Table 1. Crystal data and structure refinement for 10. S1

Empirical formula	C19 H32 B N Ru S
Formula weight	418.40
Temperature	158(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pbca
Unit cell dimensions	a = 11.906(3) A alpha = 90 deg. b = 14.607(3) A beta = 90 deg. c = 22.907(5) A gamma = 90 deg.
Volume	3983.5(15) A^3
Z, Calculated density	8, 1.395 Mg/m^3
Absorption coefficient	0.891 mm^-1
F(000)	1744
Crystal size	0.36 x 0.38 x 0.38 mm
Theta range for data collection	1.78 to 26.44 deg.
Limiting indices	-14<=h<=14, -18<=k<=18, -28<=l<=28
Reflections collected / unique	38778 / 4089 [R(int) = 0.0400]
Completeness to theta = 26.44	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.790 and 0.546
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4089 / 56 / 273
Goodness-of-fit on F^2	1.091
Final R indices [I>2sigma(I)]	R1 = 0.0348, wR2 = 0.1040
R indices (all data)	R1 = 0.0409, wR2 = 0.1080
Largest diff. peak and hole	0.755 and -0.776 e.A^-3

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

	x	y	z	U(eq)
Ru(1)	2489(1)	4038(1)	1700(1)	19(1)
N(1)	2763(3)	4259(2)	140(1)	27(1)
B(1)	3243(3)	4196(3)	703(2)	27(1)
S(1)	3660(2)	3108(2)	1058(1)	27(1)
C(1)	3613(10)	4934(4)	1120(4)	13(2)
C(2)	4164(5)	4615(3)	1642(2)	26(1)
C(3)	4229(5)	3659(4)	1695(2)	31(1)
S(1A)	3702(9)	5099(4)	1191(3)	35(2)
C(1A)	3570(20)	3294(5)	1022(7)	18(6)
C(2A)	4100(12)	3436(6)	1568(4)	15(3)
C(3A)	4241(12)	4350(7)	1741(4)	14(3)
C(4)	660(3)	4045(2)	1681(1)	22(1)
C(5)	1057(3)	4830(2)	1994(1)	23(1)
C(6)	1683(3)	4513(2)	2491(1)	24(1)
C(7)	1672(3)	3535(2)	2488(2)	24(1)
C(8)	1047(3)	3247(2)	1986(1)	22(1)
C(9)	-73(3)	4055(2)	1148(2)	29(1)
C(10)	800(3)	5820(2)	1848(2)	31(1)
C(11)	2183(3)	5100(3)	2964(2)	36(1)
C(12)	2165(3)	2928(3)	2948(2)	35(1)
C(13)	780(3)	2275(2)	1817(2)	33(1)
C(14)	2497(3)	3428(2)	-185(2)	27(1)
C(15)	3394(4)	3230(3)	-642(2)	42(1)
C(16)	1326(4)	3433(3)	-456(2)	46(1)
C(17)	2608(3)	5133(3)	-173(2)	28(1)
C(18)	1737(3)	5751(3)	122(2)	35(1)
C(19)	3703(4)	5659(3)	-270(2)	44(1)

Table 3. Bond lengths [A] and angles [deg] for 10. S3

Ru(1)-C(2A)	2.131(14)
Ru(1)-C(3A)	2.137(14)
Ru(1)-C(3)	2.144(6)
Ru(1)-C(6)	2.166(3)
Ru(1)-C(2)	2.168(6)
Ru(1)-C(5)	2.169(3)
Ru(1)-C(8)	2.171(3)
Ru(1)-C(4)	2.179(3)
Ru(1)-C(7)	2.179(3)
Ru(1)-C(1A)	2.29(3)
Ru(1)-C(1)	2.294(11)
Ru(1)-S(1A)	2.417(10)
Ru(1)-S(1)	2.439(2)
Ru(1)-B(1)	2.463(4)
N(1)-B(1)	1.416(4)
N(1)-C(14)	1.458(5)
N(1)-C(17)	1.475(5)
B(1)-C(1)	1.506(7)
B(1)-C(1A)	1.554(8)
B(1)-S(1A)	1.814(7)
B(1)-S(1)	1.853(4)
S(1)-C(3)	1.798(5)
C(1)-C(2)	1.441(7)
C(2)-C(3)	1.404(6)
S(1A)-C(3A)	1.787(8)
C(1A)-C(2A)	1.419(8)
C(2A)-C(3A)	1.403(8)
C(4)-C(5)	1.433(4)
C(4)-C(8)	1.435(5)
C(4)-C(9)	1.502(5)
C(5)-C(6)	1.438(4)
C(5)-C(10)	1.515(5)
C(6)-C(7)	1.429(5)
C(6)-C(11)	1.504(5)
C(7)-C(8)	1.433(5)
C(7)-C(12)	1.498(5)
C(8)-C(13)	1.506(5)
C(14)-C(15)	1.523(5)
C(14)-C(16)	1.527(5)
C(17)-C(19)	1.530(5)
C(17)-C(18)	1.531(5)
C(2A)-Ru(1)-C(3A)	38.4(3)
C(2A)-Ru(1)-C(3)	12.4(3)
C(3A)-Ru(1)-C(3)	27.4(3)
C(2A)-Ru(1)-C(6)	130.5(3)
C(3A)-Ru(1)-C(6)	109.1(3)
C(3)-Ru(1)-C(6)	120.99(17)
C(2A)-Ru(1)-C(2)	47.5(3)
C(3A)-Ru(1)-C(2)	12.2(3)
C(3)-Ru(1)-C(2)	38.01(18)
C(6)-Ru(1)-C(2)	109.52(15)
C(2A)-Ru(1)-C(5)	166.4(3)
C(3A)-Ru(1)-C(5)	129.8(3)
C(3)-Ru(1)-C(5)	154.05(17)
C(6)-Ru(1)-C(5)	38.74(12)
C(2)-Ru(1)-C(5)	122.33(17)
C(2A)-Ru(1)-C(8)	122.3(3)
C(3A)-Ru(1)-C(8)	150.7(3)
C(3)-Ru(1)-C(8)	128.87(17)
C(6)-Ru(1)-C(8)	64.35(12)
C(2)-Ru(1)-C(8)	162.23(16)
C(5)-Ru(1)-C(8)	64.41(13)
C(2A)-Ru(1)-C(4)	154.0(3)
C(3A)-Ru(1)-C(4)	167.4(3)
C(3)-Ru(1)-C(4)	165.20(18)
C(6)-Ru(1)-C(4)	64.64(12)
C(2)-Ru(1)-C(4)	156.40(17)
C(5)-Ru(1)-C(4)	38.50(12)
C(8)-Ru(1)-C(4)	38.52(12)
C(2A)-Ru(1)-C(7)	112.3(3)
C(3A)-Ru(1)-C(7)	118.1(3)

