Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

μ-Carbonyl-1:2κ^2C-carbonyl-1κC-(1η^5-cyclopentadienyl)(μ-phenylvinylidene)-bis(triphenylphosphine-2κP)manganese-platinum(*Mn—Pt*)

Alexander D. Vasiliev,[a]* Alla B. Antonova[b] and Oleg S. Chudin[b]

[a]Institute of Physics, SB RAS, Krasnoyarsk 660036, Russian Federation, and [b]Institute of Chemistry and Chemical Technology, SB RAS, Karl Marx Street 42, Krasnoyarsk 660049, Russian Federation
Correspondence e-mail: adva@iph.krasn.ru

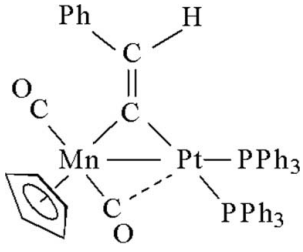
Received 9 June 2007; accepted 2 July 2007

Key indicators: single-crystal X-ray study; T = 283 K; mean σ(C–C) = 0.005 Å; R factor = 0.020; wR factor = 0.045; data-to-parameter ratio = 22.3.

The title compound, $[MnPt(C_5H_5)(C_8H_6)(C_{18}H_{15}P)_2(CO)_2]$, is a dinuclear heterometallic Mn—Pt(μ-C═CHPh) complex obtained as a product of the addition of $[Pt(PPh_3)]_2$ to $(\eta^5$-$C_5H_5)(CO)_2Mn{=}C{=}CHPh$. The two metal atoms are bridged by the μ-phenylvinylidene ligand and semibridged by a carbonyl group. The central fragment of the molecule is an almost planar methylenedimetallacyclopropane Mn—Pt(μ-C═CHPh) system. The coordination of the Mn atom is formed by two parallel planes: the first plane consists of three carbonyl C atoms and the second is the cyclopentadienyl plane. A distorted square-planar coordination of the Pt atom is formed by two P atoms of PPh_3 and C atoms of the semi-bridging and C═CHPh ligands.

Related literature

Corresponding geometry in the related MnPt complex with the chelating bis(diphenylphosphino)methane ligand was reported by Dolgushin *et al.* (2001). For crystal structures of related μ-carbene complexes containing the Mn—Pt-μ-C triangle system, see: Jeffery *et al.* (1981). For details of the synthesis, see: Antonova *et al.* (1985).



Experimental

Crystal data

$[MnPt(C_5H_5)(C_8H_6)(C_{18}H_{15}P)_2(CO)_2]$
M_r = 997.81
Orthorhombic, $P2_12_12_1$
a = 11.1320 (4) Å
b = 19.4463 (7) Å
c = 19.5174 (7) Å
V = 4225.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.72 mm^{-1}
T = 283 (2) K
0.29 × 0.17 × 0.14 mm

Data collection

Bruker SMART 4 K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.352, T_{max} = 0.624
37385 measured reflections
9675 independent reflections
8974 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.045
S = 0.95
9675 reflections
433 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), with 4291 Friedel pairs
Flack parameter: −0.007 (3)

Table 1
Selected bond lengths (Å).

Pt—C1	2.006 (3)	Mn—C4	1.761 (4)
Pt—C3	2.397 (3)	Mn—C11	2.129 (3)
Pt—P1	2.2745 (7)	Mn—C12	2.127 (3)
Pt—P2	2.3548 (8)	Mn—C13	2.158 (3)
Pt—Mn	2.6344 (4)	Mn—C14	2.167 (3)
Mn—C1	1.972 (3)	Mn—C15	2.149 (3)
Mn—C3	1.811 (3)		

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2004); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported by the Council of the President of the Russian Federation for Support of Young Scientists and Leading Scientific Schools (project No. NSh-4137.2006.2) and the Krasnoyarsk Regional Science Foundation (grant Nos. 10TS145 and 17 G002).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2263).

References

Antonova, A. B., Kovalenko, S. V., Korniyets, E. D., Petrovskii, P. V., Gulbis, G. R. & Johansson, A. A. (1985). *Inorg. Chim. Acta*, **96**, 1–7.
Bruker (1998). *SAINT* (Version 7.34a) and *SMART* (Version 5.059). Bruker AXS Inc., Madison, Wisconsin, USA.
Dolgushin, F. M., Deykhina, N. A., Pogrebnyakov, D. A. & Antonova, A. B. (2001). *Acta Cryst.* E**57**, m541–m542.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Jeffery, J. C., Navarro, R., Razay, H. & Stone, F. G. A. (1981). *J. Chem. Soc. Dalton Trans.* pp. 2471–2478.
Sheldrick, G. M. (2004). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2004). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

 doi:10.1107/S1600536807032254

supplementary materials

Acta Cryst. (2007). E**63**, m2097 [**doi:10.1107/S1600536807032254**]

