Dialkyl and Methyl Alkylzirconocenes - Precursors to Propagating Species Models in Zirconocene-Catalyzed Alkene Polymerization

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Table 1. Crystal data and structure refinement for 1 (CCDC 181777).

Empirical formula	$C_{25}H_{42}Zr$
Formula weight	433.81
Crystallization Solvent	Pentane
Crystal Habit	Chunks
Crystal size	0.26 x 0.20 x 0.19 mm^3
Crystal color	Pale yellow

Data Collection

Preliminary Photos	Rotation
Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	98(2) K
θ range for 27315 reflections used in lattice determination	2.33 to 28.81°
Unit cell dimensions	a = 9.7467(4) Å b = 25.9839(12) Å β= 116.6710(10)° c = 10.2031(5) Å
Volume	2309.07(18) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.248 Mg/m^3
F(000)	928
Data collection program	Bruker SMART v5.054
θ range for data collection	1.57 to 28.37°
Completeness to θ = 28.37°	94.2 %
Index ranges	$-12 \le h \le 12$, $-33 \le k \le 33$, $-13 \le l \le 13$
Data collection scan type	ω scans at 7 ϕ settings
Data reduction program	Bruker SAINT v6.022
Reflections collected	46222
Independent reflections	5440 [R_{int}= 0.0466]
Absorption coefficient	0.482 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9140 and 0.8849

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	5440 / 0 / 403
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	2.059
Final R indices [$I>2\sigma(I)$, 4770 reflections]	R1 = 0.0247, *w*R2 = 0.0475
R indices (all data)	R1 = 0.0305, *w*R2 = 0.0480
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	0.473 and -0.323 e.$Å^{-3}$

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of F^2

> 2s(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 1. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Zr	3300(1)	1426(1)	6232(1)	10(1)
C(1)	4470(2)	2305(1)	6672(2)	17(1)
C(2)	2944(2)	2390(1)	6416(2)	17(1)
C(3)	2748(2)	2173(1)	7574(2)	17(1)
C(4)	4165(2)	1958(1)	8572(2)	16(1)
C(5)	5228(2)	2045(1)	8026(2)	15(1)
C(6)	5802(2)	1199(1)	6137(2)	14(1)
C(7)	4615(2)	1125(1)	4702(2)	13(1)
C(8)	3724(2)	697(1)	4743(2)	13(1)
C(9)	4351(2)	515(1)	6202(2)	13(1)
C(10)	5624(2)	831(1)	7079(2)	13(1)
C(11)	7160(2)	1545(1)	6512(2)	20(1)
C(12)	4456(2)	1416(1)	3371(2)	18(1)
C(13)	2475(2)	428(1)	3467(2)	19(1)
C(14)	3893(2)	17(1)	6637(2)	20(1)
C(15)	6701(2)	748(1)	8673(2)	18(1)
C(16)	1942(2)	981(1)	7167(2)	14(1)
C(17)	1861(2)	840(1)	8597(2)	15(1)
C(18)	3393(2)	625(1)	9744(2)	20(1)
C(19)	1429(2)	1304(1)	9259(2)	17(1)
C(20)	631(2)	424(1)	8273(2)	23(1)
C(21)	1318(2)	1620(1)	3896(2)	13(1)
C(22)	-438(2)	1684(1)	3340(2)	15(1)
C(23)	-1179(2)	1161(1)	3296(2)	21(1)
C(24)	-843(2)	2057(1)	4272(2)	19(1)
C(25)	-1147(2)	1897(1)	1771(2)	22(1)

Table 3. Selected bond lengths [Å] and angles [°] for 1.

Zr-Cent(1)	2.241(1)	Cent(1)-Zr-Cent(2)	129.1(1)
Zr-Cent(2)	2.260(1)	Pln(1)-Zr-Pln(2)	126.7(1)
Zr-Pln(1)	2.239(1)	C(16)-Zr-C(21)	99.61(5)
Zr-Pln(2)	2.260(1)		
Zr-C(16)	2.2651(14)		
Zr-C(21)	2.3524(14)		

Cent(1) is the centroid formed by C(1), C(2), C(3), C(4) and C(5).
Cent(2) is the centroid formed by C(6), C(7), C(8), C(9) and C(10).
Pln(1) is the plane formed by C(1), C(2), C(3), C(4) and C(5).
Pln(2) is the plane formed by C(6), C(7), C(8), C(9) and C(10).

Table 4. Bond lengths [Å] and angles [°] for 1.

Zr-Cent(1)	2.241(1)	C(12)-H(7B)	0.959(17)
Zr-Cent(2)	2.260(1)	C(12)-H(7C)	0.904(19)
Zr-Pln(1)	2.239(1)	C(13)-H(8A)	0.925(18)
Zr-Pln(2)	2.260(1)	C(13)-H(8B)	0.953(16)
Zr-C(16)	2.2651(14)	C(13)-H(8C)	0.959(17)
Zr-C(21)	2.3524(14)	C(14)-H(9A)	0.988(17)
Zr-C(1)	2.5024(14)	C(14)-H(9B)	0.920(17)
Zr-C(5)	2.5266(14)	C(14)-H(9C)	0.937(17)
Zr-C(10)	2.5503(13)	C(15)-H(10A)	0.947(19)
Zr-C(6)	2.5531(14)	C(15)-H(10B)	0.84(2)
Zr-C(7)	2.5473(14)	C(15)-H(10C)	0.91(2)
Zr-C(2)	2.5488(14)	C(16)-C(17)	1.5401(19)
Zr-C(4)	2.5519(14)	C(16)-H(16A)	0.944(15)
Zr-C(8)	2.5736(13)	C(16)-H(16B)	0.933(16)
Zr-C(3)	2.5691(14)	C(17)-C(19)	1.531(2)
Zr-C(9)	2.5845(13)	C(17)-C(18)	1.531(2)
C(1)-C(2)	1.408(2)	C(17)-C(20)	1.535(2)
C(1)-C(5)	1.412(2)	C(18)-H(18A)	0.958(15)
C(1)-H(1)	0.923(14)	C(18)-H(18B)	0.966(15)
C(2)-C(3)	1.398(2)	C(18)-H(18C)	0.977(17)
C(2)-H(2)	0.924(15)	C(19)-H(19A)	0.971(16)
C(3)-C(4)	1.413(2)	C(19)-H(19B)	0.976(16)
C(3)-H(3)	0.924(14)	C(19)-H(19C)	0.980(16)
C(4)-C(5)	1.397(2)	C(20)-H(20A)	0.932(15)
C(4)-H(4)	0.890(15)	C(20)-H(20B)	0.979(15)
C(5)-H(5)	0.907(15)	C(20)-H(20C)	0.953(16)
C(6)-C(7)	1.4145(19)	C(21)-C(22)	1.5517(19)
C(6)-C(10)	1.4202(19)	C(21)-H(21A)	0.985(15)
C(6)-C(11)	1.501(2)	C(21)-H(21B)	0.970(15)
C(7)-C(8)	1.4222(19)	C(22)-C(25)	1.534(2)
C(7)-C(12)	1.501(2)	C(22)-C(23)	1.530(2)
C(8)-C(9)	1.4130(19)	C(22)-C(24)	1.528(2)
C(8)-C(13)	1.4973(19)	C(23)-H(23A)	0.966(16)
C(9)-C(10)	1.4215(19)	C(23)-H(23B)	0.984(16)
C(9)-C(14)	1.499(2)	C(23)-H(23C)	0.932(15)
C(10)-C(15)	1.504(2)	C(24)-H(24A)	0.939(16)
C(11)-H(6A)	0.955(17)	C(24)-H(24B)	0.968(16)
C(11)-H(6B)	0.926(18)	C(24)-H(24C)	0.954(15)
C(11)-H(6C)	0.939(17)	C(25)-H(25A)	0.977(15)
C(12)-H(7A)	0.947(17)	C(25)-H(25B)	0.981(16)

C(25)-H(25C)	0.972(16)	C(8)-Zr-C(3)	176.57(4)
		C(16)-Zr-C(9)	81.21(5)
Cent(1)-Zr-Cent(2)	129.1(1)	C(21)-Zr-C(9)	109.48(5)
Pln(1)-Zr-Pln(2)	126.7(1)	C(1)-Zr-C(9)	133.39(5)
C(16)-Zr-C(21)	99.61(5)	C(5)-Zr-C(9)	114.96(5)
C(16)-Zr-C(1)	134.09(5)	C(10)-Zr-C(9)	32.13(4)
C(21)-Zr-C(1)	95.00(5)	C(6)-Zr-C(9)	52.99(4)
C(16)-Zr-C(5)	113.92(5)	C(7)-Zr-C(9)	53.16(4)
C(21)-Zr-C(5)	127.08(5)	C(2)-Zr-C(9)	165.73(5)
C(1)-Zr-C(5)	32.60(5)	C(4)-Zr-C(9)	122.74(5)
C(16)-Zr-C(10)	98.42(5)	C(8)-Zr-C(9)	31.80(4)
C(21)-Zr-C(10)	132.32(5)	C(3)-Zr-C(9)	151.38(5)
C(1)-Zr-C(10)	103.17(5)	C(2)-C(1)-C(5)	107.61(14)
C(5)-Zr-C(10)	83.19(5)	C(2)-C(1)-Zr	75.64(8)
C(16)-Zr-C(6)	130.33(5)	C(5)-C(1)-Zr	74.65(8)
C(21)-Zr-C(6)	112.00(5)	C(2)-C(1)-H(1)	126.8(9)
C(1)-Zr-C(6)	81.43(5)	C(5)-C(1)-H(1)	125.6(9)
C(5)-Zr-C(6)	76.21(5)	Zr-C(1)-H(1)	115.5(9)
C(10)-Zr-C(6)	32.32(4)	C(3)-C(2)-C(1)	108.26(14)
C(16)-Zr-C(7)	130.63(5)	C(3)-C(2)-Zr	74.96(8)
C(21)-Zr-C(7)	81.63(5)	C(1)-C(2)-Zr	72.01(8)
C(1)-Zr-C(7)	94.37(5)	C(3)-C(2)-H(2)	125.8(10)
C(5)-Zr-C(7)	102.96(5)	C(1)-C(2)-H(2)	126.0(10)
C(10)-Zr-C(7)	53.64(4)	Zr-C(2)-H(2)	119.3(10)
C(6)-Zr-C(7)	32.20(4)	C(2)-C(3)-C(4)	107.97(14)
C(16)-Zr-C(2)	110.27(5)	C(2)-C(3)-Zr	73.35(8)
C(21)-Zr-C(2)	77.70(5)	C(4)-C(3)-Zr	73.32(8)
C(1)-Zr-C(2)	32.35(5)	C(2)-C(3)-H(3)	124.5(9)
C(5)-Zr-C(2)	53.26(5)	C(4)-C(3)-H(3)	127.5(9)
C(10)-Zr-C(2)	134.42(5)	Zr-C(3)-H(3)	120.1(9)
C(6)-Zr-C(2)	113.17(5)	C(5)-C(4)-C(3)	107.97(13)
C(7)-Zr-C(2)	118.01(5)	C(5)-C(4)-Zr	73.04(8)
C(16)-Zr-C(4)	83.86(5)	C(3)-C(4)-Zr	74.65(8)
C(21)-Zr-C(4)	127.46(5)	C(5)-C(4)-H(4)	126.1(9)
C(1)-Zr-C(4)	53.48(5)	C(3)-C(4)-H(4)	125.9(9)
C(5)-Zr-C(4)	31.93(5)	Zr-C(4)-H(4)	120.1(9)
C(10)-Zr-C(4)	98.08(5)	C(4)-C(5)-C(1)	108.16(13)
C(6)-Zr-C(4)	103.89(5)	C(4)-C(5)-Zr	75.03(8)
C(7)-Zr-C(4)	133.92(5)	C(1)-C(5)-Zr	72.76(8)
C(2)-Zr-C(4)	52.94(5)	C(4)-C(5)-H(5)	128.9(9)
C(16)-Zr-C(8)	98.74(5)	C(1)-C(5)-H(5)	122.9(9)
C(21)-Zr-C(8)	80.54(5)	Zr-C(5)-H(5)	119.9(9)
C(1)-Zr-C(8)	126.61(5)	C(7)-C(6)-C(10)	108.45(12)
C(5)-Zr-C(8)	129.18(5)	C(7)-C(6)-C(11)	124.35(13)
C(10)-Zr-C(8)	53.22(4)	C(10)-C(6)-C(11)	126.35(13)
C(6)-Zr-C(8)	53.05(4)	C(7)-C(6)-Zr	73.67(8)
C(7)-Zr-C(8)	32.24(4)	C(10)-C(6)-Zr	73.73(8)
C(2)-Zr-C(8)	146.08(5)	C(11)-C(6)-Zr	126.90(10)
C(4)-Zr-C(8)	151.30(4)	C(6)-C(7)-C(8)	107.64(12)
C(16)-Zr-C(3)	81.95(5)	C(6)-C(7)-C(12)	124.89(13)
C(21)-Zr-C(3)	96.04(5)	C(8)-C(7)-C(12)	127.19(13)
C(1)-Zr-C(3)	53.24(5)	C(6)-C(7)-Zr	74.12(8)
C(5)-Zr-C(3)	52.97(5)	C(8)-C(7)-Zr	74.90(8)
C(10)-Zr-C(3)	130.08(4)	C(12)-C(7)-Zr	121.60(10)
C(6)-Zr-C(3)	128.81(5)	C(9)-C(8)-C(7)	108.19(12)
C(7)-Zr-C(3)	147.37(5)	C(9)-C(8)-C(13)	123.93(13)
C(2)-Zr-C(3)	31.69(5)	C(7)-C(8)-C(13)	127.37(13)
C(4)-Zr-C(3)	32.03(4)	C(9)-C(8)-Zr	74.53(8)

