

ORGANOMETALLICS

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C(32)-C(33)	1.376(10)
C(32)-H(32)	0.95
C(33)-C(34)	1.395(10)
C(33)-H(33)	0.95
C(34)-C(35)	1.398(10)
C(34)-H(34)	0.95
C(35)-C(36)	1.373(10)
C(35)-H(35)	0.95
C(36)-H(36)	0.95
C(41)-C(42)	1.374(10)
C(41)-C(46)	1.399(10)
C(42)-C(43)	1.393(11)
C(42)-H(42)	0.95
C(43)-C(44)	1.383(10)
C(43)-H(43)	0.95
C(44)-C(45)	1.362(10)
C(44)-H(44)	0.95
C(45)-C(46)	1.378(10)
C(45)-H(45)	0.95
C(46)-H(46)	0.95
N(51)-C(51)	1.138(8)
C(51)-C(52)	1.464(9)
C(52)-H(52A)	0.98
C(52)-H(52B)	0.98
C(52)-H(52C)	0.98
N(61)-C(61)	1.119(9)
C(61)-C(62)	1.465(10)
C(62)-H(62A)	0.98
C(62)-H(62B)	0.98
C(62)-H(62C)	0.98
B(1)-F(2)	1.374(10)
B(1)-F(4)	1.380(10)
B(1)-F(1)	1.383(9)
B(1)-F(3)	1.384(10)
B(2)-F(6)	1.371(10)
B(2)-F(8)	1.381(10)

B(2)-F(5)	1.382(11)
B(2)-F(7)	1.396(10)
N(61)-Mo(1)-N(51)	151.8(2)
N(61)-Mo(1)-C(2)	120.5(2)
N(51)-Mo(1)-C(2)	81.9(2)
N(61)-Mo(1)-C(3)	84.2(2)
N(51)-Mo(1)-C(3)	118.2(2)
C(2)-Mo(1)-C(3)	36.7(2)
N(61)-Mo(1)-C(1)	133.5(2)
N(51)-Mo(1)-C(1)	74.7(2)
C(2)-Mo(1)-C(1)	36.2(2)
C(3)-Mo(1)-C(1)	59.5(2)
N(61)-Mo(1)-C(4)	76.3(2)
N(51)-Mo(1)-C(4)	131.9(2)
C(2)-Mo(1)-C(4)	59.6(2)
C(3)-Mo(1)-C(4)	35.9(2)
C(1)-Mo(1)-C(4)	57.2(2)
N(61)-Mo(1)-C(5)	103.5(2)
N(51)-Mo(1)-C(5)	102.9(2)
C(2)-Mo(1)-C(5)	59.6(2)
C(3)-Mo(1)-C(5)	59.3(2)
C(1)-Mo(1)-C(5)	34.4(2)
C(4)-Mo(1)-C(5)	34.2(2)
N(61)-Mo(1)-P(1)	77.3(2)
N(51)-Mo(1)-P(1)	75.0(2)
C(2)-Mo(1)-P(1)	128.7(2)
C(3)-Mo(1)-P(1)	130.4(2)
C(1)-Mo(1)-P(1)	148.2(2)
C(4)-Mo(1)-P(1)	151.5(2)
C(5)-Mo(1)-P(1)	170.1(2)
N(61)-Mo(1)-P(2)	84.9(2)
N(51)-Mo(1)-P(2)	84.7(2)
C(2)-Mo(1)-P(2)	143.9(2)
C(3)-Mo(1)-P(2)	145.0(2)
C(1)-Mo(1)-P(2)	107.8(2)
C(4)-Mo(1)-P(2)	109.1(2)

C(5)-Mo(1)-P(2)	91.4(2)
P(1)-Mo(1)-P(2)	78.78(6)
N(61)-Mo(1)-H(1)	83(2)
N(51)-Mo(1)-H(1)	87(2)
C(2)-Mo(1)-H(1)	75(2)
C(3)-Mo(1)-H(1)	73(2)
C(1)-Mo(1)-H(1)	110(2)
C(4)-Mo(1)-H(1)	107(2)
C(5)-Mo(1)-H(1)	131(2)
P(1)-Mo(1)-H(1)	59(2)
P(2)-Mo(1)-H(1)	138(2)
C(21)-P(1)-C(11)	101.8(3)
C(21)-P(1)-C(27)	108.5(3)
C(11)-P(1)-C(27)	103.8(3)
C(21)-P(1)-Mo(1)	113.6(2)
C(11)-P(1)-Mo(1)	118.1(2)
C(27)-P(1)-Mo(1)	110.1(2)
C(41)-P(2)-C(31)	105.2(3)
C(41)-P(2)-C(28)	106.4(3)
C(31)-P(2)-C(28)	103.9(3)
C(41)-P(2)-Mo(1)	113.6(2)
C(31)-P(2)-Mo(1)	120.0(2)
C(28)-P(2)-Mo(1)	106.6(2)
C(5)-C(1)-C(2)	109.1(6)
C(5)-C(1)-C(6)	125.1(6)
C(2)-C(1)-C(6)	125.5(7)
C(5)-C(1)-Mo(1)	74.8(4)
C(2)-C(1)-Mo(1)	67.3(4)
C(6)-C(1)-Mo(1)	129.0(5)
C(3)-C(2)-C(1)	107.2(6)
C(3)-C(2)-C(7)	127.1(6)
C(1)-C(2)-C(7)	124.5(7)
C(3)-C(2)-Mo(1)	72.5(4)
C(1)-C(2)-Mo(1)	76.5(4)
C(7)-C(2)-Mo(1)	126.6(5)
C(2)-C(3)-C(4)	107.2(6)

