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trans-Bis(*tert*-butylamine)dichloropalladium(II)

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Key indicators

Single-crystal X-ray study
T = 223 K
Mean σ(C–C) = 0.008 Å
R factor = 0.038
wR factor = 0.098
Data-to-parameter ratio = 22.8

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

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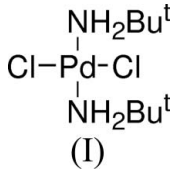
The asymmetric unit of the title complex, *trans*-$[PdCl_2(NH_2{}^tBu)_2]$, consists of two independent square-planar molecules, linked together in a hydrogen-bonding network, with the resultant alignment of the *tert*-butyl groups defining a two-dimensional layered structure approximately parallel to (001).

Comment

We have noted that the chemistry of *tert*-butylamine derivatives of palladium frequently differs from other primary amine complexes due to the steric bulk of the *tert*-butyl group. The availability of crystals of the title complex, (I), allowed comparison with other bis(primary amine)dichloro complexes of palladium to determine the structural consequences of steric bulk.



(I)

Complex (I) exists as two independent square-planar molecules in the asymmetric unit. The orientation of the *tert*-butylamine groups is such that both molecules are pseudo-centrosymmetric. Analysis of the 14 previously reported bis(primary amine)dichloropalladium(II) structures (Fletcher *et al.*, 1996) gives averages of 2.300 (8) Å and 2.047 (9) Å for the Pd—Cl and the Pd—N bonds, respectively, with a mean deviation of the N—Pd—Cl angles of *ca* 1.4° from the ideal 90°. The Pd—Cl and Pd—N bond lengths in (I) range from 2.3015 (11) to 2.3072 (12) and 2.046 (4) to 2.058 (4) Å, respectively; this indicates that, in this complex, the bulky *tert*-butyl group has no obvious structural consequence, although the average N—Pd—Cl angle in complex (I) does show a significantly smaller deviation from the 90° required by ideal square-planar geometry [0.46° (molecule 1), 0.37° (molecule 2). The molecules are linked together in a hydrogen-bonding network, resulting in the formation of a two-dimensional layered structure, externally defined by the *tert*-butyl groups and approximately parallel to (001).

Experimental

Complex (I) crystallized from a dichloromethane/hexane solution of *trans*-$[Pd(\eta^1\text{-}C_5H_5)(NH_2{}^tBu)_2Cl]$ and $[Pd(\eta^5\text{-}C_5H_5)(NH_2{}^tBu)Cl]$ and was spectroscopically identical to the material synthesized according to the literature method (Nakayama *et al.*, 1984).

Crystal data

$[PdCl_2(C_4H_{11}N)_2]$
M_r = 323.58
Triclinic, $P\overline{1}$
a = 6.2357 (10) Å
b = 10.6500 (11) Å
c = 20.472 (2) Å
α = 94.641 (8)°
β = 90.978 (13)°
γ = 93.824 (11)°
V = 1351.7 (3) Å^3
Z = 4
D_x = 1.590 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 34 reflections
θ = 5.1–12.5°
μ = 1.73 mm^{-1}
T = 223 (2) K
Block, orange
0.6 × 0.3 × 0.3 mm

