Pseudotetrahedral manganese complexes supported by the anionic tris(phosphino)borate ligand [PhBP\textsubscript{iPr}\textsubscript{3}] 

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Table 18. Atomic coordinates and equivalent isotropic displacement parameters for 4.


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Table 22. Atomic coordinates and equivalent isotropic displacement parameters for 6.

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Table 25. Crystal data and structure refinement for [PhBP<sub>i</sub>Pr<sub>3</sub>Mn(dbabh) (7).

Table 26. Atomic coordinates and equivalent isotropic displacement parameters for 7.

Table 27. Bond lengths and angles for 7.

Table 28. Anisotropic parameters for 7.

Table 29. Crystal data and structure refinement for [PhBP<sub>i</sub>Pr<sub>3</sub>Mn(1-Ph(isoindolate)) (8).

Table 30. Atomic coordinates and equivalent isotropic displacement parameters for 8.

Table 31. Bond lengths and angles for 8.

Table 32. Anisotropic parameters for 8.

Table 33. Crystal data and structure refinement for [PhBP<sub>i</sub>Pr<sub>3</sub>Tl-MnBr(CO)<sub>4</sub> (9).

Table 34. Atomic coordinates and equivalent isotropic displacement parameters for 9.

Table 35. Bond lengths and angles for 9.

Table 36. Anisotropic parameters for 9.

Table 37. Crystal data and structure refinement for [PhBP<sub>i</sub>Pr<sub>3</sub>Mn(CN<sub>t</sub>Bu)<sub>3</sub> (10).

Table 38. Atomic coordinates and equivalent isotropic displacement parameters for 10.

Table 39. Bond lengths and angles for 10.

Table 40. Anisotropic parameters for 10.

Table 41. Crystal data and structure refinement for {(Hdbabh)MnI(µ-N-dbabh)}<sub>2</sub>.

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Table 44. Anisotropic parameters for {(Hdbabh)MnI(µ-N-dbabh)}<sub>2</sub>.
Figure 1. Fully labeled drawing of \([\text{PhBP}^\text{Pr}_3]\text{MnCl (1a)}\). Displacement ellipsoid (50\%) representation. Hydrogen atoms have been omitted for clarity.
Figure 2. Fully labeled drawing of \{[\text{PhBP}^\text{Pr}_3]\text{Mn} (\mu-\text{Cl})\}_2 (1b). Displacement ellipsoid (50%) representation. Hydrogen atoms have been omitted for clarity.
Figure 3. Fully labeled drawing of [PhBP$^{\text{Pr}_3}]$MnI (2). Displacement ellipsoid (50\%) representation. Hydrogen atoms and solvent molecule have been omitted for clarity.
Figure 4. Fully labeled drawing of [PhBP$_3^{Pr_3}$]Mn(N$_3$)$_3$ (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 \([\text{PhBP}^{\text{Pr}_3}]\text{Mn(CH}_2\text{Ph})\) (4).
Figure 6. Fully labeled drawing of [PhBP\textsuperscript{Pr}_3]Mn(NH(2,6-\textsuperscript{i}Pr\textsubscript{2}-C\textsubscript{6}H\textsubscript{3}))(6). Displacement ellipsoid (50\%) representation. Hydrogen atoms have been omitted for clarity.
**Figure 7.** Fully labeled drawing of [PhBP\(^{Pr_3}\)]Mn(dbah) (7). Displacement ellipsoid (50%) representation. Hydrogen atoms have been omitted for clarity.
Figure 8. Fully labeled drawing of [PhBP$^3$Pr$_3$]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 [PhBPr\textsubscript{3}]Tl-MnBr(CO)\textsubscript{4} (9). Displacement ellipsoid (50\%) representation. Hydrogen atoms have been omitted for clarity.
Figure 10. Fully labeled drawing of [PhBP(3)]Mn(CN’Bu)_3 (10). Displacement ellipsoid (50%) representation. Hydrogen atoms have been omitted for clarity.
Figure 11. Fully labeled drawing of $\{(\text{Hdbabh})\text{MnI(}\mu-$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$_{3}$Pr$_{3}$]MnCl (1a).

