Appendix G

Crystallographic Data for

$[W\{(\eta\text{-}C_5H_4)C_2Me_4(\eta\text{-}C_5H_4)\}Me_2]$ (38)

G.1 Crystal Data and Structure Refinement for [W{(η–C_5H_4)C_2Me_4 (η–C_5H_4)}Me_2] (38)

Empirical formula	$C_{18}H_{26}W$	
Formula weight	426.26	
Temperature	125 K	
Wavelength (Mo-Kα)	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 7.350(3) Å	
	b = 13.145(3) Å	β = 105.042(2)°
	c = 12.739(4) Å	
Volume	1512.05 $Å^3$	
Z	4.00	
Density (calculated)	1.87 Mg/m^3	
Absorption coefficient	0.779 mm^{-1}	
F(000)	412	
Crystal size	0.30 x 0.20 x 0.10 mm^3	
θ range for data collection	1.68 to 26.46°.	
Index ranges	-11≤h≤11, 0≤k≤16,	
	0≤l≤15	
Reflections collected	7382	
Independent reflections	3097 [R(int) = 0.034]	
Absorption correction	Empirical (DIFABS)	
Max. and min. transmission	0.93 and 1.00	
Refinement method	Full-matrix least-squares on F	
Weighting scheme	Chebychev parameters 2.32, 0.53 and 1.82	
Data / parameters [I>3σ(I)]	2860/173	
Goodness-of-fit on F	0.8041	
Largest final shift	0.033162	
Final R indices	R = 0.0199, R_w = 0.026	
Residual density	0.927 and –0.59 e.$Å^{-3}$	

G.2 Atomic Coordinates (× 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$× 10^3) for [W{(η–C_5H_4)C_2Me_4(η–C_5H_4)}Me_2] (38)

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U_{(eq)}$
W(1)	6159(1)	2609(1)	834(1)	12
C(1)	8524(3)	2647(2)	1803(2)	18
C(2)	7684(3)	3019(2)	2523(2)	19
C(3)	7025(3)	3946(2)	2089(2)	24
C(4)	7410(3)	4165(2)	1123(2)	24
C(5)	8358(3)	3374(2)	924(2)	21
C(6)	6986(3)	1009(2)	1137(2)	16
C(7)	6676(3)	1174(2)	-20(2)	19
C(8)	5122(3)	1309(2)	-415(2)	23
C(9)	4470(3)	1260(2)	452(2)	24
C(10)	5597(3)	1076(2)	1430(2)	19
C(21)	9522(3)	1709(2)	1964(2)	20
C(22)	8487(3)	746(2)	1909(2)	18
C(23)	10376(3)	1682(2)	1084(3)	29
C(24)	10703(3)	1802(2)	3067(2)	31
C(25)	9088(3)	-208(2)	1475(2)	26
C(26)	8277(3)	457(2)	3028(2)	26
C(31)	4090(3)	3275(2)	1137(2)	26
C(32)	5157(3)	3419(2)	-733(2)	25
H(21)	7583	2681	3203	19
H(31)	6376	4376	2419	23
H(41)	7075	4774	651	21
H(51)	8815	3333	297	20
H(71)	7426	1199	-458	18
H(81)	4585	1421	-1193	21
H(91)	3385	1338	395	21
H(101)	5452	1012	2180	19
H(231)	11035	1065	1194	29
H(232)	11010	2306	1144	29
H(233)	9672	1653	350	29
H(241)	11362	1193	3188	26
H(242)	11309	2430	3071	26
H(243)	10197	1850	3674	26
H(251)	10076	-393	1966	25
H(252)	9216	-66	726	25
H(253)	8386	-786	1432	25
H(261)	9257	284	3535	25
H(262)	7827	1042	3334	25
H(263)	7602	-147	2954	25
H(311)	3233	3102	525	60

H(312)	4194	4025	1200	60
H(313)	3939	2995	1821	60
H(321)	4907	4127	-579	60
H(322)	5875	3431	-1185	60
H(323)	4246	3062	-1132	60

G.3 Bond Lengths [Å] and Angles [°] for [W{(η–C_5H_4)C_2Me_4(η–C_5H_4)}Me_2] (38)