C(6)-Ru(1)-C(7)	38.39(13)
C(2)-Ru(1)-C(7)	126.32(16)
C(5)-Ru(1)-C(7)	64.57(12)
C(8)-Ru(1)-C(7)	38.45(12)
C(4)-Ru(1)-C(7)	64.59(12)
C(2A)-Ru(1)-C(1A)	37.3(4)
C(3A)-Ru(1)-C(1A)	65.5(5)
C(3)-Ru(1)-C(1A)	48.2(4)
C(6)-Ru(1)-C(1A)	165.6(3)
C(2)-Ru(1)-C(1A)	68.2(5)
C(5)-Ru(1)-C(1A)	154.8(3)
C(8)-Ru(1)-C(1A)	113.2(5)
C(4)-Ru(1)-C(1A)	123.3(5)
C(7)-Ru(1)-C(1A)	130.7(3)
C(2A)-Ru(1)-C(1)	68.2(4)
C(3A)-Ru(1)-C(1)	48.3(3)
C(3)-Ru(1)-C(1)	65.3(2)
C(6)-Ru(1)-C(1)	124.1(2)
C(2)-Ru(1)-C(1)	37.5(2)
C(5)-Ru(1)-C(1)	109.5(2)
C(8)-Ru(1)-C(1)	160.0(2)
C(4)-Ru(1)-C(1)	124.7(2)
C(7)-Ru(1)-C(1)	158.80(19)
C(1A)-Ru(1)-C(1)	63.4(5)
C(2A)-Ru(1)-S(1A)	70.1(3)
C(3A)-Ru(1)-S(1A)	45.7(3)
C(3)-Ru(1)-S(1A)	65.6(3)
C(6)-Ru(1)-S(1A)	117.6(2)
C(2)-Ru(1)-S(1A)	34.1(2)
C(5)-Ru(1)-S(1A)	106.1(2)
C(8)-Ru(1)-S(1A)	163.6(2)
C(4)-Ru(1)-S(1A)	125.8(2)
C(7)-Ru(1)-S(1A)	151.91(18)
C(1A)-Ru(1)-S(1A)	69.1(5)
C(1)-Ru(1)-S(1A)	6.9(3)
C(2A)-Ru(1)-S(1)	34.0(3)
C(3A)-Ru(1)-S(1)	65.7(3)
C(3)-Ru(1)-S(1)	45.64(15)
C(6)-Ru(1)-S(1)	159.39(10)
C(2)-Ru(1)-S(1)	69.78(14)
C(5)-Ru(1)-S(1)	159.11(10)
C(8)-Ru(1)-S(1)	109.70(10)
C(4)-Ru(1)-S(1)	124.21(10)
C(7)-Ru(1)-S(1)	124.50(10)
C(1A)-Ru(1)-S(1)	6.5(3)
C(1)-Ru(1)-S(1)	68.7(2)
S(1A)-Ru(1)-S(1)	74.1(2)
C(2A)-Ru(1)-B(1)	65.1(3)
C(3A)-Ru(1)-B(1)	70.5(3)
C(3)-Ru(1)-B(1)	70.59(15)
C(6)-Ru(1)-B(1)	155.16(13)
C(2)-Ru(1)-B(1)	64.68(14)
C(5)-Ru(1)-B(1)	121.69(12)
C(8)-Ru(1)-B(1)	128.14(12)
C(4)-Ru(1)-B(1)	110.24(12)
C(7)-Ru(1)-B(1)	164.16(12)
C(1A)-Ru(1)-B(1)	38.0(3)
C(1)-Ru(1)-B(1)	36.70(18)
S(1A)-Ru(1)-B(1)	43.64(17)
S(1)-Ru(1)-B(1)	44.41(10)
B(1)-N(1)-C(14)	119.9(3)
B(1)-N(1)-C(17)	123.3(3)
C(14)-N(1)-C(17)	116.5(3)
N(1)-B(1)-C(1)	130.5(4)
N(1)-B(1)-C(1A)	125.7(5)
C(1)-B(1)-C(1A)	103.7(5)
N(1)-B(1)-S(1A)	129.5(3)
C(1)-B(1)-S(1A)	1.3(7)
C(1A)-B(1)-S(1A)	104.7(4)
N(1)-B(1)-S(1)	124.4(3)
C(1)-B(1)-S(1)	104.9(3)
C(1A)-B(1)-S(1)	2.2(11)
S(1A)-B(1)-S(1)	105.8(3)
N(1)-B(1)-Ru(1)	134.8(3)
C(1)-B(1)-Ru(1)	65.6(4)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 10.
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
Ru(1)	17(1)	23(1)	16(1)	0(1)	-1(1)	1(1)
N(1)	32(2)	28(2)	22(1)	1(1)	2(1)	2(1)
B(1)	19(2)	37(2)	24(2)	0(2)	5(1)	1(2)
S(1)	30(1)	27(1)	25(1)	4(1)	2(1)	11(1)
C(1)	14(2)	11(2)	14(2)	-3(2)	-3(2)	-2(2)
C(2)	22(2)	30(2)	25(2)	3(2)	-2(2)	-1(2)
C(3)	25(2)	40(2)	26(2)	-1(2)	-9(2)	2(2)
S(1A)	42(3)	34(3)	29(3)	-14(2)	2(2)	-10(3)
C(1A)	19(6)	17(6)	18(6)	1(2)	-1(2)	1(3)
C(2A)	14(4)	16(4)	14(4)	-2(2)	0(2)	1(2)
C(3A)	14(4)	17(4)	13(4)	5(2)	-4(2)	2(2)
C(4)	17(2)	28(2)	21(2)	0(1)	2(1)	1(1)
C(5)	22(2)	25(2)	21(2)	-1(1)	2(1)	2(1)
C(6)	24(2)	30(2)	18(1)	-2(1)	2(1)	2(1)
C(7)	23(2)	28(2)	20(2)	2(1)	2(1)	0(1)
C(8)	20(2)	23(2)	24(2)	0(1)	4(1)	-1(1)
C(9)	22(2)	38(2)	26(2)	2(1)	-3(1)	-2(1)
C(10)	30(2)	29(2)	33(2)	0(2)	-1(2)	4(2)
C(11)	42(2)	40(2)	26(2)	-8(2)	-5(2)	-2(2)
C(12)	37(2)	41(2)	27(2)	7(2)	-3(2)	4(2)
C(13)	31(2)	25(2)	42(2)	-2(2)	-2(2)	-3(2)
C(14)	31(2)	28(2)	21(2)	-1(1)	0(1)	5(1)
C(15)	49(3)	42(2)	35(2)	-6(2)	8(2)	14(2)
C(16)	41(2)	41(2)	56(3)	-19(2)	-13(2)	6(2)
C(17)	31(2)	30(2)	24(2)	4(1)	1(1)	4(2)
C(18)	34(2)	35(2)	35(2)	0(2)	2(2)	7(2)
C(19)	36(2)	47(2)	49(2)	18(2)	7(2)	-3(2)

