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Chloro{1-[(dimethylamino)methyl-κN]-1*H*-indolyl-κC^2}(triphenylphosphine-κP)-palladium(II) dichloromethane solvate

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Key indicators

Single-crystal X-ray study
T = 190 K
Mean σ(C–C) = 0.003 Å
R factor = 0.025
wR factor = 0.059
Data-to-parameter ratio = 19.7

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

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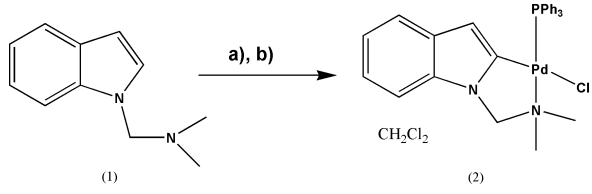
The title compound, $[Pd(C_{11}H_{13}N_2)Cl(C_{18}H_{15}P)]\cdot CH_2Cl_2$, crystallizes readily from a mixture of dichloromethane and light petroleum. The structure is one of few examples of palladacycles that incorporate the *N*-substituent in five-membered ring heterocycles [Nonoyama & Nakajima (1998). *Polyhedron* **18**, 533–543.].

Comment

Cyclometallation represents one of the most useful methods for the activation and *ortho*-functionalization of Csp^2—H bonds in aromatic compounds (Ryabov *et al.*, 1993). The presence of a tethered donor group allows the initial coordination of the ligand to the metal and favourable intramolecular cyclization. Whereas heteroatom-directed cyclometallation of benzenoid and heteroaromatic systems has been exhaustively investigated, the chemistry of the analogous indole derivatives has remained virtually unexplored (Valk *et al.*, 1994; Tollari *et al.*, 1997). Palladacycles are amongst the most active catalysts for C—C and C—heteroatom bond formation (Herrmann *et al.*, 1999; Albrecht & van Koten, 2001; Dupont *et al.*, 2001). In addition to their high activity, they permit easy synthesis, facile modification and comparative stability. We report here the synthesis and structure of a five-membered indole-fused *ortho*-palladacycle, (2), which incorporates *N*-isogramine, (1), as a *C,N*-bidentate ligand.



(1) (2)

a) $PdCl_2$, LiCl, AcONa, EtOH
b) PPh_3, CH_2Cl_2

The coordination geometry of the Pd atom closely approximates planarity. The mean plane through the Pd/C/Cl/N/P atoms intersects that of the ring system of the *N*-isogramine ligand (atoms C1–C5/N6/C7–C10) at an angle of 26.69 (6)°. The structure of a related six-membered indole-fused *ortho*-palladacycle which incorporates an *N*-methyleneoxazoline as the *C,N*-bidentate ligand has also been reported (Cowley *et al.*, 2005).

Experimental

A suspension of $PdCl_2$ (0.135 g, 0.76 mmol) and LiCl (0.064 g, 1.52 mmol) in ethanol (5 ml) was heated under reflux condition for

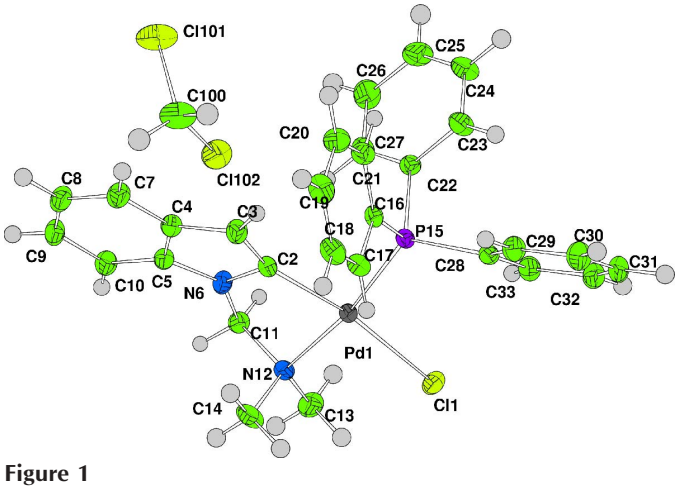


Figure 1
The molecular structure of (2), drawn with 50% probability ellipsoids for the anisotropically refined atoms.