C(7)-C(8)-Zr	72.86(8)	H(18A)-C(18)-H(18B)	108.9(12)
C(13)-C(8)-Zr	124.98(9)	C(17)-C(18)-H(18C)	109.0(9)
C(8)-C(9)-C(10)	108.15(12)	H(18A)-C(18)-H(18C)	108.8(12)
C(8)-C(9)-C(14)	123.76(13)	H(18B)-C(18)-H(18C)	107.8(12)
C(10)-C(9)-C(14)	127.23(13)	C(17)-C(19)-H(19A)	111.2(9)
C(8)-C(9)-Zr	73.68(8)	C(17)-C(19)-H(19B)	112.6(9)
C(10)-C(9)-Zr	72.61(8)	H(19A)-C(19)-H(19B)	108.0(12)
C(14)-C(9)-Zr	127.91(10)	C(17)-C(19)-H(19C)	113.8(9)
C(9)-C(10)-C(6)	107.52(12)	H(19A)-C(19)-H(19C)	102.6(13)
C(9)-C(10)-C(15)	125.80(13)	H(19B)-C(19)-H(19C)	108.0(12)
C(6)-C(10)-C(15)	126.25(13)	C(17)-C(20)-H(20A)	110.7(9)
C(9)-C(10)-Zr	75.26(8)	C(17)-C(20)-H(20B)	112.2(8)
C(6)-C(10)-Zr	73.95(8)	H(20A)-C(20)-H(20B)	107.4(13)
C(15)-C(10)-Zr	122.45(10)	C(17)-C(20)-H(20C)	111.4(9)
C(6)-C(11)-H(6A)	109.3(10)	H(20A)-C(20)-H(20C)	107.4(13)
C(6)-C(11)-H(6B)	114.8(10)	H(20B)-C(20)-H(20C)	107.5(13)
H(6A)-C(11)-H(6B)	106.8(14)	C(22)-C(21)-Zr	131.47(10)
C(6)-C(11)-H(6C)	111.6(10)	C(22)-C(21)-H(21A)	103.6(9)
H(6A)-C(11)-H(6C)	108.0(13)	Zr-C(21)-H(21A)	104.2(9)
H(6B)-C(11)-H(6C)	106.0(14)	C(22)-C(21)-H(21B)	107.9(8)
C(7)-C(12)-H(7A)	110.2(10)	Zr-C(21)-H(21B)	100.9(8)
C(7)-C(12)-H(7B)	112.4(10)	H(21A)-C(21)-H(21B)	107.0(12)
H(7A)-C(12)-H(7B)	107.8(14)	C(25)-C(22)-C(23)	107.71(12)
C(7)-C(12)-H(7C)	113.0(11)	C(25)-C(22)-C(24)	107.39(12)
H(7A)-C(12)-H(7C)	108.1(15)	C(23)-C(22)-C(24)	109.31(13)
H(7B)-C(12)-H(7C)	105.1(14)	C(25)-C(22)-C(21)	109.06(12)
C(8)-C(13)-H(8A)	110.7(10)	C(23)-C(22)-C(21)	110.11(12)
C(8)-C(13)-H(8B)	111.7(9)	C(24)-C(22)-C(21)	113.08(12)
H(8A)-C(13)-H(8B)	106.2(14)	C(22)-C(23)-H(23A)	109.9(9)
C(8)-C(13)-H(8C)	113.2(10)	C(22)-C(23)-H(23B)	113.1(9)
H(8A)-C(13)-H(8C)	105.1(14)	H(23A)-C(23)-H(23B)	105.9(13)
H(8B)-C(13)-H(8C)	109.5(13)	C(22)-C(23)-H(23C)	111.4(9)
C(9)-C(14)-H(9A)	109.2(9)	H(23A)-C(23)-H(23C)	108.1(13)
C(9)-C(14)-H(9B)	112.6(10)	H(23B)-C(23)-H(23C)	108.2(13)
H(9A)-C(14)-H(9B)	109.3(14)	C(22)-C(24)-H(24A)	112.3(9)
C(9)-C(14)-H(9C)	114.4(10)	C(22)-C(24)-H(24B)	110.3(9)
H(9A)-C(14)-H(9C)	105.8(14)	H(24A)-C(24)-H(24B)	105.8(13)
H(9B)-C(14)-H(9C)	105.2(14)	C(22)-C(24)-H(24C)	109.9(9)
C(10)-C(15)-H(10A)	112.6(11)	H(24A)-C(24)-H(24C)	109.7(12)
C(10)-C(15)-H(10B)	113.1(13)	H(24B)-C(24)-H(24C)	108.7(13)
H(10A)-C(15)-H(10B)	105.5(16)	C(22)-C(25)-H(25A)	109.7(9)
C(10)-C(15)-H(10C)	114.2(12)	C(22)-C(25)-H(25B)	110.8(9)
H(10A)-C(15)-H(10C)	103.2(15)	H(25A)-C(25)-H(25B)	108.3(12)
H(10B)-C(15)-H(10C)	107.3(17)	C(22)-C(25)-H(25C)	111.9(9)
C(17)-C(16)-Zr	143.89(10)	H(25A)-C(25)-H(25C)	108.4(12)
C(17)-C(16)-H(16A)	108.5(9)	H(25B)-C(25)-H(25C)	107.6(13)
Zr-C(16)-H(16A)	98.7(9)		
C(17)-C(16)-H(16B)	108.9(10)		
Zr-C(16)-H(16B)	85.7(10)		
H(16A)-C(16)-H(16B)	104.9(13)		
C(19)-C(17)-C(18)	108.47(12)		
C(19)-C(17)-C(16)	111.88(12)		
C(18)-C(17)-C(16)	111.32(12)		
C(19)-C(17)-C(20)	107.83(12)		
C(18)-C(17)-C(20)	107.92(13)		
C(16)-C(17)-C(20)	109.27(12)		
C(17)-C(18)-H(18A)	110.3(9)		
C(17)-C(18)-H(18B)	112.1(9)		

Cent(1) is the centroid formed by C(1), C(2), C(3), C(4) and C(5).
Cent(2) is the centroid formed by C(6), C(7), C(8), C(9) and C(10).
Pln(1) is the plane formed by C(1), C(2), C(3), C(4) and C(5).
Pln(2) is the plane formed by C(6), C(7), C(8), C(9) and C(10).

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr	108(1)	81(1)	94(1)	-2(1)	35(1)	0(1)
C(1)	230(8)	107(7)	171(8)	-23(6)	86(7)	-60(6)
C(2)	226(8)	60(7)	169(8)	-4(6)	37(6)	11(6)
C(3)	182(8)	102(7)	205(8)	-62(6)	78(7)	-5(6)
C(4)	226(8)	107(7)	105(7)	-32(6)	49(6)	-18(6)
C(5)	151(8)	114(7)	155(7)	-49(6)	31(6)	-30(6)
C(6)	119(7)	120(7)	170(7)	-12(6)	66(6)	8(6)
C(7)	130(7)	132(7)	147(7)	3(6)	76(6)	32(6)
C(8)	126(7)	113(7)	149(7)	-34(6)	69(6)	19(6)
C(9)	147(7)	87(7)	184(7)	2(6)	91(6)	36(5)
C(10)	121(7)	128(7)	149(7)	6(6)	57(6)	44(6)
C(11)	140(8)	220(9)	248(9)	-16(7)	83(7)	-28(6)
C(12)	195(8)	201(8)	174(8)	24(7)	104(7)	31(7)
C(13)	177(8)	168(8)	212(9)	-68(7)	73(7)	-2(6)
C(14)	249(9)	117(8)	264(9)	14(7)	153(7)	28(7)
C(15)	161(8)	190(8)	141(8)	18(7)	29(6)	42(7)
C(16)	153(7)	98(7)	133(7)	-3(6)	46(6)	16(6)
C(17)	160(7)	140(7)	163(8)	15(6)	85(6)	7(6)
C(18)	223(8)	200(9)	175(8)	55(7)	98(7)	52(7)
C(19)	185(8)	206(9)	143(8)	6(6)	85(7)	20(6)
C(20)	259(9)	208(9)	262(9)	4(7)	155(8)	-46(7)
C(21)	148(7)	126(7)	131(7)	-8(6)	64(6)	-10(6)
C(22)	135(7)	160(8)	133(7)	14(6)	39(6)	18(6)
C(23)	146(8)	221(9)	217(9)	-9(7)	45(7)	-17(7)
C(24)	156(8)	214(9)	193(9)	6(7)	64(7)	37(7)
C(25)	152(8)	305(10)	155(8)	41(7)	22(6)	28(7)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 1.

	x	y	z	U_{iso}
H(1)	4906(16)	2399(6)	6070(15)	14(4)
H(2)	2199(17)	2562(6)	5622(17)	23(4)
H(3)	1841(16)	2181(5)	7656(15)	13(4)
H(4)	4356(16)	1804(5)	9417(16)	13(4)
H(5)	6244(17)	1968(5)	8440(15)	14(4)
H(6A)	7840(20)	1392(6)	6177(17)	28(5)
H(6B)	6922(19)	1870(7)	6099(19)	33(5)
H(6C)	7711(19)	1596(6)	7528(19)	28(5)
H(7A)	5047(19)	1257(6)	2958(18)	30(5)
H(7B)	3410(20)	1431(6)	2625(19)	31(5)
H(7C)	4758(19)	1748(7)	3566(18)	34(5)
H(8A)	2796(19)	106(7)	3335(18)	36(5)
H(8B)	1590(18)	374(6)	3618(17)	26(5)
H(8C)	2185(17)	604(6)	2552(18)	26(4)
H(9A)	4255(18)	-272(7)	6245(18)	31(5)
H(9B)	4282(17)	-18(6)	7637(19)	27(5)
H(9C)	2830(20)	-29(6)	6269(17)	32(5)
H(10A)	7530(20)	529(7)	8814(19)	44(5)
H(10B)	7100(20)	1021(8)	9120(20)	47(6)
H(10C)	6270(20)	588(7)	9190(20)	45(6)
H(16A)	1736(16)	682(6)	6582(16)	16(4)
H(16B)	1139(18)	1205(6)	6624(17)	25(4)
H(18A)	3654(16)	319(6)	9385(16)	17(4)
H(18B)	4219(16)	871(6)	10005(15)	14(4)
H(18C)	3299(16)	541(6)	10634(18)	24(4)
H(19A)	1278(16)	1205(6)	10103(17)	19(4)
H(19B)	494(18)	1475(6)	8557(17)	22(4)
H(19C)	2240(18)	1565(6)	9671(17)	18(4)
H(20A)	-332(17)	545(6)	7608(17)	19(4)
H(20B)	841(16)	113(6)	7852(16)	17(4)
H(20C)	560(17)	325(6)	9140(18)	22(4)
H(21A)	1395(16)	1348(6)	3257(17)	18(4)
H(21B)	1707(16)	1934(6)	3672(15)	18(4)
H(23A)	-2274(18)	1201(6)	2933(16)	20(4)
H(23B)	-810(17)	1001(6)	4270(18)	23(4)
H(23C)	-1009(17)	931(6)	2683(16)	17(4)
H(24A)	-467(17)	1946(6)	5250(18)	18(4)
H(24B)	-1947(18)	2080(6)	3898(17)	23(4)
H(24C)	-450(16)	2391(6)	4246(15)	16(4)
H(25A)	-2263(18)	1915(5)	1385(16)	17(4)
H(25B)	-762(17)	2245(6)	1753(16)	24(4)
H(25C)	-909(16)	1683(6)	1119(16)	15(4)

Table 7. Crystal data and structure refinement for 2 (CCDC 181778).

Empirical formula	$C_{23}H_{42}Si_2Zr$
Formula weight	465.97
Crystallization Solvent	Pentane
Crystal Habit	Block
Crystal size	0.26 x 0.26 x 0.21 mm^3

Crystal color	Colorless

Data Collection

Preliminary Photos	Rotation
Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKa
Data Collection Temperature	98(2) K
q range for 29725 reflections used in lattice determination	2.28 to 28.24°
Unit cell dimensions	a = 9.9621(5) Å b = 26.8264(13) Å b= 116.3020(10)° c = 10.4769(5) Å
Volume	2510.0(2) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.233 Mg/m^3
F(000)	992
Data collection program	Bruker SMART v5.054
q range for data collection	1.52 to 28.36°
Completeness to q = 28.36°	95.3 %
Index ranges	$-13 \le h \le 13$, $-35 \le k \le 35$, $-13 \le l \le 13$
Data collection scan type	w scans at 7 f settings
Data reduction program	Bruker SAINT v6.022
Reflections collected	51027
Independent reflections	5985 [R_{int}= 0.0515]
Absorption coefficient	0.539 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.8953 and 0.8726

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	5985 / 0 / 403
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	2.088
Final R indices [I>2s(I), 5352 reflections]	R1 = 0.0302, *w*R2 = 0.0514
R indices (all data)	R1 = 0.0362, *w*R2 = 0.0518
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/s^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	0.480 and -0.327 $e.Å^{-3}$

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2s(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles

and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Zr	3381(1)	1429(1)	6079(1)	13(1)
Si(1)	1933(1)	864(1)	8605(1)	17(1)
Si(2)	-485(1)	1640(1)	3253(1)	17(1)
C(1)	4428(2)	2296(1)	6510(2)	24(1)
C(2)	2929(2)	2356(1)	6266(2)	24(1)
C(3)	2766(2)	2136(1)	7397(2)	21(1)
C(4)	4167(2)	1940(1)	8357(2)	19(1)
C(5)	5194(2)	2044(1)	7821(2)	20(1)
C(6)	5865(2)	1183(1)	6120(2)	18(1)
C(7)	4763(2)	1119(1)	4697(2)	18(1)
C(8)	3827(2)	716(1)	4683(2)	17(1)
C(9)	4343(2)	538(1)	6097(2)	17(1)
C(10)	5591(2)	833(1)	6990(2)	17(1)
C(11)	7231(2)	1507(1)	6559(2)	25(1)
C(12)	4709(2)	1405(1)	3443(2)	25(1)
C(13)	2619(2)	471(1)	3403(2)	25(1)
C(14)	3790(2)	72(1)	6496(2)	24(1)
C(15)	6575(2)	744(1)	8552(2)	24(1)
C(16)	1911(2)	1011(1)	6866(2)	16(1)
C(17)	3777(2)	633(1)	9987(2)	27(1)
C(18)	1436(2)	1422(1)	9387(2)	22(1)
C(19)	527(3)	370(1)	8386(2)	33(1)
C(20)	1562(2)	1622(1)	3830(2)	18(1)
C(21)	-1502(2)	1869(1)	1376(2)	33(1)
C(22)	-1255(2)	1006(1)	3262(2)	28(1)
C(23)	-1031(2)	2076(1)	4333(2)	24(1)

Table 9. Selected bond lengths [Å] and angles [°] for 2.

Zr-Cent(1)	2.246(1)	Cent(1)-Zr-Cent(2)	131.1(1)
Zr-Cent(2)	2.247(1)	Pln(1)-Zr-Pln(2)	128.9(1)
Zr-Pln(1)	2.248(1)	C(16)-Zr-C(20)	98.09(6)
Zr-Pln(2)	2.248(1)		
Zr-C(16)	2.2691(16)		
Zr-C(20)	2.3066(16)		

Cent(1) is the centroid formed by C(1), C(2), C(3), C(4) and C(5).
Cent(2) is the centroid formed by C(6), C(7), C(8), C(9) and C(10).
Pln(1) is the plane formed by C(1), C(2), C(3), C(4) and C(5).
Pln(2) is the plane formed by C(6), C(7), C(8), C(9) and C(10).

