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

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Acta Cryst. (2018). E74, 998–1001
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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)ethylen (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 P21/c, with one complex molecule in the asymmetric unit along with two solvate chloroform molecules. The PtII 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)ethylen (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.
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 PtII 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., 1998) 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 PtII 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 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)°. The $\tau_4$ 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 $D\cdot\cdot\cdotA$ distances range from 3.616 (9) to 3.789 (10) Å, while the $D\cdot\cdot\cdotH$ 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 chloride anions.

![Figure 1](image1.png)

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.

![Figure 2](image2.png)

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 1

| Compound | (I) | HINCIQ$^b$ | ZOLYII$^c$ |
|----------|-----|------------|------------|
| Pt1–Cl1  | 2.358 (2) | 2.364 (2)  | 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) |
| $\tau_4$ | 0.02  | 0.05       | 0.0        |

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

Table 2

| $D\cdot\cdot\cdotA$ $D\cdot\cdot\cdotH$ $H\cdot\cdot\cdotA$ |
|-----------------|-----------------|-----------------|
| C1S–H1S···Cl1  | 1.00            | 3.04            | 3.782 (11)     | 132 |
| C1S–H1S···Cl2  | 1.00            | 2.84            | 3.789 (10)     | 158 |
| C2S–H2S···Cl1i | 1.00            | 2.80            | 3.616 (9)      | 139 |
| C2S–H2S···Cl2i | 1.00            | 2.77            | 3.649 (9)      | 147 |

Symmetry code: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$.
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) Å, while the C—Cl⋯ring centroid angles range from 139.2 (5) to 160.3 (4)°.

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 Cg2⋯Cg2 = 4.096 (6) Å [Cg2 is the centroid of ring C9–C14, α = 0.0 (5)°], interplanar distance = 3.917 (4) Å, slippage = 1.20 Å, symmetry code (ii) −x + 2, −y, −z + 1, and Cg3⋯Cg4 = 3.770 (6) Å [Cg3 and Cg4 are the centroids of rings C15–C20 and C21–C26, respectively, α = 5.3 (5)°, interplanar distances are 3.326 (4) and 3.439 (4) Å, slippage = 1.544 Å, symmetry code (iii) −x + 1, y − ½, −z + ½].

The closely related polymorph ZOLYII, which contains one CH3Cl2 solvent molecule and one CHCl3 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 PtII complex, and is disordered in the crystal lattice.

![Figure 3](image_url)

**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 3

| Face-on Cl⋯π interactions (Å, °) |
|-------------------------------|
| 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⋯C1S⋯C1 | 1.706 (11) | 3.441 (7) | 4.862 (11) | 139.2 (5) |
| C2S⋯C4S⋯C2 | 1.737 (8) | 3.242 (5) | 4.775 (9) | 145.4 (3) |
| C2S⋯C6S⋯C3G | 1.735 (8) | 3.349 (5) | 5.017 (9) | 160.3 (4) |

### Table 4

**Experimental details.**

| Crystal data | Chemical formula |
|--------------|-----------------|
| [PtCl2(C6H12P2)]·2CHCl3 |