2 h to give a dark red solution of $Li_2[PdCl_4]$. The solution was cooled to room temperature and *N*-isogramine (Swaminathan & Narasimhan, 1966) (0.11 g, 0.63 mmol) in ethanol (2 ml) and sodium acetate trihydrate (0.086 g, 0.63 mmol) were added. The resulting suspension was stirred at room temperature for 1.5 h. The insoluble brown solid was filtered off, washed with ethanol and dried *in vacuo*. Degassed CH_2Cl_2 (8 ml) and PPh_3 (0.413 g, 1.58 mmol) were then added to the solid and the mixture was stirred at room temperature for 1 h under an argon atmosphere. Addition of pentane to the solution resulted in precipitation of a yellow solid. Recrystallization of the crude product from dichloromethane–pentane gave the yellow product, (2) (m.p. 398–402 K); full spectroscopic and physical characterization will be reported elsewhere.

Crystal data

$[Pd(C_{11}H_{13}N_2)Cl(C_{18}H_{15}P)]\cdot CH_2Cl_2$	D_x = 1.518 Mg m^{-3}
M_r = 662.31	Mo Kα radiation
Monoclinic, $P2_1/n$	Cell parameters from 6527 reflections
a = 11.0324 (1) Å	θ = 1–27°
b = 23.9623 (3) Å	μ = 1.00 mm^{-1}
c = 11.2437 (1) Å	T = 190 K
β = 102.9338 (8)°	Block, yellow
V = 2896.99 (5) Å^3	0.28 × 0.20 × 0.20 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	R_{int} = 0.012
ω scans	θ_{max} = 27.5°
Absorption correction: none	$h = -14 \rightarrow 14$
12861 measured reflections	$k = -31 \rightarrow 31$
6622 independent reflections	$l = -14 \rightarrow 14$
5789 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H-atom parameters not refined
$R[F^2 > 2\sigma(F^2)]$ = 0.025	$w = 1/[\sigma^2(F^2) + 0.02 + 2.41P]$ where $P = [\max(F_o^2,0) + 2F_c^2]/3$
$wR(F^2)$ = 0.059	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.00	$\Delta\rho_{max}$ = 0.81 e Å^{-3}
6593 reflections	$\Delta\rho_{min}$ = −0.64 e Å^{-3}
334 parameters	

Table 1
Selected geometric parameters (Å, °).

Pd1—C2	1.9974 (18)	Pd1—P15	2.2536 (5)
Pd1—N12	2.1867 (15)	Pd1—Cl1	2.3618 (5)
C2—Pd1—N12	80.76 (7)	N12—Pd1—Cl1	91.59 (4)
C2—Pd1—P15	91.69 (5)	P15—Pd1—Cl1	96.583 (17)
N12—Pd1—P15	169.10 (4)	Pd1—C2—C3	142.04 (14)
C2—Pd1—Cl1	170.75 (5)	Pd1—C2—N6	110.00 (12)

The 29 reflections below $[\sin(\theta)/\lambda]^2$ of 0.011 (= ∼4.27°) were not used in the refinement. It was suspected that some of them may have been partially obscured by the beam stop. 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 at 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: *SIR*92 (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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References

