

## Crystal structure of bis[1,3-bis(diphenylphosphanyl)propane- $\kappa^2P,P'$ ]platinum(II) dichloride chloroform pentasolvate

Bradley G. Anderson, Sarah A. Hoyte\* and John L. Spencer

School of Chemical and Physical Sciences, Victoria University of Wellington, Wellington, New Zealand. \*Correspondence e-mail: sarah.hoyte@vuw.ac.nz

Received 20 October 2014; accepted 21 January 2015

Edited by J. F. Gallagher, Dublin City University, Ireland

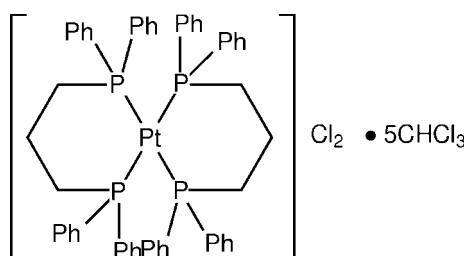
In the title compound,  $[\text{Pt}(\text{Ph}_2\text{P}(\text{CH}_2)_3\text{PPh}_2)_2]\text{Cl}_2 \cdot 5\text{CHCl}_3$ , the Pt<sup>II</sup> cations, located on a centre of inversion, is coordinated by two chelating diphosphane ligands in a geometry which is close to square-planar. The chelate rings adopt a chair conformation. The Pt<sup>II</sup> cations are arranged in layers separated by Cl<sup>-</sup> anions as well as CHCl<sub>3</sub> solvent molecules. While this complex has been reported previously [Anderson *et al.* (1983). *Inorg. Chim. Acta*, **76**, L251–L252], this is the first time a structure has been determined.

**Keywords:** crystal structure; 1,3-bis(diphenylphosphanyl)propane; platinum(II) complex.

**CCDC reference:** 1044833

### 1. Related literature

For structures of related group 10 M<sup>2+</sup> bis-diphosphane complexes, see: Pahor & Bruno (1977); Engelhardt *et al.* (1984); Ferguson *et al.* (1993); Berning *et al.* (1999); Raebiger *et al.* (2004); Fischer (2006). The corresponding Pt<sup>0</sup> complex  $[\text{Pt}(\text{dppp})_2]$  [dppp is 1,3-bis(diphenylphosphanyl)propane] has been reported by Asker *et al.* (1990). For a previous report of the title compound, see: Anderson *et al.* (1983).



### 2. Experimental

#### 2.1. Crystal data

[Pt(C<sub>27</sub>H<sub>26</sub>P<sub>2</sub>)<sub>2</sub>]Cl<sub>2</sub>·5CHCl<sub>3</sub>  
 $M_r = 1687.67$   
 Orthorhombic,  $Pccn$   
 $a = 26.2042 (9)$  Å  
 $b = 15.3120 (5)$  Å  
 $c = 16.7930 (5)$  Å

$V = 6738.0 (4)$  Å<sup>3</sup>  
 $Z = 4$   
 Mo K $\alpha$  radiation  
 $\mu = 2.89$  mm<sup>-1</sup>  
 $T = 160$  K  
 $0.60 \times 0.38 \times 0.28$  mm

#### 2.2. Data collection

Bruker APEXII CCD  
 diffractometer  
 Absorption correction: multi-scan  
 (*SADABS*; Bruker, 2007)  
 $T_{\min} = 0.562$ ,  $T_{\max} = 0.746$

179974 measured reflections  
 10325 independent reflections  
 7580 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.063$

#### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.073$   
 $S = 1.20$   
 10325 reflections

385 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.73$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.97$  e Å<sup>-3</sup>

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2015); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97*.

### Acknowledgements

We thank Dr Jan Wikaira at the University of Canterbury, New Zealand, for collection of the single-crystal X-ray data.

Supporting information for this paper is available from the IUCr electronic archives (Reference: GG2144).

