research communications

Crystal structures of (Z)-(ethene-1,2-diyl)bis(diphenylphosphine sulfide) and its complex with Pt[II] dichloride

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The crystal structures of (Z)-(ethene-1,2-diyl)bis(diphenylphosphine sulfide), $C_{26}H_{22}P_2S_2$ (**I**), along with its complex with Pt[II] dichloride, dichlorido-[(Z)-(ethene-1,2-diyl)bis(diphenylphosphine sulfide)-$\kappa^2 S,S'$]platinum(II), [PtCl$_2$(C$_{26}$H$_{22}$P$_2$S$_2$)] (**II**), are described here. Compound **I** features P═S bond lengths of 1.9571 (15) and 1.9529 (15) Å, with a torsion angle of 166.24 (7)° between the two phosphine sulfide groups. The crystal of compound **I** features both intramolecular C—H$\cdots$S hydrogen bonds and π–π interactions. Molecules of compound **I** are held together with intermolecular π–π and C—H$\cdots\pi$ interactions to form chains that run parallel to the z-axis. The intermolecular C—H$\cdots\pi$ interaction has a H$\cdots$Cg distance of 2.63 Å, a D$\cdots$Cg distance of 3.573 (5) Å and a D—H$\cdots$Cg angle of 171° (where Cg refers to the centroid of one of the phenyl rings). These chains are linked by relatively long C—H$\cdots$S hydrogen bonds with D$\cdots$A distances of 3.367 (4) and 3.394 (4) Å with D—H$\cdots$A angles of 113 and 115°. Compound **II** features Pt—Cl and Pt—S bond lengths of 2.3226 (19) and 2.2712 (19) Å, with a P═S bond length of 2.012 (3) Å. The Pt[II] center adopts a square-planar geometry, with Cl—Pt—Cl and S—Pt—S bond angles of 90.34 (10) and 97.19 (10)°, respectively. Molecules of compound **II** are linked in the crystal by intermolecular C—H$\cdots$Cl and C—H$\cdots$S hydrogen bonds.

1. Chemical context

The diphosphine compound cis-bis(diphenylphosphino)-ethylene (cis-dppe, Fig. 1) has been used by many research groups as a ligand in organometallic chemistry (Hirano & Miura, 2017; Price & Walton, 1987). While the bisphosphine oxide derivative has found use in the coordination chemistry of both d-block and f-block metals (Jarrett & Sadler, 1991; Banda & Pritchard, 2008; Morse, et al., 2016), the bisphosphine sulfide and bisphosphineselenide derivatives have been less studied. Our group is interested in developing new organic compounds that can facilitate the separation of actinide (An) metals from lanthanide (Ln) metals in liquid–liquid extraction processes (Gorden et al., 2013). Since the An metals have a
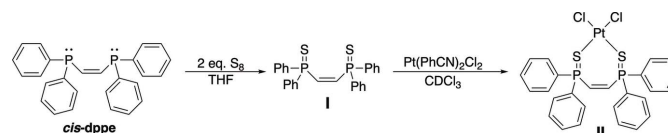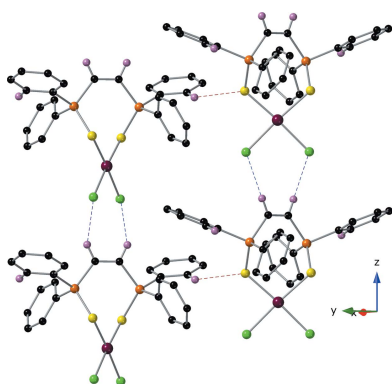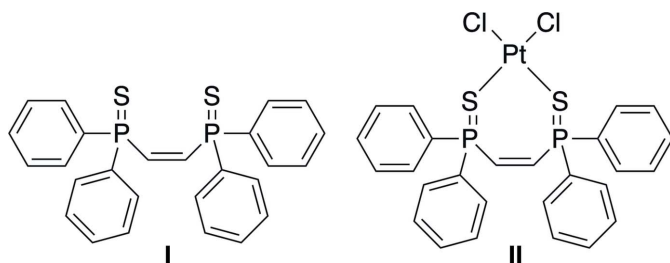

Figure 1
Reaction conditions used to prepare the title compounds.

greater preference for soft-donor atoms than the Ln metals (Cotton, 2006), there have been some successes with the use of phosphine sulfide compounds as actinide extraction agents (*e.g.* Cyanex 301; Zhu *et al.*, 1996). To this end, we prepared compound **I** from *cis*-dppe using elemental sulfur (Fig. 1; Aguiar & Daigle, 1964; Duncan & Gallagher, 1981). Unfortunately, our efforts in this area were plagued by the ease of isomerization of the *cis*-alkene to a *trans*-alkene when the systems were heated for even short lengths of time. In an effort to understand the ability of this ligand to form complexes with metals, we also reacted compound **I** with Pt(PhCN)$_2$Cl$_2$ to give compound **II**.

Table 1
Hydrogen-bond geometry (Å, °) for **I**.

Cg is the centroid of the C15–C20 ring.

$D-\mathrm{H}\cdots A$	$D-\mathrm{H}$	$\mathrm{H}\cdots A$	$D\cdots A$	$D-\mathrm{H}\cdots A$
C1—H1···S2^i	0.95	2.86	3.742 (4)	155
C7—H7···S2^{ii}	0.95	2.82	3.561 (5)	135
C8—H8···S1	0.95	2.86	3.344 (4)	113
C10—H10···S1	0.95	2.84	3.360 (4)	116
C20—H20···S2	0.95	2.89	3.367 (4)	113
C26—H26···S2	0.95	2.89	3.394 (4)	115
C11—H11···Cg^{iii}	0.95	2.63	3.573 (5)	171

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, -z$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, -y+1, z+\frac{1}{2}$.

molecular π–π interaction is present between the C9–C14 and C21–C26 rings with an intercentroid distance of 3.737 (3) Å, slippage of 3.370 Å and a dihedral angle of 5.6 (2)°. Both C8(H8) and C10(H10) are engaged in intramolecular C—H···S hydrogen bonds with S1 (Ghosh *et al.*, 2020; Table 1).

