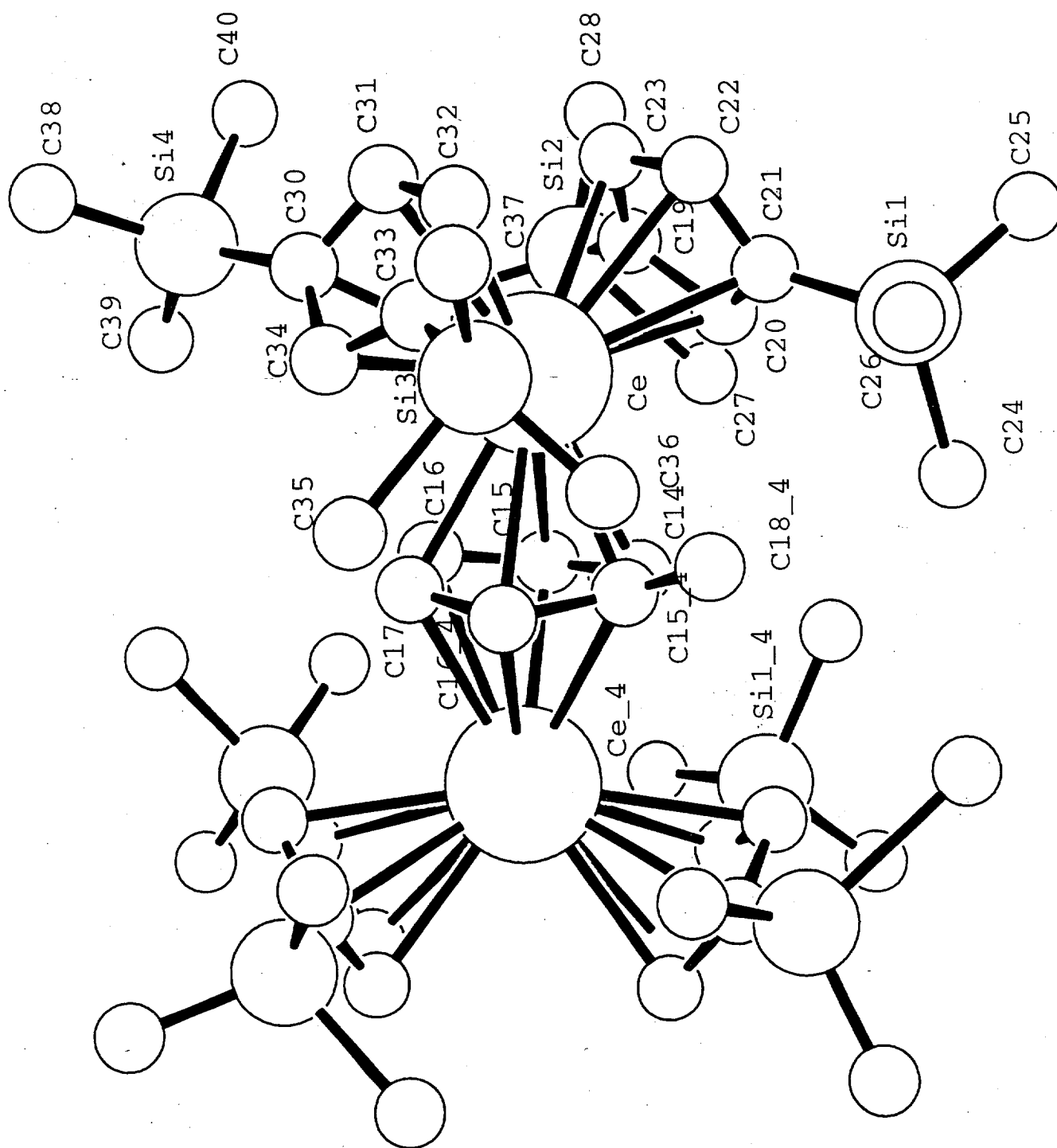
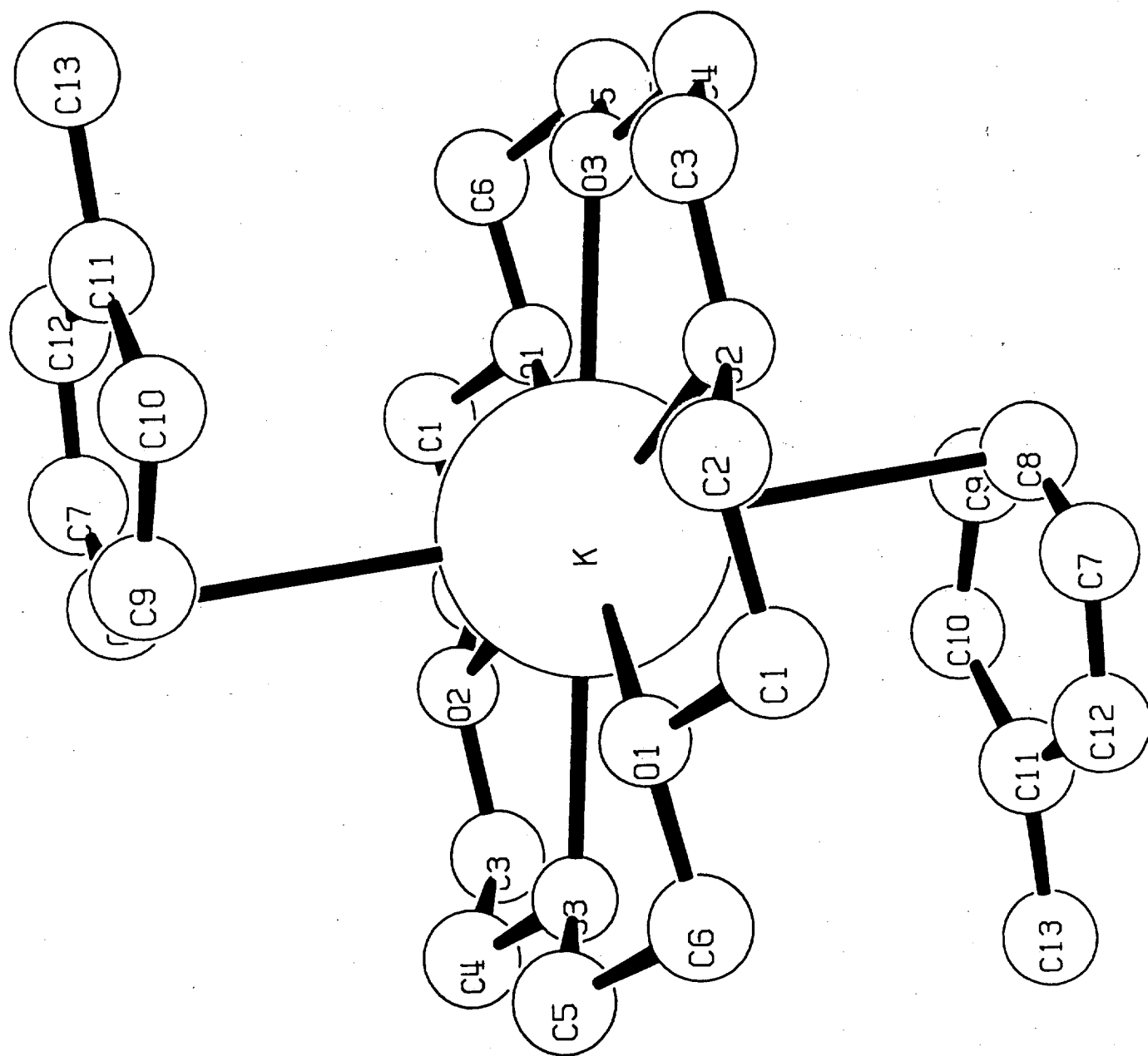






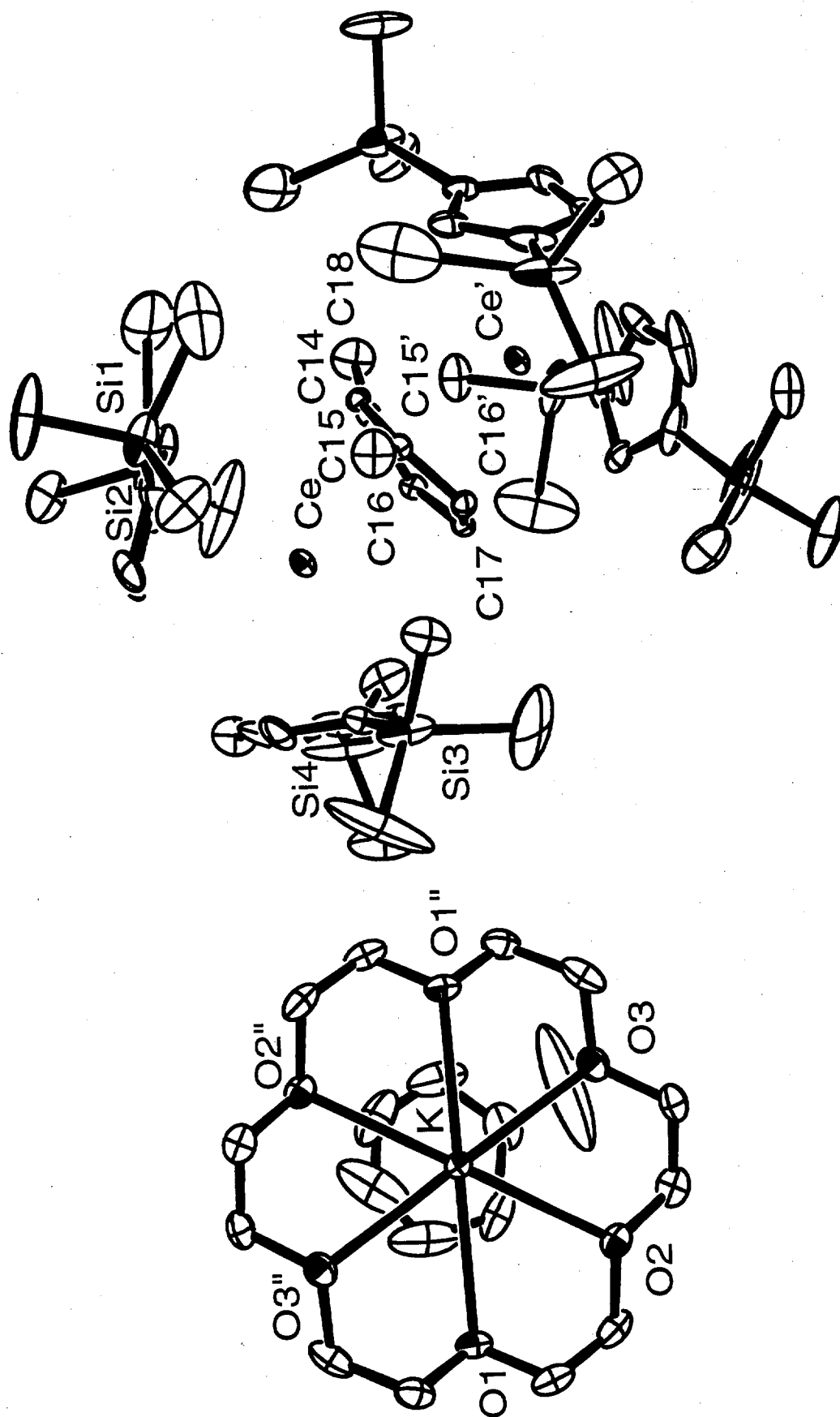


Table 1. Crystal data and structure refinement for

[CeCp ² (toluene)CeCp ²][K(18crown6)(toluene)2].toluene			1 a
Identification code	C84 H140 Ce2 K O6 Si8		
Empirical formula	1790.02		
Formula weight	180(2) K		
Temperature	0.71073 Å		
Wavelength	Monoclinic		
Crystal system	C2/c		
Space group	a = 11.9825(10) Å		α = 90°.
Unit cell dimensions	b = 33.5451(10) Å		β = 101.064(10)°.
	c = 26.302(2) Å		γ = 90°.
	10375.6(12) Å ³		
Volume	4		
Z	1.15 Mg/m ³		
Density (calculated)	1.04 mm ⁻¹		
Absorption coefficient	3756		
F(000)	0.25 x 0.25 x 0.20 mm ³		
Crystal size	1.21 to 28.68°.		
Theta range for data collection	-15<=h<=15, -23<=k<=45, -35<=l<=30		
Index ranges	30358		
Reflections collected	11872 [R(int) = 0.057]		
Independent reflections	5618		
Reflections with I>2sigma(I)	Empirical		
Absorption correction	0.928 and 0.623		
Tmax. and Tmin.	Full-matrix least-squares on F ²		
Refinement method	11869 / 0 / 443		
Data / restraints / parameters	1.02		
Goodness-of-fit on F ²	R1 = 0.097, wR2 = 0.275		
Final R indices [I>2sigma(I)]	R1 = 0.184, wR2 = 0.344		
R indices (all data)	1.90 and -1.70 e.Å ⁻³		
Largest diff. peak and hole	Data collection Siemens SMART area detector		
Data collection	Refinement using SHELXL-93		
Refinement	Drawing using ORTEP-3 for Windows		

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{C}_{22}\text{H}_{16}\text{CeK}$. U(eq) is defined as one third of the trace of the orthogonalized U^i tensor.

