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)rhenium-platinum(*Re—Pt*) diethyl ether hemisolvate

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

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

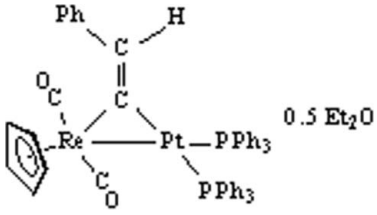
Received 16 July 2007; accepted 27 July 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.008 Å; disorder in solvent or counterion; R factor = 0.031; wR factor = 0.073; data-to-parameter ratio = 23.0.

The title compound, $[PtRe(C_5H_5)(C_8H_6)(C_{18}H_{15}P)_2(CO)_2]\cdot 0.5C_4H_{10}O$, represents the first example of a structurally characterized μ-vinylidene Re–Pt complex, and was obtained as a product of the addition of $[Pt(PPh_3)]_2$ to $(\eta^5\text{-}C_5H_5)(CO)_2Re{=}C{=}CHPh$. The two metal atoms are bridged by the μ-phenylvinylidene ligand. The central fragment of the molecule is an almost planar methylenedimetallacyclopropane RePt(μ-C=CHPh) system. The Re atom is bonded to the η^5-C_5H_5 ring and two CO groups, one of which has a tendency to a weak semi-bridging interaction with the Pt atom. The distorted square-planar coordination of the Pt atom is formed by the two P atoms of the PPh_3 ligands, and by two C atoms of the C=CHPh ligand and one of the CO ligands. The solvent molecule is disordered equally over two positions.

Related literature

The corresponding geometry in the analogous MnPt complex was reported by Vasiliev *et al.* (2007). For crystal structures of related μ-carbene complexes containing the Re–Pt–μ-C triangle system, see: Casey *et al.* (1992); Bergamo *et al.* (2000). For related literature, see: Allen *et al.* (1987).



Experimental

Crystal data

$[PtRe(C_5H_5)(C_8H_6)(C_{18}H_{15}P)_2(CO)_2]\cdot 0.5C_4H_{10}O$
M_r = 1166.13
Monoclinic, $P2_1/c$
a = 22.529 (1) Å
b = 9.1786 (5) Å
c = 21.941 (1) Å
β = 92.469 (1)°
V = 4532.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.86 mm^{-1}
T = 296 (2) K
0.36 × 0.21 × 0.18 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.278, T_{max} = 0.418
(expected range = 0.231–0.348)
38759 measured reflections
10402 independent reflections
7336 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.073
S = 1.00
10402 reflections
453 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 3.11 e Å^{-3}
$\Delta\rho_{min}$ = −1.48 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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 (grants Nos. 10TS145 and 17G002).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2027).

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Vasiliev, A. D., Antonova, A. B. & Chudin, O. S. (2007). *Acta Cryst.* E**63**, m2097.

  doi:10.1107/S1600536807036902

supplementary materials

Acta Cryst. (2007). E**63**, m2272 [**doi:10.1107/S1600536807036902**]

μ-Carbonyl-1:2κ^2C-carbonyl-1κC-(1η^5-cyclopentadienyl)(μ-phenylvinylidene)bis(triphenylphosphine-2κP)rheniumplatinum(*Re-Pt*) diethyl ether hemisolvate

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

Comment

The molecule of the title compound, [η^5-C_5H_5)$(CO)_2$RePt (μ-C═CH*Ph*)(PPh_3)$_2$] Et_2O, is the dinuclear complex containing the Re and Pt atoms bridged by the μ-phenylvinylidene ligand. The phenyl ring and the C═C bond of vinylidene coupled with the Re—Pt-μ-C triangle form an almost planar system. Corresponding geometry was found for the analogous MnPt complex (Vasiliev *et al.*, 2007). The structures of some μ-carbene (Casey *et al.*, 1992; Bergamo *et al.*, 2000) and μ-carbyne (Bergamo *et al.*, 2000) complexes containing the Re—Pt-μ-C triangle system as the central fragment of molecule were reported.

Experimental

The title compound was prepared by the interaction between *Cp*$(CO)_2$Re═C═CH*Ph* and Pt(PPh_3)$_4$ in benzene and at 298 K, 3 h. Suitable single crystals were obtained by recrystallization from ether at 298 K.

Refinement

Seven phenyl cycles 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) = 1.2U_{eq}(C).

There are the difference density maximum of 3.11 e/Å^3 at a distance of 0.87Å from Re atom and the minimum of −1.48 e/Å^3 at a distance of 0.68Å from the same atom.

The solvate diethyl ether molecule is situated close to the inversion center (the distance from the center to the oxygen atom about 0.5 Å) with the statistical occupancy of 0.5. A l l non-hydrogen 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 1.43 and 1.50 Å respectively (Allen *et al.*, 1987).

Figures

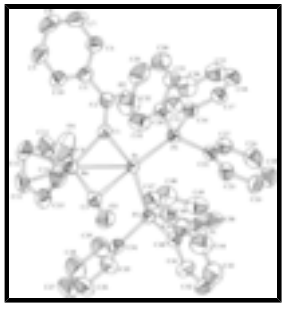


Fig. 1. The molecular structure of title compound, with atom labels and 50% probability displacement ellipsoids for non-H atoms. H atoms, except for H2 atom, omitted for clarity.