Table 10. Bond lengths [Å] and angles [°] for 2.

Zr-Cent(1)	2.246(1)	Zr-Pln(1)	2.248(1)
Zr-Cent(2)	2.247(1)	Zr-Pln(2)	2.248(1)

Zr-C(16)	2.2691(16)	C(17)-H(17B)	0.930(19)
Zr-C(20)	2.3066(16)	C(17)-H(17C)	0.96(2)
Zr-C(1)	2.5075(16)	C(18)-H(19)	0.94(2)
Zr-C(5)	2.5296(16)	C(18)-H(19B)	0.925(19)
Zr-C(7)	2.5391(15)	C(18)-H(19C)	0.980(18)
Zr-C(10)	2.5393(15)	C(19)-H(18)	0.96(2)
Zr-C(6)	2.5427(15)	C(19)-H(18B)	0.95(2)
Zr-C(2)	2.5520(16)	C(19)-H(18C)	0.95(2)
Zr-C(4)	2.5562(16)	C(20)-H(20A)	0.938(18)
Zr-C(8)	2.5623(15)	C(20)-H(20B)	0.947(17)
Zr-C(3)	2.5742(16)	C(21)-H(21A)	0.92(2)
Zr-C(9)	2.5718(15)	C(21)-H(21B)	0.98(2)
Si(1)-C(16)	1.8543(16)	C(21)-H(21C)	0.89(2)
Si(1)-C(17)	1.8702(18)	C(22)-H(22A)	0.915(19)
Si(1)-C(18)	1.8750(18)	C(22)-H(22B)	0.91(2)
Si(1)-C(19)	1.8672(19)	C(22)-H(22C)	0.90(2)
Si(2)-C(20)	1.8528(17)	C(23)-H(23A)	0.951(18)
Si(2)-C(22)	1.8682(19)	C(23)-H(23B)	0.940(19)
Si(2)-C(23)	1.8700(18)	C(23)-H(23C)	0.931(19)
Si(2)-C(21)	1.8728(19)		
C(1)-C(2)	1.408(2)	Cent(1)-Zr-Cent(2)	131.1(1)
C(1)-C(5)	1.412(2)	Pln(1)-Zr-Pln(2)	128.9(1)
C(1)-H(1)	0.904(16)	C(16)-Zr-C(20)	98.09(6)
C(2)-C(3)	1.398(2)	C(16)-Zr-C(1)	132.58(6)
C(2)-H(2)	0.929(16)	C(20)-Zr-C(1)	92.97(6)
C(3)-C(4)	1.411(2)	C(16)-Zr-C(5)	115.46(6)
C(3)-H(3)	0.953(16)	C(20)-Zr-C(5)	125.25(6)
C(4)-C(5)	1.397(2)	C(1)-Zr-C(5)	32.56(5)
C(4)-H(4)	0.940(16)	C(16)-Zr-C(7)	130.23(6)
C(5)-H(5)	0.911(16)	C(20)-Zr-C(7)	82.51(5)
C(6)-C(7)	1.416(2)	C(1)-Zr-C(7)	96.82(6)
C(6)-C(10)	1.418(2)	C(5)-Zr-C(7)	103.32(5)
C(6)-C(11)	1.505(2)	C(16)-Zr-C(10)	98.29(5)
C(7)-C(8)	1.423(2)	C(20)-Zr-C(10)	133.07(6)
C(7)-C(12)	1.501(2)	C(1)-Zr-C(10)	107.08(5)
C(8)-C(9)	1.419(2)	C(5)-Zr-C(10)	85.20(5)
C(8)-C(13)	1.500(2)	C(7)-Zr-C(10)	53.83(5)
C(9)-C(10)	1.421(2)	C(16)-Zr-C(6)	130.23(6)
C(9)-C(14)	1.499(2)	C(20)-Zr-C(6)	113.15(5)
C(10)-C(15)	1.508(2)	C(1)-Zr-C(6)	85.01(6)
C(11)-H(11A)	0.98(2)	C(5)-Zr-C(6)	77.19(5)
C(11)-H(11B)	0.974(19)	C(7)-Zr-C(6)	32.37(5)
C(11)-H(11C)	0.891(19)	C(10)-Zr-C(6)	32.39(5)
C(12)-H(12A)	0.92(2)	C(16)-Zr-C(2)	106.84(6)
C(12)-H(12B)	0.99(2)	C(20)-Zr-C(2)	76.96(6)
C(12)-H(12C)	0.93(2)	C(1)-Zr-C(2)	32.30(6)
C(13)-H(13A)	0.929(19)	C(5)-Zr-C(2)	53.26(5)
C(13)-H(13B)	0.953(19)	C(7)-Zr-C(2)	121.40(5)
C(13)-H(13C)	1.000(18)	C(10)-Zr-C(2)	137.53(5)
C(14)-H(14A)	0.960(19)	C(6)-Zr-C(2)	117.03(5)
C(14)-H(14B)	0.959(17)	C(16)-Zr-C(4)	84.60(6)
C(14)-H(14C)	0.946(19)	C(20)-Zr-C(4)	127.63(6)
C(15)-H(15A)	0.90(2)	C(1)-Zr-C(4)	53.34(6)
C(15)-H(15B)	0.91(2)	C(5)-Zr-C(4)	31.87(5)
C(15)-H(15C)	0.93(2)	C(7)-Zr-C(4)	133.51(5)
C(16)-H(16A)	0.937(17)	C(10)-Zr-C(4)	97.50(5)
C(16)-H(16B)	0.921(19)	C(6)-Zr-C(4)	103.29(5)
C(17)-H(17)	0.94(2)	C(2)-Zr-C(4)	52.89(5)

C(16)-Zr-C(8)	98.17(5)	C(4)-C(3)-H(3)	125.8(10)
C(20)-Zr-C(8)	80.82(6)	Zr-C(3)-H(3)	120.7(10)
C(1)-Zr-C(8)	129.15(6)	C(3)-C(4)-C(5)	107.98(15)
C(5)-Zr-C(8)	130.51(5)	C(3)-C(4)-Zr	74.74(9)
C(7)-Zr-C(8)	32.40(5)	C(5)-C(4)-Zr	73.02(9)
C(10)-Zr-C(8)	53.46(5)	C(3)-C(4)-H(4)	123.3(10)
C(6)-Zr-C(8)	53.33(5)	C(5)-C(4)-H(4)	128.7(10)
C(2)-Zr-C(8)	148.46(5)	Zr-C(4)-H(4)	117.7(10)
C(4)-Zr-C(8)	150.96(5)	C(4)-C(5)-C(1)	108.06(15)
C(16)-Zr-C(3)	79.84(6)	C(4)-C(5)-Zr	75.11(9)
C(20)-Zr-C(3)	96.71(6)	C(1)-C(5)-Zr	72.86(9)
C(1)-Zr-C(3)	53.05(6)	C(4)-C(5)-H(5)	126.8(10)
C(5)-Zr-C(3)	52.84(6)	C(1)-C(5)-H(5)	125.1(10)
C(7)-Zr-C(3)	149.85(5)	Zr-C(5)-H(5)	116.7(10)
C(10)-Zr-C(3)	129.39(5)	C(7)-C(6)-C(10)	108.43(14)
C(6)-Zr-C(3)	130.01(5)	C(7)-C(6)-C(11)	124.50(15)
C(2)-Zr-C(3)	31.64(5)	C(10)-C(6)-C(11)	126.27(15)
C(4)-Zr-C(3)	31.93(5)	C(7)-C(6)-Zr	73.67(8)
C(8)-Zr-C(3)	176.62(5)	C(10)-C(6)-Zr	73.67(8)
C(16)-Zr-C(9)	80.60(5)	C(11)-C(6)-Zr	126.70(12)
C(20)-Zr-C(9)	109.71(6)	C(6)-C(7)-C(8)	107.56(14)
C(1)-Zr-C(9)	137.47(5)	C(6)-C(7)-C(12)	124.73(15)
C(5)-Zr-C(9)	117.17(5)	C(8)-C(7)-C(12)	127.52(15)
C(7)-Zr-C(9)	53.55(5)	C(6)-C(7)-Zr	73.96(9)
C(10)-Zr-C(9)	32.27(5)	C(8)-C(7)-Zr	74.70(9)
C(6)-Zr-C(9)	53.31(5)	C(12)-C(7)-Zr	120.98(11)
C(2)-Zr-C(9)	169.56(5)	C(9)-C(8)-C(7)	108.24(13)
C(4)-Zr-C(9)	122.19(5)	C(9)-C(8)-C(13)	124.17(15)
C(8)-Zr-C(9)	32.08(5)	C(7)-C(8)-C(13)	127.21(15)
C(3)-Zr-C(9)	148.98(5)	C(9)-C(8)-Zr	74.33(9)
C(16)-Si(1)-C(17)	114.27(8)	C(7)-C(8)-Zr	72.91(9)
C(16)-Si(1)-C(18)	111.73(8)	C(13)-C(8)-Zr	124.33(11)
C(17)-Si(1)-C(18)	106.57(9)	C(10)-C(9)-C(8)	107.82(14)
C(16)-Si(1)-C(19)	110.36(9)	C(10)-C(9)-C(14)	127.17(15)
C(17)-Si(1)-C(19)	106.58(10)	C(8)-C(9)-C(14)	124.39(15)
C(18)-Si(1)-C(19)	106.92(9)	C(10)-C(9)-Zr	72.61(9)
C(20)-Si(2)-C(22)	111.69(8)	C(8)-C(9)-Zr	73.59(9)
C(20)-Si(2)-C(23)	113.13(8)	C(14)-C(9)-Zr	126.57(11)
C(22)-Si(2)-C(23)	109.67(9)	C(9)-C(10)-C(6)	107.91(13)
C(20)-Si(2)-C(21)	110.87(9)	C(9)-C(10)-C(15)	125.75(15)
C(22)-Si(2)-C(21)	105.79(10)	C(6)-C(10)-C(15)	125.86(15)
C(23)-Si(2)-C(21)	105.24(10)	C(9)-C(10)-Zr	75.12(8)
C(2)-C(1)-C(5)	107.75(16)	C(6)-C(10)-Zr	73.94(9)
C(2)-C(1)-Zr	75.59(9)	C(15)-C(10)-Zr	123.14(11)
C(5)-C(1)-Zr	74.58(9)	C(6)-C(11)-H(11A)	109.6(11)
C(2)-C(1)-H(1)	127.3(10)	C(6)-C(11)-H(11B)	112.3(10)
C(5)-C(1)-H(1)	124.9(11)	H(11A)-C(11)-H(11B)	105.8(14)
Zr-C(1)-H(1)	116.3(11)	C(6)-C(11)-H(11C)	113.0(11)
C(3)-C(2)-C(1)	108.04(15)	H(11A)-C(11)-H(11C)	108.2(15)
C(3)-C(2)-Zr	75.06(9)	H(11B)-C(11)-H(11C)	107.6(15)
C(1)-C(2)-Zr	72.11(9)	C(7)-C(12)-H(12A)	111.6(12)
C(3)-C(2)-H(2)	126.5(10)	C(7)-C(12)-H(12B)	113.8(12)
C(1)-C(2)-H(2)	125.4(10)	H(12A)-C(12)-H(12B)	109.3(16)
Zr-C(2)-H(2)	118.2(11)	C(7)-C(12)-H(12C)	112.5(12)
C(2)-C(3)-C(4)	108.15(16)	H(12A)-C(12)-H(12C)	107.1(16)
C(2)-C(3)-Zr	73.30(9)	H(12B)-C(12)-H(12C)	102.0(16)
C(4)-C(3)-Zr	73.33(9)	C(8)-C(13)-H(13A)	110.7(11)
C(2)-C(3)-H(3)	126.0(10)	C(8)-C(13)-H(13B)	112.0(11)

H(13A)-C(13)-H(13B)	106.4(15)	H(19)-C(18)-H(19C)	105.8(15)
C(8)-C(13)-H(13C)	112.1(10)	H(19B)-C(18)-H(19C)	107.4(16)
H(13A)-C(13)-H(13C)	107.1(14)	Si(1)-C(19)-H(18)	109.8(12)
H(13B)-C(13)-H(13C)	108.2(14)	Si(1)-C(19)-H(18B)	113.1(13)
C(9)-C(14)-H(14A)	109.4(10)	H(18)-C(19)-H(18B)	106.3(17)
C(9)-C(14)-H(14B)	113.0(11)	Si(1)-C(19)-H(18C)	110.9(12)
H(14A)-C(14)-H(14B)	105.3(15)	H(18)-C(19)-H(18C)	112.3(17)
C(9)-C(14)-H(14C)	114.1(11)	H(18B)-C(19)-H(18C)	104.4(17)
H(14A)-C(14)-H(14C)	108.6(15)	Si(2)-C(20)-Zr	126.29(8)
H(14B)-C(14)-H(14C)	106.1(14)	Si(2)-C(20)-H(20A)	103.9(11)
C(10)-C(15)-H(15A)	112.6(13)	Zr-C(20)-H(20A)	107.6(11)
C(10)-C(15)-H(15B)	114.7(12)	Si(2)-C(20)-H(20B)	107.9(9)
H(15A)-C(15)-H(15B)	100.1(17)	Zr-C(20)-H(20B)	104.9(9)
C(10)-C(15)-H(15C)	114.8(13)	H(20A)-C(20)-H(20B)	104.4(14)
H(15A)-C(15)-H(15C)	107.1(17)	Si(2)-C(21)-H(21A)	109.5(13)
H(15B)-C(15)-H(15C)	106.2(17)	Si(2)-C(21)-H(21B)	109.9(12)
Si(1)-C(16)-Zr	137.14(8)	H(21A)-C(21)-H(21B)	111.1(17)
Si(1)-C(16)-H(16A)	107.7(10)	Si(2)-C(21)-H(21C)	111.8(14)
Zr-C(16)-H(16A)	104.8(10)	H(21A)-C(21)-H(21C)	108.6(18)
Si(1)-C(16)-H(16B)	103.6(11)	H(21B)-C(21)-H(21C)	105.8(18)
Zr-C(16)-H(16B)	94.7(11)	Si(2)-C(22)-H(22A)	109.9(12)
H(16A)-C(16)-H(16B)	104.0(15)	Si(2)-C(22)-H(22B)	115.8(14)
Si(1)-C(17)-H(17)	111.3(12)	H(22A)-C(22)-H(22B)	106.1(18)
Si(1)-C(17)-H(17B)	111.3(12)	Si(2)-C(22)-H(22C)	110.1(14)
H(17)-C(17)-H(17B)	108.0(16)	H(22A)-C(22)-H(22C)	105.6(17)
Si(1)-C(17)-H(17C)	110.5(11)	H(22B)-C(22)-H(22C)	108.7(19)
H(17)-C(17)-H(17C)	108.8(16)	Si(2)-C(23)-H(23A)	114.4(11)
H(17B)-C(17)-H(17C)	106.9(16)	Si(2)-C(23)-H(23B)	107.6(11)
Si(1)-C(18)-H(19)	110.8(11)	H(23A)-C(23)-H(23B)	107.7(15)
Si(1)-C(18)-H(19B)	113.0(11)	Si(2)-C(23)-H(23C)	111.0(11)
H(19)-C(18)-H(19B)	107.7(16)	H(23A)-C(23)-H(23C)	105.6(15)
Si(1)-C(18)-H(19C)	111.8(10)	H(23B)-C(23)-H(23C)	110.5(16)

Cent(1) is the centroid formed by C(1), C(2), C(3), C(4) and C(5).
Cent(2) is the centroid formed by C(6), C(7), C(8), C(9) and C(10).
Pln(1) is the plane formed by C(1), C(2), C(3), C(4) and C(5).
Pln(2) is the plane formed by C(6), C(7), C(8), C(9) and C(10).

