ORGANOMETALLICS
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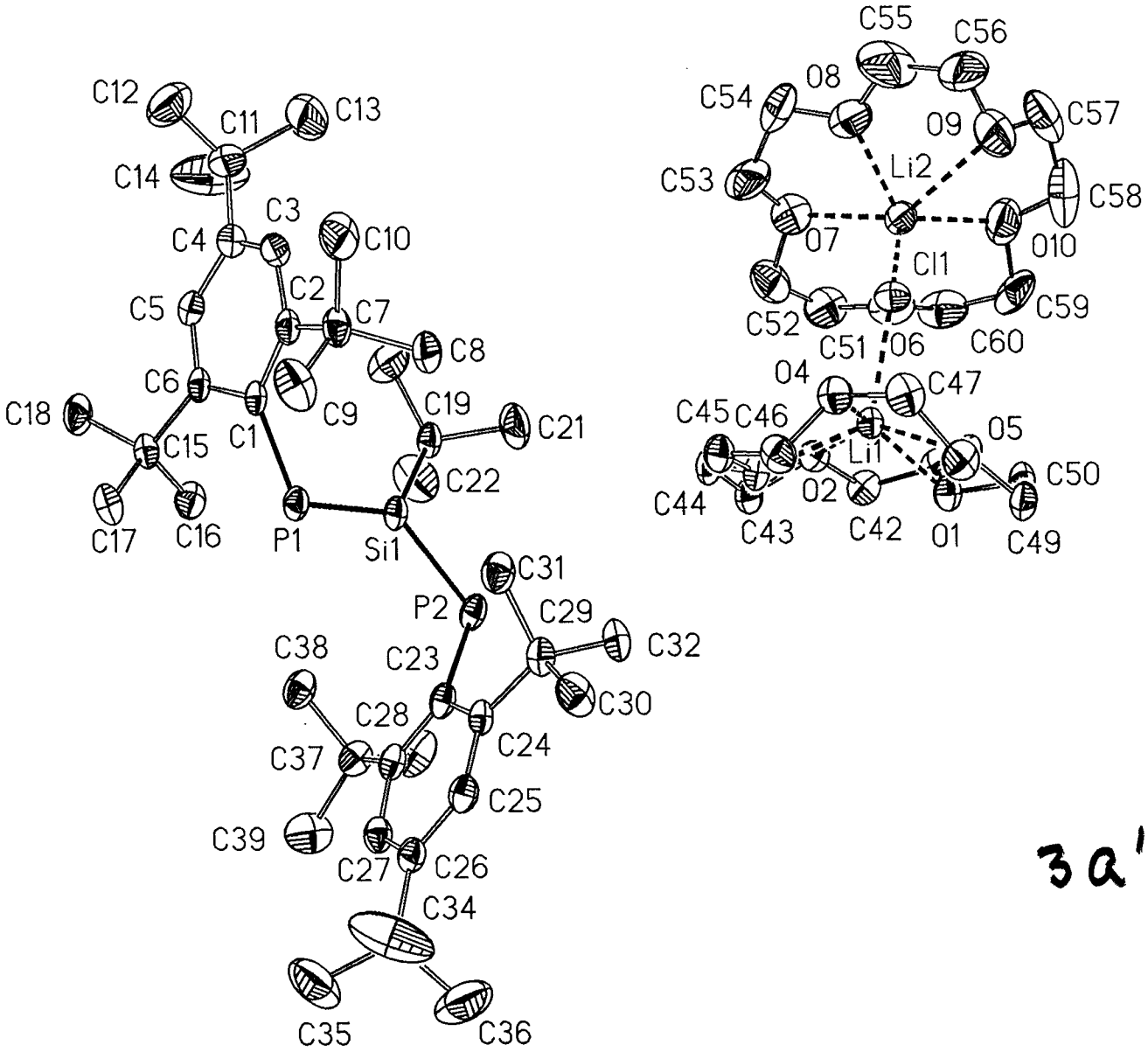
% probability level
without H-atoms



3a'

HB05 - H.Bender

STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{67}\ H_{115}\ Cl\ Li_2\ O_{10}\ P_2\ Si$
Color; Habit	red blocks
Crystal Size (mm)	0.3 x 0.4 x 0.4
Crystal System	Monoclinic
Space Group	$P2_1/c$
Unit Cell Dimensions	a = 15.403(2) Å
	b = 25.337(2) Å
	c = 19.214(3) Å
	β = 101.04(1)°
Volume	7360(2) Å^3
Z	4
Formula weight	1219.9
Density(calc.)	1.101 Mg/m^3
Absorption Coefficient	1.417 mm^{-1}
F(000)	2656

Solution and Refinement

System Used	Siemens SHELXTL PLUS (VMS)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Absolute Structure	N/A
Extinction Correction	N/A
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0005F^2$
Number of Parameters refined	701
Final R indices (obs. data)	R = 8.59 %, wR = 12.12 %
R Indices (all data)	R = 9.84 %, wR = 12.38 %
Goodness-of-Fit	3.83
Largest and Mean Δ/σ	0.012, 0.002
Data-to-Parameter Ratio	12.7:1
Largest Difference Peak	1.19 $e\text{Å}^{-3}$
Largest Difference Hole	-0.75 $e\text{Å}^{-3}$

Data Collection

Diffractometer Used	Enraf Nonius CAD4
Radiation	CuKα (λ = 1.54178 Å)
Temperature (K)	193
Monochromator	Highly oriented graphite crystal
2θ Range	4.7 to 120.0^{o}
Scan Type	ω
Prescan Limit, σ-Option	σ=1.00 I, 0.030
Prescan Speed parameter	3
Maximum scan time	30.00 sec
Scan Range (ω)	(0.75 + 0.15 tg θ)^{o}
Intensity Reflections	2 measured every 60 minutes
Orientation Reflections	3 measured every 300 reflections
Index Ranges	$-17 \leq h \leq 16$, $0 \leq k \leq 28$ $0 \leq \ell \leq 21$
Reflections Collected	11781
Independent Reflections	10917 (R_{int} = 0.74%)
Observed Reflections	8905 ($F > 4.0\sigma(F)$)
Absorption Correction	N/A

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
P(1)	4096(1)	1514(1)	2174(1)	44(1)
C(1)	2951(3)	1242(2)	1877(2)	39(1)
C(2)	2210(3)	1481(2)	2100(2)	45(2)
C(3)	1366(3)	1379(2)	1704(3)	53(2)
C(4)	1205(3)	1042(2)	1135(3)	52(2)
C(5)	1920(3)	745(2)	1016(3)	49(2)
C(6)	2782(3)	820(2)	1389(2)	42(2)
C(7)	2264(3)	1844(2)	2759(2)	52(2)
C(8)	2518(4)	2410(2)	2604(3)	69(2)
C(9)	2891(4)	1613(2)	3388(3)	79(2)
C(10)	1369(4)	1883(2)	2999(3)	84(3)
C(11)	290(4)	988(2)	668(3)	72(2)
C(12)	-269(5)	643(3)	1019(5)	129(4)
C(13)	-192(5)	1534(3)	573(5)	124(4)
C(14)	337(5)	799(5)	-78(4)	169(6)
C(15)	3501(3)	429(2)	1223(2)	47(2)
C(16)	4051(3)	671(2)	733(3)	60(2)
C(17)	4095(4)	240(2)	1908(3)	65(2)
C(18)	3075(4)	-74(2)	863(3)	67(2)
Si(1)	4207(1)	2134(1)	1454(1)	41(1)
C(19)	3382(3)	2337(2)	604(2)	49(2)
C(20)	2498(4)	2061(3)	507(4)	96(3)
C(21)	3226(5)	2931(2)	617(3)	83(3)
C(22)	3808(5)	2212(3)	-31(3)	96(3)
P(2)	5308(1)	2649(1)	1511(1)	48(1)
C(23)	6239(3)	2462(2)	2247(2)	43(2)
C(24)	6376(3)	2731(2)	2923(2)	42(2)
C(25)	7138(3)	2628(2)	3418(2)	46(2)
C(26)	7801(3)	2285(2)	3307(2)	46(2)
C(27)	7670(3)	2039(2)	2653(2)	48(2)
C(28)	6932(3)	2115(2)	2120(2)	45(2)
C(29)	5714(3)	3127(2)	3148(2)	48(2)
C(30)	6059(4)	3351(2)	3902(3)	69(2)
C(31)	4832(3)	2859(2)	3178(3)	61(2)
C(32)	5571(4)	3619(2)	2658(3)	60(2)
C(33)	8641(3)	2199(2)	3868(3)	57(2)
C(34)	8459(5)	2213(5)	4600(3)	155(5)
C(35)	9099(6)	1674(3)	3763(5)	147(4)
C(36)	9313(5)	2621(4)	3781(5)	144(4)
C(37)	6961(3)	1828(2)	1407(2)	55(2)
C(38)	6185(3)	1437(2)	1198(3)	62(2)
C(39)	7806(4)	1495(3)	1442(3)	90(3)
C(40)	6973(4)	2225(2)	812(3)	77(2)
Cl(1)	1744(1)	5616(1)	-242(1)	60(1)
Li(1)	3212(5)	5430(3)	296(4)	50(3)
O(1)	4025(2)	6022(1)	-177(2)	56(1)
C(41)	3698(4)	6009(2)	-918(3)	62(2)
C(42)	3944(4)	5490(2)	-1165(3)	60(2)
O(2)	3566(2)	5094(1)	-771(2)	59(1)
C(43)	4036(4)	4618(2)	-689(3)	62(2)
C(44)	3683(4)	4307(2)	-144(3)	62(2)
O(3)	3770(2)	4623(1)	483(2)	54(1)
C(45)	3564(4)	4342(2)	1071(3)	64(2)
C(46)	3590(4)	4720(2)	1660(3)	63(2)

O(4)	2945(2)	5112(1)	1415(2)	62(1)
C(47)	2968(4)	5552(2)	1873(3)	70(2)
C(48)	3675(4)	5930(2)	1798(3)	65(2)
O(5)	3581(2)	6036(1)	1067(2)	56(1)
C(49)	4124(4)	6450(2)	907(3)	66(2)
C(50)	3901(4)	6519(2)	132(3)	66(2)
Li(2)	736(6)	5750(4)	-1293(5)	62(3)
O(6)	1696(3)	5750(2)	-2111(2)	101(2)
C(51)	1679(5)	5272(3)	-2495(4)	105(3)
C(52)	1399(6)	4828(3)	-2034(4)	104(4)
O(7)	615(3)	4975(2)	-1903(3)	104(2)
C(53)	249(6)	4634(4)	-1500(5)	128(4)
C(54)	-550(6)	4848(3)	-1311(4)	107(4)
O(8)	-379(3)	5355(2)	-1060(3)	115(2)
C(55)	-950(7)	5598(6)	-798(6)	170(7)
C(56)	-834(7)	6127(5)	-603(8)	192(8)
O(9)	-169(4)	6381(2)	-859(4)	142(3)
C(57)	-420(7)	6778(4)	-1267(5)	130(5)
C(58)	429(9)	6970(3)	-1550(5)	143(5)
O(10)	719(4)	6561(2)	-1897(3)	119(3)
C(59)	1549(6)	6671(3)	-2043(4)	111(4)
C(60)	1710(5)	6175(4)	-2524(4)	115(4)
C(1T)	-2843(5)	6054(2)	6518(4)	139(3)
C(2T)	-3532	5698	6297	165(4)
C(3T)	-3348	5165	6220	158(4)
C(4T)	-2475	4987	6364	177(4)
C(5T)	-1786	5343	6585	144(3)
C(6T)	-1970	5876	6662	228(6)
C(7T)	-1237(7)	6227(5)	6821(8)	234(6)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 2. Bond lengths (Å)

