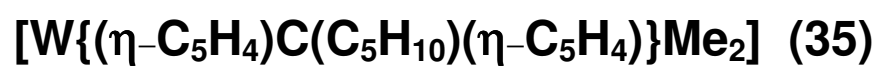


Appendix F

Crystallographic Data for



**F.1 Crystal Data and Structure Refinement for [W{(η -C₅H₄)C(C₅H₁₀)
(η -C₅H₄)}Me₂] (35)**

Empirical formula	C ₁₈ H ₂₄ W	
Formula weight	424.24	
Temperature	150 K	
Wavelength (Mo-K α)	0.71073 Å	
Crystal system	Triclinic	
Space group	P $\bar{1}$	
Unit cell dimensions	a = 7.6070(2) Å b = 8.0780(3) Å c = 12.6730(5) Å	$\alpha = 92.750(2)^\circ$ $\beta = 104.933(2)^\circ$ $\gamma = 104.765(2)^\circ$
Volume	722.20(4) Å ³	
Z	2.00	
Density (calculated)	1.951 Mg/m ³	
Absorption coefficient	7.982 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	-9 ≤ h ≤ 8, -10 ≤ k ≤ 10, -0 ≤ l ≤ 15	
Reflections collected	6923	
Independent reflections	2760 [R(int) = 0.067]	
Absorption correction	Empirical (DIFABS)	
Max. and min. transmission	0.4014 and 0.3074	
Refinement method	Full-matrix least-squares on F ²	
Weighting scheme	Statistical	
Data / parameters [I > 3 σ (I)]	2757/174	
Goodness-of-fit on F	1.106	
Largest final shift	0.002	
Final R indices	R = 0.0367, R _w = 0.1019	
Residual density	1.575 and -2.210 e.Å ⁻³	

F.2 Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{W}\{(\eta\text{-C}_5\text{H}_4)\text{C}(\text{C}_5\text{H}_{10})(\eta\text{-C}_5\text{H}_4)\}\text{Me}_2]$ (35)

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

	x	y	z	$U(\text{eq})$
W(1)	13721(1)	2129(1)	2001(1)	21(1)
C(1)	15391(9)	4488(8)	1516(5)	25(1)
C(2)	15264(11)	3049(9)	749(5)	34(2)
C(3)	13360(16)	2433(12)	129(7)	50(2)
C(4)	12302(14)	3379(12)	502(7)	46(2)
C(5)	13509(10)	4655(9)	1368(6)	33(1)
C(6)	16352(10)	3705(8)	3202(5)	23(1)
C(7)	16542(10)	1996(8)	3046(6)	27(1)
C(8)	15214(12)	879(10)	3475(7)	30(2)
C(9)	14202(11)	1849(9)	3879(6)	29(1)
C(10)	14814(9)	3584(8)	3704(5)	25(1)
C(11)	16995(9)	5176(7)	2548(5)	21(1)
C(12)	18933(10)	5257(9)	2389(6)	31(1)
C(13)	20472(10)	5815(10)	3469(6)	35(2)
C(14)	20502(12)	7544(10)	4003(7)	42(2)
C(15)	18588(11)	7534(9)	4128(6)	34(1)
C(16)	17030(9)	6924(8)	3056(5)	26(1)
C(17)	10755(10)	1304(10)	2091(7)	37(2)
C(18)	12825(12)	-629(9)	1301(6)	41(2)

F.3 Bond Lengths [Å] and Angles [°] for [W{(η-C₅H₄)C(C₅H₁₀)(η-C₅H₄)}Me₂]

(35)

