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cis-Dichlorido[bis(dicyclohexylphosphino)methane-κ^2P,P']palladium(II) dichloromethane solvate

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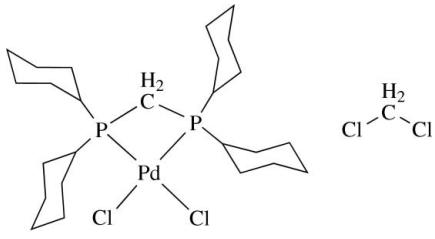
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in solvent or counterion; R factor = 0.026; wR factor = 0.058; data-to-parameter ratio = 25.7.

The title compound, $[PdCl_2(C_{25}H_{46}P_2)]\cdot CH_2Cl_2$, exhibits a distorted square-planar coordination about the Pd^{II} atom. The major distortion, seen in the P—Pd—P angle, is the result of the small bite angle of the diphosphine ligand. There is also a slight tetrahedral distortion from planarity, as measured by the dihedral angle of 2.26 (3)° between the PdP_2 and $PdCl_2$ planes. The dichloromethane solvent molecule is disordered over two sites with approximate occupancies of 0.58 and 0.42.

Related literature

For related structures see: Reid *et al.* (2001); Palenik, *et al.* (1975); Lee *et al.* (1986); Braun *et al.* (2007). For related literature, see: Zhuravel *et al.* (2000).



Experimental

Crystal data

$[PdCl_2(C_{25}H_{46}P_2)]\cdot CH_2Cl_2$
M_r = 670.78
Monoclinic, $P2_1/c$
a = 10.6978 (4) Å
b = 20.2154 (7) Å
c = 15.0333 (5) Å
β = 107.641 (1)°
V = 3098.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.06 mm^{-1}
T = 100 (2) K
0.19 × 0.15 × 0.11 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.803, T_{max} = 0.894
54228 measured reflections
7832 independent reflections
6992 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.058
S = 1.04
7832 reflections
305 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.11 e Å^{-3}
$\Delta\rho_{min}$ = −1.05 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pd1—P1	2.2205 (4)	Pd1—Cl2	2.3756 (4)
Pd1—P2	2.2345 (5)	Pd1—Cl1	2.3815 (4)
P1—Pd1—P2	73.816 (16)	P1—Pd1—Cl1	93.670 (16)
P1—Pd1—Cl2	170.092 (17)	P2—Pd1—Cl1	167.313 (16)
P2—Pd1—Cl2	96.291 (16)	Cl2—Pd1—Cl1	96.195 (16)

Data collection: *APEX2* (Bruker, 2007); cell refinement: *APEX2*; data reduction: *SAINT-Plus* (Bruker, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *APEX2*; software used to prepare material for publication: *APEX2*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2561).

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supplementary materials

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cis-Dichlorido[bis(dicyclohexylphosphino)methane-κ^2P,P']palladium(II) dichloromethane solvate

J. T. Mague, D. H. Pool and M. J. Fink

Comment

cis-Dichloro(bis(dicyclohexylphosphino)methanepalladium(II), (dcpm)$PdCl_2$ (I), has received brief mention as an intermediate in the synthesis of (dcpm)PdI_2 (Zhuravel *et al.*, 2000) but appears not to have been fully characterized. The present sample was obtained following prolonged exposure of a dichloromethane/diethyl ether solution of oxalato(bis(dicyclohexylphosphino)methanepalladium(II) to light in an attempt to grow crystals of the latter. Complex (I) exhibits distorted square planar coordination about the metal, the major distortion being the P1—Pd1—P2 angle of 73.82 (2)° which is the consequence of the small bite angle of the dcpm ligand. Additionally there is a slight tetrahedral distortion from planarity as indicated by a dihedral angle of 2.26 (3)° between the PdP_2 and $PdCl_2$ planes. These two metrical parameters are essentially the same as seen in the only other structurally characterized palladium dcpm complex (dcpm)$Pd(CH_3)_2$ (Reid *et al.*, 2001) where they are, respectively 73.34 and 2.69°. The Pd—P and Pd—Cl distances differ only slightly in each case and compare favorably with those in the related complexes $(RCH(PPh_2)_2)PdCl_2$ (*R* = H (Palenik *et al.*, 1975), CH_3 (Lee *et al.*, 1986), CN (Braun *et al.*, 2007)).

