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Pentacarbonyl-2 κ^5 C-chlorido-1 κ Cl-bis-[1(η^5)-cyclopentadienyl][μ_2 -oxido-(methyl)methylene-1:2 κ^2 O:C]-tungsten(0)zirconium(IV)

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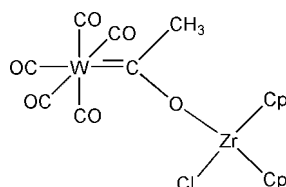
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Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.015$ Å; R factor = 0.032; wR factor = 0.093; data-to-parameter ratio = 14.1.

The title compound, $[\text{ZrW}(\text{C}_5\text{H}_5)_2(\text{C}_2\text{H}_3\text{O})\text{Cl}(\text{CO})_5]$ or $[\text{W}(\text{CO})_5\text{C}(\text{CH}_3)\text{OZr}(\text{C}_5\text{H}_5)_2\text{Cl}]$, consists of two metal centres, with a (tungsten pentacarbonyl)oxymethylcarbene group coordinating as a monodentate ligand to the chloridozirconocene. The two halves of the molecule are related by a crystallographic mirror plane. Delocalization through the $\text{Zr}-\text{O}-\text{C}=\text{W}$ unit is indicated by a short $\text{Zr}-\text{O}$ distance and a nearly linear $\text{Zr}-\text{O}-\text{C}$ angle.

Related literature

For related literature regarding catalytic data of the title compound, see: Sinn *et al.* (1980); Brüll *et al.* (2001); Luruli *et al.* (2004, 2006). For comparable structures, see: Erker *et al.* (1989); Wolczanski *et al.* (1983); Esterhuysen *et al.* (2008). For a description of the Cambridge Structural Database, see: Allen (2002).



Experimental

Crystal data

$[\text{ZrW}(\text{C}_5\text{H}_5)_2(\text{C}_2\text{H}_3\text{O})\text{Cl}(\text{CO})_5]$ $M_r = 623.79$

Orthorhombic, $Pnma$
 $a = 22.3794$ (8) Å
 $b = 12.3852$ (7) Å
 $c = 7.2404$ (3) Å
 $V = 2006.85$ (16) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 6.41$ mm⁻¹
 $T = 273$ (2) K
 $0.34 \times 0.31 \times 0.29$ mm

Data collection

Philips PW1100 diffractometer
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 $T_{\min} = 0.219$, $T_{\max} = 0.258$
 (expected range = 0.133–0.156)
 2070 measured reflections

1851 independent reflections
 1521 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.042$
 3 standard reflections
 every 50 reflections
 intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.092$
 $S = 1.08$
 1851 reflections

131 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 1.15$ e Å⁻³
 $\Delta\rho_{\min} = -1.14$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

W1—C4	2.192 (9)	Zr1—O4	2.026 (6)
O4—C4	1.270 (10)		
C4—O4—Zr1	177.4 (7)		

Data collection: *PWPC* (Gomm, 1998); cell refinement: *PWPC*; data reduction: *Xtal3.4* (Hall *et al.*, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001; Atwood & Barbour, 2003); software used to prepare material for publication: *pubCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2260).

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supporting information

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Pentacarbonyl-2 κ^5 C-chlorido-1 κ Cl-bis[1(η^5)-cyclopentadienyl][μ_2 -oxido(methyl)methylene-1:2 κ^2 O:C]tungsten(0)zirconium(IV)

Catharine Esterhuysen, Arno Neveling, Nyambeni Luruli, Gert J. Kruger and Stephanie Cronje

S1. Comment

Homogeneous equivalents of the heterogeneous catalysts used in Ziegler–Natta polymerization of alkenes are of interest in efforts to understand the mechanism of polymerization. Cp₂TiCl₂ (I) has been shown to polymerize ethylene when activated by MAO (Sinn *et al.*, 1980). In our ongoing studies into finding improved catalysts for the oligomerization of α -olefins we have studied zirconocene equivalents to (I) where we replaced one of the Cl ligands with a number of different ligands (Brüll *et al.*, 2001). In particular, the use of a tungsten–carbene moiety as a ligand, (II), has been proven to result in an effective catalyst for the oligomerization of 1-pentene, as well as the copolymerization of ethene and 1-pentene, in the presence of MAO (Luruli *et al.*, 2004; Luruli *et al.*, 2006). Herein we report the crystal structure of the title zirconocene complex, (II).

