Appendix E

Crystallographic Data for

$[V\{(\eta\text{-}C_5H_4)C_2Me_4(\eta\text{-}C_5H_4)\}(\eta^2\text{-}BH_4)]$ (12)

E.1 Crystal Data and Structure Refinement for [V{(η–C_5H_4)C_2Me_4(η–C_5H_4)}(η^2–BH_4)] (12)

Empirical formula	$C_{16}H_{24}BV$	
Formula weight	278.12	
Temperature	150 K	
Wavelength (Mo-Kα)	0.71069 Å	
Crystal system	Triclinic	
Space group	PI	
Unit cell dimensions	a = 7.4060(3) Å	α= 98.190(3)°
	B = 9.6410(6) Å	β= 106.382(4)°
	c = 11.3520(8) Å	γ= 107.820(3)°
Volume	716.7 $Å^3$	
Z	2	
Density (calculated)	1.29 Mg/m^3	
Absorption coefficient	0.65 mm^{-1}	
F(000)	296.56	
Crystal size	0.50 x 0.25 x 0.22 mm^3	
θ for data collection	1.92 to 26.57°.	
Index ranges	-9≤h≤8, -12≤k≤11, 0≤l≤14	
Reflections collected	4099	
Independent reflections	2626 [R(int) = 0.018]	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F	
Weighting scheme	Chebychev parameters 1.94, 0.472 and 1.35	
Data / parameters [I>3σ(I)]	2518/175	
Goodness-of-fit on F	0.9038	
Largest final shift	0.000690	
Final R indices	R = 0.0369, R_w = 0.0386	
Residual density	0.36 and -0.29 e.$Å^{-3}$	

E.2 Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters (Å^{2}x 10^3) for [V{(η–C_5H_4)C_2Me_4(η–C_5H_4)}(η^2–BH_4)] (12)

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

	x	y	z	U(eq)
V(1)	7425(1)	369(1)	7722(1)	12
C(1)	10293(2)	1610(2)	7471(2)	15
C(2)	10763(2)	1075(2)	8594(2)	18
C(3)	10010(3)	-512(2)	8215(2)	21
C(4)	9063(3)	-977(2)	6895(2)	20
C(5)	9202(2)	317(2)	6417(2)	16
C(6)	7332(3)	2552(2)	7377(2)	18
C(7)	5481(3)	1380(2)	6579(2)	20
C(8)	4467(3)	759(2)	7379(2)	25
C(9)	5656(3)	1510(2)	8648(2)	27
C(10)	7441(3)	2602(2)	8666(2)	22
C(21)	10906(3)	3262(2)	7425(2)	18
C(22)	8892(3)	3583(2)	6935(2)	19
C(23)	12305(3)	4260(2)	8749(2)	25
C(24)	12177(3)	3542(2)	6556(2)	26
C(25)	9157(3)	5228(2)	7445(2)	30
C(26)	8038(3)	3247(2)	5478(2)	26
B(1)	5636(3)	-1818(2)	8067(2)	25
H(1)	6890(50)	-710(30)	8790(30)	50
H(2)	5600(50)	-1380(30)	7080(30)	50
H(3)	6110(50)	-2750(30)	8110(30)	50
H(4)	4270(50)	-1980(30)	8230(30)	50
H(21)	11492	1722	9483	18
H(31)	10148	-1197	8800	22
H(41)	8389	-2043	6374	20
H(51)	8633	325	5504	16
H(71)	5003	1055	5631	22
H(81)	3111	-75	7085	26
H(91)	5302	1297	9415	28
H(101)	8600	3303	9445	23
H(231)	12716	5344	8735	27
H(232)	13547	3999	9028	27
H(233)	11584	4090	9376	27
H(241)	12590	4621	6520	26
H(242)	13431	3307	6901	26
H(243)	11378	2882	5681	26
H(251)	10179	5929	7171	32
H(252)	9636	5491	8400	32
H(253)	7837	5376	7122	32
H(261)	9028	3906	5164	26
H(262)	7755	2166	5099	26
H(263)	6740	3441	5209	26