C(2)-C(3)-C(8)	127.0(6)
C(4)-C(3)-C(8)	125.0(6)
C(2)-C(3)-Mo(1)	70.8(4)
C(4)-C(3)-Mo(1)	76.2(4)
C(8)-C(3)-Mo(1)	126.5(5)
C(5)-C(4)-C(3)	109.2(6)
C(5)-C(4)-C(9)	126.1(7)
C(3)-C(4)-C(9)	124.3(7)
C(5)-C(4)-Mo(1)	74.4(4)
C(3)-C(4)-Mo(1)	67.9(4)
C(9)-C(4)-Mo(1)	129.5(5)
C(4)-C(5)-C(1)	107.1(6)
C(4)-C(5)-C(10)	126.4(7)
C(1)-C(5)-C(10)	125.1(7)
C(4)-C(5)-Mo(1)	71.4(4)
C(1)-C(5)-Mo(1)	70.9(4)
C(10)-C(5)-Mo(1)	133.2(5)
C(1)-C(6)-H(6A)	109.5(4)
C(1)-C(6)-H(6B)	109.5(4)
H(6A)-C(6)-H(6B)	109.5
C(1)-C(6)-H(6C)	109.5(4)
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(2)-C(7)-H(7A)	109.5(4)
C(2)-C(7)-H(7B)	109.5(4)
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5(4)
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(3)-C(8)-H(8A)	109.5(4)
C(3)-C(8)-H(8B)	109.5(4)
H(8A)-C(8)-H(8B)	109.5
C(3)-C(8)-H(8C)	109.5(4)
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(4)-C(9)-H(9A)	109.5(4)

C(4)-C(9)-H(9B)	109.5(5)
H(9A)-C(9)-H(9B)	109.5
C(4)-C(9)-H(9C)	109.5(4)
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(5)-C(10)-H(10A)	109.5(4)
C(5)-C(10)-H(10B)	109.5(4)
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5(4)
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-C(16)	119.2(7)
C(12)-C(11)-P(1)	120.6(5)
C(16)-C(11)-P(1)	120.1(5)
C(11)-C(12)-C(13)	121.0(7)
C(11)-C(12)-H(12)	119.5(4)
C(13)-C(12)-H(12)	119.5(4)
C(14)-C(13)-C(12)	118.9(7)
C(14)-C(13)-H(13)	120.5(4)
C(12)-C(13)-H(13)	120.5(4)
C(15)-C(14)-C(13)	119.8(7)
C(15)-C(14)-H(14)	120.1(5)
C(13)-C(14)-H(14)	120.1(4)
C(14)-C(15)-C(16)	121.6(8)
C(14)-C(15)-H(15)	119.2(5)
C(16)-C(15)-H(15)	119.2(5)
C(15)-C(16)-C(11)	119.5(7)
C(15)-C(16)-H(16)	120.3(5)
C(11)-C(16)-H(16)	120.3(4)
C(26)-C(21)-C(22)	118.4(6)
C(26)-C(21)-P(1)	123.2(6)
C(22)-C(21)-P(1)	118.4(5)
C(23)-C(22)-C(21)	120.5(7)
C(23)-C(22)-H(22)	119.8(5)
C(21)-C(22)-H(22)	119.8(4)
C(24)-C(23)-C(22)	120.3(8)

