

ORGANOMETALLICS

Organometallics, 1998, 17(6), 1004-1006, DOI:[10.1021/om971044s](https://doi.org/10.1021/om971044s)

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1998 American Chemical Society

General Experimental Procedures

All manipulations are performed under dried nitrogen using standard vacuum line techniques described elsewhere.¹ $[(C_5H_5)_2YCl]_2$,² $[(C_5H_4SiMe_3)_2YCl]_2$,³ $[(C_5H_5)_2YMe]_2$,⁴ $B(C_6F_5)_3$,⁵ and $[CPh_3][B(C_6F_5)_4]$ ^{6,7} were prepared according to literature procedures.

- (1) Jiménez Pindado, G.; Thornton-Pett, M.; Bochmann, M. *J. Chem. Soc., Dalton Trans.* **1997**, 3115.
- (2) Evans, W.J.; Meadows, J.H.; Wayda, A.L.; Hunter, W.E.; Atwood, J.L. *J. Am. Chem. Soc.* **1982**, *104*, 2008.
- (3) Lappert, M.F.; Singh, A.; Atwood, J.L.; Hunter, W.E. *J. Chem. Soc., Chem. Commun.* **1981**, 1190.
- (4) Evans, W.J.; Meadows, J.H.; Hunter, W.E.; Atwood, J.L. *J. Am. Chem. Soc.* **1984**, *106*, 1291.
- (5) Massey, A.G.; Park, A.J. *J. Organomet. Chem.* **1964**, *2*, 245.
- (6) Bochmann, M.; Lancaster, S.J. *J. Organomet. Chem.* **1992**, *434*, C1.
- (7) Chien, J.C.W.; Tsai, W.M.; Rausch, M.D. *J. Am. Chem. Soc.* **1991**, *113*, 8570.

Spectroscopic and analytical data of THF complexes:

4a: 1H NMR (THF- d_8 , 25°C): δ 1.69 (8 H, THF), 3.53 (8 H, THF), 6.18 (s, 10 H, Cp). ^{13}C NMR (THF- d_8 , 25°C): δ 26.4, 68.2 (THF), 112.5 (Cp). ^{11}B NMR (THF- d_8 , 25°C): δ -15.6. ^{19}F NMR (THF- d_8 , 25°C): δ -132.5 (br, 6 F, *o*-F); -164.7 (t, J = 20.1 Hz, 3 F, *p*-F), -168.3 (br, 6 F, *m*-F). Anal. Calcd (found) for $C_{42}H_{26}BF_{20}O_2Y$: C 49.57 (49.45), H 3.05 (3.00).

5a: From **2a** by recrystallization from THF/light petroleum at -20°C as a microcrystalline white solid (0.73 g, 60%). 1H NMR (CD_2Cl_2 , -20°C): δ 0.13 (br, 3 H, Me-B), 1.78 (8 H, THF), 3.68 (8 H, THF), 6.09 (s, 10 H, Cp). ^{13}C NMR (THF- d_8 , 25°C): δ 11.0 (br, Me-B); 26.4, 68.2 (THF), 112.5 (Cp). ^{11}B NMR (THF- d_8 , 25°C): δ -14.3. ^{19}F NMR (CD_2Cl_2 , -20°C): δ -134.0 (d, J = 20.7 Hz, 6 F, *o*-F); -165.1 (t, J = 20.7 Hz, 3 F, *p*-F), -167.9 (t, J = 20.7 Hz, 6 F, *m*-F). Anal. Calcd (found) for $C_{37}H_{29}BF_{15}O_2Y$: C 49.89 (49.90), H 3.26 (3.95), F 32.03 (31.55).

5b: Obtained as a pale-yellow oil by layering a solution of **2b** (0.3 g (0.34mmol) in THF with light petroleum at -20°C (yield 0.30g, 86%). ^1H NMR (CD_2Cl_2 , -20°C): δ 0.29 (SiMe_3), 0.43 (br, 3 H, Me-B), 2.07, 4.00 (THF), 6.29 (t, 4 H, $J = 2.8$ Hz, Cp'), 6.72 (t, 4 H, $J = 2.8$ Hz, Cp'). ^{13}C NMR (CD_2Cl_2 , -20°C): δ -0.12 (SiMe_3), 10.1 (br, Me-B); 25.6, 74.0 (THF), 116.1, 122.4, 124.1 (Cp'). ^{11}B NMR (CD_2Cl_2 , -60°C): δ -14.9 . ^{19}F NMR (CD_2Cl_2 , -60°C): δ -134.0 (d, $J = 20.7$ Hz, 6 F, *o*-F); -164.8 (t, $J = 20.7$ Hz, 3 F, *p*-F), -167.7 (t, $J = 20.7$ Hz, 6 F, *m*-F).

