

Syntheses of 2,5-Dimethylcyclopentadienyl *Ansa*-Zirconocene Complexes and Their Reactivity for Ethylene/Norbornene Copolymerization

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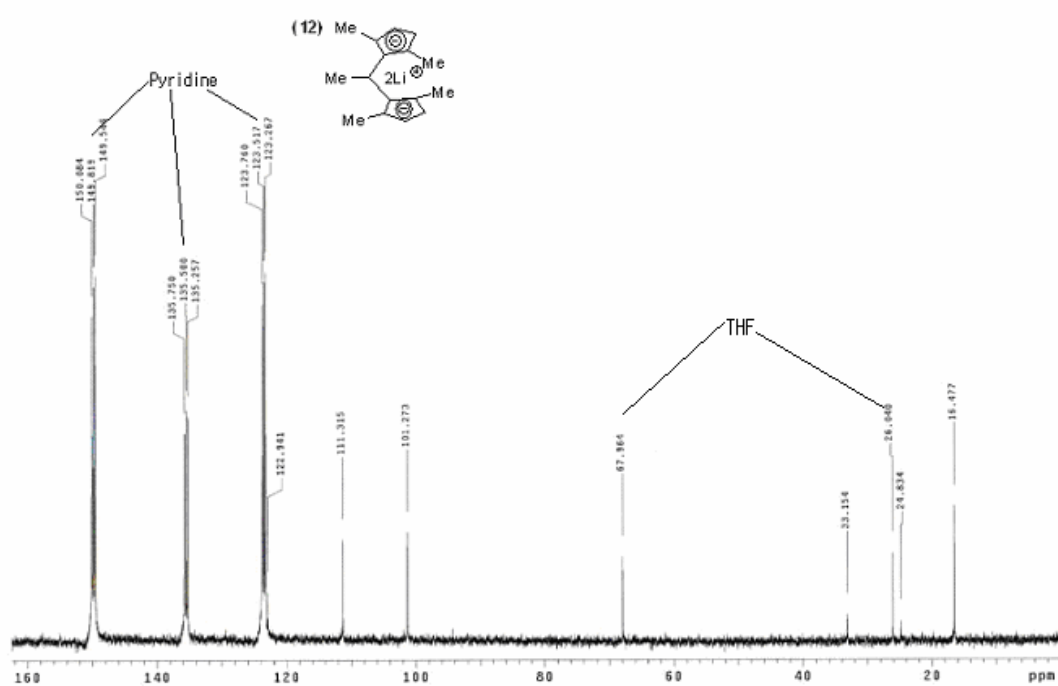
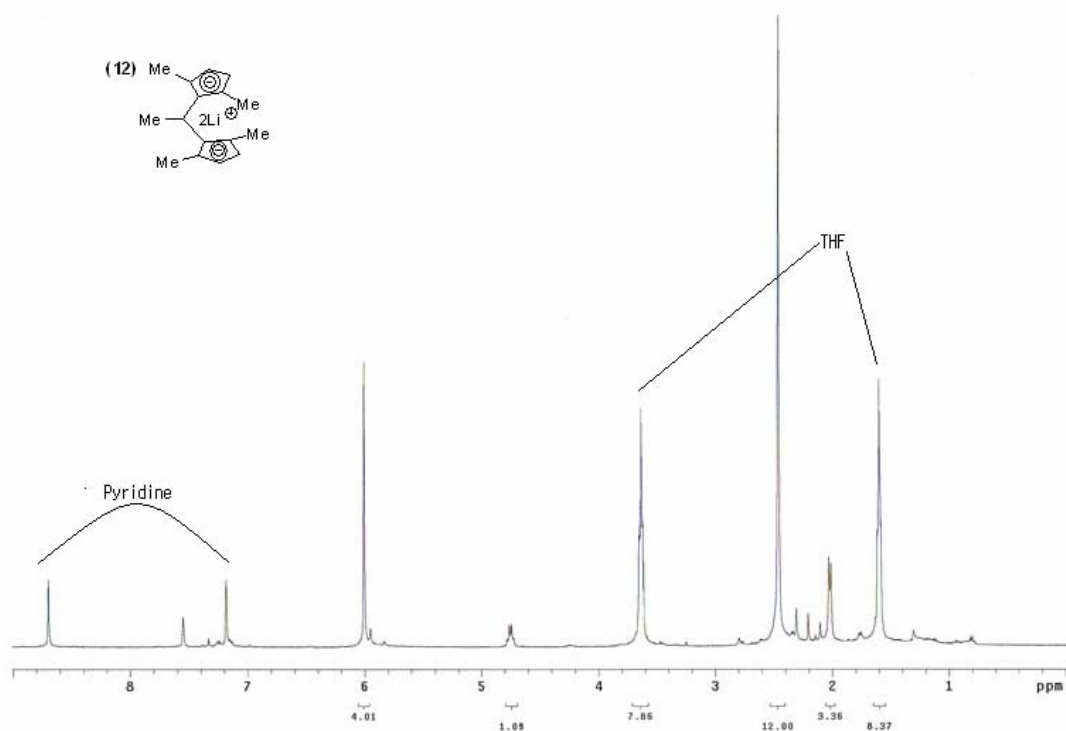
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Supporting Information

