

Octa- and Nonamethylfluorenyl Complexes of Zr(II), Zr(IV), and Hf(IV). Investigation of Steric and Electronic Effects

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Supporting Information

Contains details concerning the synthesis of mixed-ligand zirconocene dichloride derivatives **9**, **10**, and **11** along with crystallographic data (tables and CIF files) for **2**, **6**, and **7**.

Cp''Cp*ZrCl₂ (8) This was synthesized using an alternate route than the published procedure, starting with Cp''ZrCl₃ instead of Cp*ZrCl₃.¹ A Schlenk flask was charged with LiCp* (0.210 g, 1.48 mmol) and Cp''ZrCl₃ (0.600 g, 1.47 mmol). Benzene (50 mL) was cannula transferred into the flask at room temperature and the reaction mixture was stirred for 14 h. All volatiles were removed under vacuum and the product was extracted into toluene (20 mL). The extracts were filtered through Celite and concentrated under vacuum. The solution was cooled to -35 °C to yield the desired product as needle shaped crystals (0.20 g, 27%). ¹H NMR (benzene-*d*₆, 400 MHz, 25 °C): δ 6.90 (t, 1H, CH), 5.97 (d, 2H, CH), 1.82 (s, 15H, Cp*CH₃), 0.30 (s, 18H, SiCH₃). ¹³C{¹H} NMR (benzene-*d*₆, 100 MHz, 25 °C): δ 138.8 (Cp''), 127.0 (Cp''), 124.4 (Cp*), 119.6 (Cp''), 12.6 (Cp*CH₃), 0.25 (SiCH₃).

¹ Pool, J. A.; Bradley, C. A.; Chirik, P. J. *Organometallics* **2002**, *21*, 1271.

Cp''IndZrCl₂ (9) A toluene (8 mL) suspension of LiInd (0.240 g, 2.0 mmol) was added dropwise to a toluene (12 mL) solution of Cp''ZrCl₃ (0.800 g, 2.0 mmol) at room temperature. The reaction mixture quickly turned yellow and was stirred for an additional 12 h after which time all volatiles were removed under vacuum. The product was extracted into toluene (15 mL). The extracts were filtered through Celite and concentrated under vacuum (3 mL). The solution was cooled to -35 °C to yield the desired product as yellow crystals (0.601 g, 63%). ¹H NMR (benzene-*d*₆, 400 MHz, 25 °C): δ 7.44 (dd, 2H, CH), 7.01 (dd, 2H, CH), 6.76 (t, 1H, CH), 6.36 (t, 1H, CH), 6.32 (d, 2H, CH), 6.16 (d, 2H, CH), 0.23 (s, 18H, CH₃). ¹³C{¹H} NMR (benzene-*d*₆, 100 MHz, 25 °C): δ 131.2 (CH), 129.3 (C), 128.8 (C), 126.9 (2 CH), 126.4 (2 CH), 125.5 (2 CH), 117.5 (CH), 103.1 (2 CH), 0.1 (6 CH₃). Anal. Calcd for C₂₀H₂₈Cl₂Si₂Zr: C, 49.35; H, 5.80. Found: C, 49.70; H, 6.05.

Cp''Ind*ZrCl₂ (10) This complex was synthesized in a manner analogous to that of compound **9**. A suspension of LiInd* (0.410 g, 1.9 mmol) was added to Cp''ZrCl₃ (0.758, 1.9 mmol). The product was crystallized from a concentrated toluene solution at -35 °C and obtained as orange crystals (0.392 g, 36%). ¹H NMR (benzene-*d*₆, 400 MHz, 25 °C): δ 6.75 (t, 1H, CH), 5.63 (d, 2H, CH), 2.48 (s, 6H, CH₃), 2.41 (s, 6H, CH₃), 2.04 (s, 6H, CH₃), 1.99 (s, 3H, CH₃), 0.24 (s, 18H, CH₃). ¹³C{¹H} NMR (benzene-*d*₆, 100 MHz, 25 °C): δ 138.9 (C), 132.5 (C), 130.4 (C), 127.9 (C), 126.2 (C), 125.3 (C), 120.5 (2 CH), 112.1 (CH), 17.7 (2 CH₃), 16.6 (CH₃), 15.8 (CH₃), 13.6 (CH₃), 0.0 (6 CH₃). Anal. Calcd for C₂₇H₄₂Cl₂Si₂Zr: C, 55.44; H, 7.24. Found: C, 55.09; H, 7.27.

Cp''FluZrCl₂ (11) This complex was synthesized in a manner analogous to that of compound **9**. A solution of LiFlu(THF)₃ (prepared by reaction of fluorene with BuLi followed by removal of all volatiles. The THF ratio was determined via ¹H NMR in benzene-*d*₆) (0.953 g, 2.46 mmol) was added to Cp''ZrCl₃ (1.00, 2.46 mmol). The product was extracted into dichloromethane (40 mL), and crystallized from a concentrated dichloromethane solution at -35 °C. The product was obtained as

orange crystals (0.780 g, 60%). ^1H NMR (dichloromethane- d_2 , 400 MHz, 25 °C): δ 8.14-8.11 (m, 2H, CH), 7.61-7.56 (m, 2H, CH), 7.43-7.39 (m, 4H, CH), 6.56 (s, 1H, CH), 6.53 (t, 1 H, CH), 6.13 (d, 2 H, CH), 0.19 (s, 18 H, CH_3). ^{13}C NMR (dichloromethane- d_2 , 400 MHz, 25 °C): δ 134.2 (C), 131.1 (CH), 129.8 (C), 128.6 (2 CH), 125.56 (2 CH), 125.46 (2 CH), 125.42 (2 CH), 124.5 (C), 122.5 (2 CH), 84.9 (CH), 0.1 (CH_3). Anal. Calcd for $\text{C}_{24}\text{H}_{30}\text{Cl}_2\text{Si}_2\text{Zr}$: C, 53.70; H, 5.63. Found: C, 53.53; H, 5.77.

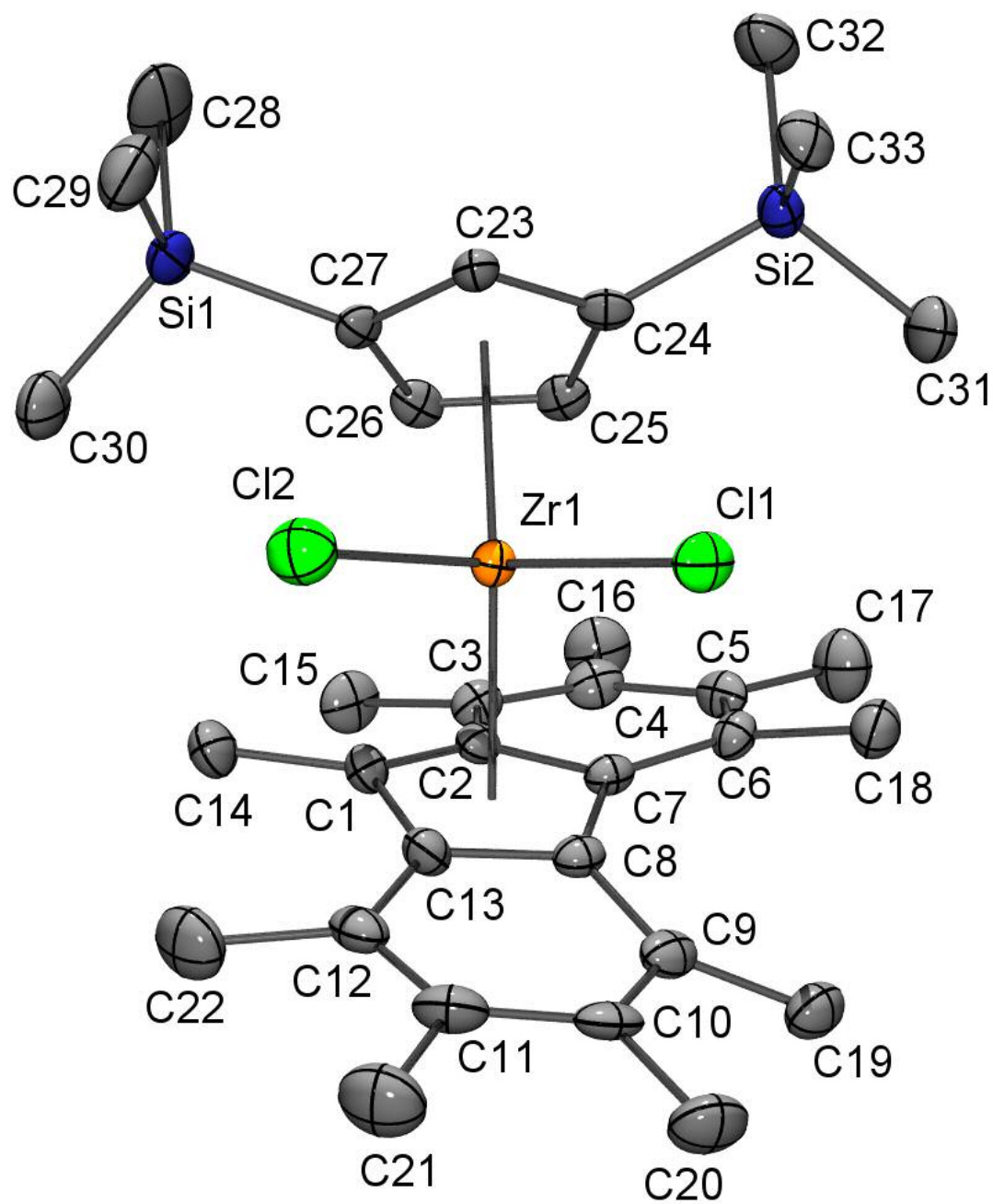


Figure 1. Thermal ellipsoid plot for compound **2**. Hydrogen atoms have been omitted for clarity.

Thermal ellipsoids are drawn at 50% probability.

A. Crystal data and structure refinement for Cp"Flu*ZrCl₂ (2).

Empirical formula	C ₃₃ H ₄₈ Cl ₂ Si ₂ Zr
Formula weight	663.01
Temperature	145(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C 2/c
Lattice Parameters	$a = 15.7039(16)$ Å $\alpha = 90^\circ$ $b = 13.2091(14)$ Å $\beta = 101.991(2)^\circ$ $c = 32.361(3)$ Å $\gamma = 90^\circ$
Volume	6566.3(12) Å ³
Z	8
Calculated density	1.341 Mg/m ³
Absorption coefficient	0.592 mm ⁻¹
F(000)	2784
Crystal size	0.4 x 0.3 x 0.25 mm
Theta range for data collection	2.03 to 23.30°
Limiting indices	-17 < h < 16, -14 < k < 9, -35 < l < 33
Reflections collected	13331
Independent reflections	4722 (R _{int} = 0.0627)
Completeness to theta = 23.30°	99.4%
Absorption correction	semi-empirical from equivalents
Max. and min. transmission	0.864 and 0.779
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4722 / 0 / 343
Goodness-of-fit on F ²	1.047
Final R indices [I > 2sigma(I)]	R1 = 0.0524, wR2 = 0.1254
R indices (all data)	R1 = 0.0761, wR2 = 0.1363
Largest diff. peak and hole	0.652 and -0.753 eÅ ⁻³

Table 1. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for Cp"Flu*ZrCl₂ (2). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zr(1)	2196(1)	4899(1)	3880(1)	17(1)
Cl(1)	3558(1)	4264(1)	3735(1)	29(1)
Si(1)	937(1)	7581(1)	3560(1)	27(1)
C(1)	1445(3)	4547(4)	4454(2)	21(1)
Cl(2)	2832(1)	6406(1)	4248(1)	37(1)
Si(2)	2334(1)	4511(1)	2637(1)	23(1)
C(2)	1096(3)	3745(4)	4168(2)	20(1)
C(3)	221(3)	3487(4)	3966(2)	22(1)
C(4)	97(3)	2688(4)	3693(2)	27(1)
C(5)	811(3)	2126(4)	3588(2)	24(1)
C(6)	1659(3)	2339(4)	3784(2)	21(1)
C(7)	1807(3)	3105(4)	4109(2)	19(1)
C(8)	2556(3)	3380(4)	4437(2)	21(1)
C(9)	3355(3)	2861(4)	4605(2)	26(1)
C(10)	3957(4)	3332(4)	4910(2)	28(1)
C(11)	3770(4)	4253(5)	5102(2)	31(1)
C(12)	2953(4)	4697(4)	4987(2)	26(1)
C(13)	2336(3)	4266(4)	4645(2)	22(1)
C(14)	936(4)	5392(4)	4604(2)	29(1)
C(15)	-549(3)	4011(5)	4091(2)	32(1)
C(16)	-812(4)	2350(5)	3476(2)	41(2)
C(17)	618(4)	1282(5)	3271(2)	42(2)
C(18)	2405(4)	1833(4)	3634(2)	31(1)
C(19)	3465(4)	1748(4)	4511(2)	31(1)
C(20)	4840(4)	2852(5)	5074(2)	39(2)
C(21)	4448(4)	4688(5)	5454(2)	45(2)
C(22)	2688(4)	5559(5)	5244(2)	41(2)
C(23)	1909(3)	6016(4)	3222(2)	19(1)
C(24)	1815(3)	5000(4)	3068(2)	20(1)
C(25)	1103(3)	4597(4)	3223(2)	22(1)
C(26)	754(3)	5375(4)	3440(2)	22(1)
C(27)	1248(3)	6259(4)	3441(2)	19(1)
C(28)	72(5)	7942(6)	3104(2)	60(2)
C(29)	1867(4)	8460(4)	3582(2)	45(2)
C(30)	513(4)	7649(5)	4046(2)	37(2)
C(31)	2445(4)	3118(4)	2651(2)	36(2)
C(32)	1571(4)	4903(5)	2144(2)	38(2)
C(33)	3393(3)	5145(4)	2652(2)	29(1)

Table 2. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for Cp"Flu*ZrCl₂ (**2**). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2hka^*b^*U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Zr(1)	14(1)	20(1)	18(1)	1(1)	3(1)	0(1)
Cl(1)	18(1)	38(1)	33(1)	8(1)	9(1)	7(1)
Si(1)	27(1)	26(1)	26(1)	3(1)	6(1)	11(1)
C(1)	22(3)	23(3)	20(3)	0(2)	8(2)	2(2)
Cl(2)	38(1)	37(1)	35(1)	2(1)	3(1)	-3(1)
Si(2)	22(1)	25(1)	21(1)	-2(1)	4(1)	1(1)
C(2)	20(3)	23(3)	18(3)	5(2)	9(2)	3(2)
C(3)	16(3)	22(3)	28(3)	4(3)	6(2)	-4(2)
C(4)	20(3)	28(3)	33(3)	7(3)	6(3)	-6(2)
C(5)	29(3)	18(3)	22(3)	-1(2)	3(3)	-9(2)
C(6)	21(3)	16(3)	27(3)	2(2)	7(3)	-1(2)
C(7)	17(3)	21(3)	20(3)	6(2)	4(2)	0(2)
C(8)	20(3)	22(3)	21(3)	7(2)	6(2)	0(2)
C(9)	23(3)	33(3)	25(3)	10(3)	12(3)	5(3)
C(10)	26(3)	38(4)	19(3)	15(3)	5(3)	2(3)
C(11)	31(3)	38(4)	21(3)	9(3)	-1(3)	-6(3)
C(12)	36(3)	26(3)	18(3)	4(2)	7(3)	-5(3)
C(13)	24(3)	26(3)	17(3)	0(2)	5(2)	1(2)
C(14)	31(3)	32(3)	26(3)	-1(3)	11(3)	4(3)
C(15)	15(3)	41(4)	42(4)	5(3)	8(3)	2(3)
C(16)	27(3)	47(4)	45(4)	1(3)	1(3)	-5(3)
C(17)	41(4)	39(4)	45(4)	-10(3)	6(3)	-5(3)
C(18)	33(3)	26(3)	36(3)	2(3)	13(3)	4(3)
C(19)	27(3)	32(3)	35(4)	9(3)	8(3)	7(3)
C(20)	30(4)	48(4)	34(4)	13(3)	-2(3)	7(3)
C(21)	45(4)	53(4)	33(4)	0(3)	-3(3)	-10(3)
C(22)	46(4)	43(4)	31(4)	-9(3)	1(3)	-9(3)
C(23)	21(3)	19(3)	17(3)	3(2)	3(2)	2(2)
C(24)	17(3)	25(3)	16(3)	5(2)	-2(2)	-2(2)
C(25)	20(3)	23(3)	19(3)	1(2)	-4(2)	-3(2)
C(26)	12(3)	32(3)	19(3)	2(2)	0(2)	1(2)
C(27)	15(3)	23(3)	18(3)	4(2)	1(2)	6(2)
C(28)	62(5)	64(5)	45(4)	-2(4)	-13(4)	42(4)
C(29)	51(4)	27(4)	63(5)	5(3)	27(4)	7(3)
C(30)	35(4)	33(4)	44(4)	1(3)	15(3)	10(3)
C(31)	47(4)	26(3)	35(4)	-5(3)	10(3)	1(3)
C(32)	37(4)	53(4)	22(3)	4(3)	1(3)	10(3)
C(33)	28(3)	31(3)	32(3)	1(3)	15(3)	-2(3)

Table 3. Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for Cp"Flu*ZrCl₂ (2).

	x	y	z	U(eq)
H(14A)	674	5149	4828	43
H(14B)	489	5620	4373	43
H(14C)	1321	5944	4705	43
H(15A)	-1081	3752	3923	48
H(15B)	-514	4726	4045	48
H(15C)	-539	3885	4384	48
H(16A)	-1237	2766	3569	61
H(16B)	-897	1656	3546	61
H(16C)	-877	2414	3175	61
H(17A)	1154	987	3231	63
H(17B)	303	1546	3006	63
H(17C)	273	775	3371	63
H(18A)	2178	1349	3418	46
H(18B)	2773	1494	3867	46
H(18C)	2736	2336	3522	46
H(19A)	4035	1527	4650	47
H(19B)	3396	1655	4212	47
H(19C)	3033	1358	4611	47
H(20A)	4887	2240	4920	58
H(20B)	4903	2699	5368	58
H(20C)	5290	3315	5036	58
H(21A)	4234	5304	5552	68
H(21B)	4969	4826	5353	68
H(21C)	4575	4210	5682	68
H(22A)	3177	5756	5460	62
H(22B)	2221	5340	5373	62
H(22C)	2498	6125	5062	62
H(23A)	2326	6505	3151	23
H(25A)	820	3946	3138	26
H(26A)	199	5334	3533	26
H(28A)	-416	7494	3087	91
H(28B)	291	7896	2849	91
H(28C)	-110	8625	3140	91
H(29A)	1694	9132	3641	67
H(29B)	2043	8454	3315	67
H(29C)	2345	8247	3800	67
H(30A)	35	7186	4027	55
H(30B)	316	8325	4082	55
H(30C)	965	7471	4283	55

H(31A)	2842	2919	2905	54
H(31B)	2664	2895	2410	54
H(31C)	1886	2815	2644	54
H(32A)	1789	4677	1903	57
H(32B)	1520	5627	2137	57
H(32C)	1009	4607	2136	57
H(33A)	3795	4958	2907	44
H(33B)	3312	5866	2646	44
H(33C)	3620	4940	2412	44

Table 4. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for $\text{Cp}^*\text{Flu}^*\text{ZrCl}_2$ (**2**).

