0\sigma(F_o^2)$
data with $I>2.0\sigma(I)$	6093
number of variables	671
largest shift/esd in final cycle	0.00
$R(F_o)$	0.055
$R_w(F_o^2)$	0.124
goodness of fit	1.085
absolute structure determination	Flack parameter[b] (0.0(2))

[a] Otwinowski Z. & Minor, W. Methods Enzymol.,**1996**, 276, 307.
[b] Flack, H. D. Acta Cryst., Sect. A **1983**, A39, 876.

Positional Parameters and Their Estimated Standard Deviations

for $C_{65}H_{57}AlLiN_3O_2Si_2$

Atom	x	y	z	U(Å²)
Si(1)	0.91934(10)	1.19030(7)	0.89726(6)	0.0354(4)
Si(2)	0.78819(10)	0.79613(7)	1.09736(5)	0.0301(3)
Al	0.87485(10)	1.02962(7)	1.04028(6)	0.0323(4)
O(1)	0.9075(2)	1.04537(16)	0.96505(13)	0.0335(9)
O(2)	0.7875(2)	0.95388(15)	1.03518(13)	0.0298(8)
N(3)	0.9878(3)	1.0142(2)	1.08108(16)	0.0397(12)
N(4)	0.7809(3)	1.0904(2)	1.07515(17)	0.0433(12)
N(911)	0.5460(3)	0.9929(2)	1.0559(2)	0.0487(15)
C(11)	0.8349(3)	1.0483(2)	0.92294(18)	0.0287(14)
C(12)	0.8233(3)	1.1161(2)	0.89205(19)	0.0300(12)
C(13)	0.7430(3)	1.1217(3)	0.8530(2)	0.0340(15)
C(14)	0.6739(3)	1.0638(2)	0.84370(19)	0.0307(14)
C(15)	0.5892(4)	1.0718(3)	0.8066(2)	0.0363(15)
C(16)	0.5248(4)	1.0154(3)	0.7981(2)	0.0403(15)
C(17)	0.5411(4)	0.9481(3)	0.8249(2)	0.0403(15)
C(18)	0.6231(3)	0.9380(3)	0.86095(19)	0.0337(15)
C(19)	0.6921(3)	0.9950(2)	0.87214(18)	0.0293(14)
C(1A)	0.7775(3)	0.9872(2)	0.91027(18)	0.0280(12)
C(21)	0.7997(3)	0.8977(2)	0.99517(19)	0.0290(15)
C(22)	0.8067(3)	0.8254(2)	1.01770(19)	0.0303(15)
C(23)	0.8252(3)	0.7698(2)	0.9765(2)	0.0327(14)
C(24)	0.8377(3)	0.7831(2)	0.9152(2)	0.0300(12)
C(25)	0.8618(3)	0.7261(3)	0.8743(2)	0.0360(15)
C(26)	0.8717(4)	0.7400(3)	0.8153(2)	0.0410(15)
C(27)	0.8598(4)	0.8112(3)	0.7941(2)	0.0407(15)
C(28)	0.8380(3)	0.8684(2)	0.8321(2)	0.0333(15)
C(29)	0.8256(3)	0.8554(2)	0.8936(2)	0.0290(12)
C(2A)	0.8005(3)	0.9139(2)	0.93450(19)	0.0290(14)
C(31)	0.9989(4)	1.0082(3)	1.1453(2)	0.0553(17)
C(32)	1.0846(4)	1.0048(3)	1.0526(2)	0.0580(17)
C(41)	0.8056(5)	1.1402(3)	1.1254(3)	0.071(2)
C(42)	0.7095(4)	1.1293(3)	1.0346(3)	0.0553(17)
C(111)	0.9477(4)	1.2299(3)	0.9733(2)	0.0457(17)
C(112)	1.0071(4)	1.1905(3)	1.0131(2)	0.0560(17)
C(113)	1.0340(5)	1.2208(4)	1.0682(3)	0.069(2)
C(114)	1.0054(6)	1.2903(4)	1.0828(3)	0.072(2)
C(115)	0.9508(6)	1.3283(3)	1.0450(3)	0.072(2)
C(116)	0.9191(5)	1.2994(3)	0.9897(2)	0.0567(17)
C(121)	1.0388(4)	1.1538(3)	0.8651(2)	0.0383(15)
C(122)	1.0401(4)	1.0948(3)	0.8262(2)	0.0467(15)
C(123)	1.1263(4)	1.0726(3)	0.7982(2)	0.0480(17)
C(124)	1.2138(5)	1.1078(3)	0.8069(3)	0.057(2)
C(125)	1.2169(5)	1.1647(4)	0.8464(4)	0.080(2)
C(126)	1.1308(4)	1.1890(3)	0.8735(3)	0.071(2)