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<th>Property</th>
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<td>C$<em>{27}$H$</em>{53}$BCl$<em>{0.98}$Mn$</em>{0.98}$P$<em>{3}$Tl$</em>{0.02}$</td>
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<td>Formula weight</td>
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**Data Collection**

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<td>in lattice determination</td>
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**Table 1 (cont.)**

**Structure Solution and Refinement**

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<td>Secondary solution method</td>
<td>difference map</td>
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<td>Hydrogen placement</td>
<td>calculated</td>
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<td>Refinement method</td>
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<td>Data / restraints / parameters</td>
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<td>Treatment of hydrogen atoms</td>
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<td>Goodness-of-fit on $F^2$</td>
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<td>Final R indices [$I&gt;2\sigma(I)$, 6237 reflections]</td>
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<td>R indices (all data)</td>
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<td>Type of weighting scheme used</td>
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**Programs Used**

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</table>

**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 ($wR$) 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 ($\text{Å}^2$ $10^3$) for [PhBP$_3$Pr$_i$]$\text{MnCl}$ (1a). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

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<th>$x$</th>
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Table 3. Bond lengths [Å] and angles [°] for [PhBP$_{3}^{+}$]MnCl (1a).

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<th>Length [Å]</th>
<th>Angles [°]</th>
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P(2)-C(1)-C(2)  90.55(2)  
P(2)-C(1)-B  90.55(2)  
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P(3)-C(1)-B  90.55(2)  
C(2)-B-C(1)  90.55(2)  

S18
Symmetry transformations used to generate equivalent atoms:

S19
Table 4. Anisotropic displacement parameters ($\AA^2 \times 10^4$) for [PhBP\textsuperscript{Pr\textsubscript{3}}]MnCl (1a). The anisotropic displacement factor exponent takes the form: 

\[-2\pi^2 [ h^2a^*2U_{11} + ... + 2hk a^* b^* U_{12} ] \]

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Table 5. Crystal Data and Structure Analysis Details for \{[\text{PhBP}^{iPr_3}]\text{Mn}(\mu-\text{Cl})\}_2 \text{(1b)}.

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**Data Collection**

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<td></td>
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Table 5 (cont.)

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Programs Used

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| 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 (wR) 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 > 2σ(Fo^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 (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for \([[\text{PhBP}_{\mu_3}]\text{Mn(µ-Cl)}\]_2 (1b). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

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Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1
Table 8. Anisotropic displacement parameters (Å² x 10⁴) for \([\text{PhBP}^{\text{iPr}}]_3\text{Mn(µ-Cl)}\)₂ (1b). The anisotropic displacement factor exponent takes the form: 


\[
-2\pi^2 [ h^2 a^* U_{11} + ... + 2 h k a^* b^* U_{12} ]
\]

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Table 9. Crystal Data and Structure Analysis Details for [PhBP$_{3}$]MnI (2).

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<td>Crystallization solvent</td>
<td>benzene/petroleum ether</td>
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<td>Crystal shape</td>
<td>plate</td>
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<td>Crystal color</td>
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<td>Crystal size</td>
<td>0.20 x 0.22 x 0.30 mm</td>
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**Data Collection**

- **Preliminary photograph(s):** rotation
- **Type of diffractometer:** Bruker SMART 1000
- **Wavelength:** 0.71073 Å MoK$_α$
- **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  $\alpha = 89.780(1)^°$
  - $b = 9.9006(8)$ Å  $\beta = 89.920(1)^°$
  - $c = 19.668(2)$ Å  $\gamma = 82.662(1)^°$
- **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:**
  - $-12 \leq h \leq 12, -13 \leq k \leq 13, -25 \leq l \leq 25$
- **Data collection scan type:** $\omega$ 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

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<td>Secondary solution method</td>
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<td>Hydrogen placement</td>
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<td>Refinement method</td>
<td>Full-matrix least-squares on $F^2$</td>
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<tr>
<td>Data / restraints / parameters</td>
<td>8473 / 0 / 364</td>
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<tr>
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<td>Final R indices [$I&gt;2\sigma(I)$, 6869 reflections]</td>
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<tr>
<td>R indices (all data)</td>
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<td>sigma</td>
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<td>Average shift/error</td>
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<td>Largest diff. peak and hole</td>
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#### Programs Used

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#### Special Refinement Details

One benzene solvent molecule was present in the asymmetric unit.

Refinement of $F^2$ against ALL reflections. The weighted R-factor ($wR$) 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.

