

Reaction of the Lewis Acids $B(C_6F_5)_3$ and $(AlMe_2Cl)_2$ with Azazirconacycles

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Table S-1. Atomic coordinates [$\times 10^3$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $\text{Cp}_2\text{ZrN}(\text{tBu})\text{C}(\text{CH}_2\text{BCF})\text{CH}_2\text{CH}_2$. U (one third of the trace of the orthogonalized σ_{ij} tensor).

	x	y	z	U(eq)
Zr	4709(1)	2644(1)	7684(1)	38(1)
N	6489(1)	2601(1)	8883(1)	34(1)
C(1)	7710(2)	1990(1)	10272(1)	33(1)
C(2)	6673(2)	2128(1)	9426(1)	32(1)
C(3)	5670(2)	1712(1)	9236(1)	38(1)
C(4)	4816(2)	1684(1)	8228(2)	44(1)
C(11)	2736(2)	2810(2)	7558(2)	73(1)
C(12)	3129(3)	3370(2)	7472(2)	70(1)
C(13)	4008(3)	3514(2)	8347(3)	88(1)
C(14)	4095(3)	3014(2)	8923(2)	84(1)
C(15)	3307(3)	2599(2)	8431(3)	85(1)
C(21)	3946(3)	2096(2)	6150(2)	67(1)
C(22)	5130(2)	2014(1)	6496(2)	57(1)
C(23)	5626(2)	2576(1)	6540(2)	55(1)
C(24)	4763(3)	3016(1)	6215(2)	59(1)
C(25)	3730(3)	2725(2)	5955(2)	65(1)
C(31)	9496(2)	1304(1)	11432(1)	33(1)
C(32)	10151(2)	777(1)	11676(1)	42(1)
C(33)	10963(2)	654(1)	12547(2)	53(1)
C(34)	11183(2)	1075(1)	13238(1)	51(1)
C(35)	10576(2)	1609(1)	13043(1)	44(1)
C(36)	9758(2)	1709(1)	12160(1)	39(1)
C(41)	7714(2)	724(1)	10316(1)	32(1)
C(42)	7599(2)	214(1)	9767(1)	38(1)
C(43)	6969(2)	-291(1)	9778(2)	50(1)
C(44)	6435(2)	-320(1)	10369(2)	54(1)
C(45)	6533(2)	158(1)	10942(2)	49(1)
C(46)	7167(2)	659(1)	10913(1)	38(1)
C(51)	8986(2)	1375(1)	9568(1)	33(1)
C(52)	8271(2)	1326(1)	8638(1)	36(1)
C(53)	8611(2)	1360(1)	7918(1)	42(1)
C(54)	9731(2)	1454(1)	8102(2)	46(1)
C(55)	10483(2)	1516(1)	8998(2)	47(1)
C(56)	10101(2)	1482(1)	9702(1)	41(1)
C(61)	7302(2)	3129(1)	9073(1)	40(1)
C(62)	6723(2)	3591(1)	8301(2)	58(1)
C(63)	8426(2)	2953(1)	9028(2)	56(1)
C(64)	7461(3)	3439(1)	9984(2)	60(1)
F(32)	10003(1)	346(1)	11030(1)	59(1)
F(33)	11552(2)	130(1)	12721(1)	87(1)
F(34)	11975(1)	971(1)	14090(1)	75(1)
F(35)	10788(1)	2029(1)	13707(1)	64(1)
F(36)	9206(1)	2248(1)	12058(1)	60(1)
F(42)	8122(1)	177(1)	9183(1)	51(1)
F(43)	6878(2)	-762(1)	9203(1)	75(1)
F(44)	5821(2)	-814(1)	10375(1)	84(1)

Table S-1.	F(46)	7226(1)	1111(1)	11513(1)	49(1)
	F(52)	7146(1)	1228(1)	8394(1)	46(1)
	F(53)	7841(1)	1302(1)	7039(1)	63(1)
	F(54)	10088(1)	1490(1)	7412(1)	67(1)
	F(55)	11593(1)	1612(1)	9196(1)	71(1)
	F(56)	10916(1)	1575(1)	10562(1)	63(1)
	B	8468(2)	1349(1)	10371(1)	30(1)
	C(01)	5160(12)	5025(10)	9859(8)	123(6)
	C(02)	4040(10)	5076(7)	9762(8)	145(8)
	C(03)	3765(7)	4957(4)	10511(10)	154(7)
	C(04)	4610(11)	4788(5)	11355(8)	290(20)
	C(05)	5730(9)	4737(3)	11452(6)	119(3)
	C(06)	6005(8)	4856(7)	10703(9)	129(5)
	C(07)	5330(13)	5206(7)	8953(16)	168(7)
	C(001)	11486(15)	342(10)	16983(8)	236(12)
	C(002)	10581(15)	392(8)	16151(12)	195(9)
	C(003)	10322(12)	130(20)	15284(13)	380(30)
	C(004)	9396(15)	16(9)	14506(11)	162(7)
	C(005)	8978(17)	-385(12)	13775(18)	440(40)
	C(006)	8328(16)	-909(9)	13571(18)	279(14)

Zr-C(4)	2.262 (2)	Zr-N	2.3113 (17)
Zr-C(11)	2.489 (3)	Zr-C(24)	2.491 (2)
Zr-C(12)	2.497 (2)	Zr-C(25)	2.512 (2)
Zr-C(13)	2.516 (3)	Zr-C(15)	2.524 (3)
Zr-C(14)	2.524 (2)	Zr-C(21)	2.525 (3)
Zr-C(23)	2.531 (2)	Zr-C(22)	2.561 (2)
N-C(2)	1.308 (2)	N-C(61)	1.508 (3)
C(1)-C(2)	1.489 (3)	C(1)-B	1.685 (3)
C(2)-C(3)	1.509 (3)	C(3)-C(4)	1.529 (3)
C(11)-C(15)	1.358 (5)	C(11)-C(12)	1.358 (5)
C(12)-C(13)	1.425 (5)	C(13)-C(14)	1.404 (5)
C(14)-C(15)	1.352 (5)	C(21)-C(22)	1.406 (4)
C(21)-C(25)	1.419 (4)	C(22)-C(23)	1.379 (4)
C(23)-C(24)	1.403 (4)	C(24)-C(25)	1.380 (4)
C(31)-C(36)	1.387 (3)	C(31)-C(32)	1.392 (3)
C(31)-B	1.667 (3)	C(32)-F(32)	1.350 (2)
C(32)-C(33)	1.378 (3)	C(33)-F(33)	1.345 (3)
C(33)-C(34)	1.371 (4)	C(34)-F(34)	1.341 (2)
C(34)-C(35)	1.372 (3)	C(35)-F(35)	1.342 (3)
C(35)-C(36)	1.385 (3)	C(36)-F(36)	1.355 (2)
C(41)-C(42)	1.388 (3)	C(41)-C(46)	1.393 (2)
C(41)-B	1.663 (3)	C(42)-F(42)	1.347 (2)
C(42)-C(43)	1.378 (3)	C(43)-F(43)	1.351 (3)
C(43)-C(44)	1.367 (3)	C(44)-F(44)	1.344 (3)
C(44)-C(45)	1.359 (3)	C(45)-F(45)	1.350 (2)
C(45)-C(46)	1.382 (3)	C(46)-F(46)	1.354 (2)
C(51)-C(56)	1.383 (3)	C(51)-C(52)	1.389 (3)
C(51)-B	1.655 (3)	C(52)-F(52)	1.354 (2)
C(52)-C(53)	1.377 (3)	C(53)-F(53)	1.348 (2)
C(53)-C(54)	1.365 (3)	C(54)-F(54)	1.346 (2)
C(54)-C(55)	1.363 (3)	C(55)-F(55)	1.349 (2)
C(55)-C(56)	1.388 (3)	C(56)-F(56)	1.355 (2)
C(61)-C(63)	1.525 (3)	C(61)-C(62)	1.530 (3)
C(61)-C(64)	1.531 (3)	C(01)-C(02)	1.3900
C(01)-C(06)	1.3900	C(01)-C(07)	1.58 (3)
C(02)-C(03)	1.3900	C(03)-C(04)	1.3900
C(04)-C(05)	1.3900	C(05)-C(06)	1.3900
C(001)-C(002)	1.365 (14)	C(002)-C(003)	1.394 (12)
C(003)-C(004)	1.348 (11)	C(004)-C(005)	1.378 (11)
C(005)-C(006)	1.382 (16)		
C(4)-Zr-N	76.19 (7)	C(4)-Zr-C(11)	94.07 (10)
N-Zr-C(11)	135.32 (9)	C(4)-Zr-C(24)	129.87 (9)
N-Zr-C(24)	112.82 (8)	C(11)-Zr-C(24)	106.77 (10)
C(4)-Zr-C(12)	124.65 (9)	N-Zr-C(12)	128.21 (9)
C(11)-Zr-C(12)	31.60 (11)	C(24)-Zr-C(12)	89.59 (9)
C(4)-Zr-C(25)	113.99 (10)	N-Zr-C(25)	142.29 (8)
C(11)-Zr-C(25)	81.73 (10)	C(24)-Zr-C(25)	32.01 (10)
C(12)-Zr-C(25)	77.67 (9)	C(4)-Zr-C(13)	121.84 (11)
N-Zr-C(13)	95.24 (10)	C(11)-Zr-C(13)	52.96 (12)
C(24)-Zr-C(13)	106.78 (12)	C(12)-Zr-C(13)	33.02 (11)
C(25)-Zr-C(13)	107.10 (12)	C(4)-Zr-C(15)	74.37 (10)
N-Zr-C(15)	105.74 (11)	C(11)-Zr-C(15)	31.42 (11)
C(24)-Zr-C(15)	138.07 (11)	C(12)-Zr-C(15)	52.57 (10)
C(25)-Zr-C(15)	111.96 (12)	C(13)-Zr-C(15)	52.53 (12)
C(4)-Zr-C(14)	89.71 (12)	N-Zr-C(14)	83.79 (9)

Table S-2.

C(12)-Zr-C(14)	53.58(9)	C(25)-Zr-C(14)	130.27(9)
C(13)-Zr-C(14)	32.35(12)	C(15)-Zr-C(14)	31.06(12)
C(4)-Zr-C(21)	81.99(10)	N-Zr-C(21)	129.86(8)
C(11)-Zr-C(21)	90.28(11)	C(24)-Zr-C(21)	53.64(10)
C(12)-Zr-C(21)	101.35(11)	C(25)-Zr-C(21)	32.71(10)
C(13)-Zr-C(21)	134.23(13)	C(15)-Zr-C(21)	110.92(14)
C(14)-Zr-C(21)	141.03(12)	C(4)-Zr-C(23)	104.03(8)
N-Zr-C(23)	89.53(7)	C(11)-Zr-C(23)	134.81(10)
C(24)-Zr-C(23)	32.44(8)	C(12)-Zr-C(23)	122.02(8)
C(25)-Zr-C(23)	53.08(9)	C(13)-Zr-C(23)	133.71(11)
C(15)-Zr-C(23)	163.48(13)	C(14)-Zr-C(23)	162.86(13)
C(21)-Zr-C(23)	52.97(9)	C(4)-Zr-C(22)	77.08(8)
N-Zr-C(22)	98.49(7)	C(11)-Zr-C(22)	122.05(10)
C(24)-Zr-C(22)	53.09(9)	C(12)-Zr-C(22)	130.43(9)
C(25)-Zr-C(22)	53.20(8)	C(13)-Zr-C(22)	159.03(12)
C(15)-Zr-C(22)	136.41(13)	C(14)-Zr-C(22)	165.53(13)
C(21)-Zr-C(22)	32.08(9)	C(23)-Zr-C(22)	31.41(9)
C(2)-N-C(61)	123.67(17)	C(2)-N-Zr	115.35(13)
C(61)-N-Zr	120.55(12)	C(2)-C(1)-B	121.87(15)
N-C(2)-C(1)	127.62(18)	N-C(2)-C(3)	115.94(17)
C(1)-C(2)-C(3)	116.03(16)	C(2)-C(3)-C(4)	115.33(16)
C(3)-C(4)-Zr	105.53(14)	C(15)-C(11)-C(12)	109.9(3)
C(15)-C(11)-Zr	75.72(16)	C(12)-C(11)-Zr	74.50(15)
C(11)-C(12)-C(13)	106.6(3)	C(11)-C(12)-Zr	73.90(15)
C(13)-C(12)-Zr	74.23(15)	C(14)-C(13)-C(12)	106.3(3)
C(14)-C(13)-Zr	74.17(16)	C(12)-C(13)-Zr	72.75(15)
C(15)-C(14)-C(13)	108.1(3)	C(15)-C(14)-Zr	74.47(17)
C(13)-C(14)-Zr	73.49(15)	C(14)-C(15)-C(11)	109.1(3)
C(14)-C(15)-Zr	74.47(16)	C(11)-C(15)-Zr	72.86(15)
C(22)-C(21)-C(25)	107.1(3)	C(22)-C(21)-Zr	75.36(15)
C(25)-C(21)-Zr	73.14(15)	C(23)-C(22)-C(21)	108.2(2)
C(23)-C(22)-Zr	73.09(13)	C(21)-C(22)-Zr	72.57(14)
C(22)-C(23)-C(24)	108.6(3)	C(22)-C(23)-Zr	75.49(13)
C(24)-C(23)-Zr	72.22(12)	C(25)-C(24)-C(23)	108.1(3)
C(25)-C(24)-Zr	74.84(14)	C(23)-C(24)-Zr	75.34(13)
C(24)-C(25)-C(21)	108.0(2)	C(24)-C(25)-Zr	73.15(14)
C(21)-C(25)-Zr	74.15(14)	C(36)-C(31)-C(32)	112.74(18)
C(36)-C(31)-B	128.82(17)	C(32)-C(31)-B	118.26(17)
F(32)-C(32)-C(33)	116.0(2)	F(32)-C(32)-C(31)	119.26(18)
C(33)-C(32)-C(31)	124.7(2)	F(33)-C(33)-C(34)	119.8(2)
F(33)-C(33)-C(32)	120.5(2)	C(34)-C(33)-C(32)	119.6(2)
F(34)-C(34)-C(33)	120.9(2)	F(34)-C(34)-C(35)	120.2(2)
C(33)-C(34)-C(35)	118.8(2)	F(35)-C(35)-C(34)	119.71(19)
F(35)-C(35)-C(36)	120.7(2)	C(34)-C(35)-C(36)	119.6(2)
F(36)-C(36)-C(35)	114.06(19)	F(36)-C(36)-C(31)	121.42(18)
C(35)-C(36)-C(31)	124.5(2)	C(42)-C(41)-C(46)	112.68(18)
C(42)-C(41)-B	127.78(16)	C(46)-C(41)-B	119.42(16)
F(42)-C(42)-C(43)	114.71(18)	F(42)-C(42)-C(41)	121.41(18)
C(43)-C(42)-C(41)	123.88(18)	F(43)-C(43)-C(44)	119.6(2)
F(43)-C(43)-C(42)	120.1(2)	C(44)-C(43)-C(42)	120.4(2)
F(44)-C(44)-C(45)	121.0(2)	F(44)-C(44)-C(43)	120.1(2)
C(45)-C(44)-C(43)	118.9(2)	F(45)-C(45)-C(44)	120.4(2)
F(45)-C(45)-C(46)	120.2(2)	C(44)-C(45)-C(46)	119.37(19)
F(46)-C(46)-C(45)	115.33(17)	F(46)-C(46)-C(41)	119.93(18)
C(45)-C(46)-C(41)	124.73(19)	C(56)-C(51)-C(52)	112.16(16)
C(56)-C(51)-B	126.97(17)	C(52)-C(51)-B	120.74(16)
F(52)-C(52)-C(53)	115.60(17)	F(52)-C(52)-C(51)	119.17(16)
C(53)-C(52)-C(51)	125.23(19)	F(53)-C(53)-C(54)	120.43(18)

Table S-2.	F(54)-C(54)-C(55)	120.5(2)	F(54)-C(54)-C(53)	120.7(2)
	C(55)-C(54)-C(53)	118.73(18)	F(55)-C(55)-C(54)	119.70(18)
	F(55)-C(55)-C(56)	120.4(2)	C(54)-C(55)-C(56)	119.9(2)
	F(56)-C(56)-C(51)	120.86(16)	F(56)-C(56)-C(55)	114.61(18)
	C(51)-C(56)-C(55)	124.52(19)	N-C(61)-C(63)	112.89(17)
	N-C(61)-C(62)	106.09(18)	C(63)-C(61)-C(62)	107.24(19)
	N-C(61)-C(64)	110.33(17)	C(63)-C(61)-C(64)	112.8(2)
	C(62)-C(61)-C(64)	107.06(19)	C(51)-B-C(41)	113.21(15)
	C(51)-B-C(31)	111.93(14)	C(41)-B-C(31)	102.28(14)
	C(51)-B-C(1)	107.24(15)	C(41)-B-C(1)	112.52(14)
	C(31)-B-C(1)	109.68(15)	C(02)-C(01)-C(06)	120.0
	C(02)-C(01)-C(07)	113.3(9)	C(06)-C(01)-C(07)	126.6(9)
	C(03)-C(02)-C(01)	120.0	C(02)-C(03)-C(04)	120.0
	C(03)-C(04)-C(05)	120.0	C(06)-C(05)-C(04)	120.0
	C(05)-C(06)-C(01)	120.0	C(001)-C(002)-C(003)	133.5(17)
	C(004)-C(003)-C(002)	138.4(17)	C(003)-C(004)-C(005)	142.3(19)
	C(004)-C(005)-C(006)	136(2)		

Symmetry transformations used to generate equivalent atoms:

Cp2ZrN(tBu)C(CH2BCF)CH2CH2.