W(1)-C(6)	2.211(7)	W(1)-C(1)	2.214(6)
W(1)-C(17)	2.218(7)	W(1)-C(18)	2.223(7)
W(1)-C(7)	2.245(7)	W(1)-C(10)	2.250(6)
W(1)-C(2)	2.253(6)	W(1)-C(5)	2.256(7)
W(1)-C(8)	2.339(8)	W(1)-C(4)	2.340(9)
W(1)-C(9)	2.345(7)	W(1)-C(3)	2.350(8)
C(1)-C(5)	1.438(10)	C(1)-C(2)	1.446(9)
C(1)-C(11)	1.507(9)	C(2)-C(3)	1.404(13)
C(3)-C(4)	1.39(2)	C(4)-C(5)	1.414(11)
C(6)-C(7)	1.434(10)	C(6)-C(10)	1.454(8)
C(6)-C(11)	1.531(9)	C(7)-C(8)	1.413(10)
C(8)-C(9)	1.393(11)	C(9)-C(10)	1.408(9)
C(11)-C(16)	1.514(8)	C(11)-C(12)	1.524(8)
C(12)-C(13)	1.514(10)	C(13)-C(14)	1.515(11)
C(14)-C(15)	1.502(12)	C(15)-C(16)	1.518(9)
C(6)-W(1)-C(1)	61.1(2)	C(6)-W(1)-C(17)	131.5(3)
C(1)-W(1)-C(17)	132.5(3)	C(6)-W(1)-C(18)	131.4(3)
C(1)-W(1)-C(18)	132.4(3)	C(17)-W(1)-C(18)	78.1(3)
C(6)-W(1)-C(7)	37.5(3)	C(1)-W(1)-C(7)	84.4(2)
C(17)-W(1)-C(7)	135.8(3)	C(18)-W(1)-C(7)	93.9(3)
C(6)-W(1)-C(10)	38.0(2)	C(1)-W(1)-C(10)	84.8(2)
C(17)-W(1)-C(10)	93.5(3)	C(18)-W(1)-C(10)	135.6(3)
C(7)-W(1)-C(10)	62.2(2)	C(6)-W(1)-C(2)	84.0(2)
C(1)-W(1)-C(2)	37.8(2)	C(17)-W(1)-C(2)	137.9(3)
C(18)-W(1)-C(2)	94.6(3)	C(7)-W(1)-C(2)	85.6(3)
C(10)-W(1)-C(2)	118.1(2)	C(6)-W(1)-C(5)	84.9(2)
C(1)-W(1)-C(5)	37.5(2)	C(17)-W(1)-C(5)	95.1(3)
C(18)-W(1)-C(5)	136.5(3)	C(7)-W(1)-C(5)	118.1(2)
C(10)-W(1)-C(5)	87.3(2)	C(2)-W(1)-C(5)	62.1(3)
C(6)-W(1)-C(8)	60.7(3)	C(1)-W(1)-C(8)	118.7(3)
C(17)-W(1)-C(8)	100.5(3)	C(18)-W(1)-C(8)	78.5(3)
C(7)-W(1)-C(8)	35.8(3)	C(10)-W(1)-C(8)	60.0(3)
C(2)-W(1)-C(8)	118.8(3)	C(5)-W(1)-C(8)	144.2(3)
C(6)-W(1)-C(4)	118.7(3)	C(1)-W(1)-C(4)	60.3(3)
C(17)-W(1)-C(4)	81.1(3)	C(18)-W(1)-C(4)	101.2(3)
C(7)-W(1)-C(4)	142.7(3)	C(10)-W(1)-C(4)	120.8(3)
C(2)-W(1)-C(4)	59.5(3)	C(5)-W(1)-C(4)	35.8(3)
C(8)-W(1)-C(4)	178.2(3)	C(6)-W(1)-C(9)	60.4(2)
C(1)-W(1)-C(9)	118.5(2)	C(17)-W(1)-C(9)	79.2(3)
C(18)-W(1)-C(9)	100.4(3)	C(7)-W(1)-C(9)	59.4(3)
C(10)-W(1)-C(9)	35.6(2)	C(2)-W(1)-C(9)	142.5(3)
C(5)-W(1)-C(9)	120.7(3)	C(8)-W(1)-C(9)	34.6(3)
C(4)-W(1)-C(9)	146.9(3)	C(6)-W(1)-C(3)	117.8(3)
C(1)-W(1)-C(3)	60.2(3)	C(17)-W(1)-C(3)	103.0(3)
C(18)-W(1)-C(3)	80.0(3)	C(7)-W(1)-C(3)	118.5(3)
C(10)-W(1)-C(3)	143.7(3)	C(2)-W(1)-C(3)	35.4(3)

