Pseudotetrahedral manganese complexes supported by the anionic tris(phosphino)borate ligand [PhBP$^{iPr}_3$]

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Supporting Information

Figure 1. Fully labeled drawing of [PhBP$^{iPr}_3$]MnCl (**1a**). Displacement ellipsoid (50%) representation. Hydrogen atoms have been omitted for clarity.

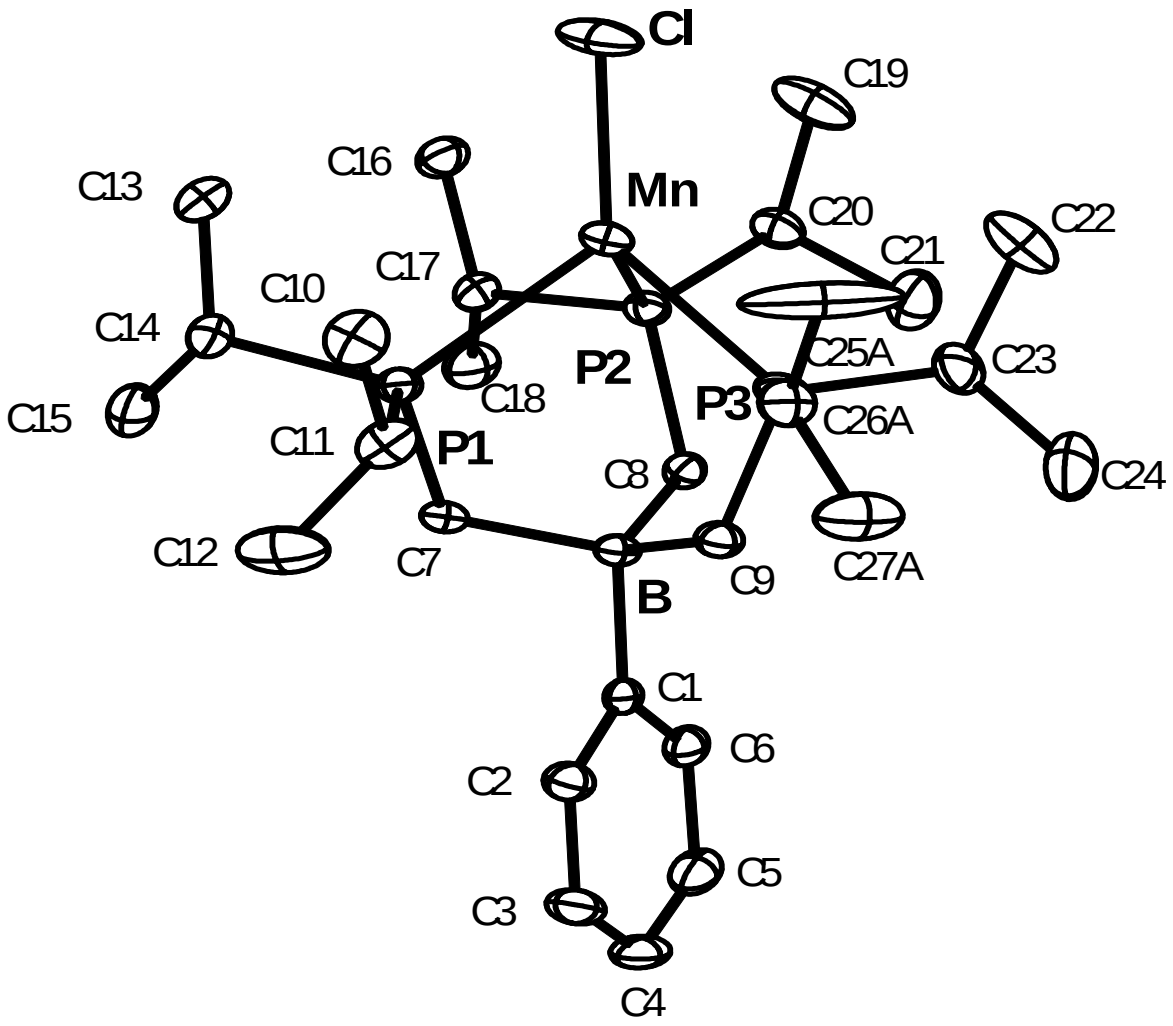

Figure 2. Fully labeled drawing of {[PhBP$^{iPr}_3$]Mn(μ-Cl)}$_2$ (**1b**). Displacement ellipsoid (50%) representation. Hydrogen atoms have been omitted for clarity.

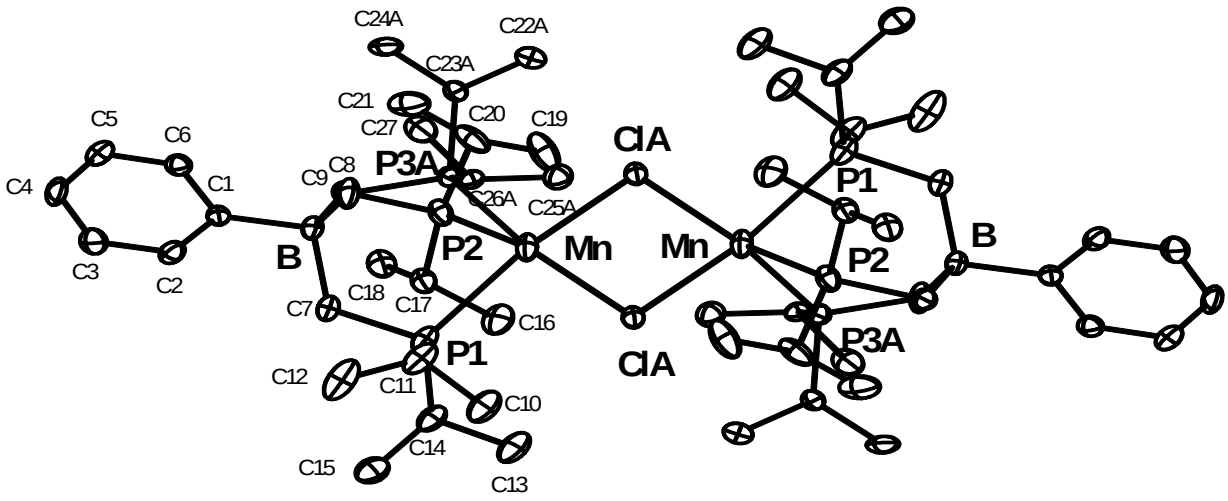

Figure 3. Fully labeled drawing of [PhBP$^{iPr}_3$]MnI (**2**). Displacement ellipsoid (50%) representation. Hydrogen atoms and solvent molecule have been omitted for clarity.

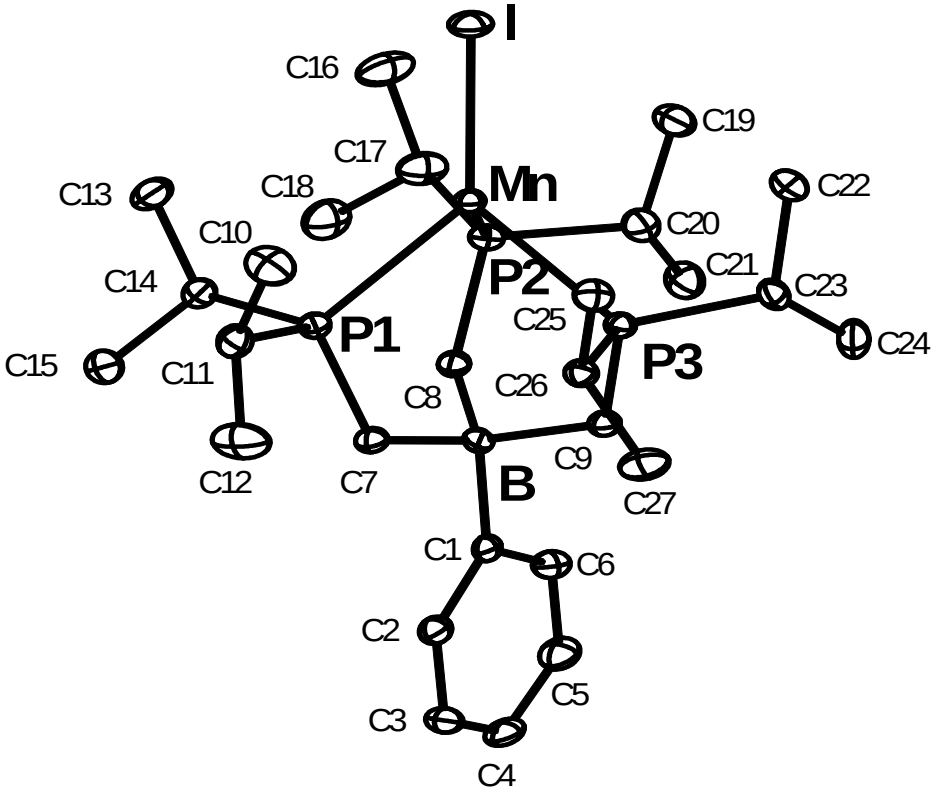

Figure 4. Fully labeled drawing of [PhBP$^{iPr}_3$]Mn(N_3) (**3**). Displacement ellipsoid (50%) representation. Two molecules were present in the asymmetric unit, but only one is shown. Hydrogen atoms have been omitted for clarity.

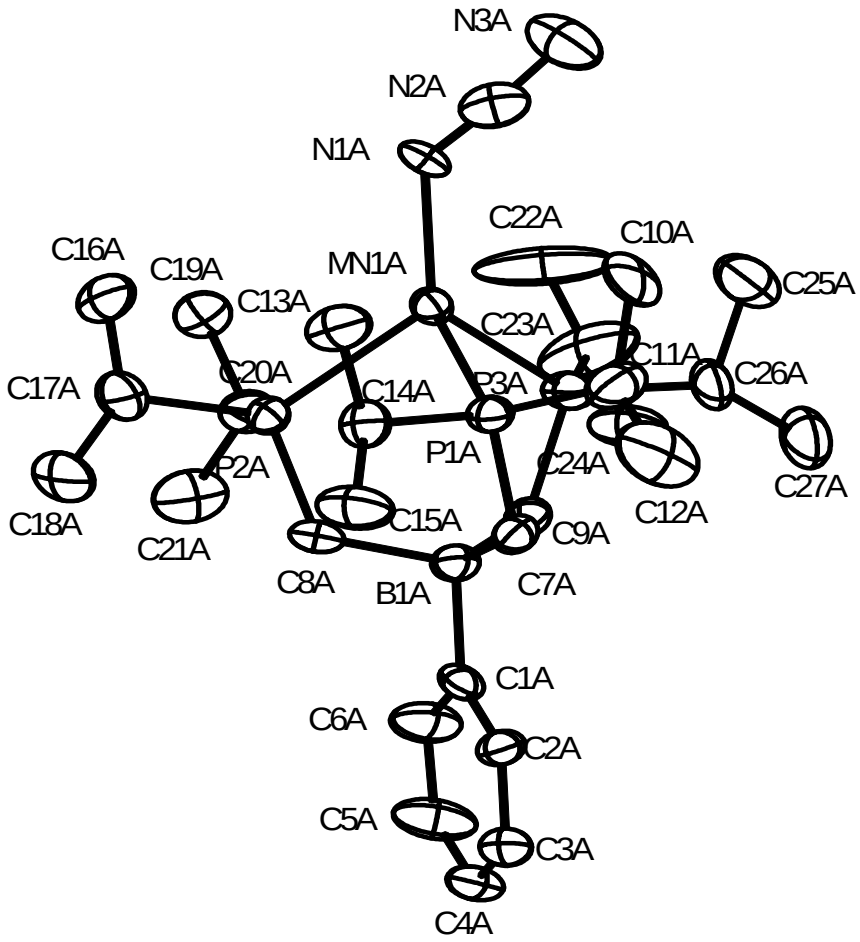

Figure 5. Fully labeled drawing of [PhBP$^{iPr}_3$]Mn(CH_2Ph) (**4**).

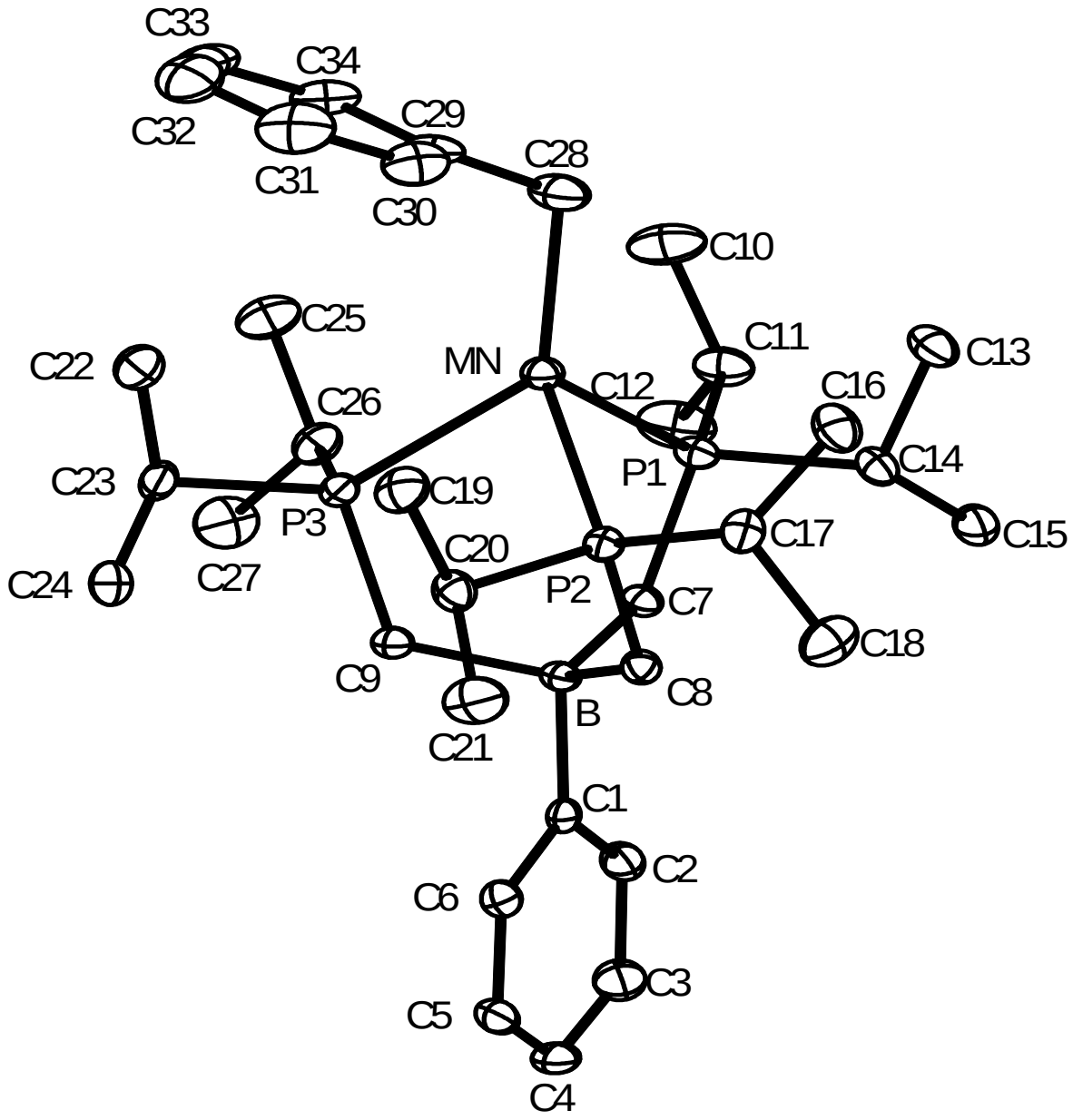

Figure 6. Fully labeled drawing of [PhBP$^{iPr}_3$]Mn(NH(2,6-^{i}Pr$_2$-C$_6$H$_3$)) (**6**). Displacement ellipsoid (50%) representation. Hydrogen atoms have been omitted for clarity.

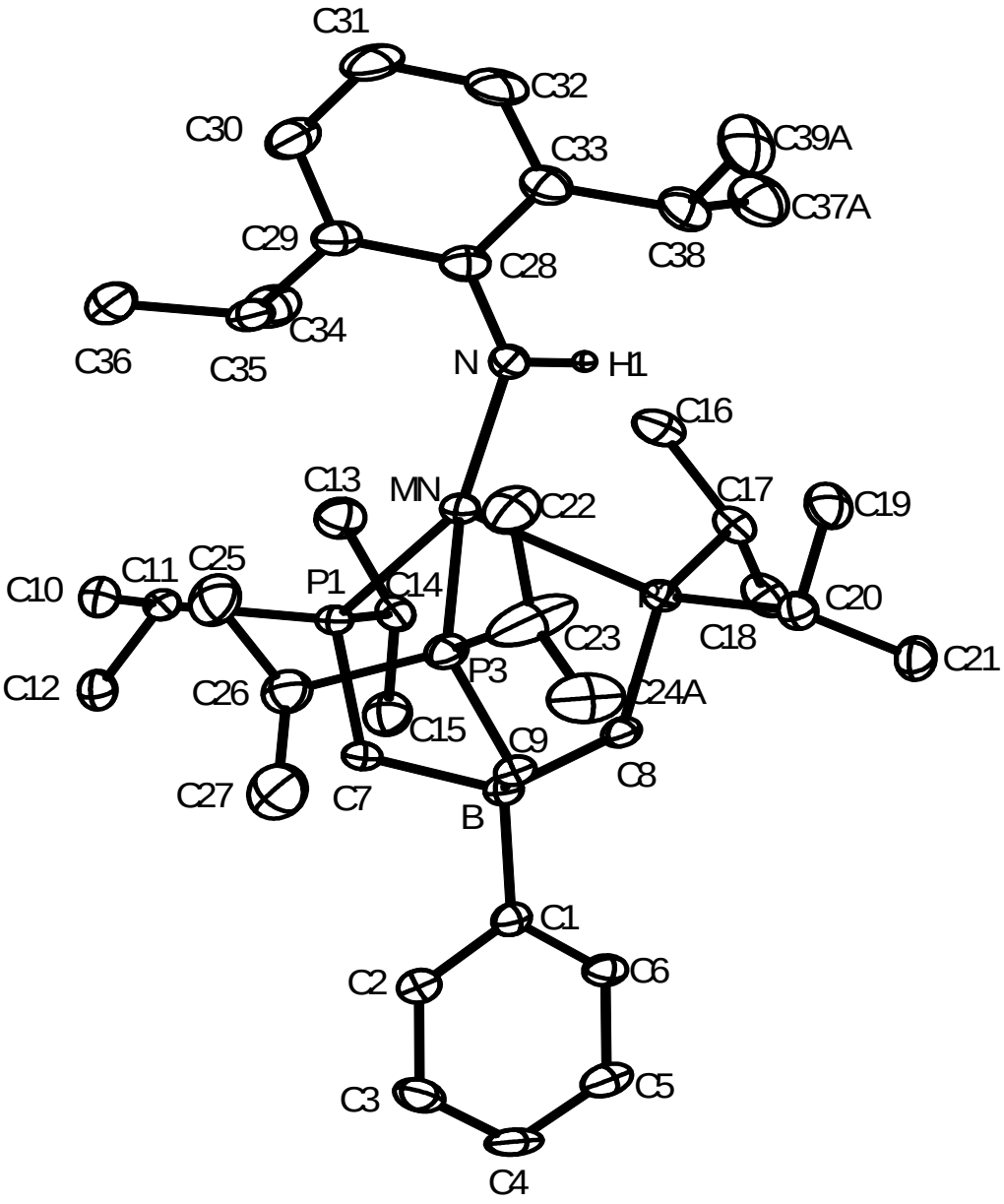

Figure 7. Fully labeled drawing of [PhBP$^{iPr}_3$]Mn(dbabh) (**7**). Displacement ellipsoid (50%) representation. Hydrogen atoms have been omitted for clarity.

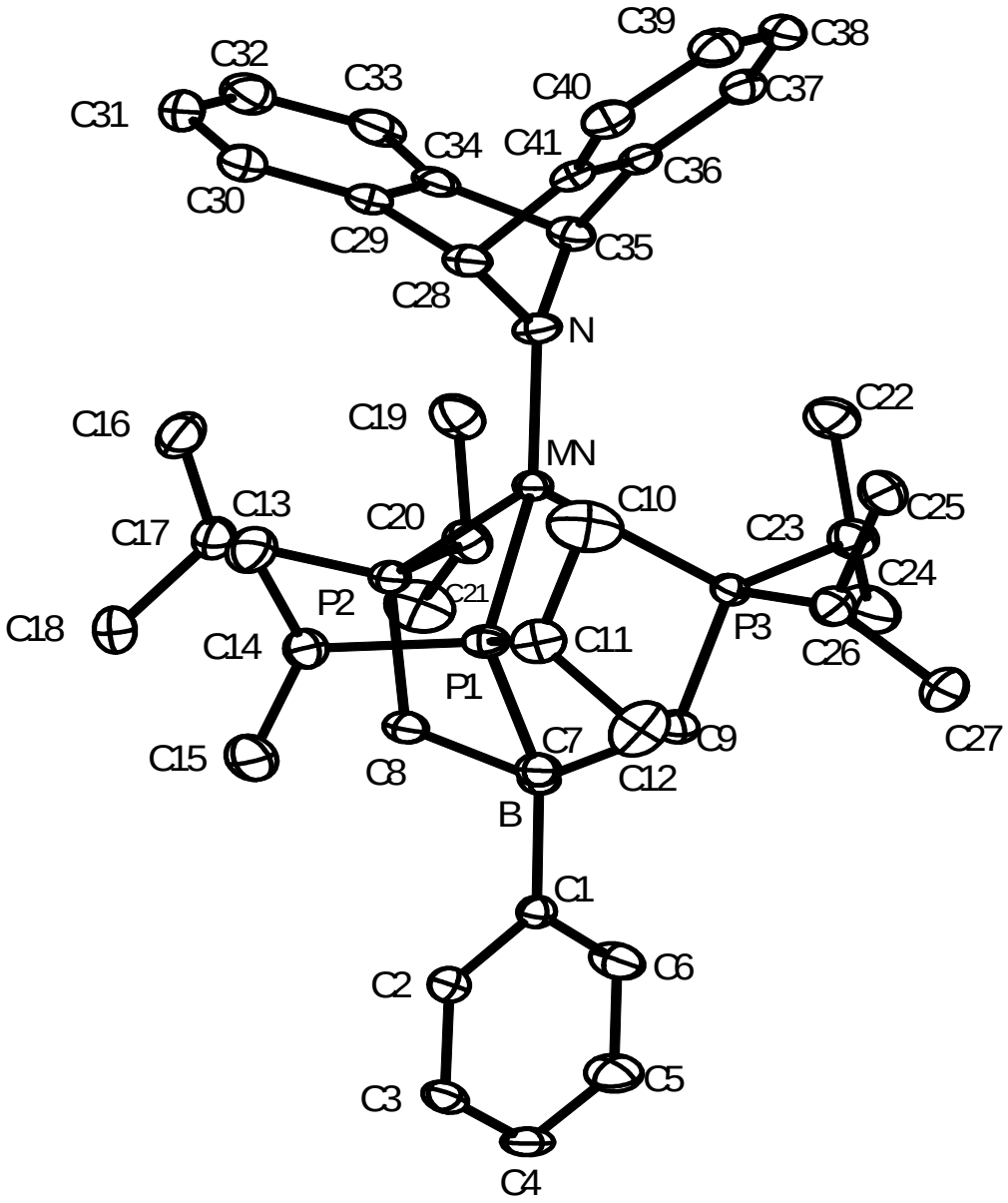

Figure 8. Fully labeled drawing of [PhBP$^{iPr}_3$]Mn(1-Ph(isoindolate)) (**8**). Displacement ellipsoid (50%) representation (C2-C6 are isotropic). Hydrogen atoms and solvent molecules have been omitted for clarity.

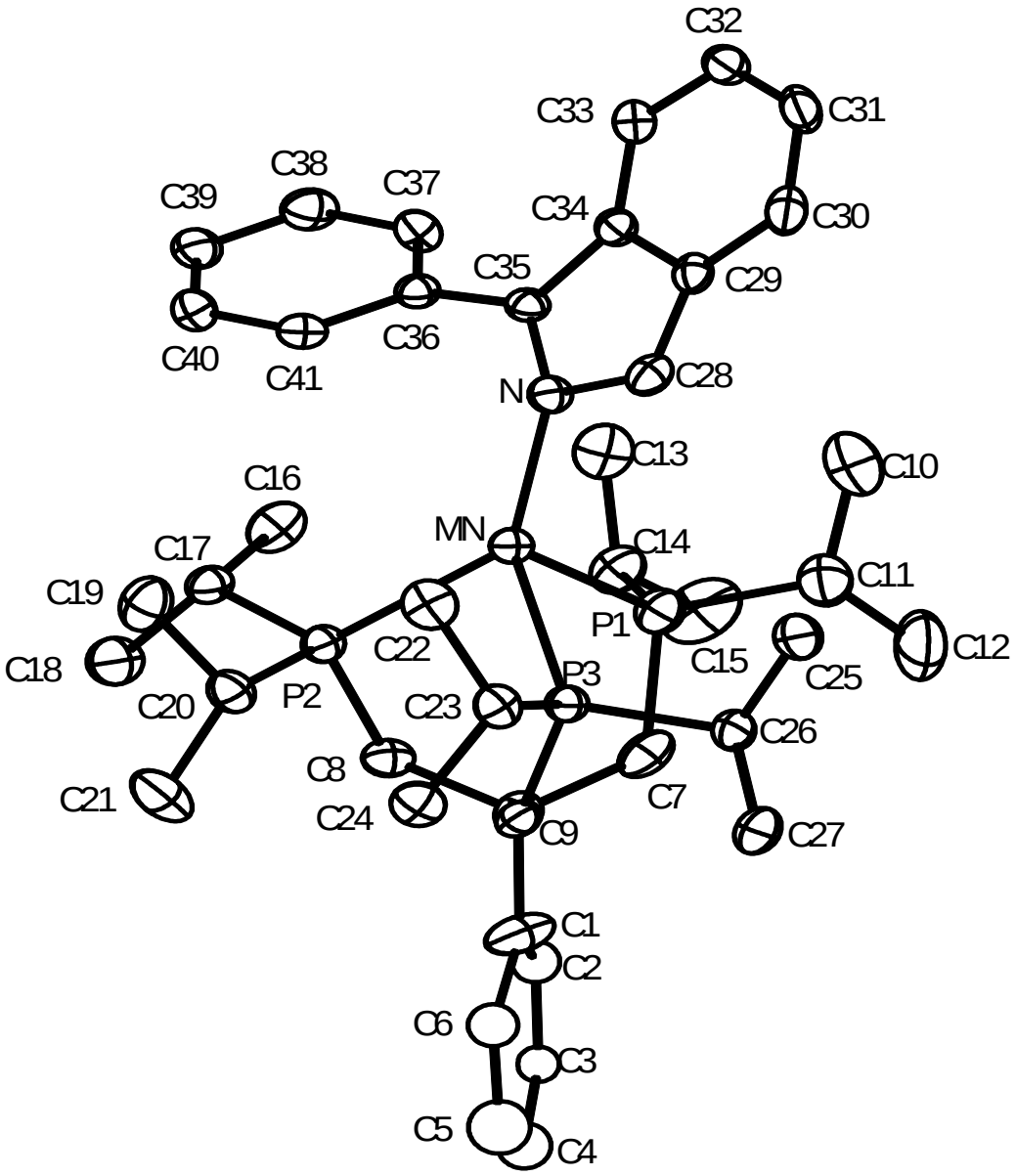

Figure 9. Fully labeled drawing of [PhBP$^{iPr}_3$]Tl-MnBr(CO)$_4$ (**9**). Displacement ellipsoid (50%) representation. Hydrogen atoms have been omitted for clarity.

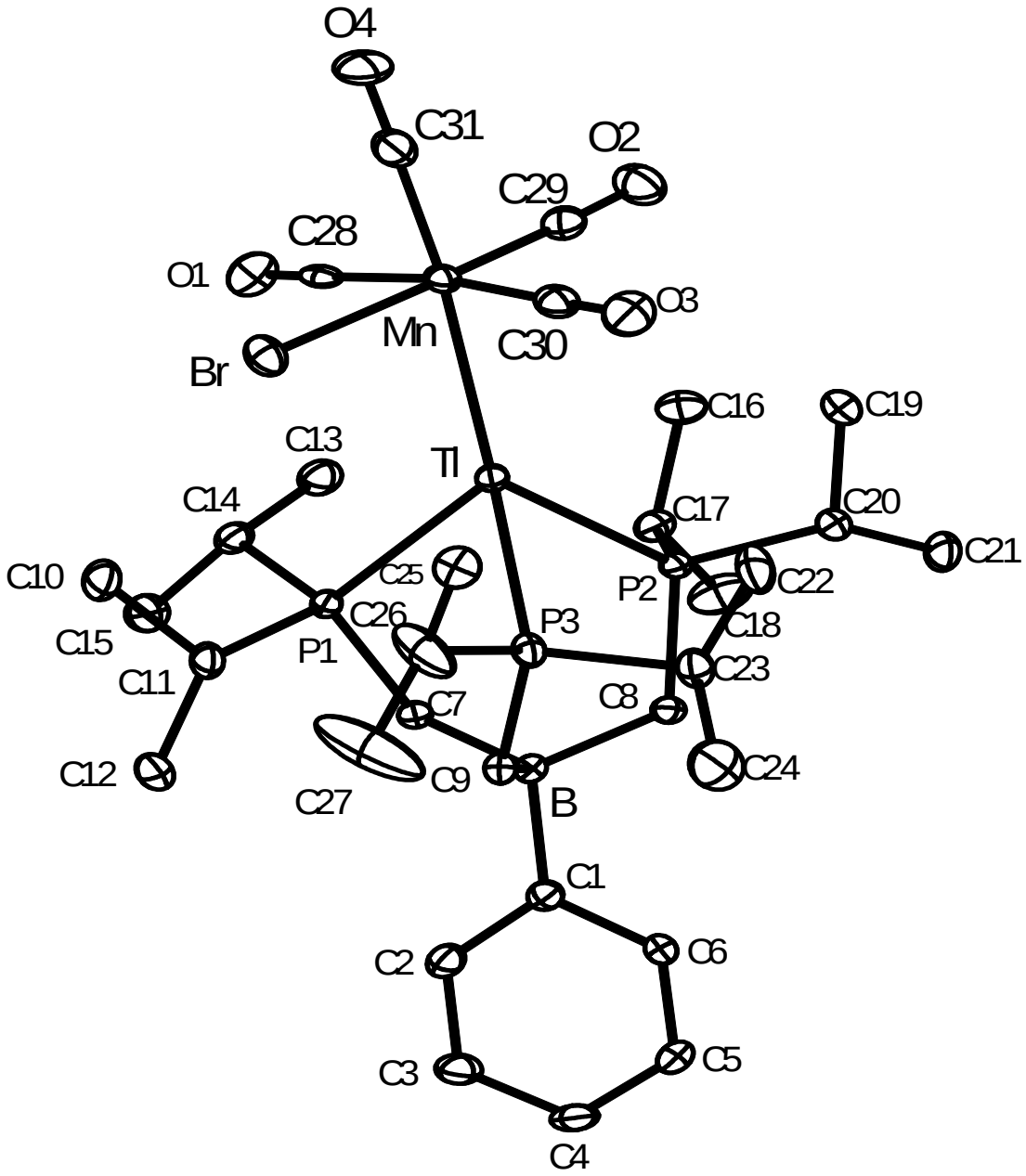

Figure 10. Fully labeled drawing of [PhBP$^{iPr}_3$]Mn(CN^{t}Bu)$_3$ (**10**). Displacement ellipsoid (50%) representation. Hydrogen atoms have been omitted for clarity.

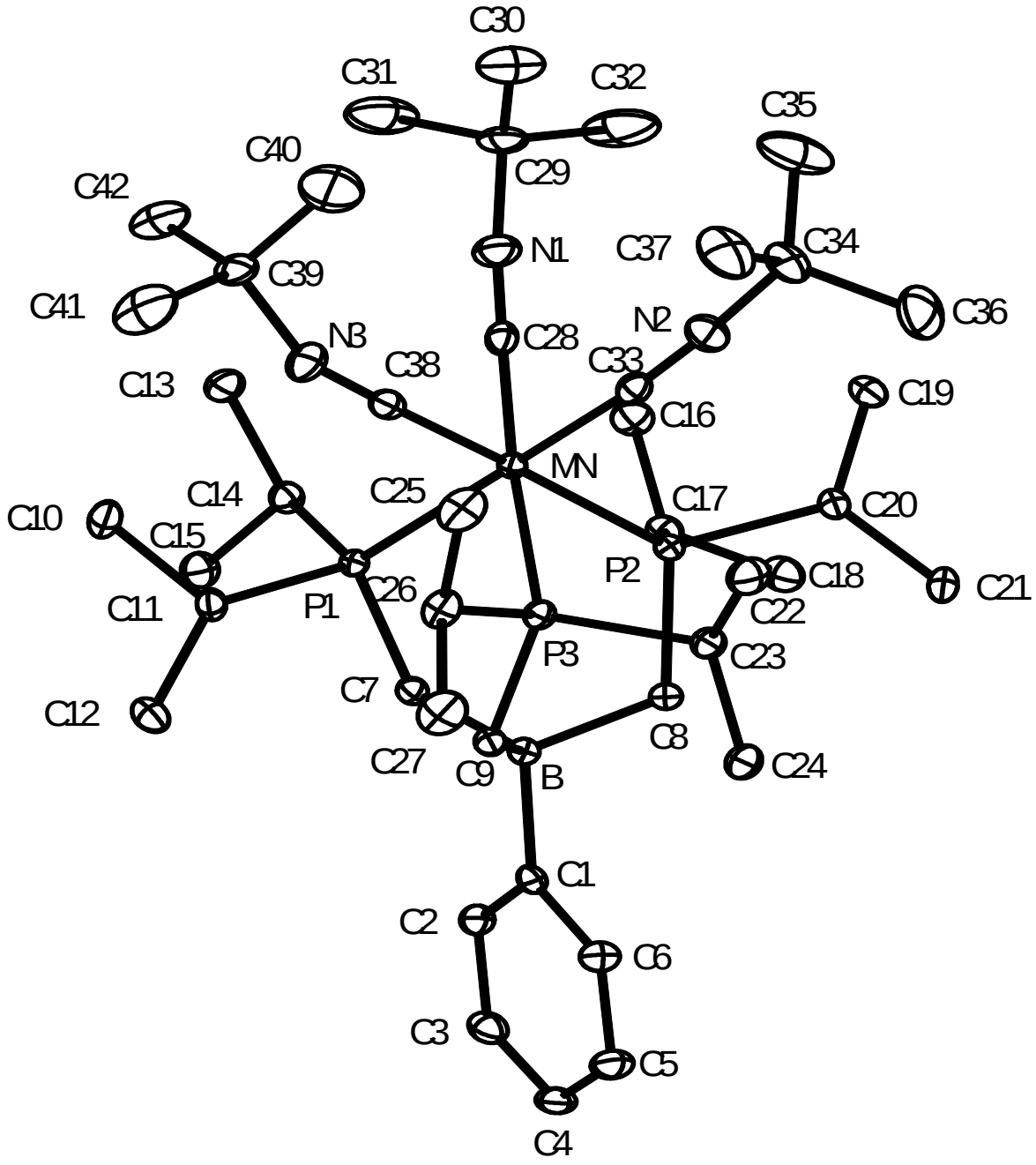

Figure 11. Fully labeled drawing of {(Hdbabh)MnI(μ-*N*-dbabh)}$_2$. Displacement ellipsoid (50%) representation for only Mn and I atoms. (The remaining atoms are isotropic.) Hydrogen and solvent atoms have been omitted for clarity.

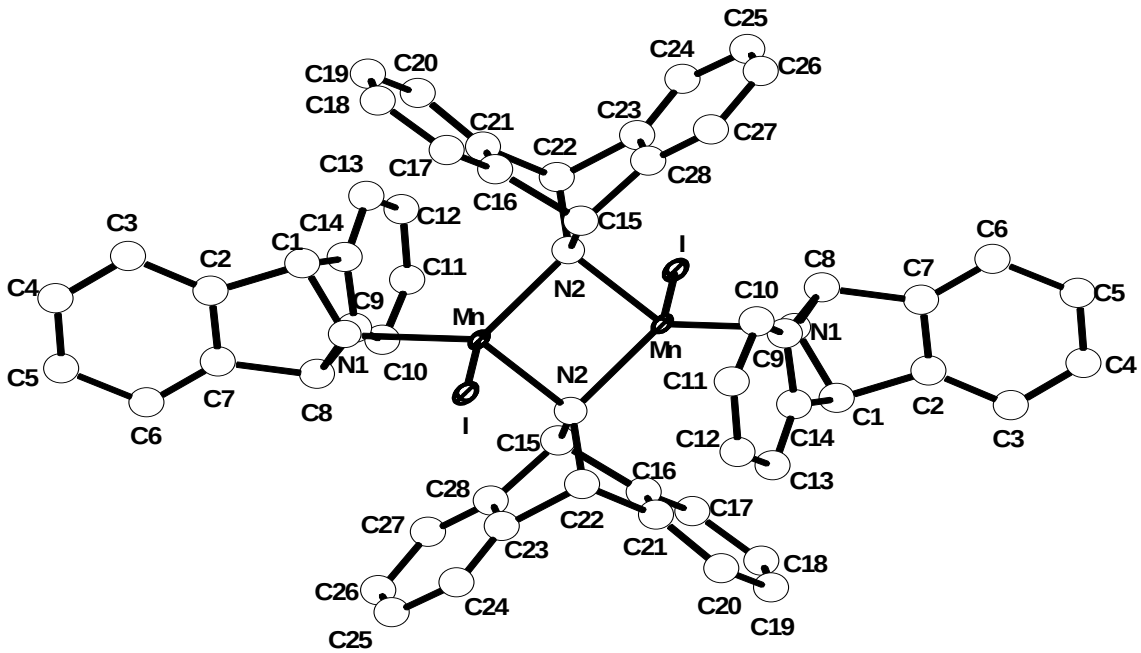

Table 1. Crystal Data and Structure Analysis Details for [PhBP$^{iPr}_3$]MnCl (1a).

Empirical formula	$C_{27}H_{53}BCl_{0.98}Mn_{0.98}P_3Tl_{0.02}$
Formula weight	573.66
Crystallization solvent	benzene/petroleum ether
Crystal shape	thin plate
Crystal color	colorless
Crystal size	0.074 x 0.30 x 0.32 mm

Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data collection temperature	100 K	
Theta range for 27512 reflections used in lattice determination	2.28 to 28.09°	
Unit cell dimensions	a = 14.493(2) Å b = 12.928(2) Å c = 34.850(5) Å	α= 90° β= 100.344(3)° γ = 90°
Volume	6423.8(16) Å^3	
Z	8	
Crystal system	monoclinic	
Space group	C 2/c (# 15)	
Density (calculated)	1.186 g/cm^3	
F(000)	2461	
Theta range for data collection	2.1 to 28.6°	
Completeness to theta = 28.56°	93.8%	
Index ranges	$-18 \le h \le 19$, $-17 \le k \le 16$, $-46 \le l \le 45$	
Data collection scan type	ω scans	
Reflections collected	46909	
Independent reflections	7671 [R_{int}= 0.0705]	
Reflections > 2σ(I)	6237	
Average σ(I)/(net I)	0.0414	
Absorption coefficient	0.73 mm^{-1}	
Absorption correction	none	
Reflections monitored for decay	initial data recollected at end	
Decay of standards	0%	

Table 1 (cont.)

Structure Solution and Refinement

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7671 / 0 / 345
Treatment of hydrogen atoms	not refined, U_{iso} fixed at 120% U_{eq} of attached atom
Goodness-of-fit on F^2	1.90
Final R indices [I>2σ(I), 6237 reflections]	R1 = 0.0422, wR2 = 0.0720
R indices (all data)	R1 = 0.0556, wR2 = 0.0731
Type of weighting scheme used	sigma
Weighting scheme used	calc $w=1/[\sigma^2(Fo^2)]$ where $P=(Fo^2+2Fc^2)/3$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	0.51 and -0.46 e·Å^{-3}

Programs Used

Cell refinement	Bruker SMART 5.606
Data collection	Bruker SMART 5.054
Data reduction	Bruker SAINT 6.45
Structure solution	Bruker SHELXTL 6.14
Structure refinement	Bruker SHELXTL 6.14

Special Refinement Details

A small amount of Tl[Ligand] had cocrystallized with compound **1a** and was modeled. The population for Tl[Ligand] was refined to be 1.7%, and 98.3% for **1a**. One of the isopropyl groups of the ligand was disordered in two positions and was modeled. The populations of two positions were refined to be 52.1 and 47.9 %. In the disordered isopropyl unit, C25B and C26B were given a BIND constraint.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for [PhBP$^{iPr}_3$]MnCl (1a). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Mn	2102.8(2)	4035.2(3)	1412.5(1)	19.0(1)
P(1)	1376.4(3)	2599.7(3)	1752.2(1)	17.1(1)
P(2)	1241.7(3)	3412.0(3)	757.1(1)	16.4(1)
P(3)	3534.7(3)	2955.3(4)	1368.1(1)	22.1(1)
Cl	2095.5(4)	5738.1(4)	1569.1(2)	39.6(2)
B	1977.4(13)	1389.7(14)	1098.7(5)	15.6(4)
Tl	2209(4)	4565(5)	1493.3(15)	27(2)
C(1)	1983.4(11)	155.5(12)	982.7(5)	17.0(4)
C(2)	2242.0(12)	-585.2(13)	1276.7(6)	22.4(4)
C(3)	2307.0(13)	-1636.4(14)	1201.0(6)	29.7(5)
C(4)	2125.6(13)	-1987.3(14)	821.5(6)	32.0(5)
C(5)	1869.2(13)	-1288.3(15)	521.7(6)	29.0(5)
C(6)	1794.6(12)	-235.3(14)	602.2(5)	21.2(4)
C(7)	1243.0(12)	1502.5(12)	1417.1(5)	16.3(4)
C(8)	1615.3(12)	2085.5(12)	696.5(5)	16.5(4)
C(9)	3102.9(12)	1629.1(13)	1294.0(5)	19.1(4)
C(10)	2403.2(14)	3036.9(16)	2488.2(5)	31.9(5)
C(11)	2202.7(14)	2155.3(15)	2191.0(5)	27.6(4)
C(12)	1903.2(18)	1157.6(16)	2373.7(6)	45.3(6)
C(13)	-36.5(15)	3941.2(15)	1905.9(6)	36.8(5)
C(14)	270.8(13)	2811.3(14)	1948.7(5)	23.5(4)
C(15)	-521.6(14)	2074.3(16)	1789.7(6)	32.7(5)
C(16)	-444.6(13)	4433.8(14)	778.8(5)	23.5(4)
C(17)	-30.5(12)	3344.3(13)	771.8(5)	19.4(4)
C(18)	-596.2(13)	2680.4(14)	448.2(5)	26.7(4)
C(19)	1564.6(17)	5287.0(15)	406.3(6)	41.0(6)
C(20)	1253.2(13)	4179.7(13)	301.3(5)	22.3(4)
C(21)	1838.7(16)	3707.2(18)	28.3(6)	41.2(6)
C(22)	4256.8(17)	4437.5(17)	909.0(7)	46.0(6)
C(23)	3959.4(13)	3305.1(15)	915.3(6)	29.1(5)
C(24)	4719.0(18)	2604(2)	807.3(9)	62.6(8)
C(25A)	4788(9)	3849(10)	1932(4)	96(6)
C(26A)	4450(7)	2931(7)	1823(3)	25.3(15)
C(27A)	5158(8)	2065(10)	1838(4)	45(3)
C(25B)	4876(8)	4041(8)	1923(3)	47(2)
C(26B)	4701(6)	2959(6)	1708(3)	26.6(14)
C(27B)	4887(8)	1996(10)	1957(4)	53(3)

Table 3. Bond lengths [Å] and angles [°] for [PhBP$^{iPr}_3$]MnCl (1a).

