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Pseudosymmetry in a cyclopalladated compound

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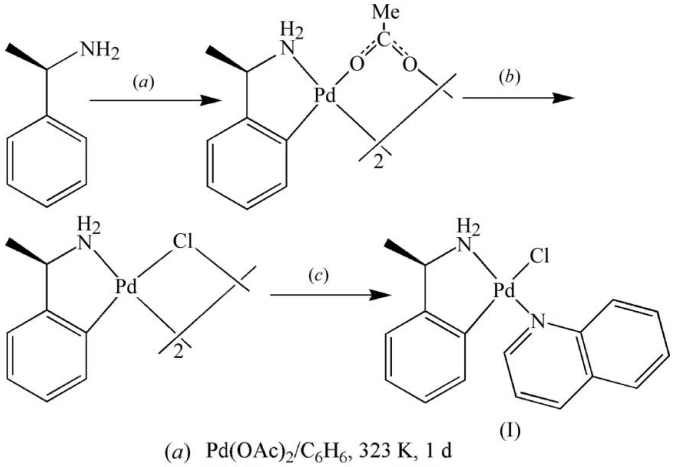
The enantiomerically pure title complex, [*SP*-4-4]-(*R*)-[2-(1-aminoethyl)phenyl-κ^2C^1,*N*]chlorido(quinoline-κN)palladium(II) acetone hemisolvate, $[Pd(C_8H_{10}N)Cl(C_9H_7N)]\cdot 0.5C_3H_6O$, crystallizes with four molecules of the organopalladium complex and two molecules of acetone in the asymmetric unit. This corresponds to a discrete hydrogen-bonded aggregate and to the content of the unit cell in the space group *P*1. Pronounced pseudo-inversion symmetry relates pairs of these objects in the asymmetric unit.

Comment

Cope & Friedrich (1968) discovered a method for cyclopalladation and cycloplatination of tertiary amines. Subsequent research by Lewis *et al.* (1973), Dunina *et al.* (1999), Fuchita & Tsuchiya (1993), Fuchita *et al.* (1995, 1997), Vicente *et al.* (1993, 1997) and Albert *et al.* (1997) indicated that the reaction can be extended to secondary and primary amines.



(*a*) $Pd(OAc)_2/C_6H_6$, 323 K, 1 d
(*b*) NaCl/acetone-water (10:1)
(*c*) Quinoline/CH_2Cl_2

In previous work by Calmuschi & Englert, all intermediates along the reaction pathway used to synthesize (I) (see Scheme) have been structurally characterized (Calmuschi & Englert, 2002; Calmuschi, Jonas & Englert, 2004). A variety of pyridine derivatives have been used successfully as σ-donor ligands (Calmuschi, Alesi & Englert, 2004; Calmuschi & Englert, 2005; Calmuschi-Cula *et al.*, 2005, 2006, 2009; Braun *et al.*, 2011). In the present case, we intended to introduce the electronically similar ligand quinoline as an approximate steric equivalent to the nucleobase guanine; guanine itself is only sparingly soluble in solvents compatible with the organopalladium starting material.

The title compound crystallizes in the space group *P*1. The centrosymmetric supergroup can be safely excluded for the following reasons: (i) a single enantiomer of the primary amine was used; (ii) the distribution of the normalized structure factors is characterized by $\langle E^2 - 1\rangle = 0.832$, a value close to that expected for a noncentrosymmetric structure; (iii) the strong anomalous signal associated with Pd results in a Flack enantiomorph polarity parameter (Flack, 1983) of 0.02 (4) and confirms the chirality of the enantiomerically pure reagent (*R*)-di-μ-chlorido-bis{[2-(1-aminoethyl)phenyl-κ^2C^1,*N*]palladium(II)}. In addition to four independent molecules of the organopalladium complex in an *R* configuration, the unit cell of the crystal contains two molecules of acetone (Fig. 1). After refinement of the structure model, the pronounced pseudo-symmetry is reflected in correlations between anisotropic displacement parameters encountered for atoms related by pseudo-inversion. We note that a search for higher symmetry (Le Page, 1987, 1988), as implemented in *PLATON* (Spek, 2009), as well as a *checkCIF* alert, suggested transformation to the supergroup which can be ruled out for the reasons given above. A graphical representation of the pseudo-inversion symmetry is provided in Fig. 2, in which the obvious exceptions, namely the methyl groups attached to the homochiral

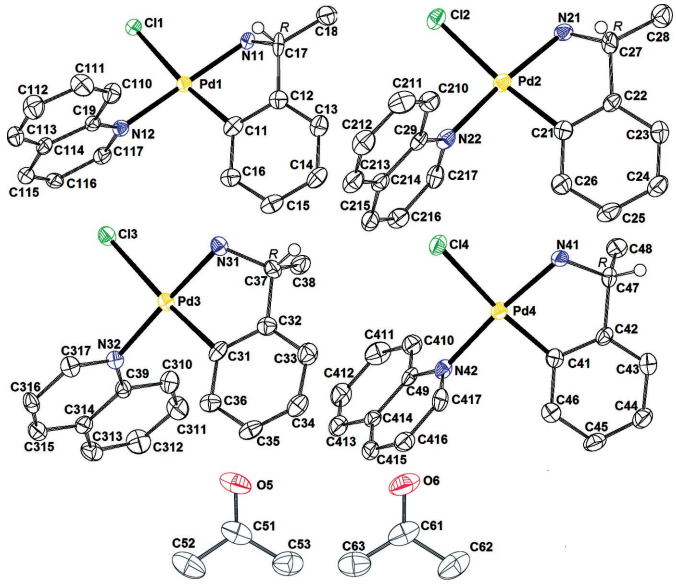


Figure 1
Displacement ellipsoid plot for all molecules in the asymmetric unit of (I); residues are not shown in a common crystallographic direction but have been aligned for better comparison. Ellipsoids have been drawn at the 50% probability level. All H atoms, except for those attached to the chiral centres, have been omitted.

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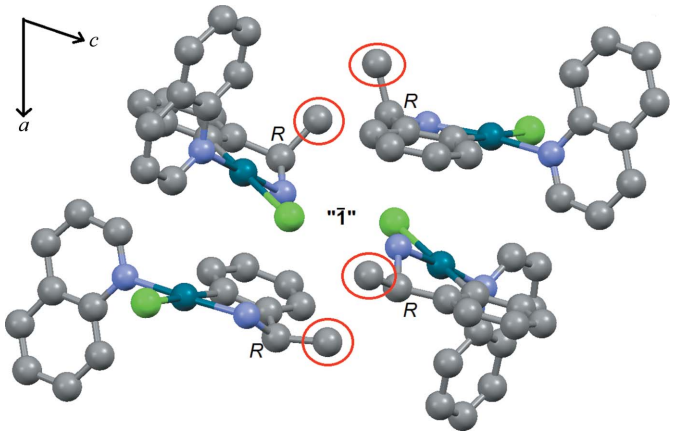

Figure 2
The pseudo-inversion in (I). Methyl substituents breaking the pseudo-symmetry have been highlighted and solvent molecules have been omitted.

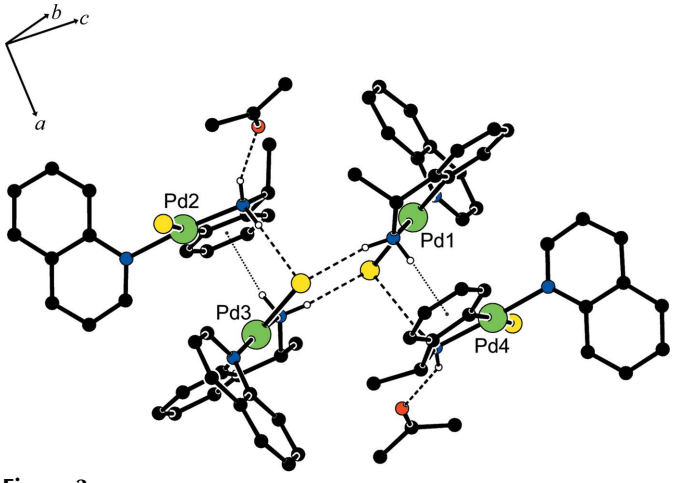

Figure 3
The hydrogen-bonded aggregate in (I). Classical hydrogen bonds are shown as dashed lines and N—H···π contacts are shown as dotted lines.

centres, have been highlighted. The symmetry-independent complex molecules differ only slightly with respect to coordination distances; they show, however, significant variation with respect to the orientation of the quinoline ligand. In agreement with the observed pseudosymmetry, two pairs of conformationally similar molecules are encountered. Coordination distances and representative torsion angles have been compiled in Table 1.

