# metal-organic compounds

Acta Crystallographica Section E **Structure Reports** Online

ISSN 1600-5368

## cis-Dichloridobis(ethyldiphenylphosphine-*κP*)platinum(II)

#### Wioleta Domanska-Babul, Jaroslaw Chojnacki\* and Jerzy **Pikies**

Chemical Department, Gdańsk University of Technology, 11/12 G. Narutowicz Street, 80952-PL Gdańsk, Poland Correspondence e-mail: jarekch@chem.pg.gda.pl

Received 13 June 2007; accepted 14 June 2007

Key indicators: single-crystal X-ray study; T = 120 K; mean  $\sigma$ (C–C) = 0.006 Å; R factor = 0.029; wR factor = 0.072; data-to-parameter ratio = 18.7.

In the title compound,  $[PtCl_2(C_{14}H_{15}P)_2]$ , the isomer from the reaction of potassium tetrachloridoplatinate(II) and ethyldiphenylphosphine, the Pt atom is in a square-planar geometry.

#### **Related literature**

For the related *cis*-dichloridobis(methyldiphenylphosphine)platinum(II), see Ho et al. (1982). For related literature, see: Domańska-Babul et al. (2007); Krautscheid et al. (1997); Porzio et al. (1980).



#### **Experimental**

m1956

| Crystal data                |  |
|-----------------------------|--|
| $[PtCl_2(C_{14}H_{15}P)_2]$ |  |
| $M_r = 694.45$              |  |
| Monoclinic, $P2_1/c$        |  |
| a = 14.2831 (6) Å           |  |

| b = 11.1025 (5) Å               |
|---------------------------------|
| c = 16.9556 (7)  Å              |
| $\beta = 106.677 \ (4)^{\circ}$ |
| $V = 2575.69 (19) \text{ Å}^3$  |
|                                 |

#### Z = 4Mo $K\alpha$ radiation $\mu = 5.80 \text{ mm}^{-1}$

#### Data collection

```
Oxford Diffraction KM-4 CCD
  diffractometer
Absorption correction: analytical
  (CrysAlis RED; Oxford Diffrac-
  tion, 2006; Clark & Reid, 1995).
  T_{\min} = 0.232, T_{\max} = 0.501
```

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.029$  $wR(F^2) = 0.072$ S = 1.105614 reflections

19512 measured reflections 5614 independent reflections

T = 120 (2) K

 $0.26 \times 0.14 \times 0.07 \text{ mm}$ 

5413 reflections with  $I > 2\sigma(I)$  $R_{\rm int}=0.032$ 

300 parameters H-atom parameters constrained  $\Delta \rho_{\rm max} = 2.88 \text{ e} \text{ Å}^ \Delta \rho_{\rm min} = -1.23 \text{ e} \text{ Å}^{-3}$ 

| Table 1  |                   |  |
|----------|-------------------|--|
| Selected | bond lengths (Å). |  |

| Pt1-P1 | 2.2633 (9) | Pt1-Cl1 | 2.3458 (9) |
|--------|------------|---------|------------|
| Pt1-P2 | 2.2517 (9) | Pt1-Cl2 | 2.3618 (9) |

Data collection: CrysAlis CCD (Oxford Diffraction, 2006); cell refinement: CrysAlis RED (Oxford Diffraction, 2006); data reduction: CrysAlis RED; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997): program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON (Spek, 2003).

WD-B and JP thank the Polish State Committee of Scientific Research (project No. 1 T09A 148 30) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2281).

#### References

- Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897.
- Domańska-Babul, W., Chojnacki, J., Matern, E. & Pikies, J. (2007). J. Organomet. Chem. doi:10.1016/j.jorganchem.2007.04.045
- Farrugia, L. J. (1997). J. Appl. Cryst. 30, 565.
- Farrugia, L. J. (1999). J. Appl. Cryst. 32, 837-838.
- Ho, K.-C., McLaughlin, G. M., McPartlin, M. & Robertson, G. B. (1982). Acta Cryst. B38, 421-425.
- Krautscheid, H., Matern, E., Kovacs, I., Fritz, G. & Pikies, J. (1997). Z. Anorg. Allg. Chem. 623, 1917-1924.
- Oxford Diffraction (2006). CrysAlis CCD and CrysAlis RED. Versions 1.171.29.9. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
- Porzio, W., Musco, A. & Immirzi, A. (1980). Inorg. Chem. 19, 2537-2540.
- Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.

Spek, A. L. (2003). J. Appl. Cryst. 36, 7-13.