### References

- Anderson, G. K., Davies, J. A. & Schoeck, D. J. (1983). *Inorg. Chim. Acta*, **76**, L251–L252.
- Asker, K., Hitchcock, P., Moulding, R. & Seddon, K. (1990). *Inorg. Chem.* **29**, 4146–4148.
- Berning, D. E., Noll, B. C. & DuBois, D. L. (1999). *J. Am. Chem. Soc.* **121**, 11432–11447.
- Bruker (2007). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Engelhardt, L. M., Patrick, J. M., Raston, C. L., Twiss, P. & White, A. H. (1984). *Aust. J. Chem.* **37**, 2193–2200.
- Ferguson, G., Lough, A. J., McAlees, A. J. & McCrindle, R. (1993). *Acta Cryst. C* **49**, 573–576.
- Fischer, R., Langer, J., Malassa, A., Walter, D., Goris, H. & Vaughan, G. (2006). *Chem. Commun.* pp. 2510–2512.
- Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
- Pahor, N. B. & Bruno, G. (1977). *Cryst. Struct. Commun.* **6**, 717–722.
- Raebiger, J. W., Miedaner, A., Curtis, C. J., Miller, S. M., Anderson, O. P. & DuBois, D. L. (2004). *J. Am. Chem. Soc.* **126**, 5502–5514.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst. C* **71**, 3–8.

# supporting information

*Acta Cryst.* (2015). E71, m37 [doi:10.1107/S205698901500136X]

## Crystal structure of bis[1,3-bis(diphenylphosphanyl)propane- $\kappa^2P,P'$ ]platinum(II) dichloride chloroform pentasolvate

Bradley G. Anderson, Sarah A. Hoyte and John L. Spencer

### S1. Comment

When  $[\text{PtCl}_2(\text{SEt}_2)_2]$  is reacted with bicyclopropylidene, this results in the formation of the  $\beta$ -chloroalkyl complex  $[\text{Pt}(\text{C}(\text{CH}_2)_2\text{C}(\text{CH}_2)_2\text{Cl})\text{Cl}(\text{SEt}_2)_2]$  after 5 days. When dppp ( $\text{Ph}_2\text{P}(\text{CH}_2)_3\text{PPh}_2$ ) was added in an attempt to make a phosphine  $\beta$ -chloroalkyl complex, the  $\beta$ -chloroalkyl ligand undergoes a  $\beta$ -chloride elimination to regenerate the alkene and  $[\text{Pt}(\text{dppp})_2]\text{Cl}_2$  is formed. While this complex has been reported previously (Anderson *et al.*, 1983), this is the first time a structure has been obtained (Fig. 1).