Table 3. Crystal data and structure refinement for 15.

Empirical formula	C16 H26 B Cl2 N S Si Zr
Formula weight	465.46
Temperature	158(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 12.421(3) A alpha = 90 deg. b = 11.317(3) A beta = 107.082(4) deg. c = 15.408(4) A gamma = 90 deg.
Volume	2070.2(8) A^3
Z, Calculated density	4, 1.493 Mg/m^3
Absorption coefficient	0.946 mm^-1
F(000)	952
Crystal size	0.10 x 0.24 x 0.42 mm
Theta range for data collection	1.86 to 26.44 deg.
Limiting indices	-14<=h<=15, -13<=k<=14, -19<=l<=19
Reflections collected / unique	19506 / 4256 [R(int) = 0.0249]
Completeness to theta = 26.44	99.7 %
Absorption correction	SADABS
Max. and min. transmission	0.932 and 0.758
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4256 / 0 / 314
Goodness-of-fit on F^2	1.054
Final R indices [I>2sigma(I)]	R1 = 0.0195, wR2 = 0.0470
R indices (all data)	R1 = 0.0227, wR2 = 0.0482
Extinction coefficient	0.00075(13)
Largest diff. peak and hole	0.351 and -0.446 e.A^-3

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 15.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
B(1)	7247(2)	7623(2)	-103(1)	22(1)
N(1)	7781(1)	7168(1)	-710(1)	24(1)
Zr(1)	6663(1)	6749(1)	1507(1)	17(1)
S(1)	5701(1)	7369(1)	-244(1)	21(1)
Si(1)	4404(1)	8450(1)	1055(1)	21(1)
Cl(1)	8294(1)	7172(1)	2790(1)	30(1)
Cl(2)	7428(1)	4998(1)	973(1)	29(1)
C(1)	7629(1)	8367(1)	756(1)	23(1)
C(2)	6738(1)	8852(1)	1028(1)	23(1)
C(3)	5654(1)	8410(1)	613(1)	22(1)
C(4)	3044(2)	8289(2)	161(1)	33(1)
C(5)	4482(2)	9775(2)	1777(1)	33(1)
C(6)	4795(1)	7070(1)	1739(1)	21(1)
C(7)	5586(1)	7016(2)	2620(1)	24(1)
C(8)	6001(1)	5848(2)	2779(1)	28(1)
C(9)	5506(1)	5171(2)	2015(1)	28(1)
C(10)	4777(1)	5917(1)	1359(1)	24(1)
C(11)	7194(2)	6400(2)	-1481(1)	28(1)
C(12)	7060(2)	7007(2)	-2393(1)	42(1)
C(13)	7747(2)	5190(2)	-1431(1)	34(1)
C(14)	8983(2)	7422(2)	-617(1)	34(1)
C(15)	9186(2)	8742(2)	-684(2)	50(1)
C(16)	9765(2)	6865(2)	235(2)	50(1)

Table 7. Bond lengths [A] and angles [deg] for 15.

