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Supporting Information

Synthesis of and Small Molecule Coordination to Highly Electrophilic Cationic Mn(I) and Re(I) Carbonyl Complexes with Tied-Back Phosphites

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1. **Crystallographic Tables for [*cis*-Mn(P(OCH$_2$)$_3$CMe)(CO)$_4$(*cis*-cyclooctene)][BAr$_F$] (5c) (pp 2-21).**
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Table 1. Crystal data and structure refinement for $Mn(CO)_4(PO_3C_5H_9)(CCO)$.

Empirical formula	$C_{49}H_{27}BF_{24}MnO_7P$	
Formula weight	1280.43	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P 2_1/n$	
Unit cell dimensions	a = 18.1505(9) Å	α= 90°.
	b = 14.6079(7) Å	β= 101.339(1)°.
	c = 21.074(1) Å	γ = 90°.
Volume	5478.6(5) $Å^3$	
Z	4	
Density (calculated)	1.552 Mg/m^3	
Absorption coefficient	0.400 mm^{-1}	
Absorption correction	empirical (SADABS, Sheldrick, 1996)	
Tmin./Tmax.	0.88/0.94	
F(000)	2552	
Crystal size	0.16 x 0.18 x 0.32 mm^3	
Theta range for data collection	1.4 to 23.4°.	
Index ranges	-20<=h<=17, -13<=k<=16, -22<=l<=23	
Reflections collected	19915	
Independent reflections	7675 [R(int) = 0.0371]	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7675 / 0 / 939	
Goodness-of-fit on F^2	1.092	
Final R indices [I>2sigma(I)]	R1 = 0.0602, wR2 = 0.1761	
R indices (all data)	R1 = 0.0826, wR2 = 0.1948	
Largest diff. peak and hole	0.937 and -0.647 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $Mn(CO)_4(PO_3C_5H_9)(CCO)$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mn	9315(1)	12342(1)	16022(1)	46(1)
P	9031(1)	13755(1)	16326(1)	45(1)
B	9021(3)	12265(3)	11083(2)	37(1)
O(1)	9022(3)	13865(2)	17061(2)	84(1)
O(2)	9573(2)	14543(2)	16186(2)	75(1)
O(3)	8236(2)	14122(2)	15988(2)	66(1)
O(4)	9760(2)	10489(3)	15627(2)	100(2)
O(5)	8199(2)	11633(3)	16771(2)	95(1)
O(6)	8072(2)	12384(3)	14871(2)	82(1)
O(7)	10255(2)	13168(3)	15152(2)	81(1)
F(1)	11659(7)	10519(8)	13067(7)	95(4)
F(2)	11910(13)	11558(16)	12450(12)	127(10)
F(3)	11467(12)	10336(13)	12093(8)	106(8)
F(1')	11873(8)	11056(16)	13081(8)	158(9)
F(2')	11827(12)	11520(20)	12161(11)	107(7)
F(3')	11457(11)	10195(10)	12236(10)	108(8)
F(4)	9676(10)	12040(30)	14045(8)	184(12)
F(5)	8625(10)	12201(16)	13446(5)	101(4)
F(6)	9015(12)	10917(8)	13667(10)	121(6)
F(4')	9145(15)	12661(8)	13671(8)	113(4)
F(5')	8610(13)	11440(30)	13449(6)	165(9)
F(6')	9652(10)	11479(15)	14050(6)	118(8)
F(7)	7983(12)	15868(14)	12214(13)	113(8)
F(8)	8949(10)	15122(10)	12541(6)	120(6)
F(9)	8904(12)	16038(10)	11789(10)	134(8)
F(7')	8010(15)	15542(15)	12331(11)	135(9)
F(8')	9127(10)	15413(18)	12303(17)	250(20)
F(9')	8429(19)	16273(10)	11645(13)	228(15)
F(10)	6163(5)	14016(10)	10080(5)	87(3)
F(11)	6799(8)	15120(12)	9803(9)	141(8)
F(12)	6906(9)	13756(18)	9473(4)	164(7)

F(10')	6242(7)	14729(16)	10298(5)	167(6)
F(11')	6859(10)	14781(14)	9587(6)	118(8)
F(12')	6479(10)	13546(11)	9830(12)	171(9)
F(13)	9075(17)	9450(20)	9442(15)	122(8)
F(14)	8469(11)	8447(11)	9774(11)	123(8)
F(15)	9497(13)	8858(19)	10314(14)	114(9)
F(13')	8780(20)	9220(20)	9409(13)	198(18)
F(14')	8654(14)	8227(13)	10151(12)	148(10)
F(15')	9614(15)	9052(18)	10244(16)	97(6)
F(16)	6169(2)	10068(3)	10313(2)	114(1)
F(17)	6402(2)	10819(2)	11185(1)	73(1)
F(18)	6624(2)	9398(3)	11185(2)	108(1)
F(19)	9136(14)	12122(19)	8540(10)	183(12)
F(20)	8667(12)	13396(12)	8613(8)	126(7)
F(21)	9768(12)	13136(17)	8402(7)	165(9)
F(19')	9263(15)	12130(13)	8545(4)	176(14)
F(20')	8527(17)	13050(20)	8606(9)	238(15)
F(21')	9538(15)	13625(18)	8443(8)	212(10)
F(22)	11815(10)	13752(15)	10356(11)	167(10)
F(23)	11156(12)	14652(13)	11041(12)	157(8)
F(22')	11818(9)	13632(13)	10683(10)	149(8)
F(23')	11438(10)	14239(12)	11230(9)	120(6)
F(24)	11288(3)	14891(3)	10245(3)	163(2)
C(1)	10513(2)	12452(3)	16741(2)	42(1)
C(2)	10045(2)	12040(3)	17083(2)	46(1)
C(3)	10098(3)	11032(3)	17270(2)	64(1)
C(4)	10638(3)	10869(4)	17924(3)	84(2)
C(5)	11438(6)	10785(7)	17781(5)	75(5)
C(6)	11770(9)	11721(10)	17722(8)	71(5)
C(5')	11380(9)	11529(10)	18080(6)	69(6)
C(6')	11947(12)	11303(16)	17614(11)	79(7)
C(7)	11879(3)	12024(3)	17054(2)	57(1)
C(8)	11161(2)	11989(3)	16528(2)	46(1)
C(9)	9589(3)	11185(4)	15782(3)	64(1)
C(10)	8632(3)	11885(3)	16490(3)	62(1)
C(11)	8543(3)	12382(3)	15317(3)	61(1)

C(12)	9913(3)	12864(3)	15500(2)	56(1)
C(13)	8043(3)	15035(3)	16204(3)	74(2)
C(14)	8843(4)	14786(4)	17262(3)	94(2)
C(15)	9374(4)	15456(3)	16382(3)	87(2)
C(16)	8693(3)	15421(3)	16694(2)	63(1)
C(17)	8491(4)	16379(4)	16907(3)	101(2)
C(18)	9520(2)	11985(2)	11789(2)	35(1)
C(19)	10248(2)	11628(2)	11870(2)	39(1)
C(20)	10650(2)	11340(3)	12470(2)	43(1)
C(21)	10340(2)	11400(3)	13014(2)	46(1)
C(22)	9620(2)	11728(3)	12950(2)	44(1)
C(23)	9217(2)	12013(3)	12352(2)	40(1)
C(24)	11431(3)	10978(4)	12514(3)	68(1)
C(25)	9254(3)	11778(4)	13529(3)	66(1)
C(26)	8475(2)	13150(2)	11113(2)	35(1)
C(27)	8670(2)	13867(3)	11552(2)	42(1)
C(28)	8269(3)	14677(3)	11516(2)	50(1)
C(29)	7660(3)	14815(3)	11025(3)	59(1)
C(30)	7460(3)	14134(3)	10573(2)	54(1)
C(31)	7856(2)	13316(3)	10621(2)	42(1)
C(32)	8523(5)	15421(4)	12000(3)	78(2)
C(33)	6804(4)	14269(4)	10028(3)	75(2)
C(34)	8538(2)	11335(3)	10827(2)	39(1)
C(35)	8865(2)	10644(3)	10514(2)	47(1)
C(36)	8491(3)	9824(3)	10323(2)	52(1)
C(37)	7784(3)	9662(3)	10437(2)	49(1)
C(38)	7443(2)	10340(3)	10752(2)	43(1)
C(39)	7823(2)	11149(3)	10938(2)	41(1)
C(40)	8870(4)	9107(4)	9993(4)	79(2)
C(41)	6680(3)	10178(3)	10858(2)	55(1)
C(42)	9524(2)	12632(3)	10572(2)	42(1)
C(43)	9258(3)	12582(3)	9906(2)	54(1)
C(44)	9612(4)	13029(4)	9467(2)	68(2)
C(45)	10254(4)	13530(4)	9676(3)	75(2)
C(46)	10542(3)	13592(3)	10333(3)	65(1)
C(47)	10177(3)	13159(3)	10769(2)	50(1)

C(48)	9268(6)	12980(6)	8764(3)	103(2)
C(49)	11254(4)	14120(5)	10579(4)	90(2)

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Table 3. Bond lengths [Å] and angles [°] for $Mn(CO)_4(PO_3C_5H_9)(CCO)$.