Crystal structure determination data and refinement for **2b**:

$\text{C}_{35}\text{H}_{29}\text{BF}_{15}\text{Si}_2\text{Y}$, $M = 890.48$; triclinic space group $P1$; $a = 11.380(2)$, $b = 12.759(4)$, $c = 14.2630(10)$ Å, $\alpha = 71.543(13)^{\circ}$, $\beta = 74.345(9)^{\circ}$, $\gamma = 82.747(11)^{\circ}$, $V = 1889.7(7)$ Å³; $Z = 2$; $D_c = 1.565$ g/cm³; $F(000) = 892$. Delft Instruments FAST TV area-detector diffractometer; MoK α radiation ($\lambda = 0.71073$ Å); $T = -123$ °C. The structure was solved *via* standard heavy-atom methods (SHELXS-86) and refined by full-matrix least-squares techniques against F^2 (SHELXL-97). Non-hydrogen atoms were assigned anisotropic displacement parameters. All hydrogen atoms were constrained to idealized positions and refined using a riding model with fixed isotropic contributions ($U_{\text{iso}} = nU_{\text{eq}}$ of the attached C atom; $n = 1.5$ for methyl and 1.2 for all others) with the exception of those of the Y-CH₃-B bridge which were located from Fourier difference syntheses and freely refined. The structure converged for 505 refined parameters to R_1 (wR_2) = 0.0432 (0.0866) for 3196 reflections with $F^2 > 2.0 \sigma(F^2)$.

Table 1. Crystal data and structure refinement.

Identification code	MB24	
Empirical formula	$C_{35}H_{29}BF_{15}Si_2Y$	
Formula weight	890.48	
Temperature	160(2) K	
Wavelength	0.71069 Å [Mo- K_α]	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	$a = 11.380(2)$ Å	$\alpha = 71.543(13)^\circ$
	$b = 12.759(4)$ Å	$\beta = 74.345(9)^\circ$
	$c = 14.2630(10)$ Å	$\gamma = 82.747(11)^\circ$
Volume	$1889.7(7)$ Å ³	
Z	2	
Density (calculated)	1.565 Mg/m ³	
Absorption coefficient	1.706 mm ⁻¹	
$F(000)$	892	
Crystal size	$0.24 \times 0.20 \times 0.16$ mm	
Data collection range	$1.86 \leq \theta \leq 24.89^\circ$	
Index ranges	$-11 \leq h \leq 13, -14 \leq k \leq 14, -16 \leq l \leq 16$	
Reflections collected	8044	
Independent reflections	5182 [$R(\text{int}) = 0.0722$]	
Max. and min. transmission	0.7719 and 0.6849	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5182 / 0 / 505	
Goodness-of-fit on F^2	0.791	
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0432, wR_2 = 0.0826$	
R indices (all data)	$R_1 = 0.0690, wR_2 = 0.0866$	
Largest diff. peak and hole	0.429 and -0.426 e.Å ⁻³	

