

# cis-(Carbonato- $\kappa^2O,O'$ )bis(triphenylphosphine- $\kappa P$ )platinum(II)–benzene–dichloromethane mixed solvate (2/1/1)

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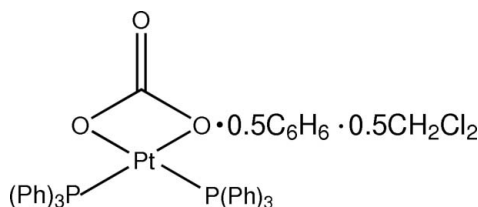
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Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(C-C) = 0.008$  Å; disorder in solvent or counterion;  $R$  factor = 0.036;  $wR$  factor = 0.060; data-to-parameter ratio = 14.9.

The title compound,  $[Pt(CO_3)(C_{18}H_{15}P)_2] \cdot 0.5C_6H_6 \cdot 0.5CH_2Cl_2$ , is isostructural with the analogous tetrahydrofuran [Gregg, Powell & Sawyer (1988). *Acta Cryst.* **C44**, 43–46] and benzene monosolvates [Scholz, Lerner & Bolte (2006). *Acta Cryst.* **E62**, m312–m313]. The Pt atom shows a distorted square-planar coordination.

## Related literature

For general background, see: Andrews *et al.* (1994, 1996); Cariati *et al.* (1967); Clarke *et al.* (1984); Davies *et al.* (1987); Dralle *et al.* (2005); Porta *et al.* (1990). For related structures, see: Abram *et al.* (1999); Gregg *et al.* (1988); Scholz *et al.* (2006). For related literature, see: Allen (2002); Bennett *et al.* (1975); Crabtree *et al.* (1985).



## Experimental

### Crystal data

$[Pt(CO_3)(C_{18}H_{15}P)_2] \cdot 0.5C_6H_6 \cdot 0.5CH_2Cl_2$   
 $M_r = 861.16$   
 Triclinic,  $P\bar{1}$   
 $a = 10.4676$  (2) Å  
 $b = 12.2005$  (3) Å  
 $c = 15.2380$  (4) Å  
 $\alpha = 85.576$  (1)°

$\beta = 71.757$  (1)°  
 $\gamma = 70.956$  (1)°  
 $V = 1746.40$  (7) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 4.22$  mm<sup>-1</sup>  
 $T = 173$  (2) K  
 $0.10 \times 0.07 \times 0.04$  mm

### Data collection

Nonius KappaCCD diffractometer  
 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 2001)  
 $T_{min} = 0.677$ ,  $T_{max} = 0.849$   
 37316 measured reflections  
 6847 independent reflections  
 5512 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.092$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.060$   
 $S = 1.05$   
 6847 reflections  
 459 parameters  
 2 restraints  
 H-atom parameters constrained  
 $\Delta\rho_{max} = 1.33$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -1.45$  e Å<sup>-3</sup>

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2113).

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**supplementary materials**

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***cis*-(Carbonato- $\kappa^2O,O'$ )bis(triphenylphosphine- $\kappa P$ )platinum(II)-benzene-dichloromethane mixed solvate (2/1/1)**

**A. Sivaramakrishna, H. Su and J. R. Moss**

**Comment**

The preparation of *cis*-(carbonato-*O,O'*)-bis(triphenylphosphine)-platinum(II) [(Ph<sub>3</sub>P)<sub>2</sub>Pt(CO<sub>3</sub>)] was first reported by Caricati *et al.* (1967). Carbonato(phosphine)platinum(II) compounds are in general good precursors for the preparation of Pt(II) diolate and alditolate complexes, as well as other Pt(0) and Pt(IV) compounds (Andrews *et al.*, 1994 and Clarke *et al.*, 1984). Platinum carbonate complexes have been observed to form from the decomposition of platinum hydride complexes (Davies *et al.*, 1987) or from the reactions of hydroxide or oxalate complexes (Porta *et al.*, 1990).

Crystal structures of [(Ph<sub>3</sub>P)<sub>2</sub>Pt(CO<sub>3</sub>)] as solvates with different solvents have been reported in the Cambridge Structural Database [CSD (Allen, 2002), version 5.28], namely the tetrahydrofuran monosolvate (FUTVOF, Gregg *et al.*, 1988), the chloroform disolvate (CISQOK, Abram *et al.*, 1999) and the benzene monosolvate (CSD Refcode CAYWIJ, Scholz *et al.*, 2006). These solvates were prepared mainly from the aerial hydrolysis of the Pt(PPh<sub>3</sub>)<sub>4</sub> complex. Here, we present a semi-benzene semi-dichloromethane solvated complex, [(Ph<sub>3</sub>P)<sub>2</sub>Pt(CO<sub>3</sub>)]·0.5C<sub>6</sub>H<sub>6</sub>·0.5CH<sub>2</sub>Cl<sub>2</sub>, Fig. 1, which was prepared by the hydrolysis of a dichloromethane solution of (PPh<sub>3</sub>)<sub>2</sub>bis(1-butenyl)platinum(II). The phenyl rings on the two P atoms are oriented such that some of the *ortho* H atoms form short Pt···H contacts (H26···Pt1 2.855 (5) Å; H42···Pt1 2.905 (5) Å; H56···Pt1 2.959 (6) Å). Similar contacts have been described as agostic (Crabtree *et al.* 1985) or non-primary valence interactions (Bennett *et al.* 1975). In addition to this, two phenyl rings from the opposite triphenylphosphine groups, the C31—C36 and C61—C66 rings, are almost overlapping, forming intramolecular  $\pi$ - $\pi$  interaction with centroid distance of 3.474 Å. The coordination geometry around Pt atom can be described as a distorted square planar. The carbonate ligand is completely planar and makes an angle of *ca* 7.2 (2)° with the PPtP plane. In CHCl<sub>3</sub> solution, the IR spectrum of the [(Ph<sub>3</sub>P)<sub>2</sub>Pt(CO<sub>3</sub>)] compound showed two peaks at 1676 (*v*) and 1632 (*m*) cm<sup>-1</sup>. Though only one fundamental carbonate vibrational mode is expected in this region, namely the C=O stretch, the extra band is attributed to an overtone of the out-of-plane carbonate bending mode as explained by Andrews *et al.* (1996).

