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Acetato[1-(oxazolin-2-ylmethyl-κN)indol-2-yl]-(triphenylphosphine)palladium(II) dichloromethane solvate

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.005 Å
R factor = 0.036
wR factor = 0.040
Data-to-parameter ratio = 12.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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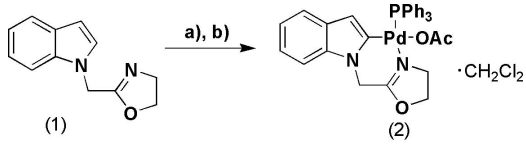
The title compound, $[Pd(C_2H_3O_2)(C_{18}H_{15}P)(C_{12}H_{11}N_2O)]\cdot CH_2Cl_2$, crystallizes readily from a mixture of dichloromethane and light petroleum. The structure is one of few examples of palladacycles that incorporate the *N*-substituent in five-membered-ring heterocycles [Nonoyama & Nakajima (1998). *Polyhedron*, **18**, 533–543].

Comment

Recently, cyclopalladated oxazoline-based complexes have attracted attention due to their catalytic efficiency and the high potential of the oxazolinyl group as an inducer of chirality (Richards & Stark, 1997; Denmark *et al.*, 1997). A few complexes based on *ortho*-palladation of an aryloxazoline in the arene, ferrocene and [2.2]*para*cyclophane series have been crystallographically characterized (Balavoine *et al.*, 1990; Bölm *et al.*, 2002; Gorunova *et al.*, 2004; Kirsch *et al.*, 2004; Smoliakova *et al.*, 2000). We report here the synthesis and structure of a six-membered indole-fused *ortho*-palladacycle, (2), which incorporates an *N*-methyleneoxazoline as a *C,N*-bidentate ligand. We found that the application of of an equimolar amount of the weak electrophilic reagent Li_2PdCl_4 in the reaction with indole-derived oxazoline, (1), in EtOH in the presence of AcONa as a base (Smoliakova *et al.*, 2000) led to the formation of a bis-oxazoline coordination complex with no traces of the desired cyclopalladated compound. On the other hand, one of the most efficient cyclopalladation methods is the use of highly electrophilic $Pd(OAc)_2$ in AcOH. By applying this method intramolecular C—H bond activation has been achieved and the desired cyclopalladated compound, (2), was obtained in good yield. This is the first crystallographically characterized oxazoline-derived palladacycle with a six-membered chelate ring, but activation of a benzylic Csp^3 atom to form a six-ring palladacycle has been reported as an alternative and controllable reaction path in the *para*-cyclophane series (Bölm *et al.*, 2002).



a) $Pd(OAc)_2$, AcONa, AcOH
b) PPh_3, CH_2Cl_2

The coordination geometry of the Pd atom closely approaches planarity. The mean plane through the reported atomic positions of the Pd/C/N/O/P atoms intersects those of the fragments C1–C9/N1, N2/O1/C10–C12 and O2/O3/C13/C14 at 39.80 (10), 36.1 (2) and 84.43 (16)°, respectively.

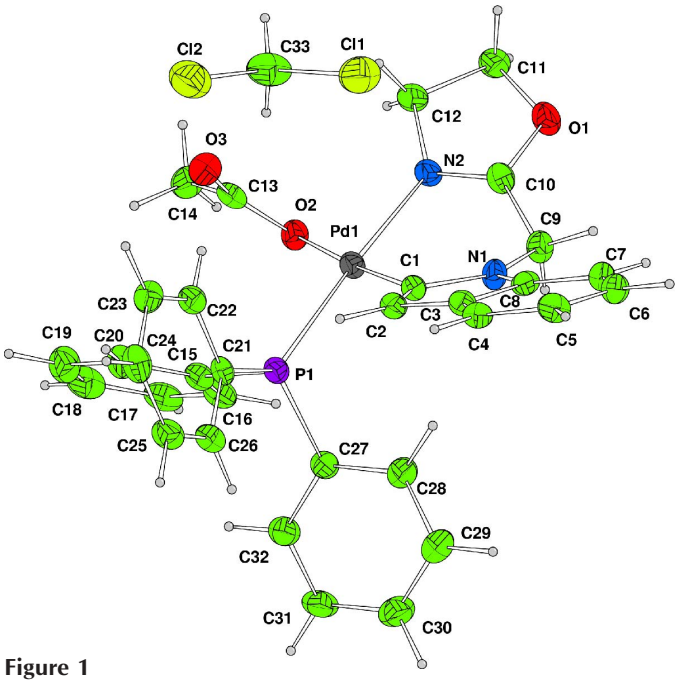


Figure 1
The molecular structure of (2). Displacement ellipsoids are drawn at the 50% probability level.