μ-Carbonyl-1:2κ^2*C*-carbonyl-1κ*C*-(1η^5-cyclopentadienyl)(μ-phenylvinylidene)bis(triphenylphosphine-2κ*P*)manganeseplatinum(*Mn-Pt*)

A. D. Vasiliev, A. B. Antonova and O. S. Chudin

Comment

The molecule of the title compound, (I), is the dinuclear complex containing the Mn and Pt atoms bridged by the μ-phenylvinylidene ligand and semi-bridged by carbonyl group. The phenyl ring and the C═C bond of vinylidene coupling with the Mn—Pt-μ-C triangle form an almost planar system. Corresponding geometry was found for the related MnPt complex with chelating bis(diphenylphosphino)methane at the Pt atom (Dolgushin *et al.*, 2001). The structures of some μ-carbene complexes containing the Mn—Pt-μ-C triangle system as a molecular central fragment were reported (Jeffery *et al.*, 1981).

Experimental

The title compound was prepared by the interaction between $Cp(CO)_2Mn{=}C{=}CHPh$ and $Pt(PPh_3)_4$ (diethyl ether, 298 K, 1 h) (Antonova *et al.*, 1985). Suitable single crystals were obtained by isothermal evaporation of an ether solution at 298 K.

Refinement

Seven phenyl rings of the title molecule were idealized and refined as rigid groups with C—C bond lengths of 1.390 Å. All H atoms were positioned geometrically (C—H 0.93 Å) and refined using a riding model with U_{iso}(H) = 1.2 U_{eq}(C).

Figures

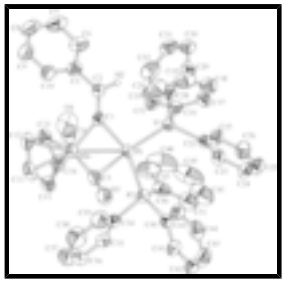


Fig. 1. The molecular structure of the title compound with atomic labels and 50% probability displacement ellipsoids. All H-atoms, except H2, omitted for clarity.

μ-Carbonyl-1:2κ^2*C*-carbonyl-1κ*C*-(1η^5-cyclopentadienyl)(μ- phenylvinylidene)bis(triphenylphosphine-2κ*P*)manganeseplatinum(Mn—Pt)

Crystal data

$[MnPt(C_5H_5)(C_8H_6)(C_{18}H_{15}P)_2(CO)_2]$	F_{000} = 1984
M_r = 997.81	D_x = 1.569 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å

Hall symbol: P 2ac 2ab	Cell parameters from 9978 reflections
a = 11.1320 (4) Å	θ = 2.4–27.5º
b = 19.4463 (7) Å	μ = 3.72 mm^{-1}
c = 19.5174 (7) Å	T = 283 (2) K
V = 4225.1 (3) $Å^3$	Block, red
Z = 4	0.29 × 0.17 × 0.14 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer	9675 independent reflections
Radiation source: sealed tube	8974 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 283(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	h = −14→14
T_{min} = 0.352, T_{max} = 0.624	k = −25→25
37385 measured reflections	l = −25→25

Refinement

Refinement on F^2	Hydrogen site location: constr
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.020	$w = 1/[\sigma^2(F_o^2) + (0.0241P)^2 + 2.8014P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.045	$(\Delta/\sigma)_{max}$ = 0.011
S = 0.95	$\Delta\rho_{max}$ = 0.63 e $Å^{-3}$
9675 reflections	$\Delta\rho_{min}$ = −0.25 e $Å^{-3}$
433 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 4291 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.007 (3)

