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REVISED

Synthesis and Characterization of Sterically Hindered Group 4 Metallocenes

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Supplemental Material

C22 H34 Cl2 Zr (2) — Page

Table 1. Crystal data and structure refinement for (2). 1

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

[Insert: Explanation of atom labels for 2.] 3a,b

Table 3. Bond lengths [Å] and angles [°] for (2). 3

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for (2). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$ 7

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (2). 8

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Table 1. Crystal data and structure refinement for (3). 9

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

Table 3. Bond lengths [Å] and angles [°] for (3). 11

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for (3). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$ 15

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (3). 16

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Table 1. Crystal data and structure refinement for (4). 17

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for (4). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor. 18

Table 3. Bond lengths [Å] and angles [°] for (4). 19

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for (4). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$ 23

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (4). 24

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Table 1. Crystal data and structure refinement for (2).

Empirical formula	C22 H34 Cl2 Zr
Formula weight	460.62
Temperature	213(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 18.4089(2) Å α= 90°.
	b = 6.6504(1) Å β= 99.950(1)°.
	c = 18.2915(1) Å γ = 90°.
Volume	2205.68(4) $Å^3$
Z	8
Density (calculated)	1.387 Mg/m^3
Absorption coefficient	0.744 mm^{-1}
F(000)	960
Crystal size	0.17 x 0.04 x 0.02 mm^3
Theta range for data collection	2.25 to 29.78°.
Index ranges	-25<h<24, -9<k<8, -24<l<24
Reflections collected	14720
Independent reflections	2975 [R(int) = 0.0768]
Absorption correction	Empirical
Max. and min. transmission	0.363381 and 0.694736
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2975 / 0 / 182
Goodness-of-fit on F^2	.974
Final R indices [I>2sigma(I)]	R1 = 0.0368, wR2 = 0.0708
R indices (all data)	R1 = 0.0587, wR2 = 0.0763
Largest diff. peak and hole	0.395 and -0.814 $e.Å^{-3}$

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

	x	y	z	U(eq)
Zr	5000	566(1)	2500	25(1)
Cl(1)	4011(1)	-1952(1)	2368(1)	39(1)
C(2)	5164(1)	3528(3)	1694(1)	28(1)
C(5)	5134(1)	475(4)	1131(1)	34(1)
C(1P)	6435(1)	2323(3)	1402(1)	30(1)
C(1)	5616(1)	2043(3)	1441(1)	27(1)
C(3)	4422(1)	2897(4)	1529(1)	32(1)
C(4P)	6478(1)	4163(4)	873(1)	36(1)
C(2P)	6752(2)	408(4)	1110(2)	42(1)
C(4)	4404(1)	1030(4)	1171(1)	38(1)
C(3P)	6876(1)	2814(4)	2172(1)	37(1)
C(6P)	7268(2)	4751(5)	803(2)	51(1)
C(5P)	6025(2)	3867(6)	99(2)	55(1)

Compound (**2**) has a labeling scheme in Fig. 6 of the text which corresponds to the format in Tables 1-4 of the text, but this is different from the labeling of (**2**) during refinement and in the supplemental data. A copy of Fig. 6 with revised labeling for the supplemental tables only is provided below (Diagram 1) including a list of the atom labeling for Fig 6 and the equivalent labels for diagram 1 below. The data is currently being refined to provide the same labeling in the supplemental as shown in Fig. 6.

Diagram 1 atom labeling	**Fig 6 atom labeling**
Zr 1	Zr
Cl 1	Cl 1
C 1	C 1
C 2	C 2
C 3	C 3
C 4	C 4
C 5	C 5
C 1P	C 6
C 2P	C 7
C 3P	C 8
C 4P	C 9
C 5P	C 10
C 6P	C 11

