Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

trans-Dichlorobis(4-cyanopyridine)palladium(II)

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Received 18 June 2002
Accepted 24 June 2002
Online 5 July 2002

In the title compound, [$PdCl_2(C_6H_4N_2)_2$], the Pd^{II} cations occupy crystallographic inversion centres and adopt a slightly distorted square-planar coordination geometry. Adjacent molecules are linked into one-dimensional chains *via* long-range pairwise Pd···Cl interactions.

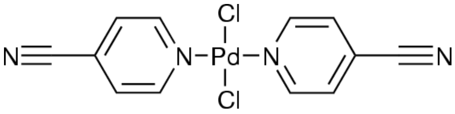
Key indicators

Single-crystal synchrotron study
T = 150 K
Mean σ(C–C) = 0.005 Å
R factor = 0.037
wR factor = 0.088
Data-to-parameter ratio = 20.9

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

Comment

The title compound, (I), isolated during our studies into the complexes of nitrile-substituted pyridine ligands, exists as an air-stable yellow–orange solid. An X-ray study confirmed the stoichiometry of the compound (Fig. 1). Each Pd^{II} centre lies on a crystallographic inversion centre and occupies a square-planar environment, with both the Cl^- and 4-cyanopyridine ligands adopting a *trans* arrangement with all Cl—Pd—N angles falling within 0.75° of 90°. Thus, each Pd^{II} cation is coordinated by two pyridyl and two Cl^- donors. The bond lengths fall within typical ranges expected for Pd—N and Pd—Cl bonds (Orpen *et al.*, 1989) and are comparable to those observed in *trans*-dichlorobis(pyridine)palladium(II) (Viossat *et al.*, 1993).



(I)

The Pd1/N1/N1^{ii}/Cl1/Cl1^{ii} plane (Fig. 1) adopts an angle of 56.5 (2)° with respect to the plane formed by the 4-cyanopyridine ligands. This arrangement allows a further long-range interaction of 3.4580 (16) Å between the Pd^{II} cation and two Cl^- ligands from two separate adjacent molecules. Taking this interaction into account, a distorted octahedral environment is observed at each Pd^{II} cation and one-dimensional chains run parallel to the crystallographic a axis (Fig. 2).

Experimental

Acicular crystals of the title compound, (I), were grown by slow diffusion of a methanolic solution of $CuCl_2{\cdot}2H_2O$ into a solution of [Pd(4-cyanopyridine)$_4$]$(PF_6)_2$ in $MeNO_2$ over 24 h. A long crystal was used for data collection as these crystals do not survive attempts to shorten them.

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DOI: 10.1107/S1600536802011248

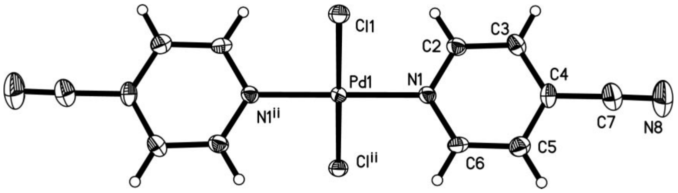

Figure 1
View of the title compound. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (ii) $-x$, $-y$, $1-z$.]

Crystal data

$[PdCl_2(C_6H_4N_2)_2]$
$M_r = 385.52$
Monoclinic, $P2_1/n$
$a = 3.8983$ (13) Å
$b = 25.651$ (14) Å
$c = 7.256$ (4) Å
$\beta = 101.33$ (5)°
$V = 711.4$ (6) Å^3
$Z = 2$
$D_x = 1.800$ Mg m^{-3}
Synchrotron radiation
$\lambda = 0.6890$ Å
Cell parameters from 2761 reflections
$\theta = 3.0$–$29.0°$
$\mu = 1.67$ mm^{-1}
$T = 150$ (2) K
Needle, yellow-orange
0.90 × 0.04 × 0.04 mm

Data collection

Bruker SMART CCD diffractometer
ω rotation with narrow frame scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.336$, $T_{max} = 0.551$
3314 measured reflections
1856 independent reflections
1452 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 29.1°$
$h = -5 \rightarrow 5$
$k = -19 \rightarrow 35$
$l = -9 \rightarrow 4$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.088$
$S = 0.93$
1856 reflections
89 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.86$ e Å^{-3}
$\Delta\rho_{min} = -1.03$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.008 (2)

Table 1
Selected geometric parameters (Å, °).

Pd1—N1	2.023 (3)	Pd1—Cl1^{i}	3.4580 (16)
Pd1—Cl1	2.3141 (14)		
N1—Pd1—Cl1	89.96 (9)	N1—Pd1—Cl1^{iii}	90.74 (8)
N1—Pd1—Cl1^{ii}	90.04 (9)	Cl1—Pd1—Cl1^{i}	82.40 (4)

Symmetry codes: (i) $1+x, y, z$; (ii) $-x, -y, 1-z$; (iii) $-1-x, -y, 1-z$.

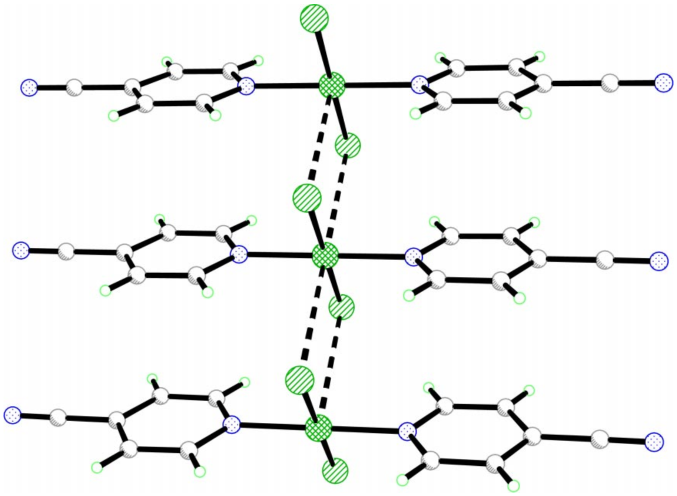

Figure 2
View of the one-dimensional chains formed by Pd···Cl interactions, which are represented by dashed lines (Pd cross-hatch, Cl left-hatch, N dotted, C shaded and H small open circles).

All H atoms were included at geometrically calculated positions; each was constrained to ride at a distance of 0.95 Å from its parent C atom. For all H atoms, displacement parameters were constrained such that $U_{iso}(H) = 1.2U_{eq}(C)$. The residual electron-density extrema lie within 1.0 Å of Pd1.

Data collection: *SMART* (Bruker, 1998); cell refinement: *LSCELL* (Clegg, 1997); data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL/*PC (Sheldrick, 1994); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2002).

The authors thank the CCLRC for access to Station 9.8 at Daresbury Laboratory.

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