P(1)-C(1)	1.877 (4)	P(1)-Si(1)	2.123 (2)
C(1)-C(2)	1.430 (7)	C(1)-C(6)	1.412 (6)
C(2)-C(3)	1.398 (6)	C(2)-C(7)	1.552 (6)
C(3)-C(4)	1.374 (7)	C(4)-C(5)	1.388 (7)
C(4)-C(11)	1.525 (7)	C(5)-C(6)	1.395 (6)
C(6)-C(15)	1.564 (7)	C(7)-C(8)	1.531 (7)
C(7)-C(9)	1.511 (7)	C(7)-C(10)	1.539 (9)
C(11)-C(12)	1.475 (11)	C(11)-C(13)	1.564 (9)
C(11)-C(14)	1.526 (11)	C(15)-C(16)	1.511 (8)
C(15)-C(17)	1.529 (7)	C(15)-C(18)	1.537 (6)
Si(1)-C(19)	1.936 (4)	Si(1)-P(2)	2.127 (2)
C(19)-C(20)	1.509 (8)	C(19)-C(21)	1.526 (7)
C(19)-C(22)	1.526 (8)	P(2)-C(23)	1.872 (4)
C(23)-C(24)	1.445 (6)	C(23)-C(28)	1.439 (7)
C(24)-C(25)	1.386 (6)	C(24)-C(29)	1.551 (7)
C(25)-C(26)	1.387 (7)	C(26)-C(27)	1.384 (6)
C(26)-C(33)	1.532 (6)	C(27)-C(28)	1.390 (6)
C(28)-C(37)	1.559 (7)	C(29)-C(30)	1.552 (6)
C(29)-C(31)	1.530 (7)	C(29)-C(32)	1.552 (6)
C(33)-C(34)	1.486 (9)	C(33)-C(35)	1.536 (10)
C(33)-C(36)	1.521 (10)	C(37)-C(38)	1.545 (7)
C(37)-C(39)	1.541 (8)	C(37)-C(40)	1.525 (7)
Cl(1)-Li(1)	2.347 (7)	Cl(1)-Li(2)	2.324 (8)
Li(1)-O(1)	2.254 (9)	Li(1)-O(2)	2.378 (9)
Li(1)-O(3)	2.220 (8)	Li(1)-O(4)	2.405 (9)
Li(1)-O(5)	2.133 (8)	O(1)-C(41)	1.417 (6)
O(1)-C(50)	1.421 (6)	C(41)-C(42)	1.473 (8)
C(42)-O(2)	1.445 (6)	O(2)-C(43)	1.400 (6)
C(43)-C(44)	1.495 (8)	C(44)-O(3)	1.432 (6)
O(3)-C(45)	1.422 (7)	C(45)-C(46)	1.477 (8)
C(46)-O(4)	1.420 (6)	O(4)-C(47)	1.417 (7)
C(47)-C(48)	1.479 (9)	C(48)-O(5)	1.410 (6)
O(5)-C(49)	1.412 (7)	C(49)-C(50)	1.472 (8)
Li(2)-O(6)	2.355 (11)	Li(2)-O(7)	2.276 (10)
Li(2)-O(8)	2.109 (11)	Li(2)-O(9)	2.375 (12)
Li(2)-O(10)	2.357 (11)	O(6)-C(51)	1.416 (10)
O(6)-C(60)	1.341 (11)	C(51)-C(52)	1.545 (12)
C(52)-O(7)	1.333 (10)	O(7)-C(53)	1.354 (11)
C(53)-C(54)	1.453 (13)	C(54)-O(8)	1.379 (9)
O(8)-C(55)	1.254 (14)	C(55)-C(56)	1.394 (18)
C(56)-O(9)	1.377 (14)	O(9)-C(57)	1.289 (11)
C(57)-C(58)	1.587 (17)	C(58)-O(10)	1.353 (11)
O(10)-C(59)	1.389 (11)	C(59)-C(60)	1.607 (12)
C(6T)-C(7T)	1.422 (13)		

Table 3. Bond angles (°)

C(1)-P(1)-Si(1)	105.2(1)	P(1)-C(1)-C(2)	120.7(3)
P(1)-C(1)-C(6)	121.5(3)	C(2)-C(1)-C(6)	117.6(4)
C(1)-C(2)-C(3)	118.1(4)	C(1)-C(2)-C(7)	125.0(4)
C(3)-C(2)-C(7)	116.9(4)	C(2)-C(3)-C(4)	123.8(5)
C(3)-C(4)-C(5)	116.1(4)	C(3)-C(4)-C(11)	122.0(5)
C(5)-C(4)-C(11)	121.9(4)	C(4)-C(5)-C(6)	123.3(4)
C(1)-C(6)-C(5)	118.8(4)	C(1)-C(6)-C(15)	124.5(4)
C(5)-C(6)-C(15)	116.7(4)	C(2)-C(7)-C(8)	111.8(4)
C(2)-C(7)-C(9)	110.5(4)	C(8)-C(7)-C(9)	111.7(4)
C(2)-C(7)-C(10)	111.7(4)	C(8)-C(7)-C(10)	105.9(4)
C(9)-C(7)-C(10)	104.9(5)	C(4)-C(11)-C(12)	109.8(5)
C(4)-C(11)-C(13)	110.8(5)	C(12)-C(11)-C(13)	105.8(6)
C(4)-C(11)-C(14)	112.0(5)	C(12)-C(11)-C(14)	112.3(7)
C(13)-C(11)-C(14)	105.9(6)	C(6)-C(15)-C(16)	111.8(4)
C(6)-C(15)-C(17)	110.7(4)	C(16)-C(15)-C(17)	110.4(4)
C(6)-C(15)-C(18)	111.1(4)	C(16)-C(15)-C(18)	107.4(4)
C(17)-C(15)-C(18)	105.1(4)	P(1)-Si(1)-C(19)	128.6(2)
P(1)-Si(1)-P(2)	125.7(1)	C(19)-Si(1)-P(2)	105.6(2)
Si(1)-C(19)-C(20)	114.4(4)	Si(1)-C(19)-C(21)	109.1(3)
C(20)-C(19)-C(21)	108.5(5)	Si(1)-C(19)-C(22)	107.9(4)
C(20)-C(19)-C(22)	108.7(5)	C(21)-C(19)-C(22)	108.1(5)
Si(1)-P(2)-C(23)	111.8(2)	P(2)-C(23)-C(24)	121.2(3)
P(2)-C(23)-C(28)	120.7(3)	C(24)-C(23)-C(28)	117.1(4)
C(23)-C(24)-C(25)	119.1(4)	C(23)-C(24)-C(29)	124.5(4)
C(25)-C(24)-C(29)	116.5(4)	C(24)-C(25)-C(26)	124.3(4)
C(25)-C(26)-C(27)	116.0(4)	C(25)-C(26)-C(33)	121.9(4)
C(27)-C(26)-C(33)	122.1(4)	C(26)-C(27)-C(28)	124.3(4)
C(23)-C(28)-C(27)	119.2(4)	C(23)-C(28)-C(37)	125.6(4)
C(27)-C(28)-C(37)	115.2(4)	C(24)-C(29)-C(30)	111.8(4)
C(24)-C(29)-C(31)	111.0(4)	C(30)-C(29)-C(31)	106.0(4)
C(24)-C(29)-C(32)	112.0(4)	C(30)-C(29)-C(32)	104.8(4)
C(31)-C(29)-C(32)	110.9(4)	C(26)-C(33)-C(34)	112.0(5)
C(26)-C(33)-C(35)	112.2(5)	C(34)-C(33)-C(35)	108.6(6)
C(26)-C(33)-C(36)	108.9(5)	C(34)-C(33)-C(36)	110.0(6)
C(35)-C(33)-C(36)	104.8(6)	C(28)-C(37)-C(38)	112.1(4)
C(28)-C(37)-C(39)	112.5(4)	C(38)-C(37)-C(39)	105.4(4)
C(28)-C(37)-C(40)	110.9(4)	C(38)-C(37)-C(40)	110.4(4)
C(39)-C(37)-C(40)	105.2(5)	Li(1)-Cl(1)-Li(2)	147.0(3)
Cl(1)-Li(1)-O(1)	104.6(3)	Cl(1)-Li(1)-O(2)	93.0(3)
O(1)-Li(1)-O(2)	69.8(3)	Cl(1)-Li(1)-O(3)	124.5(3)
O(1)-Li(1)-O(3)	116.8(4)	O(2)-Li(1)-O(3)	70.4(3)
Cl(1)-Li(1)-O(4)	98.4(3)	O(1)-Li(1)-O(4)	141.9(4)
O(2)-Li(1)-O(4)	139.2(4)	O(3)-Li(1)-O(4)	70.9(3)
Cl(1)-Li(1)-O(5)	105.5(3)	O(1)-Li(1)-O(5)	72.9(3)
O(2)-Li(1)-O(5)	141.5(4)	O(3)-Li(1)-O(5)	120.4(4)
O(4)-Li(1)-O(5)	71.9(3)	Li(1)-O(1)-C(41)	105.7(3)
Li(1)-O(1)-C(50)	107.0(4)	C(41)-O(1)-C(50)	113.1(4)
O(1)-C(41)-C(42)	106.4(4)	C(41)-C(42)-O(2)	107.2(4)
Li(1)-O(2)-C(42)	112.6(3)	Li(1)-O(2)-C(43)	114.3(3)
C(42)-O(2)-C(43)	113.9(4)	O(2)-C(43)-C(44)	106.4(5)
C(43)-C(44)-O(3)	107.9(4)	Li(1)-O(3)-C(44)	114.1(3)
Li(1)-O(3)-C(45)	116.9(4)	C(44)-O(3)-C(45)	112.9(4)
O(3)-C(45)-C(46)	107.9(4)	C(45)-C(46)-O(4)	106.5(4)
Li(1)-O(4)-C(46)	107.7(4)	Li(1)-O(4)-C(47)	107.7(4)
C(46)-O(4)-C(47)	114.3(4)	O(4)-C(47)-C(48)	112.3(5)
C(47)-C(48)-O(5)	106.5(4)	Li(1)-O(5)-C(48)	121.2(4)

