Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

trans-Bromido(pyrimidinyl-κC^2)-bis(triphenylphosphane-κP)palladium(II)

Gene-Hsiang Lee,[a]* Hsiao-Fen Wang[b] and Kuang-Hway Yih[b]*

[a]Instrumentation Center, College of Science, National Taiwan University, Taipei 106, Taiwan, and [b]Department of Applied Cosmetology, Hungkuang University, Shalu 433, Taichung, Taiwan
Correspondence e-mail: ghlee@ntu.edu.tw, khyih@sunrise.hk.edu.tw

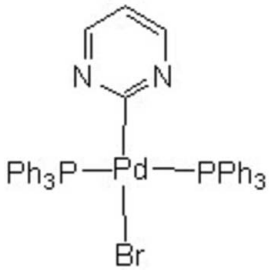
Received 21 September 2010; accepted 26 September 2010

Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.058; data-to-parameter ratio = 18.7.

In the title complex, $[PdBr(C_4H_3N_2)(C_{18}H_{15}P)_2]$, the geometry around the Pd^{II} atom is distorted square-planar with the Pd^{II} atom displaced by 0.0150 (5) Å from the least-squares BrP_2C plane. Two PPh_3 ligands are in *trans* positions [P—Pd—P = 176.743 (17)°], while the pyrimidinyl ligand and Br atom are *trans* to one another [C—Pd—Br = 176.56 (5)°]. Structural parameters from NMR, IR and mass spectra are in agreement with the crystal structure of the title compound.

Related literature

For reactions in organic synthesis that form C—C bonds, see: Steffen *et al.* (2005); Beeby *et al.* (2004); Chin *et al.* (1988); Dobrzynski & Angelici (1975). For Pd—C(carbene) bond lengths, see: Cardin *et al.* (1972) and for Pd—Br bond lengths, see: Yih & Lee (2008); Yih *et al.* (2009). For 4,6-dimethyl-2-mercaptopyrimidine, see: Hong *et al.* (2002).



Experimental

Crystal data

$[PdBr(C_4H_3N_2)(C_{18}H_{15}P)_2]$
M_r = 789.93
Triclinic, $P\overline{1}$
a = 12.1051 (8) Å
b = 12.7791 (8) Å
c = 12.8987 (8) Å
α = 90.257 (2)°
β = 117.044 (2)°
γ = 105.580 (2)°
V = 1693.11 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.86 mm^{-1}
T = 150 K
0.50 × 0.35 × 0.25 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.457, T_{max} = 0.654
22016 measured reflections
7762 independent reflections
7066 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.058
S = 1.02
7762 reflections
415 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

We thank the National Science Council of the Republic of China for financial support (NSC98–2113-M-241–011-MY2).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2211).

References

Beeby, A., Bettington, S., Fairlamb, I. J. S., Goeta, A. E., Kapdi, A. R., Niemela, E. H. & Thompson, A. L. (2004). *New J. Chem.* **28**, 600–605.
Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cardin, D. J., Cetinkaya, B. & Lappert, M. F. (1972). *Chem. Rev.* **72**, 545–574.
Chin, C. H., Yeo, S. L., Loh, Z. H., Vittal, J. J., Henderson, W. & Hor, T. S. A. (1988). *J. Chem. Soc. Dalton Trans.* pp. 3777–3784.
Dobrzynski, E. D. & Angelici, R. J. (1975). *Inorg. Chem.* **14**, 1513–1518.
Hong, F. U., Huang, Y. L., Chen, P. P. & Chang, Y. C. (2002). *J. Organomet. Chem.* **655**, 49–54.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Steffen, A., Sladek, M. I., Braun, T., Neumann, B. & Stammler, H. G. (2005). *Organometallics*, **24**, 4057–4064.
Yih, K. H. & Lee, G. H. (2008). *J. Chin. Chem. Soc.* **55**, 109–114.
Yih, K. H., Wang, H. F., Huang, K. F., Kwan, C. C. & Lee, G. H. (2009). *J. Chin. Chem. Soc.* **56**, 718–724.

supporting information

Acta Cryst. (2010). E**66**, m1345 [https://doi.org/10.1107/S1600536810038511]

trans-Bromido(pyrimidinyl-κC^2)bis(triphenylphosphane-κP)palladium(II)