B(1)-N(1)	1.395(2)
B(1)-C(1)	1.523(2)
B(1)-S(1)	1.8897(19)
N(1)-C(11)	1.478(2)
N(1)-C(14)	1.486(2)
Zr(1)-Cl(1)	2.4266(6)
Zr(1)-Cl(2)	2.4418(6)
Zr(1)-C(3)	2.4471(15)
Zr(1)-C(10)	2.4721(16)
Zr(1)-C(6)	2.4762(16)
Zr(1)-C(7)	2.4833(16)
Zr(1)-C(2)	2.5018(16)
Zr(1)-C(8)	2.5501(16)
Zr(1)-C(9)	2.5547(17)
Zr(1)-C(1)	2.6359(16)
Zr(1)-S(1)	2.7032(7)
S(1)-C(3)	1.7843(16)
Si(1)-C(4)	1.8476(19)
Si(1)-C(5)	1.8521(19)
Si(1)-C(6)	1.8671(16)
Si(1)-C(3)	1.8697(17)
C(1)-C(2)	1.404(2)
C(2)-C(3)	1.402(2)
C(6)-C(7)	1.424(2)
C(6)-C(10)	1.428(2)
C(7)-C(8)	1.413(2)
C(8)-C(9)	1.389(3)
C(9)-C(10)	1.419(2)
C(11)-C(13)	1.524(3)
C(11)-C(12)	1.528(3)
C(14)-C(16)	1.522(3)
C(14)-C(15)	1.523(3)

N(1)-B(1)-C(1)	134.39(15)
N(1)-B(1)-S(1)	122.28(13)
C(1)-B(1)-S(1)	103.34(11)
B(1)-N(1)-C(11)	122.44(14)
B(1)-N(1)-C(14)	121.75(14)
C(11)-N(1)-C(14)	115.81(13)
Cl(1)-Zr(1)-Cl(2)	96.939(19)
Cl(1)-Zr(1)-C(3)	118.27(4)
Cl(2)-Zr(1)-C(3)	128.25(4)
Cl(1)-Zr(1)-C(10)	133.79(4)
Cl(2)-Zr(1)-C(10)	96.43(4)
C(3)-Zr(1)-C(10)	85.73(5)
Cl(1)-Zr(1)-C(6)	116.53(4)
Cl(2)-Zr(1)-C(6)	129.92(4)
C(3)-Zr(1)-C(6)	67.75(5)
C(10)-Zr(1)-C(6)	33.55(5)
Cl(1)-Zr(1)-C(7)	84.46(4)
Cl(2)-Zr(1)-C(7)	132.32(4)
C(3)-Zr(1)-C(7)	90.24(5)
C(10)-Zr(1)-C(7)	54.69(6)
C(6)-Zr(1)-C(7)	33.37(5)
Cl(1)-Zr(1)-C(2)	87.60(4)
Cl(2)-Zr(1)-C(2)	128.32(4)
C(3)-Zr(1)-C(2)	32.89(5)
C(10)-Zr(1)-C(2)	116.82(5)
C(6)-Zr(1)-C(2)	91.17(5)
C(7)-Zr(1)-C(2)	99.35(5)
Cl(1)-Zr(1)-C(8)	80.42(4)
Cl(2)-Zr(1)-C(8)	100.39(4)
C(3)-Zr(1)-C(8)	120.78(5)
C(10)-Zr(1)-C(8)	53.69(5)
C(6)-Zr(1)-C(8)	54.56(5)
C(7)-Zr(1)-C(8)	32.57(5)
C(2)-Zr(1)-C(8)	130.95(5)
Cl(1)-Zr(1)-C(9)	107.40(4)
Cl(2)-Zr(1)-C(9)	81.14(5)
C(3)-Zr(1)-C(9)	117.88(6)
C(10)-Zr(1)-C(9)	32.75(5)
C(6)-Zr(1)-C(9)	54.77(5)

C(7)-Zr(1)-C(9)	33.71(6)
C(2)-Zr(1)-C(9)	145.92(5)
C(8)-Zr(1)-C(9)	31.57(6)
Cl(1)-Zr(1)-C(1)	80.89(4)
Cl(2)-Zr(1)-C(1)	98.24(4)
C(3)-Zr(1)-C(1)	56.16(5)
C(10)-Zr(1)-C(1)	139.91(5)
C(6)-Zr(1)-C(1)	121.86(5)
C(7)-Zr(1)-C(1)	128.71(5)
C(2)-Zr(1)-C(1)	31.59(5)
C(8)-Zr(1)-C(1)	154.98(6)
C(9)-Zr(1)-C(1)	171.71(5)
Cl(1)-Zr(1)-S(1)	141.285(16)
Cl(2)-Zr(1)-S(1)	88.597(18)
C(3)-Zr(1)-S(1)	40.15(4)
C(10)-Zr(1)-S(1)	82.98(4)
C(6)-Zr(1)-S(1)	87.01(4)
C(7)-Zr(1)-S(1)	119.20(4)
C(2)-Zr(1)-S(1)	60.14(4)
C(8)-Zr(1)-S(1)	136.31(4)
C(9)-Zr(1)-S(1)	111.31(4)
C(1)-Zr(1)-S(1)	60.40(4)
C(3)-S(1)-B(1)	93.90(8)
C(3)-S(1)-Zr(1)	62.17(5)
B(1)-S(1)-Zr(1)	77.79(5)
C(4)-Si(1)-C(5)	113.76(10)
C(4)-Si(1)-C(6)	111.60(8)
C(5)-Si(1)-C(6)	112.24(8)
C(4)-Si(1)-C(3)	113.64(8)
C(5)-Si(1)-C(3)	109.60(8)
C(6)-Si(1)-C(3)	94.51(7)
C(2)-C(1)-B(1)	113.80(14)
C(2)-C(1)-Zr(1)	68.93(9)
B(1)-C(1)-Zr(1)	86.08(9)
C(3)-C(2)-C(1)	117.44(14)
C(3)-C(2)-Zr(1)	71.41(9)
C(1)-C(2)-Zr(1)	79.48(9)
C(2)-C(3)-S(1)	109.64(11)
C(2)-C(3)-Si(1)	127.97(12)
S(1)-C(3)-Si(1)	119.81(9)
C(2)-C(3)-Zr(1)	75.70(9)
S(1)-C(3)-Zr(1)	77.67(6)
Si(1)-C(3)-Zr(1)	99.04(6)
C(7)-C(6)-C(10)	105.92(14)
C(7)-C(6)-Si(1)	124.56(12)
C(10)-C(6)-Si(1)	124.23(12)
C(7)-C(6)-Zr(1)	73.59(9)
C(10)-C(6)-Zr(1)	73.07(9)
Si(1)-C(6)-Zr(1)	98.11(6)
C(8)-C(7)-C(6)	108.69(15)
C(8)-C(7)-Zr(1)	76.32(9)
C(6)-C(7)-Zr(1)	73.04(9)
C(9)-C(8)-C(7)	108.72(15)
C(9)-C(8)-Zr(1)	74.40(10)
C(7)-C(8)-Zr(1)	71.11(9)
C(8)-C(9)-C(10)	107.82(15)
C(8)-C(9)-Zr(1)	74.03(10)
C(10)-C(9)-Zr(1)	70.42(9)
C(9)-C(10)-C(6)	108.79(15)
C(9)-C(10)-Zr(1)	76.83(9)
C(6)-C(10)-Zr(1)	73.38(9)
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N(1)-C(11)-C(12)	111.69(15)
C(13)-C(11)-C(12)	112.13(15)
N(1)-C(14)-C(16)	111.82(16)
N(1)-C(14)-C(15)	111.39(17)
C(16)-C(14)-C(15)	112.88(19)

