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trans-Dichloridobis(quinoline-κ*N*)-palladium(II)

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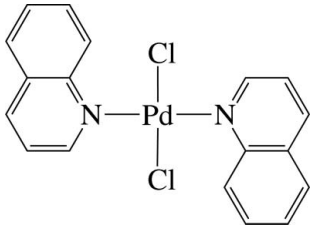
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.008 Å; R factor = 0.040; wR factor = 0.095; data-to-parameter ratio = 14.9.

In the title complex, $[PdCl_2(C_9H_7N)_2]$, the Pd^{II} ion is four-coordinated in an essentially square-planar environment defined by two N atoms from two quinoline ligands and two Cl^- anions. The Pd atom is located on an inversion centre, and thus the asymmetric unit contains one half of the complex; the PdN_2Cl_2 unit is exactly planar. The dihedral angle between the PdN_2Cl_2 unit and quinoline ligand is 85.63 (8)°. In the crystal, the complex molecules are stacked into columns along the b axis. In the columns, several intermolecular π–π interactions between the six-membered rings are present, the shortest ring centroid–centroid distance being 3.764 (3) Å between pyridine rings.

Related literature

For the crystal structure of the related Pt^{II} complex *cis*-$[PtCl_2(quinoline)_2]$·0.25DMF, see: Davies *et al.* (2001).



Experimental

Crystal data

$[PdCl_2(C_9H_7N)_2]$
M_r = 435.61
Monoclinic, $C2/c$
a = 16.430 (3) Å
b = 7.0050 (11) Å
c = 16.118 (2) Å
β = 119.532 (3)°
V = 1614.0 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.48 mm^{-1}
T = 200 K
0.31 × 0.13 × 0.11 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.869, T_{max} = 1.000
4776 measured reflections
1577 independent reflections
1125 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.095
S = 1.05
1577 reflections
106 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pd1—N1	2.035 (4)	Pd1—Cl1	2.2973 (12)
N1—Pd1—Cl1	89.53 (10)		

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 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: TK5039).

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supporting information

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trans-Dichloridobis(quinoline-κN)palladium(II)

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S1. Comment

In the title complex, $[PdCl_2(quinoline)_2]$, the Pd^{II} ion is four-coordinated in an essentially square-planar environment by two N atoms from two quinoline ligands and two Cl^- anions (Fig. 1 and Table 1). The Cl atoms are in *trans* conformation with respect to each other. By contrast, in the analogous Pt^{II} complex $[PtCl_2(quinoline)_2]$.0.25DMF (DMF = *N,N*-dimethylformamide), the Cl atoms are in *cis* conformation (Davies *et al.*, 2001).

The Pd atom is located on an inversion centre, and thus the asymmetric unit contains one half of the complex; the PdN_2Cl_2 unit is exactly planar. The nearly planar quinoline ligands, with a maximum deviation of 0.015 (4) Å from the least-squares plane, are parallel. The dihedral angle between the PdN_2Cl_2 unit and quinoline ligand is 85.63 (8)°. The Cl atoms are almost perpendicular to the quinoline planes, with the bond angle <N1—Pd1—Cl1 = 89.53 (10)°. In the crystal, the complex molecules are stacked into columns along the *b* axis (Fig. 2). In the columns, several intermolecular π-π interactions between the six-membered rings are present, the shortest ring centroid-centroid distance being 3.764 (3) Å between pyridyl rings.

S2. Experimental

To a solution of Na_2PdCl_4 (0.2943 g, 1.000 mmol) in H_2O (20 ml) was added quinoline (0.2590 g, 2.005 mmol). The mixture was stirred for 3 h at room temperature. The formed precipitate was separated by filtration, washed with H_2O and EtOH, and dried at 50 °C, to give a yellow powder (0.3706 g). Crystals suitable for X-ray analysis were obtained by slow evaporation from its dimethyl sulfoxide (DMSO) solution at 90 °C.

S3. Refinement

H atoms were positioned geometrically and allowed to ride on their respective parent atoms [C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C)]. The highest peak (1.30 e Å^{-3}) and the deepest hole (-0.40 e Å^{-3}) in the final difference Fourier map were located 1.01 Å and 1.49 Å from the atoms Pd1 and H5, respectively.

