

Appendix H

Crystallographic Data for [Re{(η-C₅H₄)CMe₂(η-C₅H₄)}Cl] (39)

H.1 Crystal Data and Structure Refinement for [Re{(η-C₅H₄)CMe₂(η-C₅H₄)}Cl] (39)

Empirical formula	C ₁₃ H ₁₄ ClRe	
Formula weight	391.91	
Temperature	150 K	
Wavelength (Mo-Kα)	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 7.125(5) Å b = 11.794(4) Å c = 13.524(8) Å	β = 103.08(3)°
Volume	1107.0 Å ³	
Z	4.00	
Density (calculated)	2.35 Mg/m ³	
Absorption coefficient	11.33 mm ⁻¹	
F(000)	730.61	
Crystal size	0.25 x 0.25 x 0.15 mm ³	
θ range for data collection	1.68 to 26.46°.	
Index ranges	-8 ≤ h ≤ 8, 0 ≤ k ≤ 14, 0 ≤ l ≤ 16	
Reflections collected	3662	
Independent reflections	2238 [R(int) = 0.08]	
Absorption correction	Empirical (DIFABS)	
Max. and min. transmission	0.94 and 1.00	
Refinement method	Full-matrix least-squares on F	
Weighting scheme	Chebychev parameters 1.59, 0.554 and 1.16	
Data / parameters [I > 3σ(I)]	1953/136	
Goodness-of-fit on F	1.1089	
Largest final shift	0.033162	
Final R indices	R = 0.035, R _w = 0.040	
Residual density	1.84 and -1.99 e.Å ⁻³	

H.2 Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Re}\{(\eta\text{-C}_5\text{H}_4)\text{CMe}_2(\eta\text{-C}_5\text{H}_4)\}\text{Cl}]$ (39)

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

	x	y	z	$U(\text{eq})$
Re(1)	5115(1)	769(1)	7463(1)	16
Cl(1)	7432(2)	-91(1)	6610(1)	31
C(1)	3089(7)	2149(4)	7463(4)	22
C(2)	4780(8)	2619(4)	7180(5)	26
C(3)	4910(9)	2110(5)	6265(4)	30
C(4)	3349(8)	1322(5)	5947(4)	30
C(5)	2222(7)	1344(5)	6685(4)	26
C(6)	4151(7)	1030(5)	8869(3)	21
C(7)	6240(7)	1084(5)	9111(4)	25
C(8)	6910(8)	11(5)	8890(4)	27
C(9)	5289(9)	-721(4)	8513(4)	28
C(10)	3601(8)	-93(4)	8499(4)	24
C(11)	2839	2087	8565	21
C(12)	749	1853	8613	28
C(13)	3593(8)	3135(5)	9180(4)	29
H(21)	5700	3215	7568	22
H(31)	5893	2285	5869	32
H(41)	3114	808	5309	26
H(51)	1015	879	6657	20
H(71)	7035	1740	9374	22
H(81)	8325	-208	9005	26
H(91)	5390	-1549	8289	25
H(101)	2263	-384	8297	21
H(131)	3426	3065	9907	26
H(132)	5010	3251	9218	26
H(133)	2881	3831	8875	26
H(121)	642	1821	9345	24
H(122)	-92	2477	8263	24
H(123)	327	1115	8282	24

H.3 Bond Lengths [Å] and Angles [°] for [Re{(η-C₅H₄)CMe₂(η-C₅H₄)}Cl] (39)