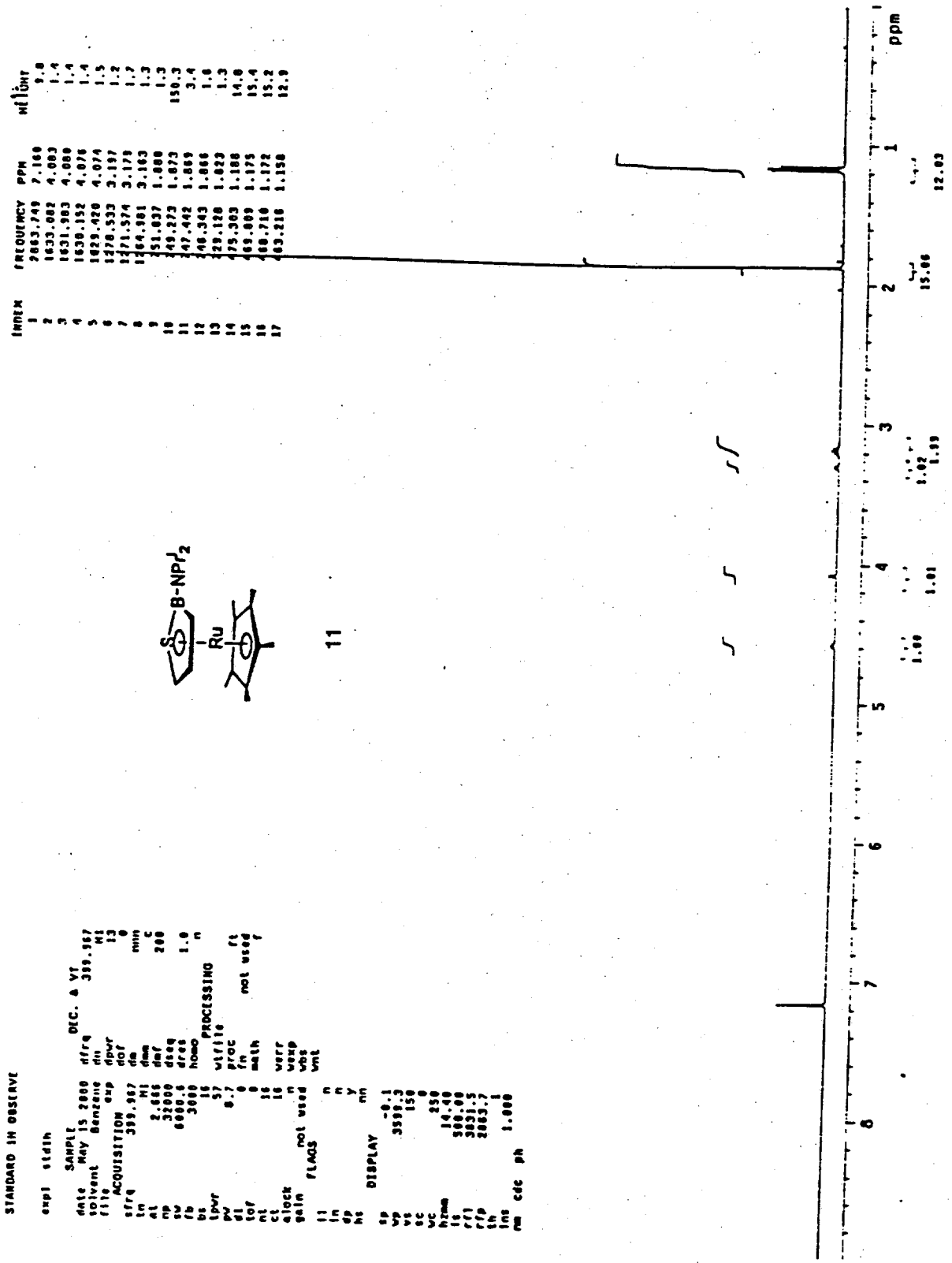
Symmetry transformations used to generate equivalent atoms:

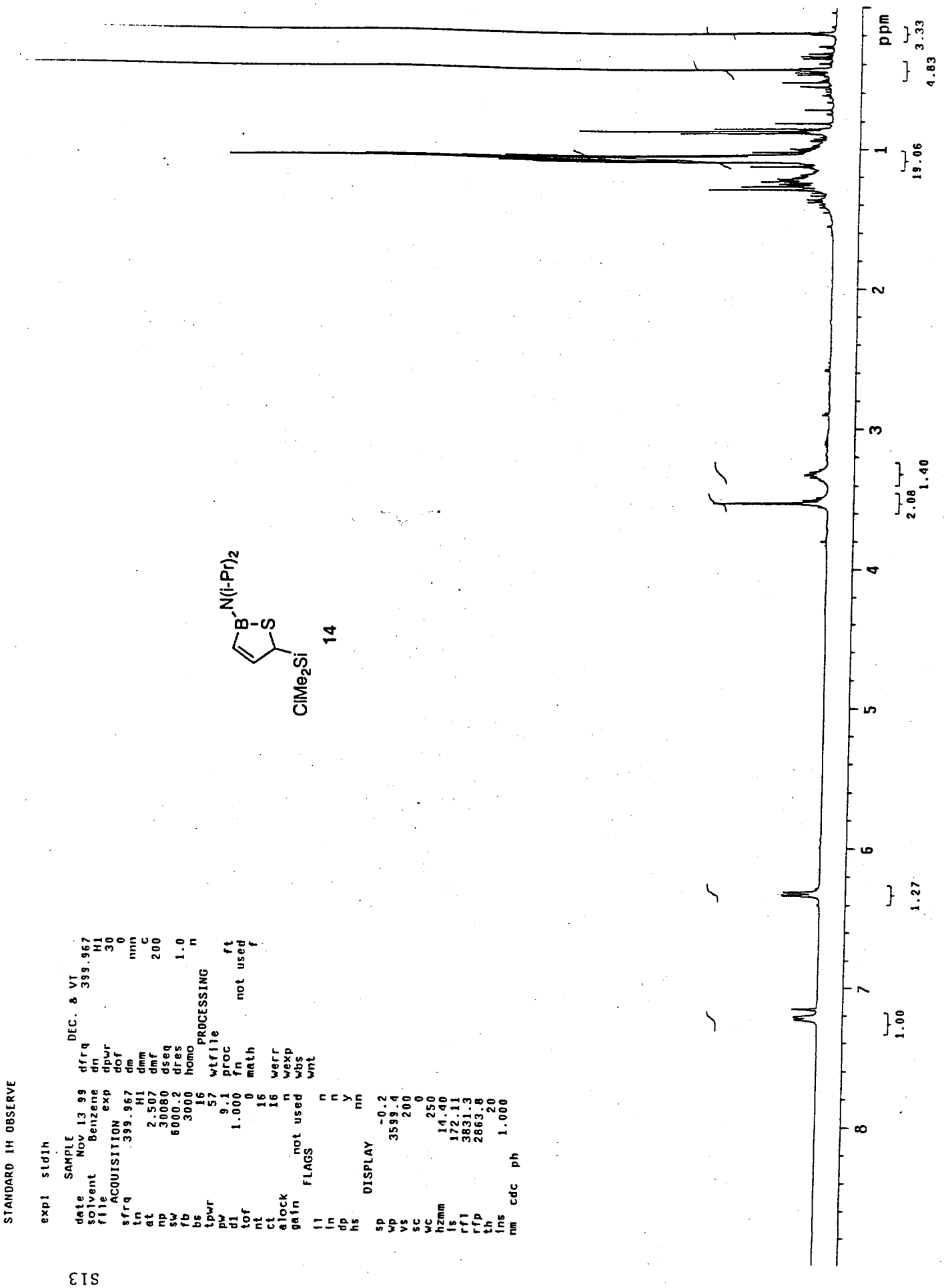
Table 8. Anisotropic displacement parameters (A^2 x 10^3) for 15.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
B(1)	23(1)	19(1)	24(1)	3(1)	8(1)	-1(1)
N(1)	23(1)	24(1)	28(1)	-5(1)	12(1)	-4(1)
Zr(1)	17(1)	16(1)	17(1)	0(1)	4(1)	-1(1)
S(1)	20(1)	24(1)	19(1)	2(1)	5(1)	0(1)
Si(1)	21(1)	20(1)	23(1)	4(1)	9(1)	3(1)
Cl(1)	26(1)	34(1)	25(1)	-1(1)	-2(1)	-6(1)
Cl(2)	38(1)	20(1)	32(1)	-1(1)	14(1)	5(1)
C(1)	23(1)	20(1)	27(1)	-2(1)	8(1)	-5(1)
C(2)	30(1)	16(1)	25(1)	1(1)	11(1)	-3(1)
C(3)	27(1)	17(1)	22(1)	3(1)	10(1)	2(1)
C(4)	26(1)	40(1)	31(1)	8(1)	6(1)	6(1)
C(5)	42(1)	24(1)	39(1)	0(1)	22(1)	2(1)
C(6)	17(1)	23(1)	25(1)	6(1)	10(1)	1(1)
C(7)	24(1)	30(1)	21(1)	3(1)	10(1)	1(1)
C(8)	25(1)	33(1)	28(1)	14(1)	10(1)	5(1)
C(9)	26(1)	19(1)	43(1)	10(1)	15(1)	1(1)
C(10)	19(1)	24(1)	30(1)	3(1)	7(1)	-4(1)
C(11)	29(1)	30(1)	28(1)	-7(1)	12(1)	-5(1)
C(12)	56(1)	42(1)	28(1)	-2(1)	13(1)	5(1)
C(13)	38(1)	29(1)	37(1)	-8(1)	18(1)	-4(1)
C(14)	28(1)	38(1)	44(1)	-15(1)	22(1)	-10(1)
C(15)	54(2)	45(1)	66(2)	-19(1)	40(1)	-26(1)
C(16)	24(1)	61(2)	63(2)	-16(1)	10(1)	0(1)

Table 9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 15.

