



Crystal structure of *cis*-[1,2-bis(diphenylphosphanyl)ethene- κ^2P,P']dichloridoplatinum(II) chloroform disolvate: a new polymorph

Jimmy Mugemana, John Bender, Richard J. Staples and Shannon M. Biros

Acta Cryst. (2018). **E74**, 998–1001



IUCr Journals

CRYSTALLOGRAPHY JOURNALS ONLINE

This open-access article is distributed under the terms of the Creative Commons Attribution Licence <http://creativecommons.org/licenses/by/2.0/uk/legalcode>, which permits unrestricted use, distribution, and reproduction in any medium, provided the original authors and source are cited.



Crystal structure of *cis*-[1,2-bis(diphenylphosphanyl)ethene- κ^2P,P']dichloridoplatinum(II) chloroform disolvate: a new polymorph

Jimmy Mugemana,^a John Bender,^a Richard J. Staples^b and Shannon M. Biros^{a*}

^aDepartment of Chemistry, Grand Valley State University, 1 Campus Dr., Allendale, MI 49401, USA, and ^bCenter for Crystallographic Research, Department of Chemistry, Michigan State University, East Lansing, MI 48824, USA.

*Correspondence e-mail: biross@gvsu.edu

Received 24 May 2018

Accepted 15 June 2018

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

Keywords: crystal structure; polymorph; *cis*-dppe; C—H...Cl hydrogen bonding; face-on C—Cl... π interactions; offset π — π interactions.

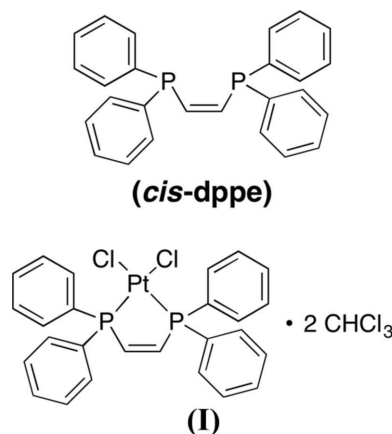
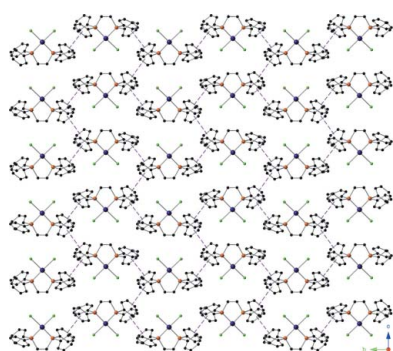
CCDC reference: 1849747

Supporting information: this article has supporting information at journals.iucr.org/e

The title compound, [PtCl₂(C₂₆H₂₂P₂)]·2CHCl₃ (I), is the third monoclinic polymorph of this platinum(II) complex involving the bidentate ligand *cis*-1,2-bis(diphenylphosphanyl)ethylene (*cis*-dppe) [for the others, see: Oberhauser *et al.* (1998a). *Inorg. Chim. Acta*, **274**, 143–154, and Oberhauser *et al.* (1995). *Inorg. Chim. Acta*, **238**, 35–43]. The structure of compound (I) was solved in the space group *P*2₁/*c*, with one complex molecule in the asymmetric unit along with two solvate chloroform molecules. The Pt^{II} atom is ligated by two P and two Cl atoms in the equatorial plane and has a perfect square-planar coordination sphere. In the crystal, the complex molecule is linked to the chloroform solvate molecules by C—H...Cl hydrogen bonds and face-on C—Cl... π interactions. There are also weak offset π — π interactions present [intercentroid distances are 3.770 (6) and 4.096 (6) Å], linking the molecules to form supramolecular sheets that lie in the *bc* plane.

1. Chemical context

The rigid compound *cis*-1,2-bis(diphenylphosphanyl)ethylene (*cis*-dppe) has been widely exploited as a bidentate ligand for transition metals. A selection of recent examples include complexes involving iron(II) (Song *et al.*, 2018), copper(I) (Trivedi *et al.*, 2017), gold(I) (Yao & Yam, 2015), nickel(II) (Schallenberg *et al.*, 2014), nickel(III) (Hwang *et al.*, 2015), and palladium(II) and platinum(II) (Song *et al.*, 2017; Oberhauser *et al.*, 1998a). The phosphorus atoms of this ligand have also been modified to give the corresponding oxide, sulfide and selenide derivatives (Morse *et al.*, 2016; Duncan & Gallagher, 1981; Colquhoun *et al.*, 1979; Aguiar & Daigle, 1964). Hence, structural studies of the parent bisphosphine are relevant to a wide array of researchers.



OPEN ACCESS

Table 1

Selected bond distances (Å), bond angles (°) and the fourfold coordination descriptor, τ_4^a , for the three polymorphs of [(*cis*-dppe)-Pt(Cl)₂].