<i>Bonds</i>	
Zr(1)-Cl(2)	2.4268(16)
Zr(1)-Cl(1)	2.4320(14)
Zr(1)-C(1)	2.444(5)
Zr(1)-C(25)	2.472(5)
Zr(1)-C(26)	2.491(5)
Zr(1)-C(23)	2.552(5)
Zr(1)-C(27)	2.565(5)
Zr(1)-C(24)	2.572(5)
Zr(1)-C(13)	2.580(5)
Zr(1)-C(7)	2.593(5)
Zr(1)-C(2)	2.617(5)
Zr(1)-C(8)	2.677(5)
Si(1)-C(30)	1.834(6)
Si(1)-C(28)	1.849(6)
Si(1)-C(29)	1.855(6)
Si(1)-C(27)	1.875(5)
C(1)-C(2)	1.438(7)
C(1)-C(13)	1.455(7)
C(1)-C(14)	1.510(7)
Si(2)-C(31)	1.848(6)
Si(2)-C(33)	1.853(5)
Si(2)-C(32)	1.860(6)
Si(2)-C(24)	1.872(5)
C(2)-C(3)	1.435(7)
C(2)-C(7)	1.445(7)
C(3)-C(4)	1.364(7)
C(3)-C(15)	1.519(7)

C(4)-C(5)	1.442(8)
C(4)-C(16)	1.523(8)
C(5)-C(6)	1.380(7)
C(5)-C(17)	1.505(7)
C(6)-C(7)	1.442(7)
C(6)-C(18)	1.513(7)
C(7)-C(8)	1.457(7)
C(8)-C(13)	1.429(7)
C(8)-C(9)	1.435(7)
C(9)-C(10)	1.365(8)
C(9)-C(19)	1.518(8)
C(10)-C(11)	1.425(8)
C(10)-C(20)	1.517(8)
C(11)-C(12)	1.389(8)
C(11)-C(21)	1.503(8)
C(12)-C(13)	1.427(8)
C(12)-C(22)	1.520(8)
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-C(27)	1.411(7)
C(23)-C(24)	1.427(7)

C(23)-H(23A)	0.9800
C(24)-C(25)	1.419(7)
C(25)-C(26)	1.418(7)
C(25)-H(25A)	0.9800
C(26)-C(27)	1.402(7)
C(26)-H(26A)	0.9800
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600
C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
C(33)-H(33A)	0.9600
C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600

Angles

Cl(2)-Zr(1)-Cl(1)	95.05(5)
Cl(2)-Zr(1)-C(1)	89.81(13)
Cl(1)-Zr(1)-C(1)	131.53(13)
Cl(2)-Zr(1)-C(25)	134.15(13)
Cl(1)-Zr(1)-C(25)	105.11(13)
C(1)-Zr(1)-C(25)	105.40(17)
Cl(2)-Zr(1)-C(26)	107.84(13)
Cl(1)-Zr(1)-C(26)	135.14(12)
C(1)-Zr(1)-C(26)	87.58(17)
C(25)-Zr(1)-C(26)	33.20(17)
Cl(2)-Zr(1)-C(23)	85.36(12)
Cl(1)-Zr(1)-C(23)	92.80(12)
C(1)-Zr(1)-C(23)	135.67(17)
C(25)-Zr(1)-C(23)	53.48(17)
C(26)-Zr(1)-C(23)	52.84(17)
Cl(2)-Zr(1)-C(27)	80.21(12)
Cl(1)-Zr(1)-C(27)	124.58(12)
C(1)-Zr(1)-C(27)	103.79(16)
C(25)-Zr(1)-C(27)	54.37(17)

C(26)-Zr(1)-C(27)	32.14(16)
C(23)-Zr(1)-C(27)	32.00(16)
Cl(2)-Zr(1)-C(24)	116.33(12)
Cl(1)-Zr(1)-C(24)	81.34(12)
C(1)-Zr(1)-C(24)	137.72(17)
C(25)-Zr(1)-C(24)	32.61(16)
C(26)-Zr(1)-C(24)	54.05(16)
C(23)-Zr(1)-C(24)	32.33(16)
C(27)-Zr(1)-C(24)	54.07(16)
Cl(2)-Zr(1)-C(13)	81.34(12)
Cl(1)-Zr(1)-C(13)	99.77(12)
C(1)-Zr(1)-C(13)	33.53(16)
C(25)-Zr(1)-C(13)	132.80(17)
C(26)-Zr(1)-C(13)	121.08(17)
C(23)-Zr(1)-C(13)	162.41(16)
C(27)-Zr(1)-C(13)	133.02(16)
C(24)-Zr(1)-C(13)	162.24(16)
Cl(2)-Zr(1)-C(7)	134.95(12)
Cl(1)-Zr(1)-C(7)	90.50(12)
C(1)-Zr(1)-C(7)	55.20(17)
C(25)-Zr(1)-C(7)	86.33(16)
C(26)-Zr(1)-C(7)	98.85(17)
C(23)-Zr(1)-C(7)	139.06(16)
C(27)-Zr(1)-C(7)	130.85(16)
C(24)-Zr(1)-C(7)	108.71(16)
C(13)-Zr(1)-C(7)	53.70(16)
Cl(2)-Zr(1)-C(2)	122.50(12)
Cl(1)-Zr(1)-C(2)	122.70(12)
C(1)-Zr(1)-C(2)	32.78(16)
C(25)-Zr(1)-C(2)	79.72(16)
C(26)-Zr(1)-C(2)	76.23(17)
C(23)-Zr(1)-C(2)	128.27(16)
C(27)-Zr(1)-C(2)	104.79(16)
C(24)-Zr(1)-C(2)	111.35(16)
C(13)-Zr(1)-C(2)	53.12(16)
C(7)-Zr(1)-C(2)	32.21(15)
Cl(2)-Zr(1)-C(8)	106.01(12)
Cl(1)-Zr(1)-C(8)	78.44(11)
C(1)-Zr(1)-C(8)	54.07(16)
C(25)-Zr(1)-C(8)	118.05(17)
C(26)-Zr(1)-C(8)	127.84(17)
C(23)-Zr(1)-C(8)	166.07(16)
C(27)-Zr(1)-C(8)	156.13(16)
C(24)-Zr(1)-C(8)	134.27(16)
C(13)-Zr(1)-C(8)	31.47(16)
C(7)-Zr(1)-C(8)	32.05(15)

C(2)-Zr(1)-C(8)	52.15(15)
C(30)-Si(1)-C(28)	109.5(3)
C(30)-Si(1)-C(29)	111.1(3)
C(28)-Si(1)-C(29)	108.1(3)
C(30)-Si(1)-C(27)	112.3(3)
C(28)-Si(1)-C(27)	104.8(3)
C(29)-Si(1)-C(27)	110.8(3)
C(2)-C(1)-C(13)	106.9(4)
C(2)-C(1)-C(14)	126.4(5)
C(13)-C(1)-C(14)	125.4(5)
C(2)-C(1)-Zr(1)	80.2(3)
C(13)-C(1)-Zr(1)	78.4(3)
C(14)-C(1)-Zr(1)	118.3(4)
C(31)-Si(2)-C(33)	111.7(3)
C(31)-Si(2)-C(32)	109.8(3)
C(33)-Si(2)-C(32)	108.2(3)
C(31)-Si(2)-C(24)	112.3(3)
C(33)-Si(2)-C(24)	110.6(2)
C(32)-Si(2)-C(24)	103.9(2)
C(3)-C(2)-C(1)	132.1(5)
C(3)-C(2)-C(7)	119.5(5)
C(1)-C(2)-C(7)	108.3(4)
C(3)-C(2)-Zr(1)	128.0(3)
C(1)-C(2)-Zr(1)	67.0(3)
C(7)-C(2)-Zr(1)	73.0(3)
C(4)-C(3)-C(2)	118.3(5)
C(4)-C(3)-C(15)	120.7(5)
C(2)-C(3)-C(15)	120.6(5)
C(3)-C(4)-C(5)	122.5(5)
C(3)-C(4)-C(16)	121.3(5)
C(5)-C(4)-C(16)	116.1(5)
C(6)-C(5)-C(4)	120.7(5)
C(6)-C(5)-C(17)	120.2(5)
C(4)-C(5)-C(17)	119.1(5)
C(5)-C(6)-C(7)	118.1(5)
C(5)-C(6)-C(18)	120.0(5)
C(7)-C(6)-C(18)	121.7(5)
C(6)-C(7)-C(2)	119.8(5)
C(6)-C(7)-C(8)	133.5(5)
C(2)-C(7)-C(8)	106.6(4)
C(6)-C(7)-Zr(1)	116.4(3)
C(2)-C(7)-Zr(1)	74.8(3)
C(8)-C(7)-Zr(1)	77.2(3)
C(13)-C(8)-C(9)	119.3(5)
C(13)-C(8)-C(7)	108.1(4)
C(9)-C(8)-C(7)	131.9(5)

C(13)-C(8)-Zr(1)	70.5(3)
C(9)-C(8)-Zr(1)	131.3(3)
C(7)-C(8)-Zr(1)	70.8(3)
C(10)-C(9)-C(8)	118.4(5)
C(10)-C(9)-C(19)	119.7(5)
C(8)-C(9)-C(19)	120.9(5)
C(9)-C(10)-C(11)	122.0(5)
C(9)-C(10)-C(20)	120.5(5)
C(11)-C(10)-C(20)	117.4(5)
C(12)-C(11)-C(10)	120.4(5)
C(12)-C(11)-C(21)	120.8(6)
C(10)-C(11)-C(21)	118.6(5)
C(11)-C(12)-C(13)	118.7(5)
C(11)-C(12)-C(22)	120.8(5)
C(13)-C(12)-C(22)	120.3(5)
C(12)-C(13)-C(8)	120.0(5)
C(12)-C(13)-C(1)	131.7(5)
C(8)-C(13)-C(1)	108.3(4)
C(12)-C(13)-Zr(1)	121.6(4)
C(8)-C(13)-Zr(1)	78.0(3)
C(1)-C(13)-Zr(1)	68.1(3)
C(1)-C(14)-H(14A)	109.5
C(1)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(1)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(3)-C(15)-H(15A)	109.5
C(3)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(3)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(4)-C(16)-H(16A)	109.5
C(4)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(4)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(5)-C(17)-H(17A)	109.5
C(5)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(5)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(6)-C(18)-H(18A)	109.5

C(6)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(6)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(9)-C(19)-H(19A)	109.5
C(9)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(9)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(10)-C(20)-H(20A)	109.5
C(10)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(10)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(11)-C(21)-H(21A)	109.5
C(11)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(11)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(12)-C(22)-H(22A)	109.5
C(12)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(12)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(27)-C(23)-C(24)	110.8(5)
C(27)-C(23)-Zr(1)	74.5(3)
C(24)-C(23)-Zr(1)	74.6(3)
C(27)-C(23)-H(23A)	124.4
C(24)-C(23)-H(23A)	124.4
Zr(1)-C(23)-H(23A)	124.4
C(25)-C(24)-C(23)	105.3(4)
C(25)-C(24)-Si(2)	129.0(4)
C(23)-C(24)-Si(2)	123.6(4)
C(25)-C(24)-Zr(1)	69.8(3)
C(23)-C(24)-Zr(1)	73.1(3)
Si(2)-C(24)-Zr(1)	134.3(2)
C(26)-C(25)-C(24)	108.4(5)
C(26)-C(25)-Zr(1)	74.2(3)
C(24)-C(25)-Zr(1)	77.6(3)
C(26)-C(25)-H(25A)	125.1
C(24)-C(25)-H(25A)	125.1

Zr(1)-C(25)-H(25A)	125.1
C(27)-C(26)-C(25)	109.5(5)
C(27)-C(26)-Zr(1)	76.8(3)
C(25)-C(26)-Zr(1)	72.6(3)
C(27)-C(26)-H(26A)	124.9
C(25)-C(26)-H(26A)	124.9
Zr(1)-C(26)-H(26A)	124.9
C(26)-C(27)-C(23)	105.9(5)
C(26)-C(27)-Si(1)	127.5(4)
C(23)-C(27)-Si(1)	124.5(4)
C(26)-C(27)-Zr(1)	71.0(3)
C(23)-C(27)-Zr(1)	73.5(3)
Si(1)-C(27)-Zr(1)	133.2(2)
Si(1)-C(28)-H(28A)	109.5
Si(1)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
Si(1)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
Si(1)-C(29)-H(29A)	109.5
Si(1)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
Si(1)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
Si(1)-C(30)-H(30A)	109.5
Si(1)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
Si(1)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
Si(2)-C(31)-H(31A)	109.5
Si(2)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
Si(2)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
Si(2)-C(32)-H(32A)	109.5
Si(2)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
Si(2)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
Si(2)-C(33)-H(33A)	109.5
Si(2)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5

Si(2)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5

Table 5. Torsion angles [deg] for Cp^{''}Flu*ZrCl₂ (**2**).

Cl(2)-Zr(1)-C(1)-C(2)	175.9(3)
Cl(1)-Zr(1)-C(1)-C(2)	-87.6(3)
C(25)-Zr(1)-C(1)-C(2)	39.7(3)
C(26)-Zr(1)-C(1)-C(2)	68.0(3)
C(23)-Zr(1)-C(1)-C(2)	92.7(3)
C(27)-Zr(1)-C(1)-C(2)	96.0(3)
C(24)-Zr(1)-C(1)-C(2)	44.9(4)
C(13)-Zr(1)-C(1)-C(2)	-109.7(4)
C(7)-Zr(1)-C(1)-C(2)	-34.5(3)
C(8)-Zr(1)-C(1)-C(2)	-74.1(3)
Cl(2)-Zr(1)-C(1)-C(13)	-74.5(3)
Cl(1)-Zr(1)-C(1)-C(13)	22.1(4)
C(25)-Zr(1)-C(1)-C(13)	149.3(3)
C(26)-Zr(1)-C(1)-C(13)	177.7(3)
C(23)-Zr(1)-C(1)-C(13)	-157.6(3)
C(27)-Zr(1)-C(1)-C(13)	-154.3(3)
C(24)-Zr(1)-C(1)-C(13)	154.6(3)
C(7)-Zr(1)-C(1)-C(13)	75.1(3)
C(2)-Zr(1)-C(1)-C(13)	109.7(4)
C(8)-Zr(1)-C(1)-C(13)	35.6(3)
Cl(2)-Zr(1)-C(1)-C(14)	49.6(4)
Cl(1)-Zr(1)-C(1)-C(14)	146.2(3)
C(25)-Zr(1)-C(1)-C(14)	-86.6(4)
C(26)-Zr(1)-C(1)-C(14)	-58.3(4)
C(23)-Zr(1)-C(1)-C(14)	-33.5(5)
C(27)-Zr(1)-C(1)-C(14)	-30.3(4)
C(24)-Zr(1)-C(1)-C(14)	-81.4(5)
C(13)-Zr(1)-C(1)-C(14)	124.1(5)
C(7)-Zr(1)-C(1)-C(14)	-160.8(5)
C(2)-Zr(1)-C(1)-C(14)	-126.3(5)
C(8)-Zr(1)-C(1)-C(14)	159.7(5)
C(13)-C(1)-C(2)-C(3)	164.2(5)
C(14)-C(1)-C(2)-C(3)	-3.1(9)
Zr(1)-C(1)-C(2)-C(3)	-121.2(6)
C(13)-C(1)-C(2)-C(7)	-13.0(6)

C(14)-C(1)-C(2)-C(7)	179.7(5)
Zr(1)-C(1)-C(2)-C(7)	61.6(4)
C(13)-C(1)-C(2)-Zr(1)	-74.6(3)
C(14)-C(1)-C(2)-Zr(1)	118.1(5)
Cl(2)-Zr(1)-C(2)-C(3)	121.4(4)
Cl(1)-Zr(1)-C(2)-C(3)	-116.4(4)
C(1)-Zr(1)-C(2)-C(3)	126.3(6)
C(25)-Zr(1)-C(2)-C(3)	-15.0(4)
C(26)-Zr(1)-C(2)-C(3)	18.8(4)
C(23)-Zr(1)-C(2)-C(3)	9.0(5)
C(27)-Zr(1)-C(2)-C(3)	33.7(5)
C(24)-Zr(1)-C(2)-C(3)	-23.1(5)
C(13)-Zr(1)-C(2)-C(3)	166.9(5)
C(7)-Zr(1)-C(2)-C(3)	-114.5(6)
C(8)-Zr(1)-C(2)-C(3)	-153.3(5)
Cl(2)-Zr(1)-C(2)-C(1)	-4.9(3)
Cl(1)-Zr(1)-C(2)-C(1)	117.3(3)
C(25)-Zr(1)-C(2)-C(1)	-141.3(3)
C(26)-Zr(1)-C(2)-C(1)	-107.5(3)
C(23)-Zr(1)-C(2)-C(1)	-117.2(3)
C(27)-Zr(1)-C(2)-C(1)	-92.6(3)
C(24)-Zr(1)-C(2)-C(1)	-149.3(3)
C(13)-Zr(1)-C(2)-C(1)	40.6(3)
C(7)-Zr(1)-C(2)-C(1)	119.2(4)
C(8)-Zr(1)-C(2)-C(1)	80.5(3)
Cl(2)-Zr(1)-C(2)-C(7)	-124.1(3)
Cl(1)-Zr(1)-C(2)-C(7)	-1.9(3)
C(1)-Zr(1)-C(2)-C(7)	-119.2(4)
C(25)-Zr(1)-C(2)-C(7)	99.6(3)
C(26)-Zr(1)-C(2)-C(7)	133.3(3)
C(23)-Zr(1)-C(2)-C(7)	123.6(3)
C(27)-Zr(1)-C(2)-C(7)	148.2(3)
C(24)-Zr(1)-C(2)-C(7)	91.5(3)
C(13)-Zr(1)-C(2)-C(7)	-78.6(3)
C(8)-Zr(1)-C(2)-C(7)	-38.7(3)
C(1)-C(2)-C(3)-C(4)	177.4(5)
C(7)-C(2)-C(3)-C(4)	-5.6(7)
Zr(1)-C(2)-C(3)-C(4)	85.3(6)
C(1)-C(2)-C(3)-C(15)	-9.5(9)
C(7)-C(2)-C(3)-C(15)	167.4(5)
Zr(1)-C(2)-C(3)-C(15)	-101.6(5)
C(2)-C(3)-C(4)-C(5)	-2.6(8)
C(15)-C(3)-C(4)-C(5)	-175.7(5)
C(2)-C(3)-C(4)-C(16)	178.3(5)
C(15)-C(3)-C(4)-C(16)	5.2(8)
C(3)-C(4)-C(5)-C(6)	4.2(8)

C(16)-C(4)-C(5)-C(6)	-176.7(5)
C(3)-C(4)-C(5)-C(17)	-177.5(5)
C(16)-C(4)-C(5)-C(17)	1.6(7)
C(4)-C(5)-C(6)-C(7)	2.7(7)
C(17)-C(5)-C(6)-C(7)	-175.5(5)
C(4)-C(5)-C(6)-C(18)	-172.5(5)
C(17)-C(5)-C(6)-C(18)	9.3(8)
C(5)-C(6)-C(7)-C(2)	-10.8(7)
C(18)-C(6)-C(7)-C(2)	164.3(5)
C(5)-C(6)-C(7)-C(8)	164.8(5)
C(18)-C(6)-C(7)-C(8)	-20.1(8)
C(5)-C(6)-C(7)-Zr(1)	-97.8(5)
C(18)-C(6)-C(7)-Zr(1)	77.4(5)
C(3)-C(2)-C(7)-C(6)	12.5(7)
C(1)-C(2)-C(7)-C(6)	-169.9(4)
Zr(1)-C(2)-C(7)-C(6)	-112.1(4)
C(3)-C(2)-C(7)-C(8)	-164.2(4)
C(1)-C(2)-C(7)-C(8)	13.4(5)
Zr(1)-C(2)-C(7)-C(8)	71.3(3)
C(3)-C(2)-C(7)-Zr(1)	124.5(4)
C(1)-C(2)-C(7)-Zr(1)	-57.9(3)
Cl(2)-Zr(1)-C(7)-C(6)	-163.2(3)
Cl(1)-Zr(1)-C(7)-C(6)	-65.5(4)
C(1)-Zr(1)-C(7)-C(6)	151.2(4)
C(25)-Zr(1)-C(7)-C(6)	39.6(4)
C(26)-Zr(1)-C(7)-C(6)	70.4(4)
C(23)-Zr(1)-C(7)-C(6)	29.3(5)
C(27)-Zr(1)-C(7)-C(6)	73.8(4)
C(24)-Zr(1)-C(7)-C(6)	15.5(4)
C(13)-Zr(1)-C(7)-C(6)	-167.3(4)
C(2)-Zr(1)-C(7)-C(6)	116.1(5)
C(8)-Zr(1)-C(7)-C(6)	-132.5(5)
Cl(2)-Zr(1)-C(7)-C(2)	80.8(3)
Cl(1)-Zr(1)-C(7)-C(2)	178.4(3)
C(1)-Zr(1)-C(7)-C(2)	35.1(3)
C(25)-Zr(1)-C(7)-C(2)	-76.5(3)
C(26)-Zr(1)-C(7)-C(2)	-45.6(3)
C(23)-Zr(1)-C(7)-C(2)	-86.7(4)
C(27)-Zr(1)-C(7)-C(2)	-42.3(4)
C(24)-Zr(1)-C(7)-C(2)	-100.6(3)
C(13)-Zr(1)-C(7)-C(2)	76.6(3)
C(8)-Zr(1)-C(7)-C(2)	111.5(4)
Cl(2)-Zr(1)-C(7)-C(8)	-30.7(3)
Cl(1)-Zr(1)-C(7)-C(8)	66.9(3)
C(1)-Zr(1)-C(7)-C(8)	-76.3(3)
C(25)-Zr(1)-C(7)-C(8)	172.1(3)

C(26)-Zr(1)-C(7)-C(8)	-157.1(3)
C(23)-Zr(1)-C(7)-C(8)	161.8(3)
C(27)-Zr(1)-C(7)-C(8)	-153.8(3)
C(24)-Zr(1)-C(7)-C(8)	148.0(3)
C(13)-Zr(1)-C(7)-C(8)	-34.8(3)
C(2)-Zr(1)-C(7)-C(8)	-111.5(4)
C(6)-C(7)-C(8)-C(13)	175.3(5)
C(2)-C(7)-C(8)-C(13)	-8.7(5)
Zr(1)-C(7)-C(8)-C(13)	60.9(4)
C(6)-C(7)-C(8)-C(9)	-14.4(9)
C(2)-C(7)-C(8)-C(9)	161.6(5)
Zr(1)-C(7)-C(8)-C(9)	-128.8(6)
C(6)-C(7)-C(8)-Zr(1)	114.4(6)
C(2)-C(7)-C(8)-Zr(1)	-69.6(3)
Cl(2)-Zr(1)-C(8)-C(13)	39.7(3)
Cl(1)-Zr(1)-C(8)-C(13)	131.7(3)
C(1)-Zr(1)-C(8)-C(13)	-38.0(3)
C(25)-Zr(1)-C(8)-C(13)	-127.2(3)
C(26)-Zr(1)-C(8)-C(13)	-89.0(3)
C(23)-Zr(1)-C(8)-C(13)	-176.4(6)
C(27)-Zr(1)-C(8)-C(13)	-62.5(5)
C(24)-Zr(1)-C(8)-C(13)	-162.7(3)
C(7)-Zr(1)-C(8)-C(13)	-118.2(4)
C(2)-Zr(1)-C(8)-C(13)	-79.3(3)
Cl(2)-Zr(1)-C(8)-C(9)	-72.6(5)
Cl(1)-Zr(1)-C(8)-C(9)	19.4(5)
C(1)-Zr(1)-C(8)-C(9)	-150.4(6)
C(25)-Zr(1)-C(8)-C(9)	120.5(5)
C(26)-Zr(1)-C(8)-C(9)	158.6(5)
C(23)-Zr(1)-C(8)-C(9)	71.2(9)
C(27)-Zr(1)-C(8)-C(9)	-174.8(4)
C(24)-Zr(1)-C(8)-C(9)	84.9(5)
C(13)-Zr(1)-C(8)-C(9)	-112.4(6)
C(7)-Zr(1)-C(8)-C(9)	129.5(6)
C(2)-Zr(1)-C(8)-C(9)	168.4(6)
Cl(2)-Zr(1)-C(8)-C(7)	157.9(3)
Cl(1)-Zr(1)-C(8)-C(7)	-110.1(3)
C(1)-Zr(1)-C(8)-C(7)	80.2(3)
C(25)-Zr(1)-C(8)-C(7)	-9.0(3)
C(26)-Zr(1)-C(8)-C(7)	29.1(4)
C(23)-Zr(1)-C(8)-C(7)	-58.2(8)
C(27)-Zr(1)-C(8)-C(7)	55.7(5)
C(24)-Zr(1)-C(8)-C(7)	-44.5(4)
C(13)-Zr(1)-C(8)-C(7)	118.2(4)
C(2)-Zr(1)-C(8)-C(7)	38.9(3)
C(13)-C(8)-C(9)-C(10)	-12.4(7)