Gene-Hsiang Lee, Hsiao-Fen Wang and Kuang-Hway Yih

S1. Comment

C—C coupling reactions of pyrimidinyl nickel complexes (Steffen *et al.*, 2005), Suzuki cross-coupling reactions of pyridyl-bridged palladium complex (Beeby, *et al.*, 2004), and intramolecular reductive elimination of Pd—N binuclear complex $[Pd(\mu\text{-}C_9H_6N)(\mu\text{-dppm})]_2(Cl)_2$ (Chin *et al.*, 1988) are some of important reactions in organic synthesis by forming C—C bond (Dobrzynski & Angelici, 1975). To our knowledge, no 2-palladiumpyrimidine crystal structure has been described.

To synthesis of 2-palladiumpyrimidine compound, complex $[Pd(PPh_3)_4]$ was used to react with 2-bromopyrimidine in dichloromethane at room temperature. As a result, a two triphenylphosphine displaced complex $[Pd(Br)(C_4H_3N_2)(PPh_3)_2]$ was isolated with 95% yield. The X-ray crystal structure analysis has been carried out to provide structural parameters.

The molecular structure of the title compound is shown in Fig. 1. In the title complex (I), the palladium atom has a distorted square planar geometry. The palladium atom is displaced by 0.0150 (5)Å from the least-squares plane of BrP1P2C1. The Pd—C1 bond distance, 1.9985 (18) Å, is longer than other Pd^{II}-carbon(carbonyl) distances, and similar to those of Pd—C(carbene) distances (Cardin *et al.*, 1972, and references therein). Two PPh_3 ligands are in *trans* position: P1—Pd—P2, 176.743 (17)°, while the pyrimidinyl ligand and bromide are *trans* to each other: C1—Pd—Br1, 176.56 (5)°. The Pd—N bond distances (2.8489 (17) and 2.8703 (16) Å) indicate no bonding interaction between the nitrogen atom and palladium metal atom. Within the pyrimidinyl ligand itself, the geometry is consistent with a significant partial double bond character in the C—C and C—N bond. The C—N bond distances (1.330 (2) ~1.340 (3) Å) are typical for a C—N bond having partial double bond character and are certainly much shorter than the normal C—N (1.47 Å) single bond. The Pd—C1 (1.9985 (18) Å) and Pd—Br (2.5353 (3) Å) lengths of (I) are in agreement with reported value (Yih *et al.*, 2008, 2009).

The $^{31}P\{^1H\}$ NMR spectra of (I) shows a singlet resonances at δ 21.4. In the ^1H NMR spectra, the 4-H and 5-H protons of the pyrimidinyl group exhibit two singlet resonances at δ 7.86 and at δ 7.52. The $^{13}C\{^1H\}$ NMR spectra of (I) reveals two singlet at δ 114.2 and at δ 154.4 which are assigned to the 5-C and 4-C carbon atom of the pyrimidinyl group. It is also noted the IR spectrum of the title complex (I) shows two stretching bands at 1546 and 1537 cm^{-1} for C═N groups. In the FAB mass spectra, base peak with the typical Pd isotope distribution is in agreement with the $[M^+]$ molecular mass of (I).

S2. Experimental

The synthesis of the title compound (I) was carried out as follows. 2-Bromo-pyrimidine (0.191 g, 1.2 mmol) was added to a flask (100 ml) containing $Pd(PPh_3)_4$ (1.155 g, 1.0 mmol) and CH_2Cl_2 (20 ml) at ambient temperature. The mixture was stirred for 2 h. The solvent was concentrated to 10 ml, and 20 ml of diethyl ether was added to the solution. The pale-yellow solids were formed which were isolated by filtration (G4), washed with n-hexane (2 *x* 10 ml) and subsequently dried under vacuum yielding 0.750 g (95%) of the complex $[Pd(PPh_3)_2(C_4H_3N_2)Br]$, (I). Spectroscopic data for (I):