The asymmetric unit of the title compound also represents a discrete hydrogen-bonded aggregate; Fig. 3 shows that the acetone molecules terminate this aggregate, in which the molecules associated with Pd2 and Pd4 act as hydrogen-bond donors *via* their amino group, and those associated with Pd1 and Pd3 act both as donors (NH) and as acceptors (chloride ligands). Classical hydrogen bonds are summarized in Table 2. The H atoms bonded to electronegative partners and not involved in conventional hydrogen bonds, *viz.* H11*A* and H31*B*, interact with the π systems of the closest benzene rings. The contact distances are H11*A*···centroid(C41–C46) = 2.68 Å and H31*B*···centroid(C21–C26) = 2.44 Å.

Experimental

Compound (I) was prepared according to the method of Vicente *et al.* (1993). (*R*)-Di-μ-chlorido-bis{[2-(1-aminoethyl)phenyl-κ^2C^1,*N*]palladium(II)} (14.0 mg, 27 µmol) and quinoline (7.2 mg, 55 µmol) were dissolved in methylene chloride (15 ml) and stirred at 300 K for 1 d. The product was dried under high vacuum and recrystallized by slow evaporation from a solution in acetone at room temperature. (I) crystallizes as colourless rods.

Crystal data

$[Pd(C_8H_{10}N)Cl(C_9H_7N)]\cdot0.5C_3H_6O$
M_r = 420.21
Triclinic, *P*1
a = 11.9699 (18) Å
b = 12.3754 (19) Å
c = 12.4793 (19) Å
α = 104.369 (3)°
β = 95.465 (3)°
γ = 95.802 (3)°
V = 1767.6 (5) Å^3
Z = 4
Mo *K*α radiation
μ = 1.20 mm^{-1}
T = 100 K
0.35 × 0.14 × 0.07 mm

Data collection

Bruker D8 goniometer with a SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.455, T_{max} = 0.745
21565 measured reflections
14570 independent reflections
11833 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.116
S = 1.01
14570 reflections
585 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.95 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}
Absolute structure: Flack (1983), 7126 Friedel pairs
Flack parameter: 0.02 (4)

After conventional refinement with anisotropic displacement parameters for all non-H atoms, correlations between displacement

Table 1
Selected geometric parameters (Å, °).

Pd1—C11	1.981 (9)	Pd3—C31	1.981 (9)
Pd1—N11	2.027 (7)	Pd3—N32	2.034 (7)
Pd1—N12	2.055 (7)	Pd3—N31	2.053 (7)
Pd1—Cl1	2.418 (2)	Pd3—Cl3	2.394 (2)
Pd2—C21	2.004 (9)	Pd4—C41	1.964 (9)
Pd2—N21	2.024 (6)	Pd4—N41	2.040 (6)
Pd2—N22	2.038 (7)	Pd4—N42	2.055 (7)
Pd2—Cl2	2.417 (2)	Pd4—Cl4	2.429 (2)
Cl1—Pd1—N12—C19	−98.1 (7)	Cl3—Pd3—N32—C39	100.2 (6)
Cl2—Pd2—N22—C29	−86.0 (7)	Cl4—Pd4—N42—C49	85.4 (6)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11—H11*B*···Cl3	0.92	2.41	3.241 (7)	151
N21—H21*A*···Cl3	0.92	2.47	3.379 (9)	171
N21—H21*B*···O6	0.92	2.20	2.983 (10)	143
N31—H31*A*···Cl1	0.92	2.45	3.301 (7)	154
N41—H41*A*···O5	0.92	2.18	3.056 (10)	160
N41—H41*B*···Cl1	0.92	2.40	3.310 (9)	171

parameters for atoms related by pseudo-inversion were encountered. Therefore, the anisotropic displacement parameters for all non-H atoms related by pseudo-inversion, *i.e.* for all non-H atoms except for the chiral centres C*X*7 (*X* = 1–4) and the methyl C atoms C*X*8 attached to them, were constrained to be equal, resulting in a total of 252 equality constraints. For the thus constrained model, an agreement factor of *wR*2 = 0.1157 for 14570 data and 585 variables was obtained, only marginally higher than for the unconstrained model with *wR*2 = 0.1136 for the same number of data and 837 variables. H atoms were treated as riding, with N—H = 0.92 Å, C—H = 0.95 Å for CH_3, C—H = 0.99 Å for aryl CH and C—H = 1.00 Å for alkyl CH groups. Isotropic displacement parameters were constrained to U_{iso}(H) = 1.5U_{eq}(C) for methyl groups or 1.2U_{eq}(C,N) otherwise. Tentative refinement of the amino H atoms with N—H distance restraints did not result in satisfactory geometries for these groups, most likely due to high correlation.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: YF3015). Services for accessing these data are described at the back of the journal.

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supplementary materials

Acta Cryst. (2012). C**68**, m223–m225 [doi:10.1107/S0108270112030776]

Pseudosymmetry in a cyclopalladated compound

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(*SP*-4–4)-(*R*)-[2-(1-aminoethyl)phenyl-κ^2C^1,*N*]- chlorido(quinoline-κN)palladium(II) acetone hemisolvate

Crystal data

$[Pd(C_8H_{10}N)Cl(C_9H_7N)]\cdot 0.5C_3H_6O$
$M_r = 420.21$
Triclinic, $P\overline{1}$
Hall symbol: P 1
$a = 11.9699\ (18)$ Å
$b = 12.3754\ (19)$ Å
$c = 12.4793\ (19)$ Å
$\alpha = 104.369\ (3)°$
$\beta = 95.465\ (3)°$
$\gamma = 95.802\ (3)°$
$V = 1767.6\ (5)$ Å^3
$Z = 4$
$F(000) = 848$
$D_x = 1.579$ Mg m^{-3}
Melting point: 413 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 21565 reflections
$\theta = 2–53.1°$
$\mu = 1.20$ mm^{-1}
$T = 100$ K
Rod, colourless
0.35 × 0.14 × 0.07 mm

Data collection

Bruker D8 goniometer with a SMART APEX CCD area-detector diffractometer
Radiation source: Incoatec microsource
Multilayer optics monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999?)
$T_{min} = 0.455$, $T_{max} = 0.745$
21565 measured reflections
14570 independent reflections
11833 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 26.6°$, $\theta_{min} = 1.7°$
$h = -15\rightarrow14$
$k = -15\rightarrow15$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.116$
$S = 1.01$
14570 reflections
585 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.0233P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.95$ e Å^{-3}
$\Delta\rho_{min} = -0.77$ e Å^{-3}
Absolute structure: Flack (1983), **???? Friedel pairs**
Flack parameter: 0.02 (4)

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	0.96980 (4)	0.77247 (4)	0.31673 (4)	0.01802 (9)
Cl1	0.9497 (2)	0.82727 (16)	0.51313 (18)	0.0222 (2)
N11	0.9792 (7)	0.9335 (5)	0.3049 (6)	0.0202 (8)
H11A	0.9084	0.9495	0.2832	0.024*
H11B	1.0066	0.9823	0.3730	0.024*
N12	0.9707 (6)	0.6083 (6)	0.3234 (6)	0.0189 (8)
C11	0.9816 (8)	0.7471 (7)	0.1553 (8)	0.0205 (9)
C12	1.0188 (8)	0.8463 (7)	0.1254 (8)	0.0231 (9)
C13	1.0138 (9)	0.8459 (8)	0.0157 (8)	0.0290 (11)
H13	1.0345	0.9144	−0.0032	0.035*
C14	0.9795 (8)	0.7487 (7)	−0.0695 (8)	0.0297 (13)
H14	0.9775	0.7505	−0.1453	0.036*
C15	0.9481 (7)	0.6485 (7)	−0.0420 (7)	0.0250 (13)
H15	0.9261	0.5805	−0.0986	0.030*
C16	0.9495 (8)	0.6498 (7)	0.0710 (7)	0.0234 (11)
H16	0.9277	0.5816	0.0900	0.028*
C17	1.0585 (9)	0.9466 (7)	0.2187 (8)	0.026 (2)
H17	1.1360	0.9376	0.2500	0.031*
C18	1.0641 (8)	1.0617 (6)	0.2017 (6)	0.038 (2)
H18A	1.1139	1.0680	0.1450	0.057*
H18B	1.0941	1.1172	0.2720	0.057*
H18C	0.9881	1.0759	0.1769	0.057*
C19	1.0685 (8)	0.5621 (6)	0.3338 (7)	0.0185 (9)
C110	1.1702 (8)	0.6227 (7)	0.3228 (8)	0.0269 (10)
H110	1.1701	0.6920	0.3028	0.032*
C111	1.2706 (9)	0.5806 (8)	0.3415 (9)	0.0311 (11)
H111	1.3402	0.6213	0.3350	0.037*
C112	1.2704 (10)	0.4783 (8)	0.3699 (9)	0.0350 (11)
H112	1.3403	0.4512	0.3838	0.042*
C113	1.1758 (9)	0.4188 (8)	0.3780 (9)	0.0276 (10)
H113	1.1782	0.3488	0.3961	0.033*
C114	1.0698 (8)	0.4583 (7)	0.3600 (7)	0.0217 (9)
C115	0.9655 (9)	0.4003 (7)	0.3716 (7)	0.0252 (10)
H115	0.9634	0.3290	0.3876	0.030*
C116	0.8680 (9)	0.4468 (7)	0.3598 (8)	0.0232 (10)
H116	0.7974	0.4089	0.3675	0.028*
C117	0.8748 (9)	0.5525 (7)	0.3359 (7)	0.0233 (9)

