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Dichlorido{[(diphenylphosphino)-methyl]bis(2-methylphenyl)phosphine-κ^2P,P'}palladium(II)

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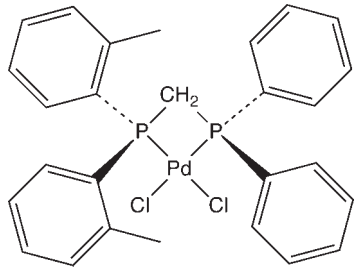
Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.030; wR factor = 0.074; data-to-parameter ratio = 13.3.

In the title compound, $[PdCl_2(C_{27}H_{26}P_2)]$ or $PdCl_2[(C_6H_5)_2PCH_2P(C_6H_4CH_3)_2]$, the palladium center has a distorted square-planar geometry. There are two crystallographically independent molecules in the asymmetric unit. The dihedral angle between the PdP_2 and $PdCl_2$ planes is 2.95 (4)° in one independent molecule and 5.15 (4)° in the other. The P—Pd—P and P—C—P bond angles are significantly distorted because of the small bite angle of the chelating (bisphosphino)methane ligand. The steric demands of the substituted rings in the mixed ligand cause a slight elongation of the Pd—$P(C_6H_4CH_3)_2$ bond relative to the Pd—$P(C_6H_5)_2$ bond. In one molecule the tolyl ring shows positional disorder in a 0.58 (2):0.42 (2) ratio, in the other molecule the phenyl ring shows positional disorder in a 0.838 (9):0.162 (9) ratio.

Related literature

For the steric effects of (bisphosphino)methane ligands, see: Filby *et al.* (2006); Dossett *et al.* (2001). For dichlorido[bis-(diphenylphosphino)methane]palladium(II), see: Shahid *et al.* (2009); Steffen & Palenik (1976). For dichlorido[bis(dicyclohexylphosphino)methane]palladium(II), see: Mague *et al.* (2007). For related literature regarding the synthesis of the title compound, see: Wass (2001); Gauthron *et al.* (1998).



Experimental

Crystal data

$[PdCl_2(C_{27}H_{26}P_2)]$
M_r = 589.72
Monoclinic, $P2_1/c$
a = 17.8761 (10) Å
b = 16.7568 (9) Å
c = 16.9407 (9) Å
β = 90.446 (3)°
V = 5074.4 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.08 mm^{-1}
T = 193 K
0.30 × 0.28 × 0.26 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: integration (*SHELXTL*/*XPREP*; Bruker, 2005 and *SADABS*; Bruker, 2007)
T_{min} = 0.728, T_{max} = 0.801
83307 measured reflections
9350 independent reflections
8400 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.074
S = 1.26
9350 reflections
702 parameters
469 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14A···Cl1	0.98	2.63	3.612 (4)	179
C34—H34A···Cl3	0.98	2.66	3.637 (4)	179

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT* and *XPREP*/*SHELXTL* (Sheldrick, 2008); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *CrystalMaker* (*CrystalMaker*, 1994); software used to prepare material for publication: *XCIF*/*SHELXTL*.

We thank the National Science Foundation (grant CHE-0548107) for support of this work. AHB thanks the NSF LSAMP Program (grant HRD-0413000) for research support. The Materials Chemistry Laboratory at the University of Illinois was supported in part by grants from the NSF (CHE 95–03145 and CHE 03–43032).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2183).

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supplementary materials

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Dichlorido{[(diphenylphosphino)methyl]bis(2-methylphenyl)phosphine-κ^2P,P'}palladium(II)

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Comment

The steric effects on the bite angles and preferred bonding modes of aromatic (bisphosphino)methane ligands have been studied (Filby *et al.*, 2006), and there is interest in their four-membered palladacyclic complexes because they have been shown to be active catalysts for reactions such as the copolymerization of CO and C_2H_4 (Dossett *et al.*, 2001).

The title compound, $PdCl_2[(C_6H_5)_2PCH_2P(C_6H_4CH_3)_2]$, crystallizes with two independent molecules in the asymmetric unit with the palladium center in each adopting a distorted square-planar geometry. The C1 to C7 *ortho*-tolyl ring in molecule 1 and the C43 to C48 phenyl ring in molecule 2 are disordered. The asymmetric unit containing both molecules showing disorder of their respective aromatic rings is shown in Fig. 1. In molecule 1 (Fig. 2) the dihedral angle between the PdP_2 and $PdCl_2$ planes is 2.95 (4)°, whereas the dihedral angle is 5.15 (4)° in molecule 2 (Fig. 3). The related symmetrical compounds $PdCl_2[(C_6H_5)_2PCH_2P(C_6H_5)_2]$ (Shahid *et al.*, 2009; Steffen & Palenik, 1976) and $PdCl_2[(C_6H_{11})_2PCH_2P(C_6H_{11})_2]$ (Mague *et al.*, 2007) show similar deviations from planarity about the palladium center due partly to the small bite angle of the chelating (bisphosphino)methane ligand and the spatial demands of the ligand substituents. The P—Pd—P bond angles of 73.75 (3)° in molecule 1 and 73.37 (3)° in molecule 2 are significantly distorted from the normal square-planar value of 90°, and the P—C—P bond angles (93.95 (13) and 92.73 (14)°, respectively) show major deviations from the normal tetrahedral value of 109.5°. Notably, the Pd—$P(C_6H_4CH_3)_2$ bond lengths of 2.2646 (8) in molecule 1 and 2.2604 (8) Å in molecule 2 are slightly longer than the Pd—$P(C_6H_5)_2$ bond lengths (2.2197 (7) and 2.2146 (8) Å in the respective molecules), which is likely a result of the steric requirements of the substituted rings.

There are two short Cl···H interactions: Cl1···H14A—C14 is 2.631 Å and Cl3···H34A—C34 is 2.658 Å. These are intramolecular Cl···H—C hydrogen bonds and they occur between the same atoms on both symmetrically independent molecules. The Cl···H—C angles are nearly linear (178.9° and 178.7°, respectively).

Experimental

The mixed ligand $Ph_2PCH_2P(C_6H_4CH_3)_2$ has been reported in the patent literature (Wass, 2001), and our synthetic procedure will be published elsewhere. The title compound, $PdCl_2[(C_6H_5)_2PCH_2P(C_6H_4CH_3)_2]$, was prepared from a procedure adapted from that described previously for the synthesis of $PdCl_2[(C_6H_5)_2PCH_2P(C_6H_5)_2]$ by Gauthron *et al.* (1998). A solid mixture of $Ph_2PCH_2P(C_6H_4CH_3)_2$ (612 mg, 1.48 mmol) and $PdCl_2$ (260 mg, 1.47 mmol) was suspended in 50% EtOH (25 ml) and concentrated HCl (25 ml). The mixture was refluxed overnight, and a yellow solid precipitated from solution. The mixture was filtered, and the yellow solid was washed with H_2O (2 × 25 ml) and EtOH (2 × 25 ml). After drying under vacuum, the title compound was obtained as a yellow powder (0.844 g, 98%). Mp: 258.1 °C (dec.). Anal. Calcd for $C_{27}H_{26}Cl_2P_2Pd$: C, 54.99; H, 4.44; P, 10.50. Found: C, 54.84; H, 4.33; P, 10.18. ^{1}H NMR ($CDCl_3$): δ 2.27 (s, C*H*$_3$), 4.30

(virtual t, $^2J_{HP}$ = 10.6, 9.0 Hz, CH_2), 7.23–8.04 (m, C$_6H_5$ and C$_6H_4$CH$_3$). ^{31}P{^{1}H} NMR ($CDCl_3$): δ -54.1 (d, $^2J_{PP}$ = 88 Hz, $P(C_6H_5)_2$ or $P(C_6H_4CH_3)_2$), -52.9 (d, $^2J_{PP}$ = 88 Hz, $P(C_6H_5)_2$ or $P(C_6H_4CH_3)_2$).

