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Bis[2,6-bis(dipiperidin-1-ylphosphanyloxy)phenyl]bromidopalladium(II)

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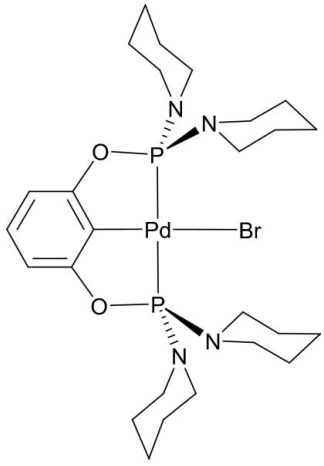
Key indicators: single-crystal X-ray study; T = 183 K; mean σ(C–C) = 0.005 Å; R factor = 0.024; wR factor = 0.065; data-to-parameter ratio = 15.4.

The title compound, [PdBr($C_{26}H_{43}N_4O_2P_2$)], a so-called palladium pincer complex, is a very efficient catalyst for the Suzuki cross-coupling reaction. The Pd atom exhibits a distorted square-planar coordination, typical for Pd^{II} complexes.

Related literature

For related literature, see: Bolliger *et al.* (2007); Miyaura *et al.* (1979); Bachechi (2003); Cross *et al.* (1995).



Experimental

Crystal data

[PdBr($C_{26}H_{43}N_4O_2P_2$)]
M_r = 691.9
Triclinic, $P\overline{1}$
a = 9.8843 (15) Å
b = 12.3457 (19) Å
c = 13.815 (2) Å
α = 76.635 (18)°
β = 70.676 (17)°
γ = 73.847 (17)°
V = 1510.0 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.07 mm^{-1}
T = 183 (2) K
0.33 × 0.32 × 0.12 mm

Data collection

Stoe IPDS diffractometer
Absorption correction: numerical (Coppens *et al.*, 1965)
T_{min} = 0.568, T_{max} = 0.797
19696 measured reflections
4989 independent reflections
4431 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.065
S = 1.02
4989 reflections
325 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pd1—C1	1.988 (2)	Pd1—P2	2.2891 (7)
Pd1—P1	2.2808 (7)	Pd1—Br1	2.5066 (7)
C1—Pd1—P1	80.14 (7)	C1—Pd1—Br1	179.28 (7)
C1—Pd1—P2	80.63 (7)	P1—Pd1—Br1	99.20 (3)
P1—Pd1—P2	160.31 (3)	P2—Pd1—Br1	100.00 (3)

Data collection: *IPDS Software* (Stoe & Cie, 1999); cell refinement: *IPDS Software*; data reduction: *IPDS Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2024).

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supplementary materials

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Bis[2,6-bis(dipiperidin-1-ylphosphanyloxy)phenyl]bromidopalladium(II)

J. L. Bolliger, O. Blacque and C. M. Frech

Comment

In a recent article, we reported a new concept for the synthesis of aminophosphine-based pincer complexes of palladium with the general formula of [Pd(Cl){C_6H_3(*XP*(piperidinyl)$_2$)$_2$}] (*X* = NH or O), which were formed by facile activation of C—H and P—N bonds (Bolliger *et al.*, 2007). These complexes proved to be extremely efficient catalysts for the Suzuki–Miyaura cross-coupling reaction (Miyaura *et al.*, 1979) and led to very high conversion rates and quantitative yields in extremely short reaction times and with very low catalyst loadings. The analogous bromo complex [Pd(Br){C_6H_3(OP(piperidinyl)$_2$)$_2$}] (I), which was found to be formed in the catalytic cycle, was independently prepared and the *x*-ray structure is presented here.

The crystal structure of (I) consists of discrete molecules with no intermolecular short contacts. The palladium atom presents a distorted square planar coordination with Br, C1, P1 and P2 as donor atoms. The main distortion affects the angle P—Pd—P of the mutually *trans* phosphorus atoms (160.31 (3)°) and is a consequence of the two five-membered rings which impose strains to the coordination sphere. The Pd—Br bond length of 2.5066 (7) Å is very similar to values found in the literature for the [Pd(Br){C_6H_3(*XPR*$_2$)$_2$}] compounds: 2.495 (1) Å, *X* = CH_2, *R* = Ph (Bachechi, 2003) and 2.514 (2) Å, *X* = CH_2, *R* = Cy (Cross *et al.*, 1995). The Pd—P bond distances of 2.2808 (7) and 2.2891 (7) Å fall in the typical range observed for compounds with the [Pd{C_6H_3(*XPR*$_2$)$_2$}] moiety.