H117	0.8070	0.5853	0.3283	0.028*
Pd2	1.36433 (5)	1.22218 (4)	0.72448 (4)	0.02090 (9)
Cl2	1.4142 (2)	1.38278 (17)	0.6531 (2)	0.0252 (2)
N21	1.3189 (7)	1.1208 (5)	0.5688 (6)	0.0215 (9)
H21A	1.2447	1.1255	0.5455	0.026*
H21B	1.3633	1.1442	0.5204	0.026*
N22	1.4034 (7)	1.3116 (6)	0.8869 (7)	0.0224 (8)
C21	1.3130 (8)	1.0801 (7)	0.7654 (8)	0.0208 (9)
C22	1.2959 (7)	0.9865 (7)	0.6737 (8)	0.0204 (11)
C23	1.2485 (8)	0.8827 (7)	0.6881 (8)	0.0274 (11)
H23	1.2324	0.8190	0.6256	0.033*
C24	1.2256 (9)	0.8723 (7)	0.7902 (8)	0.0293 (11)
H24	1.1950	0.8015	0.7990	0.035*
C25	1.2469 (8)	0.9648 (7)	0.8804 (8)	0.0308 (15)
H25	1.2306	0.9578	0.9516	0.037*
C26	1.2921 (9)	1.0689 (8)	0.8684 (8)	0.0317 (14)
H26	1.3084	1.1320	0.9315	0.038*
C27	1.3325 (6)	1.0032 (6)	0.5672 (6)	0.0222 (18)
H27	1.4153	0.9971	0.5707	0.027*
C28	1.2747 (7)	0.9185 (6)	0.4606 (6)	0.0331 (19)
H28A	1.1925	0.9169	0.4578	0.050*
H28B	1.2951	0.8436	0.4598	0.050*
H28C	1.2997	0.9407	0.3957	0.050*
C29	1.5090 (8)	1.3304 (6)	0.9449 (7)	0.0195 (10)
C210	1.5989 (8)	1.2872 (7)	0.8913 (8)	0.0275 (12)
H210	1.5855	1.2444	0.8157	0.033*
C211	1.7072 (9)	1.3066 (8)	0.9482 (9)	0.0346 (14)
H211	1.7680	1.2775	0.9114	0.041*
C212	1.7273 (9)	1.3691 (7)	1.0600 (8)	0.0317 (14)
H212	1.8021	1.3829	1.0979	0.038*
C213	1.6425 (9)	1.4101 (8)	1.1149 (8)	0.0317 (14)
H213	1.6580	1.4508	1.1911	0.038*
C214	1.5300 (8)	1.3930 (6)	1.0595 (7)	0.0219 (11)
C215	1.4399 (8)	1.4357 (7)	1.1108 (8)	0.0260 (12)
H215	1.4511	1.4794	1.1861	0.031*
C216	1.3356 (9)	1.4138 (7)	1.0513 (8)	0.0277 (12)
H216	1.2726	1.4399	1.0859	0.033*
C217	1.3203 (8)	1.3532 (6)	0.9397 (8)	0.0241 (10)
H217	1.2467	1.3411	0.8996	0.029*
Pd3	1.02955 (4)	1.22831 (4)	0.68424 (4)	0.01802 (9)
Cl3	1.0548 (2)	1.17047 (16)	0.49122 (18)	0.0222 (2)
N31	1.0305 (7)	1.0681 (5)	0.7027 (6)	0.0202 (8)
H31A	0.9985	1.0168	0.6375	0.024*
H31B	1.1038	1.0549	0.7178	0.024*
N32	1.0297 (6)	1.3898 (6)	0.6739 (6)	0.0189 (8)
C31	1.0131 (8)	1.2626 (7)	0.8453 (8)	0.0205 (9)
C32	0.9856 (8)	1.1646 (7)	0.8816 (8)	0.0231 (9)
C33	0.9764 (9)	1.1720 (8)	0.9935 (8)	0.0290 (11)
H33	0.9531	1.1070	1.0173	0.035*

C34	1.0020 (8)	1.2767 (7)	1.0694 (8)	0.0297 (13)
H34	1.0002	1.2823	1.1465	0.036*
C35	1.0296 (7)	1.3713 (7)	1.0360 (7)	0.0250 (13)
H35	1.0461	1.4420	1.0896	0.030*
C36	1.0341 (8)	1.3651 (7)	0.9226 (8)	0.0234 (11)
H36	1.0515	1.4317	0.8994	0.028*
C37	0.9665 (8)	1.0543 (7)	0.7938 (8)	0.026 (2)
H37	0.9955	0.9947	0.8261	0.031*
C38	0.8385 (6)	1.0203 (6)	0.7512 (6)	0.0289 (18)
H38A	0.8114	1.0753	0.7137	0.043*
H38B	0.7963	1.0186	0.8145	0.043*
H38C	0.8269	0.9457	0.6985	0.043*
C39	0.9283 (8)	1.4369 (6)	0.6629 (7)	0.0185 (9)
C310	0.8261 (8)	1.3771 (7)	0.6697 (8)	0.0269 (10)
H310	0.8257	1.3060	0.6857	0.032*
C311	0.7246 (9)	1.4186 (8)	0.6535 (9)	0.0311 (11)
H311	0.6554	1.3766	0.6591	0.037*
C312	0.7245 (10)	1.5230 (8)	0.6290 (9)	0.0350 (11)
H312	0.6548	1.5502	0.6142	0.042*
C313	0.8277 (9)	1.5880 (8)	0.6263 (8)	0.0276 (10)
H313	0.8276	1.6603	0.6130	0.033*
C314	0.9308 (8)	1.5452 (7)	0.6433 (7)	0.0217 (9)
C315	1.0341 (9)	1.6038 (7)	0.6361 (7)	0.0252 (10)
H315	1.0372	1.6760	0.6222	0.030*
C316	1.1314 (9)	1.5561 (7)	0.6494 (8)	0.0232 (10)
H316	1.2026	1.5965	0.6475	0.028*
C317	1.1257 (8)	1.4478 (7)	0.6656 (7)	0.0233 (9)
H317	1.1937	1.4149	0.6710	0.028*
Pd4	0.63787 (5)	0.80200 (4)	0.28935 (4)	0.02090 (9)
Cl4	0.5883 (2)	0.64003 (17)	0.3605 (2)	0.0252 (2)
N41	0.6981 (7)	0.8981 (5)	0.4460 (6)	0.0215 (9)
H41A	0.6462	0.8880	0.4936	0.026*
H41B	0.7639	0.8737	0.4697	0.026*
N42	0.5927 (7)	0.7124 (6)	0.1260 (7)	0.0224 (8)
C41	0.6846 (8)	0.9416 (7)	0.2482 (8)	0.0208 (9)
C42	0.7278 (7)	1.0346 (7)	0.3360 (8)	0.0204 (11)
C43	0.7686 (8)	1.1370 (7)	0.3222 (8)	0.0274 (11)
H43	0.7961	1.1984	0.3849	0.033*
C44	0.7687 (9)	1.1491 (7)	0.2133 (8)	0.0293 (11)
H44	0.7968	1.2195	0.2020	0.035*
C45	0.7286 (8)	1.0606 (7)	0.1234 (8)	0.0308 (15)
H45	0.7268	1.0699	0.0500	0.037*
C46	0.6900 (9)	0.9555 (8)	0.1406 (8)	0.0317 (14)
H46	0.6672	0.8928	0.0780	0.038*
C47	0.7217 (6)	1.0218 (6)	0.4532 (6)	0.0197 (17)
H47	0.7968	1.0523	0.4987	0.024*
C48	0.6317 (7)	1.0836 (6)	0.5091 (6)	0.0304 (18)
H48A	0.6465	1.1635	0.5113	0.046*
H48B	0.6330	1.0754	0.5854	0.046*