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B-C(7)-H(7B) 107.5  C(17)-C(16)-H(16C) 109.5
P(1)-C(7)-H(7B) 107.5  H(16A)-C(16)-H(16C) 109.5
Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1    #2 -x+2,-y+1,-z

S34
Table 12. Anisotropic displacement parameters (Å²x 10^4) for [PhBP^{Pr}_3]MnI (2). The anisotropic displacement factor exponent takes the form: -2π²[ h^2a*^2U_{11} + ... + 2hka*b*U_{12} ]

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Table 13. Crystal Data and Structure Analysis Details for [PhBPr\textsubscript{3}]Mn(N\textsubscript{3}) (3).

- **Empirical formula**: C\textsubscript{54}H\textsubscript{106}B\textsubscript{2}Cl\textsubscript{0.36}Mn\textsubscript{1.90}N\textsubscript{4.63}P\textsubscript{6}Tl\textsubscript{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 MoK\(\alpha\)
- **Data collection temperature**: 100 K
- **Theta range for 32076 reflections used in lattice determination**: 2.24 to 31.43°
- **Unit cell dimensions**: 
  - \(a = 11.946(2) \text{ Å}\) \(\alpha = 90°\)
  - \(b = 34.586(7) \text{ Å}\) \(\beta = 90°\)
  - \(c = 15.423(3) \text{ Å}\) \(\gamma = 90°\)

- **Volume**: 6372(2) Å\(^3\)
- **Z**: 4
- **Crystal system**: orthorhombic
- **Space group**: \(P n c 2 \quad (# 30)\)
- **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 ≤ \(h\) ≤ 17, -50 ≤ \(k\) ≤ 40, -18 ≤ \(l\) ≤ 22
- **Data collection scan type**: \(\omega\) scans
- **Reflections collected**: 75921
- **Independent reflections**: 17907 [R\(_{int}\) = 0.0716]
- **Reflections > 2\(\sigma\)(I)**: 12030
- **Average \(\sigma\)(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

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<th>Details</th>
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<td>Hydrogen placement</td>
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<td>Refinement method</td>
<td>Full-matrix least-squares on F^2</td>
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<td>Data / restraints / parameters</td>
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<td>Treatment of hydrogen atoms</td>
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<td>Goodness-of-fit on F^2</td>
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<td>Final R indices [I&gt;2σ(I), 12030 reflections]</td>
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<tr>
<td>R indices (all data)</td>
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<td>Largest diff. peak and hole</td>
<td>1.12 and -0.53 e·Å^{-3}</td>
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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 Pnca2 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 (wR) 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 > 2σ(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 ($x \times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for [PhHPr$_3$]Mn(N$_3$)$_3$ (3). U(eq) is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

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### Table 15. Bond lengths [Å] and angles [°] for [PhBP^iPr_3]Mn(N_3) (3).

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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
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B(1B)-C(7B)  1.661(6)  C(20B)-H(20B)  0.9800
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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
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C(1B)-C(2B)  1.403(5)  C(22B)-C(23B)  1.442(8)
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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
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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
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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
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C(14B)-C(15B)  1.544(5)  N(1A)-Mn(1A)-P(2A)  125.69(11)
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C(16B)-H(16D)  0.9600  C(7A)-P(1A)-C(14A)  106.9(2)
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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)
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C(18B)-H(18D)  0.9600  C(8A)-P(2A)-C(20A)  106.8(2)
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Symmetry transformations used to generate equivalent atoms:

S45
Table 16. Anisotropic displacement parameters (Å²×10⁴) for [PhBP⁺Pr₃]Mn(N₃) (3). The anisotropic displacement factor exponent takes the form: \(-2\pi^2 [ h^2a^{*2}U^{11} + \ldots + 2hk a^* b^* U^{12} ] \)

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Table 17. Crystal Data and Structure Analysis Details for [PhBP\textsuperscript{Pr}][Mn(CH\textsubscript{2}Ph)] (4).