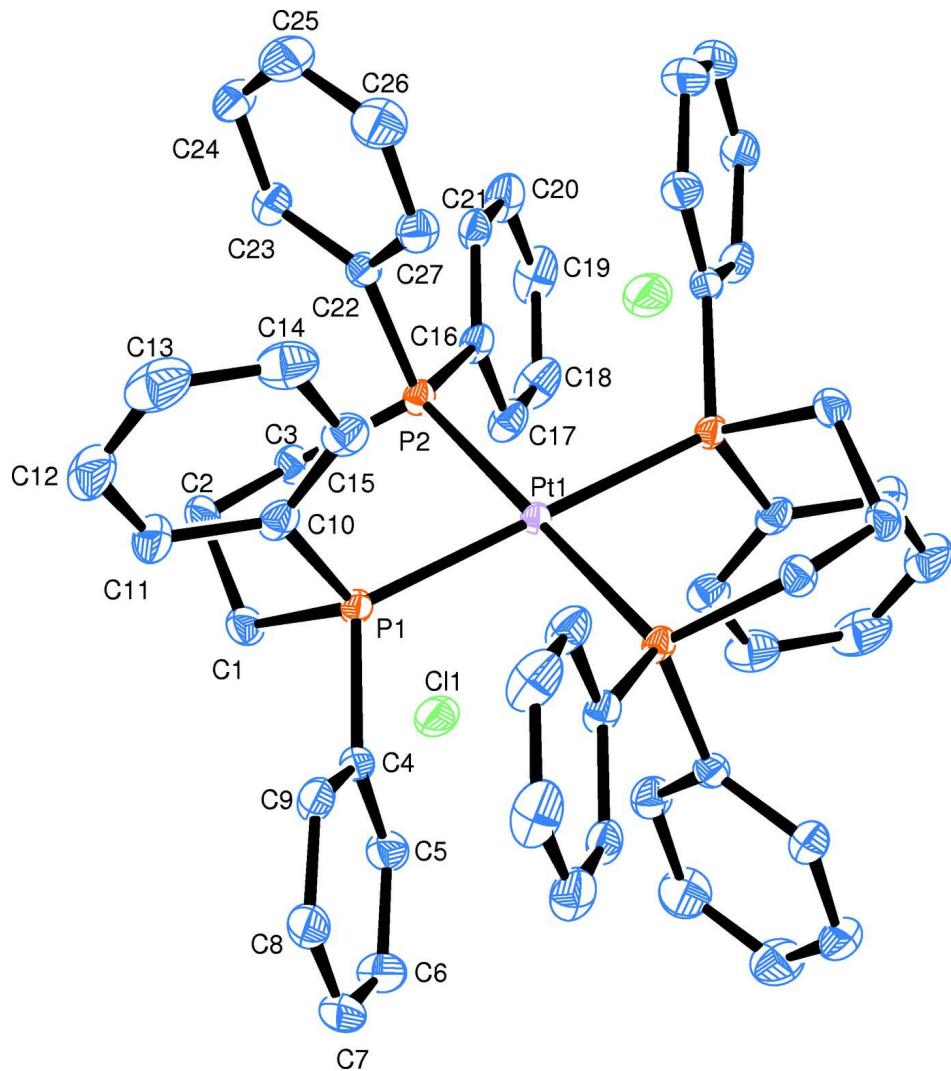
The asymmetric unit contains only half of the molecule, consisting of a complete dppp ligand as well as one of the  $\text{Cl}^-$  counter ions and half of the five  $\text{CDCl}_3$  solvent molecules. The platinum is close to square planar, with a  $\text{P1—Pt—P2}$  angle of  $87.23(3)$   $^\circ$ . This is smaller than the corresponding angle in the  $\text{Pt}(0)$  complex  $[\text{Pt}(\text{dppp})_2]$  ( $97.76(4)$   $^\circ$ ) (Asker *et al.*, 1990). The  $\text{Pt—P}$  bond lengths are  $2.3648(7)$  and  $2.3790(8)$   $\text{\AA}$ , longer than those in  $[\text{Pt}(\text{dppp})_2]$  ( $2.286(1)$   $\text{\AA}$ ). The chelate ring has a 'chair' conformation, typical for dppp complexes. In  $[\text{Pt}(\text{dppp})_2]\text{Cl}_2$ , the chelate two rings are rotated by  $180^\circ$  relative to each other, while in  $[\text{Pt}(\text{dppp})_2]$  the rings are rotated by  $87.20(2)$   $^\circ$  (according to the  $\text{PtP1P2}$  planes). While  $[\text{Pt}(\text{dppp})_2]\text{Cl}_2$  crystallized as a  $\text{CDCl}_3$  solvate in the orthorhombic  $Pccn$  space group,  $[\text{Pt}(\text{dppp})_2]$  crystallized solvent-free from tetrahydrofuran in the monoclinic  $C2/c$  space group. The  $\text{Cl}^-$  counter ion is separated by  $4.197$   $\text{\AA}$  from the Pt, showing that it is not coordinated. The  $[\text{Pt}(\text{dppp})_2]^{2+}$  ions are arranged in two-dimensional layers, with the  $\text{Cl}^-$  anions and solvent between the layers.

### S2. Experimental

$[\text{PtCl}_2(\text{SEt}_2)_2]$  (50 mg, 0.11 mmol) was dissolved in  $\text{CDCl}_3$  (0.5 ml) in an NMR tube under Ar and 5 equiv. bicyclopropylidene added (50  $\mu\text{L}$ , 0.54 mmol). The reaction was stirred for 5 days, resulting in the formation of *trans*- $[\text{Pt}(\text{C}(\text{CH}_2)_2\text{C}(\text{CH}_2)_2\text{Cl})\text{Cl}(\text{SEt}_2)_2]$ . The solution was frozen in liquid  $\text{N}_2$ , and a solution of dppp (90 mg, 0.22 mmol) in  $\text{CDCl}_3$  (0.5 ml) added. Crystals of  $[\text{Pt}(\text{dppp})_2]\text{Cl}_2$  formed as the solution warmed to RT.

### S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with aromatic C—H =  $0.93$   $\text{\AA}$ , methylene C—H =  $0.97$   $\text{\AA}$ , and tertiary C—H =  $0.98$   $\text{\AA}$ .  $U_{\text{iso}}(\text{H}) = 1.2$ . A chloroform solvent molecule was found to be disordered about a 2-fold axis, and was refined by suppressing the symmetry restriction with a 'PART -1' instruction.

**Figure 1**

ORTEP diagram of  $[\text{Pt}(\text{Ph}_2\text{P}(\text{C}_2\text{H}_5)\text{PPh}_2)_2]\text{Cl}_2$  showing 50% probability ellipsoids. H atoms have been omitted for clarity.