C(24)-C(23)-H(23)	119.8(5)
C(22)-C(23)-H(23)	119.8(5)
C(23)-C(24)-C(25)	120.1(8)
C(23)-C(24)-H(24)	120.0(5)
C(25)-C(24)-H(24)	120.0(5)
C(24)-C(25)-C(26)	119.8(7)
C(24)-C(25)-H(25)	120.1(5)
C(26)-C(25)-H(25)	120.1(4)
C(21)-C(26)-C(25)	120.9(7)
C(21)-C(26)-H(26)	119.6(4)
C(25)-C(26)-H(26)	119.6(4)
C(28)-C(27)-P(1)	112.7(5)
C(28)-C(27)-H(27A)	109.1(4)
P(1)-C(27)-H(27A)	109.1(2)
C(28)-C(27)-H(27B)	109.1(4)
P(1)-C(27)-H(27B)	109.1(2)
H(27A)-C(27)-H(27B)	107.8
C(27)-C(28)-P(2)	111.1(5)
C(27)-C(28)-H(28A)	109.4(4)
P(2)-C(28)-H(28A)	109.4(2)
C(27)-C(28)-H(28B)	109.4(4)
P(2)-C(28)-H(28B)	109.4(2)
H(28A)-C(28)-H(28B)	108.0
C(32)-C(31)-C(36)	118.2(7)
C(32)-C(31)-P(2)	122.9(6)
C(36)-C(31)-P(2)	118.6(5)
C(31)-C(32)-C(33)	122.0(7)
C(31)-C(32)-H(32)	119.0(4)
C(33)-C(32)-H(32)	119.0(5)
C(32)-C(33)-C(34)	119.5(7)
C(32)-C(33)-H(33)	120.2(5)
C(34)-C(33)-H(33)	120.2(5)
C(33)-C(34)-C(35)	119.4(7)
C(33)-C(34)-H(34)	120.3(5)
C(35)-C(34)-H(34)	120.3(4)
C(36)-C(35)-C(34)	119.8(7)

C(36)-C(35)-H(35)	120.1(4)
C(34)-C(35)-H(35)	120.1(4)
C(35)-C(36)-C(31)	121.1(7)
C(35)-C(36)-H(36)	119.5(4)
C(31)-C(36)-H(36)	119.5(4)
C(42)-C(41)-C(46)	117.8(7)
C(42)-C(41)-P(2)	123.3(6)
C(46)-C(41)-P(2)	118.4(5)
C(41)-C(42)-C(43)	121.2(8)
C(41)-C(42)-H(42)	119.4(5)
C(43)-C(42)-H(42)	119.4(5)
C(44)-C(43)-C(42)	119.5(8)
C(44)-C(43)-H(43)	120.3(5)
C(42)-C(43)-H(43)	120.3(5)
C(45)-C(44)-C(43)	120.2(8)
C(45)-C(44)-H(44)	119.9(5)
C(43)-C(44)-H(44)	119.9(5)
C(44)-C(45)-C(46)	120.1(8)
C(44)-C(45)-H(45)	120.0(5)
C(46)-C(45)-H(45)	120.0(5)
C(45)-C(46)-C(41)	121.2(7)
C(45)-C(46)-H(46)	119.4(5)
C(41)-C(46)-H(46)	119.4(4)
C(51)-N(51)-Mo(1)	174.2(6)
N(51)-C(51)-C(52)	178.6(7)
C(51)-C(52)-H(52A)	109.5(4)
C(51)-C(52)-H(52B)	109.5(4)
H(52A)-C(52)-H(52B)	109.5
C(51)-C(52)-H(52C)	109.5(4)
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(61)-N(61)-Mo(1)	175.2(6)
N(61)-C(61)-C(62)	176.8(8)
C(61)-C(62)-H(62A)	109.5(4)
C(61)-C(62)-H(62B)	109.5(4)
H(62A)-C(62)-H(62B)	109.5

C(61)-C(62)-H(62C)	109.5(4)
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
F(2)-B(1)-F(4)	109.8(6)
F(2)-B(1)-F(1)	110.7(7)
F(4)-B(1)-F(1)	108.7(7)
F(2)-B(1)-F(3)	109.6(7)
F(4)-B(1)-F(3)	109.4(7)
F(1)-B(1)-F(3)	108.6(6)
F(6)-B(2)-F(8)	111.2(7)
F(6)-B(2)-F(5)	109.5(7)
F(8)-B(2)-F(5)	109.8(8)
F(6)-B(2)-F(7)	109.1(7)
F(8)-B(2)-F(7)	107.7(6)
F(5)-B(2)-F(7)	109.4(7)

Table 14S. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Cp}^*\text{MoH}(\text{MeCN})_2(\text{dppe})][\text{BF}_4]_2$.