Table 2. Atomic co-ordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) with estimated standard deviations (e.s.d.s) in parentheses. U_{eq} is defined as $1/3$ of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Y(1)	873.2(5)	2439.2(4)	2304.7(4)	21.25(17)
C(1)	687(5)	3048(4)	426(4)	25.7(15)
C(2)	1291(5)	3900(4)	526(4)	24.3(15)
C(3)	488(6)	4418(4)	1176(4)	26.3(15)
C(4)	-606(5)	3924(4)	1496(4)	27.9(15)
C(5)	-503(5)	3075(4)	1045(4)	26.1(15)
Si(1)	1257.7(17)	2161.4(15)	-436.8(14)	39.1(5)
C(11)	1226(6)	681(5)	326(5)	58(2)
C(12)	177(7)	2391(6)	-1255(5)	65(3)
C(13)	2832(6)	2508(6)	-1166(6)	74(3)
C(6)	-428(5)	1887(4)	4152(4)	22.0(14)
C(7)	624(5)	1135(4)	4153(4)	25.5(15)
C(8)	589(6)	459(4)	3549(4)	33.8(17)
C(9)	-448(5)	748(5)	3184(5)	36.7(18)
C(10)	-1079(5)	1615(4)	3554(4)	29.9(16)
Si(6)	-917.4(15)	2872.4(13)	4930.3(13)	25.3(4)
C(61)	-820(5)	4329(4)	4077(4)	33.4(16)
C(62)	107(5)	2661(5)	5784(4)	41.8(18)
C(63)	-2506(5)	2623(4)	5651(4)	34.5(17)
B(1)	4647(6)	1916(5)	1936(5)	19.7(16)
C(111)	5506(5)	2370(4)	767(4)	19.9(14)
C(112)	5808(5)	1677(4)	136(5)	24.1(15)
C(113)	6459(5)	1977(5)	-854(5)	27.7(15)
C(114)	6829(5)	3020(5)	-1311(5)	30.8(16)
C(115)	6565(5)	3760(4)	-746(5)	28.0(15)
C(116)	5899(5)	3433(4)	256(4)	19.4(14)
F(112)	5489(3)	605(2)	545(2)	33.1(9)
F(113)	6709(3)	1246(3)	-1402(2)	49.4(11)
F(114)	7486(3)	3362(3)	-2291(3)	51.0(10)
F(115)	6950(3)	4815(2)	-1185(2)	39.5(9)
F(116)	5687(3)	4225(2)	733(2)	31.4(9)
C(121)	5211(5)	795(4)	2642(4)	15.7(13)
C(122)	6414(5)	344(4)	2409(4)	23.9(15)
C(123)	6825(5)	-634(4)	3050(5)	26.9(15)
C(124)	6086(6)	-1157(4)	3951(5)	26.9(15)
C(125)	4920(6)	-734(4)	4241(5)	28.7(15)
C(126)	4556(5)	222(4)	3564(4)	22.3(14)
F(122)	7243(3)	816(2)	1554(2)	28.7(8)
F(123)	7976(3)	-1032(2)	2756(2)	37.2(9)

Table 2 (continued)

F(124)	6487(3)	-2096(2)	4581(3)	47.7(10)
F(125)	4180(3)	-1228(2)	5147(2)	37.2(9)
F(126)	3389(3)	597(2)	3941(2)	32.0(8)
C(131)	4475(5)	2834(4)	2573(4)	18.2(13)
C(132)	3414(5)	3369(4)	2972(4)	18.0(13)
C(133)	3341(5)	4102(4)	3523(4)	23.9(15)
C(134)	4360(5)	4335(4)	3703(4)	23.5(15)
C(135)	5451(6)	3864(4)	3323(4)	26.0(15)
C(136)	5465(5)	3115(4)	2794(4)	20.1(14)
F(132)	2286(3)	3205(2)	2827(2)	24.8(8)
F(133)	2245(3)	4550(2)	3890(2)	31.9(9)
F(134)	4332(3)	5053(3)	4224(3)	45.0(10)
F(135)	6501(3)	4117(3)	3452(3)	43.9(10)
F(136)	6599(3)	2688(2)	2418(2)	31.2(9)
C(14)	3348(6)	1648(5)	1776(6)	22.0(16)

Table 3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$). The anisotropic displacement factor exponent takes the form:

$$-2\pi^2[h^2a^{*2}U_{11} + \dots + 2hk a^* b^* U_{12}]$$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Y(1)	21.1(3)	19.6(3)	21.9(4)	-3.0(3)	-6.6(3)	-2.0(3)
C(1)	35(4)	21(3)	26(4)	-5(3)	-20(3)	1(3)
C(2)	28(4)	22(3)	19(4)	1(3)	-10(3)	2(3)
C(3)	42(4)	12(3)	25(4)	-3(3)	-11(3)	0(3)
C(4)	22(4)	32(3)	29(4)	-8(3)	-12(3)	12(3)
C(5)	26(4)	30(3)	30(4)	-18(3)	-11(3)	6(3)
Si(1)	41.7(12)	49.2(11)	37.6(13)	-26.1(11)	-19.0(11)	12.8(10)
C(11)	63(5)	53(4)	77(6)	-41(5)	-33(5)	18(4)
C(12)	77(6)	84(5)	67(6)	-56(5)	-48(5)	34(5)
C(13)	60(6)	110(6)	71(7)	-62(6)	-11(5)	7(5)
C(6)	15(3)	27(3)	21(4)	-2(3)	-4(3)	-6(3)
C(7)	21(4)	25(3)	20(4)	2(3)	-1(3)	3(3)
C(8)	34(4)	16(3)	39(5)	-9(3)	11(4)	0(3)
C(9)	32(4)	41(4)	51(5)	-38(4)	-2(4)	-3(3)
C(10)	20(4)	31(3)	41(4)	-11(3)	-10(3)	-3(3)
Si(6)	26.5(10)	26.7(9)	22.2(11)	-7.5(8)	-4.3(9)	-2.7(8)
C(61)	36(4)	40(4)	30(4)	-20(3)	-10(3)	4(3)
C(62)	45(4)	41(4)	44(5)	-12(4)	-15(4)	-7(3)
C(63)	40(4)	34(3)	28(4)	-12(3)	-6(3)	3(3)
B(1)	21(4)	16(3)	21(4)	-5(3)	-3(4)	0(3)
C(111)	11(3)	24(3)	24(4)	-8(3)	-4(3)	0(3)
C(112)	23(4)	20(3)	25(4)	-2(3)	-4(3)	-3(3)
C(113)	27(4)	31(4)	25(4)	-11(4)	-5(3)	5(3)
C(114)	27(4)	48(4)	10(4)	-3(4)	1(3)	-1(3)
C(115)	22(4)	25(3)	30(4)	7(3)	-9(3)	-9(3)
C(116)	14(3)	19(3)	23(4)	-4(3)	-4(3)	-1(3)
F(112)	41(2)	25.5(17)	33(2)	-11.5(17)	-3.1(18)	-5.0(17)
F(113)	69(3)	51(2)	29(2)	-22(2)	-6(2)	7(2)
F(114)	59(3)	66(2)	17(2)	-5(2)	1(2)	-5(2)
F(115)	40(2)	36.1(19)	30(2)	5.2(18)	-0.9(18)	-14.8(18)
F(116)	45(2)	22.1(16)	23(2)	-4.2(16)	-2.4(18)	-6.4(16)
C(121)	17(3)	15(3)	13(4)	-3(3)	-1(3)	-1(3)
C(122)	34(4)	22(3)	19(4)	-8(3)	-9(3)	-5(3)
C(123)	19(4)	21(3)	46(5)	-14(3)	-14(3)	4(3)
C(124)	38(4)	14(3)	29(4)	2(3)	-20(4)	1(3)
C(125)	34(4)	26(3)	25(4)	-6(3)	-5(3)	-3(3)
C(126)	15(3)	26(3)	29(4)	-10(3)	-9(3)	3(3)
F(122)	20.2(19)	33.3(18)	26(2)	-4.4(17)	-0.1(17)	0.3(16)
F(123)	27(2)	33.5(18)	53(3)	-17.4(19)	-13.5(19)	11.5(17)

Table 3 (continued)

F(124)	60(3)	27.3(18)	51(3)	2.0(19)	-27(2)	8.4(18)
F(125)	46(2)	34.0(19)	24(2)	6.2(18)	-7.8(19)	-14.2(18)
F(126)	22.1(19)	39.3(19)	24(2)	-1.0(17)	-0.2(17)	1.5(16)
C(131)	16(3)	20(3)	13(4)	4(3)	-4(3)	-4(3)
C(132)	13(3)	23(3)	17(4)	1(3)	-8(3)	-6(3)
C(133)	23(4)	21(3)	29(4)	-13(3)	-3(3)	4(3)
C(134)	23(4)	25(3)	30(4)	-18(3)	-8(3)	2(3)
C(135)	31(4)	26(3)	28(4)	-8(3)	-18(3)	-4(3)
C(136)	11(3)	20(3)	24(4)	1(3)	-4(3)	0(3)
F(132)	16.8(18)	25.6(16)	33(2)	-12.3(16)	-0.3(16)	-5.9(15)
F(133)	22.7(19)	36.2(18)	42(2)	-23.5(18)	-4.0(18)	1.6(16)
F(134)	48(2)	52(2)	57(3)	-40(2)	-22(2)	5.0(19)
F(135)	29(2)	56(2)	66(3)	-35(2)	-26(2)	1.9(19)
F(136)	22.8(19)	35.2(18)	41(2)	-14.9(18)	-13.5(18)	2.7(16)
C(14)	20(4)	21(4)	27(5)	-14(4)	-1(4)	-2(3)