The anisotropic displacement factor exponent is $-2\pi^2 [(h a^*)^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Zr	37 (1)	50 (1)	33 (1)	11 (1)	18 (1)	14 (1)
N	39 (1)	37 (1)	32 (1)	5 (1)	20 (1)	3 (1)
C(1)	36 (1)	35 (1)	30 (1)	2 (1)	15 (1)	3 (1)
C(2)	34 (1)	35 (1)	31 (1)	1 (1)	19 (1)	5 (1)
C(3)	31 (1)	44 (1)	41 (1)	12 (1)	17 (1)	2 (1)
C(4)	31 (1)	55 (1)	44 (1)	9 (1)	13 (1)	-2 (1)
C(11)	44 (1)	97 (2)	87 (2)	1 (2)	36 (2)	18 (2)
C(12)	73 (2)	87 (2)	64 (2)	29 (2)	44 (2)	48 (2)
C(13)	77 (2)	76 (2)	140 (3)	-38 (2)	75 (2)	4 (2)
C(14)	78 (2)	139 (3)	45 (1)	16 (2)	35 (2)	57 (2)
C(15)	83 (2)	100 (3)	110 (3)	41 (2)	78 (2)	38 (2)
C(21)	71 (2)	89 (2)	44 (1)	-13 (1)	26 (1)	-15 (2)
C(22)	73 (2)	61 (2)	45 (1)	7 (1)	32 (1)	22 (1)
C(23)	59 (2)	74 (2)	46 (1)	9 (1)	36 (1)	13 (1)
C(24)	79 (2)	66 (2)	42 (1)	18 (1)	36 (1)	21 (1)
C(25)	64 (2)	96 (2)	32 (1)	13 (1)	16 (1)	33 (2)
C(31)	31 (1)	42 (1)	29 (1)	4 (1)	15 (1)	2 (1)
C(32)	36 (1)	53 (1)	39 (1)	0 (1)	15 (1)	8 (1)
C(33)	45 (1)	63 (2)	48 (1)	11 (1)	15 (1)	16 (1)
C(34)	37 (1)	79 (2)	33 (1)	12 (1)	10 (1)	5 (1)
C(35)	39 (1)	63 (1)	31 (1)	-3 (1)	14 (1)	-6 (1)
C(36)	38 (1)	45 (1)	35 (1)	2 (1)	15 (1)	1 (1)
C(41)	30 (1)	33 (1)	34 (1)	3 (1)	15 (1)	4 (1)
C(42)	40 (1)	36 (1)	45 (1)	1 (1)	24 (1)	4 (1)
C(43)	60 (1)	33 (1)	62 (1)	-6 (1)	29 (1)	-4 (1)
C(44)	56 (1)	40 (1)	74 (2)	5 (1)	35 (1)	-11 (1)
C(45)	51 (1)	52 (1)	58 (1)	10 (1)	36 (1)	-1 (1)
C(46)	42 (1)	37 (1)	40 (1)	4 (1)	23 (1)	4 (1)
C(51)	35 (1)	36 (1)	31 (1)	1 (1)	17 (1)	0 (1)
C(52)	36 (1)	39 (1)	34 (1)	-1 (1)	17 (1)	2 (1)
C(53)	52 (1)	49 (1)	27 (1)	1 (1)	17 (1)	7 (1)
C(54)	57 (1)	55 (1)	41 (1)	6 (1)	33 (1)	6 (1)
C(55)	41 (1)	59 (1)	50 (1)	4 (1)	28 (1)	-4 (1)
C(56)	37 (1)	55 (1)	33 (1)	0 (1)	16 (1)	-5 (1)
C(61)	48 (1)	35 (1)	41 (1)	3 (1)	24 (1)	-1 (1)
C(62)	72 (2)	50 (1)	58 (1)	17 (1)	33 (1)	0 (1)
C(63)	51 (1)	48 (1)	82 (2)	0 (1)	39 (1)	-10 (1)
C(64)	96 (2)	39 (1)	52 (1)	-5 (1)	36 (1)	-2 (1)
F(32)	53 (1)	64 (1)	54 (1)	-8 (1)	14 (1)	24 (1)
F(33)	78 (1)	84 (1)	72 (1)	12 (1)	4 (1)	47 (1)
F(34)	59 (1)	109 (1)	39 (1)	15 (1)	0 (1)	15 (1)
F(35)	58 (1)	87 (1)	38 (1)	-18 (1)	10 (1)	-3 (1)
F(36)	69 (1)	48 (1)	45 (1)	-12 (1)	6 (1)	12 (1)
F(42)	63 (1)	43 (1)	63 (1)	-12 (1)	43 (1)	-2 (1)
F(43)	103 (1)	40 (1)	96 (1)	-22 (1)	56 (1)	-18 (1)
F(44)	99 (1)	57 (1)	114 (1)	-1 (1)	63 (1)	-33 (1)

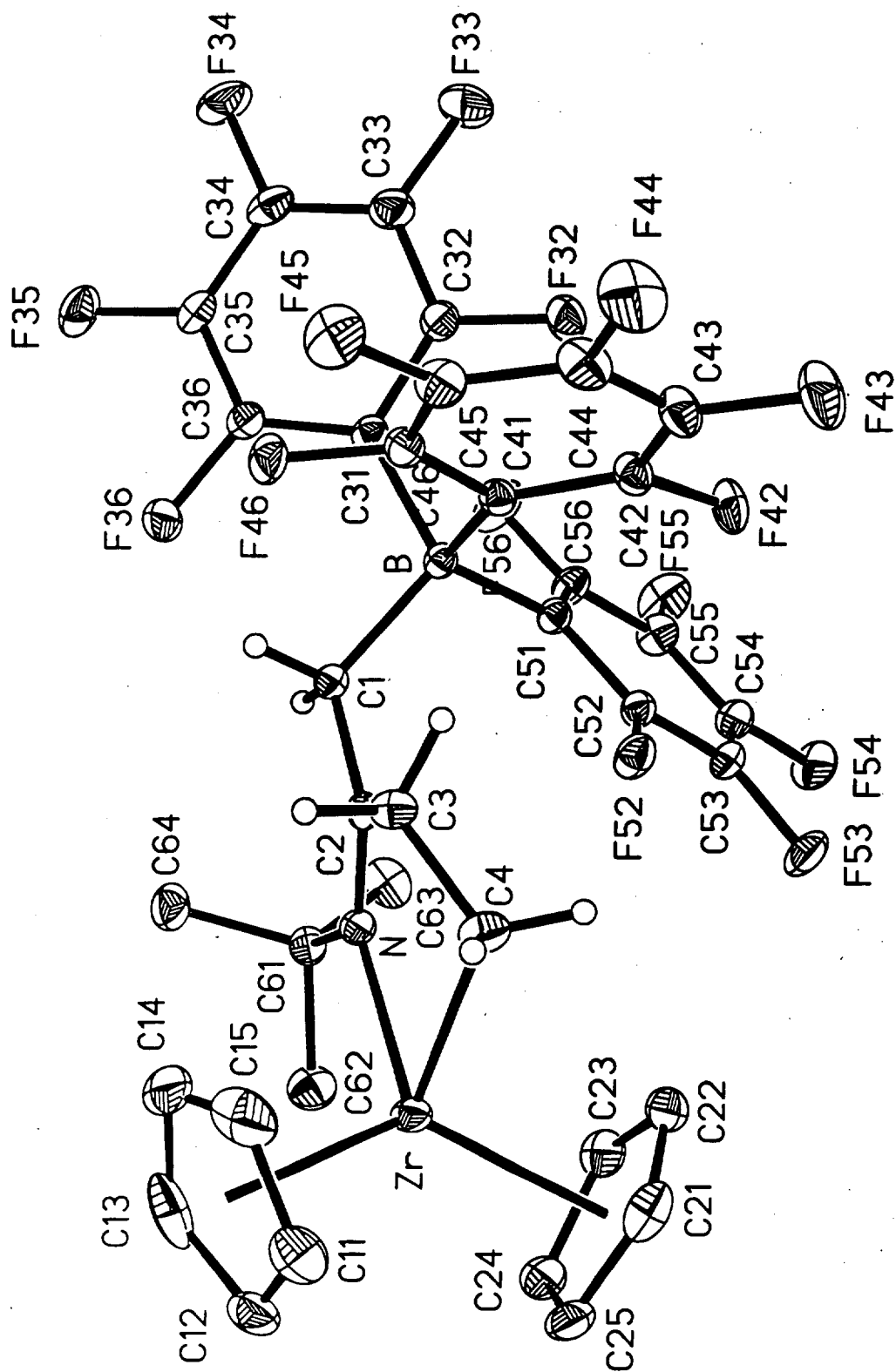
Table S-3.

F(46)	67(1)	50(1)	47(1)	-1(1)	40(1)	-1(1)
F(52)	33(1)	67(1)	35(1)	-5(1)	11(1)	2(1)
F(53)	65(1)	94(1)	27(1)	-1(1)	16(1)	11(1)
F(54)	81(1)	91(1)	51(1)	11(1)	49(1)	10(1)
F(55)	44(1)	114(1)	67(1)	6(1)	35(1)	-14(1)
F(56)	36(1)	112(1)	39(1)	-3(1)	14(1)	-20(1)
B	28(1)	36(1)	28(1)	0(1)	14(1)	-1(1)
C(01)	139(15)	47(5)	160(14)	-26(8)	36(10)	0(8)
C(02)	45(6)	69(8)	230(20)	-28(11)	-32(7)	19(5)
C(03)	111(9)	73(7)	270(20)	-61(9)	73(12)	-6(6)
C(04)	290(30)	63(9)	690(60)	75(16)	370(40)	51(11)
C(05)	128(9)	55(4)	148(9)	17(5)	28(8)	5(5)
C(06)	107(9)	54(5)	150(11)	1(7)	-27(9)	3(5)
C(07)	135(14)	78(10)	238(19)	-49(11)	20(12)	-19(9)
C(001)	181(15)	400(30)	86(7)	17(11)	9(8)	204(19)
C(002)	164(18)	190(15)	240(20)	-103(14)	93(16)	22(11)
C(003)	81(14)	400(60)	670(80)	-140(50)	180(30)	10(30)
C(004)	152(17)	195(15)	162(11)	-23(11)	89(10)	67(12)
C(005)	87(12)	840(90)	410(40)	-460(60)	108(19)	-90(20)
C(006)	186(15)	340(30)	410(30)	-260(20)	232(19)	-160(18)

displacement parameters ($\text{\AA}^2$ $\times 10^3$) for
 $\text{Cp}_2\text{ZrN}(\text{tBu})\text{C}(\text{CH}_2\text{BCF})\text{CH}_2\text{CH}_2$.

	x	y	z	U(eq)
H(1A)	7481	1995	10793	39
H(1B)	8234	2332	10364	39
H(3A)	5268	1844	9615	46
H(3B)	5955	1299	9435	46
H(4A)	4071	1547	8186	53
H(4B)	5079	1403	7874	53
H(11A)	2049	2617	7088	88
H(12A)	2773	3654	6948	83
H(13A)	4382	3914	8540	105
H(14A)	4560	2997	9597	101
H(15A)	3108	2228	8688	102
H(21A)	3368	1768	5964	81
H(22A)	5530	1618	6615	68
H(23A)	6440	2648	6685	66
H(24A)	4869	3445	6075	70
H(25A)	2975	2910	5606	78
H(62A)	6699	3431	7722	87
H(62B)	7148	3969	8446	87
H(62C)	5954	3665	8246	87
H(63A)	8856	2695	9551	85
H(63B)	8860	3318	9047	85
H(63C)	8277	2734	8458	85
H(64A)	6727	3565	9961	91
H(64B)	7947	3792	10078	91
H(64C)	7810	3155	10490	91
H(02A)	3468	5190	9191	174
H(03A)	3007	4991	10445	184
H(04A)	4424	4708	11862	349
H(05A)	6302	4623	12023	143
H(06A)	6763	4822	10768	155
H(07A)	5395	5645	8927	252
H(07B)	4682	5067	8413	252
H(07C)	6017	5017	8964	252
H(00A)	11676	-84	17121	354
H(00B)	11293	519	17462	354
H(00C)	12134	555	16958	354
H(00D)	10517	831	16030	234
H(00H)	9926	286	16290	234
H(00I)	10798	371	15052	453
H(00J)	10691	-265	15440	453
H(00K)	9280	407	14183	194
H(00L)	8799	0	14743	194
H(00M)	9661	-509	13690	531
H(00N)	8561	-120	13249	531
H(00E)	7606	-827	13608	418
H(00F)	8728	-1225	14011	418
H(00G)	8194	-1044	12952	418

Figure S-1.



displacement parameters [$\text{\AA}^2$ x 10^3] for
 $\text{Cp}_2\text{Zr}\{\text{Ph}-\text{N}[\text{C}(\text{H})(\text{Ph})\text{C}(\text{H})_2\text{B}(\text{ArF})_3\}$ one third of the trace of the
 orthogonalized σ_{ij} tensor.

	x	y	z	U(eq)
Zr(1)	3802(1)	6296(1)	7363(1)	31(1)
Zr(2)	1649(1)	3646(1)	1582(1)	39(1)
B(1)	2426(4)	4707(4)	6762(4)	33(2)
B(2)	3018(5)	5282(4)	2069(5)	43(3)
N(1)	3532(3)	6461(3)	6367(3)	29(2)
N(2)	2525(3)	3382(3)	1222(3)	29(2)
C(11)	3718(4)	7242(4)	8063(4)	41(2)
C(12)	3156(4)	7241(4)	7637(4)	42(2)
C(13)	2799(4)	6729(4)	7767(4)	44(2)
C(14)	3126(4)	6401(4)	8287(4)	48(2)
C(15)	3683(4)	6735(4)	8487(4)	41(2)
C(21)	4539(4)	5445(4)	7057(4)	42(2)
C(22)	4238(4)	5216(4)	7591(4)	46(2)
C(23)	4446(4)	5577(4)	8136(4)	49(2)
C(24)	4863(4)	6021(4)	7936(5)	55(3)
C(25)	4933(4)	5936(4)	7271(4)	49(2)
C(31)	4110(4)	6722(4)	6236(4)	39(2)
C(32)	4356(4)	7189(4)	6662(4)	46(2)
C(33)	4989(5)	7397(5)	6648(5)	67(3)
C(34)	5361(5)	7179(5)	6198(5)	79(3)
C(35)	5099(4)	6758(5)	5735(5)	67(3)
C(36)	4485(4)	6517(4)	5747(4)	50(2)
C(41)	2953(3)	6480(3)	5269(4)	34(2)
C(42)	2923(4)	6209(4)	4661(4)	53(2)
C(43)	2729(4)	6548(6)	4107(4)	72(3)
C(44)	2545(4)	7164(6)	4157(6)	78(4)
C(45)	2573(5)	7433(5)	4747(5)	69(3)
C(46)	2778(4)	7097(4)	5305(4)	53(2)
C(47)	3156(3)	6097(3)	5865(3)	31(2)
C(48)	2593(3)	5822(3)	6178(3)	34(2)
C(49)	2817(3)	5385(3)	6735(3)	37(2)
C(51)	2707(3)	4266(3)	7391(3)	28(2)
C(52)	2898(3)	3658(4)	7379(3)	32(2)
C(53)	3160(4)	3331(4)	7917(4)	40(2)
C(54)	3216(4)	3594(4)	8503(4)	46(2)
C(55)	2998(4)	4188(4)	8551(3)	39(2)
C(56)	2747(4)	4505(3)	8011(4)	38(2)
C(61)	2536(4)	4389(3)	6057(3)	34(2)
C(62)	3137(4)	4174(3)	5937(4)	36(2)
C(63)	3282(4)	3904(4)	5372(4)	52(2)
C(64)	2822(6)	3862(4)	4882(4)	61(3)
C(65)	2234(5)	4096(4)	4939(4)	56(3)
C(66)	2095(4)	4356(4)	5513(4)	39(2)
C(71)	1644(3)	4775(4)	6879(4)	34(2)
C(72)	1344(4)	5284(4)	7071(4)	36(2)
C(73)	708(4)	5293(4)	7194(4)	52(2)

Table S-5.