Li(1)-O(5)-C(49)	118.3(4)	C(48)-O(5)-C(49)	113.9(4)
O(5)-C(49)-C(50)	106.0(4)	O(1)-C(50)-C(49)	107.0(4)
Cl(1)-Li(2)-O(6)	100.4(3)	Cl(1)-Li(2)-O(7)	107.3(4)
O(6)-Li(2)-O(7)	69.9(3)	Cl(1)-Li(2)-O(8)	100.5(4)
O(6)-Li(2)-O(8)	141.5(5)	O(7)-Li(2)-O(8)	73.1(4)
Cl(1)-Li(2)-O(9)	97.6(4)	O(6)-Li(2)-O(9)	136.1(5)
O(7)-Li(2)-O(9)	139.9(4)	O(8)-Li(2)-O(9)	71.8(4)
Cl(1)-Li(2)-O(10)	119.9(4)	O(6)-Li(2)-O(10)	67.7(3)
O(7)-Li(2)-O(10)	120.4(4)	O(8)-Li(2)-O(10)	125.8(4)
O(9)-Li(2)-O(10)	68.5(3)	Li(2)-O(6)-C(51)	113.4(5)
Li(2)-O(6)-C(60)	118.6(5)	C(51)-O(6)-C(60)	112.2(6)
O(6)-C(51)-C(52)	107.6(6)	C(51)-C(52)-O(7)	105.5(6)
Li(2)-O(7)-C(52)	110.5(5)	Li(2)-O(7)-C(53)	105.0(6)
C(52)-O(7)-C(53)	114.8(6)	O(7)-C(53)-C(54)	111.6(7)
C(53)-C(54)-O(8)	108.8(7)	Li(2)-O(8)-C(54)	118.4(6)
Li(2)-O(8)-C(55)	121.0(7)	C(54)-O(8)-C(55)	119.7(8)
O(8)-C(55)-C(56)	121.0(11)	C(55)-C(56)-O(9)	114.9(11)
Li(2)-O(9)-C(56)	109.7(7)	Li(2)-O(9)-C(57)	116.1(7)
C(56)-O(9)-C(57)	115.1(8)	O(9)-C(57)-C(58)	106.0(8)
C(57)-C(58)-O(10)	107.8(7)	Li(2)-O(10)-C(58)	113.5(6)
Li(2)-O(10)-C(59)	110.5(5)	C(58)-O(10)-C(59)	110.4(7)
O(10)-C(59)-C(60)	102.0(6)	O(6)-C(60)-C(59)	105.4(7)
C(1T)-C(6T)-C(7T)	122.4(6)	C(5T)-C(6T)-C(7T)	117.3(6)

Table 4. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
P(1)	54(1)	32(1)	43(1)	-3(1)	5(1)	10(1)
C(1)	55(3)	24(2)	40(2)	0(2)	12(2)	8(2)
C(2)	58(3)	29(2)	51(3)	1(2)	17(2)	7(2)
C(3)	52(3)	42(3)	66(3)	7(2)	18(2)	6(2)
C(4)	51(3)	44(3)	62(3)	0(2)	11(2)	4(2)
C(5)	57(3)	36(2)	54(3)	-7(2)	10(2)	-1(2)
C(6)	57(3)	27(2)	45(2)	0(2)	18(2)	7(2)
C(7)	70(3)	36(2)	54(3)	3(2)	24(2)	-6(2)
C(8)	76(4)	37(3)	97(4)	3(3)	23(3)	-11(3)
C(9)	114(5)	72(4)	50(3)	25(4)	17(3)	-9(3)
C(10)	99(5)	66(4)	96(5)	5(3)	46(4)	-22(3)
C(11)	49(3)	72(4)	92(4)	-5(3)	4(3)	-5(3)
C(12)	81(5)	112(6)	178(9)	-36(5)	-14(5)	35(6)
C(13)	90(5)	93(6)	167(8)	14(4)	-27(5)	21(5)
C(14)	74(5)	325(15)	94(6)	-11(7)	-15(4)	-81(8)
C(15)	61(3)	32(2)	50(3)	5(2)	15(2)	1(2)
C(16)	72(4)	50(3)	67(3)	0(3)	32(3)	-5(3)
C(17)	78(4)	41(3)	75(4)	15(3)	13(3)	5(3)
C(18)	87(4)	36(3)	82(4)	-2(3)	30(3)	-15(3)
Si(1)	55(1)	29(1)	39(1)	-4(1)	8(1)	6(1)
C(19)	66(3)	32(2)	45(3)	-3(2)	3(2)	8(2)
C(20)	79(4)	96(5)	96(5)	-27(4)	-25(4)	54(4)
C(21)	107(5)	50(3)	83(4)	13(3)	-4(4)	20(3)
C(22)	122(6)	117(6)	46(3)	25(5)	10(3)	20(3)
P(2)	65(1)	36(1)	42(1)	-13(1)	8(1)	8(1)
C(23)	59(3)	34(2)	38(2)	-9(2)	13(2)	5(2)
C(24)	56(3)	27(2)	44(2)	-2(2)	14(2)	5(2)
C(25)	62(3)	39(2)	39(2)	-7(2)	12(2)	-4(2)
C(26)	55(3)	37(2)	46(3)	-6(2)	10(2)	7(2)
C(27)	58(3)	38(2)	52(3)	-1(2)	22(2)	5(2)
C(28)	61(3)	35(2)	43(2)	-10(2)	18(2)	1(2)
C(29)	66(3)	36(2)	41(2)	0(2)	9(2)	-1(2)
C(30)	82(4)	66(3)	56(3)	17(3)	5(3)	-20(3)
C(31)	73(4)	50(3)	64(3)	-4(3)	25(3)	-8(2)
C(32)	80(4)	33(2)	68(3)	10(2)	20(3)	6(2)
C(33)	65(3)	53(3)	53(3)	1(2)	9(2)	9(2)
C(34)	105(6)	307(14)	53(4)	88(7)	16(4)	36(6)
C(35)	137(7)	110(6)	155(8)	59(6)	-73(6)	-41(6)
C(36)	102(6)	155(8)	147(7)	-60(6)	-46(5)	55(6)
C(37)	61(3)	59(3)	48(3)	-9(2)	17(2)	-11(2)
C(38)	76(4)	51(3)	63(3)	-12(3)	25(3)	-16(2)
C(39)	80(4)	115(6)	80(4)	4(4)	27(3)	-47(4)
C(40)	109(5)	82(4)	49(3)	-37(4)	35(3)	-7(3)
Cl(1)	48(1)	74(1)	55(1)	0(1)	6(1)	4(1)
Li(1)	50(5)	38(4)	61(5)	0(3)	6(4)	1(4)
O(1)	68(2)	43(2)	56(2)	2(2)	12(2)	5(2)
C(41)	73(4)	60(3)	54(3)	-2(3)	13(3)	19(3)
C(42)	69(3)	68(3)	44(3)	-7(3)	17(2)	5(2)
O(2)	56(2)	55(2)	67(2)	0(2)	14(2)	3(2)
C(43)	69(3)	47(3)	69(3)	-1(3)	16(3)	-16(3)
C(44)	79(4)	36(3)	70(3)	-5(2)	11(3)	-17(2)
O(3)	69(2)	37(2)	56(2)	-5(2)	13(2)	-1(1)
C(45)	71(4)	46(3)	76(4)	0(3)	17(3)	15(3)
C(46)	71(4)	60(3)	58(3)	8(3)	11(3)	17(3)
O(4)	69(2)	60(2)	59(2)	0(2)	14(2)	2(2)

C(47)	87(4)	75(4)	51(3)	6(3)	22(3)	-4(3)
C(48)	78(4)	71(4)	44(3)	0(3)	6(3)	-18(3)
O(5)	65(2)	50(2)	54(2)	-13(2)	9(2)	-10(2)
C(49)	74(4)	41(3)	85(4)	-6(3)	20(3)	-15(3)
C(50)	85(4)	35(3)	81(4)	-2(3)	28(3)	4(3)
Li(2)	59(5)	61(5)	64(5)	-6(4)	7(4)	2(4)
O(6)	87(3)	135(4)	80(3)	-7(3)	11(2)	16(3)
C(51)	103(6)	127(7)	96(5)	-11(5)	46(4)	-41(5)
C(52)	113(6)	101(6)	103(6)	24(5)	36(5)	-24(5)
O(7)	95(4)	98(4)	115(4)	-2(3)	14(3)	-3(3)
C(53)	97(6)	119(7)	175(9)	-29(5)	43(6)	57(6)
C(54)	127(7)	72(5)	114(6)	-44(5)	0(5)	13(4)
O(8)	83(3)	112(4)	152(5)	-21(3)	29(3)	-25(4)
C(55)	130(9)	222(14)	174(10)	19(9)	70(7)	-84(9)
C(56)	111(8)	154(10)	346(18)	-42(7)	133(10)	-86(11)
O(9)	113(5)	96(4)	204(7)	30(4)	-4(4)	8(4)
C(57)	145(8)	99(7)	134(7)	62(6)	-2(6)	-13(6)
C(58)	255(13)	58(5)	96(6)	12(6)	-11(7)	-7(4)
O(10)	117(4)	78(3)	141(5)	-8(3)	-26(3)	-6(3)
C(59)	109(6)	85(5)	120(6)	-45(5)	-23(5)	54(5)
C(60)	88(5)	145(8)	115(6)	-9(5)	25(4)	76(6)

The anisotropic displacement exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

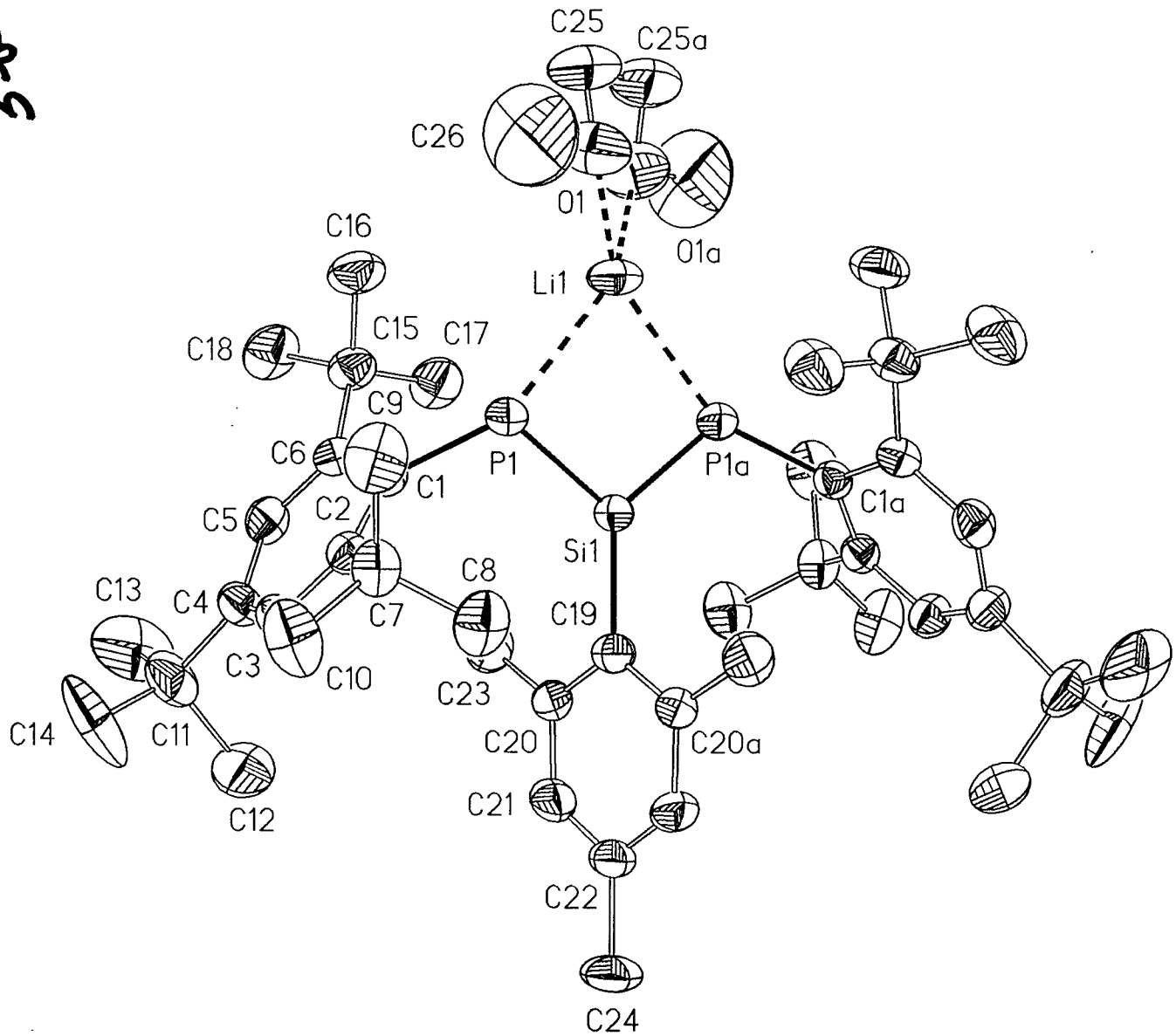
	x	y	z	U
H(3A)	875	1558	1839	64
H(5A)	1816	472	664	59
H(8A)	2545	2621	3022	83
H(8B)	3085	2410	2466	83
H(8C)	2082	2553	2226	83
H(9A)	2919	1841	3791	94
H(9B)	2696	1269	3499	94
H(9C)	3466	1588	3268	94
H(10A)	1412	2108	3406	101
H(10B)	946	2027	2613	101
H(10C)	1182	1537	3112	101
H(12A)	0	300	1069	156
H(12B)	-297	782	1479	156
H(12C)	-856	616	742	156
H(13A)	-249	1655	1035	150
H(13B)	153	1782	364	150
H(13C)	-769	1502	279	150
H(14A)	622	461	-65	197
H(14B)	-246	776	-363	197
H(14C)	676	1056	-278	197
H(16A)	3675	785	301	73
H(16B)	4367	969	964	73
H(16C)	4464	414	627	73
H(17A)	4530	-3	1800	78
H(17B)	4387	540	2152	78
H(17C)	3744	69	2203	78
H(18A)	2691	18	425	81
H(18B)	3531	-307	768	81
H(18C)	2739	-249	1168	81
H(20A)	2127	2181	77	116
H(20B)	2583	1687	481	116
H(20C)	2222	2140	902	116
H(21A)	2816	3037	199	100
H(21B)	2991	3021	1029	100
H(21C)	3779	3110	634	100
H(22A)	3411	2308	-462	116
H(22B)	4348	2408	7	116
H(22C)	3934	1841	-38	116
H(25A)	7214	2807	3866	55
H(27A)	8117	1798	2563	57
H(30A)	6616	3524	3908	83
H(30B)	5644	3600	4026	83
H(30C)	6140	3066	4237	83
H(31A)	4586	2716	2720	73
H(31B)	4926	2579	3521	73
H(31C)	4430	3113	3311	73
H(32A)	5347	3511	2178	72
H(32B)	5150	3848	2814	72
H(32C)	6120	3803	2680	72
H(34A)	8034	1945	4649	186
H(34B)	8997	2150	4934	186
H(34C)	8227	2553	4689	186
H(35A)	8704	1388	3802	175
H(35B)	9265	1663	3307	175