The solvent interacts with neighbouring molecules of the Pd complex. One of these interactions is apparently through a C—H···O hydrogen bond to the carbonyl O atom [C33···O3 = 3.129 (5) Å], while there is a second short contact between the oxazolinyl O atom and one of the Cl atoms of a second molecule of solvent [O1···Cl1^{i} = 3.030 (3) Å; symmetry code: (i) $-x, -y, 1-z$].

Experimental

A mixture of $Pd(OAc)_2$ (52 mg, 0.23 mmol) and AcONa (32 mg, 0.23 mmol) was partially dissolved in acetic acid (1 ml). Oxazoline, (1) (50 mg, 0.25 mmol), was dissolved in AcOH (1 ml). The two solutions were combined and stirred at room temperature overnight. The reaction mixture was then stirred at 323 K for 1 h and 24 h at room temperature. The mixture was filtered through Celite, the solvent removed and the yellow solid was dried *in vacuo*. Degassed CH_2Cl_2 (5 ml) and PPh_3 (66 mg, 0.25 mmol) were then added to the solid and the mixture was stirred at room temperature for 2 h under an argon atmosphere. Addition of light petroleum ether to the solution resulted in precipitation of a yellow solid. Recrystallization of the crude product from dichloromethane and hexane gave the yellow product, (2), with an overall yield of 70%. Full spectroscopic and physical characterization will be reported elsewhere.

Crystal data

$[Pd(C_2H_3O_2)(C_{18}H_{15}P)$-$(C_{12}H_{11}N_2O)]\cdot CH_2Cl_2$	$Z = 2$
$M_r = 711.90$	$D_x = 1.538$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 10.3125$ (2) Å	Cell parameters from 20892 reflections
$b = 10.9019$ (2) Å	$\theta = 5$–28°
$c = 16.4409$ (5) Å	$\mu = 0.87$ mm^{-1}
$\alpha = 71.7446$ (9)°	$T = 150$ K
$\beta = 75.0748$ (9)°	Plate, pale yellow
$\gamma = 62.0330$ (10)°	0.24 × 0.20 × 0.05 mm
$V = 1536.81$ (6) Å^3	

Data collection

Nonius KappaCCD diffractometer	6983 independent reflections
ω scans	4899 reflections with $I > 3\sigma(I)$
Absorption correction: multi-scan *DENZO/SCALEPACK* (Otwinowski & Minor, 1997)	$R_{int} = 0.053$
	$\theta_{max} = 27.5^\circ$
$T_{min} = 0.81$, $T_{max} = 0.96$	$h = -13 \rightarrow 13$
20892 measured reflections	$k = -14 \rightarrow 14$
	$l = -21 \rightarrow 21$

Refinement

Refinement on F	H-atom parameters constrained
$R = 0.036$	Weighting scheme: see text
$wR = 0.040$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.10$	$\Delta\rho_{max} = 0.61$ e Å^{-3}
4899 reflections	$\Delta\rho_{min} = -0.49$ e Å^{-3}
379 parameters	

Table 1
Selected geometric parameters (Å, °).

Pd1—C1	1.995 (3)	Pd1—O2	2.075 (2)
Pd1—N2	2.079 (3)	Pd1—P1	2.2425 (9)
C1—Pd1—N2	87.95 (12)	Pd1—C1—C2	133.7 (2)
C1—Pd1—O2	175.71 (11)	Pd1—C1—N1	118.6 (2)
N2—Pd1—O2	87.79 (10)	Pd1—P1—C15	112.13 (11)
C1—Pd1—P1	92.34 (9)	Pd1—P1—C21	114.12 (11)
N2—Pd1—P1	175.51 (9)	Pd1—P1—C27	116.38 (11)
O2—Pd1—P1	91.87 (7)		
C33···O3	3.129 (5)	O1···Cl1^{i}	3.030 (3)

Symmetry code: (i) $-x, -y, 1-z$.