Experimental

To an orange suspension of 0.709 g (1.89 mmol) of [Pd(Br)$_2$(cod)] (cod=cycloocta-1,5-diene) in 15 ml of tetrahydrofurane, 1.077 g (3.80 mmol, 2.01 equiv.) of P(NC_5H_{10})$_3$ (dissolved in 10 ml of tetrahydrofurane) was added and stirred for 5 minutes at room temperature, which quantitatively yielded the dibromo-(bis(1,1',1''-(phosphinetriyl)tripiperidine))palladium [Pd(Br)$_2${P(NC_5H_{10})$_3$}$_2$] complex. To a toluene solution (10 ml) of 262.8 mg (0.32 mmol) of [Pd(Br)$_2${P(NC_5H_{10})$_3$}$_2$], 36.0 mg (0.33 mmol, 1.01 equiv.) of resorcinol was added. The reaction mixture was placed in an oil bath and heated up to 80°C for 15 minutes, during which the solution decolorized. The solvent was removed under reduced pressure, and the solid was extracted with 20 ml of diethyl ether. After removal of the solvent in vacuo, 161.5 mg (0.24 mmol, 74%) of [Pd(Br){C_6H_3(OP(piperidinyl)$_2$)$_2$}] (I) was obtained as colorless powder.

Colorless crystals of the title compound (I) were obtained by slow evaporation of the solvent from a saturated diethyl ether solution at room temperature within three weeks.

$^{31}P\{^1H\}$-NMR (C_6D_6; δ, p.p.m.): 147.6 (s, P(NC_5H_{10})$_2$).

^1H NMR (C_6D_6; δ,p.p.m.): 6.96 (t, $^3J_{HH}$ = 8.0 Hz, 1H, Ar_{para}), 6.63 (d, $^3J_{HH}$ = 8.0 Hz, 2H, Ar_{meta}), 3.27 (m, 16H, NCH_2), 1.41 (m, 16H, NCH_2CH_2),1.27 (m, 8H, $NCH_2CH_2CH_2$).

$^{13}C\{^{1}H\}$ NMR (C_6D_6; δ, p.p.m.): 160.9 (vt, J_{PC} = 10.2 Hz, ArOP), 129.3 (s, Ar_{para}), 126.9 (unresolved t, Ar_{ipso}), 106.4 (vt, J_{PC} = 8.4 Hz, Ar_{meta}), 46.7 (vt, $^{2}J_{PC} = {}^{4}J_{PC}$ = 4.1, NCH_2), 26.6 (s, NCH_2CH_2), 24.9 (s, $NCH_2CH_2CH_2$). The assignmentof the ^{1}H and $^{13}C\{^{1}H\}$ NMR signals was confirmed by COSY and $^{13}C\{^{1}H\}$DEPT experiments.

Elemental Analysis: Calc. for $C_{26}H_{43}BrN_4O_2P_2Pd$: C, 45.13; H, 6.26; N, 8.10. Found: C, 45.08; H, 6.35; N, 8.13.

Refinement

All hydrogen atoms were included at calculated positions and treated as riding atoms with C—H distances of 0.93–0.97 Å and $U_{iso}(H) = 1.3U_{eq}(C)$].

Figures

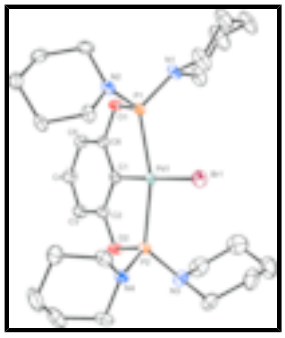

Fig. 1. The molecular structure of (I) with the atom-labeling scheme (30% probability displacement ellipsoids).

Bis[2,6-bis(dipiperidin-1-ylphosphanyloxy)phenyl]bromidopalladium(II)

Crystal data

$[PdBr(C_{26}H_{43}N_4O_2P_2)]$	$Z = 2$
M_r = 691.9	F_{000} = 708
Triclinic, $P\overline{1}$	D_x = 1.522 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 9.8843 (15) Å	Cell parameters from 8000 reflections
b = 12.3457 (19) Å	θ = 3.1–30.2°
c = 13.815 (2) Å	μ = 2.07 mm^{-1}
α = 76.635 (18)°	T = 183 (2) K
β = 70.676 (17)°	Plate, colourless
γ = 73.847 (17)°	0.33 × 0.32 × 0.12 mm
V = 1510.0 (4) Å^3	