Positional Parameters and Their Estimated Standard Deviations (cont.)

for $C_{65}H_{57}AlLiN_3O_2Si_2$

Atom	x	y	z	U(Å²)
C(131)	0.8735(4)	1.2662(2)	0.8484(2)	0.0353(14)
C(132)	0.9206(4)	1.2867(3)	0.7960(2)	0.0503(15)
C(133)	0.8842(5)	1.3401(3)	0.7589(3)	0.062(2)
C(134)	0.7996(5)	1.3776(3)	0.7737(3)	0.0570(17)
C(135)	0.7503(5)	1.3591(3)	0.8253(3)	0.0553(18)
C(136)	0.7860(4)	1.3047(3)	0.8617(2)	0.0460(15)
C(211)	0.7209(3)	0.7060(2)	1.09377(19)	0.0310(14)
C(212)	0.6286(4)	0.6994(3)	1.0649(2)	0.0383(15)
C(213)	0.5773(4)	0.6343(3)	1.0640(2)	0.0440(15)
C(214)	0.6142(4)	0.5740(3)	1.0911(2)	0.0493(17)
C(215)	0.7072(5)	0.5769(3)	1.1181(2)	0.0523(17)
C(216)	0.7596(4)	0.6428(3)	1.1199(2)	0.0403(15)
C(221)	0.9109(3)	0.7829(3)	1.1363(2)	0.0367(15)
C(222)	0.9132(4)	0.7628(3)	1.1961(2)	0.0467(15)
C(223)	1.0037(5)	0.7518(3)	1.2256(3)	0.065(2)
C(224)	1.0920(5)	0.7614(4)	1.1958(4)	0.076(3)
C(225)	1.0909(5)	0.7815(4)	1.1371(4)	0.081(3)
C(226)	1.0012(4)	0.7927(3)	1.1078(3)	0.0560(18)
C(231)	0.7138(3)	0.8628(2)	1.14398(19)	0.0317(14)
C(232)	0.7625(4)	0.9197(3)	1.1728(2)	0.0387(15)
C(233)	0.7115(4)	0.9729(3)	1.2049(2)	0.0437(15)
C(234)	0.6094(4)	0.9689(3)	1.2096(2)	0.0477(17)
C(235)	0.5591(4)	0.9108(3)	1.1842(3)	0.0527(18)
C(236)	0.6108(4)	0.8580(3)	1.1515(2)	0.0457(15)
C(911)	0.4637(4)	1.0229(3)	1.0800(3)	0.060(2)
C(913)	0.3688(5)	1.0067(3)	1.0614(3)	0.065(2)
C(914)	0.3562(4)	0.9603(4)	1.0135(3)	0.068(2)
C(915)	0.4399(4)	0.9307(4)	0.9878(3)	0.062(2)
C(916)	0.5318(4)	0.9481(3)	1.0093(2)	0.0563(17)
Li	0.6880(6)	0.9982(4)	1.0854(4)	0.040(2)

$U_{eq} = (1/3)\Sigma_i\Sigma_j\ U_{ij}a^*_i a^*_j \mathbf{a}_i \cdot \mathbf{a}_j$