Compound	(I)	HINCIQ ^b	ZOLYII ^c
Pt1—Cl1	2.358 (2)	2.36482	2.360 (2)
Pt1—Cl2	2.363 (2)	2.366 (3)	2.360 (2)
Pt1—P1	2.217 (2)	2.216 (2)	2.211 (2)
Pt1—P2	2.210 (2)	2.219 (2)	2.211 (2)
P1—Pt1—Cl2	177.58 (7)	176.35 (10)	177.92 (9)
P2—Pt1—Cl1	178.38 (7)	175.81 (10)	177.92 (9)
τ_4	0.02	0.05	0.0

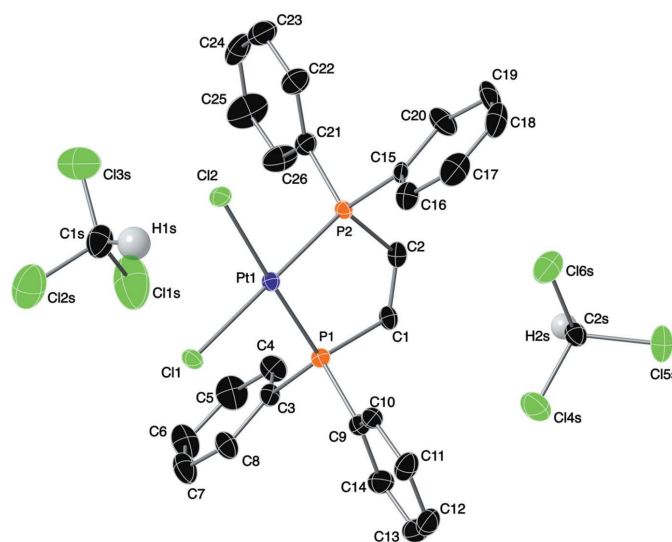
Notes: (a) Yang *et al.* (2007); (b) Oberhauser *et al.* (1998a); (c) Oberhauser *et al.* (1995).

2. Structural commentary

The molecular structures of the *cis*-dppe ligand and the title compound (I) are shown in Fig. 1. This Pt–ligand complex features a square-planar geometry around the Pt^{II} metal center with bidentate coordination by the phosphorus atoms of the *cis*-dppe ligand. The metal coordination sphere is completed by two chloride anions.

As for the previously reported polymorphs of compound (I), structure HINCIQ (Oberhauser *et al.*, 1998a) was solved in space group $P2_1/n$ without solvent in the unit cell, while structure ZOLYII (Oberhauser *et al.*, 1995) was solved in the space group $P2_1/m$ as a chloroform and methylene chloride solvate. The latter complex molecule possesses mirror symmetry with the mirror bisecting the Pt atom and central C=C bond of the *cis*-dppe ligand. Selected bond distances and bond angles for the title compound (I), and the two other monoclinic polymorphs are given in Table 1.

When comparing these two structures to the title compound, the bond lengths and angles around the Pt^{II} center of all three structures are, unsurprisingly, quite similar. The Pt–P bond lengths range from 2.210 (2) to 2.219 (2) Å, while

**Figure 1**

A view of the molecular structure of the title compound, with the atom labeling. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms bonded to the ligand have been omitted for clarity.

Table 2

Hydrogen-bond geometry (Å, °).

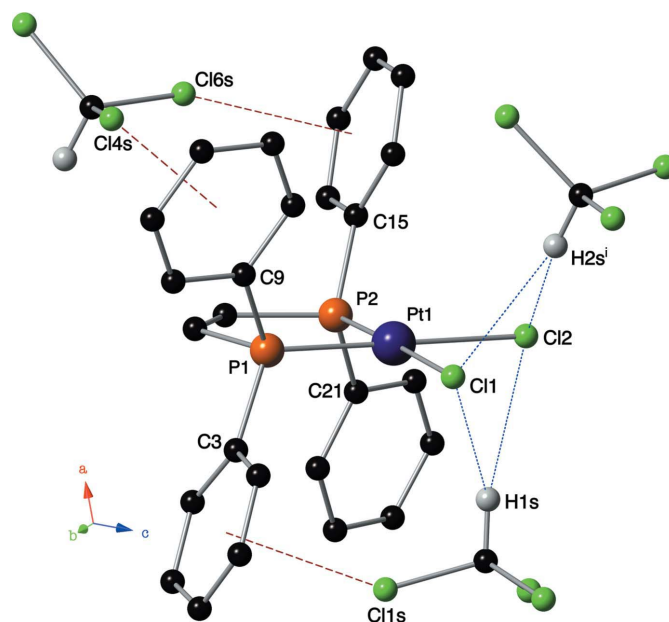
$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1S—H1S ⁱ ···Cl1	1.00	3.04	3.782 (11)	132
C1S—H1S ⁱ ···Cl2	1.00	2.84	3.789 (10)	158
C2S—H2S ⁱ ···Cl1 ⁱ	1.00	2.80	3.616 (9)	139
C2S—H2S ⁱ ···Cl2 ⁱ	1.00	2.77	3.649 (9)	147