Single crystals suitable for X-ray diffraction were grown from slow diffusion of pentane into a concentrated CH_2Cl_2 solution at room temperature.

Refinement

The proposed structural model consisting of two independent host molecules that each exhibit disorder off of the phosphines was developed. The positional disorder present in molecule 1 (Fig. 1) is located on the *ortho*-tolyl ring that contains C1 to C7. The disordered *ortho*-tolyl rings were restrained to have similar P—C bond distances, the same geometries, and to be flat using an effective standard deviation (e.s.d.) for each restraint of 0.01 Å. The final refinement showed that the *ortho*-tolyl ring is located in the primary position 57.8 (20)% of the time. The disorder present in molecule 2 (Fig. 1) is located on the phenyl ring that contains C43 to C48. The disordered phenyl rings were restrained to have similar P—C bond distances, similar C—C bond distances across the ring, and to be flat using e.s.d.'s of 0.01. The final refinement showed only a slight disorder in the phenyl ring with the primary position being 83.83 (9)% occupied. Anti bumping restraints were also used to prevent close contacts between the H atoms on the P—C—P bridged carbon and the *ortho* H atoms on the phenyl rings. Rigid-bond restraints (e.s.d. 0.01) were imposed on displacement parameters for all disordered sites and similar displacement amplitudes (e.s.d. 0.01) were imposed on disordered sites overlapping by less than the sum of Van der Waals radii. Methyl H atom positions, R—CH_3, were optimized by rotation about R—C bonds with idealized C—H, R—H and H···H distances (C—H = 0.9800 and H···H = 1.6000 Å). Remaining H atoms were included as riding idealized contributors (aromatic C-H = 0.9500 Å, and R_2CH_2 C-H = 0.9900 Å). Methyl H atom U's were assigned as 1.5 times U_{eq} of the carrier atom; remaining H atom U's were assigned as 1.2 times carrier U_{eq}.

Figures

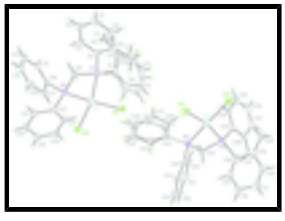


Fig. 1. Two independent molecular structures of the title compound in the asymmetric unit showing disorder of the *ortho*-tolyl ring C1 to C7 in molecule 1 (left) and the phenyl ring C43 to C48 in molecule 2 (right) with 35% probability ellipsoids for non-H atoms and circles of arbitrary size for H atoms.

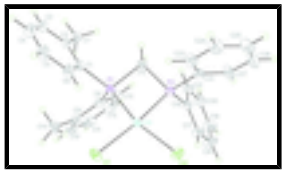


Fig. 2. Molecule 1 of the title compound showing 35% probability ellipsoids for non-H atoms and circles of arbitrary size for H atoms. Disorder of the *ortho*-tolyl ring C1 to C7 has been omitted for clarity.

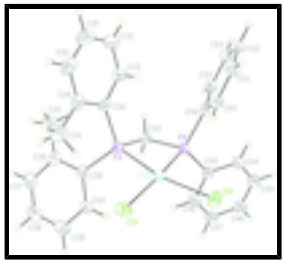


Fig. 3. Molecule 2 of the title compound showing 35% probability ellipsoids for non-H atoms and circles of arbitrary size for H atoms. Disorder of the phenyl ring C43 to C48 has been omitted for clarity.

Dichlorido{[(diphenylphosphino)methyl]bis(2-methylphenyl)phosphine- κ^2P,P'}palladium(II)

Crystal data

$[PdCl_2(C_{27}H_{26}P_2)]$	F_{000} = 2384
M_r = 589.72	D_x = 1.544 Mg m^{-3}
Monoclinic, *P*2(1)/*c*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 9741 reflections
a = 17.8761 (10) Å	θ = 2.4–27.1°
b = 16.7568 (9) Å	μ = 1.08 mm^{-1}
c = 16.9407 (9) Å	*T* = 193 K
β = 90.446 (3)°	Prism, yellow
V = 5074.4 (5) Å^3	0.30 × 0.28 × 0.26 mm
Z = 8	

Data collection

Bruker Kappa APEXII CCD diffractometer	9350 independent reflections
Radiation source: fine-focus sealed tube	8400 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.037
T = 193 K	θ_{max} = 25.4°
profile data from φ and ω scans	θ_{min} = 1.7°
Absorption correction: integration (SHELXTL/XPREP; Bruker, 2005)	*h* = −20→21
T_{min} = 0.728, T_{max} = 0.801	*k* = −20→20
83307 measured reflections	*l* = −20→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.030	H-atom parameters constrained
$wR(F^2)$ = 0.074	$w = 1/[\sigma^2(F_o^2) + (0.0262P)^2 + 5.P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.26	$(\Delta/\sigma)_{max}$ = 0.006
9350 reflections	$\Delta\rho_{max}$ = 0.66 e Å^{-3}
702 parameters	$\Delta\rho_{min}$ = −0.47 e Å^{-3}
469 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. One distinct cell was identified using *APEX2* (Bruker, 2004). Six frame series were integrated and filtered for statistical outliers using *SAINT* (Bruker, 2005) then corrected for absorption by integration using *SHELXTL*/*XPREP* V2005/2 (Bruker, 2005) before using *SAINT*/*SADABS* (Bruker, 2007) to sort, merge, and scale the combined data. No decay correction was applied.

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. Structure was phased by direct methods (Sheldrick, 2008). Systematic conditions suggested the unambiguous space group. The space group choice was confirmed by successful convergence of the full-matrix least-squares refinement on F^2. The highest peaks in the final difference Fourier map were in the vicinity of atoms Pd2, Cl4, C48, and C54; the final map had no other significant features. A final analysis of variance between observed and calculated structure factors showed some dependence on amplitude and little dependence on resolution.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Pd1	−0.003487 (12)	0.267501 (13)	0.482122 (12)	0.02435 (6)	
P1	0.08444 (4)	0.21236 (4)	0.56213 (4)	0.02565 (16)	
P2	−0.04231 (4)	0.28693 (4)	0.60477 (4)	0.02460 (16)	
Cl1	0.04979 (5)	0.24648 (5)	0.35578 (4)	0.03729 (18)	
Cl2	−0.11120 (4)	0.32869 (5)	0.42864 (5)	0.04003 (19)	
C1	0.1820 (3)	0.2426 (6)	0.5586 (6)	0.0332 (16)	0.58 (2)
C2	0.2345 (4)	0.2155 (5)	0.6137 (5)	0.0372 (16)	0.58 (2)
C3	0.3084 (4)	0.2406 (6)	0.6049 (7)	0.048 (2)	0.58 (2)
H3	0.3456	0.2234	0.6416	0.058*	0.58 (2)
C4	0.3277 (5)	0.2894 (8)	0.5444 (7)	0.053 (2)	0.58 (2)
H4	0.3786	0.3046	0.5392	0.063*	0.58 (2)
C5	0.2770 (6)	0.3175 (7)	0.4908 (6)	0.052 (2)	0.58 (2)
H5	0.2918	0.3526	0.4498	0.063*	0.58 (2)
C6	0.2030 (5)	0.2932 (7)	0.4977 (7)	0.0425 (19)	0.58 (2)
H6	0.1666	0.3113	0.4607	0.051*	0.58 (2)
C7	0.2183 (4)	0.1629 (5)	0.6826 (5)	0.0378 (18)	0.58 (2)
H7A	0.1811	0.1886	0.7164	0.057*	0.58 (2)
H7B	0.2644	0.1538	0.7129	0.057*	0.58 (2)
H7C	0.1987	0.1117	0.6637	0.057*	0.58 (2)
C1B	0.1795 (4)	0.2485 (8)	0.5497 (8)	0.033 (2)	0.42 (2)
C2B	0.2402 (6)	0.2222 (7)	0.5947 (8)	0.039 (2)	0.42 (2)
C3B	0.3100 (6)	0.2564 (7)	0.5810 (9)	0.045 (2)	0.42 (2)
H3B	0.3523	0.2395	0.6110	0.054*	0.42 (2)
C4B	0.3181 (7)	0.3139 (9)	0.5247 (9)	0.048 (2)	0.42 (2)
H4B	0.3663	0.3359	0.5158	0.057*	0.42 (2)
C5B	0.2591 (7)	0.3407 (8)	0.4811 (8)	0.042 (2)	0.42 (2)
H5B	0.2658	0.3815	0.4429	0.050*	0.42 (2)
C6B	0.1889 (7)	0.3078 (9)	0.4931 (9)	0.036 (2)	0.42 (2)
H6B	0.1473	0.3258	0.4627	0.043*	0.42 (2)

