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cis-Dichloridobis(2-isocyanophenyl 4-methoxybenzoate)palladium(II) chloroform monosolvate

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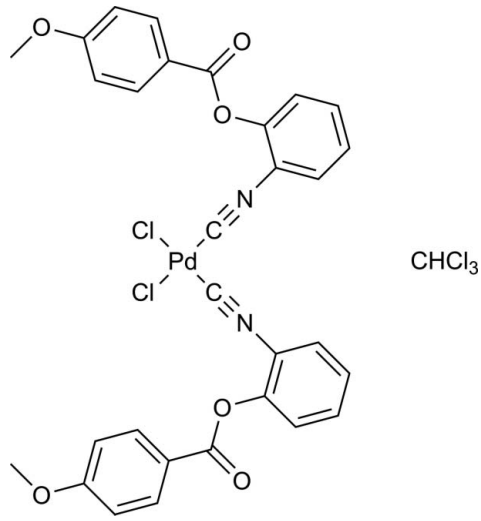
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.067; data-to-parameter ratio = 22.6.

In the title compound, $[PdCl_2(C_{15}H_{11}NO_3)_2]\cdot CHCl_3$, the Pd^{II} atom adopts a slightly distorted square-planar coordination geometry composed of two Cl atoms in *cis* positions and two C atoms from isocyanophenyl ligands. The molecular conformation is stabilized by π–π stacking interactions [shortest centroid–centroid distance = 3.600 (1) Å] between substituted benzene rings of different ligands. The crystal packing is characterized by C—H···O and C—H···Cl interactions involving the chloroform solvent molecules.

Related literature

For further information on acyclic diaminocarbenes, see: Slaughter (2012); Boyarskiy *et al.* (2012). For background to the Passerini reaction, see: Banfi & Riva (2005). For novel metal-mediated coupling as a route to cyclic carbenes and aminocarbene complexes, see: Luzyanin *et al.* (2009*a*,*b*); Tskhovrebov *et al.* (2011); Chay *et al.* (2012). For related structures, see: Davies *et al.* (1996); Bertani *et al.* (1991); Bonati & Minghetti (1970); Luzyanin *et al.* (2009*a*,*b*); Michelin *et al.* (1988*a*,*b*); Rourke (2007). For bond lengths in coordination complexes, see: Orpen *et al.* (1989).



Experimental

Crystal data

$[PdCl_2(C_{15}H_{11}NO_3)_2]\cdot CHCl_3$
M_r = 803.16
Orthorhombic, $P2_12_12_1$
a = 7.4457 (1) Å
b = 12.1352 (4) Å
c = 36.1109 (11) Å
V = 3262.80 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.02 mm^{-1}
T = 100 K
0.35 × 0.23 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008)
T_{min} = 0.717, T_{max} = 0.903
24908 measured reflections
9228 independent reflections
7397 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.067
S = 1.01
9228 reflections
408 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-3}
Absolute structure: Flack (1983), 3936 Friedel pairs
Flack parameter: −0.011 (17)

Table 1
Selected bond lengths (Å).

Pd1—C16	1.935 (3)	Pd1—Cl2	2.2979 (7)
Pd1—C1	1.947 (3)	Pd1—Cl1	2.2994 (7)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O2^{i}	0.95	2.53	3.193 (4)	127
C6—H6···O6^{ii}	0.95	2.53	3.433 (4)	158
C19—H19···O5^{iii}	0.95	2.37	3.182 (3)	143
C20—H20···Cl1^{iv}	0.95	2.80	3.622 (3)	145
C31—H31···Cl1^{v}	1.00	2.77	3.607 (3)	141
C31—H31···Cl2^{v}	1.00	2.67	3.513 (3)	142

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+2$; (iv) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+2$; (v) $x-1, y+1, z$.

Data collection: *COLLECT* (Nonius, 1997); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2184).