© 2007 International Union of Crystallography

Acta Cryst. (2007). E63, m1956 [doi:10.1107/S1600536807029200]

## cis-Dichloridobis(ethyldiphenylphosphine-KP)platinum(II)

### W. Domanska-Babul, J. Chojnacki and J. Pikies

#### Comment

In the course of our studies upon the reactivity of  $[(R_3P)_2MCl_2]$  towards  $R'_2P-P(SiMe_3)_2$  (Domańska-Babul *et al.*, 2007) we have studied the reaction of  $({}^{i}Pr_2N)_2P-P(SiMe_3)_2$  with  $[(EtPh_2P)_2PtCl_2]$ . The title compound was obtained unchanged in the synthesis.

The complex exhibits square-planar coordination that is typical for platinum(II) compounds. The platinum atom is 0.0556 (4) Å above the square plane. The structure is similar to that of  $[(MePh_2P)_2PtCl_2]$  (Ho *et al.*, 1982). The square planar geometry is characteristic of complexes having less bulky tertiary phosphines. Significant deviation from planarity is observed with sterically bulky phosphines ligands, as noted in *cis*-dichlorobis(di-*t*-butylphenylphosphine)platinum(II) (Krautscheid *et al.*, 1997; Porzio *et al.*, 1980). The bond dimensions involving the platinum atom are typical of [*cis*-(*R*<sub>3</sub>P)<sub>2</sub>PtCl<sub>2</sub>] compounds such as for [(MePh<sub>2</sub>P)<sub>2</sub>PtCl<sub>2</sub>]. Weak intermolecular C—H…Cl interactions are also present.

#### Experimental

The compound was been obtained as yellow powder by the reaction of a solution of ethyl(diphenyl)phosphane in ethanol with a solution of potassium tetrachloroplatinate(II) in water. It was obtained in a crystalline habit from the reaction of  $({}^{i}Pr_{2}N)_{2}P-P(SiMe_{3})_{2}$  with [(EtPh\_{2}P)\_{2}PtCl\_{2}] a 1:1 molar ratio in THF. Crystals were obtained by recrystallization from pentane at 249 K

#### Refinement

All C–H hydrogen atoms were refined as riding on carbon atoms with methyl C–H = 0.98 Å, methylen C–H = 0.99 Å, aromatic C–H = 0.95 Å and  $U_{iso}$ (H)=1.2  $U_{eq}$ (C) for aromatic CH, 1.3 for CH<sub>2</sub> groups and 1.5 for methyl groups.

#### Figures



Fig. 1. View of (I) (50% probability displacement ellipsoids)

## cis-Dichloridobis(ethyldiphenylphosphine-κP)platinum(II)

### Crystal data

| $[PtCl_2(C_{14}H_{15}P)_2]$     | $F_{000} = 1360$                                |
|---------------------------------|---|
| $M_r = 694.45$                  | $D_{\rm x} = 1.791 {\rm ~Mg~m}^{-3}$            |
| Monoclinic, $P2_1/c$            | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc            | Cell parameters from 9761 reflections           |
| a = 14.2831 (6) Å               | $\theta = 2.9 - 32.5^{\circ}$                   |
| b = 11.1025 (5)  Å              | $\mu = 5.80 \text{ mm}^{-1}$                    |
| c = 16.9556 (7) Å               | T = 120 (2)  K                                  |
| $\beta = 106.677 \ (4)^{\circ}$ | Prism, yellow                                   |
| $V = 2575.69 (19) \text{ Å}^3$  | $0.26 \times 0.14 \times 0.07 \text{ mm}$       |
| Z = 4                           |   |

#### Data collection

| Oxford Diffraction KM-4-CCD diffractometer   | 5413 reflections with $I > 2\sigma(I)$ |
|--|--|
| Monochromator: graphite  | $R_{\rm int} = 0.032$                  |
| $0.75^{\circ} \omega$ scans  | $\theta_{\text{max}} = 27^{\circ}$     |
| Absorption correction: Analytical<br>CrysAlis RED (Oxford Diffraction, 2006; Clark &<br>Reid, 1995). | $\theta_{\min} = 2.9^{\circ}$          |
| $T_{\min} = 0.232, \ T_{\max} = 0.501$   | $h = -18 \rightarrow 18$               |
| 19512 measured reflections   | $k = -14 \rightarrow 14$               |
| 5614 independent reflections   | $l = -21 \rightarrow 13$               |

#### Refinement

| Refinement on $F^2$             | H-atom parameters constrained   |
|---------------------------------|---|
| Least-squares matrix: full      | $w = 1/[\sigma^2(F_o^2) + (0.0399P)^2 + 6.0673P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)] = 0.029$ | $(\Delta/\sigma)_{\rm max} = 0.001$   |
| $wR(F^2) = 0.072$               | $\Delta \rho_{\text{max}} = 2.88 \text{ e} \text{ Å}^{-3}$                          |
| <i>S</i> = 1.10                 | $\Delta \rho_{\rm min} = -1.23 \text{ e} \text{ Å}^{-3}$                            |
| 5614 reflections                | Extinction correction: none   |
| 300 parameters                  |   |
|                                 |   |

