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trans-Bis(μ-benzenethiolato-κ²*S*:*S*)-bis[chlorido(triphenylphosphane-κ*P*)-palladium(II)] chloroform disolvate

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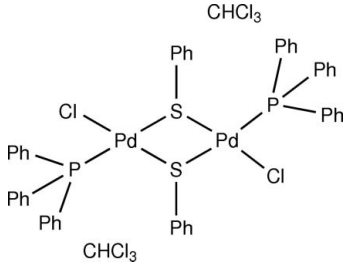
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; disorder in solvent or counterion; R factor = 0.039; wR factor = 0.088; data-to-parameter ratio = 15.3.

The title compound, $[Pd_2Cl_2(C_6H_5S)_2(C_{18}H_{15}P)_2]\cdot 2CHCl_3$, contains a centrosymmetric dinuclear palladium complex with the Pd^{II} cation in a slightly distorted square-planar coordination environment. The Pd^{II} cations are bridged by the S atoms of two benzenethiolate ligands with different Pd—S distances [2.2970 (11) and 2.3676 (11) Å]. The coordination of the metal atom is completed by a chloride anion [2.3383 (11) Å] and a triphenylphosphane ligand [2.2787 (11) Å]. Weak C—H···Cl interactions are present between complex molecules and the $CHCl_3$ solvent molecule. The latter is disordered over two positions in a 0.792 (8):0.208 (8) ratio. The crystal under investigation was found to be twinned by nonmerohedry, with a fraction of 73.4 (1)% for the major twin component.

Related literature

For related complexes in catalysis reactions, see: Yin & Liebscher (2007); Frisch & Beller (2005); Knochel & Singer (1993); Surry & Buchwald (2008). For bond lengths in a related complex, see: Estudiante-Negrete *et al.* (2007).



Experimental

Crystal data

$[Pd_2Cl_2(C_6H_5S)_2(C_{18}H_{15}P)_2]\cdot 2CHCl_3$
M_r = 1265.29
Monoclinic, $P2_1/n$
a = 10.8343 (11) Å
b = 14.2291 (15) Å
c = 17.3994 (18) Å
β = 102.095 (2)°
V = 2622.8 (5) Å³
Z = 2
Mo $K\alpha$ radiation
μ = 1.27 mm⁻¹
T = 298 K
0.36 × 0.19 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*TWINABS*; Bruker, 2007)
T_{min} = 0.707, T_{max} = 0.878
4876 measured reflections
4876 independent reflections
4577 reflections with $I > 2\sigma(I)$

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.088
S = 1.08
4876 reflections
318 parameters
96 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å⁻³
$\Delta\rho_{min}$ = −0.31 e Å⁻³

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

D—H···A	D—H	H···A	D···A	D—H···A
C25—H25···Cl1^{i}	0.98	2.79	3.744 (6)	164
C15—H15···Cl1^{ii}	0.93	2.93	3.650 (5)	135

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXL2013* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013*; molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL2013* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2753).

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supplementary materials

Acta Cryst. (2013). E**69**, m472 [doi:10.1107/S1600536813019806]

trans-Bis(*μ*-benzenethiolato-$\kappa^2 S$:*S*)bis[chlorido(triphenylphosphane-*κP*)palladium(II)] chloroform disolvate

Alcives Avila-Sorrosa, Alicia Reyes-Arellano, Juan Manuel Germán-Acacio, Reyna Reyes-Martínez and David Morales-Morales

Comment

Palladium is a transition metal well known for synthetic chemists. Thus, palladium complexes have been extensively studied and have had important applications as catalysts in a plethora of organic transformations, biological applications, material science *etc*. As catalysts, palladium complexes have shown high efficiency in different protocols of cross-coupling reactions for the construction of C—C bonds, *e.g.* through Heck reaction (Yin & Liebscher, 2007), Suzuki–Miyaura coupling (Frisch & Beller, 2005), Negishi reaction (Knochel & Singer, 1993), as well as for the formation of C-heteroatom highlighted *via* Buchwal–Hartwig reaction (Surry & Buchwald, 2008). In this context we report here the structure of the title compound, *trans*-$[PdCl(C_6H_5S)(C_{18}H_{15}P)]_2.2CHCl_3$, (I).