### Bis[1,3-bis(diphenylphosphanyl)propane- $\kappa^2P,P'$ ]platinum(II) dichloride chloroform pentasolvate

#### Crystal data

$$[\text{Pt}(\text{C}_{27}\text{H}_{26}\text{P}_2)_2]\text{Cl}_2 \cdot 5\text{CHCl}_3$$

$$M_r = 1687.67$$

Orthorhombic,  $Pccn$

Hall symbol: -P 2ab 2ac

$$a = 26.2042(9) \text{ \AA}$$

$$b = 15.3120(5) \text{ \AA}$$

$$c = 16.7930(5) \text{ \AA}$$

$$V = 6738.0(4) \text{ \AA}^3$$

$$Z = 4$$

$$F(000) = 3352.00$$

$$D_x = 1.664 \text{ Mg m}^{-3}$$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 9982 reflections

$$\theta = 2.4\text{--}30.5^\circ$$

$$\mu = 2.89 \text{ mm}^{-1}$$

$$T = 160 \text{ K}$$

Block, colourless

$$0.6 \times 0.38 \times 0.28 \text{ mm}$$

*Data collection*

Bruker APEXII CCD  
diffractometer  
Radiation source: fine-focus sealed tube  
Graphite monochromator  
 $\varphi$  and  $\omega$  scans  
Absorption correction: multi-scan  
(SADABS; Bruker, 2007)  
 $T_{\min} = 0.562$ ,  $T_{\max} = 0.746$

179974 measured reflections  
10325 independent reflections  
7580 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.063$   
 $\theta_{\max} = 30.6^\circ$ ,  $\theta_{\min} = 2.4^\circ$   
 $h = -37 \rightarrow 37$   
 $k = -21 \rightarrow 21$   
 $l = -23 \rightarrow 24$

*Refinement*

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.073$   
 $S = 1.20$   
10325 reflections  
385 parameters  
0 restraints  
Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map  
Hydrogen site location: inferred from  
neighbouring sites  
H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.P)^2 + 21.821P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.73 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.97 \text{ e } \text{\AA}^{-3}$

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^* / U_{\text{eq}}$	Occ. (<1)
Pt1	0.5000	0.0000	0.0000	0.01283 (4)	
P2	0.49876 (3)	0.10087 (5)	0.10661 (4)	0.01623 (14)	
P1	0.48568 (3)	-0.11136 (5)	0.09623 (4)	0.01524 (15)	
C4	0.41837 (12)	-0.1208 (2)	0.11952 (18)	0.0178 (6)	
C3	0.52924 (13)	0.0645 (2)	0.19883 (18)	0.0210 (6)	
H3A	0.5648	0.0519	0.1875	0.025*	
H3B	0.5284	0.1123	0.2367	0.025*	
C18	0.53826 (15)	0.3596 (2)	0.1019 (2)	0.0278 (8)	
H18	0.5219	0.4133	0.1061	0.033*	
C1	0.51746 (13)	-0.0980 (2)	0.19268 (17)	0.0194 (6)	
H1A	0.5082	-0.1472	0.2261	0.023*	
H1B	0.5540	-0.1009	0.1841	0.023*	
C21	0.58744 (13)	0.1990 (2)	0.0910 (2)	0.0234 (7)	
H21	0.6040	0.1453	0.0886	0.028*	
C2	0.50582 (13)	-0.0150 (2)	0.23790 (17)	0.0211 (7)	
H2A	0.5188	-0.0202	0.2918	0.025*	