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Acta Cryst. (2012). E**68**, m1476–m1477 [doi:10.1107/S1600536812045801]

cis-Dichloridobis(2-isocyanophenyl 4-methoxybenzoate)palladium(II) chloroform monosolvate

Alexander Tskhovrebov and Matti Haukka

S1. Comment

Isocyanides are important organic reagents used in multicomponent reactions such as, *e.g.*, Ugi and Passerini reactions (Banfi & Riva, 2005). Metal complexes of isocyanides could be used as precursors for the generation of coordinated N-heterocyclic carbenes (NHC's) and acyclic diaminocarbenes (ADS's) (Slaughter, 2012). In turn, Pd^{II}-NHC and Pd^{II}-ADC systems are particularly interesting since they are used as catalysts in a wide range of cross-coupling reactions (Boyarskiy *et al.*, 2012). Recently, it was observed that the coupling of Pd^{II}-bound isocyanides and various nucleophiles leads to the formation of cyclic carbenes (Luzyanin *et al.*, 2009*b*) and ADC complexes (Luzyanin *et al.*, 2009*a*; Tskhovrebov *et al.*, 2011; Chay *et al.*, 2012), which could not be obtained by the common methods for the generation of metal carbenes. Here we report the structure of a new isocyanide complex that could be used as a starting material for generation of various palladium carbenes.

In the title compound, the isocyanide ligands are mutually in the *cis*-position (Fig. 1) insofar as the ligated RNC species exhibit higher *trans*-effect than the chlorides (Davies *et al.*, 1996). The fragments C–N–C–Pd in both complexes are almost linear, *viz*., the angles N1–C1–Pd1 and N2–C16–Pd1 are 174.2 (2)° and 177.4 (3)°, respectively. The angles C2–N1–C1 and C17–N2–C16 are 174.3 (3)° and 172.0 (3)°, correspondingly. In the isocyanide moieties, the C≡N triple bonds [C1–N1 1.141 (3) Å and C16–N2 1.150 (3) Å] are close to those in some other palladium-isocyanide complexes (Bertani *et al.*, 1991; Bonati & Minghetti, 1970; Luzyanin *et al.*, 2009*a*,*b*; Michelin *et al.*, 1988*a*,*b*; Orpen *et al.*, 1989; Rourke, 2007). The molecular conformation is stabilized by π-π stacking interactions [shortest centroid-centroid distance = 3.600 (1) Å] between the substituted benzene rings C9–C15 and C17–C22 of different ligands. The crystal packing is characterized by intermolecular C-H···O and C-H···Cl interactions involving the chloroform solvent molecules (Table 1).

S2. Experimental

The title compound was synthesized by the addition of 2 equiv of 2-isocyanophenyl-4-methoxybenzoate into a chloroform solution of $[PdCl_2(MeCN)_2]$. The solid product was dissolved and recrystallized by slow evaporation from a solution of $Et_2O/CHCl_3$ (1:1, *v*/*v*).

S3. Refinement

All H atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H = 0.95 Å and U_{iso} = 1.2U_{eq}(C) for aromatic H atoms, with C—H = 1.00 Å and U_{iso} = 1.2U_{eq}(C) for methine H atoms, and with C—H = 0.98 Å and U_{iso} = 1.5U_{eq}(C) for methyl H atoms. The highest peak is located 1.28 Å from atom Cl6 and the deepest hole is located 0.78 Å from atom Pd1.

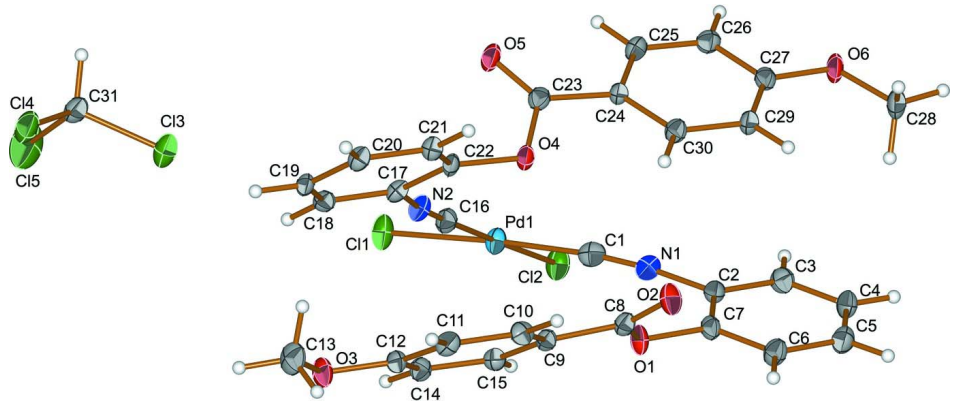

Figure 1

The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

cis-Dichloridobis(2-isocyanophenyl 4-methoxybenzoate)palladium(II) chloroform monosolvate