Diagram 1

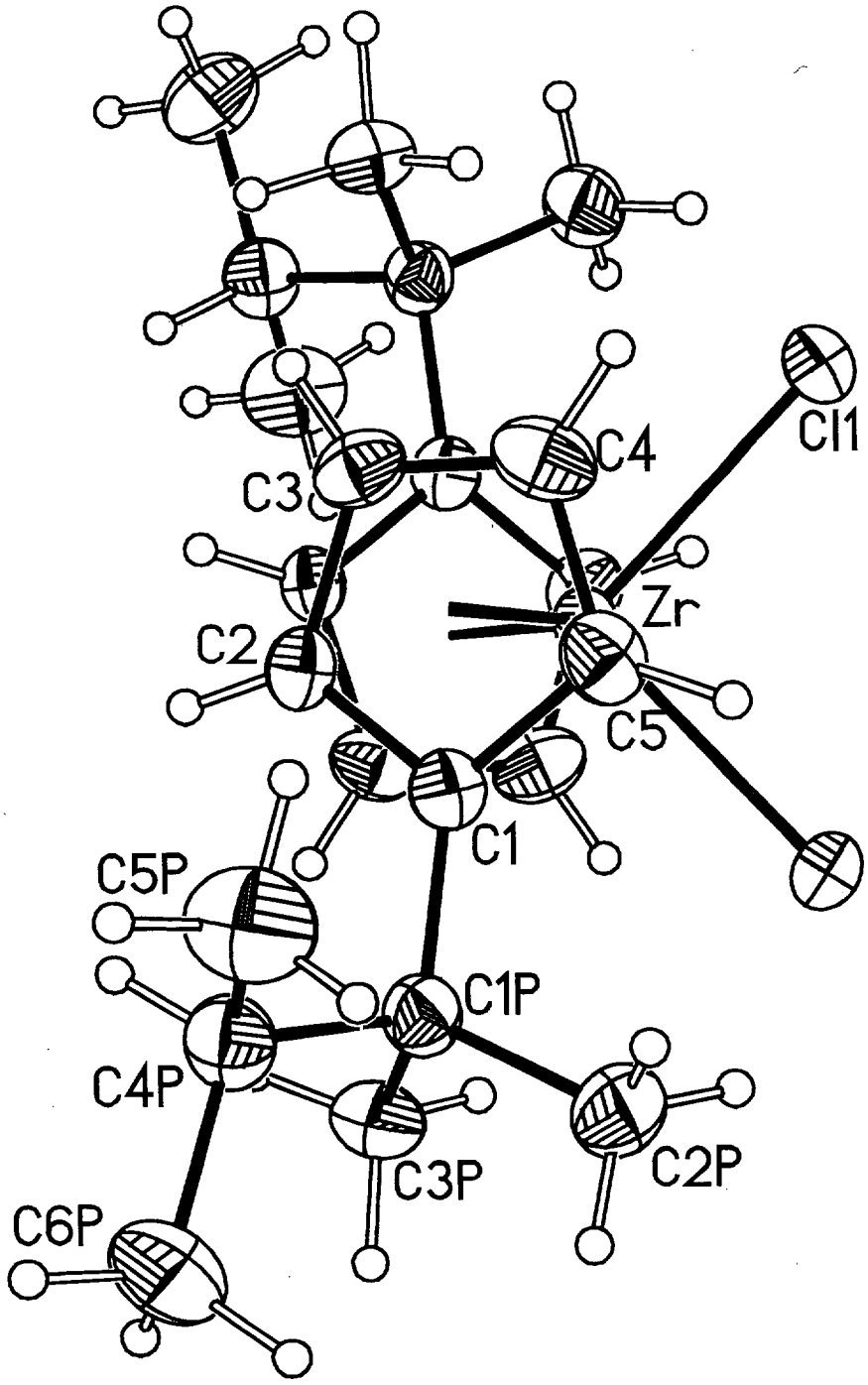


Table 3. Bond lengths [Å] and angles [°] for (2).

Zr-Cl(1)	2.4546(6)
Zr-Cl(1)#1	2.4547(6)
Zr-C(3)	2.457(2)
Zr-C(3)#1	2.457(2)
Zr-C(4)	2.507(2)
Zr-C(4)#1	2.507(2)
Zr-C(2)	2.509(2)
Zr-C(2)#1	2.510(2)
Zr-C(5)	2.560(2)
Zr-C(5)#1	2.560(2)
Zr-C(1)#1	2.600(2)
Zr-C(1)	2.601(2)
C(2)-C(3)	1.411(3)
C(2)-C(1)	1.420(3)
C(5)-C(4)	1.407(3)
C(5)-C(1)	1.422(3)
C(1P)-C(1)	1.532(3)
C(1P)-C(3P)	1.535(3)
C(1P)-C(2P)	1.535(3)
C(1P)-C(4P)	1.570(3)
C(3)-C(4)	1.402(3)
C(4P)-C(5P)	1.527(4)
C(4P)-C(6P)	1.532(4)
Cl(1)-Zr-Cl(1)#1	93.95(3)
Cl(1)-Zr-C(3)	97.94(6)
Cl(1)#1-Zr-C(3)	136.29(6)
Cl(1)-Zr-C(3)#1	136.29(6)
Cl(1)#1-Zr-C(3)#1	97.94(6)
C(3)-Zr-C(3)#1	101.77(11)
Cl(1)-Zr-C(4)	78.22(6)
Cl(1)#1-Zr-C(4)	111.84(6)
C(3)-Zr-C(4)	32.78(8)
C(3)#1-Zr-C(4)	133.28(9)