C7B	0.2347 (6)	0.1602 (8)	0.6572 (9)	0.049 (2)	0.42 (2)
H7D	0.2828	0.1556	0.6850	0.074*	0.42 (2)
H7E	0.2219	0.1088	0.6331	0.074*	0.42 (2)
H7F	0.1958	0.1753	0.6948	0.074*	0.42 (2)
C8	0.07714 (16)	0.10450 (18)	0.57255 (18)	0.0312 (7)	
C9	0.10714 (17)	0.05362 (19)	0.51544 (19)	0.0355 (7)	
C10	0.0951 (2)	−0.0281 (2)	0.5250 (2)	0.0457 (9)	
H10	0.1140	−0.0638	0.4864	0.055*	
C11	0.0573 (2)	−0.0584 (2)	0.5875 (3)	0.0521 (10)	
H11	0.0499	−0.1144	0.5916	0.063*	
C12	0.0297 (2)	−0.0090 (2)	0.6445 (2)	0.0502 (9)	
H12	0.0042	−0.0302	0.6887	0.060*	
C13	0.03945 (19)	0.07127 (18)	0.6368 (2)	0.0405 (8)	
H13	0.0200	0.1057	0.6762	0.049*	
C14	0.1503 (2)	0.0829 (2)	0.4460 (2)	0.0465 (9)	
H14A	0.1231	0.1269	0.4208	0.070*	
H14B	0.1565	0.0393	0.4081	0.070*	
H14C	0.1996	0.1016	0.4637	0.070*	
C15	0.04670 (16)	0.26069 (16)	0.65182 (16)	0.0273 (6)	
H15A	0.0409	0.2231	0.6965	0.033*	
H15B	0.0760	0.3080	0.6686	0.033*	
C16	−0.11518 (16)	0.22124 (17)	0.63808 (17)	0.0270 (6)	
C17	−0.17584 (18)	0.2076 (2)	0.58852 (19)	0.0377 (7)	
H17	−0.1784	0.2327	0.5383	0.045*	
C18	−0.2327 (2)	0.1573 (2)	0.6124 (2)	0.0505 (10)	
H18	−0.2753	0.1496	0.5794	0.061*	
C19	−0.2277 (2)	0.1185 (2)	0.6839 (2)	0.0477 (9)	
H19	−0.2660	0.0826	0.6992	0.057*	
C20	−0.1676 (2)	0.1314 (2)	0.7332 (2)	0.0430 (8)	
H20	−0.1646	0.1042	0.7823	0.052*	
C21	−0.11141 (18)	0.1838 (2)	0.71164 (18)	0.0356 (7)	
H21	−0.0707	0.1942	0.7466	0.043*	
C22	−0.06719 (17)	0.38759 (18)	0.63035 (17)	0.0294 (6)	
C23	−0.0217 (2)	0.4501 (2)	0.6063 (2)	0.0433 (8)	
H23	0.0230	0.4393	0.5783	0.052*	
C24	−0.0414 (2)	0.5281 (2)	0.6231 (2)	0.0510 (9)	
H24	−0.0095	0.5706	0.6077	0.061*	
C25	−0.1066 (2)	0.5444 (2)	0.6616 (2)	0.0505 (9)	
H25	−0.1205	0.5982	0.6717	0.061*	
C26	−0.1520 (2)	0.4832 (2)	0.6855 (3)	0.0575 (11)	
H26	−0.1971	0.4949	0.7125	0.069*	
C27	−0.1326 (2)	0.4046 (2)	0.6708 (2)	0.0460 (9)	
H27	−0.1639	0.3625	0.6884	0.055*	
Pd2	0.488381 (12)	0.480723 (13)	0.266672 (13)	0.02681 (7)	
P3	0.55839 (4)	0.58234 (4)	0.21988 (4)	0.02569 (16)	
P4	0.42890 (4)	0.59234 (5)	0.29718 (4)	0.02862 (17)	
Cl3	0.56527 (5)	0.37017 (5)	0.23698 (5)	0.0431 (2)	
Cl4	0.39319 (5)	0.39998 (6)	0.31809 (6)	0.0586 (3)	
C28	0.54532 (16)	0.60223 (19)	0.11524 (18)	0.0347 (7)	

