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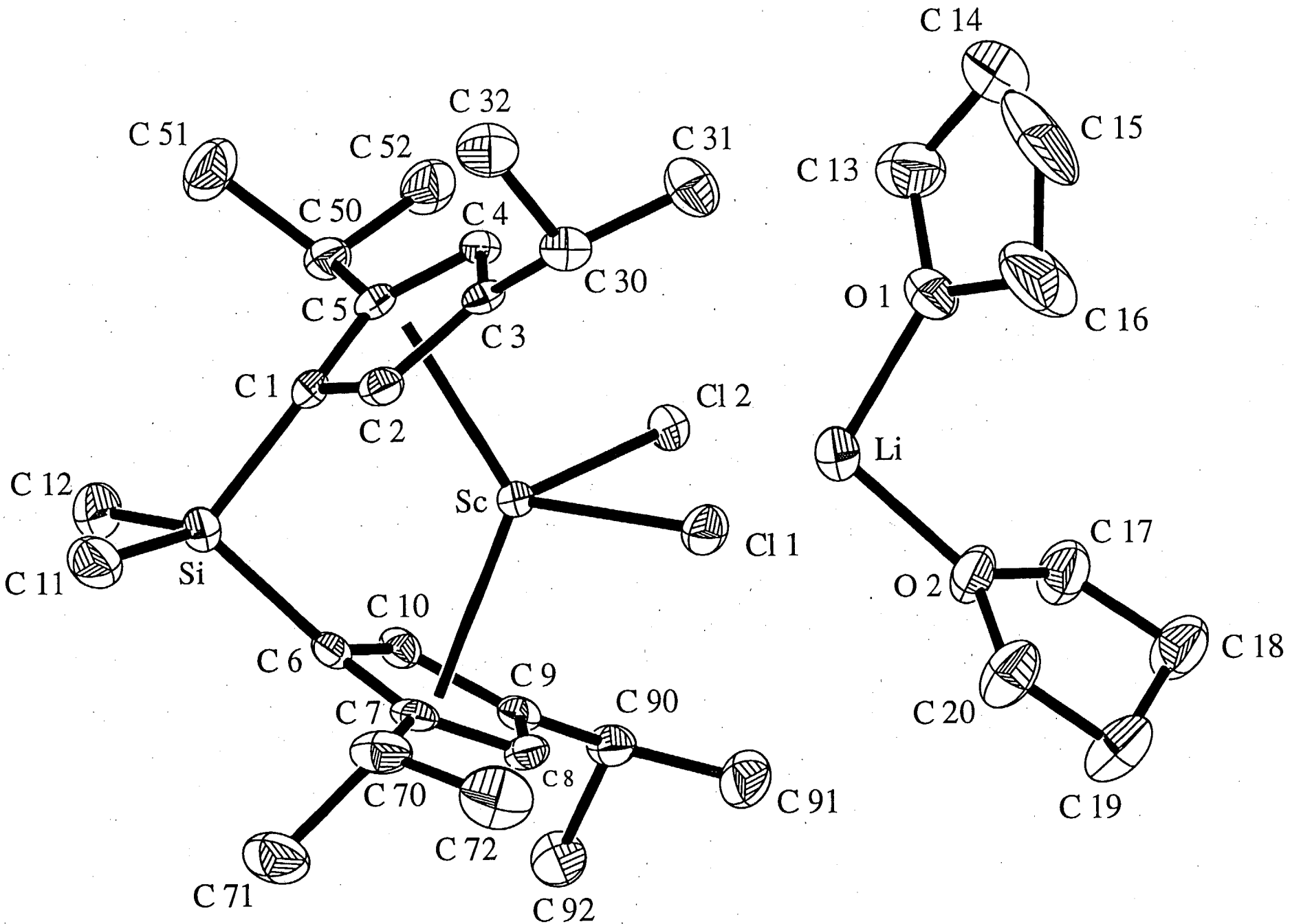


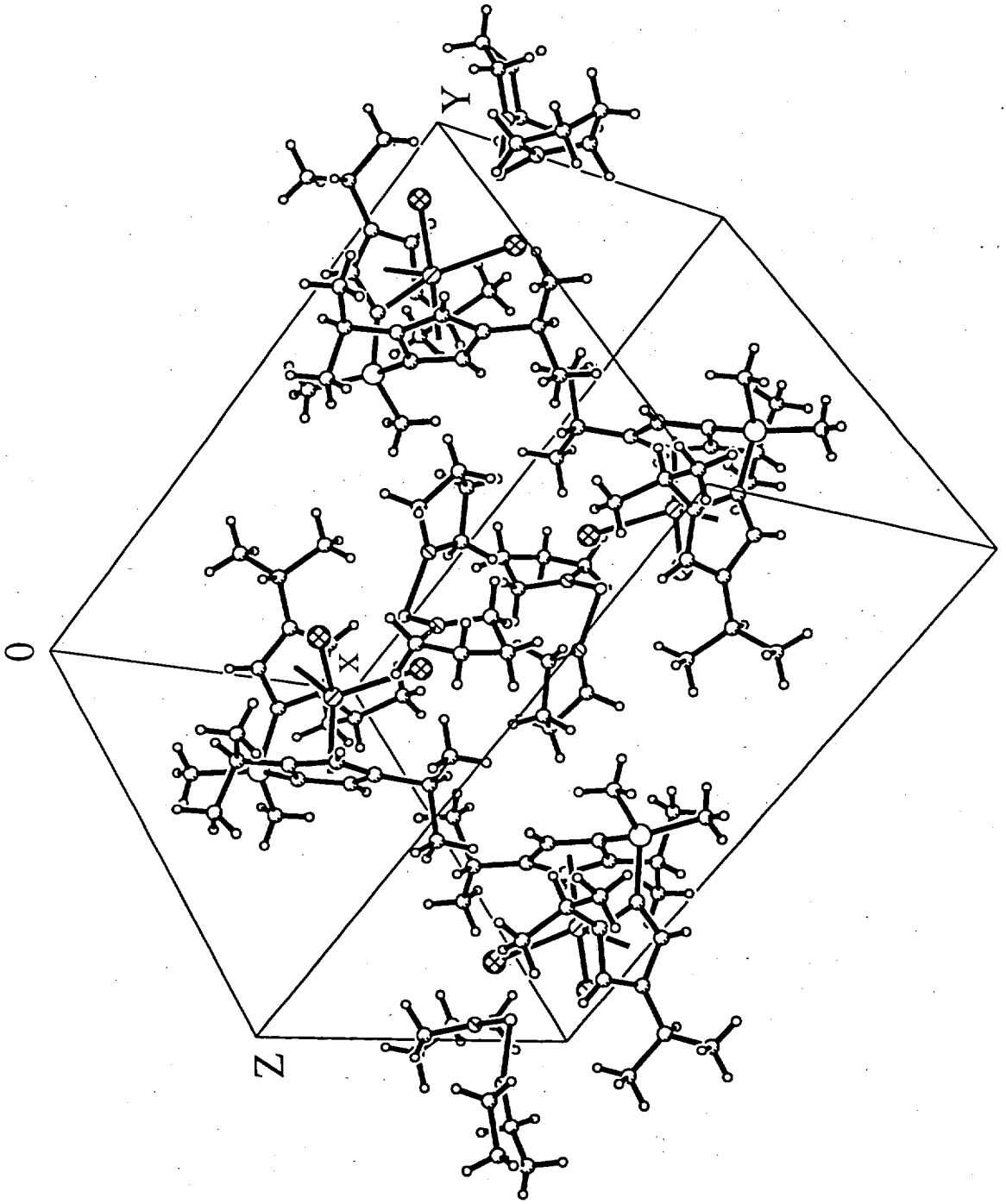

Y
O
X
Z

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

	x	y	z	U(eq)
Sc	2424(1)	2779(1)	4811(1)	17(1)
Si	2345(1)	1091(1)	4566(1)	26(1)
Cl(1)	3748(1)	3723(1)	5218(1)	28(1)
Cl(2)	983(1)	3685(1)	4633(1)	24(1)
Li	2300(4)	4514(2)	5073(3)	33(1)
O(1)	1908(2)	5018(1)	6090(1)	42(1)
O(2)	2672(1)	5247(1)	4316(1)	34(1)
C(1)	2195(2)	1661(1)	5559(2)	20(1)
C(2)	3114(2)	1985(1)	6028(2)	21(1)
C(3)	2803(2)	2543(1)	6549(1)	20(1)
C(4)	1684(2)	2589(1)	6370(2)	19(1)
C(5)	1295(2)	2055(1)	5774(1)	20(1)
C(6)	2628(2)	1799(1)	3768(1)	21(1)
C(7)	3588(2)	2196(1)	3744(1)	21(1)
C(8)	3295(2)	2828(1)	3308(2)	22(1)
C(9)	2187(2)	2851(1)	3054(1)	20(1)
C(10)	1776(2)	2222(1)	3357(2)	20(1)
C(11)	3432(3)	448(2)	4863(2)	42(1)
C(12)	1119(3)	602(2)	4110(2)	41(1)
C(13)	978(3)	4946(2)	6570(2)	47(1)
C(14)	1179(5)	5373(2)	7407(3)	78(1)
C(15)	2344(4)	5550(2)	7477(3)	81(2)
C(16)	2575(4)	5550(2)	6520(3)	79(1)
C(17)	1936(2)	5780(2)	3955(2)	42(1)
C(18)	2628(3)	6370(2)	3712(2)	44(1)
C(19)	3593(3)	6002(2)	3431(2)	46(1)
C(20)	3727(2)	5394(2)	4072(2)	42(1)
C(30)	3522(2)	2930(1)	7264(2)	25(1)
C(31)	3077(3)	3631(2)	7503(2)	36(1)
C(32)	3708(3)	2477(2)	8112(2)	34(1)
C(50)	129(2)	1866(1)	5527(2)	25(1)
C(51)	-148(3)	1230(2)	6074(2)	41(1)
C(52)	-650(2)	2444(2)	5676(2)	34(1)
C(70)	4721(2)	1949(1)	4028(2)	31(1)
C(71)	5022(3)	1382(2)	3386(2)	42(1)
C(72)	5550(2)	2524(2)	4088(2)	44(1)
C(90)	1558(2)	3397(1)	2492(2)	24(1)
C(91)	2128(3)	4091(1)	2511(2)	36(1)
C(92)	1303(3)	3148(2)	1513(2)	32(1)

Table 4. Bond lengths [A] and angles [deg] for 1.