**Crystal system, space group:** Monoclinic, P21/c

**Temperature (K):** 173

**a, b, c (Å):** 11.1441 (10), 18.0870 (17), 16.9621 (16)

**β (°):** 106.2465 (10)

**V (Å3):** 3282.4 (5)

**Z:** 4

**Mo Kα:** 5.04

**Crystal size (mm):** 0.26 × 0.14 × 0.10

**Data collection**

**Diffraughtometer:** Bruker APEXII CCD

**Absorption correction:** Multi-scan (SADABS; Bruker, 2013)

**Tmin, Tmax:** 0.503, 0.745

**No. of measured, independent and observed [I > 2σ(I)] reflections:** 26503, 6039, 3360

**Rint:** 0.069

**S:** 0.042, 0.122, 1.03

**R1:** 0.069

**No. of reflections:** 6039

**No. of parameters:** 352

**H-atom treatment:** H-atoms parameters constrained

**Δρmin (e Å⁻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 PtII center. In addition to the two polymorphs described above, the most similar cis-dppe–PtII coordination complexes include AFEXEO (Vaz et al., 2002) and FOQPUW (Lobana et al., 2000), where the PtII center is bound by two thiolate ligands (–SPh and –SPy, respectively). Another structure related to the title compound is KADQEL (Oberhauser et al., 1998b) in which the PtII center is coordinated by two acetonitrile molecules. Finally, structure ZOLYOO (Oberhauser et al., 1995) contains one PtII center coordinated by two cis-dppe ligands with two outer sphere tetraphenylborate molecules as counter-ions. 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 Pt(NCPh)2Cl2 in CDCl3 (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 $U_{iso}(H) = 1.2U_{eq}(C)$.

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.

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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-κ²P,P']dichloridoplatinum(II) chloroform disolvate

Crystal data

\[\text{[PtCl}_2\text{(C}_{26}\text{H}_{22}\text{P}_2)\text{]}\cdot 2\text{CHCl}_3\]

\[M_r = 901.10\]

Monoclinic, \(P2_1/c\)

\(a = 11.1441\ (10)\ \text{Å}\)

\(b = 18.0870\ (17)\ \text{Å}\)

\(c = 16.9621\ (16)\ \text{Å}\)

\(β = 106.2465\ (10)°\)

\(V = 3282.4\ (5)\ \text{Å}^3\)

\(Z = 4\)

\(F(000) = 1744\)

\(D_r = 1.823\ \text{Mg m}^{-3}\)

Mo Ka radiation, \(λ = 0.71073\ \text{Å}\)

Cell parameters from 6541 reflections

\(θ = 2.2–25.4°\)

\(µ = 5.04\ \text{mm}^{-1}\)

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

Needle, colorless

\(0.26 × 0.14 × 0.10\ \text{mm}\)

Data collection

Bruker APEXII CCD
diffractometer

φ and ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2013)

\(T_{\text{min}} = 0.502, T_{\text{max}} = 0.745\)

26503 measured reflections

6039 independent reflections

3360 reflections with \(I > 2σ(I)\)

\(R_{\text{int}} = 0.069\)

\(θ_{\text{max}} = 25.4°, θ_{\text{min}} = 1.7°\)

\(h = −13→13\)

\(k = −21→21\)

\(l = −20→19\)

Refinement

Refinement on \(F^2\)

Least-squares matrix: full

\(R[F^2 > 2σ(F^2)] = 0.042\)

\(wR(F^2) = 0.122\)

\(S = 1.03\)

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

\(w = 1/[(σ(F_c)^2 + (0.0396P)^2 + 10.564P)]\)

where \(P = (F_c^2 + 2F_s^2)/3\)

\((Δρ)_{\text{max}} = 0.001\)

\(Δρ_{\text{max}} = 3.44\ \text{e Å}^{-3}\)

\(Δρ_{\text{min}} = −1.00\ \text{e Å}^{-3}\)
**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 (Å²)**

| Atom | x      | y      | z      | Uiso*/Ueq |
|------|--------|--------|--------|-----------|
| Pt1  | 0.76626 (2) | 0.25106 (2) | 0.26582 (2) | 0.02442 (12) |
| C11  | 0.75592 (19) | 0.15899 (10) | 0.16572 (12) | 0.0322 (5) |
| C12  | 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) |
supporting information