Mn-Cl	2.2687(7)	C(14)-C(15)	1.518(3)
Mn-P(3)	2.5289(6)	C(14)-H(14)	1.0000
Mn-P(2)	2.5298(6)	C(15)-H(15A)	0.9800
Mn-P(1)	2.5300(6)	C(15)-H(15B)	0.9800
P(1)-C(7)	1.8252(16)	C(15)-H(15C)	0.9800
P(1)-C(11)	1.8562(18)	C(16)-C(17)	1.533(2)
P(1)-C(14)	1.8724(18)	C(16)-H(16A)	0.9800
P(1)-Tl	3.019(6)	C(16)-H(16B)	0.9800
P(2)-C(8)	1.8219(17)	C(16)-H(16C)	0.9800
P(2)-C(17)	1.8558(18)	C(17)-C(18)	1.533(2)
P(2)-C(20)	1.8759(17)	C(17)-H(17)	1.0000
P(2)-Tl	3.079(6)	C(18)-H(18A)	0.9800
P(3)-C(9)	1.8275(17)	C(18)-H(18B)	0.9800
P(3)-C(23)	1.850(2)	C(18)-H(18C)	0.9800
P(3)-C(26A)	1.877(8)	C(19)-C(20)	1.526(3)
P(3)-C(26B)	1.882(8)	C(19)-H(19A)	0.9800
P(3)-Tl	2.918(6)	C(19)-H(19B)	0.9800
B-C(1)	1.646(2)	C(19)-H(19C)	0.9800
B-C(8)	1.669(2)	C(20)-C(21)	1.512(3)
B-C(7)	1.676(2)	C(20)-H(20)	1.0000
B-C(9)	1.680(3)	C(21)-H(21A)	0.9800
C(1)-C(6)	1.399(2)	C(21)-H(21B)	0.9800
C(1)-C(2)	1.404(2)	C(21)-H(21C)	0.9800
C(2)-C(3)	1.391(2)	C(22)-C(23)	1.527(3)
C(2)-H(2)	0.9500	C(22)-H(22A)	0.9800
C(3)-C(4)	1.378(3)	C(22)-H(22B)	0.9800
C(3)-H(3)	0.9500	C(22)-H(22C)	0.9800
C(4)-C(5)	1.381(3)	C(23)-C(24)	1.524(3)
C(4)-H(4)	0.9500	C(23)-H(23)	1.0000
C(5)-C(6)	1.398(2)	C(24)-H(24A)	0.9800
C(5)-H(5)	0.9500	C(24)-H(24B)	0.9800
C(6)-H(6)	0.9500	C(24)-H(24C)	0.9800
C(7)-H(7A)	0.9900	C(25A)-C(26A)	1.314(16)
C(7)-H(7B)	0.9900	C(25A)-H(25A)	0.9800
C(8)-H(8A)	0.9900	C(25A)-H(25B)	0.9800
C(8)-H(8B)	0.9900	C(25A)-H(25C)	0.9800
C(9)-H(9A)	0.9900	C(26A)-C(27A)	1.512(16)
C(9)-H(9B)	0.9900	C(26A)-H(26A)	1.0000
C(10)-C(11)	1.532(3)	C(27A)-H(27A)	0.9800
C(10)-H(10A)	0.9800	C(27A)-H(27B)	0.9800
C(10)-H(10B)	0.9800	C(27A)-H(27C)	0.9800
C(10)-H(10C)	0.9800	C(25B)-C(26B)	1.586(14)
C(11)-C(12)	1.535(3)	C(25B)-H(25D)	0.9800
C(11)-H(11)	1.0000	C(25B)-H(25E)	0.9800
C(12)-H(12A)	0.9800	C(25B)-H(25F)	0.9800
C(12)-H(12B)	0.9800	C(26B)-C(27B)	1.514(16)
C(12)-H(12C)	0.9800	C(26B)-H(26B)	1.0000
C(13)-C(14)	1.527(3)	C(27B)-H(27D)	0.9800
C(13)-H(13A)	0.9800	C(27B)-H(27E)	0.9800
C(13)-H(13B)	0.9800	C(27B)-H(27F)	0.9800
C(13)-H(13C)	0.9800	Cl-Mn-P(3)	126.14(2)

Cl-Mn-P(2)	120.22(2)	P(3)-Mn-P(2)	92.64(2)
Cl-Mn-P(1)	125.38(2)	C(4)-C(3)-C(2)	119.73(18)
P(3)-Mn-P(1)	92.22(2)	C(4)-C(3)-H(3)	120.1
P(2)-Mn-P(1)	90.55(2)	C(2)-C(3)-H(3)	120.1
C(7)-P(1)-C(11)	105.38(8)	C(3)-C(4)-C(5)	119.33(18)
C(7)-P(1)-C(14)	110.38(8)	C(3)-C(4)-H(4)	120.3
C(11)-P(1)-C(14)	102.23(9)	C(5)-C(4)-H(4)	120.3
C(7)-P(1)-Mn	106.02(6)	C(4)-C(5)-C(6)	120.35(18)
C(11)-P(1)-Mn	110.57(7)	C(4)-C(5)-H(5)	119.8
C(14)-P(1)-Mn	121.28(6)	C(6)-C(5)-H(5)	119.8
C(7)-P(1)-Tl	117.71(13)	C(5)-C(6)-C(1)	122.20(17)
C(11)-P(1)-Tl	105.86(12)	C(5)-C(6)-H(6)	118.9
C(14)-P(1)-Tl	113.61(12)	C(1)-C(6)-H(6)	118.9
Mn-P(1)-Tl	11.69(11)	B-C(7)-P(1)	118.96(11)
C(8)-P(2)-C(17)	106.04(8)	B-C(7)-H(7A)	107.6
C(8)-P(2)-C(20)	110.60(8)	P(1)-C(7)-H(7A)	107.6
C(17)-P(2)-C(20)	102.02(8)	B-C(7)-H(7B)	107.6
C(8)-P(2)-Mn	107.20(6)	P(1)-C(7)-H(7B)	107.6
C(17)-P(2)-Mn	108.76(6)	H(7A)-C(7)-H(7B)	107.0
C(20)-P(2)-Mn	121.21(6)	B-C(8)-P(2)	117.72(11)
C(8)-P(2)-Tl	116.87(12)	B-C(8)-H(8A)	107.9
C(17)-P(2)-Tl	107.81(11)	P(2)-C(8)-H(8A)	107.9
C(20)-P(2)-Tl	112.19(12)	B-C(8)-H(8B)	107.9
Mn-P(2)-Tl	10.39(11)	P(2)-C(8)-H(8B)	107.9
C(9)-P(3)-C(23)	105.48(8)	H(8A)-C(8)-H(8B)	107.2
C(9)-P(3)-C(26A)	106.0(3)	B-C(9)-P(3)	120.87(11)
C(23)-P(3)-C(26A)	115.6(4)	B-C(9)-H(9A)	107.1
C(9)-P(3)-C(26B)	109.7(3)	P(3)-C(9)-H(9A)	107.1
C(23)-P(3)-C(26B)	97.9(3)	B-C(9)-H(9B)	107.1
C(26A)-P(3)-C(26B)	18.08(18)	P(3)-C(9)-H(9B)	107.1
C(9)-P(3)-Mn	105.22(6)	H(9A)-C(9)-H(9B)	106.8
C(23)-P(3)-Mn	108.65(6)	C(11)-C(10)-H(10A)	109.5
C(26A)-P(3)-Mn	114.9(3)	C(11)-C(10)-H(10B)	109.5
C(26B)-P(3)-Mn	127.9(3)	H(10A)-C(10)-H(10B)	109.5
C(9)-P(3)-Tl	118.18(14)	C(11)-C(10)-H(10C)	109.5
C(23)-P(3)-Tl	106.39(12)	H(10A)-C(10)-H(10C)	109.5
C(26A)-P(3)-Tl	105.7(3)	H(10B)-C(10)-H(10C)	109.5
C(26B)-P(3)-Tl	116.5(3)	C(10)-C(11)-C(12)	112.21(16)
Mn-P(3)-Tl	13.46(12)	C(10)-C(11)-P(1)	110.04(13)
C(1)-B-C(8)	109.33(13)	C(12)-C(11)-P(1)	114.40(14)
C(1)-B-C(7)	106.19(13)	C(10)-C(11)-H(11)	106.6
C(8)-B-C(7)	111.58(13)	C(12)-C(11)-H(11)	106.6
C(1)-B-C(9)	103.33(13)	P(1)-C(11)-H(11)	106.6
C(8)-B-C(9)	112.16(14)	C(11)-C(12)-H(12A)	109.5
C(7)-B-C(9)	113.67(14)	C(11)-C(12)-H(12B)	109.5
P(3)-Tl-P(1)	75.74(16)	H(12A)-C(12)-H(12B)	109.5
P(3)-Tl-P(2)	75.14(16)	C(11)-C(12)-H(12C)	109.5
P(1)-Tl-P(2)	72.24(16)	H(12A)-C(12)-H(12C)	109.5
C(6)-C(1)-C(2)	115.26(16)	H(12B)-C(12)-H(12C)	109.5
C(6)-C(1)-B	125.02(15)	C(14)-C(13)-H(13A)	109.5
C(2)-C(1)-B	119.63(15)	C(14)-C(13)-H(13B)	109.5
C(3)-C(2)-C(1)	123.13(18)	H(13A)-C(13)-H(13B)	109.5
C(3)-C(2)-H(2)	118.4	C(14)-C(13)-H(13C)	109.5
C(1)-C(2)-H(2)	118.4	H(13A)-C(13)-H(13C)	109.5

H(13B)-C(13)-H(13C)	109.5	C(20)-C(21)-H(21C)	109.5
C(15)-C(14)-C(13)	112.12(16)	H(21A)-C(21)-H(21C)	109.5
C(15)-C(14)-P(1)	114.57(13)	H(21B)-C(21)-H(21C)	109.5
C(13)-C(14)-P(1)	110.97(13)	C(23)-C(22)-H(22A)	109.5
C(15)-C(14)-H(14)	106.2	C(23)-C(22)-H(22B)	109.5
C(13)-C(14)-H(14)	106.2	H(22A)-C(22)-H(22B)	109.5
P(1)-C(14)-H(14)	106.2	C(23)-C(22)-H(22C)	109.5
C(14)-C(15)-H(15A)	109.5	H(22A)-C(22)-H(22C)	109.5
C(14)-C(15)-H(15B)	109.5	H(22B)-C(22)-H(22C)	109.5
H(15A)-C(15)-H(15B)	109.5	C(24)-C(23)-C(22)	110.36(18)
C(14)-C(15)-H(15C)	109.5	C(24)-C(23)-P(3)	115.53(15)
H(15A)-C(15)-H(15C)	109.5	C(22)-C(23)-P(3)	112.63(14)
H(15B)-C(15)-H(15C)	109.5	C(24)-C(23)-H(23)	105.8
C(17)-C(16)-H(16A)	109.5	C(22)-C(23)-H(23)	105.8
C(17)-C(16)-H(16B)	109.5	P(3)-C(23)-H(23)	105.8
H(16A)-C(16)-H(16B)	109.5	C(23)-C(24)-H(24A)	109.5
C(17)-C(16)-H(16C)	109.5	C(23)-C(24)-H(24B)	109.5
H(16A)-C(16)-H(16C)	109.5	H(24A)-C(24)-H(24B)	109.5
H(16B)-C(16)-H(16C)	109.5	C(23)-C(24)-H(24C)	109.5
C(18)-C(17)-C(16)	111.54(15)	H(24A)-C(24)-H(24C)	109.5
C(18)-C(17)-P(2)	114.14(12)	H(24B)-C(24)-H(24C)	109.5
C(16)-C(17)-P(2)	110.55(12)	C(26A)-C(25A)-H(25A)	109.5
C(18)-C(17)-H(17)	106.7	C(26A)-C(25A)-H(25B)	109.5
C(16)-C(17)-H(17)	106.7	H(25A)-C(25A)-H(25B)	109.5
P(2)-C(17)-H(17)	106.7	C(26A)-C(25A)-H(25C)	109.5
C(17)-C(18)-H(18A)	109.5	H(25A)-C(25A)-H(25C)	109.5
C(17)-C(18)-H(18B)	109.5	H(25B)-C(25A)-H(25C)	109.5
H(18A)-C(18)-H(18B)	109.5	C(25A)-C(26A)-C(27A)	116.3(10)
C(17)-C(18)-H(18C)	109.5	C(25A)-C(26A)-P(3)	113.5(7)
H(18A)-C(18)-H(18C)	109.5	C(27A)-C(26A)-P(3)	114.4(8)
H(18B)-C(18)-H(18C)	109.5	C(25A)-C(26A)-H(26A)	103.5
C(20)-C(19)-H(19A)	109.5	C(27A)-C(26A)-H(26A)	103.5
C(20)-C(19)-H(19B)	109.5	P(3)-C(26A)-H(26A)	103.5
H(19A)-C(19)-H(19B)	109.5	C(26A)-C(27A)-H(27A)	109.5
C(20)-C(19)-H(19C)	109.5	C(26A)-C(27A)-H(27B)	109.5
H(19A)-C(19)-H(19C)	109.5	H(27A)-C(27A)-H(27B)	109.5
H(19B)-C(19)-H(19C)	109.5	C(26A)-C(27A)-H(27C)	109.5
C(21)-C(20)-C(19)	110.77(17)	H(27A)-C(27A)-H(27C)	109.5
C(21)-C(20)-P(2)	114.22(13)	H(27B)-C(27A)-H(27C)	109.5
C(19)-C(20)-P(2)	109.91(12)	C(27B)-C(26B)-C(25B)	117.2(9)
C(21)-C(20)-H(20)	107.2	C(27B)-C(26B)-P(3)	113.9(7)
C(19)-C(20)-H(20)	107.2	C(25B)-C(26B)-P(3)	110.4(6)
P(2)-C(20)-H(20)	107.2	C(27B)-C(26B)-H(26B)	104.6
C(20)-C(21)-H(21A)	109.5	C(25B)-C(26B)-H(26B)	104.6
C(20)-C(21)-H(21B)	109.5	P(3)-C(26B)-H(26B)	104.6
H(21A)-C(21)-H(21B)	109.5		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for [PhBP$^{iPr}_3$]MnCl (1a). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn	228(2)	125(2)	204(2)	-2(1)	8(1)	-21(1)
P(1)	198(2)	143(2)	175(2)	1(2)	39(2)	15(2)
P(2)	186(2)	134(2)	169(2)	19(2)	27(2)	13(2)
P(3)	178(2)	156(2)	307(3)	10(2)	-18(2)	-40(2)
Cl	696(4)	133(2)	325(3)	-36(2)	0(3)	-50(2)
B	168(10)	111(9)	185(10)	-6(7)	17(8)	-3(8)
C(1)	94(8)	149(9)	275(10)	-20(7)	53(7)	-9(7)
C(2)	184(9)	175(9)	312(10)	4(8)	37(8)	-3(7)
C(3)	244(10)	146(9)	507(13)	42(9)	82(9)	10(8)
C(4)	228(11)	130(9)	614(15)	-88(9)	107(10)	-28(8)
C(5)	222(10)	258(10)	408(12)	-152(9)	106(9)	-59(8)
C(6)	161(9)	198(9)	286(10)	-46(7)	68(8)	-14(7)
C(7)	187(9)	110(8)	188(9)	4(7)	21(7)	1(7)
C(8)	150(9)	153(9)	196(9)	-12(7)	43(7)	1(7)
C(9)	187(9)	147(8)	235(9)	-12(7)	30(7)	-10(7)
C(10)	328(12)	394(12)	212(10)	-45(8)	-14(8)	-8(9)
C(11)	297(11)	325(11)	187(10)	-1(8)	-10(8)	92(9)
C(12)	801(18)	278(12)	230(11)	55(9)	-40(11)	141(11)
C(13)	395(13)	259(11)	516(14)	0(9)	255(11)	93(9)
C(14)	253(10)	230(10)	244(10)	4(8)	108(8)	26(8)
C(15)	253(11)	341(12)	419(12)	-45(9)	148(9)	-7(9)
C(16)	258(10)	212(9)	244(10)	16(7)	69(8)	70(8)
C(17)	180(9)	184(9)	225(9)	8(7)	53(7)	35(7)
C(18)	177(10)	256(10)	363(11)	-46(8)	31(8)	4(8)
C(19)	602(16)	263(12)	321(12)	132(9)	-35(11)	-127(10)
C(20)	265(10)	181(9)	220(9)	54(7)	38(8)	5(8)
C(21)	446(14)	468(14)	379(13)	240(10)	224(11)	210(11)
C(22)	486(15)	374(13)	510(15)	124(11)	64(12)	-191(11)
C(23)	180(10)	287(11)	412(12)	49(9)	71(9)	-46(8)
C(24)	503(16)	579(17)	930(20)	196(15)	486(15)	110(13)
C(25A)	930(80)	230(50)	1270(90)	-300(40)	-980(70)	260(50)
C(26A)	150(40)	260(30)	320(40)	-20(30)	-20(20)	-20(30)
C(27A)	250(50)	280(40)	730(70)	-60(40)	-150(30)	40(40)
C(25B)	570(50)	250(40)	540(40)	-150(30)	-40(40)	-260(30)
C(26B)	190(40)	280(20)	310(40)	-30(30)	0(20)	-10(30)
C(27B)	310(50)	430(30)	720(70)	130(40)	-270(40)	-100(40)

Table 5. Crystal Data and Structure Analysis Details for {[PhBP$^{iPr}_3$]Mn(μ-Cl)}$_2$ (1b).

Empirical formula	$C_{54}H_{106}B_2Cl_2Mn_2P_6$
Formula weight	1143.61
Crystallization solvent	benzene/petroleum ether
Crystal shape	rough block
Crystal color	colorless
Crystal size	0.22 x 0.28 x 0.37 mm

Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data collection temperature	100 K	
Theta range for 16248 reflections used in lattice determination	2.31 to 28.15°	
Unit cell dimensions	a = 10.950(2) Å b = 11.718(2) Å c = 13.432(3) Å	α= 68.000(3)° β= 76.424(4)° γ = 78.528(3)°
Volume	1541.5(5) Å^3	
Z	1	
Crystal system	triclinic	
Space group	P-1 (# 2)	
Density (calculated)	1.232 g/cm^3	
F(000)	614	
Theta range for data collection	1.9 to 28.3°	
Completeness to theta = 28.34°	91.6%	
Index ranges	$-14 \le h \le 14$, $-15 \le k \le 15$, $-17 \le l \le 17$	
Data collection scan type	ω scans	
Reflections collected	25889	
Independent reflections	7059 [R_{int}= 0.0499]	
Reflections > 2σ(I)	5553	
Average σ(I)/(net I)	0.0403	
Absorption coefficient	0.69 mm^{-1}	
Absorption correction	none	
Reflections monitored for decay	initial data recollected at end	
Decay of standards	0%	

Table 5 (cont.)

Structure Solution and Refinement

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7059 / 0 / 378
Treatment of hydrogen atoms	not refined, U_{iso} fixed at 120% U_{eq} of attached atom
Goodness-of-fit on F^2	1.83
Final R indices [I>2σ(I), 5553 reflections]	R1 = 0.0356, wR2 = 0.0674
R indices (all data)	R1 = 0.0502, wR2 = 0.0692
Type of weighting scheme used	sigma
Weighting scheme used	calc $w=1/[\sigma^2(Fo^2)]$ where $P=(Fo^2+2Fc^2)/3$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	0.78 and -0.45 e·Å^{-3}

Programs Used

Cell refinement	Bruker SMART 5.606
Data collection	Bruker SMART 5.054
Data reduction	Bruker SAINT 6.45
Structure solution	Bruker SHELXTL 6.14
Structure refinement	Bruker SHELXTL 6.14

Special Refinement Details

The chloride was disordered in two positions and was refined as such (population 51.9 and 48.1%). One P^iPr_2 unit in the ligand was also disordered and was refined in two positions (population 50.9, 49.1 %). One bad reflection (001) was omitted.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for {[PhBP$^{iPr}_3$]Mn(μ-Cl)}$_2$ (1b). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Mn	4333.2(2)	1404.6(2)	3952.1(2)	22.7(1)
P(1)	5228.7(4)	3498.1(4)	2740.8(4)	21.5(1)
P(2)	3339.0(4)	1633.7(4)	2288.1(4)	21.3(1)
P(3A)	2426(3)	2693(3)	4690(3)	16.4(5)
P(3B)	2183(3)	2466(3)	4655(3)	14.3(5)
B	2557.1(17)	4260.4(18)	2287.4(16)	17.7(4)
Cl(1)	3826.1(8)	-718.5(7)	5027.4(7)	21.3(3)
Cl(2)	5279.7(8)	919.7(8)	5578.2(7)	20.2(3)
C(1)	1700.4(14)	5538.7(15)	1650.1(12)	14.7(3)
C(2)	1954.9(15)	6714.6(15)	1529.1(14)	21.1(4)
C(3)	1217.5(16)	7807.0(16)	1049.7(15)	25.8(4)
C(4)	163.2(16)	7775.9(16)	667.8(15)	26.0(4)
C(5)	-134.2(16)	6634.0(16)	777.0(14)	24.4(4)
C(6)	611.9(15)	5550.8(16)	1261.0(13)	18.9(4)
C(7)	4078.7(14)	4479.8(15)	1873.6(13)	17.8(4)
C(8)	2273.7(14)	3092.3(15)	1987.9(14)	19.1(4)
C(9)	2059.1(17)	4094.4(16)	3608.2(14)	27.1(4)
C(10)	6581.2(16)	3906.4(18)	4104.9(15)	32.0(5)
C(11)	5353.2(17)	4357.5(18)	3631.4(15)	29.3(5)
C(12)	5145.8(19)	5773.4(19)	3156.1(17)	41.5(6)
C(13)	7803.8(17)	2497.0(18)	2226.4(16)	34.0(5)
C(14)	6742.4(15)	3491.9(17)	1760.4(14)	23.5(4)
C(15)	7211.0(16)	4757.9(17)	1155.3(15)	30.1(5)
C(16)	5738.3(16)	891.1(17)	1233.4(15)	30.2(5)
C(17)	4535.8(15)	1806.2(16)	1017.5(13)	20.8(4)
C(18)	4080.7(17)	1798.5(17)	29.0(14)	25.6(4)
C(20)	2359.1(18)	412.8(16)	2469.3(15)	31.3(5)
C(19)	3146(2)	-829.8(17)	2479.3(16)	39.9(5)
C(21)	1397.8(17)	787.0(18)	1707.3(18)	41.1(6)
C(27)	1159.0(17)	3789.5(17)	6233.9(15)	29.2(4)
C(22A)	898(3)	858(3)	6075(3)	26.7(10)
C(23A)	1026(8)	1892(7)	4945(6)	15.9(13)
C(24A)	-243(4)	2700(4)	4791(4)	25.2(11)
C(25A)	2950(3)	2003(3)	6834(3)	24.7(9)
C(26A)	2448(5)	3080(5)	5898(5)	14.0(10)
C(22B)	993(3)	295(3)	5429(3)	23.2(10)
C(23B)	788(8)	1690(7)	4795(7)	15.8(13)
C(24B)	-512(4)	2274(5)	5251(4)	25.6(12)
C(25B)	2078(4)	1568(3)	6951(3)	25.4(10)
C(26B)	2106(5)	2763(6)	5929(5)	19.3(12)

Table 7. Bond lengths [Å] and angles [°] for {[PhBP$^{iPr}_3$]Mn(μ-Cl)}$_2$ (1b).

Mn-Cl(1)	2.4625(9)	C(12)-H(12A)	0.9800
Mn-Cl(2)	2.4630(9)	C(12)-H(12B)	0.9800
Mn-Cl(2)#1	2.5247(10)	C(12)-H(12C)	0.9800
Mn-Cl(1)#1	2.5327(9)	C(13)-C(14)	1.535(2)
Mn-P(3A)	2.552(4)	C(13)-H(13A)	0.9800
Mn-P(3B)	2.580(4)	C(13)-H(13B)	0.9800
Mn-P(2)	2.6132(7)	C(13)-H(13C)	0.9800
Mn-P(1)	2.6162(7)	C(14)-C(15)	1.526(2)
P(1)-C(7)	1.8369(16)	C(14)-H(14)	1.0000
P(1)-C(14)	1.8599(17)	C(15)-H(15A)	0.9800
P(1)-C(11)	1.8701(18)	C(15)-H(15B)	0.9800
P(2)-C(8)	1.8320(16)	C(15)-H(15C)	0.9800
P(2)-C(17)	1.8621(17)	C(16)-C(17)	1.534(2)
P(2)-C(20)	1.8666(18)	C(16)-H(16A)	0.9800
P(3A)-C(9)	1.787(4)	C(16)-H(16B)	0.9800
P(3A)-C(26A)	1.848(6)	C(16)-H(16C)	0.9800
P(3A)-C(23A)	1.853(7)	C(17)-C(18)	1.527(2)
P(3B)-C(26B)	1.850(7)	C(17)-H(17)	1.0000
P(3B)-C(23B)	1.866(7)	C(18)-H(18A)	0.9800
P(3B)-C(9)	1.901(4)	C(18)-H(18B)	0.9800
B-C(1)	1.647(2)	C(18)-H(18C)	0.9800
B-C(8)	1.665(2)	C(20)-C(21)	1.528(3)
B-C(7)	1.667(2)	C(20)-C(19)	1.534(2)
B-C(9)	1.677(3)	C(20)-H(20)	1.0196
Cl(1)-Cl(2)#1	1.1637(12)	C(19)-H(19A)	0.9800
Cl(1)-Mn#1	2.5327(9)	C(19)-H(19B)	0.9800
Cl(2)-Cl(1)#1	1.1637(12)	C(19)-H(19C)	0.9800
Cl(2)-Mn#1	2.5247(10)	C(21)-H(21A)	0.9800
C(1)-C(2)	1.402(2)	C(21)-H(21B)	0.9800
C(1)-C(6)	1.405(2)	C(21)-H(21C)	0.9800
C(2)-C(3)	1.386(2)	C(27)-C(26B)	1.537(7)
C(2)-H(2)	0.9500	C(27)-C(26A)	1.550(6)
C(3)-C(4)	1.381(2)	C(27)-H(27A)	0.9461
C(3)-H(3)	0.9500	C(27)-H(27B)	0.9422
C(4)-C(5)	1.386(2)	C(27)-H(27C)	1.0027
C(4)-H(4)	0.9500	C(22A)-C(23A)	1.543(9)
C(5)-C(6)	1.386(2)	C(22A)-H(22A)	0.9800
C(5)-H(5)	0.9500	C(22A)-H(22B)	0.9800
C(6)-H(6)	0.9500	C(22A)-H(22C)	0.9800
C(7)-H(7A)	0.9900	C(23A)-C(24A)	1.527(10)
C(7)-H(7B)	0.9900	C(23A)-H(23A)	1.0000
C(8)-H(8A)	0.9900	C(24A)-H(24A)	0.9800
C(8)-H(8B)	0.9900	C(24A)-H(24B)	0.9800
C(9)-H(9A)	0.9959	C(24A)-H(24C)	0.9800
C(9)-H(9B)	0.9988	C(25A)-C(26A)	1.528(7)
C(10)-C(11)	1.536(2)	C(25A)-H(25A)	0.9800
C(10)-H(10A)	0.9800	C(25A)-H(25B)	0.9800
C(10)-H(10B)	0.9800	C(25A)-H(25C)	0.9800
C(10)-H(10C)	0.9800	C(26A)-H(26A)	1.0000
C(11)-C(12)	1.528(3)	C(22B)-C(23B)	1.533(9)
C(11)-H(11)	1.0000	C(22B)-H(22D)	0.9800

C(22B)-H(22E)	0.9800
C(22B)-H(22F)	0.9800
C(23B)-C(24B)	1.544(11)
C(23B)-H(23B)	1.0000
C(24B)-H(24D)	0.9800
C(24B)-H(24E)	0.9800
C(24B)-H(24F)	0.9800
C(25B)-C(26B)	1.550(7)
C(25B)-H(25D)	0.9800
C(25B)-H(25E)	0.9800
C(25B)-H(25F)	0.9800
C(26B)-H(26B)	1.0000
Cl(1)-Mn-Cl(2)	77.95(3)
Cl(1)-Mn-Cl(2)#1	26.95(3)
Cl(2)-Mn-Cl(2)#1	82.95(3)
Cl(1)-Mn-Cl(1)#1	83.15(3)
Cl(2)-Mn-Cl(1)#1	26.89(3)
Cl(2)#1-Mn-Cl(1)#1	75.55(3)
Cl(1)-Mn-P(3A)	101.39(8)
Cl(2)-Mn-P(3A)	91.05(8)
Cl(2)#1-Mn-P(3A)	128.11(7)
Cl(1)#1-Mn-P(3A)	116.17(8)
Cl(1)-Mn-P(3B)	94.72(8)
Cl(2)-Mn-P(3B)	96.53(8)
Cl(2)#1-Mn-P(3B)	120.78(7)
Cl(1)#1-Mn-P(3B)	122.74(8)
P(3A)-Mn-P(3B)	9.65(7)
Cl(1)-Mn-P(2)	95.64(2)
Cl(2)-Mn-P(2)	173.17(2)
Cl(2)#1-Mn-P(2)	90.26(2)
Cl(1)#1-Mn-P(2)	151.00(3)
P(3A)-Mn-P(2)	92.55(8)
P(3B)-Mn-P(2)	86.26(7)
Cl(1)-Mn-P(1)	171.13(2)
Cl(2)-Mn-P(1)	99.61(3)
Cl(2)#1-Mn-P(1)	144.74(3)
Cl(1)#1-Mn-P(1)	90.90(2)
P(3A)-Mn-P(1)	87.13(7)
P(3B)-Mn-P(1)	94.03(7)
P(2)-Mn-P(1)	86.375(18)
C(7)-P(1)-C(14)	103.70(8)
C(7)-P(1)-C(11)	105.92(8)
C(14)-P(1)-C(11)	108.46(8)
C(7)-P(1)-Mn	108.61(6)
C(14)-P(1)-Mn	119.76(6)
C(11)-P(1)-Mn	109.46(7)
C(8)-P(2)-C(17)	104.89(8)
C(8)-P(2)-C(20)	105.56(8)
C(17)-P(2)-C(20)	108.26(8)
C(8)-P(2)-Mn	107.52(6)
C(17)-P(2)-Mn	112.67(6)
C(20)-P(2)-Mn	117.01(7)
C(9)-P(3A)-C(26A)	108.7(2)
C(9)-P(3A)-C(23A)	101.1(3)
C(26A)-P(3A)-C(23A)	109.5(4)
C(9)-P(3A)-Mn	108.98(18)
C(26A)-P(3A)-Mn	120.0(2)
C(23A)-P(3A)-Mn	106.9(3)
C(26B)-P(3B)-C(23B)	109.1(4)
C(26B)-P(3B)-C(9)	102.5(2)
C(23B)-P(3B)-C(9)	110.4(3)
C(26B)-P(3B)-Mn	115.0(2)
C(23B)-P(3B)-Mn	114.8(3)
C(9)-P(3B)-Mn	104.21(16)
C(1)-B-C(8)	108.88(13)
C(1)-B-C(7)	108.26(13)
C(8)-B-C(7)	110.79(13)
C(1)-B-C(9)	103.57(13)
C(8)-B-C(9)	112.67(14)
C(7)-B-C(9)	112.29(13)
Cl(2)#1-Cl(1)-Mn	79.50(6)
Cl(2)#1-Cl(1)-Mn#1	73.21(6)
Mn-Cl(1)-Mn#1	96.85(3)
Cl(1)#1-Cl(2)-Mn	79.89(6)
Cl(1)#1-Cl(2)-Mn#1	73.55(6)
Mn-Cl(2)-Mn#1	97.05(3)
C(2)-C(1)-C(6)	114.37(15)
C(2)-C(1)-B	121.71(13)
C(6)-C(1)-B	123.74(14)
C(3)-C(2)-C(1)	123.46(15)
C(3)-C(2)-H(2)	118.3
C(1)-C(2)-H(2)	118.3
C(4)-C(3)-C(2)	120.20(16)
C(4)-C(3)-H(3)	119.9
C(2)-C(3)-H(3)	119.9
C(3)-C(4)-C(5)	118.51(16)
C(3)-C(4)-H(4)	120.7
C(5)-C(4)-H(4)	120.7
C(6)-C(5)-C(4)	120.52(15)
C(6)-C(5)-H(5)	119.7
C(4)-C(5)-H(5)	119.7
C(5)-C(6)-C(1)	122.93(15)
C(5)-C(6)-H(6)	118.5
C(1)-C(6)-H(6)	118.5
B-C(7)-P(1)	118.92(11)
B-C(7)-H(7A)	107.6
P(1)-C(7)-H(7A)	107.6
B-C(7)-H(7B)	107.6
P(1)-C(7)-H(7B)	107.6
H(7A)-C(7)-H(7B)	107.0
B-C(8)-P(2)	119.77(11)
B-C(8)-H(8A)	107.4
P(2)-C(8)-H(8A)	107.4
B-C(8)-H(8B)	107.4
P(2)-C(8)-H(8B)	107.4
H(8A)-C(8)-H(8B)	106.9
B-C(9)-P(3A)	122.81(17)

B-C(9)-P(3B)	118.06(16)	C(18)-C(17)-H(17)	105.4
P(3A)-C(9)-P(3B)	13.01(12)	C(16)-C(17)-H(17)	105.4
B-C(9)-H(9A)	107.0	P(2)-C(17)-H(17)	105.4
P(3A)-C(9)-H(9A)	111.6	C(17)-C(18)-H(18A)	109.5
P(3B)-C(9)-H(9A)	104.1	C(17)-C(18)-H(18B)	109.5
B-C(9)-H(9B)	106.9	H(18A)-C(18)-H(18B)	109.5
P(3A)-C(9)-H(9B)	101.3	C(17)-C(18)-H(18C)	109.5
P(3B)-C(9)-H(9B)	114.1	H(18A)-C(18)-H(18C)	109.5
H(9A)-C(9)-H(9B)	105.8	H(18B)-C(18)-H(18C)	109.5
C(11)-C(10)-H(10A)	109.5	C(21)-C(20)-C(19)	110.70(16)
C(11)-C(10)-H(10B)	109.5	C(21)-C(20)-P(2)	115.89(13)
H(10A)-C(10)-H(10B)	109.5	C(19)-C(20)-P(2)	113.31(14)
C(11)-C(10)-H(10C)	109.5	C(21)-C(20)-H(20)	106.1
H(10A)-C(10)-H(10C)	109.5	C(19)-C(20)-H(20)	102.7
H(10B)-C(10)-H(10C)	109.5	P(2)-C(20)-H(20)	106.9
C(12)-C(11)-C(10)	110.83(16)	C(20)-C(19)-H(19A)	109.5
C(12)-C(11)-P(1)	116.92(13)	C(20)-C(19)-H(19B)	109.5
C(10)-C(11)-P(1)	111.82(12)	H(19A)-C(19)-H(19B)	109.5
C(12)-C(11)-H(11)	105.4	C(20)-C(19)-H(19C)	109.5
C(10)-C(11)-H(11)	105.4	H(19A)-C(19)-H(19C)	109.5
P(1)-C(11)-H(11)	105.4	H(19B)-C(19)-H(19C)	109.5
C(11)-C(12)-H(12A)	109.5	C(20)-C(21)-H(21A)	109.5
C(11)-C(12)-H(12B)	109.5	C(20)-C(21)-H(21B)	109.5
H(12A)-C(12)-H(12B)	109.5	H(21A)-C(21)-H(21B)	109.5
C(11)-C(12)-H(12C)	109.5	C(20)-C(21)-H(21C)	109.5
H(12A)-C(12)-H(12C)	109.5	H(21A)-C(21)-H(21C)	109.5
H(12B)-C(12)-H(12C)	109.5	H(21B)-C(21)-H(21C)	109.5
C(14)-C(13)-H(13A)	109.5	C(26B)-C(27)-C(26A)	21.02(16)
C(14)-C(13)-H(13B)	109.5	C(26B)-C(27)-H(27A)	87.0
H(13A)-C(13)-H(13B)	109.5	C(26A)-C(27)-H(27A)	105.6
C(14)-C(13)-H(13C)	109.5	C(26B)-C(27)-H(27B)	108.4
H(13A)-C(13)-H(13C)	109.5	C(26A)-C(27)-H(27B)	107.6
H(13B)-C(13)-H(13C)	109.5	H(27A)-C(27)-H(27B)	115.9
C(15)-C(14)-C(13)	111.58(14)	C(26B)-C(27)-H(27C)	122.9
C(15)-C(14)-P(1)	114.88(12)	C(26A)-C(27)-H(27C)	106.1
C(13)-C(14)-P(1)	114.46(13)	H(27A)-C(27)-H(27C)	110.4
C(15)-C(14)-H(14)	104.9	H(27B)-C(27)-H(27C)	110.7
C(13)-C(14)-H(14)	104.9	C(24A)-C(23A)-C(22A)	110.2(6)
P(1)-C(14)-H(14)	104.9	C(24A)-C(23A)-P(3A)	117.3(4)
C(14)-C(15)-H(15A)	109.5	C(22A)-C(23A)-P(3A)	110.9(4)
C(14)-C(15)-H(15B)	109.5	C(24A)-C(23A)-H(23A)	105.9
H(15A)-C(15)-H(15B)	109.5	C(22A)-C(23A)-H(23A)	105.9
C(14)-C(15)-H(15C)	109.5	P(3A)-C(23A)-H(23A)	105.9
H(15A)-C(15)-H(15C)	109.5	C(25A)-C(26A)-C(27)	114.8(4)
H(15B)-C(15)-H(15C)	109.5	C(25A)-C(26A)-P(3A)	114.8(4)
C(17)-C(16)-H(16A)	109.5	C(27)-C(26A)-P(3A)	110.4(3)
C(17)-C(16)-H(16B)	109.5	C(25A)-C(26A)-H(26A)	105.2
H(16A)-C(16)-H(16B)	109.5	C(27)-C(26A)-H(26A)	105.2
C(17)-C(16)-H(16C)	109.5	P(3A)-C(26A)-H(26A)	105.2
H(16A)-C(16)-H(16C)	109.5	C(23B)-C(22B)-H(22D)	109.5
H(16B)-C(16)-H(16C)	109.5	C(23B)-C(22B)-H(22E)	109.5
C(18)-C(17)-C(16)	111.00(14)	H(22D)-C(22B)-H(22E)	109.5
C(18)-C(17)-P(2)	116.86(11)	C(23B)-C(22B)-H(22F)	109.5
C(16)-C(17)-P(2)	111.71(12)	H(22D)-C(22B)-H(22F)	109.5

H(22E)-C(22B)-H(22F)	109.5	C(26B)-C(25B)-H(25D)	109.5
C(22B)-C(23B)-C(24B)	110.6(6)	C(26B)-C(25B)-H(25E)	109.5
C(22B)-C(23B)-P(3B)	111.7(5)	H(25D)-C(25B)-H(25E)	109.5
C(24B)-C(23B)-P(3B)	116.3(4)	C(26B)-C(25B)-H(25F)	109.5
C(22B)-C(23B)-H(23B)	105.8	H(25D)-C(25B)-H(25F)	109.5
C(24B)-C(23B)-H(23B)	105.8	H(25E)-C(25B)-H(25F)	109.5
P(3B)-C(23B)-H(23B)	105.8	C(27)-C(26B)-C(25B)	108.2(4)
C(23B)-C(24B)-H(24D)	109.5	C(27)-C(26B)-P(3B)	122.2(4)
C(23B)-C(24B)-H(24E)	109.5	C(25B)-C(26B)-P(3B)	113.1(4)
H(24D)-C(24B)-H(24E)	109.5	C(27)-C(26B)-H(26B)	103.7
C(23B)-C(24B)-H(24F)	109.5	C(25B)-C(26B)-H(26B)	103.7
H(24D)-C(24B)-H(24F)	109.5	P(3B)-C(26B)-H(26B)	103.7
H(24E)-C(24B)-H(24F)	109.5		

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1

Table 8. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for {[PhBP$^{iPr}_3$]Mn(μ-Cl)}$_2$ (1b). 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	263(2)	205(2)	135(2)	-33(1)	-22(1)	79(1)
P(1)	187(2)	282(3)	186(2)	-118(2)	-71(2)	70(2)
P(2)	270(2)	132(2)	187(3)	-55(2)	16(2)	19(2)
P(3A)	160(12)	140(11)	178(7)	-56(7)	-9(7)	-9(7)
P(3B)	169(13)	131(12)	116(6)	-52(7)	-22(7)	23(7)
B	183(10)	148(10)	187(11)	-54(9)	-52(8)	26(8)
Cl(1)	205(5)	157(4)	255(5)	-15(4)	-86(4)	-29(3)
Cl(2)	270(6)	154(5)	214(5)	-72(4)	-125(4)	17(4)
C(1)	148(8)	154(9)	119(8)	-53(7)	8(6)	-2(7)
C(2)	181(9)	200(10)	282(10)	-102(8)	-86(8)	0(7)
C(3)	283(10)	153(10)	338(11)	-100(9)	-40(8)	-11(8)
C(4)	238(10)	183(10)	301(11)	-53(9)	-87(8)	88(8)
C(5)	179(9)	282(11)	285(11)	-106(9)	-97(8)	22(8)
C(6)	184(9)	167(9)	221(10)	-77(8)	-16(7)	-31(7)
C(7)	207(9)	181(9)	160(9)	-85(8)	-69(7)	41(7)
C(8)	162(8)	137(9)	239(10)	-66(8)	14(7)	9(7)
C(9)	285(10)	227(10)	197(10)	-42(8)	-30(8)	121(8)
C(10)	292(10)	436(13)	305(11)	-214(10)	-146(9)	76(9)
C(11)	235(10)	465(13)	258(11)	-248(10)	-105(8)	103(9)
C(12)	425(12)	504(14)	482(14)	-372(12)	-279(11)	215(11)
C(13)	236(10)	410(13)	385(12)	-210(10)	-83(9)	117(9)
C(14)	179(9)	322(11)	225(10)	-155(9)	-48(7)	61(8)
C(15)	227(10)	364(12)	318(11)	-168(10)	-12(8)	9(9)
C(16)	281(10)	310(12)	311(11)	-172(10)	-29(9)	77(9)
C(17)	234(9)	172(9)	181(9)	-61(8)	8(7)	5(7)
C(18)	295(10)	233(10)	217(10)	-81(8)	-16(8)	-8(8)
C(20)	405(11)	154(10)	303(11)	-92(9)	148(9)	-83(9)
C(19)	683(15)	146(10)	299(12)	-82(9)	20(11)	-13(10)
C(21)	251(10)	258(12)	763(17)	-279(12)	48(11)	-75(9)
C(27)	301(10)	216(11)	306(11)	-110(9)	67(8)	-21(8)
C(22A)	220(19)	260(20)	270(20)	-34(18)	-1(16)	-81(17)
C(23A)	180(30)	100(30)	220(30)	-73(19)	-30(20)	-30(20)
C(24A)	150(20)	280(30)	350(30)	-120(20)	0(20)	-89(19)
C(25A)	230(20)	280(20)	220(20)	-81(17)	-43(16)	-12(17)
C(26A)	130(30)	180(30)	140(20)	-80(20)	-34(18)	-20(18)
C(22B)	219(19)	190(20)	280(20)	-72(17)	-30(16)	-48(16)
C(23B)	170(30)	150(30)	180(30)	-60(20)	-30(20)	-80(20)
C(24B)	120(20)	230(30)	370(30)	-60(20)	-10(20)	-35(19)
C(25B)	290(20)	270(20)	170(20)	-80(17)	-16(16)	14(18)
C(26B)	120(30)	250(30)	250(20)	-100(20)	-30(20)	-76(19)

Table 9. Crystal Data and Structure Analysis Details for [PhBP$^{iPr}_3$]MnI (2).