Albrecht, M. & Van Koten, G. (2001). *Angew. Chem. Int. Ed.* **40**, 3750–3753.
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
Cowley, A. R., Cooper, R. I., Capito, E., Brown, J. M., Ricci, A. (2005). *Acta Cryst.* E**61**, m582–m584.
Dupont, J., Pfeffer, M. & Spencer, J. (2001). *Eur. J. Inorg. Chem.* pp. 1917–1927.
Herrmann, W. A., Böhm, V. P. W. & Reisinger, C. P. (1999). *J. Organomet. Chem.* **576**, 23–41.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Nonoyama, M. & Nakajima, K. (1998). *Polyhedron* 18, 533–543.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr and R. M. Sweet, pp. 307–326. New York: Academic Press.
Ryabov, A. D., van Eldik, R., Le Borgue, G. & Pfeffer, M. (1993). *Organometallics*, **12**, 1386–1393.
Swaminathan, S. & Narasimhan, K. (1966). *Chem. Ber.* **99**, 889–894.
Tollari, S., Demartin, F., Cenini, S., Palmisano, G. & Raimondi, P. (1997). *J. Organomet. Chem.* **527**, 93–102.
Valk, J., Maassarani, F., van der Sluis, P., Spek, A. L., Boersma, J. & van Koten, G. (1994). *Organometallics*, **13**, 2320–2329.
Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*. Chemical Crystallography Laboratory, Oxford, England.

supporting information

Acta Cryst. (2005). E**61**, m585–m586 [https://doi.org/10.1107/S1600536804033227]

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$b = 23.9623$ (3) Å
$c = 11.2437$ (1) Å
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$V = 2896.99$ (5) Å^3
$Z = 4$

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$D_x = 1.518$ Mg m^{-3}
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Cell parameters from 6527 reflections
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0.28 × 0.20 × 0.20 mm

Data collection

Nonius Kappa CCD diffractometer
Graphite monochromator
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12861 measured reflections
6622 independent reflections

5789 reflections with $I > 2\sigma(I)$
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$h = -14 \rightarrow 14$
$k = -31 \rightarrow 31$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.059$
$S = 1.00$
6593 reflections
334 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters not refined
$w = 1/[\sigma^2(F^2) + 0.02 + 2.41P]$ where $P = [\max(F_o^2,0) + 2F_c^2]/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.81$ e Å^{-3}
$\Delta\rho_{min} = -0.64$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pd1	0.379810 (12)	0.172059 (6)	0.040211 (12)	0.0171
C2	0.41809 (17)	0.16280 (8)	0.22133 (17)	0.0209
C3	0.36227 (18)	0.15409 (9)	0.31727 (17)	0.0255