$^{31}P\{^{1}H\}$ NMR: δ 21.4 (s, PPh_3). ^{1}H NMR: δ 7.23–7.66 (m, 30H, $2PPh_3$), 7.52 (s, 1H, 5-H of pyrimidinyl), 7.86 (s, 2H, 4-H of pyrimidinyl). $^{13}C\{^{1}H\}$ NMR: δ 128.0 (m, *o*-C of Ph), 129.9 (m, *p*-C of Ph), 134.8 (m, *m*-C of Ph), 114.2 (s, 4-C of pyrimidinyl), 154.4 (s, 5-C of pyrimidinyl). MS (FAB, NBA, m/*z*): 789 [M^+]. Anal. Calcd. for $C_{40}H_{33}BrN_2P_2Pd$: C, 60.82; H, 4.21; N, 3.55. Found: C, 60.94; H, 4.31; N, 3.18.

S3. Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å and with U_{iso}(H) = 1.2 times U_{eq}(C).

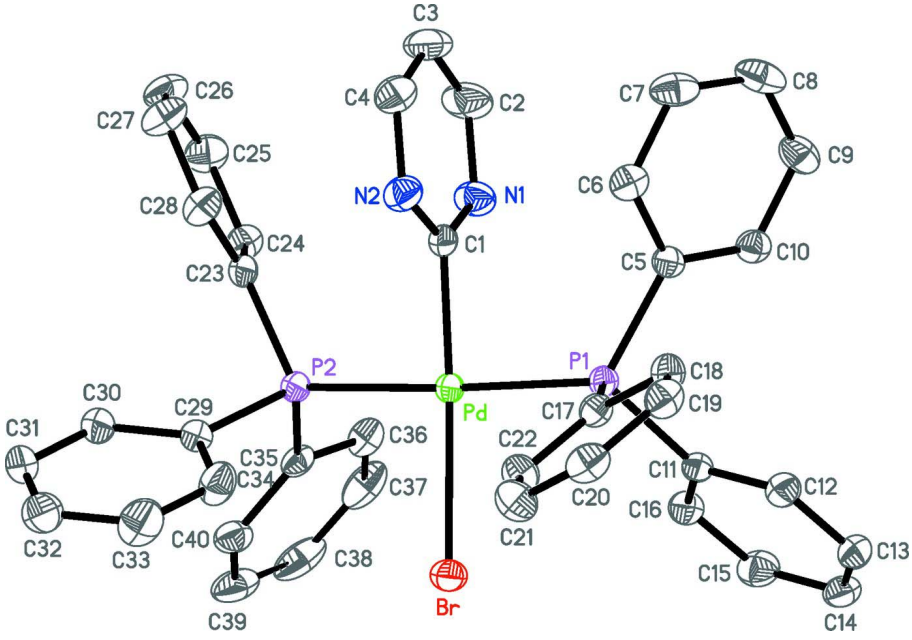


Figure 1

The molecular structure of title compound, with atom labels and 50% probability displacement ellipsoids for non-H atoms.

***trans*-Bromido(pyrimidinyl-κC^2)bis(triphenylphosphane- κP)palladium(II)**

Crystal data

$[PdBr(C_4H_3N_2)(C_{18}H_{15}P)_2]$
M_r = 789.93
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 12.1051 (8) Å
b = 12.7791 (8) Å
c = 12.8987 (8) Å
α = 90.257 (2)°
β = 117.044 (2)°
γ = 105.580 (2)°
V = 1693.11 (19) Å^3
Z = 2
F(000) = 796
D_x = 1.549 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5205 reflections
θ = 2.2–27.5°
μ = 1.86 mm^{-1}
T = 150 K
Rod, light yellow
0.50 × 0.35 × 0.25 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.457, T_{max} = 0.654
22016 measured reflections
7762 independent reflections
7066 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°, θ_{min} = 1.9°
h = −15→15
k = −16→16
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.058
S = 1.02
7762 reflections
415 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0252P)^2 + 0.8169P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 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. 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Pd	0.373889 (12)	0.223763 (11)	0.271056 (12)	0.01685 (4)
Br	0.402981 (18)	0.428222 (15)	0.282253 (18)	0.02526 (5)
P1	0.16970 (4)	0.18272 (4)	0.26328 (4)	0.01688 (9)
P2	0.57904 (4)	0.25675 (4)	0.28544 (4)	0.01794 (9)
N1	0.31551 (17)	0.01119 (14)	0.15413 (15)	0.0285 (4)
N2	0.40272 (16)	0.02238 (14)	0.36125 (15)	0.0265 (4)
C1	0.36051 (17)	0.06436 (15)	0.26102 (16)	0.0195 (3)
C2	0.3112 (2)	−0.09446 (18)	0.1485 (2)	0.0391 (5)
H2	0.2787	−0.1355	0.0736	0.047*
C3	0.3515 (2)	−0.14614 (18)	0.2462 (2)	0.0387 (5)
H3	0.3476	−0.2213	0.2406	0.046*
C4	0.3980 (2)	−0.08343 (17)	0.35255 (19)	0.0324 (5)
H4	0.4277	−0.1162	0.4222	0.039*
C5	0.06796 (17)	0.03960 (15)	0.21717 (16)	0.0191 (4)
C6	0.10631 (19)	−0.03726 (16)	0.29124 (17)	0.0245 (4)
H6	0.1829	−0.0140	0.3651	0.029*