^1H and ^{13}C NMR spectra of $[(\text{Me})(\text{H})\text{C}(1,3\text{-Me}_2\text{C}_5\text{H}_2)_2]\text{Li}_2$ (12)



X-Ray Report for Me(H)C(C₅H₄)(1,3-Me₂C₅H₂)ZrCl₂(6)

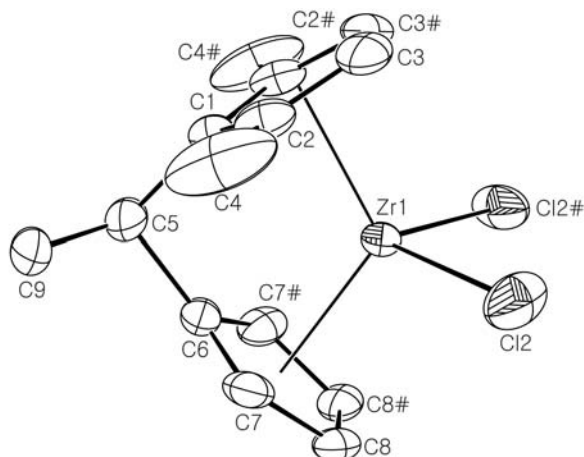


Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zr(1)	4328(1)	7500	5679(1)	38(1)
Cl(2)	4352(1)	8865(1)	7370(1)	84(1)
C(1)	3276(3)	7500	3329(5)	50(1)
C(2)	2854(3)	6679(2)	4108(4)	58(1)
C(3)	2182(3)	7006(3)	5289(4)	74(1)
C(4)	2982(5)	5635(3)	3708(9)	139(3)
C(5)	4311(5)	7500	2246(7)	81(2)
C(6)	5361(4)	7500	3311(5)	59(1)
C(7)	5780(3)	6685(3)	4088(4)	60(1)
C(8)	6494(2)	7003(2)	5280(4)	52(1)
C(9)	4327(6)	6443(8)	1255(8)	82(3)

Table 2. Bond lengths [\AA] and angles [deg]

Zr(1)-Cl(2)	2.4353(10)	Zr(1)-Cl(2)#1	2.4353(10)
Zr(1)-C(1)	2.436(4)	Zr(1)-C(6)	2.439(4)
Zr(1)-C(7)#1	2.455(3)	Zr(1)-C(7)	2.455(3)
Zr(1)-C(2)	2.466(3)	Zr(1)-C(2)#1	2.466(3)

Zr(1)-C(3)	2.538(3)	Zr(1)-C(3)#1	2.538(3)
Zr(1)-C(8)	2.560(3)	Zr(1)-C(8)#1	2.560(3)
C(1)-C(2)#1	1.422(4)	C(1)-C(2)	1.422(4)
C(1)-C(5)	1.523(7)	C(2)-C(3)	1.387(5)
C(2)-C(4)	1.500(5)	C(3)-C(3)#1	1.370(9)
C(5)-C(6)	1.527(7)	C(5)-C(9)	1.720(10)
C(5)-C(9)#1	1.720(10)	C(6)-C(7)#1	1.413(5)
C(6)-C(7)	1.413(5)	C(7)-C(8)	1.416(4)
C(8)-C(8)#1	1.380(7)		
Cl(2)-Zr(1)-Cl(2)#1	102.11(7)	Cl(2)-Zr(1)-C(1)	123.66(5)
Cl(2)#1-Zr(1)-C(1)	123.66(5)	Cl(2)-Zr(1)-C(6)	123.18(5)
Cl(2)#1-Zr(1)-C(6)	123.18(5)	C(1)-Zr(1)-C(6)	57.59(15)
Cl(2)-Zr(1)-C(7)#1	90.20(11)	Cl(2)#1-Zr(1)-C(7)#1	136.04(9)
C(1)-Zr(1)-C(7)#1	79.12(12)	C(6)-Zr(1)-C(7)#1	33.55(11)
Cl(2)-Zr(1)-C(7)	136.04(9)	Cl(2)#1-Zr(1)-C(7)	90.20(11)
C(1)-Zr(1)-C(7)	79.12(12)	C(6)-Zr(1)-C(7)	33.55(11)
C(7)#1-Zr(1)-C(7)	54.8(2)	Cl(2)-Zr(1)-C(2)	136.82(9)
Cl(2)#1-Zr(1)-C(2)	90.61(9)	C(1)-Zr(1)-C(2)	33.71(10)
C(6)-Zr(1)-C(2)	79.27(13)	C(7)#1-Zr(1)-C(2)	108.81(13)
C(7)-Zr(1)-C(2)	84.09(13)	Cl(2)-Zr(1)-C(2)#1	90.61(9)
Cl(2)#1-Zr(1)-C(2)#1	136.82(9)	C(1)-Zr(1)-C(2)#1	33.71(10)
C(6)-Zr(1)-C(2)#1	79.27(13)	C(7)#1-Zr(1)-C(2)#1	84.09(13)
C(7)-Zr(1)-C(2)#1	108.81(13)	C(2)-Zr(1)-C(2)#1	55.03(16)
Cl(2)-Zr(1)-C(3)	107.92(11)	Cl(2)#1-Zr(1)-C(3)	83.55(9)
C(1)-Zr(1)-C(3)	54.19(13)	C(6)-Zr(1)-C(3)	109.39(14)
C(7)#1-Zr(1)-C(3)	132.62(12)	C(7)-Zr(1)-C(3)	115.37(13)
C(2)-Zr(1)-C(3)	32.15(12)	C(2)#1-Zr(1)-C(3)	53.33(12)
Cl(2)-Zr(1)-C(3)#1	83.55(9)	Cl(2)#1-Zr(1)-C(3)#1	107.92(11)
C(1)-Zr(1)-C(3)#1	54.19(13)	C(6)-Zr(1)-C(3)#1	109.39(14)
C(7)#1-Zr(1)-C(3)#1	115.37(13)	C(7)-Zr(1)-C(3)#1	132.62(12)
C(2)-Zr(1)-C(3)#1	53.33(12)	C(2)#1-Zr(1)-C(3)#1	32.15(12)
C(3)-Zr(1)-C(3)#1	31.3(2)	Cl(2)-Zr(1)-C(8)	106.75(8)
Cl(2)#1-Zr(1)-C(8)	82.47(8)	C(1)-Zr(1)-C(8)	109.88(12)
C(6)-Zr(1)-C(8)	54.66(12)	C(7)#1-Zr(1)-C(8)	53.62(12)
C(7)-Zr(1)-C(8)	32.71(10)	C(2)-Zr(1)-C(8)	115.81(11)