Data collection

Siemens P4 diffractometer
Profile fitting of $\omega/2\theta$ scans
Absorption correction: ψ scan (*XSCANS*; Siemens, 1996).
T_{min} = 0.537, T_{max} = 0.594
7873 measured reflections
6177 independent reflections
5913 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 27.5°
$h = -8 \rightarrow 1$
$k = -13 \rightarrow 13$
$l = -26 \rightarrow 26$
3 standard reflections
every 97 reflections
intensity decay: 4%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.098
S = 1.23
6177 reflections
271 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0118P)^2 + 6.285P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.01 e Å^{-3}
$\Delta\rho_{min}$ = −1.24 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pd1—N12	2.046 (4)	Pd2—N21	2.057 (4)
Pd1—N11	2.050 (4)	Pd2—N22	2.058 (4)
Pd1—Cl11	2.3015 (11)	Pd2—Cl22	2.3051 (12)
Pd1—Cl12	2.3030 (11)	Pd2—Cl21	2.3072 (12)
N12—Pd1—N11	179.27 (16)	N21—Pd2—N22	179.06 (16)
N12—Pd1—Cl11	90.17 (12)	N21—Pd2—Cl22	89.93 (12)
N11—Pd1—Cl11	89.35 (12)	N22—Pd2—Cl22	90.71 (12)
N12—Pd1—Cl12	89.74 (12)	N21—Pd2—Cl21	90.04 (12)
N11—Pd1—Cl12	90.74 (12)	N22—Pd2—Cl21	89.32 (12)
Cl11—Pd1—Cl12	179.34 (5)	Cl22—Pd2—Cl21	179.26 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N11—H112···Cl11^{i}	0.81 (6)	2.62 (6)	3.408 (4)	163 (5)
N12—H121···Cl21^{ii}	0.82 (6)	2.75 (6)	3.416 (4)	140 (5)
N12—H122···Cl12^{iii}	0.84 (6)	2.60 (6)	3.423 (4)	165 (5)
N21—H211···Cl11	0.79 (6)	2.59 (6)	3.327 (4)	157 (5)
N21—H212···Cl22^{iii}	0.84 (6)	2.76 (6)	3.502 (4)	148 (5)
N22—H221···Cl21^{i}	0.80 (6)	2.71 (6)	3.481 (4)	164 (5)
N22—H222···Cl12^{iv}	0.92 (6)	2.52 (6)	3.347 (4)	149 (4)

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

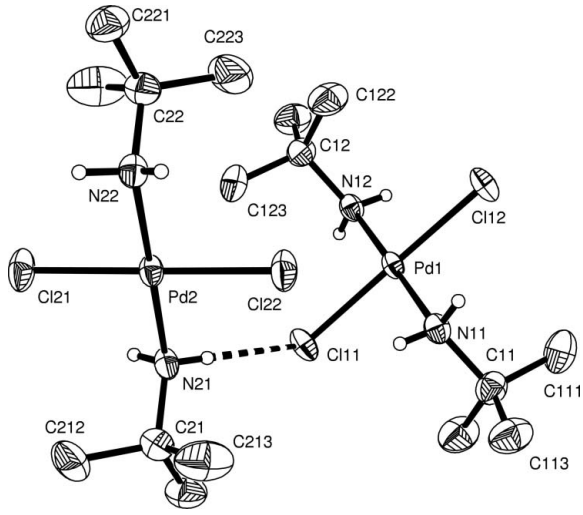


Figure 1
A view of the two independent molecules in (I). Displacement ellipsoids are drawn at the 50% probability level. *tert*-Butyl H atoms have been omitted. The dashed line indicates a hydrogen bond.

Methyl-H atoms were placed in calculated positions and subsequently constrained to an ideal geometry, with C—H distances of 0.97 Å and $U_{iso}(H) = 1.5U_{eq}(C)$, with each group allowed to rotate freely about its C—C bond. The positions of the amine H atoms were identified from a difference Fourier map and allowed to refine freely with fixed isotropic displacement parameters; N—H = 0.79 (6)–0.92 (6) Å. The highest peak is located 1.21 Å from atom Cl21 and the deepest hole 1.47 Å from atom Cl12.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-Plus* (Siemens, 1995); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus*; software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

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References

Fletcher, D. A., McMeeking, R. F. & Parkin, D. (1996). *J. Chem. Inf. Comput. Sci.* **36**, 746–749.
Nakayama, K., Komorita, T. & Shimura, Y. (1984). *Bull. Chem. Soc. Jpn*, **57**, 1336–1347.
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supporting information

Acta Cryst. (2005). E**61**, m2172–m2173 [doi:10.1107/S1600536805030047]