2. Structural commentary

The structure of compound **I** was solved in the orthorhombic space group $P2_12_12_1$. The molecular structure of this compound is shown in Fig. 2 along with the atom numbering scheme. The structure of disulfide **I** has P=S bond lengths of 1.9571 (15) and 1.9529 (15) Å, P—C bond lengths that range from 1.804 (4) to 1.824 (4) Å and a C=C bond length of 1.338 (5) Å. The P=S bonds are oriented in opposite directions with a S1—P1—P2—S2 torsion angle of 166.24 (7)°. The τ_4 descriptor for fourfold coordination around both phosphorus atoms P1 and P2 is 0.94, indicating a near tetrahedral geometry of the phosphine sulfide groups (where 0.00 = square-planar, 0.85 = trigonal–pyramidal, and 1.00 = tetrahedral; Yang *et al.*, 2007). The bond angles around both phosphorus atoms range from 100.75 (18) to 115.48 (14)°, with the largest angles involving the sulfur atom. One intra-
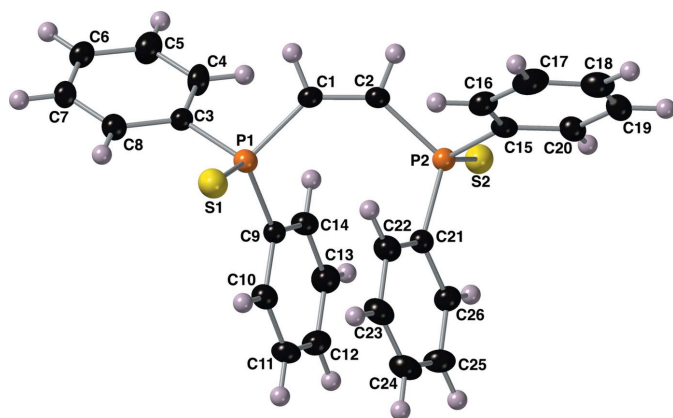

Figure 2
The molecular structure of compound **I**, with the atom-labeling scheme. Displacement ellipsoids are drawn at the 40% probability level using standard CPK colors.

Figure 3
A figure depicting the intra- and intermolecular interactions found in crystals of compound **I** using a ball-and-stick model with standard CPK colors. Hydrogen bonds are drawn using blue dotted lines while π–π and C—H···π interactions are drawn with red dashed lines. Only hydrogen atoms involved in an interaction are shown for clarity. Symmetry codes: (i) $-x+\frac{1}{2}, -y+1, z+\frac{1}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.
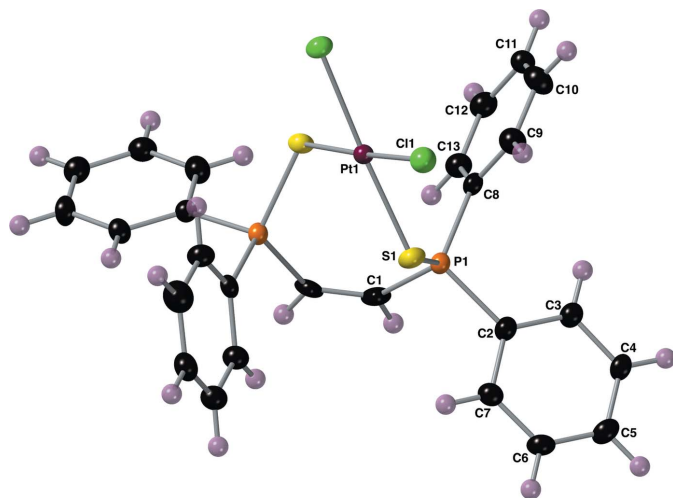
Figure 4
The complete molecular structure of compound **II**, with the atom-labeling scheme. Unlabeled atoms are related to labeled atoms by a crystallographic twofold axis. Displacement ellipsoids are drawn at the 40% probability level using standard CPK colors (Pt = maroon).

These interactions have $D \cdots A$ distances of 3.344 (4) and 3.360 (4) Å with $D-H \cdots A$ dihedral angles of 113 and 116°, respectively (Table 1, Fig. 3). In a similar fashion, S2 hosts two intramolecular C—H hydrogen bonds with C20(H20) and C26(H26). These interactions have $D \cdots A$ distances of 3.367 (4) and 3.394 (4) Å with $D-H \cdots A$ dihedral angles of 113 and 115°, respectively. The Flack parameter for this structure is −0.10 (5) (Parsons et al., 2013).

For the Pt^{II} complex **II**, the structure was solved in the orthorhombic space group Fdd2. Since the entire molecule straddles a twofold symmetry axis, the asymmetric unit is composed of half of the molecule. The complete molecular structure of compound **II** is shown in Fig. 4 along with the atom-numbering scheme. The Pt—Cl and Pt—S bond lengths are 2.3226 (19) and 2.2712 (19) Å, respectively. The Cl1—Pt1—Cl1^i and S1—Pt1—S1^i bond angles are 90.34 (10) and 97.19 (10)°, respectively [symmetry code: (i) $-x + 1, -y + 1, z$]. The τ_4 descriptor for fourfold coordination around the Pt^{II} center is 0.05, indicating a nearly perfect square-planar orientation of the sulfur and chlorine atoms around the metal (Yang et al., 2007). The P=S bond length is 2.012 (3) Å, which is slightly longer than what was observed for compound **I**. The complex has P—C bond lengths that range from 1.799 (8) to 1.816 (9) Å, with a C=C bond length of 1.312 (18) Å. The τ_4 descriptor for fourfold coordination of the phosphorus atom P1 is 0.91, indicating a slightly distorted tetrahedral geometry of the groups bonded to this atom, and that this tetrahedron is more distorted than what was observed for compound **I**.

3. Supramolecular features

Molecules of compound **I** are held together in the crystal by intermolecular π–π and C—H⋯π interactions (Table 1 and Fig. 3). Ring C9–C14 is engaged in an intermolecular π–π interaction with a screw-related C21–C26 ring (symmetry

Table 2
Hydrogen-bond geometry (Å, °) for **II**.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C1—H1⋯Cl1^i	0.95	2.73	3.515 (10)	141
C3—H3⋯S1^{ii}	0.95	2.82	3.538 (9)	133

Symmetry codes: (i) $-x + 1, -y + 1, z + 1$; (ii) $x + \frac{1}{4}, -y + \frac{5}{4}, z + \frac{1}{4}$.

code: $-x + \frac{1}{2}, -y + 1, z - \frac{1}{2}$). The centroid–centroid distance of this interaction is 3.896 (3) Å, with a slippage of 3.598 Å and a dihedral angle of 10.80 (14) °. Hydrogen atom C11(H11) is engaged in an intermolecular C—H⋯π interaction with ring C15–C20 (symmetry code $-x + \frac{1}{2}, -y + 1, z + \frac{1}{2}$) with an H⋯Cg distance of 2.63 Å, a $D \cdots Cg$ distance of 3.573 (5) Å and a $D-H \cdots Cg$ angle of 171° (Cg is the centroid of the C15–C20 ring). Together, these intermolecular π–π and C—H⋯π interactions link the molecules into chains that propagate parallel to the z-axis (Fig. 5). Two potential intermolecular C—H⋯S interactions exist between C1(H1) and C7(H7) and S2. These interactions have relatively long $D \cdots A$ distances of 3.742 (4) and 3.561 (5) Å with $D-H \cdots A$ angles of 155 and 135°, respectively. These hydrogen-bonding interactions occur between the supramolecular chains of compound **I**.