Positional Parameters and Their Estimated Standard Deviations

for $C_{65}H_{57}AlLiN_3O_2Si_2$

Atom	x	y	z	U(Å²)
H(13)	0.734	1.166	0.832	0.041
H(15)	0.577	1.117	0.787	0.044
H(16)	0.468	1.022	0.773	0.048
H(17)	0.496	0.909	0.818	0.049
H(18)	0.634	0.891	0.879	0.040
H(23)	0.830	0.721	0.990	0.040
H(25)	0.871	0.678	0.889	0.043
H(26)	0.887	0.701	0.788	0.049
H(27)	0.867	0.821	0.753	0.049
H(28)	0.831	0.917	0.817	0.040
H(112)	1.030	1.143	1.003	0.067
H(113)	1.072	1.193	1.096	0.083
H(114)	1.025	1.311	1.120	0.087
H(115)	0.932	1.377	1.055	0.086
H(116)	0.878	1.328	0.964	0.068
H(122)	0.980	1.069	0.819	0.056
H(123)	1.124	1.031	0.772	0.058
H(124)	1.272	1.093	0.786	0.068
H(125)	1.279	1.188	0.855	0.096
H(126)	1.134	1.231	0.899	0.086
H(132)	0.981	1.263	0.785	0.060
H(133)	0.918	1.351	0.723	0.074
H(134)	0.775	1.416	0.749	0.068
H(135)	0.691	1.384	0.836	0.066
H(136)	0.750	1.293	0.897	0.055
H(212)	0.601	0.741	1.045	0.046
H(213)	0.515	0.632	1.044	0.053
H(214)	0.577	0.530	1.092	0.059
H(215)	0.735	0.534	1.135	0.063
H(216)	0.823	0.645	1.139	0.049
H(222)	0.852	0.757	1.217	0.056
H(223)	1.004	0.737	1.266	0.078
H(224)	1.154	0.754	1.216	0.091
H(225)	1.152	0.788	1.116	0.097
H(226)	1.002	0.807	1.067	0.067
H(232)	0.833	0.922	1.171	0.047
H(233)	0.747	1.012	1.224	0.052
H(234)	0.574	1.006	1.230	0.057
H(235)	0.489	0.907	1.189	0.063
H(236)	0.575	0.818	1.134	0.055
H(31A)	1.029	0.961	1.155	0.083
H(31B)	0.933	1.012	1.164	0.083
H(31C)	1.042	1.048	1.160	0.083
H(32A)	1.130	1.043	1.066	0.087

Positional Parameters and Their Estimated Standard Deviations (cont.)

for $C_{65}H_{57}AlLiN_3O_2Si_2$

Atom	x	y	z	U(Å²)
H(32B)	1.077	1.008	1.009	0.087
H(32C)	1.112	0.957	1.063	0.087
H(41A)	0.828	1.188	1.110	0.106
H(41B)	0.859	1.118	1.150	0.106
H(41C)	0.746	1.148	1.150	0.106
H(42A)	0.649	1.143	1.057	0.083
H(42B)	0.691	1.097	1.001	0.083
H(42C)	0.741	1.174	1.019	0.083
H(911)	0.472	1.057	1.112	0.071
H(913)	0.313	1.027	1.081	0.078
H(914)	0.292	0.949	0.999	0.081
H(915)	0.434	0.898	0.955	0.075
H(916)	0.589	0.928	0.990	0.067