E.3 Bond Lengths [Å] and Angles [°]for [V{(η–C_5H_4)C_2Me_4(η–C_5H_4)}(η^2–BH_4)] (12)

V(1)-C(1)	2.2159(15)	V(1)-C(2)	2.2257(17)
V(1)-C(3)	2.2861(18)	V(1)-C(4)	2.3008(16)
V(1)-C(5)	2.2474(15)	V(1)-C(6)	2.2128(16)
V(1)-C(7)	2.2076(17)	V(1)-C(8)	2.2708(19)
V(1)-C(9)	2.3151(18)	V(1)-C(10)	2.2590(16)
V(1)-B(1)	2.2735(19)	V(1)-H(1)	1.76(3)
V(1)-H(2)	1.70(3)	C(1)-C(2)	1.435(2)
C(1)-C(5)	1.433(2)	C(1)-C(21)	1.529(2)
C(2)-C(3)	1.412(2)	C(2)-H(21)	1.0031(16)
C(3)-C(4)	1.400(3)	C(3)-H(31)	1.0077(16)
C(4)-C(5)	1.417(2)	C(4)-H(41)	1.0011(16)
C(5)-H(51)	1.0040(16)	C(6)-C(7)	1.427(2)
C(6)-C(10)	1.436(2)	C(6)-C(22)	1.530(2)
C(7)-C(8)	1.419(2)	C(7)-H(71)	1.0011(17)
C(8)-C(9)	1.404(3)	C(8)-H(81)	1.0030(19)
C(9)-C(10)	1.409(3)	C(9)-H(91)	1.0080(18)
C(10)-H(101)	1.0106(18)	C(21)-C(22)	1.579(2)
C(21)-C(23)	1.536(2)	C(21)-C(24)	1.542(2)
C(22)-C(25)	1.540(2)	C(22)-C(26)	1.539(2)
C(23)-H(231)	0.9992(18)	C(23)-H(232)	1.005(2)
C(23)-H(233)	1.0054(19)	C(24)-H(241)	1.0017(17)
C(24)-H(242)	1.008(2)	C(24)-H(243)	0.9997(19)
C(25)-H(251)	1.003(2)	C(25)-H(252)	1.008(2)
C(25)-H(253)	1.005(2)	C(26)-H(261)	0.9983(18)
C(26)-H(262)	1.001(2)	C(26)-H(263)	1.007(2)
B(1)-H(1)	1.18(3)	B(1)-H(2)	1.25(3)
B(1)-H(3)	1.06(3)	B(1)-H(4)	1.05(3)

C(1)-V(1)-C(2)	37.70(6)	C(1)-V(1)-C(3)	61.33(6)
C(2)-V(1)-C(3)	36.43(6)	C(1)-V(1)-C(4)	61.17(6)
C(2)-V(1)-C(4)	60.70(6)	C(3)-V(1)-C(4)	35.55(6)
C(1)-V(1)-C(5)	37.44(6)	C(2)-V(1)-C(5)	62.18(6)
C(3)-V(1)-C(5)	60.61(6)	C(4)-V(1)-C(5)	36.29(6)
C(1)-V(1)-C(6)	71.89(6)	C(2)-V(1)-C(6)	97.80(6)
C(3)-V(1)-C(6)	131.95(6)	C(4)-V(1)-C(6)	125.12(6)
C(5)-V(1)-C(6)	88.89(6)	C(1)-V(1)-C(7)	98.29(6)
C(2)-V(1)-C(7)	132.56(6)	C(3)-V(1)-C(7)	154.71(6)
C(4)-V(1)-C(7)	123.09(6)	C(5)-V(1)-C(7)	94.14(6)
C(1)-V(1)-C(8)	132.45(6)	C(2)-V(1)-C(8)	153.07(7)
C(3)-V(1)-C(8)	166.22(6)	C(4)-V(1)-C(8)	144.58(7)
C(5)-V(1)-C(8)	128.90(6)	C(1)-V(1)-C(9)	124.03(7)
C(2)-V(1)-C(9)	120.74(7)	C(3)-V(1)-C(9)	141.82(7)
C(4)-V(1)-C(9)	173.84(6)	C(5)-V(1)-C(9)	149.82(6)
C(1)-V(1)-C(10)	88.19(6)	C(2)-V(1)-C(10)	92.66(7)
C(3)-V(1)-C(10)	126.70(7)	C(4)-V(1)-C(10)	149.00(6)
C(5)-V(1)-C(10)	119.18(6)	C(1)-V(1)-B(1)	144.20(7)

