## metal-organic compounds

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# [1,2-Bis(diphenylphosphanyl)ethane- $\kappa^2 P, P'$ ]dichloridopalladium(II) dimethyl sulfoxide monosolvate

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Key indicators: single-crystal X-ray study; T = 293 K; mean  $\sigma$ (C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.027; wR factor = 0.069; data-to-parameter ratio = 20.3.

In the title compound,  $[PdCl_2(C_{26}H_{24}P_2)]\cdot C_2H_6OS$ , the Pd<sup>II</sup> atom adopts a distorted *cis*-PdCl\_2P\_2 square-planar coordination geometry. The five-membered chelate ring adopts an envelope conformation with a methylene C atom in the flap position. The S and C atoms of the dimethyl sulfoxide (DMSO) solvent molecule are disordered over two sets of sites in a 0.8976 (18):0.1024 (18) ratio. The DMSO O atom accepts three C-H···O hydrogen bonds from an adjacent complex molecule.

## **Related literature**

For the previous reports of crystal structures of this metal complex (unsolvated or with other solvents), see: Xu *et al.* (2008); Batsanov *et al.* (2001); Steffen & Palenik (1976); Singh *et al.* (1995).



## Experimental

#### Crystal data

 $\begin{array}{l} [\mathrm{PdCl}_2(\mathrm{C}_{26}\mathrm{H}_{24}\mathrm{P}_2)]\cdot\mathrm{C}_2\mathrm{H}_6\mathrm{OS} \\ M_r = 653.82 \\ \mathrm{Triclinic}, \ P\overline{1} \\ a = 8.4091 \ (3) \ \text{\AA} \\ b = 11.4745 \ (4) \ \text{\AA} \\ c = 16.8098 \ (6) \ \text{\AA} \\ \alpha = 73.674 \ (1)^\circ \\ \beta = 79.066 \ (1)^\circ \end{array}$ 

#### Data collection

Bruker SMART APEX CCD diffractometer Absorption correction: multi-scan (*SADABS*; Bruker, 2000)  $T_{\rm min} = 0.747, T_{\rm max} = 0.895$ 

### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.027$   $wR(F^2) = 0.069$  S = 1.036610 reflections 326 parameters V = 1442.67 (9) Å<sup>3</sup> Z = 2Mo K $\alpha$  radiation  $\mu = 1.03$  mm<sup>-1</sup> T = 293 K  $0.30 \times 0.23 \times 0.11$  mm

 $\gamma = 68.634 \ (1)^{\circ}$ 

19016 measured reflections 6610 independent reflections 5863 reflections with  $I > 2\sigma(I)$  $R_{int} = 0.022$ 

3 restraints H-atom parameters constrained 
$$\begin{split} &\Delta\rho_{max}=0.50\ e\ \text{\AA}^{-3}\\ &\Delta\rho_{min}=-0.32\ e\ \text{\AA}^{-3} \end{split}$$

## Table 1

Selected bond lengths (Å).

Pd1-P2	2.2336 (5)	Pd1-Cl1	2.3481 (6)
Pd1-P1	2.2355 (5)	Pd1-Cl2	2.3613 (5)

## Table 2

H	[yd	lrogen-	bond	geometry	(/	<b>٩</b> , °	).
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$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
$C2 - H2 \cdots O1$	0.93	2.49	3.348 (4)	153
C20−H20···O1	0.93	2.59	3.495 (4)	165
$C26-H26A\cdots O1$	0.97	2.44	3.410 (3)	174

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for

publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6864).

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# supplementary materials

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# [1,2-Bis(diphenylphosphanyl)ethane- $\kappa^2 P$ ,P']dichloridopalladium(II) dimethyl sulfoxide monosolvate

## Ismail Warad, Abdullah S. Aldwayyan, Fahad M. Al-Jekhedab, M. Iqbal Choudhary and Sammer Yousuf

## Comment

Metal complexes containing chelating diphosphines as ligands have been employed in numerous catalytic processes. A major advantage of these ligands is variation in their potential catalytic reactivity by varying the molecular properties of the phosphine. The title compound was synthesized as a part of our ongoing research to study the properties of metal complexes with chelating ligands.

The crystal structure of title compound,  $[PdCl_2C_{26}H_{24}P_2)].C_6H_6SO$ , consists of a bidentate diphenyl phosphine ligand and two chloride atoms coordinated with Pd(II) to adapt a distorted square planner geometry, along with an independent molecule of dimethyl sulfoxide (DMSO) as solvent (Fig. 1). The five membered metallocycle (Pd1/P1/P2/C25—C26) adopts an envelop conformation [Q= 0.466 (19) Å and  $\varphi = 301.14 (17)^\circ]$  with maximum deviation of 0.318 (2) Å for C26 atom from the least square plane. The Structural report of the compound is similar to many previously published reports with the difference that it has a DMSO solvate (Xu *et al.* 2008, Batsanov *et al.* 2001,Steffen & Palenik, 1976, Singh *et al.* 1995). The coordination environment around the Pd(II) ion is such that the two phosphorous atoms of the bidentate diphenyl phosphine ligand [Pd1–P1 = 2.2355 (5) Å, Pd1–P2 = 2.2336 (5) Å] and two chloride atoms [Pd1–C11= 2.3481 (6) Å, Pd1–C12= 2.3613 (5) Å] are assembled at four corners of square to adapt square pyramidal arrangement. The S1, C28 and C29 atoms of DMSO molecule are disordered at two positions,with relative occupancies of 0.89 (18):0.10 (18) for the isotropically refined major (S1/C27/C28) and minor (S1'/C27'/C28') components, respectively. All bond lengths are in agreement with the previously reported crystal structures (Xu *et al.* 2008, Batsanov *et al.* 2001, Steffen & Palenik, 1976, Singh *et al.* 1995). The oxygen atom of DMSO playing an important role in the crystal structure by forming C2— H2…O1, C20—H20…O1 and C26—H26A…O1 hydrogen bonds (Table 2, Fig. 2).

The compound was evaluated for its b-glucoronidase inhibiton activity against D-saccharic acid as standard (IC<sub>50</sub> 45.75  $\pm$  2.16 mM) and found as weak inhibitor (IC<sub>50</sub> 197.3  $\pm$  12.2 mM)

## Experimental

Equimolar amounts of dichlorobis(acetonitrile) palladium(II) (0.10 g, 0.26 mmol) was dissolved in 10 ml dry dichloromethane and mixed with equivalent amount of 1,2-ethanediylbis(diphenylphosphine) (0.11 g, 0.27 mmol). The resultant mixture was stirred under inert atmosphere (Ar) for about one hour. The solution was concentrated under reduced pressure to 1 ml volume. The product was precipitated by the addition of 30 ml of hexane. Then filtered off, washed with 40 ml of diethyl ether and dried under vacuum to obtained 0.12 g of title compound I (yield 78%). 20 mg of the product was dissolved in 5 ml of dry DMSO for crystallization. After one week, light orange color crystals were obtained which were found to be suitable for X-ray diffraction data collection. All chemicals were purchased from Acros (Belgium).

## Refinement

H Atoms on methyl, methylene and methine were positioned geometrically with C—H = 0.96 Å, 0.97 Å and 0.93 Å respectively, and constrained to ride on their parent atoms with  $U_{iso}(H)=1.2U_{eq}$  (CH<sub>2</sub>, CH) and  $1.5U_{eq}$ (CH<sub>3</sub>).

## **Computing details**

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008), *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).



## Figure 1

The molecular structure of (I) with displacement ellipsoids drawn at 30% probability level.



## Figure 2

The crystal packing of the title compound I. Only hydrogen atoms involved in hydrogen bonding are shown.

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Crystal data	
$[PdCl_2(C_{26}H_{24}P_2)] \cdot C_2H_6OS$	Z = 2
$M_r = 653.82$	F(000) = 664
Triclinic, P1	$D_{\rm x} = 1.505 {\rm ~Mg} {\rm ~m}^{-3}$
a = 8.4091 (3) Å	Mo <i>K</i> $\alpha$ radiation, $\lambda = 0.71073$ Å
b = 11.4745 (4) Å	Cell parameters from 8463 reflections
c = 16.8098 (6) Å	$\theta = 2.5 - 28.3^{\circ}$
$\alpha = 73.674 \ (1)^{\circ}$	$\mu = 1.03 \text{ mm}^{-1}$
$\beta = 79.066 \ (1)^{\circ}$	T = 293  K
$\gamma = 68.634 \ (1)^{\circ}$	Block, orange
$V = 1442.67 (9) Å^3$	$0.30 \times 0.23 \times 0.11 \text{ mm}$

Data collection

Bruker SMART APEX CCD diffractometer Radiation source: fine-focus sealed tube Graphite monochromator $\omega$ scan Absorption correction: multi-scan ( <i>SADABS</i> ; Bruker, 2000) $T_{min} = 0.747, T_{max} = 0.895$ <i>Refinement</i>	19016 measured reflections 6610 independent reflections 5863 reflections with $I > 2\sigma(I)$ $R_{int} = 0.022$ $\theta_{max} = 27.5^{\circ}, \ \theta_{min} = 1.3^{\circ}$ $h = -10 \rightarrow 10$ $k = -14 \rightarrow 14$ $l = -21 \rightarrow 21$
Refinement on $F^2$	Secondary atom site location: difference Fourier
Least-squares matrix: full	map
$R[F^2 > 2\sigma(F^2)] = 0.027$	Hydrogen site location: inferred from
$wR(F^2) = 0.069$	neighbouring sites
S = 1.03	H-atom parameters constrained
6610 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0363P)^2 + 0.3766P]$
326 parameters	where $P = (F_o^2 + 2F_c^2)/3$
3 restraints	$(\Delta/\sigma)_{max} = 0.003$
Primary atom site location: structure-invariant	$\Delta\rho_{max} = 0.50$ e Å <sup>-3</sup>
direct methods	$\Delta\rho_{min} = -0.32$ e Å <sup>-3</sup>