Special details

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

Refinement. 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 $F^2 > \sigma(F^2)$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Pt	0.442096 (9)	0.414461 (5)	0.378591 (5)	0.03419 (3)
Mn	0.22734 (4)	0.46992 (2)	0.36592 (2)	0.03741 (10)
C3	0.2363 (3)	0.37832 (16)	0.38176 (18)	0.0476 (7)
O3	0.2169 (2)	0.32086 (12)	0.39299 (14)	0.0623 (7)
C4	0.1687 (3)	0.47710 (18)	0.44942 (19)	0.0527 (8)
O4	0.1316 (3)	0.48242 (15)	0.50469 (14)	0.0829 (9)
C11	0.0687 (3)	0.48385 (18)	0.30666 (18)	0.0572 (9)
H11	−0.0055	0.4656	0.3190	0.069*
C12	0.1152 (3)	0.54915 (18)	0.32649 (17)	0.0523 (8)
H12	0.0768	0.5811	0.3543	0.063*
C13	0.2283 (3)	0.55672 (17)	0.29704 (16)	0.0465 (7)
H13	0.2784	0.5947	0.3015	0.056*
C14	0.2538 (3)	0.49653 (17)	0.25917 (15)	0.0476 (7)
H14	0.3236	0.4877	0.2345	0.057*
C15	0.1545 (3)	0.45249 (17)	0.26547 (17)	0.0535 (9)
H15	0.1473	0.4093	0.2454	0.064*
C1	0.3757 (2)	0.50564 (15)	0.40819 (14)	0.0367 (6)
C2	0.4220 (3)	0.56321 (15)	0.43342 (16)	0.0451 (7)
H2	0.4997	0.5584	0.4502	0.054*
C5	0.37250 (19)	0.63388 (8)	0.43978 (11)	0.0466 (7)
C6	0.45344 (16)	0.68831 (12)	0.43990 (13)	0.0639 (9)
H6	0.5355	0.6797	0.4372	0.077*
C7	0.4117 (2)	0.75556 (10)	0.44408 (13)	0.0756 (12)
H7	0.4659	0.7920	0.4442	0.091*
C8	0.2891 (3)	0.76837 (8)	0.44814 (13)	0.0763 (13)
H8	0.2612	0.8134	0.4509	0.092*
C9	0.20817 (18)	0.71395 (12)	0.44802 (12)	0.0665 (11)
H9	0.1261	0.7225	0.4507	0.080*
C10	0.24987 (17)	0.64670 (10)	0.44383 (11)	0.0509 (8)
H10	0.1957	0.6103	0.4438	0.061*
P1	0.61667 (6)	0.41618 (4)	0.43912 (3)	0.03333 (14)
C16	0.58867 (16)	0.41181 (11)	0.53218 (7)	0.0375 (6)
C17	0.67643 (14)	0.38760 (11)	0.57673 (10)	0.0492 (8)
H17	0.7493	0.3718	0.5596	0.059*
C18	0.65531 (19)	0.38708 (12)	0.64692 (9)	0.0590 (9)
H18	0.7140	0.3709	0.6767	0.071*
C19	0.5464 (2)	0.41076 (13)	0.67256 (7)	0.0680 (10)
H19	0.5323	0.4104	0.7195	0.082*
C20	0.45865 (17)	0.43497 (12)	0.62802 (10)	0.0678 (10)
H20	0.3858	0.4508	0.6452	0.081*
C21	0.47977 (15)	0.43550 (11)	0.55783 (10)	0.0505 (8)
H21	0.4210	0.4517	0.5280	0.061*
C22	0.73105 (14)	0.34921 (8)	0.42635 (11)	0.0349 (6)
C23	0.71731 (16)	0.28461 (10)	0.45581 (10)	0.0481 (8)
H23	0.6498	0.2750	0.4822	0.058*

C24	0.8044 (2)	0.23441 (8)	0.44583 (12)	0.0587 (9)
H24	0.7953	0.1912	0.4655	0.070*
C25	0.90533 (17)	0.24880 (10)	0.40639 (12)	0.0617 (10)
H25	0.9636	0.2152	0.3997	0.074*
C26	0.91907 (14)	0.31340 (11)	0.37693 (12)	0.0617 (9)
H26	0.9866	0.3230	0.3505	0.074*
C27	0.83193 (17)	0.36360 (8)	0.38691 (11)	0.0512 (8)
H27	0.8411	0.4068	0.3672	0.061*
C28	0.70882 (17)	0.49435 (9)	0.42915 (11)	0.0394 (7)
C29	0.7922 (2)	0.51345 (10)	0.47865 (10)	0.0567 (9)
H29	0.8022	0.4867	0.5177	0.068*
C30	0.86057 (18)	0.57258 (11)	0.46976 (12)	0.0675 (11)
H30	0.9163	0.5854	0.5029	0.081*
C31	0.8456 (2)	0.61260 (9)	0.41137 (13)	0.0636 (10)
H31	0.8914	0.6522	0.4054	0.076*
C32	0.7623 (2)	0.59349 (10)	0.36187 (10)	0.0669 (10)
H32	0.7523	0.6203	0.3228	0.080*
C33	0.69389 (18)	0.53437 (11)	0.37076 (10)	0.0524 (8)
H33	0.6381	0.5216	0.3376	0.063*
P2	0.47665 (7)	0.32551 (4)	0.29914 (4)	0.03942 (18)
C34	0.36562 (19)	0.32082 (12)	0.22906 (10)	0.0497 (8)
C35	0.2647 (2)	0.27973 (11)	0.23820 (12)	0.0650 (11)
H35	0.2570	0.2532	0.2776	0.078*
C36	0.1754 (2)	0.27830 (14)	0.18846 (17)	0.0879 (15)
H36	0.1079	0.2508	0.1946	0.105*
C37	0.1870 (3)	0.31797 (17)	0.12958 (14)	0.107 (2)
H37	0.1272	0.3170	0.0963	0.128*
C38	0.2879 (3)	0.35906 (15)	0.12044 (10)	0.0996 (16)
H38	0.2956	0.3856	0.0810	0.120*
C39	0.3772 (2)	0.36048 (12)	0.17018 (12)	0.0717 (11)
H39	0.4447	0.3880	0.1641	0.086*
C40	0.48294 (18)	0.23474 (8)	0.32309 (10)	0.0408 (7)
C41	0.4953 (2)	0.18370 (11)	0.27372 (8)	0.0534 (8)
H41	0.4983	0.1954	0.2276	0.064*
C42	0.5033 (2)	0.11515 (9)	0.29336 (12)	0.0644 (10)
H42	0.5116	0.0810	0.2603	0.077*
C43	0.4989 (2)	0.09763 (8)	0.36236 (14)	0.0696 (11)
H43	0.5042	0.0518	0.3755	0.083*
C44	0.4865 (2)	0.14866 (12)	0.41172 (9)	0.0654 (10)
H44	0.4835	0.1369	0.4579	0.079*
C45	0.47853 (19)	0.21722 (10)	0.39209 (9)	0.0514 (8)
H45	0.4702	0.2514	0.4251	0.062*
C46	0.61840 (18)	0.34361 (13)	0.25456 (11)	0.0539 (9)
C47	0.6366 (3)	0.41109 (12)	0.23350 (14)	0.0776 (12)
H47	0.5772	0.4439	0.2408	0.093*
C48	0.7435 (3)	0.42947 (15)	0.20160 (15)	0.112 (2)
H48	0.7557	0.4746	0.1875	0.134*
C49	0.8322 (2)	0.3804 (2)	0.19075 (15)	0.124 (3)
H49	0.9038	0.3927	0.1694	0.149*