C(2)-V(1)-B(1)	114.47(7)	C(3)-V(1)-B(1)	83.62(7)
C(4)-V(1)-B(1)	86.46(7)	C(5)-V(1)-B(1)	119.69(7)
C(1)-V(1)-H(1)	132.3(10)	C(2)-V(1)-H(1)	94.8(10)
C(3)-V(1)-H(1)	76.4(10)	C(4)-V(1)-H(1)	96.8(10)
C(5)-V(1)-H(1)	132.8(10)	C(1)-V(1)-H(2)	135.7(10)
C(2)-V(1)-H(2)	130.4(10)	C(3)-V(1)-H(2)	93.9(10)
C(4)-V(1)-H(2)	77.3(10)	C(5)-V(1)-H(2)	99.1(10)
C(6)-V(1)-C(7)	37.67(6)	C(6)-V(1)-C(8)	61.46(6)
C(7)-V(1)-C(8)	36.90(6)	C(6)-V(1)-C(9)	61.03(6)
C(7)-V(1)-C(9)	61.04(7)	C(8)-V(1)-C(9)	35.64(7)
C(6)-V(1)-C(10)	37.43(6)	C(7)-V(1)-C(10)	62.21(6)
C(8)-V(1)-C(10)	60.41(7)	C(9)-V(1)-C(10)	35.85(7)
C(6)-V(1)-B(1)	143.89(8)	C(7)-V(1)-B(1)	112.98(7)
C(8)-V(1)-B(1)	82.72(7)	C(9)-V(1)-B(1)	87.61(7)
C(10)-V(1)-B(1)	121.13(7)	C(6)-V(1)-H(1)	137.1(10)
C(7)-V(1)-H(1)	127.6(10)	C(8)-V(1)-H(1)	90.9(10)
C(9)-V(1)-H(1)	77.3(10)	C(10)-V(1)-H(1)	101.3(10)
C(6)-V(1)-H(2)	129.1(10)	C(7)-V(1)-H(2)	91.4(10)
C(8)-V(1)-H(2)	75.4(10)	C(9)-V(1)-H(2)	98.5(10)
C(10)-V(1)-H(2)	133.4(10)	B(1)-V(1)-H(1)	30.7(10)
B(1)-V(1)-H(2)	32.8(10)	H(1)-V(1)-H(2)	63.5(14)
V(1)-C(1)-C(2)	71.52(9)	V(1)-C(1)-C(5)	72.47(9)
C(2)-C(1)-C(5)	107.31(14)	V(1)-C(1)-C(21)	122.57(11)
C(2)-C(1)-C(21)	125.67(14)	C(5)-C(1)-C(21)	127.00(14)
V(1)-C(2)-C(1)	70.78(9)	V(1)-C(2)-C(3)	74.1(1)
C(1)-C(2)-C(3)	107.57(14)	V(1)-C(2)-H(21)	120.51(12)
C(1)-C(2)-H(21)	125.63(16)	C(3)-C(2)-H(21)	126.80(16)
V(1)-C(3)-C(2)	69.5(1)	V(1)-C(3)-C(4)	72.8(1)
C(2)-C(3)-C(4)	108.92(14)	V(1)-C(3)-H(31)	124.40(12)
C(2)-C(3)-H(31)	125.43(17)	C(4)-C(3)-H(31)	125.65(17)
V(1)-C(4)-C(3)	71.7(1)	V(1)-C(4)-C(5)	69.81(9)
C(3)-C(4)-C(5)	108.59(14)	V(1)-C(4)-H(41)	124.09(13)
C(3)-C(4)-H(41)	125.92(17)	C(5)-C(4)-H(41)	125.49(17)
V(1)-C(5)-C(1)	70.09(8)	V(1)-C(5)-C(4)	73.91(9)
C(1)-C(5)-C(4)	107.58(14)	V(1)-C(5)-H(51)	121.29(12)
C(1)-C(5)-H(51)	126.27(15)	C(4)-C(5)-H(51)	126.15(15)
V(1)-C(6)-C(7)	70.96(9)	V(1)-C(6)-C(10)	73.03(9)
C(7)-C(6)-C(10)	107.44(15)	V(1)-C(6)-C(22)	122.35(11)
C(7)-C(6)-C(22)	126.14(15)	C(10)-C(6)-C(22)	126.41(15)
V(1)-C(7)-C(6)	71.4(1)	V(1)-C(7)-C(8)	74.0(1)
C(6)-C(7)-C(8)	107.26(15)	V(1)-C(7)-H(71)	119.64(13)
C(6)-C(7)-H(71)	125.99(16)	C(8)-C(7)-H(71)	126.74(17)
V(1)-C(8)-C(7)	69.1(1)	V(1)-C(8)-C(9)	73.90(11)
C(7)-C(8)-C(9)	109.05(16)	V(1)-C(8)-H(81)	123.59(14)
C(7)-C(8)-H(81)	125.45(19)	C(9)-C(8)-H(81)	125.50(17)
V(1)-C(9)-C(8)	70.5(1)	V(1)-C(9)-C(10)	69.9(1)
C(8)-C(9)-C(10)	108.23(15)	V(1)-C(9)-H(91)	124.80(14)
C(8)-C(9)-H(91)	125.96(19)	C(10)-C(9)-H(91)	125.80(19)
V(1)-C(10)-C(6)	69.54(9)	V(1)-C(10)-C(9)	74.2(1)
C(6)-C(10)-C(9)	107.97(15)	V(1)-C(10)-H(101)	121.96(13)
C(6)-C(10)-H(101)	125.65(17)	C(9)-C(10)-H(101)	126.38(16)