Cl(1)-Zr-C(4)#1	111.83(6)
Cl(1)#1-Zr-C(4)#1	78.22(6)
C(3)-Zr-C(4)#1	133.28(9)
C(3)#1-Zr-C(4)#1	32.78(8)
C(4)-Zr-C(4)#1	165.87(12)
Cl(1)-Zr-C(2)	129.81(5)
Cl(1)#1-Zr-C(2)	115.53(5)
C(3)-Zr-C(2)	32.99(7)
C(3)#1-Zr-C(2)	81.28(8)
C(4)-Zr-C(2)	53.90(8)
C(4)#1-Zr-C(2)	113.34(8)
Cl(1)-Zr-C(2)#1	115.53(5)
Cl(1)#1-Zr-C(2)#1	129.81(5)
C(3)-Zr-C(2)#1	81.28(8)
C(3)#1-Zr-C(2)#1	32.99(7)
C(4)-Zr-C(2)#1	113.34(8)
C(4)#1-Zr-C(2)#1	53.90(8)
C(2)-Zr-C(2)#1	76.57(10)
Cl(1)-Zr-C(5)	94.75(6)
Cl(1)#1-Zr-C(5)	83.39(6)
C(3)-Zr-C(5)	53.88(8)
C(3)#1-Zr-C(5)	128.27(8)
C(4)-Zr-C(5)	32.23(8)
C(4)#1-Zr-C(5)	148.40(8)
C(2)-Zr-C(5)	53.28(8)
C(2)#1-Zr-C(5)	129.43(8)
Cl(1)-Zr-C(5)#1	83.39(6)
Cl(1)#1-Zr-C(5)#1	94.75(6)
C(3)-Zr-C(5)#1	128.27(8)
C(3)#1-Zr-C(5)#1	53.88(8)
C(4)-Zr-C(5)#1	148.40(8)
C(4)#1-Zr-C(5)#1	32.23(8)
C(2)-Zr-C(5)#1	129.43(8)
C(2)#1-Zr-C(5)#1	53.28(8)
C(5)-Zr-C(5)#1	177.29(12)
Cl(1)-Zr-C(1)#1	85.39(5)

Cl(1)#1-Zr-C(1)#1	126.56(5)
C(3)-Zr-C(1)#1	96.33(7)
C(3)#1-Zr-C(1)#1	54.08(7)
C(4)-Zr-C(1)#1	120.14(7)
C(4)#1-Zr-C(1)#1	53.49(7)
C(2)-Zr-C(1)#1	104.68(7)
C(2)#1-Zr-C(1)#1	32.20(7)
C(5)-Zr-C(1)#1	150.01(8)
C(5)#1-Zr-C(1)#1	31.97(7)
Cl(1)-Zr-C(1)	126.57(5)
Cl(1)#1-Zr-C(1)	85.39(5)
C(3)-Zr-C(1)	54.08(7)
C(3)#1-Zr-C(1)	96.33(7)
C(4)-Zr-C(1)	53.49(7)
C(4)#1-Zr-C(1)	120.14(7)
C(2)-Zr-C(1)	32.20(7)
C(2)#1-Zr-C(1)	104.68(7)
C(5)-Zr-C(1)	31.97(7)
C(5)#1-Zr-C(1)	150.01(8)
C(1)#1-Zr-C(1)	135.63(9)
C(3)-C(2)-C(1)	108.9(2)
C(3)-C(2)-Zr	71.48(13)
C(1)-C(2)-Zr	77.43(12)
C(4)-C(5)-C(1)	108.8(2)
C(4)-C(5)-Zr	71.83(13)
C(1)-C(5)-Zr	75.59(12)
C(1)-C(1P)-C(3P)	110.6(2)
C(1)-C(1P)-C(2P)	110.6(2)
C(3P)-C(1P)-C(2P)	108.8(2)
C(1)-C(1P)-C(4P)	106.2(2)
C(3P)-C(1P)-C(4P)	

108.9(2)**********
****
****
****
****

**********.65(13)

C(5)-C(4)-Zr 75.95(13)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for (2). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr	25(1)	21(1)	28(1)	0	3(1)	0
Cl(1)	31(1)	26(1)	58(1)	1(1)	6(1)	-5(1)
C(2)	33(1)	23(1)	26(1)	2(1)	6(1)	2(1)
C(5)	40(1)	35(1)	29(1)	-9(1)	7(1)	-4(1)
C(1P)	32(1)	28(1)	32(1)	-2(1)	9(1)	0(1)
C(1)	31(1)	28(1)	24(1)	-2(1)	5(1)	-1(1)
C(3)	29(1)	40(1)	26(1)	7(1)	4(1)	7(1)
C(4P)	40(1)	35(1)	36(1)	1(1)	14(1)	-1(1)
C(2P)	41(2)	40(2)	49(2)	-5(1)	18(1)	4(1)
C(4)	33(1)	51(2)	28(1)	-3(1)	-1(1)	-9(1)
C(3P)	30(1)	44(2)	36(1)	1(1)	4(1)	-4(1)
C(6P)	48(2)	57(2)	50(2)	2(2)	17(1)	-14(1)
C(5P)	55(2)	72(2)	39(2)	13(2)	8(1)	-3(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (2).