**Experimental**

The [(Ph<sub>3</sub>P)<sub>2</sub>Pt(CO<sub>3</sub>)] compound was prepared by the hydrolysis of a dichloromethane solution of (PPh<sub>3</sub>)<sub>2</sub>bis(1-butenyl)platinum(II) (Dralle *et al.*, 2005) on exposure to air. This is probably due to either oxidation of organic chain under these conditions by forming the C—O bonds or absorption of CO<sub>2</sub> from the air. The colour of the reaction mixture changed to yellow brown from colourless. It was also observed that the nature of ligand showed a marked effect on this oxidation reaction: the presence of diphosphine ligands like dppp, dppe did not show any signs of oxidation under these conditions. <sup>1</sup>H-NMR showed only phenyl proton signals and <sup>31</sup>P-NMR indicated a singlet at 27.2 p.p.m. with platinum satellites (*J*<sub>Pt—P</sub> = 3998 Hz). A solution (326 mg, 1.072 mmol) of *cis*-(PPh<sub>3</sub>)<sub>2</sub>Pt(CH<sub>2</sub>CH<sub>2</sub>CH=CH<sub>2</sub>)<sub>2</sub> in 20 ml of CH<sub>2</sub>Cl<sub>2</sub> was exposed to air for 45 days. Removal of solvent in high vacuum and recrystallize from a mixture of CH<sub>2</sub>Cl<sub>2</sub> and n-hexane (1:1) led

## supplementary materials

to the isolation of compound  $[(\text{Ph}_3\text{P})_2\text{Pt}(\text{CO}_3)]$  as colourless crystals (166 mg, 54%). Anal. Calc. for  $[(\text{Ph}_3\text{P})_2\text{Pt}(\text{CO}_3)]$  ( $\text{C}_{37}\text{H}_{30}\text{O}_3\text{P}_2\text{Pt}$ ): C, 57.00, H, 3.88, found: C, 56.92, H, 3.91. MS:  $M^+ = 779.6$ ,  $\text{Pt}(\text{PPh}_3)_2^+ = 719.6$ . Recrystallization from a mixture of dichloromethane and benzene (1:1) yielded colourless crystals of the title compound I which was subjected to X-ray analysis.

### Refinement

The non-H atoms of the molecule  $[(\text{Ph}_3\text{P})_2\text{Pt}(\text{CO}_3)]$  were refined anisotropically. The solvent molecules, benzene and dichloromethane are located with well defined unambiguous atomic positions in the difference electron density maps in the same solvent area and then each was assigned site occupancy factor of 0.50. The non-H atoms of both solvent molecules were refined anisotropically with the C—Cl bond being constrained lengthly and the carbon atoms of the benzene being fitted to a regular pentagon. The hydrogen atoms were placed geometrically in idealized positions riding with their respective parent atoms. The highest peak ( $1.33 \text{ e } \text{\AA}^{-3}$ ) is located at  $1.29 \text{\AA}$  from H5B and the deepest hole ( $-1.45 \text{ e } \text{\AA}^{-3}$ ) is at  $0.02 \text{\AA}$  from Pt1.

### Figures

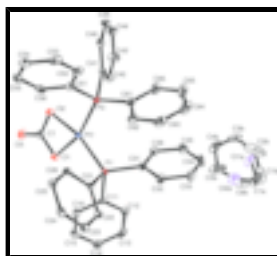


Fig. 1. ORTEP drawing of structure I, showing atomic labelling scheme. Displacement ellipsoids are drawn at 30% probability level and all H atoms are omitted for clarity. The solvent molecules, benzene and dichloromethane, occupy the same area with site occupancy factors to be 0.50 each.

### *cis*-(Carbonato- $\kappa^2\text{O},\text{O}'$ )bis(triphenylphosphine- $\kappa\text{P}$ )platinum(II)–benzene– dichloromethane (2/1/1)

#### Crystal data

$[\text{Pt}(\text{CO}_3)(\text{C}_{18}\text{H}_{15}\text{P})_2] \cdot 0.5\text{C}_6\text{H}_6 \cdot 0.5\text{CH}_2\text{Cl}_2$

$M_r = 861.16$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 10.4676 (2) \text{\AA}$