C(75)	630(4)	4242(4)	6916(4)	49(2)
C(76)	1262(4)	4244(3)	6809(4)	36(2)
C(81)	1179(5)	2818(4)	2268(5)	59(3)
C(82)	1826(4)	2842(4)	2482(4)	53(2)
C(83)	1956(5)	3423(5)	2772(4)	61(3)
C(84)	1374(6)	3761(5)	2736(5)	74(3)
C(85)	906(5)	3373(5)	2437(5)	72(3)
C(91)	1249(4)	4692(4)	1174(5)	59(3)
C(92)	1440(4)	4374(4)	639(4)	48(2)
C(93)	1027(4)	3867(4)	507(4)	49(2)
C(94)	588(4)	3858(5)	969(6)	68(3)
C(95)	711(5)	4379(5)	1380(5)	71(3)
C(101)	2258(3)	3034(4)	716(4)	34(2)
C(102)	1778(4)	2614(3)	866(4)	41(2)
C(103)	1369(4)	2315(4)	370(5)	57(3)
C(104)	1467(5)	2395(4)	-258(5)	70(3)
C(105)	1977(4)	2773(4)	-410(4)	59(3)
C(106)	2360(4)	3098(4)	48(4)	49(2)
C(111)	3668(3)	3347(3)	976(3)	30(2)
C(112)	3819(4)	2793(4)	1315(4)	43(2)
C(113)	4338(4)	2455(4)	1184(5)	52(2)
C(114)	4729(4)	2647(4)	738(5)	56(3)
C(115)	4593(4)	3191(5)	400(4)	55(3)
C(116)	4061(4)	3548(4)	526(4)	42(2)
C(117)	3111(3)	3751(3)	1139(3)	31(2)
C(118)	3259(3)	4089(3)	1782(3)	36(2)
C(119)	2735(4)	4569(3)	1910(4)	39(2)
C(121)	3487(3)	5332(4)	2752(4)	37(2)
C(122)	3578(4)	4895(4)	3231(4)	50(2)
C(123)	3980(5)	4967(4)	3783(4)	51(2)
C(124)	4312(4)	5500(5)	3895(4)	54(3)
C(125)	4223(4)	5944(4)	3452(6)	62(3)
C(126)	3820(4)	5872(4)	2897(4)	41(2)
C(131)	3379(5)	5456(4)	1424(4)	49(2)
C(132)	2987(6)	5514(4)	809(5)	71(4)
C(133)	3277(7)	5617(5)	267(8)	102(5)
C(134)	3883(8)	5626(5)	264(5)	90(4)
C(135)	4314(6)	5547(5)	795(6)	81(3)
C(136)	4027(5)	5467(4)	1379(4)	60(3)
C(141)	2420(4)	5779(4)	2186(5)	50(2)
C(142)	2305(4)	6378(5)	1870(5)	62(3)
C(143)	1788(6)	6724(5)	2085(6)	80(4)
C(144)	1465(5)	6507(11)	2536(10)	158(10)
C(145)	1492(11)	6049(8)	2891(8)	177(12)
C(146)	2020(5)	5613(6)	2686(6)	82(5)
C(151)	-504(12)	4075(8)	5116(8)	142(6)
C(152)	-1008(6)	3746(8)	4854(11)	111(5)
C(153)	-958(9)	3440(6)	4307(10)	116(6)
C(154)	-431(13)	3447(9)	4011(8)	137(8)
C(155)	43(9)	3771(12)	4243(14)	181(13)
C(156)	70(11)	4120(10)	4804(15)	188(14)
C(161)	-1362(6)	1115(7)	5499(8)	134(6)
C(162)	-1099(7)	1566(8)	5130(8)	138(6)
C(163)	-840(7)	2064(7)	5302(8)	134(5)
C(164)	-777(6)	2235(7)	5955(7)	123(5)
C(165)	-1047(5)	1798(5)	6392(6)	89(3)
C(166)	-1320(5)	1266(6)	6161(6)	96(4)
C(171)	633(6)	3345(6)	-1555(6)	103(4)

Table S-5.

C(173)	1115 (5)	4332 (5)	-1339 (5)	89 (3)
C(174)	584 (5)	4523 (5)	-1032 (5)	80 (3)
C(175)	87 (5)	4127 (5)	-994 (5)	81 (3)
C(176)	110 (5)	3541 (5)	-1265 (5)	93 (4)
F(52)	2845 (2)	3314 (2)	6819 (2)	42 (1)
F(53)	3346 (2)	2718 (2)	7845 (2)	57 (1)
F(54)	3469 (2)	3278 (2)	9032 (2)	64 (1)
F(55)	3024 (2)	4465 (2)	9153 (2)	69 (2)
F(56)	2520 (2)	5088 (2)	8118 (2)	48 (1)
F(62)	3635 (2)	4208 (2)	6409 (2)	47 (1)
F(63)	3879 (3)	3694 (2)	5306 (2)	73 (2)
F(64)	2942 (2)	3586 (3)	4296 (3)	81 (2)
F(65)	1773 (2)	4080 (2)	4422 (3)	74 (2)
F(66)	1494 (2)	4582 (2)	5531 (2)	54 (1)
F(72)	1650 (2)	5846 (2)	7177 (2)	51 (1)
F(73)	442 (2)	5834 (2)	7405 (2)	65 (1)
F(74)	-266 (2)	4780 (2)	7252 (2)	74 (2)
F(75)	284 (2)	3706 (2)	6838 (2)	70 (1)
F(76)	1505 (2)	3693 (2)	6636 (2)	49 (1)
F(122)	3280 (2)	4332 (2)	3176 (2)	73 (2)
F(123)	4051 (3)	4503 (3)	4237 (3)	84 (2)
F(124)	4710 (3)	5576 (3)	4443 (3)	79 (2)
F(125)	4560 (3)	6497 (3)	3534 (3)	93 (2)
F(126)	3765 (2)	6354 (2)	2472 (2)	60 (1)
F(132)	2362 (3)	5521 (2)	778 (3)	72 (2)
F(133)	2899 (3)	5712 (3)	-314 (3)	105 (2)
F(134)	4210 (3)	5717 (3)	-309 (4)	128 (2)
F(135)	4962 (3)	5573 (3)	827 (3)	109 (2)
F(136)	4447 (2)	5392 (2)	1919 (3)	70 (2)
F(142)	2666 (3)	6581 (2)	1438 (3)	71 (2)
F(143)	1711 (3)	7284 (3)	1726 (3)	115 (2)
F(144)	961 (4)	6979 (4)	2655 (4)	135 (3)
F(145)	1223 (3)	5880 (4)	3376 (4)	120 (2)
F(146)	2117 (3)	5123 (3)	3043 (3)	85 (2)

Zr(1)-N(1)	2.112(5)	Zr(1)-C(24)	2.490(8)
Zr(1)-C(14)	2.497(7)	Zr(1)-C(11)	2.503(7)
Zr(1)-C(21)	2.503(7)	Zr(1)-C(22)	2.508(8)
Zr(1)-C(13)	2.514(8)	Zr(1)-C(23)	2.514(7)
Zr(1)-C(25)	2.517(8)	Zr(1)-C(12)	2.526(7)
Zr(1)-C(15)	2.541(7)	Zr(1)-C(31)	2.638(7)
Zr(2)-N(2)	2.126(6)	Zr(2)-C(94)	2.494(8)
Zr(2)-C(92)	2.499(8)	Zr(2)-C(91)	2.504(8)
Zr(2)-C(93)	2.511(8)	Zr(2)-C(95)	2.517(8)
Zr(2)-C(84)	2.519(9)	Zr(2)-C(83)	2.529(8)
Zr(2)-C(81)	2.525(9)	Zr(2)-C(85)	2.533(9)
Zr(2)-C(82)	2.533(8)	Zr(2)-C(101)	2.643(8)
B(1)-C(61)	1.644(11)	B(1)-C(51)	1.667(11)
B(1)-C(49)	1.668(11)	B(1)-C(71)	1.686(11)
B(2)-C(131)	1.637(12)	B(2)-C(121)	1.644(12)
B(2)-C(119)	1.656(11)	B(2)-C(141)	1.679(12)
N(1)-C(31)	1.384(8)	N(1)-C(47)	1.466(8)
N(2)-C(101)	1.359(8)	N(2)-C(117)	1.484(8)
C(11)-C(12)	1.402(10)	C(11)-C(15)	1.400(10)
C(12)-C(13)	1.364(10)	C(13)-C(14)	1.406(11)
C(14)-C(15)	1.397(10)	C(21)-C(25)	1.381(11)
C(21)-C(22)	1.410(10)	C(22)-C(23)	1.401(11)
C(23)-C(24)	1.382(11)	C(24)-C(25)	1.409(11)
C(31)-C(32)	1.396(10)	C(31)-C(36)	1.409(10)
C(32)-C(33)	1.404(11)	C(33)-C(34)	1.352(13)
C(34)-C(35)	1.387(13)	C(35)-C(36)	1.389(11)
C(41)-C(46)	1.372(10)	C(41)-C(42)	1.380(10)
C(41)-C(47)	1.505(9)	C(42)-C(43)	1.382(12)
C(43)-C(44)	1.378(13)	C(44)-C(45)	1.344(13)
C(45)-C(46)	1.393(11)	C(47)-C(48)	1.517(9)
C(48)-C(49)	1.521(9)	C(51)-C(52)	1.360(9)
C(51)-C(56)	1.375(10)	C(52)-F(52)	1.367(7)
C(52)-C(53)	1.382(10)	C(53)-C(54)	1.329(10)
C(53)-F(53)	1.379(8)	C(54)-F(54)	1.349(8)
C(54)-C(55)	1.355(10)	C(55)-C(56)	1.367(10)
C(55)-F(55)	1.375(8)	C(56)-F(56)	1.358(8)
C(61)-C(66)	1.387(9)	C(61)-C(62)	1.386(10)
C(62)-F(62)	1.362(8)	C(62)-C(63)	1.364(11)
C(63)-C(64)	1.333(12)	C(63)-F(63)	1.347(9)
C(64)-C(65)	1.347(12)	C(64)-F(64)	1.392(9)
C(65)-C(66)	1.366(11)	C(65)-F(65)	1.370(8)
C(66)-F(66)	1.355(8)	C(71)-C(72)	1.335(10)
C(71)-C(76)	1.389(10)	C(72)-F(72)	1.368(8)
C(72)-C(73)	1.384(10)	C(73)-C(74)	1.333(11)
C(73)-F(73)	1.372(8)	C(74)-C(75)	1.348(11)
C(74)-F(74)	1.369(8)	C(75)-F(75)	1.357(8)
C(75)-C(76)	1.365(10)	C(76)-F(76)	1.342(8)
C(81)-C(85)	1.376(12)	C(81)-C(82)	1.388(11)
C(82)-C(83)	1.394(11)	C(83)-C(84)	1.414(13)
C(84)-C(85)	1.385(13)	C(91)-C(92)	1.391(11)
C(91)-C(95)	1.412(12)	C(92)-C(93)	1.398(11)
C(93)-C(94)	1.389(12)	C(94)-C(95)	1.408(12)
C(101)-C(102)	1.405(10)	C(101)-C(106)	1.422(10)
C(102)-C(103)	1.424(11)	C(103)-C(104)	1.344(12)
C(104)-C(105)	1.398(12)	C(105)-C(106)	1.371(10)
C(111)-C(116)	1.370(10)	C(111)-C(112)	1.396(10)

Table S-6.

C(113)-C(114)	1.354(11)	C(114)-C(115)	1.372(11)
C(115)-C(116)	1.397(11)	C(117)-C(118)	1.519(9)
C(118)-C(119)	1.546(9)	C(121)-C(122)	1.361(10)
C(121)-C(126)	1.367(10)	C(122)-F(122)	1.355(8)
C(122)-C(123)	1.361(11)	C(123)-C(124)	1.343(11)
C(123)-F(123)	1.362(9)	C(124)-C(125)	1.320(12)
C(124)-F(124)	1.350(8)	C(125)-C(126)	1.367(12)
C(125)-F(125)	1.378(9)	C(126)-F(126)	1.350(8)
C(131)-C(136)	1.373(11)	C(131)-C(132)	1.452(13)
C(132)-F(132)	1.308(12)	C(132)-C(133)	1.342(17)
C(133)-C(134)	1.272(15)	C(133)-F(133)	1.389(13)
C(134)-C(135)	1.364(15)	C(134)-F(134)	1.438(11)
C(135)-F(135)	1.356(11)	C(135)-C(136)	1.409(13)
C(136)-F(136)	1.364(10)	C(141)-C(146)	1.437(15)
C(141)-C(142)	1.444(12)	C(142)-F(142)	1.298(11)
C(142)-C(143)	1.419(14)	C(143)-C(144)	1.29(2)
C(143)-F(143)	1.409(11)	C(144)-C(145)	1.22(3)
C(144)-F(144)	1.498(16)	C(145)-F(145)	1.251(18)
C(145)-C(146)	1.54(3)	C(146)-F(146)	1.286(13)
C(151)-C(152)	1.339(19)	C(151)-C(156)	1.42(3)
C(152)-C(153)	1.318(18)	C(153)-C(154)	1.315(19)
C(154)-C(155)	1.27(2)	C(155)-C(156)	1.37(3)
C(161)-C(162)	1.377(18)	C(161)-C(166)	1.400(16)
C(162)-C(163)	1.231(17)	C(163)-C(164)	1.392(16)
C(164)-C(165)	1.451(14)	C(165)-C(166)	1.340(13)
C(171)-C(172)	1.348(14)	C(171)-C(176)	1.365(14)
C(172)-C(173)	1.335(13)	C(173)-C(174)	1.395(12)
C(174)-C(175)	1.351(12)	C(175)-C(176)	1.373(13)
N(1)-Zr(1)-C(24)	130.4(3)	N(1)-Zr(1)-C(14)	127.7(3)
C(24)-Zr(1)-C(14)	101.8(3)	N(1)-Zr(1)-C(11)	113.6(2)
C(24)-Zr(1)-C(11)	91.4(3)	C(14)-Zr(1)-C(11)	53.7(3)
N(1)-Zr(1)-C(21)	89.4(2)	C(24)-Zr(1)-C(21)	53.5(3)
C(14)-Zr(1)-C(21)	131.9(3)	C(11)-Zr(1)-C(21)	144.2(3)
N(1)-Zr(1)-C(22)	113.4(3)	C(24)-Zr(1)-C(22)	53.2(3)
C(14)-Zr(1)-C(22)	99.4(3)	C(11)-Zr(1)-C(22)	132.7(3)
C(21)-Zr(1)-C(22)	32.7(2)	N(1)-Zr(1)-C(13)	96.1(2)
C(24)-Zr(1)-C(13)	131.8(3)	C(14)-Zr(1)-C(13)	32.6(2)
C(11)-Zr(1)-C(13)	53.3(3)	C(21)-Zr(1)-C(13)	155.1(3)
C(22)-Zr(1)-C(13)	125.3(3)	N(1)-Zr(1)-C(23)	143.1(3)
C(24)-Zr(1)-C(23)	32.1(3)	C(14)-Zr(1)-C(23)	83.0(3)
C(11)-Zr(1)-C(23)	100.9(3)	C(21)-Zr(1)-C(23)	53.9(3)
C(22)-Zr(1)-C(23)	32.4(2)	C(13)-Zr(1)-C(23)	115.4(3)
N(1)-Zr(1)-C(25)	98.3(3)	C(24)-Zr(1)-C(25)	32.7(3)
C(14)-Zr(1)-C(25)	133.9(3)	C(11)-Zr(1)-C(25)	114.2(3)
C(21)-Zr(1)-C(25)	31.9(2)	C(22)-Zr(1)-C(25)	53.5(3)
C(13)-Zr(1)-C(25)	164.2(3)	C(23)-Zr(1)-C(25)	53.8(3)
N(1)-Zr(1)-C(12)	89.1(2)	C(24)-Zr(1)-C(12)	123.7(3)
C(14)-Zr(1)-C(12)	53.1(3)	C(11)-Zr(1)-C(12)	32.4(2)
C(21)-Zr(1)-C(12)	173.5(3)	C(22)-Zr(1)-C(12)	152.4(3)
C(13)-Zr(1)-C(12)	31.4(2)	C(23)-Zr(1)-C(12)	127.7(3)
C(25)-Zr(1)-C(12)	142.2(3)	N(1)-Zr(1)-C(15)	142.1(2)
C(24)-Zr(1)-C(15)	79.2(3)	C(14)-Zr(1)-C(15)	32.2(2)
C(11)-Zr(1)-C(15)	32.2(2)	C(21)-Zr(1)-C(15)	128.0(3)
C(22)-Zr(1)-C(15)	103.5(3)	C(13)-Zr(1)-C(15)	53.2(3)
C(23)-Zr(1)-C(15)	74.8(3)	C(25)-Zr(1)-C(15)	111.0(3)
C(12)-Zr(1)-C(15)	52.9(2)	N(1)-Zr(1)-C(31)	31.5(2)
C(24)-Zr(1)-C(31)	102.6(3)	C(14)-Zr(1)-C(31)	148.1(3)

Table S-6.