Table 11. Anisotropic displacement parameters ($Å^2 x 10^4$) for 2. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr	145(1)	115(1)	131(1)	4(1)	52(1)	-8(1)
Si(1)	209(2)	131(2)	188(2)	9(2)	116(2)	11(2)
Si(2)	158(2)	178(2)	163(2)	16(2)	56(2)	15(2)
C(1)	315(10)	151(9)	234(9)	1(7)	107(8)	-85(7)
C(2)	296(10)	93(8)	249(9)	8(7)	40(8)	13(7)
C(3)	239(9)	120(8)	260(9)	-62(7)	97(8)	-4(7)
C(4)	263(9)	129(8)	160(8)	-35(7)	71(7)	-21(7)
C(5)	200(9)	158(8)	201(9)	-42(7)	46(7)	-48(7)
C(6)	144(8)	187(8)	209(8)	-3(7)	84(7)	5(6)
C(7)	163(8)	209(9)	186(8)	-7(7)	102(7)	7(6)
C(8)	149(8)	188(8)	197(8)	-45(7)	88(7)	9(6)
C(9)	169(8)	138(8)	247(9)	-9(7)	123(7)	30(6)
C(10)	153(8)	177(8)	182(8)	19(6)	77(7)	48(6)
C(11)	185(9)	287(11)	279(10)	13(8)	105(8)	-43(8)

C(12)	219(9)	327(11)	219(9)	34(8)	123(8)	17(8)
C(13)	205(9)	257(10)	286(10)	-110(8)	102(8)	-16(8)
C(14)	266(10)	145(9)	354(11)	10(8)	190(9)	26(7)
C(15)	230(10)	261(10)	201(9)	49(8)	79(8)	54(8)
C(16)	168(8)	121(8)	175(8)	-11(7)	64(7)	9(7)
C(17)	326(11)	292(11)	219(10)	88(8)	156(8)	123(9)
C(18)	234(9)	224(9)	198(9)	-6(8)	101(8)	23(8)
C(19)	435(13)	248(11)	428(13)	-53(9)	306(11)	-104(9)
C(20)	202(8)	182(8)	179(8)	5(7)	99(7)	-3(7)
C(21)	227(11)	471(14)	234(11)	83(9)	51(9)	40(10)
C(22)	182(10)	243(10)	350(12)	-12(9)	59(9)	-24(8)
C(23)	232(10)	236(10)	280(10)	0(8)	129(8)	19(8)

Table 12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 2.

	x	y	z	U_{iso}
H(1)	4849(17)	2399(6)	5949(17)	24(5)
H(2)	2185(18)	2513(7)	5481(17)	25(5)
H(3)	1871(18)	2127(6)	7515(17)	21(4)
H(4)	4323(17)	1769(6)	9194(17)	17(4)
H(5)	6182(18)	1960(6)	8221(17)	17(4)
H(11A)	7920(20)	1357(7)	6238(19)	33(5)
H(11B)	7790(20)	1536(6)	7590(20)	30(5)
H(11C)	7018(19)	1814(7)	6203(18)	25(5)
H(12A)	5390(20)	1284(7)	3150(20)	40(6)
H(12B)	4860(20)	1767(9)	3610(20)	51(6)
H(12C)	3770(20)	1390(7)	2660(20)	37(5)
H(13A)	2907(18)	153(7)	3277(18)	30(5)
H(13B)	1710(20)	433(7)	3497(18)	33(5)
H(13C)	2384(18)	661(6)	2508(19)	27(5)
H(14A)	4270(19)	-212(7)	6318(17)	31(5)
H(14B)	2740(20)	18(7)	5934(18)	28(5)
H(14C)	3955(19)	62(7)	7460(20)	34(5)
H(15A)	7440(20)	592(8)	8710(20)	48(6)
H(15B)	6200(20)	521(8)	8970(20)	39(6)
H(15C)	6820(20)	1029(9)	9120(20)	50(7)
H(16A)	1614(17)	723(6)	6306(17)	21(4)
H(16B)	1110(20)	1223(7)	6441(19)	33(5)
H(17)	4080(20)	342(7)	9680(20)	40(6)
H(17B)	4520(20)	872(7)	10198(19)	35(6)
H(17C)	3719(19)	562(7)	10860(20)	35(5)
H(18)	760(20)	71(8)	8020(20)	47(6)
H(18B)	-460(20)	460(8)	7730(20)	46(6)
H(18C)	470(20)	313(7)	9260(20)	45(6)
H(19)	1210(20)	1327(7)	10140(20)	35(5)
H(19B)	620(20)	1595(7)	8730(20)	34(5)
H(19C)	2270(20)	1658(7)	9799(18)	29(5)
H(20A)	1668(19)	1400(7)	3189(19)	27(5)
H(20B)	1853(17)	1934(6)	3615(16)	18(4)
H(21A)	-2510(20)	1852(7)	1090(20)	44(6)
H(21B)	-1210(20)	1672(8)	750(20)	47(6)
H(21C)	-1260(20)	2184(9)	1290(20)	59(8)
H(22A)	-2270(20)	1023(7)	2929(19)	34(5)

H(22B)	-900(20)	853(8)	4120(20)	52(7)
H(22C)	-1100(20)	804(8)	2650(20)	53(7)
H(23A)	-661(19)	1986(6)	5310(20)	28(5)
H(23B)	-2080(20)	2079(7)	3930(20)	38(5)
H(23C)	-667(19)	2396(7)	4333(18)	31(5)

Table 13. Crystal data and structure refinement for 6 (CCDC 251491).

Empirical formula	$C_{20}H_{31}ClZr$
Formula weight	398.12
Crystallization Solvent	Diethylether/petroleum ether
Crystal Habit	Fragment
Crystal size	0.36 x 0.26 x 0.26 mm^3
Crystal color	Yellow

Data Collection

Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKa	
Data Collection Temperature	100(2) K	
q range for 22335 reflections used in lattice determination	2.37 to 45.84°	
Unit cell dimensions	a = 8.9772(2) Å	a= 101.6260(10)°
	b = 13.5673(4) Å	b= 104.3560(10)°
	c = 17.2242(5) Å	g = 100.4190(10)°
Volume	1930.85(9) $Å^3$	
Z	4	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.370 Mg/m^3	
F(000)	832	
Data collection program	Bruker SMART v5.054	
q range for data collection	1.58 to 46.45°	
Completeness to q = 46.45°	83.0 %	
Index ranges	$-18 \le h \le 18$, $-27 \le k \le 27$, $-32 \le l \le 35$	
Data collection scan type	w scans at 7 f settings	
Data reduction program	Bruker SAINT v6.45	
Reflections collected	54797	
Independent reflections	28459 [R_{int}= 0.0515]	
Absorption coefficient	0.704 mm^{-1}	
Absorption correction	None	
Max. and min. transmission	0.8382 and 0.7857	

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	28459 / 0 / 413
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.157
Final R indices [I>2s(I), 18839 reflections]	R1 = 0.0390, *w*R2 = 0.0748
R indices (all data)	R1 = 0.0668, *w*R2 = 0.0786
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/s^2(Fo^2)$
Max shift/error	0.004
Average shift/error	0.000
Largest diff. peak and hole	1.282 and -0.693 e.$Å^{-3}$

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 6. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Zr(1)	7828(1)	1533(1)	2617(1)	10(1)
Cl(1)	6552(1)	-316(1)	2014(1)	18(1)
C(1A)	9056(2)	1180(1)	1433(1)	21(1)
C(2A)	10164(2)	1130(1)	2156(1)	22(1)
C(3A)	10706(2)	2122(1)	2700(1)	20(1)
C(4A)	9908(2)	2794(1)	2328(1)	17(1)
C(5A)	8908(2)	2207(1)	1537(1)	17(1)
C(6A)	7530(1)	979(1)	3910(1)	12(1)
C(7A)	9119(1)	1560(1)	4099(1)	12(1)
C(8A)	9081(1)	2610(1)	4109(1)	12(1)
C(9A)	7468(1)	2669(1)	3909(1)	11(1)
C(10A)	6508(1)	1657(1)	3782(1)	11(1)
C(11A)	7026(2)	-123(1)	3949(1)	18(1)
C(12A)	10566(2)	1154(1)	4364(1)	18(1)
C(13A)	10466(2)	3546(1)	4436(1)	18(1)
C(14A)	6933(2)	3660(1)	3939(1)	16(1)
C(15A)	4743(1)	1345(1)	3609(1)	17(1)
C(16A)	5817(1)	2255(1)	2018(1)	14(1)
C(17A)	4471(2)	1835(1)	1178(1)	16(1)
C(18A)	5080(2)	1603(1)	424(1)	27(1)
C(19A)	3508(2)	2660(1)	1081(1)	30(1)
C(20A)	3349(2)	843(1)	1178(1)	25(1)
Zr(2)	9100(1)	3103(1)	7450(1)	10(1)
Cl(2)	10383(1)	4421(1)	6888(1)	16(1)
C(1B)	8565(2)	1952(1)	5996(1)	19(1)
C(2B)	10079(2)	1917(1)	6464(1)	22(1)
C(3B)	9906(2)	1435(1)	7092(1)	21(1)
C(4B)	8260(2)	1167(1)	7014(1)	20(1)
C(5B)	7448(2)	1472(1)	6330(1)	18(1)
C(6B)	11036(1)	4325(1)	8790(1)	14(1)
C(7B)	11255(1)	3315(1)	8781(1)	14(1)
C(8B)	9845(2)	2713(1)	8861(1)	16(1)
C(9B)	8755(2)	3356(1)	8892(1)	16(1)
C(10B)	9502(2)	4356(1)	8854(1)	14(1)
C(11B)	12325(2)	5225(1)	8820(1)	23(1)
C(12B)	12793(2)	3010(1)	8804(1)	22(1)
C(13B)	9638(2)	1663(1)	9038(1)	27(1)
C(14B)	7185(2)	3034(1)	9050(1)	27(1)
C(15B)	8857(2)	5312(1)	8950(1)	22(1)
C(16B)	6573(1)	3406(1)	7193(1)	16(1)

C(17B)	5585(1)	3758(1)	6472(1)	16(1)
C(18B)	5091(2)	2957(1)	5634(1)	35(1)
C(19B)	4072(2)	3937(2)	6670(1)	35(1)
C(20B)	6471(2)	4784(1)	6383(1)	35(1)

Table 15. Selected bond lengths [Å] and angles [°] for 6.

Zr(1)-Cent1A	2.232	Zr(2)-Cent1B	2.224
Zr(1)-Cent2A	2.241	Zr(2)-Cent2B	2.240
Zr(1)-C(16A)	2.3258(12)	Zr(2)-C(16B)	2.3287(12)
Zr(1)-Cl(1)	2.4503(3)	Zr(2)-Cl(2)	2.4432(3)
Cent1A-Zr(1)-Cent2A	129.5	Cent1B-Zr(2)-Cent2B	129.8
C(16A)-Zr(1)-Cl(1)	100.18(3)	C(16B)-Zr(2)-Cl(2)	99.91(3)

Table 16. Bond lengths [Å] and angles [°] for 6.