Experimental

Crystals of (dcpm)$PdCl_2$ (dcpm = bis(dicyclohexylphosphino)methane) were obtained from a methylene chloride/diethyl ether solution of (dcpm)PdC_2O_4 which was exposed to fluorescent lighting for seven days in an attempt to crystallize the latter. The $^{31}P\{^1H\}$ NMR spectrum of the material remaining after selection of the crystal for *x*-ray diffraction exhibits a single resonance at −33.3 p.p.m. and no visible carbonyl resonance in the $^{13}C\{^1H\}$ NMR spectrum·The same −33.3 p.p.m. resonance is observed after treatment of an authentic sample of (dcpm)PdC_2O_4 with HCl suggesting that the prolonged exposure of (dcpm)PdC_2O_4 to the chlorinated solvent and light generated sufficient HCl to convert the (dcpm)PdC_2O_4 to (dcpm)$PdCl_2$. Additional evidence for this proposal comes from the observation of a small peak at −33.3 p.p.m. in the $^{31}P\{^1H\}$ NMR spectrum of the product initially obtained in the synthesis of (dcpm)PdC_2O_4 by ligand displacement from (tmeda)PdC_2O_4 (tmeda = *N*,*N*',*N*'',*N*'''-tetramethylethylenediamine) with dcpm in methylene chloride with stirring over three days. ^1H NMR (CD_2Cl_2): δ 1.2–2.4 (m, 44 H, Cy), 2.85 (t, J_{PH} = 10 Hz, 2 H, PCH_2P). $^{31}P\{^1H\}$ NMR (CD_2Cl_2): δ −33.3. $^{13}C\{^1H\}$ NMR (CD_2Cl_2): δ 19.37 (t, J_{PC} = 21 Hz, PCH_2P), 26.18 (s, Cy), 27.13 (t, J_{PC} = 6 Hz Cy), 27.42 (t, JPC = 7 Hz Cy), 28.70 (s, Cy), 29.52 (s, Cy), 35.94 (t, J_{PC} = 10 Hz, –CHP–).

Refinement

H-atoms were placed in calculated positions (C—H = 0.99 − 1.00 Å) and included as riding contributions with isotropic displacement parameters 1.2 times those of the attached carbon atoms. The solvent dichloromethane molecule is disordered

over two sites having one chlorine (Cl3) in common in a 5755 (15):4245 (15) ratio of refined occupancies. Refinement was completed with the disordered model constrained to have C—Cl distances of 1.72 (1) Å.

Figures

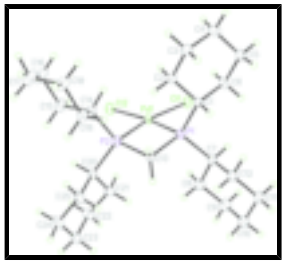

Fig. 1. The molecular structure with displacement ellipsoids drawn at the 50% probability level and H-atoms are represented by spheres of arbitrary radius. The dichloromethane solvent is not shown.

cis-Dichlorido[bis(dicyclohexylphosphino)methane-κ^2*P*,*P*']palladium(II) dichloromethane solvate