Sc-Cl(1)	2.4964(8)
Sc-Cl(2)	2.5089(8)
Sc-X(1A)	2.2385(5)
Sc-X(1B)	2.2356(6)
Pln1-Sc	2.228(2)
Pln2-Sc	2.229(2)
Sc-C(2)	2.456(2)
Sc-C(1)	2.461(2)
Sc-C(10)	2.471(2)
Sc-C(6)	2.479(2)
Sc-C(7)	2.539(2)
Sc-C(5)	2.544(2)
Sc-C(8)	2.601(2)
Sc-C(9)	2.604(2)
Sc-C(3)	2.618(2)
Sc-C(4)	2.622(2)
Si-C(11)	1.862(3)
Si-C(12)	1.865(3)
Si-C(1)	1.870(2)
Si-C(6)	1.873(2)
Cl(1)-Li	2.364(4)
Cl(2)-Li	2.341(4)
Li-O(2)	1.900(4)
Li-O(1)	1.911(4)
O(1)-C(16)	1.430(4)
O(1)-C(13)	1.442(3)
O(2)-C(20)	1.440(3)
O(2)-C(17)	1.446(3)
C(1)-C(2)	1.424(3)
C(1)-C(5)	1.428(3)
C(2)-C(3)	1.408(3)
C(2)-H(2)	0.90(2)
C(3)-C(4)	1.402(3)
C(3)-C(30)	1.513(3)
C(4)-C(5)	1.412(3)
C(4)-H(4)	0.89(2)
C(5)-C(50)	1.512(3)
C(6)-C(10)	1.426(3)
C(6)-C(7)	1.430(3)
C(7)-C(8)	1.412(3)
C(7)-C(70)	1.514(3)
C(8)-C(9)	1.400(3)
C(8)-H(8)	0.88(2)
C(9)-C(10)	1.413(3)
C(9)-C(90)	1.512(3)
C(10)-H(10)	0.91(2)
C(11)-H(11A)	0.91(3)
C(11)-H(11B)	0.96(3)
C(11)-H(11C)	0.95(3)
C(12)-H(12A)	0.93(3)
C(12)-H(12B)	0.93(3)
C(12)-H(12C)	0.95(3)
C(13)-C(14)	1.491(5)
C(13)-H(13A)	0.98(3)
C(13)-H(13B)	0.96(3)
C(14)-C(15)	1.495(6)
C(14)-H(14A)	0.94(4)
C(14)-H(14B)	0.91(5)
C(15)-C(16)	1.486(6)
C(15)-H(15A)	0.88(3)
C(15)-H(15B)	0.98(4)
C(16)-H(16A)	0.96(3)

C(16)-H(16B)	0.94(4)
C(17)-C(18)	1.503(4)
C(17)-H(17A)	1.01(3)
C(17)-H(17B)	0.98(3)
C(18)-C(19)	1.503(4)
C(18)-H(18A)	1.04(3)
C(18)-H(18B)	0.93(3)
C(19)-C(20)	1.509(4)
C(19)-H(19A)	0.97(3)
C(19)-H(19B)	0.91(3)
C(20)-H(20A)	0.96(3)
C(20)-H(20A)	0.99(3)
C(30)-C(31)	1.523(4)
C(30)-C(32)	1.532(4)
C(30)-H(30)	0.96(2)
C(31)-H(31A)	1.02(3)
C(31)-H(31B)	0.98(3)
C(31)-H(31C)	0.97(3)
C(32)-H(32A)	0.99(3)
C(32)-H(32B)	0.94(2)
C(32)-H(32C)	1.00(3)
C(50)-C(52)	1.518(4)
C(50)-C(51)	1.537(4)
C(50)-H(50)	0.93(2)
C(51)-H(51A)	0.93(3)
C(51)-H(51B)	1.02(3)
C(51)-H(51C)	0.97(3)
C(52)-H(52A)	1.00(3)
C(52)-H(52B)	0.92(3)
C(52)-H(52C)	0.99(2)
C(70)-C(72)	1.518(4)
C(70)-C(71)	1.530(4)
C(70)-H(70)	0.93(2)
C(71)-H(71A)	0.99(3)
C(71)-H(71B)	0.99(3)
C(71)-H(71C)	0.92(3)
C(72)-H(72A)	0.93(3)
C(72)-H(72B)	0.95(3)
C(72)-H(72C)	0.96(3)
C(90)-C(91)	1.517(4)
C(90)-C(92)	1.534(3)
C(90)-H(90)	0.92(2)
C(91)-H(91A)	0.99(3)
C(91)-H(91B)	0.99(3)
C(91)-H(91C)	0.95(3)
C(92)-H(92A)	0.98(2)
C(92)-H(92B)	0.99(3)
C(92)-H(92C)	0.96(3)

X(1A)-Sc-X(1B)	127.91(2)
Pln1-Sc-Pln2	118.42(7)
Cl(1)-Sc-Cl(2)	88.14(3)
C(2)-Sc-C(1)	33.66(8)
C(2)-Sc-C(10)	115.39(8)
C(1)-Sc-C(10)	88.36(8)
C(2)-Sc-C(6)	86.21(8)
C(1)-Sc-C(6)	68.92(7)
C(10)-Sc-C(6)	33.48(7)
C(2)-Sc-Cl(1)	96.15(6)
C(1)-Sc-Cl(1)	129.75(6)
C(10)-Sc-Cl(1)	132.47(6)
C(6)-Sc-Cl(1)	126.64(6)
C(2)-Sc-Cl(2)	134.69(6)
C(1)-Sc-Cl(2)	122.72(6)
C(10)-Sc-Cl(2)	92.84(6)
C(6)-Sc-Cl(2)	126.18(6)

C(2)-Sc-C(7)	90.31(8)
C(1)-Sc-C(7)	89.95(8)
C(10)-Sc-C(7)	54.15(8)
C(6)-Sc-C(7)	33.09(7)
Cl(1)-Sc-C(7)	93.56(6)
Cl(2)-Sc-C(7)	134.56(6)
C(2)-Sc-C(5)	54.09(8)
C(1)-Sc-C(5)	33.09(7)
C(10)-Sc-C(5)	96.07(8)
C(6)-Sc-C(5)	92.16(8)
Cl(1)-Sc-C(5)	131.47(6)
Cl(2)-Sc-C(5)	90.15(6)
C(7)-Sc-C(5)	120.34(8)
C(2)-Sc-C(8)	120.71(8)
C(1)-Sc-C(8)	120.25(8)
C(10)-Sc-C(8)	52.48(8)
C(6)-Sc-C(8)	53.54(8)
Cl(1)-Sc-C(8)	81.32(6)
Cl(2)-Sc-C(8)	104.55(6)
C(7)-Sc-C(8)	31.87(7)
C(5)-Sc-C(8)	145.08(8)
C(2)-Sc-C(9)	139.99(8)
C(1)-Sc-C(9)	119.73(7)
C(10)-Sc-C(9)	32.20(7)
C(6)-Sc-C(9)	54.48(7)
Cl(1)-Sc-C(9)	101.69(6)
Cl(2)-Sc-C(9)	81.80(6)
C(7)-Sc-C(9)	53.37(7)
C(5)-Sc-C(9)	126.01(7)
C(8)-Sc-C(9)	31.22(7)
C(2)-Sc-C(3)	32.03(7)
C(1)-Sc-C(3)	54.37(7)
C(10)-Sc-C(3)	142.72(8)
C(6)-Sc-C(3)	117.84(7)
Cl(1)-Sc-C(3)	81.07(6)
Cl(2)-Sc-C(3)	105.91(6)
C(7)-Sc-C(3)	119.23(7)
C(5)-Sc-C(3)	53.00(7)
C(8)-Sc-C(3)	144.07(8)
C(9)-Sc-C(3)	171.98(7)
C(2)-Sc-C(4)	52.37(8)
C(1)-Sc-C(4)	53.51(7)
C(10)-Sc-C(4)	126.93(8)
C(6)-Sc-C(4)	121.35(7)
Cl(1)-Sc-C(4)	100.33(6)
Cl(2)-Sc-C(4)	82.44(6)
C(7)-Sc-C(4)	141.09(8)
C(5)-Sc-C(4)	31.67(7)
C(8)-Sc-C(4)	172.91(8)
C(9)-Sc-C(4)	152.36(8)
C(3)-Sc-C(4)	31.04(7)
C(11)-Si-C(12)	107.5(2)
C(11)-Si-C(1)	109.92(13)
C(12)-Si-C(1)	115.69(13)
C(11)-Si-C(6)	116.85(14)
C(12)-Si-C(6)	110.28(13)
C(1)-Si-C(6)	96.65(10)
C(11)-Si-Sc	128.64(12)
C(12)-Si-Sc	123.84(12)
C(1)-Si-Sc	48.08(7)
C(6)-Si-Sc	48.64(7)
Li-Cl(1)-Sc	88.07(10)
Li-Cl(2)-Sc	88.29(11)
O(2)-Li-O(1)	101.1(2)
O(2)-Li-Cl(2)	123.8(2)
O(1)-Li-Cl(2)	109.5(2)