## Special details

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

**Refinement**. Refinement of  $F^2$  against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on  $F^2$ , conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating *R*-factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. *R*-factors based on  $F^2$  are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	X	У	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	Occ. (<1)
Pd1	0.505146 (17)	0.668916 (13)	0.771823 (8)	0.02941 (5)	
C11	0.25945 (8)	0.81046 (6)	0.82912 (5)	0.06129 (17)	
Cl2	0.34922 (7)	0.55828 (5)	0.73749 (4)	0.04605 (13)	
P1	0.74985 (6)	0.53495 (5)	0.72429 (3)	0.03260 (11)	
P2	0.67020 (6)	0.76776 (5)	0.79571 (3)	0.03221 (11)	
C1	0.7524 (3)	0.5243 (2)	0.61872 (13)	0.0396 (5)	
C2	0.7793 (3)	0.6212 (3)	0.55295 (15)	0.0558 (6)	
H2	0.8028	0.6887	0.5630	0.067*	
C3	0.7714 (4)	0.6179 (3)	0.47218 (17)	0.0725 (8)	
Н3	0.7894	0.6834	0.4281	0.087*	
C4	0.7375 (3)	0.5199 (4)	0.45682 (18)	0.0749 (9)	
H4	0.7309	0.5189	0.4024	0.090*	
C5	0.7133 (4)	0.4230 (3)	0.5210(2)	0.0759 (9)	
Н5	0.6921	0.3552	0.5099	0.091*	
C6	0.7196 (3)	0.4237 (3)	0.60288 (17)	0.0587 (6)	
H6	0.7020	0.3575	0.6465	0.070*	
C7	0.8124 (3)	0.37111 (19)	0.78653 (14)	0.0411 (5)	

C8	0.9678 (4)	0.2825(2)	0.76568 (18)	0.0645(7)	
H8	1.0381	0.3068	0.7189	0.077*	
C9	1.0188 (4)	0.1582(3)	0.8140(2)	0.0783(9)	
H9	1.1229	0.0991	0.7995	0.094*	
C10	0.9171 (5)	0.1225 (3)	0.8827(2)	0.0771 (9)	
H10	0.9504	0.0383	0.9143	0.093*	
C11	0.7664 (4)	0.2098 (3)	0.9054 (2)	0.0791 (9)	
H11	0.6995	0.1858	0.9537	0.095*	
C12	0.7125 (3)	0.3341 (2)	0.85681 (17)	0.0583 (6)	
H12	0.6083	0.3925	0.8719	0.070*	
C13	0.7402 (3)	0.7045 (2)	0.89926 (12)	0.0377 (4)	
C14	0.8598 (3)	0.7441 (3)	0.92091 (17)	0.0590 (6)	
H14	0.9046	0.8027	0.8821	0.071*	
C15	0.9125 (4)	0.6965 (4)	1.0000 (2)	0.0791 (10)	
H15	0.9929	0.7230	1.0147	0.095*	
C16	0.8465 (4)	0.6107 (3)	1.05672 (18)	0.0801 (10)	
H16	0.8803	0.5805	1.1104	0.096*	
C17	0.7318 (4)	0.5686 (3)	1.03572 (16)	0.0731 (9)	
H17	0.6912	0.5073	1.0743	0.088*	
C18	0.6754 (3)	0.6170(2)	0.95701 (14)	0.0533 (6)	
H18	0.5942	0.5905	0.9432	0.064*	
C19	0.5851 (3)	0.9401 (2)	0.78165 (15)	0.0441 (5)	
C20	0.5855 (4)	1.0192 (2)	0.70303 (19)	0.0670 (7)	
H20	0.6291	0.9842	0.6566	0.080*	
C21	0.5198 (5)	1.1521 (3)	0.6938 (3)	0.0915 (11)	
H21	0.5215	1.2056	0.6408	0.110*	
C22	0.4539 (5)	1.2048 (3)	0.7599 (3)	0.0980 (13)	
H22	0.4109	1.2938	0.7524	0.118*	
C23	0.4503 (5)	1.1276 (3)	0.8380 (3)	0.0906 (11)	
H23	0.4042	1.1641	0.8836	0.109*	
C24	0.5150 (4)	0.9944 (3)	0.8497 (2)	0.0661 (7)	
H24	0.5113	0.9420	0.9030	0.079*	
C25	0.9282 (3)	0.5915 (2)	0.72475 (14)	0.0420 (5)	
H25A	0.9877	0.5425	0.7739	0.050*	
H25B	1.0091	0.5765	0.6762	0.050*	
C26	0.8655 (3)	0.7338 (2)	0.72412 (13)	0.0398 (5)	
H26A	0.8417	0.7850	0.6683	0.048*	
H26B	0.9529	0.7552	0.7416	0.048*	
O1	0.8108 (4)	0.9128 (2)	0.52539 (14)	0.1089 (9)	
S1	0.76772 (16)	0.97151 (11)	0.43853 (6)	0.0890 (3)	0.8976 (18)
C27	0.9635 (7)	0.9661 (6)	0.3762 (3)	0.1181 (18)	0.8976 (18)
H27A	1.0259	0.8793	0.3716	0.177*	0.8976 (18)
H27B	1.0304	0.9957	0.4015	0.177*	0.8976 (18)
H27C	0.9405	1.0204	0.3218	0.177*	0.8976 (18)
C28	0.6941 (10)	1.1385 (4)	0.4309 (3)	0.173 (3)	0.8976 (18)
H28A	0.5839	1.1627	0.4621	0.259*	0.8976 (18)
H28B	0.6844	1.1833	0.3735	0.259*	0.8976 (18)
H28C	0.7739	1.1605	0.4529	0.259*	0.8976 (18)
S1′	0.8125 (14)	1.0323 (6)	0.4620 (5)	0.0890 (3)	0.1024 (18)

# supplementary materials

C27′	0.880 (7)	0.957 (6)	0.378 (3)	0.1181 (18)	0.1024 (18)
H27D	1.0007	0.9093	0.3777	0.177*	0.1024 (18)
H27E	0.8594	1.0212	0.3264	0.177*	0.1024 (18)
H27F	0.8176	0.8996	0.3830	0.177*	0.1024 (18)
C28′	0.622 (4)	1.075 (5)	0.416 (3)	0.173 (3)	0.1024 (18)
H28D	0.5292	1.1302	0.4454	0.259*	0.1024 (18)
H28E	0.5966	0.9987	0.4188	0.259*	0.1024 (18)
H28F	0.6355	1.1193	0.3589	0.259*	0.1024 (18)

Atomic displacement parameters  $(Å^2)$ 

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	U <sup>23</sup>
Pd1	0.02598 (8)	0.02756 (8)	0.03349 (9)	-0.00798 (6)	-0.00470 (5)	-0.00518 (6)
C11	0.0388 (3)	0.0489 (3)	0.0917 (5)	-0.0079 (2)	0.0116 (3)	-0.0302 (3)
Cl2	0.0400 (3)	0.0497 (3)	0.0574 (3)	-0.0209 (2)	-0.0106 (2)	-0.0140 (2)
P1	0.0292 (2)	0.0319 (2)	0.0360 (3)	-0.0073 (2)	-0.00501 (19)	-0.0095 (2)
P2	0.0341 (3)	0.0296 (2)	0.0341 (3)	-0.0124 (2)	-0.0048 (2)	-0.0057 (2)
C1	0.0316 (10)	0.0470 (12)	0.0391 (11)	-0.0070 (9)	-0.0028 (8)	-0.0168 (9)
C2	0.0657 (16)	0.0572 (15)	0.0435 (13)	-0.0190 (12)	-0.0054 (11)	-0.0119 (11)
C3	0.076 (2)	0.094 (2)	0.0397 (14)	-0.0225 (17)	-0.0052 (13)	-0.0122 (14)
C4	0.0483 (15)	0.125 (3)	0.0518 (16)	-0.0118 (16)	-0.0026 (12)	-0.0455 (18)
C5	0.0706 (19)	0.100 (2)	0.081 (2)	-0.0303 (18)	-0.0044 (16)	-0.056 (2)
C6	0.0609 (16)	0.0675 (17)	0.0606 (15)	-0.0280 (13)	-0.0019 (12)	-0.0280 (13)
C7	0.0420 (11)	0.0322 (10)	0.0478 (12)	-0.0070 (9)	-0.0131 (9)	-0.0085 (9)
C8	0.0594 (16)	0.0461 (14)	0.0703 (17)	0.0026 (12)	-0.0053 (13)	-0.0137 (13)
C9	0.078 (2)	0.0410 (15)	0.101 (2)	0.0086 (14)	-0.0300 (18)	-0.0182 (15)
C10	0.094 (2)	0.0361 (13)	0.100 (2)	-0.0154 (15)	-0.052 (2)	0.0062 (15)
C11	0.084 (2)	0.0604 (18)	0.081 (2)	-0.0317 (17)	-0.0205 (17)	0.0196 (16)
C12	0.0531 (15)	0.0455 (13)	0.0656 (16)	-0.0131 (11)	-0.0091 (12)	0.0014 (12)
C13	0.0366 (11)	0.0408 (11)	0.0351 (10)	-0.0087 (9)	-0.0056 (8)	-0.0117 (8)
C14	0.0565 (15)	0.0703 (17)	0.0601 (15)	-0.0226 (13)	-0.0163 (12)	-0.0210 (13)
C15	0.0661 (19)	0.104 (3)	0.076 (2)	-0.0095 (18)	-0.0327 (16)	-0.043 (2)
C16	0.071 (2)	0.102 (3)	0.0429 (15)	0.0130 (18)	-0.0222 (14)	-0.0224 (16)
C17	0.0649 (18)	0.086 (2)	0.0373 (13)	-0.0029 (15)	-0.0014 (12)	0.0021 (13)
C18	0.0480 (13)	0.0631 (15)	0.0407 (12)	-0.0158 (12)	-0.0032 (10)	-0.0036 (11)
C19	0.0403 (11)	0.0307 (10)	0.0646 (14)	-0.0139 (9)	-0.0121 (10)	-0.0085 (10)
C20	0.0733 (18)	0.0414 (13)	0.0762 (19)	-0.0169 (13)	-0.0125 (15)	0.0028 (13)
C21	0.089 (2)	0.0416 (16)	0.124 (3)	-0.0207 (16)	-0.023 (2)	0.0172 (18)
C22	0.075 (2)	0.0347 (15)	0.183 (4)	-0.0124 (15)	-0.031 (3)	-0.019 (2)
C23	0.084 (2)	0.0547 (18)	0.140 (3)	-0.0040 (16)	-0.019 (2)	-0.054 (2)
C24	0.0710 (18)	0.0453 (14)	0.0830 (19)	-0.0094 (13)	-0.0119 (15)	-0.0267 (14)
C25	0.0282 (10)	0.0505 (12)	0.0492 (12)	-0.0116 (9)	-0.0042 (9)	-0.0158 (10)
C26	0.0379 (11)	0.0453 (12)	0.0392 (11)	-0.0205 (9)	-0.0014 (8)	-0.0070 (9)
01	0.171 (3)	0.0846 (16)	0.0628 (14)	-0.0520 (18)	-0.0197 (15)	0.0146 (12)
S1	0.1244 (9)	0.0899 (7)	0.0686 (6)	-0.0583 (7)	-0.0235 (6)	-0.0026 (5)
C27	0.119 (4)	0.164 (5)	0.083 (3)	-0.062 (4)	0.002 (3)	-0.033 (3)
C28	0.277 (8)	0.071 (3)	0.097 (4)	0.021 (4)	-0.036 (4)	0.000 (3)
S1′	0.1244 (9)	0.0899 (7)	0.0686 (6)	-0.0583 (7)	-0.0235 (6)	-0.0026 (5)
C27′	0.119 (4)	0.164 (5)	0.083 (3)	-0.062 (4)	0.002 (3)	-0.033 (3)