Table 4. Hydrogen atom co-ordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) with e.s.d.s in parentheses.

	x	y	z	U_{eq}
H(2)	2114	4085	198	29
H(3)	667	5017	1368	32
H(4)	-1317	4122	1947	33
H(5)	-1131	2599	1141	31
H(11a)	1471	218	-133	86
H(11b)	398	511	747	86
H(11c)	1794	533	766	86
H(12a)	331	1820	-1604	97
H(12b)	291	3121	-1762	97
H(12c)	-662	2354	-833	97
H(13a)	3313	2551	-704	111
H(13b)	2822	3223	-1689	111
H(13c)	3200	1935	-1493	111
H(7)	1238	1100	4502	31
H(8)	1183	-103	3415	41
H(9)	-693	419	2759	44
H(10)	-1830	1965	3421	36
H(61a)	-969	4839	4490	50
H(61b)	-1434	4478	3679	50
H(61c)	-4	4434	3614	50
H(62a)	-152	3168	6202	63
H(62b)	945	2806	5377	63
H(62c)	71	1896	6229	63
H(63a)	-2560	1867	6115	52
H(63b)	-3023	2718	5178	52
H(63c)	-2786	3150	6047	52
H(81)	284(4)	144(4)	235(4)	9(16)
H(82)	272(5)	227(4)	139(4)	53(18)
H(83)	349(4)	118(3)	154(3)	0(15)

Table 5. Interatomic distances (Å) with e.s.d.s in parentheses.

Y(1)-F(132)	2.366(3)	Y(1)-C(10)	2.546(6)
Y(1)-C(9)	2.565(6)	Y(1)-C(6)	2.571(5)
Y(1)-C(5)	2.572(5)	Y(1)-C(4)	2.572(5)
Y(1)-C(3)	2.586(5)	Y(1)-C(8)	2.587(5)
Y(1)-C(2)	2.592(5)	Y(1)-C(7)	2.596(5)
Y(1)-C(1)	2.603(5)	Y(1)-C(14)	2.853(7)
Y(1)-H(81)	2.43(4)	Y(1)-H(82)	2.18(5)
C(1)-C(5)	1.406(7)	C(1)-C(2)	1.419(7)
C(1)-Si(1)	1.865(5)	C(2)-C(3)	1.382(7)
C(3)-C(4)	1.365(8)	C(4)-C(5)	1.404(6)
Si(1)-C(13)	1.842(7)	Si(1)-C(12)	1.851(6)
Si(1)-C(11)	1.857(6)		
C(6)-C(10)	1.410(7)	C(6)-C(7)	1.436(6)
C(7)-C(8)	1.409(7)	C(8)-C(9)	1.378(7)
C(9)-C(10)	1.409(6)	Si(6)-C(63)	1.834(6)
Si(6)-C(62)	1.842(5)	Si(6)-C(61)	1.870(5)
Si(6)-C(6)	1.870(5)		
B(1)-C(121)	1.636(7)	B(1)-C(14)	1.647(8)
B(1)-C(111)	1.649(8)	B(1)-C(131)	1.660(7)
C(111)-C(116)	1.386(7)	C(111)-C(112)	1.405(7)
C(112)-F(112)	1.360(6)	C(112)-C(113)	1.362(7)
C(113)-C(114)	1.348(8)	C(113)-F(113)	1.355(6)
C(114)-F(114)	1.355(6)	C(114)-C(115)	1.382(7)
C(115)-F(115)	1.365(6)	C(115)-C(116)	1.382(7)
C(116)-F(116)	1.352(5)		
C(121)-C(126)	1.349(7)	C(121)-C(122)	1.411(7)
C(122)-F(122)	1.341(6)	C(122)-C(123)	1.404(7)
C(123)-C(124)	1.349(8)	C(123)-F(123)	1.349(6)
C(124)-F(124)	1.362(6)	C(124)-C(125)	1.374(7)
C(125)-F(125)	1.345(6)	C(125)-C(126)	1.390(7)
C(126)-F(126)	1.377(6)		
C(131)-C(136)	1.365(7)	C(131)-C(132)	1.385(6)
C(132)-C(133)	1.381(6)	C(132)-F(132)	1.405(6)
C(133)-C(134)	1.339(7)	C(133)-F(133)	1.347(5)
C(134)-F(134)	1.344(5)	C(134)-C(135)	1.361(7)
C(135)-F(135)	1.349(6)	C(135)-C(136)	1.388(7)
C(136)-F(136)	1.372(5)		
C(14)-H(81)	0.85(5)	C(14)-H(82)	1.11(5)
C(14)-H(83)	0.76(4)		