Mn-C(11)	1.832(6)
Mn-C(12)	1.854(5)
Mn-C(10)	1.855(5)
Mn-C(9)	1.859(5)
Mn-P	2.2511(12)
Mn-C(1)	2.399(4)
Mn-C(2)	2.406(4)
P-O(1)	1.560(3)
P-O(3)	1.573(3)
P-O(2)	1.579(4)
B-C(42)	1.632(6)
B-C(18)	1.635(6)
B-C(26)	1.637(6)
B-C(34)	1.649(6)
O(1)-C(14)	1.466(6)
O(2)-C(15)	1.462(6)
O(3)-C(13)	1.474(6)
O(4)-C(9)	1.130(5)
O(5)-C(10)	1.134(6)
O(6)-C(11)	1.140(6)
O(7)-C(12)	1.139(5)
F(1)-C(24)	1.338(13)
F(2)-C(24)	1.24(2)
F(3)-C(24)	1.301(18)
F(1')-C(24)	1.308(15)
F(2')-C(24)	1.38(2)
F(3')-C(24)	1.289(18)
F(4)-C(25)	1.259(13)
F(5)-C(25)	1.279(10)
F(6)-C(25)	1.379(12)
F(4')-C(25)	1.347(11)
F(5')-C(25)	1.247(12)
F(6')-C(25)	1.268(10)
F(7)-C(32)	1.33(2)

F(8)-C(32)	1.321(15)
F(9)-C(32)	1.269(13)
F(7')-C(32)	1.28(3)
F(8')-C(32)	1.156(19)
F(9')-C(32)	1.445(19)
F(10)-C(33)	1.245(11)
F(11)-C(33)	1.329(16)
F(12)-C(33)	1.431(15)
F(10')-C(33)	1.430(12)
F(11')-C(33)	1.213(13)
F(12')-C(33)	1.241(15)
F(13)-C(40)	1.38(3)
F(14)-C(40)	1.241(18)
F(15)-C(40)	1.26(2)
F(13')-C(40)	1.22(3)
F(14')-C(40)	1.40(2)
F(15')-C(40)	1.35(3)
F(16)-C(41)	1.337(6)
F(17)-C(41)	1.320(5)
F(18)-C(41)	1.346(5)
F(19)-C(48)	1.34(2)
F(20)-C(48)	1.236(19)
F(21)-C(48)	1.315(19)
F(19')-C(48)	1.32(2)
F(20')-C(48)	1.32(3)
F(21')-C(48)	1.31(2)
F(22)-C(49)	1.317(18)
F(23)-C(49)	1.29(2)
F(23)-F(24)	1.78(3)
F(22')-C(49)	1.231(16)
F(22')-F(23')	1.70(3)
F(23')-C(49)	1.36(2)
F(24)-C(49)	1.336(8)
C(1)-C(2)	1.359(6)
C(1)-C(8)	1.500(5)
C(2)-C(3)	1.523(6)

C(3)-C(4)	1.544(8)
C(4)-C(5)	1.546(14)
C(4)-C(5')	1.637(18)
C(5)-C(6)	1.51(2)
C(6)-C(7)	1.53(2)
C(5')-C(6')	1.59(3)
C(6')-C(7)	1.57(2)
C(7)-C(8)	1.535(6)
C(13)-C(16)	1.514(7)
C(14)-C(16)	1.496(7)
C(15)-C(16)	1.511(8)
C(16)-C(17)	1.536(7)
C(18)-C(19)	1.399(5)
C(18)-C(23)	1.402(5)
C(19)-C(20)	1.395(6)
C(20)-C(21)	1.376(6)
C(20)-C(24)	1.499(7)
C(21)-C(22)	1.373(6)
C(22)-C(23)	1.391(5)
C(22)-C(25)	1.503(6)
C(26)-C(31)	1.391(5)
C(26)-C(27)	1.397(5)
C(27)-C(28)	1.384(6)
C(28)-C(29)	1.372(7)
C(28)-C(32)	1.499(7)
C(29)-C(30)	1.377(7)
C(30)-C(31)	1.387(6)
C(30)-C(33)	1.496(7)
C(34)-C(39)	1.391(6)
C(34)-C(35)	1.400(5)
C(35)-C(36)	1.397(6)
C(36)-C(37)	1.371(6)
C(36)-C(40)	1.497(7)
C(37)-C(38)	1.402(6)
C(38)-C(39)	1.385(6)
C(38)-C(41)	1.465(6)

C(42)-C(43)	1.393(6)
C(42)-C(47)	1.405(6)
C(43)-C(44)	1.389(7)
C(44)-C(45)	1.374(8)
C(44)-C(48)	1.492(9)
C(45)-C(46)	1.382(8)
C(46)-C(47)	1.386(6)
C(46)-C(49)	1.507(9)

C(11)-Mn-C(12)	87.1(2)
C(11)-Mn-C(10)	87.5(2)
C(12)-Mn-C(10)	173.9(2)
C(11)-Mn-C(9)	90.7(2)
C(12)-Mn-C(9)	89.7(2)
C(10)-Mn-C(9)	93.4(2)
C(11)-Mn-P	91.15(15)
C(12)-Mn-P	89.18(15)
C(10)-Mn-P	87.88(16)
C(9)-Mn-P	177.77(15)
C(11)-Mn-C(1)	164.64(19)
C(12)-Mn-C(1)	77.51(17)
C(10)-Mn-C(1)	107.81(19)
C(9)-Mn-C(1)	88.56(17)
P-Mn-C(1)	89.33(10)
C(11)-Mn-C(2)	162.4(2)
C(12)-Mn-C(2)	110.35(18)
C(10)-Mn-C(2)	75.08(19)
C(9)-Mn-C(2)	87.59(19)
P-Mn-C(2)	91.01(11)
C(1)-Mn-C(2)	32.86(13)
O(1)-P-O(3)	103.1(2)
O(1)-P-O(2)	103.8(2)
O(3)-P-O(2)	102.5(2)
O(1)-P-Mn	115.19(13)
O(3)-P-Mn	115.12(13)
O(2)-P-Mn	115.39(14)

C(42)-B-C(18)	113.7(3)
C(42)-B-C(26)	100.8(3)
C(18)-B-C(26)	113.2(3)
C(42)-B-C(34)	112.7(3)
C(18)-B-C(34)	104.7(3)
C(26)-B-C(34)	112.1(3)
C(14)-O(1)-P	115.3(3)
C(15)-O(2)-P	114.5(3)
C(13)-O(3)-P	114.9(3)
C(49)-F(23)-F(24)	48.6(10)
C(49)-F(22')-F(23')	52.2(10)
C(49)-F(23')-F(22')	45.7(9)
C(49)-F(24)-F(23)	46.2(7)
C(2)-C(1)-C(8)	124.6(4)
C(2)-C(1)-Mn	73.8(3)
C(8)-C(1)-Mn	116.6(3)
C(1)-C(2)-C(3)	123.5(4)
C(1)-C(2)-Mn	73.3(2)
C(3)-C(2)-Mn	114.4(3)
C(2)-C(3)-C(4)	112.1(4)
C(3)-C(4)-C(5)	107.1(6)
C(3)-C(4)-C(5')	116.3(6)
C(5)-C(4)-C(5')	47.0(6)
C(6)-C(5)-C(4)	110.5(10)
C(5)-C(6)-C(7)	117.7(12)
C(6')-C(5')-C(4)	111.1(13)
C(7)-C(6')-C(5')	111.2(13)
C(6)-C(7)-C(8)	114.2(6)
C(6)-C(7)-C(6')	27.8(7)
C(8)-C(7)-C(6')	116.8(10)
C(1)-C(8)-C(7)	111.9(3)
O(4)-C(9)-Mn	178.7(5)
O(5)-C(10)-Mn	177.6(5)
O(6)-C(11)-Mn	177.9(5)
O(7)-C(12)-Mn	176.5(4)
O(3)-C(13)-C(16)	110.3(4)