C28'         0.277 (8)         0.071 (3)         0.097 (4)         0.021 (4) $-0.036 (4)$ 0.000 (3)           Geometric parameters (J. 7)           Pall—P2         2.2336 (5)         C16—H16         0.9300           Pall—P1         2.2355 (5)         C17—C18         1.384 (3)           Pall—C11         2.3481 (6)         C17—H17         0.9300           P1—C1         1.808 (2)         C19—C20         1.377 (3)           P1—C7         1.813 (2)         C20—C21         1.344 (5)           P2—C19         1.802 (2)         C21—H21         0.9300           P2—C13         1.898 (2)         C12—C22         0.344 (5)           P2—C14         1.381 (3)         C22—C23         1.344 (5)           P2—C15         1.384 (4)         C23—C24         0.9300           C1—C6         1.382 (3)         C22—H23         0.9300           C2—C41         0.9300         C25—C26         1.520 (3)           C3—C4         1.385 (5)         C24—H24         0.9300           C3—C4         1.385 (6)         C25—H25A         0.9700           C3—C4         1.386 (3)         S1—C27         1.765 (5)           C3—H2         0.9300         C25—H25A						supplem	entary materials
Geometric parameters (Å, ?)           Pd1-P2         2.2336 (5)         C16-H16         0.9300           Pd1-P1         2.2355 (5)         C17-C18         1.384 (3)           Pd1-C1         2.3481 (6)         C17-H17         0.9300           P1-C1         1.808 (2)         C19-C20         1.377 (3)           P1-C2         2.3613 (5)         C18-H18         0.9300           P1-C2         1.810 (2)         C20         C21         1.384 (4)           P2-C19         1.808 (2)         C21         C22         1.344 (5)           P2-C19         1.808 (2)         C21         P2         0.9300           C1-C2         1.381 (3)         C22-C23         1.364 (5)           C1-C4         1.352 (5)         C24         P2         0.9300           C2-C3         1.384 (4)         C23         C24         1.391 (4)           C2-C4         1.352 (5)         C24         P2         0.9300           C3-C4         1.352 (5)         C24         P2         0.9300           C3-C4         1.355 (5)         C24         P2         0.9300           C3-C4         1.355 (5)         C24         P2         0.9700           C4-C5	C28′	0.277 (8)	0.071 (3)	0.097 (4)	0.021 (4)	-0.036 (4)	0.000 (3)
Pail-P2         2.2336 (5)         C16-H16         0.9300           Pail-P1         2.2355 (5)         C17-C18         1.334 (3)           Pail-C11         2.3481 (6)         C17-H17         0.9300           Pail-C12         2.3613 (5)         C18-H18         0.9300           PI-C1         1.808 (2)         C19-C24         1.337 (4)           PI-C25         1.840 (2)         C20-H20         0.9300           P2-C19         1.802 (2)         C20-H20         0.9300           P2-C13         1.808 (2)         C21-C22         1.344 (5)           P2-C26         1.829 (2)         C21-H21         0.9300           C2-C3         1.384 (4)         C23-C24         1.391 (4)           C2-C3         1.384 (4)         C23-C24         1.391 (4)           C2-C4         1.391 (4)         C23-C24         1.391 (4)           C3-H3         0.9300         C25-H22         0.9300           C3-H3         0.9300         C25-H23         0.9700           C4-H4         0.9300         C25-H25         0.9700           C4-H4         0.9300         C25-H25         0.9700           C5-H5         0.9300         C25-H25         0.9600	Geome	tric parameters (	(Å, °)				
NII—PI         2.2355 (s)         C17—C18         1.384 (3)           Nail—C11         2.3355 (s)         C17—C18         1.384 (3)           Pail—C12         2.361 (s)         C18—H18         0.9300           PI—C1         1.808 (2)         C19—C20         1.377 (3)           PI—C7         1.813 (2)         C19—C24         1.387 (4)           PI—C25         1.840 (2)         C20—C21         1.344 (4)           P2—C13         1.808 (2)         C21—C22         1.344 (5)           P2—C26         1.829 (2)         C21—H21         0.9300           C1—C6         1.382 (3)         C22—H22         0.9300           C2=-C3         1.384 (4)         C23—C24         1.391 (4)           C3—C4         1.355 (s)         C24—H24         0.9300           C3—C4         1.355 (s)         C24—H24         0.9300           C3—H3         0.9300         C25—C26         1.520 (3)           C4—C5         1.360 (s)         C25—H25A         0.9700           C5—C6         1.390 (4)         C26—H26A         0.9700           C5—C46         1.390 (3)         S1—C28         1.766 (5)           C8—C6         1.390 (4)         C26—H26A         0.9600 <td>Pd1—F</td> <td>2</td> <td>2.2336</td> <td>5 (5)</td> <td>C16—H16</td> <td></td> <td>0.9300</td>	Pd1—F	2	2.2336	5 (5)	C16—H16		0.9300
Pd1-Cl1       2.3481 (6)       C17-H17       0.9300         Pa1-Cl       2.3613 (5)       C18-H18       0.9300         P1-Cl       1.808 (2)       C19-C20       1.377 (3)         P1-C2       1.813 (2)       C19-C20       1.337 (4)         P1-C3       1.813 (2)       C20-C21       1.394 (4)         P2-C19       1.800 (2)       C20-C21       1.394 (4)         P2-C13       1.808 (2)       C21-H21       0.9300         C1-C2       1.381 (3)       C22-C23       1.364 (5)         C1-C4       1.382 (3)       C22-H22       0.9300         C2-C4       1.355 (5)       C24-H24       0.9300         C3-C4       1.355 (5)       C24-H24       0.9300         C3-C4       1.350 (5)       C25-H25A       0.9700         C4-C5       1.360 (5)       C25-H25A       0.9700         C5-C6       1.390 (4)       C26-H26A       0.9700         C5-C4       1.336 (3)       S1-C27       1.766 (5)         C7-C12       1.373 (3)       01-S1'       1.484 (2)         C7-C42       1.335 (5)       C27-H27A       0.9600         C5-C6       1.390 (3)       S1-C27       1.766 (5)	Pd1—F	<b>P</b> 1	2.2355	5 (5)	C17—C18		1.384 (3)
Pall—Cl2       2.3613 (5)       C18—H18       0.9300         PI—C1       1.808 (2)       C19—C20       1.377 (3)         PI—C7       1.813 (2)       C19—C24       1.387 (4)         PI—C7       1.813 (2)       C20—C21       1.394 (4)         P2—C13       1.808 (2)       C20—C21       1.394 (4)         P2—C13       1.808 (2)       C21—C22       1.344 (5)         P2—C26       1.829 (2)       C21—H21       0.9300         C1—C2       1.381 (3)       C22—C23       1.364 (5)         C2—H2       0.9300       C23—H23       0.9300         C2=-H2       0.9300       C23—H23       0.9300         C3—H3       0.9300       C25—C26       1.520 (3)         C4—C5       1.366 (5)       C25—H25A       0.9700         C4—H4       0.9300       C25—H25B       0.9700         C4—H4       0.9300       C26—H26A       0.9700         C5—H5       0.9300       C26—H26B       0.9700         C5—H5       0.9300       C26—H26B       0.9700         C5—H5       0.9300       C27—H27A       0.9600         C7—C12       1.373 (3)       OI—S1       1.479 (2)         C7—C28 <th< td=""><td>Pd1—C</td><td>C11</td><td>2.3481</td><td>(6)</td><td>С17—Н17</td><td></td><td>0.9300</td></th<>	Pd1—C	C11	2.3481	(6)	С17—Н17		0.9300
P1-C1       1.808 (2)       C19-C20       1.377 (3)         P1-C7       1.813 (2)       C19-C24       1.387 (4)         P2-C19       1.802 (2)       C20-H20       0.9300         P2-C13       1.808 (2)       C21-C22       1.344 (5)         P2-C26       1.829 (2)       C21-H21       0.9300         C1-C2       1.381 (3)       C22-C23       1.364 (5)         C1-C6       1.382 (3)       C22-L122       0.9300         C2-C3       1.384 (4)       C23-C24       1.391 (4)         C2-C3       1.384 (4)       C23-C24       1.391 (4)         C2-H2       0.9300       C23-H23       0.9300         C3-H3       0.9300       C25-C26       1.520 (3)         C4-C5       1.360 (5)       C25-H25A       0.9700         C5-C6       1.390 (4)       C26-H26A       0.9700         C5-H5       0.9300       C26-H26B       0.9700         C5-H5       0.9300       C26-H26B       0.9700         C5-H5       0.9300       C27-H27A       0.9600         C7-C12       1.378 (3)       S1-C27       1.766 (5)         C3-H6       0.9300       C27-H27A       0.9600         C9-H10	Pd1—C	C12	2.3613	3 (5)	C18—H18		0.9300
P1-C7       1.813 (2)       C19-C24       1.387 (4)         P1-C25       1.840 (2)       C20-C21       1.394 (4)         P2-C19       1.802 (2)       C21-H20       0.9300         P2-C13       1.808 (2)       C21-C22       1.344 (5)         P2-C26       1.829 (2)       C21-H21       0.9300         C1-C2       1.381 (3)       C22-C23       1.364 (5)         C1-C6       1.382 (3)       C22-H22       0.9300         C2-C3       1.384 (4)       C23-H23       0.9300         C2-C4       1.391 (4)       C23-H23       0.9300         C3-H3       0.9300       C25-C26       1.520 (3)         C4-C5       1.360 (5)       C25-H25A       0.9700         C5-C6       1.390 (4)       C26-H26A       0.9700         C5-H4       0.9300       C26-H26B       0.9700         C5-H5       0.9300       C1-S1'       1.484 (2)         C7-C12       1.373 (3)       01-S1'       1.484 (2)         C7-C28       1.386 (3)       S1-C28       1.760 (5)         C8-H6       0.9300       C27-H27A       0.9600         C9-C10       1.359 (5)       C27-H27A       0.9600         C9-C10	P1—C1	1	1.808	(2)	C19—C20		1.377 (3)