Molecules of compound **II** are held together by C—H⋯Cl (Aullón et al., 1998) and C—H⋯S hydrogen bonds (Ghosh et al., 2020; Table 2 and Fig. 6). The C—H⋯Cl interaction is between hydrogen atom C1(H1) and Cl1 and has a $D \cdots A$ distance of 3.515 (10) Å with a $D-H \cdots A$ angle of 141° (symmetry code: $-x + 1, -y + 1, z + 1$). Sulfur atom S1 hosts the other intermolecular hydrogen bond with atom C3(H3) (symmetry code: $x + \frac{1}{4}, -y + \frac{5}{4}, z + \frac{1}{4}$). This interaction has a slightly longer $D \cdots A$ distance of 3.538 (9) with a $D-H \cdots A$ angle of 133°. The intermolecular C—H⋯Cl interactions

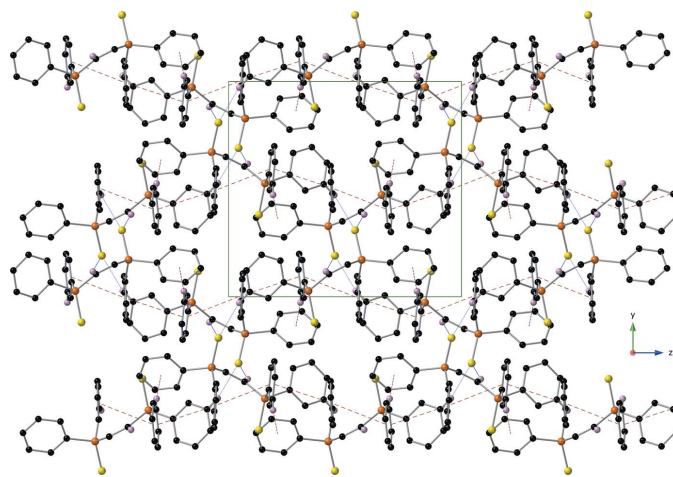**Figure 5**
A packing diagram of compound **I** viewed down the x-axis using a ball-and-stick model with standard CPK colors. All π–π and C—H⋯π interactions are drawn with red dashed lines and intermolecular C—H⋯S hydrogen bonds are drawn with blue dotted lines. Intramolecular C—H⋯S hydrogen bonds and any hydrogen atom not involved in an interaction have been omitted for clarity.
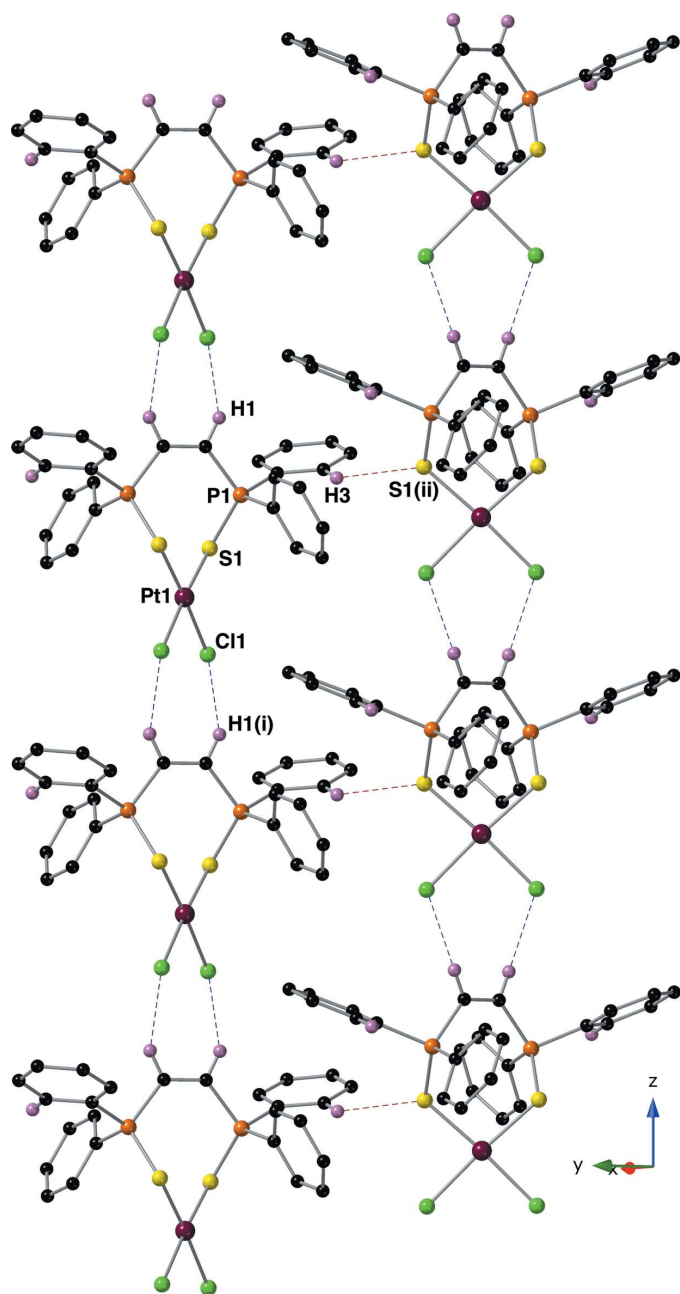
Figure 6
This figure shows the intermolecular C—H···Cl and C—H···S hydrogen bonds present in the crystal of compound **II** using a ball-and-stick model with standard CPK colors (Pt = maroon). Hydrogen bonds are drawn with blue (C—H···Cl) or red (C—H···S) dashed lines, and only hydrogen atoms H1 and H3 are shown for clarity. Symmetry codes: (i) $-x + 1, -y + 1, z - 1$; (ii) $x + \frac{1}{4}, -y + \frac{5}{4}, z + \frac{1}{4}$.

form chains of compound **II** that run parallel to the z-axis. These chains are then linked into a three-dimensional network through the intermolecular C—H···S hydrogen bonds.

4. Database survey

A search of the Cambridge Structural Database (CSD version 5.42, Sep. 2021; Groom *et al.*, 2016) for structures similar to

compound **I** resulted in 17 hits. The majority of these hits were metal–ligand complexes, where the ligand was a triazole ring bearing two diphenylphosphine sulfide groups. Crystal structures of this ligand bonded to copper(II), zinc(II), palladium(II), and cadmium(II) were reported (KOBJOC, KOBKAP, KOBKUJ, KOBKIX; Pastor-Medrano, *et al.*, 2014), along with complexes containing zirconium(IV) and hafnium(IV) (PUKNAM, PUKNEQ; Bernabe-Pablo *et al.*, 2016). A structure closely related to compound **I**, where the alkene bears a phenyl ring and is bonded to the phosphine sulfide groups with a *trans* relationship, has also been deposited in the CSD as a private communication (GOLXAI; Rybakov and Afanas'ev, 2010).