Re(1)-Cl(1)	2.4383(13)	Re(1)-C(1)	2.175(5)
Re(1)-C(2)	2.218(5)	Re(1)-C(3)	2.245(5)
Re(1)-C(4)	2.245(5)	Re(1)-C(5)	2.199(5)
Re(1)-C(9)	2.246(5)	Re(1)-C(8)	2.246(5)
Re(1)-C(7)	2.223(5)	Re(1)-C(6)	2.186(5)
Re(1)-C(10)	2.202(5)	C(1)-C(2)	1.454(7)
C(1)-C(5)	1.448(7)	C(1)-C(11)	1.542(5)
C(2)-C(3)	1.398(8)	C(2)-H(21)	1.022(6)
C(3)-C(4)	1.439(9)	C(3)-H(31)	0.995(5)
C(4)-C(5)	1.416(8)	C(4)-H(41)	1.037(6)
C(5)-H(51)	1.013(5)	C(6)-C(10)	1.439(7)
C(6)-C(11)	1.556(5)	C(7)-C(6)	1.451(7)
C(7)-H(71)	0.977(6)	C(8)-C(7)	1.408(8)
C(8)-H(81)	1.018(5)	C(9)-C(8)	1.440(8)
C(9)-C(10)	1.409(8)	C(9)-H(91)	1.031(6)
C(10)-H(101)	0.992(5)	C(12)-C(11)	1.531
C(12)-H(121)	1.011	C(12)-H(122)	0.998
C(12)-H(123)	0.994	C(13)-C(11)	1.519(5)
C(13)-H(131)	1.020(5)	C(13)-H(132)	1.009(6)
C(13)-H(133)	1.003(6)		
Cl(1)-Re(1)-C(1)	146.29(13)	Cl(1)-Re(1)-C(2)	112.70(14)
C(1)-Re(1)-C(2)	38.64(18)	Cl(1)-Re(1)-C(3)	83.83(14)
C(1)-Re(1)-C(3)	62.52(19)	C(2)-Re(1)-C(3)	36.5(2)
Cl(1)-Re(1)-C(4)	89.36(15)	C(1)-Re(1)-C(4)	63.15(19)
C(2)-Re(1)-C(4)	62.7(2)	C(3)-Re(1)-C(4)	37.4(2)
Cl(1)-Re(1)-C(5)	124.34(15)	C(1)-Re(1)-C(5)	38.6(2)
C(2)-Re(1)-C(5)	64.0(2)	C(3)-Re(1)-C(5)	62.4(2)
C(4)-Re(1)-C(5)	37.1(2)	Cl(1)-Re(1)-C(9)	91.55(17)
C(1)-Re(1)-C(9)	121.8(2)	C(2)-Re(1)-C(9)	150.1(2)
C(3)-Re(1)-C(9)	173.3(2)	C(4)-Re(1)-C(9)	138.1(2)
Cl(1)-Re(1)-C(8)	85.74(15)	C(1)-Re(1)-C(8)	123.12(19)
C(2)-Re(1)-C(8)	123.9(2)	C(3)-Re(1)-C(8)	146.3(2)
C(4)-Re(1)-C(8)	173.0(2)	Cl(1)-Re(1)-C(7)	114.49(14)
C(1)-Re(1)-C(7)	87.9(2)	C(2)-Re(1)-C(7)	90.5(2)
C(3)-Re(1)-C(7)	123.8(2)	C(4)-Re(1)-C(7)	150.2(2)
Cl(1)-Re(1)-C(6)	148.19(14)	C(1)-Re(1)-C(6)	63.58(19)
C(2)-Re(1)-C(6)	88.2(2)	C(3)-Re(1)-C(6)	123.1(2)
C(4)-Re(1)-C(6)	122.1(2)	Cl(1)-Re(1)-C(10)	126.20(15)
C(1)-Re(1)-C(10)	85.7(2)	C(2)-Re(1)-C(10)	121.0(2)
C(3)-Re(1)-C(10)	145.4(2)	C(4)-Re(1)-C(10)	117.5(2)
C(5)-Re(1)-C(9)	117.1(2)	C(5)-Re(1)-C(8)	145.5(2)
C(5)-Re(1)-C(7)	121.0(2)	C(5)-Re(1)-C(6)	85.8(2)
C(5)-Re(1)-C(10)	84.6(2)	C(6)-Re(1)-C(10)	38.28(19)
C(7)-Re(1)-C(6)	38.42(18)	C(7)-Re(1)-C(10)	63.63(19)
C(8)-Re(1)-C(6)	62.5(2)	C(8)-Re(1)-C(7)	36.7(2)
C(8)-Re(1)-C(10)	62.3(2)	C(9)-Re(1)-C(6)	62.8(2)