Zr(1)-Cent1A	2.232	Zr(2)-C(7B)	2.5329(12)
Zr(1)-Cent2A	2.241	Zr(2)-C(9B)	2.5406(12)
Zr(1)-C(16A)	2.3258(12)	Zr(2)-C(8B)	2.5438(12)
Zr(1)-Cl(1)	2.4503(3)	Zr(2)-C(5B)	2.5477(12)
Zr(1)-C(4A)	2.5125(12)	Zr(2)-C(1B)	2.5490(13)
Zr(1)-C(7A)	2.5172(11)	Zr(2)-C(6B)	2.5537(12)
Zr(1)-C(3A)	2.5211(12)	Zr(2)-C(10B)	2.5593(12)
Zr(1)-C(2A)	2.5286(13)	C(1B)-C(5B)	1.3998(18)
Zr(1)-C(8A)	2.5419(11)	C(1B)-C(2B)	1.412(2)
Zr(1)-C(6A)	2.5482(11)	C(2B)-C(3B)	1.397(2)
Zr(1)-C(5A)	2.5485(12)	C(3B)-C(4B)	1.422(2)
Zr(1)-C(1A)	2.5523(13)	C(4B)-C(5B)	1.4041(19)
Zr(1)-C(10A)	2.5642(11)	C(6B)-C(10B)	1.4157(17)
Zr(1)-C(9A)	2.5656(11)	C(6B)-C(7B)	1.4171(17)
C(1A)-C(5A)	1.4027(19)	C(6B)-C(11B)	1.5049(17)
C(1A)-C(2A)	1.410(2)	C(7B)-C(8B)	1.4306(17)
C(2A)-C(3A)	1.398(2)	C(7B)-C(12B)	1.5050(18)
C(3A)-C(4A)	1.4151(19)	C(8B)-C(9B)	1.4275(18)
C(4A)-C(5A)	1.4114(18)	C(8B)-C(13B)	1.5046(18)
C(6A)-C(7A)	1.4225(16)	C(9B)-C(10B)	1.4223(17)
C(6A)-C(10A)	1.4228(16)	C(9B)-C(14B)	1.5053(18)
C(6A)-C(11A)	1.5016(16)	C(10B)-C(15B)	1.5102(18)
C(7A)-C(8A)	1.4276(16)	C(16B)-C(17B)	1.5505(17)
C(7A)-C(12A)	1.5051(17)	C(17B)-C(18B)	1.529(2)
C(8A)-C(9A)	1.4238(16)	C(17B)-C(19B)	1.5290(19)
C(8A)-C(13A)	1.5074(16)	C(17B)-C(20B)	1.530(2)
C(9A)-C(10A)	1.4259(16)		
C(9A)-C(14A)	1.5034(16)	Cent1A-Zr(1)-Cent2A	129.5
C(10A)-C(15A)	1.5002(16)	C(16A)-Zr(1)-Cl(1)	100.18(3)
C(16A)-C(17A)	1.5591(17)	C(16A)-Zr(1)-C(4A)	92.35(4)
C(17A)-C(18A)	1.5267(18)	Cl(1)-Zr(1)-C(4A)	133.87(3)
C(17A)-C(20A)	1.5287(19)	C(16A)-Zr(1)-C(7A)	132.33(4)
C(17A)-C(19A)	1.5431(19)	Cl(1)-Zr(1)-C(7A)	101.39(3)
Zr(2)-Cent1B	2.224	C(4A)-Zr(1)-C(7A)	102.15(4)
Zr(2)-Cent2B	2.240	C(16A)-Zr(1)-C(3A)	124.98(4)
Zr(2)-C(16B)	2.3287(12)	Cl(1)-Zr(1)-C(3A)	117.26(4)
Zr(2)-Cl(2)	2.4432(3)	C(4A)-Zr(1)-C(3A)	32.66(4)
Zr(2)-C(4B)	2.4974(12)	C(7A)-Zr(1)-C(3A)	79.87(4)
Zr(2)-C(3B)	2.5049(13)	C(16A)-Zr(1)-C(2A)	130.58(4)
Zr(2)-C(2B)	2.5294(13)	Cl(1)-Zr(1)-C(2A)	86.01(3)

C(4A)-Zr(1)-C(2A)	53.75(4)	C(3A)-C(2A)-Zr(1)	73.63(7)
C(7A)-Zr(1)-C(2A)	92.97(4)	C(1A)-C(2A)-Zr(1)	74.82(8)
C(3A)-Zr(1)-C(2A)	32.15(5)	C(2A)-C(3A)-C(4A)	108.18(12)
C(16A)-Zr(1)-C(8A)	107.10(4)	C(2A)-C(3A)-Zr(1)	74.22(7)
Cl(1)-Zr(1)-C(8A)	132.24(3)	C(4A)-C(3A)-Zr(1)	73.34(7)
C(4A)-Zr(1)-C(8A)	83.82(4)	C(5A)-C(4A)-C(3A)	107.37(12)
C(7A)-Zr(1)-C(8A)	32.78(4)	C(5A)-C(4A)-Zr(1)	75.21(7)
C(3A)-Zr(1)-C(8A)	76.90(4)	C(3A)-C(4A)-Zr(1)	74.01(7)
C(2A)-Zr(1)-C(8A)	103.72(4)	C(1A)-C(5A)-C(4A)	108.33(12)
C(16A)-Zr(1)-C(6A)	114.08(4)	C(1A)-C(5A)-Zr(1)	74.19(7)
Cl(1)-Zr(1)-C(6A)	79.56(3)	C(4A)-C(5A)-Zr(1)	72.41(7)
C(4A)-Zr(1)-C(6A)	134.26(4)	C(7A)-C(6A)-C(10A)	108.29(10)
C(7A)-Zr(1)-C(6A)	32.61(4)	C(7A)-C(6A)-C(11A)	125.89(11)
C(3A)-Zr(1)-C(6A)	111.35(4)	C(10A)-C(6A)-C(11A)	125.37(11)
C(2A)-Zr(1)-C(6A)	115.26(4)	C(7A)-C(6A)-Zr(1)	72.50(6)
C(8A)-Zr(1)-C(6A)	53.76(4)	C(10A)-C(6A)-Zr(1)	74.46(6)
C(16A)-Zr(1)-C(5A)	78.64(4)	C(11A)-C(6A)-Zr(1)	125.00(8)
Cl(1)-Zr(1)-C(5A)	107.41(3)	C(6A)-C(7A)-C(8A)	107.69(10)
C(4A)-Zr(1)-C(5A)	32.38(4)	C(6A)-C(7A)-C(12A)	124.80(11)
C(7A)-Zr(1)-C(5A)	132.36(4)	C(8A)-C(7A)-C(12A)	126.92(11)
C(3A)-Zr(1)-C(5A)	53.39(4)	C(6A)-C(7A)-Zr(1)	74.89(6)
C(2A)-Zr(1)-C(5A)	53.19(4)	C(8A)-C(7A)-Zr(1)	74.56(6)
C(8A)-Zr(1)-C(5A)	115.81(4)	C(12A)-C(7A)-Zr(1)	123.39(8)
C(6A)-Zr(1)-C(5A)	164.71(4)	C(9A)-C(8A)-C(7A)	108.18(10)
C(16A)-Zr(1)-C(1A)	100.00(5)	C(9A)-C(8A)-C(13A)	123.69(11)
Cl(1)-Zr(1)-C(1A)	80.50(3)	C(7A)-C(8A)-C(13A)	127.09(11)
C(4A)-Zr(1)-C(1A)	53.54(4)	C(9A)-C(8A)-Zr(1)	74.73(6)
C(7A)-Zr(1)-C(1A)	125.18(4)	C(7A)-C(8A)-Zr(1)	72.66(6)
C(3A)-Zr(1)-C(1A)	53.29(5)	C(13A)-C(8A)-Zr(1)	127.69(8)
C(2A)-Zr(1)-C(1A)	32.21(5)	C(8A)-C(9A)-C(10A)	107.84(10)
C(8A)-Zr(1)-C(1A)	130.11(4)	C(8A)-C(9A)-C(14A)	124.58(10)
C(6A)-Zr(1)-C(1A)	142.92(4)	C(10A)-C(9A)-C(14A)	127.15(11)
C(5A)-Zr(1)-C(1A)	31.92(4)	C(8A)-C(9A)-Zr(1)	72.90(6)
C(16A)-Zr(1)-C(10A)	82.95(4)	C(10A)-C(9A)-Zr(1)	73.81(6)
Cl(1)-Zr(1)-C(10A)	93.10(3)	C(14A)-C(9A)-Zr(1)	124.94(8)
C(4A)-Zr(1)-C(10A)	132.65(4)	C(6A)-C(10A)-C(9A)	107.98(10)
C(7A)-Zr(1)-C(10A)	53.97(4)	C(6A)-C(10A)-C(15A)	124.38(10)
C(3A)-Zr(1)-C(10A)	129.58(4)	C(9A)-C(10A)-C(15A)	127.49(11)
C(2A)-Zr(1)-C(10A)	146.13(4)	C(6A)-C(10A)-Zr(1)	73.22(6)
C(8A)-Zr(1)-C(10A)	53.62(4)	C(9A)-C(10A)-Zr(1)	73.92(6)
C(6A)-Zr(1)-C(10A)	32.32(4)	C(15A)-C(10A)-Zr(1)	122.13(8)
C(5A)-Zr(1)-C(10A)	154.45(4)	C(17A)-C(16A)-Zr(1)	130.50(8)
C(1A)-Zr(1)-C(10A)	173.32(4)	C(18A)-C(17A)-C(20A)	108.16(12)
C(16A)-Zr(1)-C(9A)	78.86(4)	C(18A)-C(17A)-C(19A)	108.38(11)
Cl(1)-Zr(1)-C(9A)	125.38(3)	C(20A)-C(17A)-C(19A)	107.97(12)
C(4A)-Zr(1)-C(9A)	100.51(4)	C(18A)-C(17A)-C(16A)	113.58(11)
C(7A)-Zr(1)-C(9A)	54.04(4)	C(20A)-C(17A)-C(16A)	110.45(10)
C(3A)-Zr(1)-C(9A)	105.93(4)	C(19A)-C(17A)-C(16A)	108.14(11)
C(2A)-Zr(1)-C(9A)	135.59(4)	Cent1B-Zr(2)-Cent2B	129.8
C(8A)-Zr(1)-C(9A)	32.37(4)	C(16B)-Zr(2)-Cl(2)	99.91(3)
C(6A)-Zr(1)-C(9A)	53.57(4)	C(16B)-Zr(2)-C(4B)	97.26(5)
C(5A)-Zr(1)-C(9A)	125.25(4)	Cl(2)-Zr(2)-C(4B)	134.21(3)
C(1A)-Zr(1)-C(9A)	154.05(4)	C(16B)-Zr(2)-C(3B)	129.35(5)
C(10A)-Zr(1)-C(9A)	32.28(4)	Cl(2)-Zr(2)-C(3B)	111.53(4)
C(5A)-C(1A)-C(2A)	107.85(13)	C(4B)-Zr(2)-C(3B)	33.02(4)
C(5A)-C(1A)-Zr(1)	73.89(7)	C(16B)-Zr(2)-C(2B)	126.33(5)
C(2A)-C(1A)-Zr(1)	72.97(7)	Cl(2)-Zr(2)-C(2B)	82.32(3)
C(3A)-C(2A)-C(1A)	108.25(12)	C(4B)-Zr(2)-C(2B)	53.69(5)

C(3B)-Zr(2)-C(2B)	32.22(5)	C(1B)-Zr(2)-C(10B)	175.18(4)
C(16B)-Zr(2)-C(7B)	132.37(4)	C(6B)-Zr(2)-C(10B)	32.15(4)
Cl(2)-Zr(2)-C(7B)	100.44(3)	C(5B)-C(1B)-C(2B)	107.70(12)
C(4B)-Zr(2)-C(7B)	98.49(4)	C(5B)-C(1B)-Zr(2)	74.01(7)
C(3B)-Zr(2)-C(7B)	80.45(4)	C(2B)-C(1B)-Zr(2)	73.10(7)
C(2B)-Zr(2)-C(7B)	98.82(5)	C(3B)-C(2B)-C(1B)	108.71(12)
C(16B)-Zr(2)-C(9B)	79.35(4)	C(3B)-C(2B)-Zr(2)	72.93(8)
Cl(2)-Zr(2)-C(9B)	126.92(3)	C(1B)-C(2B)-Zr(2)	74.63(7)
C(4B)-Zr(2)-C(9B)	97.81(4)	C(2B)-C(3B)-C(4B)	107.29(12)
C(3B)-Zr(2)-C(9B)	108.54(5)	C(2B)-C(3B)-Zr(2)	74.85(8)
C(2B)-Zr(2)-C(9B)	140.19(5)	C(4B)-C(3B)-Zr(2)	73.20(7)
C(7B)-Zr(2)-C(9B)	54.13(4)	C(5B)-C(4B)-C(3B)	107.97(12)
C(16B)-Zr(2)-C(8B)	108.58(4)	C(5B)-C(4B)-Zr(2)	75.82(7)
Cl(2)-Zr(2)-C(8B)	131.85(3)	C(3B)-C(4B)-Zr(2)	73.78(7)
C(4B)-Zr(2)-C(8B)	80.12(4)	C(1B)-C(5B)-C(4B)	108.30(12)
C(3B)-Zr(2)-C(8B)	78.85(4)	C(1B)-C(5B)-Zr(2)	74.11(7)
C(2B)-Zr(2)-C(8B)	108.58(5)	C(4B)-C(5B)-Zr(2)	71.88(7)
C(7B)-Zr(2)-C(8B)	32.73(4)	C(10B)-C(6B)-C(7B)	108.93(10)
C(9B)-Zr(2)-C(8B)	32.61(4)	C(10B)-C(6B)-C(11B)	127.03(12)
C(16B)-Zr(2)-C(5B)	78.07(5)	C(7B)-C(6B)-C(11B)	123.71(12)
Cl(2)-Zr(2)-C(5B)	112.65(3)	C(10B)-C(6B)-Zr(2)	74.14(7)
C(4B)-Zr(2)-C(5B)	32.30(4)	C(7B)-C(6B)-Zr(2)	73.02(7)
C(3B)-Zr(2)-C(5B)	53.79(4)	C(11B)-C(6B)-Zr(2)	124.14(8)
C(2B)-Zr(2)-C(5B)	53.12(4)	C(6B)-C(7B)-C(8B)	107.49(11)
C(7B)-Zr(2)-C(5B)	130.33(4)	C(6B)-C(7B)-C(12B)	124.48(11)
C(9B)-Zr(2)-C(5B)	118.81(4)	C(8B)-C(7B)-C(12B)	127.53(12)
C(8B)-Zr(2)-C(5B)	110.73(4)	C(6B)-C(7B)-Zr(2)	74.63(7)
C(16B)-Zr(2)-C(1B)	94.27(5)	C(8B)-C(7B)-Zr(2)	74.05(7)
Cl(2)-Zr(2)-C(1B)	83.02(3)	C(12B)-C(7B)-Zr(2)	123.44(9)
C(4B)-Zr(2)-C(1B)	53.52(4)	C(9B)-C(8B)-C(7B)	107.75(11)
C(3B)-Zr(2)-C(1B)	53.69(5)	C(9B)-C(8B)-C(13B)	124.93(12)
C(2B)-Zr(2)-C(1B)	32.27(5)	C(7B)-C(8B)-C(13B)	126.46(13)
C(7B)-Zr(2)-C(1B)	130.66(4)	C(9B)-C(8B)-Zr(2)	73.57(7)
C(9B)-Zr(2)-C(1B)	149.95(4)	C(7B)-C(8B)-Zr(2)	73.21(7)
C(8B)-Zr(2)-C(1B)	130.76(4)	C(13B)-C(8B)-Zr(2)	127.24(9)
C(5B)-Zr(2)-C(1B)	31.88(4)	C(10B)-C(9B)-C(8B)	108.08(11)
C(16B)-Zr(2)-C(6B)	112.63(4)	C(10B)-C(9B)-C(14B)	127.57(13)
Cl(2)-Zr(2)-C(6B)	80.04(3)	C(8B)-C(9B)-C(14B)	123.91(12)
C(4B)-Zr(2)-C(6B)	130.25(4)	C(10B)-C(9B)-Zr(2)	74.53(7)
C(3B)-Zr(2)-C(6B)	111.21(4)	C(8B)-C(9B)-Zr(2)	73.82(7)
C(2B)-Zr(2)-C(6B)	120.43(4)	C(14B)-C(9B)-Zr(2)	123.52(9)
C(7B)-Zr(2)-C(6B)	32.35(4)	C(6B)-C(10B)-C(9B)	107.72(11)
C(9B)-Zr(2)-C(6B)	53.47(4)	C(6B)-C(10B)-C(15B)	125.41(12)
C(8B)-Zr(2)-C(6B)	53.55(4)	C(9B)-C(10B)-C(15B)	126.61(12)
C(5B)-Zr(2)-C(6B)	162.51(4)	C(6B)-C(10B)-Zr(2)	73.71(7)
C(1B)-Zr(2)-C(6B)	150.21(4)	C(9B)-C(10B)-Zr(2)	73.08(7)
C(16B)-Zr(2)-C(10B)	82.01(4)	C(15B)-C(10B)-Zr(2)	123.51(8)
Cl(2)-Zr(2)-C(10B)	94.56(3)	C(17B)-C(16B)-Zr(2)	131.01(8)
C(4B)-Zr(2)-C(10B)	129.82(4)	C(18B)-C(17B)-C(19B)	107.55(12)
C(3B)-Zr(2)-C(10B)	131.12(4)	C(18B)-C(17B)-C(20B)	108.39(13)
C(2B)-Zr(2)-C(10B)	151.65(4)	C(19B)-C(17B)-C(20B)	107.30(13)
C(7B)-Zr(2)-C(10B)	53.83(4)	C(18B)-C(17B)-C(16B)	113.45(11)
C(9B)-Zr(2)-C(10B)	32.39(4)	C(19B)-C(17B)-C(16B)	108.08(11)
C(8B)-Zr(2)-C(10B)	53.75(4)	C(20B)-C(17B)-C(16B)	111.80(11)
C(5B)-Zr(2)-C(10B)	148.51(4)		