Crystal data

$[PdCl_2(C_{15}H_{11}NO_3)_2]\cdot CHCl_3$
$M_r = 803.16$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 7.4457\ (1)$ Å
$b = 12.1352\ (4)$ Å
$c = 36.1109\ (11)$ Å
$V = 3262.80\ (15)$ Å^3
$Z = 4$
$F(000) = 1608$
$D_x = 1.635$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 24908 reflections
$\theta = 3.2–30.0°$
$\mu = 1.02$ mm^{-1}
$T = 100$ K
Block, colourless
0.35 × 0.23 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Horizontally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm^{-1}
φ scans and ω scans with κ offset
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008)
$T_{min} = 0.717$, $T_{max} = 0.903$
24908 measured reflections
9228 independent reflections
7397 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 30.0°$, $\theta_{min} = 3.2°$
$h = -10\rightarrow10$
$k = -17\rightarrow15$
$l = -50\rightarrow41$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.067$
$S = 1.01$
9228 reflections
408 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0262P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.61$ e Å^{-3}
$\Delta\rho_{min} = -0.79$ e Å^{-3}
Absolute structure: Flack (1983), 3936 Friedel pairs
Absolute structure parameter: −0.011 (17)

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}
Pd1	0.70069 (3)	0.468290 (17)	0.888077 (5)	0.01742 (5)
Cl1	0.77179 (10)	0.36814 (6)	0.940105 (18)	0.02588 (17)
Cl2	0.78655 (11)	0.32749 (5)	0.849385 (18)	0.02437 (15)
Cl3	0.19677 (12)	1.19482 (6)	0.947449 (18)	0.02811 (16)
Cl4	0.16546 (10)	1.10483 (7)	0.873361 (19)	0.03021 (18)
Cl5	0.30198 (14)	1.32462 (7)	0.88439 (2)	0.0512 (2)
O1	0.7349 (2)	0.81404 (15)	0.82187 (5)	0.0201 (4)
O2	0.5584 (2)	0.96590 (18)	0.81736 (5)	0.0243 (4)
O3	0.8859 (2)	0.99125 (16)	0.98090 (5)	0.0236 (5)
O4	0.3493 (2)	0.79408 (15)	0.89629 (5)	0.0176 (4)
O5	0.1775 (3)	0.65489 (16)	0.91802 (5)	0.0243 (5)
O6	0.0757 (3)	0.58547 (17)	0.74567 (5)	0.0231 (5)
N1	0.6421 (3)	0.60184 (19)	0.81643 (6)	0.0197 (5)
N2	0.5755 (3)	0.66170 (19)	0.93709 (6)	0.0181 (5)
C1	0.6542 (3)	0.5533 (2)	0.84336 (8)	0.0202 (6)
C2	0.6443 (3)	0.6656 (2)	0.78406 (7)	0.0181 (6)
C3	0.6047 (4)	0.6183 (3)	0.75010 (7)	0.0213 (6)
H3	0.5760	0.5422	0.7484	0.026*
C4	0.6076 (4)	0.6834 (3)	0.71872 (8)	0.0242 (7)
H4	0.5802	0.6522	0.6953	0.029*
C5	0.6502 (4)	0.7939 (3)	0.72142 (8)	0.0246 (7)
H5	0.6505	0.8383	0.6997	0.030*
C6	0.6925 (4)	0.8410 (2)	0.75529 (7)	0.0220 (6)
H6	0.7245	0.9166	0.7567	0.026*
C7	0.6877 (4)	0.7772 (2)	0.78685 (7)	0.0175 (6)
C8	0.6627 (4)	0.9124 (2)	0.83496 (7)	0.0175 (6)
C9	0.7281 (3)	0.9349 (2)	0.87254 (7)	0.0158 (6)
C10	0.6814 (3)	1.0340 (2)	0.88931 (7)	0.0187 (5)
H10	0.6137	1.0867	0.8758	0.022*
C11	0.7323 (3)	1.0570 (2)	0.92547 (7)	0.0186 (6)
H11	0.7003	1.1252	0.9366	0.022*
C12	0.8307 (3)	0.9794 (2)	0.94535 (7)	0.0185 (6)
C13	0.8259 (4)	1.0869 (2)	1.00095 (7)	0.0293 (7)
H13A	0.8686	1.1536	0.9884	0.044*
H13B	0.8739	1.0847	1.0262	0.044*