W(1)-C(1)	2.236(3)	W(1)-C(2)	2.315(2)
W(1)-C(3)	2.372(3)	W(1)-C(4)	2.337(3)
W(1)-C(5)	2.264(2)	W(1)-C(6)	2.240(2)
W(1)-C(7)	2.291(3)	W(1)-C(8)	2.365(3)
W(1)-C(9)	2.340(3)	W(1)-C(10)	2.263(3)
W(1)-C(31)	2.246(2)	W(1)-C(32)	2.242(3)
C(1)-C(2)	1.439(4)	C(1)-C(5)	1.449(4)
C(1)-C(21)	1.527(4)	C(2)-C(3)	1.412(4)
C(2)-H(21)	1.000(3)	C(3)-C(4)	1.398(4)
C(3)-H(31)	0.999(3)	C(4)-C(5)	1.430(4)
C(4)-H(41)	1.002(3)	C(5)-H(51)	1.001(3)
C(6)-C(7)	1.443(3)	C(6)-C(10)	1.445(3)
C(6)-C(22)	1.530(3)	C(7)-C(8)	1.420(4)
C(7)-H(71)	1.003(2)	C(8)-C(9)	1.395(4)
C(8)-H(81)	0.999(3)	C(9)-C(10)	1.428(4)
C(9)-H(91)	1.003(3)	C(10)-H(101)	1.003(2)
C(21)-C(22)	1.584(3)	C(21)-C(23)	1.537(4)
C(21)-C(24)	1.550(3)	C(22)-C(25)	1.535(4)
C(22)-C(26)	1.536(4)	C(23)-H(231)	1.007(3)
C(23)-H(232)	1.003(3)	C(23)-H(233)	0.994(3)
C(24)-H(241)	0.998(3)	C(24)-H(242)	1.002(3)
C(24)-H(243)	1.007(3)	C(25)-H(251)	1.001(3)
C(25)-H(252)	1.009(3)	C(25)-H(253)	0.996(3)
C(26)-H(261)	1.000(3)	C(26)-H(262)	1.003(3)
C(26)-H(263)	1.003(3)	C(31)-H(311)	0.988(3)
C(31)-H(312)	0.991(3)	C(31)-H(313)	0.990(3)
C(32)-H(321)	0.991(3)	C(32)-H(322)	0.991(3)
C(32)-H(323)	0.990(3)	C(1)-W(1)-C(2)	36.8(1)
C(1)-W(1)-C(3)	59.74(9)	C(2)-W(1)-C(3)	35.04(9)
C(1)-W(1)-C(4)	60.71(9)	C(2)-W(1)-C(4)	59.17(9)
C(3)-W(1)-C(4)	34.5(1)	C(1)-W(1)-C(5)	37.6(1)
C(2)-W(1)-C(5)	61.14(9)	C(3)-W(1)-C(5)	59.3(1)
C(4)-W(1)-C(5)	36.2(1)	C(1)-W(1)-C(6)	71.21(9)
C(2)-W(1)-C(6)	87.51(9)	C(3)-W(1)-C(6)	122.5(1)
C(4)-W(1)-C(6)	131.17(9)	C(5)-W(1)-C(6)	98.1(1)
C(1)-W(1)-C(7)	88.86(9)	C(2)-W(1)-C(7)	118.55(9)
C(3)-W(1)-C(7)	148.52(9)	C(4)-W(1)-C(7)	129.5(1)
C(5)-W(1)-C(7)	95.1(1)	C(1)-W(1)-C(8)	124.2(1)
C(2)-W(1)-C(8)	147.1(1)	C(3)-W(1)-C(8)	175.89(9)