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S1. Comment

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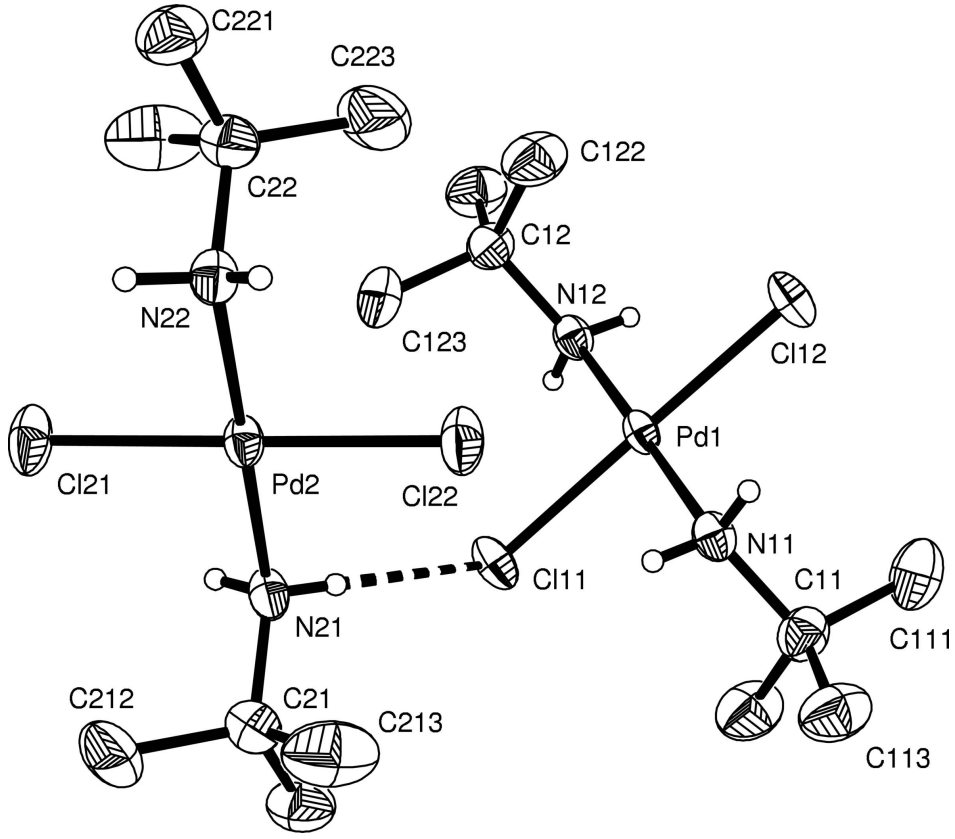
Complex (I) exists as two independent square-planar molecules in the unit cell. The orientation of the *tert*-butylamine groups is such that both molecules are pseudo-centrosymmetric. Analysis of the 14 previous bis(primary amine)-dichloride palladium structures (Fletcher *et al.*, 1996) gives averages of 2.300 (8) Å and 2.047 (9) Å for the Pd—Cl and the Pd—N bonds, respectively, with a mean deviation of the N—Pd—Cl angles of *ca* 1.4° from the ideal 90°. The Pd—Cl and Pd—N bond lengths in (I) range from 2.3015 (11) to 2.3072 (12) and 2.046 (4) to 2.058 (4) Å, respectively; this indicates that, in this complex, the bulky *tert*-butyl group has no obvious structural consequence, although complex (I) does show a significantly smaller deviation from the 90° required by ideal square-planar geometry, [0.455° (molecule 1) 0.375° (molecule 2)]. The molecules are linked together in a hydrogen-bonding network, resulting in the formation of a two-dimensional layered structure, externally defined by the *tert*-butyl groups and approximately parallel to the c face.

S2. Experimental

Complex (I) crystallized from a dichloromethane/hexane reaction mixture of *trans*-[Pd(η^1-C_5H_5)($NH_2Bu t$)$_2$Cl] and [Pd(η^5-C_5H_5)($NH_2Bu t$)Cl] (amounts? ratio?) and was spectroscopically identical to the material synthesized according to the literature method (Nakayama *et al.*, 1984).

S3. Refinement

The methyl-H atoms were placed in calculated positions and subsequently constrained to an ideal geometry, with C—H distances of 0.97 Å and U_{iso}(H) = 1.5U_{eq}(C), with each group allowed to rotate freely about its C—C bond. The positions of the amine-H atoms were identified from a difference Fourier map and allowed to refine freely with isotropic displacement parameters, N—H = 0.79 (6)–0.92 (6) Å.