C4	0.45169 (18)	0.16494 (8)	0.42884 (17)	0.0234
C5	0.56341 (18)	0.18089 (8)	0.39618 (17)	0.0218
N6	0.54108 (14)	0.17869 (7)	0.27108 (14)	0.0223
C7	0.44971 (19)	0.16240 (9)	0.55305 (18)	0.0289
C8	0.5571 (2)	0.17567 (9)	0.63891 (18)	0.0306
C9	0.66611 (19)	0.19166 (9)	0.60417 (18)	0.0294
C10	0.67149 (18)	0.19471 (9)	0.48235 (18)	0.0267
C11	0.62266 (17)	0.19418 (8)	0.19382 (17)	0.0215
N12	0.54648 (14)	0.22409 (6)	0.08783 (14)	0.0208
C13	0.62260 (19)	0.23157 (10)	−0.00399 (19)	0.0325
C14	0.5127 (2)	0.28011 (9)	0.1271 (2)	0.0342
P15	0.22953 (4)	0.106624 (19)	0.01567 (4)	0.0176
C16	0.12054 (16)	0.11533 (8)	0.11426 (16)	0.0199
C17	0.06807 (18)	0.16813 (8)	0.11899 (18)	0.0256
C18	−0.01287 (19)	0.17783 (9)	0.1953 (2)	0.0307
C19	−0.0400 (2)	0.13526 (10)	0.2682 (2)	0.0334
C20	0.0112 (2)	0.08273 (9)	0.26349 (19)	0.0316
C21	0.09117 (18)	0.07243 (8)	0.18677 (18)	0.0251
C22	0.29387 (17)	0.03644 (8)	0.04571 (16)	0.0203
C23	0.22890 (19)	−0.01008 (8)	−0.00876 (19)	0.0289
C24	0.2785 (2)	−0.06323 (9)	0.0141 (2)	0.0333
C25	0.3946 (2)	−0.07024 (9)	0.0911 (2)	0.0370
C26	0.4591 (2)	−0.02442 (10)	0.1459 (2)	0.0410
C27	0.41016 (19)	0.02890 (9)	0.12341 (19)	0.0306
C28	0.12718 (17)	0.09811 (8)	−0.13571 (17)	0.0212
C29	−0.00183 (18)	0.09930 (9)	−0.15329 (18)	0.0285
C30	−0.0770 (2)	0.08776 (10)	−0.2680 (2)	0.0364
C31	−0.0241 (2)	0.07545 (9)	−0.36462 (19)	0.0356
C32	0.1041 (2)	0.07464 (9)	−0.34823 (19)	0.0326
C33	0.17974 (18)	0.08590 (8)	−0.23477 (18)	0.0267
Cl1	0.34696 (4)	0.19778 (2)	−0.16733 (4)	0.0261
C100	0.6360 (2)	0.04871 (11)	0.4578 (2)	0.0438
Cl102	0.71605 (5)	0.05440 (3)	0.33911 (5)	0.0403
Cl101	0.67962 (6)	−0.01180 (3)	0.54647 (7)	0.0529
H31	0.2741	0.1422	0.3106	0.0304*
H71	0.3723	0.1512	0.5792	0.0350*
H81	0.5566	0.1738	0.7276	0.0363*
H91	0.7417	0.2011	0.6685	0.0336*
H101	0.7492	0.2063	0.4573	0.0311*
H111	0.6901	0.2191	0.2390	0.0256*
H112	0.6605	0.1601	0.1658	0.0256*
H131	0.5728	0.2517	−0.0765	0.0390*
H132	0.6985	0.2538	0.0324	0.0390*
H133	0.6479	0.1942	−0.0299	0.0390*
H141	0.4612	0.3003	0.0556	0.0387*
H142	0.5901	0.3019	0.1606	0.0387*
H143	0.4640	0.2758	0.1916	0.0387*
H171	0.0888	0.1991	0.0672	0.0307*