H48C	0.5573	1.0519	0.4671	0.046*
C49	0.4823 (7)	0.6965 (6)	0.0745 (7)	0.0195 (10)
C410	0.3965 (9)	0.7406 (7)	0.1315 (8)	0.0275 (12)
H410	0.4125	0.7828	0.2072	0.033*
C411	0.2875 (9)	0.7228 (8)	0.0775 (9)	0.0346 (14)
H411	0.2282	0.7517	0.1168	0.041*
C412	0.2634 (9)	0.6620 (7)	−0.0354 (8)	0.0317 (14)
H412	0.1885	0.6521	−0.0724	0.038*
C413	0.3467 (9)	0.6178 (8)	−0.0911 (8)	0.0317 (14)
H413	0.3291	0.5747	−0.1664	0.038*
C414	0.4589 (8)	0.6348 (6)	−0.0392 (7)	0.0219 (11)
C415	0.5451 (8)	0.5906 (7)	−0.0955 (8)	0.0260 (12)
H415	0.5292	0.5479	−0.1710	0.031*
C416	0.6528 (9)	0.6085 (7)	−0.0421 (8)	0.0277 (12)
H416	0.7134	0.5801	−0.0796	0.033*
C417	0.6710 (8)	0.6703 (7)	0.0700 (8)	0.0241 (10)
H417	0.7458	0.6821	0.1075	0.029*
O5	0.5728 (6)	0.9002 (6)	0.6486 (6)	0.0504 (14)
C51	0.5371 (9)	0.8401 (9)	0.7048 (9)	0.0409 (17)
C52	0.5376 (10)	0.8843 (11)	0.8267 (10)	0.056 (2)
H52A	0.6020	0.8612	0.8662	0.084*
H52B	0.4670	0.8543	0.8489	0.084*
H52C	0.5442	0.9666	0.8456	0.084*
C53	0.4838 (11)	0.7175 (9)	0.6489 (11)	0.0497 (15)
H53A	0.4015	0.7116	0.6487	0.075*
H53B	0.5146	0.6673	0.6905	0.075*
H53C	0.5016	0.6958	0.5720	0.075*
O6	1.3783 (6)	1.1240 (6)	0.3427 (6)	0.0504 (14)
C61	1.4333 (9)	1.1773 (9)	0.2930 (9)	0.0409 (17)
C62	1.4341 (11)	1.1364 (11)	0.1703 (10)	0.056 (2)
H62A	1.3858	1.0640	0.1423	0.084*
H62B	1.5117	1.1269	0.1544	0.084*
H62C	1.4055	1.1913	0.1336	0.084*
C63	1.5070 (11)	1.2813 (9)	0.3502 (11)	0.0497 (15)
H63A	1.4922	1.3049	0.4279	0.075*
H63B	1.4919	1.3403	0.3129	0.075*
H63C	1.5863	1.2684	0.3480	0.075*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.01729 (16)	0.01804 (17)	0.01815 (16)	−0.00008 (13)	−0.00123 (12)	0.00586 (13)
Cl1	0.0267 (5)	0.0208 (5)	0.0180 (5)	−0.0008 (5)	−0.0010 (4)	0.0062 (4)
N11	0.023 (2)	0.0207 (19)	0.0174 (17)	0.0014 (15)	−0.0017 (14)	0.0079 (15)
N12	0.0167 (17)	0.0205 (19)	0.0192 (18)	0.0018 (15)	0.0003 (14)	0.0058 (15)
C11	0.008 (2)	0.034 (2)	0.021 (2)	0.0073 (17)	0.0043 (16)	0.0065 (18)
C12	0.020 (2)	0.024 (2)	0.025 (2)	0.0048 (18)	0.0028 (17)	0.0053 (18)
C13	0.033 (3)	0.033 (3)	0.024 (2)	0.005 (2)	0.004 (2)	0.011 (2)
C14	0.031 (3)	0.041 (3)	0.017 (2)	0.006 (2)	0.003 (2)	0.007 (2)
C15	0.014 (3)	0.035 (3)	0.023 (3)	0.009 (2)	0.001 (2)	0.000 (2)

C16	0.017 (3)	0.025 (2)	0.026 (3)	0.006 (2)	0.001 (2)	0.003 (2)
C17	0.030 (5)	0.032 (4)	0.026 (4)	0.009 (4)	0.005 (4)	0.022 (4)
C18	0.050 (6)	0.034 (5)	0.026 (4)	−0.015 (4)	0.003 (4)	0.011 (4)
C19	0.020 (2)	0.020 (2)	0.015 (2)	−0.0007 (17)	0.0009 (16)	0.0054 (17)
C110	0.024 (2)	0.032 (3)	0.026 (3)	0.003 (2)	0.003 (2)	0.011 (2)
C111	0.015 (2)	0.033 (3)	0.046 (3)	0.002 (2)	0.004 (2)	0.011 (2)
C112	0.028 (3)	0.038 (3)	0.042 (3)	0.011 (2)	0.002 (2)	0.014 (2)
C113	0.034 (3)	0.022 (2)	0.028 (2)	0.0077 (19)	−0.0001 (19)	0.0089 (18)
C114	0.029 (2)	0.023 (2)	0.0130 (19)	0.0037 (18)	0.0021 (16)	0.0050 (16)
C115	0.036 (3)	0.021 (2)	0.018 (2)	−0.0006 (19)	−0.0001 (18)	0.0057 (17)
C116	0.024 (2)	0.021 (2)	0.022 (2)	−0.0084 (18)	−0.0019 (17)	0.0065 (18)
C117	0.021 (2)	0.026 (2)	0.022 (2)	−0.0002 (19)	−0.0030 (17)	0.0069 (18)
Pd2	0.01798 (17)	0.0236 (2)	0.02035 (17)	−0.00272 (14)	−0.00156 (13)	0.00796 (14)
Cl2	0.0214 (5)	0.0242 (6)	0.0299 (6)	−0.0031 (4)	0.0008 (4)	0.0098 (5)
N21	0.021 (2)	0.026 (2)	0.0175 (18)	−0.0021 (16)	−0.0001 (15)	0.0082 (15)
N22	0.0144 (18)	0.026 (2)	0.0271 (19)	−0.0023 (16)	−0.0025 (15)	0.0115 (17)
C21	0.013 (2)	0.026 (2)	0.023 (2)	0.0013 (17)	−0.0003 (16)	0.0059 (18)
C22	0.015 (3)	0.023 (2)	0.025 (2)	−0.001 (2)	0.001 (2)	0.0102 (19)
C23	0.026 (3)	0.024 (2)	0.029 (2)	−0.001 (2)	0.000 (2)	0.0033 (19)
C24	0.030 (3)	0.028 (3)	0.032 (2)	−0.002 (2)	0.002 (2)	0.014 (2)
C25	0.030 (4)	0.038 (3)	0.029 (3)	−0.001 (3)	0.003 (2)	0.020 (2)
C26	0.037 (4)	0.031 (3)	0.025 (2)	−0.005 (2)	0.001 (2)	0.007 (2)
C27	0.016 (4)	0.023 (4)	0.023 (4)	−0.004 (3)	−0.008 (3)	0.004 (3)
C28	0.032 (5)	0.033 (4)	0.032 (4)	−0.002 (4)	−0.003 (4)	0.010 (4)
C29	0.013 (2)	0.019 (2)	0.028 (2)	−0.0015 (18)	0.0010 (19)	0.0119 (19)
C210	0.025 (2)	0.030 (3)	0.027 (3)	0.000 (2)	0.000 (2)	0.010 (2)
C211	0.019 (2)	0.047 (3)	0.044 (3)	0.009 (2)	0.010 (2)	0.018 (3)
C212	0.019 (3)	0.038 (3)	0.038 (3)	−0.002 (2)	−0.006 (2)	0.015 (3)
C213	0.028 (3)	0.036 (3)	0.029 (3)	−0.010 (2)	−0.009 (2)	0.017 (2)
C214	0.023 (3)	0.022 (2)	0.021 (2)	−0.003 (2)	−0.001 (2)	0.0109 (19)
C215	0.031 (3)	0.022 (2)	0.024 (2)	−0.004 (2)	−0.002 (2)	0.0088 (19)
C216	0.025 (3)	0.031 (3)	0.029 (2)	0.000 (2)	0.003 (2)	0.012 (2)
C217	0.013 (2)	0.023 (2)	0.034 (2)	−0.0025 (18)	−0.0033 (19)	0.007 (2)
Pd3	0.01729 (16)	0.01804 (17)	0.01815 (16)	−0.00008 (13)	−0.00123 (12)	0.00586 (13)
Cl3	0.0267 (5)	0.0208 (5)	0.0180 (5)	−0.0008 (5)	−0.0010 (4)	0.0062 (4)
N31	0.023 (2)	0.0207 (19)	0.0174 (17)	0.0014 (15)	−0.0017 (14)	0.0079 (15)
N32	0.0167 (17)	0.0205 (19)	0.0192 (18)	0.0018 (15)	0.0003 (14)	0.0058 (15)
C31	0.008 (2)	0.034 (2)	0.021 (2)	0.0073 (17)	0.0043 (16)	0.0065 (18)
C32	0.020 (2)	0.024 (2)	0.025 (2)	0.0048 (18)	0.0028 (17)	0.0053 (18)
C33	0.033 (3)	0.033 (3)	0.024 (2)	0.005 (2)	0.004 (2)	0.011 (2)
C34	0.031 (3)	0.041 (3)	0.017 (2)	0.006 (2)	0.003 (2)	0.007 (2)
C35	0.014 (3)	0.035 (3)	0.023 (3)	0.009 (2)	0.001 (2)	0.000 (2)
C36	0.017 (3)	0.025 (2)	0.026 (3)	0.006 (2)	0.001 (2)	0.003 (2)
C37	0.025 (5)	0.018 (4)	0.034 (5)	−0.001 (3)	0.010 (4)	0.005 (4)
C38	0.030 (4)	0.030 (4)	0.021 (4)	−0.005 (3)	0.006 (3)	−0.003 (3)
C39	0.020 (2)	0.020 (2)	0.015 (2)	−0.0007 (17)	0.0009 (16)	0.0054 (17)
C310	0.024 (2)	0.032 (3)	0.026 (3)	0.003 (2)	0.003 (2)	0.011 (2)
C311	0.015 (2)	0.033 (3)	0.046 (3)	0.002 (2)	0.004 (2)	0.011 (2)
C312	0.028 (3)	0.038 (3)	0.042 (3)	0.011 (2)	0.002 (2)	0.014 (2)