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Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 34 reflections
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$T = 223$ K
Block, orange
0.6 × 0.3 × 0.3 mm

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Radiation source: fine-focus sealed tube
Graphite monochromator
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Absorption correction: ψ scan (*XSCANS*; Siemens, 1996).
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$k = -13 \rightarrow 13$
$l = -26 \rightarrow 26$

3 standard reflections every 97 reflections
intensity decay: 4%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.098$
$S = 1.23$
6177 reflections
271 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0118P)^2 + 6.285P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.01$ e Å^{-3}
$\Delta\rho_{min} = -1.24$ e Å^{-3}

Special details

Experimental. 13 reflections having 2θ between 8.98 and 45.57 degrees giving 231 ψ scans for parameter estimation,
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.
Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)
− 1.7720 (0.0053) x − 8.6655 (0.0040) y + 11.1351 (0.0205) z = 0.5317 (0.0088)
* −0.0014 (0.0012) Pd1 * 0.0119 (0.0012) Cl11 * 0.0118 (0.0012) Cl12 * −0.0111 (0.0017) N11 * −0.0112 (0.0017) N12
Rms deviation of fitted atoms = 0.0103
2.0951 (0.0059) x + 6.3911 (0.0067) y + 13.2261 (0.0209) z = 8.6109 (0.0031)
Angle to previous plane (with approximate e.s.d.) = 73.56 (0.07)
* 0.0010 (0.0012) Pd2 * −0.0139 (0.0013) Cl21 * −0.0138 (0.0013) Cl22 * 0.0133 (0.0018) N21 * 0.0133 (0.0018) N22
Rms deviation of fitted atoms = 0.0121
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	0.65182 (5)	0.13377 (3)	0.255462 (16)	0.02147 (8)
Cl11	0.39061 (17)	0.24895 (11)	0.30472 (6)	0.0327 (2)
Cl12	0.91142 (17)	0.01643 (11)	0.20664 (6)	0.0339 (2)
N11	0.8572 (6)	0.1923 (4)	0.33284 (19)	0.0255 (7)
C11	0.8717 (8)	0.1205 (5)	0.3928 (3)	0.0360 (11)
C111	0.9665 (12)	−0.0050 (6)	0.3730 (3)	0.0598 (17)
H11A	0.8688	−0.0554	0.3424	0.090*
H11B	0.9874	−0.0502	0.4117	0.090*
H11C	1.1036	0.0106	0.3524	0.090*
C112	0.6494 (10)	0.0987 (7)	0.4208 (3)	0.0522 (15)
H11D	0.5930	0.1794	0.4340	0.078*
H11E	0.6589	0.0498	0.4586	0.078*
H11F	0.5543	0.0530	0.3877	0.078*
C113	1.0205 (10)	0.1981 (7)	0.4430 (3)	0.0507 (15)