H181	−0.0514	0.2155	0.1976	0.0374*
H191	−0.0967	0.1424	0.3246	0.0415*
H201	−0.0097	0.0520	0.3157	0.0389*
H211	0.1276	0.0344	0.1835	0.0299*
H231	0.1455	−0.0052	−0.0650	0.0339*
H241	0.2307	−0.0964	−0.0249	0.0399*
H251	0.4313	−0.1084	0.1068	0.0442*
H261	0.5421	−0.0296	0.2026	0.0458*
H271	0.4584	0.0619	0.1630	0.0347*
H291	−0.0408	0.1085	−0.0835	0.0332*
H301	−0.1695	0.0884	−0.2799	0.0411*
H311	−0.0782	0.0671	−0.4466	0.0395*
H321	0.1424	0.0659	−0.4187	0.0382*
H331	0.2722	0.0853	−0.2237	0.0313*
H1001	0.6551	0.0822	0.5117	0.0541*
H1002	0.5446	0.0472	0.4214	0.0541*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.01732 (7)	0.01693 (7)	0.01648 (8)	−0.00230 (5)	0.00276 (5)	−0.00053 (5)
C2	0.0212 (9)	0.0200 (9)	0.0201 (9)	−0.0033 (7)	0.0017 (7)	−0.0017 (7)
C3	0.0225 (10)	0.0309 (11)	0.0227 (10)	−0.0054 (8)	0.0041 (7)	−0.0014 (8)
C4	0.0256 (10)	0.0237 (10)	0.0209 (9)	−0.0003 (8)	0.0055 (7)	−0.0011 (7)
C5	0.0249 (10)	0.0207 (9)	0.0191 (9)	0.0007 (7)	0.0031 (7)	−0.0006 (7)
N6	0.0200 (8)	0.0282 (9)	0.0181 (8)	−0.0032 (6)	0.0029 (6)	−0.0001 (6)
C7	0.0308 (11)	0.0335 (12)	0.0232 (10)	−0.0011 (9)	0.0078 (8)	0.0002 (8)
C8	0.0387 (12)	0.0328 (11)	0.0193 (10)	0.0031 (9)	0.0043 (8)	−0.0002 (8)
C9	0.0315 (11)	0.0311 (11)	0.0215 (10)	0.0010 (9)	−0.0030 (8)	−0.0027 (8)
C10	0.0233 (10)	0.0290 (11)	0.0255 (10)	−0.0001 (8)	0.0005 (8)	0.0000 (8)
C11	0.0189 (9)	0.0230 (9)	0.0222 (9)	−0.0003 (7)	0.0034 (7)	0.0015 (7)
N12	0.0199 (8)	0.0192 (8)	0.0221 (8)	−0.0044 (6)	0.0021 (6)	0.0009 (6)
C13	0.0291 (11)	0.0404 (13)	0.0279 (10)	−0.0114 (9)	0.0059 (8)	0.0064 (9)
C14	0.0295 (11)	0.0182 (10)	0.0491 (13)	−0.0008 (8)	−0.0036 (9)	−0.0029 (9)
P15	0.0161 (2)	0.0169 (2)	0.0189 (2)	−0.00120 (17)	0.00187 (17)	−0.00088 (17)
C16	0.0166 (9)	0.0214 (9)	0.0200 (9)	−0.0025 (7)	0.0010 (7)	−0.0027 (7)
C17	0.0267 (10)	0.0212 (10)	0.0288 (10)	−0.0022 (8)	0.0062 (8)	−0.0020 (8)
C18	0.0275 (10)	0.0279 (11)	0.0380 (12)	0.0017 (8)	0.0105 (9)	−0.0079 (9)
C19	0.0289 (11)	0.0396 (13)	0.0354 (12)	−0.0045 (9)	0.0151 (9)	−0.0081 (10)
C20	0.0307 (11)	0.0343 (12)	0.0322 (11)	−0.0063 (9)	0.0121 (9)	0.0023 (9)
C21	0.0232 (9)	0.0233 (10)	0.0283 (10)	−0.0018 (8)	0.0051 (8)	0.0001 (8)
C22	0.0220 (9)	0.0186 (9)	0.0210 (9)	0.0013 (7)	0.0060 (7)	0.0000 (7)
C23	0.0253 (10)	0.0225 (10)	0.0370 (11)	−0.0010 (8)	0.0028 (8)	−0.0019 (9)
C24	0.0361 (12)	0.0209 (10)	0.0428 (13)	−0.0023 (9)	0.0087 (10)	−0.0028 (9)
C25	0.0448 (13)	0.0234 (11)	0.0422 (13)	0.0118 (10)	0.0087 (10)	0.0043 (10)
C26	0.0379 (13)	0.0332 (12)	0.0434 (13)	0.0128 (10)	−0.0087 (10)	−0.0012 (10)
C27	0.0303 (11)	0.0252 (11)	0.0313 (11)	0.0041 (8)	−0.0040 (8)	−0.0035 (9)
C28	0.0213 (9)	0.0171 (9)	0.0224 (9)	0.0007 (7)	−0.0012 (7)	0.0009 (7)