$b = 12.2005 (3) \text{\AA}$

$c = 15.2380 (4) \text{\AA}$

$\alpha = 85.576 (1)^\circ$

$\beta = 71.757 (1)^\circ$

$\gamma = 70.956 (1)^\circ$

$V = 1746.40 (7) \text{\AA}^3$

$Z = 2$

$F_{000} = 852$

$D_x = 1.638 \text{ Mg m}^{-3}$

Melting point: 188–190°C K

Mo  $K\alpha$  radiation

$\lambda = 0.71073 \text{\AA}$

Cell parameters from 37316 reflections

$\theta = 3.1\text{--}21.6^\circ$

$\mu = 4.22 \text{ mm}^{-1}$

$T = 173 (2) \text{ K}$

Prism, colourless

$0.10 \times 0.07 \times 0.04 \text{ mm}$

#### Data collection

Nonius Kappa CCD  
diffractometer

6847 independent reflections

Radiation source: fine-focus sealed tube	5512 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.092$
$T = 173(2)$ K	$\theta_{\text{max}} = 26.0^\circ$
$1.2^\circ$ $\varphi$ scans and $\omega$ scans	$\theta_{\text{min}} = 3.1^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$h = -12 \rightarrow 12$
$T_{\text{min}} = 0.677$ , $T_{\text{max}} = 0.849$	$k = -15 \rightarrow 15$
37316 measured reflections	$l = -18 \rightarrow 18$

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.036$	H-atom parameters constrained
$wR(F^2) = 0.060$	$w = 1/[\sigma^2(F_o^2) + (0.0097P)^2 + 1.8518P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
6847 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
459 parameters	$\Delta\rho_{\text{max}} = 1.33 \text{ e } \text{\AA}^{-3}$
2 restraints	$\Delta\rho_{\text{min}} = -1.45 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL, $F_c^* = kFc[1 + 0.001x \text{Fc}^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.00138 (16)

### Special details

**Experimental.** Half sphere of data collected using *COLLECT* strategy (Nonius, 2000). Crystal to detector distance = 30 mm; combination of  $\varphi$  and  $\omega$  scans of  $1.2^\circ$ , 30 s per  $^\circ$ , 2 iterations.

**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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Pt1	0.68157 (2)	0.619084 (16)	0.722116 (14)	0.01730 (7)	
Cl1A	-0.2308 (4)	1.2485 (3)	1.0422 (3)	0.0629 (12)	0.50
Cl2A	0.0109 (4)	1.2327 (3)	0.8803 (3)	0.0590 (10)	0.50
P1	0.61853 (12)	0.77338 (9)	0.63764 (8)	0.0169 (3)	
P2	0.79888 (13)	0.68445 (10)	0.79647 (9)	0.0208 (3)	

## supplementary materials

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O1	0.6013 (3)	0.5118 (3)	0.6748 (2)	0.0230 (7)
O2	0.7197 (3)	0.4556 (2)	0.7765 (2)	0.0231 (7)
O3	0.6483 (3)	0.3258 (3)	0.7215 (2)	0.0320 (8)
C1	0.6555 (5)	0.4223 (4)	0.7241 (3)	0.0214 (11)
C11	0.4805 (5)	0.7670 (4)	0.5907 (3)	0.0183 (10)
C12	0.3494 (5)	0.8540 (4)	0.6099 (3)	0.0242 (11)
H12	0.3284	0.9169	0.6507	0.029*
C13	0.2493 (5)	0.8491 (4)	0.5694 (4)	0.0325 (13)
H13	0.1603	0.9090	0.5824	0.039*
C14	0.2782 (5)	0.7585 (4)	0.5108 (4)	0.0321 (13)
H14	0.2100	0.7565	0.4824	0.039*
C15	0.4063 (5)	0.6700 (4)	0.4929 (3)	0.0264 (11)
H15	0.4251	0.6061	0.4536	0.032*
C16	0.5070 (5)	0.6744 (4)	0.5321 (3)	0.0217 (11)
H16	0.5952	0.6137	0.5190	0.026*
C21	0.7630 (5)	0.7745 (4)	0.5340 (3)	0.0183 (10)
C22	0.7417 (5)	0.8449 (4)	0.4596 (3)	0.0232 (11)
H22	0.6500	0.8976	0.4640	0.028*
C23	0.8533 (5)	0.8383 (4)	0.3797 (3)	0.0278 (12)
H23	0.8381	0.8878	0.3301	0.033*
C24	0.9874 (5)	0.7599 (4)	0.3715 (3)	0.0251 (11)
H24	1.0639	0.7563	0.3168	0.030*
C25	1.0086 (5)	0.6873 (4)	0.4431 (3)	0.0227 (11)
H25	1.0994	0.6320	0.4370	0.027*
C26	0.8986 (5)	0.6947 (4)	0.5237 (3)	0.0202 (10)
H26	0.9150	0.6449	0.5729	0.024*
C31	0.5409 (5)	0.9146 (4)	0.6962 (3)	0.0215 (11)
C32	0.5610 (5)	1.0156 (4)	0.6548 (4)	0.0280 (12)
H32	0.6250	1.0127	0.5944	0.034*
C33	0.4857 (5)	1.1221 (4)	0.7033 (4)	0.0370 (14)
H33	0.5012	1.1914	0.6764	0.044*
C34	0.3900 (6)	1.1266 (5)	0.7892 (4)	0.0459 (16)
H34	0.3367	1.1995	0.8204	0.055*
C35	0.3699 (6)	1.0267 (5)	0.8309 (4)	0.0428 (15)
H35	0.3047	1.0304	0.8910	0.051*
C36	0.4458 (5)	0.9206 (4)	0.7845 (4)	0.0328 (13)
H36	0.4325	0.8515	0.8132	0.039*
C41	0.7442 (5)	0.6453 (4)	0.9163 (3)	0.0222 (11)
C42	0.6065 (5)	0.6427 (4)	0.9562 (4)	0.0343 (13)
H42	0.5439	0.6586	0.9199	0.041*
C43	0.5593 (6)	0.6170 (5)	1.0493 (4)	0.0397 (14)
H43	0.4648	0.6156	1.0762	0.048*
C44	0.6494 (6)	0.5940 (4)	1.1017 (4)	0.0372 (13)
H44	0.6175	0.5762	1.1650	0.045*
C45	0.7866 (6)	0.5965 (4)	1.0630 (4)	0.0351 (13)
H45	0.8485	0.5807	1.0998	0.042*
C46	0.8341 (5)	0.6221 (4)	0.9709 (3)	0.0280 (12)
H46	0.9286	0.6238	0.9447	0.034*
C51	0.9892 (5)	0.6088 (4)	0.7531 (3)	0.0201 (10)