Symmetry code: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$.

the Pt–Cl bond lengths range from 2.358 (2) to 2.366 (3) Å. The P–Pt–P bond angles range from 86.66 (11) to 87.08 (5)°, while the Cl–Pt–Cl bond angles range from 90.33 (7) to 91.03 (5)°. The τ_4 descriptor for fourfold coordination (where, for the extreme forms $\tau_4 = 0.00$ for square-planar, 1.00 for tetrahedral and 0.85 for trigonal-pyramidal; Yang *et al.*, 2007) of the Pt atoms range from 0.02 for compound (I), 0.05 for HINCIQ and 0.0 for ZOLYII, indicating perfect square-planar coordination spheres for each Pt atom.

3. Supramolecular features

In the crystal of (I), the metal–ligand complex is linked to the chloroform solvate molecules by C–H···Cl hydrogen bonds and Cl··· π interactions. The hydrogen atoms of both chloroform molecules are engaged in weak hydrogen bonds with the metal-bound chlorine atoms (Fig. 2 and Table 2). The $D\cdots A$ distances range from 3.616 (9) to 3.789 (10) Å, while the $D-H\cdots A$ bond angles range from 132 to 158°. Three face-on Cl··· π interactions (Imai *et al.*, 2008) are also present involving the chlorine atoms of the chloroform molecules and the

**Figure 2**

A view along the b axis of the title compound showing the C–H···Cl hydrogen bonds (blue dotted lines) and chlorine··· π interactions (red dashed lines) found in the crystal lattice [symmetry code: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$].

Table 3

Face-on Cl... π interactions ($\text{\AA}$, $^\circ$).

Cg1, Cg2 and Cg3 are the centroids of the phenyl rings C3–C8, C9–C14 and C15–C20, respectively.

C—Cl...Cg	C—Cl	Cl...Cg	C...Cg	C—Cl...Cg
C1S—Cl1S...Cg1	1.706 (11)	3.441 (7)	4.862 (11)	139.2 (5)
C2S—Cl4S...Cg2	1.737 (8)	3.242 (5)	4.775 (9)	145.4 (3)
C2S—Cl6S...Cg3	1.735 (8)	3.349 (5)	5.017 (9)	160.3 (4)

aromatic rings of the *cis*-dppe ligand (Fig. 2 and Table 3). The Cl...ring centroid distances for these interactions range from 3.242 (5) to 3.441 (7) $\text{\AA}$, while the C—Cl...ring centroid angles range from 139.2 (5) to 160.3 (4) $^\circ$.

The complex molecules are also linked by weak offset π – π interactions, forming sheets that lie in the *bc* plane, as shown in Fig. 3. The intercentroid distances are $\text{Cg2}\cdots\text{Cg2}^{\text{ii}} = 4.096$ (6) $\text{\AA}$ [Cg2 is the centroid of ring C9–C14, $\alpha = 0.0$ (5) $^\circ$, interplanar distance = 3.917 (4) $\text{\AA}$, slippage = 1.20 $\text{\AA}$, symmetry code (ii) $-x + 2, -y, -z + 1$], and $\text{Cg3}\cdots\text{Cg4}^{\text{iii}} = 3.770$ (6) $\text{\AA}$ [Cg3 and Cg4 are the centroids of rings C15–C20 and C21–C26, respectively, $\alpha = 5.3$ (5) $^\circ$, interplanar distances are 3.326 (4) and 3.439 (4) $\text{\AA}$, slippage = 1.544 $\text{\AA}$, symmetry code (iii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$].

The closely related polymorph ZOLYII, which contains one CH_2Cl_2 solvent molecule and one CHCl_3 solvent molecule in the unit cell, also shows Cl... π interactions. However, the methylene chloride solvent molecule is not engaged in a hydrogen bond with a chlorine atom of the Pt^{II} complex, and is disordered in the crystal lattice.