5. Synthesis and crystallization

Compound **I**: *cis*-dppe (500 mg, 1.25 mmol) and elemental sulfur (S_8, 80 mg, 0.31 mmol) were combined in a round-bottom flask and dissolved in tetrahydrofuran (5 mL). The reaction mixture was stirred for three h at room temperature. The solvent was removed under reduced pressure to give a white, gelatinous solid. The crude product was recrystallized from benzene (5 mL) at 333 K and isolated by vacuum filtration with a Hirsch funnel to give a white solid. Analysis of the solid by ^{31}P NMR (CDCl$_3$) showed that the target compound **I** was present along with *trans*-dppeS$_2$ and unreacted starting material. Single crystals of compound **I** grew serendipitously upon slow evaporation of this solution. ^{31}P NMR (CDCl$_3$, 121 MHz): Compound **I**: 32.3 ppm; *trans*-dppeS2: 36.6 ppm; *cis*-dppe: −22 ppm.

Compound **II**: Equimolar amounts of compound **I** (10.0 mg, 0.022 mmol) and Pt(PhCN)$_2$Cl$_2$ (10.4 mg, 0.022 mmol) were combined in a small vial and dissolved in 1 mL CDCl$_3$. Crystals of compound **II** formed serendipitously *via* slow evaporation of the solvent.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. For compounds **I** and **II**, all hydrogen atoms bonded to carbon atoms were placed in calculated positions and refined as riding: C—H = 0.95–1.00 Å with $U_{iso}(H) = 1.2U_{eq}(C)$ for vinylic and aromatic hydrogen atoms.

Table 3
Experimental details.

	I	II
Crystal data		
Chemical formula	$C_{26}H_{22}P_2S_2$	$[PtCl_2(C_{26}H_{22}P_2S_2)]$
M_r	460.49	726.48
Crystal system, space group	Orthorhombic, $P2_12_12_1$	Orthorhombic, $Fdd2$
Temperature (K)	173	173
a, b, c (Å)	12.315 (3), 13.092 (3), 14.211 (4)	18.0724 (12), 30.163 (2), 9.3697 (6)
V (Å^3)	2291.2 (10)	5107.5 (6)
Z	4	8
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.38	6.01
Crystal size (mm)	$0.22 \times 0.17 \times 0.11$	$0.35 \times 0.14 \times 0.10$
Data collection		
Diffractometer	Bruker APEXII CCD	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.655, 0.745	0.543, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18678, 4213, 3676	20596, 2324, 2227
R_{int}	0.057	0.039
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.603	0.603
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.088, 1.04	0.023, 0.061, 1.09
No. of reflections	4213	2324
No. of parameters	271	150
No. of restraints	0	1
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.37, −0.20	1.82, −0.48
Absolute structure	Flack x determined using 1430 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)	Flack x determined using 1010 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.* 2013)
Absolute structure parameter	−0.10 (5)	−0.006 (4)

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *OLEX2.solve* (Bourhis *et al.*, 2015), *SHELXS* (Sheldrick, 2008), *SHELXL2019/2* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009; Bourhis *et al.*, 2015), and *CrystalMaker* (Palmer, 2007).

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supporting information

Crystal structures of (*Z*)-(ethene-1,2-diyl)bis(diphenylphosphine sulfide) and its complex with Pt[II] dichloride

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Computing details

For both structures, data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013). Program(s) used to solve structure: *olex2.solve* (Bourhis *et al.*, 2015) for (I); *SHELXS* (Sheldrick, 2008) for (II). For both structures, program(s) used to refine structure: *SHELXL2019/2* (Sheldrick, 2015); molecular graphics: Olex2 (Dolomanov *et al.*, 2009; Bourhis *et al.*, 2015); software used to prepare material for publication: *CrystalMaker* (Palmer, 2007).

(*Z*)-(Ethene-1,2-diyl)bis(diphenylphosphine sulfide (I)

Crystal data

$C_{26}H_{22}P_2S_2$	$D_x = 1.335$ Mg m^{-3}
$M_r = 460.49$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 7213 reflections
$a = 12.315$ (3) Å	$\theta = 2.2–25.3°$
$b = 13.092$ (3) Å	$\mu = 0.38$ mm^{-1}
$c = 14.211$ (4) Å	$T = 173$ K
$V = 2291.2$ (10) Å^3	Chunk, yellow
$Z = 4$	$0.22 \times 0.17 \times 0.11$ mm
$F(000) = 960$	

Data collection

Bruker APEXII CCD diffractometer	4213 independent reflections
	3676 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.057$
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)	$\theta_{max} = 25.4°$, $\theta_{min} = 2.1°$
	$h = -14 \rightarrow 14$
$T_{min} = 0.655$, $T_{max} = 0.745$	$k = -15 \rightarrow 15$
18678 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.038$	H-atom parameters constrained
$wR(F^2) = 0.088$	$w = 1/[\sigma^2(F_o^2) + (0.0374P)^2 + 0.5294P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
4213 reflections	$(\Delta/\sigma)_{max} < 0.001$
271 parameters	$\Delta\rho_{max} = 0.37$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.20$ e Å^{-3}
Primary atom site location: iterative	

Absolute structure: Flack x determined using
1430 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.10 (5)

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)

	x	y	z	U_{iso}*/U_{eq}
S1	0.55697 (10)	0.38129 (8)	0.13055 (8)	0.0420 (3)
S2	0.39195 (10)	0.80901 (8)	−0.04312 (8)	0.0398 (3)
P1	0.53899 (8)	0.52703 (8)	0.15692 (7)	0.0300 (3)
P2	0.44444 (9)	0.67175 (8)	−0.07181 (7)	0.0281 (2)
C1	0.6036 (3)	0.6052 (3)	0.0686 (3)	0.0306 (9)
H1	0.677946	0.617631	0.082123	0.037*
C2	0.5716 (3)	0.6497 (3)	−0.0115 (3)	0.0297 (9)
H2	0.631332	0.676857	−0.045572	0.036*
C3	0.6119 (3)	0.5670 (3)	0.2624 (3)	0.0299 (9)
C4	0.6408 (4)	0.6679 (3)	0.2775 (3)	0.0415 (11)
H4	0.621187	0.718677	0.232846	0.050*
C5	0.6981 (4)	0.6949 (4)	0.3576 (3)	0.0476 (12)
H5	0.717475	0.764283	0.367629	0.057*
C6	0.7273 (3)	0.6222 (4)	0.4226 (3)	0.0397 (10)
H6	0.767874	0.640847	0.476863	0.048*
C7	0.6973 (3)	0.5225 (4)	0.4085 (3)	0.0445 (12)
H7	0.716344	0.472267	0.453822	0.053*
C8	0.6397 (3)	0.4940 (3)	0.3292 (3)	0.0382 (10)
H8	0.619223	0.424702	0.320333	0.046*
C9	0.3997 (3)	0.5681 (3)	0.1732 (3)	0.0285 (9)
C10	0.3184 (3)	0.4950 (3)	0.1773 (3)	0.0358 (10)
H10	0.336454	0.424670	0.171665	0.043*
C11	0.2115 (3)	0.5236 (4)	0.1896 (3)	0.0398 (11)
H11	0.155785	0.473502	0.191199	0.048*
C12	0.1863 (4)	0.6263 (4)	0.1997 (3)	0.0421 (11)
H12	0.112958	0.646480	0.208632	0.051*
C13	0.2669 (4)	0.6990 (3)	0.1967 (3)	0.0406 (11)
H13	0.248927	0.769140	0.203727	0.049*
C14	0.3735 (3)	0.6705 (3)	0.1836 (3)	0.0345 (10)
H14	0.428998	0.720940	0.181615	0.041*
C15	0.4870 (3)	0.6581 (3)	−0.1938 (3)	0.0322 (9)
C16	0.5569 (4)	0.5795 (3)	−0.2208 (3)	0.0391 (10)
H16	0.585269	0.533863	−0.174979	0.047*
C17	0.5849 (4)	0.5681 (4)	−0.3153 (3)	0.0514 (13)
H17	0.633985	0.515797	−0.333780	0.062*