In the molecular structure the Zr—O distance is shorter than all other zirconocene complexes containing a Zr—O—C(R)=M (where M = any transition metal) group reported to date (Cambridge Structural Database, v. 5.29; Allen, 2002), except when R = H [1.971 (4) Å; Wolczanski *et al.*, 1983]. The Zr—O—C angle, on the other hand, is more linear than the previously published structures, with a larger value than that of the benzoxycarbene W(CO)₅C(C₆H₅)OZr(C₅H₅)₂OC₆H₅ (166.1 (5)°; Erker *et al.*, 1989). This, together with the short [1.27 (1)Å] C(carbene)—O distance, suggests that the bridging group forms an acyl-type structure, W—C(Me)=O, with a typical hard–hard bond involving σ and π -donation from the O-atom to the Zr-fragment. This is similar to the hafnocene complex W(CO)₅C(C₆H₅)OHf(C₅H₅)₂Cl (Esterhuysen *et al.*, 2008), where the Hf—O—C angle is also nearly linear [171.4 (3)°].

No intermolecular interactions are observed in the crystal structure, with the molecules packing in columns parallel to the *a* axis.

S2. Experimental

To a well stirred suspension of W(CO)₆ (8.906 g) in 80 ml diethylether a solution of LiCH₃ (17 ml, 1.6M in diethylether) in 50 ml diethylether was added. After solvent removal, dissolution of the residue in 100 ml cold water and filtration, a solution of Et₄NCl (8.306 g) in 25 ml cold water was added to the filtrate. Upon filtration 1.015 g of the product {[W(CO)₅C(CH₃)O][N(Et₄)]} was dissolved in 30 ml dichloromethane and added to a solution of Cp₂ZrCl₂ (0.585 g) in 70 ml dichloromethane. After stirring for 30 min at -40°C AgBF₄ (0.389 g) was added and stirred for 90 min at -40°C. After reaching room temperature the solvent was removed and the residue extracted in 5 portions of 10 ml toluene. The extract was filtered, and the filtrate dried over anhydrous MgSO₄. The solution was layered with pentane to yield red crystals suitable for X-ray diffraction analysis.

S3. Refinement

H atoms were positioned geometrically, with C—H = 0.95–0.98 Å, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{C})$.

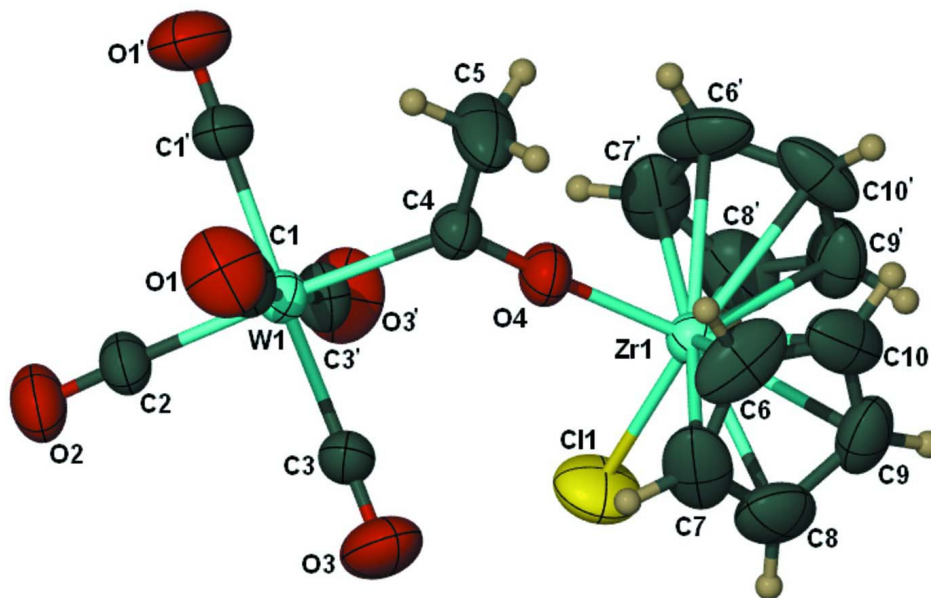


Figure 1

The molecular structure of (II) showing the atomic labelling scheme and displacement ellipsoids drawn at the 50% probability level.