μ-Carbonyl-1:2κ^2*C*-carbonyl-1κ*C*-(1η^5– cyclopentadienyl)(μ- phenylvinylidene)bis(triphenylphosphine-2κ*P*)rheniumplatinum(Re—Pt) diethyl ether hemisolvate

Crystal data

$[PtRe(C_5H_5)(C_8H_6)(C_{18}H_{15}P)_2(CO)_2]\cdot 0.5C_4H_{10}O$	F_{000} = 2268
M_r = 1166.13	D_x = 1.709 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 9791 reflections
a = 22.529 (1) Å	θ = 2.4–27.4º
b = 9.1786 (5) Å	μ = 5.86 mm^{-1}
c = 21.941 (1) Å	T = 296 (2) K
β = 92.469 (1)º	Block, orange
V = 4532.9 (4) Å^3	0.36 × 0.21 × 0.18 mm
Z = 4	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	10402 independent reflections
Radiation source: fine-focus sealed tube	7336 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.038
T = 296(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	h = −29→29
T_{min} = 0.278, T_{max} = 0.418	k = −11→11
38759 measured reflections	l = −28→28

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: constr
$R[F^2 > 2\sigma(F^2)]$ = 0.031	H-atom parameters constrained
$wR(F^2)$ = 0.073	$w = 1/[\sigma^2(F_o^2) + (0.0315P)^2 + 4.6963P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max}$ = 0.002
10402 reflections	$\Delta\rho_{max}$ = 3.11 e Å^{-3}
453 parameters	$\Delta\rho_{min}$ = −1.48 e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\sigma(F^2)$ 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}	Occ. (<1)
Pt	0.248866 (8)	0.446207 (18)	0.314347 (8)	0.03293 (5)	
Re	0.186644 (9)	0.56086 (2)	0.215806 (8)	0.04006 (6)	
C11	0.1165 (3)	0.5152 (8)	0.1403 (3)	0.0688 (17)	
H11	0.0868	0.5833	0.1314	0.083*	
C12	0.1711 (3)	0.5085 (8)	0.1141 (2)	0.0674 (17)	
H12	0.1843	0.5712	0.0843	0.081*	
C13	0.2037 (3)	0.3910 (7)	0.1401 (3)	0.0668 (17)	
H13	0.2421	0.3633	0.1311	0.080*	
C14	0.1675 (3)	0.3247 (7)	0.1818 (3)	0.0712 (18)	
H14	0.1777	0.2430	0.2051	0.085*	
C15	0.1135 (3)	0.3995 (8)	0.1833 (3)	0.0707 (18)	
H15	0.0819	0.3779	0.2077	0.085*	
P1	0.34065 (5)	0.38572 (13)	0.35326 (6)	0.0352 (3)	
P2	0.18454 (5)	0.31895 (13)	0.37882 (5)	0.0371 (3)	
C1	0.2770 (2)	0.5451 (5)	0.2392 (2)	0.0387 (10)	
C2	0.3310 (2)	0.5629 (5)	0.2158 (2)	0.0462 (12)	
H2	0.3619	0.5207	0.2390	0.055*	
C3	0.1518 (2)	0.6161 (6)	0.2899 (2)	0.0512 (13)	
O3	0.12681 (18)	0.6630 (5)	0.33088 (18)	0.0728 (12)	
C4	0.1973 (3)	0.7638 (7)	0.2106 (2)	0.0580 (15)	
O4	0.2019 (3)	0.8908 (5)	0.2078 (2)	0.0956 (17)	
C5	0.35039 (15)	0.6378 (4)	0.15943 (13)	0.0445 (12)	
C6	0.41017 (14)	0.6250 (4)	0.14714 (16)	0.0579 (15)	
H6	0.4351	0.5677	0.1721	0.069*	
C7	0.43266 (13)	0.6977 (4)	0.09758 (18)	0.0716 (18)	
H7	0.4727	0.6891	0.0894	0.086*	
C8	0.39537 (19)	0.7832 (4)	0.06030 (14)	0.075 (2)	
H8	0.4104	0.8318	0.0271	0.090*	
C9	0.33558 (18)	0.7960 (4)	0.07259 (15)	0.0668 (17)	
H9	0.3106	0.8533	0.0476	0.080*	
C10	0.31309 (12)	0.7233 (4)	0.12215 (16)	0.0547 (14)	
H10	0.2731	0.7319	0.1304	0.066*	
C16	0.39374 (13)	0.5381 (3)	0.36984 (15)	0.0417 (11)	

