Pentacarbonyl-2κ⁵C-chlorido-1κCl-bis[1(η⁵)-cyclopentadienyl](μ-1-oxido-ethylene-1:2κ²O:C)chromium(0)-zirconium(IV)

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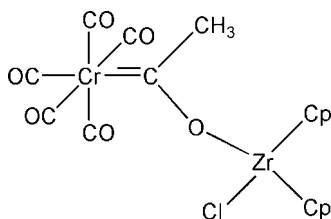
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The title compound, $[CrZr(C_5H_5)_2(C_2H_3O)Cl(CO)_5]$, consists of two metal centres, with a (pentacarbonylchromium)-oxymethylcarbene group coordinating as a monodentate ligand to the zirconocene chloride. π-Delocalization through the Zr—O—C=Cr unit is indicated by a short Zr—O distance [2.041 (3) Å] and a nearly linear Zr—O—C angle [170.5 (3)°]. Molecules are aligned with their molecular planes (through Zr, Cl, carbene and Cr) parallel to the ab plane. C—H···Cl interactions result in zigzag chains of molecules propagating parallel to the b axis.

Related literature

For related literature regarding catalytic data of the title compound, see: Sinn *et al.* (1980); Luruli *et al.* (2004, 2006). For other cases of anionic Fischer-type carbenes being used as monodentate ligands, see: Barluenga & Fañanás (2000). For comparable structures, see: Esterhuysen, Nel & Cronje (2008); Esterhuysen, Neveling *et al.* (2008).

Experimental

Crystal data

$[CrZr(C_5H_5)_2(C_2H_3O)Cl(CO)_5]$	V = 1937.71 (18) Å³
M_r = 491.94	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 12.7395 (7) Å	μ = 1.27 mm⁻¹
b = 12.1117 (6) Å	T = 173 (2) K
c = 12.7859 (7) Å	0.30 × 0.28 × 0.08 mm
β = 100.826 (5)°	

Data collection

Philips PW1100 diffractometer	3423 independent reflections
Absorption correction: ψ scan	2332 reflections with $I > 2\sigma(I)$
(North *et al.*, 1968)	3 standard reflections
T_{min} = 0.68, T_{max} = 0.88	every 50 reflections
3423 measured reflections	intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039	235 parameters
$wR(F^2)$ = 0.109	H-atom parameters constrained
S = 1.06	$\Delta\rho_{max}$ = 0.55 e Å⁻³
3423 reflections	$\Delta\rho_{min}$ = −0.58 e Å⁻³

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···Cl1[i]	0.95	2.74	3.581 (8)	149

Symmetry code: (i) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$.

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: *publCIF* (Westrip, 2009).

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supporting information

Pentacarbonyl-2κ⁵*C*-chlorido-1κ*Cl*-bis[1(η⁵)-cyclopentadienyl](μ-1-oxidoethylene-1:2κ²*O*:*C*)chromium(0)zirconium(IV)

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S1. Comment

Since Cp_2TiCl_2 was shown to polymerize ethylene when activated by methylaluminoxane, MAO (Sinn *et al.*, 1980), derivatives of this compound have been synthesized where a Cl ligand was replaced by a monodentate anionic Fischer-type carbene ligand (Barluenga and Fañanás, 2000). We have shown that zirconocene equivalents of this family of homogeneous catalysts, $Cp_2Zr(Cl)OC(R)M(CO)_5$ (where M = W or Cr), catalyze 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, (I).

In the molecular structure the Zr—O and O—C distances are similar to those found in the equivalent tungsten penta-carbonyl complex (Esterhuysen, Nel & Cronje, 2008). The Zr—O—C angle, on the other hand, is less linear than the previously published tungsten structure [177.4 (7)°], but similar to the hafnocene complex $W(CO)_5C(C_6H_5)OHf(C_5H_5)_2Cl$ (Esterhuysen, Neveling *et al.*, 2008), where the Hf—O—C angle deviates slightly more from linearity [171.4 (3)°]. These results are indicative of π delocalization through the Zr—O—C = W unit.