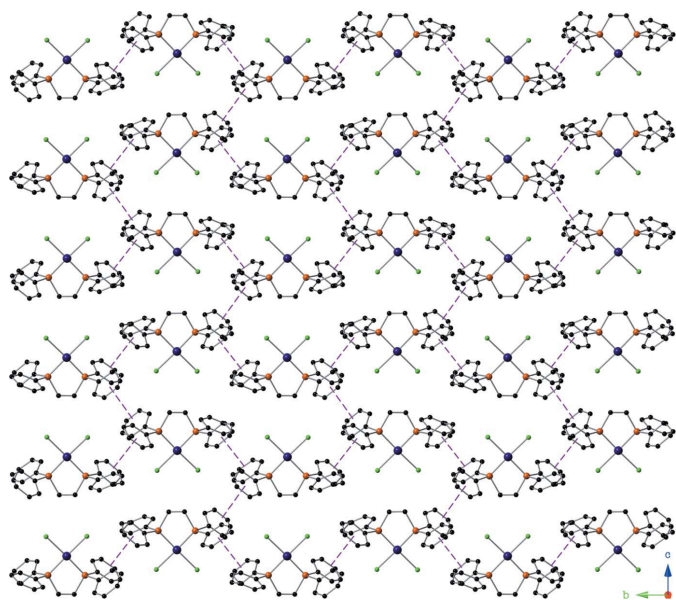


Figure 3

A view along the *a* axis of the weak offset π – π interactions (purple dashed lines) between aromatic rings of the title compound, resulting in the formation of supramolecular sheets. Chloroform solvent molecules have been omitted for clarity.

Table 4

Experimental details.

Crystal data	
Chemical formula	$[\text{PtCl}_2(\text{C}_{26}\text{H}_{22}\text{P}_2)] \cdot 2\text{CHCl}_3$
M_r	901.10
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, b, c ($\text{\AA}$)	11.1441 (10), 18.0870 (17), 16.9621 (16)
β ($^\circ$)	106.2465 (10)
V ($\text{\AA}^3$)	3282.4 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	5.04
Crystal size (mm)	$0.26 \times 0.14 \times 0.10$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2013)
$T_{\text{min}}, T_{\text{max}}$	0.503, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26503, 6039, 3360
R_{int}	0.069
$(\sin \theta/\lambda)_{\text{max}}$ ($\text{\AA}^{-1}$)	0.603
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.042, 0.122, 1.03
No. of reflections	6039
No. of parameters	352
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ ($\text{e \AA}^{-3}$)	3.44, -1.01

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009; Bourhis *et al.*, 2015), *CrystalMaker* (Palmer, 2007).

4. Database survey

The Cambridge Structural Database (CSD, version 5.39, February 2018; Groom *et al.*, 2016) contains 21 structures in which the *cis*-dppe ligand is coordinated to a Pt^{II} center. In addition to the two polymorphs described above, the most similar *cis*-dppe– Pt^{II} coordination complexes include AFEXEO (Vaz *et al.*, 2002) and FOQPUW (Lobana *et al.*, 2000), where the Pt^{II} center is bound by two thiolate ligands ($-\text{SPh}$ and $-\text{SPy}$, respectively). Another structure related to the title compound is KADQEL (Oberhauser *et al.*, 1998b) in which the Pt^{II} center is coordinated by two acetonitrile molecules. Finally, structure ZOLYOO (Oberhauser *et al.*, 1995) contains one Pt^{II} center coordinated by two *cis*-dppe ligands with two outer sphere tetraphenylborate molecules as counter-anions. In each of these structures, the bond lengths and angles are similar to those described above for the title compound.

5. Synthesis and crystallization

The title compound was prepared serendipitously by mixing 20.5 mg of *cis*-1,2-dppeSe₂ (Colquhoun *et al.*, 1979) with 8 mg of $\text{Pt}(\text{NCPH})_2\text{Cl}_2$ in CDCl_3 (0.7 ml) in a NMR tube. This solution was left to stand at room temperature, and colorless needle-like crystals of compound (I) were obtained within a few days.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. The hydrogen atoms were placed in calculated positions and refined as riding: C–H = 0.95–1.00 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Acknowledgements

The authors thank Pfizer, Inc. for the donation of a Varian INOVA 400 FT NMR. The CCD-based X-ray diffractometers at Michigan State University were upgraded and/or replaced by departmental funds.

Funding information

Funding for this research was provided by: National Science Foundation [grant Nos. CCLI CHE-0087655, MRI CHE-1725699 and REU CHE-1559886 (to J. Mugemana)]; GVSU OURS, CSCE and the Chemistry Department's Weldon Fund.