C52	1.0905 (5)	0.6579 (4)	0.7568 (4)	0.0317 (13)	
H52	1.0613	0.7345	0.7813	0.038*	
C53	1.2324 (5)	0.5957 (4)	0.7250 (4)	0.0346 (13)	
H53	1.3005	0.6306	0.7268	0.042*	
C54	1.2770 (5)	0.4851 (5)	0.6911 (3)	0.0347 (13)	
H54	1.3755	0.4432	0.6700	0.042*	
C55	1.1791 (5)	0.4336 (4)	0.6873 (4)	0.0337 (13)	
H55	1.2098	0.3564	0.6637	0.040*	
C56	1.0350 (5)	0.4960 (4)	0.7183 (3)	0.0276 (12)	
H56	0.9673	0.4611	0.7156	0.033*	
C61	0.7872 (5)	0.8355 (4)	0.8016 (4)	0.0263 (12)	
C62	0.8509 (5)	0.8877 (4)	0.7226 (4)	0.0335 (13)	
H62	0.9021	0.8431	0.6667	0.040*	
C63	0.8402 (7)	1.0033 (5)	0.7248 (5)	0.0501 (18)	
H63	0.8854	1.0375	0.6711	0.060*	
C64	0.7638 (7)	1.0693 (5)	0.8053 (6)	0.058 (2)	
H64	0.7548	1.1492	0.8066	0.070*	
C65	0.7008 (6)	1.0193 (5)	0.8836 (5)	0.0528 (17)	
H65	0.6490	1.0644	0.9391	0.063*	
C66	0.7127 (6)	0.9029 (4)	0.8816 (4)	0.0390 (14)	
H66	0.6690	0.8689	0.9360	0.047*	
C1A	-0.1603 (13)	1.3141 (13)	0.9414 (10)	0.046 (5)	0.50
H1A1	-0.2220	1.3264	0.9014	0.056*	0.50
H1A2	-0.1601	1.3911	0.9576	0.056*	0.50
C1B	-0.1889 (14)	1.3178 (7)	0.9804 (9)	0.055 (6)	0.50
H1B	-0.2442	1.3947	0.9725	0.065*	0.50
C2B	-0.2077 (12)	1.2719 (10)	1.0681 (7)	0.117 (12)	0.50
H2B	-0.2759	1.3174	1.1202	0.141*	0.50
C3B	-0.1268 (12)	1.1593 (10)	1.0797 (6)	0.055 (4)	0.50
H3B	-0.1396	1.1279	1.1397	0.067*	0.50
C4B	-0.0270 (11)	1.0926 (7)	1.0035 (9)	0.082 (5)	0.50
H4B	0.0283	1.0157	1.0114	0.098*	0.50
C5B	-0.0082 (10)	1.1386 (11)	0.9158 (7)	0.086 (6)	0.50
H5B	0.0600	1.0930	0.8637	0.103*	0.50
C6B	-0.0891 (13)	1.2511 (11)	0.9042 (7)	0.070 (5)	0.50
H6B	-0.0763	1.2825	0.8442	0.084*	0.50

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Pt1	0.01714 (10)	0.01846 (10)	0.01863 (11)	-0.00798 (7)	-0.00715 (8)	0.00441 (7)
Cl1A	0.045 (2)	0.061 (2)	0.057 (3)	-0.0059 (19)	0.004 (2)	0.016 (2)
Cl2A	0.043 (2)	0.074 (2)	0.053 (2)	-0.015 (2)	-0.009 (2)	0.0072 (18)
P1	0.0156 (6)	0.0182 (6)	0.0172 (7)	-0.0055 (5)	-0.0051 (5)	0.0007 (5)
P2	0.0229 (7)	0.0188 (6)	0.0248 (8)	-0.0089 (5)	-0.0120 (6)	0.0058 (5)
O1	0.0217 (18)	0.0280 (18)	0.024 (2)	-0.0127 (14)	-0.0095 (16)	0.0048 (15)
O2	0.0232 (18)	0.0262 (17)	0.0223 (19)	-0.0117 (15)	-0.0078 (16)	0.0071 (14)
O3	0.034 (2)	0.0233 (18)	0.042 (2)	-0.0129 (16)	-0.0135 (18)	0.0061 (16)