C(2)#1-Zr(1)-C(8)	133.20(12)	C(3)-Zr(1)-C(8)	144.60(13)
C(3)#1-Zr(1)-C(8)	163.88(12)	Cl(2)-Zr(1)-C(8)#1	82.47(8)
Cl(2)#1-Zr(1)-C(8)#1	106.75(8)	C(1)-Zr(1)-C(8)#1	109.88(12)
C(6)-Zr(1)-C(8)#1	54.66(12)	C(7)#1-Zr(1)-C(8)#1	32.71(10)
C(7)-Zr(1)-C(8)#1	53.62(12)	C(2)-Zr(1)-C(8)#1	133.20(12)
C(2)#1-Zr(1)-C(8)#1	115.81(11)	C(3)-Zr(1)-C(8)#1	163.88(12)
C(3)#1-Zr(1)-C(8)#1	144.60(13)	C(8)-Zr(1)-C(8)#1	31.27(15)
C(2)#1-C(1)-C(2)	106.5(4)	C(2)#1-C(1)-C(5)	125.1(2)
C(2)-C(1)-C(5)	125.1(2)	C(2)#1-C(1)-Zr(1)	74.3(2)
C(2)-C(1)-Zr(1)	74.3(2)	C(5)-C(1)-Zr(1)	101.0(3)
C(3)-C(2)-C(1)	107.6(3)	C(3)-C(2)-C(4)	123.7(5)
C(1)-C(2)-C(4)	128.5(5)	C(3)-C(2)-Zr(1)	76.79(19)
C(1)-C(2)-Zr(1)	72.0(2)	C(4)-C(2)-Zr(1)	121.4(3)
C(3)#1-C(3)-C(2)	109.1(2)	C(3)#1-C(3)-Zr(1)	74.34(10)
C(2)-C(3)-Zr(1)	71.06(18)	C(1)-C(5)-C(6)	100.7(4)
C(1)-C(5)-C(9)	110.2(4)	C(6)-C(5)-C(9)	108.7(3)
C(1)-C(5)-C(9)#1	110.2(4)	C(6)-C(5)-C(9)#1	108.7(3)
C(9)-C(5)-C(9)#1	117.1(8)	C(7)#1-C(6)-C(7)	106.3(4)
C(7)#1-C(6)-C(5)	125.0(2)	C(7)-C(6)-C(5)	125.0(2)
C(7)#1-C(6)-Zr(1)	73.8(2)	C(7)-C(6)-Zr(1)	73.8(2)
C(5)-C(6)-Zr(1)	100.7(3)	C(6)-C(7)-C(8)	108.7(3)
C(6)-C(7)-Zr(1)	72.6(2)	C(8)-C(7)-Zr(1)	77.73(18)
C(8)#1-C(8)-C(7)	108.1(2)	C(8)#1-C(8)-Zr(1)	74.36(8)
C(7)-C(8)-Zr(1)	69.56(16)		

Symmetry transformations used to generate equivalent atoms:

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

	U11	U22	U33	U23	U13	U12
Zr(1)	28(1)	45(1)	42(1)	0	1(1)	0
Cl(2)	63(1)	99(1)	90(1)	-51(1)	-8(1)	16(1)
C(1)	31(2)	69(3)	50(2)	0	-8(2)	0

C(2)	41(2)	51(2)	84(2)	-3(2)	-21(2)	-7(1)
C(3)	33(1)	117(3)	72(2)	21(2)	-6(2)	-17(2)
C(4)	109(4)	58(3)	251(7)	-42(4)	-98(5)	6(3)
C(5)	40(3)	160(8)	44(3)	0	-1(2)	0
C(6)	30(2)	105(4)	43(2)	0	4(2)	0
C(7)	34(1)	77(2)	70(2)	-25(2)	-1(1)	12(1)
C(8)	29(1)	66(2)	61(2)	-3(2)	-5(1)	8(1)
C(9)	47(4)	153(9)	46(4)	-30(5)	-5(3)	7(4)

Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{Å}^2 \times 10^3$).

	x	y	z	U(eq)
H(3)	1793	6618	5972	89
H(4A)	3101	5262	4589	209
H(4B)	3652	5555	3064	209
H(4C)	2276	5419	3216	209
H(5A)	4360(50)	7860(50)	1710(70)	28(17)
H(7)	5615	6046	3855	72
H(8)	6893	6609	5947	63
H(9A)	4955	6465	538	123
H(9B)	3580	6363	759	123
H(9C)	4456	5911	1913	123

X-Ray Report for [(Me)(H)C(1,3-Me₂C₅H₂)₂]ZrCl₂ (13).