The structure of (I) contains a centrosymmetric dimeric Pd^{II} complex with the Pd^{II} atom within a slightly distorted square-planar coordination environment (Fig. 1). The two Pd^{II} atoms are bridged by two $–SC_6H_5$ ligands, and the coordination environment is completed by one Cl^- and one PPh_3 ligand. The asymmetric unit is composed of half of the complex and one disordered $CHCl_3$ solvent molecule; the full molecule is completed by application of inversion symmetry.

The two bridging $–SC_6H_5$ ligands exhibit different Pd1—S1 bond lengths, 2.2970 (11) and 2.3676 (11) Å; these distances are comparable to those found in the structure of the related compound $[Pd(PPh_3)(SC_6F_5)(\mu\text{-}SC_6F_5)]_2$ (Estudiante-Negrete *et al.*, 2007). The Pd1—P1 and Pd1—Cl1 bonds lengths are 2.2787 (11) and 2.3383 (11) Å, respectively. The Cl^- and the PPh_3 ligands are arranged in a mutually *trans* conformation.

The complex molecules are packed in rows parallel to [010]. The structure is stabilized by weak C—H···Cl hydrogen-bonding interactions between complex molecules and interstitial solvent molecules (Fig. 2).

Experimental

To a suspension of $PdCl_2$ (0.078 g, 0.442 mmol) and Na_2CO_3 (0.050 g, 0.047 mmol) in 15 ml of toluene a solution of 1-ethenyl-[(phenylsulfanyl)methyl]-benzene (isomeric mix 60:40), 1-ethenyl-3-[(phenylsulfanyl)methyl]-benzene and 1-ethenyl-4-[(phenylsulfanyl)methyl]-benzene) (0.100 g, 0.442 mmol) in 5 ml of toluene was added. The resulting mixture was set to reflux for 4 h. After this time the reaction mixture was allowed to cool down to room temperature and filtered. The solid residue was further washed twice with $CHCl_3$ (5 ml) attaining a yellow solid. This solid was further treated with PPh_3 (0.232 g, 0.884 mmol) in 15 ml of $CHCl_3$. The reaction mixture was stirred until all solid was dissolved and the resulting solution was filtered through a short plug of Celite. The filtrate was left to evaporate at room temperature yielding yellow crystals of (I) suitable for X-ray diffraction analysis.

Refinement

H atoms were included in calculated positions (C—H = 0.93 Å for aromatic H) and refined using a riding model with U_{iso}(H) = 1.2 U_{eq} of the carrier atoms. In the refinement five reflections, (1 16 4), (-11 4 5), (-2 15 8), (8 11 5) and (-9 12 5), were considered as disagreeable and were omitted. The $CHCl_3$ solvent is disordered over two sets of sites in a 0.792 (8):0.208 (8) ratio. Twinning by non-merohedy was detected in the cell determination and two orientation matrices were determined. The data were then processed and corrected for absorption effects with the *TWINABS* program (Bruker, 2007). The refinement of the *BASF* parameter was 26.6 (1)%, indicating a fraction of 73.4 (1)% for the major twin component.

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXL2013* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL2013* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