Table 17. Anisotropic displacement parameters ($Å^2 x 10^4$) for 6. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr(1)	103(1)	91(1)	97(1)	28(1)	32(1)	30(1)
Cl(1)	245(2)	109(1)	161(1)	6(1)	39(1)	18(1)
C(1A)	275(7)	197(6)	184(6)	21(5)	150(5)	43(5)
C(2A)	229(6)	225(6)	313(8)	127(6)	182(6)	135(5)
C(3A)	124(5)	294(7)	222(6)	104(5)	89(5)	62(5)
C(4A)	163(5)	152(5)	220(6)	61(4)	101(5)	23(4)
C(5A)	187(5)	206(6)	173(6)	97(5)	91(5)	48(5)
C(6A)	141(5)	106(4)	100(5)	29(3)	35(4)	24(4)
C(7A)	122(4)	137(5)	103(5)	31(4)	22(4)	37(4)
C(8A)	127(4)	109(4)	109(5)	15(4)	24(4)	14(4)
C(9A)	134(5)	104(4)	104(5)	21(3)	34(4)	33(4)
C(10A)	113(4)	124(4)	100(5)	25(4)	36(3)	18(4)
C(11A)	222(6)	123(5)	198(6)	73(4)	78(5)	32(5)
C(12A)	157(5)	210(6)	178(6)	76(5)	25(4)	81(5)
C(13A)	145(5)	148(5)	179(6)	9(4)	9(4)	-20(4)
C(14A)	196(6)	118(5)	180(6)	27(4)	51(4)	60(4)
C(15A)	124(5)	196(6)	191(6)	46(5)	54(4)	24(4)
C(16A)	143(5)	161(5)	113(5)	35(4)	26(4)	52(4)
C(17A)	141(5)	209(6)	130(5)	53(4)	19(4)	31(4)
C(18A)	223(7)	418(9)	127(6)	46(6)	22(5)	17(6)
C(19A)	256(7)	356(9)	262(7)	112(6)	-31(6)	135(7)
C(20A)	153(6)	312(8)	250(7)	88(6)	19(5)	-11(5)
Zr(2)	93(1)	90(1)	100(1)	20(1)	27(1)	17(1)
Cl(2)	168(1)	162(1)	191(1)	85(1)	89(1)	42(1)
C(1B)	239(6)	171(5)	136(5)	-4(4)	62(5)	24(5)
C(2B)	187(6)	167(6)	265(7)	-51(5)	103(5)	35(5)
C(3B)	212(6)	127(5)	238(7)	-23(4)	0(5)	71(5)
C(4B)	243(6)	102(5)	198(6)	8(4)	38(5)	-3(5)
C(5B)	158(5)	137(5)	173(6)	-17(4)	10(4)	-6(4)
C(6B)	156(5)	120(5)	119(5)	18(4)	19(4)	10(4)
C(7B)	143(5)	140(5)	129(5)	30(4)	11(4)	33(4)
C(8B)	193(5)	144(5)	121(5)	54(4)	25(4)	10(4)
C(9B)	162(5)	207(6)	106(5)	45(4)	49(4)	23(4)
C(10B)	177(5)	150(5)	93(5)	10(4)	33(4)	47(4)
C(11B)	223(6)	157(5)	227(7)	24(5)	21(5)	-45(5)
C(12B)	174(6)	235(6)	228(7)	38(5)	13(5)	88(5)
C(13B)	364(9)	171(6)	234(7)	111(5)	34(6)	2(6)
C(14B)	216(6)	422(9)	199(7)	109(6)	121(5)	30(6)
C(15B)	284(7)	205(6)	178(6)	10(5)	52(5)	118(5)
C(16B)	116(5)	205(6)	151(5)	35(4)	41(4)	49(4)
C(17B)	111(5)	202(6)	172(6)	40(4)	33(4)	49(4)
C(18B)	398(10)	384(9)	200(7)	36(6)	-49(6)	201(8)
C(19B)	165(6)	578(12)	400(10)	228(9)	111(6)	184(7)
C(20B)	188(7)	292(8)	555(11)	224(8)	3(7)	58(6)

Table 18. Crystal data and structure refinement for 22 (CCDC 172586).

Empirical formula	$C_{19}H_{30}Zr$
Formula weight	349.65
Crystallization Solvent	Pentane
Crystal Habit	Block
Crystal size	0.26 x 0.19 x 0.15 mm^3
Crystal color	Pale yellow

Data Collection

Preliminary Photos	Rotation
Type of diffractometer	CCD area detector
Wavelength	0.71073 Å MoKa
Data Collection Temperature	98(2) K
q range for 19519 reflections used in lattice determination	2.38 to 28.50°
Unit cell dimensions	a = 17.658(3) Å b = 8.2098(13) Å b= 109.532(2)° c = 25.878(4) Å
Volume	3535.7(10) $Å^3$
Z	8
Crystal system	Monoclinic
Space group	P2/c
Density (calculated)	1.314 Mg/m^3
F(000)	1472
Data collection program	Bruker SMART
q range for data collection	1.71 to 28.52°
Completeness to q = 28.52°	94.4 %
Index ranges	$-22 \le h \le 23$, $-10 \le k \le 10$, $-34 \le l \le 34$
Data collection scan type	w scans at 9 f settings
Data reduction program	Bruker SAINT v6.2
Reflections collected	81002
Independent reflections	8478 [R_{int}= 0.2107]
Absorption coefficient	0.613 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9148 and 0.8575

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Patterson method
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	8478 / 0 / 369
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.217
Final R indices [$I>2\sigma(I)$, 5799 reflections]	R1 = 0.0571, *w*R2 = 0.0876
R indices (all data)	R1 = 0.0991, *w*R2 = 0.0958
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	1.045 and -1.567 $e.Å^{-3}$

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2s(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 19. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 22. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Zr(1)	7499(1)	6176(1)	3699(1)	16(1)
C(1A)	7214(2)	4999(4)	4509(1)	26(1)
C(2A)	6529(2)	5925(4)	4220(1)	28(1)
C(3A)	6155(2)	5140(4)	3715(2)	26(1)
C(4A)	6606(2)	3735(4)	3692(1)	24(1)
C(5A)	7255(2)	3639(4)	4189(1)	23(1)
C(6A)	7973(2)	8511(4)	4371(2)	35(1)
C(7A)	7448(2)	9169(4)	3878(2)	37(1)
C(8A)	7821(2)	9050(4)	3483(2)	34(1)
C(9A)	8557(2)	8311(4)	3717(1)	26(1)
C(10A)	8656(2)	7961(4)	4265(2)	27(1)
C(11A)	6636(2)	6584(4)	2823(1)	25(1)
C(12A)	8321(2)	4514(4)	3444(1)	19(1)
C(13A)	9124(2)	3566(4)	3610(1)	18(1)
C(14A)	9183(2)	2435(4)	4099(1)	20(1)
C(15A)	9332(2)	3273(4)	4650(1)	26(1)
C(16A)	9829(2)	4785(4)	3762(1)	21(1)
C(17A)	10678(2)	4030(4)	3956(2)	28(1)
C(18A)	9148(2)	2431(4)	3136(1)	24(1)
C(19A)	8992(2)	3240(4)	2576(1)	31(1)
Zr(2)	6056(1)	10989(1)	1393(1)	16(1)
C(1B)	4551(2)	10569(4)	1036(1)	23(1)
C(2B)	4864(2)	9595(4)	709(1)	21(1)
C(3B)	5317(2)	8336(4)	1040(1)	24(1)
C(4B)	5281(2)	8527(4)	1566(1)	25(1)
C(5B)	4808(2)	9910(4)	1570(1)	26(1)
C(6B)	5702(2)	13873(4)	1097(2)	38(1)
C(7B)	5695(2)	13062(4)	625(2)	34(1)
C(8B)	6487(2)	12607(4)	695(2)	28(1)
C(9B)	6981(2)	13136(4)	1212(2)	26(1)
C(10B)	6503(3)	13935(4)	1464(2)	37(1)
C(11B)	6277(2)	11609(4)	2301(1)	25(1)
C(12B)	7151(2)	9398(4)	1562(1)	19(1)
C(13B)	7741(2)	8512(3)	1327(1)	16(1)
C(14B)	7266(2)	7369(4)	856(1)	21(1)
C(15B)	6741(2)	8187(4)	327(1)	26(1)
C(16B)	8222(2)	9780(4)	1127(1)	22(1)

C(17B)	8843(2)	9074(4)	891(2)	31(1)
C(18B)	8312(2)	7406(4)	1779(1)	23(1)
C(19B)	8860(2)	8267(4)	2289(1)	29(1)

Table 20. Selected bond lengths [Å] and angles [°] for 22.

Zr(1)-C(12A)	2.248(3)	Zr(2)-C(12B)	2.252(3)
Zr(1)-C(11A)	2.294(3)	Zr(2)-C(11B)	2.306(3)
C(12A)-Zr(1)-C(11A)	94.54(12)	C(12B)-Zr(2)-C(11B)	95.07(12)
Zr(1)-Cent(1A)	2.23	Zr(2)-Cent(1B)	2.25
Zr(1)-Cent(2A)	2.24	Zr(2)-Cent(2B)	2.24
Zr(1)-Pln(1A)	2.23	Zr(2)-Pln(1B)	2.25
Zr(1)-Pln(2A)	2.24	Zr(2)-Pln(2B)	2.24
Cent(1A)-Zr1-Cent(2A)	130.9	Cent(2A)-Zr2-Cent(2B)	130.9
Pln(1A)-Zr1-Pln(2A)	129.0	Pln(1B)-Zr2-Pln(2B)	129.1

Cent(1A) is the centroid formed by C(1A), C(2A), C(3A), C(4A) and C(5A).
Cent(2A) is the centroid formed by C(6A), C(7A), C(8A), C(9A) and C(10A).
Pln(1A) is the plane formed by C(1A), C(2A), C(3A), C(4A) and C(5A).
Pln(2A) is the plane formed by C(6A), C(7A), C(8A), C(9A) and C(10A).
Cent(1B) is the centroid formed by C(1B), C(2B), C(3B), C(4B) and C(5B).
Cent(2B) is the centroid formed by C(6B), C(7B), C(8B), C(9B) and C(10B).
Pln(1B) is the plane formed by C(1B), C(2B), C(3B), C(4B) and C(5B).
Pln(2B) is the plane formed by C(6B), C(7B), C(8B), C(9B) and C(10B).

Table 21. Bond lengths [Å] and angles [°] for 22

Zr(1)-C(12A)	2.248(3)	C(4A)-H(4A)	0.9500
Zr(1)-C(11A)	2.294(3)	C(5A)-H(5A)	0.9500
Zr(1)-C(1A)	2.506(3)	C(6A)-C(10A)	1.398(5)
Zr(1)-C(7A)	2.507(3)	C(6A)-C(7A)	1.409(5)
Zr(1)-C(2A)	2.517(4)	C(6A)-H(6A)	0.9500
Zr(1)-C(8A)	2.533(3)	C(7A)-C(8A)	1.393(6)
Zr(1)-C(3A)	2.534(3)	C(7A)-H(7A)	0.9500
Zr(1)-C(6A)	2.535(3)	C(8A)-C(9A)	1.378(5)
Zr(1)-C(10A)	2.542(3)	C(8A)-H(8A)	0.9500
Zr(1)-C(4A)	2.547(3)	C(9A)-C(10A)	1.399(5)
Zr(1)-C(5A)	2.548(3)	C(9A)-H(9A)	0.9500
Zr(1)-C(9A)	2.552(3)	C(10A)-H(10A)	0.9500
C(1A)-C(5A)	1.406(5)	C(11A)-H(11A)	0.9800
C(1A)-C(2A)	1.413(5)	C(11A)-H(11B)	0.9800
C(1A)-H(1A)	0.9500	C(11A)-H(11C)	0.9800
C(2A)-C(3A)	1.408(5)	C(12A)-C(13A)	1.547(4)
C(2A)-H(2A)	0.9500	C(12A)-H(12A)	0.9900
C(3A)-C(4A)	1.414(5)	C(12A)-H(12B)	0.9900
C(3A)-H(3A)	0.9500	C(13A)-C(16A)	1.543(4)
C(4A)-C(5A)	1.410(5)	C(13A)-C(14A)	1.546(4)