Empirical formula	$C_{33}H_{59}BIMnP_3$
Formula weight	741.36
Crystallization solvent	benzene/petroleum ether
Crystal shape	plate
Crystal color	colorless
Crystal size	0.20 x 0.22 x 0.30 mm

Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data collection temperature	100 K	
Theta range for 21436 reflections used in lattice determination	2.152 to 28.255°	
Unit cell dimensions	a = 9.5424(8) Å b = 9.9006(8) Å c = 19.668(2) Å	α= 89.780(1)° β= 89.920(1)° γ = 82.662(1)°
Volume	1842.9(3) Å^3	
Z	2	
Crystal system	triclinic	
Space group	P-1 (# 2)	
Density (calculated)	1.336 g/cm^3	
F(000)	770	
Theta range for data collection	2.1 to 28.5°	
Completeness to theta = 28.46°	90.9%	
Index ranges	$-12 \le h \le 12$, $-13 \le k \le 13$, $-25 \le l \le 25$	
Data collection scan type	ω scans	
Reflections collected	33155	
Independent reflections	8473 [R_{int}= 0.0674]	
Reflections > 2σ(I)	6869	
Average σ(I)/(net I)	0.0494	
Absorption coefficient	1.35 mm^{-1}	
Absorption correction	none	
Reflections monitored for decay	initial data recollected at end	
Decay of standards	0%	

Table 9 (cont.)

Structure Solution and Refinement

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8473 / 0 / 364
Treatment of hydrogen atoms	not refined, U_{iso} fixed at 120% U_{eq} of attached atom
Goodness-of-fit on F^2	1.33
Final R indices [I>2σ(I), 6869 reflections]	R1 = 0.0305, wR2 = 0.0586
R indices (all data)	R1 = 0.0417, wR2 = 0.0602
Type of weighting scheme used	sigma
Weighting scheme used	calc $w=1/[\sigma^2(Fo^2)]$ where $P=(Fo^2+2Fc^2)/3$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	0.94 and -0.61 e·Å^{-3}

Programs Used

Cell refinement	Bruker SMART 5.606
Data collection	Bruker SMART 5.054
Data reduction	Bruker SAINT 6.45
Structure solution	Bruker SHELXTL 6.14
Structure refinement	Bruker SHELXTL 6.14

Special Refinement Details

One benzene solvent molecule was present in the asymmetric unit.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	y	z	U_{eq}
Mn	144.5(3)	-637.5(3)	6988.6(2)	13.1(1)
P(1)	-29.1(6)	1937.7(6)	7026.7(3)	14.6(1)
P(2)	315.2(6)	-794.4(6)	8267.6(3)	14.8(1)
P(3)	2815.4(5)	-836.7(6)	6892.7(3)	13.1(1)
B	2372(2)	1250(3)	8014.9(12)	13.8(5)
I	-1445.8(2)	-2108.9(2)	6277.7(1)	22.7(1)
C(1)	3416(2)	2047(2)	8499.4(10)	14.0(5)
C(2)	3812(2)	3329(2)	8346.5(11)	16.3(5)
C(3)	4690(2)	3980(2)	8766.8(12)	21.9(5)
C(4)	5205(2)	3373(3)	9366.3(12)	22.6(5)
C(5)	4868(2)	2091(2)	9526.9(12)	22.3(5)
C(6)	4003(2)	1449(2)	9100.2(11)	19.3(5)
C(7)	1537(2)	2372(2)	7474.8(10)	14.8(5)
C(8)	1225(2)	619(2)	8542.4(10)	14.3(5)
C(9)	3470(2)	38(2)	7622.1(10)	14.1(4)
C(10)	-662(3)	2159(3)	5637.8(11)	28.7(6)
C(11)	-386(2)	3026(2)	6249.2(11)	20.4(5)
C(12)	732(3)	3949(3)	6085.9(13)	35.8(7)
C(13)	-2926(2)	2139(3)	7263.6(13)	27.5(6)
C(14)	-1567(2)	2549(2)	7572.3(11)	18.1(5)
C(15)	-1737(2)	4072(2)	7734.7(12)	26.0(6)
C(16)	-2394(2)	-1501(3)	8503.2(13)	34.2(7)
C(17)	-1145(2)	-1008(3)	8873.5(12)	25.1(6)
C(18)	-1626(2)	233(3)	9304.9(12)	30.7(6)
C(19)	850(2)	-3620(2)	8283.2(12)	23.9(5)
C(20)	1571(2)	-2366(2)	8412.3(11)	21.3(5)
C(21)	2343(2)	-2435(2)	9091.7(11)	23.4(5)
C(22)	3041(2)	-3605(2)	6555.2(13)	26.0(6)
C(23)	3956(2)	-2491(2)	6732.4(11)	16.4(5)
C(24)	4987(2)	-2957(2)	7304.8(12)	25.5(6)
C(25)	2651(2)	-494(2)	5493.8(11)	19.2(5)
C(26)	3157(2)	178(2)	6129.8(10)	15.0(5)
C(27)	4685(2)	473(3)	6051.7(12)	25.8(6)
C(28)	4365(3)	3815(3)	4989.4(12)	27.5(6)
C(29)	5579(3)	3879(3)	5372.7(12)	28.9(6)
C(30)	6203(3)	5057(3)	5385.0(13)	29.4(6)
C(31)	8588(3)	5347(3)	-133.5(14)	35.4(7)
C(32)	9272(3)	6139(3)	285.2(13)	35.2(7)
C(33)	10690(3)	5812(3)	421.2(13)	35.9(7)

Table 11. Bond lengths [Å] and angles [°] for [PhBP$^{iPr}_3$]MnI (2).

Mn-P(2)	2.5238(7)	C(15)-H(15C)	0.9800
Mn-P(1)	2.5351(7)	C(16)-C(17)	1.531(3)
Mn-P(3)	2.5379(6)	C(16)-H(16A)	0.9800
Mn-I	2.6394(4)	C(16)-H(16B)	0.9800
P(1)-C(7)	1.835(2)	C(16)-H(16C)	0.9800
P(1)-C(14)	1.856(2)	C(17)-C(18)	1.518(3)
P(1)-C(11)	1.874(2)	C(17)-H(17)	1.0000
P(2)-C(8)	1.822(2)	C(18)-H(18A)	0.9800
P(2)-C(20)	1.860(2)	C(18)-H(18B)	0.9800
P(2)-C(17)	1.865(2)	C(18)-H(18C)	0.9800
P(3)-C(9)	1.830(2)	C(19)-C(20)	1.517(3)
P(3)-C(26)	1.854(2)	C(19)-H(19A)	0.9800
P(3)-C(23)	1.875(2)	C(19)-H(19B)	0.9800
B-C(1)	1.653(3)	C(19)-H(19C)	0.9800
B-C(7)	1.663(3)	C(20)-C(21)	1.524(3)
B-C(9)	1.679(3)	C(20)-H(20)	1.0000
B-C(8)	1.683(3)	C(21)-H(21A)	0.9800
C(1)-C(2)	1.402(3)	C(21)-H(21B)	0.9800
C(1)-C(6)	1.404(3)	C(21)-H(21C)	0.9800
C(2)-C(3)	1.394(3)	C(22)-C(23)	1.533(3)
C(2)-H(2)	0.9500	C(22)-H(22A)	0.9800
C(3)-C(4)	1.383(3)	C(22)-H(22B)	0.9800
C(3)-H(3)	0.9500	C(22)-H(22C)	0.9800
C(4)-C(5)	1.384(3)	C(23)-C(24)	1.527(3)
C(4)-H(4)	0.9500	C(23)-H(23)	1.0000
C(5)-C(6)	1.389(3)	C(24)-H(24A)	0.9800
C(5)-H(5)	0.9500	C(24)-H(24B)	0.9800
C(6)-H(6)	0.9500	C(24)-H(24C)	0.9800
C(7)-H(7A)	0.9900	C(25)-C(26)	1.526(3)
C(7)-H(7B)	0.9900	C(25)-H(25A)	0.9800
C(8)-H(8A)	0.9900	C(25)-H(25B)	0.9800
C(8)-H(8B)	0.9900	C(25)-H(25C)	0.9800
C(9)-H(9A)	0.9900	C(26)-C(27)	1.531(3)
C(9)-H(9B)	0.9900	C(26)-H(26)	1.0000
C(10)-C(11)	1.523(3)	C(27)-H(27A)	0.9800
C(10)-H(10A)	0.9800	C(27)-H(27B)	0.9800
C(10)-H(10B)	0.9800	C(27)-H(27C)	0.9800
C(10)-H(10C)	0.9800	C(28)-C(30)#1	1.387(3)
C(11)-C(12)	1.524(3)	C(28)-C(29)	1.392(3)
C(11)-H(11)	1.0000	C(28)-H(28)	0.9500
C(12)-H(12A)	0.9800	C(29)-C(30)	1.376(3)
C(12)-H(12B)	0.9800	C(29)-H(29)	0.9500
C(12)-H(12C)	0.9800	C(30)-C(28)#1	1.387(3)
C(13)-C(14)	1.534(3)	C(30)-H(30)	0.9500
C(13)-H(13A)	0.9800	C(31)-C(32)	1.363(4)
C(13)-H(13B)	0.9800	C(31)-C(33)#2	1.383(4)
C(13)-H(13C)	0.9800	C(31)-H(31)	0.9500
C(14)-C(15)	1.531(3)	C(32)-C(33)	1.377(4)
C(14)-H(14)	1.0000	C(32)-H(32)	0.9500
C(15)-H(15A)	0.9800	C(33)-C(31)#2	1.383(4)
C(15)-H(15B)	0.9800	C(33)-H(33)	0.9500

P(2)-Mn-P(1)	91.39(2)
P(2)-Mn-P(3)	90.68(2)
P(1)-Mn-P(3)	90.95(2)
P(2)-Mn-I	122.273(18)
P(1)-Mn-I	127.190(18)
P(3)-Mn-I	124.095(17)
C(7)-P(1)-C(14)	106.16(10)
C(7)-P(1)-C(11)	110.60(10)
C(14)-P(1)-C(11)	101.84(10)
C(7)-P(1)-Mn	107.53(7)
C(14)-P(1)-Mn	107.12(7)
C(11)-P(1)-Mn	122.35(7)
C(8)-P(2)-C(20)	106.13(10)
C(8)-P(2)-C(17)	109.38(10)
C(20)-P(2)-C(17)	102.72(11)
C(8)-P(2)-Mn	106.57(7)
C(20)-P(2)-Mn	103.38(7)
C(17)-P(2)-Mn	126.81(8)
C(9)-P(3)-C(26)	106.50(10)
C(9)-P(3)-C(23)	110.63(10)
C(26)-P(3)-C(23)	102.30(10)
C(9)-P(3)-Mn	107.80(6)
C(26)-P(3)-Mn	105.14(7)
C(23)-P(3)-Mn	123.07(7)
C(1)-B-C(7)	108.47(18)
C(1)-B-C(9)	104.48(16)
C(7)-B-C(9)	112.67(17)
C(1)-B-C(8)	106.37(16)
C(7)-B-C(8)	111.08(17)
C(9)-B-C(8)	113.25(18)
C(2)-C(1)-C(6)	114.80(19)
C(2)-C(1)-B	123.99(19)
C(6)-C(1)-B	121.19(19)
C(3)-C(2)-C(1)	122.7(2)
C(3)-C(2)-H(2)	118.6
C(1)-C(2)-H(2)	118.6
C(4)-C(3)-C(2)	120.5(2)
C(4)-C(3)-H(3)	119.7
C(2)-C(3)-H(3)	119.7
C(3)-C(4)-C(5)	118.5(2)
C(3)-C(4)-H(4)	120.7
C(5)-C(4)-H(4)	120.7
C(4)-C(5)-C(6)	120.3(2)
C(4)-C(5)-H(5)	119.8
C(6)-C(5)-H(5)	119.8
C(5)-C(6)-C(1)	123.1(2)
C(5)-C(6)-H(6)	118.5
C(1)-C(6)-H(6)	118.5
B-C(7)-P(1)	119.08(15)
B-C(7)-H(7A)	107.5
P(1)-C(7)-H(7A)	107.5
B-C(7)-H(7B)	107.5
P(1)-C(7)-H(7B)	107.5
H(7A)-C(7)-H(7B)	107.0
B-C(8)-P(2)	119.80(14)
B-C(8)-H(8A)	107.4
P(2)-C(8)-H(8A)	107.4
B-C(8)-H(8B)	107.4
P(2)-C(8)-H(8B)	107.4
H(8A)-C(8)-H(8B)	106.9
B-C(9)-P(3)	118.83(14)
B-C(9)-H(9A)	107.6
P(3)-C(9)-H(9A)	107.6
B-C(9)-H(9B)	107.6
P(3)-C(9)-H(9B)	107.6
H(9A)-C(9)-H(9B)	107.0
C(11)-C(10)-H(10A)	109.5
C(11)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(11)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(10)-C(11)-C(12)	111.00(19)
C(10)-C(11)-P(1)	110.63(16)
C(12)-C(11)-P(1)	115.07(16)
C(10)-C(11)-H(11)	106.5
C(12)-C(11)-H(11)	106.5
P(1)-C(11)-H(11)	106.5
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(14)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(13)	111.00(19)
C(15)-C(14)-P(1)	115.07(15)
C(13)-C(14)-P(1)	110.09(15)
C(15)-C(14)-H(14)	106.7
C(13)-C(14)-H(14)	106.7
P(1)-C(14)-H(14)	106.7
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(17)-C(16)-H(16A)	109.5
C(17)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(17)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5

H(16B)-C(16)-H(16C)	109.5	C(23)-C(24)-H(24A)	109.5
C(18)-C(17)-C(16)	111.07(19)	C(23)-C(24)-H(24B)	109.5
C(18)-C(17)-P(2)	114.79(17)	H(24A)-C(24)-H(24B)	109.5
C(16)-C(17)-P(2)	110.79(16)	C(23)-C(24)-H(24C)	109.5
C(18)-C(17)-H(17)	106.6	H(24A)-C(24)-H(24C)	109.5
C(16)-C(17)-H(17)	106.6	H(24B)-C(24)-H(24C)	109.5
P(2)-C(17)-H(17)	106.6	C(26)-C(25)-H(25A)	109.5
C(17)-C(18)-H(18A)	109.5	C(26)-C(25)-H(25B)	109.5
C(17)-C(18)-H(18B)	109.5	H(25A)-C(25)-H(25B)	109.5
H(18A)-C(18)-H(18B)	109.5	C(26)-C(25)-H(25C)	109.5
C(17)-C(18)-H(18C)	109.5	H(25A)-C(25)-H(25C)	109.5
H(18A)-C(18)-H(18C)	109.5	H(25B)-C(25)-H(25C)	109.5
H(18B)-C(18)-H(18C)	109.5	C(25)-C(26)-C(27)	111.36(17)
C(20)-C(19)-H(19A)	109.5	C(25)-C(26)-P(3)	109.88(15)
C(20)-C(19)-H(19B)	109.5	C(27)-C(26)-P(3)	114.84(15)
H(19A)-C(19)-H(19B)	109.5	C(25)-C(26)-H(26)	106.8
C(20)-C(19)-H(19C)	109.5	C(27)-C(26)-H(26)	106.8
H(19A)-C(19)-H(19C)	109.5	P(3)-C(26)-H(26)	106.8
H(19B)-C(19)-H(19C)	109.5	C(26)-C(27)-H(27A)	109.5
C(19)-C(20)-C(21)	112.40(19)	C(26)-C(27)-H(27B)	109.5
C(19)-C(20)-P(2)	110.33(15)	H(27A)-C(27)-H(27B)	109.5
C(21)-C(20)-P(2)	115.20(16)	C(26)-C(27)-H(27C)	109.5
C(19)-C(20)-H(20)	106.1	H(27A)-C(27)-H(27C)	109.5
C(21)-C(20)-H(20)	106.1	H(27B)-C(27)-H(27C)	109.5
P(2)-C(20)-H(20)	106.1	C(30)#1-C(28)-C(29)	119.5(2)
C(20)-C(21)-H(21A)	109.5	C(30)#1-C(28)-H(28)	120.3
C(20)-C(21)-H(21B)	109.5	C(29)-C(28)-H(28)	120.3
H(21A)-C(21)-H(21B)	109.5	C(30)-C(29)-C(28)	120.2(2)
C(20)-C(21)-H(21C)	109.5	C(30)-C(29)-H(29)	119.9
H(21A)-C(21)-H(21C)	109.5	C(28)-C(29)-H(29)	119.9
H(21B)-C(21)-H(21C)	109.5	C(29)-C(30)-C(28)#1	120.3(2)
C(23)-C(22)-H(22A)	109.5	C(29)-C(30)-H(30)	119.9
C(23)-C(22)-H(22B)	109.5	C(28)#1-C(30)-H(30)	119.9
H(22A)-C(22)-H(22B)	109.5	C(32)-C(31)-C(33)#2	120.2(3)
C(23)-C(22)-H(22C)	109.5	C(32)-C(31)-H(31)	119.9
H(22A)-C(22)-H(22C)	109.5	C(33)#2-C(31)-H(31)	119.9
H(22B)-C(22)-H(22C)	109.5	C(31)-C(32)-C(33)	120.8(2)
C(24)-C(23)-C(22)	110.92(19)	C(31)-C(32)-H(32)	119.6
C(24)-C(23)-P(3)	114.71(15)	C(33)-C(32)-H(32)	119.6
C(22)-C(23)-P(3)	110.31(15)	C(32)-C(33)-C(31)#2	119.1(2)
C(24)-C(23)-H(23)	106.8	C(32)-C(33)-H(33)	120.5
C(22)-C(23)-H(23)	106.8	C(31)#2-C(33)-H(33)	120.5
P(3)-C(23)-H(23)	106.8		

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1 #2 -x+2,-y+1,-z

Table 12. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for [PhBP$^{iPr}_3$]MnI (2). 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	122(2)	136(2)	140(2)	-21(1)	-9(1)	-36(1)
P(1)	132(3)	142(3)	164(3)	-14(2)	-30(2)	-20(2)
P(2)	156(3)	149(3)	147(3)	-11(2)	-1(2)	-47(2)
P(3)	128(3)	131(3)	138(3)	-18(2)	3(2)	-26(2)
B	140(12)	118(13)	158(13)	-39(10)	-17(9)	-17(10)
I	216(1)	243(1)	241(1)	-56(1)	-50(1)	-97(1)
C(1)	110(10)	153(12)	152(11)	-57(9)	17(8)	-3(8)
C(2)	139(10)	180(12)	168(11)	-24(9)	-10(8)	-16(9)
C(3)	172(11)	172(13)	323(14)	-70(11)	26(10)	-60(10)
C(4)	142(11)	285(15)	256(13)	-114(11)	-42(9)	-43(10)
C(5)	196(11)	274(15)	201(12)	-25(10)	-60(9)	-33(10)
C(6)	177(11)	196(13)	215(12)	-10(10)	-22(9)	-52(9)
C(7)	131(10)	160(12)	155(11)	-26(9)	-25(8)	-26(9)
C(8)	134(10)	151(12)	146(11)	-32(9)	-20(8)	-21(9)
C(9)	131(10)	150(12)	144(11)	-20(9)	-5(8)	-29(9)
C(10)	391(15)	277(15)	196(13)	6(11)	-84(11)	-58(12)
C(11)	193(11)	205(13)	209(12)	15(10)	-48(9)	0(10)
C(12)	451(16)	303(16)	354(16)	187(13)	-164(12)	-179(13)
C(13)	141(11)	316(15)	370(15)	-100(12)	-14(10)	-33(10)
C(14)	145(11)	183(13)	212(12)	-25(10)	-9(9)	-15(9)
C(15)	205(12)	222(14)	349(15)	-87(11)	19(10)	-12(10)
C(16)	220(13)	497(19)	340(15)	-77(13)	61(11)	-164(12)
C(17)	233(12)	332(15)	210(13)	-41(11)	77(10)	-120(11)
C(18)	235(13)	390(17)	298(14)	-79(12)	86(11)	-47(12)
C(19)	261(13)	175(13)	291(14)	-25(11)	12(10)	-58(10)
C(20)	218(12)	180(13)	240(13)	3(10)	-23(9)	-19(10)
C(21)	271(13)	209(13)	214(13)	22(10)	-47(10)	-5(10)
C(22)	232(12)	166(13)	382(15)	-91(11)	-16(11)	-19(10)
C(23)	182(11)	127(12)	179(11)	-20(9)	32(9)	-3(9)
C(24)	214(12)	210(14)	317(14)	-22(11)	-5(10)	60(10)
C(25)	210(11)	208(13)	162(12)	-20(10)	14(9)	-41(10)
C(26)	153(10)	144(12)	156(11)	8(9)	-4(8)	-30(9)
C(27)	232(12)	321(15)	245(13)	50(11)	2(10)	-129(11)
C(28)	316(14)	211(14)	298(14)	-61(11)	-2(11)	-38(11)
C(29)	365(14)	218(14)	265(14)	23(11)	-65(11)	29(11)
C(30)	284(13)	251(15)	337(15)	-32(12)	-85(11)	6(11)
C(31)	268(13)	316(17)	479(17)	167(14)	89(12)	-42(12)
C(32)	507(17)	191(14)	347(15)	-8(12)	242(13)	0(13)
C(33)	535(18)	312(17)	267(15)	20(12)	31(13)	-196(14)

Table 13. Crystal Data and Structure Analysis Details for [PhBP$^{iPr}_3$]Mn(N_3) (3).

Empirical formula	$C_{54}H_{106}B_2Cl_{0.36}Mn_{1.90}N_{4.63}P_6Tl_{0.10}$
Formula weight	1165.21
Crystallization solvent	benzene/petroleum ether
Crystal shape	rough plate
Crystal color	colorless
Crystal size	0.30 x 0.30 x 0.37 mm

Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data collection temperature	100 K	
Theta range for 32076 reflections used in lattice determination	2.24 to 31.43°	
Unit cell dimensions	a = 11.946(2) Å b = 34.586(7) Å c = 15.423(3) Å	α= 90° β= 90° γ = 90°
Volume	6372(2) Å^3	
Z	4	
Crystal system	orthorhombic	
Space group	P n c 2 (# 30)	
Density (calculated)	1.215 g/cm^3	
F(000)	2496	
Theta range for data collection	1.5 to 32.1°	
Completeness to theta = 32.12°	89.6%	
Index ranges	$-17 \le h \le 17$, $-50 \le k \le 40$, $-18 \le l \le 22$	
Data collection scan type	ω scans	
Reflections collected	75921	
Independent reflections	17907 [R_{int}= 0.0716]	
Reflections > 2σ(I)	12030	
Average σ(I)/(net I)	0.0713	
Absorption coefficient	0.83 mm^{-1}	
Absorption correction	none	
Reflections monitored for decay	initial data recollected at end	
Decay of standards	0%	

Table 13 (cont.)

Structure Solution and Refinement

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	17907 / 2 / 654
Treatment of hydrogen atoms	not refined, U_{iso} fixed at 120% U_{eq} of attached atom
Goodness-of-fit on F^2	1.49
Final R indices [I>2σ(I), 12030 reflections]	R1 = 0.0573, wR2 = 0.0751
R indices (all data)	R1 = 0.0938, wR2 = 0.0783
Type of weighting scheme used	sigma
Weighting scheme used	calc $w=1/[\sigma^2(Fo^2)]$ where $P=(Fo^2+2Fc^2)/3$
Max shift/error	0.017
Average shift/error	0.000
Absolute structure parameter	0.013(8)
Largest diff. peak and hole	1.12 and -0.53 e·Å^{-3}

Programs Used

Cell refinement	Bruker SMART 5.606
Data collection	Bruker SMART 5.054
Data reduction	Bruker SAINT 6.45
Structure solution	Bruker SHELXTL 6.14
Structure refinement	Bruker SHELXTL 6.14

Special Refinement Details

One bad reflection (200) was omitted. A small amount of Tl[ligand] and [ligand]MnCl had cocrystallized with **3** and their population were refined to 5 and 18 % respectively per [ligand]Mn(N_3). This structure was problematic because the crystal may have undergone a phase transition at low temperatures. It was initially solved in the Pbcn space group but there were 302 systematic absence violations as a result. The structure refined in this space group with a final GOOF of 3.58 and R1 = 0.1375, wR2 = 0.1525. The poor solution led us to remove the c-glide and to resolve the structure in the Pnc2 space group. Much better values for GOOF and the R indices were obtained and this is the solution that is presented.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for [PhBP$^{iPr}_3$]Mn(N_3) (3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Mn(1A)	2646(1)	8543(1)	5378(1)	27(1)
P(1A)	4359(1)	8130(1)	5666(1)	30(1)
P(2A)	3461(1)	8807(1)	3992(1)	26(1)
P(3A)	3438(1)	9084(1)	6284(1)	39(1)
B(1A)	5468(3)	8877(2)	5185(4)	32(1)
N(1A)	1044(2)	8346(1)	5537(2)	28(1)
N(2A)	544(3)	8323(1)	6143(3)	44(1)
N(3A)	-68(4)	8291(1)	6757(3)	67(1)
C(1A)	6740(3)	9067(1)	5057(3)	29(1)
C(2A)	7731(3)	8886(1)	5262(3)	34(1)
C(3A)	8776(3)	9061(2)	5154(4)	45(1)
C(4A)	8856(4)	9429(1)	4868(3)	40(1)
C(5A)	7873(4)	9623(1)	4655(4)	56(2)
C(6A)	6861(4)	9435(2)	4730(4)	51(1)
C(7A)	5566(3)	8457(1)	5681(3)	30(1)
C(8A)	4966(3)	8830(1)	4181(3)	29(1)
C(9A)	4776(3)	9208(1)	5794(3)	33(1)
C(10A)	3384(4)	7646(2)	6925(4)	54(2)
C(11A)	4461(4)	7837(2)	6653(4)	58(2)
C(12A)	5505(4)	7648(2)	6865(4)	102(3)
C(13A)	3586(3)	7512(2)	4655(3)	51(1)
C(14A)	4530(3)	7811(1)	4714(3)	37(1)
C(15A)	5644(4)	7645(2)	4518(4)	61(2)
C(16A)	2213(4)	8305(2)	2949(3)	54(2)
C(17A)	3182(4)	8570(2)	2925(3)	63(2)
C(18A)	4124(4)	8479(2)	2372(3)	76(2)
C(19A)	1738(3)	9324(1)	3644(3)	38(1)
C(20A)	2971(4)	9314(1)	3842(3)	38(1)
C(21A)	3686(4)	9565(1)	3285(4)	56(1)
C(22A)	1537(4)	9552(2)	6272(6)	117(3)
C(23A)	2633(4)	9539(2)	6489(6)	92(3)
C(24A)	3296(3)	9898(1)	6671(4)	56(2)
C(25A)	2731(4)	8710(2)	7783(4)	75(2)
C(26A)	3757(4)	8892(2)	7367(3)	52(1)
C(27A)	4310(4)	9185(2)	7992(4)	71(2)
Mn(1B)	7584(1)	6439(1)	5146(1)	23(1)
P(1B)	9305(1)	6842(1)	4838(1)	22(1)
P(2B)	8389(1)	6200(1)	6565(1)	24(1)
P(3B)	8364(1)	5878(1)	4298(1)	30(1)
B(1B)	10409(3)	6099(1)	5391(3)	23(1)
N(1B)	6097(8)	6635(3)	5036(7)	61(4)
N(2B)	5471(4)	6669(2)	4363(4)	18(1)
N(3B)	4893(6)	6717(2)	3776(6)	50(2)
Cl	5778(3)	6650(1)	4920(3)	39(1)
Tl	7076(2)	6508(1)	5122(1)	25(1)
C(1B)	11649(3)	5916(1)	5526(3)	29(1)

C(2B)	12663(3)	6087(2)	5274(4)	39(1)
C(3B)	13699(3)	5908(1)	5381(4)	45(1)
C(4B)	13756(4)	5545(2)	5788(3)	45(1)
C(5B)	12796(4)	5373(1)	6067(3)	46(1)
C(6B)	11766(4)	5552(1)	5943(3)	41(1)
C(7B)	10515(3)	6516(1)	4862(3)	26(1)
C(8B)	9903(3)	6172(1)	6396(3)	24(1)
C(9B)	9711(3)	5764(1)	4817(3)	28(1)
C(10B)	8371(3)	7316(2)	3523(4)	51(1)
C(11B)	9438(3)	7112(1)	3802(3)	32(1)
C(12B)	10456(3)	7369(1)	3720(3)	48(1)
C(13B)	8609(3)	7502(1)	5741(3)	37(1)
C(14B)	9476(3)	7176(1)	5746(3)	36(1)
C(15B)	10654(3)	7329(1)	5973(3)	38(1)
C(16B)	7226(4)	6756(2)	7505(4)	52(1)
C(17B)	8071(4)	6433(1)	7625(3)	37(1)
C(18B)	9066(3)	6562(1)	8142(3)	41(1)
C(19B)	6659(3)	5685(1)	6919(3)	38(1)
C(20B)	7917(4)	5692(1)	6751(3)	36(1)
C(21B)	8578(4)	5476(1)	7444(4)	64(2)
C(22B)	6476(4)	5404(2)	4389(5)	81(2)
C(23B)	7542(5)	5456(2)	3965(5)	17(2)
C(23C)	7669(6)	5382(2)	4411(6)	28(2)
C(24B)	8235(3)	5062(1)	3986(3)	41(1)
C(25B)	7669(3)	6240(2)	2753(4)	55(2)
C(26B)	8702(3)	6052(1)	3205(3)	39(1)
C(27B)	9275(4)	5764(2)	2589(4)	62(2)

Table 15. Bond lengths [Å] and angles [°] for [PhBP$^{iPr}_3$]Mn(N$_3$) (3).

Mn(1A)-N(1A)	2.046(3)	C(15A)-H(15A)	0.9600
Mn(1A)-P(3A)	2.5205(15)	C(15A)-H(15B)	0.9600
Mn(1A)-P(2A)	2.5217(14)	C(15A)-H(15C)	0.9600
Mn(1A)-P(1A)	2.5339(13)	C(16A)-C(17A)	1.477(7)
P(1A)-C(7A)	1.831(4)	C(16A)-H(16A)	0.9600
P(1A)-C(11A)	1.834(5)	C(16A)-H(16B)	0.9600
P(1A)-C(14A)	1.850(5)	C(16A)-H(16C)	0.9600
P(2A)-C(8A)	1.823(4)	C(17A)-C(18A)	1.447(6)
P(2A)-C(20A)	1.862(5)	C(17A)-H(17A)	0.9800
P(2A)-C(17A)	1.868(5)	C(18A)-H(18A)	0.9600
P(3A)-C(9A)	1.819(4)	C(18A)-H(18B)	0.9600
P(3A)-C(26A)	1.838(5)	C(18A)-H(18C)	0.9600
P(3A)-C(23A)	1.871(6)	C(19A)-C(20A)	1.505(6)
B(1A)-C(7A)	1.648(7)	C(19A)-H(19A)	0.9600
B(1A)-C(1A)	1.666(5)	C(19A)-H(19B)	0.9600
B(1A)-C(8A)	1.668(7)	C(19A)-H(19C)	0.9600
B(1A)-C(9A)	1.694(7)	C(20A)-C(21A)	1.490(6)
N(1A)-N(2A)	1.112(5)	C(20A)-H(20A)	0.9800
N(2A)-N(3A)	1.202(6)	C(21A)-H(21A)	0.9600
C(1A)-C(2A)	1.376(5)	C(21A)-H(21B)	0.9600
C(1A)-C(6A)	1.377(6)	C(21A)-H(21C)	0.9600
C(2A)-C(3A)	1.397(5)	C(22A)-C(23A)	1.352(6)
C(2A)-H(2A)	0.9300	C(22A)-H(22A)	0.9600
C(3A)-C(4A)	1.350(6)	C(22A)-H(22B)	0.9600
C(3A)-H(3A)	0.9300	C(22A)-H(22C)	0.9600
C(4A)-C(5A)	1.391(6)	C(23A)-C(24A)	1.498(7)
C(4A)-H(4A)	0.9300	C(23A)-H(23A)	0.9800
C(5A)-C(6A)	1.378(6)	C(24A)-H(24A)	0.9600
C(5A)-H(5A)	0.9300	C(24A)-H(24B)	0.9600
C(6A)-H(6A)	0.9300	C(24A)-H(24C)	0.9600
C(7A)-H(7A1)	0.9700	C(25A)-C(26A)	1.519(7)
C(7A)-H(7A2)	0.9700	C(25A)-H(25A)	0.9600
C(8A)-H(8A1)	0.9700	C(25A)-H(25B)	0.9600
C(8A)-H(8A2)	0.9700	C(25A)-H(25C)	0.9600
C(9A)-H(9A1)	0.9700	C(26A)-C(27A)	1.547(7)
C(9A)-H(9A2)	0.9700	C(26A)-H(26A)	0.9800
C(10A)-C(11A)	1.505(6)	C(27A)-H(27A)	0.9600
C(10A)-H(10A)	0.9600	C(27A)-H(27B)	0.9600
C(10A)-H(10B)	0.9600	C(27A)-H(27C)	0.9600
C(10A)-H(10C)	0.9600	Mn(1B)-N(1B)	1.909(10)
C(11A)-C(12A)	1.445(6)	Mn(1B)-Cl	2.304(4)
C(11A)-H(11A)	0.9800	Mn(1B)-P(3B)	2.5162(15)
C(12A)-H(12A)	0.9600	Mn(1B)-P(1B)	2.5298(13)
C(12A)-H(12B)	0.9600	Mn(1B)-P(2B)	2.5302(16)
C(12A)-H(12C)	0.9600	P(1B)-C(14B)	1.826(5)
C(13A)-C(14A)	1.532(6)	P(1B)-C(7B)	1.834(4)
C(13A)-H(13A)	0.9600	P(1B)-C(11B)	1.857(4)
C(13A)-H(13B)	0.9600	P(1B)-Tl	2.9366(19)
C(13A)-H(13C)	0.9600	P(2B)-C(8B)	1.830(4)
C(14A)-C(15A)	1.480(6)	P(2B)-C(17B)	1.861(5)
C(14A)-H(14A)	0.9800	P(2B)-C(20B)	1.865(4)

P(2B)-Tl	2.923(2)	C(18B)-H(18E)	0.9600
P(3B)-C(23B)	1.834(7)	C(18B)-H(18F)	0.9600
P(3B)-C(26B)	1.835(5)	C(19B)-C(20B)	1.526(6)
P(3B)-C(9B)	1.841(4)	C(19B)-H(19D)	0.9600
P(3B)-C(23C)	1.915(8)	C(19B)-H(19E)	0.9600
P(3B)-Tl	2.953(2)	C(19B)-H(19F)	0.9600
B(1B)-C(1B)	1.623(5)	C(20B)-C(21B)	1.526(6)
B(1B)-C(7B)	1.661(6)	C(20B)-H(20B)	0.9800
B(1B)-C(9B)	1.680(6)	C(21B)-H(21D)	0.9600
B(1B)-C(8B)	1.683(7)	C(21B)-H(21E)	0.9600
N(1B)-N(2B)	1.285(13)	C(21B)-H(21F)	0.9600
N(2B)-N(3B)	1.150(9)	C(22B)-C(23C)	1.428(8)
C(1B)-C(2B)	1.403(5)	C(22B)-C(23B)	1.442(8)
C(1B)-C(6B)	1.423(6)	C(22B)-H(22D)	0.9570
C(2B)-C(3B)	1.394(5)	C(22B)-H(22E)	0.9725
C(2B)-H(2B)	0.9300	C(22B)-H(22F)	0.9385
C(3B)-C(4B)	1.405(7)	C(22B)-H(22G)	0.9827
C(3B)-H(3B)	0.9300	C(22B)-H(22H)	0.9481
C(4B)-C(5B)	1.363(6)	C(22B)-H(22I)	0.9492
C(4B)-H(4B)	0.9300	C(23B)-C(24B)	1.595(8)
C(5B)-C(6B)	1.390(6)	C(23B)-H(22G)	1.5659
C(5B)-H(5B)	0.9300	C(23B)-H(23B)	0.9685
C(6B)-H(6B)	0.9300	C(23C)-C(24B)	1.453(9)
C(7B)-H(7B1)	0.9700	C(23C)-H(22F)	1.5789
C(7B)-H(7B2)	0.9700	C(23C)-H(23C)	0.9931
C(8B)-H(8B1)	0.9700	C(24B)-H(24D)	0.9618
C(8B)-H(8B2)	0.9700	C(24B)-H(24E)	0.9559
C(9B)-H(9B1)	0.9700	C(24B)-H(24F)	0.9560
C(9B)-H(9B2)	0.9700	C(24B)-H(24G)	0.9570
C(10B)-C(11B)	1.519(6)	C(24B)-H(24H)	0.9590
C(10B)-H(10D)	0.9600	C(24B)-H(24I)	0.9567
C(10B)-H(10E)	0.9600	C(25B)-C(26B)	1.560(6)
C(10B)-H(10F)	0.9600	C(25B)-H(25D)	0.9600
C(11B)-C(12B)	1.513(6)	C(25B)-H(25E)	0.9600
C(11B)-H(11B)	0.9800	C(25B)-H(25F)	0.9600
C(12B)-H(12D)	0.9600	C(26B)-C(27B)	1.538(7)
C(12B)-H(12E)	0.9600	C(26B)-H(26B)	0.9800
C(12B)-H(12F)	0.9600	C(27B)-H(27D)	0.9600
C(13B)-C(14B)	1.531(6)	C(27B)-H(27E)	0.9600
C(13B)-H(13D)	0.9600	C(27B)-H(27F)	0.9600
C(13B)-H(13E)	0.9600		
C(13B)-H(13F)	0.9600	N(1A)-Mn(1A)-P(3A)	122.17(10)
C(14B)-C(15B)	1.544(5)	N(1A)-Mn(1A)-P(2A)	125.69(11)
C(14B)-H(14B)	0.9800	P(3A)-Mn(1A)-P(2A)	93.21(5)
C(15B)-H(15D)	0.9600	N(1A)-Mn(1A)-P(1A)	123.13(10)
C(15B)-H(15E)	0.9600	P(3A)-Mn(1A)-P(1A)	91.04(5)
C(15B)-H(15F)	0.9600	P(2A)-Mn(1A)-P(1A)	92.33(4)
C(16B)-C(17B)	1.518(7)	C(7A)-P(1A)-C(11A)	106.2(2)
C(16B)-H(16D)	0.9600	C(7A)-P(1A)-C(14A)	106.9(2)
C(16B)-H(16E)	0.9600	C(11A)-P(1A)-C(14A)	108.7(2)
C(16B)-H(16F)	0.9600	C(7A)-P(1A)-Mn(1A)	106.92(14)
C(17B)-C(18B)	1.500(6)	C(11A)-P(1A)-Mn(1A)	120.70(17)
C(17B)-H(17B)	0.9800	C(14A)-P(1A)-Mn(1A)	106.68(15)
C(18B)-H(18D)	0.9600	C(8A)-P(2A)-C(20A)	106.8(2)