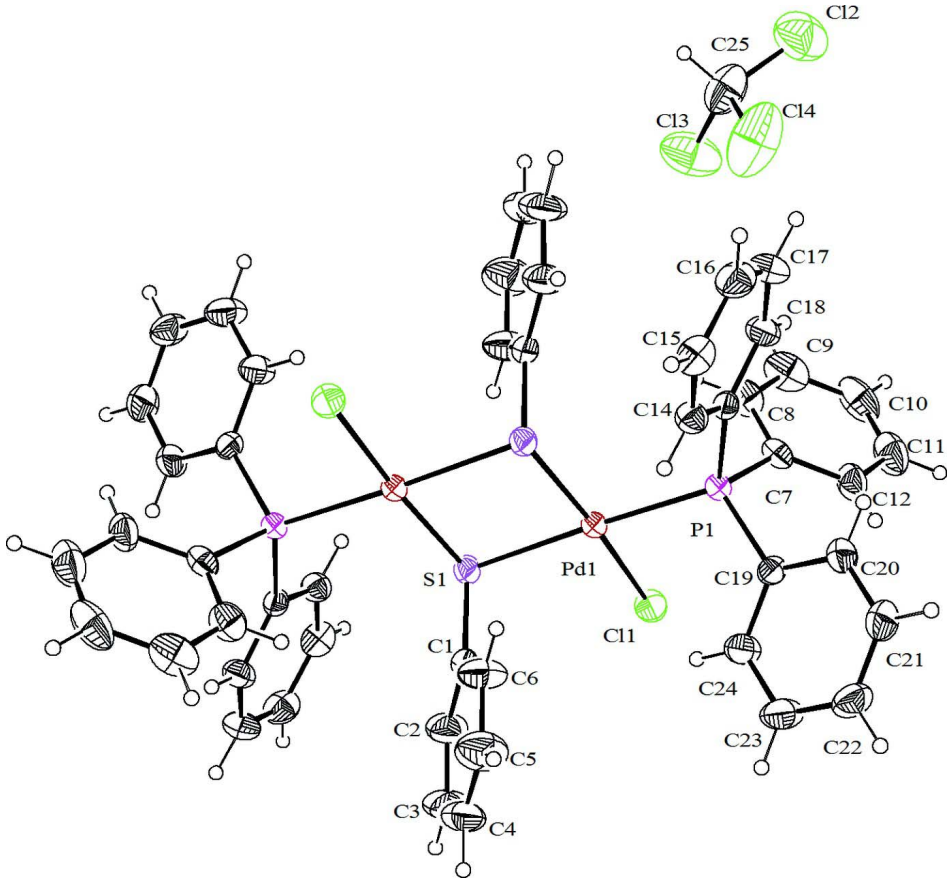

Figure 1

The molecular structure of the title compound, showing the displacement parameters of atoms at the 30% probability level. Only the major component of the disordered solvent molecule is displayed.

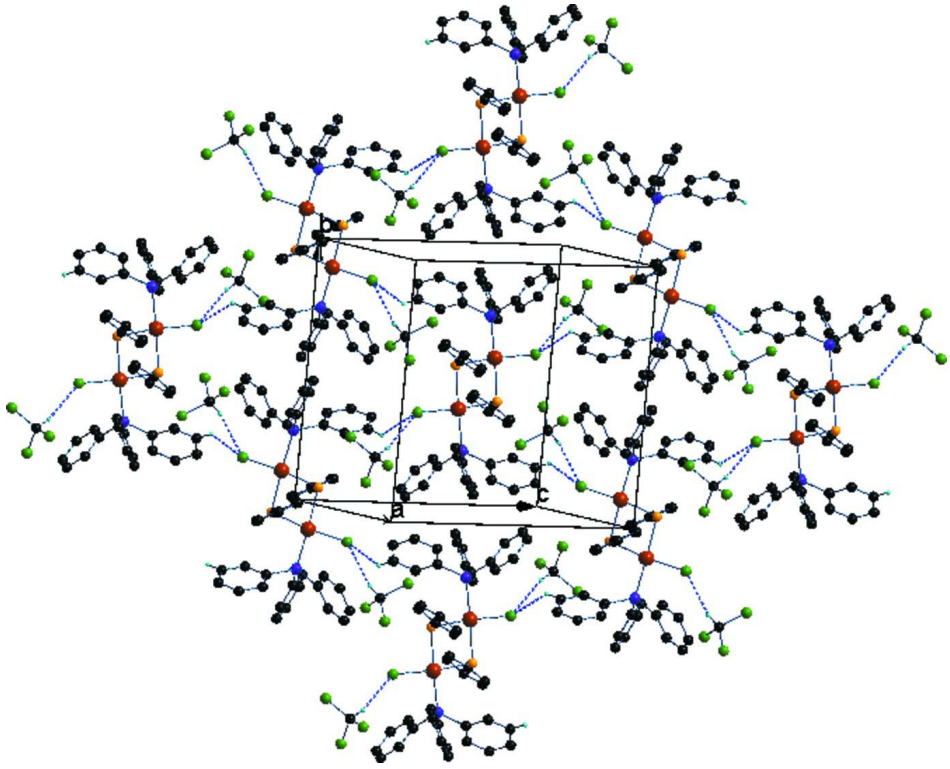

Figure 2

Packing of the molecular entities in the structure of (I). C—H···Cl interactions are shown by dashed lines.