	x	y	z	U(eq)
Ce	-76(1)	108(1)	1587(1)	65(1)
K	2500	2500	0	91(1)
Si(1)	1346(3)	-1012(2)	1373(2)	148(2)
Si(2)	-3289(3)	-458(2)	1137(3)	235(5)
Si(3)	2992(3)	691(2)	1495(3)	169(3)
Si(4)	-1783(5)	1128(3)	996(5)	366(9)
O(1)	3054(6)	3120(3)	-609(3)	95(2)
O(2)	3290(7)	3223(2)	461(4)	95(2)
O(3)	2304(7)	2652(3)	1017(3)	104(2)
C(1)	3739(12)	3421(4)	-353(7)	122(5)
C(2)	3284(12)	3544(4)	99(7)	122(5)
C(3)	2900(12)	3302(5)	916(7)	120(5)
C(4)	2953(12)	2984(5)	1255(5)	116(5)
C(5)	2274(15)	2294(6)	1322(6)	148(7)
C(6)	3500(13)	3003(5)	-1034(6)	121(5)
C(7)	-702(30)	2514(9)	-376(21)	231(29)
C(8)	-290(43)	2707(22)	-651(17)	358(45)
C(9)	-30(19)	3053(17)	-614(23)	297(33)
C(10)	-40(21)	3241(8)	-172(15)	175(15)
C(11)	-543(19)	3005(13)	197(10)	172(10)
C(12)	-910(20)	2625(14)	66(19)	230(23)
C(13)	-842(28)	3145(27)	655(17)	858(103)
C(14)	0	-297(4)	2500	57(3)
C(15)	-1052(8)	-98(3)	2477(4)	64(2)
C(16)	-1047(7)	327(3)	2401(3)	64(2)
C(17)	0	524(4)	2500	66(3)
C(18)	-1964(22)	-262(13)	2614(15)	155(13)
C(19)	-1745(11)	-454(6)	1065(8)	160(9)
C(20)	-909(9)	-698(4)	1387(5)	105(4)
C(21)	102(9)	-685(4)	1183(5)	92(4)
C(22)	-138(16)	-450(5)	745(6)	132(6)

C(23)	-1209(20)	-303(6)	683(6)	146(7)
C(24)	1260(29)	-1223(10)	2085(10)	379(29)
C(25)	1213(14)	-1447(7)	946(10)	286(19)
C(26)	2710(13)	-787(7)	1358(10)	215(11)
C(27)	-3280(30)	-993(11)	1733(15)	391(28)
C(28)	-4103(14)	-628(7)	493(8)	201(10)
C(29)	-3703(18)	2(10)	1312(20)	474(43)
C(30)	-447(14)	862(6)	1093(9)	152(10)
C(31)	-191(18)	627(11)	733(9)	253(20)
C(32)	906(15)	516(6)	828(5)	139(7)
C(33)	1425(8)	694(4)	1277(4)	86(3)
C(34)	656(12)	907(3)	1460(5)	97(4)
C(35)	3124(27)	1091(13)	2080(14)	452(34)
C(36)	3637(11)	352(6)	1958(6)	148(6)
C(37)	3637(13)	850(16)	1035(11)	535(43)
C(38)	-1678(16)	1628(7)	771(11)	274(17)
C(39)	-2642(17)	1131(7)	1425(9)	201(9)
C(40)	-2877(16)	819(10)	443(11)	153(14)
C(41)	5000	2029(14)	2500	232(17)
C(42)	4133(27)	2124(11)	2731(12)	249(12)
C(43)	4179(23)	2568(9)	2708(10)	213(10)
C(44)	5000	2715(9)	2500	170(10)

Table 3. Bond lengths [Å] and angles [°] for 1a.

Ce-C(15)#1	2.663(9)
Ce-C(16)	2.728(8)
Ce-C(14)	2.745(6)
Ce-C(17)	2.765(7)
Ce-C(31)	2.82(2)
Ce-C(16)#1	2.839(9)
Ce-C(30)	2.84(2)
Ce-C(32)	2.855(12)
Ce-C(23)	2.855(15)
Ce-C(34)	2.861(11)
Ce-C(33)	2.887(10)
Ce-C(22)	2.888(13)
Ce-C(21)	2.886(11)
Ce-C(15)	2.894(10)
Ce-C(19)	2.895(14)
Ce-C(20)	2.895(12)
K-O(3)	2.776(9)
K-O(3)#2	2.776(9)
K-O(1)	2.781(7)
K-O(1)#2	2.781(7)
K-O(2)	2.794(8)
K-O(2)#2	2.794(8)
Si(1)-C(26)	1.81(2)
Si(1)-C(25)	1.83(2)
Si(1)-C(21)	1.840(12)
Si(1)-C(24)	2.03(3)
Si(2)-C(29)	1.71(2)
Si(2)-C(28)	1.87(2)
Si(2)-C(19)	1.90(2)
Si(2)-C(27)	2.38(4)
Si(3)-C(37)	1.64(2)
Si(3)-C(36)	1.74(2)
Si(3)-C(33)	1.855(10)
Si(3)-C(35)	2.03(3)

Si(4)-C(39)	1.66(2)
Si(4)-C(38)	1.79(2)
Si(4)-C(30)	1.807(14)
Si(4)-C(40)	2.04(3)
O(1)-C(6)	1.38(2)
O(1)-C(1)	1.39(2)
O(2)-C(3)	1.39(2)
O(2)-C(2)	1.438(15)
O(3)-C(4)	1.43(2)
O(3)-C(5)	1.45(2)
C(1)-C(2)	1.46(2)
C(3)-C(4)	1.38(2)
C(5)-C(6)#2	1.47(2)
C(6)-C(5)#2	1.47(2)
C(7)-C(8)	1.15(5)
C(7)-C(12)	1.29(5)
C(8)-C(9)	1.20(8)
C(9)-C(10)	1.32(7)
C(10)-C(11)	1.47(4)
C(11)-C(12)	1.37(4)
C(11)-C(13)	1.40(4)
C(14)-C(15)#1	1.417(11)
C(14)-C(15)	1.417(11)
C(14)-Ce#1	2.745(6)
C(15)-C(18)	1.33(3)
C(15)-C(16)	1.438(13)
C(15)-Ce#1	2.663(9)
C(16)-C(17)	1.398(11)
C(16)-Ce#1	2.839(9)
C(17)-C(16)#1	1.398(11)
C(17)-Ce#1	2.765(7)
C(18)-Ce#1	3.16(3)
C(19)-C(23)	1.39(3)
C(19)-C(20)	1.44(2)
C(20)-C(21)	1.42(2)
C(21)-C(22)	1.38(2)

C(22)-C(23)	1.36(2)
C(30)-C(31)	1.31(4)
C(30)-C(34)	1.49(2)
C(31)-C(32)	1.34(3)
C(32)-C(33)	1.36(2)
C(33)-C(34)	1.33(2)
C(41)-C(42)#3	1.34(3)
C(41)-C(42)	1.34(3)
C(42)-C(43)	1.49(4)
C(43)-C(44)	1.31(3)
C(44)-C(43)#3	1.31(3)

O(3)-K-O(3)#2	180.0
O(3)-K-O(1)	119.4(3)
O(3)#2-K-O(1)	60.6(3)
O(3)-K-O(1)#2	60.6(3)
O(3)#2-K-O(1)#2	119.4(3)
O(1)-K-O(1)#2	180.0
O(3)-K-O(2)	60.4(3)
O(3)#2-K-O(2)	119.6(3)
O(1)-K-O(2)	60.2(3)
O(1)#2-K-O(2)	119.8(3)
O(3)-K-O(2)#2	119.6(3)
O(3)#2-K-O(2)#2	60.4(3)
O(1)-K-O(2)#2	119.8(3)
O(1)#2-K-O(2)#2	60.2(3)
O(2)-K-O(2)#2	180.0
C(26)-Si(1)-C(25)	107.0(11)
C(26)-Si(1)-C(21)	115.7(9)
C(25)-Si(1)-C(21)	109.8(7)
C(26)-Si(1)-C(24)	111.9(13)
C(25)-Si(1)-C(24)	105.9(14)
C(21)-Si(1)-C(24)	106.1(9)
C(29)-Si(2)-C(28)	113.0(15)
C(29)-Si(2)-C(19)	111.1(12)
C(28)-Si(2)-C(19)	105.1(8)

C(29)-Si(2)-C(27)	117.9(22)
C(28)-Si(2)-C(27)	107.5(11)
C(19)-Si(2)-C(27)	100.9(12)
C(37)-Si(3)-C(36)	121.3(11)
C(37)-Si(3)-C(33)	111.2(7)
C(36)-Si(3)-C(33)	120.6(6)
C(37)-Si(3)-C(35)	111.4(21)
C(36)-Si(3)-C(35)	86.7(15)
C(33)-Si(3)-C(35)	99.1(11)
C(39)-Si(4)-C(38)	108.0(13)
C(39)-Si(4)-C(30)	123.6(10)
C(38)-Si(4)-C(30)	113.1(9)
C(39)-Si(4)-C(40)	95.2(12)
C(38)-Si(4)-C(40)	108.4(14)
C(30)-Si(4)-C(40)	106.2(14)
C(6)-O(1)-C(1)	108.2(11)
C(6)-O(1)-K	115.2(8)
C(1)-O(1)-K	116.6(8)
C(3)-O(2)-C(2)	117.9(11)
C(3)-O(2)-K	113.5(8)
C(2)-O(2)-K	113.8(7)
C(4)-O(3)-C(5)	118.1(12)
C(4)-O(3)-K	115.2(8)
C(5)-O(3)-K	113.4(9)
O(1)-C(1)-C(2)	108.7(11)
O(2)-C(2)-C(1)	112.0(11)
C(4)-C(3)-O(2)	115.1(13)
C(3)-C(4)-O(3)	111.4(11)
O(3)-C(5)-C(6)#2	110.9(11)
O(1)-C(6)-C(5)#2	107.7(12)
C(8)-C(7)-C(12)	125.8(46)
C(7)-C(8)-C(9)	128.9(61)
C(8)-C(9)-C(10)	119.1(46)
C(9)-C(10)-C(11)	113.3(26)
C(12)-C(11)-C(10)	119.3(26)
C(12)-C(11)-C(13)	114.0(56)

C(10)-C(11)-C(13)	126.1(52)
C(7)-C(12)-C(11)	112.8(33)
C(15)#1-C(14)-C(15)	123.8(12)
C(18)-C(15)-C(14)	124.3(19)
C(18)-C(15)-C(16)	118.0(20)
C(14)-C(15)-C(16)	116.5(8)
C(17)-C(16)-C(15)	118.0(8)
C(16)-C(17)-C(16)#1	123.5(12)
C(23)-C(19)-C(20)	105.5(13)
C(23)-C(19)-Si(2)	132.1(17)
C(20)-C(19)-Si(2)	121.5(18)
C(21)-C(20)-C(19)	108.1(15)
C(22)-C(21)-C(20)	106.1(12)
C(22)-C(21)-Si(1)	126.5(11)
C(20)-C(21)-Si(1)	125.8(12)
C(23)-C(22)-C(21)	110.5(16)
C(22)-C(23)-C(19)	109.7(16)
C(31)-C(30)-C(34)	103.1(13)
C(31)-C(30)-Si(4)	121.2(21)
C(34)-C(30)-Si(4)	134.0(18)
C(30)-C(31)-C(32)	112.9(21)
C(31)-C(32)-C(33)	107.8(20)
C(34)-C(33)-C(32)	108.5(12)
C(34)-C(33)-Si(3)	128.6(11)
C(32)-C(33)-Si(3)	122.1(12)
C(33)-C(34)-C(30)	107.6(13)
C(42)#3-C(41)-C(42)	152.7(57)
C(41)-C(42)-C(43)	100.3(35)
C(44)-C(43)-C(42)	115.5(30)
C(43)-C(44)-C(43)#3	135.7(40)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2 #2 -x+1/2,-y+1/2,-z #3 -x+1,y,-z+1/2

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **12**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ce	58(1)	89(1)	49(1)	1(1)	13(1)	0(1)
K	123(3)	72(2)	75(2)	1(2)	15(2)	-21(2)
Si(1)	67(2)	132(4)	228(6)	-76(4)	-15(3)	19(2)
Si(2)	62(2)	273(8)	344(9)	-233(8)	-28(4)	29(3)
Si(3)	51(2)	167(4)	282(7)	131(5)	14(3)	5(2)
Si(4)	137(5)	334(10)	686(20)	390(13)	229(9)	147(6)
O(1)	78(5)	94(6)	114(6)	34(5)	18(4)	-3(4)
O(2)	83(5)	78(5)	118(6)	-3(5)	8(5)	9(4)
O(3)	93(5)	122(7)	91(5)	4(5)	6(4)	9(5)
C(1)	88(9)	82(9)	199(17)	39(10)	38(10)	0(8)
C(2)	98(9)	68(8)	184(15)	8(9)	-10(10)	-13(7)
C(3)	95(10)	114(11)	145(13)	-15(11)	13(9)	11(8)
C(4)	107(10)	148(14)	83(9)	-21(9)	-4(7)	0(10)
C(5)	135(13)	223(21)	89(10)	56(12)	33(9)	60(14)
C(6)	96(10)	154(14)	114(11)	40(10)	25(9)	-11(10)
C(7)	172(31)	94(14)	382(73)	-33(31)	-56(39)	47(16)
C(8)	303(51)	568(102)	246(35)	201(53)	163(37)	326(62)
C(9)	54(10)	399(63)	415(63)	277(52)	-16(21)	-28(23)
C(10)	102(15)	119(14)	287(38)	-76(22)	-8(20)	-1(12)
C(11)	84(12)	260(33)	171(20)	-35(21)	22(12)	22(15)
C(12)	76(12)	230(38)	352(56)	172(36)	-35(23)	-22(20)
C(13)	144(23)	2000(284)	382(52)	-635(111)	-66(29)	212(66)
C(14)	62(7)	47(6)	61(7)	0	13(6)	0
C(15)	67(6)	64(6)	58(5)	1(4)	8(4)	1(5)
C(16)	59(5)	70(6)	68(6)	7(5)	21(4)	17(5)
C(17)	103(11)	49(7)	49(7)	0	25(7)	0
C(18)	63(15)	204(35)	202(35)	18(29)	39(18)	-19(19)
C(19)	74(8)	208(20)	173(16)	-138(16)	-36(10)	34(10)
C(20)	69(7)	113(10)	123(10)	-62(8)	-6(7)	-14(7)
C(21)	63(6)	105(9)	104(9)	-45(7)	5(6)	21(6)
C(22)	168(15)	160(15)	76(9)	-29(9)	41(9)	59(13)