	x	y	z	U(eq)
H(2)	5309(11)	4734(31)	1933(11)	20(5)
H(2PC)	7225(17)	666(45)	1087(16)	58(9)
H(3PC)	7409(14)	2902(34)	2142(13)	37(6)
H(5)	5291(13)	-760(36)	940(13)	34(6)
H(3PB)	6816(14)	1776(41)	2487(14)	46(8)
H(2PB)	6492(16)	136(41)	620(16)	53(8)
H(2PA)	6708(14)	-773(40)	1449(15)	47(7)
H(6PC)	7247(16)	5987(47)	458(16)	62(9)
H(3)	4030(14)	3598(39)	1635(13)	39(7)
H(4P)	6256(13)	5301(36)	1099(13)	34(6)
H(5PB)	5529(16)	3510(43)	123(14)	54(8)
H(5PA)	5997(18)	5075(55)	-152(19)	70(10)
H(3PA)	6713(16)	4104(44)	2373(16)	56(8)
H(6B)	7537(16)	3560(50)	572(16)	66(9)
H(5PC)	6273(18)	2865(51)	-153(17)	71(10)
H(6A)	7552(20)	5089(49)	1243(20)	74(11)
H(4)	4012(15)	302(39)	1020(14)	43(7)

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Table 1. Crystal data and structure refinement for (3).

Empirical formula	C22 H34 Cl2 Hf	
Formula weight	547.88	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 18.3679(2) Å	α= 90°.
	b = 6.6420(1) Å	β= 100.464(1)°.
	c = 18.2908(1) Å	γ = 90°.
Volume	2194.36(4) $Å^3$	
Z	4	
Density (calculated)	1.658 Mg/m^3	
Absorption coefficient	5.000 mm^{-1}	
F(000)	1088	
Crystal size	0.38 x 0.20 x 0.20 mm^3	
Theta range for data collection	2.26 to 29.87°.	
Index ranges	-25<=h<=24, 0<=k<=9, 0<=l<=24	
Reflections collected	24058	
Independent reflections	3021 [R(int) = 0.041]	
Absorption correction	Empirical, sadabs	
Max. and min. transmission	0.91 and 0.53	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3018 / 0 / 183	
Goodness-of-fit on F^2	1.127	
Final R indices [I>2sigma(I)]	R1 = 0.0153, wR2 = 0.0308	
R indices (all data)	R1 = 0.0165, wR2 = 0.0328	
Extinction coefficient	0.00526(12)	
Largest diff. peak and hole	0.706 and -0.989 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Hf	0	-9397(1)	2500	21(1)
Cl	978(1)	-11903(1)	2626(1)	36(1)
C(1)	-614(1)	-7942(2)	3554(1)	24(1)
C(2)	-166(1)	-6454(2)	3299(1)	25(1)
C(3)	585(1)	-7080(2)	3462(1)	30(1)
C(4)	604(1)	-8954(3)	3824(1)	35(1)
C(5)	-128(1)	-9514(2)	3861(1)	32(1)
C(6)	-1433(1)	-7670(2)	3597(1)	27(1)
C(7)	-1881(1)	-7166(3)	2828(1)	33(1)
C(8)	-1749(1)	-9588(3)	3891(1)	40(1)
C(9)	-1468(1)	-5841(3)	4131(1)	34(1)
C(10)	-2260(1)	-5224(4)	4200(1)	48(1)
C(11)	-1014(2)	-6165(5)	4908(1)	53(1)

Table 3. Bond lengths [Å] and angles [°] for (3).