C(7)-C(8)-C(9)-C(10)	178.2(5)
Zr(1)-C(8)-C(9)-C(10)	76.6(6)
C(13)-C(8)-C(9)-C(19)	156.4(5)
C(7)-C(8)-C(9)-C(19)	-13.0(8)
Zr(1)-C(8)-C(9)-C(19)	-114.6(5)
C(8)-C(9)-C(10)-C(11)	8.4(8)
C(19)-C(9)-C(10)-C(11)	-160.5(5)
C(8)-C(9)-C(10)-C(20)	-175.1(5)
C(19)-C(9)-C(10)-C(20)	16.0(8)
C(9)-C(10)-C(11)-C(12)	0.9(8)
C(20)-C(10)-C(11)-C(12)	-175.7(5)
C(9)-C(10)-C(11)-C(21)	176.1(5)
C(20)-C(10)-C(11)-C(21)	-0.5(8)
C(10)-C(11)-C(12)-C(13)	-6.0(8)
C(21)-C(11)-C(12)-C(13)	178.9(5)
C(10)-C(11)-C(12)-C(22)	168.2(5)
C(21)-C(11)-C(12)-C(22)	-6.9(8)
C(11)-C(12)-C(13)-C(8)	1.7(8)
C(22)-C(12)-C(13)-C(8)	-172.5(5)
C(11)-C(12)-C(13)-C(1)	179.7(5)
C(22)-C(12)-C(13)-C(1)	5.5(9)
C(11)-C(12)-C(13)-Zr(1)	-92.5(5)
C(22)-C(12)-C(13)-Zr(1)	93.2(5)
C(9)-C(8)-C(13)-C(12)	7.5(7)
C(7)-C(8)-C(13)-C(12)	179.2(4)
Zr(1)-C(8)-C(13)-C(12)	-119.7(5)
C(9)-C(8)-C(13)-C(1)	-170.9(4)
C(7)-C(8)-C(13)-C(1)	0.8(6)
Zr(1)-C(8)-C(13)-C(1)	61.9(3)
C(9)-C(8)-C(13)-Zr(1)	127.2(4)
C(7)-C(8)-C(13)-Zr(1)	-61.1(3)
C(2)-C(1)-C(13)-C(12)	-170.7(5)
C(14)-C(1)-C(13)-C(12)	-3.2(9)
Zr(1)-C(1)-C(13)-C(12)	113.4(6)
C(2)-C(1)-C(13)-C(8)	7.5(6)
C(14)-C(1)-C(13)-C(8)	175.0(5)
Zr(1)-C(1)-C(13)-C(8)	-68.4(4)
C(2)-C(1)-C(13)-Zr(1)	75.9(3)
C(14)-C(1)-C(13)-Zr(1)	-116.6(5)
Cl(2)-Zr(1)-C(13)-C(12)	-23.5(4)
Cl(1)-Zr(1)-C(13)-C(12)	70.2(4)
C(1)-Zr(1)-C(13)-C(12)	-126.4(6)
C(25)-Zr(1)-C(13)-C(12)	-168.5(4)
C(26)-Zr(1)-C(13)-C(12)	-129.2(4)
C(23)-Zr(1)-C(13)-C(12)	-64.8(8)
C(27)-Zr(1)-C(13)-C(12)	-91.3(5)

C(24)-Zr(1)-C(13)-C(12)	162.2(5)
C(7)-Zr(1)-C(13)-C(12)	153.5(5)
C(2)-Zr(1)-C(13)-C(12)	-166.1(5)
C(8)-Zr(1)-C(13)-C(12)	118.0(6)
Cl(2)-Zr(1)-C(13)-C(8)	-141.6(3)
Cl(1)-Zr(1)-C(13)-C(8)	-47.9(3)
C(1)-Zr(1)-C(13)-C(8)	115.5(4)
C(25)-Zr(1)-C(13)-C(8)	73.4(4)
C(26)-Zr(1)-C(13)-C(8)	112.8(3)
C(23)-Zr(1)-C(13)-C(8)	177.2(5)
C(27)-Zr(1)-C(13)-C(8)	150.6(3)
C(24)-Zr(1)-C(13)-C(8)	44.2(7)
C(7)-Zr(1)-C(13)-C(8)	35.5(3)
C(2)-Zr(1)-C(13)-C(8)	75.9(3)
Cl(2)-Zr(1)-C(13)-C(1)	102.9(3)
Cl(1)-Zr(1)-C(13)-C(1)	-163.4(3)
C(25)-Zr(1)-C(13)-C(1)	-42.1(4)
C(26)-Zr(1)-C(13)-C(1)	-2.7(4)
C(23)-Zr(1)-C(13)-C(1)	61.7(7)
C(27)-Zr(1)-C(13)-C(1)	35.1(4)
C(24)-Zr(1)-C(13)-C(1)	-71.3(6)
C(7)-Zr(1)-C(13)-C(1)	-80.0(3)
C(2)-Zr(1)-C(13)-C(1)	-39.6(3)
C(8)-Zr(1)-C(13)-C(1)	-115.5(4)
Cl(2)-Zr(1)-C(23)-C(27)	-78.9(3)
Cl(1)-Zr(1)-C(23)-C(27)	-173.8(3)
C(1)-Zr(1)-C(23)-C(27)	6.0(4)
C(25)-Zr(1)-C(23)-C(27)	79.5(3)
C(26)-Zr(1)-C(23)-C(27)	37.6(3)
C(24)-Zr(1)-C(23)-C(27)	117.3(4)
C(13)-Zr(1)-C(23)-C(27)	-38.1(7)
C(7)-Zr(1)-C(23)-C(27)	92.2(4)
C(2)-Zr(1)-C(23)-C(27)	49.6(4)
C(8)-Zr(1)-C(23)-C(27)	135.8(6)
Cl(2)-Zr(1)-C(23)-C(24)	163.8(3)
Cl(1)-Zr(1)-C(23)-C(24)	69.0(3)
C(1)-Zr(1)-C(23)-C(24)	-111.2(3)
C(25)-Zr(1)-C(23)-C(24)	-37.8(3)
C(26)-Zr(1)-C(23)-C(24)	-79.6(3)
C(27)-Zr(1)-C(23)-C(24)	-117.3(4)
C(13)-Zr(1)-C(23)-C(24)	-155.3(5)
C(7)-Zr(1)-C(23)-C(24)	-25.0(4)
C(2)-Zr(1)-C(23)-C(24)	-67.7(3)
C(8)-Zr(1)-C(23)-C(24)	18.5(8)
C(27)-C(23)-C(24)-C(25)	-3.6(6)
Zr(1)-C(23)-C(24)-C(25)	62.8(3)

C(27)-C(23)-C(24)-Si(2)	161.3(4)
Zr(1)-C(23)-C(24)-Si(2)	-132.4(4)
C(27)-C(23)-C(24)-Zr(1)	-66.4(4)
C(31)-Si(2)-C(24)-C(25)	-40.8(6)
C(33)-Si(2)-C(24)-C(25)	-166.4(5)
C(32)-Si(2)-C(24)-C(25)	77.8(5)
C(31)-Si(2)-C(24)-C(23)	158.2(4)
C(33)-Si(2)-C(24)-C(23)	32.6(5)
C(32)-Si(2)-C(24)-C(23)	-83.3(5)
C(31)-Si(2)-C(24)-Zr(1)	59.0(4)
C(33)-Si(2)-C(24)-Zr(1)	-66.6(4)
C(32)-Si(2)-C(24)-Zr(1)	177.5(3)
Cl(2)-Zr(1)-C(24)-C(25)	-132.0(3)
Cl(1)-Zr(1)-C(24)-C(25)	136.7(3)
C(1)-Zr(1)-C(24)-C(25)	-9.4(4)
C(26)-Zr(1)-C(24)-C(25)	-38.3(3)
C(23)-Zr(1)-C(24)-C(25)	-113.9(4)
C(27)-Zr(1)-C(24)-C(25)	-78.3(3)
C(13)-Zr(1)-C(24)-C(25)	41.7(7)
C(7)-Zr(1)-C(24)-C(25)	49.1(3)
C(2)-Zr(1)-C(24)-C(25)	14.8(3)
C(8)-Zr(1)-C(24)-C(25)	72.2(4)
Cl(2)-Zr(1)-C(24)-C(23)	-18.1(3)
Cl(1)-Zr(1)-C(24)-C(23)	-109.4(3)
C(1)-Zr(1)-C(24)-C(23)	104.5(3)
C(25)-Zr(1)-C(24)-C(23)	113.9(4)
C(26)-Zr(1)-C(24)-C(23)	75.6(3)
C(27)-Zr(1)-C(24)-C(23)	35.6(3)
C(13)-Zr(1)-C(24)-C(23)	155.6(5)
C(7)-Zr(1)-C(24)-C(23)	163.0(3)
C(2)-Zr(1)-C(24)-C(23)	128.7(3)
C(8)-Zr(1)-C(24)-C(23)	-173.9(3)
Cl(2)-Zr(1)-C(24)-Si(2)	102.7(3)
Cl(1)-Zr(1)-C(24)-Si(2)	11.3(3)
C(1)-Zr(1)-C(24)-Si(2)	-134.7(3)
C(25)-Zr(1)-C(24)-Si(2)	-125.3(5)
C(26)-Zr(1)-C(24)-Si(2)	-163.7(4)
C(23)-Zr(1)-C(24)-Si(2)	120.8(5)
C(27)-Zr(1)-C(24)-Si(2)	156.4(4)
C(13)-Zr(1)-C(24)-Si(2)	-83.7(6)
C(7)-Zr(1)-C(24)-Si(2)	-76.2(4)
C(2)-Zr(1)-C(24)-Si(2)	-110.5(3)
C(8)-Zr(1)-C(24)-Si(2)	-53.1(4)
C(23)-C(24)-C(25)-C(26)	3.3(6)
Si(2)-C(24)-C(25)-C(26)	-160.4(4)
Zr(1)-C(24)-C(25)-C(26)	68.4(4)

C(23)-C(24)-C(25)-Zr(1)	-65.1(3)
Si(2)-C(24)-C(25)-Zr(1)	131.2(4)
Cl(2)-Zr(1)-C(25)-C(26)	-45.3(4)
Cl(1)-Zr(1)-C(25)-C(26)	-158.2(3)
C(1)-Zr(1)-C(25)-C(26)	59.9(3)
C(23)-Zr(1)-C(25)-C(26)	-76.0(3)
C(27)-Zr(1)-C(25)-C(26)	-36.2(3)
C(24)-Zr(1)-C(25)-C(26)	-113.5(4)
C(13)-Zr(1)-C(25)-C(26)	82.5(4)
C(7)-Zr(1)-C(25)-C(26)	112.3(3)
C(2)-Zr(1)-C(25)-C(26)	80.5(3)
C(8)-Zr(1)-C(25)-C(26)	117.1(3)
Cl(2)-Zr(1)-C(25)-C(24)	68.2(3)
Cl(1)-Zr(1)-C(25)-C(24)	-44.6(3)
C(1)-Zr(1)-C(25)-C(24)	173.5(3)
C(26)-Zr(1)-C(25)-C(24)	113.5(4)
C(23)-Zr(1)-C(25)-C(24)	37.5(3)
C(27)-Zr(1)-C(25)-C(24)	77.3(3)
C(13)-Zr(1)-C(25)-C(24)	-164.0(3)
C(7)-Zr(1)-C(25)-C(24)	-134.2(3)
C(2)-Zr(1)-C(25)-C(24)	-166.0(3)
C(8)-Zr(1)-C(25)-C(24)	-129.4(3)
C(24)-C(25)-C(26)-C(27)	-2.0(6)
Zr(1)-C(25)-C(26)-C(27)	68.7(4)
C(24)-C(25)-C(26)-Zr(1)	-70.7(4)
Cl(2)-Zr(1)-C(26)-C(27)	32.0(3)
Cl(1)-Zr(1)-C(26)-C(27)	-85.0(3)
C(1)-Zr(1)-C(26)-C(27)	121.0(3)
C(25)-Zr(1)-C(26)-C(27)	-115.6(4)
C(23)-Zr(1)-C(26)-C(27)	-37.5(3)
C(24)-Zr(1)-C(26)-C(27)	-78.0(3)
C(13)-Zr(1)-C(26)-C(27)	122.5(3)
C(7)-Zr(1)-C(26)-C(27)	175.3(3)
C(2)-Zr(1)-C(26)-C(27)	152.2(3)
C(8)-Zr(1)-C(26)-C(27)	160.1(3)
Cl(2)-Zr(1)-C(26)-C(25)	147.6(3)
Cl(1)-Zr(1)-C(26)-C(25)	30.6(4)
C(1)-Zr(1)-C(26)-C(25)	-123.4(3)
C(23)-Zr(1)-C(26)-C(25)	78.1(3)
C(27)-Zr(1)-C(26)-C(25)	115.6(4)
C(24)-Zr(1)-C(26)-C(25)	37.6(3)
C(13)-Zr(1)-C(26)-C(25)	-121.8(3)
C(7)-Zr(1)-C(26)-C(25)	-69.1(3)
C(2)-Zr(1)-C(26)-C(25)	-92.2(3)
C(8)-Zr(1)-C(26)-C(25)	-84.3(3)
C(25)-C(26)-C(27)-C(23)	-0.2(6)

Zr(1)-C(26)-C(27)-C(23)	65.8(3)
C(25)-C(26)-C(27)-Si(1)	163.7(4)
Zr(1)-C(26)-C(27)-Si(1)	-130.4(4)
C(25)-C(26)-C(27)-Zr(1)	-65.9(4)
C(24)-C(23)-C(27)-C(26)	2.3(6)
Zr(1)-C(23)-C(27)-C(26)	-64.1(3)
C(24)-C(23)-C(27)-Si(1)	-162.1(4)
Zr(1)-C(23)-C(27)-Si(1)	131.4(4)
C(24)-C(23)-C(27)-Zr(1)	66.4(4)
C(30)-Si(1)-C(27)-C(26)	48.3(5)
C(28)-Si(1)-C(27)-C(26)	-70.4(5)
C(29)-Si(1)-C(27)-C(26)	173.2(5)
C(30)-Si(1)-C(27)-C(23)	-150.6(4)
C(28)-Si(1)-C(27)-C(23)	90.7(5)
C(29)-Si(1)-C(27)-C(23)	-25.7(5)
C(30)-Si(1)-C(27)-Zr(1)	-50.8(4)
C(28)-Si(1)-C(27)-Zr(1)	-169.5(4)
C(29)-Si(1)-C(27)-Zr(1)	74.1(4)
Cl(2)-Zr(1)-C(27)-C(26)	-149.2(3)
Cl(1)-Zr(1)-C(27)-C(26)	121.4(3)
C(1)-Zr(1)-C(27)-C(26)	-61.8(3)
C(25)-Zr(1)-C(27)-C(26)	37.4(3)
C(23)-Zr(1)-C(27)-C(26)	113.9(4)
C(24)-Zr(1)-C(27)-C(26)	77.9(3)
C(13)-Zr(1)-C(27)-C(26)	-80.9(4)
C(7)-Zr(1)-C(27)-C(26)	-6.2(4)
C(2)-Zr(1)-C(27)-C(26)	-28.0(3)
C(8)-Zr(1)-C(27)-C(26)	-41.6(5)
Cl(2)-Zr(1)-C(27)-C(23)	97.0(3)
Cl(1)-Zr(1)-C(27)-C(23)	7.6(3)
C(1)-Zr(1)-C(27)-C(23)	-175.7(3)
C(25)-Zr(1)-C(27)-C(23)	-76.4(3)
C(26)-Zr(1)-C(27)-C(23)	-113.9(4)
C(24)-Zr(1)-C(27)-C(23)	-36.0(3)
C(13)-Zr(1)-C(27)-C(23)	165.2(3)
C(7)-Zr(1)-C(27)-C(23)	-120.1(3)
C(2)-Zr(1)-C(27)-C(23)	-141.8(3)
C(8)-Zr(1)-C(27)-C(23)	-155.5(4)
Cl(2)-Zr(1)-C(27)-Si(1)	-25.1(3)
Cl(1)-Zr(1)-C(27)-Si(1)	-114.5(3)
C(1)-Zr(1)-C(27)-Si(1)	62.3(4)
C(25)-Zr(1)-C(27)-Si(1)	161.5(4)
C(26)-Zr(1)-C(27)-Si(1)	124.1(5)
C(23)-Zr(1)-C(27)-Si(1)	-122.1(5)
C(24)-Zr(1)-C(27)-Si(1)	-158.0(4)
C(13)-Zr(1)-C(27)-Si(1)	43.2(4)

C(7)-Zr(1)-C(27)-Si(1)	117.9(3)
C(2)-Zr(1)-C(27)-Si(1)	96.1(3)
C(8)-Zr(1)-C(27)-Si(1)	82.5(5)

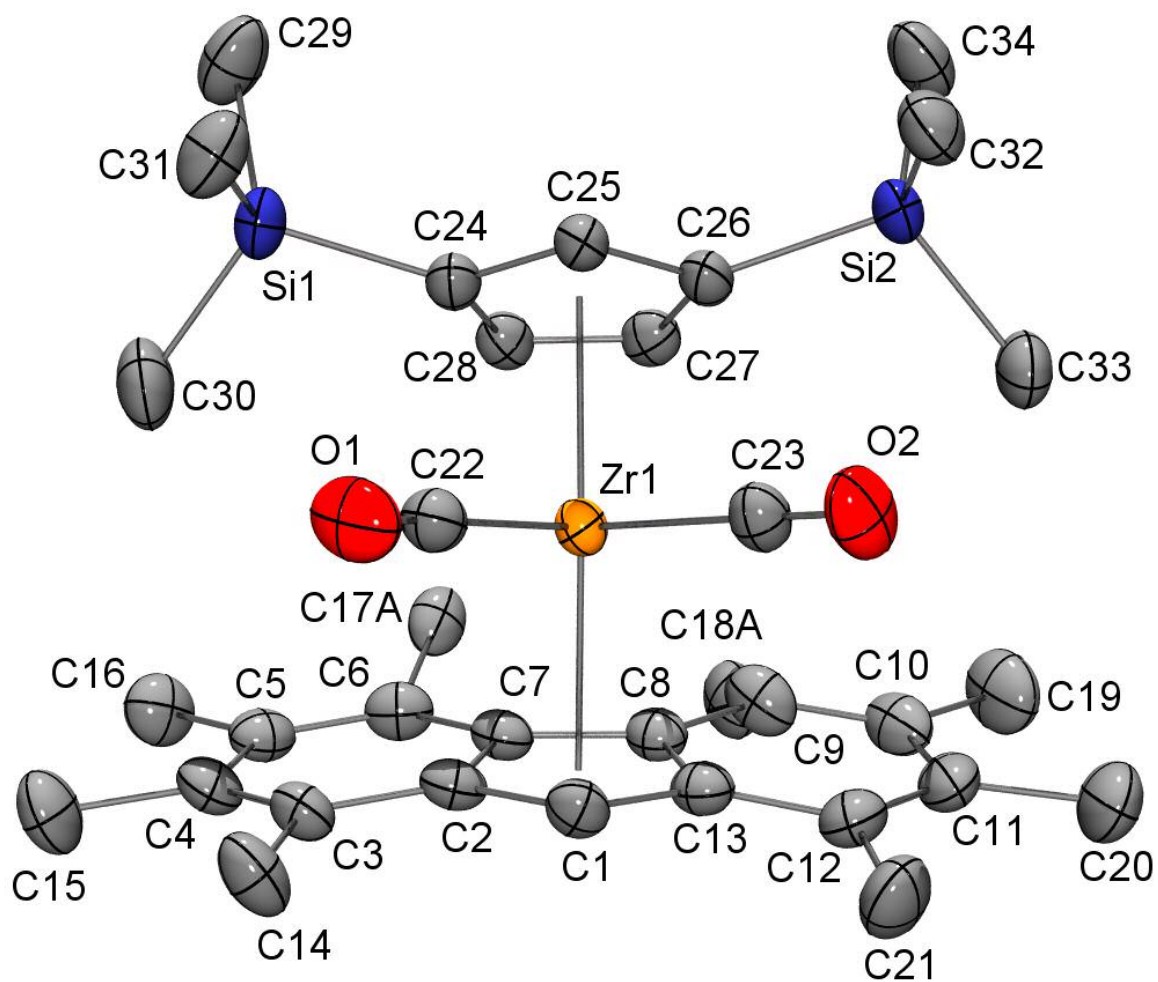


Figure 2. Thermal ellipsoid plot for compound **6**. Hydrogen atoms and one set of disordered atoms (C17B and C18B) have been omitted for clarity. Thermal ellipsoids are drawn at 50% probability.