## supplementary materials

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C1	0.020 (3)	0.019 (3)	0.023 (3)	-0.008 (2)	-0.003 (2)	0.003 (2)
C11	0.019 (2)	0.018 (2)	0.020 (3)	-0.008 (2)	-0.009 (2)	0.006 (2)
C12	0.024 (3)	0.021 (2)	0.029 (3)	-0.011 (2)	-0.006 (2)	0.001 (2)
C13	0.020 (3)	0.025 (3)	0.053 (4)	-0.005 (2)	-0.016 (3)	0.009 (3)
C14	0.031 (3)	0.036 (3)	0.042 (4)	-0.017 (3)	-0.022 (3)	0.008 (3)
C15	0.028 (3)	0.032 (3)	0.022 (3)	-0.015 (2)	-0.006 (2)	0.001 (2)
C16	0.019 (2)	0.024 (2)	0.022 (3)	-0.009 (2)	-0.004 (2)	0.003 (2)
C21	0.022 (3)	0.017 (2)	0.017 (3)	-0.008 (2)	-0.006 (2)	-0.0039 (19)
C22	0.023 (3)	0.020 (2)	0.022 (3)	-0.002 (2)	-0.007 (2)	0.003 (2)
C23	0.033 (3)	0.025 (3)	0.019 (3)	-0.007 (2)	-0.001 (2)	0.005 (2)
C24	0.022 (3)	0.027 (3)	0.023 (3)	-0.011 (2)	0.001 (2)	-0.004 (2)
C25	0.017 (2)	0.024 (2)	0.026 (3)	-0.007 (2)	-0.005 (2)	-0.003 (2)
C26	0.022 (3)	0.022 (2)	0.020 (3)	-0.009 (2)	-0.010 (2)	0.002 (2)
C31	0.018 (2)	0.020 (2)	0.026 (3)	-0.004 (2)	-0.008 (2)	0.000 (2)
C32	0.021 (3)	0.024 (3)	0.039 (3)	-0.005 (2)	-0.011 (2)	0.001 (2)
C33	0.032 (3)	0.021 (3)	0.055 (4)	-0.002 (2)	-0.013 (3)	-0.005 (3)
C34	0.041 (4)	0.030 (3)	0.057 (4)	0.008 (3)	-0.015 (3)	-0.024 (3)
C35	0.032 (3)	0.052 (4)	0.027 (3)	0.007 (3)	-0.005 (3)	-0.013 (3)
C36	0.033 (3)	0.028 (3)	0.032 (3)	-0.001 (2)	-0.011 (3)	-0.003 (2)
C41	0.027 (3)	0.018 (2)	0.024 (3)	-0.004 (2)	-0.015 (2)	-0.002 (2)
C42	0.035 (3)	0.041 (3)	0.033 (3)	-0.014 (3)	-0.018 (3)	0.005 (3)
C43	0.036 (3)	0.056 (4)	0.025 (3)	-0.020 (3)	-0.002 (3)	0.008 (3)
C44	0.039 (3)	0.044 (3)	0.019 (3)	-0.004 (3)	-0.007 (3)	0.003 (2)
C45	0.040 (3)	0.038 (3)	0.021 (3)	0.003 (3)	-0.015 (3)	-0.003 (2)
C46	0.025 (3)	0.027 (3)	0.029 (3)	-0.001 (2)	-0.011 (2)	-0.006 (2)
C51	0.018 (2)	0.024 (2)	0.020 (3)	-0.010 (2)	-0.007 (2)	0.008 (2)
C52	0.033 (3)	0.026 (3)	0.048 (4)	-0.017 (2)	-0.024 (3)	0.014 (2)
C53	0.032 (3)	0.042 (3)	0.041 (4)	-0.022 (3)	-0.021 (3)	0.020 (3)
C54	0.021 (3)	0.058 (4)	0.023 (3)	-0.013 (3)	-0.004 (2)	0.004 (3)
C55	0.023 (3)	0.042 (3)	0.033 (3)	-0.001 (2)	-0.011 (3)	-0.012 (3)
C56	0.027 (3)	0.037 (3)	0.025 (3)	-0.016 (2)	-0.011 (2)	-0.001 (2)
C61	0.026 (3)	0.024 (3)	0.040 (3)	-0.011 (2)	-0.024 (3)	0.008 (2)
C62	0.043 (3)	0.027 (3)	0.045 (4)	-0.020 (3)	-0.027 (3)	0.011 (3)
C63	0.072 (5)	0.035 (3)	0.074 (5)	-0.036 (3)	-0.052 (4)	0.031 (3)
C64	0.066 (5)	0.024 (3)	0.107 (7)	-0.022 (3)	-0.056 (5)	0.019 (4)
C65	0.051 (4)	0.024 (3)	0.083 (5)	-0.008 (3)	-0.023 (4)	-0.004 (3)
C66	0.038 (3)	0.024 (3)	0.058 (4)	-0.011 (2)	-0.019 (3)	0.005 (3)
C1A	0.061 (12)	0.039 (10)	0.025 (11)	-0.001 (8)	-0.010 (8)	0.001 (6)
C1B	0.072 (12)	0.051 (10)	0.060 (15)	-0.032 (9)	-0.035 (11)	0.001 (10)
C2B	0.14 (2)	0.16 (3)	0.084 (19)	-0.082 (19)	-0.029 (15)	-0.035 (16)
C3B	0.075 (10)	0.066 (9)	0.057 (10)	-0.048 (8)	-0.044 (9)	0.032 (8)
C4B	0.061 (10)	0.052 (8)	0.132 (16)	0.018 (8)	-0.069 (11)	0.007 (10)
C5B	0.048 (9)	0.126 (15)	0.055 (11)	0.014 (10)	-0.023 (8)	0.014 (10)
C6B	0.060 (13)	0.125 (18)	0.037 (11)	-0.041 (12)	-0.024 (11)	0.018 (10)

### *Geometric parameters (Å, °)*

Pt1—O1	2.045 (3)	C36—H36	0.9500
Pt1—O2	2.063 (3)	C41—C42	1.388 (7)