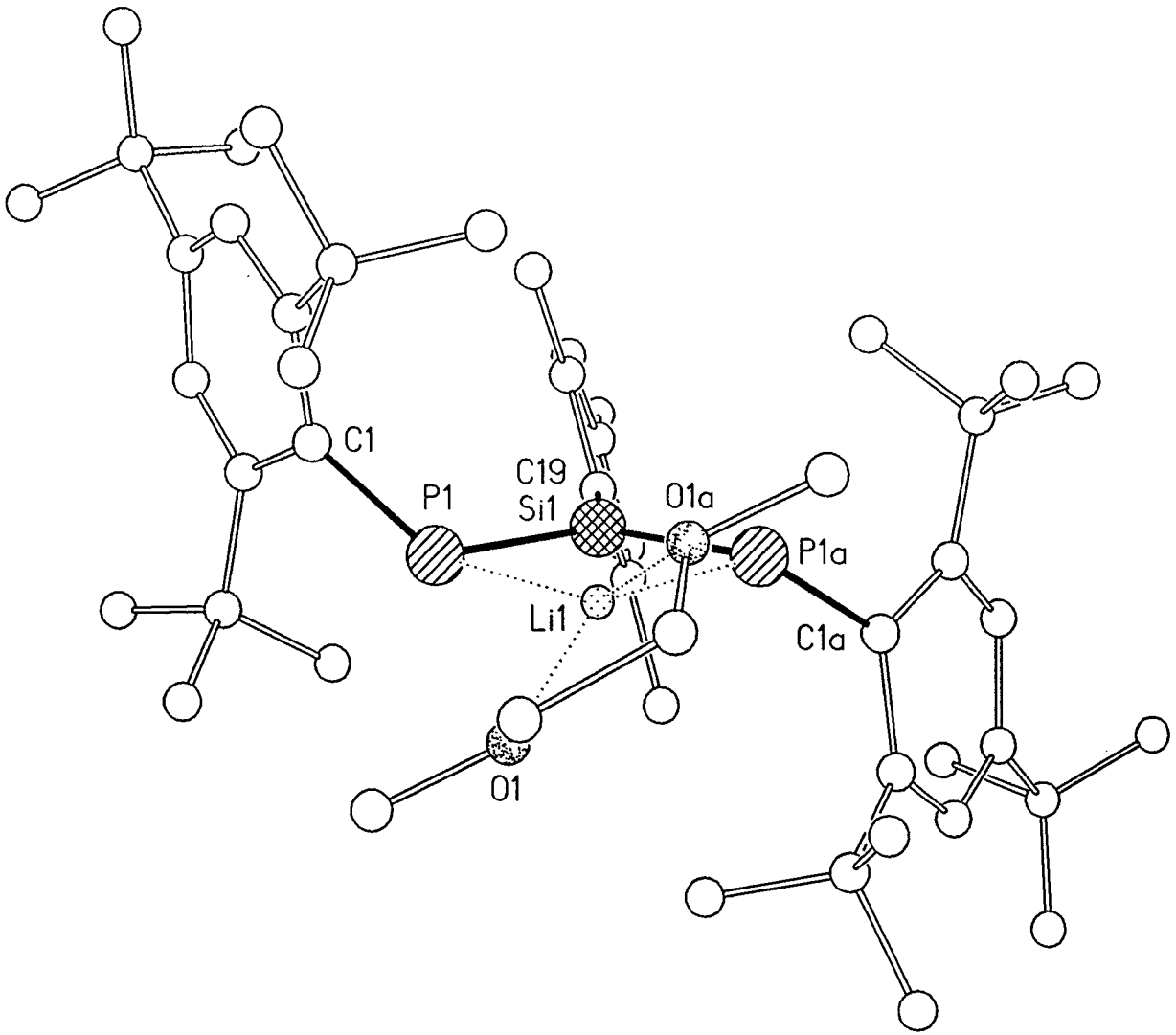
H(35C)	9618	1644	4128	175
H(36A)	9841	2565	4130	170
H(36B)	9453	2607	3316	170
H(36C)	9070	2961	3854	170
H(38A)	5634	1623	1156	74
H(38B)	6220	1276	752	74
H(38C)	6219	1169	1555	74
H(39A)	7810	1324	997	107
H(39B)	8312	1723	1556	107
H(39C)	7828	1234	1807	107
H(40A)	6452	2440	759	93
H(40B)	7488	2444	931	93
H(40C)	6985	2043	376	93
H(41A)	3943	6290	-1154	74
H(41B)	3066	6042	-1010	74
H(42A)	4576	5458	-1077	72
H(42B)	3723	5446	-1664	72
H(43A)	4654	4688	-525	73
H(43B)	3964	4431	-1132	73
H(44A)	4008	3984	-40	75
H(44B)	3073	4222	-319	75
H(45A)	3980	4061	1207	76
H(45B)	2983	4193	945	76
H(46A)	4165	4879	1781	76
H(46B)	3460	4545	2072	76
H(47A)	3054	5430	2354	85
H(47B)	2408	5731	1767	85
H(48A)	4244	5778	1978	78
H(48B)	3620	6252	2051	78
H(49A)	4736	6355	1050	79
H(49B)	4017	6769	1145	79
H(50A)	3297	6631	-4	79
H(50B)	4274	6780	-23	79
H(51A)	2245	5207	-2618	125
H(51B)	1243	5296	-2924	125
H(52A)	1821	4807	-1597	126
H(52B)	1369	4493	-2270	126
H(53A)	659	4570	-1065	149
H(53B)	125	4302	-1739	149
H(54A)	-749	4637	-957	129
H(54B)	-1006	4856	-1729	129
H(55A)	-1029	5397	-391	203
H(55B)	-1495	5578	-1137	203
H(56A)	-675	6144	-96	233
H(56B)	-1375	6319	-747	233
H(57A)	-637	7054	-1004	156
H(57B)	-876	6684	-1663	156
H(58A)	886	7061	-1154	173
H(58B)	310	7270	-1858	173
H(59A)	1989	6672	-1615	134
H(59B)	1566	7001	-2285	134
H(60A)	1235	6157	-2928	137
H(60B)	2260	6202	-2686	137
H(1TA)	-2969	6421	6571	167
H(2TA)	-4133	5821	6198	198
H(3TA)	-3822	4920	6068	187
H(4TA)	-2348	4620	6310	213
H(5TA)	-1185	5220	6684	171
H(7TA)	-692	6032	6899	276

H(7TB)	-1247	6469	6437	276
H(7TC)	-1284	6418	7244	276

X probability level
Most H-atoms
Most solvat
Most disordered part
tBu-groups

3b




C1
P1
C19
Si1
O1a
P1a
Li1
C1a
O1

STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{53}\ H_{89}\ Li\ O_2\ Si\ P_2$
Color; Habit	red prisms
Crystal size (mm)	0.5 x 0.6 x 0.7
Crystal System	Monoclinic
Space Group	C2/c
Unit Cell Dimensions	$\underline{a}$ = 24.636(5) Å
	$\underline{b}$ = 15.852(3) Å
	$\underline{c}$ = 18.025(3) Å
	β = 124.200(10)°
Volume	5822(2) $Å^3$
Z	4
Formula weight	855.2
Density(calc.)	0.976 Mg/m^3
Absorption Coefficient	0.124 mm^{-1}
F(000)	1880

Data Collection

Diffractometer Used	Siemens R3m/V
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	298
Monochromator	Highly oriented graphite crystal
2θ Range	6.0 to 50.0^{o}
Scan Type	ω
Scan Speed	Variable; 1.50 to 14.65^{o}/min. in ω
Scan Range (ω)	1.20^{o}
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 147 reflections
Index Ranges	$-29 \leq h \leq 24$, $0 \leq k \leq 18$ $0 \leq l \leq 21$
Reflections Collected	5332
Independent Reflections	4970 (R_{int} = 5.17%)
Observed Reflections	3005 ($F > 4.0\sigma(F)$)
Absorption Correction	N/A

Solution and Refinement

System Used	Siemens SHELXTL PLUS (MicroVAX II)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\Sigma w(F_o-F_c)^2$
Absolute Configuration	N/A
Extinction Correction	N/A
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0000F^2$
Number of parameters refined	287
Final R indices (obs. data)	R = 9.28 %, wR = 8.46 %
R Indices (all data)	R = 14.10 %, wR = 10.13 %
Goodness-of-Fit	2.51
Largest and Mean Δ/σ	0.193, 0.016
Data-to-Parameter Ratio	10.5:1
Largest Difference Peak	0.42 $e\text{Å}^{-3}$
Largest Difference Hole	-0.29 $e\text{Å}^{-3}$

