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Bis[(1*RS*,2*RS*)-4,4′-(1-azaniumyl-2-hydroxyethane-1,2-diyl)dipyridinium] tris[tetrachloridopalladate(II)]

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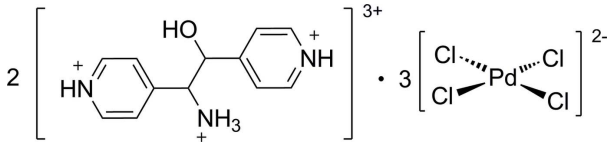
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.007 Å; R factor = 0.032; wR factor = 0.077; data-to-parameter ratio = 13.5.

The asymmetric unit of the title compound, $(C_{12}H_{16}N_3O)_2[PdCl_4]_3$, consists of a 4,4′-(1-azaniumyl-2-hydroxyethane-1,2-diyl)dipyridinium dication and one and a half tetrachloridopalladate(II) anions; the latter has inversion symmetry. In the cation, the pyridinium rings attached to the central 1-azaniumyl-2-hydroxyethane fragment show an *anti* conformation, as indicated by the central C—C—C—C torsion angle of −178.1 (4)°, and they are inclined to one another by 25.7 (2)°. In the crystal, the cations and anions are linked through N—H···Cl and O—H···Cl hydrogen bonds. There are also π–π contacts [centroid–centroid distance = 3.788 (3) Å] and a number of C—H···O and C—H···Cl interactions are present, consolidating the formation of a three-dimensional structure.

Related literature

For potential applications of organic–inorganic hybrid materials with magnetic, optical and electrical properties, see: Yao *et al.* (2010); Sanchez *et al.* (2011); Pardo *et al.* (2011). For related tetrachloridopalladate(II) compounds, see: Kumar *et al.* (2006); Adams *et al.* (2005, 2006); Maris (2008). For the synthesis of the ligand, see: Campos-Gaxiola *et al.* (2012).



Experimental

Crystal data

$(C_{12}H_{16}N_3O)_2[PdCl_4]_3$
M_r = 1181.161
Triclinic, $P\overline{1}$
a = 7.6970 (7) Å
b = 7.7339 (7) Å
c = 15.7254 (13) Å
α = 84.541 (2)°
β = 81.314 (2)°
γ = 78.717 (1)°
V = 905.40 (14) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 2.40 mm^{-1}
T = 100 K
0.29 × 0.22 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.543, T_{max} = 0.686
5043 measured reflections
3143 independent reflections
2927 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.077
S = 1.07
3143 reflections
232 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1′···Cl5	0.84 (4)	2.22 (4)	3.047 (3)	168 (4)
N1—H1A···Cl3^{i}	0.86 (3)	2.62 (2)	3.355 (4)	145 (4)
N1—H1A···Cl4^{i}	0.86 (3)	2.54 (4)	3.203 (4)	135 (4)
N1—H1B···Cl6^{ii}	0.86 (4)	2.49 (5)	3.310 (4)	160 (4)
N1—H1C···Cl1^{ii}	0.86 (2)	2.22 (2)	3.080 (3)	177 (6)
N2—H2′···Cl2^{iii}	0.84 (4)	2.35 (4)	3.137 (4)	157 (4)
N3—H3′···Cl5^{iv}	0.84 (4)	2.44 (4)	3.150 (4)	143 (4)
N3—H3′···Cl6^{iv}	0.84 (4)	2.71 (5)	3.353 (4)	135 (3)
C4—H4···Cl5^{v}	0.95	2.64	3.406 (5)	139
C6—H6···O1^{vi}	0.95	2.54	3.454 (6)	161
C9—H9···Cl3^{ii}	0.95	2.78	3.599 (5)	145
C10—H10···Cl2^{vii}	0.95	2.75	3.649 (5)	159
C11—H11···Cl1	0.95	2.61	3.486 (5)	154
C11—H11···Cl1^{viii}	0.95	2.80	3.422 (5)	124

Symmetry codes: (i) $x-1, y+1, z$; (ii) $x-1, y, z$; (iii) $x, y-1, z$; (iv) $-x, -y+2, -z$; (v) $-x, -y+1, -z$; (vi) $x, y+1, z$; (vii) $-x, -y+1, -z+1$; (viii) $-x+1, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2540).