C29	0.58273 (19)	0.5576 (2)	0.0591 (2)	0.0418 (8)	
C30	0.5684 (2)	0.5757 (2)	−0.0217 (2)	0.0530 (10)	
H30	0.5937	0.5467	−0.0616	0.064*	
C31	0.5194 (3)	0.6337 (3)	−0.0426 (2)	0.0617 (12)	
H31	0.5105	0.6440	−0.0970	0.074*	
C32	0.4827 (2)	0.6775 (3)	0.0124 (2)	0.0603 (11)	
H32	0.4485	0.7181	−0.0031	0.072*	
C33	0.4957 (2)	0.6623 (2)	0.08936 (19)	0.0497 (9)	
H33	0.4703	0.6934	0.1277	0.060*	
C34	0.6361 (2)	0.4946 (2)	0.0783 (2)	0.0529 (10)	
H34A	0.6162	0.4615	0.1209	0.079*	
H34B	0.6835	0.5186	0.0955	0.079*	
H34C	0.6445	0.4615	0.0316	0.079*	
C35	0.65584 (16)	0.58542 (18)	0.25143 (18)	0.0307 (7)	
C36	0.70975 (19)	0.6366 (2)	0.2212 (2)	0.0391 (8)	
C37	0.78383 (19)	0.6289 (2)	0.2510 (2)	0.0480 (9)	
H37	0.8226	0.6612	0.2301	0.058*	
C38	0.7998 (2)	0.5756 (2)	0.3093 (2)	0.0524 (10)	
H38	0.8499	0.5714	0.3279	0.063*	
C39	0.7466 (2)	0.5281 (2)	0.3418 (2)	0.0503 (9)	
H39	0.7588	0.4929	0.3840	0.060*	
C40	0.67476 (18)	0.5321 (2)	0.3125 (2)	0.0386 (7)	
H40	0.6373	0.4983	0.3338	0.046*	
C41	0.6961 (2)	0.6991 (3)	0.1625 (3)	0.0609 (11)	
H41A	0.6526	0.7309	0.1781	0.091*	
H41B	0.6863	0.6745	0.1109	0.091*	
H41C	0.7401	0.7337	0.1591	0.091*	
C42	0.50777 (17)	0.65964 (18)	0.27665 (17)	0.0318 (7)	
H42A	0.5349	0.6768	0.3249	0.038*	
H42B	0.4933	0.7065	0.2443	0.038*	
C43	0.4046 (2)	0.60883 (11)	0.3993 (2)	0.0342 (9)	0.838 (9)
C44	0.3333 (3)	0.6318 (3)	0.4212 (2)	0.0477 (12)	0.838 (9)
H44	0.2956	0.6395	0.3821	0.057*	0.838 (9)
C45	0.3168 (3)	0.6437 (3)	0.5005 (3)	0.0557 (15)	0.838 (9)
H45	0.2678	0.6588	0.5158	0.067*	0.838 (9)
C46	0.3716 (3)	0.6337 (2)	0.5561 (2)	0.0484 (13)	0.838 (9)
H46	0.3606	0.6430	0.6101	0.058*	0.838 (9)
C47	0.4423 (3)	0.6103 (3)	0.5352 (2)	0.0474 (12)	0.838 (9)
H47	0.4797	0.6032	0.5748	0.057*	0.838 (9)
C48	0.4594 (3)	0.5970 (3)	0.4567 (3)	0.0421 (10)	0.838 (9)
H48	0.5081	0.5801	0.4423	0.050*	0.838 (9)
C43B	0.3923 (12)	0.6025 (5)	0.3961 (7)	0.041 (3)	0.162 (9)
C44B	0.3159 (11)	0.5970 (13)	0.4095 (9)	0.043 (3)	0.162 (9)
H44B	0.2826	0.5878	0.3665	0.052*	0.162 (9)
C45B	0.2882 (11)	0.6049 (15)	0.4854 (10)	0.050 (3)	0.162 (9)
H45B	0.2359	0.6010	0.4944	0.060*	0.162 (9)
C46B	0.3361 (14)	0.6182 (11)	0.5473 (10)	0.050 (3)	0.162 (9)
H46B	0.3169	0.6237	0.5991	0.060*	0.162 (9)
C47B	0.4113 (14)	0.6237 (13)	0.5349 (10)	0.047 (3)	0.162 (9)

H47B	0.4441	0.6330	0.5783	0.057*	0.162 (9)
C48B	0.4406 (12)	0.6158 (12)	0.4593 (11)	0.044 (3)	0.162 (9)
H48B	0.4930	0.6195	0.4512	0.052*	0.162 (9)
C49	0.35162 (16)	0.61621 (19)	0.23292 (17)	0.0313 (7)	
C50	0.32022 (19)	0.5565 (2)	0.1869 (2)	0.0418 (8)	
H50	0.3380	0.5032	0.1912	0.050*	
C51	0.2627 (2)	0.5748 (2)	0.1346 (2)	0.0537 (10)	
H51	0.2412	0.5343	0.1024	0.064*	
C52	0.2368 (2)	0.6517 (3)	0.1295 (2)	0.0527 (10)	
H52	0.1971	0.6638	0.0939	0.063*	
C53	0.2674 (2)	0.7115 (2)	0.1749 (2)	0.0465 (9)	
H53	0.2489	0.7645	0.1705	0.056*	
C54	0.32488 (19)	0.6945 (2)	0.2270 (2)	0.0424 (8)	
H54	0.3462	0.7356	0.2585	0.051*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.02804 (12)	0.02685 (12)	0.01816 (11)	−0.00370 (9)	0.00142 (8)	−0.00013 (8)
P1	0.0263 (4)	0.0273 (4)	0.0233 (4)	−0.0031 (3)	0.0014 (3)	−0.0008 (3)
P2	0.0238 (4)	0.0290 (4)	0.0211 (3)	−0.0058 (3)	0.0023 (3)	−0.0014 (3)
Cl1	0.0511 (5)	0.0393 (4)	0.0215 (3)	0.0050 (4)	0.0079 (3)	0.0004 (3)
Cl2	0.0319 (4)	0.0551 (5)	0.0330 (4)	−0.0009 (4)	−0.0036 (3)	0.0092 (4)
C1	0.030 (3)	0.033 (3)	0.037 (3)	−0.004 (3)	0.009 (3)	−0.009 (3)
C2	0.030 (3)	0.043 (3)	0.039 (4)	0.000 (2)	0.003 (2)	−0.013 (3)
C3	0.034 (3)	0.060 (4)	0.049 (5)	−0.002 (3)	0.005 (3)	−0.011 (3)
C4	0.036 (3)	0.065 (5)	0.058 (5)	−0.008 (3)	0.007 (3)	−0.009 (4)
C5	0.044 (4)	0.058 (5)	0.055 (4)	−0.009 (4)	0.013 (3)	−0.001 (4)
C6	0.038 (3)	0.049 (4)	0.041 (3)	−0.007 (3)	0.010 (3)	−0.007 (3)
C7	0.029 (3)	0.047 (3)	0.037 (4)	0.005 (3)	−0.002 (3)	−0.003 (3)
C1B	0.028 (3)	0.038 (4)	0.032 (4)	−0.005 (3)	0.006 (3)	−0.012 (3)
C2B	0.033 (3)	0.046 (4)	0.039 (4)	−0.002 (3)	0.007 (3)	−0.014 (3)
C3B	0.033 (3)	0.057 (4)	0.045 (5)	−0.006 (3)	0.005 (4)	−0.010 (4)
C4B	0.034 (4)	0.057 (5)	0.052 (5)	−0.011 (4)	0.011 (4)	−0.008 (4)
C5B	0.037 (4)	0.042 (5)	0.046 (4)	−0.010 (4)	0.016 (4)	−0.009 (4)
C6B	0.032 (4)	0.039 (4)	0.037 (4)	−0.005 (3)	0.011 (3)	−0.010 (3)
C7B	0.040 (4)	0.059 (4)	0.049 (5)	0.003 (4)	−0.001 (4)	−0.010 (4)
C8	0.0303 (15)	0.0284 (16)	0.0348 (16)	−0.0030 (13)	−0.0090 (13)	0.0020 (13)
C9	0.0317 (16)	0.0336 (17)	0.0411 (18)	0.0027 (13)	−0.0133 (14)	−0.0029 (14)
C10	0.045 (2)	0.0321 (18)	0.060 (2)	0.0054 (15)	−0.0196 (18)	−0.0081 (17)
C11	0.048 (2)	0.0297 (18)	0.079 (3)	−0.0077 (16)	−0.023 (2)	0.0061 (19)
C12	0.051 (2)	0.042 (2)	0.057 (2)	−0.0136 (17)	−0.0108 (18)	0.0180 (18)
C13	0.0424 (19)	0.0363 (18)	0.0427 (19)	−0.0055 (15)	−0.0046 (15)	0.0062 (15)
C14	0.054 (2)	0.040 (2)	0.046 (2)	0.0088 (17)	0.0043 (17)	−0.0100 (16)
C15	0.0266 (14)	0.0339 (16)	0.0212 (14)	−0.0057 (12)	0.0004 (11)	−0.0032 (12)
C16	0.0267 (15)	0.0286 (15)	0.0257 (14)	−0.0070 (12)	0.0053 (11)	−0.0037 (12)
C17	0.0372 (18)	0.0421 (19)	0.0336 (17)	−0.0103 (15)	−0.0037 (14)	0.0057 (14)
C18	0.041 (2)	0.062 (2)	0.049 (2)	−0.0247 (18)	−0.0103 (16)	0.0066 (19)