Data collection

Stoe IPDS diffractometer	R_{int} = 0.056
φ oscillation scans	θ_{max} = 25°

Absorption correction: numerical (Coppens *et al.*, 1965)
T_{min} = 0.568, T_{max} = 0.797
19696 measured reflections
4989 independent reflections
4431 reflections with $I > 2\sigma(I)$

θ_{min} = 3.1°
h = −11→11
k = −14→14
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.065
S = 1.02
4989 reflections
325 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 0.1788P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Extinction correction: none

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pd1	0.595039 (18)	0.296726 (15)	0.253679 (13)	0.02177 (7)
Br1	0.37214 (3)	0.32621 (3)	0.40672 (2)	0.03958 (9)
P1	0.59392 (7)	0.11866 (5)	0.23383 (5)	0.02443 (14)
P2	0.67472 (7)	0.45960 (5)	0.23525 (4)	0.02443 (14)
C1	0.7721 (3)	0.2712 (2)	0.13281 (17)	0.0232 (5)
C2	0.8616 (3)	0.3495 (2)	0.09128 (18)	0.0266 (5)
C3	0.9860 (3)	0.3337 (2)	0.0074 (2)	0.0332 (6)
H3	1.0454	0.3866	−0.0178	0.043*
C4	1.0193 (3)	0.2369 (2)	−0.0377 (2)	0.0344 (6)
H4	1.1021	0.2252	−0.0943	0.045*
C5	0.9317 (3)	0.1564 (2)	−0.00032 (19)	0.0302 (5)
H5	0.9542	0.0922	−0.0319	0.039*
C6	0.8106 (3)	0.1747 (2)	0.08503 (17)	0.0238 (5)
O1	0.72162 (19)	0.09514 (15)	0.12318 (13)	0.0288 (4)
O2	0.8238 (2)	0.44822 (15)	0.13463 (13)	0.0334 (4)
N1	0.4599 (2)	0.07942 (19)	0.21028 (15)	0.0307 (5)
C7	0.4193 (3)	0.1359 (3)	0.1142 (2)	0.0449 (8)
H7A	0.5074	0.1394	0.0565	0.058*
H7B	0.364	0.2133	0.1218	0.058*

C8	0.3280 (4)	0.0702 (5)	0.0927 (3)	0.0780 (14)
H8A	0.3862	−0.0054	0.0807	0.101*
H8B	0.3	0.1085	0.0302	0.101*
C9	0.1899 (4)	0.0598 (4)	0.1828 (3)	0.0644 (11)
H9A	0.1253	0.1345	0.1897	0.084*
H9B	0.1377	0.0115	0.1695	0.084*
C10	0.2330 (4)	0.0087 (3)	0.2823 (3)	0.0585 (9)
H10A	0.145	0.0094	0.3406	0.076*
H10B	0.2853	−0.0701	0.2787	0.076*
C11	0.3273 (4)	0.0728 (4)	0.2992 (2)	0.0551 (9)
H11A	0.2714	0.1494	0.3099	0.072*
H11B	0.3565	0.0357	0.3614	0.072*
N2	0.6376 (2)	0.01734 (18)	0.32605 (16)	0.0306 (5)
C12	0.6752 (3)	0.0430 (3)	0.41152 (19)	0.0321 (6)
H12A	0.6247	0.0029	0.4768	0.042*
H12B	0.6422	0.1242	0.4145	0.042*
C13	0.8394 (3)	0.0077 (2)	0.3971 (2)	0.0340 (6)
H13A	0.8605	0.0202	0.4569	0.044*
H13B	0.8892	0.0544	0.3362	0.044*
C14	0.8968 (3)	−0.1179 (3)	0.3840 (2)	0.0432 (7)
H14A	1.0029	−0.1373	0.3691	0.056*
H14B	0.8563	−0.1652	0.4481	0.056*
C15	0.8537 (4)	−0.1412 (3)	0.2961 (3)	0.0448 (7)
H15A	0.8843	−0.2222	0.2921	0.058*
H15B	0.904	−0.1009	0.2308	0.058*
C16	0.6882 (3)	−0.1029 (2)	0.3126 (2)	0.0424 (7)
H16A	0.6644	−0.1136	0.2533	0.055*
H16B	0.6382	−0.1493	0.3736	0.055*
N3	0.5935 (3)	0.59172 (19)	0.19468 (17)	0.0358 (5)
C17	0.5694 (4)	0.6169 (3)	0.0915 (2)	0.0574 (9)
H17A	0.6409	0.5631	0.0482	0.075*
H17B	0.5839	0.6929	0.0591	0.075*
C18	0.4161 (5)	0.6095 (4)	0.0985 (3)	0.0741 (13)
H18A	0.4058	0.5311	0.1227	0.096*
H18B	0.4016	0.6318	0.0299	0.096*
C19	0.2992 (4)	0.6858 (4)	0.1717 (3)	0.0727 (12)
H19A	0.3011	0.7651	0.1433	0.095*
H19B	0.2029	0.6746	0.1786	0.095*
C20	0.3262 (4)	0.6582 (3)	0.2774 (3)	0.0606 (9)
H20A	0.3103	0.5825	0.3099	0.079*
H20B	0.2571	0.7124	0.3213	0.079*
C21	0.4819 (4)	0.6631 (3)	0.2676 (2)	0.0458 (7)
H21A	0.4924	0.7416	0.2448	0.06*
H21B	0.4988	0.6387	0.3354	0.06*
N4	0.7223 (2)	0.47366 (18)	0.33326 (16)	0.0297 (5)
C22	0.7178 (3)	0.3868 (2)	0.4260 (2)	0.0388 (7)
H22A	0.6579	0.3358	0.4275	0.05*
H22B	0.6726	0.4235	0.4874	0.05*
C23	0.8690 (4)	0.3190 (3)	0.4275 (3)	0.0586 (9)