B. Crystal data and structure refinement for Cp"Flu"Zr(CO)₂ (**6**).

Empirical formula	C ₃₄ H ₄₆ O ₂ Si ₂ Zr
Formula weight	634.11
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/n
Unit cell dimensions	a = 11.8741(9) Å α = 90° b = 15.1861(11) Å β = 103.3300(10)° c = 18.4029(14) Å γ = 90°
Volume	3229.0(4) Å ³
Z	4
Calculated density	1.304 Mg/m ³
Absorption coefficient	0.443 mm ⁻¹
F(000)	1336
Crystal size	0.4 x 0.3 x 0.25 mm
Theta range for data collection	1.76 to 23.27 deg.
Limiting indices	-13 ≤ h ≤ 13, -16 ≤ k ≤ 14, -20 ≤ l ≤ 20
Reflections collected	14314
Independent reflections	4634 (R _{int} = 0.0226)
Completeness to theta = 23.27°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.890 and 0.781
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4634 / 0 / 370
Goodness-of-fit on F ²	1.032
Final R indices [I > 2sigma(I)]	R1 = 0.0364, wR2 = 0.0981
R indices (all data)	R1 = 0.0434, wR2 = 0.1026
Largest diff. peak and hole	1.237 and -0.476 eÅ ⁻³

Table 6. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for Cp"Flu"Zr(CO)₂ (**6**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zr(1)	4508(1)	6480(1)	2588(1)	25(1)
Si(1)	1590(1)	5373(1)	1499(1)	33(1)
O(1)	2097(2)	7574(2)	2627(1)	54(1)
C(1)	5034(3)	7084(2)	3865(2)	31(1)
Si(2)	5765(1)	6855(1)	769(1)	33(1)
O(2)	5343(3)	8442(2)	2122(2)	50(1)
C(2)	4475(3)	6276(2)	3956(2)	30(1)
C(3)	3441(3)	6132(2)	4212(2)	32(1)
C(4)	3093(3)	5287(2)	4285(2)	36(1)
C(5)	3744(3)	4565(2)	4100(2)	35(1)
C(6)	4749(3)	4676(2)	3857(2)	35(1)
C(7)	5159(3)	5559(2)	3778(2)	30(1)
C(8)	6206(3)	5953(2)	3604(2)	31(1)
C(9)	7223(3)	5634(2)	3389(2)	42(1)
C(10)	8079(3)	6224(3)	3327(2)	42(1)
C(11)	8003(3)	7144(3)	3462(2)	43(1)
C(12)	7044(3)	7482(2)	3662(2)	37(1)
C(13)	6121(3)	6892(2)	3709(2)	32(1)
C(14)	2813(3)	6926(2)	4411(2)	45(1)
C(15)	2007(4)	5093(3)	4555(2)	49(1)
C(16)	3286(4)	3646(2)	4180(2)	47(1)
C(19)	9166(4)	5888(3)	3113(3)	61(1)
C(20)	8974(3)	7744(3)	3360(2)	57(1)
C(21)	6906(4)	8437(2)	3861(2)	53(1)
C(22)	2911(3)	7174(2)	2609(2)	34(1)
C(23)	5050(3)	7764(2)	2279(2)	34(1)
C(24)	3131(3)	5690(2)	1579(2)	29(1)
C(25)	3607(3)	6403(2)	1243(2)	27(1)
C(26)	4811(3)	6270(2)	1293(2)	30(1)
C(28)	4082(3)	5107(2)	1847(2)	30(1)
C(27)	5080(3)	5456(2)	1674(2)	31(1)
C(29)	1262(4)	4496(3)	768(2)	55(1)
C(30)	1439(4)	4916(3)	2403(2)	54(1)
C(31)	578(3)	6308(2)	1190(2)	46(1)
C(32)	5031(3)	7880(2)	345(2)	43(1)
C(33)	7211(3)	7081(3)	1391(2)	46(1)
C(34)	5967(4)	6081(3)	18(2)	51(1)
C(17A)	5216(9)	3902(7)	3452(7)	38(2)
C(18A)	7645(10)	4687(8)	3525(7)	50(3)

C(17B)	5509(6)	3858(4)	3883(4)	39(2)
C(18B)	7250(6)	4683(5)	3056(4)	43(2)

Table 7. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Cp"Flu"Zr(CO)₂ (**6**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \dots + 2hka^*b^*U^{12}]$.

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Zr(1)	26(1)	25(1)	26(1)	0(1)	8(1)	2(1)
Si(1)	27(1)	31(1)	41(1)	0(1)	10(1)	-4(1)
O(1)	46(2)	68(2)	49(2)	-2(1)	12(1)	24(2)
C(1)	36(2)	28(2)	30(2)	-5(1)	10(2)	2(1)
Si(2)	31(1)	39(1)	31(1)	1(1)	13(1)	-4(1)
O(2)	68(2)	32(2)	59(2)	-3(1)	29(2)	-8(1)
C(2)	39(2)	28(2)	21(2)	1(1)	5(1)	5(1)
C(3)	37(2)	35(2)	26(2)	1(1)	11(2)	6(2)
C(4)	45(2)	40(2)	25(2)	4(2)	10(2)	1(2)
C(5)	44(2)	33(2)	24(2)	4(1)	2(2)	0(2)
C(6)	40(2)	29(2)	32(2)	-2(1)	4(2)	8(2)
C(7)	33(2)	35(2)	21(2)	0(1)	4(1)	6(2)
C(8)	31(2)	36(2)	24(2)	1(1)	3(1)	5(2)
C(9)	44(2)	43(2)	41(2)	5(2)	14(2)	15(2)
C(10)	27(2)	64(3)	33(2)	5(2)	4(2)	14(2)
C(11)	30(2)	64(3)	31(2)	0(2)	0(2)	-8(2)
C(12)	35(2)	42(2)	31(2)	-4(2)	0(2)	-2(2)
C(13)	31(2)	38(2)	25(2)	-2(1)	3(1)	4(2)
C(14)	58(3)	39(2)	46(2)	2(2)	30(2)	6(2)
C(15)	56(3)	45(2)	53(2)	9(2)	27(2)	-2(2)
C(16)	58(3)	35(2)	47(2)	5(2)	13(2)	-2(2)
C(19)	37(2)	86(3)	62(3)	6(2)	16(2)	15(2)
C(20)	36(2)	78(3)	57(3)	-1(2)	7(2)	-13(2)
C(21)	50(3)	47(2)	61(3)	-14(2)	13(2)	-16(2)
C(22)	36(2)	37(2)	30(2)	-1(2)	7(2)	1(2)
C(23)	38(2)	31(2)	35(2)	-3(2)	14(2)	0(2)
C(24)	31(2)	31(2)	27(2)	-3(1)	8(1)	-3(1)
C(25)	27(2)	31(2)	25(2)	0(1)	6(1)	-1(1)
C(26)	32(2)	33(2)	26(2)	-4(1)	10(1)	-5(1)
C(28)	36(2)	26(2)	30(2)	-3(1)	10(2)	-1(1)
C(27)	31(2)	31(2)	30(2)	-6(1)	8(1)	4(1)
C(29)	41(2)	47(2)	72(3)	-18(2)	8(2)	-8(2)

C(30)	41(2)	64(3)	64(3)	15(2)	23(2)	-4(2)
C(31)	34(2)	40(2)	60(2)	-2(2)	3(2)	0(2)
C(32)	46(2)	48(2)	38(2)	8(2)	15(2)	-2(2)
C(33)	33(2)	60(3)	48(2)	7(2)	13(2)	-7(2)
C(34)	64(3)	54(3)	44(2)	-1(2)	31(2)	-4(2)
C(17A)	35(6)	32(5)	45(7)	13(6)	3(6)	0(4)
C(18A)	36(7)	62(7)	56(7)	3(7)	19(6)	4(5)
C(17B)	48(5)	32(3)	35(4)	4(3)	9(4)	6(3)
C(18B)	39(4)	51(4)	41(4)	7(4)	14(3)	18(3)

Table 8. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Cp"Flu"Zr(CO)₂ (6).

	x	y	z	U(eq)
H(1A)	4799	7663	4011	37
H(14A)	2139	6739	4573	67
H(14B)	2584	7299	3981	67
H(14C)	3317	7247	4805	67
H(15A)	1663	5637	4659	74
H(15B)	2202	4744	5001	74
H(15C)	1469	4776	4176	74
H(16A)	3793	3219	4039	70
H(16B)	2526	3587	3862	70
H(16C)	3249	3549	4689	70
H(19A)	9110	5262	3040	92
H(19B)	9830	6022	3505	92
H(19C)	9242	6167	2659	92
H(20A)	8799	8340	3469	86
H(20B)	9054	7706	2854	86
H(20C)	9685	7566	3693	86
H(21A)	7574	8764	3807	79
H(21B)	6830	8475	4368	79
H(21C)	6227	8676	3534	79
H(25A)	3148	6877	956	33
H(28A)	4021	4519	2055	36
H(27A)	5826	5152	1750	37
H(29A)	1778	4008	916	82
H(29B)	1361	4728	302	82
H(29C)	477	4301	713	82
H(30A)	1607	5366	2779	82

H(30B)	1971	4436	2544	82
H(30C)	663	4708	2357	82
H(31A)	730	6765	1559	69
H(31B)	-205	6107	1127	69
H(31C)	688	6533	723	69
H(32A)	4932	8273	735	65
H(32B)	4287	7734	36	65
H(32C)	5494	8160	48	65
H(33A)	7126	7478	1780	69
H(33B)	7707	7341	1105	69
H(33C)	7547	6539	1608	69
H(34A)	6448	6354	-271	76
H(34B)	5227	5943	-300	76
H(34C)	6329	5551	241	76
H(17A)	4875	3931	2926	58
H(17B)	5019	3352	3647	58
H(17C)	6043	3949	3534	58
H(18A)	8067	4623	4034	75
H(18B)	8140	4545	3197	75
H(18C)	6992	4295	3431	75
H(17D)	5914	3746	4389	58
H(17E)	6057	3953	3580	58
H(17F)	5031	3360	3694	58
H(18D)	6842	4684	2541	64
H(18E)	6887	4277	3330	64
H(18F)	8039	4509	3093	64

Table 9. Bond lengths [$\text{\AA}$] and angles [deg] for Cp"Flu"Zr(CO)₂ (**6**).

<i>Bonds</i>	
Zr(1)-C(23)	2.169(4)
Zr(1)-C(22)	2.178(4)
Zr(1)-C(25)	2.463(3)
Zr(1)-C(1)	2.464(3)
Zr(1)-C(28)	2.479(3)
Zr(1)-C(24)	2.482(3)
Zr(1)-C(27)	2.498(3)
Zr(1)-C(26)	2.510(3)
Zr(1)-C(8)	2.543(3)
Zr(1)-C(2)	2.547(3)
Zr(1)-C(13)	2.548(3)

Zr(1)-C(7)	2.563(3)
Si(1)-C(30)	1.850(4)
Si(1)-C(31)	1.861(4)
Si(1)-C(24)	1.865(3)
Si(1)-C(29)	1.868(4)
O(1)-C(22)	1.149(4)
C(1)-C(13)	1.415(5)
C(1)-C(2)	1.423(5)
C(1)-H(1A)	0.9800
Si(2)-C(33)	1.863(4)
Si(2)-C(32)	1.865(4)
Si(2)-C(34)	1.869(4)
Si(2)-C(26)	1.874(3)
O(2)-C(23)	1.145(4)
C(2)-C(3)	1.429(5)
C(2)-C(7)	1.441(5)
C(3)-C(4)	1.364(5)
C(3)-C(14)	1.507(5)
C(4)-C(5)	1.426(5)
C(4)-C(15)	1.515(5)
C(5)-C(6)	1.378(5)
C(5)-C(16)	1.518(5)
C(6)-C(7)	1.445(5)
C(6)-C(17B)	1.531(7)
C(6)-C(17A)	1.561(12)
C(7)-C(8)	1.480(5)
C(8)-C(9)	1.439(5)
C(8)-C(13)	1.446(5)
C(9)-C(10)	1.379(5)
C(9)-C(18A)	1.525(12)
C(9)-C(18B)	1.571(8)
C(10)-C(11)	1.425(6)
C(10)-C(19)	1.522(5)
C(11)-C(12)	1.374(5)
C(11)-C(20)	1.515(5)
C(12)-C(13)	1.433(5)
C(12)-C(21)	1.514(5)
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600

C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(24)-C(25)	1.426(4)
C(24)-C(28)	1.431(5)
C(25)-C(26)	1.426(5)
C(25)-H(25A)	0.9800
C(26)-C(27)	1.420(5)
C(28)-C(27)	1.401(5)
C(28)-H(28A)	0.9800
C(27)-H(27A)	0.9800
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600
C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
C(33)-H(33A)	0.9600
C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600
C(17A)-H(17A)	0.9600
C(17A)-H(17B)	0.9600
C(17A)-H(17C)	0.9600
C(18A)-H(18A)	0.9600
C(18A)-H(18B)	0.9600
C(18A)-H(18C)	0.9600
C(17B)-H(17D)	0.9600
C(17B)-H(17E)	0.9600
C(17B)-H(17F)	0.9600
C(18B)-H(18D)	0.9600
C(18B)-H(18E)	0.9600

C(18B)-H(18F) 0.9600

Angles

C(23)-Zr(1)-C(22)	83.22(13)
C(23)-Zr(1)-C(25)	82.34(12)
C(22)-Zr(1)-C(25)	82.12(11)
C(23)-Zr(1)-C(1)	83.69(12)
C(22)-Zr(1)-C(1)	80.38(12)
C(25)-Zr(1)-C(1)	158.74(11)
C(23)-Zr(1)-C(28)	130.38(11)
C(22)-Zr(1)-C(28)	110.42(12)
C(25)-Zr(1)-C(28)	54.61(11)
C(1)-Zr(1)-C(28)	144.24(11)
C(23)-Zr(1)-C(24)	115.01(12)
C(22)-Zr(1)-C(24)	79.70(12)
C(25)-Zr(1)-C(24)	33.51(10)
C(1)-Zr(1)-C(24)	150.60(11)
C(28)-Zr(1)-C(24)	33.52(11)
C(23)-Zr(1)-C(27)	103.93(11)
C(22)-Zr(1)-C(27)	133.38(12)
C(25)-Zr(1)-C(27)	54.26(11)
C(1)-Zr(1)-C(27)	145.61(11)
C(28)-Zr(1)-C(27)	32.69(11)
C(24)-Zr(1)-C(27)	55.22(11)
C(23)-Zr(1)-C(26)	75.54(11)
C(22)-Zr(1)-C(26)	113.26(12)
C(25)-Zr(1)-C(26)	33.31(11)
C(1)-Zr(1)-C(26)	153.13(11)
C(28)-Zr(1)-C(26)	55.03(11)
C(24)-Zr(1)-C(26)	56.10(10)
C(27)-Zr(1)-C(26)	32.95(11)
C(23)-Zr(1)-C(8)	104.04(12)
C(22)-Zr(1)-C(8)	133.23(11)
C(25)-Zr(1)-C(8)	144.24(10)
C(1)-Zr(1)-C(8)	55.39(11)
C(28)-Zr(1)-C(8)	99.57(11)
C(24)-Zr(1)-C(8)	132.22(11)
C(27)-Zr(1)-C(8)	90.39(10)
C(26)-Zr(1)-C(8)	113.28(11)
C(23)-Zr(1)-C(2)	116.20(11)
C(22)-Zr(1)-C(2)	80.14(11)
C(25)-Zr(1)-C(2)	152.34(11)
C(1)-Zr(1)-C(2)	32.94(11)
C(28)-Zr(1)-C(2)	113.15(10)
C(24)-Zr(1)-C(2)	121.53(11)

C(27)-Zr(1)-C(2)	131.19(10)
C(26)-Zr(1)-C(2)	163.97(11)
C(8)-Zr(1)-C(2)	54.87(10)
C(23)-Zr(1)-C(13)	77.19(12)
C(22)-Zr(1)-C(13)	111.18(11)
C(25)-Zr(1)-C(13)	153.76(10)
C(1)-Zr(1)-C(13)	32.74(10)
C(28)-Zr(1)-C(13)	132.20(11)
C(24)-Zr(1)-C(13)	165.20(11)
C(27)-Zr(1)-C(13)	115.34(11)
C(26)-Zr(1)-C(13)	123.67(10)
C(8)-Zr(1)-C(13)	33.00(11)
C(2)-Zr(1)-C(13)	53.80(11)
C(23)-Zr(1)-C(7)	131.69(12)
C(22)-Zr(1)-C(7)	109.93(11)
C(25)-Zr(1)-C(7)	143.89(10)
C(1)-Zr(1)-C(7)	55.13(10)
C(28)-Zr(1)-C(7)	89.61(10)
C(24)-Zr(1)-C(7)	113.07(11)
C(27)-Zr(1)-C(7)	99.20(10)
C(26)-Zr(1)-C(7)	131.31(11)
C(8)-Zr(1)-C(7)	33.69(11)
C(2)-Zr(1)-C(7)	32.76(10)
C(13)-Zr(1)-C(7)	54.57(11)
C(30)-Si(1)-C(31)	111.82(19)
C(30)-Si(1)-C(24)	108.81(17)
C(31)-Si(1)-C(24)	112.32(16)
C(30)-Si(1)-C(29)	109.4(2)
C(31)-Si(1)-C(29)	108.12(19)
C(24)-Si(1)-C(29)	106.22(16)
C(13)-C(1)-C(2)	108.6(3)
C(13)-C(1)-Zr(1)	76.87(18)
C(2)-C(1)-Zr(1)	76.72(18)
C(13)-C(1)-H(1A)	124.8
C(2)-C(1)-H(1A)	124.8
Zr(1)-C(1)-H(1A)	124.8
C(33)-Si(2)-C(32)	112.28(18)
C(33)-Si(2)-C(34)	108.23(19)
C(32)-Si(2)-C(34)	110.08(18)
C(33)-Si(2)-C(26)	110.59(16)
C(32)-Si(2)-C(26)	109.31(16)
C(34)-Si(2)-C(26)	106.16(16)
C(1)-C(2)-C(3)	129.1(3)
C(1)-C(2)-C(7)	108.8(3)
C(3)-C(2)-C(7)	122.1(3)
C(1)-C(2)-Zr(1)	70.34(17)

C(3)-C(2)-Zr(1)	123.7(2)
C(7)-C(2)-Zr(1)	74.25(17)
C(4)-C(3)-C(2)	118.6(3)
C(4)-C(3)-C(14)	123.5(3)
C(2)-C(3)-C(14)	117.9(3)
C(3)-C(4)-C(5)	120.5(3)
C(3)-C(4)-C(15)	121.0(3)
C(5)-C(4)-C(15)	118.5(3)
C(6)-C(5)-C(4)	122.7(3)
C(6)-C(5)-C(16)	120.0(3)
C(4)-C(5)-C(16)	117.3(3)
C(5)-C(6)-C(7)	119.0(3)
C(5)-C(6)-C(17B)	116.0(4)
C(7)-C(6)-C(17B)	123.1(4)
C(5)-C(6)-C(17A)	119.5(5)
C(7)-C(6)-C(17A)	119.0(5)
C(17B)-C(6)-C(17A)	29.6(4)
C(2)-C(7)-C(6)	117.2(3)
C(2)-C(7)-C(8)	106.8(3)
C(6)-C(7)-C(8)	135.8(3)
C(2)-C(7)-Zr(1)	72.99(17)
C(6)-C(7)-Zr(1)	123.4(2)
C(8)-C(7)-Zr(1)	72.40(17)
C(9)-C(8)-C(13)	117.3(3)
C(9)-C(8)-C(7)	136.3(3)
C(13)-C(8)-C(7)	106.4(3)
C(9)-C(8)-Zr(1)	118.5(2)
C(13)-C(8)-Zr(1)	73.68(18)
C(7)-C(8)-Zr(1)	73.91(17)
C(10)-C(9)-C(8)	119.0(3)
C(10)-C(9)-C(18A)	114.0(5)
C(8)-C(9)-C(18A)	122.5(5)
C(10)-C(9)-C(18B)	118.9(4)
C(8)-C(9)-C(18B)	120.8(4)
C(18A)-C(9)-C(18B)	33.1(4)
C(9)-C(10)-C(11)	123.1(3)
C(9)-C(10)-C(19)	119.2(4)
C(11)-C(10)-C(19)	117.7(4)
C(12)-C(11)-C(10)	120.1(3)
C(12)-C(11)-C(20)	120.7(4)
C(10)-C(11)-C(20)	119.2(4)
C(11)-C(12)-C(13)	118.4(3)
C(11)-C(12)-C(21)	124.4(3)
C(13)-C(12)-C(21)	117.2(3)
C(1)-C(13)-C(12)	129.0(3)
C(1)-C(13)-C(8)	108.9(3)

C(12)-C(13)-C(8)	122.0(3)
C(1)-C(13)-Zr(1)	70.39(18)
C(12)-C(13)-Zr(1)	123.1(2)
C(8)-C(13)-Zr(1)	73.32(18)
C(3)-C(14)-H(14A)	109.5
C(3)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(3)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(4)-C(15)-H(15A)	109.5
C(4)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(4)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(5)-C(16)-H(16A)	109.5
C(5)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(5)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(10)-C(19)-H(19A)	109.5
C(10)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(10)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(11)-C(20)-H(20A)	109.5
C(11)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(11)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(12)-C(21)-H(21A)	109.5
C(12)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(12)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
O(1)-C(22)-Zr(1)	177.0(3)
O(2)-C(23)-Zr(1)	179.4(4)
C(25)-C(24)-C(28)	105.1(3)
C(25)-C(24)-Si(1)	129.9(2)
C(28)-C(24)-Si(1)	123.3(2)
C(25)-C(24)-Zr(1)	72.49(18)

C(28)-C(24)-Zr(1)	73.12(18)
Si(1)-C(24)-Zr(1)	130.48(15)
C(24)-C(25)-C(26)	110.8(3)
C(24)-C(25)-Zr(1)	74.00(18)
C(26)-C(25)-Zr(1)	75.16(18)
C(24)-C(25)-H(25A)	124.3
C(26)-C(25)-H(25A)	124.3
Zr(1)-C(25)-H(25A)	124.3
C(27)-C(26)-C(25)	105.3(3)
C(27)-C(26)-Si(2)	124.9(3)
C(25)-C(26)-Si(2)	128.0(2)
C(27)-C(26)-Zr(1)	73.05(17)
C(25)-C(26)-Zr(1)	71.53(17)
Si(2)-C(26)-Zr(1)	131.65(16)
C(27)-C(28)-C(24)	109.2(3)
C(27)-C(28)-Zr(1)	74.38(18)
C(24)-C(28)-Zr(1)	73.36(18)
C(27)-C(28)-H(28A)	125.1
C(24)-C(28)-H(28A)	125.1
Zr(1)-C(28)-H(28A)	125.1
C(28)-C(27)-C(26)	109.6(3)
C(28)-C(27)-Zr(1)	72.94(18)
C(26)-C(27)-Zr(1)	74.00(18)
C(28)-C(27)-H(27A)	125.0
C(26)-C(27)-H(27A)	125.0
Zr(1)-C(27)-H(27A)	125.0
Si(1)-C(29)-H(29A)	109.5
Si(1)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
Si(1)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
Si(1)-C(30)-H(30A)	109.5
Si(1)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
Si(1)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
Si(1)-C(31)-H(31A)	109.5
Si(1)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
Si(1)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
Si(2)-C(32)-H(32A)	109.5
Si(2)-C(32)-H(32B)	109.5

H(32A)-C(32)-H(32B)	109.5
Si(2)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
Si(2)-C(33)-H(33A)	109.5
Si(2)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
Si(2)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
Si(2)-C(34)-H(34A)	109.5
Si(2)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
Si(2)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(6)-C(17A)-H(17A)	109.5
C(6)-C(17A)-H(17B)	109.5
H(17A)-C(17A)-H(17B)	109.5
C(6)-C(17A)-H(17C)	109.5
H(17A)-C(17A)-H(17C)	109.5
H(17B)-C(17A)-H(17C)	109.5
C(9)-C(18A)-H(18A)	109.5
C(9)-C(18A)-H(18B)	109.5
H(18A)-C(18A)-H(18B)	109.5
C(9)-C(18A)-H(18C)	109.5
H(18A)-C(18A)-H(18C)	109.5
H(18B)-C(18A)-H(18C)	109.5
C(6)-C(17B)-H(17D)	109.5
C(6)-C(17B)-H(17E)	109.5
H(17D)-C(17B)-H(17E)	109.5
C(6)-C(17B)-H(17F)	109.5
H(17D)-C(17B)-H(17F)	109.5
H(17E)-C(17B)-H(17F)	109.5
C(9)-C(18B)-H(18D)	109.5
C(9)-C(18B)-H(18E)	109.5
H(18D)-C(18B)-H(18E)	109.5
C(9)-C(18B)-H(18F)	109.5
H(18D)-C(18B)-H(18F)	109.5
H(18E)-C(18B)-H(18F)	109.5

Table 10. Torsion angles [deg] for Cp^{Flu}Zr(CO)₂ (**6**).