C17	0.44538 (14)	0.5143 (3)	0.40541 (15)	0.0501 (13)
H17	0.4541	0.4215	0.4203	0.060*
C18	0.48397 (12)	0.6292 (4)	0.41877 (16)	0.0584 (15)
H18	0.5185	0.6133	0.4426	0.070*
C19	0.47092 (15)	0.7679 (3)	0.39656 (18)	0.0671 (17)
H19	0.4967	0.8447	0.4055	0.081*
C20	0.41928 (17)	0.7917 (3)	0.36100 (17)	0.0654 (17)
H20	0.4105	0.8845	0.3461	0.078*
C21	0.38069 (13)	0.6768 (3)	0.34764 (15)	0.0503 (13)
H21	0.3461	0.6927	0.3238	0.060*
C22	0.35058 (15)	0.2911 (3)	0.42695 (11)	0.0381 (11)
C23	0.33064 (15)	0.3641 (3)	0.47767 (15)	0.0492 (13)
H23	0.3110	0.4527	0.4729	0.059*
C24	0.34009 (17)	0.3046 (4)	0.53554 (12)	0.0646 (16)
H24	0.3268	0.3535	0.5695	0.078*
C25	0.36947 (18)	0.1722 (4)	0.54270 (13)	0.0702 (18)
H25	0.3758	0.1324	0.5814	0.084*
C26	0.38941 (16)	0.0991 (3)	0.49198 (18)	0.0691 (18)
H26	0.4091	0.0105	0.4968	0.083*
C27	0.37996 (15)	0.1586 (3)	0.43411 (15)	0.0518 (13)
H27	0.3933	0.1098	0.4002	0.062*
C28	0.37716 (14)	0.2656 (3)	0.29846 (14)	0.0406 (11)
C29	0.43784 (14)	0.2665 (4)	0.28940 (17)	0.0656 (16)
H29	0.4626	0.3297	0.3118	0.079*
C30	0.46151 (14)	0.1729 (5)	0.24695 (19)	0.085 (2)
H30	0.5021	0.1736	0.2409	0.103*
C31	0.4245 (2)	0.0784 (4)	0.21355 (17)	0.084 (2)
H31	0.4403	0.0158	0.1852	0.100*
C32	0.3638 (2)	0.0775 (4)	0.22261 (18)	0.085 (2)
H32	0.3390	0.0143	0.2003	0.102*
C33	0.34014 (13)	0.1711 (4)	0.26506 (18)	0.0662 (17)
H33	0.2995	0.1704	0.2711	0.079*
C34	0.10755 (13)	0.2813 (4)	0.34826 (16)	0.0471 (12)
C35	0.06360 (18)	0.3827 (4)	0.35975 (18)	0.0692 (17)
H35	0.0724	0.4630	0.3844	0.083*
C36	0.00648 (16)	0.3642 (6)	0.3344 (2)	0.098 (3)
H36	−0.0229	0.4321	0.3421	0.118*
C37	−0.00669 (16)	0.2442 (7)	0.2976 (2)	0.112 (3)
H37	−0.0449	0.2318	0.2807	0.134*
C38	0.0373 (2)	0.1428 (5)	0.2861 (2)	0.110 (3)
H38	0.0285	0.0625	0.2615	0.132*
C39	0.0944 (2)	0.1614 (4)	0.31145 (19)	0.081 (2)
H39	0.1238	0.0935	0.3038	0.097*
C40	0.16695 (16)	0.4012 (3)	0.45167 (13)	0.0417 (11)
C41	0.13200 (16)	0.3307 (3)	0.49323 (16)	0.0573 (14)
H41	0.1171	0.2381	0.4846	0.069*
C42	0.11924 (18)	0.3986 (5)	0.54776 (15)	0.0769 (19)
H42	0.0959	0.3514	0.5756	0.092*
C43	0.1414 (2)	0.5370 (5)	0.56073 (15)	0.091 (2)

H43	0.1329	0.5824	0.5972	0.110*	
C44	0.1764 (2)	0.6075 (4)	0.51916 (19)	0.085 (2)	
H44	0.1912	0.7001	0.5278	0.102*	
C45	0.18914 (16)	0.5396 (3)	0.46463 (16)	0.0554 (14)	
H45	0.2125	0.5868	0.4368	0.066*	
C46	0.21387 (15)	0.1359 (3)	0.39821 (14)	0.0416 (11)	
C47	0.22624 (17)	0.0446 (4)	0.34983 (12)	0.0588 (15)	
H47	0.2169	0.0738	0.3100	0.071*	
C48	0.25250 (18)	−0.0904 (3)	0.36103 (16)	0.0685 (17)	
H48	0.2608	−0.1515	0.3287	0.082*	
C49	0.26641 (16)	−0.1340 (3)	0.4206 (2)	0.0686 (18)	
H49	0.2840	−0.2243	0.4281	0.082*	
C50	0.25405 (16)	−0.0427 (4)	0.46898 (14)	0.0599 (15)	
H50	0.2633	−0.0719	0.5088	0.072*	
C51	0.22778 (16)	0.0922 (3)	0.45779 (13)	0.0485 (13)	
H51	0.2195	0.1533	0.4902	0.058*	
O5	0.0180 (7)	0.0325 (16)	0.5073 (8)	0.143 (5)*	0.50
C52	−0.0330 (11)	0.033 (3)	0.5424 (10)	0.165 (10)*	0.50
H52A	−0.0289	−0.0314	0.5773	0.198*	0.50
H52B	−0.0686	0.0083	0.5181	0.198*	0.50
C53	−0.0324 (14)	0.190 (3)	0.5609 (13)	0.186 (11)*	0.50
H53A	−0.0655	0.2095	0.5859	0.224*	0.50
H53B	−0.0353	0.2507	0.5252	0.224*	0.50
H53C	0.0040	0.2115	0.5836	0.224*	0.50
C54	0.0247 (11)	−0.115 (2)	0.4895 (11)	0.154 (9)*	0.50
H54A	−0.0133	−0.1533	0.4742	0.185*	0.50
H54B	0.0381	−0.1731	0.5244	0.185*	0.50
C55	0.0689 (12)	−0.124 (3)	0.4409 (12)	0.174 (10)*	0.50
H55A	0.0735	−0.2236	0.4288	0.209*	0.50
H55B	0.1064	−0.0868	0.4564	0.209*	0.50
H55C	0.0552	−0.0671	0.4064	0.209*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt	0.03140 (10)	0.03758 (9)	0.02984 (10)	0.00111 (8)	0.00179 (7)	0.00230 (8)
Re	0.04179 (12)	0.04866 (12)	0.02939 (10)	0.00440 (9)	−0.00239 (8)	0.00195 (8)
C11	0.061 (4)	0.092 (5)	0.052 (4)	0.001 (3)	−0.020 (3)	−0.013 (3)
C12	0.079 (5)	0.093 (4)	0.030 (3)	−0.009 (4)	0.001 (3)	−0.005 (3)
C13	0.061 (4)	0.085 (4)	0.054 (4)	0.005 (3)	−0.006 (3)	−0.027 (3)
C14	0.101 (6)	0.054 (3)	0.057 (4)	−0.008 (4)	−0.015 (4)	−0.009 (3)
C15	0.064 (4)	0.097 (5)	0.050 (4)	−0.020 (4)	−0.007 (3)	−0.004 (3)
P1	0.0319 (6)	0.0366 (6)	0.0369 (7)	0.0020 (5)	0.0011 (5)	0.0019 (5)
P2	0.0382 (7)	0.0398 (6)	0.0333 (6)	−0.0039 (5)	0.0024 (5)	0.0007 (5)
C1	0.039 (3)	0.046 (3)	0.031 (2)	0.001 (2)	0.003 (2)	0.002 (2)
C2	0.044 (3)	0.050 (3)	0.044 (3)	0.000 (2)	0.001 (2)	0.009 (2)
C3	0.042 (3)	0.065 (3)	0.046 (3)	0.008 (3)	−0.003 (3)	0.004 (3)
O3	0.067 (3)	0.097 (3)	0.055 (3)	0.024 (2)	0.015 (2)	−0.004 (2)