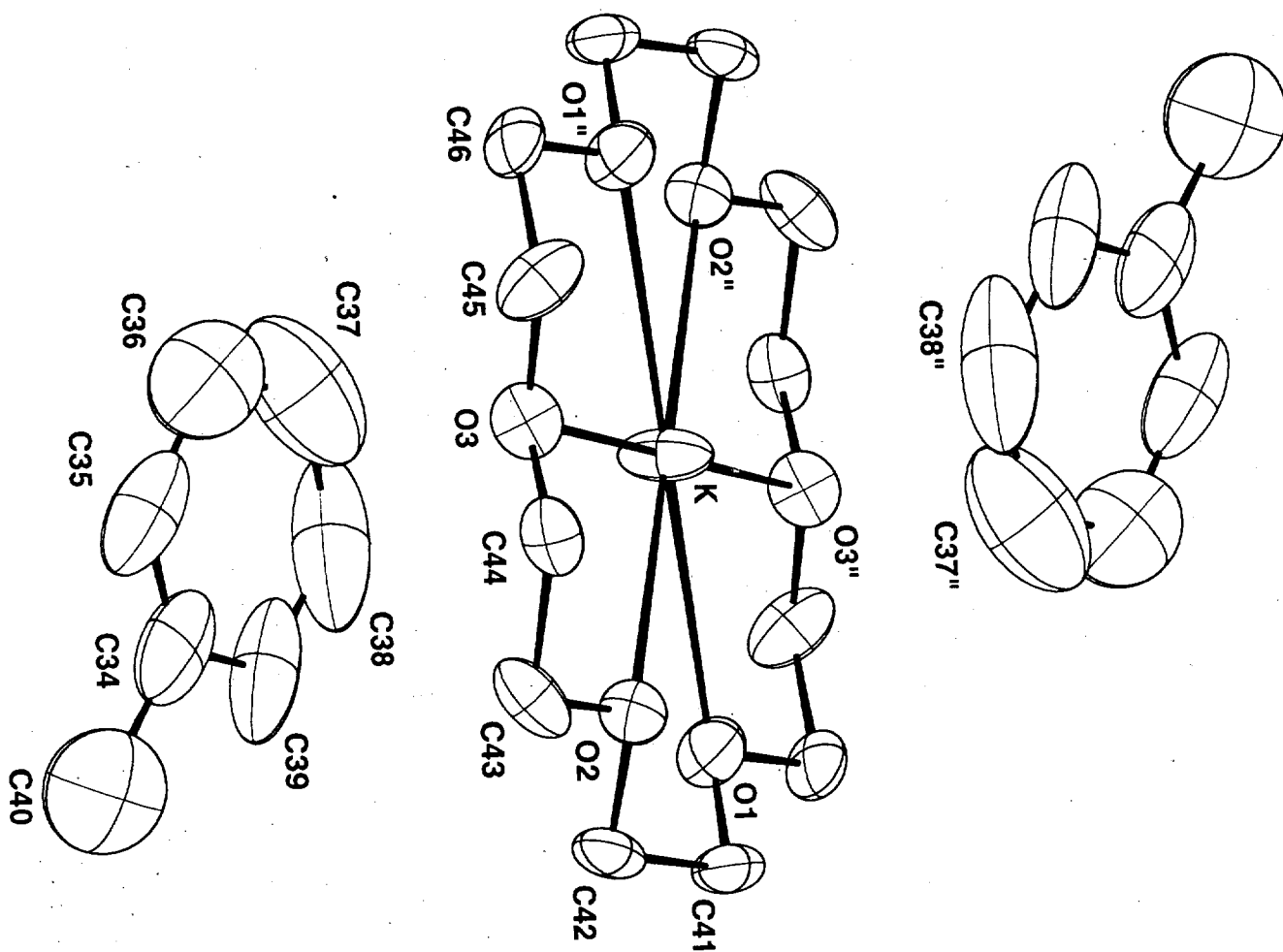
C(23)	199(20)	155(15)	68(9)	-33(10)	-16(11)	63(15)
C(24)	393(46)	355(45)	300(37)	-101(32)	-155(33)	265(41)
C(25)	107(12)	289(28)	415(35)	-277(28)	-70(17)	82(16)
C(26)	85(11)	172(19)	378(34)	-3(22)	21(16)	26(12)
C(27)	380(46)	427(56)	450(47)	-148(43)	290(39)	-270(44)
C(28)	97(11)	205(21)	273(24)	-46(18)	-39(14)	-22(13)
C(29)	70(12)	374(42)	935(102)	-451(59)	-7(28)	41(18)
C(30)	84(10)	176(16)	217(22)	137(17)	82(13)	64(11)
C(31)	109(15)	457(50)	162(19)	210(27)	-51(13)	-126(22)
C(32)	131(12)	228(19)	68(8)	5(10)	44(8)	-74(13)
C(33)	49(5)	123(9)	83(7)	33(7)	5(5)	-2(6)
C(34)	120(10)	69(7)	118(9)	37(7)	62(8)	13(7)
C(35)	285(37)	537(70)	547(63)	-306(55)	110(39)	-310(46)
C(36)	69(8)	205(18)	165(14)	59(14)	8(8)	1(10)
C(37)	65(10)	1235(115)	324(30)	522(53)	84(14)	118(27)
C(38)	122(14)	275(29)	442(39)	233(30)	98(19)	114(17)
C(39)	158(17)	156(17)	307(28)	26(19)	90(18)	20(14)
C(40)	26(10)	229(36)	178(28)	67(26)	-49(13)	15(14)

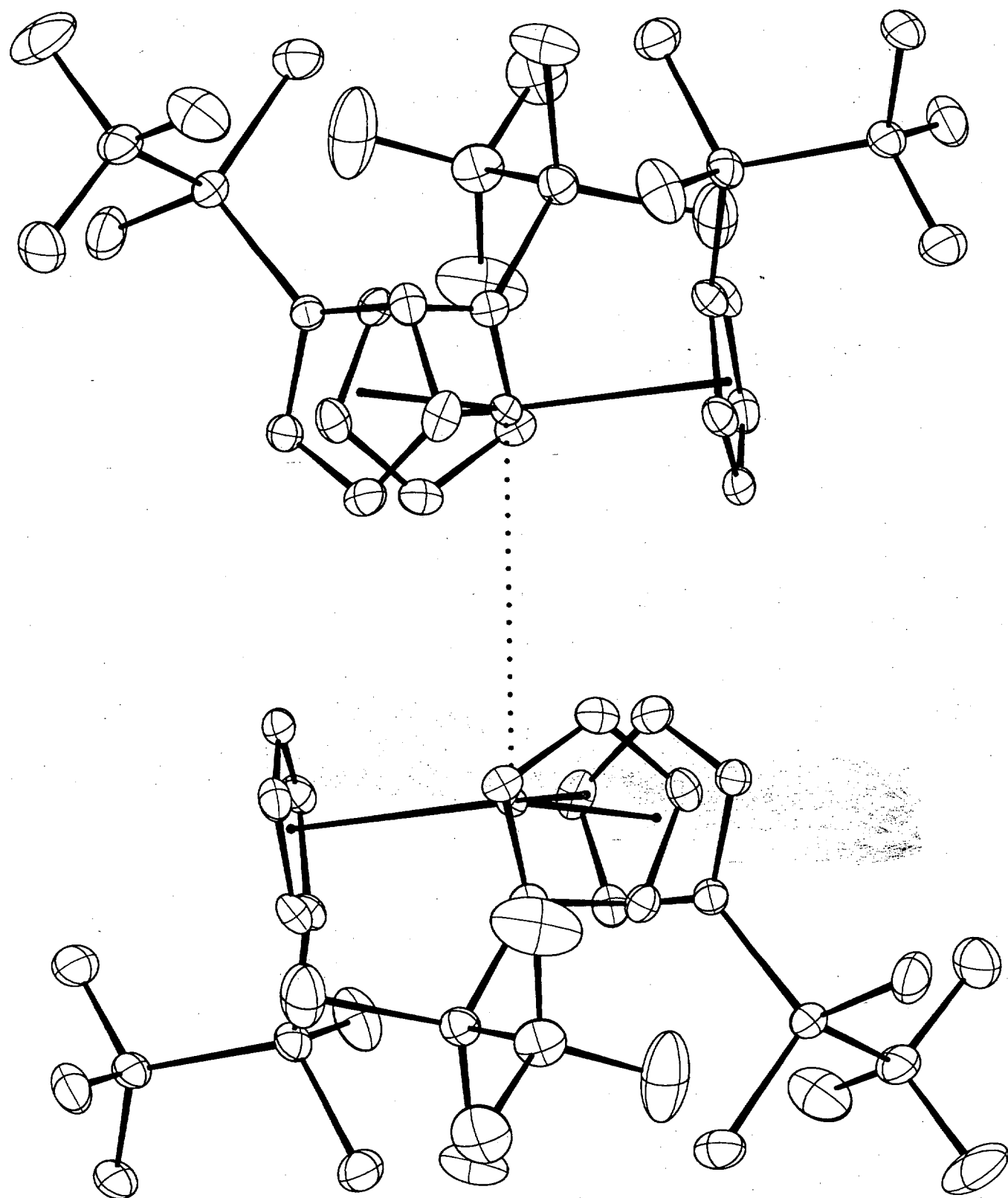
Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\mathbf{1} \cdot \mathbf{2}$.

	x	y	z	U(eq)
H(1A)	3750(12)	3651(4)	-588(7)	146
H(1B)	4528(12)	3323(4)	-243(7)	146
H(2A)	3744(12)	3768(4)	273(7)	146
H(2B)	2495(12)	3640(4)	-16(7)	146
H(3A)	3353(12)	3524(5)	1098(7)	144
H(3B)	2101(12)	3393(5)	824(7)	144
H(4A)	2657(12)	3067(5)	1565(5)	139
H(4B)	3755(12)	2902(5)	1369(5)	139
H(5A)	2019(15)	2362(6)	1648(6)	177
H(5B)	3049(15)	2180(6)	1413(6)	177
H(6A)	4266(13)	2886(5)	-919(6)	145
H(6B)	3568(13)	3236(5)	-1257(6)	145
H(7)	-906(30)	2249(9)	-483(21)	277
H(8)	-134(43)	2574(22)	-949(17)	429
H(9)	179(19)	3190(17)	-898(23)	357
H(10)	250(21)	3503(8)	-100(15)	211
H(12)	-1279(20)	2461(14)	278(19)	275
H(13F)	-565(28)	3419(27)	721(17)	1286
H(13E)	-498(28)	2975(27)	945(17)	1286
H(13D)	-1671(28)	3141(27)	619(17)	1286
H(13C)	-1258(28)	2937(27)	803(17)	1286
H(13B)	-1324(28)	3382(27)	578(17)	1286
H(13A)	-151(28)	3215(27)	904(17)	1286
H(14)	0	-580(4)	2500	68
H(16)	-1736(7)	469(3)	2288(3)	77
H(17)	0	807(4)	2500	79
H(20)	-1015(9)	-843(4)	1684(5)	126
H(22)	376(16)	-399(5)	519(6)	159
H(23)	-1542(20)	-123(6)	418(6)	175
H(24A)	511(29)	-1343(10)	2078(10)	568

H(24B)	1375(29)	-1003(10)	2336(10)	568
H(24C)	1852(29)	-1425(10)	2188(10)	568
H(25A)	479(14)	-1577(7)	943(10)	429
H(25B)	1830(14)	-1635(7)	1074(10)	429
H(25C)	1259(14)	-1362(7)	595(10)	429
H(26A)	2814(13)	-552(7)	1583(10)	323
H(26B)	2740(13)	-708(7)	1002(10)	323
H(26C)	3316(13)	-980(7)	1480(10)	323
H(27A)	-3034(30)	-1238(11)	1585(15)	587
H(27B)	-4047(30)	-1030(11)	1803(15)	587
H(27C)	-2754(30)	-931(11)	2057(15)	587
H(28A)	-3799(14)	-884(7)	403(8)	302
H(28B)	-4029(14)	-430(7)	228(8)	302
H(28C)	-4908(14)	-659(7)	512(8)	302
H(29A)	-3242(18)	77(10)	1647(20)	711
H(29B)	-4507(18)	-7(10)	1339(20)	711
H(29C)	-3597(18)	198(10)	1049(20)	711
H(31)	-726(18)	544(11)	437(9)	304
H(32)	1259(15)	344(6)	619(5)	167
H(33)	2206(8)	671(4)	1433(4)	103
H(34)	786(12)	1060(3)	1769(5)	116
H(35A)	2734(27)	988(13)	2348(14)	678
H(35B)	2775(27)	1344(13)	1946(14)	678
H(35C)	3929(27)	1136(13)	2230(14)	678
H(36A)	3121(11)	290(6)	2194(6)	223
H(36B)	4341(11)	467(6)	2155(6)	223
H(36C)	3815(11)	107(6)	1786(6)	223
H(37A)	3145(13)	1040(16)	814(11)	803
H(37B)	3799(13)	624(16)	826(11)	803
H(37C)	4351(13)	982(16)	1191(11)	803
H(38A)	-1175(16)	1633(7)	518(11)	411
H(38B)	-1366(16)	1801(7)	1065(11)	411
H(38C)	-2434(16)	1723(7)	608(11)	411
H(39A)	-2715(17)	860(7)	1553(9)	301
H(39B)	-3393(17)	1230(7)	1258(9)	301
H(39C)	-2323(17)	1306(7)	1715(9)	301