C(4)-W(1)-C(8)	147.1(1)	C(5)-W(1)-C(8)	124.3(1)
C(1)-W(1)-C(9)	130.48(9)	C(2)-W(1)-C(9)	126.1(1)
C(3)-W(1)-C(9)	142.7(1)	C(4)-W(1)-C(9)	168.2(1)
C(5)-W(1)-C(9)	154.4(1)	C(1)-W(1)-C(10)	96.74(9)
C(2)-W(1)-C(10)	92.08(9)	C(3)-W(1)-C(10)	120.1(1)
C(4)-W(1)-C(10)	151.25(9)	C(5)-W(1)-C(10)	131.7(1)
C(1)-W(1)-C(31)	132.01(11)	C(2)-W(1)-C(31)	95.75(9)
C(3)-W(1)-C(31)	75.8(1)	C(4)-W(1)-C(31)	92.87(11)
C(5)-W(1)-C(31)	128.99(12)	C(1)-W(1)-C(32)	127.3(1)
C(2)-W(1)-C(32)	137.0(1)	C(3)-W(1)-C(32)	103.8(1)
C(4)-W(1)-C(32)	78.5(1)	C(5)-W(1)-C(32)	89.9(1)
C(6)-W(1)-C(7)	37.13(9)	C(6)-W(1)-C(8)	60.02(9)
C(7)-W(1)-C(8)	35.48(9)	C(6)-W(1)-C(9)	60.57(9)
C(7)-W(1)-C(9)	59.45(9)	C(8)-W(1)-C(9)	34.5(1)
C(6)-W(1)-C(10)	37.42(9)	C(7)-W(1)-C(10)	61.46(9)
C(8)-W(1)-C(10)	59.45(9)	C(9)-W(1)-C(10)	36.10(9)
C(6)-W(1)-C(31)	127.6(1)	C(7)-W(1)-C(31)	134.4(1)
C(8)-W(1)-C(31)	100.1(1)	C(9)-W(1)-C(31)	76.5(1)
C(10)-W(1)-C(31)	90.2(1)	C(6)-W(1)-C(32)	130.2(1)
C(7)-W(1)-C(32)	93.4(1)	C(8)-W(1)-C(32)	75.0(1)
C(9)-W(1)-C(32)	94.1(1)	C(10)-W(1)-C(32)	129.9(1)
C(31)-W(1)-C(32)	77.76(11)	W(1)-C(1)-C(2)	74.59(16)
W(1)-C(1)-C(5)	72.28(15)	C(2)-C(1)-C(5)	107.5(2)
W(1)-C(1)-C(21)	122.58(16)	C(2)-C(1)-C(21)	127.1(2)
C(5)-C(1)-C(21)	125.2(3)	W(1)-C(2)-C(1)	68.60(15)
W(1)-C(2)-C(3)	74.68(15)	C(1)-C(2)-C(3)	107.4(2)
W(1)-C(2)-H(21)	121.84(18)	C(1)-C(2)-H(21)	126.3(3)
C(3)-C(2)-H(21)	126.3(3)	W(1)-C(3)-C(2)	70.28(15)
W(1)-C(3)-C(4)	71.36(15)	C(2)-C(3)-C(4)	109.6(2)
W(1)-C(3)-H(31)	124.41(19)	C(2)-C(3)-H(31)	125.1(3)
C(4)-C(3)-H(31)	125.3(3)	W(1)-C(4)-C(3)	74.10(16)
W(1)-C(4)-C(5)	69.14(14)	C(3)-C(4)-C(5)	108.6(2)
W(1)-C(4)-H(41)	122.62(19)	C(3)-C(4)-H(41)	125.5(3)
C(5)-C(4)-H(41)	125.9(3)	W(1)-C(5)-C(1)	70.15(15)
W(1)-C(5)-C(4)	74.68(14)	C(1)-C(5)-C(4)	106.9(2)
W(1)-C(5)-H(51)	120.38(19)	C(1)-C(5)-H(51)	126.7(3)
C(4)-C(5)-H(51)	126.4(3)	W(1)-C(6)-C(7)	73.38(15)
W(1)-C(6)-C(10)	72.17(15)	C(7)-C(6)-C(10)	107.4(2)
W(1)-C(6)-C(22)	122.76(16)	C(7)-C(6)-C(22)	126.7(2)
C(10)-C(6)-C(22)	125.8(2)	W(1)-C(7)-C(6)	69.49(14)
W(1)-C(7)-C(8)	75.07(15)	C(6)-C(7)-C(8)	107.2(2)
W(1)-C(7)-H(71)	120.0(2)	C(6)-C(7)-H(71)	126.1(2)
C(8)-C(7)-H(71)	126.7(2)	W(1)-C(8)-C(7)	69.45(14)
W(1)-C(8)-C(9)	71.81(15)	C(7)-C(8)-C(9)	109.4(2)
W(1)-C(8)-H(81)	125.0(2)	C(7)-C(8)-H(81)	125.0(3)
C(9)-C(8)-H(81)	125.6(3)	W(1)-C(9)-C(8)	73.71(15)
W(1)-C(9)-C(10)	69.00(14)	C(8)-C(9)-C(10)	108.9(2)
W(1)-C(9)-H(91)	123.6(2)	C(8)-C(9)-H(91)	125.4(3)
C(10)-C(9)-H(91)	125.7(3)	W(1)-C(10)-C(6)	70.41(14)
W(1)-C(10)-C(9)	74.90(15)	C(6)-C(10)-C(9)	107.1(2)
W(1)-C(10)-H(101)	119.65(19)	C(6)-C(10)-H(101)	126.4(2)