Crystal data

$[PdCl_2(C_{25}H_{46}P_2)]\cdot CH_2Cl_2$	F_{000} = 1392.1
M_r = 670.78	D_x = 1.438 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 9765 reflections
a = 10.6978 (4) Å	θ = 2.3–29.3º
b = 20.2154 (7) Å	μ = 1.06 mm^{-1}
c = 15.0333 (5) Å	T = 100 (2) K
β = 107.641 (1)º	Block, colourless
V = 3098.2 (2) Å^3	0.19 × 0.15 × 0.11 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	7832 independent reflections
Radiation source: fine-focus sealed tube	6992 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.033
T = 100(2) K	θ_{max} = 28.5º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 2007)	h = −14→14
T_{min} = 0.803, T_{max} = 0.894	k = −27→27
54228 measured reflections	l = −19→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.026$	H-atom parameters constrained
$wR(F^2) = 0.058$	$w = 1/[\sigma^2(F_o^2) + (0.0171P)^2 + 3.7026P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
7832 reflections	$\Delta\rho_{max} = 1.11$ e Å^{-3}
305 parameters	$\Delta\rho_{min} = -1.05$ e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5 °. in omega, colllected at phi = 0.00, 90.00 and 180.00 °. and 2 sets of 800 frames, each of width 0.45 ° in phi, collected at omega = −30.00 and 210.00 °. The scan time was 10 sec/frame.

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. H-atoms were placed in calculated positions (C—H = 0.99 − 1.00 Å) and included as riding contributions with isotropic displacement parameters 1.2 times those of the attached carbon atoms. The solvent dichloromethane molecule is disordered over two sites having one chlorine (Cl3) in common in a 58:42 ratio. Refinement was completed with the disordered model constrained to have C—Cl distances of 1.72 (1) Å.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Pd1	0.448118 (12)	0.231722 (6)	0.766483 (9)	0.01362 (4)	
Cl1	0.28057 (4)	0.23668 (2)	0.62016 (3)	0.01973 (9)	
Cl2	0.60824 (4)	0.18028 (2)	0.70938 (3)	0.02113 (9)	
P1	0.32599 (4)	0.28077 (2)	0.84313 (3)	0.01365 (8)	
P2	0.57527 (4)	0.24148 (2)	0.91426 (3)	0.01433 (9)	
C1	0.19916 (16)	0.23196 (8)	0.87199 (12)	0.0150 (3)	
H1	0.1687	0.2579	0.9182	0.018*	
C2	0.25493 (17)	0.16610 (9)	0.91832 (13)	0.0183 (3)	
H2A	0.2875	0.1396	0.8746	0.022*	
H2B	0.3298	0.1749	0.9747	0.022*	
C3	0.14985 (19)	0.12702 (9)	0.94548 (13)	0.0224 (4)	
H3A	0.1868	0.0842	0.9731	0.027*	
H3B	0.1226	0.1520	0.9932	0.027*	
C4	0.03056 (19)	0.11457 (10)	0.86100 (14)	0.0247 (4)	
H4A	−0.0379	0.0914	0.8811	0.030*	
H4B	0.0558	0.0858	0.8159	0.030*	