C50	0.8140 (2)	0.31289 (19)	0.21181 (15)	0.1025 (18)
H50	0.8734	0.2800	0.2046	0.123*
C51	0.7071 (2)	0.29451 (12)	0.24372 (13)	0.0691 (11)
H51	0.6950	0.2494	0.2578	0.083*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt	0.02976 (5)	0.03379 (5)	0.03903 (5)	0.00328 (4)	−0.00323 (5)	−0.00160 (5)
Mn	0.0300 (2)	0.0391 (2)	0.0431 (3)	0.00275 (17)	−0.00165 (19)	0.0078 (2)
C3	0.0390 (15)	0.0498 (18)	0.0541 (19)	−0.0004 (13)	−0.0131 (16)	0.0089 (17)
O3	0.0487 (13)	0.0455 (13)	0.093 (2)	−0.0087 (10)	−0.0133 (13)	0.0173 (13)
C4	0.0438 (18)	0.055 (2)	0.059 (2)	0.0040 (16)	0.0026 (17)	0.0154 (17)
O4	0.090 (2)	0.097 (2)	0.0622 (17)	0.0087 (17)	0.0326 (16)	0.0184 (15)
C11	0.0343 (17)	0.069 (2)	0.068 (2)	−0.0031 (18)	−0.0116 (18)	0.0224 (18)
C12	0.0473 (18)	0.057 (2)	0.053 (2)	0.0162 (16)	−0.0060 (15)	0.0099 (16)
C13	0.0469 (18)	0.0446 (17)	0.0480 (18)	0.0006 (14)	−0.0064 (15)	0.0105 (14)
C14	0.0517 (19)	0.054 (2)	0.0376 (16)	0.0057 (16)	−0.0038 (14)	0.0048 (14)
C15	0.059 (2)	0.0473 (19)	0.054 (2)	−0.0007 (16)	−0.0217 (17)	0.0066 (15)
C1	0.0316 (14)	0.0388 (16)	0.0396 (15)	0.0069 (12)	0.0003 (12)	−0.0027 (12)
C2	0.0403 (17)	0.0436 (16)	0.0514 (17)	0.0076 (13)	−0.0065 (14)	−0.0063 (13)
C5	0.056 (2)	0.0446 (18)	0.0386 (17)	0.0059 (15)	−0.0002 (14)	−0.0043 (14)
C6	0.072 (3)	0.051 (2)	0.068 (2)	−0.010 (2)	0.005 (2)	−0.0109 (17)
C7	0.106 (3)	0.041 (2)	0.080 (3)	−0.008 (2)	0.003 (2)	−0.0045 (19)
C8	0.120 (4)	0.043 (2)	0.066 (3)	0.017 (2)	−0.013 (3)	−0.0073 (18)
C9	0.080 (3)	0.061 (2)	0.058 (2)	0.027 (2)	−0.010 (2)	−0.0063 (18)
C10	0.059 (2)	0.0469 (19)	0.0462 (19)	0.0103 (16)	−0.0040 (15)	−0.0026 (15)
P1	0.0283 (3)	0.0347 (3)	0.0370 (4)	0.0017 (3)	−0.0003 (3)	−0.0014 (3)
C16	0.0362 (14)	0.0360 (14)	0.0403 (14)	−0.0019 (13)	0.0017 (11)	−0.0037 (14)
C17	0.0465 (18)	0.057 (2)	0.0438 (18)	0.0013 (15)	−0.0061 (14)	−0.0044 (14)
C18	0.076 (2)	0.058 (2)	0.0427 (18)	−0.0018 (18)	−0.0076 (17)	−0.0030 (15)
C19	0.100 (3)	0.068 (2)	0.0370 (16)	−0.004 (3)	0.0128 (19)	−0.0091 (17)
C20	0.074 (2)	0.074 (2)	0.056 (2)	0.0110 (19)	0.023 (2)	−0.0104 (18)
C21	0.0527 (19)	0.0512 (19)	0.0475 (18)	0.0101 (15)	0.0081 (15)	−0.0024 (14)
C22	0.0291 (14)	0.0395 (16)	0.0363 (15)	0.0046 (12)	−0.0008 (11)	−0.0031 (12)
C23	0.0418 (18)	0.0488 (19)	0.054 (2)	0.0067 (14)	0.0009 (15)	0.0010 (15)
C24	0.067 (2)	0.0404 (18)	0.069 (2)	0.0173 (17)	−0.0057 (19)	−0.0005 (16)
C25	0.053 (2)	0.059 (2)	0.073 (2)	0.0256 (17)	−0.0055 (17)	−0.0111 (19)
C26	0.0396 (17)	0.071 (2)	0.075 (2)	0.0102 (15)	0.0130 (18)	−0.010 (2)
C27	0.0396 (16)	0.0487 (17)	0.065 (2)	0.0065 (13)	0.0086 (17)	0.0031 (17)
C28	0.0326 (15)	0.0343 (15)	0.0513 (18)	0.0027 (12)	0.0053 (13)	−0.0041 (13)
C29	0.055 (2)	0.0459 (19)	0.069 (2)	−0.0013 (16)	−0.0159 (17)	0.0033 (17)
C30	0.056 (2)	0.041 (2)	0.106 (3)	−0.0062 (16)	−0.017 (2)	−0.0147 (19)
C31	0.055 (2)	0.0401 (18)	0.095 (3)	−0.0094 (16)	0.014 (2)	−0.0115 (19)
C32	0.081 (2)	0.050 (2)	0.070 (2)	−0.0014 (19)	0.019 (2)	0.0101 (19)
C33	0.0588 (19)	0.0487 (17)	0.0497 (19)	−0.0058 (15)	0.0030 (17)	0.0020 (16)
P2	0.0405 (4)	0.0372 (4)	0.0406 (4)	0.0017 (3)	−0.0012 (3)	−0.0043 (3)
C34	0.062 (2)	0.0414 (18)	0.0456 (18)	0.0124 (16)	−0.0118 (16)	−0.0120 (14)