### 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.

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

|      | x            | У             | Ζ            | Uiso*/Ueq    |
|------|--------------|---------------|--------------|--------------|
| Pt1  | 0.270906 (9) | 0.459023 (11) | 0.282544 (7) | 0.01446 (6)  |
| P1   | 0.15530 (6)  | 0.41497 (8)   | 0.34561 (5)  | 0.01523 (17) |
| P2   | 0.36679 (6)  | 0.29500 (8)   | 0.31639 (5)  | 0.01523 (17) |
| Cl1  | 0.36472 (8)  | 0.53298 (8)   | 0.20004 (6)  | 0.0278 (2)   |
| Cl2  | 0.17113 (7)  | 0.62945 (9)   | 0.23685 (6)  | 0.0308 (2)   |
| C1   | 0.1445 (3)   | 0.5374 (3)    | 0.4142 (2)   | 0.0167 (7)   |
| C2   | 0.0551 (3)   | 0.5606 (3)    | 0.4295 (2)   | 0.0221 (7)   |
| H2   | -0.0001      | 0.5119        | 0.4043       | 0.027*       |
| C3   | 0.0462 (3)   | 0.6541 (3)    | 0.4811 (2)   | 0.0256 (8)   |
| Н3   | -0.0152      | 0.6699        | 0.4904       | 0.031*       |
| C4   | 0.1265 (3)   | 0.7245 (3)    | 0.5193 (2)   | 0.0268 (8)   |
| H4   | 0.1207       | 0.7873        | 0.5557       | 0.032*       |
| C5   | 0.2154 (3)   | 0.7028 (4)    | 0.5043 (2)   | 0.0287 (8)   |
| H5   | 0.2705       | 0.7513        | 0.5301       | 0.034*       |
| C6   | 0.2243 (3)   | 0.6101 (3)    | 0.4515 (2)   | 0.0244 (8)   |
| Н6   | 0.2852       | 0.5964        | 0.441        | 0.029*       |
| C7   | 0.1573 (3)   | 0.2795 (3)    | 0.4077 (2)   | 0.0179 (7)   |
| C8   | 0.0867 (3)   | 0.1887 (3)    | 0.3837 (2)   | 0.0258 (8)   |
| H8   | 0.0362       | 0.1962        | 0.3333       | 0.031*       |
| C9   | 0.0898 (4)   | 0.0879 (4)    | 0.4328 (3)   | 0.0357 (10)  |
| Н9   | 0.0402       | 0.0284        | 0.4168       | 0.043*       |
| C10  | 0.1648 (4)   | 0.0736 (4)    | 0.5049 (3)   | 0.0386 (11)  |
| H10  | 0.1679       | 0.0031        | 0.5373       | 0.046*       |
| C11  | 0.2353 (4)   | 0.1624 (4)    | 0.5297 (2)   | 0.0316 (9)   |
| H11  | 0.2874       | 0.1524        | 0.5788       | 0.038*       |
| C12  | 0.2297 (3)   | 0.2667 (3)    | 0.4825 (2)   | 0.0227 (7)   |
| H12  | 0.2758       | 0.3296        | 0.5016       | 0.027*       |
| C13  | 0.0365 (3)   | 0.4052 (4)    | 0.2677 (2)   | 0.0225 (7)   |
| H13A | -0.0121      | 0.3729        | 0.2937       | 0.029*       |
| H13B | 0.0152       | 0.4873        | 0.2475       | 0.029*       |
| C14  | 0.0376 (3)   | 0.3256 (4)    | 0.1944 (2)   | 0.0300 (9)   |
| H14A | 0.0771       | 0.3641        | 0.1629       | 0.045*       |
| H14B | -0.0294      | 0.3148        | 0.159        | 0.045*       |
| H14C | 0.0657       | 0.247         | 0.2144       | 0.045*       |
| C15  | 0.2996 (3)   | 0.1563 (3)    | 0.2819 (2)   | 0.0181 (7)   |
| C16  | 0.2805 (3)   | 0.0686 (3)    | 0.3338 (2)   | 0.0212 (7)   |
| H16  | 0.2992       | 0.0818        | 0.3916       | 0.025*       |
| C17  | 0.2339 (3)   | -0.0384 (3)   | 0.3015 (3)   | 0.0237 (8)   |
| H17  | 0.2212       | -0.098        | 0.3373       | 0.028*       |