References

- Aguiar, A. M. & Daigle, D. (1964). *J. Am. Chem. Soc.* **86**, 5354–5355.
- Bourhis, L. J., Dolomanov, O. V., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2015). *Acta Cryst. A* **71**, 59–75.
- Bruker (2013). *APEX2, SAINT, XPREP and SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Colquhoun, I. J., McFarlane, H. C. E., McFarlane, W., Nash, J. A., Keat, R., Rycroft, D. S. & Thompson, D. G. (1979). *Org. Magn. Reson.* **12**, 473–475.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Duncan, M. & Gallagher, M. J. (1981). *Org. Magn. Reson.* **15**, 37–42.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst. B* **72**, 171–179.
- Hwang, S. J., Anderson, B. L., Powers, D. C., Maher, A. G., Hadt, R. G. & Nocera, D. G. (2015). *Organometallics*, **34**, 4766–4774.
- Imai, Y. N., Inoue, Y., Nakanishi, I. & Kitaura, K. (2008). *Protein Sci.* **17**, 1129–1137.
- Lobana, T. S., Verma, R., Hundal, G. & Castineiras, A. (2000). *Polyhedron*, **19**, 899–906.
- Morse, P. T., Staples, R. J. & Biros, S. M. (2016). *Polyhedron*, **114**, 2–12.
- Oberhauser, W., Bachmann, C. & Brüggeller, P. (1995). *Inorg. Chim. Acta*, **238**, 35–43.
- Oberhauser, W., Bachmann, C., Stampfl, T., Haid, R., Langes, C., Rieder, A. & Brüggeller, P. (1998a). *Inorg. Chim. Acta*, **274**, 143–154.
- Oberhauser, W., Bachmann, C., Stampfl, T., Haid, R., Langes, C., Rieder, A. & Brüggeller, P. (1998b). *Polyhedron*, **17**, 3211–3220.
- Palmer, D. (2007). *CrystalMaker*. CrystalMaker Software Ltd, Yarnton, Oxfordshire, England.
- Schallenberg, D., Neubauer, A., Erdmann, E., Tänzler, M., Villinger, A., Lochbrunner, S. & Seidel, W. W. (2014). *Inorg. Chem.* **53**, 8859–8873.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst. C* **71**, 3–8.
- Song, L.-C., Gao, X.-Y., Liu, W.-B., Zhang, H.-T. & Cao, M. (2018). *Organometallics*, **37**, 1050–1061.
- Song, L.-C., Zhang, L.-D., Liu, B.-B., Ding, S.-D., Chen, H., Xu, X.-F. & Fan, G.-L. (2017). *Organometallics*, **36**, 1419–1429.
- Trivedi, M., Smreker, J. R., Singh, G., Kumar, A. & Rath, N. P. (2017). *New J. Chem.* **41**, 14145–14151.
- Vaz, R. H., Silva, R. M., Reibenspies, J. H. & Serra, O. A. (2002). *J. Braz. Chem. Soc.* **13**, 82–87.
- Yang, L., Powell, D. R. & Houser, R. P. (2007). *Dalton Trans.* pp. 955–964.
- Yao, L.-Y. & Yam, V. W.-W. (2015). *J. Am. Chem. Soc.* **137**, 3506–3509.

supporting information

Acta Cryst. (2018). E74, 998-1001 [https://doi.org/10.1107/S2056989018008836]

Crystal structure of *cis*-[1,2-bis(diphenylphosphanyl)ethene- κ^2P,P']dichloridoplatinum(II) chloroform disolvate: a new polymorph

Jimmy Mugemana, John Bender, Richard J. Staples and Shannon M. Biros

Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009; Bourhis *et al.*, 2015); software used to prepare material for publication: *CrystalMaker* (Palmer, 2007).

cis-[1,2-Bis(diphenylphosphanyl)ethene- κ^2P,P']dichloridoplatinum(II) chloroform disolvate

Crystal data

[PtCl₂(C₂₆H₂₂P₂)]·2CHCl₃
 $M_r = 901.10$
 Monoclinic, $P2_1/c$
 $a = 11.1441$ (10) Å
 $b = 18.0870$ (17) Å
 $c = 16.9621$ (16) Å
 $\beta = 106.2465$ (10)°
 $V = 3282.4$ (5) Å³
 $Z = 4$

$F(000) = 1744$
 $D_x = 1.823$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 6541 reflections
 $\theta = 2.2$ – 25.4°
 $\mu = 5.04$ mm⁻¹
 $T = 173$ K
 Needle, colorless
 $0.26 \times 0.14 \times 0.10$ mm

Data collection

Bruker APEXII CCD
 diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2013)
 $T_{\min} = 0.502$, $T_{\max} = 0.745$
 26503 measured reflections

6039 independent reflections
 3360 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.069$
 $\theta_{\max} = 25.4^\circ$, $\theta_{\min} = 1.7^\circ$
 $h = -13 \rightarrow 13$
 $k = -21 \rightarrow 21$
 $l = -20 \rightarrow 19$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.122$
 $S = 1.03$
 6039 reflections
 352 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
 $w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 10.564P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 3.44$ e Å⁻³
 $\Delta\rho_{\min} = -1.00$ e Å⁻³