O(2)-Li-Cl(1)	107.3(2)
O(1)-Li-Cl(1)	121.4(2)
Cl(2)-Li-Cl(1)	95.4(2)
O(2)-Li-Sc	130.7(2)
O(1)-Li-Sc	128.0(2)
Cl(2)-Li-Sc	47.90(7)
Cl(1)-Li-Sc	47.57(7)
C(16)-O(1)-C(13)	108.2(2)
C(16)-O(1)-Li	122.1(2)
C(13)-O(1)-Li	129.7(2)
C(20)-O(2)-C(17)	109.4(2)
C(20)-O(2)-Li	126.3(2)
C(17)-O(2)-Li	124.1(2)
C(2)-C(1)-C(5)	105.8(2)
C(2)-C(1)-Si	119.9(2)
C(5)-C(1)-Si	130.0(2)
C(2)-C(1)-Sc	72.98(13)
C(5)-C(1)-Sc	76.64(13)
Si-C(1)-Sc	97.50(9)
C(3)-C(2)-C(1)	110.3(2)
C(3)-C(2)-Sc	80.32(14)
C(1)-C(2)-Sc	73.36(13)
C(3)-C(2)-H(2)	123.8(13)
C(1)-C(2)-H(2)	125.9(13)
Sc-C(2)-H(2)	115.2(12)
C(4)-C(3)-C(2)	106.1(2)
C(4)-C(3)-C(30)	127.4(2)
C(2)-C(3)-C(30)	125.8(2)
C(4)-C(3)-Sc	74.63(13)
C(2)-C(3)-Sc	67.65(12)
C(30)-C(3)-Sc	129.6(2)
C(3)-C(4)-C(5)	110.0(2)
C(3)-C(4)-Sc	74.33(13)
C(5)-C(4)-Sc	71.14(12)
C(3)-C(4)-H(4)	127.5(14)
C(5)-C(4)-H(4)	122.5(14)
Sc-C(4)-H(4)	120.8(13)
C(4)-C(5)-C(1)	107.7(2)
C(4)-C(5)-C(50)	125.9(2)
C(1)-C(5)-C(50)	125.8(2)
C(4)-C(5)-Sc	77.19(13)
C(1)-C(5)-Sc	70.26(12)
C(50)-C(5)-Sc	125.5(2)
C(10)-C(6)-C(7)	106.0(2)
C(10)-C(6)-Si	120.2(2)
C(7)-C(6)-Si	128.8(2)
C(10)-C(6)-Sc	72.95(13)
C(7)-C(6)-Sc	75.76(13)
Si-C(6)-Sc	96.82(9)
C(8)-C(7)-C(6)	107.4(2)
C(8)-C(7)-C(70)	126.0(2)
C(6)-C(7)-C(70)	126.2(2)
C(8)-C(7)-Sc	76.48(13)
C(6)-C(7)-Sc	71.14(12)
C(70)-C(7)-Sc	123.6(2)
C(9)-C(8)-C(7)	110.4(2)
C(9)-C(8)-Sc	74.50(13)
C(7)-C(8)-Sc	71.65(13)
C(9)-C(8)-H(8)	124.1(13)
C(7)-C(8)-H(8)	125.4(13)
Sc-C(8)-H(8)	120.6(13)
C(8)-C(9)-C(10)	105.9(2)
C(8)-C(9)-C(90)	127.7(2)
C(10)-C(9)-C(90)	126.2(2)
C(8)-C(9)-Sc	74.28(13)
C(10)-C(9)-Sc	68.72(12)

C(90)-C(9)-Sc	125.9(2)
C(9)-C(10)-C(6)	110.2(2)
C(9)-C(10)-Sc	79.07(13)
C(6)-C(10)-Sc	73.56(13)
C(9)-C(10)-H(10)	124.7(14)
C(6)-C(10)-H(10)	125.1(14)
Sc-C(10)-H(10)	115.4(14)
Si-C(11)-H(11A)	110(2)
Si-C(11)-H(11B)	111(2)
H(11A)-C(11)-H(11B)	110(2)
Si-C(11)-H(11C)	114(2)
H(11A)-C(11)-H(11C)	109(3)
H(11B)-C(11)-H(11C)	103(2)
Si-C(12)-H(12A)	107(2)
Si-C(12)-H(12B)	108(2)
H(12A)-C(12)-H(12B)	108(2)
Si-C(12)-H(12C)	114(2)
H(12A)-C(12)-H(12C)	109(2)
H(12B)-C(12)-H(12C)	112(3)
O(1)-C(13)-C(14)	106.9(3)
O(1)-C(13)-H(13A)	104(2)
C(14)-C(13)-H(13A)	114(2)
O(1)-C(13)-H(13B)	108(2)
C(14)-C(13)-H(13B)	117(2)
H(13A)-C(13)-H(13B)	106(3)
C(13)-C(14)-C(15)	104.9(3)
C(13)-C(14)-H(14A)	106(3)
C(15)-C(14)-H(14A)	102(3)
C(13)-C(14)-H(14B)	111(3)
C(15)-C(14)-H(14B)	114(3)
H(14A)-C(14)-H(14B)	117(4)
C(16)-C(15)-C(14)	103.2(4)
C(16)-C(15)-H(15A)	108(2)
C(14)-C(15)-H(15A)	119(2)
C(16)-C(15)-H(15B)	109(2)
C(14)-C(15)-H(15B)	110(3)
H(15A)-C(15)-H(15B)	107(3)
O(1)-C(16)-C(15)	105.2(4)
O(1)-C(16)-H(16A)	106(3)
C(15)-C(16)-H(16A)	115(2)
O(1)-C(16)-H(16B)	108(2)
C(15)-C(16)-H(16B)	114(2)
H(16A)-C(16)-H(16B)	108(3)
O(2)-C(17)-C(18)	105.5(2)
O(2)-C(17)-H(17A)	109(2)
C(18)-C(17)-H(17A)	109(2)
O(2)-C(17)-H(17B)	110(2)
C(18)-C(17)-H(17B)	114(2)
H(17A)-C(17)-H(17B)	109(3)
C(19)-C(18)-C(17)	102.3(3)
C(19)-C(18)-H(18A)	112(2)
C(17)-C(18)-H(18A)	106(2)
C(19)-C(18)-H(18B)	113(2)
C(17)-C(18)-H(18B)	111(2)
H(18A)-C(18)-H(18B)	112(2)
C(18)-C(19)-C(20)	103.2(3)
C(18)-C(19)-H(19A)	108(2)
C(20)-C(19)-H(19A)	108(2)
C(18)-C(19)-H(19B)	111(2)
C(20)-C(19)-H(19B)	110(2)
H(19A)-C(19)-H(19B)	115(3)
O(2)-C(20)-C(19)	105.8(2)
O(2)-C(20)-H(20A)	110(2)
C(19)-C(20)-H(20A)	115(2)
O(2)-C(20)-H(20A)	106(2)
C(19)-C(20)-H(20A)	113(2)