Molecules are linked by C—H···Cl interactions into zigzag chains along the *b* axis. All molecules in a chain point in the same direction, with their molecular planes parallel. Neighbouring chains in the a-direction have the same orientation, thus forming a layer parallel to the *ab*-plane. Molecules in neighbouring layers in the c-direction have alternating orientations.

S2. Experimental

A solution of $LiCH_3$ (11 ml, 1.5*M* in diethylether, 16.5 mmol) in 10 ml diethylether was added to a well stirred suspension of $Cr(CO)_6$ (3.30 g, 15.0 mmol) in 100 ml of diethylether over the period of 1.5 h. The mixture was stripped of solvent *in vacuo*. The residue was dried for 3 h, extracted with cold (273 K), degassed water (1 × 40 ml, 2 × 20 ml) and the formed solution filtered. The aqueous solution was treated with a solution of $[NEt_4]Cl$ (2.49 g, 15 mmol) in cold, degassed water (4 ml) and the formed precipitate was isolated and dried overnight *in vacuo*. The precipitate was dissolved in warm CH_2Cl_2 (5 ml) layered with penatne and cooled to 258 K to yield yellow crystals of $(CO)_5Cr\{=C(Me)O\}[NEt_4]$. A solution of 0.61 g (2.0 mmol) of the product in 30 ml of CH_2Cl_2 was added to a solution of Cp_2ZrCl_2 (0.58 g, 2.0 mmol) in 70 ml of diethylether at 233 K over a period of 40 min. $AgBF_4$ (0.39 g, 2.0 mmol) was then added to the mixture and stirred for an hour at 233 K. After reaching room temperature the solvent was removed in vacuo and the residue extracted in 5 portions of 10 ml of toluene. The extract was filtered, and the filtrate dried over anhydrous $MgSO_4$. The solution was layered with pentane and kept at 258 K to yield orange crystals suitable for X-ray diffraction analysis.

S3. Refinement

H atoms were positioned geometrically, with C—H = 0.95 Å and 0.98 Å, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$. Large anisotropy on atoms C16 and C17 suggests the presence of disorder in the C13–C17 Cp ring, however this could not be modeled. Highest peak: 1.03 Å from Zr1; deepest hole: 1.04 Å from Zr1.
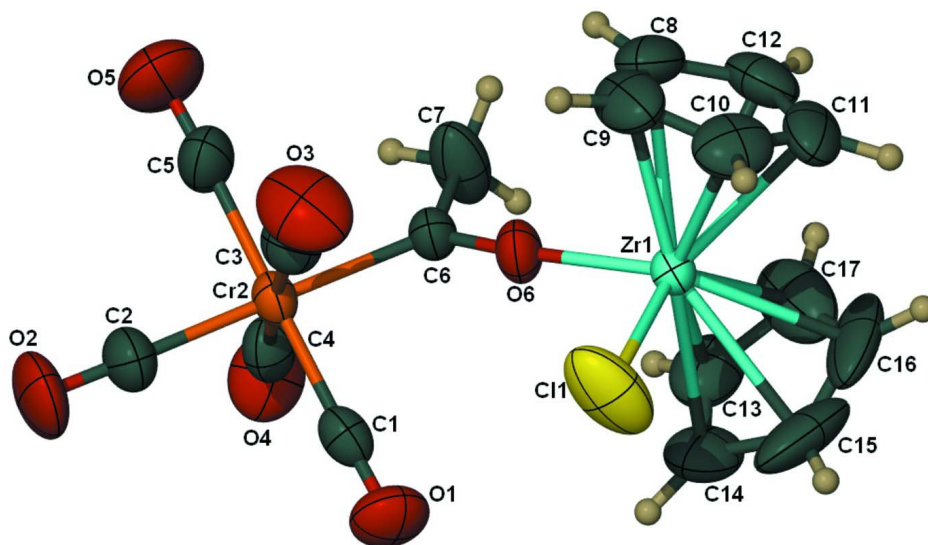