| C18  | 0.2061 (3) | -0.0577 (4) | 0.2169 (3) | 0.0249 (8)  |
|------|------------|-------------|------------|-------------|
| H18  | 0.1767     | -0.1319     | 0.1951     | 0.03*       |
| C19  | 0.2210 (3) | 0.0305 (4)  | 0.1648 (3) | 0.0298 (9)  |
| H19  | 0.1994     | 0.0187      | 0.1069     | 0.036*      |
| C20  | 0.2678 (3) | 0.1370 (4)  | 0.1970 (2) | 0.0280 (8)  |
| H20  | 0.2782     | 0.1974      | 0.1607     | 0.034*      |
| C21  | 0.4359 (2) | 0.2718 (3)  | 0.4232 (2) | 0.0184 (7)  |
| C22  | 0.4926 (3) | 0.1674 (4)  | 0.4455 (3) | 0.0284 (8)  |
| H22  | 0.4899     | 0.1057      | 0.4061     | 0.034*      |
| C23  | 0.5528 (3) | 0.1547 (4)  | 0.5254 (3) | 0.0332 (9)  |
| H23  | 0.5913     | 0.0839      | 0.5402     | 0.04*       |
| C24  | 0.5576 (3) | 0.2429 (4)  | 0.5837 (2) | 0.0333 (10) |
| H24  | 0.5987     | 0.2325      | 0.6383     | 0.04*       |
| C25  | 0.5021 (3) | 0.3470 (4)  | 0.5622 (2) | 0.0295 (9)  |
| H25  | 0.5046     | 0.4077      | 0.6023     | 0.035*      |
| C26  | 0.4427 (3) | 0.3623 (3)  | 0.4817 (2) | 0.0225 (7)  |
| H26  | 0.4066     | 0.4348      | 0.4666     | 0.027*      |
| C27  | 0.4649 (3) | 0.2823 (4)  | 0.2668 (2) | 0.0232 (7)  |
| H27A | 0.4863     | 0.1972      | 0.2697     | 0.03*       |
| H27B | 0.4379     | 0.3034      | 0.2079     | 0.03*       |
| C28  | 0.5551 (3) | 0.3615 (4)  | 0.3040 (3) | 0.0313 (9)  |
| H28A | 0.5372     | 0.4465      | 0.2938     | 0.047*      |
| H28B | 0.6065     | 0.3414      | 0.2783     | 0.047*      |
| H28C | 0.5791     | 0.3472      | 0.3634     | 0.047*      |

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

|     | $U^{11}$    | $U^{22}$    | U <sup>33</sup> | $U^{12}$     | $U^{13}$     | U <sup>23</sup> |
|-----|-------------|-------------|-----------------|--------------|--------------|-----------------|
| Pt1 | 0.01654 (8) | 0.01163 (8) | 0.01519 (8)     | -0.00052 (4) | 0.00450 (5)  | 0.00112 (4)     |
| P1  | 0.0155 (4)  | 0.0138 (4)  | 0.0161 (4)      | 0.0003 (3)   | 0.0041 (3)   | -0.0004 (3)     |
| P2  | 0.0140 (4)  | 0.0137 (4)  | 0.0174 (4)      | -0.0005 (3)  | 0.0037 (3)   | -0.0013 (3)     |
| Cl1 | 0.0330 (5)  | 0.0240 (5)  | 0.0315 (5)      | -0.0059 (4)  | 0.0174 (4)   | 0.0040 (3)      |
| Cl2 | 0.0351 (5)  | 0.0213 (4)  | 0.0369 (5)      | 0.0105 (4)   | 0.0121 (4)   | 0.0129 (4)      |
| C1  | 0.0216 (17) | 0.0132 (16) | 0.0164 (16)     | 0.0034 (12)  | 0.0072 (14)  | 0.0024 (12)     |
| C2  | 0.0253 (19) | 0.0192 (17) | 0.0244 (18)     | -0.0008 (14) | 0.0111 (15)  | 0.0020 (14)     |
| C3  | 0.034 (2)   | 0.0206 (18) | 0.0275 (19)     | 0.0058 (15)  | 0.0176 (16)  | 0.0023 (15)     |
| C4  | 0.045 (2)   | 0.0164 (17) | 0.0201 (17)     | 0.0039 (16)  | 0.0118 (16)  | -0.0002 (14)    |
| C5  | 0.033 (2)   | 0.0226 (19) | 0.027 (2)       | -0.0041 (16) | 0.0029 (16)  | -0.0045 (16)    |
| C6  | 0.0220 (18) | 0.0225 (18) | 0.0272 (18)     | 0.0005 (14)  | 0.0045 (15)  | -0.0034 (15)    |
| C7  | 0.0203 (16) | 0.0157 (16) | 0.0198 (16)     | -0.0002 (13) | 0.0090 (13)  | -0.0010 (13)    |
| C8  | 0.0266 (19) | 0.0230 (19) | 0.030 (2)       | -0.0086 (15) | 0.0116 (16)  | -0.0073 (15)    |
| C9  | 0.051 (3)   | 0.024 (2)   | 0.040 (2)       | -0.0164 (19) | 0.024 (2)    | -0.0079 (18)    |
| C10 | 0.074 (3)   | 0.0173 (19) | 0.032 (2)       | -0.006 (2)   | 0.028 (2)    | 0.0026 (17)     |
| C11 | 0.052 (3)   | 0.0221 (19) | 0.0204 (18)     | 0.0032 (18)  | 0.0101 (17)  | -0.0003 (15)    |
| C12 | 0.0294 (19) | 0.0163 (17) | 0.0228 (17)     | 0.0001 (14)  | 0.0081 (15)  | -0.0020 (14)    |
| C13 | 0.0164 (16) | 0.0253 (19) | 0.0225 (17)     | 0.0018 (14)  | 0.0003 (13)  | -0.0030 (14)    |
| C14 | 0.0258 (19) | 0.036 (2)   | 0.0238 (19)     | 0.0035 (17)  | -0.0006 (15) | -0.0048 (17)    |
| C15 | 0.0174 (16) | 0.0125 (16) | 0.0232 (17)     | 0.0018 (13)  | 0.0036 (13)  | -0.0027 (13)    |