trans-Bis(_μ_-benzenethiolato-_κ_^{2}_S_:_S_)bis[chlorido(triphenylphosphane-_κP_)palladium(II)] chloroform disolvate

Crystal data

$[Pd_2Cl_2(C_6H_5S)_2(C_{18}H_{15}P)_2]\cdot 2CHCl_3$
M_r = 1265.29
Monoclinic, $P2_1/n$
a = 10.8343 (11) Å
b = 14.2291 (15) Å
c = 17.3994 (18) Å
β = 102.095 (2)°
V = 2622.8 (5) Å^3
Z = 2
$F(000)$ = 1264
D_x = 1.602 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9960 reflections
θ = 2.4–25.3°
μ = 1.27 mm^{-1}
T = 298 K
Prism, yellow
0.36 × 0.19 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Detector resolution: 0.83 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*TWINABS*; Bruker, 2007)
T_{min} = 0.707, T_{max} = 0.878
4876 measured reflections
4876 independent reflections
4577 reflections with $I > 2\sigma(I)$
θ_{max} = 25.4°, θ_{min} = 1.9°
h = −13→12
k = 0→17
l = 0→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.088$
$S = 1.08$
4876 reflections
318 parameters
96 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0394P)^2 + 2.3327P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

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. Refined as a 2-component twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Pd1	0.42887 (3)	0.39507 (2)	0.46354 (2)	0.03549 (10)	
S1	0.38706 (10)	0.55845 (7)	0.45393 (6)	0.0405 (2)	
P1	0.46454 (10)	0.23806 (7)	0.48206 (6)	0.0366 (2)	
Cl1	0.24145 (11)	0.36353 (8)	0.37296 (7)	0.0532 (3)	
C1	0.2753 (4)	0.5666 (3)	0.5147 (3)	0.0471 (11)	
C2	0.1625 (5)	0.6099 (4)	0.4860 (4)	0.0754 (17)	
H2	0.1468	0.6365	0.4361	0.090*	
C3	0.0705 (6)	0.6143 (5)	0.5317 (6)	0.108 (3)	
H3	−0.0064	0.6434	0.5117	0.129*	
C4	0.0927 (7)	0.5769 (5)	0.6043 (6)	0.100 (3)	
H4	0.0312	0.5804	0.6344	0.120*	
C5	0.2049 (8)	0.5339 (5)	0.6339 (5)	0.101 (2)	
H5	0.2205	0.5086	0.6843	0.121*	
C6	0.2949 (5)	0.5280 (5)	0.5889 (4)	0.0769 (17)	
H6	0.3706	0.4974	0.6090	0.092*	
C7	0.4562 (4)	0.1762 (3)	0.3897 (3)	0.0456 (10)	
C8	0.5280 (5)	0.2094 (4)	0.3396 (3)	0.0633 (14)	
H8	0.5778	0.2625	0.3532	0.076*	
C9	0.5273 (7)	0.1650 (5)	0.2693 (3)	0.0813 (18)	
H9	0.5761	0.1882	0.2355	0.098*	
C10	0.4542 (8)	0.0859 (5)	0.2490 (4)	0.087 (2)	
H10	0.4540	0.0553	0.2018	0.104*	
C11	0.3825 (7)	0.0528 (4)	0.2986 (4)	0.0807 (19)	
H11	0.3327	−0.0003	0.2847	0.097*	
C12	0.3829 (5)	0.0970 (3)	0.3692 (3)	0.0595 (13)	
H12	0.3340	0.0737	0.4028	0.071*	
C13	0.6143 (4)	0.2023 (3)	0.5438 (3)	0.0389 (9)	
C14	0.6401 (4)	0.2303 (3)	0.6217 (3)	0.0473 (10)	
H14	0.5818	0.2671	0.6404	0.057*	
C15	0.7505 (5)	0.2047 (4)	0.6720 (3)	0.0587 (13)	