O(1)-C(14)-C(16)	110.7(4)
O(2)-C(15)-C(16)	111.2(4)
C(14)-C(16)-C(15)	109.5(5)
C(14)-C(16)-C(13)	108.0(5)
C(15)-C(16)-C(13)	108.0(5)
C(14)-C(16)-C(17)	110.4(5)
C(15)-C(16)-C(17)	111.0(5)
C(13)-C(16)-C(17)	109.9(4)
C(19)-C(18)-C(23)	115.2(3)
C(19)-C(18)-B	123.0(3)
C(23)-C(18)-B	121.6(3)
C(20)-C(19)-C(18)	122.4(4)
C(21)-C(20)-C(19)	120.6(4)
C(21)-C(20)-C(24)	120.5(4)
C(19)-C(20)-C(24)	118.9(4)
C(22)-C(21)-C(20)	118.5(4)
C(21)-C(22)-C(23)	120.9(4)
C(21)-C(22)-C(25)	120.1(4)
C(23)-C(22)-C(25)	118.9(4)
C(22)-C(23)-C(18)	122.3(4)
F(2)-C(24)-F(3')	117.9(16)
F(2)-C(24)-F(3)	106.8(16)
F(3')-C(24)-F(3)	16.4(15)
F(2)-C(24)-F(1')	73.8(15)
F(3')-C(24)-F(1')	114.9(14)
F(3)-C(24)-F(1')	125.6(13)
F(2)-C(24)-F(1)	109.4(13)
F(3')-C(24)-F(1)	85.3(11)
F(3)-C(24)-F(1)	100.6(10)
F(1')-C(24)-F(1)	38.5(10)
F(2)-C(24)-F(2')	25.8(19)
F(3')-C(24)-F(2')	101.4(15)
F(3)-C(24)-F(2')	87.0(16)
F(1')-C(24)-F(2')	98.7(13)
F(1)-C(24)-F(2')	130.7(11)
F(2)-C(24)-C(20)	115.3(11)

F(3')-C(24)-C(20)	113.8(10)
F(3)-C(24)-C(20)	112.7(10)
F(1')-C(24)-C(20)	115.4(9)
F(1)-C(24)-C(20)	111.0(7)
F(2')-C(24)-C(20)	110.4(11)
F(5')-C(25)-F(4)	129.2(11)
F(5')-C(25)-F(6')	110.0(12)
F(4)-C(25)-F(6')	37.8(12)
F(5')-C(25)-F(5)	52.0(11)
F(4)-C(25)-F(5)	110.4(11)
F(6')-C(25)-F(5)	128.9(9)
F(5')-C(25)-F(4')	103.4(13)
F(4)-C(25)-F(4')	67.1(11)
F(6')-C(25)-F(4')	102.8(9)
F(5)-C(25)-F(4')	53.3(7)
F(5')-C(25)-F(6)	49.2(13)
F(4)-C(25)-F(6)	104.9(13)
F(6')-C(25)-F(6)	69.7(9)
F(5)-C(25)-F(6)	99.3(10)
F(4')-C(25)-F(6)	139.5(8)
F(5')-C(25)-C(22)	115.0(7)
F(4)-C(25)-C(22)	115.0(9)
F(6')-C(25)-C(22)	114.8(8)
F(5)-C(25)-C(22)	115.9(6)
F(4')-C(25)-C(22)	109.5(6)
F(6)-C(25)-C(22)	109.5(7)
C(31)-C(26)-C(27)	115.2(3)
C(31)-C(26)-B	121.0(3)
C(27)-C(26)-B	122.7(3)
C(28)-C(27)-C(26)	122.8(4)
C(29)-C(28)-C(27)	120.3(4)
C(29)-C(28)-C(32)	120.0(5)
C(27)-C(28)-C(32)	119.6(5)
C(28)-C(29)-C(30)	118.6(4)
C(29)-C(30)-C(31)	120.6(4)
C(29)-C(30)-C(33)	119.8(4)

C(31)-C(30)-C(33)	119.6(5)
C(30)-C(31)-C(26)	122.4(4)
F(8')-C(32)-F(9)	71.1(17)
F(8')-C(32)-F(7')	114(2)
F(9)-C(32)-F(7')	126.7(13)
F(8')-C(32)-F(8)	36(2)
F(9)-C(32)-F(8)	105.7(14)
F(7')-C(32)-F(8)	86.5(15)
F(8')-C(32)-F(7)	120.0(16)
F(9)-C(32)-F(7)	105.0(13)
F(7')-C(32)-F(7)	23.5(19)
F(8)-C(32)-F(7)	102.4(15)
F(8')-C(32)-F(9')	107.3(19)
F(9)-C(32)-F(9')	39.0(13)
F(7')-C(32)-F(9')	98.0(16)
F(8)-C(32)-F(9')	136.2(14)
F(7)-C(32)-F(9')	74.5(15)
F(8')-C(32)-C(28)	120.0(10)
F(9)-C(32)-C(28)	113.2(9)
F(7')-C(32)-C(28)	108.2(12)
F(8)-C(32)-C(28)	113.4(8)
F(7)-C(32)-C(28)	116.1(12)
F(9')-C(32)-C(28)	106.5(11)
F(11')-C(33)-F(12')	111.8(14)
F(11')-C(33)-F(10)	118.0(10)
F(12')-C(33)-F(10)	52.3(11)
F(11')-C(33)-F(11)	31.4(12)
F(12')-C(33)-F(11)	134.9(11)
F(10)-C(33)-F(11)	111.5(9)
F(11')-C(33)-F(10')	100.9(10)
F(12')-C(33)-F(10')	101.9(13)
F(10)-C(33)-F(10')	49.7(7)
F(11)-C(33)-F(10')	75.3(11)
F(11')-C(33)-F(12)	69.7(10)
F(12')-C(33)-F(12)	53.7(11)
F(10)-C(33)-F(12)	101.0(12)

F(11)-C(33)-F(12)	101.1(11)
F(10')-C(33)-F(12)	142.1(9)
F(11')-C(33)-C(30)	119.8(10)
F(12')-C(33)-C(30)	113.5(7)
F(10)-C(33)-C(30)	120.7(6)
F(11)-C(33)-C(30)	110.2(9)
F(10')-C(33)-C(30)	106.2(6)
F(12)-C(33)-C(30)	110.2(6)
C(39)-C(34)-C(35)	115.8(4)
C(39)-C(34)-B	124.0(3)
C(35)-C(34)-B	120.0(4)
C(36)-C(35)-C(34)	121.8(4)
C(37)-C(36)-C(35)	121.1(4)
C(37)-C(36)-C(40)	119.5(4)
C(35)-C(36)-C(40)	119.4(5)
C(36)-C(37)-C(38)	118.4(4)
C(39)-C(38)-C(37)	119.7(4)
C(39)-C(38)-C(41)	121.8(4)
C(37)-C(38)-C(41)	118.5(4)
C(38)-C(39)-C(34)	123.2(4)
F(13')-C(40)-F(14)	77.3(19)
F(13')-C(40)-F(15)	121(2)
F(14)-C(40)-F(15)	112.2(18)
F(13')-C(40)-F(15')	109(2)
F(14)-C(40)-F(15')	124.5(14)
F(15)-C(40)-F(15')	17(2)
F(13')-C(40)-F(13)	27(3)
F(14)-C(40)-F(13)	101.7(17)
F(15)-C(40)-F(13)	101(2)
F(15')-C(40)-F(13)	86(2)
F(13')-C(40)-F(14')	112(2)
F(14)-C(40)-F(14')	37.4(13)
F(15)-C(40)-F(14')	82.7(18)
F(15')-C(40)-F(14')	99.0(15)
F(13)-C(40)-F(14')	131.7(15)
F(13')-C(40)-C(36)	112.8(14)

F(14)-C(40)-C(36)	115.3(11)
F(15)-C(40)-C(36)	113.7(14)
F(15')-C(40)-C(36)	112.0(13)
F(13)-C(40)-C(36)	111.2(14)
F(14')-C(40)-C(36)	110.8(11)
F(17)-C(41)-F(16)	105.2(4)
F(17)-C(41)-F(18)	105.0(4)
F(16)-C(41)-F(18)	103.2(4)
F(17)-C(41)-C(38)	115.8(4)
F(16)-C(41)-C(38)	113.9(4)
F(18)-C(41)-C(38)	112.6(4)
C(43)-C(42)-C(47)	115.5(4)
C(43)-C(42)-B	121.3(4)
C(47)-C(42)-B	122.3(3)
C(44)-C(43)-C(42)	122.2(5)
C(45)-C(44)-C(43)	120.7(5)
C(45)-C(44)-C(48)	120.5(6)
C(43)-C(44)-C(48)	118.8(7)
C(44)-C(45)-C(46)	119.1(5)
C(45)-C(46)-C(47)	119.9(5)
C(45)-C(46)-C(49)	120.5(5)
C(47)-C(46)-C(49)	119.6(5)
C(46)-C(47)-C(42)	122.7(4)
F(20)-C(48)-F(21')	85.0(14)
F(20)-C(48)-F(21)	116.2(14)
F(21')-C(48)-F(21)	37.3(12)
F(20)-C(48)-F(19')	115.2(16)
F(21')-C(48)-F(19')	118.3(13)
F(21)-C(48)-F(19')	85.4(13)
F(20)-C(48)-F(20')	25(2)
F(21')-C(48)-F(20')	106.3(17)
F(21)-C(48)-F(20')	128.6(14)
F(19')-C(48)-F(20')	92.5(18)
F(20)-C(48)-F(19)	106.3(18)
F(21')-C(48)-F(19)	123.3(16)
F(21)-C(48)-F(19)	93.1(15)