H(40A)	-2528(16)	780(10)	139(11)	230
H(40B)	-3586(16)	970(10)	343(11)	230
H(40C)	-3042(16)	559(10)	581(11)	230





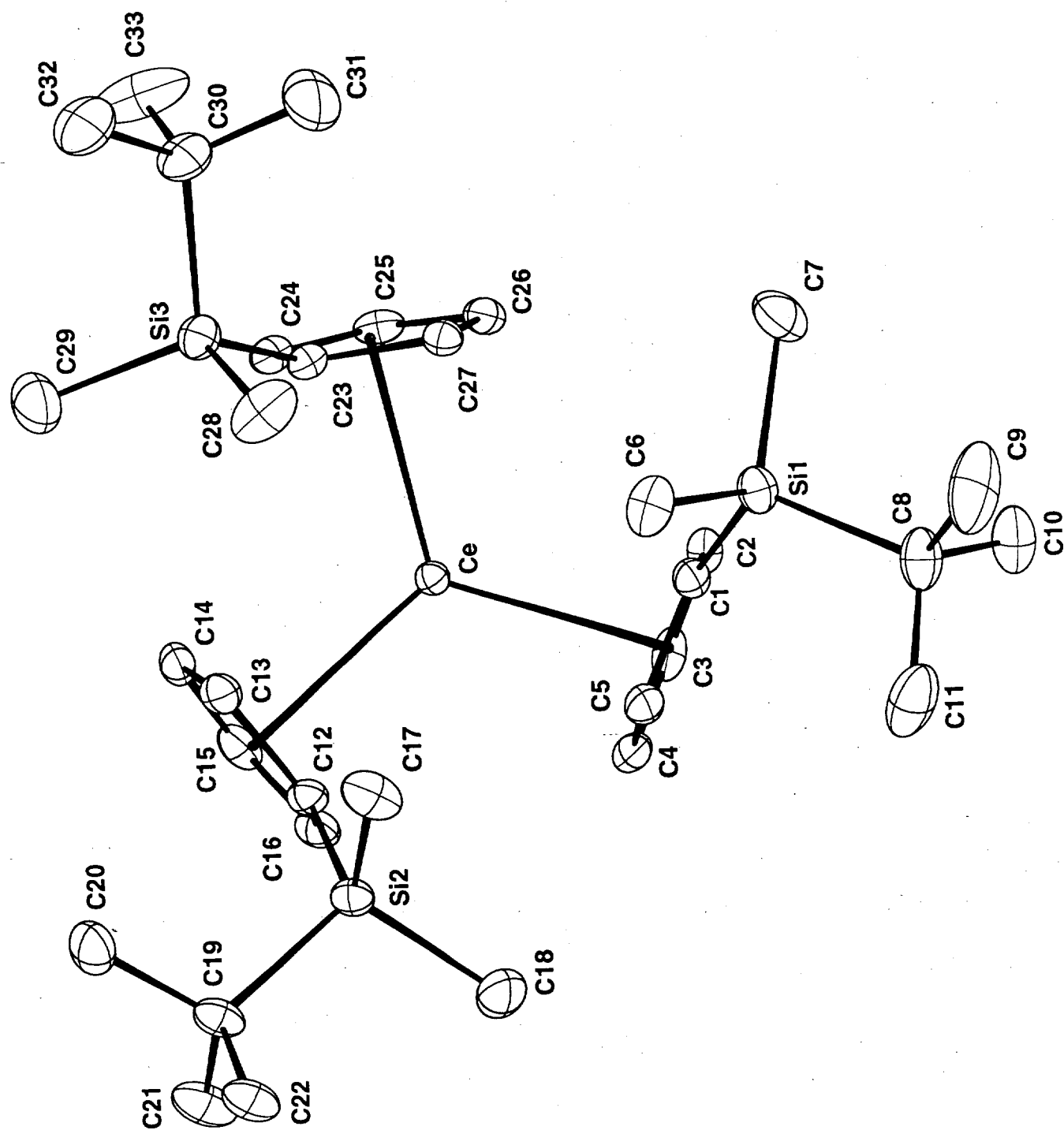


Table 1. Crystal data and structure refinement for
 $[K(18\text{-crown-6})(\text{toluene})_2][\text{Ce}(\text{C}_5\text{H}_4\text{SiMe}_2\text{tBu})_3]_2 \cdot \text{toluene}$

Identification code	2.0
Empirical formula	C ₉₉ H ₁₆₃ Ce ₂ K O ₆ Si ₆
Formula weight	1937.2
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁ /c (No.14)
Unit cell dimensions	a = 14.404(4) Å alpha = 90 deg. b = 12.704(4) Å beta = 92.97(2) deg. c = 29.271(6) Å gamma = 90 deg.
Volume	5349(3) Å ³
Z	2
Density (calculated)	1.20 Mg/m ³
Absorption coefficient	0.99 mm ⁻¹
F(000)	2048
Crystal size	0.40 x 0.30 x 0.15 mm
Theta range for data collection	2 to 28 deg.
Index ranges	0 ≤ h ≤ 19, 0 ≤ k ≤ 16, -38 ≤ l ≤ 38
Reflections collected	13350
Independent reflections	12870 [R(int) = 0.034]
Reflections with I > 2σ(I)	9666
Structure solution	Direct methods
Refinement method	Full-matrix least-squares on all F ²
Data / restraints / parameters	12867 / 0 / 543
Goodness-of-fit on F	1.016
Final R indices [I > 2σ(I)]	R1 = 0.046, wR2 = 0.102
R indices (all data)	R1 = 0.071, wR2 = 0.115
Largest diff. peak and hole	1.24 and -0.80 e.Å ⁻³ (near Ce)
Abs.correction from psi scans	Tmax=1.00 , Tmin=0.87
Maximum shift/e.s.d.	0.003

All non-H atoms were anisotropic. H's were included in riding mode with $U_{iso}(H)$ equal to $1.2U_{eq}(C)$ or $1.5U_{eq}(C)$ for methyl groups. The crown ether ligand appears to be disordered in an 0.86:0.14 ratio over two orientations related by a 30 degree rotation in the coordination plane. For the lower occupancy sites only the oxygen atoms were located. The $[K(crown)(toluene)_2]$ cation lies on an inversion centre. The $[Ce(Cp-SiMe_2tBu)_3]$ groups lie in pairs related by another inversion centre. There is a molecule of toluene solvate disordered across another inversion centre.

Programs used were :

Data collection - Enraf-Nonius CAD4 software
Structure solution - SHELXS-86
Structure refinement - SHELXL-93
Interactive graphics and final drawings - CAMERON

References :

Enraf-Nonius(1989) CAD4 Software. Version 5.0. Enraf-Nonius, The Netherlands.
Sheldrick,G.M.(1985) SHELXS-86. Program for the Solution of Crystal Structures. Univ. of Gottingen, Germany.
Sheldrick,G.M.(1993) SHELXL-93. Program for Crystal Structure Refinement. Univ. of Gottingen, Germany.
Watkin,D.J. and Pearce,L.J.(1993) CAMERON. An Interactive Graphics Editor. Univ. of Oxford, England.

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1a. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ce	14.0(1)	500.4(2)	739.9(1)	21(1)
K	5000	5000	0	64(1)
Si(1)	-1934(1)	-510(1)	1743(1)	33(1)
Si(2)	-187(1)	3672(1)	1302(1)	31(1)
Si(3)	2263(1)	-125(1)	1788(1)	33(1)
O(1)	6853(3)	5634(4)	172(2)	62(1) a
O(2)	5360(3)	7034(3)	314(1)	60(1) a
O(3)	3546(3)	6218(4)	319(2)	62(1) a
C(1)	-1736(3)	39(3)	1168(1)	27(1)
C(2)	-1791(3)	-494(3)	743(1)	31(1)
C(3)	-1828(3)	229(4)	386(1)	35(1)
C(4)	-1801(3)	1246(3)	581(2)	37(1)
C(5)	-1729(3)	1130(3)	1058(2)	33(1)
C(6)	-1205(3)	210(4)	2187(2)	47(1)
C(7)	-1667(4)	-1953(4)	1762(2)	52(1)
C(8)	-3211(3)	-331(4)	1875(2)	46(1)
C(9)	-3369(4)	-748(6)	2358(2)	85(2)
C(10)	-3824(4)	-966(5)	1532(2)	59(1)
C(11)	-3499(4)	822(5)	1837(2)	70(2)
C(12)	336(3)	2732(3)	905(1)	28(1)
C(13)	1194(3)	2202(3)	998(1)	31(1)
C(14)	1528(3)	1823(3)	584(2)	34(1)
C(15)	875(3)	2098(3)	232(1)	35(1)
C(16)	157(3)	2658(3)	425(1)	32(1)
C(17)	-24(4)	3166(4)	1898(2)	49(1)
C(18)	-1446(3)	3927(4)	1152(2)	59(2)
C(19)	429(3)	4989(3)	1255(1)	34(1)
C(20)	1473(3)	4854(4)	1364(2)	48(1)
C(21)	281(4)	5424(4)	765(2)	51(1)
C(22)	35(4)	5781(3)	1589(2)	43(1)
C(23)	1433(3)	-535(3)	1319(1)	27(1)
C(24)	1664(3)	-770(3)	867(1)	30(1)
C(25)	982(3)	-1427(3)	659(1)	32(1)
C(26)	305(3)	-1608(3)	979(1)	33(1)
C(27)	572(3)	-1064(3)	1381(1)	28(1)
C(28)	1674(4)	580(5)	2248(2)	62(2)
C(29)	3202(4)	724(5)	1566(2)	67(2)
C(30)	2818(3)	-1383(4)	2031(2)	47(1)
C(31)	2103(5)	-2057(6)	2249(3)	100(3)
C(32)	3603(4)	-1132(5)	2387(2)	67(2)
C(33)	3238(5)	-1999(6)	1644(2)	99(3)
C(34)	5226(7)	5188(8)	1548(3)	109(3)
C(35)	4364(7)	4904(10)	1496(4)	122(4)
C(36)	4124(9)	4062(13)	1207(5)	151(5)
C(37)	4787(15)	3552(13)	968(5)	196(7)
C(38)	5714(12)	3924(17)	1039(5)	210(10)
C(39)	5945(7)	4722(12)	1336(4)	145(6)
C(40)	5485(9)	6073(8)	1871(4)	170(5)
C(41)	6987(5)	6678(6)	221(2)	75(2) a
C(42)	6228(4)	7194(4)	523(2)	54(2) a
C(43)	4707(5)	7477(5)	566(2)	61(2) a

C(44)	3693(4)	7270(4)	346(2)	52(2) a
C(45)	2683(4)	6010(6)	141(3)	71(2) a
C(46)	2506(4)	4787(6)	97(2)	58(2) a
C(47)	-5058(7)	881(11)	652(4)	141(5)
C(48)	-4192(9)	334(9)	413(5)	64(3) c
C(49)	-4176(5)	-46(9)	46(4)	98(3)
C(50)	-5874(10)	390(13)	311(7)	88(5) c
C(51)	-4947(8)	-479(10)	-279(6)	74(4) c
O(1A)	6293(10)	6581(11)	244(5)	7(3) b
O(2A)	4413(10)	6794(11)	453(5)	7(3) b
O(3A)	3066(10)	5403(12)	37(5)	10(3) b

a occupancy 0.86

b occupancy 0.14

c occupancy 0.5

Table 3. Bond lengths [Å] and angles [deg] for **2a**

Ce-M(1)	2.592(4)	Ce-M(2)	2.594(4)
Ce-M(3)	2.596(4)	Ce-C(1)	2.931(4)
Ce-C(2)	2.891(4)	Ce-C(3)	2.819(4)
Ce-C(4)	2.797(4)	Ce-C(5)	2.838(4)
Ce-C(12)	2.909(4)	Ce-C(13)	2.828(4)
Ce-C(14)	2.809(4)	Ce-C(15)	2.839(4)
Ce-C(16)	2.903(4)	Ce-C(23)	2.902(4)
Ce-C(24)	2.880(4)	Ce-C(25)	2.834(4)
Ce-C(26)	2.795(4)	Ce-C(27)	2.822(4)
Ce...Ce'	4.513(1)	K-O(1)	2.809(4)
K-O(2)	2.782(4)	K-O(3)	2.803(4)
K-O(1A)	2.806(14)	K-O(2A)	2.790(14)
K-O(3A)	2.84(2)	K...C(37)	3.404(15)
K...C(38)	3.444(12)	Si(1)-C(1)	1.857(4)
Si(1)-C(6)	1.868(5)	Si(1)-C(7)	1.874(5)
Si(1)-C(8)	1.913(5)	Si(2)-C(12)	1.854(4)
Si(2)-C(17)	1.863(5)	Si(2)-C(18)	1.872(5)
Si(2)-C(19)	1.902(4)	Si(3)-C(23)	1.848(4)
Si(3)-C(28)	1.860(5)	Si(3)-C(29)	1.872(5)
Si(3)-C(30)	1.908(5)	O(1)-C(41)	1.347(8)
O(1)-C(46)"	1.354(7)	O(2)-C(43)	1.348(7)
O(2)-C(42)	1.378(7)	O(3)-C(45)	1.349(8)
O(3)-C(44)	1.355(7)	C(1)-C(2)	1.413(5)
C(1)-C(5)	1.423(5)	C(2)-C(3)	1.391(6)
C(3)-C(4)	1.412(6)	C(4)-C(5)	1.403(6)
C(8)-C(11)	1.525(8)	C(8)-C(10)	1.531(7)
C(8)-C(9)	1.538(7)	C(12)-C(16)	1.418(5)
C(12)-C(13)	1.421(5)	C(13)-C(14)	1.410(6)
C(14)-C(15)	1.405(6)	C(15)-C(16)	1.399(6)
C(19)-C(20)	1.531(6)	C(19)-C(22)	1.531(5)
C(19)-C(21)	1.542(6)	C(23)-C(24)	1.413(5)
C(23)-C(27)	1.430(5)	C(24)-C(25)	1.404(6)
C(25)-C(26)	1.406(6)	C(26)-C(27)	1.401(5)
C(30)-C(31)	1.506(8)	C(30)-C(33)	1.526(8)
C(30)-C(32)	1.532(7)	C(34)-C(35)	1.295(12)
C(34)-C(39)	1.370(13)	C(34)-C(40)	1.503(14)
C(35)-C(36)	1.39(2)	C(36)-C(37)	1.38(2)
C(37)-C(38)	1.42(2)	C(38)-C(39)	1.36(2)
C(41)-C(42)	1.583(9)	C(43)-C(44)	1.588(9)
C(45)-C(46)	1.579(10)	C(46)-O(1)"	1.354(7)
C(47)-C(48)	1.62(2)	C(47)-C(50)	1.63(2)
C(48)-C(49)	1.18(2)	C(49)-C(51)	1.53(2)
C(51)-C(47)"	1.21(2)	C(51)-C(49)"	1.61(2)
C(50)-C(49)"	1.14(2)		
M(1)-Ce-M(2)	119.29(9)	M(1)-Ce-M(3)	120.96(9)
M(2)-Ce-M(3)	118.77(9)	M(1)-Ce...Ce'	94.71(9)
M(2)-Ce...Ce'	96.32(9)	M(3)-Ce...Ce'	88.88(9)
O(2)-K-O(3)	60.46(13)	O(2)-K-O(3)"	119.54(14)
O(2A)-K-O(1A)	60.5(4)	O(2A)-K-O(1A)"	119.5(4)
O(2)-K-O(1)"	118.98(13)	O(3)-K-O(1)"	59.88(14)
O(2)-K-O(1)	61.02(13)	O(3)-K-O(1)	120.12(14)
O(2A)-K-O(3A)	60.8(4)	O(1A)-K-O(3A)	120.0(4)
O(2A)-K-O(3A)"	119.2(4)	O(1A)-K-O(3A)"	60.0(4)
C(1)-Si(1)-C(6)	109.9(2)	C(1)-Si(1)-C(7)	110.7(2)
C(6)-Si(1)-C(7)	110.5(2)	C(1)-Si(1)-C(8)	109.5(2)
C(6)-Si(1)-C(8)	108.2(2)	C(7)-Si(1)-C(8)	107.9(2)