C(8A)-P(2A)-C(17A)	109.7(2)	H(9A1)-C(9A)-H(9A2)	106.9
C(20A)-P(2A)-C(17A)	104.4(3)	C(11A)-C(10A)-H(10A)	109.5
C(8A)-P(2A)-Mn(1A)	105.10(15)	C(11A)-C(10A)-H(10B)	109.5
C(20A)-P(2A)-Mn(1A)	108.96(16)	H(10A)-C(10A)-H(10B)	109.5
C(17A)-P(2A)-Mn(1A)	121.21(19)	C(11A)-C(10A)-H(10C)	109.5
C(9A)-P(3A)-C(26A)	106.3(2)	H(10A)-C(10A)-H(10C)	109.5
C(9A)-P(3A)-C(23A)	108.9(3)	H(10B)-C(10A)-H(10C)	109.5
C(26A)-P(3A)-C(23A)	105.0(4)	C(12A)-C(11A)-C(10A)	118.4(5)
C(9A)-P(3A)-Mn(1A)	105.90(15)	C(12A)-C(11A)-P(1A)	119.7(4)
C(26A)-P(3A)-Mn(1A)	108.17(17)	C(10A)-C(11A)-P(1A)	114.7(3)
C(23A)-P(3A)-Mn(1A)	121.7(2)	C(12A)-C(11A)-H(11A)	99.0
C(7A)-B(1A)-C(1A)	109.7(3)	C(10A)-C(11A)-H(11A)	99.0
C(7A)-B(1A)-C(8A)	111.7(4)	P(1A)-C(11A)-H(11A)	99.0
C(1A)-B(1A)-C(8A)	104.8(4)	C(11A)-C(12A)-H(12A)	109.5
C(7A)-B(1A)-C(9A)	111.9(4)	C(11A)-C(12A)-H(12B)	109.5
C(1A)-B(1A)-C(9A)	104.2(3)	H(12A)-C(12A)-H(12B)	109.5
C(8A)-B(1A)-C(9A)	113.9(3)	C(11A)-C(12A)-H(12C)	109.5
N(2A)-N(1A)-Mn(1A)	128.8(3)	H(12A)-C(12A)-H(12C)	109.5
N(1A)-N(2A)-N(3A)	174.8(5)	H(12B)-C(12A)-H(12C)	109.5
C(2A)-C(1A)-C(6A)	114.4(4)	C(14A)-C(13A)-H(13A)	109.5
C(2A)-C(1A)-B(1A)	125.4(4)	C(14A)-C(13A)-H(13B)	109.5
C(6A)-C(1A)-B(1A)	120.2(4)	H(13A)-C(13A)-H(13B)	109.5
C(1A)-C(2A)-C(3A)	123.1(4)	C(14A)-C(13A)-H(13C)	109.5
C(1A)-C(2A)-H(2A)	118.5	H(13A)-C(13A)-H(13C)	109.5
C(3A)-C(2A)-H(2A)	118.5	H(13B)-C(13A)-H(13C)	109.5
C(4A)-C(3A)-C(2A)	120.7(4)	C(15A)-C(14A)-C(13A)	112.9(4)
C(4A)-C(3A)-H(3A)	119.7	C(15A)-C(14A)-P(1A)	119.5(3)
C(2A)-C(3A)-H(3A)	119.7	C(13A)-C(14A)-P(1A)	111.7(3)
C(3A)-C(4A)-C(5A)	118.1(4)	C(15A)-C(14A)-H(14A)	103.5
C(3A)-C(4A)-H(4A)	120.9	C(13A)-C(14A)-H(14A)	103.5
C(5A)-C(4A)-H(4A)	120.9	P(1A)-C(14A)-H(14A)	103.5
C(6A)-C(5A)-C(4A)	119.6(4)	C(14A)-C(15A)-H(15A)	109.5
C(6A)-C(5A)-H(5A)	120.2	C(14A)-C(15A)-H(15B)	109.5
C(4A)-C(5A)-H(5A)	120.2	H(15A)-C(15A)-H(15B)	109.5
C(1A)-C(6A)-C(5A)	124.0(4)	C(14A)-C(15A)-H(15C)	109.5
C(1A)-C(6A)-H(6A)	118.0	H(15A)-C(15A)-H(15C)	109.5
C(5A)-C(6A)-H(6A)	118.0	H(15B)-C(15A)-H(15C)	109.5
B(1A)-C(7A)-P(1A)	118.9(3)	C(17A)-C(16A)-H(16A)	109.5
B(1A)-C(7A)-H(7A1)	107.6	C(17A)-C(16A)-H(16B)	109.5
P(1A)-C(7A)-H(7A1)	107.6	H(16A)-C(16A)-H(16B)	109.5
B(1A)-C(7A)-H(7A2)	107.6	C(17A)-C(16A)-H(16C)	109.5
P(1A)-C(7A)-H(7A2)	107.6	H(16A)-C(16A)-H(16C)	109.5
H(7A1)-C(7A)-H(7A2)	107.0	H(16B)-C(16A)-H(16C)	109.5
B(1A)-C(8A)-P(2A)	120.5(3)	C(18A)-C(17A)-C(16A)	119.3(5)
B(1A)-C(8A)-H(8A1)	107.2	C(18A)-C(17A)-P(2A)	118.4(4)
P(2A)-C(8A)-H(8A1)	107.2	C(16A)-C(17A)-P(2A)	113.0(3)
B(1A)-C(8A)-H(8A2)	107.2	C(18A)-C(17A)-H(17A)	100.2
P(2A)-C(8A)-H(8A2)	107.2	C(16A)-C(17A)-H(17A)	100.2
H(8A1)-C(8A)-H(8A2)	106.8	P(2A)-C(17A)-H(17A)	100.2
B(1A)-C(9A)-P(3A)	120.0(3)	C(17A)-C(18A)-H(18A)	109.5
B(1A)-C(9A)-H(9A1)	107.3	C(17A)-C(18A)-H(18B)	109.5
P(3A)-C(9A)-H(9A1)	107.3	H(18A)-C(18A)-H(18B)	109.5
B(1A)-C(9A)-H(9A2)	107.3	C(17A)-C(18A)-H(18C)	109.5
P(3A)-C(9A)-H(9A2)	107.3	H(18A)-C(18A)-H(18C)	109.5

H(18B)-C(18A)-H(18C)	109.5	H(27B)-C(27A)-H(27C)	109.5
C(20A)-C(19A)-H(19A)	109.5	N(1B)-Mn(1B)-Cl	4.2(4)
C(20A)-C(19A)-H(19B)	109.5	N(1B)-Mn(1B)-P(3B)	124.9(3)
H(19A)-C(19A)-H(19B)	109.5	Cl-Mn(1B)-P(3B)	120.85(12)
C(20A)-C(19A)-H(19C)	109.5	N(1B)-Mn(1B)-P(1B)	122.9(3)
H(19A)-C(19A)-H(19C)	109.5	Cl-Mn(1B)-P(1B)	123.87(11)
H(19B)-C(19A)-H(19C)	109.5	P(3B)-Mn(1B)-P(1B)	91.52(5)
C(21A)-C(20A)-C(19A)	115.4(4)	N(1B)-Mn(1B)-P(2B)	123.2(3)
C(21A)-C(20A)-P(2A)	116.1(3)	Cl-Mn(1B)-P(2B)	126.18(12)
C(19A)-C(20A)-P(2A)	110.9(3)	P(3B)-Mn(1B)-P(2B)	93.27(5)
C(21A)-C(20A)-H(20A)	104.3	P(1B)-Mn(1B)-P(2B)	91.92(5)
C(19A)-C(20A)-H(20A)	104.3	C(14B)-P(1B)-C(7B)	106.58(18)
P(2A)-C(20A)-H(20A)	104.3	C(14B)-P(1B)-C(11B)	109.4(2)
C(20A)-C(21A)-H(21A)	109.5	C(7B)-P(1B)-C(11B)	104.94(19)
C(20A)-C(21A)-H(21B)	109.5	C(14B)-P(1B)-Mn(1B)	107.24(14)
H(21A)-C(21A)-H(21B)	109.5	C(7B)-P(1B)-Mn(1B)	107.31(13)
C(20A)-C(21A)-H(21C)	109.5	C(11B)-P(1B)-Mn(1B)	120.52(13)
H(21A)-C(21A)-H(21C)	109.5	C(14B)-P(1B)-Tl	103.69(14)
H(21B)-C(21A)-H(21C)	109.5	C(7B)-P(1B)-Tl	118.00(13)
C(23A)-C(22A)-H(22A)	109.5	C(11B)-P(1B)-Tl	113.84(13)
C(23A)-C(22A)-H(22B)	109.5	Mn(1B)-P(1B)-Tl	10.76(3)
H(22A)-C(22A)-H(22B)	109.5	C(8B)-P(2B)-C(17B)	110.5(2)
C(23A)-C(22A)-H(22C)	109.5	C(8B)-P(2B)-C(20B)	105.7(2)
H(22A)-C(22A)-H(22C)	109.5	C(17B)-P(2B)-C(20B)	102.2(2)
H(22B)-C(22A)-H(22C)	109.5	C(8B)-P(2B)-Mn(1B)	105.62(14)
C(22A)-C(23A)-C(24A)	122.2(5)	C(17B)-P(2B)-Mn(1B)	122.74(17)
C(22A)-C(23A)-P(3A)	118.9(5)	C(20B)-P(2B)-Mn(1B)	108.98(16)
C(24A)-C(23A)-P(3A)	117.1(3)	C(8B)-P(2B)-Tl	116.16(14)
C(22A)-C(23A)-H(23A)	94.5	C(17B)-P(2B)-Tl	113.65(17)
C(24A)-C(23A)-H(23A)	94.5	C(20B)-P(2B)-Tl	107.30(16)
P(3A)-C(23A)-H(23A)	94.5	Mn(1B)-P(2B)-Tl	11.00(3)
C(23A)-C(24A)-H(24A)	109.5	C(23B)-P(3B)-C(26B)	97.0(3)
C(23A)-C(24A)-H(24B)	109.5	C(23B)-P(3B)-C(9B)	114.7(3)
H(24A)-C(24A)-H(24B)	109.5	C(26B)-P(3B)-C(9B)	106.11(19)
C(23A)-C(24A)-H(24C)	109.5	C(23B)-P(3B)-C(23C)	22.9(2)
H(24A)-C(24A)-H(24C)	109.5	C(26B)-P(3B)-C(23C)	118.2(3)
H(24B)-C(24A)-H(24C)	109.5	C(9B)-P(3B)-C(23C)	98.4(3)
C(26A)-C(25A)-H(25A)	109.5	C(23B)-P(3B)-Mn(1B)	124.1(2)
C(26A)-C(25A)-H(25B)	109.5	C(26B)-P(3B)-Mn(1B)	107.83(16)
H(25A)-C(25A)-H(25B)	109.5	C(9B)-P(3B)-Mn(1B)	105.30(14)
C(26A)-C(25A)-H(25C)	109.5	C(23C)-P(3B)-Mn(1B)	118.9(3)
H(25A)-C(25A)-H(25C)	109.5	C(23B)-P(3B)-Tl	115.4(2)
H(25B)-C(25A)-H(25C)	109.5	C(26B)-P(3B)-Tl	105.58(15)
C(25A)-C(26A)-C(27A)	110.7(4)	C(9B)-P(3B)-Tl	115.30(14)
C(25A)-C(26A)-P(3A)	111.5(4)	C(23C)-P(3B)-Tl	113.3(2)
C(27A)-C(26A)-P(3A)	114.6(4)	Mn(1B)-P(3B)-Tl	10.22(3)
C(25A)-C(26A)-H(26A)	106.5	C(1B)-B(1B)-C(7B)	109.4(3)
C(27A)-C(26A)-H(26A)	106.5	C(1B)-B(1B)-C(9B)	104.6(3)
P(3A)-C(26A)-H(26A)	106.5	C(7B)-B(1B)-C(9B)	112.2(4)
C(26A)-C(27A)-H(27A)	109.5	C(1B)-B(1B)-C(8B)	105.5(3)
C(26A)-C(27A)-H(27B)	109.5	C(7B)-B(1B)-C(8B)	110.5(3)
H(27A)-C(27A)-H(27B)	109.5	C(9B)-B(1B)-C(8B)	114.2(3)
C(26A)-C(27A)-H(27C)	109.5	N(2B)-N(1B)-Mn(1B)	130.2(8)
H(27A)-C(27A)-H(27C)	109.5	N(3B)-N(2B)-N(1B)	176.6(8)

P(2B)-Tl-P(1B)	76.73(5)	C(11B)-C(12B)-H(12F)	109.5
P(2B)-Tl-P(3B)	77.27(6)	H(12D)-C(12B)-H(12F)	109.5
P(1B)-Tl-P(3B)	75.73(5)	H(12E)-C(12B)-H(12F)	109.5
C(2B)-C(1B)-C(6B)	114.4(4)	C(14B)-C(13B)-H(13D)	109.5
C(2B)-C(1B)-B(1B)	126.0(4)	C(14B)-C(13B)-H(13E)	109.5
C(6B)-C(1B)-B(1B)	119.5(3)	H(13D)-C(13B)-H(13E)	109.5
C(3B)-C(2B)-C(1B)	123.1(5)	C(14B)-C(13B)-H(13F)	109.5
C(3B)-C(2B)-H(2B)	118.4	H(13D)-C(13B)-H(13F)	109.5
C(1B)-C(2B)-H(2B)	118.4	H(13E)-C(13B)-H(13F)	109.5
C(2B)-C(3B)-C(4B)	119.6(4)	C(13B)-C(14B)-C(15B)	111.5(4)
C(2B)-C(3B)-H(3B)	120.2	C(13B)-C(14B)-P(1B)	112.7(3)
C(4B)-C(3B)-H(3B)	120.2	C(15B)-C(14B)-P(1B)	119.5(3)
C(5B)-C(4B)-C(3B)	119.4(4)	C(13B)-C(14B)-H(14B)	103.7
C(5B)-C(4B)-H(4B)	120.3	C(15B)-C(14B)-H(14B)	103.7
C(3B)-C(4B)-H(4B)	120.3	P(1B)-C(14B)-H(14B)	103.7
C(4B)-C(5B)-C(6B)	120.5(5)	C(14B)-C(15B)-H(15D)	109.5
C(4B)-C(5B)-H(5B)	119.8	C(14B)-C(15B)-H(15E)	109.5
C(6B)-C(5B)-H(5B)	119.8	H(15D)-C(15B)-H(15E)	109.5
C(5B)-C(6B)-C(1B)	122.9(4)	C(14B)-C(15B)-H(15F)	109.5
C(5B)-C(6B)-H(6B)	118.5	H(15D)-C(15B)-H(15F)	109.5
C(1B)-C(6B)-H(6B)	118.5	H(15E)-C(15B)-H(15F)	109.5
B(1B)-C(7B)-P(1B)	118.9(2)	C(17B)-C(16B)-H(16D)	109.5
B(1B)-C(7B)-H(7B1)	107.6	C(17B)-C(16B)-H(16E)	109.5
P(1B)-C(7B)-H(7B1)	107.6	H(16D)-C(16B)-H(16E)	109.5
B(1B)-C(7B)-H(7B2)	107.6	C(17B)-C(16B)-H(16F)	109.5
P(1B)-C(7B)-H(7B2)	107.6	H(16D)-C(16B)-H(16F)	109.5
H(7B1)-C(7B)-H(7B2)	107.0	H(16E)-C(16B)-H(16F)	109.5
B(1B)-C(8B)-P(2B)	119.6(3)	C(18B)-C(17B)-C(16B)	111.8(4)
B(1B)-C(8B)-H(8B1)	107.4	C(18B)-C(17B)-P(2B)	115.7(3)
P(2B)-C(8B)-H(8B1)	107.4	C(16B)-C(17B)-P(2B)	110.3(3)
B(1B)-C(8B)-H(8B2)	107.4	C(18B)-C(17B)-H(17B)	106.1
P(2B)-C(8B)-H(8B2)	107.4	C(16B)-C(17B)-H(17B)	106.1
H(8B1)-C(8B)-H(8B2)	106.9	P(2B)-C(17B)-H(17B)	106.1
B(1B)-C(9B)-P(3B)	120.9(3)	C(17B)-C(18B)-H(18D)	109.5
B(1B)-C(9B)-H(9B1)	107.1	C(17B)-C(18B)-H(18E)	109.5
P(3B)-C(9B)-H(9B1)	107.1	H(18D)-C(18B)-H(18E)	109.5
B(1B)-C(9B)-H(9B2)	107.1	C(17B)-C(18B)-H(18F)	109.5
P(3B)-C(9B)-H(9B2)	107.1	H(18D)-C(18B)-H(18F)	109.5
H(9B1)-C(9B)-H(9B2)	106.8	H(18E)-C(18B)-H(18F)	109.5
C(11B)-C(10B)-H(10D)	109.5	C(20B)-C(19B)-H(19D)	109.5
C(11B)-C(10B)-H(10E)	109.5	C(20B)-C(19B)-H(19E)	109.5
H(10D)-C(10B)-H(10E)	109.5	H(19D)-C(19B)-H(19E)	109.5
C(11B)-C(10B)-H(10F)	109.5	C(20B)-C(19B)-H(19F)	109.5
H(10D)-C(10B)-H(10F)	109.5	H(19D)-C(19B)-H(19F)	109.5
H(10E)-C(10B)-H(10F)	109.5	H(19E)-C(19B)-H(19F)	109.5
C(12B)-C(11B)-C(10B)	112.1(4)	C(19B)-C(20B)-C(21B)	112.5(4)
C(12B)-C(11B)-P(1B)	115.9(3)	C(19B)-C(20B)-P(2B)	109.8(3)
C(10B)-C(11B)-P(1B)	113.9(3)	C(21B)-C(20B)-P(2B)	114.4(3)
C(12B)-C(11B)-H(11B)	104.5	C(19B)-C(20B)-H(20B)	106.5
C(10B)-C(11B)-H(11B)	104.5	C(21B)-C(20B)-H(20B)	106.5
P(1B)-C(11B)-H(11B)	104.5	P(2B)-C(20B)-H(20B)	106.5
C(11B)-C(12B)-H(12D)	109.5	C(20B)-C(21B)-H(21D)	109.5
C(11B)-C(12B)-H(12E)	109.5	C(20B)-C(21B)-H(21E)	109.5
H(12D)-C(12B)-H(12E)	109.5	H(21D)-C(21B)-H(21E)	109.5

C(20B)-C(21B)-H(21F)	109.5	P(3B)-C(23C)-H(23C)	102.3
H(21D)-C(21B)-H(21F)	109.5	H(22F)-C(23C)-H(23C)	64.8
H(21E)-C(21B)-H(21F)	109.5	C(23C)-C(24B)-C(23B)	28.0(3)
C(23C)-C(22B)-C(23B)	30.3(3)	C(23C)-C(24B)-H(24D)	83.1
C(23C)-C(22B)-H(22D)	114.8	C(23B)-C(24B)-H(24D)	109.3
C(23B)-C(22B)-H(22D)	108.4	C(23C)-C(24B)-H(24E)	129.1
C(23C)-C(22B)-H(22E)	126.9	C(23B)-C(24B)-H(24E)	108.8
C(23B)-C(22B)-H(22E)	107.6	H(24D)-C(24B)-H(24E)	109.7
H(22D)-C(22B)-H(22E)	108.7	C(23C)-C(24B)-H(24F)	110.9
C(23C)-C(22B)-H(22F)	80.9	C(23B)-C(24B)-H(24F)	109.3
C(23B)-C(22B)-H(22F)	110.2	H(24D)-C(24B)-H(24F)	109.7
H(22D)-C(22B)-H(22F)	111.6	H(24E)-C(24B)-H(24F)	110.2
H(22E)-C(22B)-H(22F)	110.2	C(23C)-C(24B)-H(24G)	109.6
C(23C)-C(22B)-H(22G)	107.4	C(23B)-C(24B)-H(24G)	129.9
C(23B)-C(22B)-H(22G)	77.9	H(24D)-C(24B)-H(24G)	64.0
H(22D)-C(22B)-H(22G)	89.1	H(24E)-C(24B)-H(24G)	120.4
H(22E)-C(22B)-H(22G)	43.7	H(24F)-C(24B)-H(24G)	46.1
H(22F)-C(22B)-H(22G)	152.6	C(23C)-C(24B)-H(24H)	108.8
C(23C)-C(22B)-H(22H)	110.5	C(23B)-C(24B)-H(24H)	110.5
C(23B)-C(22B)-H(22H)	127.9	H(24D)-C(24B)-H(24H)	65.3
H(22D)-C(22B)-H(22H)	123.0	H(24E)-C(24B)-H(24H)	46.6
H(22E)-C(22B)-H(22H)	65.1	H(24F)-C(24B)-H(24H)	139.0
H(22F)-C(22B)-H(22H)	45.3	H(24G)-C(24B)-H(24H)	109.8
H(22G)-C(22B)-H(22H)	108.6	C(23C)-C(24B)-H(24I)	108.7
C(23C)-C(22B)-H(22I)	110.3	C(23B)-C(24B)-H(24I)	82.5
C(23B)-C(22B)-H(22I)	115.0	H(24D)-C(24B)-H(24I)	168.2
H(22D)-C(22B)-H(22I)	19.7	H(24E)-C(24B)-H(24I)	63.6
H(22E)-C(22B)-H(22I)	120.5	H(24F)-C(24B)-H(24I)	66.3
H(22F)-C(22B)-H(22I)	92.1	H(24G)-C(24B)-H(24I)	110.0
H(22G)-C(22B)-H(22I)	108.5	H(24H)-C(24B)-H(24I)	109.8
H(22H)-C(22B)-H(22I)	111.4	C(26B)-C(25B)-H(25D)	109.5
C(22B)-C(23B)-C(24B)	110.1(5)	C(26B)-C(25B)-H(25E)	109.5
C(22B)-C(23B)-P(3B)	116.3(5)	H(25D)-C(25B)-H(25E)	109.5
C(24B)-C(23B)-P(3B)	113.4(4)	C(26B)-C(25B)-H(25F)	109.5
C(22B)-C(23B)-H(22G)	37.9	H(25D)-C(25B)-H(25F)	109.5
C(24B)-C(23B)-H(22G)	134.0	H(25E)-C(25B)-H(25F)	109.5
P(3B)-C(23B)-H(22G)	111.7	C(27B)-C(26B)-C(25B)	110.2(4)
C(22B)-C(23B)-H(23B)	105.4	C(27B)-C(26B)-P(3B)	116.9(4)
C(24B)-C(23B)-H(23B)	105.4	C(25B)-C(26B)-P(3B)	111.9(3)
P(3B)-C(23B)-H(23B)	105.2	C(27B)-C(26B)-H(26B)	105.6
H(22G)-C(23B)-H(23B)	70.7	C(25B)-C(26B)-H(26B)	105.6
C(22B)-C(23C)-C(24B)	119.7(6)	P(3B)-C(26B)-H(26B)	105.6
C(22B)-C(23C)-P(3B)	112.4(6)	C(26B)-C(27B)-H(27D)	109.5
C(24B)-C(23C)-P(3B)	116.1(5)	C(26B)-C(27B)-H(27E)	109.5
C(22B)-C(23C)-H(22F)	35.9	H(27D)-C(27B)-H(27E)	109.5
C(24B)-C(23C)-H(22F)	128.8	C(26B)-C(27B)-H(27F)	109.5
P(3B)-C(23C)-H(22F)	115.0	H(27D)-C(27B)-H(27F)	109.5
C(22B)-C(23C)-H(23C)	100.6	H(27E)-C(27B)-H(27F)	109.5
C(24B)-C(23C)-H(23C)	101.8		

Symmetry transformations used to generate equivalent atoms:

Table 16. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for [PhBP$^{iPr}_3$]Mn(N_3) (3). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(1A)	280(3)	285(4)	235(4)	-22(3)	32(3)	-30(2)
P(1A)	264(5)	333(7)	304(7)	47(6)	-19(5)	-49(5)
P(2A)	254(6)	282(7)	256(7)	10(6)	-16(5)	13(5)
P(3A)	312(6)	446(8)	402(8)	-203(6)	92(5)	-92(5)
B(1A)	240(20)	380(30)	340(30)	-40(30)	10(20)	-7(18)
N(1A)	271(16)	247(16)	311(18)	44(13)	146(14)	39(12)
N(2A)	397(18)	215(16)	700(30)	-62(17)	-19(17)	-43(13)
N(3A)	780(30)	530(20)	700(30)	-157(19)	350(20)	-173(19)
C(1A)	310(20)	300(20)	270(30)	30(20)	79(19)	-75(16)
C(2A)	265(19)	410(30)	340(30)	90(30)	-60(20)	-93(18)
C(3A)	280(20)	700(40)	380(30)	60(30)	10(20)	-50(20)
C(4A)	270(20)	480(30)	450(30)	30(20)	110(20)	-52(19)
C(5A)	430(30)	310(30)	950(40)	150(30)	220(30)	-50(20)
C(6A)	280(20)	530(30)	710(30)	130(30)	80(20)	60(20)
C(7A)	290(20)	310(20)	310(30)	40(20)	-63(17)	-36(18)
C(8A)	219(19)	250(20)	400(30)	20(20)	84(18)	-7(16)
C(9A)	340(20)	340(30)	310(30)	0(20)	-40(18)	-118(18)
C(10A)	700(30)	540(30)	390(30)	240(30)	140(20)	-120(30)
C(11A)	460(30)	720(40)	560(30)	270(30)	-180(20)	-200(20)
C(12A)	690(40)	1510(70)	860(50)	870(50)	60(40)	370(40)
C(13A)	370(20)	520(30)	620(30)	-80(30)	-30(20)	-20(20)
C(14A)	430(20)	320(30)	360(30)	-130(20)	10(20)	0(20)
C(15A)	380(30)	630(40)	820(50)	-90(30)	180(30)	-10(20)
C(16A)	370(30)	760(40)	500(30)	-390(30)	0(20)	20(30)
C(17A)	520(30)	1010(50)	350(30)	-260(30)	130(20)	-150(30)
C(18A)	660(30)	1120(50)	500(30)	-590(30)	280(30)	-340(30)
C(19A)	350(20)	330(30)	460(30)	-10(20)	-10(20)	90(20)
C(20A)	280(20)	400(30)	450(30)	40(20)	-10(20)	90(20)
C(21A)	490(30)	380(30)	810(40)	190(30)	-80(20)	80(20)
C(22A)	230(30)	430(30)	2840(100)	-30(50)	200(40)	50(20)
C(23A)	520(30)	700(40)	1540(70)	-670(40)	-120(40)	0(20)
C(24A)	360(30)	480(30)	850(40)	-240(30)	200(20)	-40(20)
C(25A)	730(40)	1000(50)	530(40)	-90(40)	240(30)	-270(30)
C(26A)	650(30)	680(40)	220(30)	-110(30)	70(20)	-290(30)
C(27A)	980(40)	810(40)	340(30)	-130(30)	60(30)	-390(30)
Mn(1B)	231(4)	190(4)	280(5)	-16(4)	12(4)	19(3)
P(1B)	265(5)	215(5)	196(6)	19(5)	3(4)	-2(4)
P(2B)	260(5)	217(6)	253(7)	-2(5)	25(5)	-21(4)
P(3B)	229(5)	301(6)	365(7)	-111(5)	-6(5)	-4(4)
B(1B)	280(20)	200(20)	220(30)	50(20)	-10(20)	27(16)
Tl	137(8)	237(8)	377(8)	-9(6)	7(7)	67(6)
C(1B)	280(20)	330(20)	260(30)	-110(20)	4(18)	-71(16)
C(2B)	370(20)	450(30)	340(30)	130(30)	20(20)	70(20)
C(3B)	260(20)	590(30)	490(30)	100(30)	160(20)	80(20)
C(4B)	360(30)	520(30)	480(30)	-130(30)	-70(20)	200(20)
C(5B)	390(20)	320(30)	680(30)	-30(20)	-210(20)	20(20)

C(6B)	330(20)	200(20)	710(30)	20(20)	-140(20)	-3(17)
C(7B)	197(17)	340(20)	230(20)	-30(20)	3(15)	4(17)
C(8B)	290(20)	280(20)	160(20)	50(20)	21(16)	-82(17)
C(9B)	272(19)	300(20)	260(20)	-10(20)	-47(17)	18(16)
C(10B)	430(30)	600(30)	510(30)	190(30)	-40(20)	-30(20)
C(11B)	350(20)	360(20)	240(20)	100(20)	-42(18)	-44(18)
C(12B)	460(30)	500(30)	470(30)	170(30)	-40(20)	-80(20)
C(13B)	430(20)	290(20)	390(20)	-130(20)	-28(19)	60(20)
C(14B)	210(20)	420(30)	430(30)	40(20)	-42(18)	-14(18)
C(15B)	490(30)	300(30)	370(30)	-170(20)	-30(20)	-40(20)
C(16B)	300(20)	700(40)	560(30)	-300(30)	70(20)	60(20)
C(17B)	430(20)	370(30)	300(30)	-90(20)	150(20)	-160(20)
C(18B)	510(20)	310(20)	400(30)	80(20)	30(20)	-70(20)
C(19B)	230(20)	320(30)	610(40)	-40(30)	140(20)	-13(18)
C(20B)	260(20)	190(20)	620(30)	150(20)	-50(20)	-16(19)
C(21B)	420(30)	470(30)	1030(40)	470(30)	-350(30)	-190(20)
C(22B)	410(30)	420(30)	1600(60)	70(40)	70(30)	130(20)
C(24B)	380(20)	340(20)	500(30)	-70(20)	-90(20)	67(18)
C(25B)	390(30)	920(40)	340(30)	-110(30)	-90(20)	240(30)
C(26B)	300(20)	420(30)	460(30)	-130(20)	-90(20)	30(18)
C(27B)	620(30)	870(40)	390(30)	-200(30)	50(30)	240(30)

Table 17. Crystal Data and Structure Analysis Details for $[PhBP^{iPr}_3]Mn(CH_2Ph)$ (4).

Empirical formula	$C_{34}H_{60}BMnP_3$
Formula weight	627.48
Crystallization solvent	cyclopentane
Crystal shape	block
Crystal color	yellow
Crystal size	0.26 x 0.37 x 0.44 mm

Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data collection temperature	100 K	
Theta range for 23623 reflections used in lattice determination	2.13 to 32.75°	
Unit cell dimensions	a = 9.4120(6) Å b = 11.8746(8) Å c = 16.736(1) Å	α= 90° β= 105.605(1)° γ = 90°
Volume	1801.6(2) $Å^3$	
Z	2	
Crystal system	monoclinic	
Space group	P 21 (# 4)	
Density (calculated)	1.157 g/cm^3	
F(000)	678	
Theta range for data collection	2.1 to 32.9°	
Completeness to theta = 32.90°	91.0%	
Index ranges	$-14 \le h \le 12$, $-17 \le k \le 18$, $-24 \le l \le 24$	
Data collection scan type	ω scans	
Reflections collected	30165	
Independent reflections	10967 [R_{int}= 0.0446]	
Reflections > 2σ(I)	9835	
Average σ(I)/(net I)	0.0459	
Absorption coefficient	0.52 mm^{-1}	
Absorption correction	none	
Reflections monitored for decay	initial data recollected at end	
Decay of standards	0%	

Table 17 (cont.)

Structure Solution and Refinement

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10967 / 1 / 365
Treatment of hydrogen atoms	not refined, U_{iso} fixed at 120% U_{eq} of attached atom
Goodness-of-fit on F^2	1.53
Final R indices [I>2σ(I), 9835 reflections]	R1 = 0.0328, wR2 = 0.0570
R indices (all data)	R1 = 0.0394, wR2 = 0.0578
Type of weighting scheme used	sigma
Weighting scheme used	calc $w=1/[\sigma^2(Fo^2)]$ where $P=(Fo^2+2Fc^2)/3$
Max shift/error	0.001
Average shift/error	0.000
Absolute structure parameter	0.048(8)
Largest diff. peak and hole	1.00 and -0.32 e·Å^{-3}

Programs Used

Cell refinement	Bruker SMART 5.606
Data collection	Bruker SMART 5.054
Data reduction	Bruker SAINT 6.45
Structure solution	Bruker SHELXTL 6.14
Structure refinement	Bruker SHELXTL 6.14

Special Refinement Details

A twin card was used in the refinement with a BASF value of 0.04845.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for [PhBP$^{iPr}_3$]Mn(CH_2Ph) (4). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Mn	9078.8(2)	94.2(2)	6964.4(1)	15.9(1)
P(1)	9741.6(4)	-741.3(3)	8433.6(2)	15.6(1)
P(2)	8961.1(4)	2077.1(3)	7529.1(2)	14.7(1)
P(3)	6333.2(4)	-161.4(3)	6863.6(2)	15.7(1)
B	7336.6(19)	824.2(13)	8599.3(10)	14.1(3)
C(1)	6509.9(16)	1229.5(12)	9301.8(9)	14.6(3)
C(2)	6594.5(17)	662.5(14)	10047.8(9)	20.0(3)
C(3)	5841.4(19)	1021.9(15)	10615.6(10)	26.1(4)
C(4)	4954.3(17)	1968.3(15)	10452.2(10)	24.3(4)
C(5)	4843.7(17)	2549.4(13)	9725.4(10)	22.0(4)
C(6)	5601.9(16)	2188.8(13)	9170.0(9)	18.0(3)
C(7)	8317.9(16)	-336.6(12)	8935.7(9)	14.7(3)
C(8)	8418.5(16)	1915.1(12)	8493.9(9)	15.1(3)
C(9)	5957.3(16)	573.3(13)	7745.6(9)	15.8(3)
C(10)	10381(2)	-2818.8(16)	7818.7(11)	35.7(5)
C(11)	10195.4(19)	-2278.6(13)	8606.4(10)	24.1(4)
C(12)	9191(2)	-2945.7(15)	8994.5(12)	35.1(4)
C(13)	12752.9(17)	-346.6(14)	8690.5(10)	23.6(4)
C(14)	11471.3(15)	-97.1(13)	9073.9(9)	18.1(3)
C(15)	11888.8(18)	-430.0(14)	9988.7(9)	24.3(4)
C(16)	11993.0(18)	2408.9(14)	7734.3(11)	25.7(4)
C(17)	10576.6(17)	3046.8(13)	7706.2(10)	19.3(3)
C(18)	10799(2)	3802.0(15)	8467.3(11)	30.0(4)
C(19)	7708(2)	3002.2(15)	5965.2(9)	26.5(4)
C(20)	7470.1(17)	2918.8(13)	6836.4(9)	19.9(3)
C(21)	7204(2)	4083.6(15)	7156.6(11)	33.6(4)
C(22)	5404.4(18)	106.6(17)	5139.4(9)	27.8(3)
C(23)	4805.5(16)	120.7(15)	5903.6(8)	19.2(3)
C(24)	3931.0(19)	1202.1(15)	5912.3(10)	27.4(4)
C(25)	6308(2)	-2403.6(14)	6341.8(11)	30.3(4)
C(26)	6066.8(18)	-1682.0(13)	7051.3(10)	21.4(3)
C(27)	4611(2)	-1986.2(15)	7237.4(12)	32.8(4)
C(28)	10347.2(19)	-430.2(15)	6145.9(10)	27.9(4)
C(29)	9533.5(18)	-249.3(13)	5264.4(10)	22.7(3)
C(30)	9524(2)	795.3(14)	4879.1(11)	29.9(4)
C(31)	8712(2)	979.9(17)	4067.4(13)	39.3(5)
C(32)	7868(2)	138(2)	3615.0(11)	39.9(5)
C(33)	7857(2)	-905.9(17)	3979.4(11)	36.2(5)
C(34)	8675(2)	-1094.5(14)	4784.8(11)	27.9(4)

Table 9. Bond lengths [Å] and angles [°] for [$PhBP^{iPr}_3$]Mn(CH_2Ph) (4).

Mn-C(28)	2.138(2)	C(15)-H(15C)	0.9800
Mn-P(2)	2.5507(5)	C(16)-C(17)	1.523(2)
Mn-P(3)	2.5620(5)	C(16)-H(16A)	0.9800
Mn-P(1)	2.5679(4)	C(16)-H(16B)	0.9800
P(1)-C(7)	1.8273(14)	C(16)-H(16C)	0.9800
P(1)-C(14)	1.8561(15)	C(17)-C(18)	1.525(2)
P(1)-C(11)	1.8793(15)	C(17)-H(17)	1.0000
P(2)-C(8)	1.8300(14)	C(18)-H(18A)	0.9800
P(2)-C(20)	1.8539(15)	C(18)-H(18B)	0.9800
P(2)-C(17)	1.8663(16)	C(18)-H(18C)	0.9800
P(3)-C(9)	1.8293(14)	C(19)-C(20)	1.537(2)
P(3)-C(26)	1.8613(16)	C(19)-H(19A)	0.9800
P(3)-C(23)	1.8756(14)	C(19)-H(19B)	0.9800
B-C(1)	1.647(2)	C(19)-H(19C)	0.9800
B-C(7)	1.670(2)	C(20)-C(21)	1.528(2)
B-C(9)	1.679(2)	C(20)-H(20)	1.0000
B-C(8)	1.686(2)	C(21)-H(21A)	0.9800
C(1)-C(2)	1.402(2)	C(21)-H(21B)	0.9800
C(1)-C(6)	1.405(2)	C(21)-H(21C)	0.9800
C(2)-C(3)	1.396(2)	C(22)-C(23)	1.530(2)
C(2)-H(2)	0.9500	C(22)-H(22A)	0.9800
C(3)-C(4)	1.383(2)	C(22)-H(22B)	0.9800
C(3)-H(3)	0.9500	C(22)-H(22C)	0.9800
C(4)-C(5)	1.378(2)	C(23)-C(24)	1.527(2)
C(4)-H(4)	0.9500	C(23)-H(23)	1.0000
C(5)-C(6)	1.383(2)	C(24)-H(24A)	0.9800
C(5)-H(5)	0.9500	C(24)-H(24B)	0.9800
C(6)-H(6)	0.9500	C(24)-H(24C)	0.9800
C(7)-H(7A)	0.9900	C(25)-C(26)	1.530(2)
C(7)-H(7B)	0.9900	C(25)-H(25A)	0.9800
C(8)-H(8A)	0.9900	C(25)-H(25B)	0.9800
C(8)-H(8B)	0.9900	C(25)-H(25C)	0.9800
C(9)-H(9A)	0.9900	C(26)-C(27)	1.528(2)
C(9)-H(9B)	0.9900	C(26)-H(26)	1.0000
C(10)-C(11)	1.518(2)	C(27)-H(27A)	0.9800
C(10)-H(10A)	0.9800	C(27)-H(27B)	0.9800
C(10)-H(10B)	0.9800	C(27)-H(27C)	0.9800
C(10)-H(10C)	0.9800	C(28)-C(29)	1.484(2)
C(11)-C(12)	1.508(2)	C(28)-H(28A)	0.9900
C(11)-H(11)	1.0000	C(28)-H(28B)	0.9900
C(12)-H(12A)	0.9800	C(29)-C(30)	1.397(2)
C(12)-H(12B)	0.9800	C(29)-C(34)	1.399(2)
C(12)-H(12C)	0.9800	C(30)-C(31)	1.385(3)
C(13)-C(14)	1.540(2)	C(30)-H(30)	0.9500
C(13)-H(13A)	0.9800	C(31)-C(32)	1.372(3)
C(13)-H(13B)	0.9800	C(31)-H(31)	0.9500
C(13)-H(13C)	0.9800	C(32)-C(33)	1.383(3)
C(14)-C(15)	1.527(2)	C(32)-H(32)	0.9500
C(14)-H(14)	1.0000	C(33)-C(34)	1.379(3)
C(15)-H(15A)	0.9800	C(33)-H(33)	0.9500
C(15)-H(15B)	0.9800	C(34)-H(34)	0.9500

C(28)-Mn-P(2)	126.42(5)
C(28)-Mn-P(3)	130.59(5)
P(2)-Mn-P(3)	89.439(14)
C(28)-Mn-P(1)	117.86(5)
P(2)-Mn-P(1)	91.458(14)
P(3)-Mn-P(1)	89.899(14)
C(7)-P(1)-C(14)	105.30(7)
C(7)-P(1)-C(11)	110.43(7)
C(14)-P(1)-C(11)	100.59(8)
C(7)-P(1)-Mn	108.63(5)
C(14)-P(1)-Mn	110.06(5)
C(11)-P(1)-Mn	120.61(5)
C(8)-P(2)-C(20)	105.34(7)
C(8)-P(2)-C(17)	109.48(7)
C(20)-P(2)-C(17)	102.36(7)
C(8)-P(2)-Mn	106.27(5)
C(20)-P(2)-Mn	111.53(5)
C(17)-P(2)-Mn	120.91(5)
C(9)-P(3)-C(26)	105.21(7)
C(9)-P(3)-C(23)	109.63(7)
C(26)-P(3)-C(23)	102.17(7)
C(9)-P(3)-Mn	107.51(5)
C(26)-P(3)-Mn	106.44(5)
C(23)-P(3)-Mn	124.23(5)
C(1)-B-C(7)	108.97(12)
C(1)-B-C(9)	104.70(11)
C(7)-B-C(9)	111.80(12)
C(1)-B-C(8)	105.35(11)
C(7)-B-C(8)	112.00(12)
C(9)-B-C(8)	113.45(12)
C(2)-C(1)-C(6)	114.55(14)
C(2)-C(1)-B	124.82(13)
C(6)-C(1)-B	120.60(13)
C(3)-C(2)-C(1)	122.80(15)
C(3)-C(2)-H(2)	118.6
C(1)-C(2)-H(2)	118.6
C(4)-C(3)-C(2)	120.25(16)
C(4)-C(3)-H(3)	119.9
C(2)-C(3)-H(3)	119.9
C(5)-C(4)-C(3)	118.68(14)
C(5)-C(4)-H(4)	120.7
C(3)-C(4)-H(4)	120.7
C(4)-C(5)-C(6)	120.54(15)
C(4)-C(5)-H(5)	119.7
C(6)-C(5)-H(5)	119.7
C(5)-C(6)-C(1)	123.18(15)
C(5)-C(6)-H(6)	118.4
C(1)-C(6)-H(6)	118.4
B-C(7)-P(1)	117.99(10)
B-C(7)-H(7A)	107.8
P(1)-C(7)-H(7A)	107.8
B-C(7)-H(7B)	107.8
P(1)-C(7)-H(7B)	107.8
H(7A)-C(7)-H(7B)	107.1
B-C(8)-P(2)	119.53(10)
B-C(8)-H(8A)	107.4
P(2)-C(8)-H(8A)	107.4
B-C(8)-H(8B)	107.4
P(2)-C(8)-H(8B)	107.4
H(8A)-C(8)-H(8B)	107.0
B-C(9)-P(3)	119.89(10)
B-C(9)-H(9A)	107.3
P(3)-C(9)-H(9A)	107.3
B-C(9)-H(9B)	107.3
P(3)-C(9)-H(9B)	107.3
H(9A)-C(9)-H(9B)	106.9
C(11)-C(10)-H(10A)	109.5
C(11)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(11)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-C(10)	112.58(15)
C(12)-C(11)-P(1)	115.71(12)
C(10)-C(11)-P(1)	110.57(11)
C(12)-C(11)-H(11)	105.7
C(10)-C(11)-H(11)	105.7
P(1)-C(11)-H(11)	105.7
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(14)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(13)	110.42(12)
C(15)-C(14)-P(1)	114.92(11)
C(13)-C(14)-P(1)	110.11(10)
C(15)-C(14)-H(14)	107.0
C(13)-C(14)-H(14)	107.0
P(1)-C(14)-H(14)	107.0
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(17)-C(16)-H(16A)	109.5
C(17)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(17)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5