C(13A)-C(18A)	1.552(4)	C(13B)-C(14B)	1.544(4)
C(14A)-C(15A)	1.523(4)	C(13B)-C(18B)	1.556(4)
C(14A)-H(14A)	0.9900	C(14B)-C(15B)	1.529(4)
C(14A)-H(14B)	0.9900	C(14B)-H(14C)	0.9900
C(15A)-H(15A)	0.9800	C(14B)-H(14D)	0.9900
C(15A)-H(15B)	0.9800	C(15B)-H(15D)	0.9800
C(15A)-H(15C)	0.9800	C(15B)-H(15E)	0.9800
C(16A)-C(17A)	1.543(4)	C(15B)-H(15F)	0.9800
C(16A)-H(16A)	0.9900	C(16B)-C(17B)	1.534(5)
C(16A)-H(16B)	0.9900	C(16B)-H(16C)	0.9900
C(17A)-H(17A)	0.9800	C(16B)-H(16D)	0.9900
C(17A)-H(17B)	0.9800	C(17B)-H(17D)	0.9800
C(17A)-H(17C)	0.9800	C(17B)-H(17E)	0.9800
C(18A)-C(19A)	1.532(5)	C(17B)-H(17F)	0.9800
C(18A)-H(18A)	0.9900	C(18B)-C(19B)	1.524(4)
C(18A)-H(18B)	0.9900	C(18B)-H(18C)	0.9900
C(19A)-H(19A)	0.9800	C(18B)-H(18D)	0.9900
C(19A)-H(19B)	0.9800	C(19B)-H(19D)	0.9800
C(19A)-H(19C)	0.9800	C(19B)-H(19E)	0.9800
Zr(2)-C(12B)	2.252(3)	C(19B)-H(19F)	0.9800
Zr(2)-C(11B)	2.306(3)		
Zr(2)-C(6B)	2.502(3)	C(12A)-Zr(1)-C(11A)	94.54(12)
Zr(2)-C(2B)	2.526(3)	C(12A)-Zr(1)-C(1A)	109.97(11)
Zr(2)-C(1B)	2.528(3)	C(11A)-Zr(1)-C(1A)	129.04(12)
Zr(2)-C(10B)	2.531(3)	C(12A)-Zr(1)-C(7A)	135.72(13)
Zr(2)-C(7B)	2.531(3)	C(11A)-Zr(1)-C(7A)	89.25(13)
Zr(2)-C(3B)	2.547(3)	C(1A)-Zr(1)-C(7A)	101.17(13)
Zr(2)-C(9B)	2.551(3)	C(12A)-Zr(1)-C(2A)	136.88(11)
Zr(2)-C(8B)	2.554(3)	C(11A)-Zr(1)-C(2A)	101.25(12)
Zr(2)-C(5B)	2.555(3)	C(1A)-Zr(1)-C(2A)	32.67(10)
Zr(2)-C(4B)	2.563(3)	C(7A)-Zr(1)-C(2A)	84.75(13)
C(1B)-C(2B)	1.403(5)	C(12A)-Zr(1)-C(8A)	106.60(13)
C(1B)-C(5B)	1.412(5)	C(11A)-Zr(1)-C(8A)	76.70(12)
C(1B)-H(1B)	0.9500	C(1A)-Zr(1)-C(8A)	131.80(12)
C(2B)-C(3B)	1.408(4)	C(7A)-Zr(1)-C(8A)	32.09(13)
C(2B)-H(2B)	0.9500	C(2A)-Zr(1)-C(8A)	115.97(13)
C(3B)-C(4B)	1.394(5)	C(12A)-Zr(1)-C(3A)	120.10(11)
C(3B)-H(3B)	0.9500	C(11A)-Zr(1)-C(3A)	75.44(12)
C(4B)-C(5B)	1.412(5)	C(1A)-Zr(1)-C(3A)	53.60(11)
C(4B)-H(4B)	0.9500	C(7A)-Zr(1)-C(3A)	103.56(12)
C(5B)-H(5B)	0.9500	C(2A)-Zr(1)-C(3A)	32.38(11)
C(6B)-C(7B)	1.390(5)	C(8A)-Zr(1)-C(3A)	126.66(12)
C(6B)-C(10B)	1.415(6)	C(12A)-Zr(1)-C(6A)	124.28(12)
C(6B)-H(6B)	0.9500	C(11A)-Zr(1)-C(6A)	121.71(12)
C(7B)-C(8B)	1.399(5)	C(1A)-Zr(1)-C(6A)	80.24(12)
C(7B)-H(7B)	0.9500	C(7A)-Zr(1)-C(6A)	32.46(12)
C(8B)-C(9B)	1.400(5)	C(2A)-Zr(1)-C(6A)	79.76(12)
C(8B)-H(8B)	0.9500	C(8A)-Zr(1)-C(6A)	53.15(13)
C(9B)-C(10B)	1.392(5)	C(3A)-Zr(1)-C(6A)	109.82(12)
C(9B)-H(9B)	0.9500	C(12A)-Zr(1)-C(10A)	92.60(11)
C(10B)-H(10B)	0.9500	C(11A)-Zr(1)-C(10A)	128.72(11)
C(11B)-H(11D)	0.9800	C(1A)-Zr(1)-C(10A)	95.04(12)
C(11B)-H(11E)	0.9800	C(7A)-Zr(1)-C(10A)	53.16(11)
C(11B)-H(11F)	0.9800	C(2A)-Zr(1)-C(10A)	107.36(12)
C(12B)-C(13B)	1.551(4)	C(8A)-Zr(1)-C(10A)	52.69(11)
C(12B)-H(12C)	0.9900	C(3A)-Zr(1)-C(10A)	139.53(12)
C(12B)-H(12D)	0.9900	C(6A)-Zr(1)-C(10A)	31.98(12)
C(13B)-C(16B)	1.540(4)	C(12A)-Zr(1)-C(4A)	88.83(11)

C(11A)-Zr(1)-C(4A)	84.43(11)	Zr(1)-C(5A)-H(5A)	119.7
C(1A)-Zr(1)-C(4A)	53.52(11)	C(10A)-C(6A)-C(7A)	107.2(4)
C(7A)-Zr(1)-C(4A)	135.41(12)	C(10A)-C(6A)-Zr(1)	74.31(19)
C(2A)-Zr(1)-C(4A)	53.75(11)	C(7A)-C(6A)-Zr(1)	72.68(19)
C(8A)-Zr(1)-C(4A)	156.34(11)	C(10A)-C(6A)-H(6A)	126.4
C(3A)-Zr(1)-C(4A)	32.31(10)	C(7A)-C(6A)-H(6A)	126.4
C(6A)-Zr(1)-C(4A)	131.41(12)	Zr(1)-C(6A)-H(6A)	118.6
C(10A)-Zr(1)-C(4A)	146.50(11)	C(8A)-C(7A)-C(6A)	108.0(3)
C(12A)-Zr(1)-C(5A)	83.27(11)	C(8A)-C(7A)-Zr(1)	75.0(2)
C(11A)-Zr(1)-C(5A)	116.35(11)	C(6A)-C(7A)-Zr(1)	74.86(19)
C(1A)-Zr(1)-C(5A)	32.30(11)	C(8A)-C(7A)-H(7A)	126.0
C(7A)-Zr(1)-C(5A)	133.36(13)	C(6A)-C(7A)-H(7A)	126.0
C(2A)-Zr(1)-C(5A)	53.75(11)	Zr(1)-C(7A)-H(7A)	116.3
C(8A)-Zr(1)-C(5A)	163.51(12)	C(9A)-C(8A)-C(7A)	108.4(3)
C(3A)-Zr(1)-C(5A)	53.35(11)	C(9A)-C(8A)-Zr(1)	75.04(19)
C(6A)-Zr(1)-C(5A)	110.41(12)	C(7A)-C(8A)-Zr(1)	72.9(2)
C(10A)-Zr(1)-C(5A)	114.91(11)	C(9A)-C(8A)-H(8A)	125.8
C(4A)-Zr(1)-C(5A)	32.12(10)	C(7A)-C(8A)-H(8A)	125.8
C(12A)-Zr(1)-C(9A)	83.17(12)	Zr(1)-C(8A)-H(8A)	118.1
C(11A)-Zr(1)-C(9A)	99.13(11)	C(8A)-C(9A)-C(10A)	108.4(3)
C(1A)-Zr(1)-C(9A)	126.86(11)	C(8A)-C(9A)-Zr(1)	73.51(19)
C(7A)-Zr(1)-C(9A)	52.75(12)	C(10A)-C(9A)-Zr(1)	73.70(19)
C(2A)-Zr(1)-C(9A)	132.21(11)	C(8A)-C(9A)-H(9A)	125.8
C(8A)-Zr(1)-C(9A)	31.45(11)	C(10A)-C(9A)-H(9A)	125.8
C(3A)-Zr(1)-C(9A)	156.16(11)	Zr(1)-C(9A)-H(9A)	118.9
C(6A)-Zr(1)-C(9A)	52.85(12)	C(9A)-C(10A)-C(6A)	108.0(3)
C(10A)-Zr(1)-C(9A)	31.87(11)	C(9A)-C(10A)-Zr(1)	74.43(18)
C(4A)-Zr(1)-C(9A)	171.46(11)	C(6A)-C(10A)-Zr(1)	73.71(19)
C(5A)-Zr(1)-C(9A)	142.81(11)	C(9A)-C(10A)-H(10A)	126.0
C(5A)-C(1A)-C(2A)	108.6(3)	C(6A)-C(10A)-H(10A)	126.0
C(5A)-C(1A)-Zr(1)	75.50(19)	Zr(1)-C(10A)-H(10A)	117.8
C(2A)-C(1A)-Zr(1)	74.08(19)	Zr(1)-C(11A)-H(11A)	109.5
C(5A)-C(1A)-H(1A)	125.7	Zr(1)-C(11A)-H(11B)	109.5
C(2A)-C(1A)-H(1A)	125.7	H(11A)-C(11A)-H(11B)	109.5
Zr(1)-C(1A)-H(1A)	116.7	Zr(1)-C(11A)-H(11C)	109.5
C(3A)-C(2A)-C(1A)	107.3(3)	H(11A)-C(11A)-H(11C)	109.5
C(3A)-C(2A)-Zr(1)	74.5(2)	H(11B)-C(11A)-H(11C)	109.5
C(1A)-C(2A)-Zr(1)	73.2(2)	C(13A)-C(12A)-Zr(1)	147.8(2)
C(3A)-C(2A)-H(2A)	126.3	C(13A)-C(12A)-H(12A)	99.8
C(1A)-C(2A)-H(2A)	126.3	Zr(1)-C(12A)-H(12A)	99.8
Zr(1)-C(2A)-H(2A)	118.0	C(13A)-C(12A)-H(12B)	99.8
C(2A)-C(3A)-C(4A)	108.4(3)	Zr(1)-C(12A)-H(12B)	99.8
C(2A)-C(3A)-Zr(1)	73.1(2)	H(12A)-C(12A)-H(12B)	104.1
C(4A)-C(3A)-Zr(1)	74.35(19)	C(16A)-C(13A)-C(14A)	110.7(2)
C(2A)-C(3A)-H(3A)	125.8	C(16A)-C(13A)-C(12A)	109.3(2)
C(4A)-C(3A)-H(3A)	125.8	C(14A)-C(13A)-C(12A)	109.5(3)
Zr(1)-C(3A)-H(3A)	118.6	C(16A)-C(13A)-C(18A)	111.1(3)
C(5A)-C(4A)-C(3A)	107.8(3)	C(14A)-C(13A)-C(18A)	106.0(2)
C(5A)-C(4A)-Zr(1)	73.99(18)	C(12A)-C(13A)-C(18A)	110.3(2)
C(3A)-C(4A)-Zr(1)	73.34(18)	C(15A)-C(14A)-C(13A)	116.0(2)
C(5A)-C(4A)-H(4A)	126.1	C(15A)-C(14A)-H(14A)	108.3
C(3A)-C(4A)-H(4A)	126.1	C(13A)-C(14A)-H(14A)	108.3
Zr(1)-C(4A)-H(4A)	118.5	C(15A)-C(14A)-H(14B)	108.3
C(1A)-C(5A)-C(4A)	107.8(3)	C(13A)-C(14A)-H(14B)	108.3
C(1A)-C(5A)-Zr(1)	72.21(18)	H(14A)-C(14A)-H(14B)	107.4
C(4A)-C(5A)-Zr(1)	73.89(18)	C(14A)-C(15A)-H(15A)	109.5
C(1A)-C(5A)-H(5A)	126.1	C(14A)-C(15A)-H(15B)	109.5
C(4A)-C(5A)-H(5A)	126.1	H(15A)-C(15A)-H(15B)	109.5