Pentacarbonyl-2 κ^5 C-chlorido-1 κ Cl-bis[1(η^5)-cyclopentadienyl][μ_2 -oxido(methyl)methylene-1:2 κ^2 O:C]tungsten(IV)zirconium(0)

Crystal data

[ZrW(C₅H₅)₂(C₂H₃O)Cl(CO)₅]

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Orthorhombic, *Pnma*

$a = 22.3794$ (8) Å

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$c = 7.2404$ (3) Å

$V = 2006.85$ (16) Å³

$Z = 4$

$F(000) = 1176$

Data collection

Philips PW1100

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega/2\theta$ scans

Absorption correction: ψ scan

(North *et al.*, 1968)

$T_{\text{min}} = 0.219$, $T_{\text{max}} = 0.258$

2070 measured reflections

$D_x = 2.065$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 2\text{--}17^\circ$

$\mu = 6.41$ mm⁻¹

$T = 273$ K

Prism, red

$0.34 \times 0.31 \times 0.29$ mm

1851 independent reflections

1521 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.5^\circ$

$h = 0\text{--}26$

$k = 0\text{--}14$

$l = -8\text{--}0$

3 standard reflections every 50 reflections

intensity decay: none

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H-atom parameters constrained
$wR(F^2) = 0.092$	$w = 1/[\sigma^2(F_o^2) + (0.053P)^2 + 1.7971P]$
$S = 1.08$	where $P = (F_o^2 + 2F_c^2)/3$
1851 reflections	$(\Delta/\sigma)_{\max} = 0.001$
131 parameters	$\Delta\rho_{\max} = 1.15 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\min} = -1.14 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR 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 $F^2 > \sigma(F^2)$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
W1	0.812162 (16)	0.2500	0.32704 (5)	0.04133 (16)	
Cl1	0.60410 (18)	0.2500	0.5194 (4)	0.0896 (10)	
O1	0.8874 (3)	0.0780 (5)	0.1035 (9)	0.092 (2)	
C1	0.8601 (3)	0.1384 (6)	0.1848 (10)	0.0573 (18)	
Zr1	0.59893 (4)	0.2500	0.18263 (11)	0.0388 (2)	
O2	0.9032 (3)	0.2500	0.6604 (11)	0.078 (2)	
C2	0.8712 (4)	0.2500	0.5381 (14)	0.053 (2)	
O3	0.7386 (3)	0.0625 (5)	0.5187 (10)	0.094 (2)	
C3	0.7643 (3)	0.1307 (6)	0.4506 (10)	0.0529 (17)	
O4	0.6885 (3)	0.2500	0.1422 (10)	0.0535 (17)	
C4	0.7442 (4)	0.2500	0.1090 (13)	0.045 (2)	
C5	0.7572 (6)	0.2500	-0.0914 (16)	0.089 (5)	
H5A	0.8006	0.2500	-0.1105	0.134*	
H5B	0.7399	0.3146	-0.1482	0.134*	0.50
H5C	0.7399	0.1854	-0.1482	0.134*	0.50
C6	0.6081 (5)	0.0817 (7)	-0.0048 (16)	0.088 (3)	
H6	0.6406	0.0757	-0.0886	0.106*	
C7	0.6081 (5)	0.0484 (6)	0.1785 (16)	0.085 (3)	
H7	0.6407	0.0169	0.2432	0.102*	
C8	0.5524 (5)	0.0696 (8)	0.2486 (16)	0.083 (3)	
H8	0.5392	0.0535	0.3703	0.100*	
C9	0.5185 (4)	0.1185 (7)	0.1117 (15)	0.074 (2)	
H9	0.4785	0.1430	0.1246	0.088*	
C10	0.5523 (5)	0.1253 (7)	-0.0444 (13)	0.079 (3)	
H11	0.5399	0.1546	-0.1595	0.095*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
W1	0.0383 (2)	0.0444 (2)	0.0413 (2)	0.000	0.00042 (16)	0.000
Cl1	0.118 (3)	0.107 (2)	0.0435 (15)	0.000	0.0088 (17)	0.000
O1	0.099 (4)	0.091 (4)	0.087 (4)	0.026 (4)	0.009 (4)	-0.027 (4)
C1	0.059 (4)	0.058 (4)	0.055 (4)	0.010 (4)	-0.003 (3)	-0.011 (4)
Zr1	0.0376 (5)	0.0378 (5)	0.0408 (5)	0.000	0.0006 (4)	0.000
O2	0.056 (5)	0.109 (7)	0.068 (5)	0.000	-0.016 (4)	0.000
C2	0.044 (5)	0.069 (6)	0.047 (5)	0.000	-0.007 (5)	0.000
O3	0.089 (4)	0.083 (4)	0.111 (5)	-0.019 (4)	0.009 (4)	0.034 (4)
C3	0.051 (4)	0.050 (4)	0.057 (4)	-0.006 (3)	-0.007 (3)	0.014 (3)
O4	0.039 (4)	0.066 (5)	0.055 (4)	0.000	-0.002 (3)	0.000
C4	0.037 (5)	0.050 (5)	0.046 (5)	0.000	0.000 (4)	0.000
C5	0.061 (7)	0.162 (14)	0.045 (6)	0.000	0.000 (6)	0.000
C6	0.096 (7)	0.052 (5)	0.117 (8)	-0.019 (5)	0.039 (7)	-0.040 (6)
C7	0.092 (7)	0.033 (4)	0.130 (10)	0.004 (4)	-0.036 (7)	0.004 (5)
C8	0.104 (7)	0.055 (5)	0.091 (6)	-0.026 (5)	-0.002 (7)	0.015 (5)
C9	0.051 (4)	0.058 (5)	0.112 (7)	-0.013 (4)	-0.013 (5)	-0.002 (5)
C10	0.123 (8)	0.050 (5)	0.062 (5)	-0.031 (5)	-0.027 (6)	0.000 (4)

