Supporting Information

Synthesis and Structure of CpMo(CO)(dppe)H, and its Oxidation by Ph_3C^+

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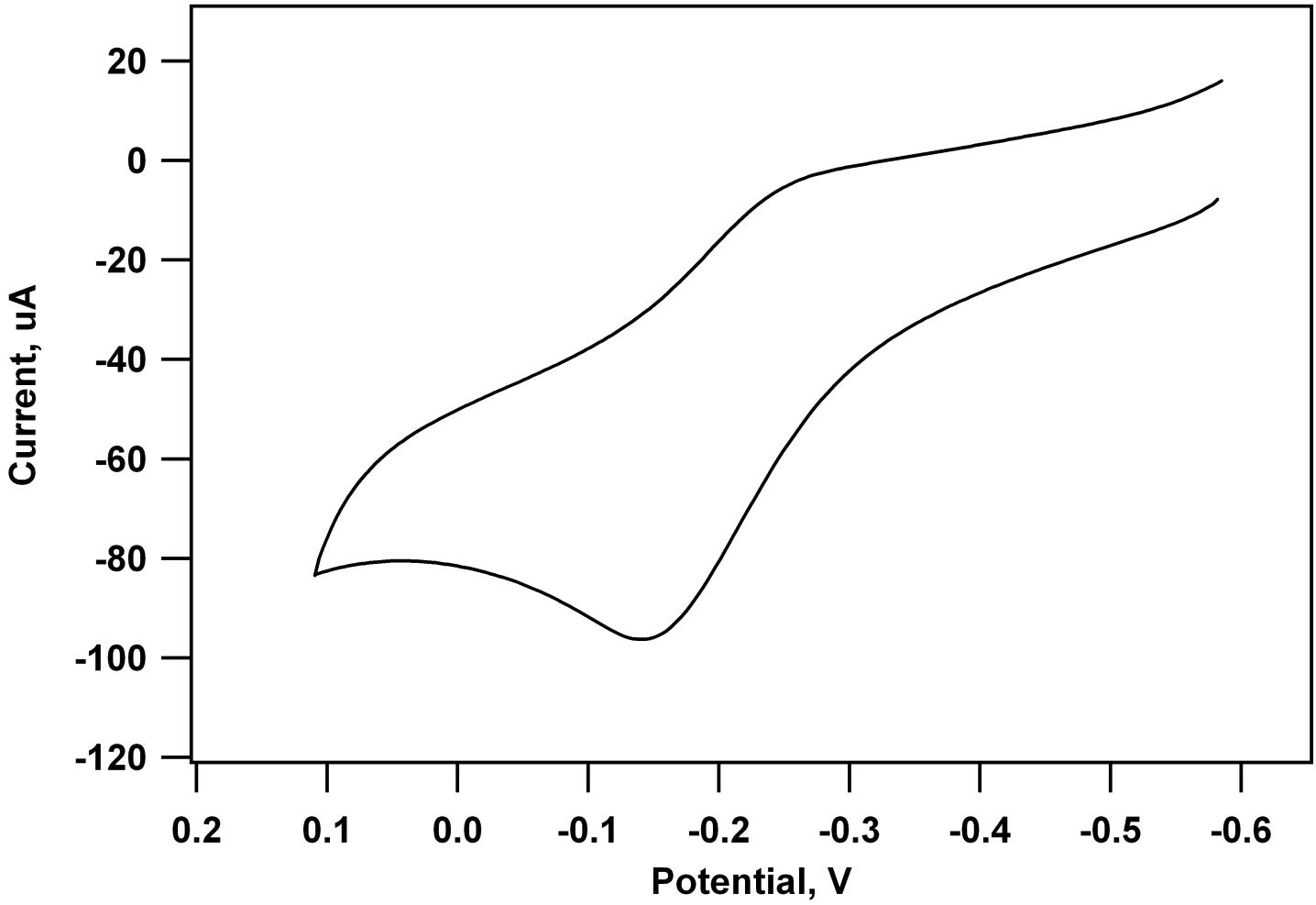
A plot of the cyclic voltammetry experiment, and additional details on the crystal structure of CpMo(CO)(dppe)H.