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<tr>
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<td>cyclopentane</td>
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<tr>
<td>Crystal shape</td>
<td>block</td>
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<td>Crystal color</td>
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<tr>
<td>Crystal size</td>
<td>0.26 x 0.37 x 0.44 mm</td>
</tr>
</tbody>
</table>

**Data Collection**

- Preliminary photograph(s)                   | rotation                                   |
- Type of diffractometer                      | Bruker SMART 1000                         |
- Wavelength                                  | 0.71073 Å MoK\textalpha                   |
- Data collection temperature                 | 100 K                                     |
- Theta range for 23623 reflections used in lattice determination | 2.13 to 32.75° |
- Unit cell dimensions                        | \begin{align*}a &= 9.4120(6) \text{ Å} \\ b &= 11.8746(8) \text{ Å} \\ c &= 16.736(1) \text{ Å} \end{align*} \begin{align*} \alpha &= 90^\circ \\ \beta &= 105.605(1)^\circ \\ \gamma &= 90^\circ \end{align*} |
- Volume                                       | 1801.6(2) Å\textsuperscript{3}             |
- Z                                            | 2                                         |
- Crystal system                              | monoclinic                                 |
- Space group                                  | P 21 (\# 4)                               |
- Density (calculated)                        | 1.157 g/cm\textsuperscript{3}              |
- F(000)                                       | 678                                       |
- Theta range for data collection             | 2.1 to 32.9°                               |
- Completeness to theta = 32.9°               | 91.0%                                     |
- Index ranges                                | -14 \leq h \leq 12, -17 \leq k \leq 18, -24 \leq l \leq 24 |
- Data collection scan type                   | \omega scans                              |
- Reflections collected                       | 30165                                     |
- Independent reflections                     | 10967 [R\textsub{int} = 0.0446]            |
- Reflections > 2\sigma(I)                    | 9835                                      |
- Average \sigma(I)/(net I)                   | 0.0459                                    |
- Absorption coefficient                      | 0.52 mm\textsuperscript{-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/[σ^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 (wR) 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 > 2σ(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 [PhBPiPr]^+Mn(CH_2Ph) (4). U(eq) is defined as one third of the trace of the orthogonalized U_ij tensor.

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Table 9. Bond lengths [Å] and angles [°] for [PhBPPr₃]Mn(CH₂Ph) (4).

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S52
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Symmetry transformations used to generate equivalent atoms:
Table 20. Anisotropic displacement parameters (Å² x 10⁴) for [PhBP\textsuperscript{Pr₃}Mn(CH₂Ph) (4). The anisotropic displacement factor exponent takes the form: -2π² [ h²a²U₁₁ + ... + 2 h k a* b* U₁₂ ]

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Table 21. Crystal Data and Structure Analysis Details for [PhBP\(^{Pr_3}\)]Mn(NH(2,6-\(^{Pr_2}\)-C\(_6\)H\(_3\)) (6).

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<th>Property</th>
<th>Value</th>
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<tr>
<td>Empirical formula</td>
<td>(C_{39}H_{71}BMnP_3)</td>
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<td>TMS(_2)O/petroleum ether</td>
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<td>Crystal shape</td>
<td>rough slab</td>
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<tr>
<td>Crystal color</td>
<td>yellow</td>
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<tr>
<td>Crystal size</td>
<td>0.11 x 0.26 x 0.37 mm</td>
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</table>

**Data Collection**

- Preliminary photograph(s): rotation
- Type of diffractometer: Bruker SMART 1000
- Wavelength: 0.71073 Å MoK\(_\alpha\)
- 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 \(\alpha = 98.393(2)^\circ\)
  - \(b = 11.249(1)\) Å \(\beta = 101.614(2)^\circ\)
  - \(c = 18.718(2)\) Å \(\gamma = 107.482(2)^\circ\)
  - 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: 
  - \(-14 \leq h \leq 14, -15 \leq k \leq 14, -24 \leq l \leq 24\)
- Data collection scan type: \(\omega\) scans
- Reflections collected: 42790
- Independent reflections: 9504 \([R_{int} = 0.0690]\)
- Reflections > 2\(\sigma(I)\): 6761
- Average \(\sigma(I)/(net I)\): 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

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<th>Primary solution method</th>
<th>direct methods</th>
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<td>Hydrogen placement</td>
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<td>Refinement method</td>
<td>Full-matrix least-squares on F^2</td>
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<tr>
<td>Data / restraints / parameters</td>
<td>9504 / 0 / 458</td>
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<tr>
<td>Treatment of hydrogen atoms</td>
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<tr>
<td>Goodness-of-fit on F^2</td>
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<td>Final R indices [I&gt;2σ(I), 6761 reflections]</td>
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</tr>
<tr>
<td>R indices (all data)</td>
<td>R1 = 0.0701, wR2 = 0.0726</td>
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<tr>
<td>Type of weighting scheme used</td>
<td>sigma</td>
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<tr>
<td>Weighting scheme used</td>
<td>calc w=1/([σ^2(Fo^2)] where P=(Fo^2+2Fc^2)/3</td>
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<tr>
<td>Max shift/error</td>
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<tr>
<td>Average shift/error</td>
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<tr>
<td>Largest diff. peak and hole</td>
<td>0.74 and -0.48 e·Å^3</td>
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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 (wR) 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 > 2σ(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 ($x \times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 x 10^3$) for [PhBP$^{iPr}_3$]Mn(NH(2,6-$^iPr_2$C$_6$H$_3$)) (6). $U_{eq}$ is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