C313	0.034 (3)	0.022 (2)	0.028 (2)	0.0077 (19)	−0.0001 (19)	0.0089 (18)
C314	0.029 (2)	0.023 (2)	0.0130 (19)	0.0037 (18)	0.0021 (16)	0.0050 (16)
C315	0.036 (3)	0.021 (2)	0.018 (2)	−0.0006 (19)	−0.0001 (18)	0.0057 (17)
C316	0.024 (2)	0.021 (2)	0.022 (2)	−0.0084 (18)	−0.0019 (17)	0.0065 (18)
C317	0.021 (2)	0.026 (2)	0.022 (2)	−0.0002 (19)	−0.0030 (17)	0.0069 (18)
Pd4	0.01798 (17)	0.0236 (2)	0.02035 (17)	−0.00272 (14)	−0.00156 (13)	0.00796 (14)
Cl4	0.0214 (5)	0.0242 (6)	0.0299 (6)	−0.0031 (4)	0.0008 (4)	0.0098 (5)
N41	0.021 (2)	0.026 (2)	0.0175 (18)	−0.0021 (16)	−0.0001 (15)	0.0082 (15)
N42	0.0144 (18)	0.026 (2)	0.0271 (19)	−0.0023 (16)	−0.0025 (15)	0.0115 (17)
C41	0.013 (2)	0.026 (2)	0.023 (2)	0.0013 (17)	−0.0003 (16)	0.0059 (18)
C42	0.015 (3)	0.023 (2)	0.025 (2)	−0.001 (2)	0.001 (2)	0.0102 (19)
C43	0.026 (3)	0.024 (2)	0.029 (2)	−0.001 (2)	0.000 (2)	0.0033 (19)
C44	0.030 (3)	0.028 (3)	0.032 (2)	−0.002 (2)	0.002 (2)	0.014 (2)
C45	0.030 (4)	0.038 (3)	0.029 (3)	−0.001 (3)	0.003 (2)	0.020 (2)
C46	0.037 (4)	0.031 (3)	0.025 (2)	−0.005 (2)	0.001 (2)	0.007 (2)
C47	0.018 (4)	0.015 (3)	0.025 (4)	0.001 (3)	−0.001 (3)	0.005 (3)
C48	0.040 (5)	0.026 (4)	0.027 (4)	0.002 (4)	0.003 (4)	0.011 (3)
C49	0.013 (2)	0.019 (2)	0.028 (2)	−0.0015 (18)	0.0010 (19)	0.0119 (19)
C410	0.025 (2)	0.030 (3)	0.027 (3)	0.000 (2)	0.000 (2)	0.010 (2)
C411	0.019 (2)	0.047 (3)	0.044 (3)	0.009 (2)	0.010 (2)	0.018 (3)
C412	0.019 (3)	0.038 (3)	0.038 (3)	−0.002 (2)	−0.006 (2)	0.015 (3)
C413	0.028 (3)	0.036 (3)	0.029 (3)	−0.010 (2)	−0.009 (2)	0.017 (2)
C414	0.023 (3)	0.022 (2)	0.021 (2)	−0.003 (2)	−0.001 (2)	0.0109 (19)
C415	0.031 (3)	0.022 (2)	0.024 (2)	−0.004 (2)	−0.002 (2)	0.0088 (19)
C416	0.025 (3)	0.031 (3)	0.029 (2)	0.000 (2)	0.003 (2)	0.012 (2)
C417	0.013 (2)	0.023 (2)	0.034 (2)	−0.0025 (18)	−0.0033 (19)	0.007 (2)
O5	0.046 (4)	0.074 (3)	0.041 (3)	0.001 (3)	0.014 (3)	0.031 (2)
C51	0.029 (5)	0.065 (4)	0.042 (3)	0.021 (3)	0.011 (3)	0.031 (3)
C52	0.042 (5)	0.093 (5)	0.040 (4)	0.009 (4)	0.005 (3)	0.032 (3)
C53	0.051 (4)	0.050 (4)	0.061 (4)	0.018 (3)	0.017 (3)	0.031 (3)
O6	0.046 (4)	0.074 (3)	0.041 (3)	0.001 (3)	0.014 (3)	0.031 (2)
C61	0.029 (5)	0.065 (4)	0.042 (3)	0.021 (3)	0.011 (3)	0.031 (3)
C62	0.042 (5)	0.093 (5)	0.040 (4)	0.009 (4)	0.005 (3)	0.032 (3)
C63	0.051 (4)	0.050 (4)	0.061 (4)	0.018 (3)	0.017 (3)	0.031 (3)

Geometric parameters (Å, º)

Pd1—C11	1.981 (9)	C31—C36	1.373 (11)
Pd1—N11	2.027 (7)	C31—C32	1.416 (13)
Pd1—N12	2.055 (7)	C32—C33	1.393 (14)
Pd1—Cl1	2.418 (2)	C32—C37	1.504 (11)
N11—C17	1.528 (12)	C33—C34	1.388 (12)
N11—H11A	0.9200	C33—H33	0.9500
N11—H11B	0.9200	C34—C35	1.358 (13)
N12—C117	1.322 (12)	C34—H34	0.9500
N12—C19	1.362 (12)	C35—C36	1.405 (13)
C11—C16	1.380 (11)	C35—H35	0.9500
C11—C12	1.412 (13)	C36—H36	0.9500
C12—C13	1.364 (14)	C37—C38	1.553 (11)
C12—C17	1.477 (12)	C37—H37	1.0000

C13—C14	1.388 (12)	C38—H38A	0.9800
C13—H13	0.9500	C38—H38B	0.9800
C14—C15	1.391 (13)	C38—H38C	0.9800
C14—H14	0.9500	C39—C310	1.385 (13)
C15—C16	1.405 (13)	C39—C314	1.420 (11)
C15—H15	0.9500	C310—C311	1.382 (14)
C16—H16	0.9500	C310—H310	0.9500
C17—C18	1.488 (11)	C311—C312	1.399 (14)
C17—H17	1.0000	C311—H311	0.9500
C18—H18A	0.9800	C312—C313	1.413 (16)
C18—H18B	0.9800	C312—H312	0.9500
C18—H18C	0.9800	C313—C314	1.409 (14)
C19—C110	1.401 (13)	C313—H313	0.9500
C19—C114	1.404 (12)	C314—C315	1.390 (14)
C110—C111	1.380 (14)	C315—C316	1.372 (14)
C110—H110	0.9500	C315—H315	0.9500
C111—C112	1.396 (14)	C316—C317	1.400 (12)
C111—H111	0.9500	C316—H316	0.9500
C112—C113	1.313 (16)	C317—H317	0.9500
C112—H112	0.9500	Pd4—C41	1.964 (9)
C113—C114	1.424 (14)	Pd4—N41	2.040 (6)
C113—H113	0.9500	Pd4—N42	2.055 (7)
C114—C115	1.413 (14)	Pd4—Cl4	2.429 (2)
C115—C116	1.364 (14)	N41—C47	1.507 (9)
C115—H115	0.9500	N41—H41A	0.9200
C116—C117	1.409 (13)	N41—H41B	0.9200
C116—H116	0.9500	N42—C417	1.296 (12)
C117—H117	0.9500	N42—C49	1.387 (11)
Pd2—C21	2.004 (9)	C41—C42	1.392 (11)
Pd2—N21	2.024 (6)	C41—C46	1.402 (14)
Pd2—N22	2.038 (7)	C42—C43	1.368 (12)
Pd2—Cl2	2.417 (2)	C42—C47	1.516 (12)
N21—C27	1.476 (9)	C43—C44	1.404 (14)
N21—H21A	0.9200	C43—H43	0.9500
N21—H21B	0.9200	C44—C45	1.367 (12)
N22—C217	1.322 (12)	C44—H44	0.9500
N22—C29	1.363 (11)	C45—C46	1.410 (13)
C21—C26	1.370 (14)	C45—H45	0.9500
C21—C22	1.394 (11)	C46—H46	0.9500
C22—C23	1.411 (12)	C47—C48	1.509 (11)
C22—C27	1.494 (12)	C47—H47	1.0000
C23—C24	1.362 (14)	C48—H48A	0.9800
C23—H23	0.9500	C48—H48B	0.9800
C24—C25	1.375 (12)	C48—H48C	0.9800
C24—H24	0.9500	C49—C410	1.385 (13)
C25—C26	1.395 (13)	C49—C414	1.421 (12)
C25—H25	0.9500	C410—C411	1.380 (14)
C26—H26	0.9500	C410—H410	0.9500
C27—C28	1.527 (9)	C411—C412	1.410 (14)