P1-C25 $1.840$ (2) $C20-C21$ $1.394$ (4) $P2-C19$ $1.802$ (2) $C20-H20$ $0.9300$ $P2-C13$ $1.808$ (2) $C21-C22$ $1.344$ (5) $P2-C13$ $1.829$ (2) $C21-H21$ $0.9300$ $C1-C2$ $1.384$ (3) $C22-C23$ $1.364$ (5) $C1-C4$ $1.352$ (3) $C22-H22$ $0.9300$ $C2-C3$ $1.384$ (4) $C23-C24$ $1.391$ (4) $C2-C3$ $1.355$ (5) $C24-H24$ $0.9300$ $C3-H2$ $0.9300$ $C25-H25A$ $0.9700$ $C4-C5$ $1.360$ (5) $C25-H25A$ $0.9700$ $C4-H4$ $0.9300$ $C25-H25A$ $0.9700$ $C5-C6$ $1.390$ (4) $C26-H26B$ $0.9700$ $C5-H5$ $0.9300$ $C1-S1$ $1.479$ (2) $C7-C12$ $1.373$ (3) $01-S1$ $0.9600$	P1C2	7	1.813	(2)	C19—C24		1.387 (4)
P2-C19 $1.802(2)$ $C20-H20$ $0.9300$ $P2-C13$ $1.808(2)$ $C21-C22$ $1.344(5)$ $P2-C26$ $1.829(2)$ $C21-H21$ $0.9300$ $C1-C2$ $1.381(3)$ $C22-C23$ $1.364(5)$ $C1-C6$ $1.382(3)$ $C22-H22$ $0.9300$ $C2-C3$ $1.384(4)$ $C23-C24$ $1.391(4)$ $C2-H2$ $0.9300$ $C23-H23$ $0.9300$ $C3-H3$ $0.9300$ $C25-C26$ $1.520(3)$ $C3-H3$ $0.9300$ $C25-H25A$ $0.9700$ $C4-C5$ $1.350(5)$ $C24-H24$ $0.9700$ $C5-C6$ $1.390(4)$ $C26-H26B$ $0.9700$ $C5-H5$ $0.9300$ $C1-S1$ $1.479(2)$ $C7-C8$ $1.386(3)$ $S1-C28$ $1.760(5)$ $C8-C9$ $1.383(4)$ $S1-C28$ $1.760(5)$ $C8-H8$ $0.9300$ $C27-H27A$ $0.9600$ $C9-C10$ $1.359(5)$ $C27-H27B$ $0.9600$ $C9-H9$ $0.9300$ $C27-H27B$ $0.9600$ $C1-C11$	P1-C2	25	1.840	(2)	C20—C21		1.394 (4)
P2-C13       1.808 (2)       C21-C22       1.344 (5)         P2-C26       1.829 (2)       C21-H21       0.9300         C1-C2       1.381 (3)       C22-C23       1.364 (5)         C2-C3       1.384 (4)       C23-C24       1.391 (4)         C2-H2       0.9300       C23-H23       0.9300         C3-C4       1.355 (5)       C24-H24       0.9300         C3-H3       0.9300       C25-C26       1.520 (3)         C4-C5       1.360 (5)       C25-H25A       0.9700         C5-C6       1.390 (4)       C26-H26A       0.9700         C5-C6       1.390 (3)       I-C28       1.479 (2)         C7-C12       1.373 (3)       O1-S1'       1.444 (2)         C7-C8       1.384 (3)       S1-C28       1.760 (5)         C8-H8       0.9300       C27-H27A       0.9600         C10-C11       1.365 (5)       C28-H28A       0.9600         C10-H10	P2-C	19	1.802	(2)	C20—H20		0.9300
P2-C26       1.829 (2)       C21-H21       0.9300         C1-C2       1.381 (3)       C22-C23       1.364 (5)         C1-C6       1.382 (3)       C22-H22       0.9300         C2-C3       1.384 (4)       C23-C24       1.391 (4)         C2-C3       1.384 (4)       C23-C24       1.391 (4)         C2-H2       0.9300       C23-H23       0.9300         C3-C4       1.355 (5)       C24-H24       0.9300         C3-H3       0.9300       C25-C26       1.520 (3)         C4-C5       1.360 (5)       C25-H25A       0.9700         C5-C6       1.390 (4)       C26-H26B       0.9700         C5-H5       0.9300       C26-H26B       0.9700         C6-H6       0.9300       OI-S1       1.479 (2)         C7-C12       1.373 (3)       OI-S1'       1.484 (2)         C7-C28       1.386 (3)       S1-C28       1.760 (5)         C8-H8       0.9300       C27-H27A       0.9600         C9-C10       1.359 (5)       C27-H27B       0.9600         C10-H10       0.9300       C28-H28A       0.9600         C10-H10       0.9300       C28-H28D       0.9600         C11-C12	P2C1	13	1.808	(2)	C21—C22		1.344 (5)
C1-C2       1.381 (3)       C2-C23       1.364 (5)         C1-C6       1.382 (3)       C22-H22       0.9300         C2-C3       1.384 (4)       C23-C24       1.391 (4)         C2-H2       0.9300       C23-H23       0.9300         C3-C4       1.355 (5)       C24-H24       0.9300         C3-C4       1.355 (5)       C24-H24       0.9300         C3-C4       1.350 (5)       C25-H25       0.9700         C4-C5       1.360 (5)       C25-H25B       0.9700         C5-C6       1.390 (4)       C26-H26B       0.9700         C5-H5       0.9300       C26-H26B       0.9700         C6-H6       0.9300       C1-S1       1.479 (2)         C7-C12       1.373 (3)       01-S1'       1.484 (2)         C7-C28       1.386 (3)       S1-C28       1.760 (5)         C8-C9       1.383 (4)       S1-C27       1.766 (5)         C8-C9       1.385 (5)       C27-H27A       0.9600         C10-C11       1.355 (5)       C28-H28A       0.9600         C10-H10       0.9300       C28-H28B       0.9600         C10-H10       0.9300       C28-H28C       0.9600         C11-H11 <td< td=""><td>P2-C2</td><td>26</td><td>1.829</td><td>(2)</td><td>C21—H21</td><td></td><td>0.9300</td></td<>	P2-C2	26	1.829	(2)	C21—H21		0.9300
C1—C6       1.382 (3)       C2—H22       0.9300         C2—C3       1.384 (4)       C23—C24       1.391 (4)         C2—H2       0.9300       C23—H23       0.9300         C3—C4       1.355 (5)       C24—H24       0.9300         C3—H3       0.9300       C25—C26       1.520 (3)         C4—C5       1.360 (5)       C25—H25A       0.9700         C5—C6       1.390 (4)       C26—H26B       0.9700         C5—C6       1.390 (4)       C26—H26B       0.9700         C5—C6       1.390 (4)       C26—H26B       0.9700         C5—C6       1.390 (3)       OI—S1       1.479 (2)         C7—C12       1.373 (3)       OI—S1'       1.484 (2)         C7—C8       1.386 (3)       S1—C28       1.760 (5)         C8—H8       0.9300       C27—H27A       0.9600         C9—C10       1.359 (5)       C27—H27A       0.9600         C10—C11       1.355 (5)       C28—H28A       0.9600         C10—C11       1.356 (4)       C28—H28C       0.9600         C10—C11       0.9300       S1—C28'       1.759 (5)         C12—H12       0.9300       S1—C28'       1.759 (5)         C12—H14	C1C	2	1.381	(3)	C22—C23		1.364 (5)
C2-C3       1.384 (4)       C23-C24       1.391 (4)         C2-L3       0.9300       C23-H23       0.9300         C3-C4       1.355 (5)       C24-H24       0.9300         C3-H3       0.9300       C25-C26       1.520 (3)         C4-C5       1.360 (5)       C25-H25A       0.9700         C4-H4       0.9300       C26-H26B       0.9700         C5-C6       1.390 (4)       C26-H26B       0.9700         C5-H5       0.9300       C1-H11       1.479 (2)         C7-C12       1.373 (3)       O1-S1       1.448 (2)         C7-C5       1.386 (3)       SI-C27       1.766 (5)         C8-C9       1.383 (4)       S1-C27       1.766 (5)         C8-H8       0.9300       C27-H27A       0.9600         C9-C10       1.359 (5)       C28-H28A       0.9600         C10-C11       1.365 (5)       C28-H28A       0.9600         C10-C11       1.365 (5)       C28-H28A       0.9600         C10-H10       0.9300       C27-H27B       0.9600         C10-L11       1.365 (5)       C28-H28B       0.9600         C11-C12       1.380 (4)       C27-H27F       0.9600         C13-C14	C1-C	6	1.382	(3)	C22—H22		0.9300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2-C	3	1.384	(4)	$C_{23}$ — $C_{24}$		1.391 (4)
C3-C4       1.355 (5)       C24-H24       0.9300         C3-H3       0.9300       C25-C26       1.520 (3)         C4-C5       1.360 (5)       C25-H25A       0.9700         C5-C6       1.390 (4)       C26-H26A       0.9700         C5-C6       1.390 (4)       C26-H26B       0.9700         C5-H5       0.9300       C26-H26B       0.9700         C6-H6       0.9300       O1-S1       1.479 (2)         C7-C12       1.373 (3)       OI-S1       1.484 (2)         C7-C8       1.386 (3)       S1-C28       1.760 (5)         C8-H8       0.9300       C27-H27A       0.9600         C9-C10       1.359 (5)       C27-H27B       0.9600         C9-C10       1.356 (5)       C28-H28A       0.9600         C10-C11       1.365 (5)       C28-H28A       0.9600         C10-H10       0.9300       C28-H28A       0.9600         C11-C12       1.386 (4)       C28-H28A       0.9600         C11-H11       0.9300       S1'-C28'       1.759 (5)         C12-H12       0.9300       S1'-C28'       1.759 (5)         C12-H12       0.9300       C27'-H27E       0.9600         C13-C14	С2—Н	2	0.9300	)	C23—H23		0.9300
C3—H3       0.9300       C25—C26       1.520 (3)         C4—C5       1.360 (5)       C25—H25A       0.9700         C5—C6       1.390 (4)       C26—H26A       0.9700         C5—C6       1.390 (4)       C26—H26B       0.9700         C5—C6       1.390 (4)       C26—H26B       0.9700         C6—H6       0.9300       O1—S1       1.479 (2)         C7—C12       1.373 (3)       O1—S1'       1.484 (2)         C7—C8       1.386 (3)       S1—C28       1.766 (5)         C8—C9       1.383 (4)       S1—C27       1.766 (5)         C8—C9       1.359 (5)       C27—H27A       0.9600         C9—H9       0.9300       C28—H28A       0.9600         C10—C11       1.365 (5)       C28—H28A       0.9600         C10—H10       0.9300       C27—H27B       0.9600         C11—C12       1.386 (4)       C28—H28A       0.9600         C11—C12       1.386 (4)       C28—H28       0.9600         C12—H11       0.9300       S1—C28'       1.759 (5)         C13—C18       1.377 (3)       C27'—H27D       0.9600         C14—C15       1.380 (4)       C27'—H27E       0.9600         C14—C14<	C3-C	4	1.355	(5)	C24—H24		0.9300
C4 — C5       1.360 (5)       C25—H25A       0.9700         C4—H4       0.9300       C25—H25B       0.9700         C5—C6       1.390 (4)       C26—H26A       0.9700         C5—H5       0.9300       C1—H26A       0.9700         C6—H6       0.9300       C1—S1       1.479 (2)         C7—C12       1.373 (3)       O1—S1       1.479 (2)         C7—C8       1.386 (3)       S1—C28       1.760 (5)         C8—H8       0.9300       C27—H27A       0.9600         C9—C10       1.355 (5)       C27—H27B       0.9600         C9—H9       0.9300       C27—H27B       0.9600         C10—C11       1.365 (5)       C28—H28A       0.9600         C10—C11       1.366 (4)       C28—H28B       0.9600         C10—C11       0.9300       S1—C27'       1.759 (5)         C11—H11       0.9300       S1—C28'       1.759 (5)         C12—H12       0.9300       S1—C28'       1.759 (5)         C13—C18       1.377 (3)       C27—H27D       0.9600         C11—H11       0.9300       S1—C27'       1.762 (5)         C13—C18       1.377 (3)       C27—H27D       0.9600         C14—C15	С3—Н	3	0.9300	)	$C_{25}$ — $C_{26}$		1.520 (3)