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
P(1)	10(1)	1491(1)	1571(1)	61(1)
C(1)	-472(3)	2004(3)	457(3)	52(3)
C(2)	-206(3)	2645(3)	206(4)	54(3)
C(3)	-614(3)	3187(4)	-471(4)	66(4)
C(4)	-1294(3)	3099(4)	-1012(4)	67(4)
C(5)	-1539(3)	2380(4)	-866(4)	67(3)
C(6)	-1158(3)	1817(3)	-172(4)	58(3)
C(7)	549(3)	2753(4)	643(4)	70(4)
C(8)	917(3)	3185(4)	1564(4)	92(4)
C(9)	864(3)	1886(5)	721(5)	105(5)
C(10)	670(3)	3295(5)	41(5)	109(5)
C(11)	-1749(4)	3763(5)	-1727(5)	102(5)
C(12)	-1714(15)	4582(15)	-1113(17)	156(20)
C(13)	-2438(10)	3531(18)	-2303(23)	177(21)
C(14)	-1437(12)	4088(25)	-2225(19)	178(23)
C(12A)	-1408(19)	4549(19)	-1634(24)	212(28)
C(13A)	-2369(17)	3912(25)	-1688(24)	157(31)
C(14A)	-2050(17)	3282(17)	-2681(11)	149(20)
C(15)	-1503(3)	1021(4)	-129(4)	74(4)
C(16)	-1115(3)	216(4)	14(5)	97(5)
C(17)	-1665(3)	1116(4)	573(5)	99(5)
C(18)	-2166(3)	847(5)	-1038(5)	107(5)
Si(1)	0	2303(1)	2500	54(1)
C(19)	0	3500(5)	2500	60(5)
C(20)	-567(3)	3937(4)	1861(4)	65(4)
C(21)	-550(4)	4811(4)	1877(4)	86(5)
C(22)	0	5262(6)	2500	84(8)
C(23)	-1186(3)	3495(4)	1171(4)	88(4)
C(24)	0	6250(6)	2500	126(10)
Li(1)	0	275(9)	2500	100(14)
O(1)	471(6)	-724(5)	2396(6)	217(9)
C(25)	201(8)	-1449(6)	2262(9)	213(15)
C(26)	797(7)	-739(10)	1926(10)	274(18)
C(27)	2524(8)	8673(12)	4652(10)	285(8)
C(28)	2240(12)	7759(18)	4746(17)	385(12)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 2. Bond lengths (Å)

P(1)-C(1)	1.852 (5)	P(1)-Si(1)	2.123 (2)
P(1)-Li(1)	2.562 (11)	C(1)-C(2)	1.414 (9)
C(1)-C(6)	1.440 (7)	C(2)-C(3)	1.363 (7)
C(2)-C(7)	1.569 (9)	C(3)-C(4)	1.393 (8)
C(4)-C(5)	1.382 (10)	C(4)-C(11)	1.550 (9)
C(5)-C(6)	1.386 (8)	C(6)-C(15)	1.548 (10)
C(7)-C(8)	1.535 (9)	C(7)-C(9)	1.546 (10)
C(7)-C(10)	1.539 (12)	C(11)-C(12)	1.678 (31)
C(11)-C(13)	1.454 (22)	C(11)-C(14)	1.561 (41)
C(11)-C(12A)	1.460 (37)	C(11)-C(13A)	1.585 (50)
C(11)-C(14A)	1.628 (22)	C(12)-C(12A)	1.500 (71)
C(12)-C(13A)	1.710 (45)	C(13)-C(13A)	1.187 (60)
C(13)-C(14A)	1.505 (58)	C(14)-C(12A)	1.260 (59)
C(14)-C(14A)	1.787 (46)	C(15)-C(16)	1.527 (9)
C(15)-C(17)	1.533 (14)	C(15)-C(18)	1.556 (8)
Si(1)-C(19)	1.898 (8)	Si(1)-P(1A)	2.123 (2)
C(19)-C(20)	1.395 (7)	C(19)-C(20A)	1.395 (7)
C(20)-C(21)	1.387 (8)	C(20)-C(23)	1.495 (8)
C(21)-C(22)	1.377 (8)	C(22)-C(24)	1.565 (13)
C(22)-C(21A)	1.377 (8)	Li(1)-O(1)	2.033 (16)
Li(1)-P(1A)	2.562 (11)	Li(1)-O(1A)	2.033 (16)
O(1)-C(25)	1.280 (15)	O(1)-C(26)	1.459 (27)
C(25)-C(25A)	1.637 (44)	C(27)-C(28)	1.660 (36)
C(28)-C(28A)	1.355 (49)		

Table 3. Bond angles (°)

C(1)-P(1)-Si(1)	107.7(2)	C(1)-P(1)-Li(1)	143.5(2)
Si(1)-P(1)-Li(1)	86.1(2)	P(1)-C(1)-C(2)	122.2(3)
P(1)-C(1)-C(6)	121.1(5)	C(2)-C(1)-C(6)	116.5(5)
C(1)-C(2)-C(3)	119.8(5)	C(1)-C(2)-C(7)	123.3(5)
C(3)-C(2)-C(7)	116.8(6)	C(2)-C(3)-C(4)	123.8(6)
C(3)-C(4)-C(5)	115.5(5)	C(3)-C(4)-C(11)	122.5(6)
C(5)-C(4)-C(11)	122.0(6)	C(4)-C(5)-C(6)	123.8(5)
C(1)-C(6)-C(5)	118.5(6)	C(1)-C(6)-C(15)	124.2(5)
C(5)-C(6)-C(15)	117.2(5)	C(2)-C(7)-C(8)	113.9(7)
C(2)-C(7)-C(9)	110.0(5)	C(8)-C(7)-C(9)	109.7(5)
C(2)-C(7)-C(10)	110.6(5)	C(8)-C(7)-C(10)	106.5(6)
C(9)-C(7)-C(10)	105.9(7)	C(4)-C(11)-C(12)	103.4(9)
C(4)-C(11)-C(13)	115.5(14)	C(12)-C(11)-C(13)	105.8(19)
C(4)-C(11)-C(14)	110.1(13)	C(12)-C(11)-C(14)	105.3(20)
C(13)-C(11)-C(14)	115.3(19)	C(4)-C(11)-C(12A)	112.6(13)
C(12)-C(11)-C(12A)	56.6(25)	C(13)-C(11)-C(12A)	131.6(18)
C(14)-C(11)-C(12A)	49.2(25)	C(4)-C(11)-C(13A)	109.2(16)
C(12)-C(11)-C(13A)	63.2(19)	C(13)-C(11)-C(13A)	45.7(21)
C(14)-C(11)-C(13A)	140.7(19)	C(12A)-C(11)-C(13A)	111.9(25)
C(4)-C(11)-C(14A)	104.4(11)	C(12)-C(11)-C(14A)	152.0(13)
C(13)-C(11)-C(14A)	58.1(23)	C(14)-C(11)-C(14A)	68.1(19)
C(12A)-C(11)-C(14A)	114.3(23)	C(13A)-C(11)-C(14A)	103.8(20)
C(11)-C(12)-C(12A)	54.3(17)	C(11)-C(12)-C(13A)	55.8(18)
C(12A)-C(12)-C(13A)	103.5(26)	C(11)-C(13)-C(13A)	73.0(24)
C(11)-C(13)-C(14A)	66.7(17)	C(13A)-C(13)-C(14A)	139.5(28)
C(11)-C(14)-C(12A)	61.2(27)	C(11)-C(14)-C(14A)	57.7(16)
C(12A)-C(14)-C(14A)	115.8(35)	C(11)-C(12A)-C(12)	69.0(25)
C(11)-C(12A)-C(14)	69.6(23)	C(12)-C(12A)-C(14)	137.7(35)
C(11)-C(13A)-C(12)	61.1(20)	C(11)-C(13A)-C(13)	61.3(26)
C(12)-C(13A)-C(13)	118.3(41)	C(11)-C(14A)-C(13)	55.1(14)
C(11)-C(14A)-C(14)	54.2(15)	C(13)-C(14A)-C(14)	101.1(21)
C(6)-C(15)-C(16)	112.4(7)	C(6)-C(15)-C(17)	111.5(6)
C(16)-C(15)-C(17)	111.9(6)	C(6)-C(15)-C(18)	111.9(5)
C(16)-C(15)-C(18)	102.5(5)	C(17)-C(15)-C(18)	106.2(7)
P(1)-Si(1)-C(19)	127.3(1)	P(1)-Si(1)-P(1A)	105.3(1)
C(19)-Si(1)-P(1A)	127.3(1)	Si(1)-C(19)-C(20)	119.7(4)
Si(1)-C(19)-C(20A)	119.7(4)	C(20)-C(19)-C(20A)	120.6(7)
C(19)-C(20)-C(21)	118.3(5)	C(19)-C(20)-C(23)	122.3(5)
C(21)-C(20)-C(23)	119.4(5)	C(20)-C(21)-C(22)	122.7(6)
C(21)-C(22)-C(24)	121.3(4)	C(21)-C(22)-C(21A)	117.5(8)
C(24)-C(22)-C(21A)	121.3(4)	P(1)-Li(1)-O(1)	108.1(4)
P(1)-Li(1)-P(1A)	82.4(4)	O(1)-Li(1)-P(1A)	149.5(2)
P(1)-Li(1)-O(1A)	149.5(2)	O(1)-Li(1)-O(1A)	77.7(9)
P(1A)-Li(1)-O(1A)	108.1(4)	Li(1)-O(1)-C(25)	117.0(13)
Li(1)-O(1)-C(26)	126.6(8)	C(25)-O(1)-C(26)	105.8(13)
O(1)-C(25)-C(25A)	107.7(11)	C(27)-C(28)-C(28A)	107.7(30)

Table 4. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
P(1)	74(1)	47(1)	61(1)	9(1)	37(1)	2(1)
C(1)	53(3)	49(3)	53(3)	4(3)	29(3)	-3(3)
C(2)	51(3)	54(3)	55(3)	1(3)	28(3)	-2(3)
C(3)	58(4)	64(4)	68(4)	-6(3)	31(3)	8(3)
C(4)	65(4)	64(4)	65(4)	3(3)	32(4)	10(3)
C(5)	52(4)	75(4)	62(4)	-6(3)	25(3)	-8(3)
C(6)	60(4)	50(3)	66(4)	-1(3)	36(3)	-6(3)
C(7)	51(4)	91(5)	67(4)	-2(4)	33(3)	-1(4)
C(8)	57(4)	121(6)	87(5)	-29(4)	34(4)	-15(5)
C(9)	68(5)	139(7)	108(6)	16(5)	50(5)	-5(5)
C(10)	67(5)	164(8)	97(6)	-10(5)	45(4)	26(5)
C(11)	86(6)	102(6)	83(5)	22(5)	26(5)	38(5)
C(12)	184(28)	89(16)	124(20)	73(18)	43(18)	20(13)
C(13)	58(13)	149(26)	177(32)	17(14)	-23(18)	48(24)
C(14)	103(19)	274(43)	126(23)	26(24)	45(20)	137(27)
C(12A)	220(39)	88(20)	118(28)	-57(22)	-33(26)	68(20)
C(13A)	136(33)	177(38)	157(32)	108(31)	83(30)	69(28)
C(14A)	177(34)	153(22)	35(9)	86(22)	10(13)	27(11)
C(15)	75(4)	63(4)	83(5)	-16(4)	43(4)	-10(4)
C(16)	117(6)	56(4)	118(6)	-24(4)	67(5)	-15(4)
C(17)	107(6)	94(6)	110(6)	-39(5)	70(5)	-17(5)
C(18)	88(5)	104(6)	113(6)	-44(5)	48(5)	-29(5)
Si(1)	60(1)	43(1)	53(1)	0	28(1)	0
C(19)	69(6)	49(5)	69(5)	0	44(5)	0
C(20)	81(4)	54(4)	60(4)	9(3)	39(4)	-1(3)
C(21)	129(7)	56(4)	81(5)	32(4)	63(5)	12(4)
C(22)	149(10)	45(5)	84(7)	0	80(8)	0
C(23)	76(5)	90(5)	82(5)	25(4)	35(4)	1(4)
C(24)	227(14)	40(5)	144(11)	0	124(11)	0
Li(1)	155(18)	40(8)	114(15)	0	81(14)	0
O(1)	306(12)	95(5)	175(8)	54(6)	89(8)	16(5)
C(25)	370(23)	67(6)	195(14)	26(10)	154(12)	-2(8)
C(26)	327(20)	324(22)	302(19)	90(16)	258(18)	29(16)