C5	−0.02433 (18)	0.17960 (10)	0.81380 (14)	0.0232 (4)
H5A	−0.0584	0.2061	0.8568	0.028*
H5B	−0.0985	0.1702	0.7572	0.028*
C6	0.07970 (17)	0.21976 (10)	0.78645 (13)	0.0203 (4)
H6A	0.0420	0.2627	0.7595	0.024*
H6B	0.1073	0.1955	0.7384	0.024*
C7	0.25300 (17)	0.35974 (9)	0.79393 (12)	0.0175 (3)
H7	0.1803	0.3496	0.7358	0.021*
C8	0.35254 (19)	0.40298 (10)	0.76581 (14)	0.0237 (4)
H8A	0.3830	0.3795	0.7184	0.028*
H8B	0.4296	0.4109	0.8211	0.028*
C9	0.2918 (2)	0.46947 (10)	0.72597 (15)	0.0300 (4)
H9A	0.3599	0.4975	0.7126	0.036*
H9B	0.2217	0.4618	0.6665	0.036*
C10	0.2346 (2)	0.50554 (10)	0.79358 (15)	0.0291 (4)
H10A	0.1930	0.5472	0.7647	0.035*
H10B	0.3059	0.5169	0.8510	0.035*
C11	0.1332 (2)	0.46278 (10)	0.81885 (16)	0.0293 (4)
H11A	0.0582	0.4547	0.7623	0.035*
H11B	0.1000	0.4865	0.8647	0.035*
C12	0.19240 (19)	0.39641 (9)	0.86022 (14)	0.0222 (4)
H12A	0.1231	0.3686	0.8723	0.027*
H12B	0.2608	0.4042	0.9205	0.027*
C13	0.45996 (16)	0.29384 (8)	0.95274 (11)	0.0147 (3)
H13A	0.4399	0.2761	1.0083	0.018*
H13B	0.4883	0.3406	0.9629	0.018*
C14	0.60524 (17)	0.16181 (9)	0.97685 (12)	0.0168 (3)
H14	0.5288	0.1331	0.9448	0.020*
C15	0.7263 (2)	0.12752 (9)	0.96282 (13)	0.0231 (4)
H15A	0.7189	0.1268	0.8956	0.028*
H15B	0.8064	0.1526	0.9960	0.028*
C16	0.7371 (2)	0.05674 (10)	1.00019 (14)	0.0300 (5)
H16A	0.8185	0.0363	0.9947	0.036*
H16B	0.6619	0.0305	0.9619	0.036*
C17	0.7388 (2)	0.05499 (11)	1.10233 (14)	0.0320 (5)
H17A	0.7388	0.0084	1.1227	0.038*
H17B	0.8201	0.0762	1.1418	0.038*
C18	0.6198 (2)	0.09083 (9)	1.11558 (13)	0.0243 (4)
H18A	0.6259	0.0907	1.1826	0.029*
H18B	0.5389	0.0669	1.0811	0.029*
C19	0.61176 (19)	0.16234 (9)	1.08058 (12)	0.0195 (4)
H19A	0.6898	0.1874	1.1174	0.023*
H19B	0.5327	0.1841	1.0881	0.023*
C20	0.73094 (17)	0.28521 (9)	0.93334 (12)	0.0173 (3)
H20	0.7951	0.2521	0.9237	0.021*
C21	0.71984 (19)	0.33969 (10)	0.86050 (13)	0.0220 (4)
H21A	0.6856	0.3207	0.7970	0.026*
H21B	0.6576	0.3740	0.8676	0.026*
C22	0.8540 (2)	0.37096 (10)	0.87262 (14)	0.0259 (4)