C(22)-Zr(1)-C(31)	111.6(3)	C(13)-Zr(1)-C(31)	116.7(3)
C(23)-Zr(1)-C(31)	127.7(3)	C(25)-Zr(1)-C(31)	74.2(3)
C(12)-Zr(1)-C(31)	96.0(3)	C(15)-Zr(1)-C(31)	137.2(3)
N(2)-Zr(2)-C(94)	129.0(3)	N(2)-Zr(2)-C(92)	89.1(3)
C(94)-Zr(2)-C(92)	53.8(3)	N(2)-Zr(2)-C(91)	113.1(3)
C(94)-Zr(2)-C(91)	54.1(3)	C(92)-Zr(2)-C(91)	32.3(3)
N(2)-Zr(2)-C(93)	97.6(3)	C(94)-Zr(2)-C(93)	32.2(3)
C(92)-Zr(2)-C(93)	32.4(2)	C(91)-Zr(2)-C(93)	53.6(3)
N(2)-Zr(2)-C(95)	142.7(3)	C(94)-Zr(2)-C(95)	32.6(3)
C(92)-Zr(2)-C(95)	53.7(3)	C(91)-Zr(2)-C(95)	32.7(3)
C(93)-Zr(2)-C(95)	53.5(3)	N(2)-Zr(2)-C(84)	129.9(3)
C(94)-Zr(2)-C(84)	100.9(4)	C(92)-Zr(2)-C(84)	129.8(3)
C(91)-Zr(2)-C(84)	97.6(3)	C(93)-Zr(2)-C(84)	132.3(4)
C(95)-Zr(2)-C(84)	81.4(4)	N(2)-Zr(2)-C(83)	98.2(3)
C(94)-Zr(2)-C(83)	131.3(3)	C(92)-Zr(2)-C(83)	152.3(3)
C(91)-Zr(2)-C(83)	122.8(4)	C(93)-Zr(2)-C(83)	163.5(3)
C(95)-Zr(2)-C(83)	113.7(4)	C(84)-Zr(2)-C(83)	32.5(3)
N(2)-Zr(2)-C(81)	114.1(3)	C(94)-Zr(2)-C(81)	92.0(3)
C(92)-Zr(2)-C(81)	145.6(3)	C(91)-Zr(2)-C(81)	132.7(3)
C(93)-Zr(2)-C(81)	115.5(3)	C(95)-Zr(2)-C(81)	100.8(3)
C(84)-Zr(2)-C(81)	53.1(3)	C(83)-Zr(2)-C(81)	53.0(3)
N(2)-Zr(2)-C(85)	142.6(3)	C(94)-Zr(2)-C(85)	79.5(4)
C(92)-Zr(2)-C(85)	127.9(3)	C(91)-Zr(2)-C(85)	103.4(3)
C(93)-Zr(2)-C(85)	111.0(3)	C(95)-Zr(2)-C(85)	74.7(3)
C(84)-Zr(2)-C(85)	31.8(3)	C(83)-Zr(2)-C(85)	52.7(3)
C(81)-Zr(2)-C(85)	31.6(3)	N(2)-Zr(2)-C(82)	90.3(2)
C(94)-Zr(2)-C(82)	123.9(3)	C(92)-Zr(2)-C(82)	175.6(3)
C(91)-Zr(2)-C(82)	150.8(3)	C(93)-Zr(2)-C(82)	143.6(3)
C(95)-Zr(2)-C(82)	127.0(3)	C(84)-Zr(2)-C(82)	53.3(3)
C(83)-Zr(2)-C(82)	32.0(3)	C(81)-Zr(2)-C(82)	31.9(3)
C(85)-Zr(2)-C(82)	52.3(3)	N(2)-Zr(2)-C(101)	30.8(2)
C(94)-Zr(2)-C(101)	102.2(3)	C(92)-Zr(2)-C(101)	80.7(3)
C(91)-Zr(2)-C(101)	112.4(3)	C(93)-Zr(2)-C(101)	74.7(3)
C(95)-Zr(2)-C(101)	128.0(3)	C(84)-Zr(2)-C(101)	149.2(3)
C(83)-Zr(2)-C(101)	118.1(3)	C(81)-Zr(2)-C(101)	105.9(3)
C(85)-Zr(2)-C(101)	136.7(3)	C(82)-Zr(2)-C(101)	96.6(3)
C(61)-B(1)-C(51)	112.9(6)	C(61)-B(1)-C(49)	102.6(6)
C(51)-B(1)-C(49)	112.2(6)	C(61)-B(1)-C(71)	112.6(6)
C(51)-B(1)-C(71)	102.3(6)	C(49)-B(1)-C(71)	114.7(6)
C(131)-B(2)-C(121)	113.6(7)	C(131)-B(2)-C(119)	103.4(6)
C(121)-B(2)-C(119)	113.8(7)	C(131)-B(2)-C(141)	112.5(7)
C(121)-B(2)-C(141)	103.3(6)	C(119)-B(2)-C(141)	110.5(7)
C(31)-N(1)-C(47)	119.8(6)	C(31)-N(1)-Zr(1)	95.7(4)
C(47)-N(1)-Zr(1)	132.6(4)	C(101)-N(2)-C(117)	119.1(6)
C(101)-N(2)-Zr(2)	96.2(4)	C(117)-N(2)-Zr(2)	130.8(4)
C(12)-C(11)-C(15)	107.4(7)	C(12)-C(11)-Zr(1)	74.7(4)
C(15)-C(11)-Zr(1)	75.4(4)	C(13)-C(12)-C(11)	108.8(7)
C(13)-C(12)-Zr(1)	73.8(5)	C(11)-C(12)-Zr(1)	72.9(4)
C(12)-C(13)-C(14)	108.2(7)	C(12)-C(13)-Zr(1)	74.8(5)
C(14)-C(13)-Zr(1)	73.0(4)	C(15)-C(14)-C(13)	107.7(7)
C(15)-C(14)-Zr(1)	75.6(5)	C(13)-C(14)-Zr(1)	74.4(4)
C(14)-C(15)-C(11)	107.6(7)	C(14)-C(15)-Zr(1)	72.2(4)
C(11)-C(15)-Zr(1)	72.4(4)	C(25)-C(21)-C(22)	108.2(8)
C(25)-C(21)-Zr(1)	74.6(5)	C(22)-C(21)-Zr(1)	73.9(4)
C(23)-C(22)-C(21)	108.1(8)	C(23)-C(22)-Zr(1)	74.0(5)
C(21)-C(22)-Zr(1)	73.5(4)	C(24)-C(23)-C(22)	107.1(8)
C(24)-C(23)-Zr(1)	73.0(5)	C(22)-C(23)-Zr(1)	73.6(4)
C(23)-C(24)-C(25)	109.3(8)	C(23)-C(24)-Zr(1)	74.9(4)

Table S-6.

C(21)-C(25)-Zr(1)	73.5(4)	C(24)-C(25)-Zr(1)	72.6(5)
N(1)-C(31)-C(32)	116.2(7)	N(1)-C(31)-C(36)	125.1(8)
C(32)-C(31)-C(36)	118.4(7)	N(1)-C(31)-Zr(1)	52.8(3)
C(32)-C(31)-Zr(1)	78.3(5)	C(36)-C(31)-Zr(1)	136.6(6)
C(31)-C(32)-C(33)	120.5(8)	C(31)-C(32)-Zr(1)	71.6(4)
C(33)-C(32)-Zr(1)	133.3(6)	C(34)-C(33)-C(32)	120.9(9)
C(33)-C(34)-C(35)	118.8(9)	C(36)-C(35)-C(34)	122.3(9)
C(35)-C(36)-C(31)	118.7(8)	C(46)-C(41)-C(42)	117.5(8)
C(46)-C(41)-C(47)	122.2(7)	C(42)-C(41)-C(47)	120.2(7)
C(41)-C(42)-C(43)	121.3(9)	C(44)-C(43)-C(42)	120.1(9)
C(45)-C(44)-C(43)	119.1(10)	C(44)-C(45)-C(46)	121.0(10)
C(41)-C(46)-C(45)	120.9(9)	N(1)-C(47)-C(41)	112.4(6)
N(1)-C(47)-C(48)	106.9(6)	C(41)-C(47)-C(48)	112.9(6)
C(47)-C(48)-C(49)	111.4(6)	C(48)-C(49)-B(1)	116.2(6)
C(52)-C(51)-C(56)	112.3(7)	C(52)-C(51)-B(1)	127.5(6)
C(56)-C(51)-B(1)	120.2(6)	C(51)-C(52)-F(52)	121.9(6)
C(51)-C(52)-C(53)	124.3(7)	F(52)-C(52)-C(53)	113.9(7)
C(54)-C(53)-C(52)	120.9(7)	C(54)-C(53)-F(53)	119.9(8)
C(52)-C(53)-F(53)	119.2(7)	C(53)-C(54)-F(54)	121.4(8)
C(53)-C(54)-C(55)	117.4(7)	F(54)-C(54)-C(55)	121.2(8)
C(54)-C(55)-C(56)	120.7(7)	C(54)-C(55)-F(55)	118.9(7)
C(56)-C(55)-F(55)	120.4(7)	F(56)-C(56)-C(55)	115.8(7)
F(56)-C(56)-C(51)	120.0(7)	C(55)-C(56)-C(51)	124.2(7)
C(66)-C(61)-C(62)	112.7(7)	C(66)-C(61)-B(1)	126.9(7)
C(62)-C(61)-B(1)	120.2(7)	F(62)-C(62)-C(63)	114.7(7)
F(62)-C(62)-C(61)	120.2(7)	C(63)-C(62)-C(61)	125.1(8)
C(64)-C(63)-F(63)	120.9(9)	C(64)-C(63)-C(62)	118.3(8)
F(63)-C(63)-C(62)	120.8(8)	C(63)-C(64)-C(65)	120.9(8)
C(63)-C(64)-F(64)	120.7(10)	C(65)-C(64)-F(64)	118.4(10)
C(64)-C(65)-C(66)	119.9(8)	C(64)-C(65)-F(65)	120.5(9)
C(66)-C(65)-F(65)	119.6(9)	F(66)-C(66)-C(65)	116.4(7)
F(66)-C(66)-C(61)	120.7(7)	C(65)-C(66)-C(61)	123.0(8)
C(72)-C(71)-C(76)	114.4(7)	C(72)-C(71)-B(1)	127.2(7)
C(76)-C(71)-B(1)	118.3(7)	C(71)-C(72)-F(72)	122.4(7)
C(71)-C(72)-C(73)	123.9(7)	F(72)-C(72)-C(73)	113.7(7)
C(74)-C(73)-F(73)	120.5(8)	C(74)-C(73)-C(72)	119.5(8)
F(73)-C(73)-C(72)	120.0(8)	C(73)-C(74)-C(75)	119.8(7)
C(73)-C(74)-F(74)	119.2(8)	C(75)-C(74)-F(74)	120.9(8)
C(74)-C(75)-F(75)	120.6(8)	C(74)-C(75)-C(76)	119.4(7)
F(75)-C(75)-C(76)	120.0(7)	F(76)-C(76)-C(75)	116.1(7)
F(76)-C(76)-C(71)	120.8(7)	C(75)-C(76)-C(71)	123.0(7)
C(85)-C(81)-C(82)	107.8(9)	C(85)-C(81)-Zr(2)	74.5(5)
C(82)-C(81)-Zr(2)	74.4(5)	C(81)-C(82)-C(83)	108.3(8)
C(81)-C(82)-Zr(2)	73.7(5)	C(83)-C(82)-Zr(2)	73.9(5)
C(82)-C(83)-C(84)	107.5(9)	C(82)-C(83)-Zr(2)	74.2(5)
C(84)-C(83)-Zr(2)	73.3(5)	C(85)-C(84)-C(83)	106.9(10)
C(85)-C(84)-Zr(2)	74.7(6)	C(83)-C(84)-Zr(2)	74.1(5)
C(81)-C(85)-C(84)	109.5(10)	C(81)-C(85)-Zr(2)	73.9(5)
C(84)-C(85)-Zr(2)	73.5(5)	C(92)-C(91)-C(95)	107.9(9)
C(92)-C(91)-Zr(2)	73.7(5)	C(95)-C(91)-Zr(2)	74.2(5)
C(91)-C(92)-C(93)	108.3(9)	C(91)-C(92)-Zr(2)	74.0(5)
C(93)-C(92)-Zr(2)	74.3(5)	C(94)-C(93)-C(92)	108.4(9)
C(94)-C(93)-Zr(2)	73.2(5)	C(92)-C(93)-Zr(2)	73.3(5)
C(93)-C(94)-C(95)	108.0(9)	C(93)-C(94)-Zr(2)	74.5(5)
C(95)-C(94)-Zr(2)	74.6(5)	C(94)-C(95)-C(91)	107.4(9)
C(94)-C(95)-Zr(2)	72.8(5)	C(91)-C(95)-Zr(2)	73.1(5)
N(2)-C(101)-C(102)	115.5(7)	N(2)-C(101)-C(106)	127.2(7)
C(102)-C(101)-C(106)	116.9(7)	N(2)-C(101)-Zr(2)	53.1(3)

Table S-6.	C(101)-C(102)-C(103)	121.5(8)	C(101)-C(102)-Zr(2)	73.2(4)
	C(103)-C(102)-Zr(2)	132.8(6)	C(104)-C(103)-C(102)	120.0(9)
	C(103)-C(104)-C(105)	118.7(9)	C(106)-C(105)-C(104)	123.2(9)
	C(105)-C(106)-C(101)	119.3(8)	C(116)-C(111)-C(112)	118.9(7)
	C(116)-C(111)-C(117)	119.9(7)	C(112)-C(111)-C(117)	121.0(7)
	C(113)-C(112)-C(111)	120.0(8)	C(114)-C(113)-C(112)	121.7(9)
	C(113)-C(114)-C(115)	119.5(8)	C(114)-C(115)-C(116)	119.8(8)
	C(111)-C(116)-C(115)	120.0(8)	N(2)-C(117)-C(111)	112.8(6)
	N(2)-C(117)-C(118)	104.6(6)	C(111)-C(117)-C(118)	111.6(6)
	C(117)-C(118)-C(119)	112.1(6)	C(118)-C(119)-B(2)	113.3(6)
	C(122)-C(121)-C(126)	112.6(7)	C(122)-C(121)-B(2)	127.8(7)
	C(126)-C(121)-B(2)	119.6(7)	F(122)-C(122)-C(121)	121.0(7)
	F(122)-C(122)-C(123)	114.4(8)	C(121)-C(122)-C(123)	124.6(8)
	C(124)-C(123)-F(123)	118.4(8)	C(124)-C(123)-C(122)	120.6(8)
	F(123)-C(123)-C(122)	121.0(8)	C(125)-C(124)-C(123)	116.9(8)
	C(125)-C(124)-F(124)	122.1(9)	C(123)-C(124)-F(124)	121.0(9)
	C(124)-C(125)-C(126)	122.5(8)	C(124)-C(125)-F(125)	119.5(9)
	C(126)-C(125)-F(125)	117.9(9)	F(126)-C(126)-C(125)	117.8(8)
	F(126)-C(126)-C(121)	119.3(8)	C(125)-C(126)-C(121)	122.8(8)
	C(136)-C(131)-C(132)	114.9(8)	C(136)-C(131)-B(2)	126.6(8)
	C(132)-C(131)-B(2)	117.8(9)	F(132)-C(132)-C(133)	119.3(11)
	F(132)-C(132)-C(131)	121.6(8)	C(133)-C(132)-C(131)	118.8(11)
	C(134)-C(133)-C(132)	122.6(14)	C(134)-C(133)-F(133)	118.8(16)
	C(132)-C(133)-F(133)	118.6(12)	C(133)-C(134)-C(135)	125.4(11)
	C(133)-C(134)-F(134)	124.2(15)	C(135)-C(134)-F(134)	110.4(13)
	F(135)-C(135)-C(134)	128.2(11)	F(135)-C(135)-C(136)	118.1(10)
	C(134)-C(135)-C(136)	113.6(11)	C(131)-C(136)-F(136)	120.6(8)
	C(131)-C(136)-C(135)	124.5(10)	F(136)-C(136)-C(135)	114.9(9)
	C(146)-C(141)-C(142)	117.4(9)	C(146)-C(141)-B(2)	116.3(9)
	C(142)-C(141)-B(2)	126.1(8)	F(142)-C(142)-C(143)	123.7(10)
	F(142)-C(142)-C(141)	121.5(8)	C(143)-C(142)-C(141)	114.8(10)
	C(144)-C(143)-F(143)	130.1(16)	C(144)-C(143)-C(142)	120.6(13)
	F(143)-C(143)-C(142)	109.3(12)	C(145)-C(144)-C(143)	136(2)
	C(145)-C(144)-F(144)	115.7(19)	C(143)-C(144)-F(144)	108(2)
	C(144)-C(145)-F(145)	136(3)	C(144)-C(145)-C(146)	108.3(19)
	F(145)-C(145)-C(146)	116.0(14)	F(146)-C(146)-C(141)	122.9(9)
	F(146)-C(146)-C(145)	114.4(12)	C(141)-C(146)-C(145)	122.3(13)
	C(152)-C(151)-C(156)	121.4(17)	C(153)-C(152)-C(151)	118.8(16)
	C(152)-C(153)-C(154)	122.2(17)	C(155)-C(154)-C(153)	120(2)
	C(154)-C(155)-C(156)	126(3)	C(155)-C(156)-C(151)	112.2(17)
	C(162)-C(161)-C(166)	112.9(14)	C(163)-C(162)-C(161)	129.3(18)
	C(162)-C(163)-C(164)	120.3(18)	C(163)-C(164)-C(165)	115.4(14)
	C(166)-C(165)-C(164)	120.2(12)	C(165)-C(166)-C(161)	121.9(13)
	C(172)-C(171)-C(176)	117.6(13)	C(173)-C(172)-C(171)	123.4(13)
	C(172)-C(173)-C(174)	118.5(11)	C(175)-C(174)-C(173)	119.9(11)
	C(174)-C(175)-C(176)	119.3(11)	C(171)-C(176)-C(175)	121.4(12)

Symmetry transformations used to generate equivalent atoms:

$\text{Cp}_2\text{Zr}\{\text{Ph}-\text{N}[\text{C}(\text{H})(\text{Ph})\text{C}(\text{H})_2\text{B}(\text{ArF})_3]\}$.