Cyclic Voltammogram (vs. Fc/Fc^+) of CpMo(CO)(dppe)H in CH_3CN with 0.1 M $Bu_4N^+PF_6^-$ electrolyte.

Cyclic voltammetry was carried out using a BAS 100B electrochemical analyzer using glassy carbon as the working electrode, Pt wire as counter electrode, and Ag/Ag^+ (0.1 M $AgNO_3$) as the reference electrode in CH_3CN solution containing 0.1 M of $Bu_4N^+PF_6^-$. The concentration of CpMo(CO)(dppe)H was 0.01 M, and sweep rates up to 2 V s^{-1} were used. The potential was calibrated using the Cp_2Fe/Cp_2Fe^+ (Fc/Fc^+) couple.

Table 1. Crystal data and structure refinement for CpMo(CO)(dppe)H.

Empirical formula	C39 H38 Mo O P2
Formula weight	680.57
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 10.830(3) A alpha = 96.65(2) deg. b = 11.307(3) A beta = 105.50(2) deg. c = 14.309(4) A gamma = 96.43(2) deg.
Volume	1658.3(8) A^3
Z, Calculated density	2, 1.363 Mg/m^3
Absorption coefficient	0.522 mm^-1
F(000)	704
Crystal size	.20 x .20 x .17 mm
Theta range for data collection	2.75 to 27.52 deg.
Limiting indices	0<=h<=14, -14<=k<=14, -18<=l<=17
Reflections collected / unique	7590 / 7590 [R(int) = 0.0000]
Completeness to theta = 27.52	99.4 %
Absorption correction	GAUSSIAN
Max. and min. transmission	0.93111 and 0.91010
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7590 / 0 / 397
Goodness-of-fit on F^2	0.945
Final R indices [I>2sigma(I)]	R1 = 0.0579, wR2 = 0.1196
R indices (all data)	R1 = 0.2393, wR2 = 0.1578
Largest diff. peak and hole	0.618 and -1.041 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for CpMo(CO)(dppe)H. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mo	1615(1)	1640(1)	2371(1)	40(1)
C(1)	3298(7)	1166(6)	2573(5)	51(2)
O(1)	4326(5)	881(5)	2684(4)	80(2)
P(1)	364(2)	-230(1)	2403(1)	38(1)
C(11)	-1379(6)	-440(5)	1785(4)	42(2)
C(12)	-1774(7)	-486(6)	791(5)	56(2)
C(13)	-3060(8)	-676(7)	273(6)	75(2)
C(14)	-3976(7)	-807(7)	756(6)	74(2)
C(15)	-3615(8)	-750(8)	1735(7)	81(3)
C(16)	-2334(7)	-584(7)	2251(5)	69(2)
C(21)	765(6)	-1651(5)	1886(4)	39(1)
C(22)	-27(7)	-2731(5)	1834(5)	60(2)
C(23)	253(10)	-3815(6)	1451(6)	76(2)
C(24)	1326(9)	-3844(6)	1125(6)	76(3)
C(25)	2111(8)	-2791(7)	1170(5)	69(2)
C(26)	1834(7)	-1711(5)	1540(4)	50(2)
C(10)	423(6)	-528(5)	3661(4)	47(2)
C(20)	1728(6)	34(5)	4344(4)	44(2)
P(2)	2116(2)	1574(1)	4112(1)	38(1)
C(31)	1194(6)	2436(5)	4782(4)	38(1)
C(32)	1748(7)	3179(6)	5669(5)	52(2)
C(33)	999(8)	3850(6)	6110(5)	66(2)
C(34)	-305(9)	3753(6)	5694(6)	66(2)
C(35)	-865(7)	3022(6)	4837(5)	61(2)
C(36)	-134(7)	2374(6)	4382(5)	52(2)
C(41)	3780(6)	2040(5)	4895(4)	45(2)
C(42)	4335(7)	1450(7)	5660(5)	60(2)
C(43)	5577(8)	1866(8)	6224(6)	75(2)
C(44)	6293(7)	2838(8)	6079(6)	72(2)
C(45)	5762(7)	3419(7)	5335(6)	66(2)
C(46)	4508(7)	3038(6)	4735(5)	59(2)
C(2)	940(20)	2620(14)	988(10)	44(4)
C(3)	2165(16)	3294(15)	1644(16)	45(4)
C(4)	1820(20)	3731(13)	2548(13)	51(4)
C(5)	550(20)	3344(14)	2444(13)	36(3)
C(6)	-27(15)	2657(13)	1508(16)	45(3)
C(2')	370(20)	2546(14)	1148(15)	55(4)
C(3')	1660(20)	2962(16)	1266(14)	44(3)