H22A	0.8448	0.4071	0.8267	0.031*	
H22B	0.9139	0.3373	0.8603	0.031*	
C23	0.91271 (19)	0.39850 (10)	0.97123 (14)	0.0250 (4)	
H23A	1.0013	0.4164	0.9780	0.030*	
H23B	0.8573	0.4353	0.9813	0.030*	
C24	0.92213 (19)	0.34531 (11)	1.04445 (14)	0.0281 (4)	
H24A	0.9543	0.3654	1.1074	0.034*	
H24B	0.9864	0.3114	1.0394	0.034*	
C25	0.78904 (19)	0.31208 (11)	1.03284 (13)	0.0251 (4)	
H25A	0.8004	0.2753	1.0781	0.030*	
H25B	0.7278	0.3446	1.0461	0.030*	
Cl3	0.39612 (6)	0.01216 (3)	0.56653 (4)	0.03819 (13)	
C26	0.3451 (16)	0.0691 (4)	0.6368 (9)	0.0492 (10)	0.5755 (15)
H26A	0.4232	0.0816	0.6890	0.059*	0.5755 (15)
H26B	0.3149	0.1095	0.5992	0.059*	0.5755 (15)
Cl4	0.22199 (18)	0.04556 (6)	0.68461 (10)	0.0584 (3)	0.5755 (15)
C26A	0.350 (2)	0.0762 (5)	0.6273 (12)	0.0492 (10)	0.4245 (15)
H26C	0.4206	0.1097	0.6459	0.059*	0.4245 (15)
H26D	0.2695	0.0979	0.5873	0.059*	0.4245 (15)
Cl4A	0.3214 (3)	0.04277 (8)	0.72482 (14)	0.0584 (3)	0.4245 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.01279 (6)	0.01723 (7)	0.01114 (6)	0.00052 (5)	0.00407 (5)	0.00010 (4)
Cl1	0.0177 (2)	0.0280 (2)	0.01247 (18)	0.00222 (16)	0.00295 (15)	0.00058 (15)
Cl2	0.0178 (2)	0.0288 (2)	0.0184 (2)	0.00419 (16)	0.00797 (16)	−0.00154 (16)
P1	0.0119 (2)	0.0162 (2)	0.01268 (19)	0.00027 (15)	0.00344 (16)	0.00006 (15)
P2	0.0127 (2)	0.0175 (2)	0.01261 (19)	0.00122 (16)	0.00358 (16)	0.00073 (15)
C1	0.0129 (8)	0.0169 (8)	0.0163 (8)	−0.0011 (6)	0.0059 (6)	−0.0009 (6)
C2	0.0169 (8)	0.0174 (8)	0.0208 (9)	−0.0003 (6)	0.0058 (7)	0.0001 (6)
C3	0.0238 (9)	0.0188 (9)	0.0259 (10)	−0.0035 (7)	0.0093 (8)	−0.0001 (7)
C4	0.0233 (10)	0.0229 (9)	0.0302 (10)	−0.0073 (7)	0.0117 (8)	−0.0055 (8)
C5	0.0136 (8)	0.0283 (10)	0.0276 (10)	−0.0037 (7)	0.0060 (7)	−0.0033 (8)
C6	0.0151 (8)	0.0260 (9)	0.0185 (9)	−0.0020 (7)	0.0032 (7)	−0.0010 (7)
C7	0.0155 (8)	0.0176 (8)	0.0177 (8)	0.0011 (6)	0.0024 (7)	0.0023 (6)
C8	0.0232 (10)	0.0227 (9)	0.0268 (10)	0.0001 (7)	0.0099 (8)	0.0062 (7)
C9	0.0315 (11)	0.0263 (10)	0.0304 (11)	−0.0001 (8)	0.0066 (9)	0.0112 (8)
C10	0.0264 (10)	0.0190 (9)	0.0371 (11)	0.0027 (8)	0.0025 (9)	0.0082 (8)
C11	0.0220 (10)	0.0201 (9)	0.0449 (13)	0.0049 (7)	0.0087 (9)	0.0034 (8)
C12	0.0192 (9)	0.0196 (9)	0.0300 (10)	0.0019 (7)	0.0107 (8)	0.0015 (7)
C13	0.0129 (8)	0.0157 (8)	0.0151 (8)	0.0006 (6)	0.0039 (6)	−0.0014 (6)
C14	0.0174 (8)	0.0173 (8)	0.0156 (8)	0.0023 (6)	0.0047 (7)	0.0021 (6)
C15	0.0274 (10)	0.0239 (9)	0.0205 (9)	0.0095 (7)	0.0109 (8)	0.0041 (7)
C16	0.0436 (13)	0.0243 (10)	0.0266 (10)	0.0147 (9)	0.0172 (9)	0.0045 (8)
C17	0.0474 (13)	0.0262 (10)	0.0242 (10)	0.0160 (9)	0.0137 (9)	0.0083 (8)
C18	0.0362 (11)	0.0212 (9)	0.0174 (9)	0.0039 (8)	0.0109 (8)	0.0021 (7)
C19	0.0226 (9)	0.0205 (9)	0.0160 (8)	0.0032 (7)	0.0070 (7)	0.0009 (6)