Hf-Cl#1	2.4281(4)
Hf-Cl	2.4281(4)
Hf-C(3)#1	2.4354(15)
Hf-C(3)	2.4355(15)
Hf-C(4)	2.490(2)
Hf-C(4)#1	2.491(2)
Hf-C(2)	2.4922(14)
Hf-C(2)#1	2.4922(14)
Hf-C(5)	2.544(2)
Hf-C(5)#1	2.544(2)
Hf-C(1)	2.5906(14)
Hf-C(1)#1	2.5907(14)
C(1)-C(2)	1.418(2)
C(1)-C(5)	1.422(2)
C(1)-C(6)	1.530(2)
C(2)-C(3)	1.419(2)
C(3)-C(4)	1.407(3)
C(4)-C(5)	1.409(3)
C(6)-C(7)	1.531(2)
C(6)-C(8)	1.537(2)
C(6)-C(9)	1.568(2)
C(9)-C(11)	1.526(3)
C(9)-C(10)	1.537(3)
Cl#1-Hf-Cl	93.49(2)
Cl#1-Hf-C(3)#1	98.21(4)
Cl-Hf-C(3)#1	136.33(4)
Cl#1-Hf-C(3)	136.33(4)
Cl-Hf-C(3)	98.21(4)
C(3)#1-Hf-C(3)	101.61(8)
Cl#1-Hf-C(4)	111.37(5)
Cl-Hf-C(4)	78.33(4)
C(3)#1-Hf-C(4)	133.43(6)
C(3)-Hf-C(4)	33.17(6)

C(4)#1-Ti-C(5)	79.95(15)
C(4)-Ti-C(5)	34.70(13)
Cl-Ti-C(5)	131.77(9)
Cl#1-Ti-C(5)	114.82(9)
C(5)#1-Ti-C(5)	76.5(2)
C(4)#1-Ti-C(3)	134.6(2)
C(4)-Ti-C(3)	34.50(14)
Cl-Ti-C(3)	76.96(10)
Cl#1-Ti-C(3)	111.06(11)
C(5)#1-Ti-C(3)	113.34(14)
C(5)-Ti-C(3)	56.77(14)
C(4)#1-Ti-C(3)#1	34.50(14)
C(4)-Ti-C(3)#1	134.6(2)
Cl-Ti-C(3)#1	111.06(11)
Cl#1-Ti-C(3)#1	76.95(10)
C(5)#1-Ti-C(3)#1	56.77(14)
C(5)-Ti-C(3)#1	113.34(14)
C(3)-Ti-C(3)#1	168.9(2)
C(4)#1-Ti-C(2)#1	56.38(15)
C(4)-Ti-C(2)#1	129.30(15)
Cl-Ti-C(2)#1	81.54(11)
Cl#1-Ti-C(2)#1	93.46(10)
C(5)#1-Ti-C(2)#1	55.74(14)
C(5)-Ti-C(2)#1	131.41(14)
C(3)-Ti-C(2)#1	147.78(13)
C(3)#1-Ti-C(2)#1	33.50(13)
C(4)#1-Ti-C(2)	129.30(14)
C(4)-Ti-C(2)	56.4(2)
Cl-Ti-C(2)	93.46(10)
Cl#1-Ti-C(2)	81.54(11)
C(5)#1-Ti-C(2)	131.41(14)
C(5)-Ti-C(2)	55.74(14)
C(3)-Ti-C(2)	33.50(13)
C(3)#1-Ti-C(2)	147.78(13)
C(2)#1-Ti-C(2)	172.8(2)
C(4)#1-Ti-C(1)	95.93(14)

C(4)-Ti-C(1)	56.53(13)
Cl-Ti-C(1)	126.79(8)
Cl#1-Ti-C(1)	83.65(9)
C(5)#1-Ti-C(1)	106.27(13)
C(5)-Ti-C(1)	33.38(12)
C(3)-Ti-C(1)	55.97(12)
C(3)#1-Ti-C(1)	119.43(13)
C(2)#1-Ti-C(1)	151.54(13)
C(2)-Ti-C(1)	33.40(12)
C(4)#1-Ti-C(1)#1	56.53(13)
C(4)-Ti-C(1)#1	95.93(14)
Cl-Ti-C(1)#1	83.65(9)
Cl#1-Ti-C(1)#1	126.79(8)
C(5)#1-Ti-C(1)#1	33.38(12)
C(5)-Ti-C(1)#1	106.27(13)
C(3)-Ti-C(1)#1	119.42(13)
C(3)#1-Ti-C(1)#1	55.98(13)
C(2)#1-Ti-C(1)#1	33.40(12)
C(2)-Ti-C(1)#1	151.54(13)
C(1)-Ti-C(1)#1	138.6(2)
C(5)-C(1)-C(2)	106.2(3)
C(5)-C(1)-C(6)	124.7(3)
C(2)-C(1)-C(6)	128.3(3)
C(5)-C(1)-Ti	69.1(2)
C(2)-C(1)-Ti	71.3(2)
C(6)-C(1)-Ti	132.0(2)
C(3)-C(2)-C(1)	109.2(4)
C(3)-C(2)-Ti	71.1(2)
C(1)-C(2)-Ti	75.3(2)
C(2)-C(3)-C(4)	107.6(4)
C(2)-C(3)-Ti	75.4(2)
C(4)-C(3)-Ti	69.9(2)
C(3)-C(4)-C(5)	108.3(4)
C(3)-C(4)-Ti	75.6(2)
C(5)-C(4)-Ti	75.4(2)
C(4)-C(5)-C(1)	108.7(4)