C35	0.062 (2)	0.046 (2)	0.088 (3)	0.0081 (17)	−0.028 (2)	−0.0165 (19)
C36	0.078 (3)	0.065 (3)	0.121 (4)	0.014 (2)	−0.047 (3)	−0.040 (3)
C37	0.125 (4)	0.111 (4)	0.084 (4)	0.050 (3)	−0.063 (3)	−0.050 (3)
C38	0.143 (5)	0.111 (4)	0.044 (2)	0.042 (3)	−0.025 (3)	−0.007 (3)
C39	0.091 (3)	0.079 (3)	0.045 (2)	0.018 (2)	−0.006 (2)	−0.0082 (19)
C40	0.0361 (15)	0.0367 (16)	0.0498 (17)	0.0043 (12)	−0.0015 (12)	−0.0017 (13)
C41	0.0520 (19)	0.0454 (19)	0.063 (2)	0.0126 (15)	0.0006 (17)	−0.0043 (16)
C42	0.056 (2)	0.045 (2)	0.092 (3)	0.0104 (17)	−0.003 (2)	−0.0141 (19)
C43	0.060 (2)	0.044 (2)	0.104 (3)	0.0073 (16)	0.000 (2)	0.015 (2)
C44	0.055 (2)	0.069 (3)	0.072 (2)	−0.0015 (18)	−0.0058 (18)	0.020 (2)
C45	0.0461 (17)	0.0490 (18)	0.059 (2)	0.0055 (13)	−0.0013 (15)	0.0006 (15)
C46	0.055 (2)	0.066 (2)	0.0409 (18)	−0.0111 (18)	0.0037 (16)	−0.0115 (16)
C47	0.094 (3)	0.075 (3)	0.063 (2)	−0.031 (3)	0.013 (2)	−0.004 (2)
C48	0.137 (5)	0.121 (5)	0.076 (3)	−0.074 (4)	0.035 (3)	−0.009 (3)
C49	0.096 (4)	0.199 (7)	0.076 (3)	−0.075 (4)	0.030 (3)	−0.046 (4)
C50	0.056 (3)	0.168 (5)	0.083 (3)	−0.017 (3)	0.019 (2)	−0.045 (3)
C51	0.051 (2)	0.092 (3)	0.064 (2)	−0.005 (2)	0.0084 (18)	−0.017 (2)

Geometric parameters (Å, °)