C(12)-Si(2)-C(17)	109.2(2)	C(12)-Si(2)-C(18)	112.6(2)
C(17)-Si(2)-C(18)	110.6(3)	C(12)-Si(2)-C(19)	108.4(2)
C(17)-Si(2)-C(19)	109.5(2)	C(18)-Si(2)-C(19)	106.3(2)
C(23)-Si(3)-C(28)	111.8(2)	C(23)-Si(3)-C(29)	110.9(2)
C(28)-Si(3)-C(29)	109.8(3)	C(23)-Si(3)-C(30)	106.4(2)
C(28)-Si(3)-C(30)	109.4(2)	C(29)-Si(3)-C(30)	108.4(2)
C(41)-O(1)-C(46) "	110.6(5)	C(41)-O(1)-K	115.5(4)
C(46) "-O(1)-K	117.0(4)	C(43)-O(2)-C(42)	109.7(5)
C(43)-O(2)-K	116.5(4)	C(42)-O(2)-K	115.7(4)
C(45)-O(3)-C(44)	110.7(5)	C(45)-O(3)-K	116.9(4)
C(44)-O(3)-K	116.5(4)	C(2)-C(1)-C(5)	105.6(4)
C(2)-C(1)-Si(1)	127.8(3)	C(5)-C(1)-Si(1)	125.0(3)
C(3)-C(2)-C(1)	110.1(4)	C(2)-C(3)-C(4)	107.6(4)
C(5)-C(4)-C(3)	107.7(4)	C(4)-C(5)-C(1)	109.1(4)
C(11)-C(8)-C(10)	108.3(4)	C(11)-C(8)-C(9)	110.1(5)
C(10)-C(8)-C(9)	108.3(4)	C(11)-C(8)-Si(1)	111.1(3)
C(10)-C(8)-Si(1)	109.4(3)	C(9)-C(8)-Si(1)	109.6(4)
C(16)-C(12)-C(13)	105.7(3)	C(16)-C(12)-Si(2)	127.2(3)
C(13)-C(12)-Si(2)	124.3(3)	C(14)-C(13)-C(12)	109.3(4)
C(15)-C(14)-C(13)	107.5(4)	C(16)-C(15)-C(14)	108.1(4)
C(15)-C(16)-C(12)	109.5(4)	C(20)-C(19)-C(22)	109.5(4)
C(20)-C(19)-C(21)	108.7(4)	C(22)-C(19)-C(21)	108.7(3)
C(20)-C(19)-Si(2)	110.0(3)	C(22)-C(19)-Si(2)	110.0(3)
C(21)-C(19)-Si(2)	109.8(3)	C(24)-C(23)-C(27)	105.5(3)
C(24)-C(23)-Si(3)	125.5(3)	C(27)-C(23)-Si(3)	124.8(3)
C(25)-C(24)-C(23)	109.8(4)	C(24)-C(25)-C(26)	107.5(3)
C(27)-C(26)-C(25)	108.1(4)	C(26)-C(27)-C(23)	109.0(3)
C(31)-C(30)-C(33)	109.2(6)	C(31)-C(30)-C(32)	109.1(5)
C(33)-C(30)-C(32)	107.7(5)	C(31)-C(30)-Si(3)	110.6(4)
C(33)-C(30)-Si(3)	109.2(4)	C(32)-C(30)-Si(3)	111.1(4)
C(35)-C(34)-C(39)	124.7(13)	C(35)-C(34)-C(40)	119.2(12)
C(39)-C(34)-C(40)	116.1(12)	C(34)-C(35)-C(36)	119.4(11)
C(37)-C(36)-C(35)	120.8(14)	C(36)-C(37)-C(38)	116(2)
C(36)-C(37)-K	105.3(8)	C(38)-C(37)-K	79.6(10)
C(39)-C(38)-C(37)	123(2)	C(39)-C(38)-K	108.6(11)
C(37)-C(38)-K	76.5(8)	C(38)-C(39)-C(34)	116.4(13)
O(1)-C(41)-C(42)	111.6(5)	O(2)-C(42)-C(41)	109.1(5)
O(2)-C(43)-C(44)	111.2(5)	O(3)-C(44)-C(43)	108.9(5)
O(3)-C(45)-C(46)	111.5(5)		

M(1), M(2), and M(3) are the centroids of the rings C(1) to C(5), C(12) to C(16), and C(23) to C(27) respectively.

Symmetry transformations used to generate equivalent atoms:

' -x, -y, -z " -x+1, -y+1, -z "' -x-1, -y, -z

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 2a
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Ce	22(1)	20(1)	21(1)	-2(1)	0(1)	0(1)
K	35(1)	51(1)	107(2)	-38(1)	5(1)	-3(1)
Si(1)	33(1)	38(1)	28(1)	-2(1)	7(1)	-5(1)
Si(2)	34(1)	22(1)	37(1)	-5(1)	4(1)	2(1)
Si(3)	30(1)	37(1)	32(1)	0(1)	-3(1)	0(1)
O(1)	55(3)	66(3)	65(3)	4(2)	9(2)	-8(2)
O(2)	68(3)	57(3)	54(3)	-4(2)	2(2)	-11(2)
O(3)	65(3)	60(3)	61(3)	-1(2)	1(2)	10(2)
C(1)	26(2)	26(2)	30(2)	-4(2)	7(2)	0(2)
C(2)	25(2)	36(2)	31(2)	-4(2)	4(2)	-4(2)
C(3)	21(2)	55(3)	30(2)	-1(2)	2(2)	-4(2)
C(4)	25(2)	40(2)	47(3)	15(2)	3(2)	6(2)
C(5)	27(2)	28(2)	43(2)	-4(2)	7(2)	3(2)
C(6)	37(2)	70(3)	35(2)	-7(2)	1(2)	-1(2)
C(7)	64(3)	39(3)	56(3)	9(2)	17(3)	-6(2)
C(8)	37(2)	66(3)	36(2)	-9(2)	13(2)	-11(2)
C(9)	50(3)	162(7)	44(3)	7(4)	22(3)	-13(4)
C(10)	42(3)	73(4)	63(3)	-13(3)	7(2)	-17(3)
C(11)	40(3)	87(4)	84(4)	-38(4)	11(3)	5(3)
C(12)	31(2)	22(2)	32(2)	-3(2)	-2(2)	1(2)
C(13)	32(2)	24(2)	38(2)	-5(2)	-6(2)	-4(2)
C(14)	28(2)	26(2)	48(3)	-5(2)	10(2)	-5(2)
C(15)	46(2)	25(2)	34(2)	-4(2)	12(2)	-9(2)
C(16)	39(2)	23(2)	34(2)	0(2)	-5(2)	-3(2)
C(17)	72(3)	37(2)	40(3)	0(2)	17(2)	0(2)
C(18)	40(3)	38(3)	99(5)	-12(3)	0(3)	5(2)
C(19)	50(3)	21(2)	32(2)	-4(2)	6(2)	0(2)
C(20)	45(3)	38(2)	62(3)	-11(2)	7(2)	-9(2)
C(21)	85(4)	30(2)	40(3)	-2(2)	12(3)	0(2)
C(22)	65(3)	24(2)	39(2)	-8(2)	7(2)	0(2)
C(23)	26(2)	28(2)	27(2)	2(2)	0(1)	5(2)
C(24)	29(2)	32(2)	28(2)	3(2)	3(2)	7(2)
C(25)	40(2)	25(2)	30(2)	-2(2)	-2(2)	11(2)
C(26)	32(2)	23(2)	41(2)	3(2)	-6(2)	0(2)
C(27)	29(2)	27(2)	28(2)	7(2)	1(2)	2(2)
C(28)	58(3)	79(4)	48(3)	-26(3)	-13(2)	20(3)
C(29)	52(3)	70(4)	76(4)	23(3)	-16(3)	-19(3)
C(30)	45(3)	54(3)	41(3)	10(2)	-14(2)	8(2)
C(31)	66(4)	94(5)	137(7)	74(5)	-27(4)	-19(4)
C(32)	57(3)	78(4)	65(4)	10(3)	-25(3)	6(3)
C(33)	125(6)	88(5)	82(5)	-19(4)	-28(4)	68(5)
C(34)	103(7)	120(7)	106(7)	80(6)	13(5)	20(6)
C(35)	82(7)	148(9)	141(9)	78(8)	45(6)	36(6)
C(36)	107(9)	170(13)	172(13)	59(10)	-20(9)	28(9)
C(37)	251(19)	198(15)	132(11)	-10(10)	-63(13)	89(16)
C(38)	163(14)	381(29)	88(9)	74(12)	36(10)	123(17)
C(39)	88(7)	253(16)	98(7)	93(9)	36(6)	67(9)
C(40)	225(14)	97(8)	182(12)	67(8)	-34(10)	8(9)
C(41)	70(5)	87(5)	69(5)	-33(4)	22(4)	-48(4)
C(42)	71(4)	35(3)	54(4)	-1(3)	-19(3)	-17(3)
C(43)	83(5)	47(4)	51(4)	-19(3)	-18(3)	28(3)

C(44)	74(4)	37(3)	46(3)	-5(2)	8(3)	20(3)
C(45)	34(3)	69(5)	112(6)	21(4)	19(4)	12(3)
C(46)	30(3)	92(5)	52(4)	9(3)	10(3)	-4(3)
C(47)	82(6)	213(13)	127(9)	66(9)	-2(7)	-13(7)
C(48)	53(7)	53(7)	86(9)	32(7)	17(7)	3(5)
C(49)	36(3)	148(9)	109(7)	82(7)	-3(4)	-8(4)
C(50)	58(8)	79(10)	132(14)	60(11)	36(10)	16(7)
C(51)	36(6)	52(7)	132(13)	44(8)	-12(7)	2(5)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 2a

	x	y	z	U(eq)
H(2)	-1802(3)	-1237(3)	707(1)	37
H(3)	-1864(3)	68(4)	69(1)	42
H(4)	-1827(3)	1893(3)	418(2)	44
H(5)	-1684(3)	1690(3)	1273(2)	39
H(6C)	-1312(3)	-82(4)	2489(2)	71
H(6B)	-1372(3)	958(4)	2181(2)	71
H(6A)	-547(3)	133(4)	2123(2)	71
H(7C)	-1775(4)	-2228(4)	2067(2)	79
H(7B)	-1015(4)	-2065(4)	1694(2)	79
H(7A)	-2070(4)	-2322(4)	1534(2)	79
H(9C)	-3182(4)	-1489(6)	2378(2)	127
H(9B)	-4029(4)	-685(6)	2420(2)	127
H(9A)	-2997(4)	-336(6)	2583(2)	127
H(10C)	-3649(4)	-1711(5)	1552(2)	88
H(10B)	-3737(4)	-707(5)	1222(2)	88
H(10A)	-4477(4)	-888(5)	1604(2)	88
H(11C)	-3113(4)	1242(5)	2055(2)	105
H(11B)	-4154(4)	892(5)	1908(2)	105
H(11A)	-3414(4)	1073(5)	1526(2)	105
H(13)	1495(3)	2116(3)	1292(1)	38
H(14)	2092(3)	1450(3)	551(2)	41
H(15)	914(3)	1933(3)	-83(1)	41
H(16)	-370(3)	2945(3)	260(1)	39
H(17C)	-299(4)	3662(4)	2109(2)	74
H(17B)	642(4)	3092(4)	1979(2)	74
H(17A)	-328(4)	2480(4)	1920(2)	74
H(18C)	-1689(3)	4426(4)	1372(2)	88
H(18B)	-1793(3)	3264(4)	1164(2)	88
H(18A)	-1516(3)	4222(4)	843(2)	88
H(20C)	1725(3)	4347(4)	1151(2)	72
H(20B)	1576(3)	4594(4)	1678(2)	72
H(20A)	1786(3)	5533(4)	1334(2)	72
H(21C)	-386(4)	5514(4)	691(2)	77
H(21B)	539(4)	4928(4)	549(2)	77
H(21A)	595(4)	6105(4)	744(2)	77
H(22C)	-633(4)	5868(3)	1519(2)	64
H(22B)	348(4)	6460(3)	1559(2)	64
H(22A)	138(4)	5521(3)	1903(2)	64
H(24)	2200(3)	-520(3)	725(1)	36
H(25)	978(3)	-1700(3)	357(1)	38
H(26)	-237(3)	-2027(3)	932(1)	39
H(27)	234(3)	-1048(3)	1652(1)	34
H(28C)	2135(4)	785(5)	2490(2)	94
H(28B)	1210(4)	116(5)	2376(2)	94
H(28A)	1366(4)	1211(5)	2121(2)	94
H(29C)	3633(4)	932(5)	1820(2)	100
H(29B)	2924(4)	1354(5)	1422(2)	100
H(29A)	3539(4)	329(5)	1339(2)	100
H(31C)	1831(5)	-1664(6)	2497(3)	150
H(31B)	2400(5)	-2698(6)	2372(3)	150
H(31A)	1613(5)	-2247(6)	2019(3)	150
H(32C)	4071(4)	-694(5)	2247(2)	101