C(4)-C(5)-Ti	69.9(2)
C(1)-C(5)-Ti	77.5(2)
C(8)-C(6)-C(7)	109.4(4)
C(8)-C(6)-C(1)	110.1(3)
C(7)-C(6)-C(1)	111.0(3)
C(8)-C(6)-C(9)	109.3(3)
C(7)-C(6)-C(9)	111.5(3)
C(1)-C(6)-C(9)	105.5(3)
C(10)-C(9)-C(11)	109.3(4)
C(10)-C(9)-C(6)	113.2(4)
C(11)-C(9)-C(6)	113.6(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+3/2

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Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for (3). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Hf	20(1)	17(1)	26(1)	0	2(1)	0
Cl	27(1)	22(1)	56(1)	-1(1)	5(1)	5(1)
C(1)	25(1)	26(1)	23(1)	2(1)	4(1)	0(1)
C(2)	27(1)	24(1)	23(1)	-3(1)	5(1)	-1(1)
C(3)	25(1)	38(1)	26(1)	-8(1)	3(1)	-5(1)
C(4)	28(1)	48(1)	27(1)	3(1)	-2(1)	8(1)
C(5)	34(1)	34(1)	29(1)	10(1)	4(1)	5(1)
C(6)	25(1)	27(1)	30(1)	2(1)	8(1)	0(1)
C(7)	24(1)	41(1)	34(1)	0(1)	4(1)	3(1)
C(8)	38(1)	35(1)	51(1)	6(1)	19(1)	-5(1)
C(9)	36(1)	34(1)	35(1)	-2(1)	14(1)	0(1)
C(10)	45(1)	52(1)	50(1)	-3(1)	21(1)	11(1)
C(11)	52(1)	69(1)	36(1)	-13(1)	6(1)	4(1)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (3).

	x	y	z	U(eq)
H(2)	-340(12)	-5201(34)	3063(12)	30(5)
H(3)	1013(13)	-6355(35)	3350(12)	39(5)
H(4)	1038(16)	-9739(40)	3952(16)	49(7)
H(5)	-260(14)	-10804(30)	4064(14)	41(6)
H(7A)	-2397(13)	-7060(32)	2864(13)	42(5)
H(7B)	-1829(12)	-8207(32)	2494(12)	37(5)
H(7C)	-1731(15)	-5850(34)	2647(15)	44(7)
H(8A)	-2258(18)	-9409(31)	3922(17)	51(8)
H(8B)	-1500(15)	-9966(44)	4385(16)	49(6)
H(8C)	-1729(19)	-10628(37)	3568(19)	60(9)
H(9)	-1277(14)	-4787(37)	3883(14)	38(6)
H(10A)	-2571(22)	-4752(51)	3725(22)	79(10)
H(10B)	-2248(18)	-4094(42)	4548(18)	63(8)
H(10C)	-2505(15)	-6286(46)	4426(16)	59(7)
H(11A)	-530(16)	-6595(43)	4863(15)	63(7)
H(11B)	-1239(19)	-7159(52)	5193(19)	84(10)
H(11C)	-995(19)	-4943(56)	5199(19)	68(8)

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Table 1. Crystal data and structure refinement for (4).

Empirical formula	C22 H34 Cl2 Ti	
Formula weight	417.29	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 18.2957(3) Å	α= 90°.
	b = 6.5568(2) Å	β= 100.202(1)°.
	c = 18.1323(5) Å	γ = 90°.
Volume	2140.78(9) $Å^3$	
Z	4	
Density (calculated)	1.295 Mg/m^3	
Absorption coefficient	0.652 mm^{-1}	
F(000)	888	
Crystal size	0.40 x 0.10 x 0.02 mm^3	
Theta range for data collection	2.26 to 25.00°.	
Index ranges	-22<=h<=22, 0<=k<=8, 0<=l<=22	
Reflections collected	8840	
Independent reflections	1885 [R(int) = 0.1]	
Absorption correction	Empirical	
Max. and min. transmission	0.82 and 0.62	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1863 / 0 / 182	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0511, wR2 = 0.0895	
R indices (all data)	R1 = 0.1013, wR2 = 0.1101	
Largest diff. peak and hole	0.283 and -0.315 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Ti	5000	747(1)	7500	25(1)
Cl	5947(1)	-1747(2)	7614(1)	39(1)
C(1)	4386(2)	2090(6)	8523(2)	29(1)
C(2)	4884(2)	513(7)	8819(2)	34(1)
C(3)	5607(2)	1099(7)	8773(2)	37(1)
C(4)	5567(2)	2989(7)	8412(2)	34(1)
C(5)	4821(2)	3606(6)	8263(2)	26(1)
C(6)	3564(2)	2340(6)	8587(2)	33(1)
C(7)	3259(3)	384(7)	8879(3)	43(1)
C(8)	3105(2)	2883(8)	7824(2)	37(1)
C(9)	3542(2)	4174(7)	9144(2)	38(1)
C(10)	3999(3)	3802(11)	9913(3)	58(2)
C(11)	2757(3)	4805(9)	9224(3)	51(1)