C4-H4       0.9300       C25-H25B       0.9700         C5-C6       1.390 (4)       C26-H26A       0.9700         C5-H5       0.9300       C16-H26B       0.9700         C6-H6       0.9300       O1-S1       1.479 (2)         C7-C12       1.373 (3)       O1-S1       1.484 (2)         C7-C8       1.386 (3)       S1-C28       1.760 (5)         C8-C9       1.383 (4)       S1-C27       1.766 (5)         C9-C10       1.359 (5)       C27-H27A       0.9600         C9-H9       0.9300       C27-H27B       0.9600         C9-H9       0.9300       C28-H28A       0.9600         C10-C11       1.365 (5)       C28-H28A       0.9600         C10-H10       0.9300       C28-H28C       0.9600         C11-H11       0.9300       S1'-C28'       1.759 (5)         C12-H12       0.9300       C27'-H27E       0.9600         C13-C18	C4—C	5	1.360	(5)	C25—H25A		0.9700
C1 - L1       0.390 (4)       C26-H26A       0.9700         C5C6       1.390 (4)       C26-H26B       0.9700         C6H6       0.9300       O1S1       1.479 (2)         C7C12       1.373 (3)       O1S1       1.484 (2)         C7C8       1.386 (3)       S1C28       1.760 (5)         C8C9       1.383 (4)       S1C28       0.9600         C9C10       1.359 (5)       C27H27A       0.9600         C9C10       1.359 (5)       C27H27C       0.9600         C10C11       1.365 (5)       C28-H28A       0.9600         C10C11       1.365 (5)       C28-H28A       0.9600         C10C11       1.365 (5)       C28-H28A       0.9600         C11C12       1.386 (4)       C28-H28B       0.9600         C11C12       1.386 (4)       C28-H28B       0.9600         C11H11       0.9300       S1'C28'       1.759 (5)         C12H12       0.9300       S1'C28'       1.759 (5)         C13C14       1.384 (3)       C27'-H27E       0.9600         C13C14       1.384 (3)       C27'-H27F       0.9600         C14C15       1.380 (4)       C28'-H28E       0.9600 </td <td>C4—H</td> <td>4</td> <td>0.9300</td> <td>)</td> <td>C25—H25B</td> <td></td> <td>0.9700</td>	C4—H	4	0.9300	)	C25—H25B		0.9700
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C5-C	6	1 390	(4)	C26—H26A		0.9700
C6 - H6       0.9300       C1 - S1       1.479 (2)         C7-C12       1.373 (3)       O1-S1'       1.484 (2)         C7-C28       1.386 (3)       S1-C28       1.760 (5)         C8-H8       0.9300       C27-H27A       0.9600         C9-C10       1.359 (5)       C27-H27B       0.9600         C9-H9       0.9300       C27-H27C       0.9600         C9-H9       0.9300       C27-H27C       0.9600         C10-C11       1.365 (5)       C28-H28A       0.9600         C10-H10       0.9300       C28-H28B       0.9600         C11-H11       0.9300       S1'-C28'       1.759 (5)         C12-H12       0.9300       S1'-C28'       1.759 (5)         C12-H12       0.9300       S1'-C28'       1.759 (5)         C12-H12       0.9300       S1'-C27'       1.762 (5)         C13-C18       1.377 (3)       C27'-H27D       0.9600         C14-C15       1.380 (4)       C27'-H27E       0.9600         C14-C15       1.380 (4)       C27'-H27F       0.9600         C14-H14       0.9300       C28'-H28D       0.9600         C15-H15       0.9300       C28'-H28E       0.9600         C	С5—Н	5	0.9300	)	C26—H26B		0.9700
C7-C12       1.373 (3)       O1-S1       1.484 (2)         C7-C28       1.386 (3)       S1-C28       1.760 (5)         C8-C9       1.383 (4)       S1-C27       1.766 (5)         C8-H8       0.9300       C27-H27A       0.9600         C9-C10       1.359 (5)       C27-H27B       0.9600         C9-H9       0.9300       C27-H27C       0.9600         C10-C11       1.365 (5)       C28-H28A       0.9600         C10-C11       1.365 (5)       C28-H28B       0.9600         C11-C12       1.386 (4)       C28-H28B       0.9600         C11-H11       0.9300       S1'-C28'       1.759 (5)         C12-H12       0.9300       S1'-C27'       1.762 (5)         C13-C18       1.377 (3)       C27'-H27D       0.9600         C13-C18       1.377 (3)       C27'-H27D       0.9600         C14-C15       1.380 (4)       C27'-H27E       0.9600         C15-C16       1.362 (5)       C28'-H28D       0.9600         C15-C16       1.362 (5)       C28'-H28E       0.9600         C15-H15       0.9300       C28'-H28E       0.9600         C15-H15       0.9300       C28'-H28E       0.9600	С6—Н	5 6	0.9300	)	01 - S1		1 479 (2)
C7-C81.386 (3)S1-C281.760 (5)C8-C91.383 (4)S1-C281.766 (5)C8-C91.383 (4)S1-C271.766 (5)C8-H80.9300C27-H27A0.9600C9-C101.359 (5)C27-H27B0.9600C9-C111.365 (5)C28-H28A0.9600C10-C111.365 (5)C28-H28A0.9600C10-C121.386 (4)C28-H28C0.9600C11-H110.9300S1'-C28'1.759 (5)C12-H120.9300S1'-C27'1.762 (5)C13-C181.377 (3)C27'-H27D0.9600C14-C151.380 (4)C27'-H27E0.9600C14-C151.380 (4)C28'-H28D0.9600C15-C161.362 (5)C28'-H28E0.9600C15-C161.362 (5)C28'-H28E0.9600C15-C161.362 (5)C28'-H28E0.9600C15-C161.362 (5)C28'-H28E0.9600C15-C161.362 (5)C28'-H28E0.9600C15-C161.362 (5)C28'-H28E0.9600C15-C161.362 (5)C28'-H28E0.9600C16-C171.362 (5)C18-C17-H17120.0P2-Pd1-C1190.93 (2)C18-C17-H17120.0P1-Pd1-C11175.75 (2)C13-C18-C17119.7 (3)P2-Pd1-C12175.049 (19)C13-C18-H18120.1P1-Pd1-C1289.95 (2)C17-C18-H18120.1P1-Pd1-C1293.61 (2)C20-C19-C24119.3 (2)	C7—C	12	1 373	(3)	01 - 51'		1.179(2) 1 484(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C7—C	8	1.375	(3)	S1 - C28		1.760(5)
C8       H8       0.9300       C27—H27A       0.9600         C9       C1       1.359 (5)       C27—H27A       0.9600         C9       H9       0.9300       C27—H27C       0.9600         C10       C1       1.365 (5)       C28—H28A       0.9600         C10       C1       1.365 (5)       C28—H28A       0.9600         C10       H1       0.9300       C28—H28B       0.9600         C11       1.365 (4)       C28—H28C       0.9600         C11       0.9300       S1'—C28'       1.759 (5)         C12       1.386 (4)       C28—H28C       0.9600         C11       0.9300       S1'—C27'       1.762 (5)         C12       H1       0.9300       S1'—C27'       1.762 (5)         C13       C18       1.377 (3)       C27'—H27D       0.9600         C14       1.384 (3)       C27'—H27F       0.9600       C14—C15         C14       1.362 (5)       C28'—H28D       0.9600       C15—C16         C15       1.380 (4)       C27'—H27F       0.9600       C15—C16         C15       H28       0.9600       C28'—H28F       0.9600         C15       H28       0.9600 <td>C8-C</td> <td>9</td> <td>1 383</td> <td>(4)</td> <td>S1-C27</td> <td></td> <td>1.766 (5)</td>	C8-C	9	1 383	(4)	S1-C27		1.766 (5)
ConstructionConstructionConstructionConstructionC9-C101.359 (5)C27-H27B0.9600C9-H90.9300C27-H27C0.9600C10-C111.365 (5)C28-H28A0.9600C10-H100.9300C28-H28B0.9600C11-C121.386 (4)C28-H28C0.9600C11-H110.9300S1'-C28'1.759 (5)C12-H120.9300S1'-C27'1.762 (5)C13-C181.377 (3)C27'-H27D0.9600C14-C151.380 (4)C27'-H27F0.9600C14-C151.380 (4)C27'-H27F0.9600C14-H140.9300C28'-H28D0.9600C15-C161.362 (5)C28'-H28E0.9600C15-C161.362 (5)C28'-H28F0.9600C15-H150.9300C28'-H28F0.9600C16-C171.362 (5)C28'-H28F0.9600C16-C171.362 (5)C18-C17-H17120.0P2-Pd1-P185.603 (19)C16-C17-H17120.0P2-Pd1-C1190.93 (2)C18-C17-H17120.0P1-Pd1-C12175.75 (2)C13-C18-C17119.7 (3)P2-Pd1-C12175.049 (19)C13-C18-H18120.1P1-Pd1-C1289.95 (2)C17-C18-H18120.1C11-Pd1-C1293.61 (2)C20-C19-C24119.3 (2)	С8—Н	8	0.9300	)	C27—H27A		0.9600
C9-H9       0.9300       C27-H27C       0.9600         C10-C11       1.365 (5)       C28-H28A       0.9600         C10-H10       0.9300       C28-H28B       0.9600         C11-C12       1.386 (4)       C28-H28B       0.9600         C11-H11       0.9300       S1'-C28'       1.759 (5)         C12-H12       0.9300       S1'-C27'       1.762 (5)         C13-C18       1.377 (3)       C27'-H27D       0.9600         C14-C15       1.380 (4)       C27'-H27E       0.9600         C14-C15       1.380 (4)       C27'-H27F       0.9600         C14-H14       0.9300       C28'-H28D       0.9600         C15-C16       1.362 (5)       C28'-H28E       0.9600         C15-C16       1.362 (5)       C28'-H28E       0.9600         C15-H15       0.9300       C28'-H28F       0.9600         C16-C17       1.362 (5)       C28'-H28F       0.9600         C16-C17       1.362 (5)       C28'-H28F       0.9600         C16-C17       1.362 (5)       C18-C17-H17       120.0         P2-Pd1-C11       90.93 (2)       C18-C17-H17       120.0         P1-Pd1-C12       175.049 (19)       C13-C18-C17       119.7 (3) </td <td>C9-C</td> <td>10</td> <td>1 359</td> <td>, (5)</td> <td>C27—H27B</td> <td></td> <td>0.9600</td>	C9-C	10	1 359	, (5)	C27—H27B		0.9600