The anisotropic displacement factor $\exp -2\pi^2 [(h a^*)^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Zr(1)	32(1)	32(1)	27(1)	0(1)	2(1)	1(1)
Zr(2)	38(1)	36(1)	43(1)	2(1)	7(1)	7(1)
B(1)	34(5)	33(6)	31(5)	-5(4)	5(4)	-5(4)
B(2)	62(7)	26(6)	43(6)	-7(5)	8(5)	7(5)
N(1)	25(3)	34(4)	28(3)	0(3)	5(3)	-8(3)
N(2)	31(4)	21(3)	34(4)	-6(3)	3(3)	-1(3)
C(11)	60(6)	30(5)	35(5)	-12(4)	6(5)	-4(4)
C(12)	53(6)	41(6)	31(5)	-7(4)	6(4)	15(4)
C(13)	38(5)	49(6)	45(6)	-14(5)	9(4)	-8(4)
C(14)	79(7)	38(6)	31(5)	-6(4)	31(5)	-10(5)
C(15)	56(6)	35(5)	32(5)	-10(4)	-2(4)	1(4)
C(21)	40(5)	43(6)	41(5)	-13(4)	3(4)	11(4)
C(22)	42(5)	44(6)	54(6)	12(5)	10(5)	13(4)
C(23)	41(5)	68(7)	37(5)	11(5)	-8(4)	19(5)
C(24)	30(5)	59(6)	72(7)	-14(5)	-14(5)	-3(4)
C(25)	27(5)	62(7)	57(6)	8(5)	2(4)	6(4)
C(31)	34(5)	54(6)	30(5)	13(4)	8(4)	-3(4)
C(32)	46(6)	56(6)	36(5)	-1(5)	7(4)	-7(4)
C(33)	57(7)	76(8)	68(7)	-3(6)	6(6)	-36(6)
C(34)	60(7)	101(9)	74(8)	19(7)	-1(6)	-41(7)
C(35)	48(6)	100(9)	56(7)	21(6)	24(5)	-4(6)
C(36)	40(5)	64(7)	46(5)	-3(5)	11(4)	2(4)
C(41)	37(5)	30(5)	34(5)	8(4)	-4(4)	-11(3)
C(42)	60(6)	73(7)	26(5)	-9(5)	2(4)	4(5)
C(43)	55(6)	143(11)	18(5)	1(6)	-8(4)	6(7)
C(44)	41(6)	127(11)	66(8)	57(8)	-1(6)	-3(7)
C(45)	75(8)	61(7)	72(8)	29(6)	10(6)	4(5)
C(46)	68(6)	49(6)	40(5)	8(5)	-4(5)	2(5)
C(47)	32(4)	29(5)	33(4)	0(4)	4(4)	7(3)
C(48)	28(4)	41(5)	30(4)	6(4)	-5(4)	-6(4)
C(49)	39(5)	40(5)	32(5)	-3(4)	0(4)	0(4)
C(51)	30(4)	22(4)	32(5)	-3(4)	10(4)	0(3)
C(52)	38(4)	34(5)	25(4)	-1(4)	2(3)	-5(4)
C(53)	45(5)	33(5)	43(5)	-12(4)	11(4)	12(4)
C(54)	57(6)	53(6)	27(5)	17(5)	-6(4)	12(5)
C(55)	63(6)	40(5)	15(4)	-18(4)	10(4)	-6(4)
C(56)	49(5)	23(5)	45(5)	-2(4)	20(4)	13(4)
C(61)	43(5)	29(5)	29(4)	3(4)	2(4)	-8(4)
C(62)	45(5)	35(5)	29(5)	6(4)	10(4)	-2(4)
C(63)	48(6)	70(7)	42(6)	13(5)	16(5)	6(5)
C(64)	102(9)	47(6)	39(6)	-13(5)	40(6)	-8(6)
C(65)	58(6)	61(7)	43(6)	6(5)	-21(5)	-8(5)
C(66)	43(5)	44(5)	29(5)	-3(4)	-1(4)	7(4)
C(71)	33(5)	33(5)	38(5)	0(4)	7(4)	0(4)
C(72)	32(5)	38(5)	36(5)	-4(4)	-3(4)	-10(4)
C(73)	44(6)	41(6)	72(7)	-16(5)	9(5)	12(4)

Table S-7.

C(75)	41(5)	31(5)	75(7)	-13(5)	11(5)	-17(4)
C(76)	40(5)	29(5)	39(5)	-9(4)	4(4)	4(4)
C(81)	63(7)	39(6)	78(7)	4(5)	25(6)	4(5)
C(82)	56(6)	47(6)	59(6)	23(5)	14(5)	17(5)
C(83)	67(7)	82(8)	35(5)	8(5)	11(5)	-21(6)
C(84)	105(9)	60(8)	63(7)	-8(6)	45(7)	10(7)
C(85)	61(7)	79(8)	86(8)	19(7)	53(6)	17(6)
C(91)	58(7)	42(6)	76(7)	11(5)	-2(6)	19(5)
C(92)	45(5)	46(6)	51(6)	16(5)	-12(5)	4(5)
C(93)	47(6)	44(6)	54(6)	-2(5)	-12(5)	6(4)
C(94)	35(6)	66(8)	101(9)	15(7)	-5(6)	3(5)
C(95)	58(7)	71(8)	84(8)	17(7)	5(6)	39(6)
C(101)	35(5)	35(5)	31(5)	-2(4)	-1(4)	6(4)
C(102)	46(5)	26(5)	52(5)	-2(4)	7(4)	2(4)
C(103)	55(6)	42(6)	72(7)	0(5)	-7(6)	-11(4)
C(104)	73(8)	50(7)	79(8)	-17(6)	-26(6)	-10(5)
C(105)	74(7)	63(7)	37(5)	-13(5)	-15(5)	-6(5)
C(106)	50(6)	56(6)	38(5)	-10(5)	-8(4)	-2(4)
C(111)	31(4)	32(5)	25(4)	-3(4)	-6(4)	-1(4)
C(112)	28(5)	42(5)	60(6)	2(5)	11(4)	-3(4)
C(113)	44(6)	36(6)	74(7)	-9(5)	-8(5)	1(4)
C(114)	47(6)	61(7)	60(6)	-9(5)	5(5)	13(5)
C(115)	47(6)	93(8)	25(5)	4(5)	7(4)	-10(5)
C(116)	35(5)	57(6)	34(5)	11(4)	-1(4)	1(4)
C(117)	42(5)	23(4)	26(4)	-1(4)	-4(4)	4(4)
C(118)	38(5)	35(5)	32(5)	6(4)	-10(4)	1(4)
C(119)	54(5)	26(5)	34(5)	0(4)	-2(4)	-1(4)
C(121)	31(5)	33(5)	47(5)	-2(4)	8(4)	-9(4)
C(122)	80(7)	36(6)	33(5)	-11(4)	6(5)	-27(5)
C(123)	88(7)	37(6)	31(5)	-4(4)	15(5)	-6(5)
C(124)	51(6)	64(7)	41(6)	-22(5)	-22(5)	9(5)
C(125)	50(6)	30(6)	104(9)	-11(6)	-1(6)	-10(4)
C(126)	40(5)	38(5)	46(5)	10(4)	6(4)	3(4)
C(131)	82(7)	29(5)	40(6)	7(4)	23(5)	11(5)
C(132)	150(12)	30(6)	41(6)	11(5)	59(7)	17(6)
C(133)	77(9)	51(8)	169(15)	-5(8)	-38(10)	6(7)
C(134)	197(14)	56(7)	24(6)	18(5)	56(8)	20(9)
C(135)	106(10)	74(8)	66(8)	35(6)	17(7)	24(6)
C(136)	85(8)	49(6)	49(6)	11(5)	29(6)	13(5)
C(141)	42(6)	48(6)	61(6)	-29(5)	3(5)	2(4)
C(142)	47(6)	48(7)	86(7)	-39(6)	-21(5)	14(5)
C(143)	73(8)	43(7)	113(10)	-15(7)	-44(8)	-3(6)
C(144)	17(6)	280(20)	180(17)	-179(17)	42(8)	-26(10)
C(145)	300(30)	131(15)	76(11)	40(10)	-96(14)	-158(17)
C(146)	53(7)	89(10)	100(10)	-79(9)	-12(7)	27(6)
C(151)	144(16)	160(16)	113(12)	-15(11)	-31(14)	11(14)
C(152)	56(9)	106(13)	169(17)	39(11)	9(10)	15(8)
C(153)	128(16)	73(10)	132(15)	0(10)	-66(13)	13(9)
C(154)	162(18)	152(18)	105(12)	32(11)	55(15)	80(16)
C(155)	56(11)	180(20)	300(40)	120(20)	-4(16)	-9(13)
C(156)	104(15)	137(18)	300(30)	58(18)	-120(20)	-59(14)
C(161)	95(10)	116(12)	178(15)	-53(11)	-44(10)	46(8)

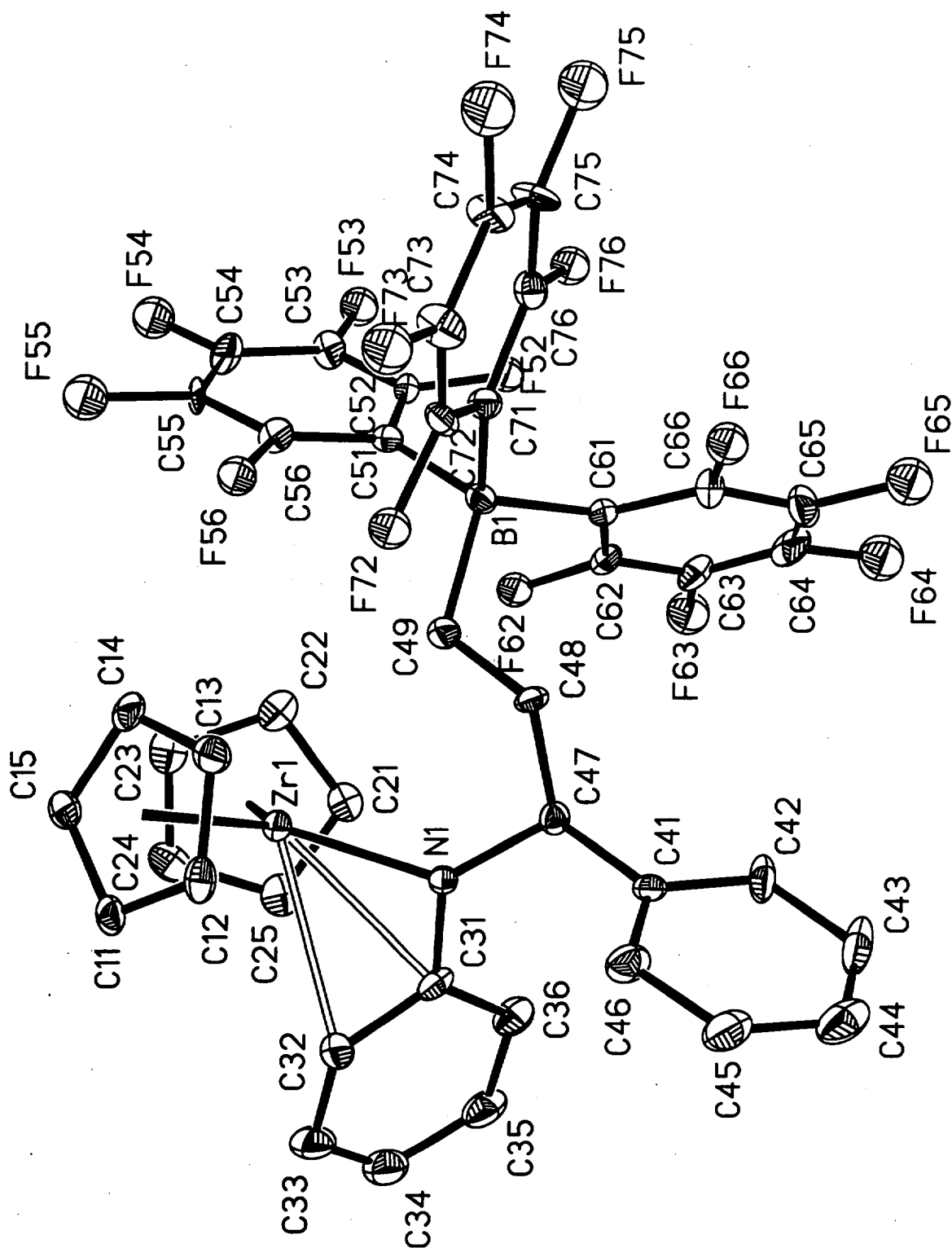
displacement parameters ($\text{\AA}^2$) for

Cp2Zr{Ph-N[C(H)(Ph)C(H)2B(ArF)3}

	x	y	z	U(eq)
H(11A)	4032	7588	8116	50
H(12A)	3016	7582	7332	50
H(13A)	2357	6643	7576	52
H(14A)	2949	6050	8526	57
H(15A)	3973	6654	8884	50
H(21A)	4527	5244	6625	50
H(22A)	3981	4827	7594	55
H(23A)	4363	5487	8591	59
H(24A)	5129	6305	8230	65
H(25A)	5252	6145	7021	59
H(32A)	4096	7365	6960	55
H(33A)	5158	7692	6956	80
H(34A)	5788	7311	6199	95
H(35A)	5345	6632	5401	80
H(36A)	4324	6222	5436	59
H(42A)	3036	5786	4623	64
H(43A)	2722	6357	3697	87
H(44A)	2403	7394	3783	94
H(45A)	2451	7854	4783	83
H(46A)	2797	7295	5712	64
H(47A)	3425	5746	5735	38
H(48A)	2318	5591	5851	40
H(48B)	2339	6163	6342	40
H(49A)	2780	5608	7145	45
H(49B)	3271	5294	6710	45
H(81A)	943	2441	2100	70
H(82A)	2128	2485	2488	64
H(83A)	2362	3547	3024	73
H(84A)	1300	4160	2960	88
H(85A)	440	3459	2401	87
H(91A)	1414	5104	1335	71
H(92A)	1764	4522	356	58
H(93A)	1014	3595	118	59
H(94A)	207	3583	959	81
H(95A)	435	4531	1709	86
H(10A)	1726	2529	1303	50
H(10B)	1029	2062	481	69
H(10C)	1199	2200	-589	84
H(10D)	2060	2805	-847	71
H(10E)	2686	3360	-77	59
H(11B)	3561	2654	1634	52
H(11C)	4430	2078	1409	63
H(11D)	5090	2408	660	67
H(11E)	4858	3324	84	66
H(11F)	3972	3926	302	51
H(11G)	3016	4064	789	37
H(11H)	3671	4305	1782	43
H(11I)	3298	3780	2135	43
H(11J)	2512	4425	2278	46

Table S-8.	H(15B)	-531	4280	5515	170
	H(15C)	-1390	3732	5057	133
	H(15D)	-1312	3210	4123	139
	H(15E)	-405	3214	3629	165
	H(15F)	408	3772	4013	217
	H(15G)	426	4360	4963	226
	H(16A)	-1550	744	5326	160
	H(16B)	-1121	1482	4682	165
	H(16C)	-683	2330	4991	161
	H(16D)	-574	2608	6103	147
	H(16E)	-1030	1888	6839	106
	H(16F)	-1488	986	6452	116
	H(17A)	652	2939	-1730	123
	H(17B)	1481	3623	-1784	117
	H(17C)	1462	4604	-1373	106
	H(17D)	572	4927	-853	96
	H(17E)	-271	4251	-785	98
	H(17F)	-241	3269	-1250	112

Figure S-2.