	x	y	z	U(eq)
H(1)	8342(16)	8580(17)	1074(12)	29(5)
H(2)	6858(15)	9390(17)	1519(12)	29(5)
H(4A)	3024(18)	7630(20)	-256(15)	50(6)
H(4B)	2900(20)	8940(30)	-171(18)	73(8)
H(4C)	2431(19)	8184(18)	431(14)	44(6)
H(5A)	4450(18)	10470(20)	1447(14)	45(6)
H(5B)	5130(20)	9810(20)	2284(16)	53(7)
H(5C)	3870(20)	9790(20)	1993(16)	59(7)
H(7)	5811(14)	7624(16)	3023(12)	23(4)
H(8)	6553(17)	5606(17)	3314(13)	37(5)
H(9)	5652(16)	4421(18)	1919(12)	34(5)
H(10)	4368(15)	5703(15)	751(12)	23(4)
H(11)	6432(15)	6291(16)	-1424(11)	25(4)
H(12A)	6664(19)	7750(20)	-2408(15)	51(6)
H(12B)	6617(19)	6500(20)	-2882(16)	49(6)
H(12C)	7760(20)	7150(20)	-2507(17)	65(8)
H(13A)	8555(17)	5245(18)	-1496(12)	36(5)
H(13B)	7296(19)	4690(20)	-1924(15)	49(6)
H(13C)	7803(17)	4836(18)	-829(14)	41(5)
H(14)	9122(16)	7035(17)	-1109(13)	30(5)
H(15A)	8670(20)	9080(30)	-1239(19)	78(9)
H(15B)	9950(20)	8890(20)	-646(16)	62(7)
H(15C)	9036(19)	9180(20)	-173(16)	55(6)
H(16A)	9720(20)	7230(20)	782(17)	60(7)
H(16B)	10530(20)	6930(20)	244(18)	70(8)
H(16C)	9621(19)	6010(20)	291(15)	57(7)





STANDARD 1H OBSERVE

expl stdlh

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tn	H1	dmm	c
at	3.335	dmf	10400
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sw	4500.5	PROCESSING	
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bs	16	proc	ft
tpwr	57	fn	not used
pw	4.8		
d1	0	werr	
tof	0	wexp	
nt	20	wbs	
ct	20	wnt	
alock	n		
gain	not used		
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in	yn		
dp	y		
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sc	0		
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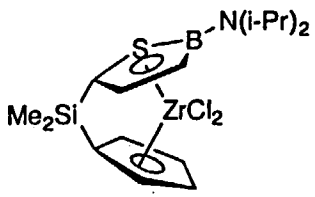
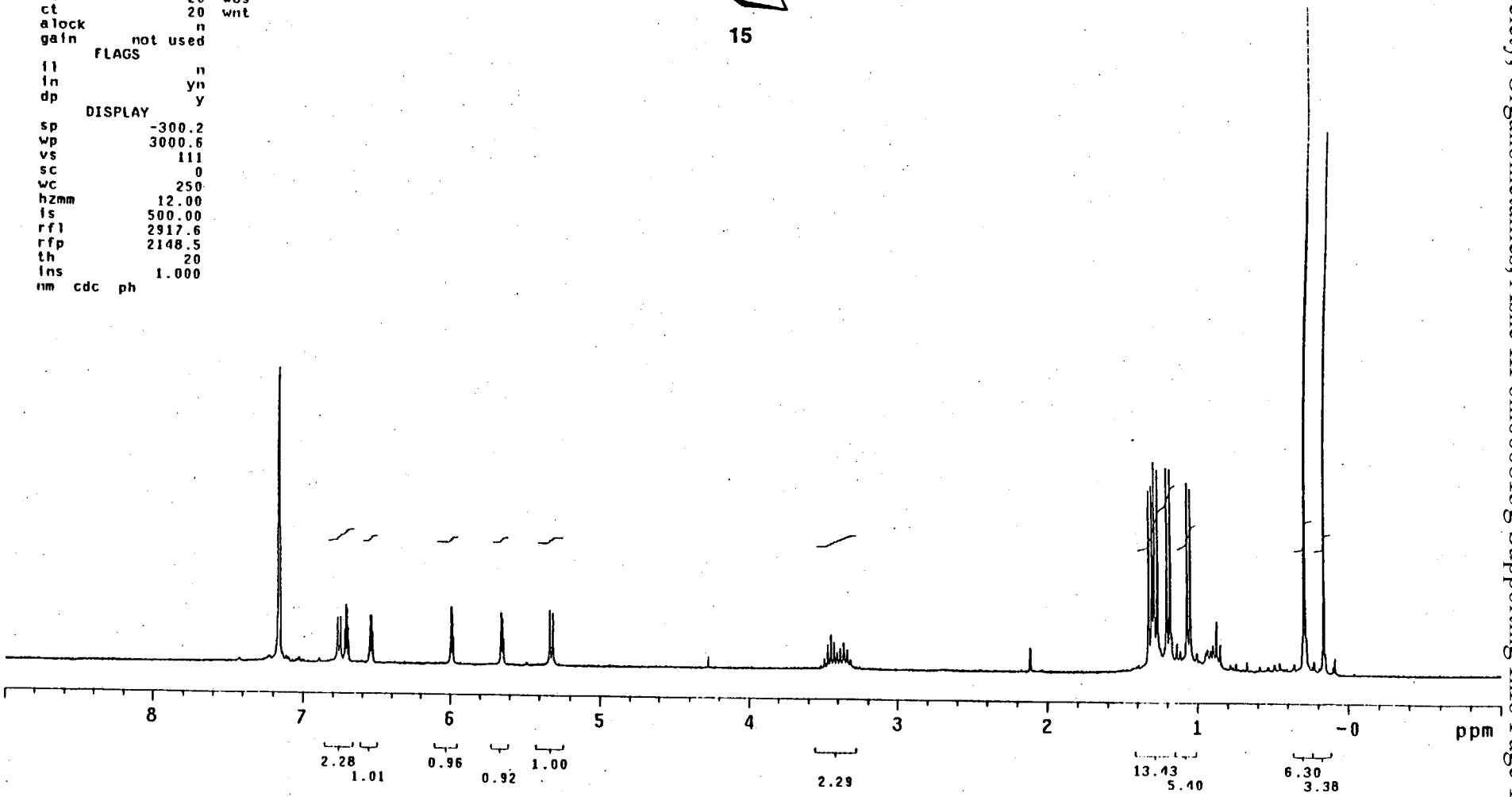
nm cdc ph			



15



Preparation of **14** and **15**.