Table 3. Bond lengths [Å] and angles [°] for (4).

Ti-C(4)#1	2.317(4)
Ti-C(4)	2.317(4)
Ti-Cl	2.3652(11)
Ti-Cl#1	2.3653(11)
Ti-C(5)#1	2.387(4)
Ti-C(5)	2.387(4)
Ti-C(3)	2.388(4)
Ti-C(3)#1	2.388(4)
Ti-C(2)#1	2.442(4)
Ti-C(2)	2.442(4)
Ti-C(1)	2.494(3)
Ti-C(1)#1	2.494(3)
C(1)-C(5)	1.406(5)
C(1)-C(2)	1.419(5)
C(1)-C(6)	1.537(5)
C(2)-C(3)	1.393(6)
C(3)-C(4)	1.397(6)
C(4)-C(5)	1.404(5)
C(6)-C(8)	1.529(5)
C(6)-C(7)	1.530(5)
C(6)-C(9)	1.574(5)
C(9)-C(10)	1.514(6)
C(9)-C(11)	1.526(6)
C(4)#1-Ti-C(4)	101.2(2)
C(4)#1-Ti-Cl	136.87(11)
C(4)-Ti-Cl	98.48(11)
C(4)#1-Ti-Cl#1	98.48(11)
C(4)-Ti-Cl#1	136.87(11)
Cl-Ti-Cl#1	92.54(6)
C(4)#1-Ti-C(5)#1	34.70(13)
C(4)-Ti-C(5)#1	79.95(15)
Cl-Ti-C(5)#1	114.82(9)
Cl#1-Ti-C(5)#1	131.77(9)

C(4)#1-Ti-C(5)	79.95(15)
C(4)-Ti-C(5)	34.70(13)
Cl-Ti-C(5)	131.77(9)
Cl#1-Ti-C(5)	114.82(9)
C(5)#1-Ti-C(5)	76.5(2)
C(4)#1-Ti-C(3)	134.6(2)
C(4)-Ti-C(3)	34.50(14)
Cl-Ti-C(3)	76.96(10)
Cl#1-Ti-C(3)	111.06(11)
C(5)#1-Ti-C(3)	113.34(14)
C(5)-Ti-C(3)	56.77(14)
C(4)#1-Ti-C(3)#1	34.50(14)
C(4)-Ti-C(3)#1	134.6(2)
Cl-Ti-C(3)#1	111.06(11)
Cl#1-Ti-C(3)#1	76.95(10)
C(5)#1-Ti-C(3)#1	56.77(14)
C(5)-Ti-C(3)#1	113.34(14)
C(3)-Ti-C(3)#1	168.9(2)
C(4)#1-Ti-C(2)#1	56.38(15)
C(4)-Ti-C(2)#1	129.30(15)
Cl-Ti-C(2)#1	81.54(11)
Cl#1-Ti-C(2)#1	93.46(10)
C(5)#1-Ti-C(2)#1	55.74(14)
C(5)-Ti-C(2)#1	131.41(14)
C(3)-Ti-C(2)#1	147.78(13)
C(3)#1-Ti-C(2)#1	33.50(13)
C(4)#1-Ti-C(2)	129.30(14)
C(4)-Ti-C(2)	56.4(2)
Cl-Ti-C(2)	93.46(10)
Cl#1-Ti-C(2)	81.54(11)
C(5)#1-Ti-C(2)	131.41(14)
C(5)-Ti-C(2)	55.74(14)
C(3)-Ti-C(2)	33.50(13)
C(3)#1-Ti-C(2)	147.78(13)
C(2)#1-Ti-C(2)	172.8(2)
C(4)#1-Ti-C(1)	95.93(14)