C20	0.0119 (8)	0.0218 (9)	0.0184 (8)	0.0009 (6)	0.0048 (7)	0.0016 (6)
C21	0.0213 (9)	0.0251 (9)	0.0177 (9)	−0.0048 (7)	0.0034 (7)	0.0022 (7)
C22	0.0259 (10)	0.0312 (11)	0.0226 (9)	−0.0083 (8)	0.0104 (8)	0.0006 (8)
C23	0.0187 (9)	0.0304 (10)	0.0243 (10)	−0.0052 (8)	0.0042 (8)	0.0015 (8)
C24	0.0172 (9)	0.0378 (12)	0.0246 (10)	−0.0061 (8)	−0.0007 (8)	0.0042 (8)
C25	0.0200 (9)	0.0364 (11)	0.0161 (9)	−0.0070 (8)	0.0015 (7)	0.0035 (8)
Cl3	0.0340 (3)	0.0310 (3)	0.0464 (3)	0.0093 (2)	0.0075 (2)	0.0033 (2)
C26	0.053 (2)	0.0254 (19)	0.078 (3)	−0.0104 (18)	0.0321 (18)	−0.0084 (19)
Cl4	0.1019 (10)	0.0379 (4)	0.0566 (7)	−0.0043 (7)	0.0557 (7)	0.0007 (5)
C26A	0.053 (2)	0.0254 (19)	0.078 (3)	−0.0104 (18)	0.0321 (18)	−0.0084 (19)
Cl4A	0.1019 (10)	0.0379 (4)	0.0566 (7)	−0.0043 (7)	0.0557 (7)	0.0007 (5)

Geometric parameters (Å, °)

Pd1—P1	2.2205 (4)	C13—H13A	0.9900
Pd1—P2	2.2345 (5)	C13—H13B	0.9900
Pd1—Cl2	2.3756 (4)	C14—C15	1.539 (2)
Pd1—Cl1	2.3815 (4)	C14—C19	1.540 (2)
P1—C7	1.8316 (18)	C14—H14	1.0000
P1—C1	1.8330 (17)	C15—C16	1.529 (3)
P1—C13	1.8459 (17)	C15—H15A	0.9900
P2—C20	1.8297 (18)	C15—H15B	0.9900
P2—C14	1.8435 (18)	C16—C17	1.531 (3)
P2—C13	1.8464 (17)	C16—H16A	0.9900
C1—C6	1.534 (2)	C16—H16B	0.9900
C1—C2	1.537 (2)	C17—C18	1.529 (3)
C1—H1	1.0000	C17—H17A	0.9900
C2—C3	1.527 (2)	C17—H17B	0.9900
C2—H2A	0.9900	C18—C19	1.532 (3)
C2—H2B	0.9900	C18—H18A	0.9900
C3—C4	1.524 (3)	C18—H18B	0.9900
C3—H3A	0.9900	C19—H19A	0.9900
C3—H3B	0.9900	C19—H19B	0.9900
C4—C5	1.525 (3)	C20—C21	1.532 (2)
C4—H4A	0.9900	C20—C25	1.535 (3)
C4—H4B	0.9900	C20—H20	1.0000
C5—C6	1.531 (3)	C21—C22	1.527 (3)
C5—H5A	0.9900	C21—H21A	0.9900
C5—H5B	0.9900	C21—H21B	0.9900
C6—H6A	0.9900	C22—C23	1.529 (3)
C6—H6B	0.9900	C22—H22A	0.9900
C7—C8	1.533 (2)	C22—H22B	0.9900
C7—C12	1.535 (3)	C23—C24	1.520 (3)
C7—H7	1.0000	C23—H23A	0.9900
C8—C9	1.533 (3)	C23—H23B	0.9900
C8—H8A	0.9900	C24—C25	1.536 (3)
C8—H8B	0.9900	C24—H24A	0.9900
C9—C10	1.522 (3)	C24—H24B	0.9900
C9—H9A	0.9900	C25—H25A	0.9900