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Pt1—P1	2.2324 (11)	C41—C46	1.392 (6)
Pt1—P2	2.2533 (12)	C42—C43	1.396 (7)
Pt1—C1	2.501 (5)	C42—H42	0.9500
C11A—C1A	1.741 (9)	C43—C44	1.367 (7)
C12A—C1A	1.733 (9)	C43—H43	0.9500
P1—C31	1.815 (4)	C44—C45	1.381 (7)
P1—C21	1.815 (5)	C44—H44	0.9500
P1—C11	1.826 (4)	C45—C46	1.382 (7)
P2—C41	1.811 (5)	C45—H45	0.9500
P2—C61	1.813 (5)	C46—H46	0.9500
P2—C51	1.824 (4)	C51—C56	1.389 (6)
O1—C1	1.348 (5)	C51—C52	1.393 (6)
O2—C1	1.349 (5)	C52—C53	1.374 (7)
O3—C1	1.208 (5)	C52—H52	0.9500
C11—C12	1.394 (6)	C53—C54	1.361 (7)
C11—C16	1.395 (6)	C53—H53	0.9500
C12—C13	1.391 (6)	C54—C55	1.382 (7)
C12—H12	0.9500	C54—H54	0.9500
C13—C14	1.369 (7)	C55—C56	1.392 (6)
C13—H13	0.9500	C55—H55	0.9500
C14—C15	1.382 (6)	C56—H56	0.9500
C14—H14	0.9500	C61—C66	1.382 (7)
C15—C16	1.381 (6)	C61—C62	1.398 (7)
C15—H15	0.9500	C62—C63	1.380 (7)
C16—H16	0.9500	C62—H62	0.9500
C21—C22	1.398 (6)	C63—C64	1.382 (9)
C21—C26	1.404 (6)	C63—H63	0.9500
C22—C23	1.384 (6)	C64—C65	1.374 (9)
C22—H22	0.9500	C64—H64	0.9500
C23—C24	1.391 (6)	C65—C66	1.385 (7)
C23—H23	0.9500	C65—H65	0.9500
C24—C25	1.377 (6)	C66—H66	0.9500
C24—H24	0.9500	C1A—H1A1	0.9900
C25—C26	1.381 (6)	C1A—H1A2	0.9900
C25—H25	0.9500	C1B—C2B	1.3900
C26—H26	0.9500	C1B—C6B	1.3900
C31—C32	1.389 (6)	C1B—H1B	0.9500
C31—C36	1.391 (7)	C2B—C3B	1.3900
C32—C33	1.404 (6)	C2B—H2B	0.9500
C32—H32	0.9500	C3B—C4B	1.3900
C33—C34	1.369 (8)	C3B—H3B	0.9500
C33—H33	0.9500	C4B—C5B	1.3900
C34—C35	1.378 (8)	C4B—H4B	0.9500
C34—H34	0.9500	C5B—C6B	1.3900
C35—C36	1.388 (7)	C5B—H5B	0.9500
C35—H35	0.9500	C6B—H6B	0.9500
O1—Pt1—O2	65.16 (11)	C35—C36—C31	120.5 (5)
O1—Pt1—P1	98.84 (9)	C35—C36—H36	119.7
O2—Pt1—P1	163.83 (9)	C31—C36—H36	119.7

## supplementary materials

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O1—Pt1—P2	161.52 (8)	C42—C41—C46	118.7 (5)
O2—Pt1—P2	96.43 (9)	C42—C41—P2	119.1 (3)
P1—Pt1—P2	99.48 (4)	C46—C41—P2	122.1 (4)
O1—Pt1—C1	32.57 (12)	C41—C42—C43	120.6 (5)
O2—Pt1—C1	32.62 (12)	C41—C42—H42	119.7
P1—Pt1—C1	131.28 (11)	C43—C42—H42	119.7
P2—Pt1—C1	128.96 (11)	C44—C43—C42	119.8 (5)
C31—P1—C21	110.5 (2)	C44—C43—H43	120.1
C31—P1—C11	102.4 (2)	C42—C43—H43	120.1
C21—P1—C11	102.5 (2)	C43—C44—C45	120.3 (5)
C31—P1—Pt1	117.35 (15)	C43—C44—H44	119.9
C21—P1—Pt1	111.32 (14)	C45—C44—H44	119.9
C11—P1—Pt1	111.45 (14)	C44—C45—C46	120.3 (5)
C41—P2—C61	104.5 (2)	C44—C45—H45	119.9
C41—P2—C51	105.7 (2)	C46—C45—H45	119.9
C61—P2—C51	103.8 (2)	C45—C46—C41	120.3 (5)
C41—P2—Pt1	107.31 (15)	C45—C46—H46	119.8
C61—P2—Pt1	123.70 (14)	C41—C46—H46	119.8
C51—P2—Pt1	110.53 (15)	C56—C51—C52	118.6 (4)
C1—O1—Pt1	92.7 (2)	C56—C51—P2	118.6 (3)
C1—O2—Pt1	91.8 (2)	C52—C51—P2	122.7 (4)
O3—C1—O1	125.0 (4)	C53—C52—C51	120.2 (5)
O3—C1—O2	124.8 (4)	C53—C52—H52	119.9
O1—C1—O2	110.2 (4)	C51—C52—H52	119.9
O3—C1—Pt1	177.0 (4)	C54—C53—C52	121.1 (5)
O1—C1—Pt1	54.7 (2)	C54—C53—H53	119.4
O2—C1—Pt1	55.5 (2)	C52—C53—H53	119.4
C12—C11—C16	118.5 (4)	C53—C54—C55	120.1 (5)
C12—C11—P1	121.8 (3)	C53—C54—H54	120.0
C16—C11—P1	119.7 (3)	C55—C54—H54	120.0
C13—C12—C11	120.2 (4)	C54—C55—C56	119.4 (5)
C13—C12—H12	119.9	C54—C55—H55	120.3
C11—C12—H12	119.9	C56—C55—H55	120.3
C14—C13—C12	120.4 (4)	C51—C56—C55	120.6 (4)
C14—C13—H13	119.8	C51—C56—H56	119.7
C12—C13—H13	119.8	C55—C56—H56	119.7
C13—C14—C15	120.1 (4)	C66—C61—C62	118.3 (5)
C13—C14—H14	119.9	C66—C61—P2	121.7 (4)
C15—C14—H14	119.9	C62—C61—P2	120.0 (4)
C16—C15—C14	120.0 (5)	C63—C62—C61	120.7 (6)
C16—C15—H15	120.0	C63—C62—H62	119.6
C14—C15—H15	120.0	C61—C62—H62	119.6
C15—C16—C11	120.7 (4)	C62—C63—C64	120.0 (6)
C15—C16—H16	119.6	C62—C63—H63	120.0
C11—C16—H16	119.6	C64—C63—H63	120.0
C22—C21—C26	118.1 (4)	C65—C64—C63	120.0 (5)
C22—C21—P1	122.3 (3)	C65—C64—H64	120.0
C26—C21—P1	119.4 (3)	C63—C64—H64	120.0
C23—C22—C21	120.4 (4)	C64—C65—C66	120.0 (6)