H(16B)-C(16)-H(16C)	109.5	C(23)-C(24)-H(24C)	109.5
C(16)-C(17)-C(18)	110.14(14)	H(24A)-C(24)-H(24C)	109.5
C(16)-C(17)-P(2)	111.53(11)	H(24B)-C(24)-H(24C)	109.5
C(18)-C(17)-P(2)	114.72(11)	C(26)-C(25)-H(25A)	109.5
C(16)-C(17)-H(17)	106.6	C(26)-C(25)-H(25B)	109.5
C(18)-C(17)-H(17)	106.6	H(25A)-C(25)-H(25B)	109.5
P(2)-C(17)-H(17)	106.6	C(26)-C(25)-H(25C)	109.5
C(17)-C(18)-H(18A)	109.5	H(25A)-C(25)-H(25C)	109.5
C(17)-C(18)-H(18B)	109.5	H(25B)-C(25)-H(25C)	109.5
H(18A)-C(18)-H(18B)	109.5	C(27)-C(26)-C(25)	110.75(14)
C(17)-C(18)-H(18C)	109.5	C(27)-C(26)-P(3)	115.64(12)
H(18A)-C(18)-H(18C)	109.5	C(25)-C(26)-P(3)	110.94(11)
H(18B)-C(18)-H(18C)	109.5	C(27)-C(26)-H(26)	106.3
C(20)-C(19)-H(19A)	109.5	C(25)-C(26)-H(26)	106.3
C(20)-C(19)-H(19B)	109.5	P(3)-C(26)-H(26)	106.3
H(19A)-C(19)-H(19B)	109.5	C(26)-C(27)-H(27A)	109.5
C(20)-C(19)-H(19C)	109.5	C(26)-C(27)-H(27B)	109.5
H(19A)-C(19)-H(19C)	109.5	H(27A)-C(27)-H(27B)	109.5
H(19B)-C(19)-H(19C)	109.5	C(26)-C(27)-H(27C)	109.5
C(21)-C(20)-C(19)	110.72(13)	H(27A)-C(27)-H(27C)	109.5
C(21)-C(20)-P(2)	115.88(12)	H(27B)-C(27)-H(27C)	109.5
C(19)-C(20)-P(2)	110.44(11)	C(29)-C(28)-Mn	111.54(11)
C(21)-C(20)-H(20)	106.4	C(29)-C(28)-H(28A)	109.3
C(19)-C(20)-H(20)	106.4	Mn-C(28)-H(28A)	109.3
P(2)-C(20)-H(20)	106.4	C(29)-C(28)-H(28B)	109.3
C(20)-C(21)-H(21A)	109.5	Mn-C(28)-H(28B)	109.3
C(20)-C(21)-H(21B)	109.5	H(28A)-C(28)-H(28B)	108.0
H(21A)-C(21)-H(21B)	109.5	C(30)-C(29)-C(34)	116.19(15)
C(20)-C(21)-H(21C)	109.5	C(30)-C(29)-C(28)	121.67(15)
H(21A)-C(21)-H(21C)	109.5	C(34)-C(29)-C(28)	122.06(15)
H(21B)-C(21)-H(21C)	109.5	C(31)-C(30)-C(29)	121.77(17)
C(23)-C(22)-H(22A)	109.5	C(31)-C(30)-H(30)	119.1
C(23)-C(22)-H(22B)	109.5	C(29)-C(30)-H(30)	119.1
H(22A)-C(22)-H(22B)	109.5	C(32)-C(31)-C(30)	120.72(17)
C(23)-C(22)-H(22C)	109.5	C(32)-C(31)-H(31)	119.6
H(22A)-C(22)-H(22C)	109.5	C(30)-C(31)-H(31)	119.6
H(22B)-C(22)-H(22C)	109.5	C(31)-C(32)-C(33)	118.81(17)
C(24)-C(23)-C(22)	109.74(14)	C(31)-C(32)-H(32)	120.6
C(24)-C(23)-P(3)	115.65(11)	C(33)-C(32)-H(32)	120.6
C(22)-C(23)-P(3)	110.13(10)	C(34)-C(33)-C(32)	120.56(18)
C(24)-C(23)-H(23)	107.0	C(34)-C(33)-H(33)	119.7
C(22)-C(23)-H(23)	107.0	C(32)-C(33)-H(33)	119.7
P(3)-C(23)-H(23)	107.0	C(33)-C(34)-C(29)	121.93(16)
C(23)-C(24)-H(24A)	109.5	C(33)-C(34)-H(34)	119.0
C(23)-C(24)-H(24B)	109.5	C(29)-C(34)-H(34)	119.0
H(24A)-C(24)-H(24B)	109.5		

Symmetry transformations used to generate equivalent atoms:

Table 20. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for [PhBP$^{iPr}_3$]Mn(CH_2Ph) (4). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn	167(1)	173(1)	149(1)	-4(1)	60(1)	10(1)
P(1)	163(2)	150(2)	169(2)	16(2)	67(2)	29(2)
P(2)	151(2)	151(2)	139(2)	6(2)	42(2)	-9(2)
P(3)	155(2)	179(2)	136(2)	-25(2)	36(2)	-13(1)
B	135(8)	152(8)	149(8)	-10(6)	59(7)	13(6)
C(1)	116(7)	168(7)	148(7)	-34(6)	23(6)	-35(6)
C(2)	174(8)	239(8)	186(8)	18(7)	48(6)	27(6)
C(3)	252(9)	366(10)	190(8)	16(7)	100(7)	6(8)
C(4)	191(8)	338(9)	234(8)	-114(7)	113(7)	-34(7)
C(5)	151(8)	226(8)	284(9)	-77(7)	58(7)	17(6)
C(6)	161(8)	198(8)	181(7)	-10(6)	46(6)	-11(6)
C(7)	141(7)	163(7)	151(7)	6(6)	63(6)	5(6)
C(8)	145(7)	155(7)	153(7)	0(6)	41(6)	-3(6)
C(9)	156(8)	174(7)	154(7)	-18(6)	61(6)	1(6)
C(10)	575(13)	212(9)	350(10)	4(8)	240(10)	87(9)
C(11)	312(10)	165(8)	274(9)	40(7)	124(8)	75(7)
C(12)	497(12)	181(8)	451(11)	120(8)	260(10)	96(8)
C(13)	175(8)	306(9)	247(8)	57(7)	90(7)	42(7)
C(14)	143(7)	200(8)	198(7)	35(6)	43(6)	36(6)
C(15)	190(8)	341(9)	193(8)	12(7)	43(6)	43(7)
C(16)	190(9)	301(9)	282(9)	54(7)	69(7)	-15(7)
C(17)	188(8)	225(8)	167(8)	30(6)	48(6)	-56(6)
C(18)	350(11)	273(9)	288(9)	-61(7)	105(8)	-141(8)
C(19)	328(10)	284(9)	172(8)	46(7)	48(7)	36(7)
C(20)	187(8)	213(8)	185(8)	39(6)	31(6)	24(6)
C(21)	453(12)	292(10)	250(9)	66(8)	73(8)	164(8)
C(22)	275(9)	384(9)	167(7)	7(8)	44(6)	27(9)
C(23)	180(7)	238(7)	137(6)	-28(7)	10(5)	-28(7)
C(24)	213(9)	367(10)	204(8)	-22(7)	-9(7)	61(7)
C(25)	421(11)	217(9)	287(10)	-60(7)	124(9)	-17(8)
C(26)	262(9)	172(8)	203(8)	-23(6)	52(7)	-33(6)
C(27)	364(11)	273(10)	386(11)	-11(8)	167(9)	-112(8)
C(28)	303(10)	319(10)	259(9)	22(7)	153(8)	86(7)
C(29)	277(9)	218(8)	251(8)	-1(7)	182(7)	55(7)
C(30)	394(11)	236(9)	324(10)	1(7)	197(9)	-44(8)
C(31)	583(14)	332(11)	329(11)	135(8)	233(10)	90(10)
C(32)	465(12)	539(12)	215(8)	46(10)	130(8)	100(11)
C(33)	422(12)	422(11)	299(10)	-142(9)	199(9)	-47(9)
C(34)	412(11)	206(8)	296(10)	-17(7)	228(9)	19(7)

Table 21. Crystal Data and Structure Analysis Details for [PhBP$^{iPr}_3$]Mn(NH(2,6-^{i}Pr$_2$-C$_6$H$_3$)) (6).

Empirical formula	$C_{39}H_{71}BMnNP_3$
Formula weight	712.63
Crystallization solvent	TMS_2O/petroleum ether
Crystal shape	rough slab
Crystal color	yellow
Crystal size	0.11 x 0.26 x 0.37 mm

Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data collection temperature	100 K	
Theta range for 20417 reflections used in lattice determination	2.53 to 27.96°	
Unit cell dimensions	a = 10.690(1) Å b = 11.249(1) Å c = 18.718(2) Å	α= 98.393(2)° β= 101.614(2)° γ = 107.482(2)°
Volume	2050.8(4) Å^3	
Z	2	
Crystal system	triclinic	
Space group	P-1 (# 2)	
Density (calculated)	1.154 g/cm^3	
F(000)	774	
Theta range for data collection	2.0 to 28.4°	
Completeness to theta = 28.40°	92.5%	
Index ranges	$-14 \le h \le 14$, $-15 \le k \le 14$, $-24 \le l \le 24$	
Data collection scan type	ω scans	
Reflections collected	42790	
Independent reflections	9504 [R_{int}= 0.0690]	
Reflections > 2σ(I)	6761	
Average σ(I)/(net I)	0.0626	
Absorption coefficient	0.47 mm^{-1}	
Absorption correction	none	
Reflections monitored for decay	initial data recollected at end	
Decay of standards	0%	

Table 21 (cont.)

Structure Solution and Refinement

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9504 / 0 / 458
Treatment of hydrogen atoms	not refined, U_{iso} fixed at 120% U_{eq} of attached atom
Goodness-of-fit on F^2	1.50
Final R indices [I>2σ(I), 6761 reflections]	R1 = 0.0419, wR2 = 0.0694
R indices (all data)	R1 = 0.0701, wR2 = 0.0726
Type of weighting scheme used	sigma
Weighting scheme used	calc $w=1/[\sigma^2(Fo^2)]$ where $P=(Fo^2+2Fc^2)/3$
Max shift/error	0.008
Average shift/error	0.000
Largest diff. peak and hole	0.74 and -0.48 e·Å^{-3}

Programs Used

Cell refinement	Bruker SMART 5.606
Data collection	Bruker SMART 5.054
Data reduction	Bruker SAINT 6.45
Structure solution	Bruker SHELXTL 6.14
Structure refinement	Bruker SHELXTL 6.14

Special Refinement Details

One methyl group of the ligand was disordered and refined in two positions with populations of 52.0 and 48 %. One isopropyl unit of the aniline was also disordered and refined in two positions with populations of 86.2 and 13.8 %.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for [PhBP$^{iPr}_3$]Mn(NH(2,6-^{i}Pr$_2$-C$_6$H$_3$)) (6). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Mn	-113.4(3)	8578.7(3)	2567.4(2)	17.9(1)
P(1)	-2241.7(5)	7635.6(4)	1443.9(3)	16.2(1)
P(2)	803.2(5)	6892.9(4)	1991.4(3)	16.7(1)
P(3)	-1161.5(5)	7067.1(5)	3355.1(3)	19.7(1)
B	-2023(2)	5195.6(19)	1871.1(12)	17.0(5)
N	1518.0(17)	10118.9(15)	3078.5(10)	23.6(4)
C(1)	-2998.4(18)	3686.9(17)	1557.5(10)	16.6(4)
C(2)	-4254.2(19)	3243.7(17)	1724.0(11)	23.3(5)
C(3)	-5131(2)	1991.1(18)	1466.7(12)	27.1(5)
C(4)	-4774(2)	1119.5(18)	1022.1(11)	27.0(5)
C(5)	-3560(2)	1508.0(17)	840.7(11)	23.4(5)
C(6)	-2686.8(19)	2772.3(16)	1108.5(10)	18.5(4)
C(7)	-3018.2(17)	6018.3(15)	1558.0(10)	16.1(4)
C(8)	-658.0(17)	5442.6(16)	1537.2(10)	16.8(4)
C(9)	-1593.7(19)	5451.0(16)	2804.6(10)	18.5(4)
C(10)	-3917.7(19)	8705.3(18)	2079.8(11)	24.2(5)
C(11)	-3596.4(18)	8357.0(17)	1332.2(10)	18.1(4)
C(12)	-4903.3(18)	7554.8(18)	741.3(11)	23.7(5)
C(13)	-1657(2)	8676.4(18)	216.0(11)	26.4(5)
C(14)	-1862.8(19)	7440.6(17)	511.1(10)	19.9(4)
C(15)	-2812(2)	6281.7(18)	-97.6(11)	27.1(5)
C(16)	1904(2)	8740.8(17)	1204.2(11)	27.0(5)
C(17)	1824.8(18)	7405.0(17)	1318.8(10)	20.0(4)
C(18)	1401.1(19)	6446.9(18)	571.7(11)	25.7(5)
C(19)	3125.7(19)	7461.3(18)	3165.8(11)	28.1(5)
C(20)	1960.8(18)	6329.8(18)	2631.9(11)	21.0(4)
C(21)	2513.4(19)	5377.7(18)	2239.7(11)	26.6(5)
C(22)	732(2)	8563.2(19)	4693.2(12)	34.9(6)
C(23)	-23(3)	7210(2)	4270.1(15)	69.3(10)
C(25)	-2587(2)	8448.9(19)	4017.4(12)	36.7(6)
C(26)	-2768(2)	7144.7(18)	3553.3(12)	28.9(5)
C(27)	-3544(2)	6069(2)	3867.1(15)	51.3(7)
C(28)	1961.3(19)	11399.2(18)	3426.4(11)	21.5(5)
C(29)	1052.0(19)	12094.9(18)	3341.0(11)	22.2(5)
C(30)	1510(2)	13391.2(18)	3679.7(12)	31.6(5)
C(31)	2835(2)	14025.2(19)	4094.3(12)	35.8(6)
C(32)	3715(2)	13350.5(19)	4184.5(12)	34.8(6)
C(33)	3325(2)	12054.1(19)	3871.6(11)	26.1(5)
C(34)	-271(2)	11431.7(19)	2014.7(12)	35.1(6)
C(35)	-355.5(19)	11465.0(18)	2824.2(12)	26.2(5)
C(36)	-1406(2)	12062.6(19)	2988.6(13)	36.9(6)
C(38)	4328(2)	11344(2)	3980.7(14)	35.6(6)
C(24B)	586(9)	6299(6)	4419(4)	25(2)
C(24A)	-90(10)	6183(5)	4612(4)	45(2)
C(37A)	4893(3)	11154(3)	3335.1(15)	39.9(8)
C(39A)	5477(3)	11922(3)	4713.9(15)	45.2(9)

C(37B)	5870(14)	12363(15)	3843(9)	38(5)
C(39B)	4438(17)	10797(17)	4453(10)	43(5)

Table 23. Bond lengths [Å] and angles [°] for [PhBP$^{iPr}_3$]Mn(NH(2,6-^{i}Pr$_2$-C$_6$H$_3$)) (6).

Mn-N	1.997(2)	C(14)-H(14)	1.0000
Mn-P(3)	2.5637(6)	C(15)-H(15A)	0.9800
Mn-P(2)	2.5813(6)	C(15)-H(15B)	0.9800
Mn-P(1)	2.5877(6)	C(15)-H(15C)	0.9800
P(1)-C(7)	1.8225(17)	C(16)-C(17)	1.528(2)
P(1)-C(11)	1.8528(18)	C(16)-H(16A)	0.9800
P(1)-C(14)	1.8674(19)	C(16)-H(16B)	0.9800
P(2)-C(8)	1.8313(17)	C(16)-H(16C)	0.9800
P(2)-C(20)	1.8616(19)	C(17)-C(18)	1.528(2)
P(2)-C(17)	1.8700(19)	C(17)-H(17)	1.0000
P(3)-C(9)	1.8267(18)	C(18)-H(18A)	0.9800
P(3)-C(23)	1.845(2)	C(18)-H(18B)	0.9800
P(3)-C(26)	1.852(2)	C(18)-H(18C)	0.9800
B-C(1)	1.647(3)	C(19)-C(20)	1.531(2)
B-C(8)	1.665(3)	C(19)-H(19A)	0.9800
B-C(9)	1.673(3)	C(19)-H(19B)	0.9800
B-C(7)	1.682(3)	C(19)-H(19C)	0.9800
N-C(28)	1.384(2)	C(20)-C(21)	1.536(2)
N-H(1)	0.826(18)	C(20)-H(20)	1.0000
C(1)-C(6)	1.393(2)	C(21)-H(21A)	0.9800
C(1)-C(2)	1.400(2)	C(21)-H(21B)	0.9800
C(2)-C(3)	1.386(2)	C(21)-H(21C)	0.9800
C(2)-H(2)	0.9500	C(22)-C(23)	1.499(3)
C(3)-C(4)	1.383(3)	C(22)-H(22A)	0.9800
C(3)-H(3)	0.9500	C(22)-H(22B)	0.9800
C(4)-C(5)	1.368(3)	C(22)-H(22C)	0.9800
C(4)-H(4)	0.9500	C(23)-C(24B)	1.402(6)
C(5)-C(6)	1.397(2)	C(23)-C(24A)	1.390(5)
C(5)-H(5)	0.9500	C(23)-H(23)	1.0454
C(6)-H(6)	0.9500	C(25)-C(26)	1.528(3)
C(7)-H(7A)	0.9900	C(25)-H(25A)	0.9800
C(7)-H(7B)	0.9900	C(25)-H(25B)	0.9800
C(8)-H(8A)	0.9900	C(25)-H(25C)	0.9800
C(8)-H(8B)	0.9900	C(26)-C(27)	1.516(3)
C(9)-H(9A)	0.9900	C(26)-H(26)	1.0000
C(9)-H(9B)	0.9900	C(27)-H(27A)	0.9800
C(10)-C(11)	1.531(3)	C(27)-H(27B)	0.9800
C(10)-H(10A)	0.9800	C(27)-H(27C)	0.9800
C(10)-H(10B)	0.9800	C(28)-C(29)	1.419(3)
C(10)-H(10C)	0.9800	C(28)-C(33)	1.431(3)
C(11)-C(12)	1.523(2)	C(29)-C(30)	1.394(3)
C(11)-H(11)	1.0000	C(29)-C(35)	1.508(3)
C(12)-H(12A)	0.9800	C(30)-C(31)	1.381(3)
C(12)-H(12B)	0.9800	C(30)-H(30)	0.9500
C(12)-H(12C)	0.9800	C(31)-C(32)	1.375(3)
C(13)-C(14)	1.541(2)	C(31)-H(31)	0.9500
C(13)-H(13A)	0.9800	C(32)-C(33)	1.389(3)
C(13)-H(13B)	0.9800	C(32)-H(32)	0.9500
C(13)-H(13C)	0.9800	C(33)-C(38)	1.517(3)
C(14)-C(15)	1.528(2)	C(34)-C(35)	1.532(3)

C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-C(36)	1.530(3)
C(35)-H(35)	1.0000
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(38)-C(39B)	1.155(19)
C(38)-C(37A)	1.472(3)
C(38)-C(39A)	1.548(3)
C(38)-C(37B)	1.795(14)
C(38)-H(38)	1.0000
C(24B)-H(23)	1.2342
C(24B)-H(24F)	0.9800
C(24B)-H(24D)	0.9800
C(24B)-H(24E)	0.9800
C(24A)-H(24A)	0.9800
C(24A)-H(24B)	0.9800
C(24A)-H(24C)	0.9800
C(37A)-H(37A)	0.9800
C(37A)-H(37B)	0.9800
C(37A)-H(37C)	0.9800
C(39A)-H(39A)	0.9800
C(39A)-H(39B)	0.9800
C(39A)-H(39C)	0.9800
C(37B)-H(37D)	0.9800
C(37B)-H(37E)	0.9800
C(37B)-H(37F)	0.9800
C(39B)-H(39D)	0.9800
C(39B)-H(39E)	0.9800
C(39B)-H(39F)	0.9800

N-Mn-P(3)	118.63(5)
N-Mn-P(2)	105.73(5)
P(3)-Mn-P(2)	89.95(2)
N-Mn-P(1)	144.77(5)
P(3)-Mn-P(1)	93.11(2)
P(2)-Mn-P(1)	87.96(2)
C(7)-P(1)-C(11)	106.54(8)
C(7)-P(1)-C(14)	105.49(8)
C(11)-P(1)-C(14)	104.83(8)
C(7)-P(1)-Mn	103.27(6)
C(11)-P(1)-Mn	121.07(6)
C(14)-P(1)-Mn	114.40(6)
C(8)-P(2)-C(20)	103.81(8)
C(8)-P(2)-C(17)	110.64(8)
C(20)-P(2)-C(17)	101.54(9)
C(8)-P(2)-Mn	107.32(6)
C(20)-P(2)-Mn	118.28(6)
C(17)-P(2)-Mn	114.68(6)
C(9)-P(3)-C(23)	108.02(10)
C(9)-P(3)-C(26)	105.14(9)
C(23)-P(3)-C(26)	105.59(13)
C(9)-P(3)-Mn	105.88(6)
C(23)-P(3)-Mn	114.75(10)
C(26)-P(3)-Mn	116.81(7)
C(1)-B-C(8)	108.83(15)
C(1)-B-C(9)	106.66(15)
C(8)-B-C(9)	111.20(15)
C(1)-B-C(7)	104.31(14)
C(8)-B-C(7)	113.10(15)
C(9)-B-C(7)	112.25(15)
C(28)-N-Mn	144.80(15)
C(28)-N-H(1)	108.3(13)
Mn-N-H(1)	106.2(13)
C(6)-C(1)-C(2)	114.97(16)
C(6)-C(1)-B	124.70(16)
C(2)-C(1)-B	120.31(16)
C(3)-C(2)-C(1)	123.09(18)
C(3)-C(2)-H(2)	118.5
C(1)-C(2)-H(2)	118.5
C(4)-C(3)-C(2)	119.70(19)
C(4)-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1
C(5)-C(4)-C(3)	119.42(17)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
C(4)-C(5)-C(6)	120.04(19)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(1)-C(6)-C(5)	122.78(18)
C(1)-C(6)-H(6)	118.6
C(5)-C(6)-H(6)	118.6
B-C(7)-P(1)	119.57(12)
B-C(7)-H(7A)	107.4
P(1)-C(7)-H(7A)	107.4
B-C(7)-H(7B)	107.4
P(1)-C(7)-H(7B)	107.4
H(7A)-C(7)-H(7B)	107.0
B-C(8)-P(2)	117.69(12)
B-C(8)-H(8A)	107.9
P(2)-C(8)-H(8A)	107.9
B-C(8)-H(8B)	107.9
P(2)-C(8)-H(8B)	107.9
H(8A)-C(8)-H(8B)	107.2
B-C(9)-P(3)	118.97(12)
B-C(9)-H(9A)	107.6
P(3)-C(9)-H(9A)	107.6
B-C(9)-H(9B)	107.6
P(3)-C(9)-H(9B)	107.6
H(9A)-C(9)-H(9B)	107.0
C(11)-C(10)-H(10A)	109.5
C(11)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(11)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5

C(12)-C(11)-C(10)	109.69(15)	C(19)-C(20)-C(21)	110.63(15)
C(12)-C(11)-P(1)	115.00(13)	C(19)-C(20)-P(2)	110.89(13)
C(10)-C(11)-P(1)	111.00(13)	C(21)-C(20)-P(2)	114.79(13)
C(12)-C(11)-H(11)	106.9	C(19)-C(20)-H(20)	106.7
C(10)-C(11)-H(11)	106.9	C(21)-C(20)-H(20)	106.7
P(1)-C(11)-H(11)	106.9	P(2)-C(20)-H(20)	106.7
C(11)-C(12)-H(12A)	109.5	C(20)-C(21)-H(21A)	109.5
C(11)-C(12)-H(12B)	109.5	C(20)-C(21)-H(21B)	109.5
H(12A)-C(12)-H(12B)	109.5	H(21A)-C(21)-H(21B)	109.5
C(11)-C(12)-H(12C)	109.5	C(20)-C(21)-H(21C)	109.5
H(12A)-C(12)-H(12C)	109.5	H(21A)-C(21)-H(21C)	109.5
H(12B)-C(12)-H(12C)	109.5	H(21B)-C(21)-H(21C)	109.5
C(14)-C(13)-H(13A)	109.5	C(23)-C(22)-H(22A)	109.5
C(14)-C(13)-H(13B)	109.5	C(23)-C(22)-H(22B)	109.5
H(13A)-C(13)-H(13B)	109.5	H(22A)-C(22)-H(22B)	109.5
C(14)-C(13)-H(13C)	109.5	C(23)-C(22)-H(22C)	109.5
H(13A)-C(13)-H(13C)	109.5	H(22A)-C(22)-H(22C)	109.5
H(13B)-C(13)-H(13C)	109.5	H(22B)-C(22)-H(22C)	109.5
C(15)-C(14)-C(13)	110.70(16)	C(24B)-C(23)-C(24A)	35.6(2)
C(15)-C(14)-P(1)	117.66(13)	C(24B)-C(23)-C(22)	117.0(3)
C(13)-C(14)-P(1)	111.46(13)	C(24A)-C(23)-C(22)	121.8(3)
C(15)-C(14)-H(14)	105.3	C(24B)-C(23)-P(3)	123.0(3)
C(13)-C(14)-H(14)	105.3	C(24A)-C(23)-P(3)	122.8(3)
P(1)-C(14)-H(14)	105.3	C(22)-C(23)-P(3)	113.80(16)
C(14)-C(15)-H(15A)	109.5	C(24B)-C(23)-H(23)	58.4
C(14)-C(15)-H(15B)	109.5	C(24A)-C(23)-H(23)	93.9
H(15A)-C(15)-H(15B)	109.5	C(22)-C(23)-H(23)	94.2
C(14)-C(15)-H(15C)	109.5	P(3)-C(23)-H(23)	94.4
H(15A)-C(15)-H(15C)	109.5	C(26)-C(25)-H(25A)	109.5
H(15B)-C(15)-H(15C)	109.5	C(26)-C(25)-H(25B)	109.5
C(17)-C(16)-H(16A)	109.5	H(25A)-C(25)-H(25B)	109.5
C(17)-C(16)-H(16B)	109.5	C(26)-C(25)-H(25C)	109.5
H(16A)-C(16)-H(16B)	109.5	H(25A)-C(25)-H(25C)	109.5
C(17)-C(16)-H(16C)	109.5	H(25B)-C(25)-H(25C)	109.5
H(16A)-C(16)-H(16C)	109.5	C(27)-C(26)-C(25)	111.23(18)
H(16B)-C(16)-H(16C)	109.5	C(27)-C(26)-P(3)	116.62(15)
C(18)-C(17)-C(16)	111.32(16)	C(25)-C(26)-P(3)	112.13(14)
C(18)-C(17)-P(2)	114.60(12)	C(27)-C(26)-H(26)	105.3
C(16)-C(17)-P(2)	112.27(13)	C(25)-C(26)-H(26)	105.3
C(18)-C(17)-H(17)	106.0	P(3)-C(26)-H(26)	105.3
C(16)-C(17)-H(17)	106.0	C(26)-C(27)-H(27A)	109.5
P(2)-C(17)-H(17)	106.0	C(26)-C(27)-H(27B)	109.5
C(17)-C(18)-H(18A)	109.5	H(27A)-C(27)-H(27B)	109.5
C(17)-C(18)-H(18B)	109.5	C(26)-C(27)-H(27C)	109.5
H(18A)-C(18)-H(18B)	109.5	H(27A)-C(27)-H(27C)	109.5
C(17)-C(18)-H(18C)	109.5	H(27B)-C(27)-H(27C)	109.5
H(18A)-C(18)-H(18C)	109.5	N-C(28)-C(29)	119.72(17)
H(18B)-C(18)-H(18C)	109.5	N-C(28)-C(33)	121.79(18)
C(20)-C(19)-H(19A)	109.5	C(29)-C(28)-C(33)	118.50(17)
C(20)-C(19)-H(19B)	109.5	C(30)-C(29)-C(28)	119.54(18)
H(19A)-C(19)-H(19B)	109.5	C(30)-C(29)-C(35)	120.31(18)
C(20)-C(19)-H(19C)	109.5	C(28)-C(29)-C(35)	119.86(17)
H(19A)-C(19)-H(19C)	109.5	C(31)-C(30)-C(29)	121.7(2)
H(19B)-C(19)-H(19C)	109.5	C(31)-C(30)-H(30)	119.1

C(29)-C(30)-H(30)	119.1	C(39B)-C(38)-C(37B)	116.8(11)
C(32)-C(31)-C(30)	118.86(19)	C(37A)-C(38)-C(37B)	53.1(5)
C(32)-C(31)-H(31)	120.6	C(33)-C(38)-C(37B)	106.0(6)
C(30)-C(31)-H(31)	120.6	C(39A)-C(38)-C(37B)	67.3(6)
C(31)-C(32)-C(33)	122.6(2)	C(39B)-C(38)-H(38)	48.1
C(31)-C(32)-H(32)	118.7	C(37A)-C(38)-H(38)	106.0
C(33)-C(32)-H(32)	118.7	C(33)-C(38)-H(38)	106.0
C(32)-C(33)-C(28)	118.78(19)	C(39A)-C(38)-H(38)	106.0
C(32)-C(33)-C(38)	121.00(19)	C(37B)-C(38)-H(38)	147.1
C(28)-C(33)-C(38)	120.20(18)	C(23)-C(24B)-H(23)	46.2
C(35)-C(34)-H(34A)	109.5	C(23)-C(24B)-H(24F)	109.5
C(35)-C(34)-H(34B)	109.5	H(23)-C(24B)-H(24F)	123.7
H(34A)-C(34)-H(34B)	109.5	C(23)-C(24B)-H(24D)	109.5
C(35)-C(34)-H(34C)	109.5	H(23)-C(24B)-H(24D)	63.3
H(34A)-C(34)-H(34C)	109.5	C(23)-C(24B)-H(24E)	109.5
H(34B)-C(34)-H(34C)	109.5	H(23)-C(24B)-H(24E)	125.9
C(29)-C(35)-C(36)	115.18(17)	C(23)-C(24A)-H(24A)	109.5
C(29)-C(35)-C(34)	109.10(17)	C(23)-C(24A)-H(24B)	109.5
C(36)-C(35)-C(34)	110.51(17)	H(24A)-C(24A)-H(24B)	109.5
C(29)-C(35)-H(35)	107.2	C(23)-C(24A)-H(24C)	109.5
C(36)-C(35)-H(35)	107.2	H(24A)-C(24A)-H(24C)	109.5
C(34)-C(35)-H(35)	107.2	H(24B)-C(24A)-H(24C)	109.5
C(35)-C(36)-H(36A)	109.5	C(38)-C(37A)-H(37A)	109.5
C(35)-C(36)-H(36B)	109.5	C(38)-C(37A)-H(37B)	109.5
H(36A)-C(36)-H(36B)	109.5	C(38)-C(37A)-H(37C)	109.5
C(35)-C(36)-H(36C)	109.5	C(38)-C(39A)-H(39A)	109.5
H(36A)-C(36)-H(36C)	109.5	C(38)-C(39A)-H(39B)	109.5
H(36B)-C(36)-H(36C)	109.5	C(38)-C(39A)-H(39C)	109.5
C(39B)-C(38)-C(37A)	122.1(8)	C(38)-C(37B)-H(37D)	109.5
C(39B)-C(38)-C(33)	122.9(8)	C(38)-C(37B)-H(37E)	109.5
C(37A)-C(38)-C(33)	113.4(2)	C(38)-C(37B)-H(37F)	109.5
C(39B)-C(38)-C(39A)	57.9(9)	C(38)-C(39B)-H(39D)	109.5
C(37A)-C(38)-C(39A)	110.7(2)	C(38)-C(39B)-H(39E)	109.5
C(33)-C(38)-C(39A)	114.06(19)	C(38)-C(39B)-H(39F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 24. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for [PhBP$^{iPr}_3$]Mn(NH(2,6-^{i}Pr$_2$-C$_6$H$_3$)) (6). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn	153(2)	135(2)	215(2)	10(1)	15(1)	34(1)
P(1)	138(3)	125(3)	202(3)	31(2)	22(2)	33(2)
P(2)	137(3)	157(3)	183(3)	18(2)	28(2)	34(2)
P(3)	223(3)	169(3)	183(3)	16(2)	30(2)	70(2)
B	162(12)	134(11)	193(13)	24(9)	24(10)	41(9)
N	154(9)	170(9)	326(11)	-2(8)	-18(8)	50(8)
C(1)	181(10)	155(10)	148(10)	51(8)	-15(8)	68(8)
C(2)	219(11)	169(10)	301(12)	40(9)	57(10)	64(9)
C(3)	194(11)	226(11)	349(13)	121(10)	35(10)	7(9)
C(4)	285(12)	120(10)	296(13)	58(9)	-38(10)	-17(9)
C(5)	304(12)	148(10)	202(11)	27(9)	-13(9)	65(9)
C(6)	201(11)	156(10)	180(11)	69(8)	18(9)	42(8)
C(7)	144(10)	128(9)	182(11)	17(8)	32(8)	20(8)
C(8)	183(10)	120(9)	177(11)	10(8)	10(8)	50(8)
C(9)	195(11)	127(10)	222(11)	26(8)	48(9)	48(8)
C(10)	218(11)	235(11)	303(13)	75(9)	66(10)	113(9)
C(11)	158(10)	142(10)	256(12)	74(9)	50(9)	59(8)
C(12)	192(11)	241(11)	279(12)	50(9)	22(9)	106(9)
C(13)	289(12)	257(11)	260(12)	96(10)	80(10)	89(10)
C(14)	155(10)	204(10)	241(12)	62(9)	55(9)	59(9)
C(15)	284(12)	277(12)	240(12)	6(9)	50(10)	114(10)
C(16)	205(11)	260(12)	302(13)	82(10)	70(10)	6(9)
C(17)	143(10)	236(11)	200(11)	40(9)	43(9)	39(9)
C(18)	195(11)	334(12)	230(12)	52(10)	72(9)	67(10)
C(19)	222(12)	341(13)	241(12)	21(10)	-4(10)	101(10)
C(20)	185(11)	220(11)	223(11)	44(9)	33(9)	80(9)
C(21)	229(11)	286(12)	296(13)	55(10)	32(10)	135(10)
C(22)	404(14)	303(13)	263(13)	-23(10)	-41(11)	132(11)
C(23)	940(20)	250(14)	527(18)	-26(13)	-459(16)	169(14)
C(25)	391(14)	359(13)	359(14)	-31(11)	105(11)	186(11)
C(26)	323(13)	270(12)	311(13)	55(10)	146(10)	117(10)
C(27)	559(17)	461(15)	770(20)	279(15)	504(16)	249(14)
C(28)	238(11)	194(11)	173(11)	35(9)	27(9)	36(9)
C(29)	231(11)	176(10)	215(12)	35(9)	23(9)	33(9)
C(30)	367(14)	211(12)	328(13)	38(10)	5(11)	106(10)
C(31)	406(14)	167(11)	357(14)	-48(10)	-44(11)	34(11)
C(32)	264(12)	262(12)	328(14)	-26(10)	-68(10)	-45(10)
C(33)	229(12)	254(12)	237(12)	10(9)	25(10)	35(10)
C(34)	352(13)	253(12)	348(14)	19(10)	-67(11)	85(10)
C(35)	234(12)	141(10)	353(14)	33(9)	0(10)	42(9)
C(36)	333(13)	231(12)	514(16)	53(11)	36(12)	118(10)
C(38)	188(12)	333(14)	406(16)	-58(12)	-53(11)	37(10)
C(24B)	300(40)	270(30)	140(30)	30(20)	10(20)	80(30)
C(24A)	570(50)	400(30)	280(30)	110(20)	-10(30)	70(30)
C(37A)	324(16)	461(18)	351(18)	6(14)	85(13)	88(14)
C(39A)	314(17)	600(20)	331(17)	-77(15)	-74(13)	181(15)

C(37B)	170(90)	420(100)	470(120)	50(90)	110(80)	0(80)
C(39B)	330(110)	550(130)	400(120)	-90(100)	0(90)	280(100)

Table 25. Crystal Data and Structure Analysis Details for [PhBP$^{iPr}_3$]Mn(dbabh) (7).

Empirical formula	$C_{41}H_{63}BMnNP_3$
Formula weight	728.58
Crystallization solvent	Et_2O
Crystal shape	rough block
Crystal color	yellow
Crystal size	0.29 x 0.33 x 0.33 mm

Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data collection temperature	100 K	
Theta range for 36539 reflections used in lattice determination	2.56 to 30.67°	
Unit cell dimensions	a = 10.4294(9) Å b = 16.812(1) Å c = 23.393(2) Å	α= 90° β= 97.476(1)° γ = 90°
Volume	4066.7(6) Å^3	
Z	4	
Crystal system	monoclinic	
Space group	P 21/c (# 14)	
Density (calculated)	1.190 g/cm^3	
F(000)	1564	
Theta range for data collection	1.5 to 30.6°	
Completeness to theta = 30.62°	89.9%	
Index ranges	$-14 \le h \le 14$, $-23 \le k \le 23$, $-32 \le l \le 30$	
Data collection scan type	ω scans	
Reflections collected	63707	
Independent reflections	11277 [R_{int}= 0.0581]	
Reflections > 2σ(I)	8678	
Average σ(I)/(net I)	0.0428	
Absorption coefficient	0.47 mm^{-1}	
Absorption correction	none	
Reflections monitored for decay	initial data recollected at end	
Decay of standards	0%	

Table 25 (cont.)

Structure Solution and Refinement

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11277 / 0 / 436
Treatment of hydrogen atoms	not refined, U_{iso} fixed at 120% U_{eq} of attached atom
Goodness-of-fit on F^2	2.04
Final R indices [I>2σ(I), 8678 reflections]	R1 = 0.0409, wR2 = 0.0724
R indices (all data)	R1 = 0.0586, wR2 = 0.0739
Type of weighting scheme used	sigma
Weighting scheme used	calc $w=1/[\sigma^2(Fo^2)]$ where $P=(Fo^2+2Fc^2)/3$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	0.97 and -0.44 e·Å^{-3}

Programs Used

Cell refinement	Bruker SMART 5.606
Data collection	Bruker SMART 5.054
Data reduction	Bruker SAINT 6.45
Structure solution	Bruker SHELXTL 6.14
Structure refinement	Bruker SHELXTL 6.14

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 26. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for [PhBP$^{iPr}_3$]Mn(dbabh) (7). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Mn	2548.7(2)	2552.7(1)	3810.9(1)	14.8(1)
P(1)	1437.0(4)	2815.4(2)	2798.9(2)	17.5(1)
P(2)	4170.9(4)	3657.2(2)	3701.3(2)	17.1(1)
P(3)	4067.2(4)	1557.0(2)	3423.7(2)	15.8(1)
B	4198.7(17)	2854.5(10)	2542.6(7)	15.6(4)
N	1697.8(12)	2348.3(8)	4489.8(5)	19.2(3)
C(1)	4934.4(14)	3021.9(8)	1973.6(6)	15.1(3)
C(2)	4416.1(15)	3548.6(9)	1537.5(6)	19.2(3)
C(3)	5002.5(15)	3698.3(9)	1048.9(6)	20.1(3)
C(4)	6154.5(16)	3336.1(9)	977.3(6)	23.4(4)
C(5)	6716.0(17)	2824.2(11)	1398.8(7)	30.5(4)
C(6)	6110.1(16)	2676.7(10)	1884.2(7)	25.9(4)
C(7)	2636.0(14)	2690.4(9)	2305.5(6)	19.3(3)
C(8)	4477.0(15)	3676.1(9)	2947.7(6)	19.6(3)
C(9)	4861.2(15)	2045.6(9)	2868.7(6)	18.6(3)
C(10)	-739.6(17)	1908.4(12)	2954.6(8)	40.2(5)
C(11)	-117.2(15)	2328.4(10)	2481.6(7)	25.2(4)
C(12)	10.0(17)	1767.9(11)	1980.6(8)	33.8(4)
C(13)	-100.9(17)	4045.7(10)	3134.6(7)	30.6(4)
C(14)	1014.5(16)	3882.7(9)	2783.2(7)	22.8(4)
C(15)	755.9(19)	4252.6(11)	2183.6(7)	36.5(5)
C(16)	2885.1(18)	4727.3(10)	4340.9(8)	33.2(4)
C(17)	3987.4(16)	4697.3(9)	3974.5(7)	24.4(4)
C(18)	3844.6(19)	5344.9(10)	3514.0(8)	34.9(5)
C(19)	5532.0(17)	3292.2(10)	4773.1(7)	29.0(4)
C(20)	5697.6(16)	3320.3(10)	4129.7(7)	24.4(4)
C(21)	6910.6(16)	3777.3(12)	4035.7(8)	37.7(5)
C(22)	5170.6(17)	948.6(10)	4488.0(6)	28.7(4)
C(23)	5292.6(16)	899.7(10)	3851.8(7)	25.4(4)
C(24)	6655.3(16)	985.3(11)	3719.8(8)	36.6(5)
C(25)	2271.5(16)	373.3(10)	3524.6(7)	25.9(4)
C(26)	2927.9(15)	813.2(9)	3067.1(7)	20.6(3)
C(27)	3467.7(17)	231.8(10)	2659.0(7)	28.8(4)
C(28)	443.8(15)	2608.7(9)	4659.3(6)	19.4(3)
C(29)	896.6(16)	3226.1(9)	5126.9(6)	21.1(4)
C(30)	392.7(18)	3930.9(10)	5297.8(7)	27.9(4)
C(31)	1126(2)	4352.4(10)	5746.2(8)	35.4(5)
C(32)	2280(2)	4058.3(11)	6012.9(7)	34.7(5)
C(33)	2770.1(17)	3332.6(10)	5848.5(7)	27.9(4)
C(34)	2073.6(16)	2928.4(9)	5399.6(6)	20.5(3)
C(35)	2283.2(15)	2146.1(9)	5084.4(6)	18.7(3)
C(36)	1262.8(15)	1573.4(9)	5255.2(6)	17.2(3)
C(37)	1305.3(16)	898.4(9)	5590.5(6)	20.5(3)
C(38)	138.0(16)	504.9(10)	5644.5(7)	24.6(4)
C(39)	-1018.9(16)	804.8(10)	5385.1(7)	25.3(4)
C(40)	-1065.2(16)	1503.0(9)	5054.2(7)	23.2(4)

C(41)	78.4(15)	1871.2(9)	4984.8(6)	18.5(3)

Table 27. Bond lengths [Å] and angles [°] for [PhBP$^{iPr}_3$]Mn(dbabh) (7).