C27—H27	1.0000	C411—H411	0.9500
C28—H28A	0.9800	C412—C413	1.353 (15)
C28—H28B	0.9800	C412—H412	0.9500
C28—H28C	0.9800	C413—C414	1.406 (13)
C29—C210	1.403 (13)	C413—H413	0.9500
C29—C214	1.432 (12)	C414—C415	1.385 (13)
C210—C211	1.385 (14)	C415—C416	1.364 (13)
C210—H210	0.9500	C415—H415	0.9500
C211—C212	1.403 (14)	C416—C417	1.403 (13)
C211—H211	0.9500	C416—H416	0.9500
C212—C213	1.349 (15)	C417—H417	0.9500
C212—H212	0.9500	O5—C51	1.217 (13)
C213—C214	1.424 (13)	C51—C52	1.482 (16)
C213—H213	0.9500	C52—H52A	0.9800
C214—C215	1.390 (13)	C52—H52B	0.9800
C215—C216	1.356 (13)	C52—H52C	0.9800
C215—H215	0.9500	C53—C51	1.546 (15)
C216—C217	1.393 (13)	C53—H53A	0.9800
C216—H216	0.9500	C53—H53B	0.9800
C217—H217	0.9500	C53—H53C	0.9800
Pd3—C31	1.981 (9)	C61—O6	1.203 (13)
Pd3—N32	2.034 (7)	C61—C63	1.462 (15)
Pd3—N31	2.053 (7)	C62—C61	1.489 (16)
Pd3—Cl3	2.394 (2)	C62—H62A	0.9800
N31—C37	1.464 (12)	C62—H62B	0.9800
N31—H31A	0.9200	C62—H62C	0.9800
N31—H31B	0.9200	C63—H63A	0.9800
N32—C317	1.319 (12)	C63—H63B	0.9800
N32—C39	1.408 (11)	C63—H63C	0.9800

C11—Pd1—N11	80.4 (3)	C36—C31—C32	119.1 (9)
C11—Pd1—N12	97.2 (3)	C36—C31—Pd3	128.1 (7)
N11—Pd1—N12	175.9 (4)	C32—C31—Pd3	112.6 (6)
C11—Pd1—Cl1	172.6 (3)	C33—C32—C31	120.7 (8)
N11—Pd1—Cl1	92.5 (2)	C33—C32—C37	122.5 (9)
N12—Pd1—Cl1	90.1 (2)	C31—C32—C37	116.8 (9)
C17—N11—Pd1	108.0 (5)	C34—C33—C32	118.3 (9)
C17—N11—H11A	110.1	C34—C33—H33	120.8
Pd1—N11—H11A	110.1	C32—C33—H33	120.8
C17—N11—H11B	110.1	C35—C34—C33	121.5 (9)
Pd1—N11—H11B	110.1	C35—C34—H34	119.2
H11A—N11—H11B	108.4	C33—C34—H34	119.2
C117—N12—C19	119.0 (8)	C34—C35—C36	120.4 (8)
C117—N12—Pd1	117.9 (6)	C34—C35—H35	119.8
C19—N12—Pd1	122.3 (6)	C36—C35—H35	119.8
C16—C11—C12	118.0 (9)	C31—C36—C35	119.9 (9)
C16—C11—Pd1	128.6 (7)	C31—C36—H36	120.1
C12—C11—Pd1	113.2 (6)	C35—C36—H36	120.1
C13—C12—C11	119.8 (8)	N31—C37—C32	107.5 (7)

C13—C12—C17	124.2 (9)	N31—C37—C38	110.7 (7)
C11—C12—C17	116.0 (8)	C32—C37—C38	110.5 (7)
C12—C13—C14	122.2 (9)	N31—C37—H37	109.4
C12—C13—H13	118.9	C32—C37—H37	109.4
C14—C13—H13	118.9	C38—C37—H37	109.4
C13—C14—C15	118.9 (9)	C37—C38—H38A	109.5
C13—C14—H14	120.5	C37—C38—H38B	109.5
C15—C14—H14	120.5	H38A—C38—H38B	109.5
C14—C15—C16	118.8 (8)	C37—C38—H38C	109.5
C14—C15—H15	120.6	H38A—C38—H38C	109.5
C16—C15—H15	120.6	H38B—C38—H38C	109.5
C11—C16—C15	122.0 (9)	C310—C39—N32	120.2 (8)
C11—C16—H16	119.0	C310—C39—C314	120.0 (9)
C15—C16—H16	119.0	N32—C39—C314	119.8 (8)
C12—C17—C18	121.0 (8)	C311—C310—C39	121.5 (9)
C12—C17—N11	102.8 (8)	C311—C310—H310	119.2
C18—C17—N11	110.6 (7)	C39—C310—H310	119.2
C12—C17—H17	107.2	C310—C311—C312	119.5 (10)
C18—C17—H17	107.2	C310—C311—H311	120.2
N11—C17—H17	107.2	C312—C311—H311	120.2
C17—C18—H18A	109.5	C311—C312—C313	120.2 (10)
C17—C18—H18B	109.5	C311—C312—H312	119.9
H18A—C18—H18B	109.5	C313—C312—H312	119.9
C17—C18—H18C	109.5	C314—C313—C312	119.8 (9)
H18A—C18—H18C	109.5	C314—C313—H313	120.1
H18B—C18—H18C	109.5	C312—C313—H313	120.1
N12—C19—C110	118.7 (8)	C315—C314—C313	121.9 (9)
N12—C19—C114	121.5 (9)	C315—C314—C39	119.2 (9)
C110—C19—C114	119.7 (9)	C313—C314—C39	118.9 (9)
C111—C110—C19	119.1 (9)	C316—C315—C314	119.3 (8)
C111—C110—H110	120.4	C316—C315—H315	120.4
C19—C110—H110	120.4	C314—C315—H315	120.4
C110—C111—C112	120.3 (10)	C315—C316—C317	120.1 (9)
C110—C111—H111	119.9	C315—C316—H316	120.0
C112—C111—H111	119.9	C317—C316—H316	120.0
C113—C112—C111	121.6 (10)	N32—C317—C316	122.6 (9)
C113—C112—H112	119.2	N32—C317—H317	118.7
C111—C112—H112	119.2	C316—C317—H317	118.7
C112—C113—C114	120.5 (9)	C41—Pd4—N41	82.7 (3)
C112—C113—H113	119.7	C41—Pd4—N42	92.8 (3)
C114—C113—H113	119.7	N41—Pd4—N42	173.8 (3)
C19—C114—C115	118.0 (9)	C41—Pd4—Cl4	173.9 (3)
C19—C114—C113	118.7 (9)	N41—Pd4—Cl4	91.2 (2)
C115—C114—C113	123.2 (9)	N42—Pd4—Cl4	93.2 (2)
C116—C115—C114	119.9 (8)	C47—N41—Pd4	113.5 (5)
C116—C115—H115	120.0	C47—N41—H41A	108.9
C114—C115—H115	120.0	Pd4—N41—H41A	108.9
C115—C116—C117	118.3 (9)	C47—N41—H41B	108.9
C115—C116—H116	120.8	Pd4—N41—H41B	108.9