Figure 1

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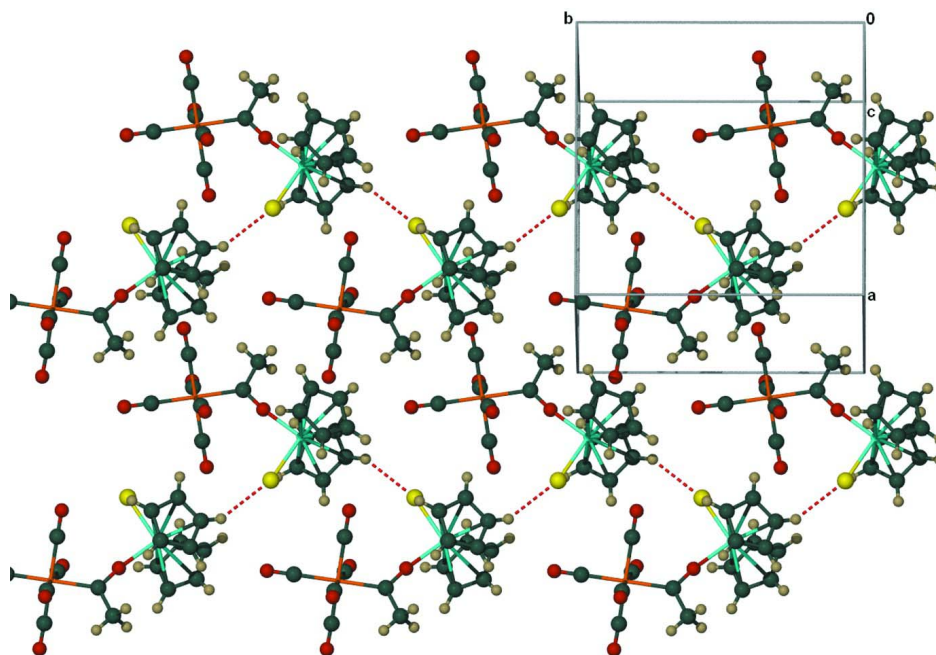

Figure 2

A portion of the packing diagram showing zigzag chains of molecules forming a layer perpendicular to the *c* axis.

Pentacarbonyl-2κ^5C-chlorido-1κCl-bis[1(η^5)-cyclopentadienyl](μ-1-oxidoethylene-1:2κ^2O:C)chromiumzirconium

Crystal data

[CrZr(C$_5$H$_5$)$_2$(C$_2$H$_3$O)Cl(CO)$_5$]	$F(000) = 976$
$M_r = 491.94$	$D_x = 1.686$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 48 reflections
$a = 12.7395$ (7) Å	$\theta = 2$–17°
$b = 12.1117$ (6) Å	$\mu = 1.27$ mm^{-1}
$c = 12.7859$ (7) Å	$T = 173$ K
$\beta = 100.826$ (5)°	Plate, orange
$V = 1937.71$ (18) Å^3	$0.30 \times 0.28 \times 0.08$ mm
$Z = 4$	

Data collection

Philips PW1100 diffractometer	3423 independent reflections
Radiation source: fine-focus sealed tube	2332 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.000$
ω–2θ scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.3°$
Absorption correction: ψ scan (North *et al.*, 1968)	$h = -15 \rightarrow 14$
	$k = 0 \rightarrow 14$
	$l = 0 \rightarrow 15$
$T_{min} = 0.68$, $T_{max} = 0.88$	3 standard reflections every 50 reflections
3423 measured reflections	intensity decay: none

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.039$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.109$	
$S = 1.06$	H-atom parameters constrained
3423 reflections	$w = 1/[\sigma^2(F_o^2) + (0.053P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
235 parameters	
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.55$ e Å^{-3}
	$\Delta\rho_{min} = -0.58$ e Å^{-3}