C(4')	2253(15)	3656(14)	2250(16)	49(4)
C(5')	1210(30)	3634(15)	2704(12)	53(4)
C(6')	10(20)	2949(19)	2020(20)	62(4)
C(51')	6640(30)	5880(20)	510(20)	168(16)
C(51)	6454(13)	5240(20)	1143(13)	162(7)
C(52)	6778(12)	4100(17)	1165(9)	126(4)
C(53')	6620(30)	2420(20)	1810(30)	174(17)
C(53)	6387(14)	3406(19)	1847(15)	160(6)
C(54)	5775(16)	3880(30)	2484(14)	186(10)
C(55)	5600(20)	5010(30)	2450(20)	222(15)
C(56)	5800(20)	5850(20)	1800(20)	200(11)

Table 3. Selected bond lengths [A] and angles [deg] for CpMo(CO)(dppe)H.

Mo-C(1)	1.916(8)
Mo-P(1)	2.3923(18)
Mo-P(2)	2.4161(17)
Mo-H(1)	1.44(6)
P(2)-Mo-C(1)	81.3(2)
P(1)-Mo-P(2)	78.4(1)
C(1)-Mo-P(1)	100.23(19)
P(2)-Mo-H(1)	131(2)
C(1)-Mo-H(1)	78(2)
P(1)-Mo-H(1)	63(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [A] and angles [deg] for CpMo(CO)(dppe)H.

Mo-C(1)	1.916(8)
Mo-C(3')	2.303(13)
Mo-C(2')	2.323(15)
Mo-C(4)	2.328(15)
Mo-C(3)	2.338(13)
Mo-C(4')	2.347(14)
Mo-C(5)	2.361(12)
Mo-C(5')	2.365(15)
Mo-C(2)	2.366(13)
Mo-C(6)	2.371(13)
Mo-P(1)	2.3923(18)
Mo-P(2)	2.4161(17)
Mo-H(1)	1.44(6)
C(1)-O(1)	1.168(8)
P(1)-C(11)	1.834(6)
P(1)-C(21)	1.836(6)
P(1)-C(10)	1.855(6)
C(11)-C(12)	1.365(8)
C(11)-C(16)	1.376(9)
C(12)-C(13)	1.371(9)
C(12)-H(12)	0.9300
C(13)-C(14)	1.357(10)
C(13)-H(13)	0.9300
C(14)-C(15)	1.342(10)
C(14)-H(14)	0.9300
C(15)-C(16)	1.366(10)
C(15)-H(15)	0.9300
C(16)-H(16)	0.9300
C(21)-C(26)	1.381(8)
C(21)-C(22)	1.393(8)
C(22)-C(23)	1.383(9)
C(22)-H(22)	0.9300
C(23)-C(24)	1.365(11)
C(23)-H(23)	0.9300
C(24)-C(25)	1.368(10)
C(24)-H(24)	0.9300
C(25)-C(26)	1.370(8)
C(25)-H(25)	0.9300
C(26)-H(26)	0.9300
C(10)-C(20)	1.508(8)
C(10)-H(101)	0.9700
C(10)-H(102)	0.9700
C(20)-P(2)	1.835(6)
C(20)-H(201)	0.9700