C(14A)-C(15A)-H(15C)	109.5	C(2B)-Zr(2)-C(9B)	128.27(11)
H(15A)-C(15A)-H(15C)	109.5	C(1B)-Zr(2)-C(9B)	133.36(11)
H(15B)-C(15A)-H(15C)	109.5	C(10B)-Zr(2)-C(9B)	31.79(11)
C(17A)-C(16A)-C(13A)	115.8(3)	C(7B)-Zr(2)-C(9B)	53.12(11)
C(17A)-C(16A)-H(16A)	108.3	C(3B)-Zr(2)-C(9B)	143.86(12)
C(13A)-C(16A)-H(16A)	108.3	C(12B)-Zr(2)-C(8B)	89.99(12)
C(17A)-C(16A)-H(16B)	108.3	C(11B)-Zr(2)-C(8B)	128.08(12)
C(13A)-C(16A)-H(16B)	108.3	C(6B)-Zr(2)-C(8B)	52.75(12)
H(16A)-C(16A)-H(16B)	107.4	C(2B)-Zr(2)-C(8B)	96.65(11)
C(16A)-C(17A)-H(17A)	109.5	C(1B)-Zr(2)-C(8B)	109.72(11)
C(16A)-C(17A)-H(17B)	109.5	C(10B)-Zr(2)-C(8B)	52.77(12)
H(17A)-C(17A)-H(17B)	109.5	C(7B)-Zr(2)-C(8B)	31.92(11)
C(16A)-C(17A)-H(17C)	109.5	C(3B)-Zr(2)-C(8B)	115.38(11)
H(17A)-C(17A)-H(17C)	109.5	C(9B)-Zr(2)-C(8B)	31.82(11)
H(17B)-C(17A)-H(17C)	109.5	C(12B)-Zr(2)-C(5B)	119.98(11)
C(19A)-C(18A)-C(13A)	116.3(3)	C(11B)-Zr(2)-C(5B)	75.86(12)
C(19A)-C(18A)-H(18A)	108.2	C(6B)-Zr(2)-C(5B)	103.96(12)
C(13A)-C(18A)-H(18A)	108.2	C(2B)-Zr(2)-C(5B)	53.26(11)
C(19A)-C(18A)-H(18B)	108.2	C(1B)-Zr(2)-C(5B)	32.25(10)
C(13A)-C(18A)-H(18B)	108.2	C(10B)-Zr(2)-C(5B)	125.82(12)
H(18A)-C(18A)-H(18B)	107.4	C(7B)-Zr(2)-C(5B)	111.63(12)
C(18A)-C(19A)-H(19A)	109.5	C(3B)-Zr(2)-C(5B)	53.04(11)
C(18A)-C(19A)-H(19B)	109.5	C(9B)-Zr(2)-C(5B)	156.43(11)
H(19A)-C(19A)-H(19B)	109.5	C(8B)-Zr(2)-C(5B)	141.82(11)
C(18A)-C(19A)-H(19C)	109.5	C(12B)-Zr(2)-C(4B)	88.98(11)
H(19A)-C(19A)-H(19C)	109.5	C(11B)-Zr(2)-C(4B)	85.09(12)
H(19B)-C(19A)-H(19C)	109.5	C(6B)-Zr(2)-C(4B)	134.95(12)
C(12B)-Zr(2)-C(11B)	95.07(12)	C(2B)-Zr(2)-C(4B)	52.87(10)
C(12B)-Zr(2)-C(6B)	135.95(12)	C(1B)-Zr(2)-C(4B)	53.06(10)
C(11B)-Zr(2)-C(6B)	92.43(13)	C(10B)-Zr(2)-C(4B)	155.88(13)
C(12B)-Zr(2)-C(2B)	109.47(11)	C(7B)-Zr(2)-C(4B)	131.19(11)
C(11B)-Zr(2)-C(2B)	129.13(12)	C(3B)-Zr(2)-C(4B)	31.65(11)
C(6B)-Zr(2)-C(2B)	98.65(12)	C(9B)-Zr(2)-C(4B)	171.54(11)
C(12B)-Zr(2)-C(1B)	136.13(11)	C(8B)-Zr(2)-C(4B)	146.75(11)
C(11B)-Zr(2)-C(1B)	101.64(12)	C(5B)-Zr(2)-C(4B)	32.02(11)
C(6B)-Zr(2)-C(1B)	83.86(12)	C(2B)-C(1B)-C(5B)	108.0(3)
C(2B)-Zr(2)-C(1B)	32.24(10)	C(2B)-C(1B)-Zr(2)	73.81(19)
C(12B)-Zr(2)-C(10B)	108.28(13)	C(5B)-C(1B)-Zr(2)	74.92(19)
C(11B)-Zr(2)-C(10B)	76.89(12)	C(2B)-C(1B)-H(1B)	126.0
C(6B)-Zr(2)-C(10B)	32.65(13)	C(5B)-C(1B)-H(1B)	126.0
C(2B)-Zr(2)-C(10B)	130.55(12)	Zr(2)-C(1B)-H(1B)	117.3
C(1B)-Zr(2)-C(10B)	114.90(12)	C(1B)-C(2B)-C(3B)	108.1(3)
C(12B)-Zr(2)-C(7B)	121.12(13)	C(1B)-C(2B)-Zr(2)	73.94(18)
C(11B)-Zr(2)-C(7B)	124.36(12)	C(3B)-C(2B)-Zr(2)	74.68(17)
C(6B)-Zr(2)-C(7B)	32.05(12)	C(1B)-C(2B)-H(2B)	125.9
C(2B)-Zr(2)-C(7B)	79.77(11)	C(3B)-C(2B)-H(2B)	125.9
C(1B)-Zr(2)-C(7B)	81.18(11)	Zr(2)-C(2B)-H(2B)	117.4
C(10B)-Zr(2)-C(7B)	53.50(13)	C(4B)-C(3B)-C(2B)	108.0(3)
C(12B)-Zr(2)-C(3B)	82.93(11)	C(4B)-C(3B)-Zr(2)	74.80(18)
C(11B)-Zr(2)-C(3B)	116.52(12)	C(2B)-C(3B)-Zr(2)	73.10(17)
C(6B)-Zr(2)-C(3B)	130.85(12)	C(4B)-C(3B)-H(3B)	126.0
C(2B)-Zr(2)-C(3B)	32.22(10)	C(2B)-C(3B)-H(3B)	126.0
C(1B)-Zr(2)-C(3B)	53.30(10)	Zr(2)-C(3B)-H(3B)	118.0
C(10B)-Zr(2)-C(3B)	162.36(12)	C(3B)-C(4B)-C(5B)	108.6(3)
C(7B)-Zr(2)-C(3B)	109.18(11)	C(3B)-C(4B)-Zr(2)	73.54(19)
C(12B)-Zr(2)-C(9B)	82.84(11)	C(5B)-C(4B)-Zr(2)	73.69(19)
C(11B)-Zr(2)-C(9B)	97.72(12)	C(3B)-C(4B)-H(4B)	125.7
C(6B)-Zr(2)-C(9B)	53.12(11)	C(5B)-C(4B)-H(4B)	125.7

Zr(2)-C(4B)-H(4B)	118.9	C(13B)-C(12B)-H(12D)	100.0
C(4B)-C(5B)-C(1B)	107.3(3)	Zr(2)-C(12B)-H(12D)	100.0
C(4B)-C(5B)-Zr(2)	74.3(2)	H(12C)-C(12B)-H(12D)	104.2
C(1B)-C(5B)-Zr(2)	72.83(19)	C(16B)-C(13B)-C(14B)	111.1(3)
C(4B)-C(5B)-H(5B)	126.4	C(16B)-C(13B)-C(12B)	109.5(2)
C(1B)-C(5B)-H(5B)	126.4	C(14B)-C(13B)-C(12B)	109.6(3)
Zr(2)-C(5B)-H(5B)	118.5	C(16B)-C(13B)-C(18B)	110.8(3)
C(7B)-C(6B)-C(10B)	108.6(3)	C(14B)-C(13B)-C(18B)	106.4(2)
C(7B)-C(6B)-Zr(2)	75.13(19)	C(12B)-C(13B)-C(18B)	109.3(3)
C(10B)-C(6B)-Zr(2)	74.79(19)	C(15B)-C(14B)-C(13B)	116.5(2)
C(7B)-C(6B)-H(6B)	125.7	C(15B)-C(14B)-H(14C)	108.2
C(10B)-C(6B)-H(6B)	125.7	C(13B)-C(14B)-H(14C)	108.2
Zr(2)-C(6B)-H(6B)	116.4	C(15B)-C(14B)-H(14D)	108.2
C(6B)-C(7B)-C(8B)	107.4(3)	C(13B)-C(14B)-H(14D)	108.2
C(6B)-C(7B)-Zr(2)	72.8(2)	H(14C)-C(14B)-H(14D)	107.3
C(8B)-C(7B)-Zr(2)	74.9(2)	C(14B)-C(15B)-H(15D)	109.5
C(6B)-C(7B)-H(7B)	126.3	C(14B)-C(15B)-H(15E)	109.5
C(8B)-C(7B)-H(7B)	126.3	H(15D)-C(15B)-H(15E)	109.5
Zr(2)-C(7B)-H(7B)	118.0	C(14B)-C(15B)-H(15F)	109.5
C(7B)-C(8B)-C(9B)	108.6(3)	H(15D)-C(15B)-H(15F)	109.5
C(7B)-C(8B)-Zr(2)	73.1(2)	H(15E)-C(15B)-H(15F)	109.5
C(9B)-C(8B)-Zr(2)	74.0(2)	C(17B)-C(16B)-C(13B)	115.3(3)
C(7B)-C(8B)-H(8B)	125.7	C(17B)-C(16B)-H(16C)	108.5
C(9B)-C(8B)-H(8B)	125.7	C(13B)-C(16B)-H(16C)	108.5
Zr(2)-C(8B)-H(8B)	119.0	C(17B)-C(16B)-H(16D)	108.5
C(10B)-C(9B)-C(8B)	108.1(3)	C(13B)-C(16B)-H(16D)	108.5
C(10B)-C(9B)-Zr(2)	73.3(2)	H(16C)-C(16B)-H(16D)	107.5
C(8B)-C(9B)-Zr(2)	74.22(19)	C(16B)-C(17B)-H(17D)	109.5
C(10B)-C(9B)-H(9B)	125.9	C(16B)-C(17B)-H(17E)	109.5
C(8B)-C(9B)-H(9B)	125.9	H(17D)-C(17B)-H(17E)	109.5
Zr(2)-C(9B)-H(9B)	118.4	C(16B)-C(17B)-H(17F)	109.5
C(9B)-C(10B)-C(6B)	107.3(4)	H(17D)-C(17B)-H(17F)	109.5
C(9B)-C(10B)-Zr(2)	74.89(19)	H(17E)-C(17B)-H(17F)	109.5
C(6B)-C(10B)-Zr(2)	72.56(19)	C(19B)-C(18B)-C(13B)	116.4(3)
C(9B)-C(10B)-H(10B)	126.4	C(19B)-C(18B)-H(18C)	108.2
C(6B)-C(10B)-H(10B)	126.4	C(13B)-C(18B)-H(18C)	108.2
Zr(2)-C(10B)-H(10B)	118.2	C(19B)-C(18B)-H(18D)	108.2
Zr(2)-C(11B)-H(11D)	109.5	C(13B)-C(18B)-H(18D)	108.2
Zr(2)-C(11B)-H(11E)	109.5	H(18C)-C(18B)-H(18D)	107.3
H(11D)-C(11B)-H(11E)	109.5	C(18B)-C(19B)-H(19D)	109.5
Zr(2)-C(11B)-H(11F)	109.5	C(18B)-C(19B)-H(19E)	109.5
H(11D)-C(11B)-H(11F)	109.5	H(19D)-C(19B)-H(19E)	109.5
H(11E)-C(11B)-H(11F)	109.5	C(18B)-C(19B)-H(19F)	109.5
C(13B)-C(12B)-Zr(2)	147.2(2)	H(19D)-C(19B)-H(19F)	109.5
C(13B)-C(12B)-H(12C)	100.0	H(19E)-C(19B)-H(19F)	109.5
Zr(2)-C(12B)-H(12C)	100.0		

Cent(1A) is the centroid formed by C(1A), C(2A), C(3A), C(4A) and C(5A).
Cent(2A) is the centroid formed by C(6A), C(7A), C(8A), C(9A) and C(10A).
Pln(1A) is the plane formed by C(1A), C(2A), C(3A), C(4A) and C(5A).
Pln(2A) is the plane formed by C(6A), C(7A), C(8A), C(9A) and C(10A).
Cent(1B) is the centroid formed by C(1B), C(2B), C(3B), C(4B) and C(5B).
Cent(2B) is the centroid formed by C(6B), C(7B), C(8B), C(9B) and C(10B).
Pln(1B) is the plane formed by C(1B), C(2B), C(3B), C(4B) and C(5B).
Pln(2B) is the plane formed by C(6B), C(7B), C(8B), C(9B) and C(10B).

Table 22. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for 22. The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr(1)	158(2)	137(1)	161(2)	10(1)	37(1)	-5(1)
C(1A)	330(20)	264(18)	222(18)	48(15)	123(16)	-8(14)
C(2A)	330(20)	238(17)	340(20)	4(16)	210(17)	30(15)
C(3A)	161(19)	297(18)	320(20)	66(16)	83(15)	-30(14)
C(4A)	290(20)	212(17)	267(18)	-11(15)	154(15)	-74(14)
C(5A)	239(19)	205(17)	276(18)	84(15)	127(15)	7(13)
C(6A)	460(30)	310(20)	340(20)	-141(18)	206(19)	-154(17)
C(7A)	210(20)	152(17)	730(30)	-135(18)	120(20)	-16(13)
C(8A)	310(20)	172(17)	420(20)	47(17)	-16(18)	-62(15)
C(9A)	260(20)	164(15)	360(20)	-26(16)	99(16)	-83(13)
C(10A)	250(20)	186(17)	281(19)	-28(15)	-50(15)	-27(13)
C(11A)	220(20)	265(17)	249(18)	14(15)	69(15)	-11(13)
C(12A)	185(18)	166(15)	213(16)	-36(14)	51(14)	-28(12)
C(13A)	187(18)	161(15)	205(16)	-5(13)	75(13)	2(12)
C(14A)	185(19)	169(15)	235(17)	1(14)	58(14)	-14(12)
C(15A)	250(20)	258(17)	238(18)	34(15)	48(15)	-6(14)
C(16A)	195(19)	159(15)	258(18)	16(14)	56(14)	-11(12)
C(17A)	210(20)	281(18)	331(19)	39(16)	58(15)	3(14)
C(18A)	250(20)	186(16)	284(19)	-42(15)	98(15)	-16(13)
C(19A)	360(20)	312(18)	271(19)	-40(17)	144(16)	13(16)
Zr(2)	162(2)	144(2)	183(2)	4(1)	62(1)	9(1)
C(1B)	160(19)	231(16)	279(18)	11(15)	57(14)	1(13)
C(2B)	197(19)	221(16)	176(16)	-5(14)	23(14)	-22(13)
C(3B)	126(18)	190(15)	350(20)	-31(15)	24(15)	-32(12)
C(4B)	168(19)	258(18)	242(18)	100(15)	-39(14)	-55(13)
C(5B)	180(20)	420(20)	191(17)	-53(16)	79(14)	-90(15)
C(6B)	390(20)	150(16)	740(30)	120(20)	380(20)	82(15)
C(7B)	290(20)	242(18)	420(20)	105(18)	48(18)	-13(15)
C(8B)	400(20)	159(16)	320(20)	76(15)	176(17)	18(14)
C(9B)	240(20)	169(16)	360(20)	68(16)	89(16)	3(13)
C(10B)	580(30)	154(16)	450(20)	-34(17)	280(20)	-95(17)
C(11B)	250(20)	262(17)	234(17)	-38(15)	67(14)	-12(14)
C(12B)	184(18)	172(15)	200(16)	29(13)	47(13)	13(12)
C(13B)	154(17)	144(15)	194(16)	5(13)	64(13)	20(11)
C(14B)	210(19)	194(16)	200(17)	1(14)	52(14)	32(12)
C(15B)	300(20)	261(17)	201(17)	-16(15)	60(15)	56(14)
C(16B)	229(19)	192(16)	248(18)	9(14)	78(14)	10(13)
C(17B)	320(20)	276(18)	420(20)	-15(17)	227(18)	19(15)
C(18B)	194(19)	207(16)	271(18)	24(15)	72(15)	51(13)
C(19B)	240(20)	301(18)	268(18)	-9(16)	8(15)	65(15)