H15	0.7665	0.2239	0.7243	0.070*	
C16	0.8373 (5)	0.1505 (4)	0.6446 (4)	0.0659 (15)	
H16	0.9120	0.1329	0.6784	0.079*	
C17	0.8141 (5)	0.1224 (4)	0.5678 (4)	0.0681 (15)	
H17	0.8727	0.0853	0.5497	0.082*	
C18	0.7030 (4)	0.1492 (3)	0.5166 (3)	0.0519 (12)	
H18	0.6885	0.1313	0.4640	0.062*	
C19	0.3518 (4)	0.1852 (3)	0.5339 (3)	0.0406 (9)	
C20	0.3754 (5)	0.0980 (3)	0.5692 (3)	0.0585 (13)	
H20	0.4467	0.0643	0.5637	0.070*	
C21	0.2941 (6)	0.0605 (4)	0.6125 (3)	0.0665 (14)	
H21	0.3116	0.0023	0.6365	0.080*	
C22	0.1881 (5)	0.1084 (4)	0.6203 (3)	0.0677 (15)	
H22	0.1331	0.0825	0.6490	0.081*	
C23	0.1633 (5)	0.1950 (4)	0.5853 (4)	0.0721 (16)	
H23	0.0913	0.2279	0.5905	0.087*	
C24	0.2451 (5)	0.2335 (3)	0.5425 (3)	0.0564 (12)	
H24	0.2280	0.2923	0.5194	0.068*	
C25	1.0053 (6)	0.1714 (4)	0.3114 (3)	0.0997 (16)	
H25	1.0794	0.2112	0.3300	0.120*	
Cl2	1.0512 (6)	0.0769 (4)	0.2630 (3)	0.1391 (18)	0.792 (8)
Cl3	0.8933 (4)	0.2375 (3)	0.24836 (19)	0.1357 (15)	0.792 (8)
Cl4	0.9460 (7)	0.1371 (4)	0.3917 (2)	0.170 (2)	0.792 (8)
Cl2A	1.0404 (19)	0.0854 (12)	0.2466 (7)	0.105 (4)	0.208 (8)
Cl3A	0.8462 (10)	0.1982 (14)	0.2823 (10)	0.170 (6)	0.208 (8)
Cl4A	1.0302 (13)	0.1208 (9)	0.4047 (4)	0.101 (3)	0.208 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.03338 (16)	0.03191 (15)	0.04120 (16)	0.00213 (13)	0.00789 (13)	0.00007 (15)
S1	0.0391 (5)	0.0340 (5)	0.0468 (6)	0.0021 (4)	0.0055 (5)	0.0027 (5)
P1	0.0345 (5)	0.0326 (5)	0.0431 (6)	0.0017 (4)	0.0086 (4)	−0.0023 (5)
Cl1	0.0462 (6)	0.0536 (6)	0.0543 (7)	0.0018 (5)	−0.0021 (5)	−0.0041 (5)
C1	0.038 (2)	0.034 (2)	0.070 (3)	−0.0019 (18)	0.014 (2)	0.000 (2)
C2	0.048 (3)	0.076 (4)	0.105 (5)	0.018 (3)	0.023 (3)	0.022 (4)
C3	0.054 (4)	0.093 (5)	0.186 (9)	0.031 (4)	0.049 (5)	0.033 (6)
C4	0.079 (5)	0.080 (4)	0.164 (8)	0.014 (4)	0.077 (5)	0.011 (5)
C5	0.098 (5)	0.123 (6)	0.096 (5)	0.011 (5)	0.053 (4)	0.014 (5)
C6	0.056 (3)	0.106 (5)	0.077 (4)	0.017 (3)	0.032 (3)	0.019 (4)
C7	0.048 (2)	0.043 (2)	0.045 (2)	0.014 (2)	0.006 (2)	−0.003 (2)
C8	0.076 (4)	0.061 (3)	0.054 (3)	0.007 (3)	0.017 (3)	0.001 (3)
C9	0.097 (5)	0.097 (5)	0.054 (3)	0.025 (4)	0.025 (3)	0.012 (3)
C10	0.118 (6)	0.081 (5)	0.056 (3)	0.033 (4)	0.004 (4)	−0.022 (3)
C11	0.090 (5)	0.061 (4)	0.081 (4)	0.007 (3)	−0.005 (4)	−0.023 (3)
C12	0.065 (3)	0.047 (3)	0.063 (3)	−0.001 (2)	0.004 (3)	−0.018 (2)
C13	0.034 (2)	0.0313 (19)	0.049 (2)	−0.0018 (16)	0.0052 (19)	0.0027 (18)
C14	0.045 (2)	0.046 (2)	0.051 (3)	0.004 (2)	0.009 (2)	0.004 (2)
C15	0.061 (3)	0.066 (3)	0.046 (3)	−0.007 (3)	0.004 (2)	0.009 (2)