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Pt1	0.76626 (2)	0.25106 (2)	0.26582 (2)	0.02442 (12)
Cl1	0.75592 (19)	0.15899 (10)	0.16572 (12)	0.0322 (5)
Cl2	0.7627 (2)	0.34405 (10)	0.16732 (12)	0.0346 (5)
P1	0.77172 (19)	0.16744 (11)	0.36235 (12)	0.0246 (5)
P2	0.78048 (19)	0.33570 (10)	0.36196 (12)	0.0243 (5)
C1	0.7832 (8)	0.2162 (5)	0.4579 (5)	0.0316 (19)
H1	0.7851	0.1901	0.5068	0.038*
C2	0.7887 (7)	0.2879 (5)	0.4572 (5)	0.0319 (19)
H2	0.7970	0.3151	0.5063	0.038*
C3	0.9055 (8)	0.1058 (4)	0.3861 (5)	0.031 (2)
C4	1.0070 (9)	0.1237 (5)	0.4509 (6)	0.053 (3)
H4	1.0036	0.1654	0.4843	0.064*
C5	1.1147 (11)	0.0803 (6)	0.4674 (7)	0.068 (3)
H5	1.1841	0.0911	0.5132	0.082*
C6	1.1195 (11)	0.0210 (6)	0.4160 (6)	0.063 (3)
H6	1.1943	−0.0068	0.4237	0.075*
C7	1.0156 (11)	0.0033 (5)	0.3545 (7)	0.059 (3)
H7	1.0171	−0.0391	0.3217	0.071*
C8	0.9087 (9)	0.0453 (5)	0.3388 (5)	0.044 (2)
H8	0.8375	0.0322	0.2952	0.053*
C9	0.6333 (8)	0.1110 (4)	0.3461 (5)	0.032 (2)
C10	0.5226 (8)	0.1331 (4)	0.2901 (5)	0.037 (2)
H10	0.5219	0.1758	0.2575	0.044*
C11	0.4138 (9)	0.0937 (5)	0.2815 (6)	0.050 (2)
H11	0.3384	0.1090	0.2430	0.060*
C12	0.4156 (11)	0.0322 (6)	0.3292 (7)	0.063 (3)
H12	0.3404	0.0055	0.3241	0.075*
C13	0.5234 (12)	0.0087 (5)	0.3838 (7)	0.059 (3)
H13	0.5233	−0.0345	0.4157	0.071*
C14	0.6331 (10)	0.0481 (5)	0.3925 (6)	0.051 (3)
H14	0.7084	0.0318	0.4304	0.061*
C15	0.6507 (8)	0.3979 (4)	0.3499 (5)	0.0290 (19)
C16	0.5387 (9)	0.3850 (5)	0.2923 (6)	0.046 (2)
H16	0.5307	0.3446	0.2554	0.055*
C17	0.4375 (10)	0.4306 (6)	0.2880 (7)	0.066 (3)
H17	0.3607	0.4217	0.2474	0.079*
C18	0.4464 (12)	0.4881 (7)	0.3410 (8)	0.066 (4)
H18	0.3761	0.5188	0.3381	0.079*
C19	0.5565 (13)	0.5010 (6)	0.3980 (8)	0.069 (4)

H19	0.5627	0.5414	0.4348	0.083*
C20	0.6601 (10)	0.4571 (5)	0.4042 (6)	0.054 (3)
H20	0.7366	0.4670	0.4446	0.065*
C21	0.9205 (8)	0.3907 (5)	0.3809 (5)	0.035 (2)
C22	0.9220 (9)	0.4607 (5)	0.3500 (6)	0.051 (3)
H22	0.8456	0.4828	0.3200	0.061*
C23	1.0324 (11)	0.4998 (6)	0.3615 (6)	0.060 (3)
H23	1.0318	0.5488	0.3414	0.072*
C24	1.1423 (10)	0.4664 (7)	0.4025 (6)	0.061 (3)
H24	1.2188	0.4922	0.4094	0.073*
C25	1.1440 (10)	0.3972 (7)	0.4336 (8)	0.085 (4)
H25	1.2209	0.3755	0.4633	0.101*
C26	1.0345 (9)	0.3588 (6)	0.4219 (7)	0.062 (3)
H26	1.0364	0.3097	0.4421	0.074*
Cl1S	1.1237 (5)	0.1975 (3)	0.2977 (2)	0.1431 (18)
Cl2S	1.0900 (3)	0.1895 (2)	0.1275 (2)	0.1086 (13)
Cl3S	1.1475 (6)	0.3253 (3)	0.2052 (5)	0.226 (4)
C1S	1.0756 (10)	0.2471 (5)	0.2089 (7)	0.066 (3)
H1S	0.9848	0.2583	0.1995	0.079*
Cl4S	0.4561 (3)	0.16565 (15)	0.48152 (18)	0.0731 (8)
Cl5S	0.3791 (3)	0.25490 (16)	0.59773 (16)	0.0679 (8)
Cl6S	0.4741 (3)	0.32216 (15)	0.47379 (18)	0.0681 (8)
C2S	0.4841 (8)	0.2468 (4)	0.5386 (5)	0.040 (2)
H2S	0.5708	0.2447	0.5764	0.048*