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

	U11	U22	U33	U23	U13	U12
Mo(1)	21(1)	14(1)	19(1)	-1(1)	-1(1)	0(1)
P(1)	27(1)	16(1)	17(1)	-1(1)	-1(1)	2(1)
P(2)	23(1)	18(1)	23(1)	1(1)	0(1)	1(1)
C(1)	28(4)	19(4)	18(4)	-10(3)	9(3)	-2(4)
C(2)	29(4)	19(4)	14(3)	-4(3)	4(3)	1(3)
C(3)	25(4)	19(4)	17(4)	-1(3)	2(3)	0(3)
C(4)	30(4)	16(4)	25(4)	-12(3)	1(3)	9(4)
C(5)	24(4)	16(3)	32(4)	-6(3)	-2(3)	5(3)
C(6)	29(5)	20(4)	34(5)	-11(4)	0(4)	-10(4)
C(7)	34(4)	36(4)	24(4)	5(4)	-8(4)	-4(4)
C(8)	28(4)	42(5)	30(4)	0(4)	2(4)	-2(4)
C(9)	39(4)	30(4)	37(4)	-9(5)	-2(5)	1(4)
C(10)	43(5)	21(3)	45(6)	-7(4)	-6(5)	0(3)
B(1)	35(6)	25(5)	25(5)	2(4)	2(4)	7(5)
F(1)	54(3)	53(3)	44(3)	-20(3)	-2(3)	5(3)
F(2)	37(3)	38(3)	48(3)	-3(2)	1(2)	-10(2)
F(3)	64(3)	41(3)	39(3)	5(2)	-9(3)	-15(3)
F(4)	53(3)	50(3)	62(3)	2(3)	-17(3)	19(3)
B(2)	40(6)	20(5)	38(6)	-4(4)	9(5)	1(4)
F(5)	73(3)	38(3)	29(3)	-3(2)	-8(2)	-11(3)
F(6)	86(4)	53(3)	39(3)	-8(3)	14(3)	-28(3)
F(7)	36(3)	31(2)	71(4)	-13(3)	-5(3)	2(2)
F(8)	33(3)	37(3)	131(5)	-30(3)	-24(3)	9(2)

Table 15S. Carbon-bonded hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Cp}^*\text{MoH}(\text{MeCN})_2(\text{dppe})][\text{BF}_4]_2$.

	x	y	z	U (eq)
H(6A)	8069(3)	4636(26)	8450(22)	41
H(6B)	7854(7)	6063(17)	8511(23)	41
H(6C)	7831(7)	5179(39)	9274(5)	41
H(7A)	8408(9)	7802(36)	8024(11)	47
H(7B)	8792(20)	6917(12)	7452(7)	47
H(7C)	9088(12)	8158(27)	7812(17)	47
H(8A)	10040(4)	8102(23)	8337(24)	50
H(8B)	10367(12)	6784(19)	8208(20)	50
H(8C)	10440(10)	7512(38)	9029(6)	50
H(9A)	10379(13)	4530(35)	9523(15)	53
H(9B)	10105(5)	4811(43)	10378(14)	53
H(9C)	10489(9)	5861(11)	9932(28)	53
H(10A)	9155(15)	3896(24)	10460(17)	54
H(10B)	8944(21)	3258(7)	9651(10)	54
H(10C)	8473(7)	4037(20)	10170(25)	54
H(12)	9959(3)	9975(6)	9594(4)	32
H(13)	10798(3)	11289(6)	9755(4)	40
H(14)	10832(3)	12663(7)	10841(4)	34
H(15)	10064(3)	12653(7)	11757(5)	40
H(16)	9230(3)	11363(6)	11602(5)	38
H(22)	8918(3)	10374(7)	8846(4)	36
H(23)	8342(4)	11643(7)	8017(5)	49

Table 15S. (continued)

	x	y	z	U(eq)
H(24)	7463(3)	12539(7)	8472(5)	40
H(25)	7147(4)	12179(7)	9764(4)	40
H(26)	7720(3)	10914(6)	10601(4)	37
H(27A)	8837(3)	9491(6)	11827(4)	29
H(27B)	8251(3)	10190(6)	11504(4)	29
H(28A)	7766(3)	8298(6)	11240(4)	30
H(28B)	8034(3)	8169(6)	12116(4)	30
H(32)	8499(4)	4531(6)	12138(5)	35
H(33)	7842(3)	2852(7)	12191(4)	38
H(34)	6973(3)	2854(7)	11398(4)	38
H(35)	6762(3)	4604(7)	10599(4)	36
H(36)	7423(3)	6280(7)	10572(4)	33
H(42)	8896(4)	7963(7)	12767(5)	43
H(43)	9740(4)	7799(7)	13584(5)	46
H(44)	10472(4)	6291(7)	13315(5)	46
H(45)	10353(3)	4943(7)	12259(5)	37
H(46)	9534(3)	5150(7)	11422(5)	34
H(52A)	6801(8)	8806(43)	9556(5)	47
H(52B)	6865(10)	7962(19)	8779(24)	47
H(52C)	7112(4)	9370(27)	8781(24)	47
H(62A)	11135(4)	8199(46)	10928(14)	64
H(62B)	10815(14)	7864(36)	11749(16)	64
H(62C)	10746(11)	9237(14)	11380(28)	64