C18	0.5419 (4)	0.6322 (4)	−0.3812 (3)	0.0547 (14)
H18	0.559414	0.622751	−0.445721	0.066*
C19	0.4738 (4)	0.7098 (4)	−0.3555 (3)	0.0481 (12)
H19	0.445533	0.754590	−0.402084	0.058*
C20	0.4456 (4)	0.7235 (3)	−0.2617 (3)	0.0396 (10)
H20	0.398261	0.777529	−0.244058	0.047*
C21	0.3463 (3)	0.5701 (3)	−0.0566 (3)	0.0302 (9)
C22	0.3761 (4)	0.4679 (3)	−0.0612 (3)	0.0359 (10)
H22	0.450739	0.449838	−0.063759	0.043*
C23	0.2974 (4)	0.3922 (3)	−0.0619 (3)	0.0422 (11)
H23	0.318214	0.322403	−0.064286	0.051*
C24	0.1897 (4)	0.4180 (4)	−0.0592 (3)	0.0486 (13)
H24	0.135887	0.366066	−0.060870	0.058*
C25	0.1589 (4)	0.5196 (4)	−0.0539 (3)	0.0493 (13)
H25	0.084124	0.537013	−0.051412	0.059*
C26	0.2363 (3)	0.5953 (3)	−0.0524 (3)	0.0384 (10)
H26	0.214848	0.664858	−0.048423	0.046*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0477 (7)	0.0281 (5)	0.0503 (6)	0.0058 (5)	0.0037 (6)	−0.0026 (5)
S2	0.0449 (7)	0.0288 (6)	0.0457 (6)	0.0060 (5)	−0.0003 (5)	−0.0047 (5)
P1	0.0292 (6)	0.0273 (5)	0.0335 (6)	0.0022 (5)	0.0029 (5)	0.0011 (4)
P2	0.0285 (5)	0.0265 (5)	0.0293 (5)	0.0007 (5)	0.0001 (5)	−0.0009 (4)
C1	0.023 (2)	0.037 (2)	0.032 (2)	−0.0012 (18)	0.0015 (17)	−0.0013 (18)
C2	0.026 (2)	0.030 (2)	0.032 (2)	−0.0026 (17)	0.0026 (17)	−0.0007 (17)
C3	0.025 (2)	0.033 (2)	0.032 (2)	0.0029 (18)	0.0009 (18)	0.0031 (18)
C4	0.051 (3)	0.034 (2)	0.039 (2)	0.005 (2)	−0.012 (2)	0.007 (2)
C5	0.055 (3)	0.039 (3)	0.050 (3)	0.001 (2)	−0.014 (2)	−0.001 (2)
C6	0.033 (2)	0.054 (3)	0.032 (2)	0.003 (2)	−0.0022 (19)	0.001 (2)
C7	0.035 (2)	0.054 (3)	0.045 (3)	0.005 (2)	−0.003 (2)	0.020 (2)
C8	0.036 (2)	0.036 (2)	0.043 (3)	0.004 (2)	0.001 (2)	0.008 (2)
C9	0.027 (2)	0.033 (2)	0.026 (2)	−0.0001 (18)	0.0009 (17)	0.0013 (17)
C10	0.037 (2)	0.032 (2)	0.038 (2)	−0.002 (2)	0.0031 (19)	0.0012 (19)
C11	0.033 (2)	0.044 (3)	0.043 (2)	−0.010 (2)	0.006 (2)	0.001 (2)
C12	0.026 (2)	0.058 (3)	0.042 (3)	0.007 (2)	0.0074 (19)	−0.001 (2)
C13	0.041 (3)	0.035 (3)	0.046 (3)	0.008 (2)	0.004 (2)	−0.003 (2)
C14	0.032 (2)	0.030 (2)	0.041 (2)	−0.0025 (19)	0.0039 (19)	−0.0013 (19)
C15	0.030 (2)	0.032 (2)	0.034 (2)	−0.0089 (18)	0.0019 (17)	−0.0035 (18)
C16	0.032 (2)	0.047 (3)	0.038 (2)	−0.004 (2)	−0.001 (2)	−0.0075 (19)
C17	0.034 (3)	0.074 (4)	0.047 (3)	−0.003 (2)	0.008 (2)	−0.021 (3)
C18	0.044 (3)	0.087 (4)	0.033 (2)	−0.020 (3)	0.007 (2)	−0.010 (3)
C19	0.048 (3)	0.064 (3)	0.032 (2)	−0.017 (3)	−0.003 (2)	0.009 (2)
C20	0.040 (3)	0.041 (3)	0.038 (2)	−0.008 (2)	0.001 (2)	0.0036 (19)
C21	0.032 (2)	0.034 (2)	0.025 (2)	−0.0023 (18)	0.0013 (17)	−0.0023 (18)
C22	0.039 (2)	0.035 (2)	0.033 (2)	0.000 (2)	0.0060 (19)	−0.0055 (19)
C23	0.051 (3)	0.037 (3)	0.038 (3)	−0.012 (2)	0.008 (2)	−0.004 (2)

C24	0.052 (3)	0.056 (3)	0.038 (3)	−0.026 (3)	0.006 (2)	−0.006 (2)
C25	0.032 (2)	0.068 (3)	0.048 (3)	−0.011 (2)	0.005 (2)	0.000 (3)
C26	0.032 (2)	0.046 (3)	0.038 (2)	0.002 (2)	0.0012 (19)	0.000 (2)

Geometric parameters (Å, º)