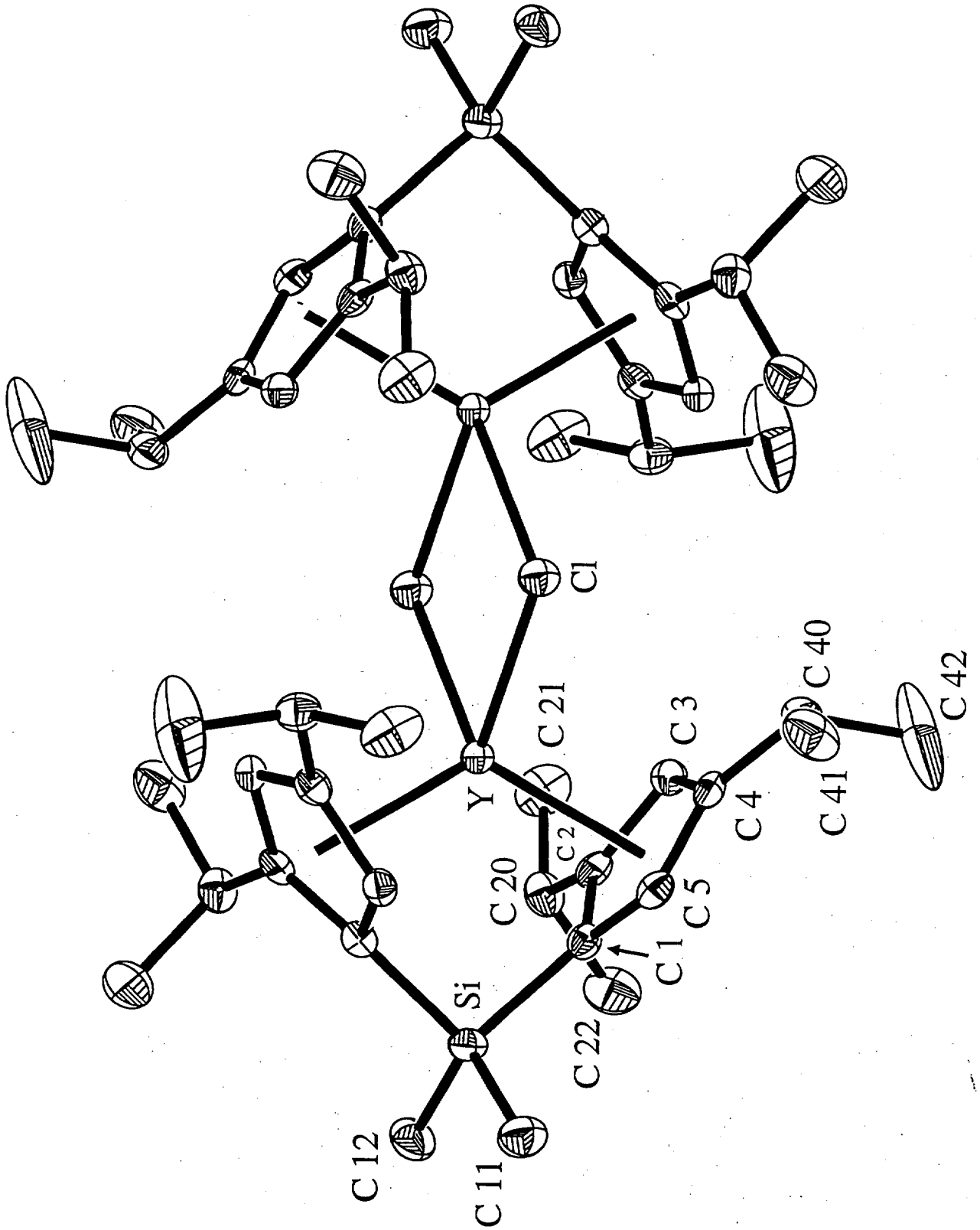
H(20A)-C(20)-H(20A)	107(2)
C(3)-C(30)-C(31)	113.5(2)
C(3)-C(30)-C(32)	108.8(2)
C(31)-C(30)-C(32)	109.9(2)
C(3)-C(30)-H(30)	106.4(13)
C(31)-C(30)-H(30)	111.3(13)
C(32)-C(30)-H(30)	106.7(13)
C(30)-C(31)-H(31A)	111(2)
C(30)-C(31)-H(31B)	110(2)
H(31A)-C(31)-H(31B)	109(2)
C(30)-C(31)-H(31C)	110(2)
H(31A)-C(31)-H(31C)	108(2)
H(31B)-C(31)-H(31C)	109(2)
C(30)-C(32)-H(32A)	109(2)
C(30)-C(32)-H(32B)	113(2)
H(32A)-C(32)-H(32B)	107(2)
C(30)-C(32)-H(32C)	110.2(14)
H(32A)-C(32)-H(32C)	112(2)
H(32B)-C(32)-H(32C)	107(2)
C(5)-C(50)-C(52)	114.1(2)
C(5)-C(50)-C(51)	109.6(2)
C(52)-C(50)-C(51)	108.8(2)
C(5)-C(50)-H(50)	109.5(14)
C(52)-C(50)-H(50)	107.0(13)
C(51)-C(50)-H(50)	107.7(13)
C(50)-C(51)-H(51A)	111(2)
C(50)-C(51)-H(51B)	109(2)
H(51A)-C(51)-H(51B)	108(2)
C(50)-C(51)-H(51C)	110(2)
H(51A)-C(51)-H(51C)	106(2)
H(51B)-C(51)-H(51C)	114(2)
C(50)-C(52)-H(52A)	110(2)
C(50)-C(52)-H(52B)	112(2)
H(52A)-C(52)-H(52B)	110(2)
C(50)-C(52)-H(52C)	110.8(14)
H(52A)-C(52)-H(52C)	108(2)
H(52B)-C(52)-H(52C)	106(2)
C(7)-C(70)-C(72)	113.7(2)
C(7)-C(70)-C(71)	110.0(2)
C(72)-C(70)-C(71)	110.2(2)
C(7)-C(70)-H(70)	109.0(14)
C(72)-C(70)-H(70)	107.3(14)
C(71)-C(70)-H(70)	106.4(14)
C(70)-C(71)-H(71A)	109(2)
C(70)-C(71)-H(71B)	110(2)
H(71A)-C(71)-H(71B)	112(2)
C(70)-C(71)-H(71C)	111(2)
H(71A)-C(71)-H(71C)	109(2)
H(71B)-C(71)-H(71C)	106(2)
C(70)-C(72)-H(72A)	112(2)
C(70)-C(72)-H(72B)	109(2)
H(72A)-C(72)-H(72B)	109(3)
C(70)-C(72)-H(72C)	110(2)
H(72A)-C(72)-H(72C)	110(2)
H(72B)-C(72)-H(72C)	107(2)
C(9)-C(90)-C(91)	113.0(2)
C(9)-C(90)-C(92)	110.4(2)
C(91)-C(90)-C(92)	110.0(2)
C(9)-C(90)-H(90)	107.4(14)
C(91)-C(90)-H(90)	111.9(14)
C(92)-C(90)-H(90)	103.8(14)
C(90)-C(91)-H(91A)	110(2)
C(90)-C(91)-H(91B)	111(2)
H(91A)-C(91)-H(91B)	108(2)
C(90)-C(91)-H(91C)	113(2)
H(91A)-C(91)-H(91C)	108(2)

H(91B)-C(91)-H(91C)	106(2)
C(90)-C(92)-H(92A)	113.3(14)
C(90)-C(92)-H(92B)	112.1(14)
H(92A)-C(92)-H(92B)	106(2)
C(90)-C(92)-H(92C)	108(2)
H(92A)-C(92)-H(92C)	110(2)
H(92B)-C(92)-H(92C)	108(2)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for 1.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Sc	21(1)	16(1)	16(1)	0(1)	5(1)	-1(1)
Si	39(1)	17(1)	23(1)	-1(1)	8(1)	2(1)
Cl(1)	29(1)	26(1)	29(1)	-2(1)	5(1)	-9(1)
Cl(2)	28(1)	20(1)	26(1)	0(1)	7(1)	3(1)
Li	44(3)	22(2)	33(3)	-3(2)	7(2)	-2(2)
O(1)	55(1)	35(1)	40(1)	-15(1)	20(1)	-10(1)
O(2)	36(1)	23(1)	45(1)	8(1)	10(1)	-3(1)
C(1)	30(1)	15(1)	17(1)	4(1)	7(1)	-1(1)
C(2)	22(2)	22(1)	21(1)	6(1)	7(1)	5(1)
C(3)	25(1)	21(1)	13(1)	4(1)	6(1)	-1(1)
C(4)	24(1)	19(1)	17(1)	1(1)	8(1)	3(1)
C(5)	26(1)	19(1)	16(1)	5(1)	7(1)	-2(1)
C(6)	31(2)	18(1)	16(1)	-3(1)	7(1)	4(1)
C(7)	26(1)	26(1)	13(1)	-2(1)	7(1)	4(1)
C(8)	26(2)	24(1)	18(1)	-1(1)	10(1)	-6(1)
C(9)	25(1)	22(1)	13(1)	-3(1)	4(1)	1(1)
C(10)	23(2)	21(1)	17(1)	-5(1)	3(1)	-1(1)
C(11)	65(2)	31(2)	32(2)	3(2)	15(2)	15(2)
C(12)	62(2)	29(2)	35(2)	-6(2)	12(2)	-13(2)
C(13)	48(2)	54(2)	42(2)	7(2)	15(2)	13(2)
C(14)	127(4)	53(3)	61(3)	-14(2)	46(3)	-5(3)
C(15)	111(4)	65(3)	60(3)	-44(2)	-15(3)	26(3)
C(16)	79(3)	75(3)	88(3)	-55(3)	32(3)	-31(3)
C(17)	41(2)	30(2)	58(2)	10(2)	13(2)	3(2)
C(18)	50(2)	36(2)	48(2)	17(2)	10(2)	2(2)
C(19)	37(2)	49(2)	52(2)	23(2)	6(2)	-3(2)
C(20)	30(2)	41(2)	56(2)	16(2)	5(2)	-4(2)
C(30)	23(1)	31(2)	22(1)	0(1)	4(1)	0(1)
C(31)	42(2)	35(2)	30(2)	-11(1)	-1(2)	-1(2)
C(32)	34(2)	44(2)	24(2)	0(1)	-2(1)	0(2)
C(50)	28(2)	26(1)	23(2)	-2(1)	8(1)	-7(1)
C(51)	36(2)	33(2)	56(2)	6(2)	14(2)	-10(2)
C(52)	25(2)	35(2)	43(2)	2(2)	10(1)	-6(1)
C(70)	28(2)	42(2)	24(2)	6(1)	8(1)	12(1)
C(71)	40(2)	49(2)	39(2)	1(2)	15(2)	16(2)
C(72)	20(2)	60(2)	51(2)	-2(2)	5(2)	5(2)
C(90)	26(2)	27(1)	20(1)	2(1)	5(1)	3(1)
C(91)	53(2)	29(2)	25(2)	6(1)	0(2)	-1(2)
C(92)	37(2)	34(2)	24(2)	4(1)	-4(1)	3(2)