Table 6. Angles between interatomic vectors (°) with e.s.d.s in parentheses

F(132)-Y(1)-C(10)	121.31(14)	F(132)-Y(1)-C(9)	132.4(2)
C(10)-Y(1)-C(9)	32.0(2)	F(132)-Y(1)-C(6)	89.43(14)
C(10)-Y(1)-C(6)	32.0(2)	C(9)-Y(1)-C(6)	53.3(2)
F(132)-Y(1)-C(5)	138.4(2)	C(10)-Y(1)-C(5)	83.1(2)
C(9)-Y(1)-C(5)	86.8(2)	C(6)-Y(1)-C(5)	110.5(2)
F(132)-Y(1)-C(4)	112.09(14)	C(10)-Y(1)-C(4)	83.7(2)
C(9)-Y(1)-C(4)	102.9(2)	C(6)-Y(1)-C(4)	98.6(2)
C(5)-Y(1)-C(4)	31.7(2)	F(132)-Y(1)-C(3)	86.9(2)
C(10)-Y(1)-C(3)	112.2(2)	C(9)-Y(1)-C(3)	133.5(2)
C(6)-Y(1)-C(3)	116.9(2)	C(5)-Y(1)-C(3)	51.6(2)
C(4)-Y(1)-C(3)	30.7(2)	F(132)-Y(1)-C(8)	104.8(2)
C(10)-Y(1)-C(8)	52.0(2)	C(9)-Y(1)-C(8)	31.0(2)
C(6)-Y(1)-C(8)	53.1(2)	C(5)-Y(1)-C(8)	116.5(2)
C(4)-Y(1)-C(8)	133.1(2)	C(3)-Y(1)-C(8)	163.7(2)
F(132)-Y(1)-C(2)	92.05(14)	C(10)-Y(1)-C(2)	132.7(2)
C(9)-Y(1)-C(2)	135.5(2)	C(6)-Y(1)-C(2)	147.5(2)
C(5)-Y(1)-C(2)	51.6(2)	C(4)-Y(1)-C(2)	51.2(2)
C(3)-Y(1)-C(2)	31.0(2)	C(8)-Y(1)-C(2)	154.8(2)
F(132)-Y(1)-C(7)	80.4(2)	C(10)-Y(1)-C(7)	52.2(2)
C(9)-Y(1)-C(7)	52.1(2)	C(6)-Y(1)-C(7)	32.28(14)
C(5)-Y(1)-C(7)	134.7(2)	C(4)-Y(1)-C(7)	130.7(2)
C(3)-Y(1)-C(7)	145.8(2)	C(8)-Y(1)-C(7)	31.6(2)
C(2)-Y(1)-C(7)	172.4(2)	F(132)-Y(1)-C(1)	122.4(2)
C(10)-Y(1)-C(1)	111.9(2)	C(9)-Y(1)-C(1)	104.4(2)
C(6)-Y(1)-C(1)	141.7(2)	C(5)-Y(1)-C(1)	31.5(2)
C(4)-Y(1)-C(1)	52.3(2)	C(3)-Y(1)-C(1)	52.2(2)
C(8)-Y(1)-C(1)	125.4(2)	C(2)-Y(1)-C(1)	31.7(2)
C(7)-Y(1)-C(1)	155.9(2)	F(132)-Y(1)-C(14)	64.64(14)
C(10)-Y(1)-C(14)	135.1(2)	C(9)-Y(1)-C(14)	107.5(2)
C(6)-Y(1)-C(14)	121.9(2)	C(5)-Y(1)-C(14)	123.5(2)
C(4)-Y(1)-C(14)	138.7(2)	C(3)-Y(1)-C(14)	112.6(2)
C(8)-Y(1)-C(14)	83.0(2)	C(2)-Y(1)-C(14)	87.6(2)
C(7)-Y(1)-C(14)	90.4(2)	C(1)-Y(1)-C(14)	92.9(2)
F(132)-Y(1)-H(81)	63.1(11)	C(10)-Y(1)-H(81)	120.6(12)
C(9)-Y(1)-H(81)	96.6(11)	C(6)-Y(1)-H(81)	106.0(11)
C(5)-Y(1)-H(81)	136.3(11)	C(4)-Y(1)-H(81)	154.7(12)
C(3)-Y(1)-H(81)	127.0(12)	C(8)-Y(1)-H(81)	69.1(12)
C(2)-Y(1)-H(81)	103.5(12)	C(7)-Y(1)-H(81)	74.3(11)
C(1)-Y(1)-H(81)	107.4(11)	C(14)-Y(1)-H(81)	16.0(11)
F(132)-Y(1)-H(82)	69.4(13)	C(10)-Y(1)-H(82)	151.6(13)
C(9)-Y(1)-H(82)	120.3(13)	C(6)-Y(1)-H(82)	142(2)
C(5)-Y(1)-H(82)	105.9(14)	C(4)-Y(1)-H(82)	118(2)
C(3)-Y(1)-H(82)	93.8(14)	C(8)-Y(1)-H(82)	101.0(14)
C(2)-Y(1)-H(82)	67.2(14)	C(7)-Y(1)-H(82)	111(2)
C(1)-Y(1)-H(82)	74.5(14)	C(14)-Y(1)-H(82)	20.5(14)
H(81)-Y(1)-H(82)	37(2)		