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Zr1	0.67690 (3)	0.45977 (3)	0.79870 (3)	0.03838 (16)
Cr2	0.82371 (6)	0.82936 (6)	0.79664 (6)	0.0441 (2)

Cl1	0.51592 (14)	0.56328 (16)	0.80604 (18)	0.1054 (7)
O1	0.6062 (3)	0.7896 (4)	0.6561 (3)	0.0785 (12)
O2	0.7878 (4)	1.0760 (3)	0.7936 (4)	0.1005 (16)
O3	0.7167 (4)	0.7914 (4)	0.9852 (4)	0.1065 (17)
O4	0.9358 (4)	0.8437 (4)	0.6086 (4)	0.0886 (14)
O5	1.0309 (4)	0.8682 (5)	0.9517 (4)	0.1162 (19)
O6	0.7769 (3)	0.5916 (3)	0.8006 (3)	0.0532 (9)
C1	0.6880 (4)	0.8052 (4)	0.7069 (4)	0.0492 (12)
C2	0.8007 (5)	0.9823 (5)	0.7944 (4)	0.0631 (15)
C3	0.7572 (5)	0.8072 (5)	0.9152 (5)	0.0627 (15)
C4	0.8933 (4)	0.8394 (4)	0.6786 (5)	0.0566 (13)
C5	0.9534 (5)	0.8515 (5)	0.8931 (5)	0.0689 (16)
C6	0.8496 (4)	0.6625 (4)	0.7962 (4)	0.0449 (11)
C7	0.9547 (4)	0.6101 (5)	0.7899 (6)	0.086 (2)
H7A	1.0080	0.6678	0.7871	0.129*
H7B	0.9469	0.5645	0.7256	0.129*
H7C	0.9780	0.5639	0.8528	0.129*
C8	0.8066 (5)	0.4232 (6)	0.9667 (5)	0.0733 (18)
H8	0.8737	0.4599	0.9772	0.088*
C9	0.7144 (6)	0.4611 (5)	0.9977 (4)	0.0769 (19)
H9	0.7065	0.5287	1.0332	0.092*
C10	0.6349 (5)	0.3814 (6)	0.9672 (4)	0.0758 (18)
H10	0.5635	0.3850	0.9787	0.091*
C11	0.6779 (6)	0.2982 (5)	0.9184 (5)	0.0762 (19)
H11	0.6414	0.2335	0.8893	0.091*
C12	0.7831 (6)	0.3228 (5)	0.9179 (5)	0.0711 (17)
H12	0.8315	0.2779	0.8887	0.085*
C13	0.7269 (6)	0.4442 (6)	0.6179 (5)	0.081 (2)
H13	0.7843	0.4867	0.6012	0.097*
C14	0.6228 (6)	0.4758 (6)	0.6006 (5)	0.084 (2)
H14	0.5943	0.5445	0.5727	0.100*
C15	0.5653 (7)	0.3857 (10)	0.6326 (6)	0.119 (3)
H15	0.4901	0.3814	0.6282	0.142*
C16	0.6386 (11)	0.3060 (7)	0.6711 (6)	0.124 (4)
H16	0.6228	0.2365	0.6989	0.149*
C17	0.7361 (9)	0.3420 (7)	0.6632 (5)	0.106 (3)
H17	0.8011	0.3027	0.6854	0.127*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zr1	0.0412 (3)	0.0306 (2)	0.0410 (3)	−0.0002 (2)	0.00175 (18)	0.0023 (2)
Cr2	0.0464 (5)	0.0299 (4)	0.0544 (5)	0.0011 (3)	0.0054 (4)	0.0004 (3)
Cl1	0.0717 (11)	0.0871 (13)	0.1666 (19)	0.0361 (10)	0.0464 (12)	0.0408 (12)
O1	0.048 (2)	0.097 (3)	0.084 (3)	0.002 (2)	−0.005 (2)	0.002 (2)
O2	0.121 (4)	0.035 (2)	0.140 (4)	0.013 (2)	0.013 (3)	−0.005 (2)
O3	0.134 (5)	0.122 (4)	0.076 (3)	0.023 (4)	0.053 (3)	0.009 (3)
O4	0.086 (3)	0.096 (3)	0.094 (3)	−0.016 (3)	0.042 (3)	−0.007 (3)