C16	0.047 (3)	0.069 (3)	0.076 (4)	0.002 (3)	−0.002 (3)	0.018 (3)
C17	0.045 (3)	0.069 (3)	0.090 (4)	0.018 (3)	0.016 (3)	0.000 (3)
C18	0.044 (3)	0.054 (3)	0.059 (3)	0.009 (2)	0.012 (2)	−0.006 (2)
C19	0.038 (2)	0.041 (2)	0.044 (2)	−0.0053 (17)	0.0111 (19)	−0.003 (2)
C20	0.063 (3)	0.040 (2)	0.077 (3)	0.003 (2)	0.026 (3)	0.005 (3)
C21	0.077 (4)	0.048 (3)	0.077 (4)	−0.006 (3)	0.023 (3)	0.011 (3)
C22	0.058 (3)	0.075 (4)	0.076 (4)	−0.009 (3)	0.029 (3)	0.013 (3)
C23	0.050 (3)	0.083 (4)	0.090 (4)	0.009 (3)	0.030 (3)	0.020 (3)
C24	0.050 (3)	0.058 (3)	0.066 (3)	0.010 (2)	0.022 (2)	0.012 (3)
C25	0.107 (4)	0.104 (4)	0.081 (3)	−0.032 (3)	0.004 (3)	0.014 (3)
Cl2	0.134 (3)	0.134 (3)	0.146 (4)	0.039 (3)	0.022 (3)	0.032 (3)
Cl3	0.129 (3)	0.178 (3)	0.108 (2)	0.060 (2)	0.0416 (18)	0.039 (2)
Cl4	0.248 (6)	0.182 (3)	0.086 (2)	−0.093 (4)	0.049 (3)	0.009 (2)
Cl2A	0.134 (9)	0.126 (8)	0.049 (4)	−0.018 (6)	0.009 (5)	0.012 (4)
Cl3A	0.136 (7)	0.199 (11)	0.155 (11)	0.039 (8)	−0.015 (7)	−0.009 (9)
Cl4A	0.107 (7)	0.130 (7)	0.061 (4)	−0.034 (6)	0.010 (4)	−0.018 (4)

Geometric parameters (Å, º)