S1—P1	1.9571 (15)	C12—H12	0.9500
S2—P2	1.9529 (15)	C12—C13	1.376 (6)
P1—C1	1.804 (4)	C13—H13	0.9500
P1—C3	1.824 (4)	C13—C14	1.378 (6)
P1—C9	1.812 (4)	C14—H14	0.9500
P2—C2	1.808 (4)	C15—C16	1.396 (6)
P2—C15	1.819 (4)	C15—C20	1.387 (6)
P2—C21	1.810 (4)	C16—H16	0.9500
C1—H1	0.9500	C16—C17	1.395 (6)
C1—C2	1.338 (5)	C17—H17	0.9500
C2—H2	0.9500	C17—C18	1.365 (7)
C3—C4	1.384 (6)	C18—H18	0.9500
C3—C8	1.389 (6)	C18—C19	1.367 (7)
C4—H4	0.9500	C19—H19	0.9500
C4—C5	1.386 (6)	C19—C20	1.390 (6)
C5—H5	0.9500	C20—H20	0.9500
C5—C6	1.375 (6)	C21—C22	1.389 (6)
C6—H6	0.9500	C21—C26	1.395 (6)
C6—C7	1.372 (6)	C22—H22	0.9500
C7—H7	0.9500	C22—C23	1.386 (6)
C7—C8	1.383 (6)	C23—H23	0.9500
C8—H8	0.9500	C23—C24	1.369 (7)
C9—C10	1.387 (6)	C24—H24	0.9500
C9—C14	1.387 (5)	C24—C25	1.384 (7)
C10—H10	0.9500	C25—H25	0.9500
C10—C11	1.380 (6)	C25—C26	1.375 (6)
C11—H11	0.9500	C26—H26	0.9500
C11—C12	1.387 (6)		
C1—P1—S1	111.69 (14)	C11—C12—H12	119.8
C1—P1—C3	101.08 (18)	C13—C12—C11	120.4 (4)
C1—P1—C9	109.73 (18)	C13—C12—H12	119.8
C3—P1—S1	112.42 (14)	C12—C13—H13	119.8
C9—P1—S1	114.89 (14)	C12—C13—C14	120.3 (4)
C9—P1—C3	106.02 (18)	C14—C13—H13	119.8
C2—P2—S2	109.54 (13)	C9—C14—H14	120.1
C2—P2—C15	100.75 (18)	C13—C14—C9	119.8 (4)
C2—P2—C21	113.85 (18)	C13—C14—H14	120.1
C15—P2—S2	112.62 (14)	C16—C15—P2	120.8 (3)
C21—P2—S2	115.48 (14)	C20—C15—P2	119.7 (3)
C21—P2—C15	103.53 (18)	C20—C15—C16	119.4 (4)
P1—C1—H1	112.4	C15—C16—H16	120.1

C2—C1—P1	135.2 (3)	C17—C16—C15	119.8 (4)
C2—C1—H1	112.4	C17—C16—H16	120.1
P2—C2—H2	111.6	C16—C17—H17	120.0
C1—C2—P2	136.7 (3)	C18—C17—C16	119.9 (5)
C1—C2—H2	111.6	C18—C17—H17	120.0
C4—C3—P1	121.8 (3)	C17—C18—H18	119.6
C4—C3—C8	119.2 (4)	C17—C18—C19	120.8 (4)
C8—C3—P1	119.0 (3)	C19—C18—H18	119.6
C3—C4—H4	120.0	C18—C19—H19	119.8
C3—C4—C5	120.1 (4)	C18—C19—C20	120.4 (4)
C5—C4—H4	120.0	C20—C19—H19	119.8
C4—C5—H5	119.7	C15—C20—C19	119.7 (4)
C6—C5—C4	120.6 (5)	C15—C20—H20	120.1
C6—C5—H5	119.7	C19—C20—H20	120.1
C5—C6—H6	120.3	C22—C21—P2	121.7 (3)
C7—C6—C5	119.3 (4)	C22—C21—C26	119.1 (4)
C7—C6—H6	120.3	C26—C21—P2	118.7 (3)
C6—C7—H7	119.5	C21—C22—H22	119.9
C6—C7—C8	121.0 (4)	C23—C22—C21	120.3 (4)
C8—C7—H7	119.5	C23—C22—H22	119.9
C3—C8—H8	120.1	C22—C23—H23	120.0
C7—C8—C3	119.8 (4)	C24—C23—C22	120.0 (4)
C7—C8—H8	120.1	C24—C23—H23	120.0
C10—C9—P1	118.9 (3)	C23—C24—H24	119.9
C10—C9—C14	119.7 (4)	C23—C24—C25	120.2 (4)
C14—C9—P1	121.4 (3)	C25—C24—H24	119.9
C9—C10—H10	119.8	C24—C25—H25	119.9
C11—C10—C9	120.4 (4)	C26—C25—C24	120.2 (4)
C11—C10—H10	119.8	C26—C25—H25	119.9
C10—C11—H11	120.3	C21—C26—H26	119.9
C10—C11—C12	119.4 (4)	C25—C26—C21	120.1 (4)
C12—C11—H11	120.3	C25—C26—H26	119.9
S1—P1—C1—C2	92.9 (4)	C4—C5—C6—C7	−1.2 (7)
S1—P1—C3—C4	158.3 (3)	C5—C6—C7—C8	1.0 (7)
S1—P1—C3—C8	−21.4 (4)	C6—C7—C8—C3	0.2 (7)
S1—P1—C9—C10	7.6 (4)	C8—C3—C4—C5	1.0 (7)
S1—P1—C9—C14	−173.9 (3)	C9—P1—C1—C2	−35.7 (5)
S2—P2—C2—C1	96.9 (4)	C9—P1—C3—C4	−75.4 (4)
S2—P2—C15—C16	159.7 (3)	C9—P1—C3—C8	104.9 (3)
S2—P2—C15—C20	−23.4 (4)	C9—C10—C11—C12	−1.3 (6)
S2—P2—C21—C22	−170.6 (3)	C10—C9—C14—C13	−0.8 (6)
S2—P2—C21—C26	17.8 (4)	C10—C11—C12—C13	0.5 (7)
P1—C1—C2—P2	9.2 (7)	C11—C12—C13—C14	0.1 (7)
P1—C3—C4—C5	−178.6 (4)	C12—C13—C14—C9	0.1 (6)
P1—C3—C8—C7	178.4 (3)	C14—C9—C10—C11	1.4 (6)
P1—C9—C10—C11	−180.0 (3)	C15—P2—C2—C1	−144.2 (4)
P1—C9—C14—C13	−179.4 (3)	C15—P2—C21—C22	65.9 (4)