O5	0.077 (3)	0.118 (4)	0.132 (4)	−0.015 (3)	−0.033 (3)	−0.002 (4)
O6	0.052 (2)	0.0333 (18)	0.073 (2)	−0.0062 (16)	0.0079 (17)	−0.0001 (16)
C1	0.058 (3)	0.039 (3)	0.054 (3)	0.008 (2)	0.018 (3)	0.005 (2)
C2	0.074 (4)	0.041 (3)	0.071 (4)	0.004 (3)	0.007 (3)	−0.003 (3)
C3	0.076 (4)	0.055 (3)	0.057 (3)	0.008 (3)	0.010 (3)	−0.005 (3)
C4	0.054 (3)	0.045 (3)	0.071 (4)	−0.008 (3)	0.014 (3)	0.000 (3)
C5	0.061 (4)	0.052 (3)	0.088 (4)	−0.007 (3)	−0.002 (3)	−0.003 (3)
C6	0.044 (3)	0.036 (3)	0.052 (3)	0.000 (2)	0.003 (2)	0.002 (2)
C7	0.048 (3)	0.049 (3)	0.160 (7)	0.008 (3)	0.016 (4)	0.004 (4)
C8	0.073 (4)	0.076 (4)	0.058 (4)	−0.007 (4)	−0.020 (3)	0.016 (3)
C9	0.115 (6)	0.071 (4)	0.041 (3)	0.015 (4)	0.004 (3)	−0.011 (3)
C10	0.083 (5)	0.099 (5)	0.047 (3)	−0.006 (4)	0.019 (3)	0.015 (3)
C11	0.124 (6)	0.049 (3)	0.050 (4)	−0.013 (4)	0.002 (4)	0.014 (3)
C12	0.084 (5)	0.065 (4)	0.061 (4)	0.026 (4)	0.005 (3)	0.020 (3)
C13	0.104 (6)	0.093 (5)	0.048 (3)	−0.021 (4)	0.019 (4)	−0.003 (3)
C14	0.100 (5)	0.094 (5)	0.048 (3)	−0.010 (5)	−0.007 (3)	0.023 (3)
C15	0.104 (6)	0.185 (10)	0.053 (4)	−0.072 (7)	−0.021 (4)	−0.008 (5)
C16	0.232 (12)	0.088 (6)	0.047 (4)	−0.088 (8)	0.009 (6)	−0.022 (4)
C17	0.188 (10)	0.076 (5)	0.058 (4)	0.042 (6)	0.032 (5)	−0.012 (4)

Geometric parameters (Å, º)

Zr1—O6	2.041 (3)	C6—C7	1.498 (7)
Zr1—Cl1	2.4205 (16)	C7—H7A	0.9800
Zr1—C16	2.463 (7)	C7—H7B	0.9800
Zr1—C17	2.470 (6)	C7—H7C	0.9800
Zr1—C12	2.476 (5)	C8—C12	1.373 (8)
Zr1—C11	2.483 (5)	C8—C9	1.387 (9)
Zr1—C15	2.490 (6)	C8—H8	0.9500
Zr1—C8	2.492 (5)	C9—C10	1.400 (9)
Zr1—C9	2.500 (5)	C9—H9	0.9500
Zr1—C10	2.503 (5)	C10—C11	1.354 (9)
Zr1—C14	2.504 (6)	C10—H10	0.9500
Zr1—C13	2.517 (6)	C11—C12	1.374 (9)
Cr2—C2	1.875 (6)	C11—H11	0.9500
Cr2—C5	1.885 (6)	C12—H12	0.9500
Cr2—C3	1.889 (6)	C13—C14	1.358 (9)
Cr2—C4	1.892 (6)	C13—C17	1.362 (9)
Cr2—C1	1.910 (6)	C13—H13	0.9500
Cr2—C6	2.048 (5)	C14—C15	1.417 (10)
O1—C1	1.135 (6)	C14—H14	0.9500
O2—C2	1.146 (6)	C15—C16	1.368 (13)
O3—C3	1.130 (6)	C15—H15	0.9500
O4—C4	1.131 (6)	C16—C17	1.338 (12)
O5—C5	1.141 (7)	C16—H16	0.9500
O6—C6	1.271 (5)	C17—H17	0.9500
O6—Zr1—Cl1	97.24 (10)	C3—Cr2—C6	87.6 (2)

