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Crystal structure of bis[(1,2,3,4,5-pentamethylcyclopentadienyl)(1,2-methylene-3,4,5-trimethylcyclopentadiene)zirconium(IV)], C₄₀H₅₆Zr₂

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Crystal structure of bis[(1,2,3,4,5-pentamethylcyclopentadienyl)-(1,2-methylene-3,4,5-trimethylcyclopentadiene)zirconium(IV)], $C_{40}H_{56}Zr_2$

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Table 1. Parameters used for the X-ray data collection

Crystal:	Yellow, plate shaped, size 0.10 x 0.25 x 0.75 mm
Wavelength:	Mo K_{α} radiation (0.71073 Å)
μ :	6.4 cm ⁻¹
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	100K
$2\theta_{\text{max}}$:	50°
$N(hkl)_{\text{unique}}$:	2727
Criterion for I_o :	$I_o > 2.5 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	296
Program:	SHELX

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{iso}
H(61)	2i	0.142(6)	-0.456(5)	0.105(3)	0.02(1)
H(62)	2i	0.265(7)	-0.509(6)	0.097(4)	0.03(1)
H(63)	2i	0.208(5)	-0.454(4)	-0.003(4)	0.016(9)
H(71)	2i	0.128(6)	-0.183(6)	0.010(4)	0.03(1)
H(72)	2i	0.201(6)	-0.021(6)	0.088(4)	0.03(1)
H(73)	2i	0.095(7)	-0.184(6)	0.129(4)	0.04(1)
H(81)	2i	0.7157(5)	0.2715(4)	0.1985(3)	0.07(2)
H(82)	2i	0.4980(5)	0.2002(4)	0.2246(3)	0.09(2)
H(83)	2i	0.5282(5)	0.2234(4)	0.0874(3)	0.10(2)
H(91)	2i	0.900(7)	0.161(7)	0.222(4)	0.04(1)
H(92)	2i	0.919(7)	0.046(6)	0.152(5)	0.04(1)
H(93)	2i	0.924(6)	0.034(5)	0.266(4)	0.03(1)
H(101)	2i	0.762(7)	-0.279(6)	0.095(4)	0.04(1)
H(102)	2i	0.751(6)	-0.312(6)	0.214(4)	0.03(1)
H(103)	2i	0.593(6)	-0.430(5)	0.128(3)	0.02(1)
H(161)	2i	0.200(5)	-0.043(4)	0.379(3)	0.003(8)
H(162)	2i	0.302(5)	0.077(5)	0.299(3)	0.02(1)
H(171)	2i	0.788(6)	0.213(5)	0.382(3)	0.02(1)
H(172)	2i	0.832(6)	0.138(5)	0.482(3)	0.02(1)
H(181)	2i	0.932(7)	0.514(6)	0.714(4)	0.04(1)
H(182)	2i	0.972(9)	0.377(8)	0.648(6)	0.07(2)
H(183)	2i	0.956(9)	0.523(8)	0.597(5)	0.07(2)
H(191)	2i	0.513(6)	0.521(5)	0.738(4)	0.03(1)
H(192)	2i	0.569(6)	0.596(6)	0.637(4)	0.04(1)
H(193)	2i	0.708(6)	0.590(6)	0.744(4)	0.03(1)
H(201)	2i	0.241(7)	0.353(7)	0.556(5)	0.05(2)
H(202)	2i	0.167(9)	0.214(8)	0.460(6)	0.08(2)
H(203)	2i	0.145(8)	0.169(8)	0.552(5)	0.06(2)

Source of material: see ref. 1.

Each Zr is tetrahedrally coordinated by two σ bonds to the methylene carbo atoms and two η -5 bonds to the cyclopentadienyl rings.

$C_{40}H_{56}Zr_2$, triclinic, $P\bar{1}$ (No. 2), $a=8.452(2)$ Å, $b=9.305(2)$ Å, $c=12.238(2)$ Å, $\alpha=97.59(2)^\circ$, $\beta=99.01(2)^\circ$, $\gamma=115.67(2)^\circ$, $V=834.9(3)$ Å³, $Z=1$, $R(F)=0.041$, $R_w(F)=0.054$.

