Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

The binuclear μ-phenylvinylidene complex $(\eta^5\text{-}C_5H_5)(CO)(\mu\text{-}CO)MnPt(\mu\text{-}C{=}CHPh)(\eta^2\text{-}Ph_2PCH_2PPh_2)\cdot Et_2O$

Fedor M. Dolgushin,[a]* Nina A. Deykhina,[b] Dmitry A. Pogrebnyakov[b] and Alla B. Antonova[b]

[a]A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Vavilov St. 28, Moscow 119991, Russian Federation, and [b]Institute of Chemistry and Chemical Technology, Russian Academy of Sciences, Siberian Branch, Karl Marx St. 42, Krasnoyarsk 660049, Russian Federation

Correspondence e-mail: fedya@xrlab.ineos.ac.ru

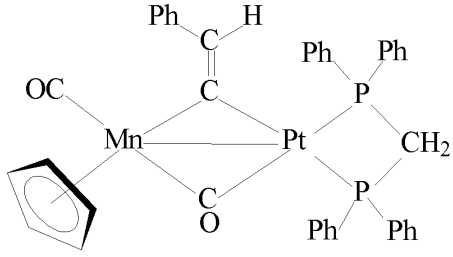
Received 10 October 2001
Accepted 16 October 2001
Online 20 October 2001

Key indicators

Single-crystal X-ray study
T = 110 K
Mean σ(C–C) = 0.010 Å
Disorder in solvent or counterion
R factor = 0.054
wR factor = 0.129
Data-to-parameter ratio = 21.0

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

The title compound, [bis(diphenylphosphino)methane-2κ^2P,P']-μ-carbonyl-1:2κC-carbonyl-1κC-[1(η^5)-cyclopentadienyl](μ-phenylvinylidene-1:2κ^2C)manganeseplatinum(*Mn—Pt*) diethyl ether solvate, $(\eta^5\text{-}C_5H_5)(CO)(\mu\text{-}CO)MnPt(\mu\text{-}C{=}CHPh)(\eta^2\text{-}Ph_2PCH_2PPh_2)\cdot Et_2O$ or $[MnPt(C_5H_5)(C_8H_6)(C_{25}H_{22}P_2)(CO)_2]\cdot C_4H_{10}O$, represents the first example of a structurally characterized μ-vinylidene Mn—Pt complex [Mn—Pt 2.6068 (10) Å]. Two metal atoms are bridged by a μ-phenylvinylidene ligand [Mn—C 1.924 (7), Pt—C 1.991 (6) and C=C 1.363 (9) Å] and an asymmetrical μ-carbonyl ligand [Mn—C 1.826 (7), Pt—C 2.212 (7), C—O 1.189 (8) Å, Mn—C—O 153.4 (6) and Pt—C—O 126.7 (5)°].



Et_2O

(I)

Experimental

The title compound was prepared according to a known procedure (Antonova *et al.*, 1991). Suitable single crystals were obtained by isothermal evaporation of a solution in benzene–ether (2:1) at 258 K.

Crystal data

$[MnPt(C_5H_5)(C_8H_6)(C_{25}H_{22}P_2)(CO)_2]\cdot C_4H_{10}O$
M_r = 931.75
Orthorhombic, *Pbca*
a = 18.3417 (18) Å
b = 18.3164 (18) Å
c = 23.547 (2) Å
V = 7910.7 (14) Å^3
Z = 8
D_x = 1.565 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 932 reflections
θ = 2–24°
μ = 3.97 mm^{-1}
T = 110 (2) K
Prism, orange
0.4 × 0.2 × 0.2 mm

Data collection

CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.443, T_{max} = 0.694
55 551 measured reflections
9557 independent reflections
5404 reflections with $I > 2\sigma(I)$
R_{int} = 0.070
θ_{max} = 28.1°
$h = -24 \rightarrow 23$
$k = -24 \rightarrow 11$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.054$	$w = 1/[\sigma^2(F_o^2) + (0.06P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.129$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.97$	$\Delta\rho_{max} = 1.91$ e Å^{-3}
9557 reflections	$\Delta\rho_{min} = -1.67$ e Å^{-3}
455 parameters	

Table 1
Selected geometric parameters (Å, °).