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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 (Å²)

|       | $U^{11}$   | $U^{22}$   | $U^{33}$   | $U^{12}$   | $U^{13}$   | $U^{23}$   |
|-------|------------|------------|------------|------------|------------|------------|
| Pt1   | 0.02528 (18)| 0.02567 (17)| 0.02229 (17)| 0.00053 (16)| 0.00661 (12)| 0.00026 (16)|
| C11   | 0.0440 (13) | 0.0263 (10) | 0.0265 (11) | 0.0004 (9)  | 0.0104 (10) | −0.0046 (9) |
| C12   | 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)  |
| 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   | 0.044 (6)   | 0.036 (5)  | 0.034 (5)  | −0.009 (4)  | 0.015 (5)   | −0.009 (4)  |
| C11   | 0.038 (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) | 0.006 (6) | 0.015 (6) |
| C11S | 0.165 (4) | 0.189 (5) | 0.087 (3) | 0.079 (4) | 0.054 (3) | 0.043 (3) |
| C12S | 0.075 (2) | 0.157 (4) | 0.097 (3) | −0.018 (2) | 0.029 (2) | −0.011 (3) |
| C13S | 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) |
| C14S | 0.104 (2) | 0.0567 (16) | 0.0630 (18) | −0.0037 (16) | 0.0315 (17) | −0.0171 (14) |
| C15S | 0.0672 (17) | 0.095 (2) | 0.0518 (16) | 0.0031 (17) | 0.0334 (14) | −0.0059 (16) |
| C16S | 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 2.217 (19)  C14—C9 1.210 (7)
Pt1—P2 2.2099 (19)  C15—C16 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)  C22—C23 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)  C26—C27 1.395 (13)
C6—C7 1.362 (14)  C27—C28 1.379 (13)
C7—C8 1.376 (12)  C28—C29 1.365 (11)
C9—C10 1.388 (11)  C29—C30 1.373 (13)
C9—C14 1.383 (11)  C30—C31 1.373 (13)
C10—C11 1.379 (11)  C31—C32 1.373 (13)
C11—C12 1.373 (13)  C32—C33 1.373 (13)

Cl1—Pt1—Cl2 90.33 (6)  C14—C9—P1 121.0 (7)
P1—Pt1—C11 92.04 (7)  C14—C9—C10 118.9 (8)
P1—Pt1—C12 177.58 (7)  C11—C10—C9 120.7 (8)
P2—Pt1—C11 178.38 (7)  C12—C11—C10 119.3 (10)

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P2—Pt1—Cl2 90.70 (7) C13—Cl2—C11 121.2 (10)
P2—Pt1—P1 86.91 (7) C12—C13—C14 119.7 (10)
C1—Pt1—Pt1 107.9 (3) C9—C14—C13 120.2 (10)
C3—Pt1—Pt1 115.7 (3) C16—C15—P2 121.2 (7)
C3—Pt1—C1 104.6 (4) C16—C15—C20 119.0 (8)
C9—Pt1—Pt1 115.3 (3) C20—C15—P2 119.7 (7)
C9—Pt1—C1 104.8 (4) C15—C16—C17 120.2 (10)
C9—Pt1—C3 107.5 (4) C18—C17—C16 120.9 (11)
C2—Pt1—Pt1 107.6 (3) C19—C18—C17 119.2 (10)
C15—Pt1—Pt1 117.4 (3) C18—C19—C20 121.8 (11)
C15—Pt1—C2 103.8 (3) C19—C20—C15 118.9 (10)
C15—Pt1—C21 107.7 (4) C22—C21—P2 123.0 (7)
C21—Pt1—Pt1 113.2 (3) C22—C21—C26 117.9 (8)
C21—Pt1—C2 106.3 (4) C26—C21—P2 118.9 (7)
C2—C1—Pt1 117.9 (7) C21—C22—C23 121.5 (10)
C1—C2—Pt2 119.6 (7) C24—C23—C22 118.7 (10)
C4—C3—Pt1 118.2 (7) C25—C24—C23 121.2 (10)
C8—C3—Pt1 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, °)

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|-------|-------|---------|
| C1S—H1S···Cl1 | 1.00 | 3.04 | 3.782 (11) | 132 |
| C1S—H1S···Cl2 | 1.00 | 2.84 | 3.789 (10) | 158 |
| C2S—H2S···Cl1i | 1.00 | 2.80 | 3.616 (9) | 139 |
| C2S—H2S···Cl2i | 1.00 | 2.77 | 3.649 (9) | 147 |

Symmetry code: (i) x, −y+1/2, z+1/2.