C(9)-Re(1)-C(7)	62.6(2)	C(9)-Re(1)-C(8)	37.4(2)
C(9)-Re(1)-C(10)	36.9(2)	Re(1)-C(1)-C(2)	72.3(3)
Re(1)-C(1)-C(5)	71.5(3)	C(2)-C(1)-C(5)	107.5(4)
Re(1)-C(1)-C(11)	100.7(2)	C(2)-C(1)-C(11)	123.8(4)
C(5)-C(1)-C(11)	123.2(4)	Re(1)-C(2)-C(1)	69.1(3)
Re(1)-C(2)-C(3)	72.8(3)	C(1)-C(2)-C(3)	107.1(5)
Re(1)-C(2)-H(21)	123.8(4)	C(1)-C(2)-H(21)	127.0(5)
C(3)-C(2)-H(21)	125.9(5)	Re(1)-C(3)-C(2)	70.7(3)
Re(1)-C(3)-C(4)	71.3(3)	C(2)-C(3)-C(4)	109.9(5)
Re(1)-C(3)-H(31)	126.5(4)	C(2)-C(3)-H(31)	125.8(6)
C(4)-C(3)-H(31)	124.3(6)	Re(1)-C(4)-C(3)	71.3(3)
Re(1)-C(4)-C(5)	69.7(3)	C(3)-C(4)-C(5)	107.5(5)
Re(1)-C(4)-H(41)	122.8(4)	C(3)-C(4)-H(41)	126.5(6)
C(5)-C(4)-H(41)	126.0(6)	Re(1)-C(5)-C(1)	69.8(3)
Re(1)-C(5)-C(4)	73.2(3)	C(1)-C(5)-C(4)	107.9(5)
Re(1)-C(5)-H(51)	123.1(4)	C(1)-C(5)-H(51)	127.0(5)
C(4)-C(5)-H(51)	125.1(6)	Re(1)-C(9)-C(8)	71.3(3)
Re(1)-C(9)-C(10)	69.8(3)	C(8)-C(9)-C(10)	107.7(5)
Re(1)-C(9)-H(91)	123.6(4)	C(8)-C(9)-H(91)	124.7(6)
C(10)-C(9)-H(91)	127.7(6)	Re(1)-C(8)-C(9)	71.3(3)
Re(1)-C(8)-C(7)	70.7(3)	C(9)-C(8)-C(7)	109.3(5)
Re(1)-C(8)-H(81)	125.7(4)	C(9)-C(8)-H(81)	126.1(5)
C(7)-C(8)-H(81)	124.6(5)	Re(1)-C(7)-C(8)	72.5(3)
Re(1)-C(7)-C(6)	69.4(3)	C(8)-C(7)-C(6)	107.0(5)
Re(1)-C(7)-H(71)	123.0(4)	C(8)-C(7)-H(71)	126.3(5)
C(6)-C(7)-H(71)	126.7(6)	Re(1)-C(6)-C(7)	72.2(3)
Re(1)-C(6)-C(10)	71.5(3)	C(7)-C(6)-C(10)	107.6(5)
Re(1)-C(6)-C(11)	99.8(2)	C(7)-C(6)-C(11)	123.3(4)
C(10)-C(6)-C(11)	123.0(4)	Re(1)-C(10)-C(9)	73.2(3)
Re(1)-C(10)-C(6)	70.3(3)	C(9)-C(10)-C(6)	108.4(5)
Re(1)-C(10)-H(101)	124.3(4)	C(9)-C(10)-H(101)	125.8(5)
C(6)-C(10)-H(101)	125.7(5)	C(11)-C(13)-H(131)	111.0(4)
C(11)-C(13)-H(132)	111.4(4)	H(131)-C(13)-H(132)	107.2(5)
C(11)-C(13)-H(133)	111.0(4)	H(131)-C(13)-H(133)	107.7(5)
H(132)-C(13)-H(133)	108.5(5)	C(11)-C(12)-H(121)	109.7(6)
C(11)-C(12)-H(122)	109.4(2)	H(121)-C(12)-H(122)	108.7(4)
C(11)-C(12)-H(123)	109.6(9)	H(121)-C(12)-H(123)	109.1(9)
H(122)-C(12)-H(123)	110.1(2)	C(1)-C(11)-C(6)	95.8(2)
C(1)-C(11)-C(13)	112.8(3)	C(6)-C(11)-C(13)	113.0(3)
C(1)-C(11)-C(12)	112.07(18)	C(6)-C(11)-C(12)	112.10(18)
C(13)-C(11)-C(12)	110.5(2)		

Symmetry transformations used to generate equivalent atoms:

H.4 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Re}\{(\eta\text{-C}_5\text{H}_4)\text{CMe}_2(\eta\text{-C}_5\text{H}_4)\}\text{Cl}]$ (39)

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
Re(1)	14(1)	18(1)	17(1)	1(1)	5(1)	0(1)
Cl(1)	28(1)	37(1)	29(1)	-2(1)	10(1)	11(1)
C(1)	15(2)	28(3)	23(2)	5(2)	5(2)	9(2)
C(2)	26(2)	19(3)	34(3)	10(2)	13(2)	2(2)
C(3)	38(3)	26(3)	31(3)	16(2)	17(2)	10(2)
C(4)	29(3)	39(4)	19(2)	5(2)	1(2)	12(2)
C(5)	17(2)	32(3)	27(3)	5(2)	-2(2)	3(2)
C(6)	21(2)	33(3)	12(2)	0(2)	9(2)	-6(2)
C(7)	19(2)	32(3)	23(2)	3(2)	5(2)	-1(2)
C(8)	26(3)	26(3)	26(3)	7(2)	0(2)	6(2)
C(9)	38(3)	20(3)	29(3)	9(2)	10(3)	-2(2)
C(10)	28(3)	25(3)	19(2)	4(2)	7(2)	-10(2)
C(13)	30(3)	32(3)	28(3)	-8(2)	14(2)	-2(2)
C(12)	18(3)	38(3)	30(3)	0(2)	8(2)	-4(2)
C(11)	14(3)	24(3)	26(3)	-2(2)	5(2)	0(2)

H.5 Additional Structural Information for $[\text{Re}\{(\eta\text{-C}_5\text{H}_4)\text{CMe}_2(\eta\text{-C}_5\text{H}_4)\}\text{Cl}]$ (39)

Re-Cp ¹ _{cent}	2.216(5) Å
Re-Cp ¹ _{ave}	2.305 Å
Re-Cp ² _{cent}	2.221(6) Å
Re-Cp ² _{ave}	2.300 Å
Between Cp planes, α	53.1°
Cp ¹ _{norm} -Re-Cp ² _{norm} , β	126.9°
Cp ¹ _{cent} -Re-Cp ² _{cent} , χ	131.3°
C _{ipso} -Cp plane, ϕ	20.9°, 22.0°
C _{ipso} -C(11)-C _{ipso} , ϵ	95.8(4)°