Hydrogens included in calculation of structure factors but not refined

Anisotropic Temperature Factor Coefficients - U's

for $C_{65}H_{57}AlLiN_3O_2Si_2$

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Si(1)	0.0395(8)	0.0241(7)	0.0427(8)	-0.0056(6)	0.0044(6)	-0.0035(6)
Si(2)	0.0273(7)	0.0256(7)	0.0374(7)	0.0003(6)	0.0011(6)	-0.0016(6)
Al	0.0337(8)	0.0244(7)	0.0389(8)	-0.0028(6)	-0.0025(7)	-0.0059(6)
O(1)	0.0341(18)	0.0294(17)	0.0370(17)	-0.0038(14)	-0.0033(15)	-0.0045(14)
O(2)	0.0307(17)	0.0213(16)	0.0375(16)	-0.0010(14)	0.0009(14)	-0.0072(14)
N(3)	0.033(2)	0.046(3)	0.040(2)	-0.0045(19)	-0.0059(19)	-0.0085(19)
N(4)	0.053(3)	0.031(2)	0.046(2)	0.001(2)	0.000(2)	-0.0156(19)
N(911)	0.037(3)	0.046(3)	0.063(3)	0.000(2)	-0.001(2)	-0.006(2)
C(11)	0.029(3)	0.028(3)	0.029(2)	0.002(2)	0.001(2)	-0.007(2)
C(12)	0.036(3)	0.023(2)	0.031(2)	0.000(2)	0.004(2)	-0.0063(19)
C(13)	0.039(3)	0.027(3)	0.036(3)	0.001(2)	0.005(2)	-0.004(2)
C(14)	0.035(3)	0.027(3)	0.030(2)	0.005(2)	0.003(2)	-0.004(2)
C(15)	0.039(3)	0.035(3)	0.035(3)	0.008(2)	-0.001(2)	-0.004(2)
C(16)	0.034(3)	0.046(3)	0.041(3)	0.007(3)	-0.008(2)	-0.008(2)
C(17)	0.031(3)	0.039(3)	0.051(3)	-0.007(2)	-0.001(2)	-0.016(2)
C(18)	0.031(3)	0.035(3)	0.035(3)	0.003(2)	0.002(2)	-0.005(2)
C(19)	0.029(3)	0.028(3)	0.031(2)	0.002(2)	0.004(2)	-0.0068(19)
C(1A)	0.030(3)	0.024(2)	0.030(2)	-0.002(2)	0.003(2)	-0.0024(19)
C(21)	0.025(3)	0.026(3)	0.036(3)	-0.002(2)	0.001(2)	-0.005(2)
C(22)	0.025(3)	0.024(3)	0.042(3)	0.003(2)	0.002(2)	-0.004(2)
C(23)	0.027(3)	0.022(2)	0.049(3)	0.002(2)	0.005(2)	-0.002(2)
C(24)	0.024(2)	0.024(2)	0.042(3)	0.0002(19)	0.003(2)	-0.005(2)
C(25)	0.032(3)	0.026(3)	0.050(3)	0.005(2)	0.006(2)	-0.011(2)
C(26)	0.040(3)	0.036(3)	0.047(3)	0.010(2)	0.003(2)	-0.021(2)
C(27)	0.046(3)	0.037(3)	0.039(3)	0.007(3)	0.007(2)	-0.008(2)
C(28)	0.033(3)	0.025(3)	0.042(3)	-0.001(2)	0.002(2)	-0.003(2)
C(29)	0.019(2)	0.026(2)	0.042(3)	-0.0014(19)	0.001(2)	-0.004(2)
C(2A)	0.026(3)	0.022(2)	0.039(3)	-0.003(2)	0.000(2)	-0.0050(19)
C(31)	0.046(3)	0.071(4)	0.049(3)	-0.015(3)	-0.005(3)	0.000(3)
C(32)	0.045(3)	0.076(4)	0.053(3)	0.002(3)	-0.005(3)	-0.020(3)
C(41)	0.070(4)	0.052(4)	0.090(5)	-0.008(3)	0.010(4)	-0.039(3)
C(42)	0.053(3)	0.043(3)	0.070(4)	0.007(3)	0.010(3)	-0.004(3)
C(111)	0.059(4)	0.033(3)	0.045(3)	-0.011(3)	0.005(3)	-0.003(2)
C(112)	0.050(3)	0.058(4)	0.060(3)	-0.008(3)	-0.010(3)	-0.012(3)
C(113)	0.071(4)	0.076(5)	0.060(4)	-0.031(4)	-0.019(3)	-0.004(3)
C(114)	0.088(5)	0.072(5)	0.057(4)	-0.034(4)	-0.009(4)	-0.016(4)
C(115)	0.107(6)	0.049(4)	0.059(4)	-0.005(4)	0.002(4)	-0.026(3)
C(116)	0.077(4)	0.037(3)	0.056(3)	0.000(3)	0.000(3)	-0.015(3)
C(121)	0.041(3)	0.030(3)	0.044(3)	-0.003(2)	0.000(2)	0.001(2)
C(122)	0.052(3)	0.035(3)	0.053(3)	-0.004(3)	-0.004(3)	-0.005(3)
C(123)	0.050(4)	0.037(3)	0.057(3)	0.014(3)	0.003(3)	-0.002(2)
C(124)	0.044(4)	0.046(4)	0.080(4)	0.007(3)	0.011(3)	0.000(3)
C(125)	0.037(4)	0.062(4)	0.141(6)	-0.012(3)	0.016(4)	-0.028(4)
C(126)	0.042(4)	0.050(4)	0.122(5)	-0.011(3)	0.011(4)	-0.037(4)