C19	0.044 (2)	0.053 (2)	0.046 (2)	−0.0241 (17)	0.0058 (16)	0.0020 (17)
C20	0.049 (2)	0.048 (2)	0.0314 (17)	−0.0174 (17)	0.0065 (15)	0.0052 (15)
C21	0.0348 (17)	0.0429 (19)	0.0293 (16)	−0.0090 (14)	0.0029 (13)	0.0005 (14)
C22	0.0319 (16)	0.0300 (16)	0.0265 (15)	−0.0049 (13)	0.0015 (12)	−0.0014 (12)
C23	0.0406 (19)	0.0427 (19)	0.047 (2)	−0.0079 (16)	0.0139 (16)	0.0009 (16)
C24	0.063 (2)	0.0328 (19)	0.058 (2)	−0.0119 (17)	0.0082 (19)	0.0061 (17)
C25	0.067 (3)	0.0334 (19)	0.051 (2)	0.0003 (18)	0.0089 (19)	−0.0042 (16)
C26	0.058 (2)	0.044 (2)	0.071 (3)	0.0016 (18)	0.028 (2)	−0.013 (2)
C27	0.046 (2)	0.0380 (19)	0.054 (2)	−0.0086 (16)	0.0223 (17)	−0.0094 (16)
Pd2	0.02488 (12)	0.02596 (12)	0.02958 (12)	−0.00231 (9)	0.00016 (9)	0.00152 (9)
P3	0.0237 (4)	0.0266 (4)	0.0268 (4)	0.0003 (3)	0.0015 (3)	0.0004 (3)
P4	0.0222 (4)	0.0352 (4)	0.0285 (4)	0.0032 (3)	0.0007 (3)	−0.0015 (3)
Cl3	0.0546 (5)	0.0288 (4)	0.0457 (5)	0.0108 (4)	−0.0038 (4)	−0.0027 (3)
Cl4	0.0459 (5)	0.0628 (6)	0.0670 (6)	−0.0236 (5)	−0.0002 (4)	0.0214 (5)
C28	0.0338 (17)	0.0390 (18)	0.0313 (16)	−0.0104 (14)	−0.0007 (13)	0.0032 (14)
C29	0.0385 (18)	0.043 (2)	0.0439 (19)	−0.0111 (15)	0.0035 (15)	−0.0048 (16)
C30	0.063 (3)	0.059 (2)	0.038 (2)	−0.021 (2)	0.0048 (18)	−0.0074 (18)
C31	0.073 (3)	0.070 (3)	0.042 (2)	−0.020 (2)	−0.011 (2)	0.010 (2)
C32	0.061 (3)	0.063 (3)	0.056 (3)	−0.004 (2)	−0.015 (2)	0.017 (2)
C33	0.048 (2)	0.053 (2)	0.048 (2)	0.0004 (18)	−0.0037 (17)	0.0134 (18)
C34	0.060 (2)	0.054 (2)	0.045 (2)	−0.0025 (19)	0.0065 (18)	−0.0048 (18)
C35	0.0266 (15)	0.0328 (16)	0.0326 (16)	0.0000 (12)	0.0046 (12)	−0.0094 (13)
C36	0.0393 (18)	0.0353 (18)	0.0427 (19)	−0.0064 (14)	0.0080 (15)	−0.0084 (15)
C37	0.0345 (18)	0.049 (2)	0.061 (2)	−0.0116 (16)	0.0045 (17)	−0.0186 (19)
C38	0.040 (2)	0.049 (2)	0.068 (3)	0.0023 (17)	−0.0109 (18)	−0.019 (2)
C39	0.050 (2)	0.048 (2)	0.053 (2)	0.0071 (18)	−0.0131 (18)	−0.0089 (18)
C40	0.0342 (17)	0.0411 (19)	0.0406 (18)	0.0063 (14)	−0.0039 (14)	−0.0046 (15)
C41	0.056 (2)	0.060 (3)	0.067 (3)	−0.016 (2)	−0.001 (2)	0.002 (2)
C42	0.0333 (16)	0.0255 (15)	0.0367 (17)	0.0019 (13)	0.0037 (13)	−0.0019 (13)
C43	0.031 (2)	0.042 (2)	0.0299 (18)	0.0071 (16)	0.0020 (15)	0.0001 (16)
C44	0.035 (2)	0.072 (3)	0.036 (2)	0.012 (2)	−0.0003 (17)	0.002 (2)
C45	0.047 (3)	0.079 (3)	0.042 (2)	0.023 (3)	0.010 (2)	0.002 (2)
C46	0.057 (3)	0.057 (3)	0.032 (2)	0.014 (2)	0.005 (2)	0.0037 (19)
C47	0.051 (3)	0.055 (3)	0.035 (2)	0.011 (2)	−0.010 (2)	0.0057 (19)
C48	0.040 (2)	0.049 (2)	0.0375 (19)	0.0142 (19)	−0.0023 (17)	0.0002 (19)
C43B	0.036 (5)	0.054 (5)	0.032 (4)	0.015 (5)	0.000 (4)	0.002 (5)
C44B	0.036 (5)	0.060 (6)	0.033 (5)	0.014 (5)	0.007 (4)	0.001 (5)
C45B	0.045 (5)	0.069 (6)	0.036 (5)	0.016 (5)	0.007 (4)	0.005 (5)
C46B	0.050 (5)	0.065 (6)	0.036 (5)	0.020 (5)	0.006 (5)	0.002 (5)
C47B	0.049 (5)	0.057 (5)	0.035 (4)	0.015 (5)	−0.001 (5)	0.002 (5)
C48B	0.041 (5)	0.053 (5)	0.036 (4)	0.014 (5)	0.000 (4)	0.000 (5)
C49	0.0237 (14)	0.0420 (18)	0.0282 (15)	0.0010 (13)	0.0032 (12)	0.0024 (13)
C50	0.0366 (18)	0.044 (2)	0.0443 (19)	−0.0012 (15)	−0.0049 (15)	0.0058 (16)
C51	0.051 (2)	0.057 (2)	0.053 (2)	−0.0087 (19)	−0.0182 (18)	−0.0015 (19)
C52	0.038 (2)	0.066 (3)	0.054 (2)	0.0007 (18)	−0.0110 (17)	0.022 (2)
C53	0.0390 (19)	0.048 (2)	0.053 (2)	0.0085 (16)	0.0016 (16)	0.0133 (18)
C54	0.0365 (18)	0.043 (2)	0.048 (2)	0.0033 (15)	−0.0014 (15)	0.0033 (16)

Geometric parameters (Å, °)