H(32B)	3892 (4)	-1790 (5)	2497 (2)	101
H(32A)	3349 (4)	-754 (5)	2644 (2)	101
H(33C)	3704 (5)	-1563 (6)	1501 (2)	149
H(33B)	2747 (5)	-2189 (6)	1415 (2)	149
H(33A)	3534 (5)	-2640 (6)	1768 (2)	149
H(35)	3899 (7)	5265 (10)	1653 (4)	147
H(36)	3494 (9)	3839 (13)	1176 (5)	181
H(37)	4635 (15)	2985 (13)	766 (5)	236
H(38)	6191 (12)	3604 (17)	875 (5)	251
H(39)	6571 (7)	4943 (12)	1391 (4)	175
H(40C)	5329 (64)	5878 (33)	2182 (7)	254
H(40B)	5142 (53)	6709 (23)	1776 (21)	254
H(40A)	6154 (15)	6208 (53)	1865 (26)	254
H(41B)	6960 (5)	7015 (6)	-85 (2)	90
H(41A)	7612 (5)	6808 (6)	366 (2)	90
H(42B)	6258 (4)	6873 (4)	831 (2)	65
H(42A)	6348 (4)	7958 (4)	557 (2)	65
H(43B)	4818 (5)	8245 (5)	587 (2)	73
H(43A)	4755 (5)	7183 (5)	879 (2)	73
H(44B)	3225 (4)	7600 (4)	536 (2)	63
H(44A)	3632 (4)	7585 (4)	36 (2)	63
H(45B)	2602 (4)	6339 (6)	-165 (3)	85
H(45A)	2219 (4)	6323 (6)	339 (3)	85
H(46B)	2555 (4)	4456 (6)	404 (2)	70
H(46A)	1873 (4)	4655 (6)	-39 (2)	70

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
 (* indicates atom used to define plane)

$$- 0.182 (0.000) x + 2.673 (0.001) y + 28.594 (0.010) z = 2.398 (0.001)$$

* 0.000 M1
 * 0.000 M2
 * 0.000 M3
 -0.149 (0.000) Ce
 -4.648 (0.002) Ce_\$1

Rms deviation of fitted atoms = 0.000

$$- 14.402 (0.005) x - 0.140 (0.026) y - 1.859 (0.057) z = 2.712 (0.005)$$

Angle to previous plane (with approximate esd) = 88.49 (0.11)

* 0.006 (0.002) C1
 * -0.001 (0.002) C2
 * -0.004 (0.002) C3
 * 0.008 (0.002) C4
 * -0.008 (0.002) C5
 -2.587 (0.002) Ce
 0.390 (0.006) Si1

Rms deviation of fitted atoms = 0.006

$$- 0.182 (0.000) x + 2.673 (0.001) y + 28.594 (0.010) z = 2.398 (0.001)$$

Angle to previous plane (with approximate esd) = 88.49 (0.11)

* 0.000 M1
 * 0.000 M2
 * 0.000 M3
 -0.149 (0.000) Ce
 -4.648 (0.002) Ce_\$1

Rms deviation of fitted atoms = 0.000

$$7.170 (0.025) x + 10.901 (0.013) y - 4.438 (0.057) z = 2.818 (0.005)$$

Angle to previous plane (with approximate esd) = 87.07 (0.11)

* 0.000 (0.002) C12
 * -0.004 (0.002) C13
 * 0.006 (0.002) C14
 * -0.006 (0.002) C15
 * 0.004 (0.002) C16
 -2.591 (0.002) Ce
 0.474 (0.006) Si2

Rms deviation of fitted atoms = 0.005

$$- 0.182 (0.000) x + 2.673 (0.001) y + 28.594 (0.010) z = 2.398 (0.001)$$

Angle to previous plane (with approximate esd) = 87.07 (0.11)

* 0.000 M1
* 0.000 M2
* 0.000 M3
-0.149 (0.000) Ce
-4.648 (0.002) Ce_\$1

Rms deviation of fitted atoms = 0.000

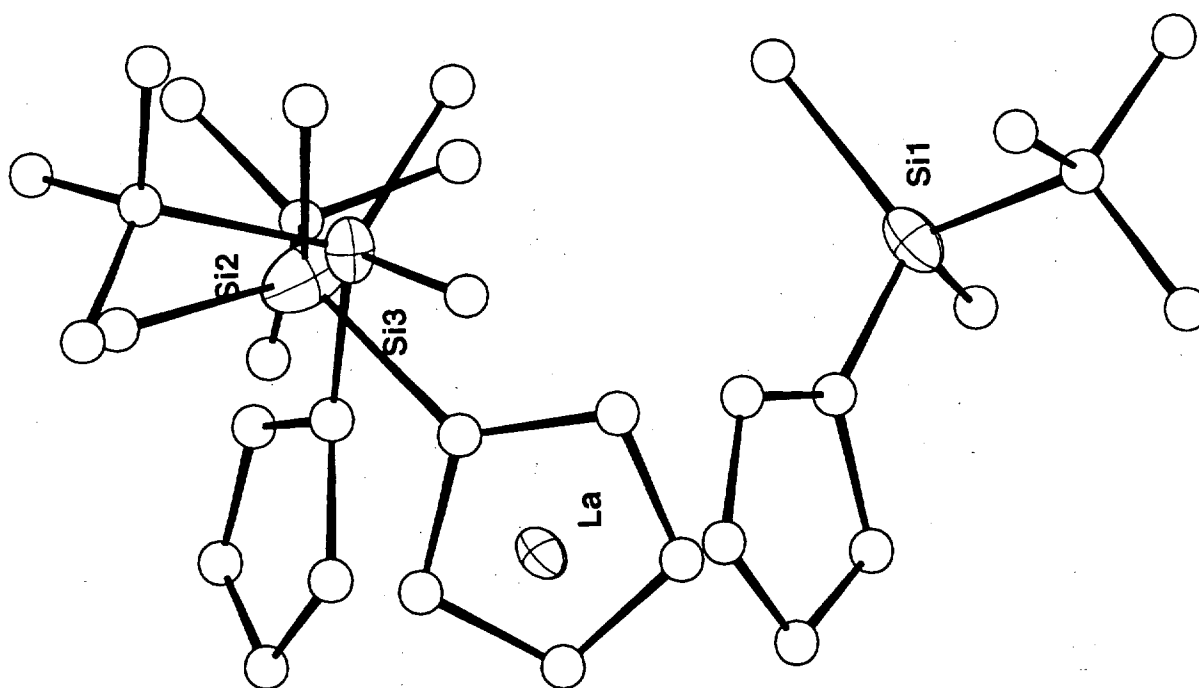
$$7.033 (0.025) x + 10.234 (0.015) y - 9.072 (0.053) z = 2.748 (0.005)$$

Angle to previous plane (with approximate esd) = 81.23 (0.11)

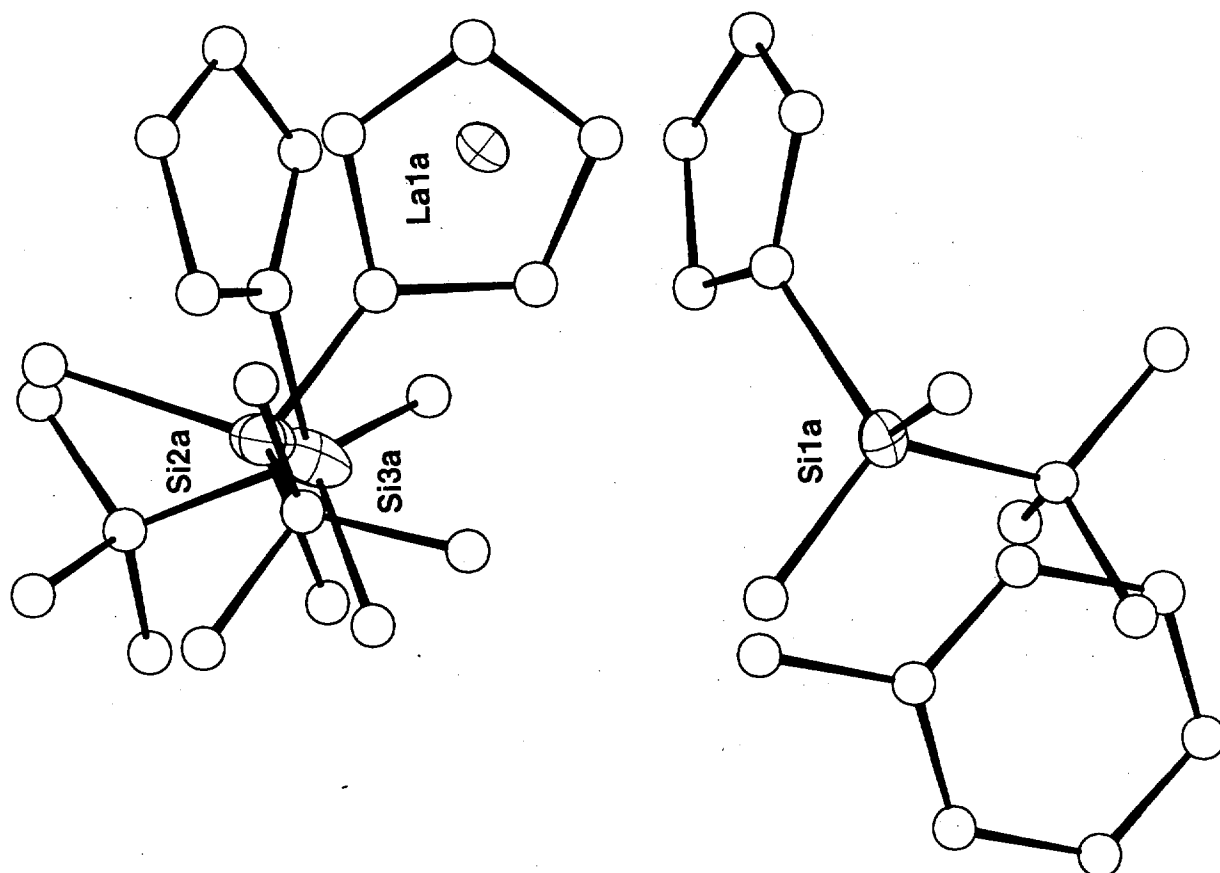
* 0.004 (0.002) C23
* -0.004 (0.002) C24
* 0.001 (0.002) C25
* 0.002 (0.002) C26
* -0.004 (0.002) C27
-2.579 (0.002) Ce
0.593 (0.006) Si3

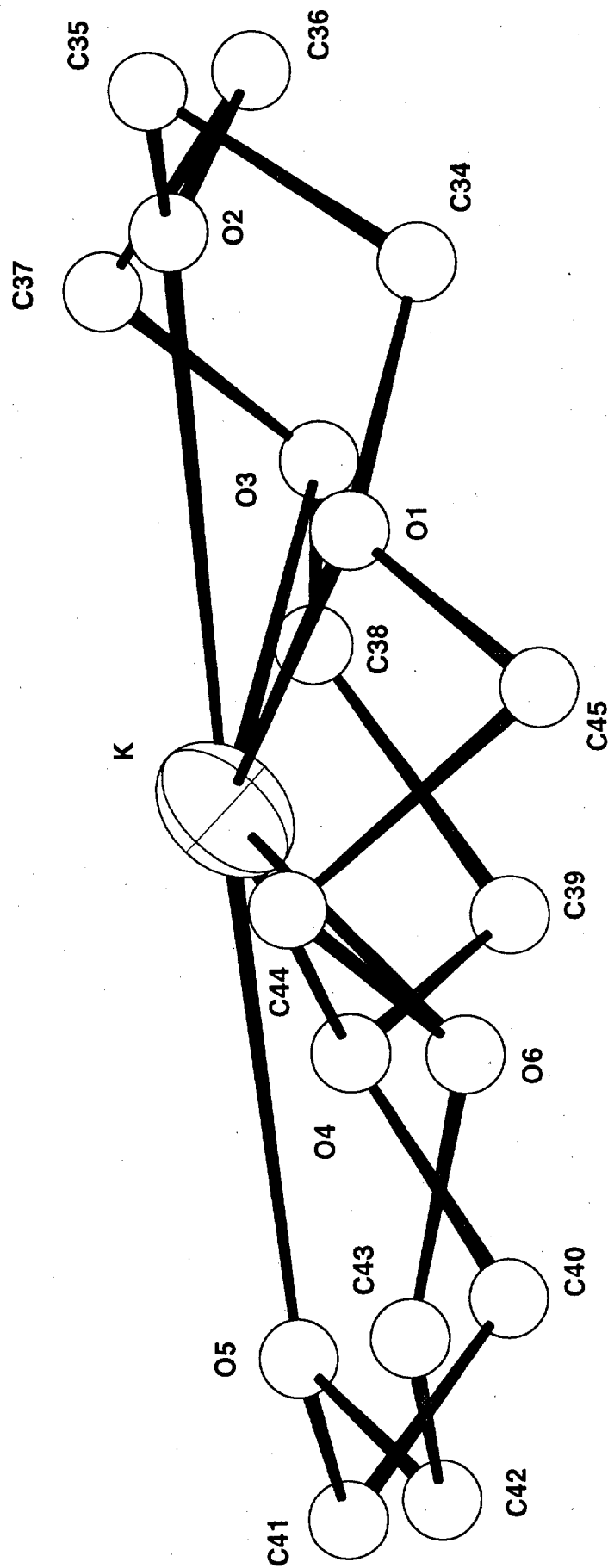
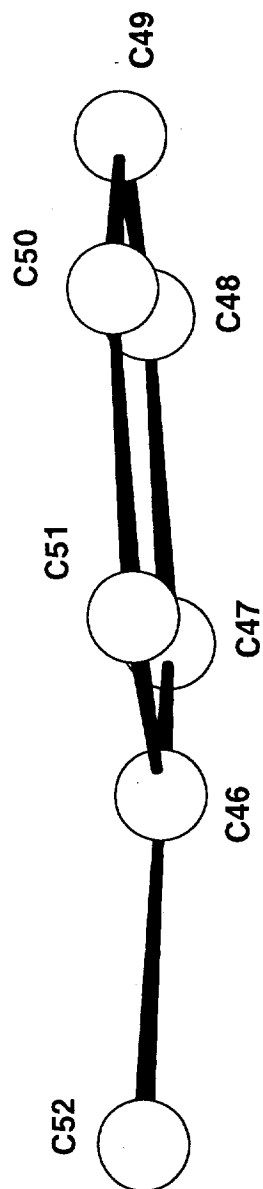
Rms deviation of fitted atoms = 0.003