C7	0.0338 (2)	−0.14719 (17)	0.25813 (19)	0.0298 (4)
H7	0.0612	−0.1993	0.3086	0.036*
C8	−0.0787 (2)	−0.18086 (17)	0.1512 (2)	0.0323 (5)
H8	−0.1295	−0.2560	0.1289	0.039*
C9	−0.1176 (2)	−0.10562 (16)	0.07663 (18)	0.0284 (4)
H9	−0.1946	−0.1292	0.0031	0.034*
C10	−0.04417 (18)	0.00417 (15)	0.10901 (17)	0.0216 (4)
H10	−0.0705	0.0555	0.0571	0.026*
C11	0.06149 (17)	0.25643 (14)	0.16714 (16)	0.0190 (4)
C12	−0.04724 (18)	0.26179 (15)	0.17709 (17)	0.0237 (4)
H12	−0.0637	0.2294	0.2368	0.028*
C13	−0.13095 (19)	0.31432 (16)	0.10011 (18)	0.0269 (4)
H13	−0.2045	0.3179	0.1075	0.032*
C14	−0.1082 (2)	0.36161 (16)	0.01236 (18)	0.0293 (4)
H14	−0.1657	0.3977	−0.0401	0.035*
C15	−0.0016 (2)	0.35582 (17)	0.00179 (18)	0.0295 (4)
H15	0.0137	0.3873	−0.0589	0.035*
C16	0.08367 (19)	0.30429 (15)	0.07917 (17)	0.0233 (4)
H16	0.1576	0.3018	0.0719	0.028*
C17	0.18063 (17)	0.21461 (15)	0.40637 (16)	0.0198 (4)
C18	0.08158 (18)	0.15884 (16)	0.43204 (17)	0.0230 (4)
H18	0.0093	0.1015	0.3757	0.028*
C19	0.08851 (19)	0.18684 (17)	0.53916 (17)	0.0257 (4)
H19	0.0212	0.1487	0.5563	0.031*
C20	0.1937 (2)	0.27055 (17)	0.62123 (17)	0.0275 (4)
H20	0.1983	0.2897	0.6947	0.033*
C21	0.2918 (2)	0.32624 (17)	0.59664 (18)	0.0300 (4)
H21	0.3635	0.3839	0.6530	0.036*
C22	0.28583 (19)	0.29816 (16)	0.48958 (17)	0.0256 (4)
H22	0.3539	0.3362	0.4733	0.031*
C23	0.63295 (17)	0.14058 (15)	0.26504 (17)	0.0205 (4)
C24	0.63245 (19)	0.10873 (16)	0.16108 (17)	0.0242 (4)
H24	0.6049	0.1493	0.0974	0.029*
C25	0.6716 (2)	0.01883 (17)	0.14949 (19)	0.0304 (4)
H25	0.6705	−0.0020	0.0782	0.036*
C26	0.7119 (2)	−0.04028 (17)	0.2415 (2)	0.0323 (5)
H26	0.7402	−0.1011	0.2342	0.039*
C27	0.7112 (2)	−0.01134 (18)	0.3444 (2)	0.0337 (5)
H27	0.7370	−0.0534	0.4070	0.040*
C28	0.67292 (19)	0.07904 (17)	0.35664 (18)	0.0270 (4)
H28	0.6740	0.0991	0.4282	0.032*
C29	0.71134 (17)	0.33035 (15)	0.42804 (16)	0.0213 (4)
C30	0.84045 (18)	0.34118 (16)	0.45735 (18)	0.0260 (4)
H30	0.8595	0.3091	0.4033	0.031*
C31	0.9408 (2)	0.39853 (17)	0.56511 (19)	0.0316 (5)
H31	1.0286	0.4063	0.5843	0.038*
C32	0.9138 (2)	0.44424 (18)	0.6445 (2)	0.0379 (5)
H32	0.9828	0.4835	0.7183	0.045*