H23A	0.9121	0.2775	0.3689	0.076*
H23B	0.8633	0.264	0.4907	0.076*
C24	0.9645 (4)	0.3990 (4)	0.4220 (4)	0.0800 (14)
H24A	1.0637	0.3558	0.4189	0.104*
H24B	0.9263	0.4347	0.4841	0.104*
C25	0.9672 (4)	0.4908 (4)	0.3267 (3)	0.0702 (11)
H25A	1.0222	0.5443	0.3275	0.091*
H25B	1.0167	0.4557	0.2645	0.091*
C26	0.8136 (3)	0.5542 (3)	0.3239 (2)	0.0428 (7)
H26A	0.769	0.5986	0.3805	0.056*
H26B	0.8181	0.6065	0.2592	0.056*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.01969 (10)	0.02554 (12)	0.01935 (10)	−0.00848 (8)	−0.00401 (7)	−0.00008 (7)
Br1	0.02724 (14)	0.04573 (19)	0.03679 (16)	−0.01067 (13)	0.00621 (11)	−0.00854 (12)
P1	0.0256 (3)	0.0282 (3)	0.0210 (3)	−0.0126 (3)	−0.0072 (2)	0.0025 (2)
P2	0.0274 (3)	0.0246 (3)	0.0212 (3)	−0.0093 (3)	−0.0055 (2)	−0.0010 (2)
C1	0.0224 (11)	0.0271 (13)	0.0203 (11)	−0.0068 (10)	−0.0082 (9)	0.0003 (9)
C2	0.0281 (12)	0.0269 (13)	0.0241 (12)	−0.0088 (11)	−0.0062 (10)	−0.0008 (10)
C3	0.0313 (13)	0.0365 (15)	0.0299 (13)	−0.0170 (12)	−0.0014 (11)	−0.0006 (11)
C4	0.0280 (13)	0.0405 (16)	0.0271 (13)	−0.0089 (13)	0.0012 (10)	−0.0024 (11)
C5	0.0341 (13)	0.0303 (14)	0.0234 (12)	−0.0066 (12)	−0.0052 (10)	−0.0039 (10)
C6	0.0251 (11)	0.0252 (13)	0.0201 (11)	−0.0079 (10)	−0.0077 (9)	0.0032 (9)
O1	0.0328 (9)	0.0291 (10)	0.0252 (8)	−0.0143 (8)	−0.0041 (7)	−0.0026 (7)
O2	0.0353 (10)	0.0318 (10)	0.0307 (9)	−0.0190 (9)	0.0050 (8)	−0.0073 (7)
N1	0.0331 (11)	0.0415 (13)	0.0233 (10)	−0.0206 (10)	−0.0130 (9)	0.0060 (9)
C7	0.0425 (16)	0.066 (2)	0.0253 (14)	−0.0202 (15)	−0.0163 (12)	0.0139 (13)
C8	0.062 (2)	0.148 (4)	0.0414 (19)	−0.045 (3)	−0.0186 (17)	−0.015 (2)
C9	0.0439 (18)	0.113 (3)	0.0499 (19)	−0.034 (2)	−0.0188 (15)	−0.010 (2)
C10	0.0436 (17)	0.080 (3)	0.057 (2)	−0.0337 (19)	−0.0175 (16)	0.0076 (18)
C11	0.0447 (17)	0.100 (3)	0.0267 (15)	−0.0359 (19)	−0.0106 (13)	0.0033 (15)
N2	0.0343 (11)	0.0334 (12)	0.0278 (11)	−0.0147 (10)	−0.0152 (9)	0.0068 (9)
C12	0.0277 (12)	0.0469 (16)	0.0203 (12)	−0.0093 (12)	−0.0078 (10)	0.0002 (10)
C13	0.0291 (13)	0.0451 (17)	0.0317 (13)	−0.0132 (13)	−0.0128 (11)	−0.0009 (11)
C14	0.0326 (14)	0.0423 (18)	0.0515 (18)	−0.0083 (14)	−0.0169 (13)	0.0062 (14)
C15	0.0546 (18)	0.0266 (15)	0.0528 (18)	−0.0091 (15)	−0.0173 (15)	−0.0020 (13)
C16	0.0568 (18)	0.0317 (15)	0.0480 (17)	−0.0222 (15)	−0.0279 (15)	0.0106 (12)
N3	0.0479 (13)	0.0310 (13)	0.0253 (11)	−0.0048 (11)	−0.0132 (10)	0.0012 (9)
C17	0.086 (3)	0.052 (2)	0.0294 (16)	−0.0068 (19)	−0.0281 (17)	0.0096 (14)
C18	0.110 (3)	0.064 (2)	0.069 (3)	−0.012 (3)	−0.068 (3)	0.004 (2)
C19	0.064 (2)	0.064 (3)	0.092 (3)	−0.007 (2)	−0.050 (2)	0.017 (2)
C20	0.0463 (18)	0.053 (2)	0.066 (2)	0.0032 (18)	−0.0169 (17)	0.0070 (18)
C21	0.0547 (18)	0.0347 (17)	0.0434 (17)	0.0031 (15)	−0.0182 (15)	−0.0063 (13)
N4	0.0347 (11)	0.0320 (12)	0.0272 (10)	−0.0135 (10)	−0.0127 (9)	−0.0001 (9)
C22	0.0485 (16)	0.0446 (17)	0.0303 (14)	−0.0199 (14)	−0.0188 (13)	0.0043 (12)
C23	0.064 (2)	0.047 (2)	0.072 (2)	−0.0073 (18)	−0.044 (2)	0.0058 (17)