Pd1—P2	2.2197 (7)	C27—H27	0.9500
Pd1—P1	2.2646 (8)	Pd2—P4	2.2146 (8)
Pd1—Cl2	2.3564 (8)	Pd2—P3	2.2604 (8)
Pd1—Cl1	2.3758 (7)	Pd2—Cl4	2.3469 (9)
P1—C1B	1.817 (6)	Pd2—Cl3	2.3632 (8)
P1—C1	1.818 (5)	P3—C28	1.817 (3)
P1—C8	1.821 (3)	P3—C35	1.819 (3)
P1—C15	1.853 (3)	P3—C42	1.853 (3)
P1—P2	2.6912 (11)	P3—P4	2.6738 (10)
P2—C22	1.798 (3)	P4—C49	1.797 (3)
P2—C16	1.800 (3)	P4—C43	1.808 (4)
P2—C15	1.828 (3)	P4—C43B	1.812 (9)
C1—C6	1.389 (7)	P4—C42	1.841 (3)
C1—C2	1.394 (7)	C28—C29	1.386 (5)
C2—C3	1.395 (7)	C28—C33	1.410 (5)
C2—C7	1.493 (7)	C29—C30	1.423 (5)
C3—C4	1.359 (9)	C29—C34	1.457 (5)
C3—H3	0.9500	C30—C31	1.353 (6)
C4—C5	1.360 (9)	C30—H30	0.9500
C4—H4	0.9500	C31—C32	1.360 (6)
C5—C6	1.390 (7)	C31—H31	0.9500
C5—H5	0.9500	C32—C33	1.346 (5)
C6—H6	0.9500	C32—H32	0.9500
C7—H7A	0.9800	C33—H33	0.9500
C7—H7B	0.9800	C34—H34A	0.9800
C7—H7C	0.9800	C34—H34B	0.9800
C1B—C6B	1.392 (8)	C34—H34C	0.9800
C1B—C2B	1.394 (8)	C35—C36	1.391 (4)
C2B—C3B	1.395 (8)	C35—C40	1.406 (5)
C2B—C7B	1.488 (9)	C36—C37	1.420 (5)
C3B—C4B	1.364 (10)	C36—C41	1.463 (5)
C3B—H3B	0.9500	C37—C38	1.359 (6)
C4B—C5B	1.360 (10)	C37—H37	0.9500
C4B—H4B	0.9500	C38—C39	1.360 (6)
C5B—C6B	1.386 (8)	C38—H38	0.9500
C5B—H5B	0.9500	C39—C40	1.375 (5)
C6B—H6B	0.9500	C39—H39	0.9500
C7B—H7D	0.9800	C40—H40	0.9500
C7B—H7E	0.9800	C41—H41A	0.9800
C7B—H7F	0.9800	C41—H41B	0.9800
C8—C13	1.399 (4)	C41—H41C	0.9800
C8—C9	1.400 (4)	C42—H42A	0.9900
C9—C10	1.396 (5)	C42—H42B	0.9900
C9—C14	1.494 (5)	C43—C44	1.385 (5)
C10—C11	1.359 (6)	C43—C48	1.390 (5)
C10—H10	0.9500	C44—C45	1.392 (5)

C11—C12	1.366 (6)	C44—H44	0.9500
C11—H11	0.9500	C45—C46	1.364 (5)
C12—C13	1.362 (5)	C45—H45	0.9500
C12—H12	0.9500	C46—C47	1.373 (5)
C13—H13	0.9500	C46—H46	0.9500
C14—H14A	0.9800	C47—C48	1.385 (5)
C14—H14B	0.9800	C47—H47	0.9500
C14—H14C	0.9800	C48—H48	0.9500
C15—H15A	0.9900	C43B—C44B	1.388 (8)
C15—H15B	0.9900	C43B—C48B	1.388 (8)
C16—C17	1.385 (4)	C44B—C45B	1.389 (9)
C16—C21	1.396 (4)	C44B—H44B	0.9500
C17—C18	1.383 (5)	C45B—C46B	1.366 (9)
C17—H17	0.9500	C45B—H45B	0.9500
C18—C19	1.378 (5)	C46B—C47B	1.366 (9)
C18—H18	0.9500	C46B—H46B	0.9500
C19—C20	1.371 (5)	C47B—C48B	1.392 (9)
C19—H19	0.9500	C47B—H47B	0.9500
C20—C21	1.386 (4)	C48B—H48B	0.9500
C20—H20	0.9500	C49—C50	1.384 (5)
C21—H21	0.9500	C49—C54	1.400 (5)
C22—C23	1.389 (4)	C50—C51	1.387 (5)
C22—C27	1.390 (4)	C50—H50	0.9500
C23—C24	1.383 (5)	C51—C52	1.370 (6)
C23—H23	0.9500	C51—H51	0.9500
C24—C25	1.367 (5)	C52—C53	1.375 (5)
C24—H24	0.9500	C52—H52	0.9500
C25—C26	1.371 (5)	C53—C54	1.379 (5)
C25—H25	0.9500	C53—H53	0.9500
C26—C27	1.385 (5)	C54—H54	0.9500
C26—H26	0.9500		
P2—Pd1—P1	73.75 (3)	P4—Pd2—P3	73.37 (3)
P2—Pd1—Cl2	92.04 (3)	P4—Pd2—Cl4	92.83 (4)
P1—Pd1—Cl2	165.68 (3)	P3—Pd2—Cl4	165.80 (4)
P2—Pd1—Cl1	174.57 (3)	P4—Pd2—Cl3	173.13 (3)
P1—Pd1—Cl1	101.39 (3)	P3—Pd2—Cl3	101.03 (3)
Cl2—Pd1—Cl1	92.88 (3)	Cl4—Pd2—Cl3	92.96 (4)
C1B—P1—C8	114.2 (5)	C28—P3—C35	113.40 (14)
C1—P1—C8	110.4 (4)	C28—P3—C42	108.57 (15)
C1B—P1—C15	107.2 (5)	C35—P3—C42	107.34 (13)
C1—P1—C15	105.1 (4)	C28—P3—Pd2	114.39 (10)
C8—P1—C15	109.11 (14)	C35—P3—Pd2	116.74 (11)
C1B—P1—Pd1	116.1 (4)	C42—P3—Pd2	94.05 (10)
C1—P1—Pd1	121.9 (3)	C28—P3—P4	111.16 (10)
C8—P1—Pd1	114.40 (9)	C35—P3—P4	133.25 (10)
C15—P1—Pd1	93.27 (9)	Pd2—P3—P4	52.53 (2)
C1B—P1—P2	131.8 (5)	C49—P4—C43	110.86 (16)
C1—P1—P2	133.6 (3)	C49—P4—C43B	104.9 (7)
C8—P1—P2	111.94 (10)	C49—P4—C42	109.60 (14)