C(1)-C(21)-C(22)	107.04(13)	C(1)-C(21)-C(23)	109.21(14)
C(22)-C(21)-C(23)	112.79(14)	C(1)-C(21)-C(24)	109.25(13)
C(22)-C(21)-C(24)	112.71(14)	C(23)-C(21)-C(24)	105.79(14)
C(6)-C(22)-C(21)	107.33(13)	C(6)-C(22)-C(25)	108.86(15)
C(21)-C(22)-C(25)	113.14(14)	C(6)-C(22)-C(26)	108.40(14)
C(21)-C(22)-C(26)	112.43(14)	C(25)-C(22)-C(26)	106.55(14)
C(21)-C(23)-H(231)	110.17(16)	C(21)-C(23)-H(232)	109.87(16)
H(231)-C(23)-H(232)	109.18(17)	C(21)-C(23)-H(233)	109.81(15)
H(231)-C(23)-H(233)	109.11(18)	H(232)-C(23)-H(233)	108.68(17)
C(21)-C(24)-H(241)	109.98(16)	C(21)-C(24)-H(242)	109.65(15)
H(241)-C(24)-H(242)	108.74(17)	C(21)-C(24)-H(243)	110.19(15)
H(241)-C(24)-H(243)	109.37(17)	H(242)-C(24)-H(243)	108.89(18)
C(22)-C(25)-H(251)	110.45(18)	C(22)-C(25)-H(252)	109.93(16)
H(251)-C(25)-H(252)	108.63(19)	C(22)-C(25)-H(253)	110.42(17)
H(251)-C(25)-H(253)	108.87(18)	H(252)-C(25)-H(253)	108.5(2)
C(22)-C(26)-H(261)	110.08(16)	C(22)-C(26)-H(262)	109.73(14)
H(261)-C(26)-H(262)	109.50(19)	C(22)-C(26)-H(263)	109.63(17)
H(261)-C(26)-H(263)	109.07(16)	H(262)-C(26)-H(263)	108.82(17)
V(1)-B(1)-H(1)	49.6(14)	V(1)-B(1)-H(2)	47.7(14)
H(1)-B(1)-H(2)	97.3(20)	V(1)-B(1)-H(3)	124.0(16)
H(1)-B(1)-H(3)	111.1(23)	H(2)-B(1)-H(3)	113.2(21)
V(1)-B(1)-H(4)	122.3(16)	H(1)-B(1)-H(4)	109.1(22)
H(2)-B(1)-H(4)	111.1(21)	H(3)-B(1)-H(4)	113.7(23)
V(1)-H(1)-B(1)	99.7(19)	V(1)-H(2)-B(1)	99.5(18)