Anisotropic Temperature Factor Coefficients - U's (Continued)

for $C_{65}H_{57}AlLiN_3O_2Si_2$

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C(131)	0.044(3)	0.021(2)	0.041(3)	-0.005(2)	0.005(2)	-0.008(2)
C(132)	0.050(3)	0.042(3)	0.059(3)	0.002(3)	0.009(3)	0.002(3)
C(133)	0.062(4)	0.058(4)	0.066(4)	0.008(3)	0.013(3)	0.021(3)
C(134)	0.072(4)	0.040(3)	0.059(3)	0.009(3)	0.000(3)	0.010(3)
C(135)	0.060(4)	0.042(3)	0.064(4)	0.009(3)	0.002(3)	-0.008(3)
C(136)	0.054(3)	0.035(3)	0.049(3)	0.002(3)	0.009(3)	-0.001(2)
C(211)	0.033(3)	0.026(3)	0.034(2)	0.000(2)	0.004(2)	-0.002(2)
C(212)	0.028(3)	0.037(3)	0.050(3)	0.001(2)	0.001(2)	-0.006(2)
C(213)	0.033(3)	0.043(3)	0.056(3)	-0.006(3)	0.002(2)	-0.013(3)
C(214)	0.059(4)	0.039(3)	0.050(3)	-0.022(3)	0.010(3)	-0.009(3)
C(215)	0.084(4)	0.024(3)	0.049(3)	-0.007(3)	0.005(3)	-0.001(2)
C(216)	0.045(3)	0.033(3)	0.043(3)	-0.002(2)	0.001(2)	0.003(2)
C(221)	0.028(3)	0.030(3)	0.052(3)	0.004(2)	-0.004(2)	-0.009(2)
C(222)	0.047(3)	0.040(3)	0.053(3)	0.014(3)	-0.011(3)	-0.011(2)
C(223)	0.077(5)	0.050(4)	0.068(4)	0.025(3)	-0.026(4)	-0.021(3)
C(224)	0.049(4)	0.067(5)	0.111(6)	0.018(3)	-0.034(4)	-0.028(4)
C(225)	0.030(4)	0.091(5)	0.123(7)	0.014(3)	-0.006(4)	-0.023(5)
C(226)	0.036(3)	0.064(4)	0.068(4)	-0.003(3)	0.001(3)	-0.009(3)
C(231)	0.029(3)	0.032(3)	0.034(2)	-0.003(2)	0.002(2)	0.000(2)
C(232)	0.037(3)	0.036(3)	0.043(3)	0.004(2)	-0.004(2)	-0.007(2)
C(233)	0.054(3)	0.034(3)	0.043(3)	-0.003(3)	0.001(3)	-0.004(2)
C(234)	0.051(4)	0.038(3)	0.054(3)	-0.005(3)	0.015(3)	-0.010(3)
C(235)	0.035(3)	0.050(4)	0.073(4)	0.000(3)	0.013(3)	-0.009(3)
C(236)	0.037(3)	0.043(3)	0.057(3)	0.000(2)	0.005(3)	-0.010(3)
C(911)	0.044(4)	0.059(4)	0.076(4)	0.010(3)	-0.004(3)	-0.023(3)
C(913)	0.040(4)	0.061(4)	0.094(5)	0.012(3)	-0.001(3)	-0.020(3)
C(914)	0.034(3)	0.091(5)	0.078(4)	-0.002(3)	-0.008(3)	-0.015(4)
C(915)	0.041(4)	0.079(4)	0.067(4)	-0.011(3)	0.001(3)	-0.027(3)
C(916)	0.041(3)	0.074(4)	0.054(3)	-0.004(3)	0.008(3)	-0.021(3)
Li	0.040(5)	0.032(4)	0.049(5)	-0.003(4)	0.011(4)	-0.013(4)

The form of the anisotropic temperature factor is:

$\exp[-2\pi \{h^2a^{*2}U(1,1) + k^2b^{*2}U(2,2) + l^2c^{*2}U(3,3) + 2hka^*b^*U(1,2) + 2hla^*c^*U(1,3) + 2klb^*c^*U(2,3)\}]$ where a^*, b^*, and c^* are reciprocal lattice constants.