C9—H9B	0.9900	C25—H25B	0.9900
C10—C11	1.523 (3)	Cl3—C26A	1.740 (9)
C10—H10A	0.9900	Cl3—C26	1.757 (6)
C10—H10B	0.9900	C26—Cl4	1.747 (9)
C11—C12	1.533 (3)	C26—H26A	0.9900
C11—H11A	0.9900	C26—H26B	0.9900
C11—H11B	0.9900	C26A—Cl4A	1.724 (9)
C12—H12A	0.9900	C26A—H26C	0.9900
C12—H12B	0.9900	C26A—H26D	0.9900
P1—Pd1—P2	73.816 (16)	P1—C13—P2	92.87 (8)
P1—Pd1—Cl2	170.092 (17)	P1—C13—H13A	113.1
P2—Pd1—Cl2	96.291 (16)	P2—C13—H13A	113.1
P1—Pd1—Cl1	93.670 (16)	P1—C13—H13B	113.1
P2—Pd1—Cl1	167.313 (16)	P2—C13—H13B	113.1
Cl2—Pd1—Cl1	96.195 (16)	H13A—C13—H13B	110.5
C7—P1—C1	108.02 (8)	C15—C14—C19	111.11 (14)
C7—P1—C13	110.87 (8)	C15—C14—P2	110.30 (12)
C1—P1—C13	107.22 (8)	C19—C14—P2	117.28 (12)
C7—P1—Pd1	115.18 (6)	C15—C14—H14	105.8
C1—P1—Pd1	118.46 (6)	C19—C14—H14	105.8
C13—P1—Pd1	96.16 (5)	P2—C14—H14	105.8
C20—P2—C14	109.44 (8)	C16—C15—C14	110.13 (16)
C20—P2—C13	109.67 (8)	C16—C15—H15A	109.6
C14—P2—C13	111.74 (8)	C14—C15—H15A	109.6
C20—P2—Pd1	116.70 (6)	C16—C15—H15B	109.6
C14—P2—Pd1	112.93 (6)	C14—C15—H15B	109.6
C13—P2—Pd1	95.67 (5)	H15A—C15—H15B	108.1
C6—C1—C2	110.56 (14)	C15—C16—C17	111.53 (17)
C6—C1—P1	112.12 (12)	C15—C16—H16A	109.3
C2—C1—P1	111.10 (12)	C17—C16—H16A	109.3
C6—C1—H1	107.6	C15—C16—H16B	109.3
C2—C1—H1	107.6	C17—C16—H16B	109.3
P1—C1—H1	107.6	H16A—C16—H16B	108.0
C3—C2—C1	110.67 (15)	C18—C17—C16	111.26 (17)
C3—C2—H2A	109.5	C18—C17—H17A	109.4
C1—C2—H2A	109.5	C16—C17—H17A	109.4
C3—C2—H2B	109.5	C18—C17—H17B	109.4
C1—C2—H2B	109.5	C16—C17—H17B	109.4
H2A—C2—H2B	108.1	H17A—C17—H17B	108.0
C4—C3—C2	111.16 (16)	C17—C18—C19	111.40 (17)
C4—C3—H3A	109.4	C17—C18—H18A	109.3
C2—C3—H3A	109.4	C19—C18—H18A	109.3
C4—C3—H3B	109.4	C17—C18—H18B	109.3
C2—C3—H3B	109.4	C19—C18—H18B	109.3
H3A—C3—H3B	108.0	H18A—C18—H18B	108.0
C3—C4—C5	110.65 (16)	C18—C19—C14	108.78 (15)
C3—C4—H4A	109.5	C18—C19—H19A	109.9
C5—C4—H4A	109.5	C14—C19—H19A	109.9
C3—C4—H4B	109.5	C18—C19—H19B	109.9