Atomic coordinates [x 10³] and equivalent isotropic displacement parameters [Å² x 10³] for Cp₂ZrN(SiMe₃)CH(Ph)CH₂CH₂B(C₆F₅) one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zr	-3714 (1)	3441 (1)	-2439 (1)	42 (1)
Si	-738 (1)	2815 (1)	-3721 (1)	50 (1)
N	-1924 (3)	2475 (2)	-3101 (2)	39 (1)
F(32)	2147 (2)	-1382 (2)	-4597 (1)	48 (1)
F(33)	3489 (3)	-297 (3)	-5297 (2)	73 (1)
F(34)	3940 (3)	899 (2)	-4305 (2)	82 (1)
F(35)	3066 (2)	905 (2)	-2586 (2)	71 (1)
F(36)	1771 (2)	-192 (2)	-1871 (2)	57 (1)
F(42)	2623 (2)	-2697 (2)	-2041 (2)	51 (1)
F(43)	2324 (2)	-2869 (2)	-409 (2)	71 (1)
F(44)	135 (3)	-1814 (3)	829 (2)	95 (1)
F(45)	-1780 (3)	-547 (3)	381 (2)	86 (1)
F(46)	-1509 (2)	-340 (2)	-1219 (2)	61 (1)
F(52)	3407 (2)	-3123 (2)	-3925 (2)	45 (1)
F(53)	3855 (2)	-5089 (2)	-4545 (2)	53 (1)
F(54)	2103 (3)	-5832 (2)	-4124 (2)	66 (1)
F(55)	-162 (2)	-4530 (2)	-3041 (2)	66 (1)
F(56)	-649 (2)	-2572 (2)	-2404 (2)	50 (1)
C(1)	-267 (3)	-624 (3)	-3021 (2)	34 (1)
C(2)	-645 (3)	602 (3)	-2874 (2)	35 (1)
C(3)	-1679 (3)	1287 (3)	-3167 (2)	34 (1)
C(11)	-4147 (8)	3940 (5)	-884 (4)	93 (2)
C(12)	-4945 (7)	4805 (6)	-1130 (5)	108 (3)
C(13)	-4265 (10)	5271 (4)	-1746 (5)	123 (4)
C(14)	-3079 (8)	4673 (6)	-1831 (4)	100 (2)
C(15)	-3049 (7)	3881 (5)	-1310 (4)	86 (2)
C(21)	-5442 (6)	3395 (7)	-2770 (4)	89 (2)
C(22)	-5650 (5)	4477 (6)	-2670 (4)	94 (2)
C(23)	-4733 (7)	4636 (4)	-3321 (5)	90 (2)
C(24)	-3995 (5)	3635 (5)	-3843 (3)	66 (1)
C(25)	-4441 (5)	2918 (4)	-3483 (4)	67 (1)
C(31)	1900 (3)	-896 (3)	-3185 (2)	35 (1)
C(32)	2385 (3)	-857 (3)	-4062 (3)	40 (1)
C(33)	3070 (4)	-296 (3)	-4447 (3)	49 (1)
C(34)	3307 (4)	313 (3)	-3953 (3)	55 (1)
C(35)	2857 (4)	311 (3)	-3085 (3)	50 (1)
C(36)	2185 (3)	-272 (3)	-2732 (3)	41 (1)
C(41)	590 (3)	-1492 (3)	-1737 (2)	36 (1)
C(42)	1500 (3)	-2144 (3)	-1452 (3)	41 (1)
C(43)	1372 (4)	-2237 (3)	-617 (3)	51 (1)
C(44)	279 (5)	-1706 (4)	9 (3)	61 (1)
C(45)	-672 (4)	-1072 (4)	-222 (3)	59 (1)
C(46)	-500 (4)	-985 (3)	-1072 (3)	45 (1)
C(51)	1325 (3)	-2693 (3)	-3172 (2)	33 (1)
C(52)	2458 (3)	-3406 (3)	-3700 (2)	35 (1)
C(53)	2733 (3)	-4446 (3)	-4024 (2)	39 (1)

Table S-9.	C(55)	708(4)	-4166(3)	-3271(3)	44(1)
	C(56)	490(3)	-3140(3)	-2965(2)	37(1)
	C(62)	194(5)	1852(5)	-4725(3)	74(2)
	C(63)	221(5)	2821(4)	-3126(4)	68(1)
	C(64)	-1329(5)	4205(4)	-4078(4)	77(2)
	C(71)	-2802(3)	1129(3)	-2657(3)	41(1)
	C(72)	-3460(4)	1610(3)	-1815(3)	50(1)
	C(73)	-4557(5)	1525(4)	-1360(4)	75(2)
	C(74)	-4949(5)	932(5)	-1723(5)	88(2)
	C(75)	-4260(5)	406(4)	-2531(5)	78(2)
	C(76)	-3219(4)	503(3)	-2986(3)	56(1)
	B	886(4)	-1414(3)	-2772(3)	33(1)
	C(01)	4895(10)	-1785(8)	-1192(8)	224(8)
	C(02)	5545(7)	-2066(5)	-2093(8)	134(4)
	C(03)	4926(8)	-2086(8)	-2613(11)	174(8)
	C(04)	5579(17)	-2377(11)	-3517(13)	233(11)
	C(05)	6689(12)	-2610(6)	-3805(8)	154(4)
	C(06)	7315(7)	-2595(5)	-3292(6)	102(2)
	C(07)	6725(5)	-2333(5)	-2454(6)	88(2)
	C(001)	-1259(7)	-4072(8)	1697(5)	131(3)
	C(002)	-1597(6)	-3970(7)	961(4)	97(2)
	C(003)	-1534(6)	-4898(6)	573(5)	98(2)
	C(004)	-1833(8)	-4802(9)	-122(6)	132(3)
	C(005)	-2160(7)	-3865(7)	-515(5)	110(2)
	C(006)	-2194(6)	-2978(7)	-127(5)	110(2)
	C(007)	-1912(5)	-3016(5)	605(4)	81(2)

Zr-N	2.062 (3)	Zr-C(23)	2.464 (4)
Zr-C(13)	2.492 (5)	Zr-C(22)	2.515 (5)
Zr-C(24)	2.516 (4)	Zr-C(12)	2.518 (5)
Zr-C(14)	2.519 (5)	Zr-C(25)	2.519 (5)
Zr-C(21)	2.533 (6)	Zr-C(15)	2.537 (5)
Zr-C(11)	2.546 (5)	Zr-C(72)	2.580 (4)
Si-N	1.752 (3)	Si-C(63)	1.867 (5)
Si-C(62)	1.876 (5)	Si-C(64)	1.881 (5)
N-C(3)	1.501 (4)	F(32)-C(32)	1.359 (4)
F(33)-C(33)	1.345 (5)	F(34)-C(34)	1.336 (5)
F(35)-C(35)	1.352 (5)	F(36)-C(36)	1.354 (5)
F(42)-C(42)	1.362 (4)	F(43)-C(43)	1.354 (4)
F(44)-C(44)	1.341 (5)	F(45)-C(45)	1.354 (5)
F(46)-C(46)	1.361 (4)	F(52)-C(52)	1.360 (4)
F(53)-C(53)	1.346 (4)	F(54)-C(54)	1.344 (4)
F(55)-C(55)	1.338 (4)	F(56)-C(56)	1.361 (4)
C(1)-C(2)	1.527 (5)	C(1)-B	1.646 (5)
C(2)-C(3)	1.535 (5)	C(3)-C(71)	1.506 (5)
C(11)-C(15)	1.326 (9)	C(11)-C(12)	1.382 (9)
C(12)-C(13)	1.412 (11)	C(13)-C(14)	1.387 (11)
C(14)-C(15)	1.349 (9)	C(21)-C(25)	1.361 (8)
C(21)-C(22)	1.377 (9)	C(22)-C(23)	1.392 (9)
C(23)-C(24)	1.411 (8)	C(24)-C(25)	1.335 (7)
C(31)-C(36)	1.393 (5)	C(31)-C(32)	1.398 (5)
C(31)-B	1.660 (6)	C(32)-C(33)	1.368 (6)
C(33)-C(34)	1.383 (6)	C(34)-C(35)	1.373 (7)
C(35)-C(36)	1.369 (6)	C(41)-C(46)	1.382 (5)
C(41)-C(42)	1.397 (5)	C(41)-B	1.660 (6)
C(42)-C(43)	1.366 (6)	C(43)-C(44)	1.360 (6)
C(44)-C(45)	1.375 (6)	C(45)-C(46)	1.381 (6)
C(51)-C(56)	1.379 (5)	C(51)-C(52)	1.384 (5)
C(51)-B	1.672 (5)	C(52)-C(53)	1.384 (5)
C(53)-C(54)	1.359 (6)	C(54)-C(55)	1.388 (6)
C(55)-C(56)	1.380 (5)	C(71)-C(76)	1.392 (6)
C(71)-C(72)	1.398 (6)	C(72)-C(73)	1.412 (7)
C(73)-C(74)	1.365 (8)	C(74)-C(75)	1.372 (8)
C(75)-C(76)	1.357 (7)	C(01)-C(02)	1.436 (14)
C(02)-C(07)	1.335 (9)	C(02)-C(03)	1.40 (2)
C(03)-C(04)	1.44 (2)	C(04)-C(05)	1.26 (2)
C(05)-C(06)	1.392 (11)	C(06)-C(07)	1.334 (9)
C(001)-C(002)	1.444 (9)	C(002)-C(007)	1.366 (9)
C(002)-C(003)	1.397 (10)	C(003)-C(004)	1.351 (10)
C(004)-C(005)	1.382 (11)	C(005)-C(006)	1.366 (10)
C(006)-C(007)	1.404 (9)		
N-Zr-C(23)	113.7 (2)	N-Zr-C(13)	118.7 (3)
C(23)-Zr-C(13)	79.2 (2)	N-Zr-C(22)	141.1 (2)
C(23)-Zr-C(22)	32.5 (2)	C(13)-Zr-C(22)	80.9 (3)
N-Zr-C(24)	87.8 (2)	C(23)-Zr-C(24)	32.9 (2)
C(13)-Zr-C(24)	109.6 (2)	C(22)-Zr-C(24)	53.3 (2)
N-Zr-C(12)	137.5 (2)	C(23)-Zr-C(12)	93.5 (3)
C(13)-Zr-C(12)	32.7 (3)	C(22)-Zr-C(12)	77.6 (2)
C(24)-Zr-C(12)	126.0 (2)	N-Zr-C(14)	88.7 (2)
C(23)-Zr-C(14)	101.9 (2)	C(13)-Zr-C(14)	32.1 (2)
C(22)-Zr-C(14)	112.2 (3)	C(24)-Zr-C(14)	123.2 (2)
C(12)-Zr-C(14)	52.6 (3)	N-Zr-C(25)	94.8 (2)

Table S-10.

C(22)-Zr-C(25)	52.0(2)	C(24)-Zr-C(25)	30.8(2)
C(12)-Zr-C(25)	127.6(2)	C(14)-Zr-C(25)	153.1(2)
N-Zr-C(21)	124.7(2)	C(23)-Zr-C(21)	53.1(2)
C(13)-Zr-C(21)	110.8(3)	C(22)-Zr-C(21)	31.7(2)
C(24)-Zr-C(21)	52.3(2)	C(12)-Zr-C(21)	97.6(3)
C(14)-Zr-C(21)	142.9(3)	C(25)-Zr-C(21)	31.3(2)
N-Zr-C(15)	86.6(2)	C(23)-Zr-C(15)	130.6(2)
C(13)-Zr-C(15)	52.2(2)	C(22)-Zr-C(15)	128.3(2)
C(24)-Zr-C(15)	153.6(2)	C(12)-Zr-C(15)	51.4(2)
C(14)-Zr-C(15)	30.9(2)	C(25)-Zr-C(15)	175.7(2)
C(21)-Zr-C(15)	146.2(3)	N-Zr-C(11)	112.4(2)
C(23)-Zr-C(11)	125.1(2)	C(13)-Zr-C(11)	53.0(2)
C(22)-Zr-C(11)	106.1(2)	C(24)-Zr-C(11)	157.6(2)
C(12)-Zr-C(11)	31.7(2)	C(14)-Zr-C(11)	51.5(2)
C(25)-Zr-C(11)	146.4(3)	C(21)-Zr-C(11)	116.2(3)
C(15)-Zr-C(11)	30.2(2)	N-Zr-C(72)	77.61(12)
C(23)-Zr-C(72)	140.3(2)	C(13)-Zr-C(72)	130.7(2)
C(22)-Zr-C(72)	116.6(2)	C(24)-Zr-C(72)	117.6(2)
C(12)-Zr-C(72)	102.5(3)	C(14)-Zr-C(72)	116.8(2)
C(25)-Zr-C(72)	90.0(2)	C(21)-Zr-C(72)	88.5(2)
C(15)-Zr-C(72)	86.2(2)	C(11)-Zr-C(72)	77.6(2)
N-Si-C(63)	112.1(2)	N-Si-C(62)	110.1(2)
C(63)-Si-C(62)	110.4(3)	N-Si-C(64)	110.7(2)
C(63)-Si-C(64)	108.0(2)	C(62)-Si-C(64)	105.4(3)
C(3)-N-Si	116.0(2)	C(3)-N-Zr	112.2(2)
Si-N-Zr	130.9(2)	C(2)-C(1)-B	116.3(3)
C(1)-C(2)-C(3)	113.5(3)	N-C(3)-C(71)	110.0(3)
N-C(3)-C(2)	111.5(3)	C(71)-C(3)-C(2)	110.7(3)
C(15)-C(11)-C(12)	108.1(7)	C(15)-C(11)-Zr	74.5(3)
C(12)-C(11)-Zr	73.1(3)	C(11)-C(12)-C(13)	107.2(7)
C(11)-C(12)-Zr	75.3(3)	C(13)-C(12)-Zr	72.6(3)
C(14)-C(13)-C(12)	105.8(6)	C(14)-C(13)-Zr	75.0(3)
C(12)-C(13)-Zr	74.7(3)	C(15)-C(14)-C(13)	108.1(7)
C(15)-C(14)-Zr	75.3(3)	C(13)-C(14)-Zr	72.9(3)
C(11)-C(15)-C(14)	110.7(7)	C(11)-C(15)-Zr	75.3(3)
C(14)-C(15)-Zr	73.8(3)	C(25)-C(21)-C(22)	107.3(6)
C(25)-C(21)-Zr	73.8(3)	C(22)-C(21)-Zr	73.4(3)
C(21)-C(22)-C(23)	107.5(5)	C(21)-C(22)-Zr	74.9(3)
C(23)-C(22)-Zr	71.8(3)	C(22)-C(23)-C(24)	107.2(5)
C(22)-C(23)-Zr	75.8(3)	C(24)-C(23)-Zr	75.6(3)
C(25)-C(24)-C(23)	106.6(5)	C(25)-C(24)-Zr	74.7(3)
C(23)-C(24)-Zr	71.5(3)	C(24)-C(25)-C(21)	111.3(5)
C(24)-C(25)-Zr	74.5(3)	C(21)-C(25)-Zr	74.9(3)
C(36)-C(31)-C(32)	111.5(3)	C(36)-C(31)-B	125.8(3)
C(32)-C(31)-B	121.5(3)	F(32)-C(32)-C(33)	115.3(4)
F(32)-C(32)-C(31)	119.2(3)	C(33)-C(32)-C(31)	125.5(4)
F(33)-C(33)-C(32)	121.2(4)	F(33)-C(33)-C(34)	119.1(4)
C(32)-C(33)-C(34)	119.6(4)	F(34)-C(34)-C(35)	120.8(4)
F(34)-C(34)-C(33)	121.3(5)	C(35)-C(34)-C(33)	117.9(4)
F(35)-C(35)-C(36)	120.6(4)	F(35)-C(35)-C(34)	119.3(4)
C(36)-C(35)-C(34)	120.1(4)	F(36)-C(36)-C(35)	114.6(3)
F(36)-C(36)-C(31)	120.1(4)	C(35)-C(36)-C(31)	125.3(4)
C(46)-C(41)-C(42)	112.0(3)	C(46)-C(41)-B	127.9(3)
C(42)-C(41)-B	120.1(3)	F(42)-C(42)-C(43)	116.5(3)
F(42)-C(42)-C(41)	118.3(3)	C(43)-C(42)-C(41)	125.1(4)
F(43)-C(43)-C(44)	119.6(4)	F(43)-C(43)-C(42)	120.4(4)
C(44)-C(43)-C(42)	120.0(4)	F(44)-C(44)-C(43)	120.5(4)
F(44)-C(44)-C(45)	121.2(4)	C(43)-C(44)-C(45)	118.2(4)

Table S-10.