The weighting scheme was $w = [1 - \{||F_o| - |F_c||/6\sigma(F_o)\}^2]^2/[0.391T_0(x) + 0.126\,T_1(x) + 0.171T_2(x)]$, using a second-order Chebychev polymial, with $x = F_c/F_{max}$ (Watkin, 1994; Prince, 1982).

All H atoms were placed in geometrically calculated positions after each refinement cycle, with X—H = 1.0 Å; U_{iso}(H) values were set equal to $1.2U_{eq}$ of the connected atom.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *CRYSTALS*.

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Triclinic, $P\overline{1}$
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$\beta = 75.0748$ (9)°
$\gamma = 62.033$ (1)°
$V = 1536.81$ (6) Å^3
$Z = 2$
$F(000) = 724$
$D_x = 1.538$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 20892 reflections
$\theta = 5$–28°
$\mu = 0.87$ mm^{-1}
$T = 150$ K
Plate, pale yellow
0.24 × 0.20 × 0.05 mm

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Graphite monochromator
ω scans
Absorption correction: multi-scan DENZO/SCALEPACK (Otwinowski & Minor, 1997)
$T_{min} = 0.81$, $T_{max} = 0.96$
20892 measured reflections
6983 independent reflections
4899 reflections with $I > 3\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 27.6°$, $\theta_{min} = 5.2°$
$h = -13\rightarrow13$
$k = -14\rightarrow14$
$l = -21\rightarrow21$

Refinement

Refinement on F
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.040$
$S = 1.10$
4899 reflections
379 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters not refined
Method, part 1: Chebychev polynomial (Watkin, 1994; *P*rince, 1982) [*w*eight] = 1/[0.391T_0(x) + 0.126T_1(x) + 0.171T_2(x)] where T_i are the Chebychev polynomials of degree i and x = F/F_{max}. Method, part 2: Robust *w*eight modifier (*P*rince, 1982) W = [*w*eight] [1-{$\Delta F/6\sigma(F)$}^{2}]^2
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.61$ e Å^{-3}
$\Delta\rho_{min} = -0.49$ e Å^{-3}

Special details

Refinement. The hydrogen atoms were all positioned geometrically. The preferred orientation of the methyl group C14, H141—H143 was identified by examination of a difference Fourier map

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pd1	0.33058 (3)	0.19723 (3)	0.322879 (17)	0.0218
C1	0.2342 (4)	0.1180 (3)	0.2752 (2)	0.0223
C2	0.1370 (4)	0.1760 (3)	0.2159 (2)	0.0234
C3	0.0852 (3)	0.0736 (3)	0.2181 (2)	0.0228
C4	−0.0132 (4)	0.0723 (4)	0.1735 (2)	0.0251
C5	−0.0378 (4)	−0.0495 (4)	0.1920 (2)	0.0294
C6	0.0355 (4)	−0.1703 (4)	0.2542 (2)	0.0296
C7	0.1332 (4)	−0.1723 (3)	0.2992 (2)	0.0255
C8	0.1566 (4)	−0.0500 (3)	0.2809 (2)	0.0233
N1	0.2458 (3)	−0.0206 (3)	0.31444 (18)	0.0239
C9	0.3262 (4)	−0.1165 (4)	0.3867 (2)	0.0280
C10	0.2899 (4)	−0.0404 (3)	0.4567 (2)	0.0248
O1	0.2683 (3)	−0.1101 (3)	0.53787 (16)	0.0316
C11	0.2468 (4)	−0.0168 (4)	0.5928 (2)	0.0335
C12	0.2467 (5)	0.1200 (4)	0.5291 (2)	0.0325
N2	0.2804 (3)	0.0839 (3)	0.44470 (17)	0.0243
O2	0.4286 (3)	0.2698 (2)	0.38144 (15)	0.0256
C13	0.3541 (4)	0.3952 (4)	0.3952 (2)	0.0248
O3	0.2237 (3)	0.4733 (3)	0.38191 (17)	0.0311
C14	0.4362 (4)	0.4490 (4)	0.4298 (2)	0.0323
P1	0.40209 (9)	0.30494 (9)	0.19079 (5)	0.0215
C15	0.4937 (4)	0.4111 (4)	0.1951 (2)	0.0250
C16	0.6338 (4)	0.3408 (4)	0.2225 (2)	0.0298
C17	0.7046 (4)	0.4179 (4)	0.2287 (2)	0.0339
C18	0.6360 (5)	0.5655 (5)	0.2083 (3)	0.0380
C19	0.4966 (4)	0.6367 (4)	0.1822 (3)	0.0369
C20	0.4257 (4)	0.5597 (4)	0.1753 (2)	0.0300
C21	0.2502 (3)	0.4336 (3)	0.1293 (2)	0.0219
C22	0.1210 (4)	0.5185 (4)	0.1743 (2)	0.0255
C23	0.0027 (4)	0.6216 (4)	0.1305 (2)	0.0288
C24	0.0113 (4)	0.6374 (4)	0.0428 (2)	0.0323
C25	0.1387 (4)	0.5521 (4)	−0.0020 (2)	0.0313
C26	0.2593 (4)	0.4506 (4)	0.0409 (2)	0.0260
C27	0.5345 (4)	0.1887 (3)	0.1198 (2)	0.0252
C28	0.5335 (4)	0.0582 (4)	0.1262 (3)	0.0336
C29	0.6280 (5)	−0.0262 (4)	0.0678 (3)	0.0411
C30	0.7252 (5)	0.0170 (4)	0.0044 (3)	0.0404
C31	0.7299 (4)	0.1444 (4)	−0.0008 (2)	0.0382
C32	0.6348 (4)	0.2300 (4)	0.0560 (2)	0.0316
C33	−0.0756 (5)	0.4430 (5)	0.4306 (3)	0.0447
Cl1	−0.11210 (12)	0.29973 (13)	0.43171 (7)	0.0474