C29	0.0228 (10)	0.0310 (11)	0.0293 (11)	−0.0025 (8)	0.0005 (8)	0.0004 (8)
C30	0.0251 (11)	0.0405 (13)	0.0372 (12)	−0.0034 (9)	−0.0066 (9)	0.0014 (10)
C31	0.0408 (13)	0.0314 (12)	0.0265 (11)	−0.0027 (10)	−0.0093 (9)	−0.0012 (9)
C32	0.0440 (13)	0.0276 (11)	0.0239 (10)	0.0032 (9)	0.0027 (9)	−0.0026 (8)
C33	0.0264 (10)	0.0253 (10)	0.0265 (10)	0.0035 (8)	0.0019 (8)	−0.0028 (8)
Cl1	0.0253 (2)	0.0321 (3)	0.0201 (2)	−0.00170 (19)	0.00353 (17)	0.00504 (19)
C100	0.0375 (13)	0.0391 (14)	0.0588 (16)	0.0054 (11)	0.0192 (11)	0.0105 (12)
Cl102	0.0352 (3)	0.0439 (3)	0.0416 (3)	0.0006 (2)	0.0082 (2)	0.0036 (3)
Cl101	0.0463 (4)	0.0434 (4)	0.0730 (5)	0.0037 (3)	0.0220 (3)	0.0208 (3)

Geometric parameters (Å, º)

Pd1—C2	1.9974 (18)	C17—C18	1.390 (3)
Pd1—N12	2.1867 (15)	C17—H171	1.000
Pd1—P15	2.2536 (5)	C18—C19	1.383 (3)
Pd1—Cl1	2.3618 (5)	C18—H181	1.000
C2—C3	1.373 (3)	C19—C20	1.385 (3)
C2—N6	1.400 (2)	C19—H191	1.000
C3—C4	1.435 (3)	C20—C21	1.387 (3)
C3—H31	1.000	C20—H201	1.000
C4—C5	1.415 (3)	C21—H211	1.000
C4—C7	1.403 (3)	C22—C23	1.391 (3)
C5—N6	1.374 (2)	C22—C27	1.393 (3)
C5—C10	1.398 (3)	C23—C24	1.388 (3)
N6—C11	1.433 (2)	C23—H231	1.000
C7—C8	1.388 (3)	C24—C25	1.386 (3)
C7—H71	1.000	C24—H241	1.000
C8—C9	1.398 (3)	C25—C26	1.377 (3)
C8—H81	1.000	C25—H251	1.000
C9—C10	1.386 (3)	C26—C27	1.388 (3)
C9—H91	1.000	C26—H261	1.000
C10—H101	1.000	C27—H271	1.000
C11—N12	1.481 (2)	C28—C29	1.393 (3)
C11—H111	1.000	C28—C33	1.397 (3)
C11—H112	1.000	C29—C30	1.396 (3)
N12—C13	1.480 (3)	C29—H291	1.000
N12—C14	1.487 (3)	C30—C31	1.375 (3)
C13—H131	1.000	C30—H301	1.000
C13—H132	1.000	C31—C32	1.386 (3)
C13—H133	1.000	C31—H311	1.000
C14—H141	1.000	C32—C33	1.385 (3)
C14—H142	1.000	C32—H321	1.000
C14—H143	1.000	C33—H331	1.000
P15—C16	1.8207 (19)	C100—Cl102	1.762 (2)
P15—C22	1.8273 (19)	C100—Cl101	1.765 (3)
P15—C28	1.8312 (18)	C100—H1001	1.000
C16—C17	1.397 (3)	C100—H1002	1.000
C16—C21	1.394 (3)		