2b



La... La1a 4.523(3) Å





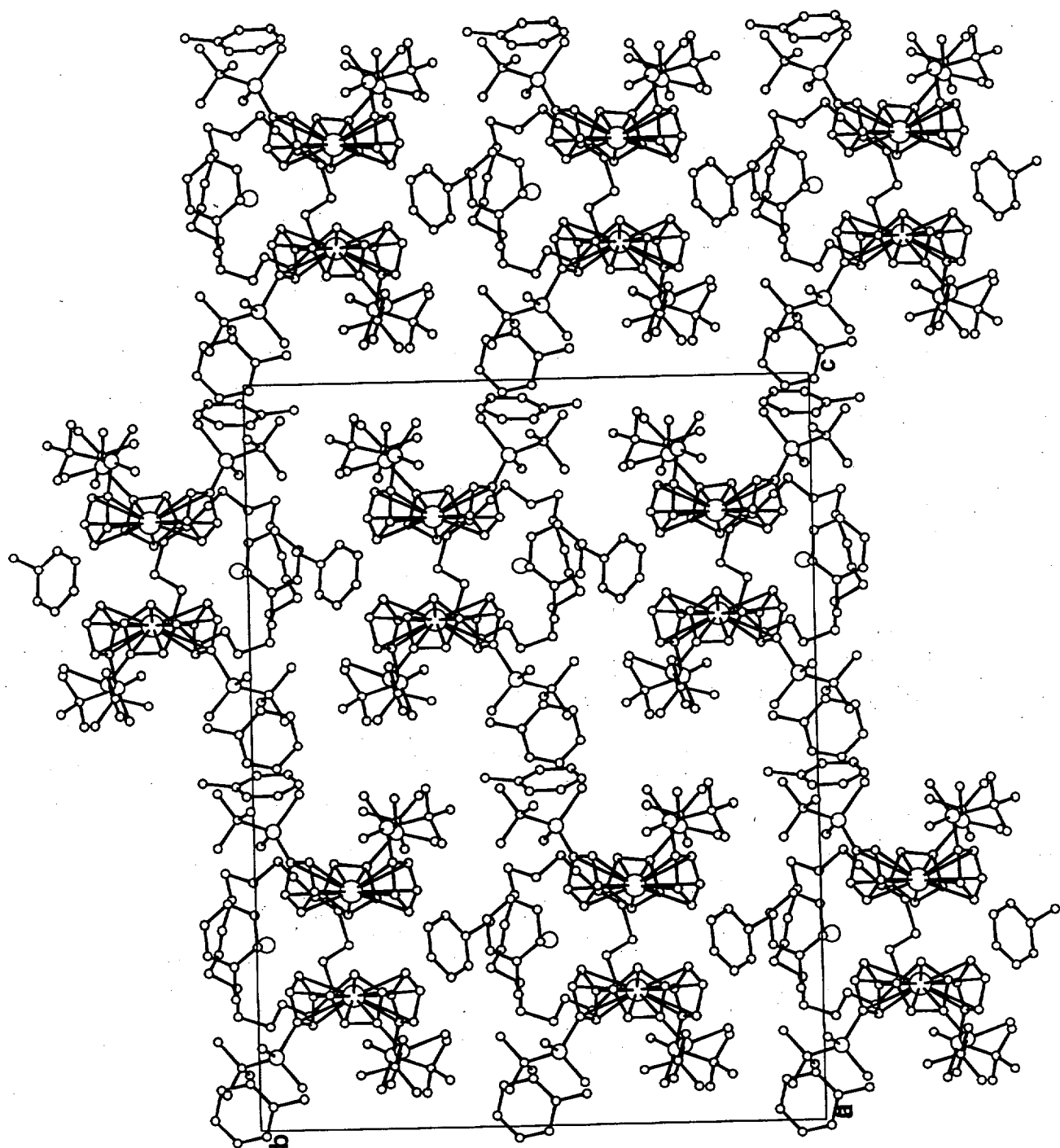


Table 1. Crystal data and structure refinement for
 $[K(18\text{-crown-6})][H\{La(C_6H_3(SiMe_3)_2)_3\}_2] \cdot 4(\text{toluene})$

Identification code	2b
Empirical formula	C ₁₀₆ H ₁₇₀ K La ₂ O ₆ Si ₆
Formula weight	2025.88
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, Cc (No.9)
Unit cell dimensions(Å and deg.)	a=14.029(2) alpha=90 b=24.648(7) beta=98.21(3) c=33.00(2) gamma=90
Volume	11293(9) Å ³
Z, Calculated density	4, 1.19 Mg.m ⁻³
Absorption coefficient	0.89 mm ⁻¹
F(000)	4284
Crystal size	0.30 x 0.20 x 0.05 mm
Theta range for data collection	2 to 23 deg.
Limiting indices	0 ≤ h ≤ 15 0 ≤ k ≤ 27 -36 ≤ l ≤ 35
Reflections collected / unique	8200 / 8200
Reflections with I > 2σ(I)	4678
Completeness to theta = 22.99	99.7 %
Abs. correction from psi-scans	Tmax.=1.00 , Tmin.=0.63
Refinement method	Full-matrix on all F ²
Data / restraints / parameters	8200 / 852 / 482
Goodness-of-fit on F ²	1.039
Final R indices [I > 2σ(I)]	R1 = 0.100, wR2 = 0.236
R indices (all data)	R1 = 0.180, wR2 = 0.290
Absolute structure parameter	0.00(6)
Largest diff. peak and hole	2.30 and -1.56 e.Å ⁻³
Maximum shift/e.s.d.	0.025

La, Si, K atoms were anisotropic. H's were included in riding mode with Uiso(H) equal to 1.2Ueq(C) or 1.5Ueq(C) for methyl groups. The hydride H was not located.

Programs used were :

Data collection - Enraf-Nonius CAD4 software
 Structure solution - SHELXS-97
 Structure refinement - SHELXL-97
 Interactive graphics and final drawings - CAMERON

References :

- Enraf-Nonius(1989) CAD4 Software. Version 5.0. Enraf-Nonius, The Netherlands.
- Sheldrick, G.M. (1997) SHELXS-97. Program for Crystal Structure Solution. Univ. of Gottingen, Germany.
- Sheldrick, G.M. (1997) SHELXL-97. Program for Crystal Structure Refinement. Univ. of Gottingen, Germany.
- Watkin, D.J. and Pearce, L.J. (1993) CAMERON. An Interactive Graphics Editor. Univ. of Oxford, England.

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
La(1)	5282(1)	6708(1)	8186(1)	38(1)
K	10460(4)	5176(2)	7500(2)	66(2)
Si(1)	5761(6)	5332(3)	8995(2)	46(2)
Si(2)	7646(6)	7519(4)	8953(3)	72(3)
Si(3)	3442(5)	7355(3)	9022(2)	40(2)
O(1)	11908(14)	4400(10)	7708(4)	117(8)
O(2)	11169(17)	4967(6)	8328(6)	125(9)
O(3)	10529(15)	6060(6)	8123(6)	136(10)
O(4)	9781(19)	6176(8)	7266(4)	139(10)
O(5)	9814(14)	5423(7)	6707(6)	146(11)
O(6)	11452(17)	4642(7)	6933(5)	118(8)
C(1)	5078(10)	5634(7)	8583(4)	28(5)
C(2)	5044(11)	5521(8)	8162(4)	35(6)
C(3)	4269(11)	5798(8)	7925(5)	54(7)
C(4)	3710(12)	6050(8)	8198(4)	36(6)
C(5)	4253(11)	5965(8)	8587(5)	39(6)
C(6)	6074(19)	5812(10)	9493(7)	51(7)
C(7)	6930(20)	5115(13)	8808(9)	76(10)
C(8)	5064(9)	4717(6)	9163(3)	35(6)
C(9)	4127(9)	4949(8)	9275(5)	75(9)
C(10)	4829(16)	4361(8)	8785(4)	79(10)
C(11)	5542(15)	4372(9)	9518(5)	116(14)
C(12)	7297(16)	6985(5)	8510(4)	34(5)
C(13)	7298(15)	6417(5)	8554(4)	33(5)
C(14)	7185(19)	6205(6)	8155(4)	52(7)
C(15)	7149(15)	6644(5)	7880(5)	30(5)
C(16)	7194(16)	7141(6)	8092(4)	33(6)
C(17)	6920(20)	7495(11)	9413(8)	59(8)
C(18)	7570(20)	8191(10)	8828(8)	64(8)
C(19)	8914(13)	7523(5)	9104(4)	58(7)
C(20)	9200(20)	6954(4)	9251(5)	96(11)
C(21)	9231(18)	7931(5)	9442(4)	64(8)
C(22)	9422(19)	7656(9)	8735(5)	112(13)
C(23)	3961(10)	7439(9)	8563(4)	45(6)
C(24)	3750(12)	7462(8)	8131(4)	46(6)
C(25)	4423(10)	7701(8)	7904(5)	36(5)
C(26)	5227(12)	7853(9)	8187(4)	47(6)
C(27)	4843(11)	7716(7)	8550(4)	26(5)
C(28)	4112(16)	6967(9)	9454(6)	34(5)
C(29)	2280(30)	6943(15)	8888(11)	89(12)
C(30)	2981(9)	8097(8)	9161(4)	102(13)
C(31)	3835(9)	8480(9)	9253(6)	93(11)
C(32)	2463(12)	8051(10)	9533(4)	67(9)
C(33)	2300(12)	8314(10)	8798(4)	70(8)
C(34)	12348(18)	4580(20)	8099(6)	230(30)
C(35)	11670(20)	4484(11)	8456(10)	190(20)
C(36)	11319(15)	5408(9)	8604(8)	120(13)
C(37)	10281(19)	5667(13)	8401(11)	190(20)
C(38)	9930(20)	6474(11)	7933(7)	135(15)
C(39)	10150(30)	6646(11)	7478(8)	176(17)
C(40)	9900(30)	6353(11)	6866(5)	144(16)
C(41)	9390(20)	5907(8)	6535(8)	90(10)
C(42)	10330(20)	5211(11)	6396(9)	200(20)
C(43)	10880(20)	4645(12)	6544(8)	139(15)
C(44)	11400(20)	4140(11)	7136(12)	250(30)
C(45)	12450(19)	4330(20)	7380(8)	210(30)

C(46)	8198(15)	4595(7)	7213(4)	170(20)
C(47)	8046(17)	5016(8)	7476(5)	82(9)
C(48)	8380(20)	4974(11)	7892(5)	115(13)
C(49)	8880(20)	4511(13)	8044(5)	290(40)
C(50)	9030(30)	4090(12)	7781(7)	260(40)
C(51)	8690(20)	4132(9)	7365(6)	200(20)
C(52)	7740(20)	4607(10)	6782(5)	85(10)
C(53)	10514(13)	8698(8)	7579(5)	166(19)
C(54)	10124(16)	8350(8)	7843(6)	88(10)
C(55)	9318(16)	8040(9)	7700(9)	103(11)
C(56)	8903(17)	8079(11)	7292(10)	158(18)
C(57)	9290(20)	8426(13)	7028(7)	1700(500)
C(58)	10100(20)	8736(10)	7171(5)	290(40)
C(59)	11160(30)	9138(14)	7757(9)	250(30)
C(60)	11183(10)	4705(5)	9607(5)	81(9)
C(61)	10255(10)	4886(7)	9470(6)	102(11)
C(62)	10042(13)	5436(7)	9479(7)	111(12)
C(63)	10759(17)	5806(5)	9625(7)	139(16)
C(64)	11687(15)	5625(5)	9762(6)	89(10)
C(65)	11899(10)	5074(6)	9753(5)	69(8)
C(66)	11371(15)	4117(7)	9658(9)	87(10)
C(67)	8340(16)	5223(7)	5315(5)	103(12)
C(68)	8488(19)	4835(8)	5624(6)	137(15)
C(69)	8810(20)	4319(8)	5540(9)	141(16)
C(70)	8980(20)	4191(8)	5146(10)	170(20)
C(71)	8830(30)	4578(10)	4838(8)	230(30)
C(72)	8510(20)	5094(9)	4922(5)	164(19)
C(73)	8040(30)	5772(9)	5405(7)	122(14)
La(1A)	4715(1)	6708(1)	6802(1)	38(1)
Si(1A)	4248(5)	5302(3)	5981(2)	34(2)
Si(2A)	2428(7)	7529(4)	6033(2)	52(3)
Si(3A)	6630(6)	7361(4)	5978(3)	57(3)
C(1A)	5028(11)	5683(9)	6455(4)	50(8)
C(2A)	4982(10)	5559(8)	6868(4)	25(6)
C(3A)	5877(10)	5724(9)	7085(5)	46(7)
C(4A)	6414(14)	5978(10)	6805(4)	51(8)
C(5A)	5883(11)	5962(9)	6405(5)	32(6)
C(6A)	4067(19)	5742(10)	5558(7)	44(7)
C(7A)	3095(15)	5058(9)	6099(6)	31(6)
C(8A)	4932(9)	4688(6)	5847(3)	51(8)
C(9A)	5927(8)	4824(8)	5740(5)	42(6)
C(10A)	5057(13)	4278(7)	6200(4)	42(6)
C(11A)	4340(10)	4420(7)	5478(4)	27(5)
C(12A)	2842(16)	7105(5)	6426(4)	33(5)
C(13A)	2872(19)	6534(5)	6428(5)	51(7)
C(14A)	2907(18)	6284(6)	6816(4)	40(7)
C(15A)	2960(20)	6730(5)	7090(5)	59(8)
C(16A)	2890(20)	7202(8)	6848(4)	65(9)
C(17A)	2991(19)	7318(11)	5584(7)	51(7)
C(18A)	2767(18)	8293(9)	6252(7)	44(6)
C(19A)	991(13)	7396(5)	5833(4)	63(8)
C(20A)	770(20)	6808(4)	5713(6)	124(15)
C(21A)	669(19)	7764(6)	5471(4)	77(9)
C(22A)	442(16)	7545(8)	6184(4)	70(9)
C(23A)	5863(9)	7488(8)	6432(4)	34(6)
C(24A)	6449(12)	7361(8)	6808(4)	44(6)
C(25A)	5933(11)	7617(8)	7092(5)	40(6)
C(26A)	5130(13)	7866(9)	6857(4)	46(6)
C(27A)	4953(12)	7740(9)	6432(4)	45(7)
C(28A)	5770(20)	7155(11)	5519(8)	60(8)
C(29A)	7668(19)	6931(11)	6137(8)	45(7)
C(30A)	6977(8)	8030(7)	5796(4)	41(6)
C(31A)	6093(9)	8363(9)	5628(5)	78(9)
C(32A)	7612(12)	7955(12)	5463(5)	114(15)
C(33A)	7536(14)	8317(11)	6159(5)	131(17)