*5-Chlorodimethylsilyl-2,5-dihydro-2-(N,N-Diisopropylamino)-1,2-thiaborole (**14**).* A solution of **3** (0.62g, 3.27 mmol) in 20 mL of THF was added dropwise to a solution of Me_2SiCl_2 (10 equiv.) in 10 mL of THF at –78 °C. The color turned to bright yellow. The mixture was stirred at –78 °C for 1 h and at 25 °C for 4 h. A white solid formed gradually. After removal of the volatiles, the residue was extracted with 2 x 20 mL of pentane. After filtration and removal of the solvent, the product was obtained as a light yellow solid (0.83 g, 93%). ^{1}H NMR (C_6D_6, 400 MHz): δ 7.23 (d, 1H, J= 7.2 Hz, BCH), 6.35 (dd, 1H, J= 7.2, 1.4 Hz, =CHCSi), 3.55 (m, 1H, CHSi), 3.54 (sept, 1H, J= 6.6 Hz, NCH), 3.36 (sept, 1H, J= 6.6 Hz, NCH), 1.07 (m, 12H, Me), 0.43 (s, 3H, SiMe), 0.20 (s, 3H, SiMe). ^{13}C NMR (C_6D_6, 100.6 MHz): δ 154.8, 132.6 (br, CSi), 51.8 (br, BC), 47.5 (NC), 45.1 (NC), 23.9, 23.8, 21.9, 21.8 (Me). ^{11}B NMR (C_6D_6, 115.5 MHz): δ 43.2. HRMS (EI, m/z): calcd for $C_{11}H_{23}{}^{11}B^{35}ClNSSi$ (M^+), 275.1102; found, 275.1105. (g) *1,5-Dimethylsilyl[cyclopentadienyl][η^4-N,N-diisopropyl-2-amino-1,2-thiaboryl] zirconium (IV) dichloride (**15**).* A solution of **14** (0.83 g, 3.0 mmol) in 10 mL of ether was treated with a solution of CpLi (216 mg, 3.0 mmol) in 5 mL of THF at –78 °C. The mixture was stirred at –78 °C for 1 h and at 25 °C for 4 h. A white solid formed gradually. The volatiles were removed under reduced pressure. The residue was extracted with 2 x 20 mL of pentane. After filtration and removal of the solvent the product was obtained as a yellow oil. The oil was further dissolved in 15 mL of ether and added dropwise to tBuLi (0.42 g, 6.6 mmol) at –78 °C. The mixture was stirred at –78 °C for 2 h and at 25 °C for 10 h. A fine solid formed gradually. The volatiles were removed under reduced pressure. The residue was washed with 3 x 20 mL of pentane and dried under vacuum. The dianion intermediate could be isolated as a light yellow solid, which was characterized by ^{1}H and ^{11}B NMR spectra. ^{1}H NMR (THF-d_8, 400 MHz): δ 7.06 (d, 1H, J= 6.4 Hz, H_4), 5.96 (m, 2H, CpH), 5.81 (m, 2H, CpH), 4.17 (d, 1H, J= 6.4 Hz, H_3), 3.42 (sept, 2H, J= 6.6 Hz, NCH), 1.18 (d, 12H, J= 6.6 Hz, Me), 0.30 (s, 6H, SiMe). ^{11}B NMR (THF-d_8, 115.5 MHz): δ 41.4. To the dianion intermediate was added $ZrCl_4$ (1.0 equiv.) followed by 10 mL of toluene at –78 °C. The mixture was stirred at –78 °C for 2 h and at 25 °C for 15 h. After filtration and removal of toluene the residue was extracted

with 3 x 20 mL of hexane. The solution was concentrated and the recrystallization was performed at –30 °C. The product was obtained as red crystals (0.32 g, 23% from **14**), mp = 164 °C (dec.). ^{1}H NMR (C_6D_6, 400 MHz): δ 6.76 (d, 1H, J= 6.6 Hz, H4), 6.71 (m, 1H, CpH), 6.54 (m, 1H, CpH), 5.99 (m, 1H, CpH), 6.66 (m, 1H, CpH), 5.33 (d, 1H, J= 6.6 Hz, H3), 3.45 (sept, 1H, J= 7.0 Hz, NCH), 3.36 (sept, 1H, J= 7.0 Hz, NCH), 1.33 (d, 3H, J= 7.0 Hz, Me), 1.28 (d, 3H, J= 7.0 Hz, Me), 1.21 (d, 3H, J= 7.0 Hz, Me), 1.06 (d, 3H, J= 7.0 Hz, Me). ^{13}C NMR (C_6D_6, 100.6 MHz): δ 152.5, 124.8, 124.2, 123.9, 123.1 (Cp), 98.7 (br), 46.5, 45.4 (NCH), 22.4, 22.0, 20.8, 20.2 (Me), 2.6, -2.3 (SiMe). ^{11}B NMR (C_6D_6, 115.5 MHz): δ 37.7. HRMS (EI, m/z): calcd for $C_{16}H_{26}{}^{11}B^{35}Cl_2NSSi^{90}Zr$ (M^+), 463.0072; found, 463.0079.