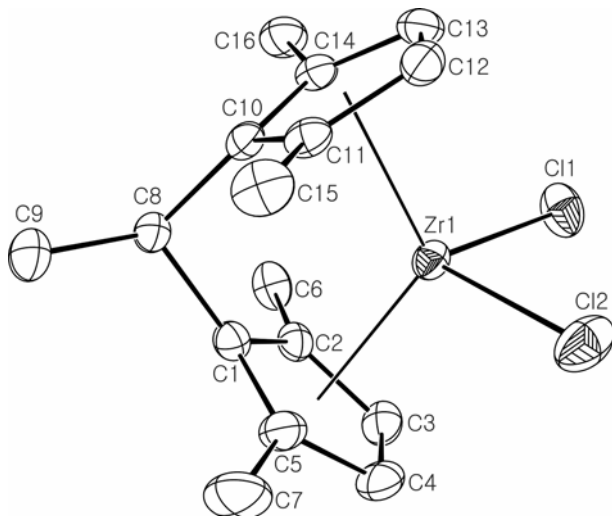


Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Zr(1)	4063(1)	12495(1)	-2127(1)	32(1)
Cl(1)	3776(1)	13870(1)	-3129(1)	55(1)
Cl(2)	4156(1)	9915(1)	-2544(1)	60(1)
C(1)	3549(2)	13120(5)	-1062(2)	35(1)
C(2)	3114(2)	14018(5)	-1519(2)	35(1)
C(3)	2666(2)	13018(5)	-1902(2)	44(1)
C(4)	2802(2)	11553(5)	-1691(2)	48(1)
C(5)	3348(2)	11591(5)	-1164(2)	42(1)
C(6)	3032(2)	15694(5)	-1572(2)	47(1)
C(7)	3515(3)	10172(5)	-770(2)	67(2)
C(8)	4279(2)	13727(5)	-721(2)	35(1)
C(9)	4474(2)	13139(5)	-29(2)	51(1)
C(10)	4880(2)	13467(4)	-1239(2)	31(1)
C(11)	5222(2)	12074(4)	-1421(2)	34(1)
C(12)	5511(2)	12278(5)	-2053(2)	40(1)
C(13)	5361(2)	13748(5)	-2255(2)	41(1)
C(14)	4979(2)	14504(4)	-1762(2)	34(1)

C(15)	5376(2)	10661(5)	-1031(2)	51(1)
C(16)	4838(3)	16185(5)	-1769(2)	49(1)
Zr(2)	2143(1)	6837(1)	874(1)	36(1)
Cl(3)	3248(1)	6730(1)	178(1)	57(1)
Cl(4)	2322(1)	9261(1)	1411(1)	73(1)
C(17)	1612(2)	4695(5)	1454(2)	36(1)
C(18)	1804(2)	5749(5)	1949(2)	43(1)
C(19)	2609(3)	5860(6)	1977(2)	50(1)
C(21)	2307(3)	4155(5)	1188(2)	46(1)
C(20)	2907(3)	4915(5)	1523(2)	52(1)
C(22)	1313(3)	6533(5)	2430(2)	59(1)
C(23)	2465(3)	2918(5)	710(2)	65(1)
C(24)	815(2)	4617(5)	1130(2)	40(1)
C(25)	519(3)	3071(5)	918(2)	60(1)
C(26)	868(2)	5848(5)	601(2)	41(1)
C(27)	1275(2)	5778(5)	5(2)	44(1)
C(28)	1412(3)	7267(6)	-198(2)	55(1)
C(29)	1102(3)	8255(6)	243(2)	58(1)
C(30)	748(3)	7415(5)	739(2)	48(1)
C(31)	1427(3)	4446(6)	-442(2)	63(1)
C(32)	260(3)	8126(6)	1253(2)	75(2)

Table 2. Bond lengths [Å] and angles [deg] .

Zr(1)-Cl(1)	2.4338(11)	Zr(1)-Cl(2)	2.4469(12)
Zr(1)-C(1)	2.448(4)	Zr(1)-C(10)	2.448(3)
Zr(1)-C(11)	2.498(3)	Zr(1)-C(5)	02.498(4)
Zr(1)-C(2)	2.502(4)	Zr(1)-C(14)	2.502(4)
Zr(1)-C(4)	2.551(4)	Zr(1)-C(3)	2.551(4)
Zr(1)-C(12)	2.552(4)	Zr(1)-C(13)	2.556(4)
C(1)-C(5)	1.414(5)	C(1)-C(2)	1.436(5)
C(1)-C(8)	1.544(5)	C(2)-C(3)	1.411(5)
C(2)-C(6)	1.496(5)	C(3)-C(4)	1.387(6)
C(4)-C(5)	1.428(5)	C(5)-C(7)	1.519(6)
C(8)-C(10)	1.533(5)	C(8)-C(9)	1.543(5)