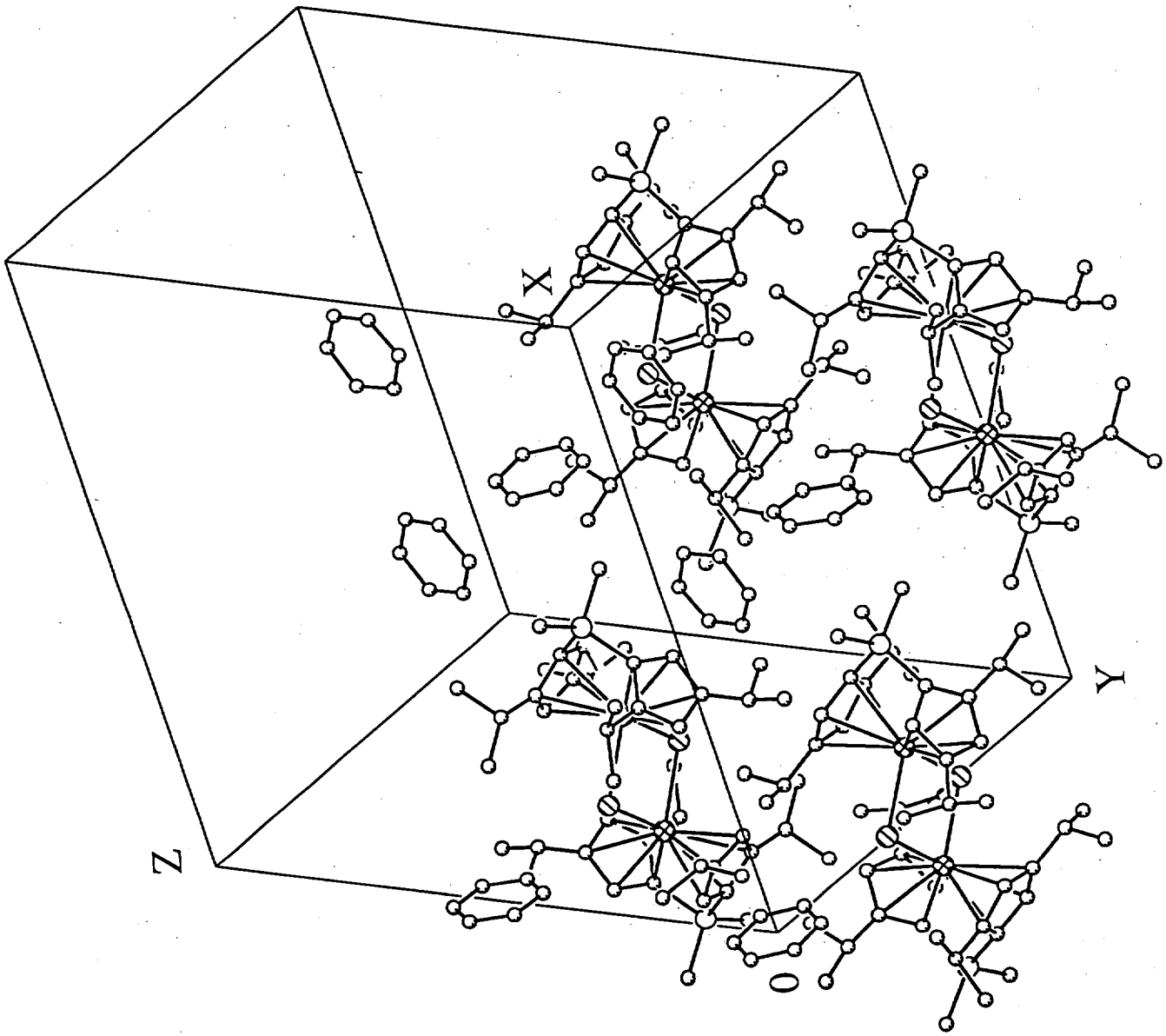

X
Y
Z
O

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

	x	y	z	U(eq)
Y	4038(1)	-26(1)	5000	16(1)
Cl	4980(1)	1226(1)	5000	23(1)
Si	2459(1)	-322(1)	5000	20(1)
C(1)	3031(1)	-196(2)	5656(1)	17(1)
C(2)	3462(1)	-857(2)	5921(2)	18(1)
C(3)	3954(2)	-348(2)	6216(2)	18(1)
C(4)	3840(1)	623(2)	6153(1)	18(1)
C(5)	3280(2)	704(2)	5803(1)	18(1)
C(11)	1901(3)	694(4)	5000	32(1)
C(12)	1979(3)	-1418(4)	5000	31(1)
C(20)	3372(2)	-1918(2)	5948(2)	24(1)
C(21)	3972(2)	-2449(3)	6115(2)	34(1)
C(22)	2850(2)	-2158(3)	6410(2)	35(1)
C(40)	4216(2)	1391(2)	6464(2)	23(1)
C(41)	4067(2)	2363(3)	6218(2)	38(1)
C(42)	4115(5)	1368(5)	7147(2)	88(3)
C(70)	5024(3)	-4524(2)	5543(2)	50(1)
C(71)	5050(4)	-4046(4)	5000	52(2)
C(60)	1108(3)	-24(6)	7187(3)	107(2)
C(61)	1692(3)	-10(5)	6878(2)	87(2)
C(62)	2250(3)	5(5)	7198(2)	77(1)

Table 4. Bond lengths [A] and angles [deg] for 4.

Y-X(1A)#1	2.3441(4)
Y-X(1A)	2.3441(4)
Y-Pln1#1	2.338(1)
Y-Pln1	2.338(1)
Y-C(1)	2.570(3)
Y-C(1)#1	2.570(3)
Y-C(5)	2.587(3)
Y-C(5)#1	2.587(3)
Y-C(2)	2.625(3)
Y-C(2)#1	2.625(3)
Y-Cl	2.6682(14)
Y-Cl#2	2.6823(14)
Y-C(3)#1	2.690(3)
Y-C(3)	2.690(3)
Y-C(4)	2.707(3)
Y-C(4)#1	2.707(3)
Cl-Y#2	2.6823(14)
Si-C(12)	1.860(5)
Si-C(11)	1.864(6)
Si-C(1)	1.877(3)
Si-C(1)#1	1.877(3)
C(1)-C(5)	1.423(4)
C(1)-C(2)	1.430(4)
C(2)-C(3)	1.418(4)
C(2)-C(20)	1.526(4)
C(3)-C(4)	1.411(4)
C(3)-H(3)	0.91(3)
C(4)-C(5)	1.409(4)
C(4)-C(40)	1.511(4)
C(5)-H(5)	0.90(3)
C(11)-H(11A)	0.87(6)
C(11)-H(11B)	0.89(3)
C(12)-H(12A)	0.94(4)
C(12)-H(12B)	0.95(3)
C(20)-C(21)	1.518(5)
C(20)-C(22)	1.528(5)
C(20)-H(20)	0.98(3)
C(21)-H(21A)	0.96(3)
C(21)-H(21B)	0.95(3)
C(21)-H(21C)	0.97(3)
C(22)-H(22A)	0.96(3)
C(22)-H(22B)	0.94(3)
C(22)-H(22C)	0.89(3)
C(40)-C(42)	1.502(6)
C(40)-C(41)	1.518(5)
C(40)-H(40)	0.85(3)
C(41)-H(41A)	0.97(3)
C(41)-H(41B)	1.09(4)
C(41)-H(41C)	0.93(3)
C(42)-H(42A)	0.88(4)
C(42)-H(42B)	0.97(4)
C(42)-H(42C)	0.76(5)
C(70)-C(70)#3	1.361(7)
C(70)-C(71)	1.364(5)
C(70)-H(72)	0.84(3)
C(71)-C(70)#1	1.364(5)
C(71)-H(71)	0.93(5)
C(60)-C(60)#4	1.361(11)
C(60)-C(61)	1.401(7)
C(60)-H(60)	1.10(5)
C(61)-C(62)	1.367(7)
C(61)-H(61)	1.23(7)

C(62)-C(62)#4	1.313(9)
C(62)-H(62)	1.12(5)
X(1A)#1-Y-X(1A)	123.70(2)
Pln1#1-Y-Pln1	115.53(8)
C(1)-Y-C(1)#1	67.53(13)
C(1)-Y-C(5)	32.04(9)
C(1)#1-Y-C(5)	84.45(10)
C(1)-Y-C(5)#1	84.45(10)
C(1)#1-Y-C(5)#1	32.04(9)
C(5)-Y-C(5)#1	85.01(14)
C(1)-Y-C(2)	31.93(8)
C(1)#1-Y-C(2)	90.00(9)
C(5)-Y-C(2)	51.70(9)
C(5)#1-Y-C(2)	114.33(11)
C(1)-Y-C(2)#1	90.00(9)
C(1)#1-Y-C(2)#1	31.93(8)
C(5)-Y-C(2)#1	114.33(11)
C(5)#1-Y-C(2)#1	51.70(9)
C(2)-Y-C(2)#1	99.54(14)
C(1)-Y-Cl	132.62(6)
C(1)#1-Y-Cl	132.62(6)
C(5)-Y-Cl	100.95(8)
C(5)#1-Y-Cl	100.95(8)
C(2)-Y-Cl	130.19(7)
C(2)#1-Y-Cl	130.19(7)
C(1)-Y-Cl#2	125.19(6)
C(1)#1-Y-Cl#2	125.19(6)
C(5)-Y-Cl#2	137.10(7)
C(5)#1-Y-Cl#2	137.10(7)
C(2)-Y-Cl#2	93.94(7)
C(2)#1-Y-Cl#2	93.94(7)
Cl-Y-Cl#2	81.57(4)
C(1)-Y-C(3)#1	118.42(9)
C(1)#1-Y-C(3)#1	51.90(9)
C(5)-Y-C(3)#1	133.80(10)
C(5)#1-Y-C(3)#1	50.48(10)
C(2)-Y-C(3)#1	130.04(10)
C(2)#1-Y-C(3)#1	30.91(9)
Cl-Y-C(3)#1	99.38(7)
Cl#2-Y-C(3)#1	86.69(7)
C(1)-Y-C(3)	51.90(9)
C(1)#1-Y-C(3)	118.42(9)
C(5)-Y-C(3)	50.48(10)
C(5)#1-Y-C(3)	133.80(10)
C(2)-Y-C(3)	30.91(9)
C(2)#1-Y-C(3)	130.04(10)
Cl-Y-C(3)	99.38(7)
Cl#2-Y-C(3)	86.69(7)
C(3)#1-Y-C(3)	158.95(13)
C(1)-Y-C(4)	52.38(9)
C(1)#1-Y-C(4)	114.83(9)
C(5)-Y-C(4)	30.77(9)
C(5)#1-Y-C(4)	113.16(10)
C(2)-Y-C(4)	51.33(10)
C(2)#1-Y-C(4)	142.24(10)
Cl-Y-C(4)	83.45(7)
Cl#2-Y-C(4)	109.69(7)
C(3)#1-Y-C(4)	163.62(9)
C(3)-Y-C(4)	30.32(9)
C(1)-Y-C(4)#1	114.83(9)
C(1)#1-Y-C(4)#1	52.38(9)
C(5)-Y-C(4)#1	113.16(10)
C(5)#1-Y-C(4)#1	30.77(9)
C(2)-Y-C(4)#1	142.24(10)
C(2)#1-Y-C(4)#1	51.33(10)