P2—C15—C16—C17	177.4 (3)	C15—P2—C21—C26	−105.8 (3)
P2—C15—C20—C19	−176.7 (3)	C15—C16—C17—C18	−1.7 (7)
P2—C21—C22—C23	−171.3 (3)	C16—C15—C20—C19	0.3 (6)
P2—C21—C26—C25	171.0 (3)	C16—C17—C18—C19	2.0 (7)
C1—P1—C3—C4	39.0 (4)	C17—C18—C19—C20	−1.2 (7)
C1—P1—C3—C8	−140.6 (3)	C18—C19—C20—C15	0.0 (7)
C1—P1—C9—C10	134.4 (3)	C20—C15—C16—C17	0.5 (6)
C1—P1—C9—C14	−47.1 (4)	C21—P2—C2—C1	−34.1 (5)
C2—P2—C15—C16	43.0 (4)	C21—P2—C15—C16	−74.9 (4)
C2—P2—C15—C20	−140.0 (3)	C21—P2—C15—C20	102.0 (3)
C2—P2—C21—C22	−42.5 (4)	C21—C22—C23—C24	0.7 (6)
C2—P2—C21—C26	145.8 (3)	C22—C21—C26—C25	−0.8 (6)
C3—P1—C1—C2	−147.3 (4)	C22—C23—C24—C25	−1.2 (7)
C3—P1—C9—C10	−117.2 (3)	C23—C24—C25—C26	0.6 (7)
C3—P1—C9—C14	61.3 (4)	C24—C25—C26—C21	0.4 (7)
C3—C4—C5—C6	0.2 (7)	C26—C21—C22—C23	0.3 (6)
C4—C3—C8—C7	−1.2 (6)		

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C15–C20 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···S2[i]	0.95	2.86	3.742 (4)	155
C7—H7···S2[ii]	0.95	2.82	3.561 (5)	135
C8—H8···S1	0.95	2.86	3.344 (4)	113
C10—H10···S1	0.95	2.84	3.360 (4)	116
C20—H20···S2	0.95	2.89	3.367 (4)	113
C26—H26···S2	0.95	2.89	3.394 (4)	115
C11—H11···Cg[iii]	0.95	2.63	3.573 (5)	171

Symmetry codes: (i) $x+1/2$, $−y+3/2$, $−z$; (ii) $−x+1$, $y−1/2$, $−z+1/2$; (iii) $−x+1/2$, $−y+1$, $z+1/2$.

Dichlorido[(*Z*)-(ethene-1,2-diyl)bis(diphenylphosphine sulfide)-κ^2S,S']platinum(II) (II)

Crystal data

[PtCl$_2$(C$_{26}$H$_{22}$P$_2$S$_2$)]	$D_x = 1.890$ Mg m$^{−3}$
$M_r = 726.48$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, *Fdd*2	Cell parameters from 9927 reflections
$a = 18.0724$ (12) Å	$\theta = 2.5–25.4°$
$b = 30.163$ (2) Å	$\mu = 6.01$ mm$^{−1}$
$c = 9.3697$ (6) Å	$T = 173$ K
$V = 5107.5$ (6) Å^3	Plate, yellow
$Z = 8$	$0.35 × 0.14 × 0.10$ mm
$F(000) = 2816$	

Data collection

Bruker APEXII CCD diffractometer	Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
Radiation source: sealed tube	$T_{min} = 0.543$, $T_{max} = 0.745$
Graphite monochromator	20596 measured reflections
Detector resolution: 8 pixels mm^{-1}	2324 independent reflections
φ and ω scans	2227 reflections with $I > 2\sigma(I)$

$R_{int} = 0.039$

$\theta_{max} = 25.4°$, $\theta_{min} = 2.5°$

$h = -21 \rightarrow 21$

$k = -36 \rightarrow 36$

$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2 + 4.1023P]$
$R[F^2 > 2\sigma(F^2)] = 0.023$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.061$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.09$	$\Delta\rho_{max} = 1.82$ e Å⁻³
2324 reflections	$\Delta\rho_{min} = -0.47$ e Å⁻³
150 parameters	Absolute structure: Flack x determined using
1 restraint	1010 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et*
Primary atom site location: heavy-atom method	*al.* 2013)
Hydrogen site location: inferred from	Absolute structure parameter: −0.006 (4)
neighbouring sites	

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)

	x	y	z	$U_{iso}*/U_{eq}$
Pt1	0.500000	0.500000	−0.21568 (8)	0.02096 (13)
S1	0.44478 (10)	0.54577 (6)	−0.0554 (2)	0.0278 (4)
Cl1	0.55528 (10)	0.45658 (6)	−0.3904 (2)	0.0322 (4)
P1	0.51249 (11)	0.55887 (7)	0.1097 (2)	0.0232 (4)
C1	0.5064 (5)	0.5214 (3)	0.2610 (10)	0.027 (2)
H1	0.513340	0.534545	0.352168	0.032*
C6	0.3769 (4)	0.6526 (3)	0.2775 (10)	0.0340 (16)
H6	0.326369	0.654598	0.304722	0.041*
C4	0.4948 (5)	0.6864 (3)	0.2493 (10)	0.037 (3)
H4	0.525799	0.711707	0.258970	0.045*
C5	0.4219 (5)	0.6890 (3)	0.2897 (11)	0.0378 (18)
H5	0.402617	0.715993	0.326227	0.045*
C3	0.5238 (5)	0.6471 (3)	0.1941 (10)	0.0334 (18)
H3	0.573993	0.645788	0.164031	0.040*
C2	0.4790 (4)	0.6101 (3)	0.1836 (8)	0.0272 (16)
C7	0.4047 (5)	0.6130 (3)	0.2256 (8)	0.0340 (18)
H7	0.373423	0.587756	0.218478	0.041*
C8	0.6089 (4)	0.5641 (2)	0.0639 (8)	0.0263 (17)
C13	0.6637 (4)	0.5485 (3)	0.1545 (9)	0.0332 (18)
H13	0.650228	0.534949	0.242200	0.040*
C9	0.6287 (4)	0.5837 (3)	−0.0631 (9)	0.0358 (19)
H9	0.591769	0.594278	−0.126754	0.043*
C12	0.7374 (5)	0.5524 (3)	0.1194 (12)	0.037 (2)
H12	0.774484	0.541843	0.182621	0.044*
C11	0.7569 (5)	0.5718 (3)	−0.0084 (11)	0.035 (3)