F(19')-C(48)-F(19)	10(2)
F(20')-C(48)-F(19)	83.0(19)
F(20)-C(48)-C(44)	114.0(9)
F(21')-C(48)-C(44)	110.6(13)
F(21)-C(48)-C(44)	111.5(12)
F(19')-C(48)-C(44)	111.4(7)
F(20')-C(48)-C(44)	116.9(10)
F(19)-C(48)-C(44)	113.9(11)
F(22')-C(49)-F(23)	116.7(15)
F(22')-C(49)-F(22)	32.2(14)
F(23)-C(49)-F(22)	138.5(16)
F(22')-C(49)-F(24)	117.3(11)
F(23)-C(49)-F(24)	85.3(11)
F(22)-C(49)-F(24)	92.0(10)
F(22')-C(49)-F(23')	82.1(14)
F(23)-C(49)-F(23')	36.9(10)
F(22)-C(49)-F(23')	111.1(14)
F(24)-C(49)-F(23')	113.4(10)
F(22')-C(49)-C(46)	113.0(10)
F(23)-C(49)-C(46)	109.5(11)
F(22)-C(49)-C(46)	109.8(12)
F(24)-C(49)-C(46)	112.1(7)
F(23')-C(49)-C(46)	116.0(8)

Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Mn(CO)_4(PO_3C_5H_9)(CCO)$.

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn	48(1)	40(1)	47(1)	-6(1)	3(1)	-6(1)
P	53(1)	40(1)	39(1)	1(1)	0(1)	-2(1)
B	40(3)	38(2)	32(2)	-3(2)	5(2)	7(2)
O(1)	158(4)	50(2)	42(2)	1(2)	15(2)	29(2)
O(2)	75(2)	49(2)	101(3)	-8(2)	22(2)	-10(2)
O(3)	68(2)	54(2)	69(2)	-10(2)	-7(2)	8(2)
O(4)	71(3)	68(2)	148(4)	-62(3)	-8(2)	-1(2)
O(5)	63(2)	98(3)	131(4)	34(3)	34(2)	-7(2)
O(6)	69(2)	91(3)	71(2)	-17(2)	-25(2)	0(2)
O(7)	97(3)	100(3)	48(2)	-5(2)	18(2)	-29(2)
F(1)	74(8)	136(8)	65(7)	28(7)	-10(6)	66(6)
F(2)	59(6)	81(8)	230(30)	20(14)	0(14)	2(5)
F(3)	93(11)	150(18)	67(5)	-27(7)	-2(5)	61(11)
F(1')	64(7)	310(30)	76(8)	-39(15)	-40(6)	44(12)
F(2')	45(8)	139(13)	142(13)	63(10)	30(9)	16(7)
F(3')	77(9)	42(5)	210(20)	0(8)	52(11)	15(5)
F(4)	138(16)	350(30)	71(11)	-124(16)	32(10)	-90(20)
F(5)	108(9)	144(11)	63(6)	31(8)	49(7)	49(9)
F(6)	177(16)	109(7)	101(12)	28(7)	90(12)	-1(9)
F(4')	188(13)	85(6)	89(8)	12(5)	84(9)	45(8)
F(5')	154(16)	280(20)	72(8)	-31(15)	45(9)	-135(18)
F(6')	155(16)	173(13)	26(6)	38(8)	16(7)	83(14)
F(7)	101(9)	78(10)	166(15)	-57(9)	35(7)	35(8)
F(8)	177(18)	77(6)	79(6)	-52(5)	-41(7)	35(8)
F(9)	206(19)	66(11)	150(14)	-43(9)	84(14)	-68(12)
F(7')	177(18)	119(17)	118(11)	-82(12)	53(11)	-21(13)
F(8')	67(7)	200(30)	440(40)	-240(30)	-26(18)	-6(13)
F(9')	470(40)	40(5)	170(15)	-26(7)	60(20)	18(13)
F(10)	51(5)	121(8)	84(7)	60(6)	0(4)	-16(6)
F(11)	84(8)	107(9)	200(18)	101(11)	-53(11)	3(6)
F(12)	137(11)	280(20)	56(5)	4(8)	-31(5)	122(12)

F(10')	86(8)	336(19)	78(6)	22(10)	14(5)	111(11)
F(11')	108(8)	200(20)	48(5)	61(8)	18(5)	-27(10)
F(12')	105(12)	133(11)	220(20)	45(12)	-107(12)	-11(9)
F(13)	162(15)	117(9)	105(17)	-33(9)	67(14)	30(10)
F(14)	100(8)	66(12)	210(20)	-92(13)	40(13)	-9(10)
F(15)	94(14)	105(17)	134(12)	-16(9)	1(12)	65(14)
F(13')	270(40)	250(40)	65(13)	-56(19)	-2(16)	180(30)
F(14')	151(19)	48(6)	270(30)	-38(11)	113(18)	12(7)
F(15')	84(9)	66(7)	155(14)	-35(8)	54(9)	8(5)
F(16)	53(2)	188(4)	93(3)	-56(2)	-8(2)	-3(2)
F(17)	66(2)	67(2)	89(2)	-19(2)	26(2)	-5(1)
F(20)	143(13)	137(7)	74(8)	1(5)	-37(7)	97(8)
F(21)	183(14)	280(30)	47(7)	-19(11)	63(8)	-7(14)
F(19')	340(30)	143(12)	13(3)	-25(4)	-29(6)	119(15)
F(20')	169(17)	490(40)	46(8)	-48(14)	-6(8)	60(20)
F(21')	260(20)	300(30)	87(11)	131(15)	64(11)	62(17)
F(22)	110(12)	141(13)	290(20)	-50(14)	137(16)	-19(10)
F(23)	164(18)	120(13)	200(20)	-50(12)	76(15)	-68(10)
F(22')	85(10)	92(8)	240(20)	-29(11)	-54(11)	10(8)
F(23')	111(11)	155(16)	95(8)	-10(9)	27(7)	-71(10)
F(24)	174(5)	108(3)	219(6)	51(4)	71(4)	-34(3)
C(1)	46(2)	41(2)	36(2)	-4(2)	5(2)	-2(2)
C(2)	49(3)	44(2)	45(2)	3(2)	10(2)	0(2)
C(3)	72(3)	50(3)	73(3)	16(2)	18(3)	0(2)
C(4)	75(4)	85(4)	92(4)	54(3)	14(3)	13(3)
C(5)	77(8)	60(8)	76(7)	20(6)	-13(5)	19(6)
C(6)	55(9)	68(10)	74(10)	13(7)	-27(7)	-6(6)
C(5')	87(11)	74(11)	42(8)	9(7)	1(7)	19(8)
C(6')	69(12)	85(16)	83(12)	38(11)	18(8)	28(11)
C(7)	53(3)	59(3)	55(3)	-3(2)	1(2)	2(2)
C(8)	48(3)	48(2)	44(2)	-7(2)	13(2)	-1(2)
C(9)	50(3)	58(3)	79(4)	-27(3)	-3(2)	-13(2)
C(10)	54(3)	56(3)	76(3)	10(3)	9(3)	-2(2)
C(11)	61(3)	49(3)	69(3)	-12(2)	3(3)	-4(2)
C(12)	65(3)	60(3)	39(3)	-10(2)	2(2)	-12(2)
C(13)	77(4)	59(3)	79(4)	-13(3)	-1(3)	20(3)