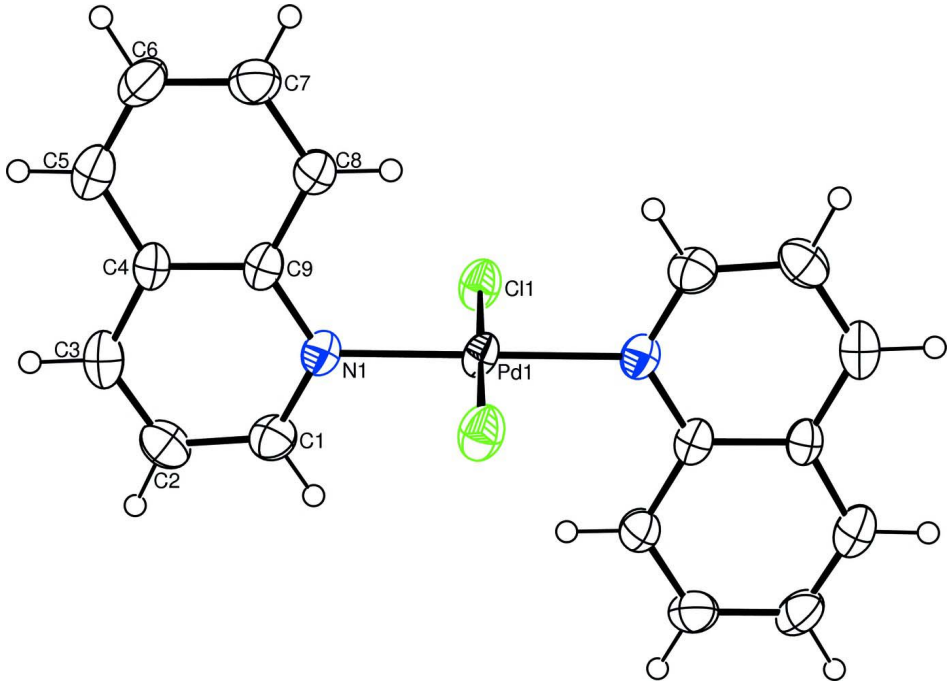

Figure 1

A view of the molecular structure of the title complex, with displacement ellipsoids drawn at the 40% probability level and the atom numbering. Unlabelled atoms are related to the reference atoms by the (-*x*, 1 - *y*, -*z*) symmetry transformation.

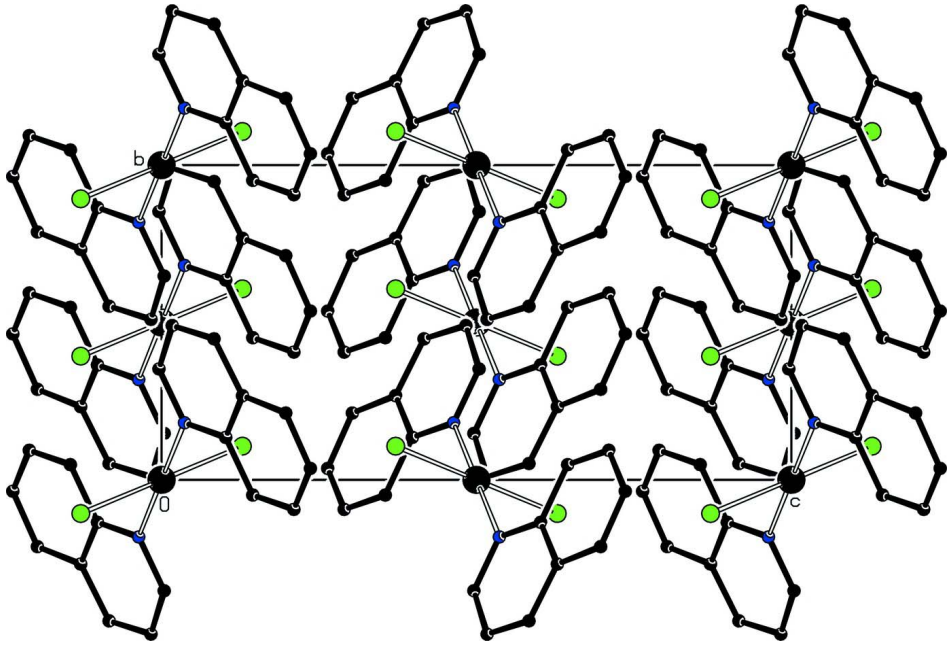

Figure 2

A view of the unit-cell contents of the title complex, along the *a* axis.