Table 3. Bond lengths [Å] and angles [deg]

La(1)-C(1)	2.986(18)	La(1)-C(2)	2.94(2)
La(1)-C(3)	2.73(2)	La(1)-C(4)	2.74(2)
La(1)-C(5)	2.78(2)	La(1)-C(12)	2.96(2)
La(1)-C(13)	3.00(2)	La(1)-C(14)	2.96(3)
La(1)-C(15)	2.94(2)	La(1)-C(16)	2.94(2)
La(1)-C(23)	2.982(19)	La(1)-C(24)	2.83(2)
La(1)-C(25)	2.828(19)	La(1)-C(26)	2.82(2)
La(1)-C(27)	2.866(18)	K-O(1)	2.80(2)
K-O(2)	2.82(2)	K-O(3)	2.99(2)
K-O(4)	2.71(2)	K-O(5)	2.71(2)
K-O(6)	2.81(2)	K-C(47)	3.40(2)
K-C(48)	3.39(3)	K-C(49)	3.46(3)
Si(1)-C(1)	1.715(15)	Si(1)-C(7)	1.91(3)
Si(1)-C(8)	1.929(16)	Si(1)-C(6)	2.02(2)
Si(2)-C(18)	1.71(3)	Si(2)-C(19)	1.78(2)
Si(2)-C(17)	1.94(3)	Si(2)-C(12)	1.976(16)
Si(3)-C(23)	1.785(16)	Si(3)-C(28)	1.86(2)
Si(3)-C(29)	1.92(4)	Si(3)-C(30)	2.02(2)
O(1)-C(45)	1.420(16)	O(1)-C(34)	1.423(16)
O(2)-C(36)	1.414(16)	O(2)-C(35)	1.416(16)
O(3)-C(38)	1.410(16)	O(3)-C(37)	1.411(17)
O(4)-C(39)	1.414(16)	O(4)-C(40)	1.420(15)
O(5)-C(41)	1.416(16)	O(5)-C(42)	1.432(16)
O(6)-C(43)	1.412(16)	O(6)-C(44)	1.414(16)
C(1)-C(2)	1.414(12)	C(1)-C(5)	1.417(12)
C(2)-C(3)	1.421(12)	C(3)-C(4)	1.418(13)
C(4)-C(5)	1.411(12)	C(8)-C(10)	1.522(12)
C(8)-C(11)	1.522(12)	C(8)-C(9)	1.527(12)
C(12)-C(13)	1.407(12)	C(12)-C(16)	1.420(12)
C(13)-C(14)	1.404(12)	C(14)-C(15)	1.407(12)
C(15)-C(16)	1.408(12)	C(19)-C(20)	1.518(12)
C(19)-C(21)	1.519(12)	C(19)-C(22)	1.531(13)
C(23)-C(24)	1.414(12)	C(23)-C(27)	1.419(13)
C(24)-C(25)	1.415(13)	C(24)-C(27)	2.01(2)
C(25)-C(26)	1.408(13)	C(26)-C(27)	1.422(12)
C(30)-C(32)	1.517(12)	C(30)-C(33)	1.519(13)
C(30)-C(31)	1.520(13)	C(34)-C(35)	1.63(2)
C(36)-C(37)	1.64(2)	C(38)-C(39)	1.63(2)
C(40)-C(41)	1.64(2)	C(42)-C(43)	1.64(2)
C(44)-C(45)	1.64(2)	C(46)-C(47)	1.3900
C(46)-C(51)	1.3900	C(46)-C(52)	1.474(17)
C(53)-C(59)	1.48(2)	C(60)-C(66)	1.479(17)
C(67)-C(73)	1.459(18)	La(1A)-C(1A)	2.83(2)
La(1A)-C(2A)	2.86(2)	La(1A)-C(3A)	2.99(2)
La(1A)-C(4A)	2.98(2)	La(1A)-C(5A)	2.90(2)
La(1A)-C(12A)	2.91(2)	La(1A)-C(13A)	2.73(3)
La(1A)-C(14A)	2.75(2)	La(1A)-C(15A)	2.76(3)
La(1A)-C(16A)	2.86(3)	La(1A)-C(23A)	2.888(19)
La(1A)-C(24A)	2.91(2)	La(1A)-C(25A)	2.897(19)
La(1A)-C(26A)	2.92(2)	La(1A)-C(27A)	2.86(2)
Si(1A)-C(6A)	1.76(2)	Si(1A)-C(7A)	1.82(2)
Si(1A)-C(8A)	1.878(17)	Si(1A)-C(1A)	2.007(18)
Si(2A)-C(12A)	1.702(16)	Si(2A)-C(17A)	1.85(3)
Si(2A)-C(18A)	2.05(2)	Si(2A)-C(19A)	2.06(2)
Si(3A)-C(29A)	1.82(3)	Si(3A)-C(30A)	1.844(18)
Si(3A)-C(28A)	1.86(3)	Si(3A)-C(23A)	1.991(18)
C(1A)-C(2A)	1.408(12)	C(1A)-C(5A)	1.412(13)
C(2A)-C(3A)	1.414(12)	C(3A)-C(4A)	1.418(13)
C(4A)-C(5A)	1.420(12)	C(8A)-C(11A)	1.524(12)
C(8A)-C(9A)	1.526(12)	C(8A)-C(10A)	1.532(12)
C(12A)-C(16A)	1.406(12)	C(12A)-C(13A)	1.408(12)
C(13A)-C(14A)	1.415(12)	C(14A)-C(15A)	1.420(12)
C(15A)-C(16A)	1.407(13)	C(19A)-C(21A)	1.517(12)
C(19A)-C(20A)	1.523(12)	C(19A)-C(22A)	1.525(13)

C(23A)-C(27A)	1.420(13)	C(23A)-C(24A)	1.421(12)
C(24A)-C(25A)	1.410(13)	C(25A)-C(26A)	1.415(13)
C(26A)-C(27A)	1.425(12)	C(30A)-C(33A)	1.511(13)
C(30A)-C(32A)	1.522(12)	C(30A)-C(31A)	1.525(12)
O(5)-K-O(4)	57.8(5)	O(5)-K-O(1)	121.3(5)
O(4)-K-O(1)	154.4(7)	O(5)-K-O(6)	66.0(5)
O(4)-K-O(6)	115.0(6)	O(1)-K-O(6)	55.5(5)
O(5)-K-O(2)	177.4(6)	O(4)-K-O(2)	120.2(5)
O(1)-K-O(2)	59.6(5)	O(6)-K-O(2)	114.8(6)
O(5)-K-O(3)	118.3(6)	O(4)-K-O(3)	60.6(5)
O(1)-K-O(3)	112.2(5)	O(6)-K-O(3)	145.9(7)
O(2)-K-O(3)	59.6(5)	C(1)-Si(1)-C(7)	106.0(11)
C(1)-Si(1)-C(8)	108.7(8)	C(7)-Si(1)-C(8)	111.5(11)
C(1)-Si(1)-C(6)	115.0(10)	C(7)-Si(1)-C(6)	109.2(13)
C(8)-Si(1)-C(6)	106.7(9)	C(18)-Si(2)-C(19)	94.9(11)
C(18)-Si(2)-C(17)	101.5(13)	C(19)-Si(2)-C(17)	113.2(10)
C(18)-Si(2)-C(12)	117.9(11)	C(19)-Si(2)-C(12)	110.1(9)
C(17)-Si(2)-C(12)	117.1(11)	C(23)-Si(3)-C(28)	119.3(10)
C(23)-Si(3)-C(29)	107.6(12)	C(28)-Si(3)-C(29)	103.0(13)
C(23)-Si(3)-C(30)	105.8(9)	C(28)-Si(3)-C(30)	115.9(8)
C(29)-Si(3)-C(30)	104.0(12)	C(45)-O(1)-C(34)	121(2)
C(45)-O(1)-K	110(2)	C(34)-O(1)-K	102(2)
C(36)-O(2)-C(35)	116(2)	C(36)-O(2)-K	118.8(14)
C(35)-O(2)-K	122.3(17)	C(38)-O(3)-C(37)	127(2)
C(38)-O(3)-K	105.2(15)	C(37)-O(3)-K	87.7(19)
C(39)-O(4)-C(40)	97.3(19)	C(39)-O(4)-K	121(2)
C(40)-O(4)-K	117.4(18)	C(41)-O(5)-C(42)	104(2)
C(41)-O(5)-K	129.7(15)	C(42)-O(5)-K	118.4(16)
C(43)-O(6)-C(44)	112(2)	C(43)-O(6)-K	109.4(19)
C(44)-O(6)-K	92(2)	C(2)-C(1)-C(5)	102.0(13)
C(2)-C(1)-Si(1)	129.1(12)	C(5)-C(1)-Si(1)	127.4(10)
C(1)-C(2)-C(3)	111.3(14)	C(4)-C(3)-C(2)	108.0(14)
C(5)-C(4)-C(3)	103.8(14)	C(4)-C(5)-C(1)	114.4(14)
C(10)-C(8)-C(11)	109.2(10)	C(10)-C(8)-C(9)	108.7(10)
C(11)-C(8)-C(9)	108.8(10)	C(10)-C(8)-Si(1)	106.1(11)
C(11)-C(8)-Si(1)	118.3(13)	C(9)-C(8)-Si(1)	105.4(11)
C(13)-C(12)-C(16)	111.7(12)	C(13)-C(12)-Si(2)	126.1(10)
C(16)-C(12)-Si(2)	121.2(10)	C(14)-C(13)-C(12)	105.9(12)
C(13)-C(14)-C(15)	107.9(13)	C(14)-C(15)-C(16)	110.8(13)
C(15)-C(16)-C(12)	103.6(12)	C(20)-C(19)-C(21)	109.9(10)
C(20)-C(19)-C(22)	108.8(11)	C(21)-C(19)-C(22)	108.8(11)
C(20)-C(19)-Si(2)	106.8(14)	C(21)-C(19)-Si(2)	112.7(13)
C(22)-C(19)-Si(2)	109.8(13)	C(24)-C(23)-C(27)	90.5(12)
C(24)-C(23)-Si(3)	143.9(12)	C(27)-C(23)-Si(3)	123.0(11)
C(23)-C(24)-C(25)	119.4(14)	C(23)-C(24)-C(27)	44.8(7)
C(25)-C(24)-C(27)	74.6(10)	C(26)-C(25)-C(24)	106.9(14)
C(25)-C(26)-C(27)	97.6(13)	C(23)-C(27)-C(26)	125.1(14)
C(23)-C(27)-C(24)	44.6(7)	C(26)-C(27)-C(24)	80.7(10)
C(32)-C(30)-C(33)	110.1(11)	C(32)-C(30)-C(31)	109.9(11)
C(33)-C(30)-C(31)	109.1(11)	C(32)-C(30)-Si(3)	108.8(13)
C(33)-C(30)-Si(3)	109.0(12)	C(31)-C(30)-Si(3)	109.8(12)
O(1)-C(34)-C(35)	113(2)	O(1)-C(34)-K	53.7(16)
C(35)-C(34)-K	90.0(16)	O(2)-C(35)-C(34)	89(2)
O(2)-C(36)-C(37)	90(2)	O(3)-C(37)-C(36)	104(2)
O(3)-C(37)-K	66.6(17)	C(36)-C(37)-K	92.8(18)
O(3)-C(38)-C(39)	115(2)	O(4)-C(39)-C(38)	97.9(19)
O(4)-C(40)-C(41)	109(2)	O(5)-C(41)-C(40)	100.4(19)
O(5)-C(42)-C(43)	111(2)	O(6)-C(43)-C(42)	117(2)
O(6)-C(44)-C(45)	83(2)	O(6)-C(44)-K	61.8(17)
C(45)-C(44)-K	89(2)	O(1)-C(45)-C(44)	82(2)
C(47)-C(46)-C(51)	120.0	C(47)-C(46)-C(52)	120.3(7)
C(51)-C(46)-C(52)	119.3(7)	C(47)-C(46)-K	74.8(9)
C(51)-C(46)-K	81.7(10)	C(52)-C(46)-K	120.5(16)
C(48)-C(47)-C(46)	120.0	C(48)-C(47)-K	77.7(8)
C(46)-C(47)-K	81.9(9)	C(47)-C(48)-C(49)	120.0
C(47)-C(48)-K	78.7(8)	C(49)-C(48)-K	81.4(10)
C(50)-C(49)-C(48)	120.0	C(50)-C(49)-K	82.1(9)
C(48)-C(49)-K	75.2(10)	C(51)-C(50)-C(49)	120.0