C33	0.7862 (2)	0.4330 (2)	0.6167 (2)	0.0397 (5)
H33	0.7677	0.4645	0.6715	0.048*
C34	0.6852 (2)	0.37604 (18)	0.50921 (18)	0.0311 (5)
H34	0.5977	0.3682	0.4909	0.037*
C35	0.59335 (18)	0.33938 (15)	0.17515 (17)	0.0210 (4)
C36	0.5034 (2)	0.29949 (17)	0.05672 (18)	0.0282 (4)
H36	0.4329	0.2344	0.0366	0.034*
C37	0.5167 (2)	0.3544 (2)	−0.0311 (2)	0.0376 (5)
H37	0.4576	0.3251	−0.1114	0.045*
C38	0.6157 (3)	0.4516 (2)	−0.0027 (2)	0.0406 (6)
H38	0.6243	0.4893	−0.0631	0.049*
C39	0.7017 (2)	0.49357 (18)	0.1138 (2)	0.0362 (5)
H39	0.7687	0.5611	0.1333	0.043*
C40	0.6914 (2)	0.43795 (16)	0.20293 (19)	0.0263 (4)
H40	0.7514	0.4674	0.2829	0.032*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd	0.01563 (7)	0.01653 (7)	0.01959 (7)	0.00490 (5)	0.00931 (6)	0.00247 (5)
Br	0.02570 (10)	0.01863 (9)	0.03430 (11)	0.00637 (7)	0.01675 (9)	0.00424 (8)
P1	0.0163 (2)	0.0174 (2)	0.0180 (2)	0.00520 (17)	0.00902 (18)	0.00283 (17)
P2	0.0165 (2)	0.0182 (2)	0.0203 (2)	0.00569 (17)	0.00951 (18)	0.00209 (18)
N1	0.0332 (9)	0.0225 (8)	0.0243 (9)	0.0072 (7)	0.0099 (7)	0.0001 (7)
N2	0.0291 (9)	0.0254 (8)	0.0253 (8)	0.0116 (7)	0.0114 (7)	0.0066 (7)
C1	0.0158 (8)	0.0193 (7)	0.0242 (9)	0.0059 (7)	0.0099 (7)	0.0045 (7)
C2	0.0500 (14)	0.0248 (11)	0.0315 (12)	0.0091 (10)	0.0115 (10)	−0.0059 (9)
C3	0.0465 (13)	0.0196 (10)	0.0445 (13)	0.0125 (9)	0.0157 (11)	0.0042 (9)
C4	0.0352 (11)	0.0293 (11)	0.0328 (11)	0.0143 (9)	0.0136 (9)	0.0122 (9)
C5	0.0199 (8)	0.0179 (8)	0.0240 (9)	0.0051 (7)	0.0144 (7)	0.0024 (7)
C6	0.0286 (10)	0.0256 (10)	0.0249 (10)	0.0107 (8)	0.0160 (8)	0.0064 (8)
C7	0.0473 (13)	0.0226 (10)	0.0344 (11)	0.0138 (9)	0.0298 (10)	0.0100 (8)
C8	0.0459 (13)	0.0191 (10)	0.0392 (12)	0.0011 (9)	0.0308 (11)	0.0006 (9)
C9	0.0296 (10)	0.0249 (10)	0.0280 (10)	0.0009 (8)	0.0156 (9)	−0.0040 (8)
C10	0.0237 (9)	0.0208 (9)	0.0239 (9)	0.0074 (7)	0.0137 (8)	0.0032 (7)
C11	0.0183 (8)	0.0162 (8)	0.0199 (9)	0.0051 (7)	0.0070 (7)	−0.0008 (7)
C12	0.0240 (9)	0.0227 (9)	0.0265 (10)	0.0085 (8)	0.0127 (8)	0.0033 (8)
C13	0.0222 (9)	0.0234 (10)	0.0342 (11)	0.0093 (8)	0.0113 (8)	−0.0004 (8)
C14	0.0286 (10)	0.0204 (9)	0.0316 (11)	0.0109 (8)	0.0064 (9)	0.0039 (8)
C15	0.0353 (11)	0.0259 (10)	0.0277 (10)	0.0111 (9)	0.0142 (9)	0.0095 (8)
C16	0.0241 (9)	0.0216 (9)	0.0241 (9)	0.0066 (7)	0.0117 (8)	0.0030 (7)
C17	0.0209 (9)	0.0218 (9)	0.0190 (9)	0.0085 (7)	0.0102 (7)	0.0037 (7)
C18	0.0212 (9)	0.0256 (10)	0.0227 (9)	0.0069 (8)	0.0110 (8)	0.0032 (8)
C19	0.0279 (10)	0.0301 (10)	0.0280 (10)	0.0118 (8)	0.0189 (9)	0.0085 (8)
C20	0.0364 (11)	0.0310 (11)	0.0209 (9)	0.0161 (9)	0.0152 (9)	0.0036 (8)
C21	0.0316 (11)	0.0297 (11)	0.0224 (10)	0.0047 (9)	0.0101 (9)	−0.0031 (8)
C22	0.0249 (10)	0.0260 (10)	0.0252 (10)	0.0054 (8)	0.0125 (8)	0.0031 (8)
C23	0.0161 (8)	0.0206 (9)	0.0256 (9)	0.0056 (7)	0.0106 (7)	0.0022 (7)