C10—C11       1.365 (5)       C28—H28A       0.9600         C10—C11       0.9300       C28—H28B       0.9600         C11—C12       1.386 (4)       C28—H28B       0.9600         C11—H11       0.9300       S1'—C28'       1.759 (5)         C12—H12       0.9300       S1'—C28'       1.762 (5)         C13—C18       1.377 (3)       C27'—H27D       0.9600         C14—C15       1.380 (4)       C27'—H27F       0.9600         C14—C15       1.380 (4)       C27'—H27F       0.9600         C14—C15       1.380 (4)       C27'—H27F       0.9600         C15—C16       1.362 (5)       C28'—H28D       0.9600         C15—C16       1.362 (5)       C28'—H28E       0.9600         C15—H15       0.9300       C28'—H28E       0.9600         C16—C17       1.362 (5)       C28'—H28E       0.9600         C16—C17       1.362 (5)       C28'—H28F       0.9600         C16—C17       1.362 (5)       C18—C17—H17       120.0         P2—Pd1—P1       85.603 (19)       C16—C17—H17       120.0         P1—Pd1—C11       175.75 (2)       C13—C18—C17       119.7 (3)         P2—Pd1—C12       175.049 (19)       C13—C18—H18	Су С С9—Н	9	0.9300	)	C27 H27C		0.9600
C10—H10       0.9300       C28—H28B       0.9600         C11—C12       1.386 (4)       C28—H28B       0.9600         C11—C12       1.386 (4)       C28—H28C       0.9600         C11—H11       0.9300       S1'—C28'       1.759 (5)         C12—H12       0.9300       S1'—C27'       1.762 (5)         C13—C18       1.377 (3)       C27'—H27D       0.9600         C14—C15       1.380 (4)       C27'—H27F       0.9600         C14—C15       1.380 (4)       C27'—H27F       0.9600         C14—C15       1.380 (4)       C28'—H28D       0.9600         C15—C16       1.362 (5)       C28'—H28D       0.9600         C15—C16       1.362 (5)       C28'—H28E       0.9600         C15—H15       0.9300       C28'—H28E       0.9600         C16—C17       1.362 (5)       C28'—H28E       0.9600         C16—C17       1.362 (5)       C18—C17—H17       120.0         P2—Pd1—P1       85.603 (19)       C16—C17—H17       120.0         P2—Pd1—C11       175.75 (2)       C13—C18—C17       119.7 (3)         P2—Pd1—C12       175.049 (19)       C13—C18—H18       120.1         P1—Pd1—C12       89.95 (2)       C17—C18—H18 <td>C10-0</td> <td>211</td> <td>1 365</td> <td>, (5)</td> <td>C28—H28A</td> <td></td> <td>0.9600</td>	C10-0	211	1 365	, (5)	C28—H28A		0.9600
C10C10C1.500C28H2B0.9600C11—C121.386 (4)C28—H28C0.9600C11—H110.9300S1'—C28'1.759 (5)C12—H120.9300S1'—C27'1.762 (5)C13—C181.377 (3)C27'—H27D0.9600C14—C151.384 (3)C27'—H27E0.9600C14—C151.380 (4)C27'—H27F0.9600C14—H140.9300C28'—H28D0.9600C15—C161.362 (5)C28'—H28E0.9600C15—H150.9300C28'—H28F0.9600C16—C171.362 (5)P2—Pd1—P185.603 (19)C16—C17—H17120.0P2—Pd1—C1190.93 (2)C18—C17—H17120.0P1—Pd1—C11175.75 (2)C13—C18—C17119.7 (3)P2—Pd1—C12175.049 (19)C13—C18—H18120.1P1—Pd1—C1289.95 (2)C17—C18—H18120.1C11—Pd1—C1293.61 (2)C20—C19—C24119.3 (2)	C10—F	H10	0.9300	)	C28—H28B		0.9600
C11C121.500 (f)C121.2000.5000C11—H110.9300S1'—C28'1.759 (5)C12—H120.9300S1'—C27'1.762 (5)C13—C181.377 (3)C27'—H27D0.9600C13—C141.384 (3)C27'—H27E0.9600C14—C151.380 (4)C27'—H27F0.9600C14—H140.9300C28'—H28D0.9600C15—C161.362 (5)C28'—H28E0.9600C15—C161.362 (5)C28'—H28F0.9600C16—C171.362 (5)C1.362 (5)P2—Pd1—P185.603 (19)C16—C17—H17120.0P2—Pd1—C1190.93 (2)C18—C17—H17120.0P1—Pd1—C11175.75 (2)C13—C18—C17119.7 (3)P2—Pd1—C12175.049 (19)C13—C18—H18120.1P1—Pd1—C1289.95 (2)C17—C18—H18120.1C11—Pd1—C1293.61 (2)C20—C19—C24119.3 (2)	$C_{11}$	712	1 386	, (4)	C28—H28C		0.9600
C11III $0.9300$ S11 $C23$ $1.159(5)$ C12—H12 $0.9300$ S11 $C27'$ $1.762(5)$ C13—C18 $1.377(3)$ $C27'$ —H27D $0.9600$ C13—C14 $1.384(3)$ $C27'$ —H27E $0.9600$ C14—C15 $1.380(4)$ $C27'$ —H27F $0.9600$ C14—H14 $0.9300$ $C28'$ —H28D $0.9600$ C15—C16 $1.362(5)$ $C28'$ —H28E $0.9600$ C15—C16 $1.362(5)$ $C28'$ —H28F $0.9600$ C16—C17 $1.362(5)$ $C16$ —C17—H17 $120.0$ P2—Pd1—C11 $90.93(2)$ $C18$ —C17—H17 $120.0$ P1—Pd1—C11 $175.75(2)$ $C13$ —C18—C17 $119.7(3)$ P2—Pd1—C12 $175.049(19)$ $C13$ —C18—H18 $120.1$ P1—Pd1—C12 $89.95(2)$ $C17$ —C18—H18 $120.1$ C13—C12 $93.61(2)$ $C20$ —C19—C24 $119.3(2)$	C11—F	411	0.9300	(-) )	S1'-C28'		1 759 (5)
C12C13C17C1711.02 (c)C13C181.377 (3)C27'-H27D0.9600C13C141.384 (3)C27'-H27E0.9600C14C151.380 (4)C27'-H27F0.9600C14C151.362 (5)C28'-H28D0.9600C15C161.362 (5)C28'-H28E0.9600C15C161.362 (5)C28'-H28F0.9600C161.362 (5)C28'-H28F0.9600C161.362 (5)C16C16P2Pd190.93 (2)C18C171.302 (2)C13C18P1Pd1C10P1.75 (2)P2Pd1C12P1.049 (19)C13C18C17119.7 (3)P2Pd1C12P1.049 (19)C13C18C18120.1P1Pd1C12P1.049 (19)C13C18L17L19.3 (2)	C12—F	412	0.9300	)	S1'-C27'		1.757 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C12	~18	1 377	(3)	С27'—Н27D		0.9600
C15       C14       C15       1.364 (5)       C27       H27E       0.9600         C14       C15       1.380 (4)       C27'-H27F       0.9600         C14       H14       0.9300       C28'-H28D       0.9600         C15       C16       1.362 (5)       C28'-H28E       0.9600         C15       H15       0.9300       C28'-H28E       0.9600         C16       1.362 (5)       C28'-H28F       0.9600         C16       1.362 (5)       C16       C10         P2       Pd1       P1       85.603 (19)       C16       C17       120.0         P2       Pd1       C11       90.93 (2)       C18       C17       120.0         P1       Pd1       C17       120.0       119.7 (3)       120.0         P1       Pd1       C12       C13       C18       120.1         P1       Pd1       C12       175.049 (19)       C13       C18       120.1         P1       Pd1       C12       89.95 (2)       C17       C18       119.3 (2)	C13 - C	~14	1.377	(3)	C27' H27E		0.9600
C14—C15       1.500 (4)       C27—H217       0.9000         C14—H14       0.9300       C28'—H28D       0.9600         C15—C16       1.362 (5)       C28'—H28E       0.9600         C15—H15       0.9300       C28'—H28F       0.9600         C16—C17       1.362 (5)       C28'—H28F       0.9600         P2—Pd1—P1       85.603 (19)       C16—C17—H17       120.0         P2—Pd1—C11       90.93 (2)       C18—C17—H17       120.0         P1—Pd1—C11       175.75 (2)       C13—C18—C17       119.7 (3)         P2—Pd1—C12       175.049 (19)       C13—C18—H18       120.1         P1—Pd1—C12       89.95 (2)       C17—C18—H18       120.1         C11—Pd1—C12       93.61 (2)       C20—C19—C24       119.3 (2)	C13 - C	~1 <b>5</b>	1.384	(3)	C27' - H27E		0.9600
C14—1114       0.7500       C23—1126D       0.7000         C15—C16       1.362 (5)       C28'—H28E       0.9600         C15—H15       0.9300       C28'—H28F       0.9600         C16—C17       1.362 (5)       C16—C17—H17       120.0         P2—Pd1—C11       90.93 (2)       C18—C17—H17       120.0         P1—Pd1—C11       175.75 (2)       C13—C18—C17       119.7 (3)         P2—Pd1—C12       175.049 (19)       C13—C18—H18       120.1         P1—Pd1—C12       89.95 (2)       C17—C18—H18       120.1         C11—Pd1—C12       93.61 (2)       C20—C19—C24       119.3 (2)	C14	H14	0.9300	)	C28'_H28D		0.9600
C15—C10       1.302 (5)       C28—1128L       0.9000         C15—H15       0.9300       C28'—H28F       0.9600         C16—C17       1.362 (5)       1.362 (5)       120.0         P2—Pd1—P1       85.603 (19)       C16—C17—H17       120.0         P2—Pd1—C11       90.93 (2)       C18—C17—H17       120.0         P1—Pd1—C11       175.75 (2)       C13—C18—C17       119.7 (3)         P2—Pd1—C12       175.049 (19)       C13—C18—H18       120.1         P1—Pd1—C12       89.95 (2)       C17—C18—H18       120.1         C11—Pd1—C12       93.61 (2)       C20—C19—C24       119.3 (2)	$C_{14}$	~16	1 362	, (5)	C28 H28E		0.9600
C15-H15       0.3500       C23-H231       0.3000         C16-C17       1.362 (5)       120.0         P2-Pd1-Cl1       90.93 (2)       C16-C17-H17       120.0         P1-Pd1-Cl1       175.75 (2)       C13-C18-C17       119.7 (3)         P2-Pd1-Cl2       175.049 (19)       C13-C18-H18       120.1         P1-Pd1-Cl2       89.95 (2)       C17-C18-H18       120.1         C11-Pd1-Cl2       93.61 (2)       C20-C19-C24       119.3 (2)	C15		0.9300	)	C28 —H28E		0.9000
P2—Pd1—P1       85.603 (19)       C16—C17—H17       120.0         P2—Pd1—Cl1       90.93 (2)       C18—C17—H17       120.0         P1—Pd1—Cl1       175.75 (2)       C13—C18—C17       119.7 (3)         P2—Pd1—Cl2       175.049 (19)       C13—C18—H18       120.1         P1—Pd1—Cl2       89.95 (2)       C17—C18—H18       120.1         Cl1—Pd1—Cl2       93.61 (2)       C20—C19—C24       119.3 (2)	C15—1	~17	1 362	, (5)	C28—11281		0.9000
P2Pd1P185.603 (19)C16C17H17120.0P2Pd1Cl190.93 (2)C18C17H17120.0P1Pd1Cl1175.75 (2)C13C18C17119.7 (3)P2Pd1Cl2175.049 (19)C13C18H18120.1P1Pd1Cl289.95 (2)C17C18H18120.1Cl1Pd1Cl293.61 (2)C20C19C24119.3 (2)	C10-C		1.502	(3)			
P2Pd1Cl1       90.93 (2)       C18C17H17       120.0         P1Pd1Cl1       175.75 (2)       C13C18C17       119.7 (3)         P2Pd1Cl2       175.049 (19)       C13C18H18       120.1         P1Pd1Cl2       89.95 (2)       C17C18H18       120.1         Cl1Pd1Cl2       93.61 (2)       C20C19C24       119.3 (2)	P2—Pc	11—P1	85.603	8 (19)	С16—С17—Н17		120.0
P1—Pd1—Cl1175.75 (2)C13—C18—Cl7119.7 (3)P2—Pd1—Cl2175.049 (19)C13—C18—H18120.1P1—Pd1—Cl289.95 (2)C17—C18—H18120.1Cl1—Pd1—Cl293.61 (2)C20—C19—C24119.3 (2)	P2—Pc	l1—Cl1	90.93	(2)	С18—С17—Н17		120.0
P2—Pd1—Cl2175.049 (19)C13—C18—H18120.1P1—Pd1—Cl289.95 (2)C17—C18—H18120.1Cl1—Pd1—Cl293.61 (2)C20—C19—C24119.3 (2)	P1—Pc	11—C11	175.75	5 (2)	C13—C18—C17		119.7 (3)
P1—Pd1—Cl2         89.95 (2)         C17—C18—H18         120.1           Cl1—Pd1—Cl2         93.61 (2)         C20—C19—C24         119.3 (2)	P2—Pc	11—Cl2	175.04	19 (19)	C13—C18—H18		120.1
Cl1—Pd1—Cl2 93.61 (2) C20—C19—C24 119.3 (2)	P1—Pc	11—Cl2	89.95	(2)	C17—C18—H18		120.1
	Cl1—P	d1—Cl2	93.61	(2)	C20—C19—C24		119.3 (2)