C(9)-C(10)-H(101)	126.4(2)	C(1)-C(21)-C(22)	107.13(19)
C(1)-C(21)-C(23)	109.6(2)	C(22)-C(21)-C(23)	112.1(2)
C(1)-C(21)-C(24)	109.0(2)	C(22)-C(21)-C(24)	112.7(2)
C(23)-C(21)-C(24)	106.3(2)	C(6)-C(22)-C(21)	107.20(19)
C(6)-C(22)-C(25)	108.3(2)	C(21)-C(22)-C(25)	113.1(2)
C(6)-C(22)-C(26)	109.6(2)	C(21)-C(22)-C(26)	112.4(2)
C(25)-C(22)-C(26)	106.2(2)	C(21)-C(23)-H(231)	109.4(3)
C(21)-C(23)-H(232)	109.5(3)	H(231)-C(23)-H(232)	108.7(2)
C(21)-C(23)-H(233)	110.2(2)	H(231)-C(23)-H(233)	109.4(3)
H(232)-C(23)-H(233)	109.7(3)	C(21)-C(24)-H(241)	110.1(3)
C(21)-C(24)-H(242)	109.8(3)	H(241)-C(24)-H(242)	109.5(3)
C(21)-C(24)-H(243)	109.6(2)	H(241)-C(24)-H(243)	109.1(3)
H(242)-C(24)-H(243)	108.8(3)	C(22)-C(25)-H(251)	109.8(2)
C(22)-C(25)-H(252)	109.5(2)	H(251)-C(25)-H(252)	108.6(3)
C(22)-C(25)-H(253)	110.2(2)	H(251)-C(25)-H(253)	109.7(3)
H(252)-C(25)-H(253)	109.1(3)	C(22)-C(26)-H(261)	109.8(2)
C(22)-C(26)-H(262)	109.8(2)	H(261)-C(26)-H(262)	109.2(3)
C(22)-C(26)-H(263)	109.7(2)	H(261)-C(26)-H(263)	109.2(3)
H(262)-C(26)-H(263)	109.0(3)	W(1)-C(31)-H(311)	109.50(19)
W(1)-C(31)-H(312)	109.34(18)	H(311)-C(31)-H(312)	109.5(3)
W(1)-C(31)-H(313)	109.4(2)	H(311)-C(31)-H(313)	109.7(3)
H(312)-C(31)-H(313)	109.4(3)	W(1)-C(32)-H(321)	109.6(2)
W(1)-C(32)-H(322)	109.58(19)	H(321)-C(32)-H(322)	109.3(3)
W(1)-C(32)-H(323)	109.6(2)	H(321)-C(32)-H(323)	109.4(3)
H(322)-C(32)-H(323)	109.3(3)		

Symmetry transformations used to generate equivalent atoms:

G.4 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for [W{(η–C_5H_4)C_2Me_4(η–C_5H_4)}Me_2] (38)

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^{14}
W(1)	11(1)	11(1)	16(1)	-1(1)	4(1)	0(1)
C(1)	13(1)	16(1)	22(1)	-2(1)	2(1)	-2(1)
C(2)	17(1)	16(1)	23(1)	-5(1)	3(1)	-3(1)
C(3)	21(1)	19(1)	30(1)	-11(1)	0(1)	3(1)
C(4)	24(1)	14(1)	30(1)	1(1)	-3(1)	-3(1)
C(5)	17(1)	19(1)	27(1)	-2(1)	4(1)	-7(1)
C(6)	17(1)	11(1)	21(1)	-2(1)	5(1)	-2(1)
C(7)	25(1)	12(1)	21(1)	-4(1)	7(1)	0(1)
C(8)	27(1)	17(1)	22(1)	-5(1)	-2(1)	-2(1)
C(9)	16(1)	20(1)	33(1)	-5(1)	2(1)	-6(1)
C(10)	22(1)	13(1)	23(1)	-1(1)	8(1)	-5(1)
C(21)	18(1)	13(1)	27(1)	0(1)	5(1)	1(1)
C(22)	18(1)	14(1)	22(1)	0(1)	4(1)	0(1)
C(23)	21(1)	25(2)	46(2)	-3(1)	17(1)	-2(1)
C(24)	22(1)	24(2)	38(2)	1(1)	-6(1)	2(1)
C(25)	26(1)	17(1)	34(1)	-2(1)	5(1)	5(1)
C(26)	26(1)	24(2)	25(1)	4(1)	4(1)	1(1)
C(31)	17(1)	27(2)	35(1)	-6(1)	10(1)	4(1)
C(32)	21(1)	25(2)	27(1)	6(1)	2(1)	3(1)

G.5 Additional Structural Information for [W{(η–C_5H_4)C_2Me_4(η–C_5H_4)}Me_2] (38)

W-Cp^1_{cent}	1.961(3) Å
W-Cp^1_{ave}	2.305 Å
W-Cp^2_{cent}	1.945(3) Å
W-Cp^2_{ave}	2.300 Å
Between Cp planes, α	50.9°
Cp^1_{norm}-W-Cp^2_{norm}, β	129.1°
Cp^1_{cent}-W-Cp^2_{cent}, χ	136.6°
C_{ipso}-Cp plane, ϕ	17.6°, 18.8°