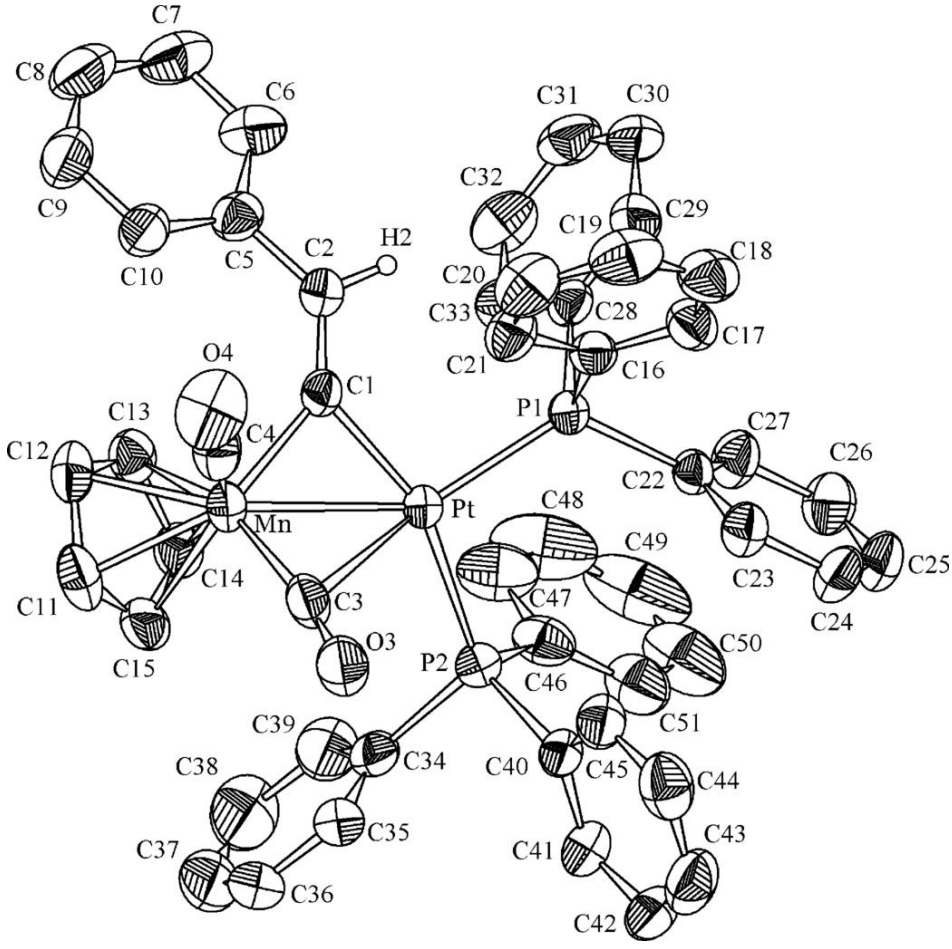
Pt—C1	2.006 (3)	C23—H23	0.9300
Pt—C3	2.397 (3)	C24—C25	1.3900
Pt—P1	2.2745 (7)	C24—H24	0.9300
Pt—P2	2.3548 (8)	C25—C26	1.3900
Pt—Mn	2.6344 (4)	C25—H25	0.9300
Mn—C1	1.972 (3)	C26—C27	1.3900
Mn—C3	1.811 (3)	C26—H26	0.9300
Mn—C4	1.761 (4)	C27—H27	0.9300
Mn—C11	2.129 (3)	C28—C29	1.3900
Mn—C12	2.127 (3)	C28—C33	1.3900
Mn—C13	2.158 (3)	C29—C30	1.3900
Mn—C14	2.167 (3)	C29—H29	0.9300
Mn—C15	2.149 (3)	C30—C31	1.3900
C3—O3	1.159 (3)	C30—H30	0.9300
C4—O4	1.160 (4)	C31—C32	1.3900
C11—C15	1.390 (5)	C31—H31	0.9300
C11—C12	1.425 (5)	C32—C33	1.3900
C11—H11	0.9300	C32—H32	0.9300
C12—C13	1.391 (5)	C33—H33	0.9300
C12—H12	0.9300	P2—C40	1.8273 (16)
C13—C14	1.413 (4)	P2—C46	1.8359 (19)
C13—H13	0.9300	P2—C34	1.8457 (18)
C14—C15	1.404 (5)	C34—C35	1.3900
C14—H14	0.9300	C34—C39	1.3900
C15—H15	0.9300	C35—C36	1.3900
C1—C2	1.327 (4)	C35—H35	0.9300
C2—C5	1.486 (3)	C36—C37	1.3900
C2—H2	0.9300	C36—H36	0.9300
C5—C6	1.3900	C37—C38	1.3900