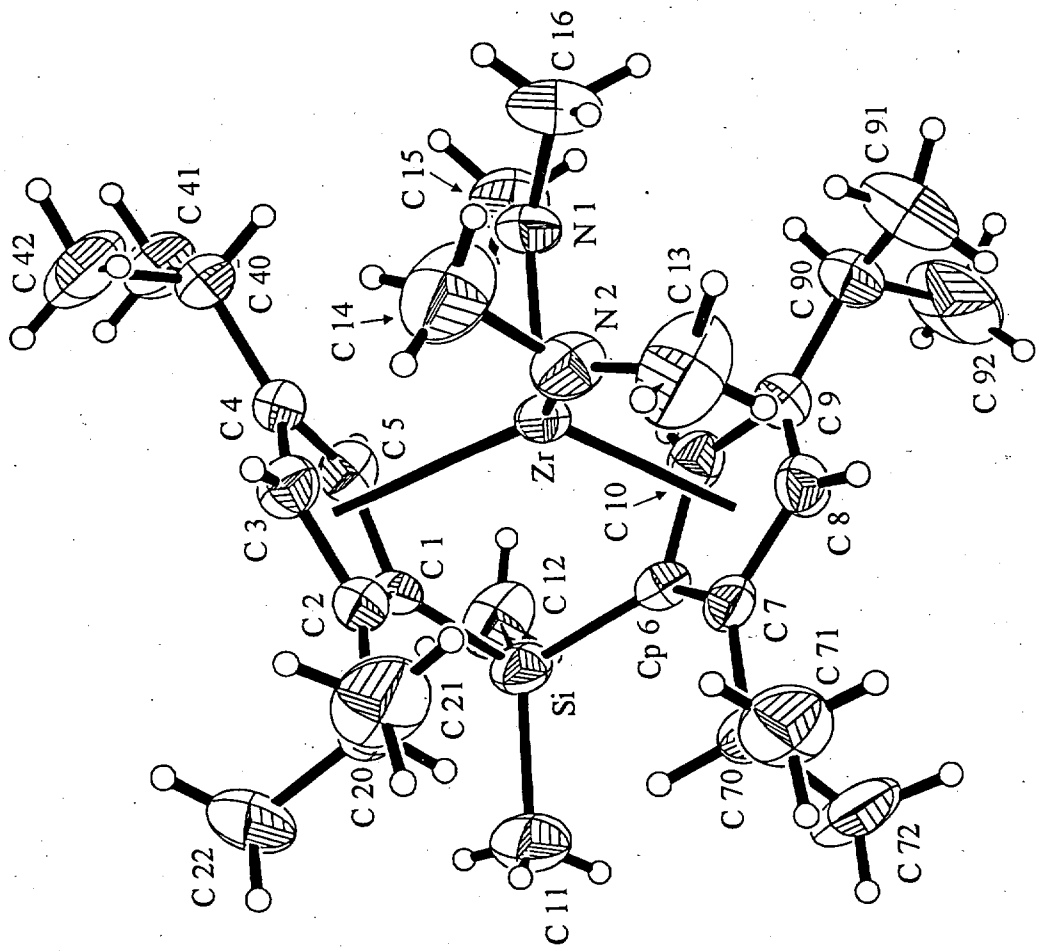
Cl-Y-C(4)#1	83.45(7)
Cl#2-Y-C(4)#1	109.69(7)
C(3)#1-Y-C(4)#1	30.32(9)
C(3)-Y-C(4)#1	163.62(9)
C(4)-Y-C(4)#1	135.92(13)
Y-Cl-Y#2	98.43(4)
C(12)-Si-C(11)	108.1(3)
C(12)-Si-C(1)	115.35(14)
C(11)-Si-C(1)	109.3(2)
C(12)-Si-C(1)#1	115.35(14)
C(11)-Si-C(1)#1	109.3(2)
C(1)-Si-C(1)#1	99.1(2)
C(12)-Si-Y	130.1(2)
C(11)-Si-Y	121.8(2)
C(1)-Si-Y	49.56(9)
C(1)#1-Si-Y	49.56(9)
C(5)-C(1)-C(2)	105.6(2)
C(5)-C(1)-Si	119.6(2)
C(2)-C(1)-Si	130.7(2)
C(5)-C(1)-Y	74.6(2)
C(2)-C(1)-Y	76.2(2)
Si-C(1)-Y	96.67(12)
C(3)-C(2)-C(1)	108.0(3)
C(3)-C(2)-C(20)	125.6(3)
C(1)-C(2)-C(20)	126.1(3)
C(3)-C(2)-Y	77.0(2)
C(1)-C(2)-Y	71.9(2)
C(20)-C(2)-Y	122.3(2)
C(4)-C(3)-C(2)	109.5(3)
C(4)-C(3)-Y	75.5(2)
C(2)-C(3)-Y	72.0(2)
C(4)-C(3)-H(3)	124(2)
C(2)-C(3)-H(3)	126(2)
Y-C(3)-H(3)	125(2)
C(5)-C(4)-C(3)	106.0(3)
C(5)-C(4)-C(40)	128.4(3)
C(3)-C(4)-C(40)	125.3(3)
C(5)-C(4)-Y	69.9(2)
C(3)-C(4)-Y	74.2(2)
C(40)-C(4)-Y	125.5(2)
C(4)-C(5)-C(1)	110.9(3)
C(4)-C(5)-Y	79.3(2)
C(1)-C(5)-Y	73.3(2)
C(4)-C(5)-H(5)	125(2)
C(1)-C(5)-H(5)	125(2)
Y-C(5)-H(5)	114(2)
Si-C(11)-H(11A)	114(4)
Si-C(11)-H(11B)	108(2)
H(11A)-C(11)-H(11B)	110(3)
Si-C(12)-H(12A)	116(3)
Si-C(12)-H(12B)	105(2)
H(12A)-C(12)-H(12B)	106(2)
C(21)-C(20)-C(2)	113.5(3)
C(21)-C(20)-C(22)	109.3(3)
C(2)-C(20)-C(22)	109.7(3)
C(21)-C(20)-H(20)	107(2)
C(2)-C(20)-H(20)	108(2)
C(22)-C(20)-H(20)	109(2)
C(20)-C(21)-H(21A)	111(2)
C(20)-C(21)-H(21B)	111(2)
H(21A)-C(21)-H(21B)	110(3)
C(20)-C(21)-H(21C)	109(2)
H(21A)-C(21)-H(21C)	105(3)
H(21B)-C(21)-H(21C)	111(3)
C(20)-C(22)-H(22A)	110(2)
C(20)-C(22)-H(22B)	108(2)

H(22A)-C(22)-H(22B)	109(3)
C(20)-C(22)-H(22C)	111(2)
H(22A)-C(22)-H(22C)	114(3)
H(22B)-C(22)-H(22C)	106(3)
C(42)-C(40)-C(4)	110.6(3)
C(42)-C(40)-C(41)	109.8(5)
C(4)-C(40)-C(41)	113.3(3)
C(42)-C(40)-H(40)	111(2)
C(4)-C(40)-H(40)	105(2)
C(41)-C(40)-H(40)	108(2)
C(40)-C(41)-H(41A)	108(2)
C(40)-C(41)-H(41B)	115(2)
H(41A)-C(41)-H(41B)	111(3)
C(40)-C(41)-H(41C)	108(2)
H(41A)-C(41)-H(41C)	105(3)
H(41B)-C(41)-H(41C)	109(3)
C(40)-C(42)-H(42A)	117(4)
C(40)-C(42)-H(42B)	109(2)
H(42A)-C(42)-H(42B)	102(4)
C(40)-C(42)-H(42C)	114(5)
H(42A)-C(42)-H(42C)	95(5)
H(42B)-C(42)-H(42C)	120(5)
C(70)#3-C(70)-C(71)	120.1(3)
C(70)#3-C(70)-H(72)	119(2)
C(71)-C(70)-H(72)	121(2)
C(70)-C(71)-C(70)#1	119.8(5)
C(70)-C(71)-H(71)	120.1(3)
C(70)#1-C(71)-H(71)	120.1(3)
C(60)#4-C(60)-C(61)	118.6(3)
C(60)#4-C(60)-H(60)	100(3)
C(61)-C(60)-H(60)	137(3)
C(62)-C(61)-C(60)	120.7(5)
C(62)-C(61)-H(61)	129(3)
C(60)-C(61)-H(61)	110(3)
C(62)#4-C(62)-C(61)	120.6(3)
C(62)#4-C(62)-H(62)	116(2)
C(61)-C(62)-H(62)	124(2)