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Table 23. Bond lengths [Å] and angles [°] for [PhBP\textsuperscript{ipr\_3}]Mn(NH(2,6-\textit{i}Pr\_2-C\textsubscript{6}H\textsubscript{3})) (6).

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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
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C(13)-C(14)-H(14) 111.46(13) C(24A)-C(23)-C(22) 121.8(3)
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Symmetry transformations used to generate equivalent atoms:
Table 24. Anisotropic displacement parameters (Å² x 10⁴) for [PhBP^(Pr)_3]Mn(NH(2,6-i-Pr_2-C_6H_3)) (6). The anisotropic displacement factor exponent takes the form: -2π² [h^2a^*2U_11 + ... + 2h k a^* b^* U_12 ]

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<tr>
<td>Space group</td>
<td>P 21/c (# 14)</td>
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<tr>
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<tr>
<td>F(000)</td>
<td>1564</td>
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<tr>
<td>Theta range for data collection</td>
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<tr>
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</tr>
<tr>
<td>Index ranges</td>
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<tr>
<td>Independent reflections</td>
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<tr>
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</tr>
<tr>
<td>Average σ(I)/(net I)</td>
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</tr>
<tr>
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Table 25 (cont.)

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<tr>
<td>Secondary solution method</td>
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<tr>
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<td>Treatment of hydrogen atoms</td>
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<tr>
<td>Goodness-of-fit on $F^2$</td>
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<td>Final R indices [I&gt;2$σ$(I), 8678 reflections]</td>
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<td>Max shift/error</td>
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<td>Average shift/error</td>
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<td>Largest diff. peak and hole</td>
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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 (wR) 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.

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<th>z</th>
<th>U_{eq}</th>
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Table 27. Bond lengths [Å] and angles [°] for [PhBP^iPr_3]Mn(dbabh) (7).

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<th>Angle [°]</th>
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Symmetry transformations used to generate equivalent atoms:
Table 28. Anisotropic displacement parameters (Å² x 10⁴) for [PhBPβPr₃]Mn(dbabh) (7). The anisotropic displacement factor exponent takes the form: -2\pi² [ h^2a^*^2U_11 + ... + 2hk a^* b^* U_12 ]

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

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Data Collection

- Preliminary photograph(s): rotation
- Type of diffractometer: Bruker SMART 1000
- Wavelength: 0.71073 Å MoK$_\alpha$
- 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, α = 90°
  - b = 77.737(4) Å, β = 90°
  - c = 11.2629(6) Å, 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 ≤ h ≤ 29, -108 ≤ k ≤ 105, -16 ≤ l ≤ 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%
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<td>R indices (all data)</td>
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<td>Type of weighting scheme used</td>
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<td>Weighting scheme used</td>
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<td>Largest diff. peak and hole</td>
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<tr>
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<td>Structure refinement</td>
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| **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 ($wR$) 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.

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S81
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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)
H(22A)-C(22)-H(22C) 109.5  N(C35)-C(34) 108.93(19)
H(22B)-C(22)-H(22C) 109.5  N(C35)-C(36) 123.10(19)
C(22)-C(23)-C(24) 112.45(19)  C(34)-C(35)-C(36) 127.22(19)
C(22)-C(23)-P(3) 110.65(16)  C(37)-C(36)-C(41) 117.01(19)
C(24)-C(23)-P(3) 114.53(15)  C(37)-C(36)-C(35) 122.12(19)
C(22)-C(23)-H(23) 106.2  C(41)-C(36)-C(35) 120.70(19)
C(24)-C(23)-H(23) 106.2  C(38)-C(37)-C(36) 121.6(2)
P(3)-C(23)-H(23) 106.2  C(38)-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)
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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
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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
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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
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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)
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C(30)-C(29)-C(34) 119.0(2)  C(1)-C(112)-H(112) 120.0
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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
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Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,-y+1/2,z
Table 32. Anisotropic displacement parameters (Å²) for [PhBP$_{3}$Pr$_{3}$]Mn(1-Ph(isoindolate)) (8). The anisotropic displacement factor exponent takes the form: \(-2\pi^2[ h^2a^*2U^{11} + \ldots + 2hka^*b^*U^{12}] \)

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<th>U$^{33}$</th>
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Table 33. Crystal Data and Structure Analysis Details for [PhBP$_{3}$]TlMnBr(CO)$_{4}$ (9).