C(20)-H(202)	0.9700
P(2)-C(41)	1.830(6)
P(2)-C(31)	1.838(6)
C(31)-C(32)	1.382(8)
C(31)-C(36)	1.388(8)
C(32)-C(33)	1.390(9)
C(32)-H(32)	0.9300
C(33)-C(34)	1.364(10)
C(33)-H(33)	0.9300
C(34)-C(35)	1.346(10)
C(34)-H(34)	0.9300
C(35)-C(36)	1.373(9)
C(35)-H(35)	0.9300
C(36)-H(36)	0.9300
C(41)-C(46)	1.380(9)
C(41)-C(42)	1.384(8)
C(42)-C(43)	1.368(9)
C(42)-H(42)	0.9300
C(43)-C(44)	1.341(10)
C(43)-H(43)	0.9300
C(44)-C(45)	1.347(10)
C(44)-H(44)	0.9300
C(45)-C(46)	1.388(9)
C(45)-H(45)	0.9300
C(46)-H(46)	0.9300
C(2)-C(6)	1.44(2)
C(2)-C(3)	1.47(2)
C(3)-C(4)	1.49(2)
C(4)-C(5)	1.36(2)
C(5)-C(6)	1.41(2)
C(2')-C(3')	1.38(2)
C(2')-C(6')	1.44(3)
C(3')-C(4')	1.47(2)
C(4')-C(5')	1.45(2)
C(5')-C(6')	1.47(2)
C(51')-C(51)	1.27(3)
C(51)-C(52)	1.37(2)
C(51)-C(56)	1.47(3)
C(52)-C(53)	1.44(2)
C(53')-C(53)	1.17(2)
C(53)-C(54)	1.36(2)
C(54)-C(55)	1.32(3)
C(55)-C(56)	1.44(3)

C(1)-Mo-C(3')	101.2(5)
C(1)-Mo-C(2')	132.3(8)
C(3')-Mo-C(2')	34.8(6)
C(1)-Mo-C(4)	109.2(6)

C(1)-Mo-C(3)	93.0(4)
C(4)-Mo-C(3)	37.2(6)
C(1)-Mo-C(4')	96.3(5)
C(3')-Mo-C(4')	36.8(5)
C(2')-Mo-C(4')	60.2(5)
C(1)-Mo-C(5)	142.6(6)
C(4)-Mo-C(5)	33.7(6)
C(3)-Mo-C(5)	59.7(5)
C(1)-Mo-C(5')	125.2(7)
C(3')-Mo-C(5')	59.1(5)
C(2')-Mo-C(5')	59.0(6)
C(4')-Mo-C(5')	35.8(6)
P(2)-Mo-C(1)	81.3(2)
C(1)-Mo-C(2)	115.0(6)
P(1)-Mo-P(2)	78.4(1)
C(4)-Mo-C(2)	59.4(5)
C(3)-Mo-C(2)	36.5(5)
C(5)-Mo-C(2)	58.6(5)
C(1)-Mo-C(6)	150.0(6)
C(3')-Mo-C(6)	49.2(5)
C(2')-Mo-C(6)	18.6(5)
C(4)-Mo-C(6)	57.6(5)
C(3)-Mo-C(6)	59.9(5)
C(5)-Mo-C(6)	34.7(5)
C(5')-Mo-C(6)	49.6(6)
C(2)-Mo-C(6)	35.4(5)
C(1)-Mo-P(1)	100.23(19)
C(3')-Mo-P(1)	137.0(7)
C(2')-Mo-P(1)	107.1(5)
C(4)-Mo-P(1)	148.3(7)
C(3)-Mo-P(1)	154.2(6)
C(4')-Mo-P(1)	163.4(4)
C(5)-Mo-P(1)	115.3(5)
C(5')-Mo-P(1)	129.9(7)
C(2)-Mo-P(1)	117.9(6)
C(6)-Mo-P(1)	100.8(3)
C(1)-Mo-C(6')	156.7(5)
C(3')-Mo-C(6')	59.1(5)
C(2')-Mo-C(6')	35.5(6)
C(4')-Mo-C(6')	60.5(6)
P(2)-Mo-H(1)	131(2)
C(6)-Mo-C(6')	18.2(5)
P(1)-Mo-C(6')	102.9(5)
C(1)-Mo-H(1)	78(2)
C(3')-Mo-H(1)	85(2)
C(2')-Mo-H(1)	80(2)
C(4)-Mo-H(1)	134(2)
C(3)-Mo-H(1)	99(2)