Table of Bond Distances in Angstroms

for $C_{65}H_{57}AlLiN_3O_2Si_2$

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
Si(1)	C(131)	1.869(5)	C(25)	C(26)	1.353(7)
Si(1)	C(12)	1.871(5)	C(26)	C(27)	1.393(7)
Si(1)	C(121)	1.876(5)	C(27)	C(28)	1.376(6)
Si(1)	C(111)	1.889(5)	C(28)	C(29)	1.410(6)
Si(2)	C(211)	1.876(4)	C(29)	C(2A)	1.445(6)
Si(2)	C(221)	1.877(5)	C(111)	C(116)	1.375(7)
Si(2)	C(22)	1.881(5)	C(111)	C(112)	1.395(8)
Si(2)	C(231)	1.888(5)	C(112)	C(113)	1.400(8)
Al	O(1)	1.766(3)	C(113)	C(114)	1.364(9)
Al	N(3)	1.790(4)	C(114)	C(115)	1.316(9)
Al	O(2)	1.813(3)	C(115)	C(116)	1.413(8)
Al	N(4)	1.849(4)	C(121)	C(122)	1.385(7)
Al	Li	2.759(8)	C(121)	C(126)	1.403(7)
O(1)	C(11)	1.356(5)	C(122)	C(123)	1.376(7)
O(2)	C(21)	1.371(5)	C(123)	C(124)	1.350(8)
O(2)	Li	1.923(8)	C(124)	C(125)	1.366(8)
N(3)	C(31)	1.452(6)	C(125)	C(126)	1.376(8)
N(3)	C(32)	1.455(7)	C(131)	C(132)	1.384(7)
N(4)	C(41)	1.485(6)	C(131)	C(136)	1.398(7)
N(4)	C(42)	1.498(7)	C(132)	C(133)	1.371(8)
N(4)	Li	2.103(9)	C(133)	C(134)	1.363(8)
N(911)	C(916)	1.340(7)	C(134)	C(135)	1.374(8)
N(911)	C(911)	1.344(7)	C(135)	C(136)	1.371(7)
N(911)	Li	2.016(9)	C(211)	C(216)	1.393(6)
C(11)	C(1A)	1.383(6)	C(211)	C(212)	1.401(7)
C(11)	C(12)	1.426(6)	C(212)	C(213)	1.373(7)
C(12)	C(13)	1.390(6)	C(213)	C(214)	1.349(7)
C(13)	C(14)	1.419(6)	C(214)	C(215)	1.386(8)
C(14)	C(15)	1.414(6)	C(215)	C(216)	1.392(7)
C(14)	C(19)	1.428(6)	C(221)	C(226)	1.380(7)
C(15)	C(16)	1.357(7)	C(221)	C(222)	1.389(7)
C(16)	C(17)	1.383(7)	C(222)	C(223)	1.395(8)
C(17)	C(18)	1.376(7)	C(223)	C(224)	1.370(10)
C(18)	C(19)	1.414(6)	C(224)	C(225)	1.366(10)
C(19)	C(1A)	1.435(6)	C(225)	C(226)	1.384(9)
C(1A)	C(2A)	1.475(6)	C(231)	C(232)	1.385(6)
C(21)	C(2A)	1.392(6)	C(231)	C(236)	1.392(7)
C(21)	C(22)	1.415(6)	C(232)	C(233)	1.387(7)
C(22)	C(23)	1.395(6)	C(232)	Li	2.625(10)
C(23)	C(24)	1.406(6)	C(233)	C(234)	1.373(7)
C(24)	C(29)	1.414(6)	C(233)	Li	2.738(9)
C(24)	C(25)	1.422(6)	C(234)	C(235)	1.378(7)

Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C(235)	C(236)	1.394(7)	Li	N(911)	2.016(9)
C(911)	C(913)	1.370(8)	Li	N(4)	2.103(9)
C(913)	C(914)	1.378(8)	Li	C(232)	2.625(10)
C(914)	C(915)	1.371(8)	Li	C(42)	2.663(10)
C(915)	C(916)	1.359(8)	Li	C(233)	2.738(9)
Li	O(2)	1.923(8)	Li	Al	2.759(8)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Bond Angles in Degrees

for $C_{65}H_{57}AlLiN_3O_2Si_2$

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C(131)	Si(1)	C(12)	105.9(2)	C(13)	C(12)	Si(1)	121.2(3)
C(131)	Si(1)	C(121)	108.5(2)	C(11)	C(12)	Si(1)	121.4(3)
C(12)	Si(1)	C(121)	107.8(2)	C(12)	C(13)	C(14)	122.9(4)
C(131)	Si(1)	C(111)	108.2(2)	C(15)	C(14)	C(13)	122.2(4)
C(12)	Si(1)	C(111)	118.1(2)	C(15)	C(14)	C(19)	119.4(4)
C(121)	Si(1)	C(111)	108.1(2)	C(13)	C(14)	C(19)	118.4(4)
C(211)	Si(2)	C(221)	109.1(2)	C(16)	C(15)	C(14)	120.9(4)
C(211)	Si(2)	C(22)	105.7(2)	C(15)	C(16)	C(17)	120.8(5)
C(221)	Si(2)	C(22)	111.3(2)	C(18)	C(17)	C(16)	120.0(5)
C(211)	Si(2)	C(231)	109.6(2)	C(17)	C(18)	C(19)	121.8(4)
C(221)	Si(2)	C(231)	106.7(2)	C(18)	C(19)	C(14)	117.1(4)
C(22)	Si(2)	C(231)	114.35(19)	C(18)	C(19)	C(1A)	123.6(4)
O(1)	Al	N(3)	107.73(17)	C(14)	C(19)	C(1A)	119.3(4)
O(1)	Al	O(2)	102.89(14)	C(11)	C(1A)	C(19)	119.0(4)
N(3)	Al	O(2)	117.24(18)	C(11)	C(1A)	C(2A)	122.6(4)
O(1)	Al	N(4)	118.32(17)	C(19)	C(1A)	C(2A)	118.4(4)
N(3)	Al	N(4)	116.93(19)	O(2)	C(21)	C(2A)	118.8(4)
O(2)	Al	N(4)	92.54(17)	O(2)	C(21)	C(22)	118.1(4)
O(1)	Al	Li	127.4(2)	C(2A)	C(21)	C(22)	123.0(4)
N(3)	Al	Li	123.1(2)	C(23)	C(22)	C(21)	116.9(4)
O(2)	Al	Li	43.96(18)	C(23)	C(22)	Si(2)	116.5(3)
N(4)	Al	Li	49.6(2)	C(21)	C(22)	Si(2)	126.5(3)
C(11)	O(1)	Al	119.6(3)	C(22)	C(23)	C(24)	122.9(4)
C(21)	O(2)	Al	122.3(3)	C(23)	C(24)	C(29)	118.8(4)
C(21)	O(2)	Li	141.2(4)	C(23)	C(24)	C(25)	122.0(4)
Al	O(2)	Li	95.2(3)	C(29)	C(24)	C(25)	119.2(4)
C(31)	N(3)	C(32)	109.6(4)	C(26)	C(25)	C(24)	121.0(4)
C(31)	N(3)	Al	127.2(4)	C(25)	C(26)	C(27)	119.8(4)
C(32)	N(3)	Al	123.2(3)	C(28)	C(27)	C(26)	121.3(4)
C(41)	N(4)	C(42)	108.2(4)	C(27)	C(28)	C(29)	120.2(4)
C(41)	N(4)	Al	122.4(4)	C(28)	C(29)	C(24)	118.5(4)
C(42)	N(4)	Al	117.5(3)	C(28)	C(29)	C(2A)	121.6(4)
C(41)	N(4)	Li	122.5(4)	C(24)	C(29)	C(2A)	119.9(4)
C(42)	N(4)	Li	93.8(4)	C(21)	C(2A)	C(29)	117.8(4)
Al	N(4)	Li	88.3(3)	C(21)	C(2A)	C(1A)	123.3(4)
C(916)	N(911)	C(911)	116.5(5)	C(29)	C(2A)	C(1A)	118.9(4)
C(916)	N(911)	Li	114.8(4)	C(116)	C(111)	C(112)	117.5(5)
C(911)	N(911)	Li	128.5(4)	C(116)	C(111)	Si(1)	122.5(4)
O(1)	C(11)	C(1A)	120.6(4)	C(112)	C(111)	Si(1)	119.7(4)
O(1)	C(11)	C(12)	116.8(4)	C(111)	C(112)	C(113)	120.6(6)
C(1A)	C(11)	C(12)	122.6(4)	C(114)	C(113)	C(112)	120.4(6)
C(13)	C(12)	C(11)	117.0(4)	C(115)	C(114)	C(113)	119.4(6)

Bond Angles (cont.)