H2B	0.4691	-0.0074	0.2410	0.025*
C9	0.40155 (13)	-0.1654 (2)	0.18772 (19)	0.0219 (7)
H9	0.4251	-0.1879	0.2237	0.026*
C22	0.43463 (13)	0.1321 (2)	0.13539 (19)	0.0203 (6)
C14	0.49389 (16)	-0.3787 (2)	0.0796 (2)	0.0299 (8)
H14	0.4719	-0.4262	0.0833	0.036*
C5	0.38263 (13)	-0.0870 (2)	0.0673 (2)	0.0239 (7)
H5	0.3934	-0.0568	0.0222	0.029*
C8	0.34994 (14)	-0.1758 (3)	0.2012 (2)	0.0294 (8)
H8	0.3389	-0.2057	0.2461	0.035*
C16	0.53416 (12)	0.2026 (2)	0.09712 (18)	0.0183 (6)
C19	0.59096 (16)	0.3563 (3)	0.0944 (2)	0.0316 (8)
H19	0.6099	0.4077	0.0932	0.038*
C17	0.50980 (13)	0.2833 (2)	0.10331 (18)	0.0217 (7)
H17	0.4745	0.2859	0.1084	0.026*
C11	0.56005 (14)	-0.2376 (2)	0.0705 (2)	0.0251 (7)
H11	0.5824	-0.1905	0.0679	0.030*
C10	0.50772 (13)	-0.22317 (19)	0.07887 (17)	0.0189 (6)
C6	0.33060 (14)	-0.0978 (3)	0.0817 (2)	0.0352 (9)
H6	0.3068	-0.0752	0.0463	0.042*
C12	0.57854 (16)	-0.3223 (3)	0.0660 (2)	0.0326 (9)
H12	0.6134	-0.3320	0.0598	0.039*
C15	0.47444 (14)	-0.2942 (2)	0.08337 (18)	0.0214 (7)
H15	0.4395	-0.2852	0.0888	0.026*
C23	0.39470 (13)	0.1199 (2)	0.0827 (2)	0.0236 (7)
H23	0.4008	0.0938	0.0336	0.028*
C20	0.61522 (15)	0.2762 (2)	0.0886 (2)	0.0291 (8)
H20	0.6505	0.2741	0.0830	0.035*
C7	0.31462 (15)	-0.1420 (3)	0.1484 (2)	0.0352 (9)
H7	0.2799	-0.1492	0.1581	0.042*
C13	0.54565 (17)	-0.3923 (3)	0.0706 (2)	0.0350 (9)
H13	0.5583	-0.4489	0.0676	0.042*
C26	0.37622 (16)	0.1975 (3)	0.2287 (3)	0.0365 (9)
H26	0.3698	0.2235	0.2778	0.044*
C24	0.34563 (15)	0.1462 (3)	0.1022 (3)	0.0343 (9)
H24	0.3189	0.1377	0.0665	0.041*
C27	0.42495 (15)	0.1714 (3)	0.2095 (2)	0.0288 (8)
H27	0.4515	0.1798	0.2455	0.035*
C25	0.33674 (16)	0.1853 (3)	0.1753 (3)	0.0414 (10)
H25	0.3039	0.2034	0.1885	0.050*
Cl1	0.35882 (4)	0.04388 (8)	-0.11105 (5)	0.0380 (2)
Cl3B	0.31059 (4)	0.01417 (7)	0.32358 (6)	0.0371 (2)
Cl2A	0.21666 (4)	0.05178 (8)	0.17673 (6)	0.0434 (3)
Cl2B	0.24294 (5)	-0.13417 (8)	0.34282 (7)	0.0475 (3)
Cl3A	0.14625 (5)	-0.09321 (7)	0.16878 (7)	0.0430 (2)
Cl1A	0.11366 (4)	0.07947 (8)	0.12128 (7)	0.0447 (3)
Cl1B	0.29044 (4)	-0.05640 (10)	0.48005 (6)	0.0523 (3)
C1B	0.26446 (14)	-0.0355 (3)	0.3849 (2)	0.0328 (8)

H1BA	0.2354	0.0042	0.3907	0.039*	
C1A	0.15290 (14)	0.0195 (3)	0.1870 (2)	0.0304 (8)	
H1AA	0.1420	0.0315	0.2417	0.036*	
C1C	0.2657 (3)	0.2740 (5)	0.4313 (4)	0.0282 (15)	0.5
H1C	0.2954	0.3115	0.4218	0.034*	0.5
Cl3C	0.23595 (11)	0.2360 (3)	0.34548 (14)	0.0622 (9)	0.5
Cl1C	0.2171 (5)	0.3222 (11)	0.4886 (6)	0.076 (3)	0.5
Cl2C	0.2802 (3)	0.1693 (9)	0.4893 (3)	0.0494 (17)	0.5