Table 6 (continued)

C(5)-C(1)-C(2)	105.5(5)	C(5)-C(1)-Si(1)	125.8(5)
C(2)-C(1)-Si(1)	128.4(5)	C(5)-C(1)-Y(1)	73.0(3)
C(2)-C(1)-Y(1)	73.7(3)	Si(1)-C(1)-Y(1)	122.8(2)
C(3)-C(2)-C(1)	109.1(5)	C(3)-C(2)-Y(1)	74.3(3)
C(1)-C(2)-Y(1)	74.6(3)	C(4)-C(3)-C(2)	108.5(5)
C(4)-C(3)-Y(1)	74.1(3)	C(2)-C(3)-Y(1)	74.8(3)
C(3)-C(4)-C(5)	108.4(5)	C(3)-C(4)-Y(1)	75.2(3)
C(5)-C(4)-Y(1)	74.2(3)	C(4)-C(5)-C(1)	108.5(5)
C(4)-C(5)-Y(1)	74.2(3)	C(1)-C(5)-Y(1)	75.5(3)
C(13)-Si(1)-C(12)	113.2(4)	C(13)-Si(1)-C(11)	109.7(3)
C(12)-Si(1)-C(11)	107.6(3)	C(13)-Si(1)-C(1)	109.5(3)
C(12)-Si(1)-C(1)	107.1(2)	C(11)-Si(1)-C(1)	109.8(3)
C(10)-C(6)-C(7)	105.4(5)	C(10)-C(6)-Si(6)	127.8(4)
C(7)-C(6)-Si(6)	126.3(4)	C(10)-C(6)-Y(1)	73.0(3)
C(7)-C(6)-Y(1)	74.8(3)	Si(6)-C(6)-Y(1)	123.3(3)
C(8)-C(7)-C(6)	108.3(5)	C(8)-C(7)-Y(1)	73.9(3)
C(6)-C(7)-Y(1)	72.9(3)	C(9)-C(8)-C(7)	108.8(5)
C(9)-C(8)-Y(1)	73.6(3)	C(7)-C(8)-Y(1)	74.6(3)
C(8)-C(9)-C(10)	107.8(5)	C(8)-C(9)-Y(1)	75.4(4)
C(10)-C(9)-Y(1)	73.3(3)	C(9)-C(10)-C(6)	109.7(5)
C(9)-C(10)-Y(1)	74.7(3)	C(6)-C(10)-Y(1)	75.0(3)
C(63)-Si(6)-C(62)	111.5(3)	C(63)-Si(6)-C(61)	109.1(2)
C(62)-Si(6)-C(61)	108.8(3)	C(63)-Si(6)-C(6)	108.4(2)
C(62)-Si(6)-C(6)	109.0(2)	C(61)-Si(6)-C(6)	110.0(2)
C(121)-B(1)-C(14)	109.5(5)	C(121)-B(1)-C(111)	113.9(4)
C(14)-B(1)-C(111)	104.3(5)	C(121)-B(1)-C(131)	104.7(4)
C(14)-B(1)-C(131)	112.8(5)	C(111)-B(1)-C(131)	111.9(4)
C(116)-C(111)-C(112)	112.3(5)	C(116)-C(111)-B(1)	127.6(5)
C(112)-C(111)-B(1)	119.7(5)	F(112)-C(112)-C(113)	116.5(5)
F(112)-C(112)-C(111)	118.4(5)	C(113)-C(112)-C(111)	125.0(5)
C(114)-C(113)-F(113)	119.2(6)	C(114)-C(113)-C(112)	120.1(5)
F(113)-C(113)-C(112)	120.7(5)	C(113)-C(114)-F(114)	122.7(5)
C(113)-C(114)-C(115)	118.7(6)	F(114)-C(114)-C(115)	118.6(6)
F(115)-C(115)-C(114)	119.8(6)	F(115)-C(115)-C(116)	120.3(5)
C(114)-C(115)-C(116)	119.9(5)	F(116)-C(116)-C(115)	114.8(5)
F(116)-C(116)-C(111)	121.2(5)	C(115)-C(116)-C(111)	123.9(5)
C(126)-C(121)-C(122)	112.2(5)	C(126)-C(121)-B(1)	121.8(5)
C(122)-C(121)-B(1)	125.9(5)	F(122)-C(122)-C(123)	115.3(5)
F(122)-C(122)-C(121)	122.2(5)	C(123)-C(122)-C(121)	122.5(6)
C(124)-C(123)-F(123)	120.6(5)	C(124)-C(123)-C(122)	120.5(5)
F(123)-C(123)-C(122)	118.9(6)	C(123)-C(124)-F(124)	120.7(5)