Pd1—P1—P2	52.36 (2)	C43—P4—C42	106.10 (13)
C22—P2—C16	108.49 (14)	C43B—P4—C42	113.6 (6)
C22—P2—C15	109.67 (13)	C49—P4—Pd2	114.51 (11)
C16—P2—C15	110.24 (14)	C43—P4—Pd2	118.15 (10)
C22—P2—Pd1	116.29 (10)	C43B—P4—Pd2	118.2 (3)
C16—P2—Pd1	115.86 (9)	C42—P4—Pd2	95.94 (10)
C15—P2—Pd1	95.48 (9)	C49—P4—P3	112.43 (10)
C22—P2—P1	135.28 (10)	C43—P4—P3	133.92 (13)
C16—P2—P1	114.41 (10)	C43B—P4—P3	141.2 (7)
Pd1—P2—P1	53.89 (2)	Pd2—P4—P3	54.10 (2)
C6—C1—C2	120.8 (5)	C29—C28—C33	118.6 (3)
C6—C1—P1	117.3 (6)	C29—C28—P3	120.7 (3)
C2—C1—P1	121.9 (6)	C33—C28—P3	120.7 (3)
C1—C2—C3	117.6 (6)	C28—C29—C30	117.4 (3)
C1—C2—C7	125.6 (6)	C28—C29—C34	123.7 (3)
C3—C2—C7	116.8 (6)	C30—C29—C34	118.8 (3)
C4—C3—C2	120.5 (7)	C31—C30—C29	121.1 (4)
C4—C3—H3	119.8	C31—C30—H30	119.4
C2—C3—H3	119.8	C29—C30—H30	119.4
C3—C4—C5	122.7 (6)	C30—C31—C32	121.5 (4)
C3—C4—H4	118.6	C30—C31—H31	119.2
C5—C4—H4	118.6	C32—C31—H31	119.2
C4—C5—C6	118.2 (7)	C33—C32—C31	118.8 (4)
C4—C5—H5	120.9	C33—C32—H32	120.6
C6—C5—H5	120.9	C31—C32—H32	120.6
C1—C6—C5	120.2 (7)	C32—C33—C28	122.6 (4)
C1—C6—H6	119.9	C32—C33—H33	118.7
C5—C6—H6	119.9	C28—C33—H33	118.7
C6B—C1B—C2B	120.3 (7)	C29—C34—H34A	109.5
C6B—C1B—P1	115.9 (8)	C29—C34—H34B	109.5
C2B—C1B—P1	123.8 (7)	H34A—C34—H34B	109.5
C1B—C2B—C3B	118.3 (8)	C29—C34—H34C	109.5
C1B—C2B—C7B	123.7 (8)	H34A—C34—H34C	109.5
C3B—C2B—C7B	118.0 (8)	H34B—C34—H34C	109.5
C4B—C3B—C2B	120.4 (8)	C36—C35—C40	120.0 (3)
C4B—C3B—H3B	119.8	C36—C35—P3	125.0 (3)
C2B—C3B—H3B	119.8	C40—C35—P3	115.0 (2)
C5B—C4B—C3B	121.8 (8)	C35—C36—C37	117.3 (3)
C5B—C4B—H4B	119.1	C35—C36—C41	125.4 (3)
C3B—C4B—H4B	119.1	C37—C36—C41	117.2 (3)
C4B—C5B—C6B	119.2 (8)	C38—C37—C36	120.5 (3)
C4B—C5B—H5B	120.4	C38—C37—H37	119.7
C6B—C5B—H5B	120.4	C36—C37—H37	119.7
C5B—C6B—C1B	120.0 (8)	C37—C38—C39	122.4 (4)
C5B—C6B—H6B	120.0	C37—C38—H38	118.8
C1B—C6B—H6B	120.0	C39—C38—H38	118.8
C2B—C7B—H7D	109.5	C38—C39—C40	118.6 (4)
C2B—C7B—H7E	109.5	C38—C39—H39	120.7
H7D—C7B—H7E	109.5	C40—C39—H39	120.7

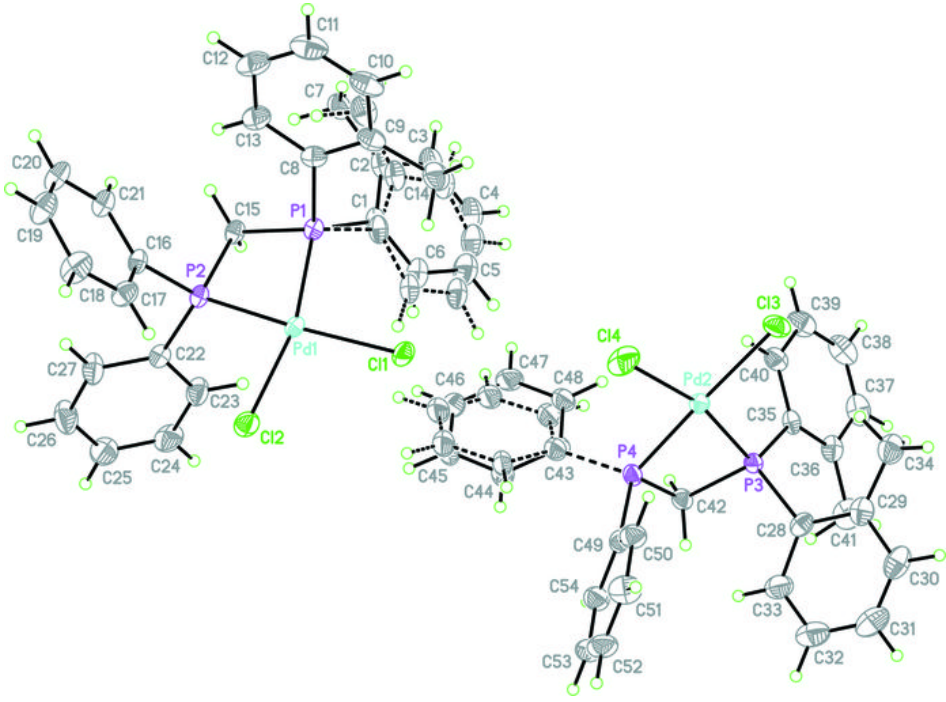
C2B—C7B—H7F	109.5	C39—C40—C35	121.0 (3)
H7D—C7B—H7F	109.5	C39—C40—H40	119.5
H7E—C7B—H7F	109.5	C35—C40—H40	119.5
C13—C8—C9	119.0 (3)	C36—C41—H41A	109.5
C13—C8—P1	120.4 (2)	C36—C41—H41B	109.5
C9—C8—P1	120.6 (2)	H41A—C41—H41B	109.5
C10—C9—C8	117.2 (3)	C36—C41—H41C	109.5
C10—C9—C14	119.6 (3)	H41A—C41—H41C	109.5
C8—C9—C14	123.2 (3)	H41B—C41—H41C	109.5
C11—C10—C9	122.3 (4)	P4—C42—P3	92.73 (14)
C11—C10—H10	118.8	P4—C42—H42A	113.2
C9—C10—H10	118.8	P3—C42—H42A	113.2
C10—C11—C12	120.5 (3)	P4—C42—H42B	113.2
C10—C11—H11	119.7	P3—C42—H42B	113.2
C12—C11—H11	119.7	H42A—C42—H42B	110.5
C13—C12—C11	118.9 (4)	C44—C43—C48	119.8 (3)
C13—C12—H12	120.5	C44—C43—P4	121.9 (3)
C11—C12—H12	120.5	C48—C43—P4	118.3 (3)
C12—C13—C8	122.0 (3)	C43—C44—C45	120.1 (4)
C12—C13—H13	119.0	C43—C44—H44	120.0
C8—C13—H13	119.0	C45—C44—H44	120.0
C9—C14—H14A	109.5	C46—C45—C44	119.5 (4)
C9—C14—H14B	109.5	C46—C45—H45	120.2
H14A—C14—H14B	109.5	C44—C45—H45	120.2
C9—C14—H14C	109.5	C45—C46—C47	121.0 (4)
H14A—C14—H14C	109.5	C45—C46—H46	119.5
H14B—C14—H14C	109.5	C47—C46—H46	119.5
P2—C15—P1	93.95 (13)	C46—C47—C48	120.3 (4)
P2—C15—H15A	112.9	C46—C47—H47	119.9
P1—C15—H15A	112.9	C48—C47—H47	119.9
P2—C15—H15B	112.9	C47—C48—C43	119.3 (4)
P1—C15—H15B	112.9	C47—C48—H48	120.3
H15A—C15—H15B	110.4	C43—C48—H48	120.3
C17—C16—C21	119.9 (3)	C44B—C43B—C48B	119.4 (10)
C17—C16—P2	118.4 (2)	C44B—C43B—P4	120.5 (12)
C21—C16—P2	121.6 (2)	C48B—C43B—P4	120.1 (13)
C18—C17—C16	119.8 (3)	C43B—C44B—C45B	120.3 (11)
C18—C17—H17	120.1	C43B—C44B—H44B	119.9
C16—C17—H17	120.1	C45B—C44B—H44B	119.9
C19—C18—C17	120.1 (3)	C46B—C45B—C44B	120.0 (11)
C19—C18—H18	120.0	C46B—C45B—H45B	120.0
C17—C18—H18	120.0	C44B—C45B—H45B	120.0
C20—C19—C18	120.5 (3)	C45B—C46B—C47B	120.4 (12)
C20—C19—H19	119.8	C45B—C46B—H46B	119.8
C18—C19—H19	119.8	C47B—C46B—H46B	119.8
C19—C20—C21	120.3 (3)	C46B—C47B—C48B	120.8 (12)
C19—C20—H20	119.8	C46B—C47B—H47B	119.6
C21—C20—H20	119.8	C48B—C47B—H47B	119.6
C20—C21—C16	119.3 (3)	C43B—C48B—C47B	119.3 (11)