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<tr>
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<td>benzene/petroleum ether</td>
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<td>Crystal shape</td>
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<td>Crystal color</td>
<td>yellow</td>
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<td>Crystal size</td>
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**Data Collection**

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<td>Data collection temperature</td>
<td>100 K</td>
</tr>
<tr>
<td>Theta range for 48690 reflections used in</td>
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</tr>
<tr>
<td>lattice determination</td>
<td></td>
</tr>
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<td>Unit cell dimensions</td>
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</tr>
<tr>
<td>Volume</td>
<td>3748.9(3) Å$^{3}$</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
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</tr>
<tr>
<td>Space group</td>
<td>P 21/n ( # 14)</td>
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<tr>
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<tr>
<td>F(000)</td>
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<td>ω scans</td>
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<td>Reflections &gt; 2σ(I)</td>
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<td>Average σ(I)/(net I)</td>
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<td>Absorption coefficient</td>
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<td>Absorption correction</td>
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<td>Max. and min. transmission</td>
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S85
## Decay of standards

0%

## Structure Solution and Refinement

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<td>Refinement method</td>
<td>Full-matrix least-squares on F^2</td>
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<tr>
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<tr>
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<tr>
<td>R indices (all data)</td>
<td>R1 = 0.0570, wR2 = 0.0555</td>
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<td>sigma</td>
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<td>Weighting scheme used</td>
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## Programs Used

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<td>Data reduction</td>
<td>Bruker SAINT 6.45</td>
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<td>Bruker SHELXTL 6.14</td>
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<tr>
<td>Structure refinement</td>
<td>Bruker SHELXTL 6.14</td>
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## Special Refinement Details

An absorption correction was applied using SADABS. Refinement of F^2 against ALL reflections. The weighted R-factor (wR) 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 > 2σ(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 (Å² x 10^3) for [PhBP_{3}^{Pr}]TlMnBr(CO)_{4} (9). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

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Table 35. Bond lengths [Å] and angles [°] for [PhBP\textsuperscript{ipr}_3]TlMnBr(CO)\textsubscript{4} (9).

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C(31)-Mn-Tl  172.74(8)  P(1)-C(7)-H(7A)  107.8
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C(28)-Mn-Tl  87.41(7)  P(1)-C(7)-H(7B)  107.8
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C(20)-P(2)-Tl  111.07(8)  P(3)-C(9)-H(9B)  107.0
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C(2)-C(3)-H(3)  120.1  C(13)-C(14)-H(14)  107.0
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Symmetry transformations used to generate equivalent atoms:
Table 36. Anisotropic displacement parameters (Å² x 10⁴) for [PhBP\textsuperscript{iPr}₃]TlMnBr(CO)₄ (9). The anisotropic displacement factor exponent takes the form: -2π²[h²a*²U\textsubscript{11} + ... + 2 h k a* b* U\textsubscript{12}]

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<th>U\textsuperscript{22}</th>
<th>U\textsuperscript{33}</th>
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<td>660(30)</td>
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Table 37. Crystal Data and Structure Analysis Details for [PhBP\textsuperscript{Pr}\textsubscript{3}]Mn(CN\textsuperscript{t}Bu)\textsubscript{3} (10).

<table>
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<tr>
<th>Property</th>
<th>Value</th>
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<tr>
<td>Empirical formula</td>
<td>C\textsubscript{42}H\textsubscript{80}BMnN\textsubscript{3}P\textsubscript{3}</td>
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<tr>
<td>Formula weight</td>
<td>785.75</td>
</tr>
<tr>
<td>Crystallization solvent</td>
<td>petroleum ether</td>
</tr>
<tr>
<td>Crystal shape</td>
<td>rough block</td>
</tr>
<tr>
<td>Crystal color</td>
<td>pale yellow</td>
</tr>
<tr>
<td>Crystal size</td>
<td>0.18 x 0.28 x 0.33 mm</td>
</tr>
</tbody>
</table>