C(23)-Zr(1)-C(1)-C(13)	-76.1(2)
C(22)-Zr(1)-C(1)-C(13)	-160.2(2)
C(25)-Zr(1)-C(1)-C(13)	-125.2(3)
C(28)-Zr(1)-C(1)-C(13)	88.0(3)
C(24)-Zr(1)-C(1)-C(13)	151.8(2)
C(27)-Zr(1)-C(1)-C(13)	29.4(3)
C(26)-Zr(1)-C(1)-C(13)	-36.8(3)
C(8)-Zr(1)-C(1)-C(13)	35.82(19)
C(2)-Zr(1)-C(1)-C(13)	113.1(3)
C(7)-Zr(1)-C(1)-C(13)	77.1(2)
C(23)-Zr(1)-C(1)-C(2)	170.9(2)
C(22)-Zr(1)-C(1)-C(2)	86.7(2)
C(25)-Zr(1)-C(1)-C(2)	121.7(3)
C(28)-Zr(1)-C(1)-C(2)	-25.0(3)
C(24)-Zr(1)-C(1)-C(2)	38.7(3)
C(27)-Zr(1)-C(1)-C(2)	-83.6(3)
C(26)-Zr(1)-C(1)-C(2)	-149.8(2)
C(8)-Zr(1)-C(1)-C(2)	-77.3(2)
C(13)-Zr(1)-C(1)-C(2)	-113.1(3)
C(7)-Zr(1)-C(1)-C(2)	-35.96(18)
C(13)-C(1)-C(2)-C(3)	171.1(3)
Zr(1)-C(1)-C(2)-C(3)	-117.9(3)
C(13)-C(1)-C(2)-C(7)	-6.2(4)
Zr(1)-C(1)-C(2)-C(7)	64.8(2)
C(13)-C(1)-C(2)-Zr(1)	-71.0(2)
C(23)-Zr(1)-C(2)-C(1)	-10.1(2)
C(22)-Zr(1)-C(2)-C(1)	-87.5(2)
C(25)-Zr(1)-C(2)-C(1)	-138.4(2)
C(28)-Zr(1)-C(2)-C(1)	164.39(18)
C(24)-Zr(1)-C(2)-C(1)	-158.87(18)
C(27)-Zr(1)-C(2)-C(1)	131.77(19)
C(26)-Zr(1)-C(2)-C(1)	124.7(4)
C(8)-Zr(1)-C(2)-C(1)	79.0(2)
C(13)-Zr(1)-C(2)-C(1)	38.07(19)
C(7)-Zr(1)-C(2)-C(1)	117.1(3)
C(23)-Zr(1)-C(2)-C(3)	114.4(3)
C(22)-Zr(1)-C(2)-C(3)	37.0(3)
C(25)-Zr(1)-C(2)-C(3)	-13.8(4)
C(1)-Zr(1)-C(2)-C(3)	124.5(4)
C(28)-Zr(1)-C(2)-C(3)	-71.1(3)
C(24)-Zr(1)-C(2)-C(3)	-34.4(3)
C(27)-Zr(1)-C(2)-C(3)	-103.7(3)
C(26)-Zr(1)-C(2)-C(3)	-110.8(4)

C(8)-Zr(1)-C(2)-C(3)	-156.5(3)
C(13)-Zr(1)-C(2)-C(3)	162.6(3)
C(7)-Zr(1)-C(2)-C(3)	-118.4(4)
C(23)-Zr(1)-C(2)-C(7)	-127.2(2)
C(22)-Zr(1)-C(2)-C(7)	155.4(2)
C(25)-Zr(1)-C(2)-C(7)	104.5(3)
C(1)-Zr(1)-C(2)-C(7)	-117.1(3)
C(28)-Zr(1)-C(2)-C(7)	47.3(2)
C(24)-Zr(1)-C(2)-C(7)	84.0(2)
C(27)-Zr(1)-C(2)-C(7)	14.7(3)
C(26)-Zr(1)-C(2)-C(7)	7.6(5)
C(8)-Zr(1)-C(2)-C(7)	-38.13(19)
C(13)-Zr(1)-C(2)-C(7)	-79.0(2)
C(1)-C(2)-C(3)-C(4)	-177.2(3)
C(7)-C(2)-C(3)-C(4)	-0.3(5)
Zr(1)-C(2)-C(3)-C(4)	91.6(3)
C(1)-C(2)-C(3)-C(14)	0.8(5)
C(7)-C(2)-C(3)-C(14)	177.8(3)
Zr(1)-C(2)-C(3)-C(14)	-90.4(3)
C(2)-C(3)-C(4)-C(5)	-0.8(5)
C(14)-C(3)-C(4)-C(5)	-178.7(3)
C(2)-C(3)-C(4)-C(15)	179.8(3)
C(14)-C(3)-C(4)-C(15)	1.9(5)
C(3)-C(4)-C(5)-C(6)	1.3(5)
C(15)-C(4)-C(5)-C(6)	-179.3(3)
C(3)-C(4)-C(5)-C(16)	-178.7(3)
C(15)-C(4)-C(5)-C(16)	0.7(5)
C(4)-C(5)-C(6)-C(7)	-0.6(5)
C(16)-C(5)-C(6)-C(7)	179.3(3)
C(4)-C(5)-C(6)-C(17B)	164.2(4)
C(16)-C(5)-C(6)-C(17B)	-15.8(5)
C(4)-C(5)-C(6)-C(17A)	-162.4(5)
C(16)-C(5)-C(6)-C(17A)	17.5(7)
C(1)-C(2)-C(7)-C(6)	178.4(3)
C(3)-C(2)-C(7)-C(6)	0.9(5)
Zr(1)-C(2)-C(7)-C(6)	-119.4(3)
C(1)-C(2)-C(7)-C(8)	2.7(3)
C(3)-C(2)-C(7)-C(8)	-174.8(3)
Zr(1)-C(2)-C(7)-C(8)	65.0(2)
C(1)-C(2)-C(7)-Zr(1)	-62.3(2)
C(3)-C(2)-C(7)-Zr(1)	120.2(3)
C(5)-C(6)-C(7)-C(2)	-0.4(5)
C(17B)-C(6)-C(7)-C(2)	-164.1(4)
C(17A)-C(6)-C(7)-C(2)	161.5(5)
C(5)-C(6)-C(7)-C(8)	173.6(3)
C(17B)-C(6)-C(7)-C(8)	9.9(6)

C(17A)-C(6)-C(7)-C(8)	-24.5(7)
C(5)-C(6)-C(7)-Zr(1)	-87.2(3)
C(17B)-C(6)-C(7)-Zr(1)	109.1(4)
C(17A)-C(6)-C(7)-Zr(1)	74.7(6)
C(23)-Zr(1)-C(7)-C(2)	73.0(2)
C(22)-Zr(1)-C(7)-C(2)	-25.9(2)
C(25)-Zr(1)-C(7)-C(2)	-130.3(2)
C(1)-Zr(1)-C(7)-C(2)	36.16(19)
C(28)-Zr(1)-C(7)-C(2)	-137.5(2)
C(24)-Zr(1)-C(7)-C(2)	-112.9(2)
C(27)-Zr(1)-C(7)-C(2)	-168.87(19)
C(26)-Zr(1)-C(7)-C(2)	-177.22(18)
C(8)-Zr(1)-C(7)-C(2)	114.5(3)
C(13)-Zr(1)-C(7)-C(2)	76.5(2)
C(23)-Zr(1)-C(7)-C(6)	-175.2(2)
C(22)-Zr(1)-C(7)-C(6)	85.9(3)
C(25)-Zr(1)-C(7)-C(6)	-18.6(4)
C(1)-Zr(1)-C(7)-C(6)	147.9(3)
C(28)-Zr(1)-C(7)-C(6)	-25.7(3)
C(24)-Zr(1)-C(7)-C(6)	-1.1(3)
C(27)-Zr(1)-C(7)-C(6)	-57.1(3)
C(26)-Zr(1)-C(7)-C(6)	-65.5(3)
C(8)-Zr(1)-C(7)-C(6)	-133.8(3)
C(2)-Zr(1)-C(7)-C(6)	111.8(3)
C(13)-Zr(1)-C(7)-C(6)	-171.8(3)
C(23)-Zr(1)-C(7)-C(8)	-41.4(2)
C(22)-Zr(1)-C(7)-C(8)	-140.32(19)
C(25)-Zr(1)-C(7)-C(8)	115.2(2)
C(1)-Zr(1)-C(7)-C(8)	-78.30(19)
C(28)-Zr(1)-C(7)-C(8)	108.06(19)
C(24)-Zr(1)-C(7)-C(8)	132.68(18)
C(27)-Zr(1)-C(7)-C(8)	76.68(19)
C(26)-Zr(1)-C(7)-C(8)	68.3(2)
C(2)-Zr(1)-C(7)-C(8)	-114.5(3)
C(13)-Zr(1)-C(7)-C(8)	-37.97(18)
C(2)-C(7)-C(8)-C(9)	-180.0(4)
C(6)-C(7)-C(8)-C(9)	5.6(7)
Zr(1)-C(7)-C(8)-C(9)	-114.6(4)
C(2)-C(7)-C(8)-C(13)	1.7(3)
C(6)-C(7)-C(8)-C(13)	-172.8(4)
Zr(1)-C(7)-C(8)-C(13)	67.1(2)
C(2)-C(7)-C(8)-Zr(1)	-65.4(2)
C(6)-C(7)-C(8)-Zr(1)	120.2(4)
C(23)-Zr(1)-C(8)-C(9)	-76.2(3)
C(22)-Zr(1)-C(8)-C(9)	-170.1(3)
C(25)-Zr(1)-C(8)-C(9)	20.2(4)

C(1)-Zr(1)-C(8)-C(9)	-148.2(3)
C(28)-Zr(1)-C(8)-C(9)	59.8(3)
C(24)-Zr(1)-C(8)-C(9)	68.4(3)
C(27)-Zr(1)-C(8)-C(9)	28.2(3)
C(26)-Zr(1)-C(8)-C(9)	3.8(3)
C(2)-Zr(1)-C(8)-C(9)	171.4(3)
C(13)-Zr(1)-C(8)-C(9)	-112.6(4)
C(7)-Zr(1)-C(8)-C(9)	134.4(4)
C(23)-Zr(1)-C(8)-C(13)	36.4(2)
C(22)-Zr(1)-C(8)-C(13)	-57.5(2)
C(25)-Zr(1)-C(8)-C(13)	132.8(2)
C(1)-Zr(1)-C(8)-C(13)	-35.54(18)
C(28)-Zr(1)-C(8)-C(13)	172.39(18)
C(24)-Zr(1)-C(8)-C(13)	-178.97(17)
C(27)-Zr(1)-C(8)-C(13)	140.86(19)
C(26)-Zr(1)-C(8)-C(13)	116.46(19)
C(2)-Zr(1)-C(8)-C(13)	-76.0(2)
C(7)-Zr(1)-C(8)-C(13)	-113.0(3)
C(23)-Zr(1)-C(8)-C(7)	149.39(18)
C(22)-Zr(1)-C(8)-C(7)	55.5(2)
C(25)-Zr(1)-C(8)-C(7)	-114.2(2)
C(1)-Zr(1)-C(8)-C(7)	77.46(19)
C(28)-Zr(1)-C(8)-C(7)	-74.61(19)
C(24)-Zr(1)-C(8)-C(7)	-66.0(2)
C(27)-Zr(1)-C(8)-C(7)	-106.14(18)
C(26)-Zr(1)-C(8)-C(7)	-130.54(18)
C(2)-Zr(1)-C(8)-C(7)	37.03(17)
C(13)-Zr(1)-C(8)-C(7)	113.0(3)
C(13)-C(8)-C(9)-C(10)	3.0(5)
C(7)-C(8)-C(9)-C(10)	-175.3(3)
Zr(1)-C(8)-C(9)-C(10)	88.4(4)
C(13)-C(8)-C(9)-C(18A)	157.6(7)
C(7)-C(8)-C(9)-C(18A)	-20.6(8)
Zr(1)-C(8)-C(9)-C(18A)	-117.0(7)
C(13)-C(8)-C(9)-C(18B)	-163.4(4)
C(7)-C(8)-C(9)-C(18B)	18.4(6)
Zr(1)-C(8)-C(9)-C(18B)	-78.0(4)
C(8)-C(9)-C(10)-C(11)	-0.4(5)
C(18A)-C(9)-C(10)-C(11)	-157.1(6)
C(18B)-C(9)-C(10)-C(11)	166.2(4)
C(8)-C(9)-C(10)-C(19)	178.9(3)
C(18A)-C(9)-C(10)-C(19)	22.2(7)
C(18B)-C(9)-C(10)-C(19)	-14.5(6)
C(9)-C(10)-C(11)-C(12)	-0.3(5)
C(19)-C(10)-C(11)-C(12)	-179.6(3)
C(9)-C(10)-C(11)-C(20)	-178.4(3)

C(19)-C(10)-C(11)-C(20)	2.3(5)
C(10)-C(11)-C(12)-C(13)	-1.7(5)
C(20)-C(11)-C(12)-C(13)	176.4(3)
C(10)-C(11)-C(12)-C(21)	176.3(3)
C(20)-C(11)-C(12)-C(21)	-5.6(6)
C(2)-C(1)-C(13)-C(12)	-171.8(3)
Zr(1)-C(1)-C(13)-C(12)	117.3(3)
C(2)-C(1)-C(13)-C(8)	7.3(4)
Zr(1)-C(1)-C(13)-C(8)	-63.6(2)
C(2)-C(1)-C(13)-Zr(1)	70.9(2)
C(11)-C(12)-C(13)-C(1)	-176.6(3)
C(21)-C(12)-C(13)-C(1)	5.3(5)
C(11)-C(12)-C(13)-C(8)	4.4(5)
C(21)-C(12)-C(13)-C(8)	-173.7(3)
C(11)-C(12)-C(13)-Zr(1)	-85.8(4)
C(21)-C(12)-C(13)-Zr(1)	96.1(3)
C(9)-C(8)-C(13)-C(1)	175.8(3)
C(7)-C(8)-C(13)-C(1)	-5.5(3)
Zr(1)-C(8)-C(13)-C(1)	61.7(2)
C(9)-C(8)-C(13)-C(12)	-5.0(5)
C(7)-C(8)-C(13)-C(12)	173.7(3)
Zr(1)-C(8)-C(13)-C(12)	-119.1(3)
C(9)-C(8)-C(13)-Zr(1)	114.1(3)
C(7)-C(8)-C(13)-Zr(1)	-67.2(2)
C(23)-Zr(1)-C(13)-C(1)	98.4(2)
C(22)-Zr(1)-C(13)-C(1)	20.9(2)
C(25)-Zr(1)-C(13)-C(1)	137.9(2)
C(28)-Zr(1)-C(13)-C(1)	-128.0(2)
C(24)-Zr(1)-C(13)-C(1)	-114.8(4)
C(27)-Zr(1)-C(13)-C(1)	-162.11(18)
C(26)-Zr(1)-C(13)-C(1)	161.03(18)
C(8)-Zr(1)-C(13)-C(1)	-117.8(3)
C(2)-Zr(1)-C(13)-C(1)	-38.31(18)
C(7)-Zr(1)-C(13)-C(1)	-79.0(2)
C(23)-Zr(1)-C(13)-C(12)	-26.1(3)
C(22)-Zr(1)-C(13)-C(12)	-103.5(3)
C(25)-Zr(1)-C(13)-C(12)	13.5(4)
C(1)-Zr(1)-C(13)-C(12)	-124.5(4)
C(28)-Zr(1)-C(13)-C(12)	107.6(3)
C(24)-Zr(1)-C(13)-C(12)	120.7(4)
C(27)-Zr(1)-C(13)-C(12)	73.4(3)
C(26)-Zr(1)-C(13)-C(12)	36.6(3)
C(8)-Zr(1)-C(13)-C(12)	117.7(4)
C(2)-Zr(1)-C(13)-C(12)	-162.8(3)
C(7)-Zr(1)-C(13)-C(12)	156.5(3)
C(23)-Zr(1)-C(13)-C(8)	-143.8(2)

C(22)-Zr(1)-C(13)-C(8)	138.76(19)
C(25)-Zr(1)-C(13)-C(8)	-104.2(3)
C(1)-Zr(1)-C(13)-C(8)	117.8(3)
C(28)-Zr(1)-C(13)-C(8)	-10.2(2)
C(24)-Zr(1)-C(13)-C(8)	3.0(5)
C(27)-Zr(1)-C(13)-C(8)	-44.3(2)
C(26)-Zr(1)-C(13)-C(8)	-81.2(2)
C(2)-Zr(1)-C(13)-C(8)	79.5(2)
C(7)-Zr(1)-C(13)-C(8)	38.81(18)
C(23)-Zr(1)-C(22)-O(1)	-26(5)
C(25)-Zr(1)-C(22)-O(1)	-110(5)
C(1)-Zr(1)-C(22)-O(1)	58(5)
C(28)-Zr(1)-C(22)-O(1)	-157(5)
C(24)-Zr(1)-C(22)-O(1)	-144(5)
C(27)-Zr(1)-C(22)-O(1)	-129(5)
C(26)-Zr(1)-C(22)-O(1)	-98(5)
C(8)-Zr(1)-C(22)-O(1)	76(5)
C(2)-Zr(1)-C(22)-O(1)	92(5)
C(13)-Zr(1)-C(22)-O(1)	47(5)
C(7)-Zr(1)-C(22)-O(1)	106(5)
C(22)-Zr(1)-C(23)-O(2)	115(36)
C(25)-Zr(1)-C(23)-O(2)	-162(100)
C(1)-Zr(1)-C(23)-O(2)	34(36)
C(28)-Zr(1)-C(23)-O(2)	-134(36)
C(24)-Zr(1)-C(23)-O(2)	-170(100)
C(27)-Zr(1)-C(23)-O(2)	-112(36)
C(26)-Zr(1)-C(23)-O(2)	-129(36)
C(8)-Zr(1)-C(23)-O(2)	-18(36)
C(2)-Zr(1)-C(23)-O(2)	40(36)
C(13)-Zr(1)-C(23)-O(2)	1(36)
C(7)-Zr(1)-C(23)-O(2)	4(36)
C(30)-Si(1)-C(24)-C(25)	-145.5(3)
C(31)-Si(1)-C(24)-C(25)	-21.2(4)
C(29)-Si(1)-C(24)-C(25)	96.9(3)
C(30)-Si(1)-C(24)-C(28)	51.9(3)
C(31)-Si(1)-C(24)-C(28)	176.2(3)
C(29)-Si(1)-C(24)-C(28)	-65.8(3)
C(30)-Si(1)-C(24)-Zr(1)	-44.1(3)
C(31)-Si(1)-C(24)-Zr(1)	80.3(2)
C(29)-Si(1)-C(24)-Zr(1)	-161.7(2)
C(23)-Zr(1)-C(24)-C(25)	13.8(2)
C(22)-Zr(1)-C(24)-C(25)	91.3(2)
C(1)-Zr(1)-C(24)-C(25)	139.3(2)
C(28)-Zr(1)-C(24)-C(25)	-112.4(3)
C(27)-Zr(1)-C(24)-C(25)	-76.17(19)
C(26)-Zr(1)-C(24)-C(25)	-36.00(18)