Geometric parameters (\AA , $^\circ$)

W1—C2	2.019 (10)	Zr1—C8	2.511 (9)
W1—C1 ⁱ	2.030 (8)	O2—C2	1.139 (11)
W1—C1	2.030 (7)	O3—C3	1.134 (8)
W1—C3 ⁱ	2.033 (7)	O4—C4	1.270 (10)
W1—C3	2.033 (7)	C4—C5	1.480 (14)
W1—C4	2.192 (9)	C5—H5A	0.9800
Cl1—Zr1	2.441 (3)	C5—H5B	0.9800
O1—C1	1.131 (9)	C5—H5C	0.9800
Zr1—O4	2.026 (6)	C6—C7	1.390 (13)
Zr1—C9	2.482 (8)	C6—C10	1.391 (13)
Zr1—C9 ⁱ	2.482 (8)	C6—H6	0.9500
Zr1—C10	2.485 (8)	C7—C8	1.373 (13)
Zr1—C10 ⁱ	2.485 (8)	C7—H7	0.9500
Zr1—C6	2.496 (8)	C8—C9	1.387 (13)
Zr1—C6 ⁱ	2.496 (8)	C8—H8	0.9500
Zr1—C7 ⁱ	2.506 (8)	C9—C10	1.362 (12)
Zr1—C7	2.506 (8)	C9—H9	0.9500
Zr1—C8 ⁱ	2.511 (9)	C10—H11	0.9500
C2—W1—C1 ⁱ	92.2 (3)	Cl1—Zr1—C8 ⁱ	80.2 (3)
C2—W1—C1	92.2 (3)	C9—Zr1—C8 ⁱ	108.8 (3)
C1 ⁱ —W1—C1	85.8 (5)	C9 ⁱ —Zr1—C8 ⁱ	32.3 (3)
C2—W1—C3 ⁱ	90.7 (3)	C10—Zr1—C8 ⁱ	120.3 (3)
C1 ⁱ —W1—C3 ⁱ	90.4 (3)	C10 ⁱ —Zr1—C8 ⁱ	53.0 (3)
C1—W1—C3 ⁱ	175.3 (3)	C6—Zr1—C8 ⁱ	151.7 (4)