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Pt1	0.01516 (6)	0.01052 (6)	0.01280 (6)	0.00000 (7)	0.00067 (6)	0.00078 (6)
P2	0.0207 (4)	0.0126 (3)	0.0154 (3)	-0.0020 (3)	0.0032 (3)	-0.0003 (3)
P1	0.0192 (4)	0.0124 (3)	0.0141 (3)	0.0011 (3)	0.0022 (3)	0.0021 (3)
C4	0.0193 (15)	0.0149 (15)	0.0190 (14)	-0.0017 (12)	0.0029 (11)	-0.0026 (11)
C3	0.0254 (17)	0.0203 (16)	0.0174 (14)	-0.0028 (13)	-0.0029 (12)	0.0006 (12)
C18	0.044 (2)	0.0149 (16)	0.0248 (17)	-0.0045 (15)	0.0073 (15)	-0.0037 (13)
C1	0.0232 (15)	0.0188 (15)	0.0163 (13)	0.0000 (13)	-0.0023 (11)	0.0029 (11)
C21	0.0261 (17)	0.0215 (17)	0.0227 (15)	-0.0029 (14)	-0.0008 (13)	0.0006 (13)
C2	0.0278 (18)	0.0213 (17)	0.0141 (12)	-0.0034 (13)	-0.0035 (12)	0.0021 (10)
C9	0.0237 (17)	0.0212 (16)	0.0208 (15)	0.0015 (13)	0.0028 (12)	0.0020 (12)
C22	0.0258 (17)	0.0141 (15)	0.0211 (15)	-0.0009 (13)	0.0056 (12)	0.0026 (12)
C14	0.049 (2)	0.0157 (15)	0.0253 (16)	-0.0002 (16)	0.0086 (16)	0.0042 (12)
C5	0.0250 (17)	0.0251 (18)	0.0216 (15)	-0.0006 (14)	-0.0015 (13)	0.0039 (13)
C8	0.0276 (19)	0.033 (2)	0.0280 (17)	-0.0057 (16)	0.0099 (14)	-0.0017 (15)
C16	0.0240 (16)	0.0164 (15)	0.0146 (13)	-0.0049 (12)	0.0009 (11)	-0.0003 (11)
C19	0.043 (2)	0.0238 (18)	0.0276 (17)	-0.0149 (17)	0.0017 (16)	-0.0028 (15)
C17	0.0293 (19)	0.0170 (15)	0.0188 (14)	0.0002 (13)	0.0070 (12)	0.0005 (11)
C11	0.0303 (19)	0.0194 (17)	0.0255 (16)	0.0025 (14)	0.0090 (14)	0.0037 (13)
C10	0.0283 (19)	0.0106 (13)	0.0179 (13)	0.0016 (12)	0.0056 (12)	0.0030 (10)
C6	0.0229 (18)	0.046 (2)	0.036 (2)	0.0016 (17)	-0.0060 (15)	0.0019 (18)
C12	0.034 (2)	0.0257 (19)	0.038 (2)	0.0122 (16)	0.0134 (16)	0.0076 (16)
C15	0.0292 (18)	0.0194 (16)	0.0156 (14)	0.0002 (13)	0.0032 (12)	0.0016 (12)
C23	0.0254 (17)	0.0175 (16)	0.0280 (17)	0.0003 (13)	0.0041 (13)	0.0015 (13)
C20	0.0284 (19)	0.0282 (19)	0.0307 (18)	-0.0084 (15)	-0.0007 (15)	0.0007 (15)
C7	0.0206 (18)	0.043 (2)	0.042 (2)	-0.0021 (17)	0.0045 (16)	-0.0016 (18)
C13	0.053 (3)	0.0189 (18)	0.0335 (19)	0.0140 (18)	0.0129 (17)	0.0048 (15)
C26	0.037 (2)	0.033 (2)	0.039 (2)	0.0013 (18)	0.0192 (18)	-0.0097 (17)
C24	0.0241 (19)	0.031 (2)	0.047 (2)	-0.0007 (16)	0.0024 (17)	0.0015 (18)
C27	0.031 (2)	0.031 (2)	0.0245 (16)	-0.0018 (16)	0.0088 (14)	-0.0058 (14)
C25	0.027 (2)	0.035 (2)	0.063 (3)	0.0041 (17)	0.018 (2)	-0.001 (2)
Cl1	0.0287 (5)	0.0622 (7)	0.0231 (4)	-0.0202 (5)	-0.0050 (3)	0.0069 (4)
Cl3B	0.0336 (5)	0.0431 (6)	0.0346 (5)	0.0032 (4)	0.0003 (4)	0.0038 (4)
Cl2A	0.0321 (5)	0.0565 (7)	0.0417 (5)	-0.0104 (5)	-0.0056 (4)	0.0056 (5)
Cl2B	0.0446 (6)	0.0378 (6)	0.0602 (7)	-0.0017 (5)	0.0086 (5)	-0.0088 (5)
Cl3A	0.0497 (6)	0.0355 (6)	0.0437 (5)	-0.0053 (5)	-0.0016 (5)	0.0020 (4)
Cl1A	0.0346 (5)	0.0484 (7)	0.0510 (6)	0.0033 (5)	-0.0021 (5)	0.0146 (5)