C5—C10	1.3900	C37—H37	0.9300
C6—C7	1.3900	C38—C39	1.3900
C6—H6	0.9300	C38—H38	0.9300
C7—C8	1.3900	C39—H39	0.9300
C7—H7	0.9300	C40—C41	1.3900
C8—C9	1.3900	C40—C45	1.3900
C8—H8	0.9300	C41—C42	1.3900
C9—C10	1.3900	C41—H41	0.9300
C9—H9	0.9300	C42—C43	1.3900
C10—H10	0.9300	C42—H42	0.9300
P1—C22	1.8382 (15)	C43—C44	1.3900
P1—C28	1.8442 (16)	C43—H43	0.9300
P1—C16	1.8448 (15)	C44—C45	1.3900
C16—C17	1.3900	C44—H44	0.9300
C16—C21	1.3900	C45—H45	0.9300
C17—C18	1.3900	C46—C47	1.3900
C17—H17	0.9300	C46—C51	1.3900
C18—C19	1.3900	C47—C48	1.3900
C18—H18	0.9300	C47—H47	0.9300
C19—C20	1.3900	C48—C49	1.3900
C19—H19	0.9300	C48—H48	0.9300
C20—C21	1.3900	C49—C50	1.3900
C20—H20	0.9300	C49—H49	0.9300
C21—H21	0.9300	C50—C51	1.3900
C22—C23	1.3900	C50—H50	0.9300
C22—C27	1.3900	C51—H51	0.9300
C23—C24	1.3900		
C1—Pt—P1	98.76 (8)	C21—C16—P1	119.12 (11)
C1—Pt—P2	154.04 (8)	C16—C17—C18	120.0
P1—Pt—P2	102.31 (3)	C16—C17—H17	120.0
C1—Pt—C3	84.23 (11)	C18—C17—H17	120.0
P1—Pt—C3	143.85 (8)	C19—C18—C17	120.0
P2—Pt—C3	87.58 (8)	C19—C18—H18	120.0
C1—Pt—Mn	47.99 (8)	C17—C18—H18	120.0
P1—Pt—Mn	144.90 (2)	C20—C19—C18	120.0
P2—Pt—Mn	112.78 (2)	C20—C19—H19	120.0
C3—Pt—Mn	41.86 (7)	C18—C19—H19	120.0
C4—Mn—C3	86.59 (16)	C21—C20—C19	120.0
C4—Mn—C1	84.00 (14)	C21—C20—H20	120.0
C3—Mn—C1	103.22 (13)	C19—C20—H20	120.0
C4—Mn—C12	93.44 (14)	C20—C21—C16	120.0
C3—Mn—C12	143.79 (13)	C20—C21—H21	120.0
C1—Mn—C12	112.80 (13)	C16—C21—H21	120.0
C4—Mn—C11	100.66 (15)	C23—C22—C27	120.0
C3—Mn—C11	105.29 (14)	C23—C22—P1	120.53 (11)
C1—Mn—C11	151.32 (13)	C27—C22—P1	119.47 (11)
C12—Mn—C11	39.13 (13)	C22—C23—C24	120.0
C4—Mn—C15	135.80 (15)	C22—C23—H23	120.0
C3—Mn—C15	91.22 (14)	C24—C23—H23	120.0

C1—Mn—C15	138.88 (13)	C25—C24—C23	120.0
C12—Mn—C15	64.06 (13)	C25—C24—H24	120.0
C11—Mn—C15	37.91 (13)	C23—C24—H24	120.0
C4—Mn—C13	121.09 (14)	C24—C25—C26	120.0
C3—Mn—C13	151.11 (15)	C24—C25—H25	120.0
C1—Mn—C13	88.91 (12)	C26—C25—H25	120.0
C12—Mn—C13	37.89 (12)	C25—C26—C27	120.0
C11—Mn—C13	64.29 (12)	C25—C26—H26	120.0
C15—Mn—C13	63.70 (12)	C27—C26—H26	120.0
C4—Mn—C14	157.10 (14)	C26—C27—C22	120.0
C3—Mn—C14	113.05 (15)	C26—C27—H27	120.0
C1—Mn—C14	101.79 (12)	C22—C27—H27	120.0
C12—Mn—C14	63.82 (13)	C29—C28—C33	120.0
C11—Mn—C14	63.89 (13)	C29—C28—P1	121.22 (12)
C15—Mn—C14	37.96 (12)	C33—C28—P1	118.79 (12)
C13—Mn—C14	38.14 (12)	C30—C29—C28	120.0
C4—Mn—Pt	106.38 (11)	C30—C29—H29	120.0
C3—Mn—Pt	62.03 (9)	C28—C29—H29	120.0
C1—Mn—Pt	49.08 (8)	C31—C30—C29	120.0
C12—Mn—Pt	149.66 (10)	C31—C30—H30	120.0
C11—Mn—Pt	148.89 (11)	C29—C30—H30	120.0
C15—Mn—Pt	111.32 (10)	C30—C31—C32	120.0
C13—Mn—Pt	111.97 (9)	C30—C31—H31	120.0
C14—Mn—Pt	93.71 (9)	C32—C31—H31	120.0
O3—C3—Mn	166.0 (3)	C33—C32—C31	120.0
O3—C3—Pt	117.7 (2)	C33—C32—H32	120.0
Mn—C3—Pt	76.11 (11)	C31—C32—H32	120.0
O4—C4—Mn	178.9 (4)	C32—C33—C28	120.0
C15—C11—C12	107.3 (3)	C32—C33—H33	120.0
C15—C11—Mn	71.82 (19)	C28—C33—H33	120.0
C12—C11—Mn	70.36 (18)	C40—P2—C46	105.87 (11)
C15—C11—H11	126.3	C40—P2—C34	99.64 (10)
C12—C11—H11	126.3	C46—P2—C34	103.53 (11)
Mn—C11—H11	123.2	C40—P2—Pt	123.19 (7)
C13—C12—C11	108.1 (3)	C46—P2—Pt	108.16 (8)
C13—C12—Mn	72.27 (18)	C34—P2—Pt	114.51 (8)
C11—C12—Mn	70.51 (18)	C35—C34—C39	120.0
C13—C12—H12	125.9	C35—C34—P2	118.32 (14)
C11—C12—H12	125.9	C39—C34—P2	121.55 (14)
Mn—C12—H12	122.9	C36—C35—C34	120.0
C12—C13—C14	108.1 (3)	C36—C35—H35	120.0
C12—C13—Mn	69.84 (18)	C34—C35—H35	120.0
C14—C13—Mn	71.28 (18)	C35—C36—C37	120.0
C12—C13—H13	126.0	C35—C36—H36	120.0
C14—C13—H13	126.0	C37—C36—H36	120.0
Mn—C13—H13	124.5	C38—C37—C36	120.0
C15—C14—C13	107.5 (3)	C38—C37—H37	120.0
C15—C14—Mn	70.31 (19)	C36—C37—H37	120.0
C13—C14—Mn	70.58 (17)	C39—C38—C37	120.0