C4	0.081 (4)	0.063 (4)	0.031 (3)	0.016 (3)	−0.002 (3)	0.002 (3)
O4	0.175 (5)	0.048 (2)	0.063 (3)	0.010 (3)	0.000 (3)	0.005 (2)
C5	0.049 (3)	0.047 (3)	0.038 (3)	−0.013 (2)	0.005 (2)	−0.004 (2)
C6	0.056 (4)	0.071 (4)	0.047 (3)	−0.018 (3)	0.007 (3)	−0.005 (3)
C7	0.065 (4)	0.086 (5)	0.066 (4)	−0.029 (4)	0.026 (3)	−0.010 (4)
C8	0.099 (6)	0.074 (4)	0.054 (4)	−0.039 (4)	0.021 (4)	0.001 (3)
C9	0.082 (5)	0.070 (4)	0.048 (3)	−0.015 (3)	0.004 (3)	0.013 (3)
C10	0.057 (4)	0.061 (3)	0.046 (3)	−0.007 (3)	0.004 (3)	0.010 (3)
C16	0.040 (3)	0.041 (3)	0.044 (3)	−0.003 (2)	0.004 (2)	−0.004 (2)
C17	0.042 (3)	0.055 (3)	0.053 (3)	−0.005 (2)	−0.003 (3)	0.003 (3)
C18	0.043 (3)	0.070 (4)	0.061 (4)	−0.011 (3)	−0.002 (3)	−0.006 (3)
C19	0.066 (4)	0.062 (4)	0.074 (4)	−0.022 (3)	0.010 (3)	−0.019 (3)
C20	0.080 (5)	0.038 (3)	0.078 (4)	−0.005 (3)	0.000 (4)	−0.003 (3)
C21	0.049 (3)	0.041 (3)	0.060 (3)	0.005 (2)	0.002 (3)	−0.004 (2)
C22	0.037 (3)	0.037 (2)	0.040 (3)	−0.004 (2)	−0.004 (2)	0.003 (2)
C23	0.054 (3)	0.047 (3)	0.046 (3)	−0.004 (2)	−0.005 (3)	−0.002 (2)
C24	0.074 (4)	0.077 (4)	0.042 (3)	−0.016 (3)	−0.004 (3)	0.004 (3)
C25	0.073 (4)	0.077 (4)	0.059 (4)	−0.013 (4)	−0.015 (3)	0.032 (3)
C26	0.064 (4)	0.056 (3)	0.086 (5)	0.003 (3)	−0.009 (4)	0.027 (3)
C27	0.051 (3)	0.047 (3)	0.057 (3)	0.003 (2)	0.004 (3)	0.011 (3)
C28	0.040 (3)	0.043 (3)	0.039 (3)	0.009 (2)	0.003 (2)	0.005 (2)
C29	0.047 (3)	0.097 (5)	0.054 (4)	0.010 (3)	0.009 (3)	−0.006 (3)
C30	0.062 (4)	0.134 (6)	0.062 (4)	0.028 (4)	0.017 (3)	−0.007 (4)
C31	0.097 (6)	0.096 (5)	0.059 (4)	0.035 (4)	0.021 (4)	−0.010 (4)
C32	0.095 (6)	0.083 (5)	0.078 (5)	−0.003 (4)	0.009 (4)	−0.032 (4)
C33	0.058 (4)	0.066 (4)	0.076 (4)	−0.002 (3)	0.017 (3)	−0.029 (3)
C34	0.046 (3)	0.058 (3)	0.037 (3)	−0.014 (3)	0.002 (2)	0.009 (2)
C35	0.040 (3)	0.098 (5)	0.070 (4)	−0.004 (3)	−0.001 (3)	0.007 (4)
C36	0.046 (4)	0.145 (8)	0.102 (6)	−0.003 (4)	−0.007 (4)	0.032 (6)
C37	0.063 (5)	0.171 (9)	0.099 (6)	−0.053 (6)	−0.025 (5)	0.040 (6)
C38	0.095 (6)	0.142 (8)	0.091 (6)	−0.057 (6)	−0.022 (5)	−0.006 (5)
C39	0.074 (5)	0.092 (5)	0.075 (5)	−0.031 (4)	−0.011 (4)	−0.010 (4)
C40	0.042 (3)	0.047 (3)	0.036 (3)	−0.001 (2)	0.004 (2)	−0.001 (2)
C41	0.065 (4)	0.060 (3)	0.048 (3)	0.001 (3)	0.017 (3)	0.005 (3)
C42	0.077 (5)	0.106 (5)	0.050 (4)	0.011 (4)	0.023 (3)	0.007 (4)
C43	0.088 (6)	0.124 (7)	0.061 (4)	0.000 (5)	0.005 (4)	−0.042 (4)
C44	0.081 (5)	0.095 (5)	0.080 (5)	−0.015 (4)	0.017 (4)	−0.046 (4)
C45	0.055 (3)	0.057 (3)	0.054 (3)	−0.004 (3)	0.004 (3)	−0.013 (3)
C46	0.044 (3)	0.038 (3)	0.043 (3)	−0.009 (2)	0.001 (2)	0.003 (2)
C47	0.066 (4)	0.054 (3)	0.057 (4)	−0.002 (3)	0.006 (3)	−0.006 (3)
C48	0.076 (5)	0.049 (3)	0.081 (5)	0.003 (3)	0.007 (4)	−0.012 (3)
C49	0.064 (4)	0.043 (3)	0.101 (5)	0.003 (3)	0.019 (4)	0.014 (3)
C50	0.055 (4)	0.059 (3)	0.067 (4)	0.001 (3)	0.014 (3)	0.026 (3)
C51	0.053 (3)	0.047 (3)	0.046 (3)	−0.004 (2)	0.008 (3)	0.010 (2)