C24	0.0260 (10)	0.0243 (10)	0.0256 (10)	0.0096 (8)	0.0137 (8)	0.0059 (8)
C25	0.0375 (11)	0.0295 (11)	0.0309 (11)	0.0131 (9)	0.0201 (9)	0.0014 (9)
C26	0.0394 (12)	0.0265 (11)	0.0409 (12)	0.0191 (9)	0.0222 (10)	0.0057 (9)
C27	0.0426 (12)	0.0340 (12)	0.0328 (11)	0.0235 (10)	0.0181 (10)	0.0130 (9)
C28	0.0298 (10)	0.0314 (11)	0.0247 (10)	0.0153 (9)	0.0135 (9)	0.0061 (8)
C29	0.0201 (9)	0.0192 (9)	0.0229 (9)	0.0057 (7)	0.0088 (8)	0.0027 (7)
C30	0.0216 (9)	0.0239 (10)	0.0313 (11)	0.0069 (8)	0.0115 (8)	0.0014 (8)
C31	0.0202 (10)	0.0261 (10)	0.0371 (12)	0.0051 (8)	0.0052 (9)	0.0020 (9)
C32	0.0346 (12)	0.0313 (12)	0.0289 (11)	0.0108 (9)	−0.0008 (9)	−0.0046 (9)
C33	0.0420 (13)	0.0459 (14)	0.0286 (11)	0.0206 (11)	0.0106 (10)	−0.0062 (10)
C34	0.0280 (10)	0.0387 (12)	0.0284 (11)	0.0161 (9)	0.0117 (9)	0.0016 (9)
C35	0.0229 (9)	0.0225 (9)	0.0261 (9)	0.0127 (7)	0.0152 (8)	0.0071 (7)
C36	0.0272 (10)	0.0320 (11)	0.0274 (10)	0.0147 (9)	0.0114 (9)	0.0074 (8)
C37	0.0454 (13)	0.0540 (15)	0.0277 (11)	0.0342 (12)	0.0185 (10)	0.0166 (10)
C38	0.0603 (16)	0.0481 (14)	0.0478 (14)	0.0406 (13)	0.0405 (13)	0.0326 (12)
C39	0.0465 (13)	0.0265 (11)	0.0590 (15)	0.0204 (10)	0.0389 (12)	0.0219 (10)
C40	0.0298 (10)	0.0218 (9)	0.0348 (11)	0.0109 (8)	0.0199 (9)	0.0061 (8)