| C16 | 0.0215 (17) | 0.0209 (17) | 0.0210 (17) | 0.0003 (14)  | 0.0060 (14)  | -0.0007 (14) |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C17 | 0.0224 (19) | 0.0180 (18) | 0.032 (2)   | -0.0005 (13) | 0.0097 (16)  | 0.0003 (14)  |
| C18 | 0.0199 (17) | 0.0193 (18) | 0.034 (2)   | -0.0024 (14) | 0.0058 (15)  | -0.0071 (15) |
| C19 | 0.033 (2)   | 0.028 (2)   | 0.025 (2)   | -0.0058 (16) | 0.0031 (17)  | -0.0062 (16) |
| C20 | 0.038 (2)   | 0.0209 (19) | 0.0211 (18) | -0.0082 (16) | 0.0017 (16)  | 0.0010 (15)  |
| C21 | 0.0155 (15) | 0.0182 (17) | 0.0182 (16) | -0.0031 (13) | -0.0006 (12) | -0.0014 (13) |
| C22 | 0.0238 (19) | 0.0234 (19) | 0.034 (2)   | 0.0019 (15)  | 0.0019 (16)  | 0.0030 (16)  |
| C23 | 0.025 (2)   | 0.030 (2)   | 0.038 (2)   | 0.0001 (16)  | -0.0030 (17) | 0.0126 (18)  |
| C24 | 0.028 (2)   | 0.042 (2)   | 0.0219 (19) | -0.0080 (18) | -0.0055 (15) | 0.0113 (18)  |
| C25 | 0.031 (2)   | 0.034 (2)   | 0.0212 (18) | -0.0110 (17) | 0.0038 (15)  | -0.0035 (16) |
| C26 | 0.0209 (17) | 0.0206 (18) | 0.0252 (18) | -0.0030 (14) | 0.0051 (14)  | -0.0007 (14) |
| C27 | 0.0213 (17) | 0.0238 (18) | 0.0263 (19) | 0.0030 (14)  | 0.0099 (15)  | -0.0041 (15) |
| C28 | 0.0193 (18) | 0.043 (2)   | 0.032 (2)   | -0.0063 (17) | 0.0092 (16)  | -0.0061 (18) |
|     |             |             |             |              |              |              |

Geometric parameters (Å, °)