C(10)-C(11)	1.426(5)	C(10)-C(14)	1.428(5)
C(11)-C(12)	1.415(5)	C(11)-C(15)	1.506(5)
C(12)-C(13)	1.390(6)	C(13)-C(14)	1.398(5)
C(14)-C(16)	1.510(5)	Zr(2)-Cl(4)	2.4304(13)
Zr(2)-C(17)	2.437(4)	Zr(2)-Cl(3)	2.4409(12)
Zr(2)-C(26)	2.457(4)	Zr(2)-C(21)	2.476(4)
Zr(2)-C(18)	2.492(4)	Zr(2)-C(27)	2.501(4)
Zr(2)-C(30)	2.512(4)	Zr(2)-C(20)	2.527(4)
Zr(2)-C(19)	2.540(4)	Zr(2)-C(29)	2.547(4)
Zr(2)-C(28)	2.549(4)	C(17)-C(18)	1.415(5)
C(17)-C(21)	1.432(6)	C(17)-C(24)	1.537(5)
C(18)-C(19)	1.417(6)	C(18)-C(22)	1.499(6)
C(19)-C(20)	1.366(6)	C(21)-C(20)	1.414(6)
C(21)-C(23)	1.502(6)	C(24)-C(25)	1.524(5)
C(24)-C(26)	1.543(5)	C(26)-C(27)	1.432(6)
C(26)-C(30)	1.433(6)	C(27)-C(28)	1.406(6)
C(27)-C(31)	1.522(6)	C(28)-C(29)	1.382(6)
C(29)-C(30)	1.416(6)	C(30)-C(32)	1.513(6)
Cl(1)-Zr(1)-Cl(2)	100.69(4)	Cl(1)-Zr(1)-C(1)	124.61(10)
Cl(2)-Zr(1)-C(1)	123.57(10)	Cl(1)-Zr(1)-C(10)	123.98(9)
Cl(2)-Zr(1)-C(10)	123.11(9)	C(1)-Zr(1)-C(10)	58.58(13)
Cl(1)-Zr(1)-C(11)	135.57(10)	Cl(2)-Zr(1)-C(11)	90.19(10)
C(1)-Zr(1)-C(11)	80.21(13)	C(10)-Zr(1)-C(11)	33.50(12)
Cl(1)-Zr(1)-C(5)	136.98(10)	Cl(2)-Zr(1)-C(5)	90.97(10)
C(1)-Zr(1)-C(5)	33.19(13)	C(10)-Zr(1)-C(5)	79.70(13)
C(11)-Zr(1)-C(5)	84.98(13)	Cl(1)-Zr(1)-C(2)	91.41(9)
Cl(2)-Zr(1)-C(2)	136.80(10)	C(1)-Zr(1)-C(2)	33.69(11)
C(11)-Zr(1)-C(2)	109.61(12)	C(5)-Zr(1)-C(2)	54.85(13)
Cl(1)-Zr(1)-C(14)	90.87(9)	Cl(2)-Zr(1)-C(14)	136.12(10)
C(1)-Zr(1)-C(14)	79.70(13)	C(10)-Zr(1)-C(14)	33.50(12)
C(11)-Zr(1)-C(14)	54.77(12)	C(5)-Zr(1)-C(14)	108.90(13)
C(2)-Zr(1)-C(14)	84.24(13)	Cl(1)-Zr(1)-C(4)	107.26(10)
Cl(2)-Zr(1)-C(4)	83.31(11)	C(1)-Zr(1)-C(4)	54.40(13)
C(10)-Zr(1)-C(4)	110.63(13)	C(11)-Zr(1)-C(4)	116.80(13)
C(5)-Zr(1)-C(4)	32.83(12)	C(2)-Zr(1)-C(4)	53.54(14)