C(4')-Mo-H(1)	120(2)
C(5)-Mo-H(1)	127(2)
C(5')-Mo-H(1)	139(2)
C(2)-Mo-H(1)	76(2)
C(6)-Mo-H(1)	92(2)
P(1)-Mo-H(1)	63(2)
C(6')-Mo-H(1)	110(2)
O(1)-C(1)-Mo	179.0(6)
C(11)-P(1)-C(21)	99.7(3)
C(11)-P(1)-C(10)	103.0(3)
C(21)-P(1)-C(10)	100.6(3)
C(11)-P(1)-Mo	117.46(19)
C(21)-P(1)-Mo	119.9(2)
C(10)-P(1)-Mo	113.5(2)
C(12)-C(11)-C(16)	116.9(6)
C(12)-C(11)-P(1)	118.4(5)
C(16)-C(11)-P(1)	124.6(5)
C(11)-C(12)-C(13)	121.9(6)
C(11)-C(12)-H(12)	119.0
C(13)-C(12)-H(12)	119.0
C(14)-C(13)-C(12)	119.6(7)
C(14)-C(13)-H(13)	120.2
C(12)-C(13)-H(13)	120.2
C(15)-C(14)-C(13)	119.7(7)
C(15)-C(14)-H(14)	120.1
C(13)-C(14)-H(14)	120.1
C(14)-C(15)-C(16)	120.8(8)
C(14)-C(15)-H(15)	119.6
C(16)-C(15)-H(15)	119.6
C(15)-C(16)-C(11)	121.1(7)
C(15)-C(16)-H(16)	119.5
C(11)-C(16)-H(16)	119.5
C(26)-C(21)-C(22)	117.3(6)
C(26)-C(21)-P(1)	122.9(5)
C(22)-C(21)-P(1)	119.8(5)
C(23)-C(22)-C(21)	121.0(7)
C(23)-C(22)-H(22)	119.5
C(21)-C(22)-H(22)	119.5
C(24)-C(23)-C(22)	120.2(8)
C(24)-C(23)-H(23)	119.9
C(22)-C(23)-H(23)	119.9
C(23)-C(24)-C(25)	119.4(7)
C(23)-C(24)-H(24)	120.3
C(25)-C(24)-H(24)	120.3
C(24)-C(25)-C(26)	120.8(8)
C(24)-C(25)-H(25)	119.6
C(26)-C(25)-H(25)	119.6
C(25)-C(26)-C(21)	121.3(7)

C(25)-C(26)-H(26)	119.4
C(21)-C(26)-H(26)	119.4
C(20)-C(10)-P(1)	108.6(4)
C(20)-C(10)-H(101)	110.0
P(1)-C(10)-H(101)	110.0
C(20)-C(10)-H(102)	110.0
P(1)-C(10)-H(102)	110.0
H(101)-C(10)-H(102)	108.4
C(10)-C(20)-P(2)	109.3(4)
C(10)-C(20)-H(201)	109.8
P(2)-C(20)-H(201)	109.8
C(10)-C(20)-H(202)	109.8
P(2)-C(20)-H(202)	109.8
H(201)-C(20)-H(202)	108.3
C(41)-P(2)-C(20)	103.0(3)
C(41)-P(2)-C(31)	102.0(3)
C(20)-P(2)-C(31)	103.0(3)
C(41)-P(2)-Mo	120.0(2)
C(20)-P(2)-Mo	110.72(19)
C(31)-P(2)-Mo	116.15(19)
C(32)-C(31)-C(36)	116.7(6)
C(32)-C(31)-P(2)	123.8(5)
C(36)-C(31)-P(2)	119.5(4)
C(31)-C(32)-C(33)	120.6(7)
C(31)-C(32)-H(32)	119.7
C(33)-C(32)-H(32)	119.7
C(34)-C(33)-C(32)	120.7(7)
C(34)-C(33)-H(33)	119.7
C(32)-C(33)-H(33)	119.7
C(35)-C(34)-C(33)	119.6(7)
C(35)-C(34)-H(34)	120.2
C(33)-C(34)-H(34)	120.2
C(34)-C(35)-C(36)	120.4(7)
C(34)-C(35)-H(35)	119.8
C(36)-C(35)-H(35)	119.8
C(35)-C(36)-C(31)	122.0(6)
C(35)-C(36)-H(36)	119.0
C(31)-C(36)-H(36)	119.0
C(46)-C(41)-C(42)	118.2(6)
C(46)-C(41)-P(2)	119.0(5)
C(42)-C(41)-P(2)	122.8(5)
C(43)-C(42)-C(41)	119.3(7)
C(43)-C(42)-H(42)	120.3
C(41)-C(42)-H(42)	120.3
C(44)-C(43)-C(42)	123.1(7)
C(44)-C(43)-H(43)	118.5
C(42)-C(43)-H(43)	118.5
C(43)-C(44)-C(45)	118.1(7)