C24	0.057 (2)	0.092 (3)	0.106 (3)	−0.024 (2)	−0.055 (2)	0.013 (3)
C25	0.045 (2)	0.095 (3)	0.085 (3)	−0.038 (2)	−0.0196 (19)	−0.013 (2)
C26	0.0592 (19)	0.0417 (17)	0.0395 (15)	−0.0290 (16)	−0.0175 (14)	−0.0022 (12)

Geometric parameters (Å, °)

Pd1—C1	1.988 (2)	C13—H13A	0.9700
Pd1—P1	2.2808 (7)	C13—H13B	0.9700
Pd1—P2	2.2891 (7)	C14—C15	1.521 (4)
Pd1—Br1	2.5066 (7)	C14—H14A	0.9700
P1—N2	1.643 (2)	C14—H14B	0.9700
P1—O1	1.6549 (19)	C15—C16	1.524 (4)
P1—N1	1.6762 (18)	C15—H15A	0.9700
P2—N4	1.631 (2)	C15—H15B	0.9700
P2—O2	1.6563 (19)	C16—H16A	0.9700
P2—N3	1.663 (2)	C16—H16B	0.9700
C1—C2	1.388 (3)	N3—C21	1.464 (4)
C1—C6	1.395 (3)	N3—C17	1.471 (3)
C2—O2	1.386 (3)	C17—C18	1.514 (6)
C2—C3	1.386 (4)	C17—H17A	0.9700
C3—C4	1.384 (4)	C17—H17B	0.9700
C3—H3	0.9300	C18—C19	1.519 (6)
C4—C5	1.397 (4)	C18—H18A	0.9700
C4—H4	0.9300	C18—H18B	0.9700
C5—C6	1.383 (4)	C19—C20	1.516 (5)
C5—H5	0.9300	C19—H19A	0.9700
C6—O1	1.397 (3)	C19—H19B	0.9700
N1—C7	1.476 (3)	C20—C21	1.517 (5)
N1—C11	1.478 (4)	C20—H20A	0.9700
C7—C8	1.502 (5)	C20—H20B	0.9700
C7—H7A	0.9700	C21—H21A	0.9700
C7—H7B	0.9700	C21—H21B	0.9700
C8—C9	1.526 (5)	N4—C22	1.465 (3)
C8—H8A	0.9700	N4—C26	1.477 (3)
C8—H8B	0.9700	C22—C23	1.500 (4)
C9—C10	1.519 (5)	C22—H22A	0.9700
C9—H9A	0.9700	C22—H22B	0.9700
C9—H9B	0.9700	C23—C24	1.520 (5)
C10—C11	1.479 (4)	C23—H23A	0.9700
C10—H10A	0.9700	C23—H23B	0.9700
C10—H10B	0.9700	C24—C25	1.524 (6)
C11—H11A	0.9700	C24—H24A	0.9700
C11—H11B	0.9700	C24—H24B	0.9700
N2—C16	1.464 (4)	C25—C26	1.511 (5)
N2—C12	1.470 (3)	C25—H25A	0.9700
C12—C13	1.515 (3)	C25—H25B	0.9700
C12—H12A	0.9700	C26—H26A	0.9700
C12—H12B	0.9700	C26—H26B	0.9700
C13—C14	1.527 (4)		