Cl1B	0.0340 (5)	0.0915 (10)	0.0314 (5)	0.0023 (6)	0.0049 (4)	0.0052 (5)
C1B	0.0246 (19)	0.038 (2)	0.0358 (19)	0.0078 (16)	0.0004 (15)	-0.0033 (17)
C1A	0.031 (2)	0.038 (2)	0.0219 (16)	-0.0022 (16)	0.0035 (14)	0.0008 (14)
C1C	0.024 (4)	0.030 (4)	0.030 (3)	0.000 (3)	-0.004 (3)	-0.001 (3)
Cl3C	0.071 (3)	0.073 (3)	0.0421 (11)	0.0157 (19)	-0.0230 (11)	-0.0151 (14)
Cl1C	0.079 (6)	0.076 (5)	0.074 (5)	0.046 (4)	0.006 (4)	-0.009 (3)
Cl2C	0.045 (3)	0.076 (4)	0.027 (2)	0.041 (3)	0.0020 (18)	0.005 (2)

Geometric parameters ( $\text{\AA}$ ,  $^{\circ}$ )

Pt1—P2	2.3648 (7)	C5—C6	1.395 (5)
Pt1—P2 <sup>i</sup>	2.3648 (7)	C8—C7	1.381 (6)
Pt1—P1	2.3790 (8)	C16—C17	1.395 (4)
Pt1—P1 <sup>i</sup>	2.3790 (8)	C19—C20	1.385 (5)
P2—C3	1.829 (3)	C11—C10	1.396 (5)
P2—C22	1.813 (3)	C11—C12	1.387 (5)
P2—C16	1.820 (3)	C10—C15	1.396 (4)
P1—C4	1.812 (3)	C6—C7	1.374 (6)
P1—C1	1.833 (3)	C12—C13	1.377 (6)
P1—C10	1.830 (3)	C23—C24	1.386 (5)
C4—C9	1.404 (4)	C26—C27	1.376 (5)
C4—C5	1.384 (5)	C26—C25	1.382 (6)
C3—C2	1.513 (4)	C24—C25	1.386 (6)
C18—C19	1.388 (5)	Cl3B—C1B	1.761 (4)
C18—C17	1.387 (5)	Cl2A—C1A	1.751 (4)
C1—C2	1.512 (4)	Cl2B—C1B	1.760 (4)
C21—C16	1.401 (5)	Cl3A—C1A	1.761 (4)
C21—C20	1.390 (5)	Cl1A—C1A	1.766 (4)
C9—C8	1.380 (5)	Cl1B—C1B	1.765 (4)
C22—C23	1.382 (5)	C1C—Cl3C	1.739 (7)
C22—C27	1.405 (5)	C1C—Cl1C	1.759 (13)
C14—C15	1.391 (5)	C1C—Cl2C	1.914 (14)
C14—C13	1.381 (6)		
P2—Pt1—P2 <sup>i</sup>	180.0	C4—C5—C6	120.5 (3)
P2 <sup>i</sup> —Pt1—P1	92.77 (3)	C9—C8—C7	120.6 (3)
P2—Pt1—P1	87.23 (3)	C21—C16—P2	118.7 (3)
P2—Pt1—P1 <sup>i</sup>	92.77 (3)	C17—C16—P2	121.2 (2)
P2 <sup>i</sup> —Pt1—P1 <sup>i</sup>	87.23 (3)	C17—C16—C21	119.8 (3)
P1 <sup>i</sup> —Pt1—P1	180.0	C20—C19—C18	119.7 (3)
C3—P2—Pt1	115.85 (11)	C18—C17—C16	119.9 (3)
C22—P2—Pt1	112.76 (11)	C12—C11—C10	119.8 (3)
C22—P2—C3	105.04 (15)	C11—C10—P1	118.3 (2)
C22—P2—C16	105.67 (15)	C11—C10—C15	119.7 (3)
C16—P2—Pt1	119.06 (10)	C15—C10—P1	121.5 (3)
C16—P2—C3	96.45 (15)	C7—C6—C5	119.9 (4)
C4—P1—Pt1	110.94 (11)	C13—C12—C11	120.4 (4)
C4—P1—C1	105.09 (15)	C14—C15—C10	119.5 (3)