**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  \(\alpha = 90^\circ\)
  - b = 17.578(1) Å  \(\beta = 93.660(2)^\circ\)
  - c = 23.108(1) Å  \(\gamma = 90^\circ\)
- Volume: 4580.4(5) Å\textsuperscript{3}
- Z: 4
- Crystal system: monoclinic
- Space group: P 21/n (# 14)
- Density (calculated): 1.139 g/cm\textsuperscript{3}
- F(000): 1712
- Theta range for data collection: 2.0 to 36.1°
- Completeness to theta = 36.13°: 89.9%
- Index ranges: -16 ≤ h ≤ 18, -28 ≤ k ≤ 28, -37 ≤ l ≤ 38
- Data collection scan type: \(\omega\) scans
- Reflections collected: 80212
- Independent reflections: 19689 \([R\text{int} = 0.0796]\)
- Reflections > 2\(\sigma(I)\): 13052
- Average \(\sigma(I)/(\text{net I})\): 0.0760
- Absorption coefficient: 0.42 mm\textsuperscript{-1}
- Absorption correction: none
- Reflections monitored for decay: initial data recollected at end
- Decay of standards: 0%
### Structure Solution and Refinement

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<th>Primary solution method</th>
<th>direct methods</th>
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<td>Secondary solution method</td>
<td>difference map</td>
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<td>Hydrogen placement</td>
<td>calculated</td>
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<td>Refinement method</td>
<td>Full-matrix least-squares on F^2</td>
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<tr>
<td>Data / restraints / parameters</td>
<td>19689 / 0 / 472</td>
</tr>
<tr>
<td>Treatment of hydrogen atoms</td>
<td>not refined, U_{iso} fixed at 120% U_{eq} of attached atom</td>
</tr>
<tr>
<td>Goodness-of-fit on F^2</td>
<td>1.28</td>
</tr>
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<td>Final R indices [I&gt;2\sigma(I), 13052 reflections]</td>
<td>( R1 = 0.0437, \ wR2 = 0.0707 )</td>
</tr>
<tr>
<td>R indices (all data)</td>
<td>( R1 = 0.0784, \ wR2 = 0.0752 )</td>
</tr>
<tr>
<td>Type of weighting scheme used</td>
<td>sigma</td>
</tr>
<tr>
<td>Weighting scheme used</td>
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<tr>
<td>Max shift/error</td>
<td>0.001</td>
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<tr>
<td>Average shift/error</td>
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<td>Largest diff. peak and hole</td>
<td>1.15 and -0.67 e\cdot\text{Å}^3</td>
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### Programs Used

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<td>Structure refinement</td>
<td>Bruker SHELXTL 6.14</td>
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### Special Refinement Details

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

Refinement of F^2 against ALL reflections. The weighted R-factor (wR) 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 ($x \times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for [PhBP$^{iPr}_3]$Mn(CN'tBu)$_3$ (10). $U_{eq}$ is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

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C(31)-H(31C)  0.9800  C(20)-P(2)-Mn  110.71(4)
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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)-Mn  114.48(4)
C(34)-C(36)  1.525(2)  C(23)-P(3)-Mn  116.51(4)
C(34)-C(37)  1.5248(19)  C(1)-B-C(7)  109.20(9)
C(35)-H(35A)  0.9800  C(1)-B-C(8)  107.10(9)
C(35)-H(35B)  0.9800  C(7)-B-C(8)  109.55(9)
C(35)-H(35C)  0.9800  C(1)-B-C(9)  109.58(9)
C(36)-H(36A)  0.9800  C(7)-B-C(9)  110.00(9)
C(36)-H(36B)  0.9800  C(8)-B-C(9)  111.35(9)
C(36)-H(36C)  0.9800  C(30)-N(1)-C(29)  173.50(14)
C(37)-H(37A)  0.9800  C(33)-N(2)-C(34)  174.29(13)
C(37)-H(37B)  0.9800  C(38)-N(3)-C(39)  153.99(12)
C(37)-H(37C)  0.9800  C(2)-C(1)-C(6)  114.56(10)
C(39)-C(40)  1.518(2)  C(2)-C(1)-B  122.86(10)
C(39)-C(41)  1.5199(18)  C(6)-C(1)-B  122.51(11)
C(39)-C(42)  1.5255(19)  C(3)-C(2)-C(1)  122.91(11)
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C(40)-H(40B)  0.9800  C(1)-C(2)-H(2)  118.5
C(40)-H(40C)  0.9800  C(4)-C(3)-C(2)  120.49(12)
C(41)-H(41A)  0.9800  C(4)-C(3)-H(3)  119.8
C(41)-H(41B)  0.9800  C(2)-C(3)-H(3)  119.8
C(41)-H(41C)  0.9800  C(5)-C(4)-C(3)  118.66(11)
C(42)-H(42A)  0.9800  C(5)-C(4)-H(4)  120.7
C(42)-H(42B)  0.9800  C(3)-C(4)-H(4)  120.7
C(42)-H(42C)  0.9800  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
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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
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Symmetry transformations used to generate equivalent atoms:
Table 40. Anisotropic displacement parameters (Å² x 10⁴) for \([\text{PhBP}^3\text{Pr}_3]Mn(\text{CN}^\text{tBu})_3\) (10). The anisotropic displacement factorexponent takes the form: 