C(8)-Zr(1)-C(24)-C(25)	-127.91(19)
C(2)-Zr(1)-C(24)-C(25)	162.87(17)
C(13)-Zr(1)-C(24)-C(25)	-130.1(4)
C(7)-Zr(1)-C(24)-C(25)	-161.33(18)
C(23)-Zr(1)-C(24)-C(28)	126.16(19)
C(22)-Zr(1)-C(24)-C(28)	-156.4(2)
C(25)-Zr(1)-C(24)-C(28)	112.4(3)
C(1)-Zr(1)-C(24)-C(28)	-108.3(3)
C(27)-Zr(1)-C(24)-C(28)	36.19(18)
C(26)-Zr(1)-C(24)-C(28)	76.4(2)
C(8)-Zr(1)-C(24)-C(28)	-15.6(2)
C(2)-Zr(1)-C(24)-C(28)	-84.8(2)
C(13)-Zr(1)-C(24)-C(28)	-17.7(5)
C(7)-Zr(1)-C(24)-C(28)	-49.0(2)
C(23)-Zr(1)-C(24)-Si(1)	-114.1(2)
C(22)-Zr(1)-C(24)-Si(1)	-36.7(2)
C(25)-Zr(1)-C(24)-Si(1)	-127.9(3)
C(1)-Zr(1)-C(24)-Si(1)	11.4(4)
C(28)-Zr(1)-C(24)-Si(1)	119.7(3)
C(27)-Zr(1)-C(24)-Si(1)	155.9(3)
C(26)-Zr(1)-C(24)-Si(1)	-163.9(3)
C(8)-Zr(1)-C(24)-Si(1)	104.2(2)
C(2)-Zr(1)-C(24)-Si(1)	34.9(3)
C(13)-Zr(1)-C(24)-Si(1)	102.0(4)
C(7)-Zr(1)-C(24)-Si(1)	70.7(2)
C(28)-C(24)-C(25)-C(26)	0.4(3)
Si(1)-C(24)-C(25)-C(26)	-164.6(2)
Zr(1)-C(24)-C(25)-C(26)	66.8(2)
C(28)-C(24)-C(25)-Zr(1)	-66.4(2)
Si(1)-C(24)-C(25)-Zr(1)	128.6(3)
C(23)-Zr(1)-C(25)-C(24)	-167.4(2)
C(22)-Zr(1)-C(25)-C(24)	-83.2(2)
C(1)-Zr(1)-C(25)-C(24)	-118.1(3)
C(28)-Zr(1)-C(25)-C(24)	38.79(18)
C(27)-Zr(1)-C(25)-C(24)	79.3(2)
C(26)-Zr(1)-C(25)-C(24)	117.3(3)
C(8)-Zr(1)-C(25)-C(24)	89.2(2)
C(2)-Zr(1)-C(25)-C(24)	-32.7(3)
C(13)-Zr(1)-C(25)-C(24)	153.8(2)
C(7)-Zr(1)-C(25)-C(24)	30.0(3)
C(23)-Zr(1)-C(25)-C(26)	75.3(2)
C(22)-Zr(1)-C(25)-C(26)	159.5(2)
C(1)-Zr(1)-C(25)-C(26)	124.6(3)
C(28)-Zr(1)-C(25)-C(26)	-78.5(2)
C(24)-Zr(1)-C(25)-C(26)	-117.3(3)
C(27)-Zr(1)-C(25)-C(26)	-38.04(18)

C(8)-Zr(1)-C(25)-C(26)	-28.1(3)
C(2)-Zr(1)-C(25)-C(26)	-150.1(2)
C(13)-Zr(1)-C(25)-C(26)	36.5(3)
C(7)-Zr(1)-C(25)-C(26)	-87.3(2)
C(24)-C(25)-C(26)-C(27)	-0.3(3)
Zr(1)-C(25)-C(26)-C(27)	65.8(2)
C(24)-C(25)-C(26)-Si(2)	165.0(2)
Zr(1)-C(25)-C(26)-Si(2)	-128.9(3)
C(24)-C(25)-C(26)-Zr(1)	-66.0(2)
C(33)-Si(2)-C(26)-C(27)	-57.3(3)
C(32)-Si(2)-C(26)-C(27)	178.6(3)
C(34)-Si(2)-C(26)-C(27)	59.9(3)
C(33)-Si(2)-C(26)-C(25)	140.1(3)
C(32)-Si(2)-C(26)-C(25)	16.0(3)
C(34)-Si(2)-C(26)-C(25)	-102.7(3)
C(33)-Si(2)-C(26)-Zr(1)	41.1(3)
C(32)-Si(2)-C(26)-Zr(1)	-83.0(2)
C(34)-Si(2)-C(26)-Zr(1)	158.3(2)
C(23)-Zr(1)-C(26)-C(27)	148.7(2)
C(22)-Zr(1)-C(26)-C(27)	-135.3(2)
C(25)-Zr(1)-C(26)-C(27)	-113.1(3)
C(1)-Zr(1)-C(26)-C(27)	108.2(3)
C(28)-Zr(1)-C(26)-C(27)	-35.97(19)
C(24)-Zr(1)-C(26)-C(27)	-76.9(2)
C(8)-Zr(1)-C(26)-C(27)	49.4(2)
C(2)-Zr(1)-C(26)-C(27)	9.8(5)
C(13)-Zr(1)-C(26)-C(27)	85.3(2)
C(7)-Zr(1)-C(26)-C(27)	15.3(2)
C(23)-Zr(1)-C(26)-C(25)	-98.1(2)
C(22)-Zr(1)-C(26)-C(25)	-22.2(2)
C(1)-Zr(1)-C(26)-C(25)	-138.7(2)
C(28)-Zr(1)-C(26)-C(25)	77.1(2)
C(24)-Zr(1)-C(26)-C(25)	36.23(18)
C(27)-Zr(1)-C(26)-C(25)	113.1(3)
C(8)-Zr(1)-C(26)-C(25)	162.55(18)
C(2)-Zr(1)-C(26)-C(25)	123.0(4)
C(13)-Zr(1)-C(26)-C(25)	-161.59(18)
C(7)-Zr(1)-C(26)-C(25)	128.41(19)
C(23)-Zr(1)-C(26)-Si(2)	26.7(2)
C(22)-Zr(1)-C(26)-Si(2)	102.6(2)
C(25)-Zr(1)-C(26)-Si(2)	124.9(3)
C(1)-Zr(1)-C(26)-Si(2)	-13.8(4)
C(28)-Zr(1)-C(26)-Si(2)	-158.0(3)
C(24)-Zr(1)-C(26)-Si(2)	161.1(3)
C(27)-Zr(1)-C(26)-Si(2)	-122.0(3)
C(8)-Zr(1)-C(26)-Si(2)	-72.6(2)

C(2)-Zr(1)-C(26)-Si(2)	-112.2(4)
C(13)-Zr(1)-C(26)-Si(2)	-36.7(3)
C(7)-Zr(1)-C(26)-Si(2)	-106.7(2)
C(25)-C(24)-C(28)-C(27)	-0.3(3)
Si(1)-C(24)-C(28)-C(27)	165.9(2)
Zr(1)-C(24)-C(28)-C(27)	-66.3(2)
C(25)-C(24)-C(28)-Zr(1)	66.0(2)
Si(1)-C(24)-C(28)-Zr(1)	-127.8(2)
C(23)-Zr(1)-C(28)-C(27)	42.3(3)
C(22)-Zr(1)-C(28)-C(27)	141.0(2)
C(25)-Zr(1)-C(28)-C(27)	77.3(2)
C(1)-Zr(1)-C(28)-C(27)	-116.8(2)
C(24)-Zr(1)-C(28)-C(27)	116.1(3)
C(26)-Zr(1)-C(28)-C(27)	36.27(19)
C(8)-Zr(1)-C(28)-C(27)	-75.5(2)
C(2)-Zr(1)-C(28)-C(27)	-131.29(19)
C(13)-Zr(1)-C(28)-C(27)	-69.9(2)
C(7)-Zr(1)-C(28)-C(27)	-107.9(2)
C(23)-Zr(1)-C(28)-C(24)	-73.8(2)
C(22)-Zr(1)-C(28)-C(24)	24.9(2)
C(25)-Zr(1)-C(28)-C(24)	-38.78(18)
C(1)-Zr(1)-C(28)-C(24)	127.1(2)
C(27)-Zr(1)-C(28)-C(24)	-116.1(3)
C(26)-Zr(1)-C(28)-C(24)	-79.8(2)
C(8)-Zr(1)-C(28)-C(24)	168.38(18)
C(2)-Zr(1)-C(28)-C(24)	112.61(19)
C(13)-Zr(1)-C(28)-C(24)	173.97(17)
C(7)-Zr(1)-C(28)-C(24)	136.05(19)
C(24)-C(28)-C(27)-C(26)	0.2(4)
Zr(1)-C(28)-C(27)-C(26)	-65.5(2)
C(24)-C(28)-C(27)-Zr(1)	65.7(2)
C(25)-C(26)-C(27)-C(28)	0.0(3)
Si(2)-C(26)-C(27)-C(28)	-165.8(2)
Zr(1)-C(26)-C(27)-C(28)	64.8(2)
C(25)-C(26)-C(27)-Zr(1)	-64.7(2)
Si(2)-C(26)-C(27)-Zr(1)	129.4(2)
C(23)-Zr(1)-C(27)-C(28)	-148.1(2)
C(22)-Zr(1)-C(27)-C(28)	-54.3(3)
C(25)-Zr(1)-C(27)-C(28)	-78.5(2)
C(1)-Zr(1)-C(27)-C(28)	112.5(2)
C(24)-Zr(1)-C(27)-C(28)	-37.15(19)
C(26)-Zr(1)-C(27)-C(28)	-117.0(3)
C(8)-Zr(1)-C(27)-C(28)	107.3(2)
C(2)-Zr(1)-C(27)-C(28)	66.6(2)
C(13)-Zr(1)-C(27)-C(28)	129.65(19)
C(7)-Zr(1)-C(27)-C(28)	74.6(2)

C(23)-Zr(1)-C(27)-C(26)	-31.2(2)
C(22)-Zr(1)-C(27)-C(26)	62.7(2)
C(25)-Zr(1)-C(27)-C(26)	38.48(18)
C(1)-Zr(1)-C(27)-C(26)	-130.5(2)
C(28)-Zr(1)-C(27)-C(26)	117.0(3)
C(24)-Zr(1)-C(27)-C(26)	79.8(2)
C(8)-Zr(1)-C(27)-C(26)	-135.7(2)
C(2)-Zr(1)-C(27)-C(26)	-176.40(18)
C(13)-Zr(1)-C(27)-C(26)	-113.4(2)
C(7)-Zr(1)-C(27)-C(26)	-168.42(19)

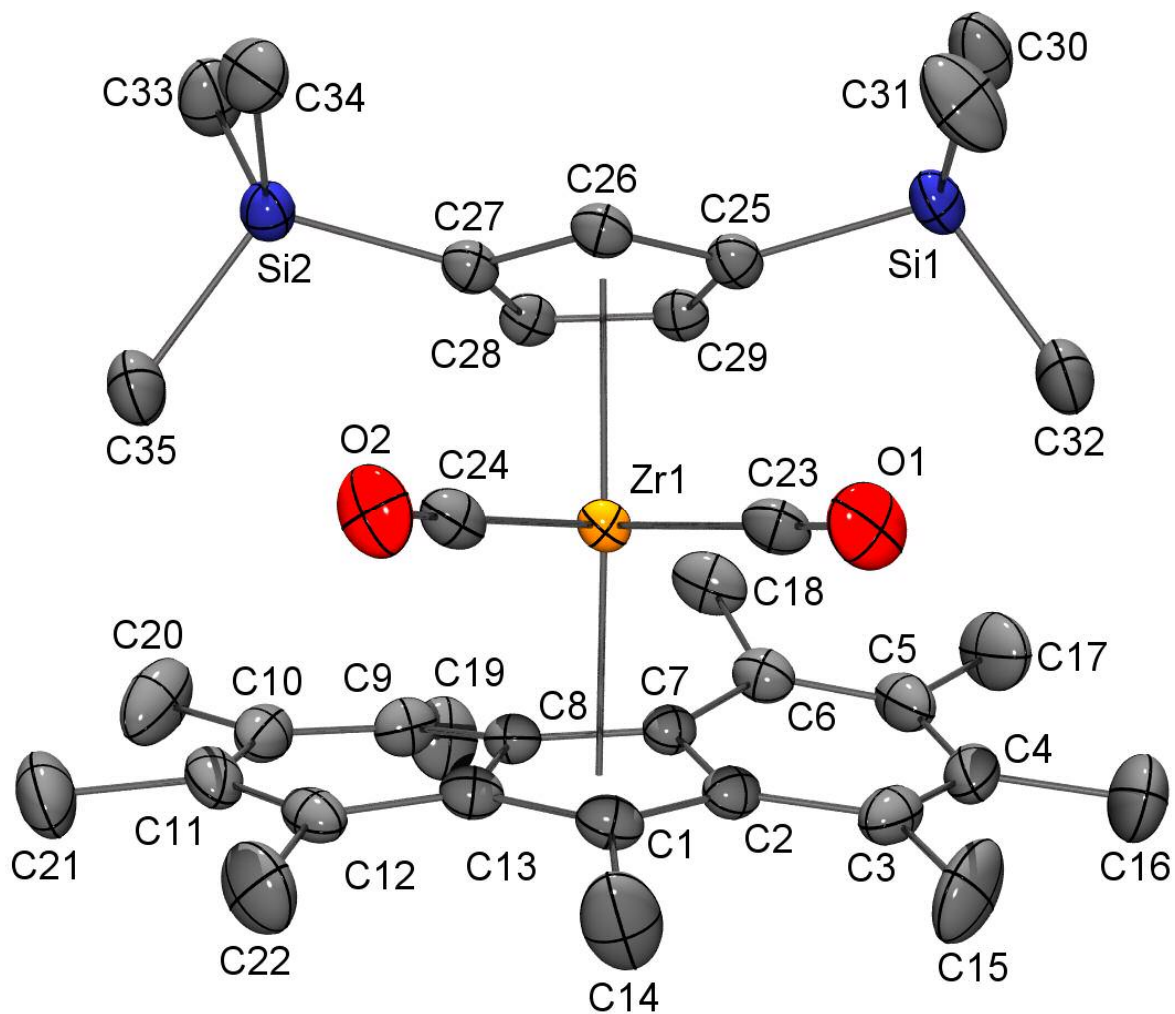


Figure 3. Thermal ellipsoid plot for compound **7**. Hydrogen atoms have been omitted for clarity.

Thermal ellipsoids are drawn at 50% probability.

C. Crystal data and structure refinement for Cp"Flu*Zr(CO)₂ (7).

Empirical formula	C ₃₅ H ₄₈ O ₂ Si ₂ Zr
Formula weight	648.13
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 2 ₁ /n
Unit cell dimensions	$a = 13.5735(19)$ Å $\alpha = 90^\circ$ $b = 16.060(2)$ Å $\beta = 100.134(2)^\circ$ $c = 15.706(2)$ Å $\gamma = 90^\circ$
Volume	3370.3(8) Å ³
Z	4
Calculated density	1.277 Mg/m ³
Absorption coefficient	0.426 mm ⁻¹
F(000)	1368
Crystal size	0.3 x 0.2 x 0.2 mm
Theta range for data collection	3.08 to 23.28°.
Limiting indices	-11 ≤ h ≤ 15, -17 ≤ k ≤ 17, -17 ≤ l ≤ 15
Reflections collected	13425
Independent reflections	4819 (R _{int} = 0.0321)
Completeness to theta = 23.28°	99.3%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.92 and 0.841
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4819 / 0 / 361
Goodness-of-fit on F ²	1.093
Final R indices [I > 2sigma(I)]	R1 = 0.0428, wR2 = 0.1043
R indices (all data)	R1 = 0.0524, wR2 = 0.1086
Largest diff. peak and hole	0.544 and -0.559 eÅ ⁻³

Table 11. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Cp"Flu*Zr(CO)₂ (7). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zr(1)	6887(1)	788(1)	2352(1)	21(1)
Si(1)	9815(1)	1175(1)	2920(1)	28(1)
O(1)	8468(2)	-779(2)	2265(2)	43(1)
C(1)	5901(3)	-23(2)	1157(2)	26(1)
Si(2)	6299(1)	1406(1)	4639(1)	26(1)
O(2)	6165(2)	-708(2)	3572(2)	40(1)
C(2)	6516(3)	508(2)	727(2)	25(1)
C(3)	7291(3)	325(2)	242(2)	33(1)
C(4)	7772(3)	973(3)	-88(2)	38(1)
C(5)	7566(3)	1819(3)	103(2)	35(1)
C(6)	6859(3)	2022(2)	587(2)	29(1)
C(12)	4331(3)	312(2)	1870(2)	30(1)
C(7)	6253(3)	1366(2)	856(2)	23(1)
C(8)	5371(3)	1363(2)	1268(2)	24(1)
C(9)	4662(3)	1991(2)	1392(2)	29(1)
C(10)	3926(3)	1787(3)	1859(2)	33(1)
C(11)	3753(3)	951(3)	2090(2)	34(1)
C(13)	5170(3)	508(2)	1463(2)	25(1)
C(14)	5822(4)	-962(3)	1066(3)	54(1)
C(15)	7556(4)	-573(3)	82(3)	55(1)
C(16)	8587(4)	802(3)	-623(3)	62(1)
C(17)	8187(4)	2505(3)	-202(3)	54(1)
C(18)	6784(3)	2912(2)	895(3)	39(1)
C(19)	4582(3)	2802(3)	884(3)	45(1)
C(20)	3246(4)	2472(3)	2095(3)	55(1)
C(21)	2873(3)	781(3)	2541(3)	51(1)
C(22)	4069(3)	-586(3)	2030(3)	49(1)
C(23)	7939(3)	-212(2)	2269(2)	29(1)
C(24)	6375(3)	-173(2)	3148(2)	29(1)
C(25)	8515(3)	1383(2)	3113(2)	25(1)
C(26)	8000(3)	1027(2)	3744(2)	24(1)
C(27)	7100(3)	1483(2)	3788(2)	24(1)
C(28)	7067(3)	2128(2)	3158(2)	23(1)
C(29)	7919(3)	2070(2)	2760(2)	24(1)
C(30)	10567(3)	2128(3)	3239(3)	43(1)
C(31)	10357(3)	295(3)	3625(3)	54(1)
C(32)	9833(3)	981(3)	1754(3)	44(1)
C(33)	6229(3)	2473(3)	5094(3)	42(1)

C(34)	6921(3)	678(3)	5489(3)	38(1)
C(35)	4994(3)	1062(3)	4233(3)	39(1)

Table 12. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cp}^*\text{Flu}^*\text{Zr}(\text{CO})_2$ (**7**). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr(1)	21(1)	15(1)	25(1)	0(1)	3(1)	0(1)
Si(1)	21(1)	25(1)	37(1)	-1(1)	4(1)	1(1)
O(1)	40(2)	26(2)	61(2)	-6(1)	5(1)	10(1)
C(1)	28(2)	18(2)	30(2)	-1(2)	-2(2)	-1(2)
Si(2)	25(1)	26(1)	28(1)	-1(1)	5(1)	-1(1)
O(2)	42(2)	29(2)	51(2)	14(1)	12(1)	-4(1)
C(2)	24(2)	25(2)	25(2)	-2(2)	-1(2)	4(2)
C(3)	34(2)	37(2)	26(2)	-5(2)	-1(2)	8(2)
C(4)	29(2)	61(3)	23(2)	-3(2)	4(2)	2(2)
C(5)	30(2)	46(3)	28(2)	6(2)	2(2)	-9(2)
C(6)	30(2)	27(2)	27(2)	5(2)	-1(2)	-2(2)
C(12)	27(2)	34(2)	24(2)	6(2)	-3(2)	-6(2)
C(7)	23(2)	22(2)	22(2)	-1(2)	1(2)	2(2)
C(8)	27(2)	23(2)	22(2)	0(2)	1(2)	-3(2)
C(9)	34(2)	22(2)	29(2)	0(2)	1(2)	6(2)
C(10)	26(2)	45(3)	27(2)	-2(2)	-1(2)	10(2)
C(11)	21(2)	51(3)	29(2)	5(2)	-1(2)	1(2)
C(13)	27(2)	22(2)	25(2)	2(2)	-2(2)	1(2)
C(14)	53(3)	25(2)	89(4)	-15(2)	24(3)	-6(2)
C(15)	70(3)	46(3)	53(3)	-3(2)	27(3)	26(3)
C(16)	52(3)	86(4)	55(3)	-16(3)	28(3)	-6(3)
C(17)	53(3)	66(3)	46(3)	9(2)	16(2)	-21(3)
C(18)	42(2)	25(2)	45(2)	8(2)	-3(2)	-6(2)
C(19)	48(3)	31(2)	56(3)	9(2)	10(2)	16(2)
C(20)	58(3)	67(3)	41(3)	4(2)	11(2)	32(3)
C(21)	29(2)	77(4)	50(3)	10(2)	11(2)	0(2)
C(22)	46(3)	44(3)	60(3)	9(2)	15(2)	-12(2)
C(23)	27(2)	25(2)	32(2)	-3(2)	-1(2)	-7(2)
C(24)	24(2)	25(2)	35(2)	-3(2)	0(2)	0(2)
C(25)	24(2)	21(2)	29(2)	-5(2)	3(2)	-2(2)
C(26)	24(2)	21(2)	26(2)	1(2)	0(2)	-2(2)
C(27)	23(2)	21(2)	26(2)	-1(2)	1(2)	-1(2)
C(28)	25(2)	14(2)	28(2)	-4(2)	2(2)	1(2)

C(29)	26(2)	18(2)	26(2)	-2(2)	3(2)	-5(2)
C(30)	32(2)	37(2)	62(3)	-13(2)	11(2)	-7(2)
C(31)	33(3)	46(3)	78(3)	15(2)	-1(2)	10(2)
C(32)	28(2)	54(3)	51(3)	-11(2)	12(2)	-3(2)
C(33)	42(3)	35(2)	51(3)	-11(2)	15(2)	-2(2)
C(34)	39(2)	41(3)	33(2)	9(2)	6(2)	-4(2)
C(35)	28(2)	45(3)	44(3)	-3(2)	11(2)	-1(2)

Table 13. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Cp"Flu*Zr(CO)₂ (**7**).

	x	y	z	U(eq)
H(14A)	5383	-1100	536	82
H(14B)	5559	-1189	1546	82
H(14C)	6473	-1192	1060	82
H(15A)	8082	-586	-254	82
H(15B)	6977	-854	-227	82
H(15C)	7776	-847	625	82
H(16A)	8648	212	-700	93
H(16B)	9213	1021	-328	93
H(16C)	8413	1065	-1178	93
H(17A)	7963	3035	-28	81
H(17B)	8113	2488	-821	81
H(17C)	8878	2428	49	81
H(18A)	7239	3258	650	58
H(18B)	6952	2931	1514	58
H(18C)	6113	3112	714	58
H(19A)	4071	3145	1056	67
H(19B)	4411	2683	277	67
H(19C)	5211	3089	999	67
H(20A)	3455	2999	1899	82
H(20B)	3287	2487	2712	82
H(20C)	2568	2362	1824	82
H(21A)	2842	197	2662	77
H(21B)	2264	950	2173	77
H(21C)	2954	1089	3072	77
H(22A)	3491	-602	2305	74
H(22B)	4623	-847	2399	74
H(22C)	3929	-878	1489	74
H(26A)	8272	585	4147	29
H(28A)	6580	2584	3074	27

H(29A)	8106	2475	2351	28
H(30A)	10576	2241	3841	65
H(30B)	10273	2591	2900	65
H(30C)	11239	2045	3143	65
H(31A)	10328	423	4217	81
H(31B)	11041	211	3562	81
H(31C)	9980	-203	3458	81
H(32A)	10508	877	1675	66
H(32B)	9577	1461	1422	66
H(32C)	9424	507	1562	66
H(33A)	5912	2842	4648	63
H(33B)	6893	2670	5316	63
H(33C)	5847	2456	5553	63
H(34A)	6949	131	5245	56
H(34B)	6547	656	5953	56
H(34C)	7588	869	5706	56
H(35A)	5000	512	3995	58
H(35B)	4681	1439	3793	58
H(35C)	4625	1057	4702	58

Table 14. Bond lengths [$\text{\AA}$] and angles [deg] for $\text{Cp}^*\text{Flu}^*\text{Zr}(\text{CO})_2$ (7).