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

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for 4.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Y	15(1)	16(1)	15(1)	0	0	0(1)
Cl	21(1)	22(1)	25(1)	0	0	0(1)
Si	16(1)	23(1)	22(1)	0	0	-2(1)
C(1)	19(1)	14(2)	18(2)	-1(1)	3(1)	0(1)
C(2)	20(2)	17(2)	18(2)	2(1)	7(1)	0(1)
C(3)	18(2)	22(2)	14(2)	3(1)	0(1)	0(1)
C(4)	19(2)	20(2)	15(2)	-3(1)	5(1)	2(1)
C(5)	19(2)	18(2)	18(2)	2(1)	4(1)	4(1)
C(11)	23(3)	41(4)	33(3)	0	0	5(2)
C(12)	28(3)	38(3)	26(3)	0	0	-15(3)
C(20)	29(2)	20(2)	22(2)	0(2)	-2(1)	-5(1)
C(21)	38(3)	20(2)	44(3)	5(2)	9(2)	-2(2)
C(22)	34(2)	30(2)	42(3)	8(2)	1(2)	-10(2)
C(40)	21(2)	23(2)	26(2)	-4(2)	-1(1)	-1(1)
C(41)	37(3)	23(2)	53(3)	-8(2)	-13(2)	1(2)
C(42)	173(8)	66(4)	25(3)	-5(2)	-10(4)	-71(5)
C(70)	63(2)	38(2)	50(2)	-11(2)	-2(3)	-4(3)
C(71)	68(4)	26(3)	62(4)	0	0	3(4)
C(60)	99(4)	132(5)	89(4)	-19(6)	-21(3)	27(6)
C(61)	129(5)	84(4)	49(3)	3(4)	-4(3)	21(5)
C(62)	105(4)	64(3)	61(3)	6(4)	11(3)	12(4)



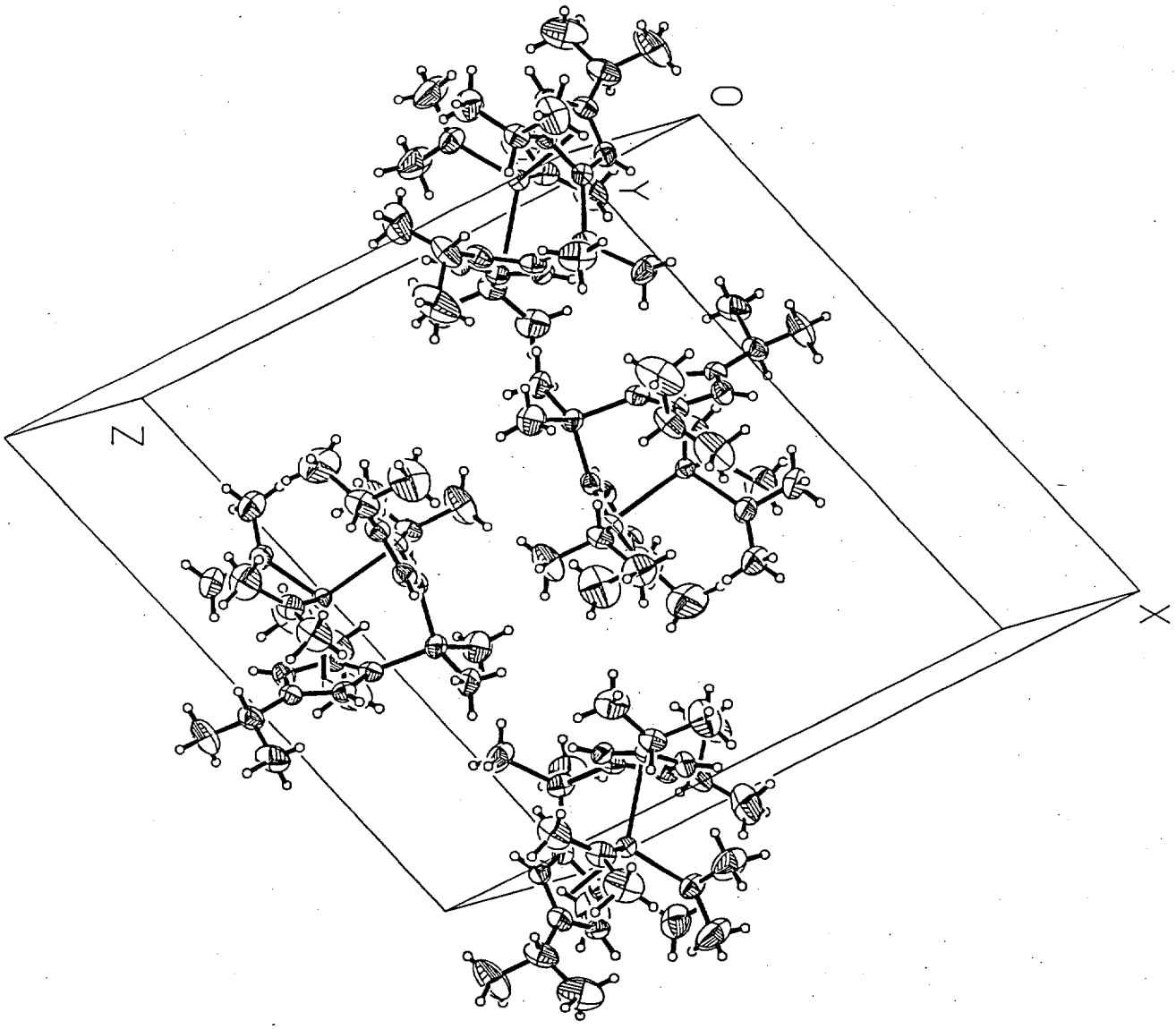


Table 2. Atomic coordinates (x 10^4) for 4. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zr	5276(1)	7477(1)	2571(1)	31(1)
Si	3834(1)	9211(1)	3048(1)	43(1)
N(1)	5281(2)	5408(3)	2524(2)	47(1)
N(2)	6316(2)	7718(3)	2244(2)	47(1)
C(1)	3929(2)	8725(4)	2071(2)	36(1)
C(2)	4397(2)	9253(4)	1609(2)	42(1)
C(3)	4491(2)	8263(4)	1075(2)	41(1)
C(4)	4098(2)	7120(3)	1173(2)	35(1)
C(5)	3766(2)	7404(5)	1799(2)	38(1)
C(6)	4848(2)	8643(4)	3662(2)	33(1)
C(7)	5617(2)	9226(4)	3739(2)	36(1)
C(8)	6208(2)	8239(4)	4012(2)	38(1)
C(9)	5848(2)	7064(4)	4116(2)	42(1)
C(10)	5016(2)	7303(4)	3885(2)	40(1)
C(11)	3604(3)	10979(4)	3169(3)	73(1)
C(12)	3035(2)	8192(5)	3267(2)	62(1)
C(13)	7142(3)	8138(6)	2613(3)	89(2)
C(14)	6287(3)	7282(7)	1442(3)	91(2)
C(15)	4677(3)	4562(4)	2681(3)	69(1)
C(16)	5939(4)	4614(6)	2429(3)	87(2)
C(20)	4640(3)	10673(4)	1563(2)	58(1)
C(22)	3939(4)	11416(5)	1003(3)	108(2)
C(21)	5400(3)	10832(5)	1310(3)	89(2)
C(40)	4009(2)	5871(4)	696(2)	44(1)
C(41)	3228(3)	5163(4)	643(3)	64(1)
C(42)	4072(3)	6132(5)	-136(2)	77(2)
C(70)	5779(2)	10686(4)	3721(2)	42(1)
C(72)	5785(4)	11289(5)	4521(3)	78(2)
C(71)	6557(3)	11034(5)	3546(3)	71(1)
C(90)	6272(3)	5816(5)	4480(2)	60(1)
C(91)	7119(3)	5693(6)	4425(4)	110(2)
C(92)	6280(4)	5723(6)	5344(3)	109(2)

Table 3. Bond lengths [A] and angles [deg] for 9.

Zr-N(2)	2.067(3)
Zr-N(1)	2.107(3)
Zr-C(10)	2.496(3)
Zr-C(6)	2.552(3)
Zr-C(5)	2.567(3)
Zr-C(1)	2.573(3)
Zr-C(2)	2.631(4)
Zr-C(9)	2.638(4)
Zr-C(7)	2.651(3)
Zr-C(8)	2.684(4)
Zr-C(3)	2.701(4)
Zr-C(4)	2.714(3)
Si-C(1)	1.847(4)
Si-C(12)	1.863(4)
Si-C(6)	1.860(4)
Si-C(11)	1.870(4)
N(1)-C(15)	1.446(5)
N(1)-C(16)	1.450(5)
N(2)-C(13)	1.450(4)
N(2)-C(14)	1.468(5)
C(1)-C(2)	1.415(5)
C(1)-C(5)	1.428(5)
C(2)-C(3)	1.421(5)
C(2)-C(20)	1.515(5)
C(3)-C(4)	1.386(5)
C(4)-C(5)	1.418(4)
C(4)-C(40)	1.506(4)
C(6)-C(10)	1.426(5)
C(6)-C(7)	1.429(4)
C(7)-C(8)	1.413(5)
C(7)-C(70)	1.515(5)
C(8)-C(9)	1.387(5)
C(9)-C(10)	1.398(4)
C(9)-C(90)	1.511(5)
C(20)-C(21)	1.522(5)
C(20)-C(22)	1.519(5)
C(40)-C(41)	1.513(5)
C(40)-C(42)	1.526(5)
C(70)-C(71)	1.516(5)
C(70)-C(72)	1.534(5)
C(90)-C(91)	1.508(6)
C(90)-C(92)	1.520(5)
N(2)-Zr-N(1)	95.38(14)
N(2)-Zr-C(10)	133.06(11)
N(1)-Zr-C(10)	88.24(14)
N(2)-Zr-C(6)	129.08(12)
N(1)-Zr-C(6)	119.97(13)
C(10)-Zr-C(6)	32.78(11)
N(2)-Zr-C(5)	133.91(11)
N(1)-Zr-C(5)	88.02(14)
C(10)-Zr-C(5)	92.91(11)
C(6)-Zr-C(5)	86.09(11)
N(2)-Zr-C(1)	128.70(12)
N(1)-Zr-C(1)	119.58(12)
C(10)-Zr-C(1)	87.42(12)
C(6)-Zr-C(1)	65.73(11)
C(5)-Zr-C(1)	32.25(11)
N(2)-Zr-C(2)	97.21(12)
N(1)-Zr-C(2)	132.03(12)
C(10)-Zr-C(2)	114.56(12)
C(6)-Zr-C(2)	85.54(12)