H13C	0.6944	1.0875	1.0019	0.044*
C14	0.8794 (3)	0.8798 (2)	0.92857 (7)	0.0176 (6)
H14	0.9465	0.8267	0.9421	0.021*
C15	0.8303 (3)	0.8586 (2)	0.89253 (7)	0.0173 (6)
H15	0.8662	0.7916	0.8811	0.021*
C16	0.6242 (4)	0.5885 (2)	0.91953 (7)	0.0194 (6)
C17	0.5048 (4)	0.7558 (2)	0.95387 (7)	0.0165 (6)
C18	0.5512 (3)	0.7851 (2)	0.98970 (7)	0.0176 (6)
H18	0.6306	0.7403	1.0038	0.021*
C19	0.4803 (3)	0.8805 (2)	1.00472 (7)	0.0173 (6)
H19	0.5105	0.9015	1.0293	0.021*
C20	0.3652 (3)	0.9456 (2)	0.98394 (7)	0.0176 (6)
H20	0.3170	1.0110	0.9944	0.021*
C21	0.3197 (4)	0.9165 (2)	0.94812 (7)	0.0171 (6)
H21	0.2407	0.9617	0.9341	0.021*
C22	0.3893 (3)	0.8223 (2)	0.93303 (7)	0.0152 (6)
C23	0.2352 (3)	0.7055 (2)	0.89214 (8)	0.0182 (6)
C24	0.1980 (4)	0.6801 (2)	0.85274 (7)	0.0153 (5)
C25	0.1211 (4)	0.5787 (2)	0.84476 (7)	0.0198 (6)
H25	0.0940	0.5293	0.8644	0.024*
C26	0.0834 (3)	0.5485 (2)	0.80881 (7)	0.0203 (6)
H26	0.0349	0.4778	0.8035	0.024*
C27	0.1174 (3)	0.6232 (2)	0.78018 (7)	0.0185 (6)
C28	0.1047 (4)	0.6582 (3)	0.71486 (7)	0.0269 (7)
H28A	0.0354	0.7260	0.7185	0.040*
H28B	0.0658	0.6221	0.6920	0.040*
H28C	0.2327	0.6763	0.7131	0.040*
C29	0.1902 (4)	0.7258 (2)	0.78777 (7)	0.0185 (6)
H29	0.2117	0.7765	0.7682	0.022*
C30	0.2316 (3)	0.7546 (2)	0.82398 (7)	0.0182 (6)
H30	0.2825	0.8247	0.8292	0.022*
C31	0.1513 (4)	1.2255 (2)	0.90068 (7)	0.0237 (7)
H31	0.0267	1.2557	0.8988	0.028*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.02268 (10)	0.01504 (10)	0.01454 (9)	0.00299 (10)	0.00058 (9)	−0.00068 (9)
Cl1	0.0409 (4)	0.0209 (4)	0.0159 (3)	0.0074 (3)	−0.0020 (3)	−0.0008 (3)
Cl2	0.0353 (4)	0.0195 (3)	0.0184 (3)	0.0051 (4)	0.0003 (3)	−0.0039 (3)
Cl3	0.0448 (4)	0.0220 (4)	0.0175 (3)	0.0023 (4)	−0.0028 (4)	0.0009 (3)
Cl4	0.0401 (4)	0.0340 (4)	0.0165 (3)	0.0044 (4)	−0.0049 (3)	−0.0018 (3)
Cl5	0.0628 (5)	0.0512 (6)	0.0397 (5)	−0.0301 (5)	−0.0031 (6)	0.0165 (4)
O1	0.0291 (11)	0.0193 (10)	0.0119 (9)	0.0024 (9)	−0.0041 (8)	−0.0030 (8)
O2	0.0310 (11)	0.0232 (11)	0.0186 (11)	0.0062 (11)	−0.0058 (8)	0.0005 (10)
O3	0.0283 (10)	0.0287 (13)	0.0139 (10)	0.0011 (9)	−0.0028 (8)	−0.0068 (9)
O4	0.0247 (10)	0.0177 (10)	0.0104 (10)	−0.0043 (8)	−0.0010 (7)	0.0006 (7)
O5	0.0324 (11)	0.0296 (12)	0.0109 (9)	−0.0083 (10)	0.0024 (9)	−0.0012 (8)