The anisotropic displacement exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(3)	-423	3650	-590	100
H(5)	-1998	2262	-1277	100
H(8A)	722	3728	1498	100
H(8B)	879	2850	1977	100
H(8C)	1372	3255	1790	100
H(9A)	1327	1935	987	100
H(9B)	791	1521	1082	100
H(9C)	654	1654	129	100
H(10A)	498	3851	-13	100
H(10B)	1132	3329	296	100
H(10C)	451	3038	-542	100
H(16A)	-694	272	572	100
H(16B)	-1334	-274	36	100
H(16C)	-1056	157	-467	100
H(17A)	-1267	1198	1154	100
H(17B)	-1943	1600	417	100
H(17C)	-1888	624	583	100
H(18A)	-2375	350	-1007	100
H(18B)	-2441	1329	-1159	100
H(18C)	-2098	784	-1510	100
H(21)	-937	5119	1443	100
H(23A)	-1529	3885	782	100
H(23B)	-1101	3132	821	100
H(23C)	-1320	3160	1485	100
H(25A)	462	-1942	2368	200
H(25B)	-155	-1434	1640	200
H(26A)	993	-1285	2010	200
H(26B)	465	-653	1300	200
H(26C)	1127	-311	2134	200

% probability level
without H-atoms

'3c

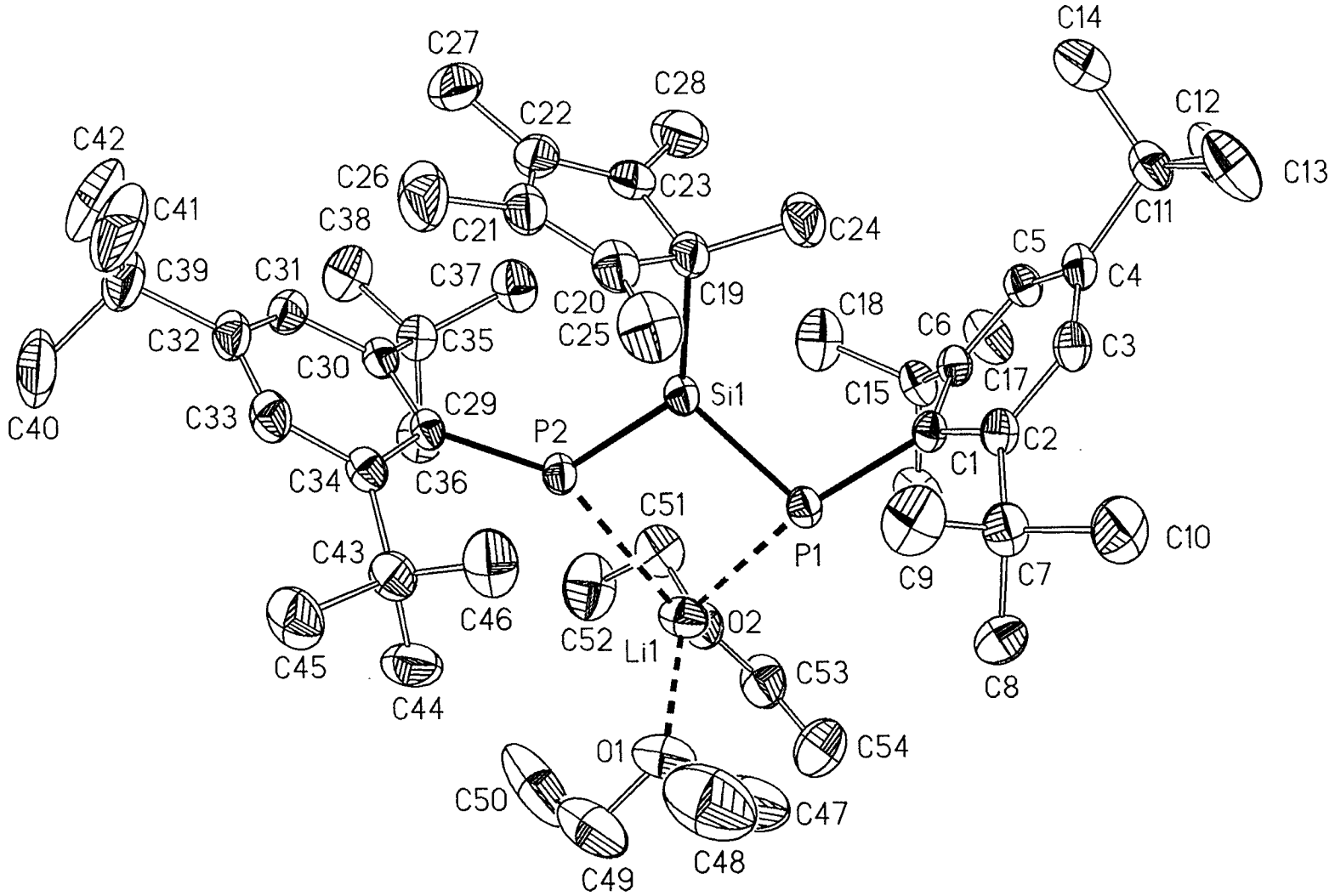
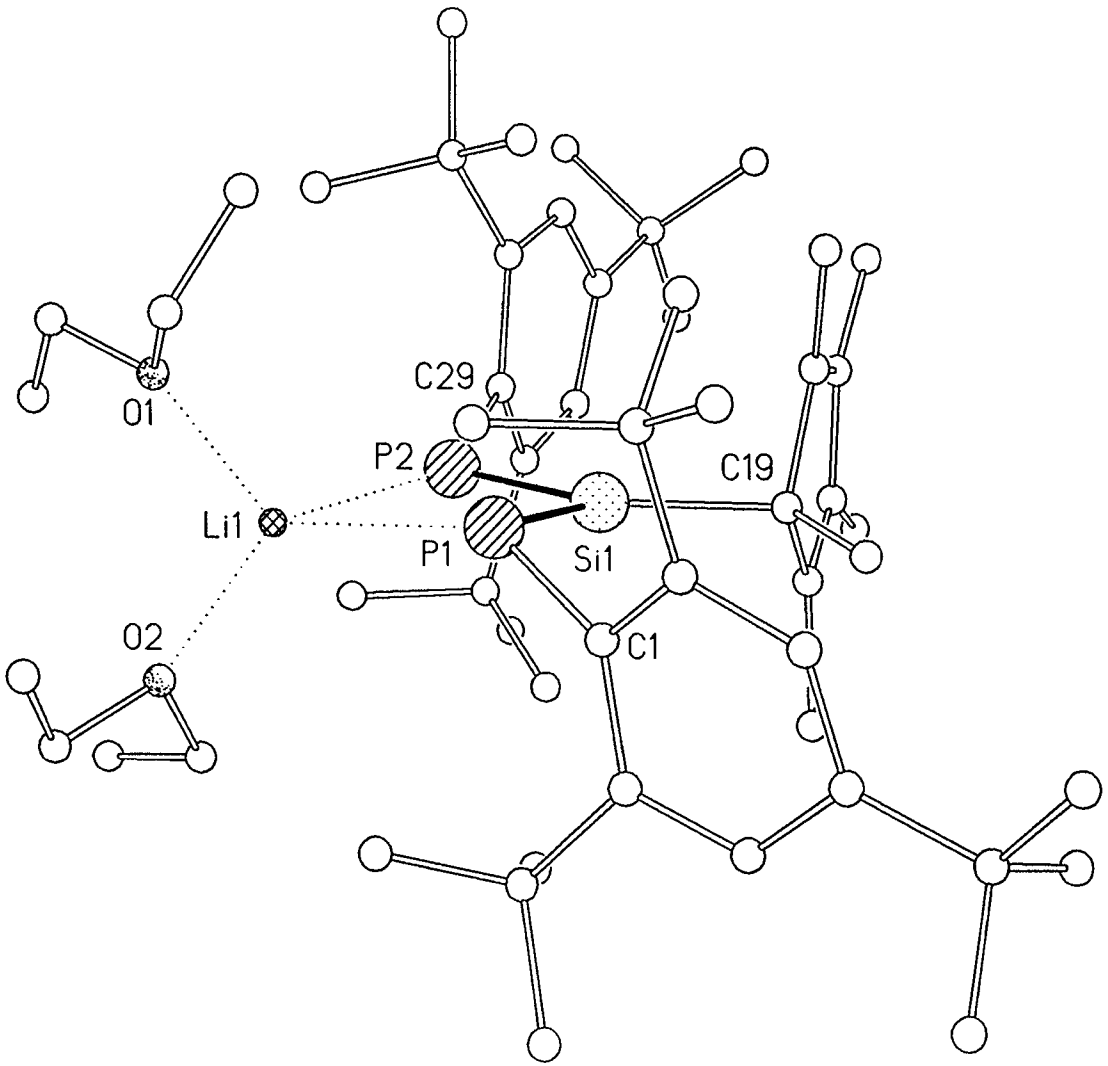


Table 1. Crystal data and structure refinement for MN13

Identification code	MN13
Empirical formula	C54 H93 O2 Si P2 Li C46 H73 P2 Si - (C4 H10 O)2 Li
Formula weight	871.3
Temperature	293(2) K
Wavelength	0.71073 A (MoKa)
Crystal system, space group	triclinic, P-1 (no.2)
Unit cell dimensions	a = 12.436(2) A alpha = 91.05(1) deg. b = 14.703(3) A beta = 95.95(1) deg. c = 14.703(3) A gamma = 93.66(1)deg.
Volume	2857.9 A^3
Z, Calculated density	2, 1.01 Mg/m^3
Absorption coefficient	0.13 mm^-1
F(000)	960
Crystal size	0.90 x 0.90 x 0.90 mm
Theta range for data collection	3 to 25 deg.
Index ranges	-14<=h<=14, -17<=k<=17, 0<=l<=22
Reflections collected / unique	10188 / 9802 [R(int) = 0.034]
Absorption correction	None
Refinement method	Full-matrix least-squares on F
Data / parameters	7556 [I>2sigma(I)] / 541
Goodness-of-fit on F^2	1.72
shift/esd (max./mean)	0.006 / 0.000
Final R indices [I>2sigma(I)]	R1 = 0.066, Rw = 0.072
weighting scheme	w = (s^2(F) + 0.0010 F^2)^-1
Largest diff. peak and hole	0.81 and -0.31 e.A^-3