H11G	1.1632	0.2087	0.4251	0.076*
H11H	1.0280	0.1546	0.4827	0.076*
H11I	0.9651	0.2802	0.4529	0.076*
N12	0.4460 (6)	0.0777 (4)	0.1782 (2)	0.0261 (7)
C12	0.4354 (8)	0.1510 (5)	0.1187 (2)	0.0336 (10)
C121	0.2900 (9)	0.0729 (6)	0.0676 (3)	0.0480 (14)
H12G	0.3488	−0.0082	0.0572	0.072*
H12H	0.2818	0.1173	0.0282	0.072*
H12I	0.1472	0.0599	0.0850	0.072*
C122	0.6580 (9)	0.1721 (7)	0.0916 (3)	0.0510 (15)
H12D	0.7486	0.2243	0.1235	0.077*
H12E	0.6487	0.2141	0.0514	0.077*
H12F	0.7194	0.0914	0.0825	0.077*
C123	0.3396 (12)	0.2755 (6)	0.1380 (3)	0.0532 (15)
H12A	0.1990	0.2594	0.1564	0.080*
H12B	0.3254	0.3223	0.0996	0.080*
H12C	0.4329	0.3245	0.1704	0.080*
Pd2	0.64561 (5)	0.63092 (3)	0.243993 (17)	0.02377 (9)
Cl21	0.39915 (19)	0.76984 (12)	0.21478 (7)	0.0401 (3)
Cl22	0.88984 (19)	0.49019 (12)	0.27219 (7)	0.0390 (3)
N21	0.4354 (6)	0.5628 (4)	0.3111 (2)	0.0272 (8)
C21	0.4302 (8)	0.6210 (5)	0.3804 (2)	0.0355 (10)
C211	0.2889 (10)	0.5330 (6)	0.4198 (3)	0.0493 (14)
H21D	0.1460	0.5212	0.3998	0.074*
H21E	0.2797	0.5701	0.4644	0.074*
H21F	0.3512	0.4520	0.4201	0.074*
C212	0.3290 (14)	0.7483 (6)	0.3792 (4)	0.067 (2)
H21G	0.4222	0.8058	0.3563	0.101*
H21H	0.3108	0.7836	0.4238	0.101*
H21I	0.1900	0.7358	0.3568	0.101*
C213	0.6562 (11)	0.6364 (8)	0.4096 (3)	0.068 (2)
H21A	0.7171	0.5548	0.4080	0.101*
H21B	0.6519	0.6711	0.4548	0.101*
H21C	0.7442	0.6931	0.3847	0.101*
N22	0.8550 (6)	0.7021 (4)	0.1774 (2)	0.0273 (8)
C22	0.8660 (8)	0.6480 (5)	0.1078 (2)	0.0357 (10)
C221	1.0054 (10)	0.7391 (6)	0.0706 (3)	0.0456 (13)
H22A	0.9351	0.8172	0.0684	0.068*
H22B	1.0265	0.7018	0.0266	0.068*
H22C	1.1437	0.7565	0.0931	0.068*
C222	0.6405 (11)	0.6331 (9)	0.0775 (3)	0.069 (2)
H22G	0.5536	0.5717	0.0998	0.103*
H22H	0.6479	0.6044	0.0314	0.103*
H22I	0.5762	0.7137	0.0818	0.103*
C223	0.9687 (14)	0.5218 (6)	0.1074 (4)	0.068 (2)
H22D	1.1079	0.5341	0.1297	0.102*
H22E	0.9867	0.4883	0.0625	0.102*
H22F	0.8767	0.4628	0.1298	0.102*