C(14)	155(6)	65(3)	56(3)	-10(3)	10(3)	33(4)
C(15)	102(5)	47(3)	108(5)	-8(3)	11(4)	-3(3)
C(16)	72(3)	43(3)	67(3)	-7(2)	-3(3)	8(2)
C(17)	129(6)	54(3)	108(5)	-26(3)	-7(4)	15(3)
C(18)	40(2)	27(2)	38(2)	-6(2)	5(2)	1(2)
C(19)	44(2)	33(2)	39(2)	-4(2)	5(2)	2(2)
C(20)	47(3)	37(2)	42(2)	1(2)	-3(2)	7(2)
C(21)	58(3)	38(2)	35(2)	4(2)	-8(2)	-1(2)
C(22)	61(3)	36(2)	33(2)	1(2)	8(2)	-3(2)
C(23)	45(2)	39(2)	36(2)	-1(2)	9(2)	0(2)
C(24)	58(3)	69(4)	70(4)	7(3)	-1(3)	14(3)
C(26)	38(2)	35(2)	34(2)	0(2)	9(2)	5(2)
C(27)	45(2)	40(2)	41(2)	-3(2)	10(2)	-1(2)
C(28)	60(3)	35(2)	61(3)	-1(2)	28(2)	6(2)
C(29)	64(3)	36(2)	84(4)	10(2)	33(3)	19(2)
C(30)	51(3)	56(3)	56(3)	21(2)	14(2)	16(2)
C(31)	46(2)	43(2)	37(2)	1(2)	6(2)	6(2)
C(32)	111(6)	40(3)	96(5)	-21(3)	50(5)	-7(3)
C(33)	66(4)	73(4)	81(4)	29(3)	2(3)	21(3)
C(34)	47(2)	38(2)	31(2)	-5(2)	1(2)	12(2)
C(35)	44(2)	48(3)	48(2)	-11(2)	2(2)	12(2)
C(36)	53(3)	44(3)	54(3)	-18(2)	0(2)	14(2)
C(37)	55(3)	36(2)	49(3)	-11(2)	-8(2)	6(2)
C(38)	44(2)	37(2)	43(2)	-1(2)	-5(2)	6(2)
C(39)	48(3)	39(2)	33(2)	-9(2)	2(2)	8(2)
C(40)	77(5)	65(4)	95(5)	-35(4)	16(4)	11(4)
C(41)	64(3)	31(2)	66(3)	3(2)	2(2)	2(2)
C(42)	52(3)	40(2)	35(2)	1(2)	13(2)	17(2)
C(43)	66(3)	59(3)	37(3)	1(2)	10(2)	30(2)
C(44)	98(4)	73(3)	41(3)	16(2)	31(3)	46(3)
C(45)	103(5)	64(3)	72(4)	22(3)	50(4)	28(3)
C(46)	81(4)	50(3)	73(4)	15(2)	38(3)	16(3)
C(47)	58(3)	45(2)	49(3)	5(2)	20(2)	13(2)
C(48)	159(8)	112(6)	43(4)	16(4)	29(4)	38(6)
C(49)	99(5)	63(4)	120(6)	9(4)	52(5)	-21(4)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $Mn(CO)_4(PO_3C_5H_9)(CCO)$.

	x	y	z	U(eq)
H(1A)	10633	13082	16884	50
H(2A)	9910	12435	17419	55
H(3A)	10272	10686	16935	77
H(3B)	9601	10808	17298	77
H(8A)	11255	12285	16140	56
H(8B)	11032	11355	16424	56
H(13A)	7602	14992	16397	89
H(13B)	7928	15443	15835	89
H(14A)	9260	15017	17582	112
H(14B)	8404	14758	17460	112
H(15A)	9269	15851	16005	104
H(15B)	9795	15713	16685	104
H(17A)	8058	16339	17104	152
H(17B)	8382	16775	16536	152
H(17C)	8906	16623	17214	152
H(19A)	10472	11581	11510	47
H(21A)	10612	11222	13416	55
H(23A)	8731	12231	12324	48
H(27A)	9088	13796	11884	50
H(29A)	7388	15358	10999	71
H(31A)	7702	12862	10314	51
H(35A)	9345	10733	10432	57
H(37A)	7537	9115	10309	59
H(39A)	7588	11590	11147	49
H(43A)	8829	12238	9751	65
H(45A)	10492	13823	9381	90
H(47A)	10371	13220	11209	60

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Table 1. Crystal data and structure refinement for $\{[Re(CO)_4(PO_3C_5H_9)]_2(\mu\text{-}H)\}BArF$.

Empirical formula	$C_{50}\ H_{31}\ B\ F_{24}\ O_{14}\ P_2\ Re_2$	
Formula weight	1756.90	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 19.707(1) Å	α= 90°.
	b = 16.5848(8) Å	β= 94.600(1)°.
	c = 18.538(1) Å	γ = 90°.
Volume	6039.5(5) $Å^3$	
Z	4	
Density (calculated)	1.932 Mg/m^3	
Absorption coefficient	4.193 mm^{-1}	
Absorption correction	empirical (SADABS, Sheldrick, 1996)	
Tmin./Tmax.	0.36/0.78	
F(000)	3376	
Crystal size	0.06 x 0.12 x 0.24 mm^3	
Theta range for data collection	1.6 to 23.3°	
Index ranges	-21<=h<=21, -18<=k<=18, -20<=l<=18	
Reflections collected	9725	
Independent reflections	4126 [R(int) = 0.0179]	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4126 / 0 / 421	
Goodness-of-fit on F^2	1.408	
Final R indices [I>2sigma(I)]	R1 = 0.0277, wR2 = 0.0811	
R indices (all data)	R1 = 0.0308, wR2 = 0.0834	
Largest diff. peak and hole	1.040 and -1.040 $e.Å^{-3}$	

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for {[$Re(CO)_4(PO_3C_5H_9)]_2(\mu$-H)}BArF. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	607(1)	5398(1)	1879(1)	33(1)
B(1)	0	1009(4)	2500	23(1)
P(1)	1434(1)	5737(1)	2832(1)	32(1)
O(1)	1669(2)	5000(2)	3340(2)	38(1)
O(2)	2130(2)	6103(2)	2606(2)	45(1)
O(3)	1186(2)	6383(2)	3388(2)	40(1)
O(4)	1682(2)	5295(4)	763(3)	93(2)
O(5)	829(2)	3602(3)	2338(2)	71(1)
O(6)	-498(2)	4925(2)	649(2)	49(1)
O(7)	413(3)	7247(3)	1603(3)	96(2)
F(1)	-681(2)	2360(2)	4994(2)	75(1)
F(2)	-120(2)	3407(3)	5081(3)	117(2)
F(3)	-903(3)	3269(4)	4256(2)	139(2)
F(4)	2207(2)	2767(3)	3209(2)	108(2)
F(5)	2343(2)	2011(3)	4096(3)	101(2)
F(6)	2115(2)	3227(3)	4253(3)	101(2)
F(7)	1936(3)	-1834(3)	2993(3)	128(2)
F(8)	1786(4)	-933(5)	3713(2)	211(4)
F(9)	2556(2)	-882(4)	2990(3)	132(2)
F(10)	279(2)	-1022(3)	309(2)	112(2)
F(11)	1060(4)	-291(3)	95(2)	148(3)
F(12)	1265(3)	-1447(4)	430(3)	160(3)
C(1)	2170(2)	5198(3)	3939(3)	42(1)
C(2)	2623(2)	6297(3)	3213(3)	41(1)
C(3)	1684(2)	6570(3)	3993(3)	41(1)
C(4)	2337(2)	6099(3)	3930(2)	37(1)
C(5)	2859(2)	6320(4)	4558(3)	51(1)
C(6)	1293(3)	5328(4)	1187(3)	59(2)
C(7)	744(3)	4248(4)	2165(3)	47(1)
C(8)	-109(2)	5094(3)	1110(3)	37(1)

C(9)	483(3)	6576(4)	1688(3)	58(2)
C(10)	302(2)	1606(2)	3144(2)	24(1)
C(11)	-128(2)	1990(3)	3604(2)	27(1)
C(12)	99(2)	2540(3)	4118(2)	30(1)
C(12A)	-400(3)	2898(3)	4603(3)	42(1)
C(13)	778(2)	2755(3)	4207(3)	39(1)
C(14)	1222(2)	2401(3)	3762(2)	30(1)
C(14A)	1959(3)	2603(3)	3832(3)	47(1)
C(15)	984(2)	1836(3)	3244(2)	27(1)
C(16)	567(2)	374(2)	2228(3)	24(1)
C(17)	1024(2)	-26(3)	2723(2)	29(1)
C(18)	1437(2)	-643(3)	2524(3)	37(1)
C(18A)	1914(3)	-1044(4)	3080(3)	61(2)
C(19)	1401(2)	-913(3)	1811(3)	40(1)
C(20)	954(2)	-538(3)	1310(3)	33(1)
C(20A)	895(2)	-832(4)	550(3)	49(1)
C(21)	551(2)	89(3)	1511(2)	28(1)

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Table 3. Bond lengths [Å] and angles [°] for $\{[Re(CO)_4(PO_3C_5H_9)]_2(\mu\text{-}H)\}BArF$.