H11	0.807545	0.574026	−0.034541	0.043*
C10	0.7034 (5)	0.5880 (3)	−0.0977 (11)	0.047 (2)
H10	0.717297	0.602202	−0.184109	0.057*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.01883 (18)	0.02136 (18)	0.02268 (19)	0.0004 (3)	0.000	0.000
S1	0.0218 (10)	0.0335 (11)	0.0283 (10)	0.0078 (8)	−0.0036 (8)	−0.0072 (8)
Cl1	0.0339 (10)	0.0340 (10)	0.0287 (11)	0.0051 (8)	0.0031 (9)	−0.0066 (8)
P1	0.0256 (9)	0.0202 (9)	0.0238 (10)	−0.0008 (7)	0.0003 (8)	−0.0017 (8)
C1	0.020 (4)	0.045 (4)	0.015 (6)	0.004 (4)	−0.004 (3)	−0.012 (4)
C6	0.024 (4)	0.041 (4)	0.036 (4)	0.006 (3)	0.004 (4)	−0.002 (4)
C4	0.037 (5)	0.023 (4)	0.052 (9)	−0.002 (4)	0.004 (5)	−0.007 (4)
C5	0.036 (4)	0.032 (4)	0.046 (5)	0.009 (3)	0.000 (4)	−0.008 (4)
C3	0.024 (4)	0.028 (4)	0.047 (5)	−0.001 (3)	−0.002 (4)	−0.007 (4)
C2	0.030 (4)	0.024 (4)	0.028 (4)	0.001 (3)	−0.003 (3)	−0.002 (3)
C7	0.031 (5)	0.036 (4)	0.035 (4)	−0.004 (4)	0.006 (3)	−0.003 (3)
C8	0.022 (4)	0.020 (3)	0.037 (5)	−0.002 (3)	−0.002 (3)	−0.008 (3)
C13	0.027 (4)	0.036 (4)	0.037 (5)	0.002 (3)	−0.002 (3)	−0.002 (3)
C9	0.026 (4)	0.039 (5)	0.042 (5)	0.002 (3)	−0.004 (4)	0.005 (4)
C12	0.028 (4)	0.037 (5)	0.045 (6)	0.004 (4)	−0.004 (4)	−0.005 (5)
C11	0.023 (5)	0.033 (5)	0.051 (8)	−0.005 (4)	0.006 (4)	−0.007 (4)
C10	0.040 (5)	0.053 (6)	0.049 (6)	−0.011 (4)	0.009 (4)	0.006 (4)

Geometric parameters (Å, º)

Pt1—S1	2.2712 (19)	C5—H5	0.9500
Pt1—S1^i	2.2712 (19)	C3—H3	0.9500
Pt1—Cl1	2.3226 (19)	C3—C2	1.382 (12)
Pt1—Cl1^i	2.3226 (19)	C2—C7	1.403 (11)
S1—P1	2.012 (3)	C7—H7	0.9500
P1—C1	1.816 (9)	C8—C13	1.387 (11)
P1—C2	1.799 (8)	C8—C9	1.377 (11)
P1—C8	1.801 (7)	C13—H13	0.9500
C1—C1^i	1.312 (18)	C13—C12	1.377 (12)
C1—H1	0.9500	C9—H9	0.9500
C6—H6	0.9500	C9—C10	1.394 (12)
C6—C5	1.370 (11)	C12—H12	0.9500
C6—C7	1.384 (11)	C12—C11	1.379 (14)
C4—H4	0.9500	C11—H11	0.9500
C4—C5	1.373 (13)	C11—C10	1.367 (14)
C4—C3	1.397 (12)	C10—H10	0.9500
S1—Pt1—S1^i	97.19 (10)	C2—C3—C4	119.5 (8)
S1^i—Pt1—Cl1	86.24 (6)	C2—C3—H3	120.3
S1^i—Pt1—Cl1^i	176.41 (8)	C3—C2—P1	121.6 (6)
S1—Pt1—Cl1	176.41 (8)	C3—C2—C7	119.5 (7)

S1—Pt1—Cl1[i]	86.24 (6)	C7—C2—P1	118.9 (6)
Cl1—Pt1—Cl1[i]	90.34 (10)	C6—C7—C2	119.9 (7)
P1—S1—Pt1	111.14 (10)	C6—C7—H7	120.0
C1—P1—S1	116.2 (3)	C2—C7—H7	120.0
C2—P1—S1	105.1 (3)	C13—C8—P1	121.0 (6)
C2—P1—C1	102.4 (4)	C9—C8—P1	119.7 (6)
C2—P1—C8	110.0 (4)	C9—C8—C13	119.2 (7)
C8—P1—S1	115.0 (3)	C8—C13—H13	119.5
C8—P1—C1	107.4 (4)	C12—C13—C8	121.1 (8)
P1—C1—H1	115.7	C12—C13—H13	119.5
C1[i]—C1—P1	128.6 (3)	C8—C9—H9	120.2
C1[i]—C1—H1	115.7	C8—C9—C10	119.5 (8)
C5—C6—H6	119.8	C10—C9—H9	120.2
C5—C6—C7	120.3 (7)	C13—C12—H12	120.3
C7—C6—H6	119.8	C13—C12—C11	119.4 (9)
C5—C4—H4	119.7	C11—C12—H12	120.3
C5—C4—C3	120.7 (8)	C12—C11—H11	119.9
C3—C4—H4	119.7	C10—C11—C12	120.1 (8)
C6—C5—C4	120.1 (7)	C10—C11—H11	119.9
C6—C5—H5	119.9	C9—C10—H10	119.7
C4—C5—H5	119.9	C11—C10—C9	120.6 (9)
C4—C3—H3	120.3	C11—C10—H10	119.7
S1—P1—C1—C1[i]	35.0 (13)	C3—C4—C5—C6	0.6 (15)
S1—P1—C2—C3	−121.8 (7)	C3—C2—C7—C6	−0.2 (12)
S1—P1—C2—C7	55.4 (7)	C2—P1—C1—C1[i]	148.8 (11)
S1—P1—C8—C13	−143.1 (5)	C2—P1—C8—C13	98.5 (7)
S1—P1—C8—C9	36.7 (7)	C2—P1—C8—C9	−81.6 (7)
P1—C2—C7—C6	−177.5 (7)	C7—C6—C5—C4	0.6 (14)
P1—C8—C13—C12	179.9 (7)	C8—P1—C1—C1[i]	−95.3 (12)
P1—C8—C9—C10	179.5 (7)	C8—P1—C2—C3	2.4 (8)
C1—P1—C2—C3	116.4 (7)	C8—P1—C2—C7	179.7 (6)
C1—P1—C2—C7	−66.4 (7)	C8—C13—C12—C11	−0.5 (13)
C1—P1—C8—C13	−12.1 (7)	C8—C9—C10—C11	1.7 (14)
C1—P1—C8—C9	167.7 (6)	C13—C8—C9—C10	−0.6 (12)
C4—C3—C2—P1	178.6 (7)	C13—C12—C11—C10	1.5 (13)
C4—C3—C2—C7	1.4 (13)	C9—C8—C13—C12	0.0 (12)
C5—C6—C7—C2	−0.8 (13)	C12—C11—C10—C9	−2.1 (14)
C5—C4—C3—C2	−1.6 (14)		

Symmetry code: (i) −x+1, −y+1, z.

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···Cl1[ii]	0.95	2.73	3.515 (10)	141
C3—H3···S1[iii]	0.95	2.82	3.538 (9)	133

Symmetry codes: (ii) −x+1, −y+1, z+1; (iii) x+1/4, −y+5/4, z+1/4.