H111	0.818 (9)	0.261 (5)	0.340 (3)	0.030*
H112	0.977 (9)	0.197 (5)	0.318 (3)	0.030*
H121	0.479 (9)	0.005 (5)	0.170 (3)	0.030*
H122	0.323 (9)	0.060 (5)	0.193 (3)	0.030*
H211	0.463 (9)	0.492 (5)	0.312 (3)	0.030*
H212	0.317 (9)	0.572 (5)	0.292 (3)	0.030*
H221	0.976 (9)	0.705 (5)	0.191 (3)	0.030*
H222	0.825 (9)	0.785 (5)	0.174 (3)	0.030*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.01610 (15)	0.01825 (15)	0.03003 (17)	0.00218 (11)	0.00305 (11)	0.00047 (11)
Cl11	0.0222 (5)	0.0288 (5)	0.0466 (6)	0.0052 (4)	0.0071 (4)	−0.0046 (5)
Cl12	0.0218 (5)	0.0307 (5)	0.0480 (7)	0.0060 (4)	0.0049 (4)	−0.0085 (5)
N11	0.0186 (17)	0.0244 (18)	0.033 (2)	0.0002 (14)	0.0026 (14)	0.0024 (15)
C11	0.033 (3)	0.039 (3)	0.037 (3)	0.001 (2)	0.001 (2)	0.010 (2)
C111	0.076 (5)	0.045 (3)	0.063 (4)	0.018 (3)	−0.001 (3)	0.023 (3)
C112	0.038 (3)	0.071 (4)	0.048 (3)	−0.008 (3)	0.007 (2)	0.019 (3)
C113	0.041 (3)	0.073 (4)	0.037 (3)	−0.005 (3)	−0.002 (2)	0.006 (3)
N12	0.0205 (18)	0.0236 (18)	0.034 (2)	0.0014 (14)	0.0037 (15)	0.0019 (15)
C12	0.030 (2)	0.038 (3)	0.033 (2)	0.002 (2)	0.0006 (19)	0.006 (2)
C121	0.040 (3)	0.065 (4)	0.038 (3)	−0.003 (3)	−0.004 (2)	0.005 (3)
C122	0.037 (3)	0.070 (4)	0.048 (3)	−0.006 (3)	0.007 (2)	0.020 (3)
C123	0.069 (4)	0.042 (3)	0.052 (3)	0.021 (3)	0.001 (3)	0.016 (3)
Pd2	0.01797 (15)	0.02036 (15)	0.03378 (18)	0.00259 (11)	0.00199 (12)	0.00589 (12)
Cl21	0.0238 (5)	0.0368 (6)	0.0638 (8)	0.0094 (4)	0.0054 (5)	0.0220 (6)
Cl22	0.0270 (5)	0.0363 (6)	0.0575 (8)	0.0113 (5)	0.0064 (5)	0.0196 (5)
N21	0.0239 (19)	0.0220 (18)	0.037 (2)	0.0051 (15)	0.0051 (15)	0.0057 (15)
C21	0.036 (3)	0.034 (3)	0.036 (3)	0.002 (2)	0.004 (2)	0.000 (2)
C211	0.052 (3)	0.056 (4)	0.041 (3)	0.000 (3)	0.014 (3)	0.004 (3)
C212	0.105 (6)	0.037 (3)	0.060 (4)	0.022 (4)	0.019 (4)	−0.005 (3)
C213	0.045 (4)	0.105 (6)	0.048 (4)	−0.012 (4)	−0.004 (3)	−0.011 (4)
N22	0.0202 (18)	0.0263 (19)	0.036 (2)	0.0006 (15)	0.0027 (15)	0.0068 (15)
C22	0.036 (3)	0.036 (3)	0.034 (2)	0.001 (2)	0.005 (2)	0.001 (2)
C221	0.044 (3)	0.052 (3)	0.042 (3)	−0.002 (3)	0.009 (2)	0.013 (2)
C222	0.044 (4)	0.109 (6)	0.048 (4)	−0.024 (4)	−0.004 (3)	−0.005 (4)
C223	0.108 (6)	0.040 (3)	0.057 (4)	0.018 (4)	0.027 (4)	−0.002 (3)

Geometric parameters (Å, º)

Pd1—N12	2.046 (4)	Pd2—N21	2.057 (4)
Pd1—N11	2.050 (4)	Pd2—N22	2.058 (4)
Pd1—Cl11	2.3015 (11)	Pd2—Cl22	2.3051 (12)
Pd1—Cl12	2.3030 (11)	Pd2—Cl21	2.3072 (12)
N11—C11	1.501 (6)	N21—C21	1.502 (6)
N11—H111	0.79 (6)	N21—H211	0.79 (6)
N11—H112	0.81 (6)	N21—H212	0.84 (6)

C11—C112	1.520 (7)	C21—C213	1.515 (8)
C11—C113	1.525 (8)	C21—C211	1.530 (7)
C11—C111	1.526 (8)	C21—C212	1.535 (8)
C111—H11A	0.9700	C211—H21D	0.9700
C111—H11B	0.9700	C211—H21E	0.9700
C111—H11C	0.9700	C211—H21F	0.9700
C112—H11D	0.9700	C212—H21G	0.9700
C112—H11E	0.9700	C212—H21H	0.9700
C112—H11F	0.9700	C212—H21I	0.9700
C113—H11G	0.9700	C213—H21A	0.9700
C113—H11H	0.9700	C213—H21B	0.9700
C113—H11I	0.9700	C213—H21C	0.9700
N12—C12	1.502 (6)	N22—C22	1.497 (6)
N12—H121	0.82 (6)	N22—H221	0.80 (6)
N12—H122	0.84 (6)	N22—H222	0.92 (6)
C12—C122	1.514 (7)	C22—C221	1.519 (7)
C12—C123	1.516 (7)	C22—C222	1.521 (8)
C12—C121	1.528 (7)	C22—C223	1.526 (8)
C121—H12G	0.9700	C221—H22A	0.9700
C121—H12H	0.9700	C221—H22B	0.9700
C121—H12I	0.9700	C221—H22C	0.9700
C122—H12D	0.9700	C222—H22G	0.9700
C122—H12E	0.9700	C222—H22H	0.9700
C122—H12F	0.9700	C222—H22I	0.9700
C123—H12A	0.9700	C223—H22D	0.9700
C123—H12B	0.9700	C223—H22E	0.9700
C123—H12C	0.9700	C223—H22F	0.9700