| Pt1—P1  | 2.2633 (9) | С13—Н13А | 0.99      |
|---------|------------|----------|-----------|
| Pt1—P2  | 2.2517 (9) | С13—Н13В | 0.99      |
| Pt1—Cl1 | 2.3458 (9) | C14—H14A | 0.98      |
| Pt1—Cl2 | 2.3618 (9) | C14—H14B | 0.98      |
| P1—C1   | 1.824 (3)  | C14—H14C | 0.98      |
| P1—C13  | 1.830 (4)  | C15—C16  | 1.391 (5) |
| P1—C7   | 1.832 (4)  | C15—C20  | 1.397 (5) |
| P2—C21  | 1.816 (4)  | C16—C17  | 1.394 (5) |
| P2—C15  | 1.820 (4)  | C16—H16  | 0.95      |
| P2—C27  | 1.835 (4)  | C17—C18  | 1.391 (6) |
| C1—C6   | 1.391 (5)  | С17—Н17  | 0.95      |
| C1—C2   | 1.398 (5)  | C18—C19  | 1.376 (6) |
| C2—C3   | 1.387 (5)  | C18—H18  | 0.95      |
| С2—Н2   | 0.95       | C19—C20  | 1.390 (5) |
| C3—C4   | 1.386 (6)  | С19—Н19  | 0.95      |
| С3—Н3   | 0.95       | C20—H20  | 0.95      |
| C4—C5   | 1.385 (6)  | C21—C26  | 1.396 (5) |
| C4—H4   | 0.95       | C21—C22  | 1.403 (5) |
| C5—C6   | 1.394 (5)  | C22—C23  | 1.388 (6) |
| С5—Н5   | 0.95       | С22—Н22  | 0.95      |
| С6—Н6   | 0.95       | C23—C24  | 1.379 (7) |
| C7—C12  | 1.395 (5)  | С23—Н23  | 0.95      |
| С7—С8   | 1.400 (5)  | C24—C25  | 1.390 (6) |
| C8—C9   | 1.388 (6)  | C24—H24  | 0.95      |
| С8—Н8   | 0.95       | C25—C26  | 1.395 (5) |
| C9—C10  | 1.385 (7)  | С25—Н25  | 0.95      |
| С9—Н9   | 0.95       | C26—H26  | 0.95      |
| C10-C11 | 1.386 (7)  | C27—C28  | 1.537 (5) |
| С10—Н10 | 0.95       | С27—Н27А | 0.99      |
| C11—C12 | 1.397 (5)  | С27—Н27В | 0.99      |
| C11—H11 | 0.95       | C28—H28A | 0.98      |
| C12—H12 | 0.95       | C28—H28B | 0.98      |
| C13—C14 | 1.529 (5)  | C28—H28C | 0.98      |
|         |            |          |           |

| P2Pt1P1                     | 100 23 (3)               | C14—C13—H13B   | 108.9                |
|-----------------------------|--------------------------|--|----------------------|
| P2—Pt1—Cl1                  | 91.45 (3)                | P1—C13—H13B  | 108.9                |
| P1Pt1C11                    | 167 54 (3)               | H13A_C13_H13B  | 107.7                |
| $P2\_Pt1\_C12$              | 175 70 (3)               | C13 - C14 - H14A                                     | 109.5                |
| $P1_Pt1_C12$                | 82 81 (3)                | C13_C14_H14B   | 109.5                |
| C11 $Pt1$ $C12$             | 85 30 (3)                | $H_{14A}$ $C_{14}$ $H_{14B}$                         | 109.5                |
| C1 - P1 - C13               | 105 86 (17)              | C13 - C14 - H14C                                     | 109.5                |
| C1  P1  C7                  | 103.60(17)<br>103.62(15) |  | 109.5                |
| $C_1 = 1 = C_7$             | 103.02(13)<br>102.05(17) | $H_{14} = C_{14} = H_{14} C_{14}$                    | 109.5                |
| $C_{1} = D_{1} = D_{1}$     | 102.93(17)<br>110.20(12) | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | 107.5<br>119.7(2)    |
| $C_1 - r_1 - r_1$           | 110.29(12)<br>108.86(12) | $C_{10} = C_{15} = C_{20}$                           | 110.7(3)<br>124.8(2) |
| $C_{13}$ $-P_{1}$ $-P_{11}$ | 108.80(13)               | C10-C15-P2   | 124.0(3)             |
| C/—PI—Pti                   | 123.80 (11)              | C20C15P2   | 116.6 (3)            |
| C21—P2—C15                  | 106.63 (16)              | C15-C16-C17  | 120.4 (3)            |
| C21—P2—C27                  | 100.27 (17)              | С15—С16—Н16  | 119.8                |
| C15—P2—C27                  | 100.92 (17)              | С17—С16—Н16  | 119.8                |
| C21—P2—Pt1                  | 119.05 (12)              | C18—C17—C16  | 120.0 (4)            |