O6—Zr1—C16	130.2 (3)	C4—Cr2—C6	87.8 (2)
Cl1—Zr1—C16	110.7 (3)	C1—Cr2—C6	88.58 (19)
O6—Zr1—C17	100.8 (3)	C6—O6—Zr1	170.5 (3)
Cl1—Zr1—C17	134.4 (2)	O1—C1—Cr2	178.0 (5)
C16—Zr1—C17	31.5 (3)	O2—C2—Cr2	179.2 (6)
O6—Zr1—C12	104.4 (2)	O3—C3—Cr2	178.3 (6)
Cl1—Zr1—C12	133.79 (17)	O4—C4—Cr2	178.7 (5)
C16—Zr1—C12	85.4 (3)	O5—C5—Cr2	177.9 (6)
C17—Zr1—C12	80.9 (2)	O6—C6—C7	112.5 (4)
O6—Zr1—C11	132.73 (19)	O6—C6—Cr2	123.2 (3)
Cl1—Zr1—C11	106.9 (2)	C7—C6—Cr2	124.3 (4)
C16—Zr1—C11	77.9 (3)	C6—C7—H7A	109.5
C17—Zr1—C11	90.6 (3)	C6—C7—H7B	109.5
C12—Zr1—C11	32.2 (2)	H7A—C7—H7B	109.5
O6—Zr1—C15	123.2 (2)	C6—C7—H7C	109.5
Cl1—Zr1—C15	82.4 (3)	H7A—C7—H7C	109.5
C16—Zr1—C15	32.1 (3)	H7B—C7—H7C	109.5
C17—Zr1—C15	52.7 (3)	C12—C8—C9	107.3 (6)
C12—Zr1—C15	116.3 (3)	C12—C8—Zr1	73.3 (3)
C11—Zr1—C15	100.2 (3)	C9—C8—Zr1	74.2 (3)
O6—Zr1—C8	79.46 (18)	C12—C8—H8	126.3
Cl1—Zr1—C8	119.22 (18)	C9—C8—H8	126.3
C16—Zr1—C8	117.0 (3)	Zr1—C8—H8	118.2
C17—Zr1—C8	105.2 (3)	C8—C9—C10	107.4 (6)
C12—Zr1—C8	32.1 (2)	C8—C9—Zr1	73.5 (3)
C11—Zr1—C8	53.3 (2)	C10—C9—Zr1	73.9 (3)
C15—Zr1—C8	148.3 (3)	C8—C9—H9	126.3
O6—Zr1—C9	89.1 (2)	C10—C9—H9	126.3
Cl1—Zr1—C9	87.62 (17)	Zr1—C9—H9	118.3
C16—Zr1—C9	130.9 (3)	C11—C10—C9	107.9 (6)
C17—Zr1—C9	133.9 (2)	C11—C10—Zr1	73.4 (3)
C12—Zr1—C9	53.1 (2)	C9—C10—Zr1	73.6 (3)
C11—Zr1—C9	53.1 (2)	C11—C10—H10	126.0
C15—Zr1—C9	147.1 (3)	C9—C10—H10	126.0
C8—Zr1—C9	32.3 (2)	Zr1—C10—H10	118.8
O6—Zr1—C10	121.38 (19)	C10—C11—C12	108.6 (6)
Cl1—Zr1—C10	81.00 (17)	C10—C11—Zr1	75.1 (3)
C16—Zr1—C10	103.6 (3)	C12—C11—Zr1	73.6 (3)
C17—Zr1—C10	121.9 (3)	C10—C11—H11	125.7
C12—Zr1—C10	52.9 (2)	C12—C11—H11	125.7
C11—Zr1—C10	31.5 (2)	Zr1—C11—H11	117.6
C15—Zr1—C10	114.7 (3)	C8—C12—C11	108.7 (6)
C8—Zr1—C10	53.5 (2)	C8—C12—Zr1	74.6 (3)
C9—Zr1—C10	32.5 (2)	C11—C12—Zr1	74.2 (3)
O6—Zr1—C14	90.23 (19)	C8—C12—H12	125.7
Cl1—Zr1—C14	85.7 (2)	C11—C12—H12	125.7
C16—Zr1—C14	53.6 (3)	Zr1—C12—H12	117.5
C17—Zr1—C14	52.9 (3)	C14—C13—C17	109.2 (7)