Re(1)-H	1.762(19)
Re(1)-C(6)	1.941(6)
Re(1)-C(8)	1.988(5)
Re(1)-C(7)	1.992(6)
Re(1)-C(9)	1.996(7)
Re(1)-P(1)	2.3735(12)
B(1)-C(10)	1.627(6)
B(1)-C(10)#1	1.627(6)
B(1)-C(16)#1	1.644(6)
B(1)-C(16)	1.644(6)
P(1)-O(2)	1.586(3)
P(1)-O(1)	1.590(4)
P(1)-O(3)	1.590(3)
O(1)-C(1)	1.463(6)
O(2)-C(2)	1.462(6)
O(3)-C(3)	1.462(6)
O(4)-C(6)	1.143(7)
O(5)-C(7)	1.127(6)
O(6)-C(8)	1.137(5)
O(7)-C(9)	1.131(7)
F(1)-C(12A)	1.301(6)
F(2)-C(12A)	1.314(6)
F(3)-C(12A)	1.293(6)
F(4)-C(14A)	1.318(6)
F(5)-C(14A)	1.310(7)
F(6)-C(14A)	1.319(6)
F(7)-C(18A)	1.322(7)
F(8)-C(18A)	1.234(7)
F(9)-C(18A)	1.316(7)
F(10)-C(20A)	1.297(6)
F(11)-C(20A)	1.291(7)
F(12)-C(20A)	1.284(6)
C(1)-C(4)	1.530(7)
C(2)-C(4)	1.521(6)

C(3)-C(4)	1.518(6)
C(4)-C(5)	1.534(6)
C(10)-C(15)	1.393(6)
C(10)-C(11)	1.404(6)
C(11)-C(12)	1.368(6)
C(12)-C(13)	1.383(6)
C(12)-C(12A)	1.506(6)
C(13)-C(14)	1.380(7)
C(14)-C(15)	1.396(6)
C(14)-C(14A)	1.486(6)
C(16)-C(17)	1.400(6)
C(16)-C(21)	1.408(7)
C(17)-C(18)	1.375(6)
C(18)-C(19)	1.393(7)
C(18)-C(18A)	1.495(7)
C(19)-C(20)	1.376(7)
C(20)-C(21)	1.378(6)
C(20)-C(20A)	1.488(7)

H-Re(1)-C(6)	172(3)
H-Re(1)-C(8)	92.3(7)
C(6)-Re(1)-C(8)	90.1(2)
H-Re(1)-C(7)	96(3)
C(6)-Re(1)-C(7)	91.8(2)
C(8)-Re(1)-C(7)	91.2(2)
H-Re(1)-C(9)	81(3)
C(6)-Re(1)-C(9)	91.3(3)
C(8)-Re(1)-C(9)	92.9(2)
C(7)-Re(1)-C(9)	174.8(2)
H-Re(1)-P(1)	85.8(7)
C(6)-Re(1)-P(1)	91.88(17)
C(8)-Re(1)-P(1)	177.71(13)
C(7)-Re(1)-P(1)	87.65(16)
C(9)-Re(1)-P(1)	88.12(17)
C(10)-B(1)-C(10)#1	104.9(5)
C(10)-B(1)-C(16)#1	112.5(2)

C(10)#1-B(1)-C(16)#1	113.4(2)
C(10)-B(1)-C(16)	113.4(2)
C(10)#1-B(1)-C(16)	112.5(2)
C(16)#1-B(1)-C(16)	100.3(4)
O(2)-P(1)-O(1)	103.56(18)
O(2)-P(1)-O(3)	103.39(19)
O(1)-P(1)-O(3)	102.93(18)
O(2)-P(1)-Re(1)	116.82(13)
O(1)-P(1)-Re(1)	114.07(14)
O(3)-P(1)-Re(1)	114.40(12)
C(1)-O(1)-P(1)	115.0(3)
C(2)-O(2)-P(1)	114.6(3)
C(3)-O(3)-P(1)	114.7(3)
O(1)-C(1)-C(4)	110.1(4)
O(2)-C(2)-C(4)	110.8(3)
O(3)-C(3)-C(4)	110.7(4)
C(3)-C(4)-C(2)	109.3(4)
C(3)-C(4)-C(1)	108.5(4)
C(2)-C(4)-C(1)	108.4(4)
C(3)-C(4)-C(5)	109.9(4)
C(2)-C(4)-C(5)	109.8(4)
C(1)-C(4)-C(5)	110.9(4)
O(4)-C(6)-Re(1)	177.9(6)
O(5)-C(7)-Re(1)	178.7(5)
O(6)-C(8)-Re(1)	177.0(4)
O(7)-C(9)-Re(1)	177.8(6)
C(15)-C(10)-C(11)	114.7(4)
C(15)-C(10)-B(1)	123.8(3)
C(11)-C(10)-B(1)	121.2(3)
C(12)-C(11)-C(10)	123.1(4)
C(11)-C(12)-C(13)	121.0(4)
C(11)-C(12)-C(12A)	119.0(4)
C(13)-C(12)-C(12A)	119.9(4)
F(3)-C(12A)-F(1)	105.0(5)
F(3)-C(12A)-F(2)	107.1(5)
F(1)-C(12A)-F(2)	103.8(4)

F(3)-C(12A)-C(12)	113.7(4)
F(1)-C(12A)-C(12)	112.9(4)
F(2)-C(12A)-C(12)	113.4(4)
C(14)-C(13)-C(12)	118.1(4)
C(13)-C(14)-C(15)	120.2(4)
C(13)-C(14)-C(14A)	120.9(4)
C(15)-C(14)-C(14A)	118.9(4)
F(5)-C(14A)-F(4)	103.8(5)
F(5)-C(14A)-F(6)	105.5(4)
F(4)-C(14A)-F(6)	105.7(5)
F(5)-C(14A)-C(14)	113.3(4)
F(4)-C(14A)-C(14)	113.6(4)
F(6)-C(14A)-C(14)	114.1(5)
C(10)-C(15)-C(14)	122.8(4)
C(17)-C(16)-C(21)	115.1(4)
C(17)-C(16)-B(1)	121.3(4)
C(21)-C(16)-B(1)	122.7(4)
C(18)-C(17)-C(16)	122.7(4)
C(17)-C(18)-C(19)	120.5(4)
C(17)-C(18)-C(18A)	120.0(5)
C(19)-C(18)-C(18A)	119.5(5)
F(8)-C(18A)-F(9)	111.2(7)
F(8)-C(18A)-F(7)	105.9(7)
F(9)-C(18A)-F(7)	98.4(5)
F(8)-C(18A)-C(18)	115.1(5)
F(9)-C(18A)-C(18)	112.4(5)
F(7)-C(18A)-C(18)	112.5(6)
C(20)-C(19)-C(18)	118.4(4)
C(19)-C(20)-C(21)	120.7(4)
C(19)-C(20)-C(20A)	119.2(4)
C(21)-C(20)-C(20A)	120.0(4)
F(12)-C(20A)-F(11)	105.2(6)
F(12)-C(20A)-F(10)	106.1(5)
F(11)-C(20A)-F(10)	102.9(6)
F(12)-C(20A)-C(20)	114.9(5)
F(11)-C(20A)-C(20)	112.7(5)

F(10)-C(20A)-C(20)	113.9(4)
C(20)-C(21)-C(16)	122.5(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

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Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for {[$Re(CO)_4(PO_3C_5H_9)]_2(\mu$-H)}BArF. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	38(1)	36(1)	25(1)	3(1)	1(1)	1(1)
B(1)	19(3)	27(4)	23(3)	0	5(2)	0
P(1)	34(1)	35(1)	27(1)	1(1)	4(1)	1(1)
O(1)	45(2)	34(2)	34(2)	5(2)	-1(1)	2(2)
O(2)	44(2)	60(2)	31(2)	4(2)	9(1)	-9(2)
O(3)	33(2)	46(2)	42(2)	-11(2)	1(1)	8(1)
O(4)	61(3)	178(6)	43(3)	-13(3)	23(2)	-12(3)
O(5)	101(3)	35(3)	74(3)	4(2)	-22(2)	4(2)
O(6)	46(2)	61(3)	37(2)	-9(2)	-1(2)	-1(2)
O(7)	122(4)	46(3)	113(4)	26(3)	-36(3)	-8(3)
F(1)	82(2)	56(2)	94(3)	-3(2)	57(2)	3(2)
F(2)	124(3)	119(4)	120(4)	-91(3)	74(3)	-54(3)
F(3)	170(4)	196(5)	56(2)	25(3)	39(3)	151(4)
F(4)	63(2)	194(5)	67(3)	2(3)	12(2)	-72(3)
F(5)	44(2)	86(3)	168(4)	18(3)	-19(2)	-6(2)
F(6)	66(2)	93(3)	141(4)	-63(3)	-1(2)	-32(2)
F(7)	159(5)	77(3)	144(5)	46(3)	-15(4)	56(3)
F(8)	257(7)	335(9)	38(2)	25(4)	4(3)	253(8)
F(9)	65(3)	181(5)	142(4)	64(4)	-32(3)	14(3)
F(10)	70(2)	183(5)	82(3)	-79(3)	-3(2)	-22(3)
F(11)	274(8)	135(5)	42(2)	-39(3)	56(3)	-110(5)
F(12)	190(5)	184(6)	97(4)	-94(4)	-42(3)	133(5)
C(1)	38(3)	50(3)	35(3)	4(2)	-4(2)	2(2)
C(2)	35(2)	46(3)	43(3)	-4(2)	6(2)	-5(2)
C(3)	43(3)	44(3)	36(3)	-9(2)	5(2)	3(2)
C(4)	33(2)	45(3)	32(3)	-5(2)	4(2)	-2(2)
C(5)	41(3)	64(4)	45(3)	-6(3)	-8(2)	-1(2)
C(6)	49(3)	92(5)	35(3)	-2(3)	-3(3)	-3(3)
C(7)	55(3)	49(4)	36(3)	1(3)	-5(2)	8(3)
C(8)	42(3)	39(3)	31(3)	8(2)	5(2)	4(2)
C(9)	66(3)	49(4)	55(3)	16(3)	-16(3)	-9(3)