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C(114)	C(115)	C(116)	122.4(6)	C(236)	C(231)	Si(2)	123.3(4)
C(111)	C(116)	C(115)	119.7(6)	C(231)	C(232)	C(233)	122.3(5)
C(122)	C(121)	C(126)	115.4(5)	C(231)	C(232)	Li	83.1(3)
C(122)	C(121)	Si(1)	121.9(4)	C(233)	C(232)	Li	79.6(3)
C(126)	C(121)	Si(1)	122.4(4)	C(234)	C(233)	C(232)	119.5(5)
C(123)	C(122)	C(121)	121.8(5)	C(234)	C(233)	Li	88.3(4)
C(124)	C(123)	C(122)	121.6(5)	C(232)	C(233)	Li	70.6(3)
C(123)	C(124)	C(125)	118.7(6)	C(233)	C(234)	C(235)	119.7(5)
C(124)	C(125)	C(126)	120.4(6)	C(234)	C(235)	C(236)	120.4(5)
C(125)	C(126)	C(121)	122.0(5)	C(231)	C(236)	C(235)	120.8(5)
C(132)	C(131)	C(136)	115.4(5)	N(911)	C(911)	C(913)	123.4(5)
C(132)	C(131)	Si(1)	123.1(4)	C(911)	C(913)	C(914)	118.9(6)
C(136)	C(131)	Si(1)	121.5(4)	C(915)	C(914)	C(913)	118.0(6)
C(133)	C(132)	C(131)	123.0(5)	C(916)	C(915)	C(914)	119.9(5)
C(134)	C(133)	C(132)	120.3(6)	N(911)	C(916)	C(915)	123.2(5)
C(133)	C(134)	C(135)	118.7(5)	O(2)	Li	N(911)	116.2(4)
C(136)	C(135)	C(134)	120.8(5)	O(2)	Li	N(4)	82.1(3)
C(135)	C(136)	C(131)	121.9(5)	N(911)	Li	N(4)	124.2(4)
C(216)	C(211)	C(212)	116.9(4)	O(2)	Li	C(232)	86.8(3)
C(216)	C(211)	Si(2)	121.9(4)	N(911)	Li	C(232)	125.2(4)
C(212)	C(211)	Si(2)	121.2(3)	N(4)	Li	C(232)	107.0(4)
C(213)	C(212)	C(211)	121.5(5)	O(2)	Li	C(42)	93.0(3)
C(214)	C(213)	C(212)	121.0(5)	N(911)	Li	C(42)	90.3(4)
C(213)	C(214)	C(215)	119.7(5)	N(4)	Li	C(42)	34.2(2)
C(214)	C(215)	C(216)	119.9(5)	C(232)	Li	C(42)	140.2(4)
C(215)	C(216)	C(211)	120.9(5)	O(2)	Li	C(233)	115.0(4)
C(226)	C(221)	C(222)	117.5(5)	N(911)	Li	C(233)	114.9(4)
C(226)	C(221)	Si(2)	122.4(4)	N(4)	Li	C(233)	100.0(3)
C(222)	C(221)	Si(2)	120.1(4)	C(232)	Li	C(233)	29.88(17)
C(221)	C(222)	C(223)	121.0(6)	C(42)	Li	C(233)	123.9(3)
C(224)	C(223)	C(222)	120.1(6)	O(2)	Li	Al	40.88(18)
C(225)	C(224)	C(223)	119.6(6)	N(911)	Li	Al	138.2(4)
C(224)	C(225)	C(226)	120.5(7)	N(4)	Li	Al	42.07(18)
C(221)	C(226)	C(225)	121.4(6)	C(232)	Li	Al	92.4(3)
C(232)	C(231)	C(236)	117.2(4)	C(42)	Li	Al	63.8(2)
C(232)	C(231)	Si(2)	119.5(4)	C(233)	Li	Al	106.8(3)

Numbers in parentheses are estimated standard deviations in the least significant digits.