C(44)-C(45)-C(46)	120.0(4)	F(46)-C(46)-C(45)	114.4(4)
F(46)-C(46)-C(41)	121.1(3)	C(45)-C(46)-C(41)	124.5(4)
C(56)-C(51)-C(52)	113.0(3)	C(56)-C(51)-B	118.7(3)
C(52)-C(51)-B	128.3(3)	F(52)-C(52)-C(51)	120.8(3)
F(52)-C(52)-C(53)	114.9(3)	C(51)-C(52)-C(53)	124.3(3)
F(53)-C(53)-C(54)	119.2(3)	F(53)-C(53)-C(52)	121.0(4)
C(54)-C(53)-C(52)	119.8(3)	F(54)-C(54)-C(53)	121.0(4)
F(54)-C(54)-C(55)	120.0(4)	C(53)-C(54)-C(55)	119.0(3)
F(55)-C(55)-C(56)	121.2(4)	F(55)-C(55)-C(54)	120.3(3)
C(56)-C(55)-C(54)	118.5(4)	F(56)-C(56)-C(51)	120.4(3)
F(56)-C(56)-C(55)	114.3(3)	C(51)-C(56)-C(55)	125.3(3)
C(76)-C(71)-C(72)	117.5(4)	C(76)-C(71)-C(3)	122.6(4)
C(72)-C(71)-C(3)	119.9(3)	C(76)-C(71)-Zr	127.0(3)
C(72)-C(71)-Zr	64.9(2)	C(3)-C(71)-Zr	79.9(2)
C(71)-C(72)-C(73)	119.7(5)	C(71)-C(72)-Zr	85.8(2)
C(73)-C(72)-Zr	113.8(3)	C(74)-C(73)-C(72)	120.4(5)
C(73)-C(74)-C(75)	119.5(5)	C(76)-C(75)-C(74)	120.9(5)
C(75)-C(76)-C(71)	121.8(5)	C(1)-B-C(31)	104.5(3)
C(1)-B-C(41)	115.1(3)	C(31)-B-C(41)	111.1(3)
C(1)-B-C(51)	108.1(3)	C(31)-B-C(51)	114.3(3)
C(41)-B-C(51)	103.9(3)	C(07)-C(02)-C(03)	118.5(11)
C(07)-C(02)-C(01)	122.7(12)	C(03)-C(02)-C(01)	118.8(9)
C(02)-C(03)-C(04)	118.9(9)	C(05)-C(04)-C(03)	118.5(12)
C(04)-C(05)-C(06)	123.1(14)	C(07)-C(06)-C(05)	119.2(9)
C(02)-C(07)-C(06)	121.8(9)	C(007)-C(002)-C(003)	118.9(6)
C(007)-C(002)-C(001)	122.4(8)	C(003)-C(002)-C(001)	118.6(8)
C(004)-C(003)-C(002)	118.4(8)	C(003)-C(004)-C(005)	125.8(9)
C(006)-C(005)-C(004)	114.3(8)	C(005)-C(006)-C(007)	123.0(8)
C(002)-C(007)-C(006)	119.7(7)		

Symmetry transformations used to generate equivalent atoms:

Cp2ZrN(SiMe3)CH(Ph)CH2CH2B(C6F5)3.

The anisotropic displacement factor $\exp -2\pi^2 [(h a^*)^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Zr	53(1)	27(1)	40(1)	1(1)	-27(1)	0(1)
Si	63(1)	42(1)	60(1)	17(1)	-34(1)	-26(1)
N	48(2)	26(2)	49(2)	7(1)	-29(2)	-12(1)
F(32)	54(1)	53(1)	42(1)	3(1)	-22(1)	-23(1)
F(33)	76(2)	94(2)	54(2)	16(2)	-14(2)	-48(2)
F(34)	75(2)	78(2)	106(2)	13(2)	-23(2)	-53(2)
F(35)	69(2)	64(2)	98(2)	-12(2)	-38(2)	-35(1)
F(36)	71(2)	56(1)	52(2)	-8(1)	-29(1)	-26(1)
F(42)	39(1)	50(1)	52(1)	5(1)	-22(1)	-3(1)
F(43)	73(2)	68(2)	67(2)	13(1)	-50(2)	-4(1)
F(44)	110(3)	93(2)	40(2)	-1(2)	-37(2)	8(2)
F(45)	76(2)	86(2)	38(2)	-6(1)	-11(1)	15(2)
F(46)	41(1)	68(2)	44(1)	4(1)	-15(1)	7(1)
F(52)	33(1)	36(1)	58(2)	0(1)	-15(1)	-7(1)
F(53)	50(1)	34(1)	50(1)	-3(1)	-11(1)	2(1)
F(54)	83(2)	32(1)	80(2)	-9(1)	-28(2)	-20(1)
F(55)	61(2)	42(1)	104(2)	7(1)	-33(2)	-27(1)
F(56)	36(1)	36(1)	69(2)	2(1)	-14(1)	-12(1)
C(1)	37(2)	27(2)	36(2)	4(1)	-18(2)	-8(2)
C(2)	35(2)	29(2)	46(2)	4(2)	-24(2)	-10(2)
C(3)	40(2)	25(2)	40(2)	6(1)	-24(2)	-9(2)
C(11)	151(7)	75(4)	45(3)	-9(3)	-41(4)	-32(5)
C(12)	98(5)	83(5)	97(5)	-58(4)	-41(4)	19(4)
C(13)	244(11)	27(3)	110(6)	-3(3)	-129(7)	-10(4)
C(14)	177(8)	83(5)	76(4)	-4(4)	-55(5)	-79(5)
C(15)	123(6)	62(3)	82(4)	-12(3)	-72(4)	-16(4)
C(21)	79(4)	133(6)	80(4)	42(4)	-54(4)	-50(4)
C(22)	66(4)	102(5)	71(4)	-25(4)	-45(3)	27(3)
C(23)	146(6)	51(3)	123(5)	44(3)	-115(5)	-35(4)
C(24)	65(3)	81(4)	46(3)	14(3)	-40(2)	-9(3)
C(25)	83(4)	54(3)	70(3)	10(3)	-57(3)	-11(3)
C(31)	33(2)	27(2)	43(2)	2(2)	-20(2)	-4(2)
C(32)	34(2)	35(2)	51(2)	2(2)	-21(2)	-10(2)
C(33)	37(2)	49(2)	55(3)	10(2)	-14(2)	-16(2)
C(34)	47(3)	47(2)	76(3)	8(2)	-24(2)	-23(2)
C(35)	43(2)	37(2)	75(3)	-3(2)	-31(2)	-14(2)
C(36)	38(2)	34(2)	48(2)	-3(2)	-23(2)	-5(2)
C(41)	38(2)	30(2)	40(2)	0(2)	-20(2)	-9(2)
C(42)	41(2)	33(2)	45(2)	1(2)	-20(2)	-8(2)
C(43)	60(3)	41(2)	48(3)	6(2)	-33(2)	-6(2)
C(44)	79(3)	54(3)	38(2)	3(2)	-31(2)	-7(2)
C(45)	61(3)	53(3)	35(2)	-9(2)	-13(2)	1(2)
C(46)	44(2)	42(2)	39(2)	-1(2)	-20(2)	-1(2)
C(51)	33(2)	25(2)	38(2)	4(1)	-22(2)	-3(1)
C(52)	37(2)	31(2)	39(2)	5(2)	-22(2)	-9(2)
C(53)	42(2)	31(2)	34(2)	4(2)	-16(2)	-2(2)

Table S-11.

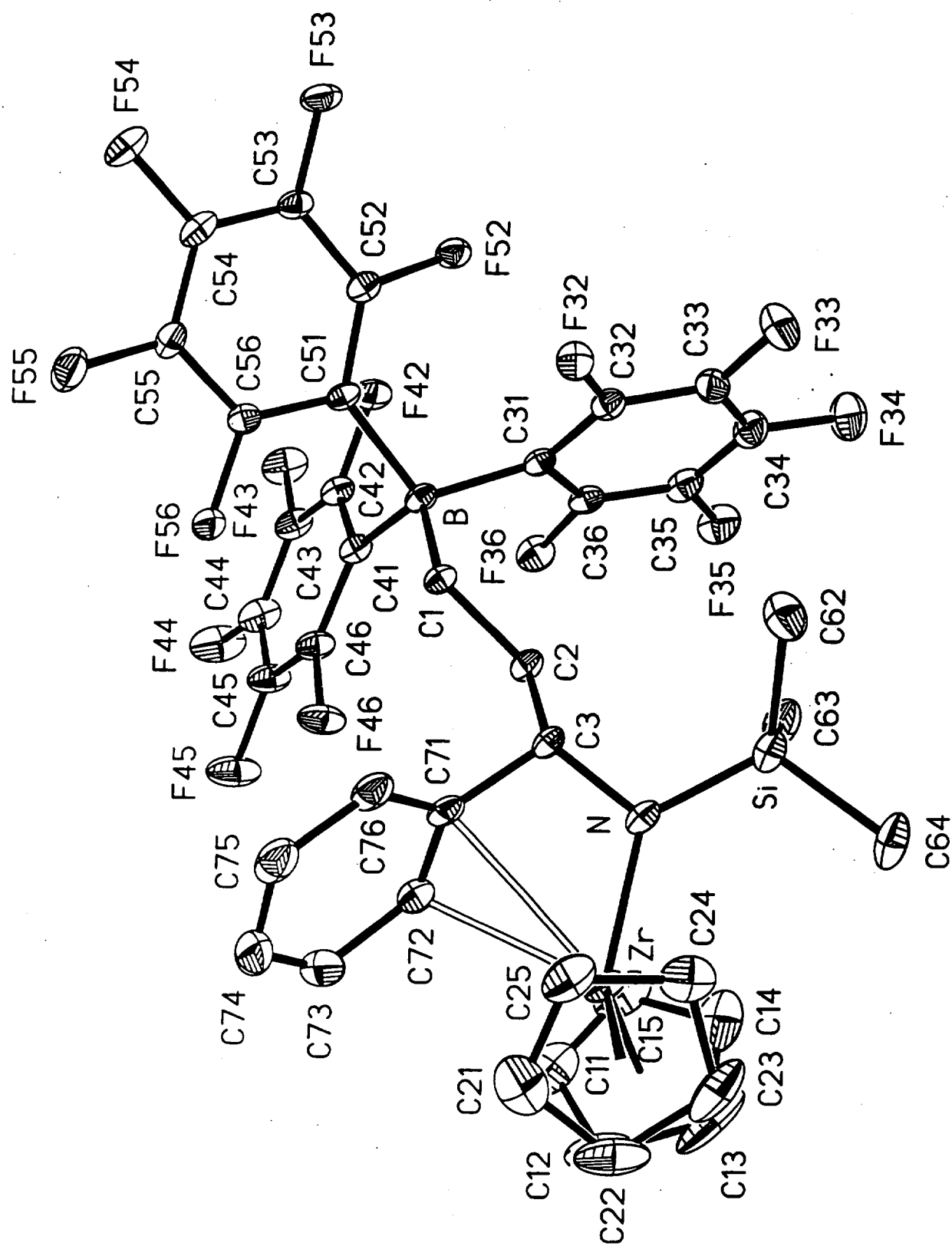
C(55)	48(2)	32(2)	60(3)	10(2)	-27(2)	-18(2)
C(56)	33(2)	33(2)	41(2)	2(2)	-15(2)	-7(2)
C(62)	77(4)	87(4)	58(3)	10(3)	-16(3)	-42(3)
C(63)	74(3)	54(3)	104(4)	26(3)	-55(3)	-36(3)
C(64)	105(4)	64(3)	95(4)	47(3)	-62(4)	-49(3)
C(71)	38(2)	26(2)	57(3)	8(2)	-28(2)	-4(2)
C(72)	46(2)	37(2)	60(3)	11(2)	-21(2)	-9(2)
C(73)	53(3)	58(3)	83(4)	9(3)	-8(3)	-7(2)
C(74)	52(3)	59(3)	147(6)	24(4)	-25(4)	-27(3)
C(75)	54(3)	45(3)	145(6)	16(3)	-50(4)	-19(2)
C(76)	45(2)	35(2)	92(4)	9(2)	-39(3)	-10(2)
B	34(2)	26(2)	41(2)	5(2)	-20(2)	-7(2)
C(01)	179(10)	99(7)	228(14)	43(8)	59(10)	-16(7)
C(02)	72(5)	61(4)	226(11)	62(5)	-18(6)	-25(3)
C(03)	79(5)	105(6)	407(22)	162(11)	-152(10)	-64(5)
C(04)	325(22)	138(10)	484(29)	203(16)	-360(24)	-171(14)
C(05)	226(12)	71(5)	236(12)	53(6)	-177(11)	-55(6)
C(06)	86(5)	74(4)	152(7)	30(5)	-63(5)	-21(4)
C(07)	55(4)	62(3)	152(7)	37(4)	-45(4)	-27(3)
C(001)	96(5)	209(9)	103(6)	32(6)	-49(5)	-66(6)
C(002)	67(4)	147(7)	74(4)	28(4)	-27(3)	-43(4)
C(003)	113(6)	96(5)	98(5)	16(4)	-39(4)	-56(4)
C(004)	149(8)	156(9)	120(7)	21(6)	-59(6)	-81(7)
C(005)	126(6)	122(6)	97(5)	8(5)	-54(5)	-54(5)
C(006)	87(5)	129(6)	102(6)	23(5)	-35(4)	-32(5)
C(007)	64(4)	82(4)	87(4)	4(3)	-18(3)	-27(3)

displacement parameters ($\text{\AA}^2$) and isotropic for

Cp2ZrN(SiMe3)CH(Ph)CH2CH2B(C6F5)

	x	y	z	U(eq)
H(1A)	-76(3)	-817(3)	-3624(2)	40
H(1B)	-958(3)	-788(3)	-2691(2)	40
H(2A)	51(3)	770(3)	-3180(2)	42
H(2B)	-890(3)	811(3)	-2265(2)	42
H(3A)	-1442(3)	1034(3)	-3771(2)	40
H(11A)	-4368(8)	3515(5)	-409(4)	112
H(12A)	-5832(7)	5119(6)	-851(5)	129
H(13A)	-4585(10)	5979(4)	-1965(5)	148
H(14A)	-2398(8)	4869(6)	-2142(4)	120
H(15A)	-2323(7)	3390(5)	-1202(4)	103
H(21A)	-5993(6)	3059(7)	-2444(4)	107
H(22A)	-6382(5)	5055(6)	-2263(4)	112
H(23A)	-4717(7)	5352(4)	-3469(5)	108
H(24A)	-3359(5)	3519(5)	-4412(3)	79
H(25A)	-4145(5)	2164(4)	-3741(4)	80
H(62A)	867(20)	2027(20)	-5053(12)	111
H(62B)	-296(11)	1920(23)	-5060(12)	111
H(62C)	492(28)	1110(5)	-4583(3)	111
H(63A)	-241(10)	3404(19)	-2660(14)	102
H(63B)	913(17)	2936(29)	-3508(6)	102
H(63C)	492(27)	2128(11)	-2901(20)	102
H(64A)	-667(7)	4410(14)	-4370(22)	115
H(64B)	-1898(26)	4731(7)	-3586(4)	115
H(64C)	-1727(31)	4190(9)	-4462(19)	115
H(72A)	-3174(4)	1988(3)	-1554(3)	60
H(73A)	-5021(5)	1878(4)	-804(4)	90
H(74A)	-5685(5)	885(5)	-1421(5)	106
H(75A)	-4512(5)	-28(4)	-2771(5)	94
H(76A)	-2767(4)	138(3)	-3540(3)	67
H(01A)	4045(17)	-1565(97)	-1069(11)	336
H(01B)	5019(91)	-1188(68)	-1000(16)	336
H(01C)	5181(79)	-2412(31)	-899(10)	336
H(03A)	4098(8)	-1914(8)	-2377(11)	209
H(04A)	5184(17)	-2391(11)	-3882(13)	279
H(05A)	7115(12)	-2803(6)	-4394(8)	184
H(06A)	8143(7)	-2768(5)	-3534(6)	123
H(07A)	7151(5)	-2336(5)	-2107(6)	105
H(00A)	-987(54)	-3510(32)	1740(23)	197
H(00B)	-615(40)	-4783(20)	1639(20)	197
H(00C)	-1947(17)	-3991(53)	2206(6)	197
H(003)	-1290(6)	-5572(6)	791(5)	117
H(004)	-1817(8)	-5428(9)	-360(6)	159
H(005)	-2344(7)	-3840(7)	-1007(5)	132
H(006)	-2416(6)	-2313(7)	-360(5)	133
H(007)	-1940(5)	-2387(5)	849(4)	97

Figure S-3.



displacement parameters [$\text{\AA}^2 \times 10^3$] for $[\text{Cp}_2\text{Zr}(\text{PhCHNPh})\text{AlMe}_2\text{Cl}]$.