C12—Zr1—C14	133.6 (2)	C14—C13—Zr1	73.8 (4)
C11—Zr1—C14	130.8 (2)	C17—C13—Zr1	72.2 (4)
C15—Zr1—C14	33.0 (2)	C14—C13—H13	125.4
C8—Zr1—C14	153.9 (3)	C17—C13—H13	125.4
C9—Zr1—C14	173.1 (2)	Zr1—C13—H13	120.3
C10—Zr1—C14	146.9 (2)	C13—C14—C15	106.2 (7)
O6—Zr1—C13	78.71 (18)	C13—C14—Zr1	74.9 (3)
Cl1—Zr1—C13	115.91 (19)	C15—C14—Zr1	73.0 (3)
C16—Zr1—C13	52.3 (3)	C13—C14—H14	126.9
C17—Zr1—C13	31.7 (2)	C15—C14—H14	126.9
C12—Zr1—C13	108.2 (2)	Zr1—C14—H14	117.5
C11—Zr1—C13	122.3 (2)	C16—C15—C14	107.0 (8)
C15—Zr1—C13	52.6 (3)	C16—C15—Zr1	72.9 (4)
C8—Zr1—C13	122.5 (3)	C14—C15—Zr1	74.1 (4)
C9—Zr1—C13	154.5 (3)	C16—C15—H15	126.5
C10—Zr1—C13	153.4 (2)	C14—C15—H15	126.5
C14—Zr1—C13	31.4 (2)	Zr1—C15—H15	118.6
C2—Cr2—C5	89.1 (2)	C17—C16—C15	108.9 (8)
C2—Cr2—C3	93.4 (2)	C17—C16—Zr1	74.5 (4)
C5—Cr2—C3	88.0 (3)	C15—C16—Zr1	75.0 (5)
C2—Cr2—C4	91.1 (2)	C17—C16—H16	125.5
C5—Cr2—C4	91.6 (3)	C15—C16—H16	125.5
C3—Cr2—C4	175.4 (2)	Zr1—C16—H16	116.8
C2—Cr2—C1	91.2 (2)	C16—C17—C13	108.7 (9)
C5—Cr2—C1	176.2 (2)	C16—C17—Zr1	74.0 (5)
C3—Cr2—C1	88.2 (2)	C13—C17—Zr1	76.1 (4)
C4—Cr2—C1	92.2 (2)	C16—C17—H17	125.7
C2—Cr2—C6	178.9 (2)	C13—C17—H17	125.6
C5—Cr2—C6	91.2 (2)	Zr1—C17—H17	116.3

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···Cl1[i]	0.95	2.74	3.581 (8)	149

Symmetry code: (i) −x+1, y−1/2, −z+3/2.