Geometric parameters (Å, º)

Pd—C1	1.9985 (18)	C18—C19	1.385 (3)
Pd—P2	2.3232 (5)	C18—H18	0.9500
Pd—P1	2.3393 (5)	C19—C20	1.385 (3)
Pd—Br	2.5353 (3)	C19—H19	0.9500
P1—C5	1.8248 (18)	C20—C21	1.381 (3)
P1—C17	1.8255 (18)	C20—H20	0.9500
P1—C11	1.8267 (18)	C21—C22	1.390 (3)
P2—C35	1.8188 (19)	C21—H21	0.9500
P2—C29	1.8247 (19)	C22—H22	0.9500
P2—C23	1.8363 (19)	C23—C28	1.393 (3)
N1—C1	1.330 (2)	C23—C24	1.397 (3)
N1—C2	1.337 (3)	C24—C25	1.386 (3)
N2—C1	1.332 (2)	C24—H24	0.9500
N2—C4	1.340 (3)	C25—C26	1.377 (3)
C2—C3	1.373 (3)	C25—H25	0.9500
C2—H2	0.9500	C26—C27	1.380 (3)
C3—C4	1.373 (3)	C26—H26	0.9500
C3—H3	0.9500	C27—C28	1.388 (3)
C4—H4	0.9500	C27—H27	0.9500
C5—C10	1.391 (3)	C28—H28	0.9500
C5—C6	1.394 (3)	C29—C34	1.390 (3)
C6—C7	1.385 (3)	C29—C30	1.397 (3)
C6—H6	0.9500	C30—C31	1.387 (3)
C7—C8	1.384 (3)	C30—H30	0.9500
C7—H7	0.9500	C31—C32	1.378 (3)
C8—C9	1.382 (3)	C31—H31	0.9500
C8—H8	0.9500	C32—C33	1.383 (3)
C9—C10	1.386 (3)	C32—H32	0.9500

C9—H9	0.9500	C33—C34	1.385 (3)
C10—H10	0.9500	C33—H33	0.9500
C11—C16	1.389 (3)	C34—H34	0.9500
C11—C12	1.398 (2)	C35—C40	1.389 (3)
C12—C13	1.386 (3)	C35—C36	1.400 (3)
C12—H12	0.9500	C36—C37	1.384 (3)
C13—C14	1.386 (3)	C36—H36	0.9500
C13—H13	0.9500	C37—C38	1.382 (4)
C14—C15	1.379 (3)	C37—H37	0.9500
C14—H14	0.9500	C38—C39	1.378 (4)
C15—C16	1.389 (3)	C38—H38	0.9500
C15—H15	0.9500	C39—C40	1.391 (3)
C16—H16	0.9500	C39—H39	0.9500
C17—C22	1.389 (3)	C40—H40	0.9500
C17—C18	1.400 (2)		