C2—W1—C3	90.7 (3)	C6 ⁱ —Zr1—C8 ⁱ	52.7 (3)
C1 ⁱ —W1—C3	175.3 (3)	C7 ⁱ —Zr1—C8 ⁱ	31.8 (3)
C1—W1—C3	90.4 (3)	C7—Zr1—C8 ⁱ	157.4 (5)
C3 ⁱ —W1—C3	93.2 (4)	O4—Zr1—C8	116.0 (3)
C2—W1—C4	176.9 (4)	Cl1—Zr1—C8	80.2 (3)
C1 ⁱ —W1—C4	90.1 (3)	C9—Zr1—C8	32.3 (3)
C1—W1—C4	90.1 (3)	C9 ⁱ —Zr1—C8	108.8 (3)
C3 ⁱ —W1—C4	87.2 (3)	C10—Zr1—C8	53.0 (3)
C3—W1—C4	87.2 (3)	C10 ⁱ —Zr1—C8	120.3 (3)
O1—C1—W1	178.5 (8)	C6—Zr1—C8	52.7 (3)
O4—Zr1—Cl1	95.6 (2)	C6 ⁱ —Zr1—C8	151.7 (4)
O4—Zr1—C9	133.5 (2)	C7 ⁱ —Zr1—C8	157.4 (5)
Cl1—Zr1—C9	104.0 (3)	C7—Zr1—C8	31.8 (3)
O4—Zr1—C9 ⁱ	133.5 (2)	C8 ⁱ —Zr1—C8	125.7 (5)
Cl1—Zr1—C9 ⁱ	104.0 (3)	O2—C2—W1	178.1 (9)
C9—Zr1—C9 ⁱ	82.1 (4)	O3—C3—W1	178.4 (7)
O4—Zr1—C10	108.7 (3)	C4—O4—Zr1	177.4 (7)
Cl1—Zr1—C10	132.9 (2)	O4—C4—C5	112.3 (9)
C9—Zr1—C10	31.8 (3)	O4—C4—W1	123.0 (7)
C9 ⁱ —Zr1—C10	88.1 (3)	C5—C4—W1	124.7 (7)
O4—Zr1—C10 ⁱ	108.7 (3)	C4—C5—H5A	109.5
Cl1—Zr1—C10 ⁱ	132.9 (2)	C4—C5—H5B	109.5
C9—Zr1—C10 ⁱ	88.1 (3)	H5A—C5—H5B	109.5
C9 ⁱ —Zr1—C10 ⁱ	31.8 (3)	C4—C5—H5C	109.5
C10—Zr1—C10 ⁱ	76.8 (4)	H5A—C5—H5C	109.5
O4—Zr1—C6	80.8 (3)	H5B—C5—H5C	109.5
Cl1—Zr1—C6	122.6 (3)	C7—C6—C10	108.2 (9)
C9—Zr1—C6	53.0 (3)	C7—C6—Zr1	74.2 (5)
C9 ⁱ —Zr1—C6	119.7 (4)	C10—C6—Zr1	73.4 (5)
C10—Zr1—C6	32.4 (3)	C7—C6—H6	125.9
C10 ⁱ —Zr1—C6	101.2 (4)	C10—C6—H6	125.9
O4—Zr1—C6 ⁱ	80.8 (3)	Zr1—C6—H6	118.4
Cl1—Zr1—C6 ⁱ	122.6 (3)	C8—C7—C6	107.2 (9)
C9—Zr1—C6 ⁱ	119.7 (4)	C8—C7—Zr1	74.3 (5)
C9 ⁱ —Zr1—C6 ⁱ	53.0 (3)	C6—C7—Zr1	73.5 (5)
C10—Zr1—C6 ⁱ	101.2 (4)	C8—C7—H7	126.4
C10 ⁱ —Zr1—C6 ⁱ	32.4 (3)	C6—C7—H7	126.4
C6—Zr1—C6 ⁱ	113.3 (6)	Zr1—C7—H7	117.8
O4—Zr1—C7 ⁱ	85.2 (3)	C7—C8—C9	108.4 (10)
Cl1—Zr1—C7 ⁱ	90.5 (3)	C7—C8—Zr1	73.9 (5)
C9—Zr1—C7 ⁱ	135.4 (3)	C9—C8—Zr1	72.7 (5)
C9 ⁱ —Zr1—C7 ⁱ	53.4 (3)	C7—C8—H8	125.8
C10—Zr1—C7 ⁱ	130.2 (3)	C9—C8—H8	125.8
C10 ⁱ —Zr1—C7 ⁱ	53.7 (3)	Zr1—C8—H8	119.4
C6—Zr1—C7 ⁱ	145.0 (5)	C10—C9—C8	108.4 (9)
C6 ⁱ —Zr1—C7 ⁱ	32.3 (3)	C10—C9—Zr1	74.2 (5)
O4—Zr1—C7	85.2 (3)	C8—C9—Zr1	75.0 (5)
Cl1—Zr1—C7	90.5 (3)	C10—C9—H9	125.8

C9—Zr1—C7	53.4 (3)	C8—C9—H9	125.8
C9 ⁱ —Zr1—C7	135.4 (3)	Zr1—C9—H9	116.9
C10—Zr1—C7	53.7 (3)	C9—C10—C6	107.7 (8)
C10 ⁱ —Zr1—C7	130.2 (3)	C9—C10—Zr1	73.9 (5)
C6—Zr1—C7	32.3 (3)	C6—C10—Zr1	74.2 (5)
C6 ⁱ —Zr1—C7	145.0 (5)	C9—C10—H11	126.2
C7 ⁱ —Zr1—C7	170.5 (6)	C6—C10—H11	126.2
O4—Zr1—C8 ⁱ	116.0 (3)	Zr1—C10—H11	117.7

Symmetry code: (i) $x, -y+1/2, z$.