Cl2	−0.18805 (15)	0.60378 (14)	0.36412 (8)	0.0545
H21	0.1071	0.2736	0.1774	0.0284*
H41	−0.0651	0.1578	0.1289	0.0296*
H51	−0.1082	−0.0510	0.1607	0.0387*
H61	0.0167	−0.2567	0.2663	0.0384*
H71	0.1852	−0.2587	0.3433	0.0308*
H91	0.4350	−0.1530	0.3664	0.0335*
H92	0.2980	−0.1984	0.4100	0.0335*
H111	0.3295	−0.0613	0.6286	0.0370*
H112	0.1503	0.0034	0.6315	0.0370*
H121	0.3245	0.1431	0.5379	0.0396*
H122	0.1477	0.2023	0.5347	0.0396*
H141	0.5391	0.3738	0.4369	0.0418*
H142	0.3831	0.4717	0.4870	0.0418*
H143	0.4404	0.5369	0.3883	0.0418*
H161	0.6832	0.2343	0.2375	0.0354*
H171	0.8050	0.3671	0.2480	0.0419*
H181	0.6875	0.6211	0.2125	0.0523*
H191	0.4471	0.7432	0.1683	0.0470*
H201	0.3252	0.6112	0.1561	0.0371*
H221	0.1135	0.5053	0.2381	0.0311*
H231	−0.0889	0.6843	0.1625	0.0346*
H241	−0.0746	0.7107	0.0116	0.0378*
H251	0.1441	0.5634	−0.0653	0.0387*
H261	0.3519	0.3902	0.0083	0.0323*
H281	0.4650	0.0252	0.1727	0.0399*
H291	0.6253	−0.1185	0.0719	0.0482*
H301	0.7919	−0.0433	−0.0377	0.0422*
H311	0.8021	0.1745	−0.0456	0.0384*
H321	0.6380	0.3223	0.0512	0.0337*
H331	−0.0962	0.4561	0.4909	0.0610*
H332	0.0310	0.4204	0.4078	0.0610*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.02423 (13)	0.02180 (12)	0.02126 (12)	−0.01224 (9)	−0.00276 (9)	−0.00357 (9)
C1	0.0235 (15)	0.0210 (15)	0.0233 (16)	−0.0120 (13)	0.0014 (12)	−0.0057 (12)
C2	0.0240 (16)	0.0242 (15)	0.0227 (16)	−0.0118 (13)	−0.0008 (12)	−0.0055 (12)
C3	0.0199 (15)	0.0246 (16)	0.0243 (16)	−0.0109 (13)	0.0003 (12)	−0.0062 (13)
C4	0.0241 (16)	0.0282 (17)	0.0218 (16)	−0.0105 (14)	−0.0012 (12)	−0.0065 (13)
C5	0.0307 (18)	0.038 (2)	0.0275 (17)	−0.0210 (16)	−0.0022 (14)	−0.0096 (15)
C6	0.0359 (19)	0.0287 (17)	0.0314 (18)	−0.0196 (15)	0.0006 (15)	−0.0107 (14)
C7	0.0277 (17)	0.0218 (15)	0.0274 (17)	−0.0112 (13)	−0.0020 (13)	−0.0061 (13)
C8	0.0224 (15)	0.0255 (16)	0.0239 (16)	−0.0108 (13)	0.0014 (12)	−0.0107 (13)
N1	0.0297 (14)	0.0208 (13)	0.0250 (14)	−0.0119 (12)	−0.0081 (11)	−0.0045 (11)
C9	0.0328 (18)	0.0230 (16)	0.0279 (17)	−0.0113 (14)	−0.0084 (14)	−0.0025 (13)
C10	0.0248 (16)	0.0246 (16)	0.0245 (16)	−0.0103 (13)	−0.0085 (13)	−0.0008 (13)