Geometric parameters (Å, °)

Pt—C1	2.008 (4)	C29—H29	0.9300
Pt—P1	2.2717 (12)	C30—C31	1.3900

Pt—P2	2.3753 (12)	C30—H30	0.9300
Pt—Re	2.7360 (3)	C31—C32	1.3900
Re—C4	1.883 (6)	C31—H31	0.9300
Re—C3	1.905 (6)	C32—C33	1.3900
Re—C1	2.083 (5)	C32—H32	0.9300
Re—C11	2.278 (6)	C33—H33	0.9300
Re—C12	2.294 (5)	C34—C35	1.3900
Re—C15	2.305 (6)	C34—C39	1.3900
Re—C13	2.322 (6)	C35—C36	1.3900
Re—C14	2.327 (6)	C35—H35	0.9300
C11—C12	1.382 (8)	C36—C37	1.3900
C11—C15	1.424 (9)	C36—H36	0.9300
C11—H11	0.9300	C37—C38	1.3900
C12—C13	1.411 (9)	C37—H37	0.9300
C12—H12	0.9300	C38—C39	1.3900
C13—C14	1.391 (9)	C38—H38	0.9300
C13—H13	0.9300	C39—H39	0.9300
C14—C15	1.398 (9)	C40—C41	1.3900
C14—H14	0.9300	C40—C45	1.3900
C15—H15	0.9300	C41—C42	1.3900
P1—C22	1.841 (3)	C41—H41	0.9300
P1—C28	1.850 (3)	C42—C43	1.3900
P1—C16	1.866 (3)	C42—H42	0.9300
P2—C40	1.827 (3)	C43—C44	1.3900
P2—C46	1.849 (3)	C43—H43	0.9300
P2—C34	1.865 (3)	C44—C45	1.3900
C1—C2	1.351 (6)	C44—H44	0.9300
C2—C5	1.497 (5)	C45—H45	0.9300
C2—H2	0.9300	C46—C47	1.3900
C3—O3	1.163 (6)	C46—C51	1.3900
C4—O4	1.171 (6)	C47—C48	1.3900
C5—C6	1.3900	C47—H47	0.9300
C5—C10	1.3900	C48—C49	1.3900
C6—C7	1.3900	C48—H48	0.9300
C6—H6	0.9300	C49—C50	1.3900
C7—C8	1.3900	C49—H49	0.9300
C7—H7	0.9300	C50—C51	1.3900
C8—C9	1.3900	C50—H50	0.9300
C8—H8	0.9300	C51—H51	0.9300
C9—C10	1.3900	O5—O5^{i}	1.05 (3)
C9—H9	0.9300	O5—C54^{i}	1.23 (3)
C10—H10	0.9300	O5—C52^{i}	1.30 (3)
C16—C17	1.3900	O5—C52	1.409 (10)
C16—C21	1.3900	O5—C54	1.420 (10)
C17—C18	1.3900	C52—C54^{i}	1.05 (3)
C17—H17	0.9300	C52—C55^{i}	1.23 (3)
C18—C19	1.3900	C52—O5^{i}	1.30 (3)
C18—H18	0.9300	C52—C53	1.498 (10)