$U(\text{eq})$ one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Zr	4748(1)	866(1)	3571(1)	42(1)
Al	3022(2)	2176(2)	4064(1)	61(1)
C(1)	2713(8)	3062(7)	4646(4)	99(4)
C(2)	1829(7)	1868(6)	3614(4)	75(3)
Cl	3611(2)	951(2)	4529(1)	73(1)
N(1)	4322(5)	2333(4)	3680(2)	39(2)
C(3)	4656(6)	2154(4)	3090(3)	37(2)
C(11)	3120(8)	62(7)	3326(5)	74(3)
C(12)	3438(10)	490(7)	2819(5)	72(3)
C(13)	4351(10)	110(7)	2644(4)	71(3)
C(14)	4576(9)	-545(6)	3023(5)	71(3)
C(15)	3849(10)	-562(6)	3451(4)	71(3)
C(21)	6184(7)	-8(6)	3956(5)	73(3)
C(22)	6119(7)	742(6)	4306(4)	67(3)
C(23)	6395(7)	1441(6)	3982(4)	59(3)
C(24)	6597(7)	1151(6)	3417(4)	56(3)
C(25)	6463(8)	271(6)	3420(4)	67(3)
C(31)	4875(7)	3018(5)	3962(3)	45(2)
C(32)	5159(7)	3728(5)	3663(4)	56(3)
C(33)	5659(8)	4408(6)	3925(5)	83(4)
C(34)	5881(10)	4350(7)	4507(6)	98(4)
C(35)	5610(10)	3662(8)	4819(5)	100(5)
C(36)	5087(8)	2965(6)	4565(4)	68(3)
C(41)	4009(7)	2453(5)	2590(3)	38(2)
C(42)	4303(7)	2210(5)	2035(3)	47(2)
C(43)	3758(8)	2501(6)	1557(4)	62(3)
C(44)	2961(9)	3034(6)	1615(4)	62(3)
C(45)	2651(7)	3273(5)	2165(5)	60(3)
C(46)	3194(7)	2987(5)	2643(4)	44(2)

Zr-C(3)	2.297(7)	Zr-N(1)	2.366(6)
Zr-C(25)	2.477(10)	Zr-C(22)	2.493(9)
Zr-C(21)	2.501(9)	Zr-C(13)	2.503(9)
Zr-C(24)	2.513(10)	Zr-C(12)	2.525(9)
Zr-C(15)	2.538(9)	Zr-C(23)	2.542(9)
Zr-C(14)	2.548(9)	Zr-C(11)	2.557(10)
Zr-Cl	2.680(3)	Zr-Al	3.269(3)
Al-C(2)	1.950(9)	Al-N(1)	1.952(7)
Al-C(1)	1.969(9)	Al-Cl	2.325(4)
N(1)-C(31)	1.449(9)	N(1)-C(3)	1.462(9)
C(3)-C(41)	1.513(10)	C(11)-C(15)	1.399(13)
C(11)-C(12)	1.413(13)	C(12)-C(13)	1.406(13)
C(13)-C(14)	1.378(12)	C(14)-C(15)	1.381(13)
C(21)-C(25)	1.363(13)	C(21)-C(22)	1.423(12)
C(22)-C(23)	1.371(11)	C(23)-C(24)	1.408(11)
C(24)-C(25)	1.383(11)	C(31)-C(32)	1.356(10)
C(31)-C(36)	1.424(11)	C(32)-C(33)	1.387(12)
C(33)-C(34)	1.379(14)	C(34)-C(35)	1.341(14)
C(35)-C(36)	1.416(13)	C(41)-C(46)	1.368(10)
C(41)-C(42)	1.392(10)	C(42)-C(43)	1.396(11)
C(43)-C(44)	1.349(12)	C(44)-C(45)	1.389(12)
C(45)-C(46)	1.390(11)		
C(3)-Zr-N(1)	36.5(2)	C(3)-Zr-C(25)	107.9(3)
N(1)-Zr-C(25)	126.5(3)	C(3)-Zr-C(22)	115.9(3)
N(1)-Zr-C(22)	100.1(3)	C(25)-Zr-C(22)	53.1(3)
C(3)-Zr-C(21)	133.5(3)	N(1)-Zr-C(21)	131.9(3)
C(25)-Zr-C(21)	31.8(3)	C(22)-Zr-C(21)	33.1(3)
C(3)-Zr-C(13)	89.1(3)	N(1)-Zr-C(13)	119.7(3)
C(25)-Zr-C(13)	84.0(4)	C(22)-Zr-C(13)	134.4(4)
C(21)-Zr-C(13)	102.0(4)	C(3)-Zr-C(24)	80.2(3)
N(1)-Zr-C(24)	94.4(3)	C(25)-Zr-C(24)	32.2(3)
C(22)-Zr-C(24)	53.2(3)	C(21)-Zr-C(24)	53.6(3)
C(13)-Zr-C(24)	99.6(4)	C(3)-Zr-C(12)	80.4(3)
N(1)-Zr-C(12)	97.7(3)	C(25)-Zr-C(12)	116.4(4)
C(22)-Zr-C(12)	162.0(3)	C(21)-Zr-C(12)	129.8(4)
C(13)-Zr-C(12)	32.5(3)	C(24)-Zr-C(12)	127.8(4)
C(3)-Zr-C(15)	133.4(3)	N(1)-Zr-C(15)	138.2(3)
C(25)-Zr-C(15)	94.9(4)	C(22)-Zr-C(15)	110.3(3)
C(21)-Zr-C(15)	85.3(4)	C(13)-Zr-C(15)	52.8(3)
C(24)-Zr-C(15)	126.6(4)	C(12)-Zr-C(15)	53.1(3)
C(3)-Zr-C(23)	85.4(3)	N(1)-Zr-C(23)	79.9(3)
C(25)-Zr-C(23)	53.0(3)	C(22)-Zr-C(23)	31.6(3)
C(21)-Zr-C(23)	53.6(3)	C(13)-Zr-C(23)	131.8(4)
C(24)-Zr-C(23)	32.3(3)	C(12)-Zr-C(23)	158.2(4)
C(15)-Zr-C(23)	138.8(3)	C(3)-Zr-C(14)	120.5(3)
N(1)-Zr-C(14)	149.9(3)	C(25)-Zr-C(14)	71.9(3)
C(22)-Zr-C(14)	109.7(3)	C(21)-Zr-C(14)	77.0(4)
C(13)-Zr-C(14)	31.7(3)	C(24)-Zr-C(14)	99.7(3)
C(12)-Zr-C(14)	52.8(3)	C(15)-Zr-C(14)	31.5(3)
C(23)-Zr-C(14)	124.5(3)	C(3)-Zr-C(11)	106.0(3)
N(1)-Zr-C(11)	107.2(3)	C(25)-Zr-C(11)	123.9(3)
C(22)-Zr-C(11)	136.6(3)	C(21)-Zr-C(11)	116.9(4)
C(13)-Zr-C(11)	53.3(4)	C(24)-Zr-C(11)	151.2(3)
C(12)-Zr-C(11)	32.3(3)	C(15)-Zr-C(11)	31.9(3)

Table S-14.

C(3)-Zr-Cl	109.1(2)	N(1)-Zr-Cl	74.3(2)
C(25)-Zr-Cl	130.5(2)	C(22)-Zr-Cl	81.4(3)
C(21)-Zr-Cl	99.2(3)	C(13)-Zr-Cl	127.8(3)
C(24)-Zr-Cl	130.9(2)	C(12)-Zr-Cl	101.2(3)
C(15)-Zr-Cl	82.5(3)	C(23)-Zr-Cl	98.9(2)
C(14)-Zr-Cl	113.8(3)	C(11)-Zr-Cl	74.6(3)
C(3)-Zr-Al	65.6(2)	N(1)-Zr-Al	36.3(2)
C(25)-Zr-Al	157.5(2)	C(22)-Zr-Al	108.6(3)
C(21)-Zr-Al	138.3(3)	C(13)-Zr-Al	116.5(3)
C(24)-Zr-Al	128.3(2)	C(12)-Zr-Al	84.6(3)
C(15)-Zr-Al	104.9(3)	C(23)-Zr-Al	104.4(2)
C(14)-Zr-Al	130.5(3)	C(11)-Zr-Al	78.1(3)
Cl-Zr-Al	44.65(7)	C(2)-Al-N(1)	120.1(4)
C(2)-Al-C(1)	111.7(5)	N(1)-Al-C(1)	114.0(4)
C(2)-Al-Cl	108.4(3)	N(1)-Al-Cl	90.9(2)
C(1)-Al-Cl	109.2(3)	C(2)-Al-Zr	103.1(3)
N(1)-Al-Zr	45.8(2)	C(1)-Al-Zr	145.1(4)
Cl-Al-Zr	54.13(8)	Al-Cl-Zr	81.22(10)
C(31)-N(1)-C(3)	114.0(6)	C(31)-N(1)-Al	109.5(5)
C(3)-N(1)-Al	131.9(5)	C(31)-N(1)-Zr	129.7(5)
C(3)-N(1)-Zr	69.2(3)	Al-N(1)-Zr	98.0(3)
N(1)-C(3)-C(41)	119.0(7)	N(1)-C(3)-Zr	74.3(4)
C(41)-C(3)-Zr	132.0(5)	C(15)-C(11)-C(12)	107.1(10)
C(15)-C(11)-Zr	73.3(6)	C(12)-C(11)-Zr	72.6(6)
C(13)-C(12)-C(11)	107.2(10)	C(13)-C(12)-Zr	72.9(5)
C(11)-C(12)-Zr	75.1(6)	C(14)-C(13)-C(12)	108.3(11)
C(14)-C(13)-Zr	76.0(6)	C(12)-C(13)-Zr	74.6(5)
C(13)-C(14)-C(15)	108.7(10)	C(13)-C(14)-Zr	72.4(5)
C(15)-C(14)-Zr	73.8(6)	C(14)-C(15)-C(11)	108.6(10)
C(14)-C(15)-Zr	74.6(5)	C(11)-C(15)-Zr	74.8(5)
C(25)-C(21)-C(22)	105.8(9)	C(25)-C(21)-Zr	73.1(6)
C(22)-C(21)-Zr	73.1(5)	C(23)-C(22)-C(21)	109.0(10)
C(23)-C(22)-Zr	76.1(5)	C(21)-C(22)-Zr	73.7(5)
C(22)-C(23)-C(24)	107.6(8)	C(22)-C(23)-Zr	72.3(5)
C(24)-C(23)-Zr	72.7(5)	C(25)-C(24)-C(23)	106.8(8)
C(25)-C(24)-Zr	72.5(6)	C(23)-C(24)-Zr	75.0(6)
C(21)-C(25)-C(24)	110.8(9)	C(21)-C(25)-Zr	75.1(6)
C(24)-C(25)-Zr	75.4(6)	C(32)-C(31)-C(36)	119.4(8)
C(32)-C(31)-N(1)	120.9(7)	C(36)-C(31)-N(1)	119.7(8)
C(31)-C(32)-C(33)	122.2(8)	C(34)-C(33)-C(32)	118.5(10)
C(35)-C(34)-C(33)	121.3(10)	C(34)-C(35)-C(36)	121.3(10)
C(35)-C(36)-C(31)	117.3(9)	C(46)-C(41)-C(42)	118.0(8)
C(46)-C(41)-C(3)	124.4(7)	C(42)-C(41)-C(3)	117.5(8)
C(41)-C(42)-C(43)	119.7(9)	C(44)-C(43)-C(42)	121.7(9)
C(43)-C(44)-C(45)	119.2(9)	C(44)-C(45)-C(46)	119.2(9)
C(41)-C(46)-C(45)	122.1(9)		

Symmetry transformations used to generate equivalent atoms:

[Cp2Zr(PhCHNPh)AlMe2Cl].

The anisotropic displacement factor exponent takes $-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Zr	54(1)	37(1)	35(1)	2(1)	-5(1)	0(1)
Al	62(2)	78(2)	44(2)	12(1)	15(2)	13(2)
C(1)	105(10)	128(10)	62(8)	-24(7)	23(7)	43(8)
C(2)	38(7)	97(7)	90(8)	23(6)	6(6)	4(6)
Cl	90(2)	84(2)	44(1)	24(1)	14(1)	2(2)
N(1)	59(5)	42(4)	17(4)	2(3)	3(3)	1(3)
C(3)	33(5)	46(5)	33(4)	-3(3)	0(4)	10(4)
C(11)	70(9)	68(7)	86(9)	0(6)	-25(7)	-16(7)
C(12)	84(10)	62(7)	69(8)	-3(6)	-50(7)	-1(7)
C(13)	106(11)	62(7)	47(7)	-20(5)	-15(6)	-29(7)
C(14)	79(9)	45(6)	89(9)	-19(6)	-10(8)	-3(6)
C(15)	102(11)	60(7)	52(7)	11(5)	-3(7)	-29(6)
C(21)	84(9)	47(6)	87(9)	12(6)	-29(7)	14(6)
C(22)	73(8)	68(7)	59(7)	12(6)	-22(5)	8(6)
C(23)	66(7)	55(6)	58(7)	-7(5)	-17(5)	8(5)
C(24)	56(7)	67(7)	45(6)	7(4)	0(5)	8(5)
C(25)	89(9)	59(7)	53(7)	4(5)	-4(6)	7(6)
C(31)	61(7)	42(5)	33(5)	-8(4)	-14(5)	12(5)
C(32)	86(8)	38(5)	43(6)	-11(4)	-12(5)	0(5)
C(33)	103(10)	71(7)	76(9)	-9(6)	4(7)	-20(6)
C(34)	123(11)	80(9)	90(10)	-31(7)	-46(9)	5(8)
C(35)	160(14)	92(9)	48(7)	-20(7)	-43(8)	28(9)
C(36)	88(9)	74(7)	40(6)	-10(5)	-12(6)	19(6)
C(41)	55(7)	26(4)	32(5)	-2(3)	0(4)	-6(4)
C(42)	56(7)	50(6)	36(5)	1(4)	2(5)	4(5)
C(43)	81(9)	60(6)	45(7)	7(5)	1(6)	-10(6)
C(44)	86(9)	57(6)	44(6)	17(5)	-22(6)	-12(6)
C(45)	58(8)	49(6)	73(7)	20(5)	-15(6)	-1(5)
C(46)	49(7)	45(5)	37(5)	8(4)	2(4)	5(5)

Table S-10. hydrogen coordinates ($\times 10^3$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Cp}_2\text{Zr}(\text{PhCHNPh})\text{AlMe}_2\text{Cl}]$.

	x	y	z	U(eq)
H(1A)	3315(8)	3198(7)	4859(4)	148
H(1B)	2206(8)	2850(7)	4907(4)	148
H(1C)	2468(8)	3569(7)	4456(4)	148
H(2A)	2006(7)	1436(6)	3336(4)	112
H(2B)	1578(7)	2367(6)	3418(4)	112
H(2C)	1317(7)	1649(6)	3868(4)	112
H(3A)	5341(6)	2380(4)	3040(3)	45
H(11A)	2466(8)	130(7)	3519(5)	89
H(12A)	3037(10)	900(7)	2594(5)	86
H(13A)	4690(10)	211(7)	2273(4)	86
H(14A)	5113(9)	-971(6)	2971(5)	85
H(15A)	3788(10)	-1004(6)	3751(4)	86
H(21A)	6154(7)	-605(6)	4089(5)	87
H(22A)	6017(7)	744(6)	4726(4)	80
H(23A)	6510(7)	2024(6)	4129(4)	71
H(24A)	6894(7)	1490(6)	3103(4)	67
H(25A)	6649(8)	-109(6)	3100(4)	80
H(32A)	5013(7)	3761(5)	3271(4)	67
H(33A)	5840(8)	4892(6)	3713(5)	100
H(34A)	6226(10)	4797(7)	4686(6)	117
H(35A)	5768(10)	3643(8)	5211(5)	120
H(36A)	4890(8)	2491(6)	4782(4)	81
H(42A)	4861(7)	1855(5)	1983(3)	57
H(43A)	3949(8)	2323(6)	1189(4)	74
H(44A)	2624(9)	3239(6)	1290(4)	75
H(45A)	2086(7)	3621(5)	2214(5)	72
H(46A)	2997(7)	3165(5)	3010(4)	52

Figure S-4.