N12—Pd1—N11	179.27 (16)	N21—Pd2—N22	179.06 (16)
N12—Pd1—Cl11	90.17 (12)	N21—Pd2—Cl22	89.93 (12)
N11—Pd1—Cl11	89.35 (12)	N22—Pd2—Cl22	90.71 (12)
N12—Pd1—Cl12	89.74 (12)	N21—Pd2—Cl21	90.04 (12)
N11—Pd1—Cl12	90.74 (12)	N22—Pd2—Cl21	89.32 (12)
Cl11—Pd1—Cl12	179.34 (5)	Cl22—Pd2—Cl21	179.26 (6)
C11—N11—Pd1	122.4 (3)	C21—N21—Pd2	122.1 (3)
C11—N11—H111	114 (4)	C21—N21—H211	109 (4)
Pd1—N11—H111	98 (4)	Pd2—N21—H211	103 (4)
C11—N11—H112	106 (4)	C21—N21—H212	109 (4)
Pd1—N11—H112	107 (4)	Pd2—N21—H212	101 (4)
H111—N11—H112	109 (5)	H211—N21—H212	113 (5)
N11—C11—C112	109.8 (4)	N21—C21—C213	109.6 (4)
N11—C11—C113	108.2 (4)	N21—C21—C211	108.1 (4)
C112—C11—C113	110.2 (5)	C213—C21—C211	110.0 (5)
N11—C11—C111	108.2 (4)	N21—C21—C212	108.1 (5)
C112—C11—C111	110.6 (5)	C213—C21—C212	111.7 (6)
C113—C11—C111	109.8 (5)	C211—C21—C212	109.3 (5)
C11—C111—H11A	109.5	C21—C211—H21D	109.5
C11—C111—H11B	109.5	C21—C211—H21E	109.5