C(10)	31(2)	20(2)	22(2)	6(2)	5(2)	1(2)
C(11)	32(2)	22(2)	26(2)	3(2)	5(2)	0(2)
C(12)	46(3)	21(3)	24(2)	0(2)	10(2)	3(2)
C(12A)	63(3)	32(3)	31(3)	-3(2)	11(2)	0(2)
C(13)	60(3)	26(3)	31(3)	1(2)	1(2)	-7(2)
C(14)	40(2)	25(3)	27(2)	3(2)	3(2)	-9(2)
C(14A)	47(3)	49(4)	44(3)	-10(3)	-5(2)	-19(3)
C(15)	32(2)	27(3)	23(2)	2(2)	5(2)	-4(2)
C(16)	25(2)	20(3)	28(2)	2(2)	5(2)	-2(2)
C(17)	31(2)	27(3)	29(2)	3(2)	5(2)	0(2)
C(18)	38(2)	34(3)	40(3)	8(2)	7(2)	10(2)
C(18A)	62(4)	59(4)	64(4)	13(3)	9(3)	31(3)
C(19)	37(2)	31(3)	54(3)	-6(2)	14(2)	4(2)
C(20)	30(2)	31(3)	37(3)	-10(2)	7(2)	-4(2)
C(20A)	43(3)	56(4)	51(3)	-22(3)	11(2)	5(2)
C(21)	26(2)	26(3)	32(2)	-2(2)	2(2)	-2(2)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $\{[Re(CO)_4(PO_3C_5H_9)]_2(\mu\text{-}H)\}BArF$.

	x	y	z	U(eq)
H	0	5620(50)	2500	80
H(1A)	2582	4887	3896	50
H(1B)	1990	5059	4395	50
H(2A)	2735	6867	3200	49
H(2B)	3038	5993	3170	49
H(3A)	1495	6436	4445	49
H(3B)	1782	7143	3995	49
H(5A)	3271	6021	4515	76
H(5B)	2677	6191	5009	76
H(5C)	2955	6887	4542	76
H(11)	-590	1865	3557	32
H(13)	932	3129	4557	47
H(15)	1293	1603	2953	33
H(17)	1050	132	3205	35
H(19)	1672	-1337	1676	48
H(21)	256	334	1160	33

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Table 1. Crystal data and structure refinement for $[Re(CO)_3(PO_3C_5H_9)_2(OEt_2)]BArF$.

Empirical formula	$C_{49}\,H_{40}\,B\,F_{24}\,O_{10}\,P_2\,Re$	
Formula weight	1503.76	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 12.9841(9) Å	α= 91.325(1)°.
	b = 14.202(1) Å	β= 98.447(1)°.
	c = 16.321(1) Å	γ = 102.836(2)°.
Volume	2897.8(4) $Å^3$	
Z	2	
Density (calculated)	1.723 Mg/m^3	
Absorption coefficient	2.283 mm^{-1}	
Absorption correction	empirical (SADABS, Sheldrick, 1996)	
Tmin./Tmax.	0.69/0.83	
F(000)	1480	
Crystal size	0.08 x 0.08 x 0.16 mm^3	
Theta range for data collection	1.26 to 23.31°.	
Index ranges	-14<=h<=14, -15<=k<=15, 0<=l<=18	
Reflections collected	10861	
Independent reflections	7597 [R(int) = 0.0397]	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7597 / 0 / 784	
Goodness-of-fit on F^2	1.275	
Final R indices [I>2sigma(I)]	R1 = 0.0644, wR2 = 0.1152	
R indices (all data)	R1 = 0.0943, wR2 = 0.1246	
Largest diff. peak and hole	0.929 and -0.797 $e.Å^{-3}$	

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[Re(CO)_3(PO_3C_5H_9)_2(OEt_2)]BArF$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B(1)	14399(8)	8514(7)	12487(6)	31(3)
Re(1)	9698(1)	6075(1)	7302(1)	40(1)
P(1)	11197(2)	5364(2)	7360(2)	39(1)
P(2)	10100(2)	6593(2)	8735(2)	42(1)
F(1)	17862(5)	8247(5)	11174(4)	82(2)
F(2)	18234(6)	9772(5)	11353(4)	85(2)
F(3)	19213(5)	8974(6)	12030(4)	105(3)
F(4)	18782(6)	9382(7)	14879(4)	132(4)
F(5)	17264(6)	9284(7)	15228(4)	119(3)
F(6)	17758(8)	8020(7)	14974(5)	135(4)
F(7)	14132(7)	12444(5)	13943(5)	123(3)
F(8)	15353(7)	11721(5)	14304(5)	117(3)
F(9)	15494(8)	12691(6)	13358(6)	140(4)
F(10)	12116(8)	10424(7)	10462(5)	142(4)
F(11)	11995(9)	11624(6)	11127(7)	187(6)
F(12)	11151(8)	10312(9)	11304(7)	173(5)
F(13)	14289(7)	7818(5)	8649(4)	121(3)
F(14)	13530(8)	8836(7)	9107(5)	136(4)
F(15)	15180(7)	9032(6)	9393(4)	108(3)
F(16)	14449(8)	4960(5)	10819(7)	151(4)
F(17)	13166(9)	4908(5)	11353(6)	150(4)
F(18)	13031(9)	4852(5)	10085(5)	168(5)
F(19)	10649(8)	7207(8)	14481(8)	180(6)
F(20)	11242(7)	8558(8)	14347(10)	210(7)
F(21)	10491(8)	7738(12)	13369(6)	217(7)
F(22)	14846(8)	5828(7)	14501(7)	173(5)
F(23)	13770(10)	5693(6)	15237(6)	162(4)
F(24)	13391(9)	4957(6)	14151(7)	197(6)
C(1)	12154(11)	4419(11)	6491(7)	108(5)
C(2)	11972(9)	3926(9)	7883(9)	90(5)

C(3)	13206(9)	5432(8)	7694(10)	103(5)
C(4)	12756(8)	4420(7)	7352(6)	44(3)
C(5)	13650(8)	3869(7)	7335(7)	62(3)
C(6)	10947(17)	7970(12)	9808(8)	208(13)
C(7)	9331(9)	6954(11)	10009(6)	95(5)
C(8)	10922(16)	6394(15)	10216(8)	202(12)
C(9)	10455(8)	7224(7)	10332(6)	40(3)
C(10)	10668(8)	7569(8)	11238(6)	63(3)
C(11)	8346(10)	6496(8)	7264(6)	54(3)
C(12)	8915(9)	4877(8)	7557(6)	46(3)
C(13)	9358(8)	5697(7)	6087(7)	44(3)
C(14)	9988(12)	8165(11)	6444(9)	110(5)
C(15)	9571(11)	8781(9)	6932(8)	91(4)
C(16)	11648(12)	8006(10)	7259(9)	101(5)
C(17)	12386(12)	8268(12)	6714(10)	135(7)
C(18)	15715(7)	8677(6)	12769(5)	32(2)
C(19)	16428(7)	8777(6)	12201(6)	35(2)
C(20)	17526(8)	8908(6)	12413(6)	38(2)
C(20A)	18201(9)	8976(9)	11734(8)	59(3)
C(21)	17965(8)	8952(7)	13244(7)	52(3)
C(22)	17299(8)	8888(7)	13833(6)	49(3)
C(22A)	17777(11)	8904(12)	14718(8)	77(4)
C(23)	16200(8)	8751(6)	13605(6)	39(2)
C(24)	14097(7)	9580(6)	12422(5)	31(2)
C(25)	14588(7)	10334(6)	13005(5)	35(2)
C(26)	14282(8)	11206(7)	13011(6)	45(3)
C(26A)	14816(11)	11994(9)	13647(9)	76(4)
C(27)	13476(8)	11363(7)	12417(6)	47(3)
C(28)	12971(8)	10631(7)	11834(6)	41(3)
C(28A)	12119(12)	10768(11)	11191(9)	77(4)
C(29)	13275(7)	9758(6)	11837(5)	33(2)
C(30)	14136(6)	7899(6)	11569(5)	29(2)
C(31)	14248(7)	8345(6)	10825(5)	35(2)
C(32)	14162(7)	7835(7)	10072(5)	37(2)
C(32A)	14308(11)	8353(10)	9302(7)	66(3)
C(33)	13944(7)	6836(8)	10042(6)	46(3)