<i>Bonds</i>	
Zr(1)-C(23)	2.169(4)
Zr(1)-C(24)	2.177(4)
Zr(1)-C(26)	2.458(3)
Zr(1)-C(1)	2.476(3)
Zr(1)-C(28)	2.486(3)
Zr(1)-C(27)	2.486(3)
Zr(1)-C(29)	2.508(3)
Zr(1)-C(25)	2.508(3)
Zr(1)-C(7)	2.531(3)
Zr(1)-C(13)	2.538(3)
Zr(1)-C(2)	2.553(3)
Zr(1)-C(8)	2.599(3)
Si(1)-C(30)	1.860(4)
Si(1)-C(32)	1.862(4)
Si(1)-C(31)	1.865(4)
Si(1)-C(25)	1.873(4)
O(1)-C(23)	1.160(4)
C(1)-C(2)	1.442(5)

C(1)-C(13)	1.453(5)
C(1)-C(14)	1.517(5)
Si(2)-C(35)	1.859(4)
Si(2)-C(34)	1.862(4)
Si(2)-C(33)	1.866(4)
Si(2)-C(27)	1.870(4)
O(2)-C(24)	1.152(4)
C(2)-C(3)	1.434(5)
C(2)-C(7)	1.446(5)
C(3)-C(4)	1.378(6)
C(3)-C(15)	1.518(6)
C(4)-C(5)	1.429(6)
C(4)-C(16)	1.528(6)
C(5)-C(6)	1.365(5)
C(5)-C(17)	1.516(6)
C(6)-C(7)	1.445(5)
C(6)-C(18)	1.518(5)
C(12)-C(11)	1.372(6)
C(12)-C(13)	1.435(5)
C(12)-C(22)	1.518(5)
C(7)-C(8)	1.458(5)
C(8)-C(9)	1.430(5)
C(8)-C(13)	1.444(5)
C(9)-C(10)	1.380(5)
C(9)-C(19)	1.521(5)
C(10)-C(11)	1.422(6)
C(10)-C(20)	1.523(6)
C(11)-C(21)	1.517(5)
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600

C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(25)-C(29)	1.422(5)
C(25)-C(26)	1.428(5)
C(26)-C(27)	1.435(5)
C(26)-H(26A)	0.9800
C(27)-C(28)	1.427(5)
C(28)-C(29)	1.411(5)
C(28)-H(28A)	0.9800
C(29)-H(29A)	0.9800
C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
C(33)-H(33A)	0.9600
C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600
C(35)-H(35A)	0.9600
C(35)-H(35B)	0.9600
C(35)-H(35C)	0.9600

Angles

C(23)-Zr(1)-C(24)	77.81(14)
C(23)-Zr(1)-C(26)	82.02(13)
C(24)-Zr(1)-C(26)	78.95(13)
C(23)-Zr(1)-C(1)	80.69(12)
C(24)-Zr(1)-C(1)	82.95(13)
C(26)-Zr(1)-C(1)	157.20(12)
C(23)-Zr(1)-C(28)	131.70(12)
C(24)-Zr(1)-C(28)	109.50(13)

C(26)-Zr(1)-C(28)	54.71(12)
C(1)-Zr(1)-C(28)	146.41(11)
C(23)-Zr(1)-C(27)	114.45(12)
C(24)-Zr(1)-C(27)	78.17(13)
C(26)-Zr(1)-C(27)	33.75(11)
C(1)-Zr(1)-C(27)	152.21(12)
C(28)-Zr(1)-C(27)	33.36(11)
C(23)-Zr(1)-C(29)	106.25(12)
C(24)-Zr(1)-C(29)	130.97(12)
C(26)-Zr(1)-C(29)	54.31(12)
C(1)-Zr(1)-C(29)	145.98(12)
C(28)-Zr(1)-C(29)	32.82(11)
C(27)-Zr(1)-C(29)	55.23(11)
C(23)-Zr(1)-C(25)	77.10(12)
C(24)-Zr(1)-C(25)	109.87(13)
C(26)-Zr(1)-C(25)	33.40(12)
C(1)-Zr(1)-C(25)	151.05(12)
C(28)-Zr(1)-C(25)	55.18(11)
C(27)-Zr(1)-C(25)	56.30(11)
C(29)-Zr(1)-C(25)	32.93(11)
C(23)-Zr(1)-C(7)	109.61(13)
C(24)-Zr(1)-C(7)	134.61(12)
C(26)-Zr(1)-C(7)	145.41(11)
C(1)-Zr(1)-C(7)	55.88(11)
C(28)-Zr(1)-C(7)	98.21(11)
C(27)-Zr(1)-C(7)	130.08(11)
C(29)-Zr(1)-C(7)	91.15(11)
C(25)-Zr(1)-C(7)	115.46(11)
C(23)-Zr(1)-C(13)	112.70(12)
C(24)-Zr(1)-C(13)	80.48(12)
C(26)-Zr(1)-C(13)	151.39(12)
C(1)-Zr(1)-C(13)	33.66(12)
C(28)-Zr(1)-C(13)	115.60(11)
C(27)-Zr(1)-C(13)	121.84(11)
C(29)-Zr(1)-C(13)	134.73(11)
C(25)-Zr(1)-C(13)	167.55(11)
C(7)-Zr(1)-C(13)	54.92(11)
C(23)-Zr(1)-C(2)	79.96(13)
C(24)-Zr(1)-C(2)	114.99(13)
C(26)-Zr(1)-C(2)	153.97(12)
C(1)-Zr(1)-C(2)	33.28(12)
C(28)-Zr(1)-C(2)	130.25(11)
C(27)-Zr(1)-C(2)	163.08(11)
C(29)-Zr(1)-C(2)	113.78(11)
C(25)-Zr(1)-C(2)	123.08(12)
C(7)-Zr(1)-C(2)	33.04(11)

C(13)-Zr(1)-C(2)	54.42(12)
C(23)-Zr(1)-C(8)	132.67(12)
C(24)-Zr(1)-C(8)	109.39(12)
C(26)-Zr(1)-C(8)	144.96(12)
C(1)-Zr(1)-C(8)	55.26(11)
C(28)-Zr(1)-C(8)	91.24(11)
C(27)-Zr(1)-C(8)	112.77(11)
C(29)-Zr(1)-C(8)	102.60(11)
C(25)-Zr(1)-C(8)	134.96(11)
C(7)-Zr(1)-C(8)	33.00(11)
C(13)-Zr(1)-C(8)	32.63(11)
C(2)-Zr(1)-C(8)	54.10(11)
C(30)-Si(1)-C(32)	107.5(2)
C(30)-Si(1)-C(31)	108.9(2)
C(32)-Si(1)-C(31)	112.7(2)
C(30)-Si(1)-C(25)	107.26(17)
C(32)-Si(1)-C(25)	111.41(17)
C(31)-Si(1)-C(25)	108.87(19)
C(2)-C(1)-C(13)	107.0(3)
C(2)-C(1)-C(14)	125.6(3)
C(13)-C(1)-C(14)	125.0(3)
C(2)-C(1)-Zr(1)	76.3(2)
C(13)-C(1)-Zr(1)	75.5(2)
C(14)-C(1)-Zr(1)	127.9(3)
C(35)-Si(2)-C(34)	110.10(19)
C(35)-Si(2)-C(33)	107.13(19)
C(34)-Si(2)-C(33)	110.5(2)
C(35)-Si(2)-C(27)	114.44(17)
C(34)-Si(2)-C(27)	107.86(17)
C(33)-Si(2)-C(27)	106.80(17)
C(3)-C(2)-C(1)	131.8(3)
C(3)-C(2)-C(7)	119.5(3)
C(1)-C(2)-C(7)	108.7(3)
C(3)-C(2)-Zr(1)	122.2(2)
C(1)-C(2)-Zr(1)	70.44(19)
C(7)-C(2)-Zr(1)	72.65(19)
C(4)-C(3)-C(2)	119.1(4)
C(4)-C(3)-C(15)	120.9(4)
C(2)-C(3)-C(15)	120.0(4)
C(3)-C(4)-C(5)	121.1(4)
C(3)-C(4)-C(16)	120.6(4)
C(5)-C(4)-C(16)	118.3(4)
C(6)-C(5)-C(4)	121.8(4)
C(6)-C(5)-C(17)	119.1(4)
C(4)-C(5)-C(17)	119.0(4)
C(5)-C(6)-C(7)	118.7(3)

C(5)-C(6)-C(18)	119.7(3)
C(7)-C(6)-C(18)	121.4(3)
C(11)-C(12)-C(13)	118.8(3)
C(11)-C(12)-C(22)	120.5(4)
C(13)-C(12)-C(22)	120.6(4)
C(6)-C(7)-C(2)	119.1(3)
C(6)-C(7)-C(8)	133.3(3)
C(2)-C(7)-C(8)	107.6(3)
C(6)-C(7)-Zr(1)	114.9(2)
C(2)-C(7)-Zr(1)	74.31(19)
C(8)-C(7)-Zr(1)	76.05(19)
C(9)-C(8)-C(13)	119.0(3)
C(9)-C(8)-C(7)	133.1(3)
C(13)-C(8)-C(7)	107.3(3)
C(9)-C(8)-Zr(1)	129.5(2)
C(13)-C(8)-Zr(1)	71.37(19)
C(7)-C(8)-Zr(1)	70.95(19)
C(10)-C(9)-C(8)	118.2(3)
C(10)-C(9)-C(19)	119.4(3)
C(8)-C(9)-C(19)	121.3(3)
C(9)-C(10)-C(11)	121.8(3)
C(9)-C(10)-C(20)	119.0(4)
C(11)-C(10)-C(20)	119.1(4)
C(12)-C(11)-C(10)	121.0(4)
C(12)-C(11)-C(21)	121.1(4)
C(10)-C(11)-C(21)	117.8(4)
C(12)-C(13)-C(8)	119.8(3)
C(12)-C(13)-C(1)	131.3(3)
C(8)-C(13)-C(1)	108.8(3)
C(12)-C(13)-Zr(1)	121.2(2)
C(8)-C(13)-Zr(1)	76.00(19)
C(1)-C(13)-Zr(1)	70.84(19)
C(1)-C(14)-H(14A)	109.5
C(1)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(1)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(3)-C(15)-H(15A)	109.5
C(3)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(3)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(4)-C(16)-H(16A)	109.5
C(4)-C(16)-H(16B)	109.5

H(16A)-C(16)-H(16B)	109.5
C(4)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(5)-C(17)-H(17A)	109.5
C(5)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(5)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(6)-C(18)-H(18A)	109.5
C(6)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(6)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(9)-C(19)-H(19A)	109.5
C(9)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(9)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(10)-C(20)-H(20A)	109.5
C(10)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(10)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(11)-C(21)-H(21A)	109.5
C(11)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(11)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(12)-C(22)-H(22A)	109.5
C(12)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(12)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
O(1)-C(23)-Zr(1)	175.2(3)
O(2)-C(24)-Zr(1)	175.4(3)
C(29)-C(25)-C(26)	105.4(3)
C(29)-C(25)-Si(1)	124.3(3)
C(26)-C(25)-Si(1)	129.1(3)
C(29)-C(25)-Zr(1)	73.52(19)

C(26)-C(25)-Zr(1)	71.39(19)
Si(1)-C(25)-Zr(1)	129.12(17)
C(25)-C(26)-C(27)	110.8(3)
C(25)-C(26)-Zr(1)	75.2(2)
C(27)-C(26)-Zr(1)	74.18(19)
C(25)-C(26)-H(26A)	124.4
C(27)-C(26)-H(26A)	124.4
Zr(1)-C(26)-H(26A)	124.4
C(28)-C(27)-C(26)	105.1(3)
C(28)-C(27)-Si(2)	126.2(3)
C(26)-C(27)-Si(2)	127.4(3)
C(28)-C(27)-Zr(1)	73.31(19)
C(26)-C(27)-Zr(1)	72.07(19)
Si(2)-C(27)-Zr(1)	129.01(17)
C(29)-C(28)-C(27)	109.3(3)
C(29)-C(28)-Zr(1)	74.44(19)
C(27)-C(28)-Zr(1)	73.32(19)
C(29)-C(28)-H(28A)	125.1
C(27)-C(28)-H(28A)	125.1
Zr(1)-C(28)-H(28A)	125.1
C(28)-C(29)-C(25)	109.5(3)
C(28)-C(29)-Zr(1)	72.74(19)
C(25)-C(29)-Zr(1)	73.55(19)
C(28)-C(29)-H(29A)	125.1
C(25)-C(29)-H(29A)	125.1
Zr(1)-C(29)-H(29A)	125.1
Si(1)-C(30)-H(30A)	109.5
Si(1)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
Si(1)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
Si(1)-C(31)-H(31A)	109.5
Si(1)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
Si(1)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
Si(1)-C(32)-H(32A)	109.5
Si(1)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
Si(1)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
Si(2)-C(33)-H(33A)	109.5
Si(2)-C(33)-H(33B)	109.5

H(33A)-C(33)-H(33B)	109.5
Si(2)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
Si(2)-C(34)-H(34A)	109.5
Si(2)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
Si(2)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
Si(2)-C(35)-H(35A)	109.5
Si(2)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
Si(2)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5

Table15. Torsion angles [deg] for Cp^{Flu}*Zr(CO)₂ (**7**).

C(23)-Zr(1)-C(1)-C(2)	-85.9(2)
C(24)-Zr(1)-C(1)-C(2)	-164.6(2)
C(26)-Zr(1)-C(1)-C(2)	-127.0(3)
C(28)-Zr(1)-C(1)-C(2)	80.5(3)
C(27)-Zr(1)-C(1)-C(2)	148.1(2)
C(29)-Zr(1)-C(1)-C(2)	19.4(3)
C(25)-Zr(1)-C(1)-C(2)	-45.6(3)
C(7)-Zr(1)-C(1)-C(2)	35.60(19)
C(13)-Zr(1)-C(1)-C(2)	112.0(3)
C(8)-Zr(1)-C(1)-C(2)	75.9(2)
C(23)-Zr(1)-C(1)-C(13)	162.1(2)
C(24)-Zr(1)-C(1)-C(13)	83.4(2)
C(26)-Zr(1)-C(1)-C(13)	121.0(3)
C(28)-Zr(1)-C(1)-C(13)	-31.5(3)
C(27)-Zr(1)-C(1)-C(13)	36.1(3)
C(29)-Zr(1)-C(1)-C(13)	-92.6(3)
C(25)-Zr(1)-C(1)-C(13)	-157.7(2)
C(7)-Zr(1)-C(1)-C(13)	-76.4(2)
C(2)-Zr(1)-C(1)-C(13)	-112.0(3)
C(8)-Zr(1)-C(1)-C(13)	-36.14(19)
C(23)-Zr(1)-C(1)-C(14)	38.8(3)
C(24)-Zr(1)-C(1)-C(14)	-39.9(3)
C(26)-Zr(1)-C(1)-C(14)	-2.3(5)

C(28)-Zr(1)-C(1)-C(14)	-154.9(3)
C(27)-Zr(1)-C(1)-C(14)	-87.3(4)
C(29)-Zr(1)-C(1)-C(14)	144.1(3)
C(25)-Zr(1)-C(1)-C(14)	79.0(4)
C(7)-Zr(1)-C(1)-C(14)	160.3(4)
C(13)-Zr(1)-C(1)-C(14)	-123.3(4)
C(2)-Zr(1)-C(1)-C(14)	124.7(4)
C(8)-Zr(1)-C(1)-C(14)	-159.5(4)
C(13)-C(1)-C(2)-C(3)	-174.0(4)
C(14)-C(1)-C(2)-C(3)	-10.9(6)
Zr(1)-C(1)-C(2)-C(3)	116.2(4)
C(13)-C(1)-C(2)-C(7)	6.9(4)
C(14)-C(1)-C(2)-C(7)	169.9(4)
Zr(1)-C(1)-C(2)-C(7)	-63.0(2)
C(13)-C(1)-C(2)-Zr(1)	69.9(2)
C(14)-C(1)-C(2)-Zr(1)	-127.1(4)
C(23)-Zr(1)-C(2)-C(3)	-39.4(3)
C(24)-Zr(1)-C(2)-C(3)	-110.8(3)
C(26)-Zr(1)-C(2)-C(3)	7.4(5)
C(1)-Zr(1)-C(2)-C(3)	-127.7(4)
C(28)-Zr(1)-C(2)-C(3)	97.9(3)
C(27)-Zr(1)-C(2)-C(3)	110.1(4)
C(29)-Zr(1)-C(2)-C(3)	64.0(3)
C(25)-Zr(1)-C(2)-C(3)	27.9(3)
C(7)-Zr(1)-C(2)-C(3)	114.4(4)
C(13)-Zr(1)-C(2)-C(3)	-166.9(4)
C(8)-Zr(1)-C(2)-C(3)	152.6(4)
C(23)-Zr(1)-C(2)-C(1)	88.3(2)
C(24)-Zr(1)-C(2)-C(1)	16.9(2)
C(26)-Zr(1)-C(2)-C(1)	135.1(3)
C(28)-Zr(1)-C(2)-C(1)	-134.4(2)
C(27)-Zr(1)-C(2)-C(1)	-122.1(4)
C(29)-Zr(1)-C(2)-C(1)	-168.26(19)
C(25)-Zr(1)-C(2)-C(1)	155.60(19)
C(7)-Zr(1)-C(2)-C(1)	-117.9(3)
C(13)-Zr(1)-C(2)-C(1)	-39.2(2)
C(8)-Zr(1)-C(2)-C(1)	-79.7(2)
C(23)-Zr(1)-C(2)-C(7)	-153.8(2)
C(24)-Zr(1)-C(2)-C(7)	134.8(2)
C(26)-Zr(1)-C(2)-C(7)	-107.0(3)
C(1)-Zr(1)-C(2)-C(7)	117.9(3)
C(28)-Zr(1)-C(2)-C(7)	-16.5(3)
C(27)-Zr(1)-C(2)-C(7)	-4.2(5)
C(29)-Zr(1)-C(2)-C(7)	-50.4(2)
C(25)-Zr(1)-C(2)-C(7)	-86.5(2)
C(13)-Zr(1)-C(2)-C(7)	78.7(2)

C(8)-Zr(1)-C(2)-C(7)	38.19(19)
C(1)-C(2)-C(3)-C(4)	-178.8(4)
C(7)-C(2)-C(3)-C(4)	0.3(5)
Zr(1)-C(2)-C(3)-C(4)	-86.9(4)
C(1)-C(2)-C(3)-C(15)	2.5(6)
C(7)-C(2)-C(3)-C(15)	-178.4(4)
Zr(1)-C(2)-C(3)-C(15)	94.3(4)
C(2)-C(3)-C(4)-C(5)	4.9(6)
C(15)-C(3)-C(4)-C(5)	-176.4(4)
C(2)-C(3)-C(4)-C(16)	-178.8(4)
C(15)-C(3)-C(4)-C(16)	-0.1(6)
C(3)-C(4)-C(5)-C(6)	-2.7(6)
C(16)-C(4)-C(5)-C(6)	-179.1(4)
C(3)-C(4)-C(5)-C(17)	174.1(4)
C(16)-C(4)-C(5)-C(17)	-2.3(6)
C(4)-C(5)-C(6)-C(7)	-4.8(6)
C(17)-C(5)-C(6)-C(7)	178.4(3)
C(4)-C(5)-C(6)-C(18)	170.0(3)
C(17)-C(5)-C(6)-C(18)	-6.7(5)
C(5)-C(6)-C(7)-C(2)	9.8(5)
C(18)-C(6)-C(7)-C(2)	-165.0(3)
C(5)-C(6)-C(7)-C(8)	-170.8(4)
C(18)-C(6)-C(7)-C(8)	14.4(6)
C(5)-C(6)-C(7)-Zr(1)	95.1(3)
C(18)-C(6)-C(7)-Zr(1)	-79.7(4)
C(3)-C(2)-C(7)-C(6)	-7.6(5)
C(1)-C(2)-C(7)-C(6)	171.7(3)
Zr(1)-C(2)-C(7)-C(6)	110.1(3)
C(3)-C(2)-C(7)-C(8)	172.9(3)
C(1)-C(2)-C(7)-C(8)	-7.8(4)
Zr(1)-C(2)-C(7)-C(8)	-69.4(2)
C(3)-C(2)-C(7)-Zr(1)	-117.7(3)
C(1)-C(2)-C(7)-Zr(1)	61.6(2)
C(23)-Zr(1)-C(7)-C(6)	-87.8(3)
C(24)-Zr(1)-C(7)-C(6)	-179.9(2)
C(26)-Zr(1)-C(7)-C(6)	17.1(4)
C(1)-Zr(1)-C(7)-C(6)	-151.2(3)
C(28)-Zr(1)-C(7)-C(6)	52.1(3)
C(27)-Zr(1)-C(7)-C(6)	63.1(3)
C(29)-Zr(1)-C(7)-C(6)	19.9(3)
C(25)-Zr(1)-C(7)-C(6)	-3.2(3)
C(13)-Zr(1)-C(7)-C(6)	167.7(3)
C(2)-Zr(1)-C(7)-C(6)	-115.3(3)
C(8)-Zr(1)-C(7)-C(6)	131.6(4)
C(23)-Zr(1)-C(7)-C(2)	27.5(2)
C(24)-Zr(1)-C(7)-C(2)	-64.6(3)