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

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.02528 (18)	0.02567 (17)	0.02229 (17)	0.00053 (16)	0.00661 (12)	0.00026 (16)
Cl1	0.0440 (13)	0.0263 (10)	0.0265 (11)	0.0004 (9)	0.0104 (10)	−0.0046 (9)
Cl2	0.0494 (14)	0.0302 (10)	0.0260 (11)	−0.0040 (10)	0.0132 (10)	0.0034 (9)
P1	0.0261 (12)	0.0261 (11)	0.0201 (11)	0.0019 (9)	0.0040 (9)	0.0028 (9)
P2	0.0289 (12)	0.0234 (10)	0.0209 (11)	0.0004 (9)	0.0075 (10)	−0.0012 (9)
C1	0.035 (5)	0.039 (5)	0.022 (5)	0.004 (4)	0.009 (4)	−0.002 (4)
C2	0.026 (5)	0.046 (5)	0.023 (5)	0.004 (4)	0.004 (4)	−0.004 (4)
C3	0.029 (5)	0.031 (4)	0.035 (5)	0.013 (4)	0.011 (4)	0.011 (4)
C4	0.053 (7)	0.050 (6)	0.057 (7)	0.006 (5)	0.016 (6)	−0.002 (5)
C5	0.064 (8)	0.078 (8)	0.056 (7)	0.020 (6)	0.005 (6)	0.013 (6)
C6	0.067 (8)	0.072 (8)	0.046 (7)	0.038 (6)	0.010 (6)	0.013 (6)
C7	0.081 (9)	0.054 (6)	0.051 (7)	0.031 (6)	0.031 (7)	0.011 (5)
C8	0.050 (6)	0.050 (5)	0.030 (5)	0.010 (5)	0.009 (5)	−0.005 (4)
C9	0.032 (5)	0.033 (5)	0.031 (5)	−0.001 (4)	0.008 (4)	0.000 (4)
C10	0.043 (6)	0.036 (5)	0.034 (5)	−0.009 (4)	0.015 (5)	−0.009 (4)
C11	0.036 (6)	0.066 (7)	0.048 (6)	−0.013 (5)	0.014 (5)	−0.004 (5)
C12	0.075 (9)	0.067 (7)	0.059 (7)	−0.035 (7)	0.040 (7)	−0.024 (6)
C13	0.092 (10)	0.040 (6)	0.055 (7)	−0.007 (6)	0.037 (7)	0.001 (5)
C14	0.075 (8)	0.042 (5)	0.039 (6)	−0.010 (5)	0.021 (5)	−0.002 (5)
C15	0.034 (5)	0.029 (4)	0.031 (5)	0.005 (4)	0.021 (4)	0.005 (4)

C16	0.040 (6)	0.057 (6)	0.044 (6)	0.002 (5)	0.015 (5)	0.003 (5)
C17	0.048 (7)	0.070 (8)	0.079 (9)	0.022 (6)	0.019 (6)	0.035 (7)
C18	0.066 (8)	0.071 (8)	0.077 (9)	0.044 (7)	0.046 (7)	0.045 (7)
C19	0.107 (10)	0.048 (6)	0.073 (8)	0.042 (7)	0.058 (8)	0.014 (6)
C20	0.062 (7)	0.045 (6)	0.051 (7)	0.024 (5)	0.010 (6)	−0.002 (5)
C21	0.039 (5)	0.040 (5)	0.026 (5)	−0.006 (4)	0.008 (4)	−0.002 (4)
C22	0.044 (6)	0.055 (6)	0.052 (7)	−0.011 (5)	0.010 (5)	0.002 (5)
C23	0.080 (9)	0.055 (7)	0.046 (7)	−0.026 (6)	0.022 (7)	−0.004 (5)
C24	0.047 (7)	0.089 (9)	0.047 (7)	−0.031 (6)	0.017 (6)	−0.006 (6)
C25	0.034 (6)	0.102 (10)	0.098 (10)	−0.007 (7)	−0.014 (7)	0.019 (8)
C26	0.032 (6)	0.059 (6)	0.085 (8)	−0.005 (5)	0.000 (6)	0.015 (6)
Cl1S	0.165 (4)	0.189 (5)	0.087 (3)	0.079 (4)	0.054 (3)	0.043 (3)
Cl2S	0.075 (2)	0.157 (4)	0.097 (3)	−0.018 (2)	0.029 (2)	−0.011 (3)
Cl3S	0.276 (7)	0.097 (3)	0.395 (10)	−0.060 (4)	0.244 (7)	−0.033 (5)
C1S	0.053 (6)	0.077 (7)	0.075 (8)	0.018 (6)	0.028 (6)	0.019 (7)
Cl4S	0.104 (2)	0.0567 (16)	0.0630 (18)	−0.0037 (16)	0.0315 (17)	−0.0171 (14)
Cl5S	0.0672 (17)	0.095 (2)	0.0518 (16)	0.0031 (17)	0.0334 (14)	−0.0059 (16)
Cl6S	0.0653 (18)	0.0624 (17)	0.080 (2)	0.0084 (14)	0.0262 (16)	0.0302 (15)
C2S	0.044 (5)	0.038 (5)	0.038 (5)	0.009 (5)	0.013 (4)	0.002 (5)