C1—P1—C7	106.37 (10)	C20—C19—P2	120.4 (2)
C1—P1—C25	106.61 (10)	C24—C19—P2	120.34 (19)
C7—P1—C25	104.57 (10)	C19—C20—C21	119.3 (3)
C1—P1—Pd1	114.01 (7)	С19—С20—Н20	120.4
C7—P1—Pd1	115.28 (8)	С21—С20—Н20	120.4
C25—P1—Pd1	109.25 (7)	C22—C21—C20	121.4 (3)
C19—P2—C13	106.06 (10)	C22—C21—H21	119.3
C19—P2—C26	106.39 (10)	C20—C21—H21	119.3
C13—P2—C26	105.79 (10)	C21—C22—C23	119.9 (3)
C19—P2—Pd1	118.01 (7)	C21—C22—H22	120.1
C13—P2—Pd1	112.48 (7)	C23—C22—H22	120.1
C26—P2—Pd1	107.32 (7)	C22—C23—C24	120.4 (3)
C2-C1-C6	119.4 (2)	C22—C23—H23	119.8
C2-C1-P1	119.55 (17)	C24—C23—H23	119.8
C6-C1-P1	121.01 (18)	C19 - C24 - C23	119.7 (3)
C1 - C2 - C3	1201(3)	C19 - C24 - H24	120.1
C1 - C2 - H2	120.1 (5)	$C_{23}$ $C_{24}$ $H_{24}$	120.1
$C_3 - C_2 - H_2$	120.0	$C_{25} = C_{25} = P_1$	120.1 111.70(14)
$C_{4}$ $C_{3}$ $C_{2}$ $C_{2}$	120.5 (3)	$C_{26} = C_{25} = H_{25A}$	109.3
$C_{4} = C_{3} = H_{3}$	110.7	P1 = C25 = H25A	109.3
C2-C3-H3	119.7	$C_{26} = C_{25} = H_{25}R$	109.3
$C_2 = C_3 = C_5$	120.0 (3)	P1H25B	109.3
$C_3 = C_4 = C_3$	120.0 (3)	$H_{25}^{-1123D}$	107.9
$C_5 = C_4 = H_4$	120.0	1125A - C25 - 1125B	107.9 108.28 (14)
$C_{4}$ $C_{5}$ $C_{6}$	120.0 (3)	$C_{25} = C_{26} = 12$	110.0
$C_4 = C_5 = H_5$	110.5	$P_2 = C_26 = H_26A$	110.0
C4 C5 H5	119.5	12 - 0.20 - 1120 A	110.0
$C_{0}$	119.5	$P_2 = C_2 C_2 C_2 C_2 C_2 C_2 C_2 C_2 C_2 C_2$	110.0
C1 = C6 = H6	119.2 (3)	$H_2 = C_2 O = H_2 O B$	108.4
$C_1 = C_0 = H_0$	120.4	1120A - C20 - 1120B	100.4
$C_{12} = C_{7} = C_{8}$	120.4	S1 = 01 = S1	43.2(4)
$C_{12} = C_7 = C_8$	110.0(2) 121.18(17)	01 - 51 - C28	104.0(2)
$C_{12} - C_{7} - F_{1}$	121.10(17) 110.80(10)	01 - 31 - 027	100.0(2)
$C_{0}$ $C_{0}$ $C_{1}$	119.89 (19)	$C_{20} = S_{1} = C_{27}$	93.9(3)
$C_{2} = C_{3} = C_{1}$	120.5 (3)	SI_C27_H27A	109.5
C7_C8_H8	119.8	SI = C27 = H27B	109.5
$C_{1} = C_{8} = H_{8}$	119.8	HZ/A = CZ/=HZ/B	109.5
C10 - C9 - C8	120.1 (3)	SI = C27 = H27C	109.5
C10 - C9 - H9	120.0	$H_2/A = C_2/=H_2/C$	109.5
$C_8 = C_9 = H_9$	120.0	$H_2/B = C_2/=H_2/C$	109.5
	120.2 (3)	SI-C28-H28A	109.5
C9—C10—H10	119.9	SI-C28-H28B	109.5
C11—C10—H10	119.9	H28A—C28—H28B	109.5
C10-C11-C12	120.3 (3)	SI-C28-H28C	109.5
CIU-CII-HII	119.9	$H_2 \otimes A \longrightarrow C_2 \otimes H_2 \otimes C_2$	109.5
CI2—CII—HII	119.9	$H_2 \times B \longrightarrow C_2 \times H_2 \times C_2$	109.5
C/C12C11	120.2 (3)	01 - 81' - C28'	102.2 (18)
C/—C12—H12	119.9	01—81′—C27′	95 (2)
C11—C12—H12	119.9	C28′—S1′—C27′	77 (3)
C18—C13—C14	119.5 (2)	S1'—C27'—H27D	109.5