C19—C20	1.3900	C52—H52A	0.97 (3)
C19—H19	0.9300	C52—H52B	0.97 (3)
C20—C21	1.3900	C53—C55^{i}	1.02 (3)
C20—H20	0.9300	C53—C54^{i}	1.32 (3)
C21—H21	0.9300	C53—H53A	0.96 (3)
C22—C23	1.3900	C53—H53B	0.96 (3)
C22—C27	1.3900	C53—H53C	0.96 (3)
C23—C24	1.3900	C54—C52^{i}	1.05 (3)
C23—H23	0.9300	C54—O5^{i}	1.23 (3)
C24—C25	1.3900	C54—C53^{i}	1.32 (3)
C24—H24	0.9300	C54—C55	1.491 (10)
C25—C26	1.3900	C54—H54A	0.97 (3)
C25—H25	0.9300	C54—H54B	0.97 (2)
C26—C27	1.3900	C55—C53^{i}	1.02 (3)
C26—H26	0.9300	C55—C52^{i}	1.23 (3)
C27—H27	0.9300	C55—H55A	0.96 (3)
C28—C29	1.3900	C55—H55B	0.96 (3)
C28—C33	1.3900	C55—H55C	0.96 (3)
C29—C30	1.3900		
C1—Pt—P1	95.99 (14)	C26—C25—C24	120.0
C1—Pt—P2	158.97 (14)	C26—C25—H25	120.0
P1—Pt—P2	102.99 (4)	C24—C25—H25	120.0
C1—Pt—Re	49.21 (14)	C25—C26—C27	120.0
P1—Pt—Re	144.89 (3)	C25—C26—H26	120.0
P2—Pt—Re	110.78 (3)	C27—C26—H26	120.0
C4—Re—C3	81.2 (2)	C26—C27—C22	120.0
C4—Re—C1	87.6 (2)	C26—C27—H27	120.0
C3—Re—C1	104.0 (2)	C22—C27—H27	120.0
C4—Re—C11	103.0 (2)	C29—C28—C33	120.0
C3—Re—C11	111.8 (2)	C29—C28—P1	123.8 (2)
C1—Re—C11	143.8 (2)	C33—C28—P1	116.2 (2)
C4—Re—C12	99.4 (2)	C30—C29—C28	120.0
C3—Re—C12	146.6 (2)	C30—C29—H29	120.0
C1—Re—C12	109.4 (2)	C28—C29—H29	120.0
C11—Re—C12	35.2 (2)	C29—C30—C31	120.0
C4—Re—C15	135.1 (3)	C29—C30—H30	120.0
C3—Re—C15	96.8 (2)	C31—C30—H30	120.0
C1—Re—C15	135.2 (2)	C32—C31—C30	120.0
C11—Re—C15	36.2 (2)	C32—C31—H31	120.0
C12—Re—C15	59.2 (2)	C30—C31—H31	120.0
C4—Re—C13	126.6 (2)	C31—C32—C33	120.0
C3—Re—C13	151.2 (2)	C31—C32—H32	120.0
C1—Re—C13	86.5 (2)	C33—C32—H32	120.0
C11—Re—C13	59.2 (2)	C32—C33—C28	120.0
C12—Re—C13	35.6 (2)	C32—C33—H33	120.0
C15—Re—C13	59.1 (2)	C28—C33—H33	120.0
C4—Re—C14	157.6 (2)	C35—C34—C39	120.0