H11A—C111—H11B	109.5	H21D—C211—H21E	109.5
C11—C111—H11C	109.5	C21—C211—H21F	109.5
H11A—C111—H11C	109.5	H21D—C211—H21F	109.5
H11B—C111—H11C	109.5	H21E—C211—H21F	109.5
C11—C112—H11D	109.5	C21—C212—H21G	109.5
C11—C112—H11E	109.5	C21—C212—H21H	109.5
H11D—C112—H11E	109.5	H21G—C212—H21H	109.5
C11—C112—H11F	109.5	C21—C212—H21I	109.5
H11D—C112—H11F	109.5	H21G—C212—H21I	109.5
H11E—C112—H11F	109.5	H21H—C212—H21I	109.5
C11—C113—H11G	109.5	C21—C213—H21A	109.5
C11—C113—H11H	109.5	C21—C213—H21B	109.5
H11G—C113—H11H	109.5	H21A—C213—H21B	109.5
C11—C113—H11I	109.5	C21—C213—H21C	109.5
H11G—C113—H11I	109.5	H21A—C213—H21C	109.5
H11H—C113—H11I	109.5	H21B—C213—H21C	109.5
C12—N12—Pd1	121.9 (3)	C22—N22—Pd2	123.5 (3)
C12—N12—H121	114 (4)	C22—N22—H221	105 (4)
Pd1—N12—H121	100 (4)	Pd2—N22—H221	111 (4)
C12—N12—H122	112 (4)	C22—N22—H222	104 (3)
Pd1—N12—H122	109 (4)	Pd2—N22—H222	107 (3)
H121—N12—H122	97 (5)	H221—N22—H222	105 (5)
N12—C12—C122	109.9 (4)	N22—C22—C221	108.3 (4)
N12—C12—C123	108.6 (4)	N22—C22—C222	109.1 (5)
C122—C12—C123	111.2 (5)	C221—C22—C222	109.5 (5)
N12—C12—C121	107.5 (4)	N22—C22—C223	108.4 (5)
C122—C12—C121	109.6 (5)	C221—C22—C223	109.6 (5)
C123—C12—C121	110.0 (5)	C222—C22—C223	111.8 (6)
C12—C121—H12G	109.5	C22—C221—H22A	109.5
C12—C121—H12H	109.5	C22—C221—H22B	109.5
H12G—C121—H12H	109.5	H22A—C221—H22B	109.5
C12—C121—H12I	109.5	C22—C221—H22C	109.5
H12G—C121—H12I	109.5	H22A—C221—H22C	109.5
H12H—C121—H12I	109.5	H22B—C221—H22C	109.5
C12—C122—H12D	109.5	C22—C222—H22G	109.5
C12—C122—H12E	109.5	C22—C222—H22H	109.5
H12D—C122—H12E	109.5	H22G—C222—H22H	109.5
C12—C122—H12F	109.5	C22—C222—H22I	109.5
H12D—C122—H12F	109.5	H22G—C222—H22I	109.5
H12E—C122—H12F	109.5	H22H—C222—H22I	109.5
C12—C123—H12A	109.5	C22—C223—H22D	109.5
C12—C123—H12B	109.5	C22—C223—H22E	109.5
H12A—C123—H12B	109.5	H22D—C223—H22E	109.5
C12—C123—H12C	109.5	C22—C223—H22F	109.5
H12A—C123—H12C	109.5	H22D—C223—H22F	109.5
H12B—C123—H12C	109.5	H22E—C223—H22F	109.5
N12—Pd1—N11—C11	139 (12)	N22—Pd2—N21—C21	−41 (10)

Cl11—Pd1—N11—C11	89.7 (4)	Cl22—Pd2—N21—C21	92.4 (4)
Cl12—Pd1—N11—C11	−89.6 (4)	Cl21—Pd2—N21—C21	−88.4 (4)
Pd1—N11—C11—C112	−53.4 (6)	Pd2—N21—C21—C213	−49.4 (6)
Pd1—N11—C11—C113	−173.8 (4)	Pd2—N21—C21—C211	−169.2 (4)
Pd1—N11—C11—C111	67.3 (5)	Pd2—N21—C21—C212	72.6 (5)
N11—Pd1—N12—C12	42 (12)	N21—Pd2—N22—C22	−139 (10)
Cl11—Pd1—N12—C12	90.8 (3)	Cl22—Pd2—N22—C22	87.5 (4)
Cl12—Pd1—N12—C12	−89.9 (3)	Cl21—Pd2—N22—C22	−91.8 (4)
Pd1—N12—C12—C122	52.9 (5)	Pd2—N22—C22—C221	169.1 (3)
Pd1—N12—C12—C123	−68.9 (5)	Pd2—N22—C22—C222	50.0 (6)
Pd1—N12—C12—C121	172.1 (3)	Pd2—N22—C22—C223	−72.0 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11—H111···Cl22	0.79 (6)	2.92 (6)	3.494 (4)	132 (5)
N11—H112···Cl11^{i}	0.81 (6)	2.62 (6)	3.408 (4)	163 (5)
N12—H121···Cl21^{ii}	0.82 (6)	2.75 (6)	3.416 (4)	140 (5)
N12—H122···Cl12^{iii}	0.84 (6)	2.60 (6)	3.423 (4)	165 (5)
N21—H211···Cl11	0.79 (6)	2.59 (6)	3.327 (4)	157 (5)
N21—H212···Cl22^{iii}	0.84 (6)	2.76 (6)	3.502 (4)	148 (5)
N22—H221···Cl21^{i}	0.80 (6)	2.71 (6)	3.481 (4)	164 (5)
N22—H222···Cl12^{iv}	0.92 (6)	2.52 (6)	3.347 (4)	149 (4)

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