C1—Pd1—P1	80.14 (7)	H13A—C13—H13B	108.1
C1—Pd1—P2	80.63 (7)	C15—C14—C13	110.3 (2)
P1—Pd1—P2	160.31 (3)	C15—C14—H14A	109.6
C1—Pd1—Br1	179.28 (7)	C13—C14—H14A	109.6
P1—Pd1—Br1	99.20 (3)	C15—C14—H14B	109.6
P2—Pd1—Br1	100.00 (3)	C13—C14—H14B	109.6
N2—P1—O1	108.07 (11)	H14A—C14—H14B	108.1
N2—P1—N1	103.23 (10)	C14—C15—C16	111.1 (3)
O1—P1—N1	97.66 (10)	C14—C15—H15A	109.4
N2—P1—Pd1	113.99 (8)	C16—C15—H15A	109.4
O1—P1—Pd1	104.72 (6)	C14—C15—H15B	109.4
N1—P1—Pd1	126.94 (9)	C16—C15—H15B	109.4
N4—P2—O2	107.57 (10)	H15A—C15—H15B	108.0
N4—P2—N3	103.59 (11)	N2—C16—C15	110.5 (2)
O2—P2—N3	97.15 (11)	N2—C16—H16A	109.5
N4—P2—Pd1	115.52 (8)	C15—C16—H16A	109.5
O2—P2—Pd1	103.76 (7)	N2—C16—H16B	109.5
N3—P2—Pd1	126.50 (8)	C15—C16—H16B	109.5
C2—C1—C6	117.1 (2)	H16A—C16—H16B	108.1
C2—C1—Pd1	121.52 (19)	C21—N3—C17	112.6 (2)
C6—C1—Pd1	121.40 (16)	C21—N3—P2	121.29 (18)
O2—C2—C3	118.6 (2)	C17—N3—P2	118.4 (2)
O2—C2—C1	118.6 (2)	N3—C17—C18	111.5 (3)
C3—C2—C1	122.8 (2)	N3—C17—H17A	109.3
C4—C3—C2	118.0 (2)	C18—C17—H17A	109.3
C4—C3—H3	121.0	N3—C17—H17B	109.3
C2—C3—H3	121.0	C18—C17—H17B	109.3
C3—C4—C5	121.6 (2)	H17A—C17—H17B	108.0
C3—C4—H4	119.2	C17—C18—C19	111.7 (3)
C5—C4—H4	119.2	C17—C18—H18A	109.3
C6—C5—C4	118.1 (2)	C19—C18—H18A	109.3
C6—C5—H5	120.9	C17—C18—H18B	109.3
C4—C5—H5	120.9	C19—C18—H18B	109.3
C5—C6—C1	122.4 (2)	H18A—C18—H18B	107.9
C5—C6—O1	118.8 (2)	C20—C19—C18	110.2 (3)
C1—C6—O1	118.8 (2)	C20—C19—H19A	109.6
C6—O1—P1	113.66 (15)	C18—C19—H19A	109.6
C2—O2—P2	115.47 (14)	C20—C19—H19B	109.6
C7—N1—C11	110.7 (2)	C18—C19—H19B	109.6
C7—N1—P1	117.55 (17)	H19A—C19—H19B	108.1
C11—N1—P1	115.22 (17)	C19—C20—C21	110.7 (3)
N1—C7—C8	109.6 (3)	C19—C20—H20A	109.5
N1—C7—H7A	109.8	C21—C20—H20A	109.5
C8—C7—H7A	109.8	C19—C20—H20B	109.5
N1—C7—H7B	109.8	C21—C20—H20B	109.5
C8—C7—H7B	109.8	H20A—C20—H20B	108.1
H7A—C7—H7B	108.2	N3—C21—C20	113.2 (3)
C7—C8—C9	111.6 (3)	N3—C21—H21A	108.9
C7—C8—H8A	109.3	C20—C21—H21A	108.9