O6	0.0312 (11)	0.0284 (12)	0.0097 (10)	−0.0021 (10)	−0.0025 (8)	−0.0009 (9)
N1	0.0214 (12)	0.0170 (13)	0.0207 (13)	0.0035 (10)	0.0028 (10)	0.0013 (10)
N2	0.0240 (12)	0.0146 (13)	0.0157 (12)	0.0036 (10)	0.0030 (10)	0.0016 (10)
C1	0.0197 (14)	0.0167 (16)	0.0240 (15)	0.0023 (11)	0.0033 (11)	−0.0053 (12)
C2	0.0170 (13)	0.0228 (16)	0.0145 (14)	0.0005 (12)	0.0000 (11)	0.0000 (12)
C3	0.0226 (14)	0.0219 (16)	0.0194 (15)	−0.0021 (13)	0.0001 (12)	−0.0042 (13)
C4	0.0263 (15)	0.0324 (19)	0.0138 (15)	−0.0011 (14)	0.0004 (12)	−0.0041 (13)
C5	0.0286 (16)	0.0288 (17)	0.0165 (15)	−0.0035 (14)	0.0008 (12)	0.0008 (13)
C6	0.0283 (14)	0.0202 (15)	0.0176 (14)	−0.0023 (15)	0.0017 (14)	−0.0017 (11)
C7	0.0188 (13)	0.0208 (14)	0.0128 (12)	0.0011 (13)	−0.0010 (12)	−0.0037 (11)
C8	0.0210 (15)	0.0163 (14)	0.0150 (13)	−0.0017 (12)	0.0016 (11)	0.0010 (11)
C9	0.0185 (13)	0.0153 (13)	0.0137 (12)	−0.0027 (11)	0.0008 (11)	−0.0002 (10)
C10	0.0196 (12)	0.0157 (12)	0.0207 (13)	0.0019 (13)	−0.0011 (13)	0.0053 (13)
C11	0.0232 (14)	0.0135 (14)	0.0190 (13)	−0.0018 (11)	0.0029 (11)	−0.0015 (10)
C12	0.0182 (13)	0.0235 (15)	0.0138 (13)	−0.0040 (13)	−0.0001 (10)	−0.0022 (12)
C13	0.0363 (18)	0.0322 (18)	0.0192 (15)	−0.0030 (16)	0.0014 (14)	−0.0105 (13)
C14	0.0184 (13)	0.0176 (15)	0.0169 (14)	0.0011 (12)	−0.0009 (11)	0.0029 (12)
C15	0.0167 (13)	0.0175 (14)	0.0177 (14)	−0.0002 (11)	0.0003 (11)	−0.0001 (11)
C16	0.0210 (14)	0.0214 (16)	0.0158 (14)	0.0002 (13)	0.0001 (11)	0.0043 (12)
C17	0.0188 (13)	0.0155 (14)	0.0152 (14)	0.0003 (12)	0.0039 (11)	0.0017 (12)
C18	0.0159 (13)	0.0190 (15)	0.0180 (15)	0.0010 (12)	0.0002 (11)	0.0040 (12)
C19	0.0202 (14)	0.0214 (16)	0.0103 (13)	−0.0052 (13)	0.0006 (11)	−0.0004 (12)
C20	0.0220 (13)	0.0147 (15)	0.0160 (13)	0.0004 (11)	0.0026 (11)	−0.0011 (11)
C21	0.0196 (13)	0.0166 (14)	0.0153 (13)	0.0003 (12)	0.0002 (11)	0.0005 (11)
C22	0.0204 (13)	0.0166 (15)	0.0087 (13)	−0.0034 (12)	0.0002 (10)	0.0009 (11)
C23	0.0189 (13)	0.0194 (14)	0.0162 (14)	0.0025 (11)	0.0020 (11)	0.0006 (12)
C24	0.0158 (12)	0.0183 (13)	0.0118 (12)	−0.0001 (13)	−0.0002 (12)	0.0015 (10)
C25	0.0218 (14)	0.0222 (16)	0.0154 (14)	−0.0002 (12)	0.0018 (11)	0.0032 (12)
C26	0.0214 (13)	0.0196 (17)	0.0198 (14)	−0.0043 (13)	0.0008 (11)	0.0002 (13)
C27	0.0157 (13)	0.0248 (16)	0.0151 (14)	0.0033 (13)	−0.0006 (11)	−0.0011 (12)
C28	0.0300 (16)	0.038 (2)	0.0127 (14)	0.0025 (15)	−0.0032 (13)	0.0035 (13)
C29	0.0196 (13)	0.0231 (15)	0.0128 (12)	0.0003 (14)	−0.0006 (12)	0.0032 (11)
C30	0.0205 (14)	0.0184 (14)	0.0157 (13)	−0.0004 (12)	0.0012 (11)	−0.0024 (11)
C31	0.0267 (15)	0.0252 (17)	0.0192 (15)	0.0005 (13)	−0.0039 (12)	0.0044 (12)