O1	0.0437 (15)	0.0287 (13)	0.0233 (12)	−0.0180 (11)	−0.0094 (11)	0.0013 (10)
C11	0.039 (2)	0.0294 (18)	0.0241 (17)	−0.0106 (16)	−0.0025 (15)	−0.0033 (14)
C12	0.049 (2)	0.0320 (18)	0.0179 (16)	−0.0193 (17)	−0.0019 (15)	−0.0060 (14)
N2	0.0322 (15)	0.0258 (14)	0.0182 (13)	−0.0155 (12)	−0.0034 (11)	−0.0041 (11)
O2	0.0293 (12)	0.0247 (12)	0.0265 (12)	−0.0135 (10)	−0.0058 (10)	−0.0053 (9)
C13	0.0260 (16)	0.0320 (17)	0.0190 (15)	−0.0180 (14)	−0.0003 (12)	−0.0018 (13)
O3	0.0248 (12)	0.0332 (13)	0.0380 (14)	−0.0123 (10)	−0.0052 (10)	−0.0108 (11)
C14	0.0303 (18)	0.0359 (19)	0.038 (2)	−0.0173 (16)	−0.0028 (15)	−0.0143 (16)
P1	0.0213 (4)	0.0207 (4)	0.0222 (4)	−0.0100 (3)	−0.0020 (3)	−0.0032 (3)
C15	0.0237 (16)	0.0292 (17)	0.0242 (16)	−0.0150 (14)	−0.0014 (13)	−0.0041 (13)
C16	0.0248 (16)	0.0369 (19)	0.0268 (17)	−0.0158 (15)	−0.0020 (13)	−0.0028 (14)
C17	0.0276 (17)	0.050 (2)	0.0269 (18)	−0.0215 (17)	0.0003 (14)	−0.0077 (16)
C18	0.040 (2)	0.056 (2)	0.035 (2)	−0.035 (2)	0.0009 (16)	−0.0137 (18)
C19	0.040 (2)	0.035 (2)	0.043 (2)	−0.0220 (17)	−0.0043 (17)	−0.0082 (17)
C20	0.0289 (17)	0.0276 (17)	0.0361 (19)	−0.0155 (15)	−0.0046 (15)	−0.0047 (14)
C21	0.0237 (15)	0.0203 (15)	0.0243 (16)	−0.0137 (13)	−0.0027 (12)	−0.0016 (12)
C22	0.0249 (16)	0.0261 (16)	0.0268 (17)	−0.0134 (14)	−0.0013 (13)	−0.0051 (13)
C23	0.0222 (16)	0.0260 (17)	0.0383 (19)	−0.0096 (14)	−0.0037 (14)	−0.0086 (14)
C24	0.0306 (18)	0.0266 (17)	0.037 (2)	−0.0111 (15)	−0.0159 (15)	0.0032 (15)
C25	0.0380 (19)	0.0354 (19)	0.0234 (17)	−0.0189 (16)	−0.0049 (14)	−0.0041 (14)
C26	0.0277 (17)	0.0310 (17)	0.0222 (16)	−0.0166 (14)	−0.0025 (13)	−0.0036 (13)
C27	0.0207 (15)	0.0235 (16)	0.0256 (16)	−0.0069 (13)	−0.0022 (13)	−0.0029 (13)
C28	0.0325 (19)	0.0288 (18)	0.038 (2)	−0.0136 (15)	0.0037 (15)	−0.0118 (15)
C29	0.044 (2)	0.032 (2)	0.045 (2)	−0.0137 (17)	0.0037 (18)	−0.0166 (17)
C30	0.038 (2)	0.034 (2)	0.033 (2)	−0.0029 (17)	−0.0012 (16)	−0.0103 (16)
C31	0.0303 (19)	0.037 (2)	0.0290 (19)	−0.0072 (16)	0.0063 (15)	−0.0030 (15)
C32	0.0279 (17)	0.0283 (17)	0.0280 (18)	−0.0071 (14)	−0.0012 (14)	−0.0025 (14)
C33	0.042 (2)	0.070 (3)	0.041 (2)	−0.037 (2)	0.0043 (18)	−0.023 (2)
Cl1	0.0473 (6)	0.0585 (7)	0.0493 (6)	−0.0301 (5)	0.0011 (5)	−0.0222 (5)
Cl2	0.0662 (7)	0.0648 (7)	0.0454 (6)	−0.0420 (6)	0.0041 (5)	−0.0152 (5)