C23—C22—H22	119.8	C64—C65—H65	120.0
C21—C22—H22	119.8	C66—C65—H65	120.0
C22—C23—C24	120.5 (4)	C61—C66—C65	121.0 (6)
C22—C23—H23	119.7	C61—C66—H66	119.5
C24—C23—H23	119.7	C65—C66—H66	119.5
C25—C24—C23	119.6 (5)	Cl2A—C1A—Cl1A	112.8 (6)
C25—C24—H24	120.2	Cl2A—C1A—H1A1	109.0
C23—C24—H24	120.2	Cl1A—C1A—H1A1	109.0
C24—C25—C26	120.3 (4)	Cl2A—C1A—H1A2	109.0
C24—C25—H25	119.8	Cl1A—C1A—H1A2	109.0
C26—C25—H25	119.8	H1A1—C1A—H1A2	107.8
C25—C26—C21	121.0 (4)	C2B—C1B—C6B	120.0
C25—C26—H26	119.5	C2B—C1B—H1B	120.0
C21—C26—H26	119.5	C6B—C1B—H1B	120.0
C32—C31—C36	119.6 (4)	C3B—C2B—C1B	120.0
C32—C31—P1	123.8 (4)	C3B—C2B—H2B	120.0
C36—C31—P1	116.3 (3)	C1B—C2B—H2B	120.0
C31—C32—C33	119.3 (5)	C2B—C3B—C4B	120.0
C31—C32—H32	120.3	C2B—C3B—H3B	120.0
C33—C32—H32	120.3	C4B—C3B—H3B	120.0
C34—C33—C32	120.3 (5)	C5B—C4B—C3B	120.0
C34—C33—H33	119.9	C5B—C4B—H4B	120.0
C32—C33—H33	119.9	C3B—C4B—H4B	120.0
C33—C34—C35	120.7 (5)	C4B—C5B—C6B	120.0
C33—C34—H34	119.6	C4B—C5B—H5B	120.0
C35—C34—H34	119.6	C6B—C5B—H5B	120.0
C34—C35—C36	119.6 (5)	C5B—C6B—C1B	120.0
C34—C35—H35	120.2	C5B—C6B—H6B	120.0
C36—C35—H35	120.2	C1B—C6B—H6B	120.0
O1—Pt1—P1—C31	135.33 (19)	C22—C23—C24—C25	0.8 (7)
O2—Pt1—P1—C31	143.2 (4)	C23—C24—C25—C26	-1.9 (7)
P2—Pt1—P1—C31	-47.15 (17)	C24—C25—C26—C21	0.9 (7)
C1—Pt1—P1—C31	138.7 (2)	C22—C21—C26—C25	1.2 (6)
O1—Pt1—P1—C21	-96.03 (17)	P1—C21—C26—C25	175.3 (3)
O2—Pt1—P1—C21	-88.2 (4)	C21—P1—C31—C32	17.0 (4)
P2—Pt1—P1—C21	81.48 (15)	C11—P1—C31—C32	-91.6 (4)
C1—Pt1—P1—C21	-92.7 (2)	Pt1—P1—C31—C32	146.0 (3)
O1—Pt1—P1—C11	17.72 (19)	C21—P1—C31—C36	-169.4 (3)
O2—Pt1—P1—C11	25.6 (4)	C11—P1—C31—C36	82.1 (4)
P2—Pt1—P1—C11	-164.77 (16)	Pt1—P1—C31—C36	-40.3 (4)
C1—Pt1—P1—C11	21.0 (2)	C36—C31—C32—C33	0.6 (7)
O1—Pt1—P2—C41	-51.4 (3)	P1—C31—C32—C33	174.1 (4)
O2—Pt1—P2—C41	-46.50 (17)	C31—C32—C33—C34	-2.2 (7)
P1—Pt1—P2—C41	136.39 (15)	C32—C33—C34—C35	2.5 (8)
C1—Pt1—P2—C41	-49.2 (2)	C33—C34—C35—C36	-1.2 (8)
O1—Pt1—P2—C61	-172.9 (3)	C34—C35—C36—C31	-0.3 (8)
O2—Pt1—P2—C61	-168.0 (2)	C32—C31—C36—C35	0.6 (7)
P1—Pt1—P2—C61	14.9 (2)	P1—C31—C36—C35	-173.3 (4)
C1—Pt1—P2—C61	-170.7 (2)	C61—P2—C41—C42	99.9 (4)