C(4)-Ti-C(1)	56.53(13)
Cl-Ti-C(1)	126.79(8)
Cl#1-Ti-C(1)	83.65(9)
C(5)#1-Ti-C(1)	106.27(13)
C(5)-Ti-C(1)	33.38(12)
C(3)-Ti-C(1)	55.97(12)
C(3)#1-Ti-C(1)	119.43(13)
C(2)#1-Ti-C(1)	151.54(13)
C(2)-Ti-C(1)	33.40(12)
C(4)#1-Ti-C(1)#1	56.53(13)
C(4)-Ti-C(1)#1	95.93(14)
Cl-Ti-C(1)#1	83.65(9)
Cl#1-Ti-C(1)#1	126.79(8)
C(5)#1-Ti-C(1)#1	33.38(12)
C(5)-Ti-C(1)#1	106.27(13)
C(3)-Ti-C(1)#1	119.42(13)
C(3)#1-Ti-C(1)#1	55.98(13)
C(2)#1-Ti-C(1)#1	33.40(12)
C(2)-Ti-C(1)#1	151.54(13)
C(1)-Ti-C(1)#1	138.6(2)
C(5)-C(1)-C(2)	106.2(3)
C(5)-C(1)-C(6)	124.7(3)
C(2)-C(1)-C(6)	128.3(3)
C(5)-C(1)-Ti	69.1(2)
C(2)-C(1)-Ti	71.3(2)
C(6)-C(1)-Ti	132.0(2)
C(3)-C(2)-C(1)	109.2(4)
C(3)-C(2)-Ti	71.1(2)
C(1)-C(2)-Ti	75.3(2)
C(2)-C(3)-C(4)	107.6(4)
C(2)-C(3)-Ti	75.4(2)
C(4)-C(3)-Ti	69.9(2)
C(3)-C(4)-C(5)	108.3(4)
C(3)-C(4)-Ti	75.6(2)
C(5)-C(4)-Ti	75.4(2)
C(4)-C(5)-C(1)	108.7(4)

C(4)-C(5)-Ti	69.9(2)
C(1)-C(5)-Ti	77.5(2)
C(8)-C(6)-C(7)	109.4(4)
C(8)-C(6)-C(1)	110.1(3)
C(7)-C(6)-C(1)	111.0(3)
C(8)-C(6)-C(9)	109.3(3)
C(7)-C(6)-C(9)	111.5(3)
C(1)-C(6)-C(9)	105.5(3)
C(10)-C(9)-C(11)	109.3(4)
C(10)-C(9)-C(6)	113.2(4)
C(11)-C(9)-C(6)	113.6(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+3/2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for (4). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ti	25(1)	20(1)	31(1)	0	3(1)	0
Cl	32(1)	25(1)	60(1)	-1(1)	6(1)	5(1)
C(1)	34(2)	28(2)	23(2)	4(2)	3(2)	2(2)
C(2)	39(3)	32(3)	31(2)	8(2)	4(2)	4(2)
C(3)	30(2)	49(3)	28(2)	3(2)	-1(2)	13(2)
C(4)	30(2)	43(3)	29(2)	-10(2)	6(2)	-6(2)
C(5)	29(2)	22(2)	28(2)	1(2)	5(2)	0(2)
C(6)	34(2)	31(2)	35(2)	5(2)	7(2)	-1(2)
C(7)	40(3)	38(3)	52(3)	9(3)	12(2)	0(2)
C(8)	25(2)	44(3)	43(3)	-2(2)	6(2)	2(2)
C(9)	41(3)	38(3)	38(2)	-2(2)	15(2)	0(2)
C(10)	55(4)	79(5)	40(3)	-13(3)	10(3)	0(3)
C(11)	48(3)	58(4)	52(3)	-3(3)	19(3)	9(3)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (4).

	x	y	z	U(eq)
H(2)	4721(19)	-644(59)	8993(20)	34(11)
H(3)	6064(20)	316(58)	8936(20)	42(11)
H(4)	5925(19)	3681(54)	8297(18)	26(11)
H(5)	4631(17)	4816(52)	8057(17)	18(9)
H(7A)	3504(17)	-56(50)	9330(19)	19(10)
H(7B)	3304(19)	-817(61)	8529(20)	40(11)
H(7C)	2726(24)	574(64)	8902(21)	54(13)
H(8A)	2593(22)	3018(54)	7864(18)	35(10)
H(8B)	3166(22)	1776(67)	7426(23)	61(13)
H(8C)	3252(21)	4292(68)	7661(21)	53(13)
H(9)	3765(18)	5373(56)	8932(18)	29(10)
H(10A)	3766(24)	2812(68)	10205(24)	58(14)
H(10B)	4487(24)	3275(67)	9912(21)	56(14)
H(10C)	4083(25)	4978(80)	10202(29)	80(18)
H(11A)	2456(24)	5184(69)	8744(26)	69(16)
H(11B)	2496(24)	3607(74)	9370(23)	62(15)
H(11C)	2762(24)	5869(73)	9575(26)	68(15)