C(5)-W(1)-C(3)	59.6(3)	C(8)-W(1)-C(3)	143.9(4)
C(4)-W(1)-C(3)	34.5(4)	C(9)-W(1)-C(3)	177.9(3)
C(5)-C(1)-C(2)	107.5(6)	C(5)-C(1)-C(11)	124.2(6)
C(2)-C(1)-C(11)	124.2(6)	C(5)-C(1)-W(1)	72.8(4)
C(2)-C(1)-W(1)	72.6(3)	C(11)-C(1)-W(1)	102.0(4)
C(3)-C(2)-C(1)	107.0(7)	C(3)-C(2)-W(1)	76.1(4)
C(1)-C(2)-W(1)	69.7(3)	C(4)-C(3)-C(2)	109.3(8)
C(4)-C(3)-W(1)	72.4(5)	C(2)-C(3)-W(1)	68.5(4)
C(3)-C(4)-C(5)	109.4(8)	C(3)-C(4)-W(1)	73.1(5)
C(5)-C(4)-W(1)	68.9(4)	C(4)-C(5)-C(1)	106.7(7)
C(4)-C(5)-W(1)	75.3(5)	C(1)-C(5)-W(1)	69.7(4)
C(7)-C(6)-C(10)	107.0(6)	C(7)-C(6)-C(11)	125.2(6)
C(10)-C(6)-C(11)	123.2(6)	C(7)-C(6)-W(1)	72.5(4)
C(10)-C(6)-W(1)	72.4(4)	C(11)-C(6)-W(1)	101.3(4)
C(8)-C(7)-C(6)	108.0(6)	C(8)-C(7)-W(1)	75.8(4)
C(6)-C(7)-W(1)	70.0(4)	C(9)-C(8)-C(7)	108.3(6)
C(9)-C(8)-W(1)	72.9(4)	C(7)-C(8)-W(1)	68.4(4)
C(8)-C(9)-C(10)	110.1(6)	C(8)-C(9)-W(1)	72.5(4)
C(10)-C(9)-W(1)	68.5(3)	C(9)-C(10)-C(6)	106.5(6)
C(9)-C(10)-W(1)	75.9(4)	C(6)-C(10)-W(1)	69.5(3)
C(1)-C(11)-C(16)	113.2(5)	C(1)-C(11)-C(12)	113.4(5)
C(16)-C(11)-C(12)	109.3(5)	C(1)-C(11)-C(6)	95.5(5)
C(16)-C(11)-C(6)	113.3(5)	C(12)-C(11)-C(6)	111.8(5)
C(13)-C(12)-C(11)	111.1(5)	C(12)-C(13)-C(14)	111.6(6)
C(15)-C(14)-C(13)	111.2(6)	C(14)-C(15)-C(16)	112.5(6)
C(11)-C(16)-C(15)	111.9(5)		

Symmetry transformations used to generate equivalent atoms:

F.4 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{W}\{(\eta\text{-C}_5\text{H}_4)\text{C}(\text{C}_5\text{H}_{10})(\eta\text{-C}_5\text{H}_4)\}\text{Me}_2]$ (35)

The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
W(1)	23(1)	18(1)	19(1)	2(1)	5(1)	1(1)
C(1)	32(3)	19(3)	21(3)	7(2)	8(3)	0(2)
C(2)	43(4)	30(3)	20(3)	-2(2)	10(3)	-7(3)
C(3)	74(7)	39(5)	21(4)	9(3)	12(4)	-10(4)
C(4)	34(5)	49(5)	32(4)	16(4)	-9(4)	-11(4)
C(5)	32(4)	30(3)	31(3)	10(3)	4(3)	1(3)
C(6)	27(3)	21(3)	20(3)	-1(2)	8(3)	2(2)
C(7)	29(3)	21(3)	30(3)	3(2)	11(3)	5(2)
C(8)	35(4)	21(3)	33(4)	9(3)	8(3)	5(3)
C(9)	37(4)	29(4)	26(3)	10(3)	15(3)	8(3)
C(10)	26(3)	29(3)	17(3)	-4(2)	9(2)	3(2)
C(11)	21(3)	14(3)	24(3)	2(2)	1(3)	2(2)
C(12)	33(4)	28(3)	37(4)	11(3)	22(3)	6(3)
C(13)	20(3)	41(4)	39(4)	13(3)	3(3)	4(3)
C(14)	39(4)	34(4)	37(4)	9(3)	-1(3)	-7(3)
C(15)	37(4)	23(3)	31(3)	2(2)	4(3)	-3(3)
C(16)	31(3)	19(3)	26(3)	-1(2)	6(3)	5(2)
C(17)	25(3)	34(4)	45(4)	8(3)	4(3)	1(3)
C(18)	53(5)	24(3)	36(4)	-7(3)	12(3)	-6(3)

F.5 Additional Structural Information for $[\text{W}\{(\eta\text{-C}_5\text{H}_4)\text{C}(\text{C}_5\text{H}_{10})(\eta\text{-C}_5\text{H}_4)\}\text{Me}_2]$ (35)

W-Cp ¹ _{cent}	1.938 Å
W-Cp ¹ _{ave}	2.323(7) Å
W-Cp ² _{cent}	1.932 Å
W-Cp ² _{ave}	2.278(6) Å
Between Cp planes, α	61.7°
Cp ¹ _{norm} -W-Cp ² _{norm} , β	118.3°
Cp ¹ _{cent} -W-Cp ² _{cent} , χ	127.6°
C _{ipso} -Cp plane, ϕ	24.1°, 25.2°
C _{ipso} -C(11)-C _{ipso} , ϵ	95.5(3)°