C2—Pd1—N12	80.76 (7)	C22—P15—C28	101.68 (8)
C2—Pd1—P15	91.69 (5)	P15—C16—C17	117.55 (14)
N12—Pd1—P15	169.10 (4)	P15—C16—C21	122.89 (14)
C2—Pd1—Cl1	170.75 (5)	C17—C16—C21	119.53 (17)
N12—Pd1—Cl1	91.59 (4)	C16—C17—C18	120.25 (18)
P15—Pd1—Cl1	96.583 (17)	C16—C17—H171	119.877
Pd1—C2—C3	142.04 (14)	C18—C17—H171	119.875
Pd1—C2—N6	110.00 (12)	C17—C18—C19	119.79 (19)
C3—C2—N6	107.02 (15)	C17—C18—H181	120.104
C2—C3—C4	108.53 (16)	C19—C18—H181	120.102
C2—C3—H31	125.734	C18—C19—C20	120.24 (19)
C4—C3—H31	125.735	C18—C19—H191	119.881
C3—C4—C5	106.87 (16)	C20—C19—H191	119.881
C3—C4—C7	134.54 (18)	C19—C20—C21	120.46 (19)
C5—C4—C7	118.59 (17)	C19—C20—H201	119.769
C4—C5—N6	106.76 (16)	C21—C20—H201	119.770
C4—C5—C10	122.80 (18)	C16—C21—C20	119.72 (19)
N6—C5—C10	130.43 (18)	C16—C21—H211	120.142
C2—N6—C5	110.81 (15)	C20—C21—H211	120.142
C2—N6—C11	120.84 (15)	P15—C22—C23	121.03 (14)
C5—N6—C11	128.17 (15)	P15—C22—C27	120.03 (14)
C4—C7—C8	118.78 (19)	C23—C22—C27	118.94 (18)
C4—C7—H71	120.608	C22—C23—C24	120.72 (18)
C8—C7—H71	120.609	C22—C23—H231	119.640
C7—C8—C9	121.49 (19)	C24—C23—H231	119.641
C7—C8—H81	119.255	C23—C24—C25	119.88 (19)
C9—C8—H81	119.255	C23—C24—H241	120.059
C8—C9—C10	121.35 (18)	C25—C24—H241	120.060
C8—C9—H91	119.327	C24—C25—C26	119.7 (2)
C10—C9—H91	119.326	C24—C25—H251	120.156
C5—C10—C9	116.99 (18)	C26—C25—H251	120.156
C5—C10—H101	121.505	C25—C26—C27	120.8 (2)
C9—C10—H101	121.505	C25—C26—H261	119.604
N6—C11—N12	107.03 (14)	C27—C26—H261	119.603
N6—C11—H111	110.079	C22—C27—C26	119.97 (19)
N12—C11—H111	110.078	C22—C27—H271	120.014
N6—C11—H112	110.078	C26—C27—H271	120.013
N12—C11—H112	110.078	P15—C28—C29	121.84 (15)
H111—C11—H112	109.467	P15—C28—C33	119.00 (14)
C11—N12—Pd1	102.46 (10)	C29—C28—C33	118.98 (17)
C11—N12—C13	108.15 (15)	C28—C29—C30	120.25 (19)
Pd1—N12—C13	118.39 (12)	C28—C29—H291	119.873
C11—N12—C14	109.44 (15)	C30—C29—H291	119.872
Pd1—N12—C14	109.54 (12)	C29—C30—C31	120.2 (2)
C13—N12—C14	108.50 (16)	C29—C30—H301	119.889
N12—C13—H131	109.466	C31—C30—H301	119.890
N12—C13—H132	109.467	C30—C31—C32	119.92 (19)

H131—C13—H132	109.475	C30—C31—H311	120.039
N12—C13—H133	109.467	C32—C31—H311	120.040
H131—C13—H133	109.475	C31—C32—C33	120.4 (2)
H132—C13—H133	109.477	C31—C32—H321	119.797
N12—C14—H141	109.467	C33—C32—H321	119.798
N12—C14—H142	109.466	C28—C33—C32	120.21 (19)
H141—C14—H142	109.475	C28—C33—H331	119.894
N12—C14—H143	109.467	C32—C33—H331	119.893
H141—C14—H143	109.476	Cl102—C100—Cl101	111.85 (13)
H142—C14—H143	109.476	Cl102—C100—H1001	108.875
Pd1—P15—C16	114.44 (6)	Cl101—C100—H1001	108.875
Pd1—P15—C22	111.90 (6)	Cl102—C100—H1002	108.875
C16—P15—C22	105.97 (8)	Cl101—C100—H1002	108.875
Pd1—P15—C28	118.36 (6)	H1001—C100—H1002	109.467
C16—P15—C28	102.99 (8)		