Pt1—Mn1	2.6068 (10)	Mn1—C12	2.112 (7)
Pt1—P1	2.3312 (16)	Mn1—C13	2.137 (7)
Pt1—P2	2.2796 (17)	Mn1—C14	2.178 (7)
Pt1—C1	1.991 (6)	Mn1—C15	2.146 (7)
Pt1—C3	2.212 (7)	O3—C3	1.189 (8)
Mn1—C1	1.924 (7)	O4—C4	1.153 (8)
Mn1—C3	1.826 (7)	C1—C2	1.363 (9)
Mn1—C4	1.775 (8)	C2—C5	1.469 (9)
Mn1—C11	2.126 (7)		
C1—Pt1—C3	89.1 (3)	C4—Mn1—C1	92.4 (3)
C1—Pt1—P2	102.7 (2)	C3—Mn1—C1	103.8 (3)
C3—Pt1—P2	166.9 (2)	C2—C1—Mn1	143.2 (5)
C1—Pt1—P1	169.4 (2)	C2—C1—Pt1	132.5 (5)
C3—Pt1—P1	96.47 (19)	Mn1—C1—Pt1	83.5 (2)
P2—Pt1—P1	72.83 (6)	C1—C2—C5	126.5 (6)
C1—Pt1—Mn1	47.17 (19)	O3—C3—Mn1	153.4 (6)
C3—Pt1—Mn1	43.57 (19)	O3—C3—Pt1	126.7 (5)
P2—Pt1—Mn1	149.17 (5)	Mn1—C3—Pt1	79.8 (3)
P1—Pt1—Mn1	135.32 (5)	O4—C4—Mn1	176.3 (6)
C4—Mn1—C3	90.8 (3)	P2—C16—P1	95.9 (3)

The solvate diethyl ether molecule is disordered over two positions with occupancies of 0.6 and 0.4. All atoms of the solvate molecule were refined isotropically and the C—O and C—C distances were restrained by *SHELXL DFIX* instructions to values of 1.426 and 1.530 Å, respectively (Allen *et al.*, 1987). H atoms were placed in calculated positions with U_{iso} constrained to be 1.2 times U_{eq} of the carrier atom. The highest peak in the final difference map is 0.91 Å from the Mn atom.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT–Plus* (Bruker, 1998); data reduction: *SAINT–Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported by the Russian Foundation for Basic Research (project Nos. 99-03-33027 and 00-03-32807) and INTAS (project No. 00-291). DAP thanks the Krasnoyarsk Regional Science Foundation for individual support.

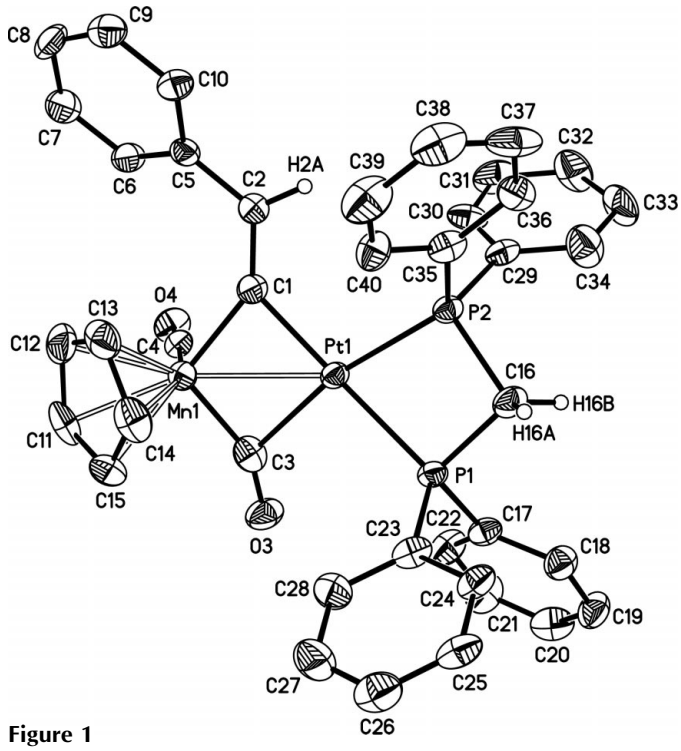


Figure 1
A view of the title compound showing the atom labeling and displacement ellipsoids at the 50% probability level. The disordered ether and the H atoms of the phenyl groups and cyclopentadienyl ligand have been omitted for clarity.

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