Geometric parameters (Å, º)

Pd1—C1	1.995 (3)	P1—C21	1.819 (3)
Pd1—N2	2.079 (3)	P1—C27	1.820 (3)
Pd1—O2	2.075 (2)	C15—C16	1.399 (5)
Pd1—P1	2.2425 (9)	C15—C20	1.395 (5)
C1—C2	1.371 (5)	C16—C17	1.384 (5)
C1—N1	1.406 (4)	C16—H161	1.000
C2—C3	1.434 (4)	C17—C18	1.386 (6)
C2—H21	1.000	C17—H171	1.000
C3—C4	1.404 (4)	C18—C19	1.384 (6)
C3—C8	1.419 (5)	C18—H181	1.000
C4—C5	1.394 (5)	C19—C20	1.389 (5)
C4—H41	1.000	C19—H191	1.000
C5—C6	1.404 (5)	C20—H201	1.000
C5—H51	1.000	C21—C22	1.394 (5)
C6—C7	1.383 (5)	C21—C26	1.390 (5)

C6—H61	1.000	C22—C23	1.389 (5)
C7—C8	1.394 (4)	C22—H221	1.000
C7—H71	1.000	C23—C24	1.381 (5)
C8—N1	1.378 (4)	C23—H231	1.000
N1—C9	1.452 (4)	C24—C25	1.385 (5)
C9—C10	1.496 (5)	C24—H241	1.000
C9—H91	1.000	C25—C26	1.393 (5)
C9—H92	1.000	C25—H251	1.000
C10—O1	1.334 (4)	C26—H261	1.000
C10—N2	1.266 (4)	C27—C28	1.399 (5)
O1—C11	1.470 (4)	C27—C32	1.399 (5)
C11—C12	1.530 (5)	C28—C29	1.396 (5)
C11—H111	1.000	C28—H281	1.000
C11—H112	1.000	C29—C30	1.383 (6)
C12—N2	1.471 (4)	C29—H291	1.000
C12—H121	1.000	C30—C31	1.387 (6)
C12—H122	1.000	C30—H301	1.000
O2—C13	1.277 (4)	C31—C32	1.385 (5)
C13—O3	1.241 (4)	C31—H311	1.000
C13—C14	1.519 (5)	C32—H321	1.000
C14—H141	1.000	C33—Cl1	1.764 (4)
C14—H142	1.000	C33—Cl2	1.777 (5)
C14—H143	1.000	C33—H331	1.000
P1—C15	1.830 (3)	C33—H332	1.000
C33···O3	3.129 (5)	O1···Cl1^{i}	3.030 (3)

C1—Pd1—N2	87.95 (12)	H142—C14—H143	109.476
C1—Pd1—O2	175.71 (11)	Pd1—P1—C15	112.13 (11)
N2—Pd1—O2	87.79 (10)	Pd1—P1—C21	114.12 (11)
C1—Pd1—P1	92.34 (9)	C15—P1—C21	103.34 (15)
N2—Pd1—P1	175.51 (9)	Pd1—P1—C27	116.38 (11)
O2—Pd1—P1	91.87 (7)	C15—P1—C27	103.71 (15)
Pd1—C1—C2	133.7 (2)	C21—P1—C27	105.85 (15)
Pd1—C1—N1	118.6 (2)	P1—C15—C16	118.9 (3)
C2—C1—N1	107.0 (3)	P1—C15—C20	122.0 (3)
C1—C2—C3	108.8 (3)	C16—C15—C20	119.1 (3)
C1—C2—H21	125.577	C15—C16—C17	120.4 (3)
C3—C2—H21	125.578	C15—C16—H161	119.792
C2—C3—C4	134.6 (3)	C17—C16—H161	119.792
C2—C3—C8	106.8 (3)	C16—C17—C18	119.9 (3)
C4—C3—C8	118.6 (3)	C16—C17—H171	120.058
C3—C4—C5	119.3 (3)	C18—C17—H171	120.059
C3—C4—H41	120.343	C17—C18—C19	120.4 (3)
C5—C4—H41	120.343	C17—C18—H181	119.787
C4—C5—C6	120.6 (3)	C19—C18—H181	119.787
C4—C5—H51	119.718	C18—C19—C20	119.9 (4)
C6—C5—H51	119.718	C18—C19—H191	120.075