C117—C116—H116	120.8	H41A—N41—H41B	107.7
N12—C117—C116	123.2 (9)	C417—N42—C49	119.5 (8)
N12—C117—H117	118.4	C417—N42—Pd4	118.3 (6)
C116—C117—H117	118.4	C49—N42—Pd4	122.2 (7)
C21—Pd2—N21	81.6 (3)	C42—C41—C46	116.1 (8)
C21—Pd2—N22	92.9 (3)	C42—C41—Pd4	116.1 (7)
N21—Pd2—N22	174.4 (3)	C46—C41—Pd4	127.4 (6)
C21—Pd2—Cl2	173.1 (2)	C43—C42—C41	123.9 (9)
N21—Pd2—Cl2	91.8 (2)	C43—C42—C47	119.0 (8)
N22—Pd2—Cl2	93.7 (2)	C41—C42—C47	117.0 (8)
C27—N21—Pd2	110.3 (5)	C42—C43—C44	118.4 (8)
C27—N21—H21A	109.6	C42—C43—H43	120.8
Pd2—N21—H21A	109.6	C44—C43—H43	120.8
C27—N21—H21B	109.6	C45—C44—C43	120.6 (9)
Pd2—N21—H21B	109.6	C45—C44—H44	119.7
H21A—N21—H21B	108.1	C43—C44—H44	119.7
C217—N22—C29	117.9 (8)	C44—C45—C46	119.5 (10)
C217—N22—Pd2	117.6 (6)	C44—C45—H45	120.3
C29—N22—Pd2	124.4 (7)	C46—C45—H45	120.3
C26—C21—C22	120.3 (9)	C41—C46—C45	121.3 (9)
C26—C21—Pd2	127.4 (6)	C41—C46—H46	119.3
C22—C21—Pd2	112.3 (7)	C45—C46—H46	119.3
C21—C22—C23	118.4 (9)	N41—C47—C48	110.1 (7)
C21—C22—C27	117.0 (8)	N41—C47—C42	108.0 (6)
C23—C22—C27	124.6 (8)	C48—C47—C42	112.4 (6)
C24—C23—C22	121.1 (8)	N41—C47—H47	108.8
C24—C23—H23	119.5	C48—C47—H47	108.8
C22—C23—H23	119.5	C42—C47—H47	108.8
C23—C24—C25	119.6 (9)	C47—C48—H48A	109.5
C23—C24—H24	120.2	C47—C48—H48B	109.5
C25—C24—H24	120.2	H48A—C48—H48B	109.5
C24—C25—C26	120.6 (10)	C47—C48—H48C	109.5
C24—C25—H25	119.7	H48A—C48—H48C	109.5
C26—C25—H25	119.7	H48B—C48—H48C	109.5
C21—C26—C25	119.9 (9)	C410—C49—N42	121.2 (8)
C21—C26—H26	120.0	C410—C49—C414	120.4 (8)
C25—C26—H26	120.0	N42—C49—C414	118.4 (8)
N21—C27—C22	105.8 (7)	C411—C410—C49	119.5 (9)
N21—C27—C28	113.2 (6)	C411—C410—H410	120.2
C22—C27—C28	116.0 (6)	C49—C410—H410	120.2
N21—C27—H27	107.1	C410—C411—C412	120.6 (10)
C22—C27—H27	107.1	C410—C411—H411	119.7
C28—C27—H27	107.1	C412—C411—H411	119.7
C27—C28—H28A	109.5	C413—C412—C411	120.1 (9)
C27—C28—H28B	109.5	C413—C412—H412	120.0
H28A—C28—H28B	109.5	C411—C412—H412	120.0
C27—C28—H28C	109.5	C412—C413—C414	121.0 (9)
H28A—C28—H28C	109.5	C412—C413—H413	119.5
H28B—C28—H28C	109.5	C414—C413—H413	119.5

N22—C29—C210	119.3 (8)	C415—C414—C413	121.5 (8)
N22—C29—C214	121.4 (9)	C415—C414—C49	120.0 (8)
C210—C29—C214	119.3 (8)	C413—C414—C49	118.4 (9)
C211—C210—C29	120.3 (9)	C416—C415—C414	119.8 (9)
C211—C210—H210	119.9	C416—C415—H415	120.1
C29—C210—H210	119.9	C414—C415—H415	120.1
C210—C211—C212	120.0 (10)	C415—C416—C417	117.6 (10)
C210—C211—H211	120.0	C415—C416—H416	121.2
C212—C211—H211	120.0	C417—C416—H416	121.2
C213—C212—C211	121.3 (9)	N42—C417—C416	124.6 (9)
C213—C212—H212	119.3	N42—C417—H417	117.7
C211—C212—H212	119.3	C416—C417—H417	117.7
C212—C213—C214	120.6 (9)	C51—C53—H53A	109.5
C212—C213—H213	119.7	C51—C53—H53B	109.5
C214—C213—H213	119.7	H53A—C53—H53B	109.5
C215—C214—C213	123.2 (8)	C51—C53—H53C	109.5
C215—C214—C29	118.4 (8)	H53A—C53—H53C	109.5
C213—C214—C29	118.4 (9)	H53B—C53—H53C	109.5
C216—C215—C214	118.7 (8)	O5—C51—C52	121.0 (11)
C216—C215—H215	120.7	O5—C51—C53	120.3 (10)
C214—C215—H215	120.7	C52—C51—C53	118.7 (10)
C215—C216—C217	120.4 (10)	C51—C52—H52A	109.5
C215—C216—H216	119.8	C51—C52—H52B	109.5
C217—C216—H216	119.8	H52A—C52—H52B	109.5
N22—C217—C216	123.2 (9)	C51—C52—H52C	109.5
N22—C217—H217	118.4	H52A—C52—H52C	109.5
C216—C217—H217	118.4	H52B—C52—H52C	109.5
C31—Pd3—N32	95.1 (3)	C61—C62—H62A	109.5
C31—Pd3—N31	82.3 (3)	C61—C62—H62B	109.5
N32—Pd3—N31	177.3 (3)	H62A—C62—H62B	109.5
C31—Pd3—Cl3	174.6 (3)	C61—C62—H62C	109.5
N32—Pd3—Cl3	90.0 (2)	H62A—C62—H62C	109.5
N31—Pd3—Cl3	92.6 (2)	H62B—C62—H62C	109.5
C37—N31—Pd3	109.9 (5)	O6—C61—C63	122.0 (10)
C37—N31—H31A	109.7	O6—C61—C62	121.1 (11)
Pd3—N31—H31A	109.7	C63—C61—C62	116.9 (11)
C37—N31—H31B	109.7	C61—C63—H63A	109.5
Pd3—N31—H31B	109.7	C61—C63—H63B	109.5
H31A—N31—H31B	108.2	H63A—C63—H63B	109.5
C317—N32—C39	119.0 (8)	C61—C63—H63C	109.5
C317—N32—Pd3	119.1 (6)	H63A—C63—H63C	109.5
C39—N32—Pd3	121.5 (6)	H63B—C63—H63C	109.5
C11—Pd1—N11—C17	−35.4 (6)	C31—Pd3—N31—C37	27.7 (6)
Cl1—Pd1—N11—C17	146.6 (5)	Cl3—Pd3—N31—C37	−153.8 (5)
C11—Pd1—N12—C117	−107.4 (7)	C31—Pd3—N32—C317	105.8 (7)
Cl1—Pd1—N12—C117	71.0 (6)	Cl3—Pd3—N32—C317	−72.7 (7)
C11—Pd1—N12—C19	83.5 (7)	C31—Pd3—N32—C39	−81.3 (7)
Cl1—Pd1—N12—C19	−98.1 (7)	Cl3—Pd3—N32—C39	100.2 (6)