O1
C29
P2
C19
Li1
P1
Si1
O2
C1

Tab. 1. Atomkoordinaten ($x10^4$) und äquivalente isotrope Thermalparameter ($pm^2 x10^{-1}$)

	x	y	z	U(eq)
Si(1)	1353(1)	2811(1)	2499(1)	41(1)
P(1)	1239(1)	1538(1)	3129(1)	44(1)
P(2)	2502(1)	3616(1)	3341(1)	43(1)
C(1)	-123(2)	949(2)	2782(2)	41(1)
C(2)	-214(2)	217(2)	2175(2)	46(1)
C(3)	-1205(2)	13(2)	1696(2)	49(1)
C(4)	-2131(2)	460(2)	1810(2)	46(1)
C(5)	-2062(2)	1041(2)	2518(2)	47(1)
C(6)	-1107(2)	1266(2)	3040(2)	41(1)
C(7)	730(3)	-404(2)	2031(2)	60(1)
C(8)	1295(3)	-675(3)	2885(3)	79(2)
C(9)	1539(4)	51(3)	1473(3)	90(2)
C(10)	292(4)	-1314(3)	1574(3)	95(2)
C(11)	-3190(3)	310(2)	1226(2)	61(1)
C(12)	-4148(3)	108(4)	1748(3)	100(2)
C(13)	-3188(3)	-486(3)	593(3)	99(2)
C(14)	-3402(4)	1174(4)	748(4)	128(3)
C(15)	-1202(2)	1785(2)	3894(2)	50(1)
C(16)	-494(3)	1389(3)	4618(2)	70(1)
C(17)	-2368(3)	1651(3)	4151(2)	74(1)
C(18)	-932(4)	2805(3)	3854(3)	82(2)
C(19)	586(3)	3080(2)	1401(2)	56(1)
C(20)	1489(3)	3206(3)	845(2)	62(1)
C(21)	1638(3)	4095(3)	685(2)	67(1)
C(22)	845(3)	4611(3)	1074(2)	68(1)
C(23)	199(3)	4017(3)	1472(2)	61(1)
C(24)	-291(3)	2337(3)	1081(2)	77(1)
C(25)	2028(4)	2410(3)	483(3)	92(2)
C(26)	2463(4)	4522(4)	150(3)	104(2)
C(27)	775(4)	5613(3)	989(3)	97(2)
C(28)	-827(3)	4209(3)	1861(3)	90(2)
C(29)	3220(2)	4602(2)	2850(2)	40(1)
C(30)	2843(2)	5492(2)	2937(2)	45(1)
C(31)	3269(3)	6194(2)	2456(2)	55(1)
C(32)	4081(3)	6080(2)	1935(2)	58(1)
C(33)	4521(3)	5254(2)	1953(2)	59(1)
C(34)	4164(2)	4511(2)	2409(2)	48(1)
C(35)	2088(3)	5780(2)	3608(2)	55(1)
C(36)	2627(3)	5561(3)	4497(2)	72(1)
C(37)	929(3)	5328(3)	3464(3)	74(1)
C(38)	1942(4)	6810(3)	3620(3)	80(2)
C(39)	4528(4)	6867(3)	1409(3)	82(2)
C(40)	5735(5)	7077(4)	1734(4)	148(3)
C(41)	4479(6)	6589(4)	490(3)	139(3)
C(42)	3972(6)	7739(3)	1505(4)	145(3)
C(43)	4865(3)	3681(3)	2468(2)	63(1)
C(44)	5168(3)	3481(3)	3405(3)	90(2)
C(45)	5959(3)	3866(3)	2091(3)	89(2)
C(46)	4316(3)	2840(3)	1978(3)	89(2)
Li(1)	2470(4)	2323(4)	4477(3)	63(2)
O(1)	3796(2)	1700(3)	4730(2)	96(1)
C(47)	3752(5)	697(6)	4401(5)	151(4)
C(48)	4268(6)	702(6)	3671(5)	176(5)
C(49)	4747(4)	2000(6)	5236(4)	131(3)

C(50)	4635(5)	2863(7)	5662(4)	170(4)
O(2)	1920(2)	2600(2)	5598(1)	64(1)
C(51)	1465(3)	3477(3)	5672(3)	82(2)
C(52)	2074(5)	4102(4)	6337(3)	120(3)
C(53)	1726(4)	2039(3)	6298(3)	91(2)
C(54)	2030(5)	1119(4)	6154(4)	117(2)

* äquivalente isotrope U berechnet als ein Drittel der Spur des orthogonalen U_{ij} Tensors

Tab. 2. Bindungsabstände (pm)

Si(1)-P(1)	213.8 (1)	Si(1)-P(2)	213.0 (1)
Si(1)-C(19)	194.6 (3)	P(1)-C(1)	187.7 (3)
P(1)-Li(1)	268.2 (5)	P(2)-C(29)	187.4 (3)
P(2)-Li(1)	263.7 (6)	C(1)-C(2)	141.7 (4)
C(1)-C(6)	143.1 (4)	C(2)-C(3)	138.9 (4)
C(2)-C(7)	156.5 (5)	C(3)-C(4)	138.9 (4)
C(4)-C(5)	138.4 (4)	C(4)-C(11)	152.8 (4)
C(5)-C(6)	139.1 (4)	C(6)-C(15)	155.3 (4)
C(7)-C(8)	152.2 (5)	C(7)-C(9)	153.4 (6)
C(7)-C(10)	154.8 (5)	C(11)-C(12)	153.4 (6)
C(11)-C(13)	152.4 (6)	C(11)-C(14)	151.1 (7)
C(15)-C(16)	151.5 (5)	C(15)-C(17)	154.7 (5)
C(15)-C(18)	152.0 (5)	C(19)-C(20)	149.9 (5)
C(19)-C(23)	149.4 (5)	C(19)-C(24)	153.4 (5)
C(20)-C(21)	134.0 (5)	C(20)-C(25)	151.6 (6)
C(21)-C(22)	146.0 (6)	C(21)-C(26)	150.7 (6)
C(22)-C(23)	135.4 (5)	C(22)-C(27)	148.8 (6)
C(23)-C(28)	151.1 (6)	C(29)-C(30)	142.7 (4)
C(29)-C(34)	143.7 (4)	C(30)-C(31)	140.1 (4)
C(30)-C(35)	155.6 (4)	C(31)-C(32)	138.2 (5)
C(32)-C(33)	136.3 (5)	C(32)-C(39)	154.4 (5)
C(33)-C(34)	139.3 (5)	C(34)-C(43)	154.2 (5)
C(35)-C(36)	153.7 (5)	C(35)-C(37)	154.0 (5)
C(35)-C(38)	153.7 (5)	C(39)-C(40)	154.5 (7)
C(39)-C(41)	149.1 (6)	C(39)-C(42)	150.7 (7)
C(43)-C(44)	152.5 (6)	C(43)-C(45)	155.1 (5)
C(43)-C(46)	152.9 (5)	Li(1)-O(1)	194.6 (7)
Li(1)-O(2)	200.3 (6)	O(1)-C(47)	155.0 (9)
O(1)-C(49)	139.8 (6)	C(47)-C(48)	137.3 (11)
C(49)-C(50)	144.6 (12)	O(2)-C(51)	144.8 (5)
O(2)-C(53)	142.1 (5)	C(51)-C(52)	149.3 (7)
C(53)-C(54)	144.9 (8)		

Tab. 3. Bindungswinkel (°)

P(1)-Si(1)-P(2)	103.0(1)	P(1)-Si(1)-C(19)	125.7(1)
P(2)-Si(1)-C(19)	131.3(1)	Si(1)-P(1)-C(1)	108.5(1)
Si(1)-P(1)-Li(1)	88.5(1)	C(1)-P(1)-Li(1)	143.4(2)
Si(1)-P(2)-C(29)	115.8(1)	Si(1)-P(2)-Li(1)	89.9(1)
C(29)-P(2)-Li(1)	150.6(1)	P(1)-C(1)-C(2)	119.8(2)
P(1)-C(1)-C(6)	122.5(2)	C(2)-C(1)-C(6)	117.4(2)
C(1)-C(2)-C(3)	118.7(3)	C(1)-C(2)-C(7)	123.8(2)
C(3)-C(2)-C(7)	117.4(3)	C(2)-C(3)-C(4)	123.4(3)
C(3)-C(4)-C(5)	115.8(2)	C(3)-C(4)-C(11)	123.6(3)
C(5)-C(4)-C(11)	120.6(3)	C(4)-C(5)-C(6)	123.8(3)
C(1)-C(6)-C(5)	117.8(2)	C(1)-C(6)-C(15)	124.8(2)
C(5)-C(6)-C(15)	117.2(2)	C(2)-C(7)-C(8)	110.4(3)
C(2)-C(7)-C(9)	111.9(3)	C(8)-C(7)-C(9)	111.2(3)
C(2)-C(7)-C(10)	111.1(3)	C(8)-C(7)-C(10)	105.2(3)
C(9)-C(7)-C(10)	106.8(3)	C(4)-C(11)-C(12)	110.8(3)
C(4)-C(11)-C(13)	113.1(3)	C(12)-C(11)-C(13)	106.9(3)
C(4)-C(11)-C(14)	109.0(3)	C(12)-C(11)-C(14)	107.2(4)
C(13)-C(11)-C(14)	109.7(4)	C(6)-C(15)-C(16)	110.6(3)
C(6)-C(15)-C(17)	110.5(2)	C(16)-C(15)-C(17)	104.9(3)
C(6)-C(15)-C(18)	113.2(3)	C(16)-C(15)-C(18)	110.0(3)
C(17)-C(15)-C(18)	107.3(3)	Si(1)-C(19)-C(20)	102.4(2)
Si(1)-C(19)-C(23)	107.5(2)	C(20)-C(19)-C(23)	103.2(3)
Si(1)-C(19)-C(24)	113.0(2)	C(20)-C(19)-C(24)	114.4(3)
C(23)-C(19)-C(24)	115.1(3)	C(19)-C(20)-C(21)	108.7(3)
C(19)-C(20)-C(25)	122.5(3)	C(21)-C(20)-C(25)	128.5(3)
C(20)-C(21)-C(22)	110.3(3)	C(20)-C(21)-C(26)	126.4(4)
C(22)-C(21)-C(26)	123.3(4)	C(21)-C(22)-C(23)	108.1(3)
C(21)-C(22)-C(27)	123.4(4)	C(23)-C(22)-C(27)	128.5(4)
C(19)-C(23)-C(22)	109.6(3)	C(19)-C(23)-C(28)	122.7(3)
C(22)-C(23)-C(28)	127.5(4)	P(2)-C(29)-C(30)	119.3(2)
P(2)-C(29)-C(34)	122.9(2)	C(30)-C(29)-C(34)	117.8(2)
C(29)-C(30)-C(31)	118.7(3)	C(29)-C(30)-C(35)	124.8(3)
C(31)-C(30)-C(35)	116.1(3)	C(30)-C(31)-C(32)	123.1(3)
C(31)-C(32)-C(33)	116.6(3)	C(31)-C(32)-C(39)	121.8(3)
C(33)-C(32)-C(39)	121.4(3)	C(32)-C(33)-C(34)	124.8(3)
C(29)-C(34)-C(33)	117.6(3)	C(29)-C(34)-C(43)	124.6(3)
C(33)-C(34)-C(43)	117.6(3)	C(30)-C(35)-C(36)	107.9(3)
C(30)-C(35)-C(37)	114.2(3)	C(36)-C(35)-C(37)	110.6(3)
C(30)-C(35)-C(38)	112.6(3)	C(36)-C(35)-C(38)	106.3(3)
C(37)-C(35)-C(38)	105.0(3)	C(32)-C(39)-C(40)	108.0(4)
C(32)-C(39)-C(41)	110.7(4)	C(40)-C(39)-C(41)	107.1(5)
C(32)-C(39)-C(42)	113.6(4)	C(40)-C(39)-C(42)	106.9(4)
C(41)-C(39)-C(42)	110.4(4)	C(34)-C(43)-C(44)	109.0(3)
C(34)-C(43)-C(45)	112.6(3)	C(44)-C(43)-C(45)	105.2(3)
C(34)-C(43)-C(46)	112.9(3)	C(44)-C(43)-C(46)	111.5(3)
C(45)-C(43)-C(46)	105.4(3)	P(1)-Li(1)-P(2)	77.8(2)
P(1)-Li(1)-O(1)	111.2(3)	P(2)-Li(1)-O(1)	116.9(3)
P(1)-Li(1)-O(2)	124.0(3)	P(2)-Li(1)-O(2)	118.4(3)
O(1)-Li(1)-O(2)	106.8(3)	Li(1)-O(1)-C(47)	115.5(3)
Li(1)-O(1)-C(49)	129.0(4)	C(47)-O(1)-C(49)	115.1(5)
O(1)-C(47)-C(48)	106.6(6)	O(1)-C(49)-C(50)	111.6(5)
Li(1)-O(2)-C(51)	115.7(3)	Li(1)-O(2)-C(53)	131.6(3)
C(51)-O(2)-C(53)	111.8(3)	O(2)-C(51)-C(52)	113.9(4)
O(2)-C(53)-C(54)	111.3(4)		