C5—C6—C7	121.5 (3)	C20—C19—H191	120.074
C5—C6—H61	119.253	C15—C20—C19	120.4 (3)
C7—C6—H61	119.253	C15—C20—H201	119.822
C6—C7—C8	117.8 (3)	C19—C20—H201	119.822
C6—C7—H71	121.113	P1—C21—C22	117.2 (2)
C8—C7—H71	121.113	P1—C21—C26	122.8 (3)
C3—C8—C7	122.2 (3)	C22—C21—C26	119.9 (3)
C3—C8—N1	106.8 (3)	C21—C22—C23	119.9 (3)
C7—C8—N1	130.9 (3)	C21—C22—H221	120.034
C1—N1—C8	110.5 (3)	C23—C22—H221	120.034
C1—N1—C9	126.0 (3)	C22—C23—C24	120.1 (3)
C8—N1—C9	123.1 (3)	C22—C23—H231	119.940
N1—C9—C10	110.4 (3)	C24—C23—H231	119.940
N1—C9—H91	109.228	C23—C24—C25	120.1 (3)
C10—C9—H91	109.228	C23—C24—H241	119.926
N1—C9—H92	109.228	C25—C24—H241	119.926
C10—C9—H92	109.228	C24—C25—C26	120.3 (3)
H91—C9—H92	109.466	C24—C25—H251	119.869
C9—C10—O1	117.3 (3)	C26—C25—H251	119.870
C9—C10—N2	125.0 (3)	C21—C26—C25	119.6 (3)
O1—C10—N2	117.7 (3)	C21—C26—H261	120.196
C10—O1—C11	105.9 (3)	C25—C26—H261	120.196
O1—C11—C12	104.5 (3)	P1—C27—C28	120.2 (3)
O1—C11—H111	110.695	P1—C27—C32	121.1 (3)
C12—C11—H111	110.695	C28—C27—C32	118.7 (3)
O1—C11—H112	110.695	C27—C28—C29	120.1 (3)
C12—C11—H112	110.695	C27—C28—H281	119.935
H111—C11—H112	109.467	C29—C28—H281	119.935
C11—C12—N2	102.7 (3)	C28—C29—C30	120.4 (4)
C11—C12—H121	111.133	C28—C29—H291	119.799
N2—C12—H121	111.133	C30—C29—H291	119.799
C11—C12—H122	111.133	C29—C30—C31	119.8 (3)
N2—C12—H122	111.133	C29—C30—H301	120.102
H121—C12—H122	109.467	C31—C30—H301	120.102
Pd1—N2—C10	121.8 (2)	C30—C31—C32	120.2 (3)
Pd1—N2—C12	128.9 (2)	C30—C31—H311	119.897
C10—N2—C12	108.9 (3)	C32—C31—H311	119.897
Pd1—O2—C13	117.5 (2)	C27—C32—C31	120.7 (3)
O2—C13—O3	125.0 (3)	C27—C32—H321	119.634
O2—C13—C14	115.4 (3)	C31—C32—H321	119.634
O3—C13—C14	119.5 (3)	Cl1—C33—Cl2	111.3 (2)
C13—C14—H141	109.467	Cl1—C33—H331	109.024
C13—C14—H142	109.467	Cl2—C33—H331	109.024
H141—C14—H142	109.476	Cl1—C33—H332	109.024
C13—C14—H143	109.466	Cl2—C33—H332	109.024
H141—C14—H143	109.476	H331—C33—H332	109.467

Symmetry code: (i) $-x$, $-y$, $-z+1$.