C20—C21—H21	120.3	C43B—C48B—H48B	120.4
C16—C21—H21	120.3	C47B—C48B—H48B	120.4
C23—C22—C27	119.1 (3)	C50—C49—C54	120.0 (3)
C23—C22—P2	119.4 (2)	C50—C49—P4	119.1 (3)
C27—C22—P2	121.5 (2)	C54—C49—P4	120.8 (3)
C24—C23—C22	120.1 (3)	C49—C50—C51	119.6 (3)
C24—C23—H23	119.9	C49—C50—H50	120.2
C22—C23—H23	119.9	C51—C50—H50	120.2
C25—C24—C23	120.4 (3)	C52—C51—C50	119.8 (4)
C25—C24—H24	119.8	C52—C51—H51	120.1
C23—C24—H24	119.8	C50—C51—H51	120.1
C24—C25—C26	120.0 (3)	C51—C52—C53	121.2 (3)
C24—C25—H25	120.0	C51—C52—H52	119.4
C26—C25—H25	120.0	C53—C52—H52	119.4
C25—C26—C27	120.6 (4)	C52—C53—C54	119.9 (3)
C25—C26—H26	119.7	C52—C53—H53	120.1
C27—C26—H26	119.7	C54—C53—H53	120.1
C26—C27—C22	119.7 (3)	C53—C54—C49	119.5 (3)
C26—C27—H27	120.1	C53—C54—H54	120.3
C22—C27—H27	120.1	C49—C54—H54	120.3

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14A···Cl1	0.98	2.63	3.612 (4)	179
C34—H34A···Cl3	0.98	2.66	3.637 (4)	179

Fig. 1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C12
C10
C7
C13
C9
C3
C8
C2
C14
C4
C20
C21
C15
P1
C1
C19
C16
P2
C6
C5
C18
C17
Pd1
Cl1
C22
C27
C23
Cl2
C26
C24
C25
Cl3
C39
Cl4
C38
C47
C46
C48
Pd2
C40
C37
C35
C34
C45
C44
C43
P4
C36
P3
C42
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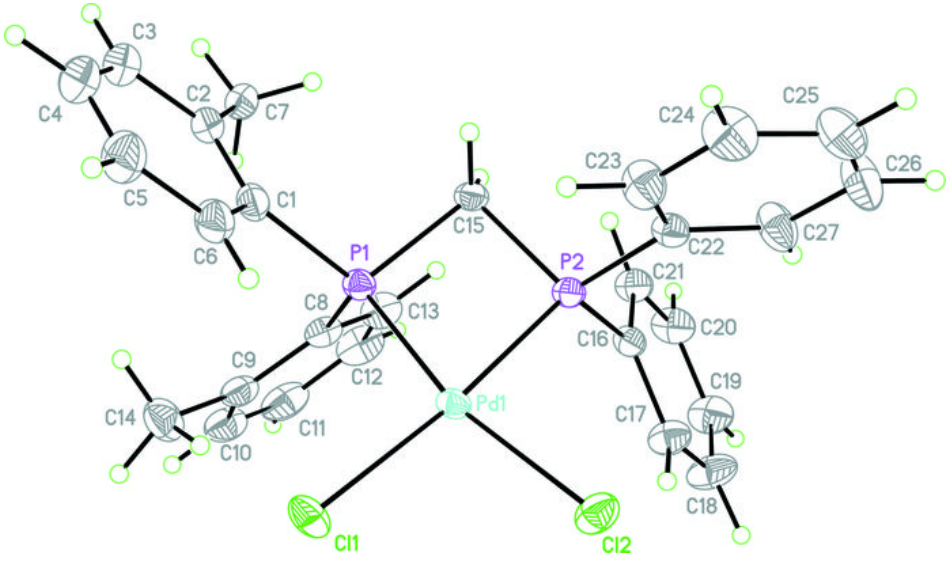
C31
C53
C52
C32

Fig. 2


C3
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C7
C5
C1
C6
C15
P1
P2
C8
C13
C21
C20
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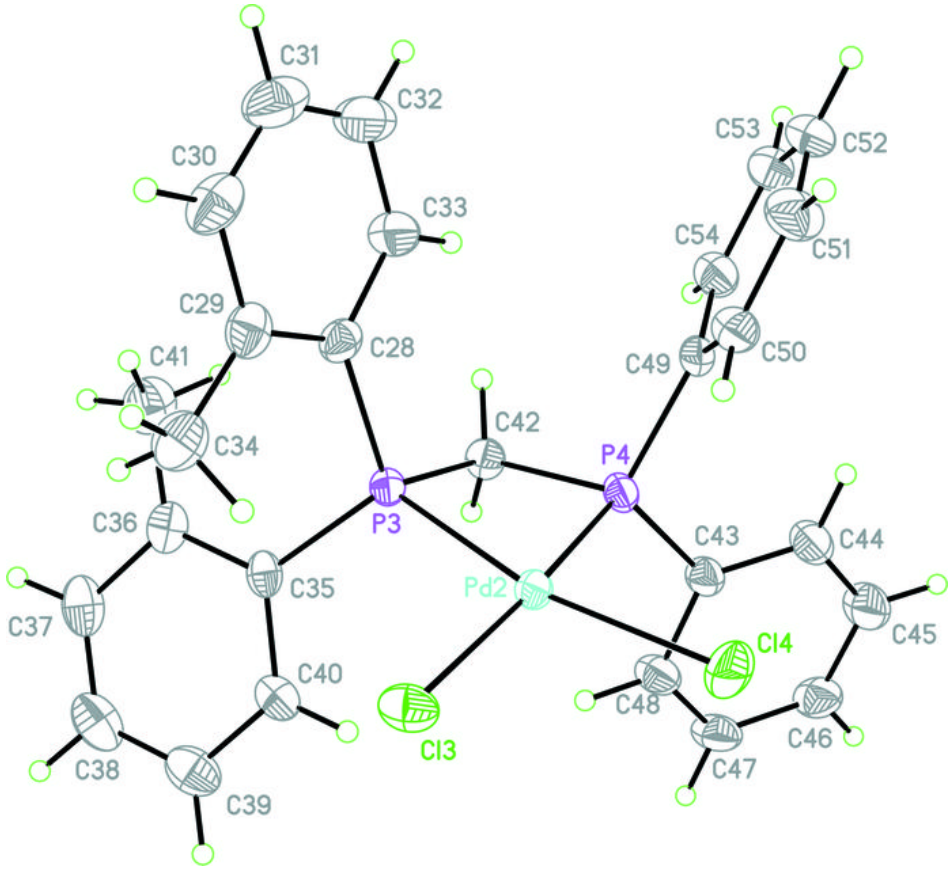
C9
C12
C19
Pd1
C14
C11
C17
C10
C18
Cl1
Cl2
C24
C25
C23
C26
C22
C27

Fig. 3


C31
C32
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P4
Pd2
Cl3
Cl4
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C52
C54
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C43
C44
C45
C48
C46
C47