Tab. 4. Anisotrope Thermalparameter ($pm^2 x 10^{-1}$)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si(1)	39(1)	45(1)	38(1)	0(1)	5(1)	-4(1)
P(1)	38(1)	45(1)	48(1)	2(1)	5(1)	-3(1)
P(2)	43(1)	46(1)	39(1)	2(1)	4(1)	-6(1)
C(1)	39(1)	39(1)	44(1)	2(1)	10(1)	-2(1)
C(2)	48(2)	43(2)	48(2)	-3(1)	12(1)	-3(1)
C(3)	54(2)	44(2)	49(2)	-11(1)	12(1)	-5(1)
C(4)	47(2)	46(2)	45(2)	-2(1)	7(1)	-11(1)
C(5)	41(1)	50(2)	49(2)	-4(1)	9(1)	1(1)
C(6)	41(1)	42(1)	40(1)	-1(1)	9(1)	-2(1)
C(7)	56(2)	54(2)	73(2)	-13(2)	16(2)	5(1)
C(8)	80(3)	55(2)	103(3)	2(2)	3(2)	20(2)
C(9)	91(3)	88(3)	102(3)	-4(2)	55(3)	23(2)
C(10)	90(3)	64(2)	129(4)	-41(2)	8(3)	17(2)
C(11)	54(2)	72(2)	52(2)	-7(2)	-4(1)	-10(2)
C(12)	53(2)	151(4)	92(3)	-27(3)	6(2)	-22(2)
C(13)	71(3)	135(4)	83(3)	-43(3)	-4(2)	-15(3)
C(14)	106(4)	126(4)	133(5)	34(4)	-59(3)	-25(3)
C(15)	42(1)	61(2)	48(2)	-12(1)	12(1)	-3(1)
C(16)	61(2)	105(3)	46(2)	-9(2)	11(2)	-1(2)
C(17)	53(2)	107(3)	62(2)	-24(2)	21(2)	-1(2)
C(18)	99(3)	67(2)	81(3)	-28(2)	37(2)	-3(2)
C(19)	60(2)	61(2)	42(2)	5(1)	-5(1)	-14(1)
C(20)	69(2)	78(2)	37(2)	-1(1)	1(1)	-12(2)
C(21)	71(2)	81(2)	43(2)	10(2)	-7(2)	-22(2)
C(22)	78(2)	66(2)	53(2)	12(2)	-21(2)	-11(2)
C(23)	56(2)	72(2)	51(2)	9(2)	-12(1)	2(2)
C(24)	81(3)	85(3)	57(2)	8(2)	-14(2)	-29(2)
C(25)	105(3)	106(3)	64(2)	-23(2)	19(2)	-2(3)
C(26)	107(3)	127(4)	72(3)	24(3)	7(2)	-45(3)
C(27)	120(4)	74(3)	85(3)	20(2)	-35(3)	-9(2)
C(28)	69(2)	110(3)	89(3)	13(3)	-6(2)	14(2)
C(29)	37(1)	47(1)	35(1)	-2(1)	4(1)	-6(1)
C(30)	43(1)	51(2)	42(1)	-1(1)	4(1)	-4(1)
C(31)	65(2)	47(2)	52(2)	2(1)	5(1)	-2(1)
C(32)	61(2)	64(2)	48(2)	8(1)	9(1)	-15(2)
C(33)	51(2)	74(2)	52(2)	5(2)	17(1)	-7(2)
C(34)	42(1)	60(2)	41(1)	-1(1)	7(1)	-1(1)
C(35)	59(2)	53(2)	53(2)	-5(1)	14(1)	2(1)
C(36)	91(3)	77(2)	49(2)	-12(2)	17(2)	-1(2)
C(37)	55(2)	75(2)	95(3)	-10(2)	26(2)	9(2)
C(38)	103(3)	60(2)	83(3)	-11(2)	29(2)	12(2)
C(39)	99(3)	80(3)	68(2)	20(2)	19(2)	-23(2)
C(40)	135(5)	153(5)	143(5)	59(4)	1(4)	-84(4)
C(41)	213(7)	123(4)	80(3)	32(3)	46(4)	-49(4)
C(42)	210(7)	80(3)	158(6)	50(4)	83(5)	3(4)
C(43)	46(2)	70(2)	75(2)	4(2)	19(2)	9(2)
C(44)	62(2)	116(4)	96(3)	30(3)	10(2)	31(2)
C(45)	58(2)	104(3)	112(3)	0(3)	37(2)	13(2)
C(46)	74(3)	74(3)	125(4)	-22(2)	39(3)	9(2)
Li(1)	55(3)	82(4)	54(3)	10(3)	6(2)	13(3)
O(1)	71(2)	118(3)	100(2)	10(2)	-6(2)	33(2)
C(47)	96(4)	215(8)	150(6)	38(6)	11(4)	59(5)
C(48)	118(5)	281(11)	137(6)	14(7)	29(5)	44(6)
C(49)	67(3)	220(8)	104(4)	21(5)	-3(3)	11(4)
C(50)	76(4)	325(12)	96(4)	-12(6)	-4(3)	-61(5)

O(2)	62(1)	77(2)	52(1)	8(1)	10(1)	-8(1)
C(51)	80(3)	92(3)	75(3)	-9(2)	17(2)	6(2)
C(52)	149(5)	109(4)	99(4)	-26(3)	19(4)	-16(4)
C(53)	92(3)	115(4)	63(2)	25(2)	6(2)	-24(3)
C(54)	126(4)	108(4)	116(4)	51(3)	17(3)	-9(3)

der Temperaturfaktorexponent hat die Form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Tab. 5. H-Atomkoordinaten ($x10^4$) und isotrope Thermalparameter ($pm^2 x10^{-1}$)

	x	y	z	U
H(3)	-1252	-467	1270	60
H(5)	-2709	1309	2652	60
H(8A)	1590	-137	3203	100
H(8B)	780	-999	3200	100
H(8C)	1869	-1059	2789	100
H(9A)	1822	621	1739	100
H(9B)	2122	-337	1419	100
H(9C)	1182	157	917	100
H(10A)	-221	-1618	1907	100
H(10B)	-57	-1199	1017	100
H(10C)	883	-1693	1519	100
H(12A)	-4195	596	2154	150
H(12B)	-4814	30	1380	150
H(12C)	-4023	-445	2046	150
H(13A)	-2611	-378	239	150
H(13B)	-3077	-1031	907	150
H(13C)	-3867	-556	241	150
H(14A)	-2810	1311	416	150
H(14B)	-4065	1094	376	150
H(14C)	-3451	1667	1148	150
H(16A)	251	1450	4506	100
H(16B)	-574	1702	5146	100
H(16C)	-715	755	4659	100
H(17A)	-2419	1977	4677	100
H(17B)	-2867	1877	3710	100
H(17C)	-2543	1014	4221	100
H(18A)	-211	2916	3698	100
H(18B)	-1439	3056	3434	100
H(18C)	-984	3088	4401	100
H(24A)	-640	2504	539	100
H(24B)	36	1768	1017	100
H(24C)	-817	2273	1484	100
H(25A)	2581	2628	141	100
H(25B)	2347	2070	948	100
H(25C)	1495	2024	139	100
H(26A)	2899	4057	-36	100
H(26B)	2100	4797	-339	100
H(26C)	2916	4979	483	100
H(27A)	192	5798	1294	100
H(27B)	1442	5924	1229	100
H(27C)	637	5762	399	100
H(28A)	-1279	4561	1481	100
H(28B)	-1211	3642	1966	100
H(28C)	-637	4542	2390	100
H(31)	2978	6782	2489	60
H(33)	5127	5180	1632	60
H(36A)	3346	5851	4572	100
H(36B)	2215	5783	4931	100
H(36C)	2665	4913	4542	100
H(37A)	604	5475	2908	100
H(37B)	956	4679	3502	100
H(37C)	506	5548	3891	100
H(38A)	2641	7135	3709	100
H(38B)	1579	6971	3081	100

H(38C)	1519	6968	4070	100
H(40A)	6035	7570	1424	150
H(40B)	5796	7241	2331	150
H(40C)	6122	6543	1654	150
H(41A)	3734	6462	273	150
H(41B)	4791	7073	174	150
H(41C)	4868	6052	431	150
H(42A)	3215	7648	1306	150
H(42B)	4053	7919	2098	150
H(42C)	4301	8207	1181	150
H(44A)	4527	3358	3686	100
H(44B)	5600	2962	3446	100
H(44C)	5578	4003	3674	100
H(45A)	5825	3994	1495	100
H(45B)	6354	4380	2387	100
H(45C)	6375	3339	2159	100
H(46A)	3627	2684	2179	100
H(46B)	4212	2966	1380	100
H(46C)	4772	2340	2065	100
H(47A)	3010	476	4270	150
H(47B)	4092	317	4825	150
H(48A)	4248	91	3440	150
H(48B)	3920	1086	3256	150
H(48C)	5008	927	3814	150
H(49A)	5347	2047	4899	150
H(49B)	4906	1568	5674	150
H(50A)	5292	3057	6011	150
H(50B)	4490	3300	5226	150
H(50C)	4045	2817	6009	150
H(51A)	733	3379	5809	150
H(51B)	1449	3769	5131	150
H(52A)	1746	4673	6369	150
H(52B)	2081	3813	6880	150
H(52C)	2803	4206	6196	150
H(53A)	972	2033	6383	150
H(53B)	2140	2282	6810	150
H(54A)	1887	745	6628	150
H(54B)	1608	875	5647	150
H(54C)	2786	1127	6077	150