Geometric parameters (Å, °)

Pt1—Cl1	2.3580 (18)	C12—C13	1.363 (14)
Pt1—Cl2	2.3632 (19)	C13—C14	1.387 (14)
Pt1—P1	2.2173 (19)	C15—C16	1.372 (12)
Pt1—P2	2.2099 (19)	C15—C20	1.397 (11)
P1—C1	1.818 (8)	C16—C17	1.383 (12)
P1—C3	1.814 (8)	C17—C18	1.360 (15)
P1—C9	1.806 (8)	C18—C19	1.353 (16)
P2—C2	1.812 (8)	C19—C20	1.382 (13)
P2—C15	1.798 (8)	C21—C22	1.371 (12)
P2—C21	1.803 (8)	C21—C26	1.392 (12)
C1—C2	1.297 (11)	C22—C23	1.384 (13)
C3—C4	1.377 (12)	C23—C24	1.368 (14)
C3—C8	1.364 (11)	C24—C25	1.355 (15)
C4—C5	1.396 (13)	C25—C26	1.370 (13)
C5—C6	1.393 (14)	Cl1S—C1S	1.706 (11)
C6—C7	1.362 (14)	Cl2S—C1S	1.773 (11)
C7—C8	1.376 (12)	Cl3S—C1S	1.636 (11)
C9—C10	1.388 (11)	Cl4S—C2S	1.737 (8)
C9—C14	1.383 (11)	Cl5S—C2S	1.748 (9)
C10—C11	1.379 (11)	Cl6S—C2S	1.735 (8)
C11—C12	1.373 (13)		
Cl1—Pt1—Cl2	90.33 (6)	C14—C9—P1	121.0 (7)
P1—Pt1—Cl1	92.04 (7)	C14—C9—C10	118.9 (8)
P1—Pt1—Cl2	177.58 (7)	C11—C10—C9	120.7 (8)
P2—Pt1—Cl1	178.38 (7)	C12—C11—C10	119.3 (10)

P2—Pt1—C12	90.70 (7)	C13—C12—C11	121.2 (10)
P2—Pt1—P1	86.91 (7)	C12—C13—C14	119.7 (10)
C1—P1—Pt1	107.9 (3)	C9—C14—C13	120.2 (10)
C3—P1—Pt1	115.7 (3)	C16—C15—P2	121.2 (7)
C3—P1—C1	104.6 (4)	C16—C15—C20	119.0 (8)
C9—P1—Pt1	115.3 (3)	C20—C15—P2	119.7 (7)
C9—P1—C1	104.8 (4)	C15—C16—C17	120.2 (10)
C9—P1—C3	107.5 (4)	C18—C17—C16	120.9 (11)
C2—P2—Pt1	107.6 (3)	C19—C18—C17	119.2 (10)
C15—P2—Pt1	117.4 (3)	C18—C19—C20	121.8 (11)
C15—P2—C2	103.8 (3)	C19—C20—C15	118.9 (10)
C15—P2—C21	107.7 (4)	C22—C21—P2	123.0 (7)
C21—P2—Pt1	113.2 (3)	C22—C21—C26	117.9 (8)
C21—P2—C2	106.3 (4)	C26—C21—P2	118.9 (7)
C2—C1—P1	117.9 (7)	C21—C22—C23	121.5 (10)
C1—C2—P2	119.6 (7)	C24—C23—C22	118.7 (10)
C4—C3—P1	118.2 (7)	C25—C24—C23	121.2 (10)
C8—C3—P1	121.1 (7)	C24—C25—C26	119.8 (11)
C8—C3—C4	120.5 (8)	C25—C26—C21	120.8 (10)
C3—C4—C5	119.7 (9)	Cl1S—C1S—Cl2S	107.7 (6)
C6—C5—C4	119.3 (11)	Cl3S—C1S—Cl1S	116.9 (8)
C7—C6—C5	119.2 (10)	Cl3S—C1S—Cl2S	109.0 (6)
C6—C7—C8	121.5 (10)	Cl4S—C2S—Cl5S	110.2 (5)
C3—C8—C7	119.5 (9)	Cl6S—C2S—Cl4S	109.9 (5)
C10—C9—P1	119.9 (6)	Cl6S—C2S—Cl5S	111.3 (4)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C1S—H1S $\cdots$ Cl1	1.00	3.04	3.782 (11)	132
C1S—H1S $\cdots$ Cl2	1.00	2.84	3.789 (10)	158
C2S—H2S $\cdots$ Cl1 ⁱ	1.00	2.80	3.616 (9)	139
C2S—H2S $\cdots$ Cl2 ⁱ	1.00	2.77	3.649 (9)	147

Symmetry code: (i) $x, -y+1/2, z+1/2$.