C9—C8—H8A	109.3	N3—C21—H21B	108.9
C7—C8—H8B	109.3	C20—C21—H21B	108.9
C9—C8—H8B	109.3	H21A—C21—H21B	107.8
H8A—C8—H8B	108.0	C22—N4—C26	112.93 (19)
C10—C9—C8	109.3 (3)	C22—N4—P2	122.37 (16)
C10—C9—H9A	109.8	C26—N4—P2	122.27 (17)
C8—C9—H9A	109.8	N4—C22—C23	111.4 (3)
C10—C9—H9B	109.8	N4—C22—H22A	109.3
C8—C9—H9B	109.8	C23—C22—H22A	109.3
H9A—C9—H9B	108.3	N4—C22—H22B	109.3
C11—C10—C9	111.5 (3)	C23—C22—H22B	109.3
C11—C10—H10A	109.3	H22A—C22—H22B	108.0
C9—C10—H10A	109.3	C22—C23—C24	109.5 (3)
C11—C10—H10B	109.3	C22—C23—H23A	109.8
C9—C10—H10B	109.3	C24—C23—H23A	109.8
H10A—C10—H10B	108.0	C22—C23—H23B	109.8
N1—C11—C10	111.8 (3)	C24—C23—H23B	109.8
N1—C11—H11A	109.3	H23A—C23—H23B	108.2
C10—C11—H11A	109.3	C23—C24—C25	110.7 (3)
N1—C11—H11B	109.3	C23—C24—H24A	109.5
C10—C11—H11B	109.3	C25—C24—H24A	109.5
H11A—C11—H11B	107.9	C23—C24—H24B	109.5
C16—N2—C12	113.5 (2)	C25—C24—H24B	109.5
C16—N2—P1	122.31 (18)	H24A—C24—H24B	108.1
C12—N2—P1	121.26 (18)	C26—C25—C24	111.3 (3)
N2—C12—C13	111.1 (2)	C26—C25—H25A	109.4
N2—C12—H12A	109.4	C24—C25—H25A	109.4
C13—C12—H12A	109.4	C26—C25—H25B	109.4
N2—C12—H12B	109.4	C24—C25—H25B	109.4
C13—C12—H12B	109.4	H25A—C25—H25B	108.0
H12A—C12—H12B	108.0	N4—C26—C25	110.7 (3)
C12—C13—C14	110.7 (2)	N4—C26—H26A	109.5
C12—C13—H13A	109.5	C25—C26—H26A	109.5
C14—C13—H13A	109.5	N4—C26—H26B	109.5
C12—C13—H13B	109.5	C25—C26—H26B	109.5
C14—C13—H13B	109.5	H26A—C26—H26B	108.1
C1—Pd1—P1—N2	109.12 (11)	Pd1—P1—N1—C11	−73.1 (2)
P2—Pd1—P1—N2	96.51 (11)	C11—N1—C7—C8	−59.2 (4)
Br1—Pd1—P1—N2	−70.58 (9)	P1—N1—C7—C8	165.5 (3)
C1—Pd1—P1—O1	−8.77 (9)	N1—C7—C8—C9	57.9 (4)
P2—Pd1—P1—O1	−21.39 (10)	C7—C8—C9—C10	−54.5 (5)
Br1—Pd1—P1—O1	171.52 (6)	C8—C9—C10—C11	53.1 (5)
C1—Pd1—P1—N1	−120.48 (11)	C7—N1—C11—C10	59.2 (4)
P2—Pd1—P1—N1	−133.10 (10)	P1—N1—C11—C10	−164.4 (2)
Br1—Pd1—P1—N1	59.81 (9)	C9—C10—C11—N1	−56.2 (4)
C1—Pd1—P2—N4	−117.13 (11)	O1—P1—N2—C16	−44.3 (2)
P1—Pd1—P2—N4	−104.54 (11)	N1—P1—N2—C16	58.5 (2)
Br1—Pd1—P2—N4	62.52 (10)	Pd1—P1—N2—C16	−160.24 (17)
C1—Pd1—P2—O2	0.34 (9)	O1—P1—N2—C12	115.2 (2)