Geometric parameters (Å, º)

Pd1—C16	1.935 (3)	C10—H10	0.9500
Pd1—C1	1.947 (3)	C11—C12	1.393 (4)
Pd1—Cl2	2.2979 (7)	C11—H11	0.9500
Pd1—Cl1	2.2994 (7)	C12—C14	1.400 (4)
Cl3—C31	1.762 (3)	C13—H13A	0.9800
Cl4—C31	1.768 (3)	C13—H13B	0.9800
Cl5—C31	1.747 (3)	C13—H13C	0.9800
O1—C7	1.387 (3)	C14—C15	1.376 (4)
O1—C8	1.392 (3)	C14—H14	0.9500
O2—C8	1.195 (3)	C15—H15	0.9500
O3—C12	1.356 (3)	C17—C18	1.386 (4)

O3—C13	1.439 (3)	C17—C22	1.400 (4)
O4—C23	1.379 (3)	C18—C19	1.383 (4)
O4—C22	1.402 (3)	C18—H18	0.9500
O5—C23	1.198 (3)	C19—C20	1.386 (4)
O6—C27	1.364 (3)	C19—H19	0.9500
O6—C28	1.437 (3)	C20—C21	1.383 (3)
N1—C1	1.141 (3)	C20—H20	0.9500
N1—C2	1.402 (3)	C21—C22	1.368 (3)
N2—C16	1.150 (3)	C21—H21	0.9500
N2—C17	1.395 (3)	C23—C24	1.482 (3)
C2—C3	1.386 (4)	C24—C25	1.387 (4)
C2—C7	1.396 (4)	C24—C30	1.400 (3)
C3—C4	1.382 (4)	C25—C26	1.378 (3)
C3—H3	0.9500	C25—H25	0.9500
C4—C5	1.381 (4)	C26—C27	1.398 (4)
C4—H4	0.9500	C26—H26	0.9500
C5—C6	1.386 (4)	C27—C29	1.385 (4)
C5—H5	0.9500	C28—H28A	0.9800
C6—C7	1.378 (3)	C28—H28B	0.9800
C6—H6	0.9500	C28—H28C	0.9800
C8—C9	1.467 (3)	C29—C30	1.388 (3)
C9—C10	1.391 (3)	C29—H29	0.9500
C9—C15	1.399 (4)	C30—H30	0.9500
C10—C11	1.388 (3)	C31—H31	1.0000