## supplementary materials

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O1—Pt1—P2—C51	63.4 (3)	C51—P2—C41—C42	-151.0 (4)
O2—Pt1—P2—C51	68.29 (17)	Pt1—P2—C41—C42	-33.0 (4)
P1—Pt1—P2—C51	-108.82 (15)	C61—P2—C41—C46	-77.5 (4)
C1—Pt1—P2—C51	65.6 (2)	C51—P2—C41—C46	31.6 (4)
O2—Pt1—O1—C1	-2.2 (2)	Pt1—P2—C41—C46	149.6 (3)
P1—Pt1—O1—C1	175.4 (2)	C46—C41—C42—C43	-0.1 (7)
P2—Pt1—O1—C1	3.1 (5)	P2—C41—C42—C43	-177.7 (4)
O1—Pt1—O2—C1	2.2 (2)	C41—C42—C43—C44	-0.1 (8)
P1—Pt1—O2—C1	-6.4 (5)	C42—C43—C44—C45	0.3 (8)
P2—Pt1—O2—C1	-176.1 (2)	C43—C44—C45—C46	-0.2 (8)
Pt1—O1—C1—O3	-176.3 (4)	C44—C45—C46—C41	-0.1 (7)
Pt1—O1—C1—O2	3.3 (4)	C42—C41—C46—C45	0.2 (7)
Pt1—O2—C1—O3	176.3 (4)	P2—C41—C46—C45	177.7 (4)
Pt1—O2—C1—O1	-3.3 (3)	C41—P2—C51—C56	86.8 (4)
O1—Pt1—C1—O3	87 (7)	C61—P2—C51—C56	-163.5 (4)
O2—Pt1—C1—O3	-97 (7)	Pt1—P2—C51—C56	-29.0 (4)
P1—Pt1—C1—O3	81 (7)	C41—P2—C51—C52	-90.6 (4)
P2—Pt1—C1—O3	-92 (7)	C61—P2—C51—C52	19.1 (5)
O2—Pt1—C1—O1	176.3 (4)	Pt1—P2—C51—C52	153.6 (4)
P1—Pt1—C1—O1	-6.1 (3)	C56—C51—C52—C53	1.0 (7)
P2—Pt1—C1—O1	-178.72 (19)	P2—C51—C52—C53	178.4 (4)
O1—Pt1—C1—O2	-176.3 (4)	C51—C52—C53—C54	-1.2 (8)
P1—Pt1—C1—O2	177.65 (18)	C52—C53—C54—C55	0.6 (8)
P2—Pt1—C1—O2	5.0 (3)	C53—C54—C55—C56	0.1 (8)
C31—P1—C11—C12	-4.8 (4)	C52—C51—C56—C55	-0.4 (7)
C21—P1—C11—C12	-119.3 (4)	P2—C51—C56—C55	-177.9 (4)
Pt1—P1—C11—C12	121.5 (3)	C54—C55—C56—C51	-0.2 (7)
C31—P1—C11—C16	173.6 (4)	C41—P2—C61—C66	-16.0 (4)
C21—P1—C11—C16	59.0 (4)	C51—P2—C61—C66	-126.5 (4)
Pt1—P1—C11—C16	-60.1 (4)	Pt1—P2—C61—C66	106.8 (4)
C16—C11—C12—C13	-1.5 (7)	C41—P2—C61—C62	165.9 (4)
P1—C11—C12—C13	176.9 (4)	C51—P2—C61—C62	55.4 (4)
C11—C12—C13—C14	0.4 (7)	Pt1—P2—C61—C62	-71.3 (4)
C12—C13—C14—C15	1.3 (8)	C66—C61—C62—C63	0.4 (7)
C13—C14—C15—C16	-1.8 (7)	P2—C61—C62—C63	178.5 (4)
C14—C15—C16—C11	0.7 (7)	C61—C62—C63—C64	-1.2 (8)
C12—C11—C16—C15	1.0 (7)	C62—C63—C64—C65	1.3 (9)
P1—C11—C16—C15	-177.5 (3)	C63—C64—C65—C66	-0.6 (9)
C31—P1—C21—C22	-63.3 (4)	C62—C61—C66—C65	0.3 (7)
C11—P1—C21—C22	45.3 (4)	P2—C61—C66—C65	-177.8 (4)
Pt1—P1—C21—C22	164.5 (3)	C64—C65—C66—C61	-0.2 (8)
C31—P1—C21—C26	122.9 (3)	C6B—C1B—C2B—C3B	0.0
C11—P1—C21—C26	-128.6 (3)	C1B—C2B—C3B—C4B	0.0
Pt1—P1—C21—C26	-9.3 (4)	C2B—C3B—C4B—C5B	0.0
C26—C21—C22—C23	-2.4 (6)	C3B—C4B—C5B—C6B	0.0
P1—C21—C22—C23	-176.3 (4)	C4B—C5B—C6B—C1B	0.0
C21—C22—C23—C24	1.4 (7)	C2B—C1B—C6B—C5B	0.0

Fig. 1