C5—C4—H4B	109.5	C14—C19—H19B	109.9
H4A—C4—H4B	108.1	H19A—C19—H19B	108.3
C4—C5—C6	111.93 (15)	C21—C20—C25	111.28 (15)
C4—C5—H5A	109.2	C21—C20—P2	111.44 (12)
C6—C5—H5A	109.2	C25—C20—P2	113.85 (12)
C4—C5—H5B	109.2	C21—C20—H20	106.6
C6—C5—H5B	109.2	C25—C20—H20	106.6
H5A—C5—H5B	107.9	P2—C20—H20	106.6
C5—C6—C1	110.42 (15)	C22—C21—C20	110.22 (15)
C5—C6—H6A	109.6	C22—C21—H21A	109.6
C1—C6—H6A	109.6	C20—C21—H21A	109.6
C5—C6—H6B	109.6	C22—C21—H21B	109.6
C1—C6—H6B	109.6	C20—C21—H21B	109.6
H6A—C6—H6B	108.1	H21A—C21—H21B	108.1
C8—C7—C12	111.66 (15)	C21—C22—C23	111.20 (16)
C8—C7—P1	111.21 (12)	C21—C22—H22A	109.4
C12—C7—P1	111.78 (12)	C23—C22—H22A	109.4
C8—C7—H7	107.3	C21—C22—H22B	109.4
C12—C7—H7	107.3	C23—C22—H22B	109.4
P1—C7—H7	107.3	H22A—C22—H22B	108.0
C7—C8—C9	111.12 (16)	C24—C23—C22	111.22 (17)
C7—C8—H8A	109.4	C24—C23—H23A	109.4
C9—C8—H8A	109.4	C22—C23—H23A	109.4
C7—C8—H8B	109.4	C24—C23—H23B	109.4
C9—C8—H8B	109.4	C22—C23—H23B	109.4
H8A—C8—H8B	108.0	H23A—C23—H23B	108.0
C10—C9—C8	111.56 (17)	C23—C24—C25	111.80 (16)
C10—C9—H9A	109.3	C23—C24—H24A	109.3
C8—C9—H9A	109.3	C25—C24—H24A	109.3
C10—C9—H9B	109.3	C23—C24—H24B	109.3
C8—C9—H9B	109.3	C25—C24—H24B	109.3
H9A—C9—H9B	108.0	H24A—C24—H24B	107.9
C9—C10—C11	110.84 (18)	C20—C25—C24	110.69 (16)
C9—C10—H10A	109.5	C20—C25—H25A	109.5
C11—C10—H10A	109.5	C24—C25—H25A	109.5
C9—C10—H10B	109.5	C20—C25—H25B	109.5
C11—C10—H10B	109.5	C24—C25—H25B	109.5
H10A—C10—H10B	108.1	H25A—C25—H25B	108.1
C10—C11—C12	111.10 (16)	Cl4—C26—Cl3	118.6 (6)
C10—C11—H11A	109.4	Cl4—C26—H26A	107.7
C12—C11—H11A	109.4	Cl3—C26—H26A	107.7
C10—C11—H11B	109.4	Cl4—C26—H26B	107.7
C12—C11—H11B	109.4	Cl3—C26—H26B	107.7
H11A—C11—H11B	108.0	H26A—C26—H26B	107.1
C11—C12—C7	111.31 (16)	Cl4A—C26A—Cl3	107.8 (6)
C11—C12—H12A	109.4	Cl4A—C26A—H26C	110.1
C7—C12—H12A	109.4	Cl3—C26A—H26C	110.1
C11—C12—H12B	109.4	Cl4A—C26A—H26D	110.1
C7—C12—H12B	109.4	Cl3—C26A—H26D	110.1

H12A—C12—H12B	108.0	H26C—C26A—H26D	108.5

Fig. 1