C(5)-Zr-C(2)	51.32(13)
C(1)-Zr-C(2)	31.53(10)
N(2)-Zr-C(9)	102.54(12)
N(1)-Zr-C(9)	82.91(12)
C(10)-Zr-C(9)	31.44(10)
C(6)-Zr-C(9)	53.17(11)
C(5)-Zr-C(9)	123.45(11)
C(1)-Zr-C(9)	117.03(11)
C(2)-Zr-C(9)	137.80(11)
N(2)-Zr-C(7)	97.27(12)
N(1)-Zr-C(7)	134.33(12)
C(10)-Zr-C(7)	52.19(12)
C(6)-Zr-C(7)	31.80(10)
C(5)-Zr-C(7)	112.71(12)
C(1)-Zr-C(7)	84.42(11)
C(2)-Zr-C(7)	89.44(11)
C(9)-Zr-C(7)	51.53(11)
N(2)-Zr-C(8)	84.31(11)
N(1)-Zr-C(8)	108.51(12)
C(10)-Zr-C(8)	50.74(11)
C(6)-Zr-C(8)	51.79(11)
C(5)-Zr-C(8)	137.73(11)
C(1)-Zr-C(8)	114.16(11)
C(2)-Zr-C(8)	118.68(11)
C(9)-Zr-C(8)	30.19(10)
C(7)-Zr-C(8)	30.71(10)
N(2)-Zr-C(3)	85.42(12)
N(1)-Zr-C(3)	105.34(12)
C(10)-Zr-C(3)	138.46(12)
C(6)-Zr-C(3)	114.96(12)
C(5)-Zr-C(3)	49.80(11)
C(1)-Zr-C(3)	51.56(11)
C(2)-Zr-C(3)	30.88(10)
C(9)-Zr-C(3)	168.12(11)
C(7)-Zr-C(3)	119.26(11)
C(8)-Zr-C(3)	145.35(11)
N(2)-Zr-C(4)	104.26(11)
N(1)-Zr-C(4)	80.86(11)
C(10)-Zr-C(4)	122.46(11)
C(6)-Zr-C(4)	115.85(10)
C(5)-Zr-C(4)	30.98(9)
C(1)-Zr-C(4)	52.77(10)
C(2)-Zr-C(4)	51.18(11)
C(9)-Zr-C(4)	149.74(12)
C(7)-Zr-C(4)	136.63(11)
C(8)-Zr-C(4)	166.92(10)
C(3)-Zr-C(4)	29.66(10)
C(1)-Si-C(12)	108.9(2)
C(1)-Si-C(6)	97.2(2)
C(12)-Si-C(6)	109.8(2)
C(1)-Si-C(11)	116.5(2)
C(12)-Si-C(11)	108.3(2)
C(6)-Si-C(11)	115.5(2)
C(15)-N(1)-C(16)	109.3(4)
C(15)-N(1)-Zr	125.2(3)
C(16)-N(1)-Zr	125.0(3)
C(13)-N(2)-C(14)	105.4(3)
C(13)-N(2)-Zr	137.6(3)
C(14)-N(2)-Zr	116.8(3)
C(2)-C(1)-C(5)	104.7(3)
C(2)-C(1)-Si	131.4(3)
C(5)-C(1)-Si	120.1(3)
C(2)-C(1)-Zr	76.5(2)
C(5)-C(1)-Zr	73.6(2)
Si-C(1)-Zr	97.94(13)
C(1)-C(2)-C(3)	108.2(3)

C(1)-C(2)-C(20)	127.6(4)
C(3)-C(2)-C(20)	123.4(4)
C(1)-C(2)-Zr	72.0(2)
C(3)-C(2)-Zr	77.3(2)
C(20)-C(2)-Zr	125.0(2)
C(4)-C(3)-C(2)	110.7(3)
C(4)-C(3)-Zr	75.7(2)
C(2)-C(3)-Zr	71.8(2)
C(3)-C(4)-C(5)	104.8(3)
C(3)-C(4)-C(40)	127.6(3)
C(5)-C(4)-C(40)	127.5(4)
C(3)-C(4)-Zr	74.6(2)
C(5)-C(4)-Zr	68.8(2)
C(40)-C(4)-Zr	122.9(2)
C(4)-C(5)-C(1)	111.6(3)
C(4)-C(5)-Zr	80.3(2)
C(1)-C(5)-Zr	74.1(2)
C(10)-C(6)-C(7)	105.3(3)
C(10)-C(6)-Si	122.6(3)
C(7)-C(6)-Si	128.3(3)
C(10)-C(6)-Zr	71.5(2)
C(7)-C(6)-Zr	77.9(2)
Si-C(6)-Zr	98.33(13)
C(8)-C(7)-C(6)	107.4(3)
C(8)-C(7)-C(70)	125.8(3)
C(6)-C(7)-C(70)	125.4(3)
C(8)-C(7)-Zr	75.9(2)
C(6)-C(7)-Zr	70.3(2)
C(70)-C(7)-Zr	130.0(2)
C(9)-C(8)-C(7)	110.4(3)
C(9)-C(8)-Zr	73.1(2)
C(7)-C(8)-Zr	73.3(2)
C(8)-C(9)-C(10)	106.1(3)
C(8)-C(9)-C(90)	126.9(4)
C(10)-C(9)-C(90)	126.8(4)
C(8)-C(9)-Zr	76.7(2)
C(10)-C(9)-Zr	68.7(2)
C(90)-C(9)-Zr	123.9(3)
C(9)-C(10)-C(6)	110.8(4)
C(9)-C(10)-Zr	79.9(2)
C(6)-C(10)-Zr	75.8(2)
C(21)-C(20)-C(2)	113.4(4)
C(21)-C(20)-C(22)	110.7(5)
C(2)-C(20)-C(22)	109.1(4)
C(4)-C(40)-C(41)	112.1(3)
C(4)-C(40)-C(42)	111.4(3)
C(41)-C(40)-C(42)	110.1(4)
C(71)-C(70)-C(7)	114.6(3)
C(71)-C(70)-C(72)	109.4(4)
C(7)-C(70)-C(72)	108.9(3)
C(9)-C(90)-C(91)	113.7(4)
C(9)-C(90)-C(92)	109.6(4)
C(91)-C(90)-C(92)	110.0(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 9.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zr	31(1)	27(1)	35(1)	-2(1)	10(1)	1(1)
Si	38(1)	43(1)	49(1)	-13(1)	12(1)	6(1)
N(1)	54(2)	27(2)	56(2)	-4(2)	7(2)	8(2)
N(2)	40(2)	51(3)	54(2)	-12(2)	19(1)	-3(2)
C(1)	35(2)	27(2)	39(2)	-1(2)	1(2)	6(2)
C(2)	50(2)	32(3)	36(2)	1(2)	2(2)	3(2)
C(3)	49(2)	39(3)	34(2)	-1(2)	15(2)	-4(2)
C(4)	36(2)	32(3)	33(2)	-3(2)	4(2)	2(2)
C(5)	31(2)	42(3)	42(2)	0(3)	11(2)	-6(3)
C(6)	37(2)	32(2)	33(2)	-6(2)	13(2)	-2(2)
C(7)	46(2)	34(2)	26(2)	-4(2)	8(2)	-4(2)
C(8)	31(2)	39(3)	41(2)	1(2)	4(2)	-2(2)
C(9)	47(2)	38(3)	36(2)	1(2)	6(2)	4(2)
C(10)	44(2)	40(3)	36(2)	-4(2)	11(2)	-11(2)
C(11)	67(3)	58(4)	87(4)	-17(3)	14(3)	26(3)
C(12)	48(3)	81(4)	65(3)	-26(2)	28(3)	-6(3)
C(13)	51(3)	128(6)	96(4)	-44(4)	33(3)	-18(3)
C(14)	60(3)	134(6)	86(3)	-34(4)	34(3)	10(4)
C(15)	98(4)	34(3)	69(4)	1(3)	16(3)	2(3)
C(16)	108(4)	49(4)	99(5)	-7(4)	26(4)	35(4)
C(20)	95(4)	30(3)	40(3)	0(2)	7(2)	-5(3)
C(22)	165(7)	32(4)	94(5)	17(3)	-11(5)	6(4)
C(21)	145(5)	45(4)	77(4)	9(3)	32(4)	-38(4)
C(40)	51(2)	35(3)	40(2)	-7(2)	5(2)	-1(2)
C(41)	70(3)	40(3)	69(3)	-17(3)	3(3)	-15(3)
C(42)	122(5)	55(4)	56(3)	-23(3)	31(3)	-14(4)
C(70)	51(2)	30(3)	40(2)	-2(2)	5(2)	-6(2)
C(72)	124(5)	41(4)	69(4)	-23(3)	29(4)	-22(3)
C(71)	77(4)	51(4)	85(4)	6(3)	27(3)	-16(3)
C(90)	72(3)	37(3)	56(3)	7(3)	-3(2)	11(3)
C(91)	96(5)	85(6)	128(6)	24(5)	2(4)	50(4)
C(92)	156(7)	83(5)	80(4)	49(4)	25(4)	40(5)