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Crystal data

$[PdCl_2(C_9H_7N)_2]$
M_r = 435.61
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 16.430 (3) Å
b = 7.0050 (11) Å
c = 16.118 (2) Å
β = 119.532 (3)°
V = 1614.0 (4) Å^3
Z = 4
F(000) = 864
D_x = 1.793 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 1841 reflections
θ = 2.9–25.6°
μ = 1.48 mm^{-1}
T = 200 K
Block, yellow
0.31 × 0.13 × 0.11 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.869, T_{max} = 1.000
4776 measured reflections
1577 independent reflections
1125 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 26.0°, θ_{min} = 2.9°
h = −19→20
k = −8→8
l = −18→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.095
S = 1.05
1577 reflections
106 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
$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.30 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Pd1	0.0000	0.5000	0.0000	0.0367 (2)
Cl1	−0.01202 (8)	0.3930 (2)	0.12827 (8)	0.0488 (3)
N1	0.1092 (2)	0.3186 (6)	0.0364 (3)	0.0381 (9)
C1	0.0916 (3)	0.1476 (7)	−0.0041 (3)	0.0451 (12)

H1	0.0288	0.1172	−0.0498	0.054*
C2	0.1606 (4)	0.0098 (7)	0.0169 (4)	0.0480 (13)
H2	0.1449	−0.1106	−0.0142	0.058*
C3	0.2514 (4)	0.0518 (7)	0.0833 (4)	0.0490 (14)
H3	0.2996	−0.0392	0.0988	0.059*
C4	0.2721 (3)	0.2324 (7)	0.1284 (3)	0.0356 (10)
C5	0.3633 (3)	0.2877 (8)	0.1971 (3)	0.0505 (13)
H5	0.4134	0.1997	0.2162	0.061*
C6	0.3806 (4)	0.4638 (8)	0.2362 (4)	0.0519 (14)
H6	0.4426	0.4991	0.2819	0.062*
C7	0.3078 (4)	0.5939 (9)	0.2100 (3)	0.0496 (13)
H7	0.3211	0.7172	0.2383	0.060*
C8	0.2180 (3)	0.5483 (7)	0.1448 (3)	0.0421 (12)
H8	0.1692	0.6384	0.1283	0.051*
C9	0.1979 (3)	0.3651 (7)	0.1018 (3)	0.0373 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.0248 (3)	0.0445 (3)	0.0377 (3)	0.0052 (2)	0.0129 (2)	0.0054 (2)
Cl1	0.0436 (7)	0.0605 (9)	0.0453 (7)	0.0101 (7)	0.0243 (6)	0.0128 (6)
N1	0.030 (2)	0.041 (2)	0.042 (2)	0.0018 (18)	0.0168 (18)	0.0036 (19)
C1	0.040 (3)	0.046 (3)	0.050 (3)	−0.008 (2)	0.023 (2)	−0.002 (2)
C2	0.065 (4)	0.033 (3)	0.054 (3)	−0.003 (3)	0.035 (3)	0.000 (2)
C3	0.048 (3)	0.047 (3)	0.061 (3)	0.014 (2)	0.033 (3)	0.016 (3)
C4	0.032 (2)	0.039 (3)	0.040 (3)	0.007 (2)	0.020 (2)	0.008 (2)
C5	0.037 (3)	0.062 (4)	0.050 (3)	0.010 (3)	0.019 (2)	0.011 (3)
C6	0.032 (3)	0.071 (4)	0.044 (3)	−0.001 (3)	0.012 (2)	−0.001 (3)
C7	0.046 (3)	0.060 (3)	0.041 (3)	−0.005 (3)	0.021 (2)	−0.008 (3)
C8	0.035 (3)	0.042 (3)	0.046 (3)	0.001 (2)	0.018 (2)	−0.002 (2)
C9	0.033 (3)	0.043 (3)	0.037 (3)	0.005 (2)	0.018 (2)	0.009 (2)