Table 6 (continued)

C(123)-C(124)-C(125)	119.7(5)	F(124)-C(124)-C(125)	119.6(6)
F(125)-C(125)-C(124)	120.6(5)	F(125)-C(125)-C(126)	122.3(5)
C(124)-C(125)-C(126)	117.1(6)	C(121)-C(126)-F(126)	119.7(4)
C(121)-C(126)-C(125)	127.8(5)	F(126)-C(126)-C(125)	112.5(5)
C(136)-C(131)-C(132)	111.4(5)	C(136)-C(131)-B(1)	119.7(5)
C(132)-C(131)-B(1)	128.8(5)	C(133)-C(132)-C(131)	125.4(5)
C(133)-C(132)-F(132)	113.8(4)	C(131)-C(132)-F(132)	120.8(4)
C(134)-C(133)-F(133)	121.1(5)	C(134)-C(133)-C(132)	119.3(5)
F(133)-C(133)-C(132)	119.5(5)	C(133)-C(134)-F(134)	121.2(5)
C(133)-C(134)-C(135)	119.5(5)	F(134)-C(134)-C(135)	119.2(5)
F(135)-C(135)-C(134)	121.1(5)	F(135)-C(135)-C(136)	120.4(5)
C(134)-C(135)-C(136)	118.6(5)	C(131)-C(136)-F(136)	118.7(5)
C(131)-C(136)-C(135)	125.8(5)	F(136)-C(136)-C(135)	115.4(5)
C(132)-F(132)-Y(1)	158.2(3)		
B(1)-C(14)-Y(1)	134.6(4)	B(1)-C(14)-H(81)	110(3)
Y(1)-C(14)-H(81)	53(3)	B(1)-C(14)-H(82)	125(3)
Y(1)-C(14)-H(82)	43(3)	H(81)-C(14)-H(82)	96(4)
B(1)-C(14)-H(83)	107(4)	Y(1)-C(14)-H(83)	119(4)
H(81)-C(14)-H(83)	109(5)	H(82)-C(14)-H(83)	109(4)
C(14)-H(81)-Y(1)	111(4)	C(14)-H(82)-Y(1)	116(4)