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Zr	2i	0.49141(3)	-0.11175(3)	0.33221(2)	0.0108(2)	0.0080(2)	0.0047(2)	0.0037(1)	0.0020(1)	0.0019(1)
C(1)	2i	0.3887(4)	-0.2647(4)	0.1253(3)	0.018(2)	0.015(2)	0.006(1)	0.007(1)	0.003(1)	0.002(1)
C(2)	2i	0.3637(5)	-0.1241(4)	0.1263(3)	0.021(2)	0.021(2)	0.003(1)	0.011(1)	0.003(1)	0.004(1)
C(3)	2i	0.5370(5)	0.0158(4)	0.1593(3)	0.023(2)	0.016(2)	0.004(1)	0.011(1)	0.007(1)	0.004(1)
C(4)	2i	0.6696(5)	-0.0389(4)	0.1790(3)	0.022(2)	0.018(2)	0.006(1)	0.010(1)	0.008(1)	0.006(1)
C(5)	2i	0.5793(5)	-0.2120(4)	0.1574(3)	0.018(2)	0.014(2)	0.006(1)	0.007(1)	0.004(1)	0.001(1)
C(6)	2i	0.2418(5)	-0.4362(5)	0.0765(3)	0.021(2)	0.019(2)	0.011(2)	0.005(2)	0.003(1)	0.000(1)
C(7)	2i	0.1846(5)	-0.1269(5)	0.0871(3)	0.025(2)	0.032(2)	0.011(2)	0.017(2)	-0.000(2)	0.003(2)
C(8)	2i	0.5736(5)	0.1902(4)	0.1631(3)	0.036(2)	0.018(2)	0.015(2)	0.014(2)	0.011(2)	0.009(1)
C(9)	2i	0.8707(5)	0.0606(5)	0.2081(3)	0.020(2)	0.019(2)	0.015(2)	0.005(2)	0.009(2)	0.003(1)
C(10)	2i	0.6740(5)	-0.3152(5)	0.1471(3)	0.020(2)	0.022(2)	0.015(2)	0.011(2)	0.005(1)	0.004(1)
C(11)	2i	0.4420(4)	0.1522(4)	0.4678(3)	0.018(2)	0.011(2)	0.006(1)	0.007(1)	0.003(1)	0.005(1)
C(12)	2i	0.6309(4)	0.2056(4)	0.4991(3)	0.016(2)	0.010(2)	0.007(1)	0.004(1)	0.004(1)	0.006(1)
C(13)	2i	0.7089(4)	0.3461(4)	0.5913(3)	0.017(2)	0.011(2)	0.010(2)	0.004(1)	0.005(1)	0.007(1)
C(14)	2i	0.5682(4)	0.3807(4)	0.6141(3)	0.018(2)	0.010(2)	0.009(1)	0.006(1)	0.006(1)	0.006(1)
C(15)	2i	0.4032(5)	0.2583(4)	0.5406(3)	0.018(2)	0.013(2)	0.009(1)	0.009(1)	0.003(1)	0.006(1)
C(16)	2i	0.3195(4)	0.0200(4)	0.3634(3)	0.013(2)	0.014(2)	0.007(1)	0.008(1)	0.002(1)	0.003(1)
C(17)	2i	0.7263(4)	0.1364(4)	0.4315(3)	0.014(2)	0.010(2)	0.009(1)	0.004(1)	0.004(1)	0.003(1)
C(18)	2i	0.9078(5)	0.4453(4)	0.6447(3)	0.016(2)	0.013(2)	0.014(2)	0.001(1)	0.003(1)	-0.001(1)
C(19)	2i	0.5925(5)	0.5369(4)	0.6858(3)	0.028(2)	0.012(2)	0.015(2)	0.010(1)	0.006(2)	0.003(1)
C(20)	2i	0.2198(5)	0.2516(5)	0.5310(3)	0.021(2)	0.020(2)	0.013(2)	0.013(2)	0.004(1)	0.005(1)

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Reference

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