Mn-N	1.948(1)	C(15)-H(15A)	0.9800
Mn-P(1)	2.5357(5)	C(15)-H(15B)	0.9800
Mn-P(2)	2.5473(5)	C(15)-H(15C)	0.9800
Mn-P(3)	2.5503(5)	C(16)-C(17)	1.522(2)
P(1)-C(7)	1.8208(15)	C(16)-H(16A)	0.9800
P(1)-C(14)	1.8469(16)	C(16)-H(16B)	0.9800
P(1)-C(11)	1.8803(16)	C(16)-H(16C)	0.9800
P(2)-C(8)	1.8321(15)	C(17)-C(18)	1.525(2)
P(2)-C(20)	1.8561(16)	C(17)-H(17)	1.0000
P(2)-C(17)	1.8800(16)	C(18)-H(18A)	0.9800
P(3)-C(9)	1.8238(15)	C(18)-H(18B)	0.9800
P(3)-C(26)	1.8475(15)	C(18)-H(18C)	0.9800
P(3)-C(23)	1.8773(16)	C(19)-C(20)	1.538(2)
B-C(1)	1.645(2)	C(19)-H(19A)	0.9800
B-C(9)	1.665(2)	C(19)-H(19B)	0.9800
B-C(7)	1.675(2)	C(19)-H(19C)	0.9800
B-C(8)	1.679(2)	C(20)-C(21)	1.520(2)
N-C(28)	1.4814(19)	C(20)-H(20)	1.0000
N-C(35)	1.4840(18)	C(21)-H(21A)	0.9800
C(1)-C(6)	1.397(2)	C(21)-H(21B)	0.9800
C(1)-C(2)	1.405(2)	C(21)-H(21C)	0.9800
C(2)-C(3)	1.388(2)	C(22)-C(23)	1.512(2)
C(2)-H(2)	0.9500	C(22)-H(22A)	0.9800
C(3)-C(4)	1.376(2)	C(22)-H(22B)	0.9800
C(3)-H(3)	0.9500	C(22)-H(22C)	0.9800
C(4)-C(5)	1.380(2)	C(23)-C(24)	1.500(2)
C(4)-H(4)	0.9500	C(23)-H(23)	1.0000
C(5)-C(6)	1.392(2)	C(24)-H(24A)	0.9800
C(5)-H(5)	0.9500	C(24)-H(24B)	0.9800
C(6)-H(6)	0.9500	C(24)-H(24C)	0.9800
C(7)-H(7A)	0.9900	C(25)-C(26)	1.533(2)
C(7)-H(7B)	0.9900	C(25)-H(25A)	0.9800
C(8)-H(8A)	0.9900	C(25)-H(25B)	0.9800
C(8)-H(8B)	0.9900	C(25)-H(25C)	0.9800
C(9)-H(9A)	0.9900	C(26)-C(27)	1.524(2)
C(9)-H(9B)	0.9900	C(26)-H(26)	1.0000
C(10)-C(11)	1.527(2)	C(27)-H(27A)	0.9800
C(10)-H(10A)	0.9800	C(27)-H(27B)	0.9800
C(10)-H(10B)	0.9800	C(27)-H(27C)	0.9800
C(10)-H(10C)	0.9800	C(28)-C(41)	1.529(2)
C(11)-C(12)	1.523(2)	C(28)-C(29)	1.537(2)
C(11)-H(11)	1.0000	C(28)-H(28)	1.0000
C(12)-H(12A)	0.9800	C(29)-C(30)	1.376(2)
C(12)-H(12B)	0.9800	C(29)-C(34)	1.400(2)
C(12)-H(12C)	0.9800	C(30)-C(31)	1.407(2)
C(13)-C(14)	1.534(2)	C(30)-H(30)	0.9500
C(13)-H(13A)	0.9800	C(31)-C(32)	1.373(3)
C(13)-H(13B)	0.9800	C(31)-H(31)	0.9500
C(13)-H(13C)	0.9800	C(32)-C(33)	1.396(2)
C(14)-C(15)	1.526(2)	C(32)-H(32)	0.9500
C(14)-H(14)	1.0000	C(33)-C(34)	1.376(2)

C(33)-H(33)	0.9500
C(34)-C(35)	1.537(2)
C(35)-C(36)	1.526(2)
C(35)-H(35)	1.0000
C(36)-C(37)	1.377(2)
C(36)-C(41)	1.405(2)
C(37)-C(38)	1.406(2)
C(37)-H(37)	0.9500
C(38)-C(39)	1.374(2)
C(38)-H(38)	0.9500
C(39)-C(40)	1.403(2)
C(39)-H(39)	0.9500
C(40)-C(41)	1.372(2)
C(40)-H(40)	0.9500

N-Mn-P(1)	126.19(4)
N-Mn-P(2)	126.13(4)
P(1)-Mn-P(2)	90.46(2)
N-Mn-P(3)	122.92(4)
P(1)-Mn-P(3)	90.71(2)
P(2)-Mn-P(3)	89.51(2)
C(7)-P(1)-C(14)	106.34(7)
C(7)-P(1)-C(11)	109.11(7)
C(14)-P(1)-C(11)	102.95(8)
C(7)-P(1)-Mn	107.66(5)
C(14)-P(1)-Mn	105.46(5)
C(11)-P(1)-Mn	123.97(5)
C(8)-P(2)-C(20)	106.27(7)
C(8)-P(2)-C(17)	110.44(7)
C(20)-P(2)-C(17)	102.61(8)
C(8)-P(2)-Mn	108.10(5)
C(20)-P(2)-Mn	104.92(5)
C(17)-P(2)-Mn	123.05(5)
C(9)-P(3)-C(26)	107.96(7)
C(9)-P(3)-C(23)	107.71(7)
C(26)-P(3)-C(23)	101.28(7)
C(9)-P(3)-Mn	108.52(5)
C(26)-P(3)-Mn	102.24(5)
C(23)-P(3)-Mn	127.45(5)
C(1)-B-C(9)	107.52(12)
C(1)-B-C(7)	107.24(11)
C(9)-B-C(7)	110.19(12)
C(1)-B-C(8)	104.56(12)
C(9)-B-C(8)	112.49(12)
C(7)-B-C(8)	114.32(12)
C(28)-N-C(35)	94.97(11)
C(28)-N-Mn	132.67(10)
C(35)-N-Mn	128.99(10)
C(6)-C(1)-C(2)	114.56(14)
C(6)-C(1)-B	124.13(13)
C(2)-C(1)-B	121.31(13)
C(3)-C(2)-C(1)	122.91(14)
C(3)-C(2)-H(2)	118.5
C(1)-C(2)-H(2)	118.5
C(4)-C(3)-C(2)	120.34(14)
C(4)-C(3)-H(3)	119.8
C(2)-C(3)-H(3)	119.8
C(5)-C(4)-C(3)	119.01(15)
C(5)-C(4)-H(4)	120.5
C(3)-C(4)-H(4)	120.5
C(4)-C(5)-C(6)	119.89(16)
C(4)-C(5)-H(5)	120.1
C(6)-C(5)-H(5)	120.1
C(5)-C(6)-C(1)	123.28(15)
C(5)-C(6)-H(6)	118.4
C(1)-C(6)-H(6)	118.4
B-C(7)-P(1)	119.34(10)
B-C(7)-H(7A)	107.5
P(1)-C(7)-H(7A)	107.5
B-C(7)-H(7B)	107.5
P(1)-C(7)-H(7B)	107.5
H(7A)-C(7)-H(7B)	107.0
B-C(8)-P(2)	119.33(10)
B-C(8)-H(8A)	107.5
P(2)-C(8)-H(8A)	107.5
B-C(8)-H(8B)	107.5
P(2)-C(8)-H(8B)	107.5
H(8A)-C(8)-H(8B)	107.0
B-C(9)-P(3)	119.62(10)
B-C(9)-H(9A)	107.4
P(3)-C(9)-H(9A)	107.4
B-C(9)-H(9B)	107.4
P(3)-C(9)-H(9B)	107.4
H(9A)-C(9)-H(9B)	106.9
C(11)-C(10)-H(10A)	109.5
C(11)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(11)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-C(10)	111.07(15)
C(12)-C(11)-P(1)	114.59(12)
C(10)-C(11)-P(1)	109.95(11)
C(12)-C(11)-H(11)	106.9
C(10)-C(11)-H(11)	106.9
P(1)-C(11)-H(11)	106.9
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(14)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5

C(15)-C(14)-C(13)	111.35(13)	C(24)-C(23)-C(22)	113.62(14)
C(15)-C(14)-P(1)	115.30(12)	C(24)-C(23)-P(3)	115.54(12)
C(13)-C(14)-P(1)	111.01(11)	C(22)-C(23)-P(3)	110.75(11)
C(15)-C(14)-H(14)	106.2	C(24)-C(23)-H(23)	105.3
C(13)-C(14)-H(14)	106.2	C(22)-C(23)-H(23)	105.3
P(1)-C(14)-H(14)	106.2	P(3)-C(23)-H(23)	105.3
C(14)-C(15)-H(15A)	109.5	C(23)-C(24)-H(24A)	109.5
C(14)-C(15)-H(15B)	109.5	C(23)-C(24)-H(24B)	109.5
H(15A)-C(15)-H(15B)	109.5	H(24A)-C(24)-H(24B)	109.5
C(14)-C(15)-H(15C)	109.5	C(23)-C(24)-H(24C)	109.5
H(15A)-C(15)-H(15C)	109.5	H(24A)-C(24)-H(24C)	109.5
H(15B)-C(15)-H(15C)	109.5	H(24B)-C(24)-H(24C)	109.5
C(17)-C(16)-H(16A)	109.5	C(26)-C(25)-H(25A)	109.5
C(17)-C(16)-H(16B)	109.5	C(26)-C(25)-H(25B)	109.5
H(16A)-C(16)-H(16B)	109.5	H(25A)-C(25)-H(25B)	109.5
C(17)-C(16)-H(16C)	109.5	C(26)-C(25)-H(25C)	109.5
H(16A)-C(16)-H(16C)	109.5	H(25A)-C(25)-H(25C)	109.5
H(16B)-C(16)-H(16C)	109.5	H(25B)-C(25)-H(25C)	109.5
C(16)-C(17)-C(18)	111.26(14)	C(27)-C(26)-C(25)	111.27(13)
C(16)-C(17)-P(2)	109.89(11)	C(27)-C(26)-P(3)	116.65(11)
C(18)-C(17)-P(2)	115.38(11)	C(25)-C(26)-P(3)	109.30(11)
C(16)-C(17)-H(17)	106.6	C(27)-C(26)-H(26)	106.3
C(18)-C(17)-H(17)	106.6	C(25)-C(26)-H(26)	106.3
P(2)-C(17)-H(17)	106.6	P(3)-C(26)-H(26)	106.3
C(17)-C(18)-H(18A)	109.5	C(26)-C(27)-H(27A)	109.5
C(17)-C(18)-H(18B)	109.5	C(26)-C(27)-H(27B)	109.5
H(18A)-C(18)-H(18B)	109.5	H(27A)-C(27)-H(27B)	109.5
C(17)-C(18)-H(18C)	109.5	C(26)-C(27)-H(27C)	109.5
H(18A)-C(18)-H(18C)	109.5	H(27A)-C(27)-H(27C)	109.5
H(18B)-C(18)-H(18C)	109.5	H(27B)-C(27)-H(27C)	109.5
C(20)-C(19)-H(19A)	109.5	N-C(28)-C(41)	100.34(12)
C(20)-C(19)-H(19B)	109.5	N-C(28)-C(29)	100.95(12)
H(19A)-C(19)-H(19B)	109.5	C(41)-C(28)-C(29)	105.47(12)
C(20)-C(19)-H(19C)	109.5	N-C(28)-H(28)	116.0
H(19A)-C(19)-H(19C)	109.5	C(41)-C(28)-H(28)	116.0
H(19B)-C(19)-H(19C)	109.5	C(29)-C(28)-H(28)	116.0
C(21)-C(20)-C(19)	111.01(14)	C(30)-C(29)-C(34)	121.37(15)
C(21)-C(20)-P(2)	116.05(12)	C(30)-C(29)-C(28)	133.99(15)
C(19)-C(20)-P(2)	109.89(12)	C(34)-C(29)-C(28)	104.65(13)
C(21)-C(20)-H(20)	106.4	C(29)-C(30)-C(31)	117.34(16)
C(19)-C(20)-H(20)	106.4	C(29)-C(30)-H(30)	121.3
P(2)-C(20)-H(20)	106.4	C(31)-C(30)-H(30)	121.3
C(20)-C(21)-H(21A)	109.5	C(32)-C(31)-C(30)	121.10(16)
C(20)-C(21)-H(21B)	109.5	C(32)-C(31)-H(31)	119.5
H(21A)-C(21)-H(21B)	109.5	C(30)-C(31)-H(31)	119.5
C(20)-C(21)-H(21C)	109.5	C(31)-C(32)-C(33)	121.35(16)
H(21A)-C(21)-H(21C)	109.5	C(31)-C(32)-H(32)	119.3
H(21B)-C(21)-H(21C)	109.5	C(33)-C(32)-H(32)	119.3
C(23)-C(22)-H(22A)	109.5	C(34)-C(33)-C(32)	117.76(16)
C(23)-C(22)-H(22B)	109.5	C(34)-C(33)-H(33)	121.1
H(22A)-C(22)-H(22B)	109.5	C(32)-C(33)-H(33)	121.1
C(23)-C(22)-H(22C)	109.5	C(33)-C(34)-C(29)	121.04(15)
H(22A)-C(22)-H(22C)	109.5	C(33)-C(34)-C(35)	134.00(15)
H(22B)-C(22)-H(22C)	109.5	C(29)-C(34)-C(35)	104.96(13)

N-C(35)-C(36)	100.02(11)	C(39)-C(38)-C(37)	120.58(15)
N-C(35)-C(34)	100.77(11)	C(39)-C(38)-H(38)	119.7
C(36)-C(35)-C(34)	105.47(12)	C(37)-C(38)-H(38)	119.7
N-C(35)-H(35)	116.1	C(38)-C(39)-C(40)	121.05(15)
C(36)-C(35)-H(35)	116.1	C(38)-C(39)-H(39)	119.5
C(34)-C(35)-H(35)	116.1	C(40)-C(39)-H(39)	119.5
C(37)-C(36)-C(41)	120.76(14)	C(41)-C(40)-C(39)	118.34(15)
C(37)-C(36)-C(35)	134.19(14)	C(41)-C(40)-H(40)	120.8
C(41)-C(36)-C(35)	105.04(13)	C(39)-C(40)-H(40)	120.8
C(36)-C(37)-C(38)	118.36(15)	C(40)-C(41)-C(36)	120.85(14)
C(36)-C(37)-H(37)	120.8	C(40)-C(41)-C(28)	134.56(14)
C(38)-C(37)-H(37)	120.8	C(36)-C(41)-C(28)	104.58(13)

Symmetry transformations used to generate equivalent atoms:

Table 28. Anisotropic displacement parameters ($Å^2$x 10^4) for [PhBP$^{iPr}_3$]Mn(dbabh) (7). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn	153(1)	165(1)	131(1)	12(1)	39(1)	4(1)
P(1)	146(2)	232(2)	148(2)	15(2)	24(2)	19(2)
P(2)	199(2)	166(2)	153(2)	-3(2)	44(2)	-21(2)
P(3)	173(2)	150(2)	161(2)	28(2)	53(2)	14(2)
B	159(9)	185(9)	128(8)	22(7)	30(7)	6(7)
N	175(7)	273(8)	133(6)	15(5)	43(5)	58(6)
C(1)	160(8)	155(8)	139(7)	-14(6)	19(6)	-23(6)
C(2)	211(8)	187(8)	184(8)	12(6)	41(6)	16(7)
C(3)	264(9)	203(8)	132(7)	33(6)	9(6)	-35(7)
C(4)	290(10)	284(9)	144(8)	1(7)	89(7)	-66(8)
C(5)	256(10)	383(11)	306(10)	75(8)	152(8)	75(8)
C(6)	223(9)	327(10)	238(9)	102(7)	68(7)	57(7)
C(7)	199(8)	223(9)	163(8)	21(6)	44(6)	15(7)
C(8)	235(9)	202(8)	160(8)	18(6)	59(6)	-21(7)
C(9)	184(8)	200(8)	186(8)	19(6)	67(6)	-3(7)
C(10)	251(10)	551(13)	403(11)	20(10)	34(8)	-155(9)
C(11)	187(8)	318(10)	243(9)	-6(7)	-7(7)	-2(7)
C(12)	220(10)	394(11)	383(11)	-110(9)	-21(8)	-7(8)
C(13)	309(10)	307(10)	309(10)	-2(8)	72(8)	100(8)
C(14)	246(9)	219(9)	217(8)	22(7)	31(7)	55(7)
C(15)	446(12)	338(11)	318(10)	112(8)	76(9)	182(9)
C(16)	417(12)	242(10)	372(11)	-94(8)	179(9)	-43(8)
C(17)	287(10)	189(9)	262(9)	-36(7)	61(7)	-16(7)
C(18)	524(13)	180(9)	367(11)	-3(8)	152(9)	5(8)
C(19)	342(10)	282(10)	224(9)	28(7)	-48(7)	-40(8)
C(20)	239(9)	242(9)	243(9)	19(7)	-2(7)	-2(7)
C(21)	223(10)	494(12)	406(11)	54(9)	14(8)	-54(9)
C(22)	316(10)	333(10)	198(9)	43(7)	-13(7)	42(8)
C(23)	268(10)	282(10)	209(9)	44(7)	24(7)	61(7)
C(24)	268(10)	444(12)	392(11)	157(9)	70(8)	132(9)
C(25)	267(10)	215(9)	299(9)	6(7)	56(8)	-66(7)
C(26)	199(9)	202(9)	220(8)	-12(7)	35(7)	-16(7)
C(27)	378(11)	235(9)	255(9)	-61(7)	55(8)	-21(8)
C(28)	179(8)	254(9)	155(8)	42(7)	42(6)	28(7)
C(29)	268(9)	209(9)	174(8)	46(7)	98(7)	-9(7)
C(30)	358(11)	244(9)	261(9)	49(7)	139(8)	23(8)
C(31)	617(14)	187(9)	291(10)	-18(8)	180(9)	-17(9)
C(32)	580(14)	255(10)	207(9)	-18(8)	53(9)	-124(9)
C(33)	365(10)	282(10)	186(8)	59(7)	26(7)	-94(8)
C(34)	271(9)	204(8)	154(8)	48(6)	72(7)	-50(7)
C(35)	159(8)	232(9)	172(8)	39(7)	34(6)	8(7)
C(36)	212(8)	187(8)	125(7)	-32(6)	51(6)	-4(7)
C(37)	241(9)	223(9)	155(8)	-16(7)	34(7)	12(7)
C(38)	349(10)	204(9)	201(9)	5(7)	99(7)	-37(8)
C(39)	238(9)	278(9)	263(9)	-38(7)	110(7)	-72(7)
C(40)	200(9)	288(10)	214(8)	-31(7)	50(7)	4(7)

C(41)	222(9)	205(8)	137(8)	-34(6)	60(6)	11(7)

Table 29. Crystal Data and Structure Analysis Details for [PhBP$^{iPr}_3$]Mn(1-Ph(isoindolate)) (8).

Empirical formula	$C_{43}H_{68}BMnNO_{0.50}P_3$
Formula weight	765.64
Crystallization solvent	Et_2O
Crystal shape	block
Crystal color	dichroic orange red
Crystal size	0.25 x 0.26 x 0.37 mm

Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data collection temperature	98 K	
Theta range for 26587 reflections used in lattice determination	2.23 to 31.51°	
Unit cell dimensions	a = 19.6218(9) Å b = 77.737(4) Å c = 11.2629(6) Å	α= 90° β= 90° γ = 90°
Volume	17179.8(15) Å^3	
Z	16	
Crystal system	orthorhombic	
Space group	Fdd2 (# 43)	
Density (calculated)	1.184 g/cm^3	
F(000)	6592	
Theta range for data collection	2.1 to 32.2°	
Completeness to theta = 32.20°	91.4%	
Index ranges	$-29 \le h \le 29$, $-108 \le k \le 105$, $-16 \le l \le 16$	
Data collection scan type	ω scans	
Reflections collected	46858	
Independent reflections	12898 [R_{int}= 0.0724]	
Reflections > 2σ(I)	9619	
Average σ(I)/(net I)	0.0769	
Absorption coefficient	0.45 mm^{-1}	
Absorption correction	none	
Reflections monitored for decay	initial data recollected at end	
Decay of standards	0%	

Table 29 (cont.)

Structure Solution and Refinement

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12898 / 2 / 479
Treatment of hydrogen atoms	not refined, U_{iso} fixed at 120% U_{eq} of attached atom
Goodness-of-fit on F^2	1.47
Final R indices [I>2σ(I), 9619 reflections]	R1 = 0.0514, wR2 = 0.0731
R indices (all data)	R1 = 0.0747, wR2 = 0.0755
Type of weighting scheme used	sigma
Weighting scheme used	calc $w=1/[\sigma^2(Fo^2)]$ where $P=(Fo^2+2Fc^2)/3$
Max shift/error	0.002
Average shift/error	0.000
Absolute structure parameter	-0.011(10)
Largest diff. peak and hole	1.02 and -0.78 e·Å^{-3}

Programs Used

Cell refinement	Bruker SMART 5.606
Data collection	Bruker SMART 5.054
Data reduction	Bruker SAINT 6.45
Structure solution	Bruker SHELXTL 6.14
Structure refinement	Bruker SHELXTL 6.14

Special Refinement Details

Four bad reflections were omitted (040, 260, 220, 080). One half of an ether molecule was present in the asymmetric unit and was disordered in a few positions. The ether molecule was kept isotropic. The phenyl ring on the borate atom was badly disordered, and three different positions were found. The phenyl ring was kept isotropic as well.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 30. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for [PhBP$^{iPr}_3$]Mn(1-Ph(isoindolate)) (8). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Mn	1595.9(2)	1761.8(1)	9777.4(3)	20.9(1)
P(1)	2062.1(3)	2054.9(1)	10320.6(6)	29.6(2)
P(2)	404.6(3)	1817.5(1)	10608.8(5)	22.0(1)
P(3)	1220.4(3)	1881.6(1)	7752.0(5)	21.8(1)
B	662.4(14)	2157.0(3)	9383(2)	27.4(6)
N	2320.5(8)	1572.4(2)	9934.8(15)	21.9(4)
C(1)	230.7(15)	2336.2(3)	9220(2)	42.3(7)
C(2)	230(5)	2464.3(14)	9981(12)	29(3)
C(3)	-126(3)	2617.8(9)	9846(9)	21.3(17)
C(4)	-513(6)	2649.5(12)	8920(8)	36(3)
C(5)	-591(5)	2519.3(10)	8064(8)	48(3)
C(6)	-253(4)	2361.9(9)	8186(7)	30(2)
C(7)	1470.2(12)	2212.2(3)	9693(2)	33.9(6)
C(8)	293.1(11)	2049.0(3)	10493.1(19)	26.3(5)
C(9)	598.0(12)	2049.5(3)	8091(2)	25.8(5)
C(10)	3478.9(13)	1993.7(3)	10230(2)	46.9(7)
C(11)	2914.5(12)	2103.8(3)	9696(3)	40.6(6)
C(12)	3119.5(16)	2292.0(4)	9641(4)	76.7(11)
C(13)	2452.0(14)	1957.6(3)	12627(2)	40.4(6)
C(14)	2072.7(13)	2096.8(3)	11943(2)	33.4(6)
C(15)	2321.1(16)	2276.1(3)	12331(3)	58.9(8)
C(16)	687.1(13)	1807.5(3)	13029(2)	34.9(6)
C(17)	142.8(11)	1754.8(3)	12128.1(19)	25.6(5)
C(18)	-552.2(13)	1822.3(3)	12507(2)	41.3(7)
C(19)	-293.5(13)	1520.9(3)	9874(2)	39.0(6)
C(20)	-222.5(11)	1714.2(3)	9592(2)	27.5(5)
C(21)	-918.8(12)	1800.7(3)	9439(2)	44.9(7)
C(22)	920.8(12)	1540.1(3)	7154(2)	32.4(5)
C(23)	857.1(12)	1722.2(3)	6673(2)	25.7(5)
C(24)	125.3(12)	1764.0(3)	6246(2)	31.5(6)
C(25)	2484.6(12)	1884.4(3)	6573(2)	37.1(6)
C(26)	1864.5(11)	1997.7(3)	6848(2)	26.8(5)
C(27)	1579.7(13)	2075.0(3)	5697(2)	36.6(6)
C(28)	2820.0(12)	1557.9(3)	9094(2)	25.3(5)
C(29)	3397.1(11)	1479.9(2)	9564.9(19)	22.0(5)
C(30)	4035.9(11)	1424.8(3)	9091(2)	29.9(6)
C(31)	4487.6(11)	1343.8(3)	9826(2)	33.7(6)
C(32)	4340.8(12)	1313.5(3)	11035(2)	30.1(6)
C(33)	3733.2(11)	1362.2(3)	11520(2)	27.9(5)
C(34)	3247.8(11)	1446.4(3)	10790(2)	22.8(5)
C(35)	2568.5(11)	1503.8(3)	10979.2(19)	21.1(5)
C(36)	2144.0(11)	1472.3(2)	12013.5(18)	21.0(5)
C(37)	2400.3(12)	1483.2(3)	13176(2)	27.0(5)
C(38)	2009.4(12)	1435.8(3)	14153(2)	32.2(6)
C(39)	1346.0(13)	1378.3(3)	13995(2)	31.4(6)
C(40)	1076.1(12)	1369.3(3)	12846(2)	29.4(5)

C(41)	1466.0(11)	1416.3(2)	11883.4(19)	22.8(5)
C(102)	203(4)	2435.4(10)	8279(7)	39(2)
C(103)	-19(4)	2605.2(9)	8248(8)	38(2)
C(104)	-86(8)	2696(2)	9329(15)	63(5)
C(105)	59(4)	2617.3(9)	10335(8)	29(2)
C(106)	302(6)	2450.9(14)	10323(10)	35(3)
C(112)	-502(5)	2316.3(11)	8689(8)	36(2)
C(113)	-892(4)	2464.5(10)	8408(7)	29(2)
C(114)	-702(4)	2619.6(11)	8757(7)	16(2)
C(115)	-94(7)	2651.4(19)	9253(14)	36(4)
C(116)	328(5)	2489.7(12)	9575(10)	37(3)
O(1)	7500	2500	495(6)	19(2)
C(42)	7935(9)	2405(2)	1609(17)	95(5)
C(43)	8712(5)	2440.0(13)	1808(10)	66(4)
O(2)	7390(4)	2435.7(7)	1376(6)	70(2)
C(44)	8037(3)	2432.7(6)	1139(5)	53.1(14)
C(45)	8451(4)	2315.1(9)	722(8)	131(3)

Table 31. Bond lengths [Å] and angles [°] for [PhBP$^{iPr}_3$]Mn(1-Ph(isoindolate)) (8).

Mn-N	2.054(2)	C(13)-H(13A)	0.9800
Mn-P(1)	2.5308(7)	C(13)-H(13B)	0.9800
Mn-P(2)	2.5550(7)	C(13)-H(13C)	0.9800
Mn-P(3)	2.5718(6)	C(14)-C(15)	1.540(3)
P(1)-C(7)	1.828(2)	C(14)-H(14)	1.0000
P(1)-C(11)	1.854(3)	C(15)-H(15A)	0.9800
P(1)-C(14)	1.856(2)	C(15)-H(15B)	0.9800
P(2)-C(8)	1.818(2)	C(15)-H(15C)	0.9800
P(2)-C(17)	1.852(2)	C(16)-C(17)	1.529(3)
P(2)-C(20)	1.863(2)	C(16)-H(16A)	0.9800
P(3)-C(9)	1.828(2)	C(16)-H(16B)	0.9800
P(3)-C(26)	1.857(2)	C(16)-H(16C)	0.9800
P(3)-C(23)	1.876(2)	C(17)-C(18)	1.522(3)
B-C(1)	1.640(4)	C(17)-H(17)	1.0000
B-C(8)	1.672(3)	C(18)-H(18A)	0.9800
B-C(7)	1.679(4)	C(18)-H(18B)	0.9800
B-C(9)	1.683(3)	C(18)-H(18C)	0.9800
N-C(28)	1.368(3)	C(19)-C(20)	1.542(3)
N-C(35)	1.380(3)	C(19)-H(19A)	0.9800
C(1)-C(116)	1.272(9)	C(19)-H(19B)	0.9800
C(1)-C(102)	1.312(8)	C(19)-H(19C)	0.9800
C(1)-C(2)	1.313(11)	C(20)-C(21)	1.532(3)
C(1)-C(6)	1.517(7)	C(20)-H(20)	1.0000
C(1)-C(106)	1.535(11)	C(21)-H(21A)	0.9800
C(1)-C(112)	1.565(9)	C(21)-H(21B)	0.9800
C(2)-C(3)	1.392(12)	C(21)-H(21C)	0.9800
C(2)-H(2)	0.9500	C(22)-C(23)	1.521(3)
C(3)-C(4)	1.314(13)	C(22)-H(22A)	0.9800
C(3)-H(3)	0.9500	C(22)-H(22B)	0.9800
C(4)-C(5)	1.406(12)	C(22)-H(22C)	0.9800
C(4)-H(4)	0.9500	C(23)-C(24)	1.549(3)
C(5)-C(6)	1.398(10)	C(23)-H(23)	1.0000
C(5)-H(5)	0.9500	C(24)-H(24A)	0.9800
C(6)-H(6)	0.9500	C(24)-H(24B)	0.9800
C(7)-H(7A)	0.9900	C(24)-H(24C)	0.9800
C(7)-H(7B)	0.9900	C(25)-C(26)	1.534(3)
C(8)-H(8A)	0.9900	C(25)-H(25A)	0.9800
C(8)-H(8B)	0.9900	C(25)-H(25B)	0.9800
C(9)-H(9A)	0.9900	C(25)-H(25C)	0.9800
C(9)-H(9B)	0.9900	C(26)-C(27)	1.535(3)
C(10)-C(11)	1.523(3)	C(26)-H(26)	1.0000
C(10)-H(10A)	0.9800	C(27)-H(27A)	0.9800
C(10)-H(10B)	0.9800	C(27)-H(27B)	0.9800
C(10)-H(10C)	0.9800	C(27)-H(27C)	0.9800
C(11)-C(12)	1.519(4)	C(28)-C(29)	1.390(3)
C(11)-H(11)	1.0000	C(28)-H(28)	0.9500
C(12)-H(12A)	0.9800	C(29)-C(30)	1.428(3)
C(12)-H(12B)	0.9800	C(29)-C(34)	1.435(3)
C(12)-H(12C)	0.9800	C(30)-C(31)	1.366(3)
C(13)-C(14)	1.523(3)	C(30)-H(30)	0.9500

C(31)-C(32)	1.412(4)	C(44)-H(44A)	0.9387
C(31)-H(31)	0.9500	C(44)-H(44B)	1.0235
C(32)-C(33)	1.365(3)	C(45)-H(45A)	0.9800
C(32)-H(32)	0.9500	C(45)-H(45B)	0.9800
C(33)-C(34)	1.418(3)	C(45)-H(45C)	0.9800
C(33)-H(33)	0.9500		
C(34)-C(35)	1.422(3)	N-Mn-P(1)	111.98(5)
C(35)-C(36)	1.453(3)	N-Mn-P(2)	136.31(5)
C(36)-C(37)	1.405(3)	P(1)-Mn-P(2)	95.13(2)
C(36)-C(41)	1.408(3)	N-Mn-P(3)	122.30(5)
C(37)-C(38)	1.392(3)	P(1)-Mn-P(3)	89.54(2)
C(37)-H(37)	0.9500	P(2)-Mn-P(3)	90.09(2)
C(38)-C(39)	1.388(3)	C(7)-P(1)-C(11)	106.85(11)
C(38)-H(38)	0.9500	C(7)-P(1)-C(14)	105.68(11)
C(39)-C(40)	1.400(3)	C(11)-P(1)-C(14)	109.12(13)
C(39)-H(39)	0.9500	C(7)-P(1)-Mn	106.20(8)
C(40)-C(41)	1.377(3)	C(11)-P(1)-Mn	114.76(8)
C(40)-H(40)	0.9500	C(14)-P(1)-Mn	113.57(7)
C(41)-H(41)	0.9500	C(8)-P(2)-C(17)	107.07(10)
C(102)-C(103)	1.390(10)	C(8)-P(2)-C(20)	107.65(10)
C(102)-H(102)	0.9500	C(17)-P(2)-C(20)	105.73(10)
C(103)-C(104)	1.413(19)	C(8)-P(2)-Mn	104.58(7)
C(103)-H(103)	0.9500	C(17)-P(2)-Mn	123.22(7)
C(104)-C(105)	1.32(2)	C(20)-P(2)-Mn	107.83(7)
C(104)-H(104)	0.9500	C(9)-P(3)-C(26)	102.82(10)
C(105)-C(106)	1.378(13)	C(9)-P(3)-C(23)	110.66(10)
C(105)-H(105)	0.9500	C(26)-P(3)-C(23)	102.98(10)
C(106)-H(106)	0.9500	C(9)-P(3)-Mn	105.36(8)
C(112)-C(113)	1.419(11)	C(26)-P(3)-Mn	117.85(7)
C(112)-H(112)	0.9500	C(23)-P(3)-Mn	116.39(7)
C(113)-C(114)	1.322(11)	C(1)-B-C(8)	106.62(19)
C(113)-H(113)	0.9500	C(1)-B-C(7)	107.10(19)
C(114)-C(115)	1.340(17)	C(8)-B-C(7)	112.43(19)
C(114)-H(114)	0.9500	C(1)-B-C(9)	106.67(19)
C(115)-C(116)	1.548(18)	C(8)-B-C(9)	111.39(18)
C(115)-H(115)	0.9500	C(7)-B-C(9)	112.21(19)
C(116)-H(116)	0.9500	C(28)-N-C(35)	107.77(17)
O(1)-C(42)	1.687(18)	C(28)-N-Mn	119.71(14)
O(1)-C(42)#1	1.687(18)	C(35)-N-Mn	126.49(14)
O(1)-H(44B)	1.1424	C(116)-C(1)-C(102)	73.1(6)
C(42)-C(43)	1.565(19)	C(116)-C(1)-C(2)	23.7(6)
C(42)-H(42A)	0.9900	C(102)-C(1)-C(2)	94.7(7)
C(42)-H(42B)	0.9900	C(116)-C(1)-C(6)	102.2(6)
C(42)-H(44A)	0.9180	C(102)-C(1)-C(6)	43.6(4)
C(42)-H(44B)	1.5880	C(2)-C(1)-C(6)	113.6(6)
C(43)-H(43A)	0.9800	C(116)-C(1)-C(106)	35.7(7)
C(43)-H(43B)	0.9800	C(102)-C(1)-C(106)	108.4(6)
C(43)-H(43C)	0.9800	C(2)-C(1)-C(106)	14.6(7)
C(43)-H(44A)	0.9301	C(6)-C(1)-C(106)	127.0(5)
O(2)-O(2)#1	1.088(11)	C(116)-C(1)-C(112)	110.5(6)
O(2)-C(44)	1.296(9)	C(102)-C(1)-C(112)	73.2(5)
O(2)-C(44)#1	1.350(8)	C(2)-C(1)-C(112)	108.9(6)
C(44)-C(45)	1.310(8)	C(6)-C(1)-C(112)	31.1(3)
C(44)-O(2)#1	1.349(8)	C(106)-C(1)-C(112)	116.7(6)

C(116)-C(1)-B	133.1(5)	C(11)-C(12)-H(12C)	109.5
C(102)-C(1)-B	127.6(4)	H(12A)-C(12)-H(12C)	109.5
C(2)-C(1)-B	124.9(6)	H(12B)-C(12)-H(12C)	109.5
C(6)-C(1)-B	121.4(3)	C(14)-C(13)-H(13A)	109.5
C(106)-C(1)-B	110.9(5)	C(14)-C(13)-H(13B)	109.5
C(112)-C(1)-B	115.6(4)	H(13A)-C(13)-H(13B)	109.5
C(1)-C(2)-C(3)	125.4(10)	C(14)-C(13)-H(13C)	109.5
C(1)-C(2)-H(2)	117.3	H(13A)-C(13)-H(13C)	109.5
C(3)-C(2)-H(2)	117.3	H(13B)-C(13)-H(13C)	109.5
C(4)-C(3)-C(2)	122.5(9)	C(13)-C(14)-C(15)	110.2(2)
C(4)-C(3)-H(3)	118.7	C(13)-C(14)-P(1)	112.29(16)
C(2)-C(3)-H(3)	118.7	C(15)-C(14)-P(1)	116.22(18)
C(3)-C(4)-C(5)	118.2(9)	C(13)-C(14)-H(14)	105.8
C(3)-C(4)-H(4)	120.9	C(15)-C(14)-H(14)	105.8
C(5)-C(4)-H(4)	120.9	P(1)-C(14)-H(14)	105.8
C(6)-C(5)-C(4)	120.8(8)	C(14)-C(15)-H(15A)	109.5
C(6)-C(5)-H(5)	119.6	C(14)-C(15)-H(15B)	109.5
C(4)-C(5)-H(5)	119.6	H(15A)-C(15)-H(15B)	109.5
C(5)-C(6)-C(1)	119.2(6)	C(14)-C(15)-H(15C)	109.5
C(5)-C(6)-H(6)	120.4	H(15A)-C(15)-H(15C)	109.5
C(1)-C(6)-H(6)	120.4	H(15B)-C(15)-H(15C)	109.5
B-C(7)-P(1)	120.65(14)	C(17)-C(16)-H(16A)	109.5
B-C(7)-H(7A)	107.2	C(17)-C(16)-H(16B)	109.5
P(1)-C(7)-H(7A)	107.2	H(16A)-C(16)-H(16B)	109.5
B-C(7)-H(7B)	107.2	C(17)-C(16)-H(16C)	109.5
P(1)-C(7)-H(7B)	107.2	H(16A)-C(16)-H(16C)	109.5
H(7A)-C(7)-H(7B)	106.8	H(16B)-C(16)-H(16C)	109.5
B-C(8)-P(2)	119.92(15)	C(18)-C(17)-C(16)	110.32(19)
B-C(8)-H(8A)	107.3	C(18)-C(17)-P(2)	114.62(16)
P(2)-C(8)-H(8A)	107.3	C(16)-C(17)-P(2)	110.42(16)
B-C(8)-H(8B)	107.3	C(18)-C(17)-H(17)	107.0
P(2)-C(8)-H(8B)	107.3	C(16)-C(17)-H(17)	107.0
H(8A)-C(8)-H(8B)	106.9	P(2)-C(17)-H(17)	107.0
B-C(9)-P(3)	119.02(16)	C(17)-C(18)-H(18A)	109.5
B-C(9)-H(9A)	107.6	C(17)-C(18)-H(18B)	109.5
P(3)-C(9)-H(9A)	107.6	H(18A)-C(18)-H(18B)	109.5
B-C(9)-H(9B)	107.6	C(17)-C(18)-H(18C)	109.5
P(3)-C(9)-H(9B)	107.6	H(18A)-C(18)-H(18C)	109.5
H(9A)-C(9)-H(9B)	107.0	H(18B)-C(18)-H(18C)	109.5
C(11)-C(10)-H(10A)	109.5	C(20)-C(19)-H(19A)	109.5
C(11)-C(10)-H(10B)	109.5	C(20)-C(19)-H(19B)	109.5
H(10A)-C(10)-H(10B)	109.5	H(19A)-C(19)-H(19B)	109.5
C(11)-C(10)-H(10C)	109.5	C(20)-C(19)-H(19C)	109.5
H(10A)-C(10)-H(10C)	109.5	H(19A)-C(19)-H(19C)	109.5
H(10B)-C(10)-H(10C)	109.5	H(19B)-C(19)-H(19C)	109.5
C(12)-C(11)-C(10)	111.4(2)	C(21)-C(20)-C(19)	111.71(19)
C(12)-C(11)-P(1)	116.85(19)	C(21)-C(20)-P(2)	117.98(16)
C(10)-C(11)-P(1)	113.03(18)	C(19)-C(20)-P(2)	110.70(15)
C(12)-C(11)-H(11)	104.7	C(21)-C(20)-H(20)	105.1
C(10)-C(11)-H(11)	104.7	C(19)-C(20)-H(20)	105.1
P(1)-C(11)-H(11)	104.7	P(2)-C(20)-H(20)	105.1
C(11)-C(12)-H(12A)	109.5	C(20)-C(21)-H(21A)	109.5
C(11)-C(12)-H(12B)	109.5	C(20)-C(21)-H(21B)	109.5
H(12A)-C(12)-H(12B)	109.5	H(21A)-C(21)-H(21B)	109.5