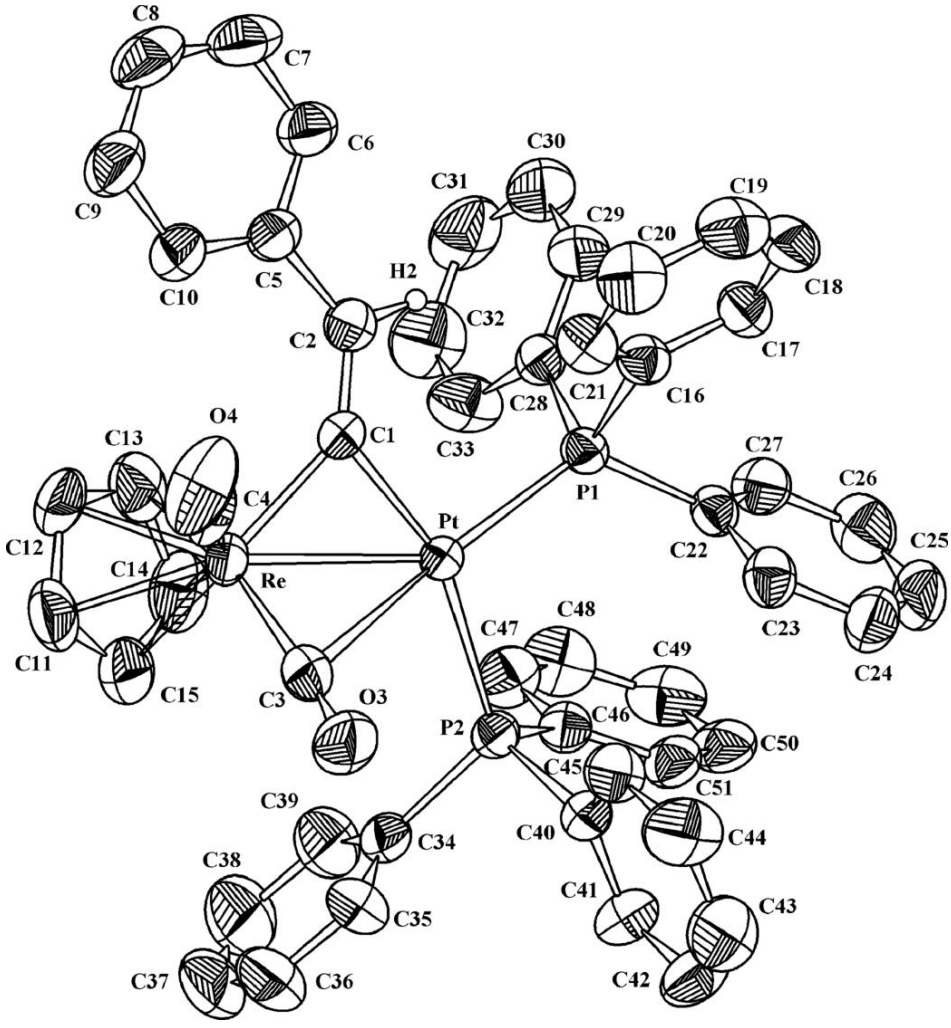
C3—Re—C14	116.4 (2)	C35—C34—P2	118.0 (2)
C1—Re—C14	100.4 (2)	C39—C34—P2	121.8 (2)
C11—Re—C14	58.8 (2)	C34—C35—C36	120.0
C12—Re—C14	58.3 (2)	C34—C35—H35	120.0
C15—Re—C14	35.1 (2)	C36—C35—H35	120.0
C13—Re—C14	34.8 (2)	C37—C36—C35	120.0
C4—Re—Pt	111.49 (16)	C37—C36—H36	120.0
C3—Re—Pt	69.14 (15)	C35—C36—H36	120.0
C1—Re—Pt	46.87 (12)	C36—C37—C38	120.0
C11—Re—Pt	145.02 (18)	C36—C37—H37	120.0
C12—Re—Pt	137.67 (18)	C38—C37—H37	120.0
C15—Re—Pt	109.39 (17)	C39—C38—C37	120.0
C13—Re—Pt	102.23 (17)	C39—C38—H38	120.0
C14—Re—Pt	88.66 (16)	C37—C38—H38	120.0
C12—C11—C15	108.1 (6)	C38—C39—C34	120.0
C12—C11—Re	73.0 (3)	C38—C39—H39	120.0
C15—C11—Re	72.9 (3)	C34—C39—H39	120.0
C12—C11—H11	126.0	C41—C40—C45	120.0
C15—C11—H11	126.0	C41—C40—P2	122.15 (19)
Re—C11—H11	119.9	C45—C40—P2	117.85 (19)
C11—C12—C13	108.8 (6)	C42—C41—C40	120.0
C11—C12—Re	71.8 (3)	C42—C41—H41	120.0
C13—C12—Re	73.3 (3)	C40—C41—H41	120.0
C11—C12—H12	125.6	C41—C42—C43	120.0
C13—C12—H12	125.6	C41—C42—H42	120.0
Re—C12—H12	121.1	C43—C42—H42	120.0
C14—C13—C12	106.9 (6)	C44—C43—C42	120.0
C14—C13—Re	72.8 (3)	C44—C43—H43	120.0
C12—C13—Re	71.1 (3)	C42—C43—H43	120.0
C14—C13—H13	126.6	C43—C44—C45	120.0
C12—C13—H13	126.6	C43—C44—H44	120.0
Re—C13—H13	121.3	C45—C44—H44	120.0
C13—C14—C15	109.6 (6)	C44—C45—C40	120.0
C13—C14—Re	72.4 (3)	C44—C45—H45	120.0
C15—C14—Re	71.6 (4)	C40—C45—H45	120.0
C13—C14—H14	125.2	C47—C46—C51	120.0
C15—C14—H14	125.2	C47—C46—P2	116.98 (19)
Re—C14—H14	122.5	C51—C46—P2	122.84 (19)
C14—C15—C11	106.5 (6)	C46—C47—C48	120.0
C14—C15—Re	73.3 (4)	C46—C47—H47	120.0
C11—C15—Re	70.9 (3)	C48—C47—H47	120.0
C14—C15—H15	126.7	C49—C48—C47	120.0
C11—C15—H15	126.7	C49—C48—H48	120.0
Re—C15—H15	120.9	C47—C48—H48	120.0
C22—P1—C28	104.41 (16)	C50—C49—C48	120.0
C22—P1—C16	97.46 (15)	C50—C49—H49	120.0
C28—P1—C16	105.92 (16)	C48—C49—H49	120.0
C22—P1—Pt	121.31 (12)	C49—C50—C51	120.0
C28—P1—Pt	108.92 (12)	C49—C50—H50	120.0