| C15—P2—Pt1                  | 112.12 (11)              | C18—C17—H17  | 120                  |
| C27—P2—Pt1                  | 115.72 (13)              | С16—С17—Н17  | 120                  |
| C6—C1—C2                    | 118.8 (3)                | C19—C18—C17  | 120.1 (4)            |
| C6—C1—P1                    | 120.9 (3)                | C19—C18—H18  | 120                  |
| C2—C1—P1                    | 120.3 (3)                | C17—C18—H18  | 120                  |
| C3—C2—C1                    | 120.6 (4)                | C18—C19—C20  | 119.9 (4)            |
| С3—С2—Н2                    | 119.7                    | С18—С19—Н19  | 120                  |
| C1—C2—H2                    | 119.7                    | С20—С19—Н19  | 120                  |
| C4—C3—C2                    | 120.2 (4)                | C19—C20—C15  | 120.9 (4)            |
| С4—С3—Н3                    | 119.9                    | С19—С20—Н20  | 119.6                |
| С2—С3—Н3                    | 119.9                    | С15—С20—Н20  | 119.6                |
| C5—C4—C3                    | 119.7 (4)                | C26—C21—C22  | 119.2 (3)            |
| С5—С4—Н4                    | 120.1                    | C26—C21—P2   | 120.9 (3)            |
| C3—C4—H4                    | 120.1                    | C22—C21—P2   | 119.5 (3)            |
| C4—C5—C6                    | 120.2 (4)                | C23—C22—C21  | 119.7 (4)            |
| C4—C5—H5                    | 119.9                    | С23—С22—Н22  | 120.2                |
| С6—С5—Н5                    | 119.9                    | C21—C22—H22  | 120.2                |
| C1—C6—C5                    | 120.5 (4)                | C24—C23—C22  | 121.1 (4)            |
| С1—С6—Н6                    | 119.8                    | C24—C23—H23  | 119.4                |
| С5—С6—Нб                    | 119.8                    | C22—C23—H23  | 119.4                |
| C12 - C7 - C8               | 118.4 (3)                | $C_{23} - C_{24} - C_{25}$                           | 119.7 (4)            |
| C12_C7_P1                   | 119.4 (3)                | $C_{23} = C_{24} = H_{24}$                           | 120.2                |
| $C_{12} = C_7 = P_1$        | 117.4(3)<br>122.2(3)     | $C_{25} = C_{24} = H_{24}$                           | 120.2                |
| $C_{0} - C_{1} - C_{1}$     | 122.2(3)<br>120.6(4)     | $C_{23} = C_{24} = 1124$                             | 110 0 (1)            |
| $C_{0} = C_{0} = C_{1}$     | 110.7                    | $C_{24} = C_{25} = C_{26}$                           | 119.9 (4)            |
| $C_{2} = C_{3} = 118$       | 119.7                    | $C_{24} = C_{25} = H_{25}$                           | 120                  |
| $C_{1} = C_{0} = C_{0}^{0}$ | 119.7                    | $C_{20} = C_{23} = M_{23}$                           | 120                  |
| C10_C9_C8                   | 120.3 (4)                | $C_{25} = C_{20} = C_{21}$                           | 120.4 (4)            |
| $C_{10} = C_{9} = H_{9}$    | 119.8                    | $C_{23} - C_{20} - H_{20}$                           | 119.0                |
|                             | 119.8                    | $C_{21} - C_{20} - H_{20}$                           | 119.8                |
| C9—C10—C11                  | 119.8 (4)                | $C_{28} = C_{27} = H_{27}$                           | 115.4 (3)            |
| С9—С10—Н10                  | 120.1                    | C28—C27—H2/A   | 108.4                |
| C11—C10—H10                 | 120.1                    | P2—C2/—H2/A  | 108.4                |
| C10-C11-C12                 | 120.0 (4)                | С28—С27—Н27В   | 108.4                |