C(20)-C(21)-H(21C)	109.5	C(32)-C(33)-C(34)	118.8(2)
H(21A)-C(21)-H(21C)	109.5	C(32)-C(33)-H(33)	120.6
H(21B)-C(21)-H(21C)	109.5	C(34)-C(33)-H(33)	120.6
C(23)-C(22)-H(22A)	109.5	C(33)-C(34)-C(35)	133.4(2)
C(23)-C(22)-H(22B)	109.5	C(33)-C(34)-C(29)	120.3(2)
H(22A)-C(22)-H(22B)	109.5	C(35)-C(34)-C(29)	106.17(19)
C(23)-C(22)-H(22C)	109.5	N-C(35)-C(34)	108.93(19)
H(22A)-C(22)-H(22C)	109.5	N-C(35)-C(36)	123.10(19)
H(22B)-C(22)-H(22C)	109.5	C(34)-C(35)-C(36)	127.22(19)
C(22)-C(23)-C(24)	112.45(19)	C(37)-C(36)-C(41)	117.01(19)
C(22)-C(23)-P(3)	110.65(16)	C(37)-C(36)-C(35)	122.12(19)
C(24)-C(23)-P(3)	114.53(15)	C(41)-C(36)-C(35)	120.70(19)
C(22)-C(23)-H(23)	106.2	C(38)-C(37)-C(36)	121.6(2)
C(24)-C(23)-H(23)	106.2	C(38)-C(37)-H(37)	119.2
P(3)-C(23)-H(23)	106.2	C(36)-C(37)-H(37)	119.2
C(23)-C(24)-H(24A)	109.5	C(39)-C(38)-C(37)	120.1(2)
C(23)-C(24)-H(24B)	109.5	C(39)-C(38)-H(38)	120.0
H(24A)-C(24)-H(24B)	109.5	C(37)-C(38)-H(38)	120.0
C(23)-C(24)-H(24C)	109.5	C(38)-C(39)-C(40)	119.3(2)
H(24A)-C(24)-H(24C)	109.5	C(38)-C(39)-H(39)	120.4
H(24B)-C(24)-H(24C)	109.5	C(40)-C(39)-H(39)	120.4
C(26)-C(25)-H(25A)	109.5	C(41)-C(40)-C(39)	120.3(2)
C(26)-C(25)-H(25B)	109.5	C(41)-C(40)-H(40)	119.8
H(25A)-C(25)-H(25B)	109.5	C(39)-C(40)-H(40)	119.8
C(26)-C(25)-H(25C)	109.5	C(40)-C(41)-C(36)	121.7(2)
H(25A)-C(25)-H(25C)	109.5	C(40)-C(41)-H(41)	119.2
H(25B)-C(25)-H(25C)	109.5	C(36)-C(41)-H(41)	119.2
C(25)-C(26)-C(27)	110.04(19)	C(1)-C(102)-C(103)	126.3(7)
C(25)-C(26)-P(3)	111.81(15)	C(1)-C(102)-H(102)	116.9
C(27)-C(26)-P(3)	113.93(16)	C(103)-C(102)-H(102)	116.9
C(25)-C(26)-H(26)	106.9	C(102)-C(103)-C(104)	118.7(10)
C(27)-C(26)-H(26)	106.9	C(102)-C(103)-H(103)	120.6
P(3)-C(26)-H(26)	106.9	C(104)-C(103)-H(103)	120.6
C(26)-C(27)-H(27A)	109.5	C(105)-C(104)-C(103)	119.3(14)
C(26)-C(27)-H(27B)	109.5	C(105)-C(104)-H(104)	120.3
H(27A)-C(27)-H(27B)	109.5	C(103)-C(104)-H(104)	120.3
C(26)-C(27)-H(27C)	109.5	C(104)-C(105)-C(106)	120.1(11)
H(27A)-C(27)-H(27C)	109.5	C(104)-C(105)-H(105)	120.0
H(27B)-C(27)-H(27C)	109.5	C(106)-C(105)-H(105)	120.0
N-C(28)-C(29)	110.85(19)	C(105)-C(106)-C(1)	121.4(9)
N-C(28)-H(28)	124.6	C(105)-C(106)-H(106)	119.3
C(29)-C(28)-H(28)	124.6	C(1)-C(106)-H(106)	119.3
C(28)-C(29)-C(30)	134.7(2)	C(113)-C(112)-C(1)	120.0(7)
C(28)-C(29)-C(34)	106.26(19)	C(113)-C(112)-H(112)	120.0
C(30)-C(29)-C(34)	119.0(2)	C(1)-C(112)-H(112)	120.0
C(31)-C(30)-C(29)	118.8(2)	C(114)-C(113)-C(112)	121.4(8)
C(31)-C(30)-H(30)	120.6	C(114)-C(113)-H(113)	119.3
C(29)-C(30)-H(30)	120.6	C(112)-C(113)-H(113)	119.3
C(30)-C(31)-C(32)	121.9(2)	C(113)-C(114)-C(115)	123.0(9)
C(30)-C(31)-H(31)	119.0	C(113)-C(114)-H(114)	118.5
C(32)-C(31)-H(31)	119.0	C(115)-C(114)-H(114)	118.5
C(33)-C(32)-C(31)	121.2(2)	C(114)-C(115)-C(116)	115.1(11)
C(33)-C(32)-H(32)	119.4	C(114)-C(115)-H(115)	122.5
C(31)-C(32)-H(32)	119.4	C(116)-C(115)-H(115)	122.5

C(1)-C(116)-C(115)	127.4(10)	H(43A)-C(43)-H(44A)	102.7
C(1)-C(116)-H(116)	116.3	H(43B)-C(43)-H(44A)	138.0
C(115)-C(116)-H(116)	116.3	H(43C)-C(43)-H(44A)	83.5
C(42)-O(1)-C(42)#1	83.9(13)	O(2)#1-O(2)-C(44)	68.3(7)
C(42)-O(1)-H(44B)	65.0	O(2)#1-O(2)-C(44)#1	63.2(7)
C(42)#1-O(1)-H(44B)	115.3	C(44)-O(2)-C(44)#1	125.5(6)
C(43)-C(42)-O(1)	121.6(12)	O(2)-C(44)-C(45)	133.8(6)
C(43)-C(42)-H(42A)	106.9	O(2)-C(44)-O(2)#1	48.5(5)
O(1)-C(42)-H(42A)	106.9	C(45)-C(44)-O(2)#1	170.2(7)
C(43)-C(42)-H(42B)	106.9	O(2)-C(44)-H(44A)	108.3
O(1)-C(42)-H(42B)	106.9	C(45)-C(44)-H(44A)	105.3
H(42A)-C(42)-H(42B)	106.7	O(2)#1-C(44)-H(44A)	80.4
C(43)-C(42)-H(44A)	32.4	O(2)-C(44)-H(44B)	101.7
O(1)-C(42)-H(44A)	103.0	C(45)-C(44)-H(44B)	100.9
H(42A)-C(42)-H(44A)	90.1	O(2)#1-C(44)-H(44B)	69.8
H(42B)-C(42)-H(44A)	139.2	H(44A)-C(44)-H(44B)	102.4
C(43)-C(42)-H(44B)	81.1	C(44)-C(45)-H(45A)	109.5
O(1)-C(42)-H(44B)	40.7	C(44)-C(45)-H(45B)	109.5
H(42A)-C(42)-H(44B)	127.8	H(45A)-C(45)-H(45B)	109.5
H(42B)-C(42)-H(44B)	120.2	C(44)-C(45)-H(45C)	109.5
H(44A)-C(42)-H(44B)	69.4	H(45A)-C(45)-H(45C)	109.5
C(42)-C(43)-H(44A)	31.9	H(45B)-C(45)-H(45C)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 -x+3/2,-y+1/2,z

Table 32. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for [PhBP$^{iPr}_3$]Mn(1-Ph(isoindolate)) (8). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn	223(2)	211(2)	194(2)	-1(1)	-1(2)	20(1)
P(1)	326(4)	246(3)	317(4)	-28(3)	-11(3)	-41(3)
P(2)	234(3)	221(3)	206(3)	-1(2)	26(2)	16(3)
P(3)	225(3)	237(3)	192(3)	16(2)	28(2)	23(2)
B	328(16)	242(14)	253(15)	-8(11)	40(12)	6(12)
N	225(10)	229(9)	203(10)	-3(8)	20(8)	21(7)
C(1)	670(20)	321(15)	281(14)	88(12)	187(13)	228(13)
C(7)	505(16)	183(11)	329(14)	-2(11)	36(13)	-38(10)
C(8)	300(13)	265(12)	224(12)	-9(10)	0(10)	59(10)
C(9)	289(13)	235(12)	251(13)	68(10)	22(10)	16(10)
C(10)	367(16)	609(17)	429(17)	-154(13)	31(13)	-66(13)
C(11)	364(15)	428(15)	425(16)	7(12)	40(14)	-25(12)
C(12)	480(20)	551(19)	1270(30)	120(20)	200(20)	-174(15)
C(13)	468(17)	445(15)	301(15)	-45(11)	2(12)	-40(13)
C(14)	425(16)	265(13)	310(14)	-32(10)	-22(11)	-51(11)
C(15)	950(20)	402(16)	417(17)	-107(14)	-118(18)	-134(15)
C(16)	516(17)	341(14)	190(13)	-18(11)	43(12)	-20(12)
C(17)	291(13)	252(12)	225(13)	34(10)	59(10)	47(10)
C(18)	412(16)	479(15)	348(16)	78(12)	172(12)	118(12)
C(19)	435(16)	375(14)	360(15)	-9(12)	-34(13)	-136(12)
C(20)	238(12)	332(13)	255(13)	-16(10)	-15(10)	-1(10)
C(21)	264(14)	705(19)	379(17)	-31(13)	-24(12)	80(13)
C(22)	354(14)	327(13)	291(14)	-106(11)	-18(11)	-22(11)
C(23)	263(13)	310(13)	198(12)	-38(10)	32(10)	8(10)
C(24)	336(14)	364(14)	246(13)	-19(10)	-39(11)	4(11)
C(25)	295(14)	421(15)	396(16)	89(12)	117(12)	52(12)
C(26)	242(13)	322(13)	239(13)	57(10)	26(10)	-4(10)
C(27)	368(15)	431(15)	298(15)	139(12)	98(12)	-7(12)
C(28)	320(14)	219(12)	221(12)	16(9)	50(10)	-3(10)
C(29)	228(12)	168(11)	266(14)	-25(9)	55(10)	-18(9)
C(30)	285(14)	242(13)	369(14)	-21(10)	111(12)	-53(11)
C(31)	187(12)	299(13)	525(17)	-13(12)	84(13)	-20(10)
C(32)	217(13)	233(13)	454(16)	15(11)	-10(11)	5(10)
C(33)	229(13)	292(13)	316(14)	31(10)	23(11)	-31(10)
C(34)	208(12)	173(11)	305(14)	-3(9)	3(10)	-11(9)
C(35)	215(12)	188(12)	230(12)	3(9)	15(9)	46(9)
C(36)	227(12)	191(11)	212(12)	10(9)	11(9)	31(9)
C(37)	224(12)	316(13)	270(14)	-15(10)	5(10)	12(10)
C(38)	370(16)	368(14)	229(13)	30(11)	10(11)	68(12)
C(39)	274(14)	360(14)	309(15)	66(11)	70(11)	75(11)
C(40)	233(13)	304(13)	345(14)	33(10)	57(11)	21(10)
C(41)	255(13)	225(11)	204(12)	-7(9)	-18(9)	49(10)

Table 33. Crystal Data and Structure Analysis Details for $[PhBP^{iPr}_3]TlMnBr(CO)_4$ (9).

Empirical formula	$C_{31}H_{53}BBrMnO_4P_3Tl$
Formula weight	932.67
Crystallization solvent	benzene/petroleum ether
Crystal shape	thick plate
Crystal color	yellow
Crystal size	0.17 x 0.30 x 0.33 mm

Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data collection temperature	100 K	
Theta range for 48690 reflections used in lattice determination	2.42 to 34.7°	
Unit cell dimensions	a = 10.2574(5) Å b = 18.6613(8) Å c = 19.9243(9) Å	α= 90° β= 100.590(1)° γ = 90°
Volume	3748.9(3) $Å^3$	
Z	4	
Crystal system	monoclinic	
Space group	P 21/n (# 14)	
Density (calculated)	1.652 g/cm^3	
F(000)	1848	
Theta range for data collection	1.5 to 34.7°	
Completeness to theta = 34.66°	94.8%	
Index ranges	$-16 \le h \le 16, -29 \le k \le 29, -29 \le l \le 31$	
Data collection scan type	ω scans	
Reflections collected	86733	
Independent reflections	15253 [R_{int}= 0.0519]	
Reflections > 2σ(I)	11838	
Average σ(I)/(net I)	0.0460	
Absorption coefficient	5.86 mm^{-1}	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.370 and 0.161	
Reflections monitored for decay	initial data recollected	

Decay of standards	0%

Structure Solution and Refinement

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15253 / 0 / 392
Treatment of hydrogen atoms	not refined, U_{iso} fixed at 120% U_{eq} of attached atom
Goodness-of-fit on F^2	1.55
Final R indices [I>2σ(I), 11838 reflections]	R1 = 0.0355, wR2 = 0.0532
R indices (all data)	R1 = 0.0570, wR2 = 0.0555
Type of weighting scheme used	sigma
Weighting scheme used	calc $w=1/[\sigma^2(Fo^2)]$ where $P=(Fo^2+2Fc^2)/3$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	3.81 and -1.85 e·Å^{-3}

Programs Used

Cell refinement	Bruker SMART 5.606
Data collection	Bruker SMART 5.054
Data reduction	Bruker SAINT 6.45
Structure solution	Bruker SHELXTL 6.14
Structure refinement	Bruker SHELXTL 6.14

Special Refinement Details

An absorption correction was applied using SADABS.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 34. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for [PhBP$^{iPr}_3$]TlMnBr(CO)$_4$ (9). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Mn	1707.4(3)	-951.4(2)	1144.9(2)	14.9(1)
P(1)	5960.8(6)	-798.2(3)	2509.3(3)	13.2(1)
P(2)	4804.9(6)	1013.3(3)	1847.1(3)	13.3(1)
P(3)	3566.4(6)	217.9(3)	3266.9(3)	15.2(1)
B	6431(3)	623.6(13)	3214.4(13)	13.4(5)
Br	1750.7(2)	-1825.9(1)	2118.9(1)	21.9(1)
Tl	3561.7(1)	-239.5(1)	1980.2(1)	13.5(1)
O(1)	3870.6(19)	-1852.6(9)	771.3(10)	28.7(4)
O(2)	1703.1(19)	17.9(10)	-21.8(10)	29.3(4)
O(3)	-222.2(18)	-5.5(10)	1687.0(11)	29.7(4)
O(4)	-403(2)	-1867.5(10)	368.9(11)	37.8(5)
C(1)	7613(2)	980.7(11)	3781.9(12)	13.8(4)
C(2)	8692(2)	600.6(12)	4141.8(13)	19.9(5)
C(3)	9658(2)	903.4(13)	4639.4(13)	22.2(5)
C(4)	9580(3)	1619.1(13)	4802.8(13)	21.0(5)
C(5)	8513(3)	2011.7(13)	4475.8(14)	29.3(6)
C(6)	7559(3)	1700.9(12)	3980.7(13)	24.6(6)
C(7)	7055(2)	-56.2(11)	2821.6(12)	14.0(4)
C(8)	5857(2)	1264.9(11)	2653.6(11)	13.5(4)
C(9)	5292(2)	362.1(11)	3671.3(12)	14.8(5)
C(10)	5354(3)	-2137.8(12)	3008.8(14)	25.1(6)
C(11)	5858(2)	-1391.1(11)	3248.2(13)	17.8(5)
C(12)	7106(3)	-1426.9(13)	3811.9(13)	23.2(5)
C(13)	6754(3)	-954.8(13)	1244.2(13)	21.2(5)
C(14)	6730(2)	-1350.8(12)	1914.8(12)	17.4(5)
C(15)	8120(2)	-1620.6(13)	2221.1(14)	23.8(6)
C(16)	5096(3)	839.6(14)	485.8(13)	23.5(5)
C(17)	5898(2)	924.4(12)	1206.7(12)	17.8(5)
C(18)	7005(3)	1477.0(15)	1224.8(15)	30.3(6)
C(19)	2375(3)	1523.7(13)	1082.2(14)	23.2(5)
C(20)	3597(2)	1745.2(11)	1605.7(12)	16.6(5)
C(21)	4192(3)	2439.8(12)	1383.9(13)	23.2(5)
C(22)	1438(3)	1202.0(14)	2871.5(15)	28.2(6)
C(23)	2807(2)	1116.5(12)	3315.6(13)	19.4(5)
C(24)	2803(3)	1374.9(16)	4040.7(16)	39.0(7)
C(28)	3098(2)	-1526.3(12)	906.9(12)	14.8(5)
C(29)	1716(2)	-349.9(12)	440.4(14)	20.7(5)
C(30)	525(2)	-368.5(13)	1487.6(13)	21.0(5)
C(31)	405(3)	-1510.1(13)	662.9(14)	24.3(6)
C(25)	1307(2)	-482.5(13)	3542.1(14)	22.4(5)
C(26)	2773(3)	-431.7(18)	3770.0(17)	43.5(9)
C(27)	3333(4)	-554(3)	4464(2)	81.6(16)

Table 35. Bond lengths [Å] and angles [°] for [PhBP$^{iPr}_3$]TlMnBr(CO)$_4$ (9).

Mn-C(29)	1.799(3)	C(12)-H(12C)	0.9800
Mn-C(31)	1.823(3)	C(13)-C(14)	1.531(3)
Mn-C(30)	1.851(3)	C(13)-H(13A)	0.9800
Mn-C(28)	1.913(3)	C(13)-H(13B)	0.9800
Mn-Br	2.5299(4)	C(13)-H(13C)	0.9800
Mn-Tl	2.6437(4)	C(14)-C(15)	1.530(3)
P(1)-C(7)	1.819(2)	C(14)-H(14)	1.0000
P(1)-C(14)	1.853(2)	C(15)-H(15A)	0.9800
P(1)-C(11)	1.860(2)	C(15)-H(15B)	0.9800
P(1)-Tl	2.7020(6)	C(15)-H(15C)	0.9800
P(2)-C(8)	1.825(2)	C(16)-C(17)	1.527(3)
P(2)-C(20)	1.847(2)	C(16)-H(16A)	0.9800
P(2)-C(17)	1.854(2)	C(16)-H(16B)	0.9800
P(2)-Tl	2.6993(6)	C(16)-H(16C)	0.9800
P(3)-C(9)	1.825(2)	C(17)-C(18)	1.530(3)
P(3)-C(26)	1.854(3)	C(17)-H(17)	1.0000
P(3)-C(23)	1.859(2)	C(18)-H(18A)	0.9800
P(3)-Tl	2.7011(6)	C(18)-H(18B)	0.9800
B-C(1)	1.640(3)	C(18)-H(18C)	0.9800
B-C(8)	1.669(3)	C(19)-C(20)	1.533(3)
B-C(7)	1.678(3)	C(19)-H(19A)	0.9800
B-C(9)	1.680(3)	C(19)-H(19B)	0.9800
O(1)-C(28)	1.073(3)	C(19)-H(19C)	0.9800
O(2)-C(29)	1.146(3)	C(20)-C(21)	1.532(3)
O(3)-C(30)	1.147(3)	C(20)-H(20)	1.0000
O(4)-C(31)	1.139(3)	C(21)-H(21A)	0.9800
C(1)-C(2)	1.396(3)	C(21)-H(21B)	0.9800
C(1)-C(6)	1.405(3)	C(21)-H(21C)	0.9800
C(2)-C(3)	1.387(3)	C(22)-C(23)	1.525(4)
C(2)-H(2)	0.9500	C(22)-H(22A)	0.9800
C(3)-C(4)	1.380(3)	C(22)-H(22B)	0.9800
C(3)-H(3)	0.9500	C(22)-H(22C)	0.9800
C(4)-C(5)	1.377(4)	C(23)-C(24)	1.524(4)
C(4)-H(4)	0.9500	C(23)-H(23)	1.0000
C(5)-C(6)	1.383(4)	C(24)-H(24A)	0.9800
C(5)-H(5)	0.9500	C(24)-H(24B)	0.9800
C(6)-H(6)	0.9500	C(24)-H(24C)	0.9800
C(7)-H(7A)	0.9900	C(25)-C(26)	1.492(4)
C(7)-H(7B)	0.9900	C(25)-H(25A)	0.9800
C(8)-H(8A)	0.9900	C(25)-H(25B)	0.9800
C(8)-H(8B)	0.9900	C(25)-H(25C)	0.9800
C(9)-H(9A)	0.9900	C(26)-C(27)	1.416(5)
C(9)-H(9B)	0.9900	C(26)-H(26)	1.0000
C(10)-C(11)	1.531(3)	C(27)-H(27A)	0.9800
C(10)-H(10A)	0.9800	C(27)-H(27B)	0.9800
C(10)-H(10B)	0.9800	C(27)-H(27C)	0.9800
C(10)-H(10C)	0.9800		
C(11)-C(12)	1.542(3)	C(29)-Mn-C(31)	93.11(11)
C(11)-H(11)	1.0000	C(29)-Mn-C(30)	91.08(11)
C(12)-H(12A)	0.9800	C(31)-Mn-C(30)	93.68(11)
C(12)-H(12B)	0.9800	C(29)-Mn-C(28)	92.61(10)

C(31)-Mn-C(28)	93.22(11)	C(4)-C(5)-H(5)	119.6
C(30)-Mn-C(28)	171.99(10)	C(6)-C(5)-H(5)	119.6
C(29)-Mn-Br	177.98(8)	C(5)-C(6)-C(1)	122.9(2)
C(31)-Mn-Br	86.73(8)	C(5)-C(6)-H(6)	118.6
C(30)-Mn-Br	90.94(8)	C(1)-C(6)-H(6)	118.6
C(28)-Mn-Br	85.39(7)	B-C(7)-P(1)	118.08(15)
C(29)-Mn-Tl	94.09(8)	B-C(7)-H(7A)	107.8
C(31)-Mn-Tl	172.74(8)	P(1)-C(7)-H(7A)	107.8
C(30)-Mn-Tl	85.23(8)	B-C(7)-H(7B)	107.8
C(28)-Mn-Tl	87.41(7)	P(1)-C(7)-H(7B)	107.8
Br-Mn-Tl	86.11(1)	H(7A)-C(7)-H(7B)	107.1
C(7)-P(1)-C(14)	109.52(11)	B-C(8)-P(2)	118.93(15)
C(7)-P(1)-C(11)	107.66(11)	B-C(8)-H(8A)	107.6
C(14)-P(1)-C(11)	105.54(11)	P(2)-C(8)-H(8A)	107.6
C(7)-P(1)-Tl	107.47(7)	B-C(8)-H(8B)	107.6
C(14)-P(1)-Tl	115.44(8)	P(2)-C(8)-H(8B)	107.6
C(11)-P(1)-Tl	110.98(8)	H(8A)-C(8)-H(8B)	107.0
C(8)-P(2)-C(20)	107.39(10)	B-C(9)-P(3)	121.21(16)
C(8)-P(2)-C(17)	107.13(11)	B-C(9)-H(9A)	107.0
C(20)-P(2)-C(17)	110.39(11)	P(3)-C(9)-H(9A)	107.0
C(8)-P(2)-Tl	110.48(7)	B-C(9)-H(9B)	107.0
C(20)-P(2)-Tl	111.07(8)	P(3)-C(9)-H(9B)	107.0
C(17)-P(2)-Tl	110.26(7)	H(9A)-C(9)-H(9B)	106.8
C(9)-P(3)-C(26)	110.12(12)	C(11)-C(10)-H(10A)	109.5
C(9)-P(3)-C(23)	103.03(11)	C(11)-C(10)-H(10B)	109.5
C(26)-P(3)-C(23)	109.40(14)	H(10A)-C(10)-H(10B)	109.5
C(9)-P(3)-Tl	107.34(8)	C(11)-C(10)-H(10C)	109.5
C(26)-P(3)-Tl	112.47(12)	H(10A)-C(10)-H(10C)	109.5
C(23)-P(3)-Tl	114.01(8)	H(10B)-C(10)-H(10C)	109.5
C(1)-B-C(8)	107.18(17)	C(10)-C(11)-C(12)	112.00(19)
C(1)-B-C(7)	109.36(18)	C(10)-C(11)-P(1)	111.08(18)
C(8)-B-C(7)	110.34(18)	C(12)-C(11)-P(1)	116.21(16)
C(1)-B-C(9)	104.14(18)	C(10)-C(11)-H(11)	105.5
C(8)-B-C(9)	112.10(18)	C(12)-C(11)-H(11)	105.5
C(7)-B-C(9)	113.33(17)	P(1)-C(11)-H(11)	105.5
Mn-Tl-P(2)	132.191(15)	C(11)-C(12)-H(12A)	109.5
Mn-Tl-P(3)	129.188(15)	C(11)-C(12)-H(12B)	109.5
P(2)-Tl-P(3)	84.322(18)	H(12A)-C(12)-H(12B)	109.5
Mn-Tl-P(1)	123.368(14)	C(11)-C(12)-H(12C)	109.5
P(2)-Tl-P(1)	87.692(18)	H(12A)-C(12)-H(12C)	109.5
P(3)-Tl-P(1)	84.777(18)	H(12B)-C(12)-H(12C)	109.5
C(2)-C(1)-C(6)	114.2(2)	C(14)-C(13)-H(13A)	109.5
C(2)-C(1)-B	124.29(19)	C(14)-C(13)-H(13B)	109.5
C(6)-C(1)-B	121.3(2)	H(13A)-C(13)-H(13B)	109.5
C(3)-C(2)-C(1)	123.7(2)	C(14)-C(13)-H(13C)	109.5
C(3)-C(2)-H(2)	118.2	H(13A)-C(13)-H(13C)	109.5
C(1)-C(2)-H(2)	118.2	H(13B)-C(13)-H(13C)	109.5
C(4)-C(3)-C(2)	119.9(2)	C(15)-C(14)-C(13)	110.1(2)
C(4)-C(3)-H(3)	120.1	C(15)-C(14)-P(1)	113.79(17)
C(2)-C(3)-H(3)	120.1	C(13)-C(14)-P(1)	111.49(15)
C(5)-C(4)-C(3)	118.6(2)	C(15)-C(14)-H(14)	107.0
C(5)-C(4)-H(4)	120.7	C(13)-C(14)-H(14)	107.0
C(3)-C(4)-H(4)	120.7	P(1)-C(14)-H(14)	107.0
C(4)-C(5)-C(6)	120.7(2)	C(14)-C(15)-H(15A)	109.5

C(14)-C(15)-H(15B)	109.5	C(23)-C(22)-H(22A)	109.5
H(15A)-C(15)-H(15B)	109.5	C(23)-C(22)-H(22B)	109.5
C(14)-C(15)-H(15C)	109.5	H(22A)-C(22)-H(22B)	109.5
H(15A)-C(15)-H(15C)	109.5	C(23)-C(22)-H(22C)	109.5
H(15B)-C(15)-H(15C)	109.5	H(22A)-C(22)-H(22C)	109.5
C(17)-C(16)-H(16A)	109.5	H(22B)-C(22)-H(22C)	109.5
C(17)-C(16)-H(16B)	109.5	C(24)-C(23)-C(22)	110.7(2)
H(16A)-C(16)-H(16B)	109.5	C(24)-C(23)-P(3)	114.16(18)
C(17)-C(16)-H(16C)	109.5	C(22)-C(23)-P(3)	114.46(17)
H(16A)-C(16)-H(16C)	109.5	C(24)-C(23)-H(23)	105.5
H(16B)-C(16)-H(16C)	109.5	C(22)-C(23)-H(23)	105.5
C(16)-C(17)-C(18)	111.2(2)	P(3)-C(23)-H(23)	105.5
C(16)-C(17)-P(2)	111.55(17)	C(23)-C(24)-H(24A)	109.5
C(18)-C(17)-P(2)	117.62(17)	C(23)-C(24)-H(24B)	109.5
C(16)-C(17)-H(17)	105.1	H(24A)-C(24)-H(24B)	109.5
C(18)-C(17)-H(17)	105.1	C(23)-C(24)-H(24C)	109.5
P(2)-C(17)-H(17)	105.1	H(24A)-C(24)-H(24C)	109.5
C(17)-C(18)-H(18A)	109.5	H(24B)-C(24)-H(24C)	109.5
C(17)-C(18)-H(18B)	109.5	O(1)-C(28)-Mn	179.4(2)
H(18A)-C(18)-H(18B)	109.5	O(2)-C(29)-Mn	177.9(2)
C(17)-C(18)-H(18C)	109.5	O(3)-C(30)-Mn	178.6(2)
H(18A)-C(18)-H(18C)	109.5	O(4)-C(31)-Mn	178.9(2)
H(18B)-C(18)-H(18C)	109.5	C(26)-C(25)-H(25A)	109.5
C(20)-C(19)-H(19A)	109.5	C(26)-C(25)-H(25B)	109.5
C(20)-C(19)-H(19B)	109.5	H(25A)-C(25)-H(25B)	109.5
H(19A)-C(19)-H(19B)	109.5	C(26)-C(25)-H(25C)	109.5
C(20)-C(19)-H(19C)	109.5	H(25A)-C(25)-H(25C)	109.5
H(19A)-C(19)-H(19C)	109.5	H(25B)-C(25)-H(25C)	109.5
H(19B)-C(19)-H(19C)	109.5	C(27)-C(26)-C(25)	119.5(3)
C(21)-C(20)-C(19)	110.6(2)	C(27)-C(26)-P(3)	119.7(2)
C(21)-C(20)-P(2)	114.62(17)	C(25)-C(26)-P(3)	113.26(19)
C(19)-C(20)-P(2)	113.79(16)	C(27)-C(26)-H(26)	99.2
C(21)-C(20)-H(20)	105.7	C(25)-C(26)-H(26)	99.2
C(19)-C(20)-H(20)	105.7	P(3)-C(26)-H(26)	99.2
P(2)-C(20)-H(20)	105.7	C(26)-C(27)-H(27A)	109.5
C(20)-C(21)-H(21A)	109.5	C(26)-C(27)-H(27B)	109.5
C(20)-C(21)-H(21B)	109.5	H(27A)-C(27)-H(27B)	109.5
H(21A)-C(21)-H(21B)	109.5	C(26)-C(27)-H(27C)	109.5
C(20)-C(21)-H(21C)	109.5	H(27A)-C(27)-H(27C)	109.5
H(21A)-C(21)-H(21C)	109.5	H(27B)-C(27)-H(27C)	109.5
H(21B)-C(21)-H(21C)	109.5		

Symmetry transformations used to generate equivalent atoms:

Table 36. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for $[PhBP^{iPr}_3]TlMnBr(CO)_4$ (9). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn	132(2)	145(2)	154(2)	14(1)	-17(1)	-25(1)
P(1)	126(3)	106(3)	152(3)	-15(2)	-5(2)	8(2)
P(2)	150(3)	111(3)	124(3)	9(2)	-12(2)	-22(2)
P(3)	142(3)	132(3)	180(3)	31(2)	27(2)	4(2)
B	151(12)	109(11)	135(13)	-9(9)	8(10)	-7(9)
Br	204(1)	228(1)	228(1)	67(1)	44(1)	0(1)
Tl	118(1)	113(1)	160(1)	-4(1)	-12(1)	-11(1)
O(1)	307(11)	244(9)	321(11)	-33(8)	80(9)	-46(8)
O(2)	302(11)	316(10)	244(11)	68(8)	2(9)	-40(8)
O(3)	183(9)	308(10)	399(12)	-49(9)	47(9)	8(8)
O(4)	337(12)	348(11)	373(13)	-6(9)	-138(10)	-150(9)
C(1)	168(11)	137(10)	115(11)	0(8)	37(9)	-19(8)
C(2)	194(12)	159(11)	231(14)	-51(9)	3(10)	19(9)
C(3)	165(12)	264(13)	212(14)	-60(10)	-29(10)	31(10)
C(4)	232(13)	232(12)	145(13)	-40(9)	-18(10)	-70(10)
C(5)	431(17)	128(11)	260(15)	-38(10)	-100(13)	-4(11)
C(6)	332(15)	142(11)	206(14)	-12(9)	-107(11)	55(10)
C(7)	135(11)	124(10)	148(12)	-8(8)	-11(9)	-12(8)
C(8)	157(11)	128(10)	111(11)	1(8)	2(9)	-16(8)
C(9)	162(11)	126(11)	152(12)	2(8)	18(9)	13(8)
C(10)	242(13)	150(11)	340(16)	27(10)	-1(12)	-24(10)
C(11)	187(12)	128(10)	213(13)	30(9)	21(10)	-3(9)
C(12)	266(14)	190(12)	214(14)	53(10)	-21(11)	10(10)
C(13)	218(13)	211(12)	207(14)	-51(10)	40(11)	17(10)
C(14)	168(12)	153(11)	193(13)	-51(9)	8(10)	11(9)
C(15)	179(12)	241(12)	282(15)	-64(10)	11(11)	63(10)
C(16)	273(14)	271(13)	154(13)	-45(10)	21(11)	-14(11)
C(17)	194(12)	161(11)	172(13)	-26(9)	16(10)	-25(9)
C(18)	290(15)	365(15)	280(16)	-90(12)	120(12)	-143(12)
C(19)	231(13)	199(12)	232(14)	7(10)	-47(11)	44(10)
C(20)	203(12)	142(10)	142(12)	15(8)	2(10)	6(9)
C(21)	359(15)	141(11)	191(13)	33(9)	36(11)	4(10)
C(22)	209(13)	212(12)	416(18)	90(11)	36(12)	59(10)
C(23)	220(13)	174(11)	195(13)	20(9)	54(10)	44(9)
C(24)	457(19)	417(17)	305(17)	-77(13)	96(14)	201(14)
C(28)	142(11)	177(11)	106(11)	34(8)	-28(9)	-107(9)
C(29)	173(12)	197(12)	235(14)	-22(10)	-5(10)	-31(9)
C(30)	165(12)	218(12)	224(14)	20(9)	-22(10)	-52(9)
C(31)	231(13)	238(13)	239(14)	46(10)	-14(11)	-6(10)
C(25)	211(13)	239(12)	245(14)	11(10)	99(11)	-25(10)
C(26)	260(15)	518(19)	480(20)	357(16)	-61(14)	-133(13)
C(27)	350(20)	1590(40)	460(20)	660(30)	-41(18)	-280(20)

Table 37. Crystal Data and Structure Analysis Details for $[PhBP^{iPr}_3]Mn(CN^tBu)_3$ (10).

Empirical formula	$C_{42}H_{80}BMnN_3P_3$
Formula weight	785.75
Crystallization solvent	petroleum ether
Crystal shape	rough block
Crystal color	pale yellow
Crystal size	0.18 x 0.28 x 0.33 mm

Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data collection temperature	100 K	
Theta range for 36474 reflections used in lattice determination	2.32 to 35.87°	
Unit cell dimensions	a = 11.2996(7) Å b = 17.578(1) Å c = 23.108(1) Å	α= 90° β= 93.660(2)° γ = 90°
Volume	4580.4(5) $Å^3$	
Z	4	
Crystal system	monoclinic	
Space group	P 21/n (# 14)	
Density (calculated)	1.139 g/cm^3	
F(000)	1712	
Theta range for data collection	2.0 to 36.1°	
Completeness to theta = 36.13°	89.9%	
Index ranges	$-16 \le h \le 18, -28 \le k \le 28, -37 \le l \le 38$	
Data collection scan type	ω scans	
Reflections collected	80212	
Independent reflections	19689 [R_{int}= 0.0796]	
Reflections > 2σ(I)	13052	
Average σ(I)/(net I)	0.0760	
Absorption coefficient	0.42 mm^{-1}	
Absorption correction	none	
Reflections monitored for decay	initial data recollected at end	
Decay of standards	0%	

Table 37 (cont.)

Structure Solution and Refinement

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	19689 / 0 / 472
Treatment of hydrogen atoms	not refined, U_{iso} fixed at 120% U_{eq} of attached atom
Goodness-of-fit on F^2	1.28
Final R indices [I>2σ(I), 13052 reflections]	R1 = 0.0437, wR2 = 0.0707
R indices (all data)	R1 = 0.0784, wR2 = 0.0752
Type of weighting scheme used	sigma
Weighting scheme used	calc $w=1/[\sigma^2(Fo^2)]$ where $P=(Fo^2+2Fc^2)/3$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	1.15 and -0.67 e·Å^{-3}

Programs Used

Cell refinement	Bruker SMART 5.606
Data collection	Bruker SMART 5.054
Data reduction	Bruker SAINT 6.45
Structure solution	Bruker SHELXTL 6.14
Structure refinement	Bruker SHELXTL 6.14

Special Refinement Details

Three bad reflections were omitted (011, 002, -103).

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 38. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for [PhBP$^{iPr}_3$]Mn(CN^{t}Bu)$_3$ (10). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Mn	7128.9(2)	2488.7(1)	847.9(1)	9.6(1)
P(1)	5523.2(3)	2949.8(2)	244.8(1)	10.2(1)
P(2)	8078.4(3)	3688.9(2)	753.3(1)	10.2(1)
P(3)	8082.7(3)	2116.3(2)	11.0(1)	11.1(1)
B	7301.5(12)	3574.4(7)	-499.5(5)	11.6(2)
N(1)	6174.5(11)	2770.3(6)	2028.2(4)	22.5(2)
N(2)	9130.9(10)	1842.8(6)	1639.7(5)	21.3(2)
N(3)	5844.2(10)	994.7(6)	959.6(5)	19.7(2)
C(1)	7396.3(11)	4068.9(6)	-1098.1(5)	12.7(2)
C(2)	6573.7(11)	4635.8(6)	-1275.2(5)	14.4(2)
C(3)	6679.1(12)	5076.2(7)	-1770.6(5)	17.0(2)
C(4)	7629.7(12)	4975.0(7)	-2112.5(5)	18.2(3)
C(5)	8463.7(12)	4425.0(7)	-1954.7(5)	18.9(3)
C(6)	8343.6(11)	3984.8(7)	-1459.8(5)	16.7(2)
C(7)	5955.8(10)	3672.9(6)	-267.0(5)	11.7(2)
C(8)	8297.5(10)	3932.6(6)	-9.8(5)	11.8(2)
C(9)	7570.9(11)	2659.0(6)	-630.4(5)	12.1(2)
C(10)	3735.3(11)	1805.7(7)	54.2(5)	18.5(3)
C(11)	4746.5(11)	2208.8(7)	-236.1(5)	13.4(2)
C(12)	4283.5(11)	2461.1(8)	-846.8(5)	19.5(3)
C(13)	3704.6(11)	3005.6(7)	1082.1(5)	17.2(2)
C(14)	4320.2(11)	3453.8(7)	615.2(5)	13.4(2)
C(15)	3395.1(11)	3852.4(7)	205.2(5)	17.3(2)
C(16)	6735.2(11)	4572.7(7)	1557.0(5)	17.8(3)
C(17)	7355.2(11)	4598.4(6)	985.3(5)	13.6(2)
C(18)	8144.1(12)	5313.8(7)	983.5(5)	18.1(3)
C(19)	9516.9(11)	3811.8(7)	1801.6(5)	16.9(2)
C(20)	9583.5(10)	3686.9(7)	1145.6(5)	13.6(2)
C(21)	10540.0(11)	4187.6(7)	896.6(5)	18.6(3)
C(22)	10423.2(12)	1558.9(8)	329.3(6)	22.1(3)
C(23)	9750.0(11)	2229.6(7)	40.4(5)	14.1(2)
C(24)	10301.5(11)	2420.8(7)	-531.3(5)	18.4(3)
C(25)	8150.0(12)	484.8(7)	233.9(6)	23.0(3)
C(26)	7800.9(12)	1103.6(7)	-217.7(5)	16.7(2)
C(27)	8252.9(13)	883.1(7)	-809.4(6)	24.8(3)
C(28)	6505.0(11)	2719.1(6)	1557.3(5)	13.9(2)
C(29)	5897.3(13)	2801.5(7)	2634.3(5)	20.5(3)
C(30)	6282.8(15)	2059.3(9)	2922.8(6)	34.0(4)
C(31)	4564.0(15)	2899.1(11)	2664.1(7)	43.3(5)
C(32)	6578(2)	3462.3(10)	2919.5(7)	55.0(6)
C(33)	8390.9(11)	2095.8(7)	1313.8(5)	14.1(2)
C(34)	9992.8(12)	1455.6(8)	2032.5(6)	22.4(3)
C(35)	9664.1(16)	1595.5(10)	2650.9(6)	43.1(4)
C(36)	11221.3(13)	1778.1(9)	1945.2(7)	36.9(4)
C(37)	9944.9(15)	609.3(8)	1888.2(7)	35.3(4)
C(38)	6355.2(11)	1576.6(7)	905.7(5)	13.2(2)

C(39)	5300.3(12)	404.4(7)	1292.0(5)	19.1(3)
C(40)	6183.6(16)	152.3(10)	1776.6(7)	44.9(4)
C(41)	4969.6(16)	-250.5(8)	883.7(7)	38.4(4)
C(42)	4181.6(14)	726.8(8)	1535.6(6)	30.7(3)

Table 39. Bond lengths [Å] and angles [°] for [PhBP$^{iPr}_3$]Mn(CN^{t}Bu)$_3$ (10).