E.4 Anisotropic Displacement Parameters ($Å^2 x\ 10^3$) for [V{(η–C_5H_4)C_2Me_4 (η–C_5H_4)}(η²–BH_4)] (12)

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
V(1)	12(1)	15(1)	12(1)	4(1)	5(1)	5(1)
C(1)	11(1)	20(1)	17(1)	6(1)	6(1)	7(1)
C(2)	14(1)	25(1)	18(1)	9(1)	6(1)	10(1)
C(3)	19(1)	24(1)	28(1)	15(1)	12(1)	13(1)
C(4)	20(1)	19(1)	28(1)	5(1)	13(1)	10(1)
C(5)	16(1)	18(1)	17(1)	4(1)	10(1)	7(1)
C(6)	18(1)	18(1)	21(1)	6(1)	7(1)	12(1)
C(7)	15(1)	24(1)	24(1)	8(1)	5(1)	12(1)
C(8)	17(1)	31(1)	36(1)	13(1)	14(1)	15(1)
C(9)	30(1)	34(1)	30(1)	10(1)	21(1)	20(1)
C(10)	27(1)	23(1)	20(1)	2(1)	11(1)	15(1)
C(21)	17(1)	16(1)	20(1)	5(1)	6(1)	5(1)
C(22)	20(1)	16(1)	20(1)	6(1)	5(1)	7(1)
C(23)	21(1)	19(1)	26(1)	2(1)	1(1)	3(1)
C(24)	25(1)	26(1)	31(1)	14(1)	15(1)	8(1)
C(25)	32(1)	17(1)	40(1)	7(1)	8(1)	11(1)
C(26)	27(1)	29(1)	22(1)	14(1)	5(1)	9(1)
B(1)	22(1)	23(1)	31(1)	10(1)	12(1)	4(1)

E.5 Additional Structural Parameters for [V{(η–C_5H_4)C_2Me_4(η–C_5H_4)}(η²–BH_4)] (12)

$V\text{-}Cp^1_{cent}$	1.9050 Å
$V\text{-}Cp^1_{ave}$	2.2552(17) Å
$V\text{-}Cp^2_{cent}$	1.9029 Å
$V\text{-}Cp^2_{ave}$	2.2530(17) Å
$C_{ipso}\text{-}C_{ipso}$	2.5996 Å
Between Cp planes, α	47.7°
$Cp^1_{norm}\text{-}V\text{-}Cp^2_{norm}$, β	132.3°
$Cp^1_{cent}\text{-}V\text{-}Cp^2_{cent}$, χ	137.71°
C_{ipso}-Cp plane, ϕ	-2.0°, -1.6°