C1—Pd—P2	86.86 (5)	C18—C17—P1	120.85 (14)
C1—Pd—P1	90.58 (5)	C19—C18—C17	120.29 (18)
P2—Pd—P1	176.743 (17)	C19—C18—H18	119.9
C1—Pd—Br	176.56 (5)	C17—C18—H18	119.9
P2—Pd—Br	89.758 (13)	C20—C19—C18	119.93 (18)
P1—Pd—Br	92.815 (13)	C20—C19—H19	120.0
C5—P1—C17	102.50 (8)	C18—C19—H19	120.0
C5—P1—C11	103.18 (8)	C21—C20—C19	120.22 (18)
C17—P1—C11	103.89 (8)	C21—C20—H20	119.9
C5—P1—Pd	117.16 (6)	C19—C20—H20	119.9
C17—P1—Pd	112.70 (6)	C20—C21—C22	120.16 (19)
C11—P1—Pd	115.70 (6)	C20—C21—H21	119.9
C35—P2—C29	106.74 (9)	C22—C21—H21	119.9
C35—P2—C23	103.18 (8)	C17—C22—C21	120.16 (18)
C29—P2—C23	102.10 (8)	C17—C22—H22	119.9
C35—P2—Pd	110.52 (6)	C21—C22—H22	119.9
C29—P2—Pd	113.50 (6)	C28—C23—C24	118.21 (17)
C23—P2—Pd	119.58 (6)	C28—C23—P2	118.41 (14)
C1—N1—C2	115.99 (18)	C24—C23—P2	123.35 (14)
C1—N2—C4	116.48 (17)	C25—C24—C23	120.97 (18)
N1—C1—N2	125.98 (17)	C25—C24—H24	119.5
N1—C1—Pd	116.27 (13)	C23—C24—H24	119.5
N2—C1—Pd	117.66 (14)	C26—C25—C24	119.89 (19)
N1—C2—C3	122.9 (2)	C26—C25—H25	120.1
N1—C2—H2	118.6	C24—C25—H25	120.1
C3—C2—H2	118.6	C25—C26—C27	120.13 (19)
C2—C3—C4	116.5 (2)	C25—C26—H26	119.9
C2—C3—H3	121.7	C27—C26—H26	119.9
C4—C3—H3	121.7	C26—C27—C28	120.1 (2)
N2—C4—C3	122.2 (2)	C26—C27—H27	119.9
N2—C4—H4	118.9	C28—C27—H27	119.9
C3—C4—H4	118.9	C27—C28—C23	120.64 (19)

C10—C5—C6	119.00 (17)	C27—C28—H28	119.7
C10—C5—P1	122.17 (14)	C23—C28—H28	119.7
C6—C5—P1	118.80 (14)	C34—C29—C30	119.03 (18)
C7—C6—C5	120.63 (19)	C34—C29—P2	120.58 (15)
C7—C6—H6	119.7	C30—C29—P2	120.39 (14)
C5—C6—H6	119.7	C31—C30—C29	120.22 (19)
C8—C7—C6	119.70 (19)	C31—C30—H30	119.9
C8—C7—H7	120.2	C29—C30—H30	119.9
C6—C7—H7	120.2	C32—C31—C30	120.2 (2)
C9—C8—C7	120.28 (19)	C32—C31—H31	119.9
C9—C8—H8	119.9	C30—C31—H31	119.9
C7—C8—H8	119.9	C31—C32—C33	120.0 (2)
C8—C9—C10	120.07 (19)	C31—C32—H32	120.0
C8—C9—H9	120.0	C33—C32—H32	120.0
C10—C9—H9	120.0	C32—C33—C34	120.3 (2)
C9—C10—C5	120.32 (18)	C32—C33—H33	119.9
C9—C10—H10	119.8	C34—C33—H33	119.9
C5—C10—H10	119.8	C33—C34—C29	120.29 (19)
C16—C11—C12	118.97 (17)	C33—C34—H34	119.9
C16—C11—P1	119.85 (14)	C29—C34—H34	119.9
C12—C11—P1	121.13 (14)	C40—C35—C36	118.88 (18)
C13—C12—C11	120.14 (18)	C40—C35—P2	123.01 (15)
C13—C12—H12	119.9	C36—C35—P2	118.08 (15)
C11—C12—H12	119.9	C37—C36—C35	120.3 (2)
C12—C13—C14	120.48 (18)	C37—C36—H36	119.8
C12—C13—H13	119.8	C35—C36—H36	119.8
C14—C13—H13	119.8	C38—C37—C36	120.3 (2)
C15—C14—C13	119.52 (18)	C38—C37—H37	119.9
C15—C14—H14	120.2	C36—C37—H37	119.9
C13—C14—H14	120.2	C39—C38—C37	119.7 (2)
C14—C15—C16	120.50 (19)	C39—C38—H38	120.1
C14—C15—H15	119.8	C37—C38—H38	120.1
C16—C15—H15	119.8	C38—C39—C40	120.6 (2)
C11—C16—C15	120.38 (18)	C38—C39—H39	119.7
C11—C16—H16	119.8	C40—C39—H39	119.7
C15—C16—H16	119.8	C35—C40—C39	120.1 (2)
C22—C17—C18	119.23 (17)	C35—C40—H40	120.0
C22—C17—P1	119.88 (14)	C39—C40—H40	120.0