C(14)-Zr(1)-C(4)	133.32(14)	Cl(1)-Zr(1)-C(3)	83.19(10)
Cl(2)-Zr(1)-C(3)	107.79(10)	C(1)-Zr(1)-C(3)	54.54(12)
C(10)-Zr(1)-C(3)	110.54(13)	C(11)-Zr(1)-C(3)	134.17(13)
C(5)-Zr(1)-C(3)	53.89(13)	C(2)-Zr(1)-C(3)	32.41(12)
C(14)-Zr(1)-C(3)	115.59(14)	C(4)-Zr(1)-C(3)	31.55(13)
Cl(1)-Zr(1)-C(12)	105.87(10)	Cl(2)-Zr(1)-C(12)	82.87(10)
C(1)-Zr(1)-C(12)	110.68(12)	C(10)-Zr(1)-C(12)	54.32(13)
C(11)-Zr(1)-C(12)	32.53(12)	C(5)-Zr(1)-C(12)	116.67(13)
C(2)-Zr(1)-C(12)	133.37(12)	C(14)-Zr(1)-C(12)	53.29(13)
C(4)-Zr(1)-C(12)	145.90(14)	C(3)-Zr(1)-C(12)	164.81(12)
Cl(1)-Zr(1)-C(13)	82.09(9)	Cl(2)-Zr(1)-C(13)	107.59(11)
C(1)-Zr(1)-C(13)	110.09(13)	C(10)-Zr(1)-C(13)	54.24(13)
C(11)-Zr(1)-C(13)	53.67(13)	C(5)-Zr(1)-C(13)	133.46(12)
C(2)-Zr(1)-C(13)	115.13(14)	C(14)-Zr(1)-C(13)	32.06(12)
C(4)-Zr(1)-C(13)	164.44(13)	C(3)-Zr(1)-C(13)	143.58(15)
C(12)-Zr(1)-C(13)	31.57(12)	C(5)-C(1)-C(2)	107.9(3)
C(5)-C(1)-C(8)	127.0(3)	C(2)-C(1)-C(8)	121.8(3)
C(5)-C(1)-Zr(1)	75.4(2)	C(2)-C(1)-Zr(1)	75.2(2)
C(8)-C(1)-Zr(1)	99.3(2)	C(3)-C(2)-C(1)	107.3(4)
C(3)-C(2)-C(6)	122.1(3)	C(1)-C(2)-C(6)	130.2(3)
C(3)-C(2)-Zr(1)	75.7(2)	C(1)-C(2)-Zr(1)	71.1(2)
C(6)-C(2)-Zr(1)	124.3(3)	C(4)-C(3)-C(2)	108.9(4)
C(4)-C(3)-Zr(1)	74.2(2)	C(2)-C(3)-Zr(1)	71.9(2)
C(3)-C(4)-C(5)	108.8(4)	C(3)-C(4)-Zr(1)	74.2(3)
C(5)-C(4)-Zr(1)	71.6(2)	C(1)-C(5)-C(4)	107.2(4)
C(1)-C(5)-C(7)	132.0(4)	C(4)-C(5)-C(7)	120.1(4)
C(1)-C(5)-Zr(1)	71.5(2)	C(4)-C(5)-Zr(1)	75.6(2)
C(7)-C(5)-Zr(1)	126.2(3)	C(10)-C(8)-C(9)	116.6(3)
C(10)-C(8)-C(1)	102.2(3)	C(9)-C(8)-C(1)	117.6(3)
C(11)-C(10)-C(14)	107.4(3)	C(11)-C(10)-C(8)	127.8(4)
C(14)-C(10)-C(8)	121.6(3)	C(11)-C(10)-Zr(1)	75.1(2)
C(14)-C(10)-Zr(1)	75.3(2)	C(8)-C(10)-Zr(1)	99.7(2)
C(12)-C(11)-C(10)	107.0(3)	C(12)-C(11)-C(15)	121.9(4)
C(10)-C(11)-C(15)	130.6(4)	C(12)-C(11)-Zr(1)	75.9(2)
C(10)-C(11)-Zr(1)	71.35(19)	C(15)-C(11)-Zr(1)	124.4(3)
C(13)-C(12)-C(11)	108.9(4)	C(13)-C(12)-Zr(1)	74.4(2)

C(11)-C(12)-Zr(1)	71.6(2)	C(12)-C(13)-C(14)	108.9(4)
C(12)-C(13)-Zr(1)	74.1(2)	C(14)-C(13)-Zr(1)	71.8(2)
C(13)-C(14)-C(10)	107.8(4)	C(13)-C(14)-C(16)	123.2(4)
C(10)-C(14)-C(16)	128.2(4)	C(13)-C(14)-Zr(1)	76.1(2)
C(10)-C(14)-Zr(1)	71.2(2)	C(16)-C(14)-Zr(1)	126.4(3)
Cl(4)-Zr(2)-C(17)	120.90(10)	Cl(4)-Zr(2)-Cl(3)	101.73(5)
C(17)-Zr(2)-Cl(3)	125.13(11)	Cl(4)-Zr(2)-C(26)	121.71(11)
C(17)-Zr(2)-C(26)	58.39(13)	Cl(3)-Zr(2)-C(26)	125.90(10)
Cl(4)-Zr(2)-C(21)	135.77(11)	C(17)-Zr(2)-C(21)	33.88(13)
Cl(3)-Zr(2)-C(21)	91.51(11)	C(26)-Zr(2)-C(21)	79.46(14)
Cl(4)-Zr(2)-C(18)	88.37(11)	C(17)-Zr(2)-C(18)	33.35(13)
Cl(3)-Zr(2)-C(18)	135.56(11)	C(26)-Zr(2)-C(18)	80.10(13)
C(21)-Zr(2)-C(18)	55.08(15)	Cl(4)-Zr(2)-C(27)	136.44(11)
C(17)-Zr(2)-C(27)	79.73(13)	Cl(3)-Zr(2)-C(27)	92.76(11)
C(26)-Zr(2)-C(27)	33.56(13)	C(21)-Zr(2)-C(27)	83.74(14)
C(18)-Zr(2)-C(27)	109.35(14)	Cl(4)-Zr(2)-C(30)	89.16(11)
C(17)-Zr(2)-C(30)	80.10(14)	Cl(3)-Zr(2)-C(30)	136.98(11)
C(26)-Zr(2)-C(30)	33.49(14)	C(21)-Zr(2)-C(30)	109.33(15)
C(18)-Zr(2)-C(30)	85.57(14)	C(27)-Zr(2)-C(30)	54.64(14)
Cl(4)-Zr(2)-C(20)	107.15(12)	C(17)-Zr(2)-C(20)	54.78(14)
Cl(3)-Zr(2)-C(20)	82.12(12)	C(26)-Zr(2)-C(20)	110.47(14)
C(21)-Zr(2)-C(20)	32.83(13)	C(18)-Zr(2)-C(20)	53.73(15)
C(27)-Zr(2)-C(20)	115.48(15)	C(30)-Zr(2)-C(20)	134.38(15)
Cl(4)-Zr(2)-C(19)	82.04(12)	C(17)-Zr(2)-C(19)	54.49(13)
Cl(3)-Zr(2)-C(19)	105.37(11)	C(26)-Zr(2)-C(19)	110.75(14)
C(21)-Zr(2)-C(19)	53.74(15)	C(18)-Zr(2)-C(19)	32.70(13)
C(27)-Zr(2)-C(19)	133.28(15)	C(30)-Zr(2)-C(19)	117.38(15)
C(20)-Zr(2)-C(19)	31.29(14)	Cl(4)-Zr(2)-C(29)	82.99(12)
C(17)-Zr(2)-C(29)	110.67(15)	Cl(3)-Zr(2)-C(29)	107.06(12)
C(26)-Zr(2)-C(29)	54.56(14)	C(21)-Zr(2)-C(29)	133.09(15)
C(18)-Zr(2)-C(29)	117.15(16)	C(27)-Zr(2)-C(29)	53.45(15)
C(30)-Zr(2)-C(29)	32.51(14)	C(20)-Zr(2)-C(29)	165.00(15)
C(19)-Zr(2)-C(29)	146.39(17)	Cl(4)-Zr(2)-C(28)	108.43(12)
C(17)-Zr(2)-C(28)	110.28(14)	Cl(3)-Zr(2)-C(28)	83.77(12)
C(26)-Zr(2)-C(28)	54.48(14)	C(21)-Zr(2)-C(28)	114.91(15)
C(18)-Zr(2)-C(28)	134.07(15)	C(27)-Zr(2)-C(28)	32.32(13)