C(26)-Zr(1)-C(7)-C(2)	132.3(2)
C(1)-Zr(1)-C(7)-C(2)	-35.9(2)
C(28)-Zr(1)-C(7)-C(2)	167.3(2)
C(27)-Zr(1)-C(7)-C(2)	178.39(19)
C(29)-Zr(1)-C(7)-C(2)	135.2(2)
C(25)-Zr(1)-C(7)-C(2)	112.1(2)
C(13)-Zr(1)-C(7)-C(2)	-77.0(2)
C(8)-Zr(1)-C(7)-C(2)	-113.1(3)
C(23)-Zr(1)-C(7)-C(8)	140.6(2)
C(24)-Zr(1)-C(7)-C(8)	48.5(3)
C(26)-Zr(1)-C(7)-C(8)	-114.5(2)
C(1)-Zr(1)-C(7)-C(8)	77.3(2)
C(28)-Zr(1)-C(7)-C(8)	-79.5(2)
C(27)-Zr(1)-C(7)-C(8)	-68.5(2)
C(29)-Zr(1)-C(7)-C(8)	-111.7(2)
C(25)-Zr(1)-C(7)-C(8)	-134.74(19)
C(13)-Zr(1)-C(7)-C(8)	36.09(19)
C(2)-Zr(1)-C(7)-C(8)	113.1(3)
C(6)-C(7)-C(8)-C(9)	15.6(7)
C(2)-C(7)-C(8)-C(9)	-165.0(4)
Zr(1)-C(7)-C(8)-C(9)	126.8(4)
C(6)-C(7)-C(8)-C(13)	-173.7(4)
C(2)-C(7)-C(8)-C(13)	5.7(4)
Zr(1)-C(7)-C(8)-C(13)	-62.5(2)
C(6)-C(7)-C(8)-Zr(1)	-111.2(4)
C(2)-C(7)-C(8)-Zr(1)	68.2(2)
C(23)-Zr(1)-C(8)-C(9)	174.9(3)
C(24)-Zr(1)-C(8)-C(9)	83.7(3)
C(26)-Zr(1)-C(8)-C(9)	-14.8(4)
C(1)-Zr(1)-C(8)-C(9)	150.0(4)
C(28)-Zr(1)-C(8)-C(9)	-27.5(3)
C(27)-Zr(1)-C(8)-C(9)	-1.2(4)
C(29)-Zr(1)-C(8)-C(9)	-58.6(3)
C(25)-Zr(1)-C(8)-C(9)	-65.7(4)
C(7)-Zr(1)-C(8)-C(9)	-130.7(4)
C(13)-Zr(1)-C(8)-C(9)	112.7(4)
C(2)-Zr(1)-C(8)-C(9)	-168.9(4)
C(23)-Zr(1)-C(8)-C(13)	62.2(3)
C(24)-Zr(1)-C(8)-C(13)	-29.0(2)
C(26)-Zr(1)-C(8)-C(13)	-127.5(2)
C(1)-Zr(1)-C(8)-C(13)	37.3(2)
C(28)-Zr(1)-C(8)-C(13)	-140.2(2)
C(27)-Zr(1)-C(8)-C(13)	-113.9(2)
C(29)-Zr(1)-C(8)-C(13)	-171.2(2)
C(25)-Zr(1)-C(8)-C(13)	-178.4(2)
C(7)-Zr(1)-C(8)-C(13)	116.6(3)

C(2)-Zr(1)-C(8)-C(13)	78.4(2)
C(23)-Zr(1)-C(8)-C(7)	-54.4(3)
C(24)-Zr(1)-C(8)-C(7)	-145.6(2)
C(26)-Zr(1)-C(8)-C(7)	115.9(2)
C(1)-Zr(1)-C(8)-C(7)	-79.3(2)
C(28)-Zr(1)-C(8)-C(7)	103.2(2)
C(27)-Zr(1)-C(8)-C(7)	129.5(2)
C(29)-Zr(1)-C(8)-C(7)	72.2(2)
C(25)-Zr(1)-C(8)-C(7)	65.0(2)
C(13)-Zr(1)-C(8)-C(7)	-116.6(3)
C(2)-Zr(1)-C(8)-C(7)	-38.23(19)
C(13)-C(8)-C(9)-C(10)	13.5(5)
C(7)-C(8)-C(9)-C(10)	-176.7(4)
Zr(1)-C(8)-C(9)-C(10)	-75.6(4)
C(13)-C(8)-C(9)-C(19)	-154.6(4)
C(7)-C(8)-C(9)-C(19)	15.2(6)
Zr(1)-C(8)-C(9)-C(19)	116.3(4)
C(8)-C(9)-C(10)-C(11)	-10.8(5)
C(19)-C(9)-C(10)-C(11)	157.6(4)
C(8)-C(9)-C(10)-C(20)	172.3(3)
C(19)-C(9)-C(10)-C(20)	-19.3(5)
C(13)-C(12)-C(11)-C(10)	5.0(5)
C(22)-C(12)-C(11)-C(10)	-173.1(4)
C(13)-C(12)-C(11)-C(21)	-178.5(3)
C(22)-C(12)-C(11)-C(21)	3.3(6)
C(9)-C(10)-C(11)-C(12)	1.4(6)
C(20)-C(10)-C(11)-C(12)	178.3(4)
C(9)-C(10)-C(11)-C(21)	-175.1(4)
C(20)-C(10)-C(11)-C(21)	1.8(5)
C(11)-C(12)-C(13)-C(8)	-2.0(5)
C(22)-C(12)-C(13)-C(8)	176.2(3)
C(11)-C(12)-C(13)-C(1)	-179.5(4)
C(22)-C(12)-C(13)-C(1)	-1.4(6)
C(11)-C(12)-C(13)-Zr(1)	89.2(4)
C(22)-C(12)-C(13)-Zr(1)	-92.6(4)
C(9)-C(8)-C(13)-C(12)	-7.3(5)
C(7)-C(8)-C(13)-C(12)	-179.6(3)
Zr(1)-C(8)-C(13)-C(12)	118.2(3)
C(9)-C(8)-C(13)-C(1)	170.8(3)
C(7)-C(8)-C(13)-C(1)	-1.5(4)
Zr(1)-C(8)-C(13)-C(1)	-63.7(2)
C(9)-C(8)-C(13)-Zr(1)	-125.5(3)
C(7)-C(8)-C(13)-Zr(1)	62.3(2)
C(2)-C(1)-C(13)-C(12)	174.5(4)
C(14)-C(1)-C(13)-C(12)	11.3(6)
Zr(1)-C(1)-C(13)-C(12)	-115.1(4)

C(2)-C(1)-C(13)-C(8)	-3.3(4)
C(14)-C(1)-C(13)-C(8)	-166.5(4)
Zr(1)-C(1)-C(13)-C(8)	67.1(2)
C(2)-C(1)-C(13)-Zr(1)	-70.4(2)
C(14)-C(1)-C(13)-Zr(1)	126.4(4)
C(23)-Zr(1)-C(13)-C(12)	108.2(3)
C(24)-Zr(1)-C(13)-C(12)	35.8(3)
C(26)-Zr(1)-C(13)-C(12)	-8.7(4)
C(1)-Zr(1)-C(13)-C(12)	127.4(4)
C(28)-Zr(1)-C(13)-C(12)	-71.3(3)
C(27)-Zr(1)-C(13)-C(12)	-33.8(3)
C(29)-Zr(1)-C(13)-C(12)	-104.5(3)
C(25)-Zr(1)-C(13)-C(12)	-111.2(5)
C(7)-Zr(1)-C(13)-C(12)	-153.1(3)
C(2)-Zr(1)-C(13)-C(12)	166.1(3)
C(8)-Zr(1)-C(13)-C(12)	-116.6(4)
C(23)-Zr(1)-C(13)-C(8)	-135.2(2)
C(24)-Zr(1)-C(13)-C(8)	152.4(2)
C(26)-Zr(1)-C(13)-C(8)	107.9(3)
C(1)-Zr(1)-C(13)-C(8)	-116.0(3)
C(28)-Zr(1)-C(13)-C(8)	45.3(2)
C(27)-Zr(1)-C(13)-C(8)	82.8(2)
C(29)-Zr(1)-C(13)-C(8)	12.1(3)
C(25)-Zr(1)-C(13)-C(8)	5.4(6)
C(7)-Zr(1)-C(13)-C(8)	-36.51(19)
C(2)-Zr(1)-C(13)-C(8)	-77.3(2)
C(23)-Zr(1)-C(13)-C(1)	-19.2(2)
C(24)-Zr(1)-C(13)-C(1)	-91.6(2)
C(26)-Zr(1)-C(13)-C(1)	-136.1(3)
C(28)-Zr(1)-C(13)-C(1)	161.28(19)
C(27)-Zr(1)-C(13)-C(1)	-161.15(19)
C(29)-Zr(1)-C(13)-C(1)	128.1(2)
C(25)-Zr(1)-C(13)-C(1)	121.4(5)
C(7)-Zr(1)-C(13)-C(1)	79.5(2)
C(2)-Zr(1)-C(13)-C(1)	38.7(2)
C(8)-Zr(1)-C(13)-C(1)	116.0(3)
C(24)-Zr(1)-C(23)-O(1)	-3(4)
C(26)-Zr(1)-C(23)-O(1)	77(4)
C(1)-Zr(1)-C(23)-O(1)	-88(4)
C(28)-Zr(1)-C(23)-O(1)	102(4)
C(27)-Zr(1)-C(23)-O(1)	68(4)
C(29)-Zr(1)-C(23)-O(1)	126(4)
C(25)-Zr(1)-C(23)-O(1)	111(4)
C(7)-Zr(1)-C(23)-O(1)	-136(4)
C(13)-Zr(1)-C(23)-O(1)	-77(4)
C(2)-Zr(1)-C(23)-O(1)	-122(4)

C(8)-Zr(1)-C(23)-O(1)	-108(4)
C(23)-Zr(1)-C(24)-O(2)	17(4)
C(26)-Zr(1)-C(24)-O(2)	-67(4)
C(1)-Zr(1)-C(24)-O(2)	99(4)
C(28)-Zr(1)-C(24)-O(2)	-113(4)
C(27)-Zr(1)-C(24)-O(2)	-102(4)
C(29)-Zr(1)-C(24)-O(2)	-84(4)
C(25)-Zr(1)-C(24)-O(2)	-54(4)
C(7)-Zr(1)-C(24)-O(2)	122(4)
C(13)-Zr(1)-C(24)-O(2)	133(4)
C(2)-Zr(1)-C(24)-O(2)	90(4)
C(8)-Zr(1)-C(24)-O(2)	148(4)
C(30)-Si(1)-C(25)-C(29)	54.9(3)
C(32)-Si(1)-C(25)-C(29)	-62.5(3)
C(31)-Si(1)-C(25)-C(29)	172.6(3)
C(30)-Si(1)-C(25)-C(26)	-111.1(3)
C(32)-Si(1)-C(25)-C(26)	131.5(3)
C(31)-Si(1)-C(25)-C(26)	6.6(4)
C(30)-Si(1)-C(25)-Zr(1)	151.3(2)
C(32)-Si(1)-C(25)-Zr(1)	33.9(3)
C(31)-Si(1)-C(25)-Zr(1)	-91.0(3)
C(23)-Zr(1)-C(25)-C(29)	151.8(2)
C(24)-Zr(1)-C(25)-C(29)	-136.4(2)
C(26)-Zr(1)-C(25)-C(29)	-113.1(3)
C(1)-Zr(1)-C(25)-C(29)	111.0(3)
C(28)-Zr(1)-C(25)-C(29)	-36.00(19)
C(27)-Zr(1)-C(25)-C(29)	-76.6(2)
C(7)-Zr(1)-C(25)-C(29)	46.0(2)
C(13)-Zr(1)-C(25)-C(29)	8.8(6)
C(2)-Zr(1)-C(25)-C(29)	83.1(2)
C(8)-Zr(1)-C(25)-C(29)	12.9(3)
C(23)-Zr(1)-C(25)-C(26)	-95.1(2)
C(24)-Zr(1)-C(25)-C(26)	-23.3(2)
C(1)-Zr(1)-C(25)-C(26)	-135.9(3)
C(28)-Zr(1)-C(25)-C(26)	77.1(2)
C(27)-Zr(1)-C(25)-C(26)	36.5(2)
C(29)-Zr(1)-C(25)-C(26)	113.1(3)
C(7)-Zr(1)-C(25)-C(26)	159.12(19)
C(13)-Zr(1)-C(25)-C(26)	121.9(5)
C(2)-Zr(1)-C(25)-C(26)	-163.81(19)
C(8)-Zr(1)-C(25)-C(26)	126.0(2)
C(23)-Zr(1)-C(25)-Si(1)	30.7(2)
C(24)-Zr(1)-C(25)-Si(1)	102.5(2)
C(26)-Zr(1)-C(25)-Si(1)	125.8(3)
C(1)-Zr(1)-C(25)-Si(1)	-10.1(4)
C(28)-Zr(1)-C(25)-Si(1)	-157.1(3)

C(27)-Zr(1)-C(25)-Si(1)	162.2(3)
C(29)-Zr(1)-C(25)-Si(1)	-121.1(3)
C(7)-Zr(1)-C(25)-Si(1)	-75.1(2)
C(13)-Zr(1)-C(25)-Si(1)	-112.3(5)
C(2)-Zr(1)-C(25)-Si(1)	-38.0(3)
C(8)-Zr(1)-C(25)-Si(1)	-108.2(2)
C(29)-C(25)-C(26)-C(27)	-0.1(4)
Si(1)-C(25)-C(26)-C(27)	167.9(3)
Zr(1)-C(25)-C(26)-C(27)	-66.3(2)
C(29)-C(25)-C(26)-Zr(1)	66.2(2)
Si(1)-C(25)-C(26)-Zr(1)	-125.8(3)
C(23)-Zr(1)-C(26)-C(25)	78.6(2)
C(24)-Zr(1)-C(26)-C(25)	157.7(2)
C(1)-Zr(1)-C(26)-C(25)	119.6(3)
C(28)-Zr(1)-C(26)-C(25)	-78.6(2)
C(27)-Zr(1)-C(26)-C(25)	-117.1(3)
C(29)-Zr(1)-C(26)-C(25)	-38.00(19)
C(7)-Zr(1)-C(26)-C(25)	-34.5(3)
C(13)-Zr(1)-C(26)-C(25)	-157.5(2)
C(2)-Zr(1)-C(26)-C(25)	32.2(4)
C(8)-Zr(1)-C(26)-C(25)	-94.2(3)
C(23)-Zr(1)-C(26)-C(27)	-164.2(2)
C(24)-Zr(1)-C(26)-C(27)	-85.2(2)
C(1)-Zr(1)-C(26)-C(27)	-123.3(3)
C(28)-Zr(1)-C(26)-C(27)	38.50(19)
C(29)-Zr(1)-C(26)-C(27)	79.1(2)
C(25)-Zr(1)-C(26)-C(27)	117.1(3)
C(7)-Zr(1)-C(26)-C(27)	82.6(3)
C(13)-Zr(1)-C(26)-C(27)	-40.4(3)
C(2)-Zr(1)-C(26)-C(27)	149.3(3)
C(8)-Zr(1)-C(26)-C(27)	22.9(3)
C(25)-C(26)-C(27)-C(28)	0.5(4)
Zr(1)-C(26)-C(27)-C(28)	-66.4(2)
C(25)-C(26)-C(27)-Si(2)	-167.2(3)
Zr(1)-C(26)-C(27)-Si(2)	125.8(3)
C(25)-C(26)-C(27)-Zr(1)	67.0(2)
C(35)-Si(2)-C(27)-C(28)	75.9(3)
C(34)-Si(2)-C(27)-C(28)	-161.2(3)
C(33)-Si(2)-C(27)-C(28)	-42.5(3)
C(35)-Si(2)-C(27)-C(26)	-118.8(3)
C(34)-Si(2)-C(27)-C(26)	4.0(4)
C(33)-Si(2)-C(27)-C(26)	122.8(3)
C(35)-Si(2)-C(27)-Zr(1)	-21.9(3)
C(34)-Si(2)-C(27)-Zr(1)	101.0(2)
C(33)-Si(2)-C(27)-Zr(1)	-140.3(2)
C(23)-Zr(1)-C(27)-C(28)	129.7(2)

C(24)-Zr(1)-C(27)-C(28)	-159.7(2)
C(26)-Zr(1)-C(27)-C(28)	112.5(3)
C(1)-Zr(1)-C(27)-C(28)	-111.5(3)
C(29)-Zr(1)-C(27)-C(28)	36.31(19)
C(25)-Zr(1)-C(27)-C(28)	76.4(2)
C(7)-Zr(1)-C(27)-C(28)	-20.2(3)
C(13)-Zr(1)-C(27)-C(28)	-89.0(2)
C(2)-Zr(1)-C(27)-C(28)	-17.1(5)
C(8)-Zr(1)-C(27)-C(28)	-53.5(2)
C(23)-Zr(1)-C(27)-C(26)	17.2(2)
C(24)-Zr(1)-C(27)-C(26)	87.8(2)
C(1)-Zr(1)-C(27)-C(26)	136.0(3)
C(28)-Zr(1)-C(27)-C(26)	-112.5(3)
C(29)-Zr(1)-C(27)-C(26)	-76.2(2)
C(25)-Zr(1)-C(27)-C(26)	-36.1(2)
C(7)-Zr(1)-C(27)-C(26)	-132.6(2)
C(13)-Zr(1)-C(27)-C(26)	158.57(19)
C(2)-Zr(1)-C(27)-C(26)	-129.6(4)
C(8)-Zr(1)-C(27)-C(26)	-165.97(19)
C(23)-Zr(1)-C(27)-Si(2)	-106.9(2)
C(24)-Zr(1)-C(27)-Si(2)	-36.3(2)
C(26)-Zr(1)-C(27)-Si(2)	-124.1(3)
C(1)-Zr(1)-C(27)-Si(2)	11.9(4)
C(28)-Zr(1)-C(27)-Si(2)	123.5(3)
C(29)-Zr(1)-C(27)-Si(2)	159.8(3)
C(25)-Zr(1)-C(27)-Si(2)	-160.1(3)
C(7)-Zr(1)-C(27)-Si(2)	103.3(2)
C(13)-Zr(1)-C(27)-Si(2)	34.5(3)
C(2)-Zr(1)-C(27)-Si(2)	106.3(4)
C(8)-Zr(1)-C(27)-Si(2)	70.0(2)
C(26)-C(27)-C(28)-C(29)	-0.8(4)
Si(2)-C(27)-C(28)-C(29)	167.2(3)
Zr(1)-C(27)-C(28)-C(29)	-66.3(2)
C(26)-C(27)-C(28)-Zr(1)	65.6(2)
Si(2)-C(27)-C(28)-Zr(1)	-126.5(3)
C(23)-Zr(1)-C(28)-C(29)	46.4(3)
C(24)-Zr(1)-C(28)-C(29)	137.2(2)
C(26)-Zr(1)-C(28)-C(29)	77.2(2)
C(1)-Zr(1)-C(28)-C(29)	-115.4(2)
C(27)-Zr(1)-C(28)-C(29)	116.2(3)
C(25)-Zr(1)-C(28)-C(29)	36.1(2)
C(7)-Zr(1)-C(28)-C(29)	-79.3(2)
C(13)-Zr(1)-C(28)-C(29)	-134.2(2)
C(2)-Zr(1)-C(28)-C(29)	-70.3(2)
C(8)-Zr(1)-C(28)-C(29)	-111.7(2)
C(23)-Zr(1)-C(28)-C(27)	-69.8(3)

C(24)-Zr(1)-C(28)-C(27)	21.1(2)
C(26)-Zr(1)-C(28)-C(27)	-39.0(2)
C(1)-Zr(1)-C(28)-C(27)	128.4(2)
C(29)-Zr(1)-C(28)-C(27)	-116.2(3)
C(25)-Zr(1)-C(28)-C(27)	-80.1(2)
C(7)-Zr(1)-C(28)-C(27)	164.5(2)
C(13)-Zr(1)-C(28)-C(27)	109.6(2)
C(2)-Zr(1)-C(28)-C(27)	173.55(19)
C(8)-Zr(1)-C(28)-C(27)	132.2(2)
C(27)-C(28)-C(29)-C(25)	0.7(4)
Zr(1)-C(28)-C(29)-C(25)	-64.9(2)
C(27)-C(28)-C(29)-Zr(1)	65.6(2)
C(26)-C(25)-C(29)-C(28)	-0.4(4)
Si(1)-C(25)-C(29)-C(28)	-169.1(2)
Zr(1)-C(25)-C(29)-C(28)	64.4(2)
C(26)-C(25)-C(29)-Zr(1)	-64.7(2)
Si(1)-C(25)-C(29)-Zr(1)	126.5(3)
C(23)-Zr(1)-C(29)-C(28)	-145.7(2)
C(24)-Zr(1)-C(29)-C(28)	-57.9(3)
C(26)-Zr(1)-C(29)-C(28)	-78.5(2)
C(1)-Zr(1)-C(29)-C(28)	116.8(2)
C(27)-Zr(1)-C(29)-C(28)	-36.93(19)
C(25)-Zr(1)-C(29)-C(28)	-117.1(3)
C(7)-Zr(1)-C(29)-C(28)	103.4(2)
C(13)-Zr(1)-C(29)-C(28)	65.6(3)
C(2)-Zr(1)-C(29)-C(28)	128.3(2)
C(8)-Zr(1)-C(29)-C(28)	72.2(2)
C(23)-Zr(1)-C(29)-C(25)	-28.6(2)
C(24)-Zr(1)-C(29)-C(25)	59.2(3)
C(26)-Zr(1)-C(29)-C(25)	38.6(2)
C(1)-Zr(1)-C(29)-C(25)	-126.1(2)
C(28)-Zr(1)-C(29)-C(25)	117.1(3)
C(27)-Zr(1)-C(29)-C(25)	80.2(2)
C(7)-Zr(1)-C(29)-C(25)	-139.5(2)
C(13)-Zr(1)-C(29)-C(25)	-177.34(19)
C(2)-Zr(1)-C(29)-C(25)	-114.6(2)
C(8)-Zr(1)-C(29)-C(25)	-170.7(2)