Pd1—P1	2.2787 (11)	C12—H12	0.9300
Pd1—S1^{i}	2.2970 (11)	C13—C18	1.383 (6)
Pd1—Cl1	2.3383 (11)	C13—C14	1.384 (6)
Pd1—S1	2.3676 (11)	C14—C15	1.375 (6)
S1—C1	1.770 (5)	C14—H14	0.9300
S1—Pd1^{i}	2.2971 (11)	C15—C16	1.376 (8)
P1—C7	1.819 (5)	C15—H15	0.9300
P1—C13	1.821 (4)	C16—C17	1.366 (8)
P1—C19	1.825 (4)	C16—H16	0.9300
C1—C2	1.366 (7)	C17—C18	1.392 (7)
C1—C6	1.378 (8)	C17—H17	0.9300
C2—C3	1.400 (9)	C18—H18	0.9300
C2—H2	0.9300	C19—C24	1.380 (6)
C3—C4	1.346 (11)	C19—C20	1.385 (6)
C3—H3	0.9300	C20—C21	1.380 (7)
C4—C5	1.362 (10)	C20—H20	0.9300
C4—H4	0.9300	C21—C22	1.365 (8)
C5—C6	1.376 (9)	C21—H21	0.9300
C5—H5	0.9300	C22—C23	1.377 (8)
C6—H6	0.9300	C22—H22	0.9300
C7—C8	1.368 (7)	C23—C24	1.385 (7)
C7—C12	1.381 (6)	C23—H23	0.9300
C8—C9	1.376 (8)	C24—H24	0.9300
C8—H8	0.9300	C25—Cl2	1.715 (6)
C9—C10	1.379 (10)	C25—Cl4	1.726 (6)
C9—H9	0.9300	C25—Cl3	1.732 (5)
C10—C11	1.359 (10)	C25—Cl3A	1.733 (7)
C10—H10	0.9300	C25—Cl4A	1.745 (7)
C11—C12	1.379 (8)	C25—Cl2A	1.759 (7)
C11—H11	0.9300	C25—H25	0.9800

P1—Pd1—S1^{i}	95.42 (4)	C11—C12—C7	119.8 (6)
P1—Pd1—Cl1	90.27 (4)	C11—C12—H12	120.1
S1^{i}—Pd1—Cl1	173.83 (4)	C7—C12—H12	120.1
P1—Pd1—S1	175.51 (4)	C18—C13—C14	118.7 (4)
S1^{i}—Pd1—S1	83.67 (4)	C18—C13—P1	123.2 (3)
Cl1—Pd1—S1	90.84 (4)	C14—C13—P1	118.1 (3)
C1—S1—Pd1^{i}	102.77 (16)	C15—C14—C13	121.2 (4)
C1—S1—Pd1	99.59 (14)	C15—C14—H14	119.4
Pd1^{i}—S1—Pd1	96.33 (4)	C13—C14—H14	119.4
C7—P1—C13	105.1 (2)	C14—C15—C16	119.6 (5)
C7—P1—C19	108.8 (2)	C14—C15—H15	120.2
C13—P1—C19	101.47 (19)	C16—C15—H15	120.2
C7—P1—Pd1	111.96 (15)	C17—C16—C15	120.3 (5)
C13—P1—Pd1	117.46 (13)	C17—C16—H16	119.9
C19—P1—Pd1	111.26 (14)	C15—C16—H16	119.9
C2—C1—C6	118.2 (5)	C16—C17—C18	120.2 (5)
C2—C1—S1	118.9 (4)	C16—C17—H17	119.9
C6—C1—S1	122.9 (4)	C18—C17—H17	119.9
C1—C2—C3	120.1 (6)	C13—C18—C17	120.0 (5)
C1—C2—H2	119.9	C13—C18—H18	120.0
C3—C2—H2	119.9	C17—C18—H18	120.0
C4—C3—C2	120.5 (6)	C24—C19—C20	118.6 (4)
C4—C3—H3	119.8	C24—C19—P1	120.7 (3)
C2—C3—H3	119.8	C20—C19—P1	120.5 (4)
C3—C4—C5	120.1 (7)	C21—C20—C19	120.6 (5)
C3—C4—H4	119.9	C21—C20—H20	119.7
C5—C4—H4	119.9	C19—C20—H20	119.7
C4—C5—C6	119.7 (7)	C22—C21—C20	120.5 (5)
C4—C5—H5	120.1	C22—C21—H21	119.7
C6—C5—H5	120.1	C20—C21—H21	119.7
C5—C6—C1	121.4 (6)	C21—C22—C23	119.6 (5)
C5—C6—H6	119.3	C21—C22—H22	120.2
C1—C6—H6	119.3	C23—C22—H22	120.2
C8—C7—C12	119.3 (5)	C22—C23—C24	120.2 (5)
C8—C7—P1	117.8 (4)	C22—C23—H23	119.9
C12—C7—P1	122.9 (4)	C24—C23—H23	119.9
C7—C8—C9	120.6 (6)	C19—C24—C23	120.5 (5)
C7—C8—H8	119.7	C19—C24—H24	119.8
C9—C8—H8	119.7	C23—C24—H24	119.8
C8—C9—C10	119.9 (6)	Cl2—C25—Cl4	111.8 (4)
C8—C9—H9	120.1	Cl2—C25—Cl3	110.6 (4)
C10—C9—H9	120.1	Cl4—C25—Cl3	109.6 (4)
C11—C10—C9	119.6 (6)	Cl3A—C25—Cl4A	108.2 (6)
C11—C10—H10	120.2	Cl3A—C25—Cl2A	107.5 (6)
C9—C10—H10	120.2	Cl4A—C25—Cl2A	107.2 (5)
C10—C11—C12	120.7 (6)	Cl2—C25—H25	108.2
C10—C11—H11	119.6	Cl4—C25—H25	108.2
C12—C11—H11	119.6	Cl3—C25—H25	108.2