C(43)-C(44)-H(44)	120.9
C(45)-C(44)-H(44)	120.9
C(44)-C(45)-C(46)	121.5(7)
C(44)-C(45)-H(45)	119.3
C(46)-C(45)-H(45)	119.3
C(41)-C(46)-C(45)	119.8(6)
C(41)-C(46)-H(46)	120.1
C(45)-C(46)-H(46)	120.1
C(6)-C(2)-C(3)	107.8(11)
C(6)-C(2)-Mo	72.5(7)
C(3)-C(2)-Mo	70.7(7)
C(2)-C(3)-C(4)	103.7(12)
C(2)-C(3)-Mo	72.8(7)
C(4)-C(3)-Mo	71.0(7)
C(5)-C(4)-C(3)	110.3(13)
C(5)-C(4)-Mo	74.5(8)
C(3)-C(4)-Mo	71.8(7)
C(4)-C(5)-C(6)	109.7(13)
C(4)-C(5)-Mo	71.8(8)
C(6)-C(5)-Mo	73.0(7)
C(5)-C(6)-C(2)	108.5(12)
C(5)-C(6)-Mo	72.3(7)
C(2)-C(6)-Mo	72.1(7)
C(3')-C(2')-C(6')	110.2(14)
C(3')-C(2')-Mo	71.8(8)
C(6')-C(2')-Mo	75.0(9)
C(2')-C(3')-C(4')	110.3(13)
C(2')-C(3')-Mo	73.4(8)
C(4')-C(3')-Mo	73.2(7)
C(5')-C(4')-C(3')	104.3(12)
C(5')-C(4')-Mo	72.8(8)
C(3')-C(4')-Mo	70.0(7)
C(4')-C(5')-C(6')	110.1(13)
C(4')-C(5')-Mo	71.4(8)
C(6')-C(5')-Mo	73.2(8)
C(2')-C(6')-C(5')	105.0(13)
C(2')-C(6')-Mo	69.5(8)
C(5')-C(6')-Mo	70.9(8)
C(51')-C(51)-C(52)	123(3)
C(51')-C(51)-C(56)	111(3)
C(52)-C(51)-C(56)	126(2)
C(51)-C(52)-C(53)	117.8(16)
C(53')-C(53)-C(54)	123(3)
C(53')-C(53)-C(52)	116(3)
C(54)-C(53)-C(52)	121(2)
C(55)-C(54)-C(53)	116(2)
C(54)-C(55)-C(56)	133(3)
C(55)-C(56)-C(51)	106(2)