C16—P1—Pt	117.11 (11)	C51—C50—H50	120.0
C40—P2—C46	105.26 (16)	C50—C51—C46	120.0
C40—P2—C34	99.07 (17)	C50—C51—H51	120.0
C46—P2—C34	103.43 (17)	C46—C51—H51	120.0
C40—P2—Pt	118.61 (11)	$O5^{i}$—O5—$C54^{i}$	76.8 (16)
C46—P2—Pt	111.27 (12)	$O5^{i}$—O5—$C52^{i}$	72.8 (14)
C34—P2—Pt	117.32 (13)	$C54^{i}$—O5—$C52^{i}$	124 (2)
C2—C1—Pt	133.5 (4)	$O5^{i}$—O5—C52	62.1 (16)
C2—C1—Re	141.6 (4)	$C54^{i}$—O5—C52	46.2 (14)
Pt—C1—Re	83.92 (17)	$C52^{i}$—O5—C52	134.8 (13)
C1—C2—C5	132.0 (4)	$O5^{i}$—O5—C54	57.4 (15)
C1—C2—H2	114.0	$C54^{i}$—O5—C54	134.2 (13)
C5—C2—H2	114.0	$C52^{i}$—O5—C54	45.0 (13)
O3—C3—Re	171.5 (5)	C52—O5—C54	104.7 (15)
O4—C4—Re	177.6 (6)	$C54^{i}$—C52—$O5^{i}$	73.4 (16)
C6—C5—C10	120.0	$C55^{i}$—C52—$O5^{i}$	140 (3)
C6—C5—C2	116.2 (3)	$C55^{i}$—C52—O5	137 (3)
C10—C5—C2	123.7 (3)	$O5^{i}$—C52—C53	132 (2)
C5—C6—C7	120.0	O5—C52—C53	99 (2)
C5—C6—H6	120.0	$C54^{i}$—C52—H52A	162 (3)
C7—C6—H6	120.0	$C55^{i}$—C52—H52A	103 (2)
C8—C7—C6	120.0	$O5^{i}$—C52—H52A	111 (2)
C8—C7—H7	120.0	O5—C52—H52A	112 (2)
C6—C7—H7	120.0	C53—C52—H52A	112 (2)
C9—C8—C7	120.0	$C54^{i}$—C52—H52B	88 (3)
C9—C8—H8	120.0	$C55^{i}$—C52—H52B	78 (2)
C7—C8—H8	120.0	$O5^{i}$—C52—H52B	70.8 (15)
C8—C9—C10	120.0	O5—C52—H52B	112.0 (19)
C8—C9—H9	120.0	C53—C52—H52B	112 (2)
C10—C9—H9	120.0	H52A—C52—H52B	110 (2)
C9—C10—C5	120.0	$C54^{i}$—C53—H53A	135 (3)
C9—C10—H10	120.0	C52—C53—H53A	109 (2)
C5—C10—H10	120.0	$C55^{i}$—C53—H53B	107 (3)
C17—C16—C21	120.0	C52—C53—H53B	109 (2)
C17—C16—P1	120.38 (18)	H53A—C53—H53B	109 (3)
C21—C16—P1	119.60 (18)	$C55^{i}$—C53—H53C	144 (4)
C16—C17—C18	120.0	$C54^{i}$—C53—H53C	114 (3)
C16—C17—H17	120.0	C52—C53—H53C	109 (3)
C18—C17—H17	120.0	H53A—C53—H53C	109 (3)
C17—C18—C19	120.0	H53B—C53—H53C	109 (3)
C17—C18—H18	120.0	$O5^{i}$—C54—$C53^{i}$	120 (3)
C19—C18—H18	120.0	$C53^{i}$—C54—O5	138 (2)
C20—C19—C18	120.0	$O5^{i}$—C54—C55	129 (2)
C20—C19—H19	120.0	O5—C54—C55	109 (2)

C18—C19—H19	120.0	$C52^{i}$—C54—H54A	102 (3)
C19—C20—C21	120.0	O5—C54—H54A	109.8 (17)
C19—C20—H20	120.0	C55—C54—H54A	110 (2)
C21—C20—H20	120.0	$O5^{i}$—C54—H54B	121 (2)
C20—C21—C16	120.0	$C53^{i}$—C54—H54B	109.0 (18)
C20—C21—H21	120.0	O5—C54—H54B	109.8 (19)
C16—C21—H21	120.0	C55—C54—H54B	110 (2)
C23—C22—C27	120.0	H54A—C54—H54B	108 (2)
C23—C22—P1	116.39 (19)	C54—C55—H55A	109 (2)
C27—C22—P1	123.46 (19)	$C52^{i}$—C55—H55B	104 (3)
C24—C23—C22	120.0	C54—C55—H55B	109 (3)
C24—C23—H23	120.0	H55A—C55—H55B	109 (3)
C22—C23—H23	120.0	C54—C55—H55C	109 (2)
C25—C24—C23	120.0	H55A—C55—H55C	109 (3)
C25—C24—H24	120.0	H55B—C55—H55C	109 (3)
C23—C24—H24	120.0		

Symmetry codes: (i) $-x$, $-y$, $-z+1$.

Fig. 1


C8
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