Pd1^{i}—S1—C1—C2	133.2 (4)	C19—P1—C13—C18	120.9 (4)
Pd1—S1—C1—C2	−128.0 (4)	Pd1—P1—C13—C18	−117.6 (4)
Pd1^{i}—S1—C1—C6	−49.3 (5)	C7—P1—C13—C14	−172.8 (3)
Pd1—S1—C1—C6	49.5 (5)	C19—P1—C13—C14	−59.4 (4)
C6—C1—C2—C3	0.0 (9)	Pd1—P1—C13—C14	62.1 (4)
S1—C1—C2—C3	177.7 (5)	C18—C13—C14—C15	−1.3 (7)
C1—C2—C3—C4	0.6 (12)	P1—C13—C14—C15	179.0 (4)
C2—C3—C4—C5	−0.3 (13)	C13—C14—C15—C16	0.2 (7)
C3—C4—C5—C6	−0.7 (13)	C14—C15—C16—C17	0.1 (8)
C4—C5—C6—C1	1.4 (12)	C15—C16—C17—C18	0.6 (9)
C2—C1—C6—C5	−1.0 (10)	C14—C13—C18—C17	2.0 (7)
S1—C1—C6—C5	−178.6 (6)	P1—C13—C18—C17	−178.3 (4)
C13—P1—C7—C8	−76.2 (4)	C16—C17—C18—C13	−1.7 (8)
C19—P1—C7—C8	175.8 (4)	C7—P1—C19—C24	−110.5 (4)
Pd1—P1—C7—C8	52.4 (4)	C13—P1—C19—C24	139.1 (4)
C13—P1—C7—C12	102.6 (4)	Pd1—P1—C19—C24	13.4 (4)
C19—P1—C7—C12	−5.5 (4)	C7—P1—C19—C20	73.2 (4)
Pd1—P1—C7—C12	−128.9 (4)	C13—P1—C19—C20	−37.2 (4)
C12—C7—C8—C9	0.3 (8)	Pd1—P1—C19—C20	−162.9 (4)
P1—C7—C8—C9	179.1 (4)	C24—C19—C20—C21	−0.4 (8)
C7—C8—C9—C10	−0.4 (9)	P1—C19—C20—C21	176.0 (4)
C8—C9—C10—C11	0.5 (10)	C19—C20—C21—C22	0.9 (9)
C9—C10—C11—C12	−0.5 (10)	C20—C21—C22—C23	−0.7 (9)
C10—C11—C12—C7	0.4 (9)	C21—C22—C23—C24	0.0 (9)
C8—C7—C12—C11	−0.3 (7)	C20—C19—C24—C23	−0.3 (8)
P1—C7—C12—C11	−179.0 (4)	P1—C19—C24—C23	−176.7 (4)
C7—P1—C13—C18	7.5 (4)	C22—C23—C24—C19	0.5 (9)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C25—H25···Cl1^{ii}	0.98	2.79	3.744 (6)	164
C15—H15···Cl1^{iii}	0.93	2.93	3.650 (5)	135

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