C16—Pd1—C1	92.00 (12)	C14—C15—C9	120.6 (3)
C16—Pd1—Cl2	178.37 (8)	C14—C15—H15	119.7
C1—Pd1—Cl2	86.52 (8)	C9—C15—H15	119.7
C16—Pd1—Cl1	89.24 (8)	N2—C16—Pd1	177.4 (3)
C1—Pd1—Cl1	176.91 (8)	C18—C17—N2	121.4 (2)
Cl2—Pd1—Cl1	92.28 (3)	C18—C17—C22	120.5 (3)
C7—O1—C8	119.2 (2)	N2—C17—C22	118.1 (2)
C12—O3—C13	117.9 (2)	C19—C18—C17	119.1 (3)
C23—O4—C22	115.11 (19)	C19—C18—H18	120.5
C27—O6—C28	117.8 (2)	C17—C18—H18	120.5
C1—N1—C2	174.3 (3)	C18—C19—C20	120.0 (3)
C16—N2—C17	172.0 (3)	C18—C19—H19	120.0
N1—C1—Pd1	174.2 (2)	C20—C19—H19	120.0
C3—C2—C7	121.0 (3)	C21—C20—C19	120.8 (3)
C3—C2—N1	120.5 (3)	C21—C20—H20	119.6
C7—C2—N1	118.5 (2)	C19—C20—H20	119.6
C4—C3—C2	119.1 (3)	C22—C21—C20	119.5 (2)
C4—C3—H3	120.5	C22—C21—H21	120.2
C2—C3—H3	120.5	C20—C21—H21	120.2
C5—C4—C3	120.1 (3)	C21—C22—C17	120.0 (2)
C5—C4—H4	120.0	C21—C22—O4	120.1 (2)
C3—C4—H4	120.0	C17—C22—O4	119.9 (2)
C4—C5—C6	120.9 (3)	O5—C23—O4	122.4 (3)

C4—C5—H5	119.5	O5—C23—C24	125.2 (2)
C6—C5—H5	119.5	O4—C23—C24	112.4 (2)
C7—C6—C5	119.5 (3)	C25—C24—C30	119.5 (2)
C7—C6—H6	120.2	C25—C24—C23	117.4 (2)
C5—C6—H6	120.2	C30—C24—C23	123.0 (2)
C6—C7—O1	124.5 (2)	C26—C25—C24	121.1 (3)
C6—C7—C2	119.4 (2)	C26—C25—H25	119.5
O1—C7—C2	115.9 (2)	C24—C25—H25	119.5
O2—C8—O1	122.4 (2)	C25—C26—C27	119.1 (3)
O2—C8—C9	127.3 (3)	C25—C26—H26	120.4
O1—C8—C9	110.2 (2)	C27—C26—H26	120.4
C10—C9—C15	118.9 (2)	O6—C27—C29	124.9 (2)
C10—C9—C8	118.7 (2)	O6—C27—C26	114.6 (2)
C15—C9—C8	122.3 (2)	C29—C27—C26	120.5 (2)
C11—C10—C9	121.0 (2)	O6—C28—H28A	109.5
C11—C10—H10	119.5	O6—C28—H28B	109.5
C9—C10—H10	119.5	H28A—C28—H28B	109.5
C10—C11—C12	119.5 (2)	O6—C28—H28C	109.5
C10—C11—H11	120.3	H28A—C28—H28C	109.5
C12—C11—H11	120.3	H28B—C28—H28C	109.5
O3—C12—C11	125.1 (2)	C27—C29—C30	120.0 (2)
O3—C12—C14	115.0 (2)	C27—C29—H29	120.0
C11—C12—C14	119.8 (2)	C30—C29—H29	120.0
O3—C13—H13A	109.5	C29—C30—C24	119.8 (3)
O3—C13—H13B	109.5	C29—C30—H30	120.1
H13A—C13—H13B	109.5	C24—C30—H30	120.1
O3—C13—H13C	109.5	Cl5—C31—Cl3	110.17 (15)
H13A—C13—H13C	109.5	Cl5—C31—Cl4	110.14 (15)
H13B—C13—H13C	109.5	Cl3—C31—Cl4	110.39 (16)
C15—C14—C12	120.1 (3)	Cl5—C31—H31	108.7
C15—C14—H14	119.9	Cl3—C31—H31	108.7
C12—C14—H14	119.9	Cl4—C31—H31	108.7

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O2^{i}	0.95	2.53	3.193 (4)	127
C6—H6···O6^{ii}	0.95	2.53	3.433 (4)	158
C19—H19···O5^{iii}	0.95	2.37	3.182 (3)	143
C20—H20···Cl1^{iv}	0.95	2.80	3.622 (3)	145
C31—H31···Cl1^{v}	1.00	2.77	3.607 (3)	141
C31—H31···Cl2^{v}	1.00	2.67	3.513 (3)	142

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+3/2; (ii) −*x*+1, *y*+1/2, −*z*+3/2; (iii) *x*+1/2, −*y*+3/2, −*z*+2; (iv) *x*−1/2, −*y*+3/2, −*z*+2; (v) *x*−1, *y*+1, *z*.