N11—Pd1—C11—C16	−158.4 (9)	N32—Pd3—C31—C36	−18.3 (9)
N12—Pd1—C11—C16	24.9 (8)	N31—Pd3—C31—C36	161.1 (9)
N11—Pd1—C11—C12	15.5 (7)	N32—Pd3—C31—C32	167.5 (7)
N12—Pd1—C11—C12	−161.2 (7)	N31—Pd3—C31—C32	−13.1 (7)
C16—C11—C12—C13	5.1 (14)	C36—C31—C32—C33	2.0 (14)
Pd1—C11—C12—C13	−169.5 (8)	Pd3—C31—C32—C33	176.7 (8)
C16—C11—C12—C17	−176.6 (9)	C36—C31—C32—C37	−178.4 (8)
Pd1—C11—C12—C17	8.9 (11)	Pd3—C31—C32—C37	−3.6 (10)
C11—C12—C13—C14	−4.0 (16)	C31—C32—C33—C34	−4.2 (15)
C17—C12—C13—C14	177.7 (10)	C37—C32—C33—C34	176.3 (9)
C12—C13—C14—C15	0.6 (15)	C32—C33—C34—C35	3.5 (15)
C13—C14—C15—C16	1.6 (14)	C33—C34—C35—C36	−0.7 (14)
C12—C11—C16—C15	−2.9 (13)	C32—C31—C36—C35	1.0 (13)
Pd1—C11—C16—C15	170.7 (7)	Pd3—C31—C36—C35	−172.9 (7)
C14—C15—C16—C11	−0.4 (13)	C34—C35—C36—C31	−1.6 (13)
C13—C12—C17—C18	18.3 (15)	Pd3—N31—C37—C32	−34.9 (8)
C11—C12—C17—C18	−160.0 (9)	Pd3—N31—C37—C38	85.9 (6)
C13—C12—C17—N11	142.2 (10)	C33—C32—C37—N31	−154.5 (9)
C11—C12—C17—N11	−36.0 (10)	C31—C32—C37—N31	25.9 (11)
Pd1—N11—C17—C12	46.4 (7)	C33—C32—C37—C38	84.6 (11)
Pd1—N11—C17—C18	176.9 (6)	C31—C32—C37—C38	−95.0 (10)
C117—N12—C19—C110	−178.7 (8)	C317—N32—C39—C310	179.1 (8)
Pd1—N12—C19—C110	−9.7 (11)	Pd3—N32—C39—C310	6.2 (11)
C117—N12—C19—C114	−1.6 (12)	C317—N32—C39—C314	0.0 (12)
Pd1—N12—C19—C114	167.4 (6)	Pd3—N32—C39—C314	−172.9 (6)
N12—C19—C110—C111	175.1 (9)	N32—C39—C310—C311	−176.6 (9)
C114—C19—C110—C111	−2.0 (13)	C314—C39—C310—C311	2.4 (14)
C19—C110—C111—C112	0.6 (15)	C39—C310—C311—C312	0.5 (16)
C110—C111—C112—C113	1.1 (17)	C310—C311—C312—C313	−3.2 (17)
C111—C112—C113—C114	−1.2 (17)	C311—C312—C313—C314	2.9 (16)
N12—C19—C114—C115	2.2 (12)	C312—C313—C314—C315	176.9 (9)
C110—C19—C114—C115	179.3 (8)	C312—C313—C314—C39	0.0 (14)
N12—C19—C114—C113	−175.2 (8)	C310—C39—C314—C315	−179.6 (8)
C110—C19—C114—C113	1.8 (13)	N32—C39—C314—C315	−0.6 (12)
C112—C113—C114—C19	−0.2 (15)	C310—C39—C314—C313	−2.6 (13)
C112—C113—C114—C115	−177.5 (10)	N32—C39—C314—C313	176.4 (8)
C19—C114—C115—C116	−1.4 (13)	C313—C314—C315—C316	−177.6 (9)
C113—C114—C115—C116	175.8 (9)	C39—C314—C315—C316	−0.7 (13)
C114—C115—C116—C117	0.1 (13)	C314—C315—C316—C317	2.4 (14)
C19—N12—C117—C116	0.2 (13)	C39—N32—C317—C316	1.8 (13)
Pd1—N12—C117—C116	−169.3 (7)	Pd3—N32—C317—C316	174.8 (7)
C115—C116—C117—N12	0.6 (14)	C315—C316—C317—N32	−3.0 (14)
C21—Pd2—N21—C27	−28.8 (6)	C41—Pd4—N41—C47	11.7 (6)
Cl2—Pd2—N21—C27	153.0 (5)	Cl4—Pd4—N41—C47	−168.6 (6)
C21—Pd2—N22—C217	−83.4 (7)	C41—Pd4—N42—C417	84.2 (7)
N21—Pd2—N22—C217	−76 (3)	Cl4—Pd4—N42—C417	−95.0 (7)
Cl2—Pd2—N22—C217	94.6 (7)	C41—Pd4—N42—C49	−95.4 (7)
C21—Pd2—N22—C29	96.0 (8)	Cl4—Pd4—N42—C49	85.4 (6)
Cl2—Pd2—N22—C29	−86.0 (7)	N41—Pd4—C41—C42	−2.9 (7)

N21—Pd2—C21—C26	−166.7 (10)	N42—Pd4—C41—C42	−178.5 (7)
N22—Pd2—C21—C26	12.6 (9)	N41—Pd4—C41—C46	170.3 (10)
N21—Pd2—C21—C22	11.6 (7)	N42—Pd4—C41—C46	−5.4 (10)
N22—Pd2—C21—C22	−169.1 (7)	C46—C41—C42—C43	3.3 (15)
C26—C21—C22—C23	4.9 (14)	Pd4—C41—C42—C43	177.2 (8)
Pd2—C21—C22—C23	−173.5 (7)	C46—C41—C42—C47	179.4 (8)
C26—C21—C22—C27	−173.5 (9)	Pd4—C41—C42—C47	−6.7 (11)
Pd2—C21—C22—C27	8.1 (10)	C41—C42—C43—C44	−0.9 (15)
C21—C22—C23—C24	−3.5 (15)	C47—C42—C43—C44	−177.0 (8)
C27—C22—C23—C24	174.7 (9)	C42—C43—C44—C45	0.2 (15)
C22—C23—C24—C25	1.2 (15)	C43—C44—C45—C46	−1.9 (16)
C23—C24—C25—C26	−0.3 (15)	C42—C41—C46—C45	−4.9 (15)
C22—C21—C26—C25	−4.0 (15)	Pd4—C41—C46—C45	−178.1 (8)
Pd2—C21—C26—C25	174.2 (7)	C44—C45—C46—C41	4.4 (16)
C24—C25—C26—C21	1.7 (16)	Pd4—N41—C47—C48	105.9 (6)
Pd2—N21—C27—C22	38.4 (7)	Pd4—N41—C47—C42	−17.2 (8)
Pd2—N21—C27—C28	166.6 (6)	C43—C42—C47—N41	−168.2 (8)
C21—C22—C27—N21	−30.6 (10)	C41—C42—C47—N41	15.5 (10)
C23—C22—C27—N21	151.1 (8)	C43—C42—C47—C48	70.2 (10)
C21—C22—C27—C28	−157.1 (8)	C41—C42—C47—C48	−106.1 (9)
C23—C22—C27—C28	24.6 (12)	C417—N42—C49—C410	−179.7 (9)
C217—N22—C29—C210	179.8 (8)	Pd4—N42—C49—C410	−0.1 (11)
Pd2—N22—C29—C210	0.5 (12)	C417—N42—C49—C414	−0.5 (12)
C217—N22—C29—C214	0.2 (13)	Pd4—N42—C49—C414	179.1 (6)
Pd2—N22—C29—C214	−179.2 (6)	N42—C49—C410—C411	−179.8 (9)
N22—C29—C210—C211	179.1 (9)	C414—C49—C410—C411	0.9 (14)
C214—C29—C210—C211	−1.2 (14)	C49—C410—C411—C412	−1.2 (15)
C29—C210—C211—C212	0.4 (15)	C410—C411—C412—C413	1.9 (16)
C210—C211—C212—C213	0.9 (16)	C411—C412—C413—C414	−2.3 (15)
C211—C212—C213—C214	−1.4 (15)	C412—C413—C414—C415	−179.6 (9)
C212—C213—C214—C215	−178.2 (9)	C412—C413—C414—C49	2.0 (14)
C212—C213—C214—C29	0.6 (14)	C410—C49—C414—C415	−179.7 (8)
N22—C29—C214—C215	−0.8 (13)	N42—C49—C414—C415	1.0 (12)
C210—C29—C214—C215	179.6 (8)	C410—C49—C414—C413	−1.3 (13)
N22—C29—C214—C213	−179.6 (8)	N42—C49—C414—C413	179.4 (8)
C210—C29—C214—C213	0.7 (13)	C413—C414—C415—C416	−179.7 (9)
C213—C214—C215—C216	−179.3 (9)	C49—C414—C415—C416	−1.4 (13)
C29—C214—C215—C216	1.9 (13)	C414—C415—C416—C417	1.2 (14)
C214—C215—C216—C217	−2.4 (14)	C49—N42—C417—C416	0.3 (14)
C29—N22—C217—C216	−0.7 (14)	Pd4—N42—C417—C416	−179.3 (7)
Pd2—N22—C217—C216	178.7 (7)	C415—C416—C417—N42	−0.7 (15)
C215—C216—C217—N22	1.9 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11—H11*B*···Cl3	0.92	2.41	3.241 (7)	151
N21—H21*A*···Cl3	0.92	2.47	3.379 (9)	171
N21—H21*B*···O6	0.92	2.20	2.983 (10)	143
N31—H31*A*···Cl1	0.92	2.45	3.301 (7)	154

N41—H41*A*···O5	0.92	2.18	3.056 (10)	160
N41—H41*B*···Cl1	0.92	2.40	3.310 (9)	171