| C10-C11-H11    | 120          | Р2—С27—Н27В     | 108.4      |
|----------------|--------------|-----------------|------------|
| C12—C11—H11    | 120          | H27A—C27—H27B   | 107.5      |
| C7—C12—C11     | 120.7 (4)    | C27—C28—H28A    | 109.5      |
| C7—C12—H12     | 119.7        | C27—C28—H28B    | 109.5      |
| C11—C12—H12    | 119.7        | H28A—C28—H28B   | 109.5      |
| C14—C13—P1     | 113.4 (3)    | C27—C28—H28C    | 109.5      |
| C14—C13—H13A   | 108.9        | H28A—C28—H28C   | 109.5      |
| P1             | 108.9        | H28B—C28—H28C   | 109.5      |
| P2—Pt1—P1—C1   | 125.44 (12)  | C7—C8—C9—C10    | -2.3 (6)   |
| Cl1—Pt1—P1—C1  | -75.1 (2)    | C8—C9—C10—C11   | 2.2 (7)    |
| Cl2—Pt1—P1—C1  | -57.64 (13)  | C9-C10-C11-C12  | 0.9 (7)    |
| P2—Pt1—P1—C13  | -118.82 (13) | C8—C7—C12—C11   | 3.9 (5)    |
| Cl1—Pt1—P1—C13 | 40.6 (2)     | P1              | -177.6 (3) |
| Cl2—Pt1—P1—C13 | 58.09 (14)   | C10-C11-C12-C7  | -4.0 (6)   |
| P2—Pt1—P1—C7   | 2.09 (14)    | C1—P1—C13—C14   | 167.9 (3)  |
| Cl1—Pt1—P1—C7  | 161.55 (18)  | C7—P1—C13—C14   | -83.7 (3)  |
| Cl2—Pt1—P1—C7  | 179.01 (14)  | Pt1—P1—C13—C14  | 49.3 (3)   |
| P1—Pt1—P2—C21  | -67.66 (14)  | C21—P2—C15—C16  | 19.0 (4)   |
| Cl1—Pt1—P2—C21 | 116.69 (14)  | C27—P2—C15—C16  | 123.3 (3)  |
| Cl2—Pt1—P2—C21 | 157.7 (4)    | Pt1—P2—C15—C16  | -112.9 (3) |
| P1—Pt1—P2—C15  | 57.73 (13)   | C21—P2—C15—C20  | -159.4 (3) |
| Cl1—Pt1—P2—C15 | -117.92 (13) | C27—P2—C15—C20  | -55.1 (3)  |
| Cl2—Pt1—P2—C15 | -76.9 (5)    | Pt1—P2—C15—C20  | 68.7 (3)   |
| P1—Pt1—P2—C27  | 172.74 (14)  | C20-C15-C16-C17 | 2.6 (5)    |
| Cl1—Pt1—P2—C27 | -2.92 (14)   | P2-C15-C16-C17  | -175.7 (3) |
| Cl2—Pt1—P2—C27 | 38.1 (5)     | C15-C16-C17-C18 | -0.2 (6)   |
| C13—P1—C1—C6   | -146.9 (3)   | C16-C17-C18-C19 | -2.5 (6)   |
| C7—P1—C1—C6    | 105.2 (3)    | C17—C18—C19—C20 | 2.8 (6)    |
| Pt1—P1—C1—C6   | -29.3 (3)    | C18—C19—C20—C15 | -0.3 (7)   |
| C13—P1—C1—C2   | 32.5 (3)     | C16-C15-C20-C19 | -2.3 (6)   |
| C7—P1—C1—C2    | -75.5 (3)    | P2-C15-C20-C19  | 176.1 (3)  |
| Pt1—P1—C1—C2   | 150.1 (3)    | C15—P2—C21—C26  | -138.3 (3) |
| C6—C1—C2—C3    | -0.2 (5)     | C27—P2—C21—C26  | 117.0 (3)  |
| P1—C1—C2—C3    | -179.6 (3)   | Pt1—P2—C21—C26  | -10.3 (3)  |
| C1—C2—C3—C4    | -1.1 (6)     | C15—P2—C21—C22  | 49.4 (3)   |
| C2—C3—C4—C5    | 1.4 (6)      | C27—P2—C21—C22  | -55.4 (3)  |
| C3—C4—C5—C6    | -0.5 (6)     | Pt1—P2—C21—C22  | 177.3 (3)  |
| C2—C1—C6—C5    | 1.1 (6)      | C26—C21—C22—C23 | 1.3 (6)    |
| P1-C1-C6-C5    | -179.5 (3)   | P2-C21-C22-C23  | 173.9 (3)  |
| C4—C5—C6—C1    | -0.8 (6)     | C21—C22—C23—C24 | 0.2 (6)    |
| C1—P1—C7—C12   | -58.4 (3)    | C22—C23—C24—C25 | -0.6(7)    |
| C13—P1—C7—C12  | -168.6 (3)   | C23—C24—C25—C26 | -0.7 (6)   |
| Pt1—P1—C7—C12  | 67.8 (3)     | C24—C25—C26—C21 | 2.3 (6)    |
| C1—P1—C7—C8    | 120.0 (3)    | C22—C21—C26—C25 | -2.6 (6)   |
| C13—P1—C7—C8   | 9.8 (3)      | P2-C21-C26-C25  | -175.0 (3) |
| Pt1—P1—C7—C8   | -113.8 (3)   | C21—P2—C27—C28  | -51.3 (3)  |
| C12—C7—C8—C9   | -0.8 (6)     | C15—P2—C27—C28  | -160.6 (3) |
| P1—C7—C8—C9    | -179.2 (3)   | Pt1-P2-C27-C28  | 78.1 (3)   |

# Hydrogen-bond geometry (Å, °)

| D—H···A                     | <i>D</i> —Н | H···A | $D \cdots A$ | D—H···A |
|-----------------------------|-------------|-------|--------------|---------|
| C13—H13B…Cl2                | 0.99        | 2.78  | 3.278 (4)    | 112     |
| C18—H18····Cl2 <sup>i</sup> | 0.95        | 2.75  | 3.539 (4)    | 141     |
| C27—H27A…Cl1 <sup>ii</sup>  | 0.99        | 2.74  | 3.622 (4)    | 149     |
| C27—H27B…Cl1                | 0.99        | 2.74  | 3.185 (4)    | 108     |
| C28—H28A…Cl1                | 0.98        | 2.70  | 3.373 (5)    | 126     |
| $\mathbf{C}_{i}$            | 1/2 = 1/2   |       |              |         |

Symmetry codes: (i) *x*, *y*-1, *z*; (ii) –*x*+1, *y*-1/2, –*z*+1/2.



Fig. 1