C4—P1—C10	105.47 (15)	C22—C23—C24	120.8 (3)
C1—P1—Pt1	116.67 (11)	C19—C20—C21	120.8 (3)
C10—P1—Pt1	120.83 (10)	C6—C7—C8	120.2 (4)
C10—P1—C1	95.82 (15)	C12—C13—C14	120.2 (3)
C9—C4—P1	121.3 (3)	C27—C26—C25	120.2 (4)
C5—C4—P1	119.5 (2)	C25—C24—C23	119.3 (4)
C5—C4—C9	119.1 (3)	C26—C27—C22	120.0 (4)
C2—C3—P2	115.8 (2)	C26—C25—C24	120.5 (4)
C17—C18—C19	120.4 (3)	Cl3B—C1B—Cl1B	110.0 (2)
C2—C1—P1	116.5 (2)	Cl2B—C1B—Cl3B	110.8 (2)
C20—C21—C16	119.4 (3)	Cl2B—C1B—Cl1B	109.4 (2)
C1—C2—C3	112.1 (3)	Cl2A—C1A—Cl3A	110.8 (2)
C8—C9—C4	119.8 (3)	Cl2A—C1A—Cl1A	110.3 (2)
C23—C22—P2	119.7 (2)	Cl3A—C1A—Cl1A	110.1 (2)
C23—C22—C27	119.2 (3)	Cl3C—C1C—Cl1C	105.6 (5)
C27—C22—P2	121.1 (3)	Cl3C—C1C—Cl2C	103.3 (5)
C13—C14—C15	120.3 (3)	Cl1C—C1C—Cl2C	102.5 (6)
Pt1—P2—C3—C2	-61.9 (3)	C21—C16—C17—C18	1.2 (5)
Pt1—P2—C22—C23	-19.8 (3)	C9—C4—C5—C6	-0.7 (5)
Pt1—P2—C22—C27	162.4 (3)	C9—C8—C7—C6	0.2 (6)
Pt1—P2—C16—C21	-64.6 (3)	C22—P2—C3—C2	63.2 (3)
Pt1—P2—C16—C17	121.4 (2)	C22—P2—C16—C21	167.4 (3)
Pt1—P1—C4—C9	-163.8 (2)	C22—P2—C16—C17	-6.6 (3)
Pt1—P1—C4—C5	19.2 (3)	C22—C23—C24—C25	0.2 (6)
Pt1—P1—C1—C2	57.5 (3)	C5—C4—C9—C8	0.8 (5)
Pt1—P1—C10—C11	62.2 (3)	C5—C6—C7—C8	-0.1 (6)
Pt1—P1—C10—C15	-125.6 (2)	C16—P2—C3—C2	171.3 (3)
P2—C3—C2—C1	72.9 (3)	C16—P2—C22—C23	111.8 (3)
P2—C22—C23—C24	-177.6 (3)	C16—P2—C22—C27	-65.9 (3)
P2—C22—C27—C26	177.6 (3)	C16—C21—C20—C19	1.8 (5)
P2—C16—C17—C18	175.1 (2)	C19—C18—C17—C16	0.0 (5)
P1—C4—C9—C8	-176.2 (3)	C17—C18—C19—C20	-0.3 (5)
P1—C4—C5—C6	176.4 (3)	C11—C10—C15—C14	0.2 (5)
P1—C1—C2—C3	-70.5 (3)	C11—C12—C13—C14	0.1 (6)
P1—C10—C15—C14	-172.0 (2)	C10—P1—C4—C9	63.7 (3)
C4—P1—C1—C2	-65.8 (3)	C10—P1—C4—C5	-113.3 (3)
C4—P1—C10—C11	-171.2 (2)	C10—P1—C1—C2	-173.6 (3)
C4—P1—C10—C15	1.1 (3)	C10—C11—C12—C13	-0.7 (6)
C4—C9—C8—C7	-0.6 (6)	C12—C11—C10—P1	173.0 (3)
C4—C5—C6—C7	0.3 (6)	C12—C11—C10—C15	0.6 (5)
C3—P2—C22—C23	-146.9 (3)	C15—C14—C13—C12	0.7 (6)
C3—P2—C22—C27	35.4 (3)	C23—C22—C27—C26	-0.2 (5)
C3—P2—C16—C21	59.8 (3)	C23—C24—C25—C26	-0.5 (6)
C3—P2—C16—C17	-114.2 (3)	C20—C21—C16—P2	-176.1 (3)
C18—C19—C20—C21	-0.6 (6)	C20—C21—C16—C17	-2.1 (5)
C1—P1—C4—C9	-36.9 (3)	C13—C14—C15—C10	-0.8 (5)
C1—P1—C4—C5	146.2 (3)	C27—C22—C23—C24	0.2 (5)

---

C1—P1—C10—C11	−63.7 (3)	C27—C26—C25—C24	0.4 (7)
C1—P1—C10—C15	108.5 (3)	C25—C26—C27—C22	−0.1 (6)

---

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