Geometric parameters (Å, º)

Pd1—N1	2.035 (4)	C3—H3	0.9500
Pd1—N1^{i}	2.035 (4)	C4—C5	1.409 (6)
Pd1—Cl1	2.2973 (12)	C4—C9	1.421 (6)
Pd1—Cl1^{i}	2.2973 (12)	C5—C6	1.350 (7)
N1—C1	1.326 (6)	C5—H5	0.9500
N1—C9	1.351 (5)	C6—C7	1.393 (8)
C1—C2	1.397 (7)	C6—H6	0.9500
C1—H1	0.9500	C7—C8	1.362 (7)
C2—C3	1.373 (7)	C7—H7	0.9500
C2—H2	0.9500	C8—C9	1.418 (7)
C3—C4	1.414 (6)	C8—H8	0.9500
N1—Pd1—N1^{i}	180.0 (2)	C5—C4—C3	122.9 (4)
N1—Pd1—Cl1	89.53 (10)	C5—C4—C9	118.6 (5)

N1^{i}—Pd1—Cl1	90.47 (10)	C3—C4—C9	118.4 (4)
N1—Pd1—Cl1^{i}	90.47 (10)	C6—C5—C4	121.0 (5)
N1^{i}—Pd1—Cl1^{i}	89.53 (10)	C6—C5—H5	119.5
Cl1—Pd1—Cl1^{i}	180.00 (9)	C4—C5—H5	119.5
C1—N1—C9	119.4 (4)	C5—C6—C7	120.3 (5)
C1—N1—Pd1	118.3 (3)	C5—C6—H6	119.8
C9—N1—Pd1	122.2 (3)	C7—C6—H6	119.8
N1—C1—C2	123.4 (5)	C8—C7—C6	121.4 (5)
N1—C1—H1	118.3	C8—C7—H7	119.3
C2—C1—H1	118.3	C6—C7—H7	119.3
C3—C2—C1	118.7 (5)	C7—C8—C9	119.5 (5)
C3—C2—H2	120.6	C7—C8—H8	120.3
C1—C2—H2	120.6	C9—C8—H8	120.3
C2—C3—C4	119.1 (5)	N1—C9—C8	120.1 (4)
C2—C3—H3	120.4	N1—C9—C4	120.9 (4)
C4—C3—H3	120.4	C8—C9—C4	119.1 (4)

Cl1—Pd1—N1—C1	93.7 (3)	C5—C6—C7—C8	−0.1 (8)
Cl1^{i}—Pd1—N1—C1	−86.3 (3)	C6—C7—C8—C9	−0.6 (8)
Cl1—Pd1—N1—C9	−84.5 (3)	C1—N1—C9—C8	179.2 (4)
Cl1^{i}—Pd1—N1—C9	95.5 (3)	Pd1—N1—C9—C8	−2.6 (6)
C9—N1—C1—C2	−0.2 (7)	C1—N1—C9—C4	−0.7 (6)
Pd1—N1—C1—C2	−178.5 (3)	Pd1—N1—C9—C4	177.5 (3)
N1—C1—C2—C3	0.5 (7)	C7—C8—C9—N1	−179.4 (4)
C1—C2—C3—C4	0.2 (7)	C7—C8—C9—C4	0.5 (7)
C2—C3—C4—C5	−179.8 (5)	C5—C4—C9—N1	−179.9 (4)
C2—C3—C4—C9	−1.1 (7)	C3—C4—C9—N1	1.4 (6)
C3—C4—C5—C6	177.8 (5)	C5—C4—C9—C8	0.2 (6)
C9—C4—C5—C6	−0.9 (7)	C3—C4—C9—C8	−178.6 (4)
C4—C5—C6—C7	0.8 (8)		

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