C18—C13—P2	120.55 (17)	S1'—C27'—H27E	109.5
C14—C13—P2	119.91 (18)	H27D—C27′—H27E	109.5
C15—C14—C13	120.0 (3)	S1'—C27'—H27F	109.5
C15—C14—H14	120.0	H27D—C27′—H27F	109.5
C13—C14—H14	120.0	H27E—C27'—H27F	109.5
C16—C15—C14	119.8 (3)	S1'—C28'—H28D	109.5
C16—C15—H15	120.1	S1'—C28'—H28E	109.5
C14—C15—H15	120.1	H28D—C28′—H28E	109.5
C17—C16—C15	120.8 (3)	S1'—C28'—H28F	109.5
C17—C16—H16	119.6	H28D—C28′—H28F	109.5
C15—C16—H16	119.6	H28E—C28'—H28F	109.5
C16—C17—C18	120.0 (3)		
P2—Pd1—P1—C1	-123.79 (8)	C8—C7—C12—C11	-0.5 (4)
Cl1—Pd1—P1—C1	-159.1 (3)	P1-C7-C12-C11	-177.2(2)
Cl2—Pd1—P1—C1	54.04 (8)	C10—C11—C12—C7	-1.6(5)
P2—Pd1—P1—C7	112.73 (8)	C19—P2—C13—C18	122.64 (19)
Cl1—Pd1—P1—C7	77.5 (3)	C26—P2—C13—C18	-124.61 (19)
Cl2—Pd1—P1—C7	-69.44 (8)	Pd1—P2—C13—C18	-7.8(2)
P2-Pd1-P1-C25	-4.64 (8)	C19 - P2 - C13 - C14	-57.4(2)
Cl1— $Pd1$ — $P1$ — $C25$	-39.9(3)	$C_{26} = P_{2} = C_{13} = C_{14}$	55.4 (2)
C12—Pd1—P1—C25	173 19 (8)	Pd1 - P2 - C13 - C14	172.25(17)
$P1_Pd1_P2_C19$	145 15 (9)	$C_{18}$ $C_{13}$ $C_{14}$ $C_{15}$	-0.4(4)
C11 - Pd1 - P2 - C19	-3730(9)	$P_{-13} - C_{14} - C_{15}$	179.6(2)
C12 - Pd1 - P2 - C19	1191(2)	$C_{13}$ $C_{14}$ $C_{15}$ $C_{16}$	179.0(2)
$P1_Pd1_P2_C13$	-90.85(7)	$C_{14}$ $C_{15}$ $C_{16}$ $C_{17}$	1.6(5)
$C_{11}$ $P_{d1}$ $P_{2}$ $C_{13}$	86 70 (7)	$C_{15}$ $C_{16}$ $C_{17}$ $C_{18}$	-26(5)
C12 Pd1 P2 C13	-1169(2)	$C_{14}$ $C_{13}$ $C_{18}$ $C_{17}$	-0.6(4)
$P_1 P_4 P_2 C_{26}$	110.9(2)	$P_2 = C_{13} = C_{16} = C_{17}$	179 4 (2)
11 - 101 - 12 - 020	-157.35(8)	12 - 013 - 013 - 017	179.4(2)
$C_{11} = 101 = 12 = C_{20}$	-0.0(2)	$C_{10} = C_{17} = C_{18} = C_{15}$	2.2(4)
$C_{12}$ $-1$ $C_{1}$ $C_{20}$	-153.83(10)	$C_{13} = 12 = C_{19} = C_{20}$	133.3(2)
$C_{1} = C_{1} = C_{2}$	-126(2)	$P_{41}$ $P_{2}$ $P_{10}$ $P_{20}$	+1.2(2)
$C_{23}$ $-F_1$ $-C_1$ $-C_2$	-42.0(2)	Pd1 - P2 - C19 - C20	-79.3(2)
PdI = PI = CI = C2	77.99 (19)	C13 - P2 - C19 - C24	-28.0(2)
C = PI = CI = Cb	29.3(2)	$C_{26}$ P2 $C_{19}$ $C_{24}$	-140.3(2)
$C_{25}$ $P_{1}$ $C_{1}$ $C_{6}$	140.52 (19)	Pa1 - P2 - C19 - C24	99.2 (2)
Pd1—P1—C1—C6	-98.85 (19)	$C_{24} = C_{19} = C_{20} = C_{21}$	1.8 (4)
C6-C1-C2-C3	0.8 (4)	P2-C19-C20-C21	-179.7 (2)
PI-CI-C2-C3	-176.1(2)	C19—C20—C21—C22	-0.9 (5)
C1 - C2 - C3 - C4	-0.1(4)	C20—C21—C22—C23	-0.1 (6)
C2—C3—C4—C5	-0.8 (5)	C21—C22—C23—C24	0.3 (6)
C3—C4—C5—C6	1.2 (5)	C20—C19—C24—C23	-1.7 (4)
C2-C1-C6-C5	-0.4(4)	P2—C19—C24—C23	179.8 (2)
P1—C1—C6—C5	176.4 (2)	C22—C23—C24—C19	0.6 (5)
C4—C5—C6—C1	-0.5 (4)	C1—P1—C25—C26	101.86 (16)
C1—P1—C7—C12	-126.3 (2)	C7—P1—C25—C26	-145.72 (15)
C25—P1—C7—C12	121.1 (2)	Pd1—P1—C25—C26	-21.79 (17)
Pd1—P1—C7—C12	1.1 (2)	P1—C25—C26—P2	42.01 (18)
C1—P1—C7—C8	56.9 (2)	C19—P2—C26—C25	-172.09 (14)

# supplementary materials

C25—P1—C7—C8	-55.7 (2)	C13—P2—C26—C25	75.39 (16)
Pd1—P1—C7—C8	-175.66 (18)	Pd1—P2—C26—C25	-44.90 (15)
С12—С7—С8—С9	1.4 (4)	S1'-O1-S1-C28	-31.7 (7)
P1—C7—C8—C9	178.3 (2)	S1'-O1-S1-C27	69.2 (7)
C7—C8—C9—C10	-0.4 (5)	S1-01-S1'-C28'	40.1 (19)
C8—C9—C10—C11	-1.7 (5)	S1—O1—S1′—C27′	-37.4 (18)
C9-C10-C11-C12	2.6 (5)		

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	H···A	D····A	D—H···A
C2—H2…O1	0.93	2.49	3.348 (4)	153
C20—H20…O1	0.93	2.59	3.495 (4)	165
C26—H26A…O1	0.97	2.44	3.410 (3)	174