C(30)-Zr(2)-C(28)	53.48(15)	C(20)-Zr(2)-C(28)	143.67(17)
C(19)-Zr(2)-C(28)	164.75(15)	C(29)-Zr(2)-C(28)	31.46(14)
C(18)-C(17)-C(21)	107.6(4)	C(18)-C(17)-C(24)	122.6(4)
C(21)-C(17)-C(24)	126.7(4)	C(18)-C(17)-Zr(2)	75.5(2)
C(21)-C(17)-Zr(2)	74.5(2)	C(24)-C(17)-Zr(2)	100.4(2)
C(17)-C(18)-C(19)	107.3(4)	C(17)-C(18)-C(22)	130.4(4)
C(19)-C(18)-C(22)	122.1(4)	C(17)-C(18)-Zr(2)	71.2(2)
C(19)-C(18)-Zr(2)	75.5(2)	C(22)-C(18)-Zr(2)	124.0(3)
C(20)-C(19)-C(18)	109.1(4)	C(20)-C(19)-Zr(2)	73.8(2)
C(18)-C(19)-Zr(2)	71.8(2)	C(20)-C(21)-C(17)	106.8(4)
C(20)-C(21)-C(23)	121.1(4)	C(17)-C(21)-C(23)	131.7(4)
C(20)-C(21)-Zr(2)	75.6(2)	C(17)-C(21)-Zr(2)	71.6(2)
C(23)-C(21)-Zr(2)	123.5(3)	C(19)-C(20)-C(21)	109.3(4)
C(19)-C(20)-Zr(2)	74.9(3)	C(21)-C(20)-Zr(2)	71.6(2)
C(25)-C(24)-C(17)	117.7(4)	C(25)-C(24)-C(26)	117.4(3)
C(17)-C(24)-C(26)	101.7(3)	C(27)-C(26)-C(30)	106.9(4)
C(27)-C(26)-C(24)	127.6(4)	C(30)-C(26)-C(24)	122.2(4)
C(27)-C(26)-Zr(2)	74.9(2)	C(30)-C(26)-Zr(2)	75.4(2)
C(24)-C(26)-Zr(2)	99.3(2)	C(28)-C(27)-C(26)	107.8(4)
C(28)-C(27)-C(31)	120.9(4)	C(26)-C(27)-C(31)	130.3(4)
C(28)-C(27)-Zr(2)	75.7(2)	C(26)-C(27)-Zr(2)	71.6(2)
C(31)-C(27)-Zr(2)	127.4(3)	C(29)-C(28)-C(27)	109.0(4)
C(29)-C(28)-Zr(2)	74.2(2)	C(27)-C(28)-Zr(2)	71.9(2)
C(28)-C(29)-C(30)	109.0(4)	C(28)-C(29)-Zr(2)	74.4(3)
C(30)-C(29)-Zr(2)	72.4(2)	C(29)-C(30)-C(26)	107.3(4)
C(29)-C(30)-C(32)	123.2(5)	C(26)-C(30)-C(32)	129.0(4)
C(29)-C(30)-Zr(2)	75.1(3)	C(26)-C(30)-Zr(2)	71.1(2)
C(32)-C(30)-Zr(2)	125.2(3)		

Symmetry transformations used to generate equivalent atoms:

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

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

U11	U22	U33	U23	U13	U12
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Zr(1)	30(1)	34(1)	33(1)	-3(1)	-4(1)	0(1)
Cl(1)	55(1)	75(1)	36(1)	7(1)	-3(1)	16(1)
Cl(2)	49(1)	45(1)	86(1)	-23(1)	-4(1)	1(1)
C(1)	36(2)	38(2)	29(2)	3(2)	1(2)	-1(2)
C(2)	29(2)	45(3)	30(2)	-1(2)	1(2)	4(2)
C(3)	30(2)	60(3)	41(2)	-6(2)	-5(2)	5(2)
C(4)	30(3)	57(3)	58(3)	-11(2)	2(2)	-10(2)
C(5)	40(3)	40(3)	47(3)	2(2)	0(2)	-9(2)
C(6)	54(3)	49(3)	39(2)	4(2)	1(2)	15(2)
C(7)	74(4)	51(3)	76(3)	24(3)	-2(3)	-22(3)
C(8)	37(2)	38(2)	29(2)	1(2)	-3(2)	-4(2)
C(9)	56(3)	60(3)	35(2)	3(2)	-9(2)	-4(3)
C(10)	30(2)	32(3)	31(2)	0(2)	-6(2)	-3(2)
C(11)	27(2)	34(3)	41(2)	4(2)	-8(2)	-1(2)
C(12)	32(2)	45(3)	44(3)	-12(2)	0(2)	1(2)
C(13)	33(2)	48(3)	41(2)	8(2)	2(2)	-8(2)
C(14)	32(2)	31(2)	39(2)	3(2)	-4(2)	-6(2)
C(15)	47(3)	45(3)	62(3)	7(2)	-7(2)	4(2)
C(16)	50(3)	42(3)	55(3)	5(2)	2(2)	-9(2)
Zr(2)	40(1)	37(1)	33(1)	4(1)	-2(1)	-8(1)
Cl(3)	53(1)	71(1)	46(1)	4(1)	11(1)	-11(1)
Cl(4)	106(1)	47(1)	66(1)	-10(1)	-4(1)	-21(1)
C(17)	37(3)	36(3)	35(2)	5(2)	4(2)	-7(2)
C(18)	44(3)	49(3)	35(2)	10(2)	0(2)	-9(2)
C(19)	45(3)	68(4)	38(3)	16(2)	-7(2)	-17(3)
C(21)	50(3)	36(3)	52(3)	16(2)	1(2)	1(2)
C(20)	36(3)	68(4)	52(3)	23(3)	-5(2)	-4(3)
C(22)	63(3)	72(4)	41(3)	-6(2)	7(2)	-17(3)
C(23)	64(4)	50(3)	83(4)	6(3)	12(3)	9(3)
C(24)	38(3)	42(3)	40(2)	-2(2)	6(2)	-10(2)
C(25)	59(3)	59(3)	61(3)	-1(3)	3(2)	-24(3)
C(26)	33(3)	50(3)	38(2)	-1(2)	-7(2)	-4(2)
C(27)	39(3)	51(3)	41(3)	1(2)	-7(2)	-4(2)
C(28)	58(3)	66(4)	40(3)	13(2)	-8(2)	-12(3)
C(29)	65(4)	43(3)	65(3)	19(3)	-18(3)	-1(3)

C(30)	46(3)	45(3)	51(3)	4(2)	-10(2)	0(2)
C(31)	65(3)	82(4)	43(3)	-11(3)	7(2)	-11(3)
C(32)	68(4)	71(4)	85(4)	-18(3)	8(3)	23(3)

Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{Å}^2 \times 10^3$).

	x	y	z	U(eq)
H(3)	2335	13296	-2241	53
H(4)	2574	10688	-1863	58
H(6A)	3274	16165	-1200	71
H(6B)	2502	15956	-1588	71
H(6C)	3268	16039	-1962	71
H(7A)	3913	10376	-453	100
H(7B)	3674	9382	-1056	100
H(7C)	3064	9863	-552	100
H(8)	4216	14822	-683	52
H(9A)	4422	12060	-20	76
H(9B)	4132	13581	276	76
H(9C)	4988	13409	89	76
H(12)	5760	11548	-2293	48
H(13)	5493	14161	-2653	49
H(15A)	5156	9809	-1256	77
H(15B)	5154	10756	-610	77
H(15C)	5915	10517	-980	77
H(16A)	5314	16710	-1730	73
H(16B)	4524	16452	-1410	73
H(16C)	4584	16462	-2171	73
H(19)	2890	6478	2260	60
H(20)	3422	4791	1446	62
H(22A)	788	6294	2338	88
H(22B)	1385	7605	2398	88
H(22C)	1450	6203	2863	88
H(23A)	2691	3342	330	98

H(23B)	1998	2423	587	98
H(23C)	2809	2199	907	98
H(24)	460	4997	1452	60
H(25A)	8	3169	746	89
H(25B)	524	2403	1286	89
H(25C)	839	2669	587	89
H(28)	1670	7542	-570	66
H(29)	1122	9303	219	70
H(31A)	1190	4625	-861	95
H(31B)	1221	3543	-257	95
H(31C)	1966	4329	-490	95
H(32A)	572	8750	1534	112
H(32B)	29	7347	1506	112
H(32C)	-129	8731	1046	112