C15—C14—H14	126.2	C39—C38—H38	120.0
C13—C14—H14	126.2	C37—C38—H38	120.0
Mn—C14—H14	124.5	C38—C39—C34	120.0
C11—C15—C14	108.9 (3)	C38—C39—H39	120.0
C11—C15—Mn	70.27 (19)	C34—C39—H39	120.0
C14—C15—Mn	71.73 (18)	C41—C40—C45	120.0
C11—C15—H15	125.5	C41—C40—P2	121.08 (12)
C14—C15—H15	125.5	C45—C40—P2	118.90 (12)
Mn—C15—H15	124.1	C42—C41—C40	120.0
C2—C1—Mn	141.0 (2)	C42—C41—H41	120.0
C2—C1—Pt	135.2 (2)	C40—C41—H41	120.0
Mn—C1—Pt	82.93 (11)	C41—C42—C43	120.0
C1—C2—C5	131.9 (3)	C41—C42—H42	120.0
C1—C2—H2	114.1	C43—C42—H42	120.0
C5—C2—H2	114.1	C44—C43—C42	120.0
C6—C5—C10	120.0	C44—C43—H43	120.0
C6—C5—C2	117.66 (18)	C42—C43—H43	120.0
C10—C5—C2	122.32 (18)	C43—C44—C45	120.0
C5—C6—C7	120.0	C43—C44—H44	120.0
C5—C6—H6	120.0	C45—C44—H44	120.0
C7—C6—H6	120.0	C44—C45—C40	120.0
C8—C7—C6	120.0	C44—C45—H45	120.0
C8—C7—H7	120.0	C40—C45—H45	120.0
C6—C7—H7	120.0	C47—C46—C51	120.0
C9—C8—C7	120.0	C47—C46—P2	116.51 (15)
C9—C8—H8	120.0	C51—C46—P2	123.45 (15)
C7—C8—H8	120.0	C48—C47—C46	120.0
C8—C9—C10	120.0	C48—C47—H47	120.0
C8—C9—H9	120.0	C46—C47—H47	120.0
C10—C9—H9	120.0	C47—C48—C49	120.0
C9—C10—C5	120.0	C47—C48—H48	120.0
C9—C10—H10	120.0	C49—C48—H48	120.0
C5—C10—H10	120.0	C50—C49—C48	120.0
C22—P1—C28	100.62 (9)	C50—C49—H49	120.0
C22—P1—C16	102.59 (9)	C48—C49—H49	120.0
C28—P1—C16	103.64 (10)	C49—C50—C51	120.0
C22—P1—Pt	120.73 (7)	C49—C50—H50	120.0
C28—P1—Pt	115.63 (7)	C51—C50—H50	120.0
C16—P1—Pt	111.49 (6)	C50—C51—C46	120.0
C17—C16—C21	120.0	C50—C51—H51	120.0
C17—C16—P1	120.84 (11)	C46—C51—H51	120.0

Fig. 1


C7
C8
C6
C9
C10
C5
C2
H2
C31
C30
C32
C29
C19
C18
C20
C33
C28
C17
C21
C16
O4
C1
P1
C13
C4
C27
C12
C26
C22
Mn
Pt
C48
C49
C14
C23
C25
C11
C3
C47
C24
O3
C50
P2
C46
C15
C51
C39
C34
C40
C45
C44
C38
C35
C43
C37
C41
C36
C42