Mn-C(38)	1.8352(12)	C(13)-C(14)	1.5377(16)
Mn-C(33)	1.8637(12)	C(13)-H(13A)	0.9800
Mn-C(28)	1.8698(12)	C(13)-H(13B)	0.9800
Mn-P(1)	2.3597(4)	C(13)-H(13C)	0.9800
Mn-P(3)	2.3655(3)	C(14)-C(15)	1.5345(17)
Mn-P(2)	2.3831(4)	C(14)-H(14)	1.0000
P(1)-C(7)	1.8240(11)	C(15)-H(15A)	0.9800
P(1)-C(14)	1.8744(12)	C(15)-H(15B)	0.9800
P(1)-C(11)	1.8914(12)	C(15)-H(15C)	0.9800
P(2)-C(8)	1.8466(11)	C(16)-C(17)	1.5349(16)
P(2)-C(20)	1.8755(12)	C(16)-H(16A)	0.9800
P(2)-C(17)	1.8888(12)	C(16)-H(16B)	0.9800
P(3)-C(9)	1.8253(11)	C(16)-H(16C)	0.9800
P(3)-C(26)	1.8782(12)	C(17)-C(18)	1.5416(16)
P(3)-C(23)	1.8914(12)	C(17)-H(17)	1.0000
B-C(1)	1.6430(17)	C(18)-H(18A)	0.9800
B-C(7)	1.6539(17)	C(18)-H(18B)	0.9800
B-C(8)	1.6676(17)	C(18)-H(18C)	0.9800
B-C(9)	1.6688(17)	C(19)-C(20)	1.5383(16)
N(1)-C(28)	1.1762(15)	C(19)-H(19A)	0.9800
N(1)-C(29)	1.4555(15)	C(19)-H(19B)	0.9800
N(2)-C(33)	1.1763(15)	C(19)-H(19C)	0.9800
N(2)-C(34)	1.4569(16)	C(20)-C(21)	1.5340(16)
N(3)-C(38)	1.1849(15)	C(20)-H(20)	1.0000
N(3)-C(39)	1.4508(15)	C(21)-H(21A)	0.9800
C(1)-C(2)	1.4056(17)	C(21)-H(21B)	0.9800
C(1)-C(6)	1.4071(16)	C(21)-H(21C)	0.9800
C(2)-C(3)	1.3934(16)	C(22)-C(23)	1.5328(17)
C(2)-H(2)	0.9500	C(22)-H(22A)	0.9800
C(3)-C(4)	1.3850(18)	C(22)-H(22B)	0.9800
C(3)-H(3)	0.9500	C(22)-H(22C)	0.9800
C(4)-C(5)	1.3828(18)	C(23)-C(24)	1.5334(16)
C(4)-H(4)	0.9500	C(23)-H(23)	1.0000
C(5)-C(6)	1.3945(16)	C(24)-H(24A)	0.9800
C(5)-H(5)	0.9500	C(24)-H(24B)	0.9800
C(6)-H(6)	0.9500	C(24)-H(24C)	0.9800
C(7)-H(7A)	0.9900	C(25)-C(26)	1.5412(18)
C(7)-H(7B)	0.9900	C(25)-H(25A)	0.9800
C(8)-H(8A)	0.9900	C(25)-H(25B)	0.9800
C(8)-H(8B)	0.9900	C(25)-H(25C)	0.9800
C(9)-H(9A)	0.9900	C(26)-C(27)	1.5395(17)
C(9)-H(9B)	0.9900	C(26)-H(26)	1.0000
C(10)-C(11)	1.5349(16)	C(27)-H(27A)	0.9800
C(10)-H(10A)	0.9800	C(27)-H(27B)	0.9800
C(10)-H(10B)	0.9800	C(27)-H(27C)	0.9800
C(10)-H(10C)	0.9800	C(29)-C(30)	1.5164(19)
C(11)-C(12)	1.5386(16)	C(29)-C(32)	1.520(2)
C(11)-H(11)	1.0000	C(29)-C(31)	1.522(2)
C(12)-H(12A)	0.9800	C(30)-H(30A)	0.9800
C(12)-H(12B)	0.9800	C(30)-H(30B)	0.9800
C(12)-H(12C)	0.9800	C(30)-H(30C)	0.9800

C(31)-H(31A)	0.9800	C(20)-P(2)-C(17)	105.05(5)
C(31)-H(31B)	0.9800	C(8)-P(2)-Mn	112.43(4)
C(31)-H(31C)	0.9800	C(20)-P(2)-Mn	110.71(4)
C(32)-H(32A)	0.9800	C(17)-P(2)-Mn	121.19(4)
C(32)-H(32B)	0.9800	C(9)-P(3)-C(26)	103.16(5)
C(32)-H(32C)	0.9800	C(9)-P(3)-C(23)	103.73(5)
C(34)-C(35)	1.519(2)	C(26)-P(3)-C(23)	105.10(6)
C(34)-C(36)	1.525(2)	C(9)-P(3)-Mn	112.45(4)
C(34)-C(37)	1.5248(19)	C(26)-P(3)-Mn	114.48(4)
C(35)-H(35A)	0.9800	C(23)-P(3)-Mn	116.51(4)
C(35)-H(35B)	0.9800	C(1)-B-C(7)	109.20(9)
C(35)-H(35C)	0.9800	C(1)-B-C(8)	107.10(9)
C(36)-H(36A)	0.9800	C(7)-B-C(8)	109.55(9)
C(36)-H(36B)	0.9800	C(1)-B-C(9)	109.58(9)
C(36)-H(36C)	0.9800	C(7)-B-C(9)	110.00(9)
C(37)-H(37A)	0.9800	C(8)-B-C(9)	111.35(9)
C(37)-H(37B)	0.9800	C(28)-N(1)-C(29)	173.50(14)
C(37)-H(37C)	0.9800	C(33)-N(2)-C(34)	174.29(13)
C(39)-C(40)	1.518(2)	C(38)-N(3)-C(39)	153.99(12)
C(39)-C(41)	1.5199(18)	C(2)-C(1)-C(6)	114.56(10)
C(39)-C(42)	1.5255(19)	C(2)-C(1)-B	122.86(10)
C(40)-H(40A)	0.9800	C(6)-C(1)-B	122.51(11)
C(40)-H(40B)	0.9800	C(3)-C(2)-C(1)	122.91(11)
C(40)-H(40C)	0.9800	C(3)-C(2)-H(2)	118.5
C(41)-H(41A)	0.9800	C(1)-C(2)-H(2)	118.5
C(41)-H(41B)	0.9800	C(4)-C(3)-C(2)	120.49(12)
C(41)-H(41C)	0.9800	C(4)-C(3)-H(3)	119.8
C(42)-H(42A)	0.9800	C(2)-C(3)-H(3)	119.8
C(42)-H(42B)	0.9800	C(5)-C(4)-C(3)	118.66(11)
C(42)-H(42C)	0.9800	C(5)-C(4)-H(4)	120.7
		C(3)-C(4)-H(4)	120.7
C(38)-Mn-C(33)	89.12(5)	C(4)-C(5)-C(6)	120.26(12)
C(38)-Mn-C(28)	85.26(5)	C(4)-C(5)-H(5)	119.9
C(33)-Mn-C(28)	83.75(5)	C(6)-C(5)-H(5)	119.9
C(38)-Mn-P(1)	89.49(4)	C(5)-C(6)-C(1)	123.12(12)
C(33)-Mn-P(1)	178.27(4)	C(5)-C(6)-H(6)	118.4
C(28)-Mn-P(1)	97.16(4)	C(1)-C(6)-H(6)	118.4
C(38)-Mn-P(3)	93.54(4)	B-C(7)-P(1)	115.32(8)
C(33)-Mn-P(3)	89.88(4)	B-C(7)-H(7A)	108.4
C(28)-Mn-P(3)	173.54(4)	P(1)-C(7)-H(7A)	108.4
P(1)-Mn-P(3)	89.173(12)	B-C(7)-H(7B)	108.4
C(38)-Mn-P(2)	178.09(4)	P(1)-C(7)-H(7B)	108.4
C(33)-Mn-P(2)	92.79(4)	H(7A)-C(7)-H(7B)	107.5
C(28)-Mn-P(2)	94.93(4)	B-C(8)-P(2)	115.75(8)
P(1)-Mn-P(2)	88.594(12)	B-C(8)-H(8A)	108.3
P(3)-Mn-P(2)	86.485(12)	P(2)-C(8)-H(8A)	108.3
C(7)-P(1)-C(14)	101.47(5)	B-C(8)-H(8B)	108.3
C(7)-P(1)-C(11)	103.44(5)	P(2)-C(8)-H(8B)	108.3
C(14)-P(1)-C(11)	105.73(5)	H(8A)-C(8)-H(8B)	107.4
C(7)-P(1)-Mn	113.23(4)	B-C(9)-P(3)	114.13(7)
C(14)-P(1)-Mn	116.44(4)	B-C(9)-H(9A)	108.7
C(11)-P(1)-Mn	114.89(4)	P(3)-C(9)-H(9A)	108.7
C(8)-P(2)-C(20)	106.81(5)	B-C(9)-H(9B)	108.7
C(8)-P(2)-C(17)	99.29(5)	P(3)-C(9)-H(9B)	108.7

H(9A)-C(9)-H(9B)	107.6	H(18B)-C(18)-H(18C)	109.5
C(11)-C(10)-H(10A)	109.5	C(20)-C(19)-H(19A)	109.5
C(11)-C(10)-H(10B)	109.5	C(20)-C(19)-H(19B)	109.5
H(10A)-C(10)-H(10B)	109.5	H(19A)-C(19)-H(19B)	109.5
C(11)-C(10)-H(10C)	109.5	C(20)-C(19)-H(19C)	109.5
H(10A)-C(10)-H(10C)	109.5	H(19A)-C(19)-H(19C)	109.5
H(10B)-C(10)-H(10C)	109.5	H(19B)-C(19)-H(19C)	109.5
C(10)-C(11)-C(12)	108.35(10)	C(21)-C(20)-C(19)	111.57(10)
C(10)-C(11)-P(1)	113.05(8)	C(21)-C(20)-P(2)	117.17(8)
C(12)-C(11)-P(1)	117.28(8)	C(19)-C(20)-P(2)	112.09(8)
C(10)-C(11)-H(11)	105.8	C(21)-C(20)-H(20)	104.9
C(12)-C(11)-H(11)	105.8	C(19)-C(20)-H(20)	104.9
P(1)-C(11)-H(11)	105.8	P(2)-C(20)-H(20)	104.9
C(11)-C(12)-H(12A)	109.5	C(20)-C(21)-H(21A)	109.5
C(11)-C(12)-H(12B)	109.5	C(20)-C(21)-H(21B)	109.5
H(12A)-C(12)-H(12B)	109.5	H(21A)-C(21)-H(21B)	109.5
C(11)-C(12)-H(12C)	109.5	C(20)-C(21)-H(21C)	109.5
H(12A)-C(12)-H(12C)	109.5	H(21A)-C(21)-H(21C)	109.5
H(12B)-C(12)-H(12C)	109.5	H(21B)-C(21)-H(21C)	109.5
C(14)-C(13)-H(13A)	109.5	C(23)-C(22)-H(22A)	109.5
C(14)-C(13)-H(13B)	109.5	C(23)-C(22)-H(22B)	109.5
H(13A)-C(13)-H(13B)	109.5	H(22A)-C(22)-H(22B)	109.5
C(14)-C(13)-H(13C)	109.5	C(23)-C(22)-H(22C)	109.5
H(13A)-C(13)-H(13C)	109.5	H(22A)-C(22)-H(22C)	109.5
H(13B)-C(13)-H(13C)	109.5	H(22B)-C(22)-H(22C)	109.5
C(15)-C(14)-C(13)	110.25(10)	C(22)-C(23)-C(24)	109.03(10)
C(15)-C(14)-P(1)	114.78(8)	C(22)-C(23)-P(3)	113.58(8)
C(13)-C(14)-P(1)	116.87(8)	C(24)-C(23)-P(3)	116.80(8)
C(15)-C(14)-H(14)	104.5	C(22)-C(23)-H(23)	105.5
C(13)-C(14)-H(14)	104.5	C(24)-C(23)-H(23)	105.5
P(1)-C(14)-H(14)	104.5	P(3)-C(23)-H(23)	105.5
C(14)-C(15)-H(15A)	109.5	C(23)-C(24)-H(24A)	109.5
C(14)-C(15)-H(15B)	109.5	C(23)-C(24)-H(24B)	109.5
H(15A)-C(15)-H(15B)	109.5	H(24A)-C(24)-H(24B)	109.5
C(14)-C(15)-H(15C)	109.5	C(23)-C(24)-H(24C)	109.5
H(15A)-C(15)-H(15C)	109.5	H(24A)-C(24)-H(24C)	109.5
H(15B)-C(15)-H(15C)	109.5	H(24B)-C(24)-H(24C)	109.5
C(17)-C(16)-H(16A)	109.5	C(26)-C(25)-H(25A)	109.5
C(17)-C(16)-H(16B)	109.5	C(26)-C(25)-H(25B)	109.5
H(16A)-C(16)-H(16B)	109.5	H(25A)-C(25)-H(25B)	109.5
C(17)-C(16)-H(16C)	109.5	C(26)-C(25)-H(25C)	109.5
H(16A)-C(16)-H(16C)	109.5	H(25A)-C(25)-H(25C)	109.5
H(16B)-C(16)-H(16C)	109.5	H(25B)-C(25)-H(25C)	109.5
C(16)-C(17)-C(18)	108.79(9)	C(27)-C(26)-C(25)	109.79(10)
C(16)-C(17)-P(2)	116.67(8)	C(27)-C(26)-P(3)	115.38(9)
C(18)-C(17)-P(2)	115.41(8)	C(25)-C(26)-P(3)	116.55(9)
C(16)-C(17)-H(17)	104.9	C(27)-C(26)-H(26)	104.5
C(18)-C(17)-H(17)	104.9	C(25)-C(26)-H(26)	104.5
P(2)-C(17)-H(17)	104.9	P(3)-C(26)-H(26)	104.5
C(17)-C(18)-H(18A)	109.5	C(26)-C(27)-H(27A)	109.5
C(17)-C(18)-H(18B)	109.5	C(26)-C(27)-H(27B)	109.5
H(18A)-C(18)-H(18B)	109.5	H(27A)-C(27)-H(27B)	109.5
C(17)-C(18)-H(18C)	109.5	C(26)-C(27)-H(27C)	109.5
H(18A)-C(18)-H(18C)	109.5	H(27A)-C(27)-H(27C)	109.5

H(27B)-C(27)-H(27C)	109.5	H(35B)-C(35)-H(35C)	109.5
N(1)-C(28)-Mn	170.91(11)	C(34)-C(36)-H(36A)	109.5
N(1)-C(29)-C(30)	108.50(11)	C(34)-C(36)-H(36B)	109.5
N(1)-C(29)-C(32)	108.18(11)	H(36A)-C(36)-H(36B)	109.5
C(30)-C(29)-C(32)	110.10(14)	C(34)-C(36)-H(36C)	109.5
N(1)-C(29)-C(31)	108.80(11)	H(36A)-C(36)-H(36C)	109.5
C(30)-C(29)-C(31)	109.53(12)	H(36B)-C(36)-H(36C)	109.5
C(32)-C(29)-C(31)	111.67(14)	C(34)-C(37)-H(37A)	109.5
C(29)-C(30)-H(30A)	109.5	C(34)-C(37)-H(37B)	109.5
C(29)-C(30)-H(30B)	109.5	H(37A)-C(37)-H(37B)	109.5
H(30A)-C(30)-H(30B)	109.5	C(34)-C(37)-H(37C)	109.5
C(29)-C(30)-H(30C)	109.5	H(37A)-C(37)-H(37C)	109.5
H(30A)-C(30)-H(30C)	109.5	H(37B)-C(37)-H(37C)	109.5
H(30B)-C(30)-H(30C)	109.5	N(3)-C(38)-Mn	177.92(10)
C(29)-C(31)-H(31A)	109.5	N(3)-C(39)-C(40)	108.58(11)
C(29)-C(31)-H(31B)	109.5	N(3)-C(39)-C(41)	107.99(11)
H(31A)-C(31)-H(31B)	109.5	C(40)-C(39)-C(41)	111.16(13)
C(29)-C(31)-H(31C)	109.5	N(3)-C(39)-C(42)	108.59(11)
H(31A)-C(31)-H(31C)	109.5	C(40)-C(39)-C(42)	110.94(12)
H(31B)-C(31)-H(31C)	109.5	C(41)-C(39)-C(42)	109.50(12)
C(29)-C(32)-H(32A)	109.5	C(39)-C(40)-H(40A)	109.5
C(29)-C(32)-H(32B)	109.5	C(39)-C(40)-H(40B)	109.5
H(32A)-C(32)-H(32B)	109.5	H(40A)-C(40)-H(40B)	109.5
C(29)-C(32)-H(32C)	109.5	C(39)-C(40)-H(40C)	109.5
H(32A)-C(32)-H(32C)	109.5	H(40A)-C(40)-H(40C)	109.5
H(32B)-C(32)-H(32C)	109.5	H(40B)-C(40)-H(40C)	109.5
N(2)-C(33)-Mn	175.09(11)	C(39)-C(41)-H(41A)	109.5
N(2)-C(34)-C(35)	108.46(11)	C(39)-C(41)-H(41B)	109.5
N(2)-C(34)-C(36)	108.79(11)	H(41A)-C(41)-H(41B)	109.5
C(35)-C(34)-C(36)	110.10(13)	C(39)-C(41)-H(41C)	109.5
N(2)-C(34)-C(37)	107.85(11)	H(41A)-C(41)-H(41C)	109.5
C(35)-C(34)-C(37)	110.86(13)	H(41B)-C(41)-H(41C)	109.5
C(36)-C(34)-C(37)	110.71(12)	C(39)-C(42)-H(42A)	109.5
C(34)-C(35)-H(35A)	109.5	C(39)-C(42)-H(42B)	109.5
C(34)-C(35)-H(35B)	109.5	H(42A)-C(42)-H(42B)	109.5
H(35A)-C(35)-H(35B)	109.5	C(39)-C(42)-H(42C)	109.5
C(34)-C(35)-H(35C)	109.5	H(42A)-C(42)-H(42C)	109.5
H(35A)-C(35)-H(35C)	109.5	H(42B)-C(42)-H(42C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 40. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for $[PhBP^{iPr}_3]Mn(CN^tBu)_3$ (10). The anisotropic displacement factorexponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn	93(1)	99(1)	96(1)	6(1)	4(1)	-2(1)
P(1)	86(1)	119(1)	102(1)	0(1)	7(1)	-4(1)
P(2)	101(2)	110(1)	94(1)	-2(1)	2(1)	-8(1)
P(3)	104(2)	106(1)	124(1)	-6(1)	18(1)	2(1)
B	115(6)	128(6)	105(6)	5(4)	4(5)	-10(5)
N(1)	283(7)	245(6)	153(5)	-15(4)	62(5)	-55(5)
N(2)	191(6)	231(6)	212(5)	54(4)	-38(5)	28(5)
N(3)	185(6)	152(5)	257(6)	25(4)	29(5)	-28(4)
C(1)	138(6)	139(5)	100(5)	-19(4)	-14(4)	-35(4)
C(2)	154(6)	144(6)	134(5)	-4(4)	8(5)	-27(5)
C(3)	209(7)	146(6)	149(6)	21(4)	-29(5)	-13(5)
C(4)	257(7)	182(6)	106(5)	27(4)	-4(5)	-72(5)
C(5)	218(7)	221(6)	131(5)	-1(5)	46(5)	-29(5)
C(6)	180(7)	181(6)	139(5)	9(4)	21(5)	-3(5)
C(7)	116(6)	120(5)	114(5)	10(4)	-5(4)	-7(4)
C(8)	119(6)	131(5)	105(5)	10(4)	8(4)	-7(4)
C(9)	108(6)	147(6)	109(5)	-8(4)	6(4)	-6(4)
C(10)	135(6)	194(6)	226(6)	-16(5)	21(5)	-46(5)
C(11)	97(6)	161(6)	142(5)	-22(4)	-3(4)	-7(4)
C(12)	188(7)	243(6)	149(5)	-24(5)	-30(5)	-20(6)
C(13)	139(6)	217(6)	164(6)	6(5)	43(5)	8(5)
C(14)	117(6)	150(5)	135(5)	-14(4)	10(4)	9(4)
C(15)	126(6)	196(6)	198(6)	16(5)	9(5)	36(5)
C(16)	179(7)	192(6)	166(6)	-26(4)	29(5)	23(5)
C(17)	155(6)	121(5)	131(5)	-7(4)	-3(5)	4(4)
C(18)	241(7)	132(6)	168(6)	-20(4)	-9(5)	-17(5)
C(19)	166(6)	216(6)	122(5)	-3(4)	-19(5)	-7(5)
C(20)	116(6)	166(6)	124(5)	-9(4)	-7(4)	-19(5)
C(21)	125(6)	251(7)	181(6)	-11(5)	-1(5)	-64(5)
C(22)	130(6)	287(7)	246(7)	67(5)	28(5)	45(5)
C(23)	116(6)	169(6)	140(5)	-2(4)	19(5)	6(5)
C(24)	112(6)	257(7)	186(6)	5(5)	35(5)	10(5)
C(25)	219(7)	143(6)	336(8)	16(5)	69(6)	31(5)
C(26)	162(6)	121(5)	223(6)	-40(4)	50(5)	-5(5)
C(27)	288(8)	189(7)	276(7)	-96(5)	86(6)	-22(6)
C(28)	123(6)	124(5)	169(6)	8(4)	-3(5)	-22(4)
C(29)	298(8)	229(6)	96(5)	-9(4)	65(5)	-18(6)
C(30)	435(10)	352(9)	244(7)	77(6)	103(7)	100(7)
C(31)	383(10)	696(12)	234(8)	112(8)	127(7)	216(9)
C(32)	1004(17)	476(11)	187(8)	-128(7)	177(9)	-394(11)
C(33)	145(6)	120(5)	159(5)	-4(4)	23(5)	-21(5)
C(34)	191(7)	239(7)	231(7)	55(5)	-75(5)	78(5)
C(35)	487(11)	581(11)	219(8)	66(7)	-34(7)	271(9)
C(36)	214(8)	431(9)	445(10)	85(7)	-111(7)	16(7)
C(37)	400(10)	245(7)	393(9)	73(6)	-146(7)	60(7)
C(38)	120(6)	161(6)	116(5)	-4(4)	9(4)	26(5)

C(39)	257(7)	153(6)	165(6)	20(4)	29(5)	-74(5)
C(40)	445(11)	483(11)	406(10)	207(8)	-61(8)	11(9)
C(41)	568(11)	208(7)	395(9)	-107(6)	175(8)	-176(7)
C(42)	363(9)	315(8)	260(7)	22(6)	142(7)	-29(7)

Table 41. Crystal Data and Structure Analysis Details for {(Hdbabh)MnI(*μ*-*N*-dbabh)}$_2$.

Empirical formula	$C_{104}H_{92}I_2Mn_2N_6O_2$
Formula weight	1821.52
Crystallization solvent	benzene/THF/petroleum ether
Crystal shape	thin blade
Crystal color	colorless
Crystal size	0.03 x 0.13 x 0.43 mm

Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data collection temperature	100 K	
Theta range for 1766 reflections used in lattice determination	2.20 to 26.94°	
Unit cell dimensions	a = 10.602(3) Å b = 12.269(3) Å c = 17.484(4) Å	α= 81.448(5)° β= 81.588(5)° γ = 76.562(5)°
Volume	2172.6(9) Å^3	
Z	1	
Crystal system	triclinic	
Space group	P-1	
Density (calculated)	1.392 g/cm^3	
F(000)	930	
Theta range for data collection	2.2 to 28.3°	
Completeness to theta = 28.33°	66.1%	
Index ranges	-13 ≤ h ≤ 14, -15 ≤ k ≤ 16,0 ≤ l ≤ 23	
Data collection scan type	ω scans	
Reflections collected	7486	
Independent reflections	7486 [R_{int}= 0.0000]	
Reflections > 2σ(I)	4104	
Average σ(I)/(net I)	0.2405	
Absorption coefficient	1.06 mm^{-1}	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.969 and 0.851	
Reflections monitored for decay	initial data recollected at end	

Decay of standards	0%

Structure Solution and Refinement

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7486 / 0 / 244
Treatment of hydrogen atoms	not refined, U_{iso} fixed at 120% U_{eq} of attached atom
Goodness-of-fit on F^2	1.28
Final R indices [I>2σ(I), 4104 reflections]	R1 = 0.0892, wR2 = 0.1213
R indices (all data)	R1 = 0.1561, wR2 = 0.1304
Type of weighting scheme used	sigma
Weighting scheme used	calc $w=1/[\sigma^2(Fo^2)]$ where $P=(Fo^2+2Fc^2)/3$
Max shift/error	0.000
Average shift/error	0.000
Largest diff. peak and hole	2.83 and -1.50 e·Å^{-3}

Programs Used

Cell refinement	Bruker SMART 5.606
Data collection	Bruker SMART 5.054
Data reduction	Bruker SAINT 6.45
Structure solution	Bruker SHELXTL 6.14
Structure refinement	Bruker SHELXTL 6.14

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 42. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for {(Hdbabh)MnI(μ-*N*-dbabh)}$_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Mn	9659(2)	847(1)	5553(1)	13(1)
N(1)	8427(9)	1627(8)	6450(5)	15(2)
N(2)	9351(8)	936(7)	4363(5)	8(2)
N(3)	723(9)	1919(8)	7634(5)	20(3)
I	11646(1)	2051(1)	5463(1)	16(1)
O	8950(8)	4286(6)	6586(4)	23(2)
C(1)	7018(11)	2197(10)	6347(7)	20(3)
C(2)	6540(11)	2519(10)	7163(6)	12(3)
C(3)	5563(11)	3412(10)	7446(7)	22(3)
C(4)	5353(12)	3431(11)	8254(7)	29(4)
C(5)	6020(12)	2651(10)	8758(8)	28(4)
C(6)	6989(11)	1724(10)	8458(7)	23(3)
C(7)	7212(11)	1706(9)	7665(6)	10(3)
C(8)	8058(12)	867(10)	7125(7)	22(3)
C(9)	7144(11)	285(10)	6810(6)	16(3)
C(10)	6806(11)	-726(10)	6964(7)	24(3)
C(11)	5845(12)	-901(11)	6563(7)	27(4)
C(12)	5196(13)	-95(11)	6051(7)	32(4)
C(13)	5496(12)	1000(11)	5929(7)	28(4)
C(14)	6496(12)	1145(10)	6312(7)	21(3)
C(15)	9832(11)	1830(9)	3815(6)	7(3)
C(16)	8648(12)	2893(10)	4006(6)	23(3)
C(17)	8665(11)	4013(10)	3971(6)	17(3)
C(18)	7398(12)	4701(11)	4148(7)	28(4)
C(19)	6360(12)	4294(10)	4268(6)	20(3)
C(20)	6351(12)	3168(10)	4297(6)	21(3)
C(21)	7610(11)	2448(10)	4181(6)	14(3)
C(22)	8015(11)	1168(10)	4096(6)	18(3)
C(23)	8365(10)	1163(9)	3208(6)	6(3)
C(24)	7727(12)	944(10)	2656(7)	22(3)
C(25)	8290(12)	1158(10)	1883(7)	31(4)
C(26)	9315(12)	1590(10)	1700(7)	29(4)
C(27)	9973(12)	1859(10)	2282(7)	25(3)
C(28)	9466(10)	1643(9)	3040(6)	9(3)
C(29)	1982(11)	2317(9)	7580(7)	17(3)
C(30)	2634(12)	1494(10)	8228(6)	14(3)
C(31)	3961(12)	1000(10)	8288(7)	22(3)
C(32)	4230(12)	289(10)	8962(7)	24(3)
C(33)	3277(11)	83(10)	9569(6)	19(3)
C(34)	1954(12)	607(10)	9509(7)	21(3)
C(35)	1678(11)	1271(10)	8838(7)	15(3)
C(36)	382(12)	1947(10)	8517(6)	22(3)
C(37)	467(12)	3228(10)	8522(7)	21(3)
C(38)	-173(13)	4015(11)	9013(7)	36(4)
C(39)	175(12)	5044(11)	8903(7)	33(4)
C(40)	1175(13)	5227(11)	8342(7)	38(4)

C(41)	1859(12)	4446(10)	7843(7)	32(4)
C(42)	1446(11)	3436(10)	7954(6)	16(3)
C(43)	8383(13)	4947(10)	7229(7)	30(4)
C(44)	7535(13)	5976(11)	6801(7)	41(4)
C(45)	7225(13)	5560(11)	6112(7)	44(4)
C(46)	8427(12)	4725(10)	5853(7)	25(4)
C(47)	5860(17)	7307(15)	8833(10)	79(6)
C(48)	5390(20)	6440(20)	8790(13)	138(9)
C(49)	6040(20)	5617(18)	9364(12)	120(8)
C(50)	6877(19)	5747(17)	9973(12)	116(8)
C(51)	7161(15)	6791(13)	9943(9)	55(5)
C(52)	6686(16)	7446(15)	9341(9)	70(5)

Table 43. Bond lengths [Å] and angles [°] for {(Hdbabh)MnI(μ-*N*-dbabh)}$_2$.

Mn-N(1)	2.085(8)	C(19)-C(20)	1.377(14)
Mn-N(2)	2.137(8)	C(19)-H(19)	0.9500
Mn-N(2)#1	2.189(8)	C(20)-C(21)	1.425(14)
Mn-I	2.8149(18)	C(20)-H(20)	0.9500
Mn-Mn#1	2.945(3)	C(21)-C(22)	1.552(14)
N(1)-C(8)	1.457(13)	C(22)-C(23)	1.543(13)
N(1)-C(1)	1.520(13)	C(22)-H(22)	1.0000
N(1)-H	0.9300	C(23)-C(24)	1.346(14)
N(2)-C(15)	1.478(12)	C(23)-C(28)	1.401(12)
N(2)-C(22)	1.507(13)	C(24)-C(25)	1.409(14)
N(2)-Mn#1	2.189(8)	C(24)-H(24)	0.9500
N(3)-C(29)	1.511(12)	C(25)-C(26)	1.295(14)
N(3)-C(36)	1.538(12)	C(25)-H(25)	0.9500
N(3)-H(3A)	0.9469	C(26)-C(27)	1.432(15)
O-C(46)	1.451(13)	C(26)-H(26)	0.9500
O-C(43)	1.459(12)	C(27)-C(28)	1.367(13)
C(1)-C(2)	1.521(13)	C(27)-H(27)	0.9500
C(1)-C(14)	1.530(14)	C(29)-C(30)	1.532(15)
C(1)-H(1)	1.0000	C(29)-C(42)	1.560(14)
C(2)-C(7)	1.366(15)	C(29)-H(29)	1.0000
C(2)-C(3)	1.414(14)	C(30)-C(35)	1.402(13)
C(3)-C(4)	1.400(14)	C(30)-C(31)	1.409(15)
C(3)-H(3)	0.9500	C(31)-C(32)	1.380(15)
C(4)-C(5)	1.346(16)	C(31)-H(31)	0.9500
C(4)-H(4)	0.9500	C(32)-C(33)	1.392(13)
C(5)-C(6)	1.449(15)	C(32)-H(32)	0.9500
C(5)-H(5)	0.9500	C(33)-C(34)	1.412(14)
C(6)-C(7)	1.374(14)	C(33)-H(33)	0.9500
C(6)-H(6)	0.9500	C(34)-C(35)	1.352(15)
C(7)-C(8)	1.539(14)	C(34)-H(34)	0.9500
C(8)-C(9)	1.531(14)	C(35)-C(36)	1.565(15)
C(8)-H(8)	1.0000	C(36)-C(37)	1.595(14)
C(9)-C(10)	1.349(14)	C(36)-H(36)	1.0000
C(9)-C(14)	1.382(16)	C(37)-C(42)	1.369(14)
C(10)-C(11)	1.389(15)	C(37)-C(38)	1.379(14)
C(10)-H(10)	0.9500	C(38)-C(39)	1.376(14)
C(11)-C(12)	1.360(16)	C(38)-H(38)	0.9500
C(11)-H(11)	0.9500	C(39)-C(40)	1.370(14)
C(12)-C(13)	1.430(14)	C(39)-H(39)	0.9500
C(12)-H(12)	0.9500	C(40)-C(41)	1.396(15)
C(13)-C(14)	1.390(15)	C(40)-H(40)	0.9500
C(13)-H(13)	0.9500	C(41)-C(42)	1.386(14)
C(15)-C(28)	1.524(13)	C(41)-H(41)	0.9500
C(15)-C(16)	1.623(15)	C(43)-C(44)	1.533(16)
C(15)-H(15)	1.0000	C(43)-H(43A)	0.9900
C(16)-C(21)	1.317(13)	C(43)-H(43B)	0.9900
C(16)-C(17)	1.371(14)	C(44)-C(45)	1.481(14)
C(17)-C(18)	1.428(15)	C(44)-H(44A)	0.9900
C(17)-H(17)	0.9500	C(44)-H(44B)	0.9900
C(18)-C(19)	1.288(14)	C(45)-C(46)	1.497(15)
C(18)-H(18)	0.9500	C(45)-H(45A)	0.9900

C(45)-H(45B)	0.9900
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-C(48)	1.29(2)
C(47)-C(52)	1.388(19)
C(47)-H(47)	0.9500
C(48)-C(49)	1.44(3)
C(48)-H(48)	0.9500
C(49)-C(50)	1.53(2)
C(49)-H(49)	0.9500
C(50)-C(51)	1.37(2)
C(50)-H(50)	0.9500
C(51)-C(52)	1.31(2)
C(51)-H(51)	0.9500
C(52)-H(52)	0.9500

N(1)-Mn-N(2)	128.7(4)
N(1)-Mn-N(2)#1	124.9(4)
N(2)-Mn-N(2)#1	94.2(3)
N(1)-Mn-I	97.2(2)
N(2)-Mn-I	103.0(2)
N(2)#1-Mn-I	105.5(2)
N(1)-Mn-Mn#1	151.5(3)
N(2)-Mn-Mn#1	47.8(2)
N(2)#1-Mn-Mn#1	46.3(2)
I-Mn-Mn#1	111.23(8)
C(8)-N(1)-C(1)	93.2(8)
C(8)-N(1)-Mn	115.4(7)
C(1)-N(1)-Mn	120.8(7)
C(8)-N(1)-H	108.8
C(1)-N(1)-H	108.8
Mn-N(1)-H	108.8
C(15)-N(2)-C(22)	96.2(8)
C(15)-N(2)-Mn	116.6(6)
C(22)-N(2)-Mn	123.2(6)
C(15)-N(2)-Mn#1	123.8(6)
C(22)-N(2)-Mn#1	113.8(6)
Mn-N(2)-Mn#1	85.8(3)
C(29)-N(3)-C(36)	95.5(8)
C(29)-N(3)-H(3A)	110.8
C(36)-N(3)-H(3A)	111.5
C(46)-O-C(43)	115.0(9)
N(1)-C(1)-C(2)	99.9(9)
N(1)-C(1)-C(14)	98.6(10)
C(2)-C(1)-C(14)	105.0(9)
N(1)-C(1)-H(1)	116.8
C(2)-C(1)-H(1)	116.8
C(14)-C(1)-H(1)	116.8
C(7)-C(2)-C(3)	120.7(11)
C(7)-C(2)-C(1)	106.9(11)
C(3)-C(2)-C(1)	132.3(12)
C(4)-C(3)-C(2)	116.9(12)
C(4)-C(3)-H(3)	121.6
C(2)-C(3)-H(3)	121.6
C(5)-C(4)-C(3)	123.4(13)
C(5)-C(4)-H(4)	118.3
C(3)-C(4)-H(4)	118.3
C(4)-C(5)-C(6)	118.8(12)
C(4)-C(5)-H(5)	120.6
C(6)-C(5)-H(5)	120.6
C(7)-C(6)-C(5)	118.1(12)
C(7)-C(6)-H(6)	120.9
C(5)-C(6)-H(6)	120.9
C(2)-C(7)-C(6)	122.0(11)
C(2)-C(7)-C(8)	103.3(10)
C(6)-C(7)-C(8)	134.6(12)
N(1)-C(8)-C(9)	102.5(9)
N(1)-C(8)-C(7)	101.5(9)
C(9)-C(8)-C(7)	107.7(9)
N(1)-C(8)-H(8)	114.6
C(9)-C(8)-H(8)	114.6
C(7)-C(8)-H(8)	114.6
C(10)-C(9)-C(14)	121.2(12)
C(10)-C(9)-C(8)	136.1(12)
C(14)-C(9)-C(8)	102.4(10)
C(9)-C(10)-C(11)	117.7(13)
C(9)-C(10)-H(10)	121.1
C(11)-C(10)-H(10)	121.1
C(12)-C(11)-C(10)	123.6(13)
C(12)-C(11)-H(11)	118.2
C(10)-C(11)-H(11)	118.2
C(11)-C(12)-C(13)	118.5(13)
C(11)-C(12)-H(12)	120.7
C(13)-C(12)-H(12)	120.7
C(14)-C(13)-C(12)	117.0(13)
C(14)-C(13)-H(13)	121.5
C(12)-C(13)-H(13)	121.5
C(9)-C(14)-C(13)	121.8(11)
C(9)-C(14)-C(1)	107.2(11)
C(13)-C(14)-C(1)	130.8(13)
N(2)-C(15)-C(28)	102.5(8)
N(2)-C(15)-C(16)	99.0(7)
C(28)-C(15)-C(16)	98.4(9)
N(2)-C(15)-H(15)	117.8
C(28)-C(15)-H(15)	117.8
C(16)-C(15)-H(15)	117.8
C(21)-C(16)-C(17)	126.1(12)
C(21)-C(16)-C(15)	104.0(10)
C(17)-C(16)-C(15)	129.8(10)
C(16)-C(17)-C(18)	112.8(11)
C(16)-C(17)-H(17)	123.6
C(18)-C(17)-H(17)	123.6
C(19)-C(18)-C(17)	122.0(12)
C(19)-C(18)-H(18)	119.0
C(17)-C(18)-H(18)	119.0
C(18)-C(19)-C(20)	124.7(13)
C(18)-C(19)-H(19)	117.7
C(20)-C(19)-H(19)	117.7

C(19)-C(20)-C(21)	114.6(11)	N(3)-C(36)-C(35)	102.4(9)
C(19)-C(20)-H(20)	122.7	N(3)-C(36)-C(37)	96.7(8)
C(21)-C(20)-H(20)	122.7	C(35)-C(36)-C(37)	102.8(9)
C(16)-C(21)-C(20)	119.5(11)	N(3)-C(36)-H(36)	117.3
C(16)-C(21)-C(22)	109.2(11)	C(35)-C(36)-H(36)	117.3
C(20)-C(21)-C(22)	130.7(10)	C(37)-C(36)-H(36)	117.3
N(2)-C(22)-C(23)	101.3(8)	C(42)-C(37)-C(38)	121.9(11)
N(2)-C(22)-C(21)	98.3(8)	C(42)-C(37)-C(36)	106.7(10)
C(23)-C(22)-C(21)	102.5(9)	C(38)-C(37)-C(36)	131.1(11)
N(2)-C(22)-H(22)	117.2	C(39)-C(38)-C(37)	117.9(12)
C(23)-C(22)-H(22)	117.2	C(39)-C(38)-H(38)	121.1
C(21)-C(22)-H(22)	117.2	C(37)-C(38)-H(38)	121.1
C(24)-C(23)-C(28)	123.4(11)	C(40)-C(39)-C(38)	119.2(13)
C(24)-C(23)-C(22)	132.0(10)	C(40)-C(39)-H(39)	120.4
C(28)-C(23)-C(22)	103.8(9)	C(38)-C(39)-H(39)	120.4
C(23)-C(24)-C(25)	115.6(11)	C(39)-C(40)-C(41)	124.5(12)
C(23)-C(24)-H(24)	122.2	C(39)-C(40)-H(40)	117.7
C(25)-C(24)-H(24)	122.2	C(41)-C(40)-H(40)	117.7
C(26)-C(25)-C(24)	123.2(13)	C(42)-C(41)-C(40)	114.3(11)
C(26)-C(25)-H(25)	118.4	C(42)-C(41)-H(41)	122.8
C(24)-C(25)-H(25)	118.4	C(40)-C(41)-H(41)	122.8
C(25)-C(26)-C(27)	121.5(13)	C(37)-C(42)-C(41)	122.1(11)
C(25)-C(26)-H(26)	119.2	C(37)-C(42)-C(29)	105.9(9)
C(27)-C(26)-H(26)	119.2	C(41)-C(42)-C(29)	131.7(10)
C(28)-C(27)-C(26)	116.8(11)	O-C(43)-C(44)	100.7(10)
C(28)-C(27)-H(27)	121.6	O-C(43)-H(43A)	111.6
C(26)-C(27)-H(27)	121.6	C(44)-C(43)-H(43A)	111.6
C(27)-C(28)-C(23)	119.4(10)	O-C(43)-H(43B)	111.6
C(27)-C(28)-C(15)	133.5(10)	C(44)-C(43)-H(43B)	111.6
C(23)-C(28)-C(15)	107.1(9)	H(43A)-C(43)-H(43B)	109.4
N(3)-C(29)-C(30)	99.9(8)	C(45)-C(44)-C(43)	105.0(11)
N(3)-C(29)-C(42)	99.2(8)	C(45)-C(44)-H(44A)	110.8
C(30)-C(29)-C(42)	104.0(9)	C(43)-C(44)-H(44A)	110.8
N(3)-C(29)-H(29)	117.0	C(45)-C(44)-H(44B)	110.8
C(30)-C(29)-H(29)	117.0	C(43)-C(44)-H(44B)	110.8
C(42)-C(29)-H(29)	117.0	H(44A)-C(44)-H(44B)	108.8
C(35)-C(30)-C(31)	120.1(11)	C(44)-C(45)-C(46)	105.5(12)
C(35)-C(30)-C(29)	109.4(11)	C(44)-C(45)-H(45A)	110.6
C(31)-C(30)-C(29)	130.5(10)	C(46)-C(45)-H(45A)	110.6
C(32)-C(31)-C(30)	116.1(11)	C(44)-C(45)-H(45B)	110.6
C(32)-C(31)-H(31)	122.0	C(46)-C(45)-H(45B)	110.6
C(30)-C(31)-H(31)	122.0	H(45A)-C(45)-H(45B)	108.8
C(31)-C(32)-C(33)	123.4(13)	O-C(46)-C(45)	101.4(9)
C(31)-C(32)-H(32)	118.3	O-C(46)-H(46A)	111.5
C(33)-C(32)-H(32)	118.3	C(45)-C(46)-H(46A)	111.5
C(32)-C(33)-C(34)	119.8(12)	O-C(46)-H(46B)	111.5
C(32)-C(33)-H(33)	120.1	C(45)-C(46)-H(46B)	111.5
C(34)-C(33)-H(33)	120.1	H(46A)-C(46)-H(46B)	109.3
C(35)-C(34)-C(33)	117.1(11)	C(48)-C(47)-C(52)	129(2)
C(35)-C(34)-H(34)	121.5	C(48)-C(47)-H(47)	115.3
C(33)-C(34)-H(34)	121.5	C(52)-C(47)-H(47)	115.3
C(34)-C(35)-C(30)	123.4(12)	C(47)-C(48)-C(49)	102(2)
C(34)-C(35)-C(36)	133.9(11)	C(47)-C(48)-H(48)	129.2
C(30)-C(35)-C(36)	102.7(10)	C(49)-C(48)-H(48)	129.2

C(48)-C(49)-C(50)	131(2)	C(52)-C(51)-C(50)	109.1(17)
C(48)-C(49)-H(49)	114.7	C(52)-C(51)-H(51)	125.5
C(50)-C(49)-H(49)	114.7	C(50)-C(51)-H(51)	125.5
C(51)-C(50)-C(49)	116(2)	C(51)-C(52)-C(47)	131.9(18)
C(51)-C(50)-H(50)	121.8	C(51)-C(52)-H(52)	114.0
C(49)-C(50)-H(50)	121.8	C(47)-C(52)-H(52)	114.0

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y,-z+1

Table 44. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for {(Hdbabh)MnI(μ-*N*-dbabh)}$_2$. 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	98(12)	103(12)	165(12)	-47(11)	-22(9)	36(10)
I	111(4)	136(5)	235(5)	-64(5)	-27(4)	21(4)