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A novel coordination mode for a phospholyl ligand: μ-phosphindolyl-$\kappa^2 P$:P-μ-1-phenylphosphindolyl-$\kappa^2 C^2$:P-bis[tetracarbonylmanganese(I)]

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Key indicators

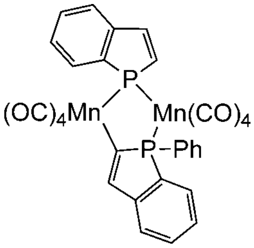
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.011 Å
R factor = 0.072
wR factor = 0.181
Data-to-parameter ratio = 13.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $[Mn_2(C_8H_6P)(C_{14}H_{11}P)(CO)_8]$, displays a novel coordination mode for a phospholyl ligand, where dinuclear coordination is observed through the P atom and the adjacent C atom of the heterocycle.

Comment

1,2-Dinuclear σ-complexes of heterocyclopentadienyls are rare and limited to a few sulfur-containing heterocycles and one example each for oxygen- (Arndt *et al.*, 2001) and nitrogen-containing (Arce *et al.*, 1998) rings. This bonding mode has not been reported for phospholyls or any benzannelated heterocyclopentadienyl ligand and is unknown for manganese complexes.



(I)

The unusual coordination mode in the title compound, (I), results in distortion from planarity of the phosphindolyl ligand; the eight C atoms of the bicyclic unit fit a least-squares plane to within 0.051 (6) Å, but P2 deviates by 0.152 (7) Å from this plane. The coordination of this ligand is twisted with respect to the Mn_2P_2 plane such that C22 is displaced from it by 0.629 (7) Å. The P2—C22 bond [1.793 (8) Å] is contracted in comparison to the P1—C2 bond [1.823 (7) Å], while the C22—Mn2 bond length [2.056 (8) Å] is comparable to the corresponding interatomic distance in $(\mu_2\text{-PPh}_2)(\sigma^1\text{-}\eta^5\text{-}C_4H_3S)Mn_2(CO)_6$ [2.079 (2) Å], the closest analogue to (I) (Deeming *et al.*, 1999). The (phosphindolyl)$Mn_2(CO)_8$ fragment is highly symmetric, such that the planar heterocycle is almost orthogonal to the Mn_2P_2 plane [dihedral angle = 88.16 (9)°] and the two $Mn(CO)_4$ moieties are slightly rotated [10.1 (4)°] from an eclipsed conformation as determined by the (OC)—Mn···Mn—(CO) dihedral angles. The Mn—P distances involving P1 [2.401 (2) and 2.382 (2) Å] are longer than those observed in the related compound bis(μ_2-dibenzophospholyl)bis[manganesetetracarbonyl(I)] [2.3670 (4) and 2.3718 (5) Å] (Decken *et al.*, 2001) that contains two phospholyl ligands that bridge the metal centers exclusively though P atoms.

Experimental

The title compound was obtained in trace quantities in the synthesis of (η^5-phosphindolyl)Mn(CO)$_3$ (Decken *et al.*, 2004).

Crystal data

[$Mn_2(C_8H_6P)(C_{14}H_{11}P)(CO)_8$]
M_r = 676.25
Monoclinic, $C2/c$
a = 20.681 (2) Å
b = 9.8850 (9) Å
c = 28.440 (2) Å
β = 100.368 (4)°
V = 5719.2 (9) Å^3
Z = 8
D_x = 1.571 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4864 reflections
θ = 2.2–30.5°
μ = 1.05 mm^{-1}
T = 173 (2) K
Irregular fragment, orange
0.25 × 0.15 × 0.10 mm

Data collection

Bruker SMART1000/P4 CCD area detector diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997*a*)
$T_{\min}$ = 0.765, $T_{\max}$ = 0.903
18 319 measured reflections
5036 independent reflections
2916 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.067
$\theta_{\max}$ = 25.0°
$h = -24 \rightarrow 24$
$k = -11 \rightarrow 11$
$l = -33 \rightarrow 33$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.072
$wR(F^2)$ = 0.181
S = 0.97
5036 reflections
379 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.097P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 1.21 e Å^{-3}
$\Delta\rho_{\min}$ = −0.51 e Å^{-3}

H atoms were placed in calculated positions (C—H = 0.93 Å) and refined as riding, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). The highest electron-density peak is 1 Å from atom P2.

Data collection: *SMART* (Bruker, 1997–1999); cell refinement: *SAINT* (Bruker, 1997–2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

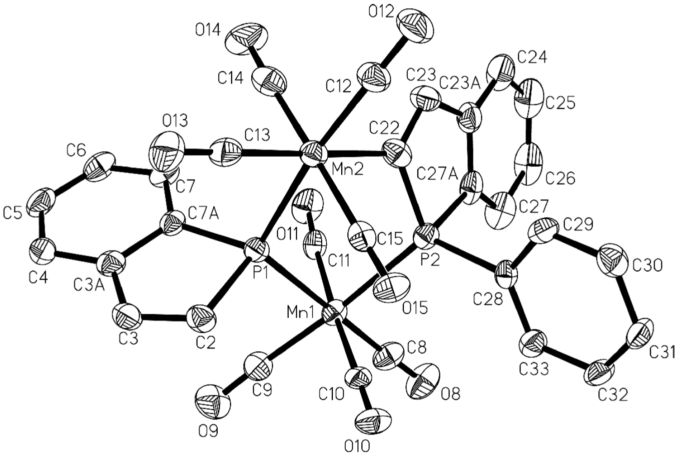


Figure 1
A view of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity.

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