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for CpMo(CO)(dppe)H.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mo	53(1)	33(1)	37(1)	12(1)	16(1)	9(1)
C(1)	65(5)	43(4)	52(4)	9(3)	29(4)	6(3)
O(1)	63(4)	82(4)	101(4)	7(3)	38(3)	17(3)
P(1)	49(1)	33(1)	34(1)	6(1)	15(1)	8(1)
C(11)	47(4)	37(3)	49(4)	10(3)	19(3)	13(3)
C(12)	45(4)	81(5)	48(4)	20(4)	18(3)	14(4)
C(13)	65(6)	105(7)	54(5)	29(4)	5(4)	21(5)
C(14)	39(5)	93(6)	84(6)	28(5)	1(4)	12(4)
C(15)	47(5)	122(7)	88(6)	36(5)	30(5)	17(5)
C(16)	61(5)	100(6)	53(4)	12(4)	27(4)	15(4)
C(21)	49(4)	38(3)	29(3)	6(2)	8(3)	15(3)
C(22)	78(5)	38(4)	70(5)	10(3)	30(4)	9(4)
C(23)	110(7)	38(4)	75(5)	9(4)	22(5)	3(4)
C(24)	118(8)	36(4)	63(5)	2(3)	3(5)	29(5)
C(25)	81(6)	72(5)	58(5)	2(4)	18(4)	41(5)
C(26)	62(5)	38(3)	44(4)	1(3)	6(3)	11(3)
C(10)	67(5)	39(3)	39(3)	9(3)	19(3)	8(3)
C(20)	59(4)	42(3)	34(3)	16(3)	14(3)	8(3)
P(2)	44(1)	37(1)	35(1)	6(1)	13(1)	7(1)
C(31)	46(4)	38(3)	37(3)	6(3)	19(3)	14(3)
C(32)	58(5)	49(4)	48(4)	2(3)	16(3)	2(3)
C(33)	87(6)	50(4)	61(5)	-9(3)	37(5)	-10(4)
C(34)	86(6)	53(4)	78(5)	6(4)	52(5)	20(4)
C(35)	59(5)	63(5)	69(5)	13(4)	23(4)	26(4)
C(36)	55(5)	50(4)	52(4)	3(3)	17(4)	7(3)
C(41)	53(4)	50(4)	35(3)	4(3)	17(3)	16(3)
C(42)	42(4)	74(5)	58(4)	22(4)	1(4)	-1(4)
C(43)	59(5)	98(6)	59(5)	17(4)	1(4)	14(5)
C(44)	44(5)	85(6)	74(5)	8(5)	1(4)	5(4)
C(45)	50(5)	68(5)	76(5)	9(4)	16(4)	-6(4)
C(46)	58(5)	59(4)	61(4)	18(4)	15(4)	8(4)
C(51')	180(30)	130(20)	140(20)	94(18)	-43(19)	-46(19)
C(51)	64(9)	210(20)	164(15)	-6(15)	-37(9)	28(11)
C(52)	87(9)	198(15)	92(8)	30(9)	20(7)	21(10)
C(53')	87(18)	73(15)	330(50)	30(20)	10(20)	-7(14)
C(53)	82(10)	202(19)	156(15)	-31(15)	14(9)	-26(12)
C(54)	97(11)	280(30)	145(14)	-47(17)	56(10)	-78(16)

C(55)	95(12)	240(30)	240(30)	-110(20)	-13(15)	-70(19)
C(56)	92(13)	190(20)	250(30)	-66(18)	-6(13)	2(13)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for CpMo(CO)(dppe)H.

	x	y	z	U(eq)
H(1)	1400(60)	710(50)	1540(40)	63(18)
H(12)	-1153	-386	455	60(4)
H(13)	-3303	-713	-406	60(4)
H(14)	-4850	-937	410	60(4)
H(15)	-4244	-823	2067	60(4)
H(16)	-2103	-567	2927	60(4)
H(22)	-755	-2722	2061	60(4)
H(23)	-290	-4527	1416	60(4)
H(24)	1521	-4573	874	60(4)
H(25)	2842	-2808	947	60(4)
H(26)	2376	-1005	1558	60(4)
H(101)	-259	-187	3872	60(4)
H(102)	293	-1390	3670	60(4)
H(201)	2386	-439	4237	60(4)
H(202)	1713	47	5020	60(4)
H(32)	2630	3231	5974	60(4)
H(33)	1390	4369	6694	60(4)
H(34)	-803	4190	6001	60(4)
H(35)	-1754	2956	4551	60(4)
H(36)	-540	1877	3789	60(4)
H(42)	3869	777	5791	60(4)
H(43)	5943	1456	6732	60(4)
H(44)	7131	3103	6480	60(4)
H(45)	6246	4091	5221	60(4)
H(46)	4160	3454	4226	60(4)