C(34)	13798(7)	6365(7)	10759(6)	38(2)
C(34A)	13572(11)	5299(9)	10735(8)	62(3)
C(35)	13895(7)	6896(6)	11510(5)	34(2)
C(36)	13746(7)	7916(6)	13150(5)	32(2)
C(37)	12782(7)	8083(6)	13329(5)	36(2)
C(38)	12193(7)	7547(7)	13854(6)	40(2)
C(38A)	11159(10)	7760(11)	13989(9)	69(4)
C(39)	12518(8)	6780(7)	14237(6)	44(3)
C(40)	13491(8)	6598(6)	14072(6)	39(2)
C(40A)	13848(11)	5769(9)	14450(8)	61(3)
C(41)	14062(7)	7138(6)	13537(5)	33(2)
O(1)	11360(6)	4986(6)	6491(4)	84(3)
O(2)	11099(6)	4428(5)	7874(5)	70(2)
O(3)	12356(6)	5959(5)	7721(6)	89(3)
O(4)	10762(11)	7621(8)	8934(6)	207(8)
O(5)	9140(6)	6632(8)	9134(4)	108(4)
O(6)	10700(11)	6042(10)	9330(5)	200(7)
O(7)	7513(7)	6644(5)	7241(5)	76(3)
O(8)	8427(6)	4137(6)	7740(4)	55(2)
O(9)	9159(6)	5470(5)	5409(4)	67(2)
O(10)	10581(6)	7505(5)	6972(4)	58(2)

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Table 3. Bond lengths [Å] and angles [°] for $[Re(CO)_3(PO_3C_5H_9)_2(OEt_2)]BArF$.

B(1)-C(36)	1.613(13)
B(1)-C(24)	1.649(13)
B(1)-C(18)	1.665(13)
B(1)-C(30)	1.669(12)
Re(1)-C(12)	1.869(12)
Re(1)-C(11)	1.969(12)
Re(1)-C(13)	2.001(11)
Re(1)-O(10)	2.220(7)
Re(1)-P(1)	2.375(3)
Re(1)-P(2)	2.383(3)
P(1)-O(1)	1.564(7)
P(1)-O(3)	1.574(7)
P(1)-O(2)	1.579(7)
P(2)-O(6)	1.499(9)
P(2)-O(5)	1.499(7)
P(2)-O(4)	1.521(9)
F(1)-C(20A)	1.318(12)
F(2)-C(20A)	1.298(12)
F(3)-C(20A)	1.332(12)
F(4)-C(22A)	1.316(13)
F(5)-C(22A)	1.314(14)
F(6)-C(22A)	1.329(15)
F(7)-C(26A)	1.340(13)
F(8)-C(26A)	1.307(14)
F(9)-C(26A)	1.317(14)
F(10)-C(28A)	1.275(14)
F(11)-C(28A)	1.265(14)
F(12)-C(28A)	1.322(16)
F(13)-C(32A)	1.289(12)
F(14)-C(32A)	1.347(14)
F(15)-C(32A)	1.301(13)
F(16)-C(34A)	1.323(13)
F(17)-C(34A)	1.286(12)
F(18)-C(34A)	1.254(13)

F(19)-C(38A)	1.286(14)
F(20)-C(38A)	1.239(14)
F(21)-C(38A)	1.227(14)
F(22)-C(40A)	1.270(13)
F(23)-C(40A)	1.308(13)
F(24)-C(40A)	1.227(13)
C(1)-O(1)	1.441(12)
C(1)-C(4)	1.505(14)
C(2)-O(2)	1.466(11)
C(2)-C(4)	1.500(14)
C(3)-O(3)	1.468(12)
C(3)-C(4)	1.488(14)
C(4)-C(5)	1.541(12)
C(6)-O(4)	1.467(13)
C(6)-C(9)	1.471(16)
C(7)-C(9)	1.439(13)
C(7)-O(5)	1.458(11)
C(8)-C(9)	1.460(15)
C(8)-O(6)	1.484(13)
C(9)-C(10)	1.513(12)
C(11)-O(7)	1.143(11)
C(12)-O(8)	1.170(11)
C(13)-O(9)	1.121(10)
C(14)-C(15)	1.413(16)
C(14)-O(10)	1.543(14)
C(16)-C(17)	1.399(16)
C(16)-O(10)	1.414(14)
C(18)-C(19)	1.391(11)
C(18)-C(23)	1.407(11)
C(19)-C(20)	1.387(11)
C(20)-C(21)	1.387(12)
C(20)-C(20A)	1.502(14)
C(21)-C(22)	1.375(13)
C(22)-C(23)	1.389(12)
C(22)-C(22A)	1.483(14)
C(24)-C(25)	1.388(11)

C(24)-C(29)	1.396(11)
C(25)-C(26)	1.382(12)
C(26)-C(27)	1.379(13)
C(26)-C(26A)	1.484(14)
C(27)-C(28)	1.371(12)
C(28)-C(29)	1.382(11)
C(28)-C(28A)	1.459(14)
C(30)-C(35)	1.387(11)
C(30)-C(31)	1.394(11)
C(31)-C(32)	1.389(11)
C(32)-C(33)	1.382(12)
C(32)-C(32A)	1.486(14)
C(33)-C(34)	1.377(12)
C(34)-C(35)	1.399(12)
C(34)-C(34A)	1.476(14)
C(36)-C(37)	1.394(11)
C(36)-C(41)	1.396(11)
C(37)-C(38)	1.363(12)
C(38)-C(39)	1.384(13)
C(38)-C(38A)	1.486(14)
C(39)-C(40)	1.405(13)
C(40)-C(41)	1.367(11)
C(40)-C(40A)	1.474(13)

C(36)-B(1)-C(24)	108.6(7)
C(36)-B(1)-C(18)	111.7(7)
C(24)-B(1)-C(18)	108.8(7)
C(36)-B(1)-C(30)	110.9(7)
C(24)-B(1)-C(30)	112.0(7)
C(18)-B(1)-C(30)	104.8(7)
C(12)-Re(1)-C(11)	85.3(4)
C(12)-Re(1)-C(13)	91.5(4)
C(11)-Re(1)-C(13)	90.9(4)
C(12)-Re(1)-O(10)	178.2(4)
C(11)-Re(1)-O(10)	93.2(4)
C(13)-Re(1)-O(10)	87.5(3)

C(12)-Re(1)-P(1)	87.5(3)
C(11)-Re(1)-P(1)	172.7(3)
C(13)-Re(1)-P(1)	88.1(3)
O(10)-Re(1)-P(1)	94.0(2)
C(12)-Re(1)-P(2)	90.5(3)
C(11)-Re(1)-P(2)	87.9(3)
C(13)-Re(1)-P(2)	177.6(3)
O(10)-Re(1)-P(2)	90.4(2)
P(1)-Re(1)-P(2)	93.34(9)
O(1)-P(1)-O(3)	101.7(5)
O(1)-P(1)-O(2)	102.6(4)
O(3)-P(1)-O(2)	102.2(5)
O(1)-P(1)-Re(1)	113.3(3)
O(3)-P(1)-Re(1)	121.1(3)
O(2)-P(1)-Re(1)	113.6(3)
O(6)-P(2)-O(5)	102.7(6)
O(6)-P(2)-O(4)	101.3(8)
O(5)-P(2)-O(4)	100.9(6)
O(6)-P(2)-Re(1)	119.3(3)
O(5)-P(2)-Re(1)	114.4(3)
O(4)-P(2)-Re(1)	115.6(4)
O(1)-C(1)-C(4)	110.4(8)
O(2)-C(2)-C(4)	110.0(9)
O(3)-C(3)-C(4)	111.1(9)
C(3)-C(4)-C(2)	108.6(10)
C(3)-C(4)-C(1)	109.9(11)
C(2)-C(4)-C(1)	107.5(10)
C(3)-C(4)-C(5)	110.8(8)
C(2)-C(4)-C(5)	110.0(8)
C(1)-C(4)-C(5)	110.0(8)
O(4)-C(6)-C(9)	111.7(10)
C(9)-C(7)-O(5)	111.7(8)
C(9)-C(8)-O(6)	110.6(10)
C(7)-C(9)-C(8)	108.7(11)
C(7)-C(9)-C(6)	107.0(12)
C(8)-C(9)-C(6)	106.2(13)