P1—Pd1—P2—O2	12.94 (10)	N1—P1—N2—C12	−142.08 (19)
Br1—Pd1—P2—O2	180.00 (7)	Pd1—P1—N2—C12	−0.8 (2)
C1—Pd1—P2—N3	110.24 (12)	C16—N2—C12—C13	56.8 (3)
P1—Pd1—P2—N3	122.84 (12)	P1—N2—C12—C13	−104.4 (2)
Br1—Pd1—P2—N3	−70.10 (11)	N2—C12—C13—C14	−54.9 (3)
P1—Pd1—C1—C2	−175.34 (19)	C12—C13—C14—C15	54.5 (3)
P2—Pd1—C1—C2	0.39 (17)	C13—C14—C15—C16	−54.8 (3)
P1—Pd1—C1—C6	5.65 (16)	C12—N2—C16—C15	−56.5 (3)
P2—Pd1—C1—C6	−178.63 (18)	P1—N2—C16—C15	104.4 (2)
C6—C1—C2—O2	177.85 (19)	C14—C15—C16—N2	55.2 (3)
Pd1—C1—C2—O2	−1.2 (3)	N4—P2—N3—C21	−47.9 (2)
C6—C1—C2—C3	−1.3 (3)	O2—P2—N3—C21	−158.0 (2)
Pd1—C1—C2—C3	179.68 (18)	Pd1—P2—N3—C21	89.0 (2)
O2—C2—C3—C4	−177.5 (2)	N4—P2—N3—C17	164.8 (2)
C1—C2—C3—C4	1.6 (4)	O2—P2—N3—C17	54.7 (2)
C2—C3—C4—C5	−0.4 (4)	Pd1—P2—N3—C17	−58.3 (3)
C3—C4—C5—C6	−1.0 (4)	C21—N3—C17—C18	−54.1 (4)
C4—C5—C6—C1	1.4 (3)	P2—N3—C17—C18	95.9 (3)
C4—C5—C6—O1	179.8 (2)	N3—C17—C18—C19	54.9 (4)
C2—C1—C6—C5	−0.3 (3)	C17—C18—C19—C20	−54.8 (4)
Pd1—C1—C6—C5	178.77 (17)	C18—C19—C20—C21	53.4 (4)
C2—C1—C6—O1	−178.70 (19)	C17—N3—C21—C20	54.1 (3)
Pd1—C1—C6—O1	0.4 (3)	P2—N3—C21—C20	−94.9 (3)
C5—C6—O1—P1	172.54 (17)	C19—C20—C21—N3	−53.7 (4)
C1—C6—O1—P1	−9.0 (2)	O2—P2—N4—C22	−113.9 (2)
N2—P1—O1—C6	−110.08 (16)	N3—P2—N4—C22	143.9 (2)
N1—P1—O1—C6	143.25 (16)	Pd1—P2—N4—C22	1.4 (3)
Pd1—P1—O1—C6	11.78 (15)	O2—P2—N4—C26	47.1 (2)
C3—C2—O2—P2	−179.37 (18)	N3—P2—N4—C26	−55.1 (2)
C1—C2—O2—P2	1.5 (3)	Pd1—P2—N4—C26	162.4 (2)
N4—P2—O2—C2	121.83 (17)	C26—N4—C22—C23	−58.1 (3)
N3—P2—O2—C2	−131.42 (17)	P2—N4—C22—C23	104.5 (3)
Pd1—P2—O2—C2	−1.04 (17)	N4—C22—C23—C24	57.4 (4)
N2—P1—N1—C7	−165.4 (2)	C22—C23—C24—C25	−55.9 (5)
O1—P1—N1—C7	−54.8 (2)	C23—C24—C25—C26	54.6 (5)
Pd1—P1—N1—C7	60.2 (2)	C22—N4—C26—C25	55.4 (3)
N2—P1—N1—C11	61.2 (2)	P2—N4—C26—C25	−107.3 (3)
O1—P1—N1—C11	171.9 (2)	C24—C25—C26—N4	−53.4 (4)

Fig. 1