\[-2\pi^2 \left[ h^2 a^{*2} U^{11} + \ldots + 2h k a^{*} b^{*} U^{12} \right] \]

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

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<tr>
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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 (wR) 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.

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

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N(1)-Mn-N(2)          | 128.7(4)   | 114.6     |
N(1)-Mn-N(2)#1        | 124.9(4)   | 114.6     |
N(2)-Mn-N(2)#1        | 94.2(3)    | 121.2(12) |
N(1)-Mn-I             | 97.2(2)    | 136.1(12) |
N(2)-Mn-I             | 103.0(2)   | 102.4(10) |
N(2)#1-Mn-I           | 105.5(2)   | 117.7(13) |
N(1)-Mn-Mn#1          | 151.5(3)   | 121.1     |
N(2)-Mn-Mn#1          | 47.8(2)    | 121.1     |
I-Mn-Mn#1             | 111.23(8)  |           |
C(8)-N(1)-C(1)        | 93.2(8)    | 118.2     |
C(8)-N(1)-Mn           | 115.4(7)   | 118.5(13) |
C(1)-N(1)-Mn          | 120.8(7)   | 120.7     |
C(8)-N(1)-H          | 108.8      | 120.7     |
C(1)-N(1)-H          | 108.8      | 117.0(13) |
Mn-N(1)-H             | 108.8      | 121.5     |
C(15)-N(2)-C(22)      | 96.2(8)    | 121.5     |
C(15)-N(2)-Mn         | 116.6(6)   | 121.8(11) |
C(22)-N(2)-Mn         | 123.2(6)   | 107.2(11) |
C(15)-N(2)-Mn#1      | 123.8(6)   | 130.8(13) |
C(22)-N(2)-Mn#1      | 113.8(6)   | 102.5(8)  |
Mn-N(2)-Mn#1         | 85.8(3)    | 99.0(7)   |
C(29)-N(3)-C(36)      | 95.5(8)    | 98.4(9)   |
C(29)-N(3)-H(3A)      | 110.8      |           |
C(36)-N(3)-H(3A)      | 111.5      | 117.8     |
C(46)-O-C(43)         | 115.0(9)   | 117.8     |
N(1)-C(1)-C(2)        | 99.9(9)    | 126.1(12) |
N(1)-C(1)-C(14)       | 98.6(10)   | 104.0(10) |
C(2)-C(1)-C(14)       | 105.0(9)   | 129.8(10) |
N(1)-C(1)-H(1)        | 116.8      | 112.8(11) |
C(2)-C(1)-H(1)        | 116.8      | 123.6     |
C(14)-C(1)-H(1)       | 116.8      | 123.6     |
C(7)-C(2)-C(3)        | 120.7(11)  | 122.0(12) |
C(7)-C(2)-C(1)        | 106.9(11)  | 119.0     |
C(3)-C(2)-C(1)        | 132.3(12)  | 119.0     |
C(4)-C(3)-C(2)        | 116.9(12)  | 124.7(13) |
C(4)-C(3)-H(3)        | 121.6      | 117.7     |
C(2)-C(3)-H(3)        | 121.6      | 117.7     |
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Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+1
Table 44. Anisotropic displacement parameters (Å² x 10⁴) for \{(Hdbabh)MnI(\mu-N-dbahh)\}_2. The anisotropic displacement factor exponent takes the form: -2\pi^2 [h²a*/h²U₁₁ + ... + 2hkab*U₁₂ ]

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