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supporting information

Acta Cryst. (2013). E**69**, m65–m66 [https://doi.org/10.1107/S1600536812050817]

Bis[(1*RS*,2*RS*)-4,4′-(1-azaniumyl-2-hydroxyethane-1,2-diyl)dipyridinium] tris-[tetrachloridopalladate(II)]

Jose J. Campos-Gaxiola, Alberto Baez-Castro, Adriana Cruz-Enriquez, Herbert Hopfl and Miguel Parra-Hake

S1. Comment

Hydrogen bond based organic–inorganic hybrid materials are receiving continuous interest because of their structural, magnetic, optical and electrical properties (Yao *et al.*, 2010; Sanchez *et al.*, 2011; Pardo *et al.*, 2011). An interesting approach for the preparation of such materials consists in the utilization of supramolecular synthons containing charge-assisted N^+–H···Cl^- hydrogen bonds, through which organic cations and anionic metal complexes are linked to form crystalline organic–inorganic hybrid solids (Kumar *et al.*, 2006; Adams *et al.*, 2005,2006; Maris, 2008). As a further contribution we report herein on the crystal structure of the title compound.

The asymmetric unit of the title compound consists of one threefold charged organic cation in a general position and two independent $[PdCl_4]^{2-}$ dianions, one of which is located on a crystallographic inversion center (Fig. 1). In the cation, the pyridinium rings attached to the central 2-ammoniumethanol fragment show an *anti* conformation, as indicated by the C8—C1—C2—C3 torsion angle of -178.1 (4)°, and form a dihedral angle of 25.7 (2)°. The Pd atoms have square-planar coordination environments with Pd—Cl distances ranging from 2.2760 (10) to 2.3056 (11) Å.

In the crystal, the cations and anions are linked by N^+—H···Cl^- and O—H···Cl^- hydrogen bonds (Table 1 and Fig. 2). There are π—π interactions present involving inversion related pyridinium rings [Cg···Cg^i distance = 3.788 (3) Å; Cg centroid of the N3,C3-C7 ring; symmetry code (i) -x, -y+2, -z]. There are also a number of C-H···O and C-H···Cl interactions present, consolidating the formation of a three-dimensional structure (Table 1 and Fig. 2).

S2. Experimental

The organic entities in the title compound are the product of partial hydrolysis starting from 2,4,5-tris(pyridin-4-yl)-4,5-dihydro-1,3-oxazole, which was synthesized according to a previously reported procedure (Campos-Gaxiola *et al.*, 2012). For the preparation of the palladium complex, a solution of 2,4,5-tris(pyridin-4-yl)-4,5-dihydro-1,3-oxazole (0.05 g, 0.16 mmol) in methanol and concentrated HCl (37%, 3 ml) was added dropwise to a stirring solution of potassium tetrachloridopalladate (0.05 g, 0.16 mmol) in water (5 ml). The resulting yellow solution was stirred for 30 min at 333 K, whereupon the solution was left to evaporate slowly at room temperature. After two weeks, red crystals were isolated [Yield: 30%]. Spectroscopic and TGA data for the title compound are available in the archived CIF.

S3. Refinement

C bound H atoms were positioned geometrically and constrained using the riding-model approximation [aryl C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C)]. The N—H and O—H hydrogen atoms were located in difference Fourier maps and were refined with distance restraints: N-H = 0.86 (1) for NH_3^+ H atoms and 0.84 (1) Å for O—H and pyN-H^+ H atoms, with U_{iso}(H) = 1.2U_{eq}(O,N).

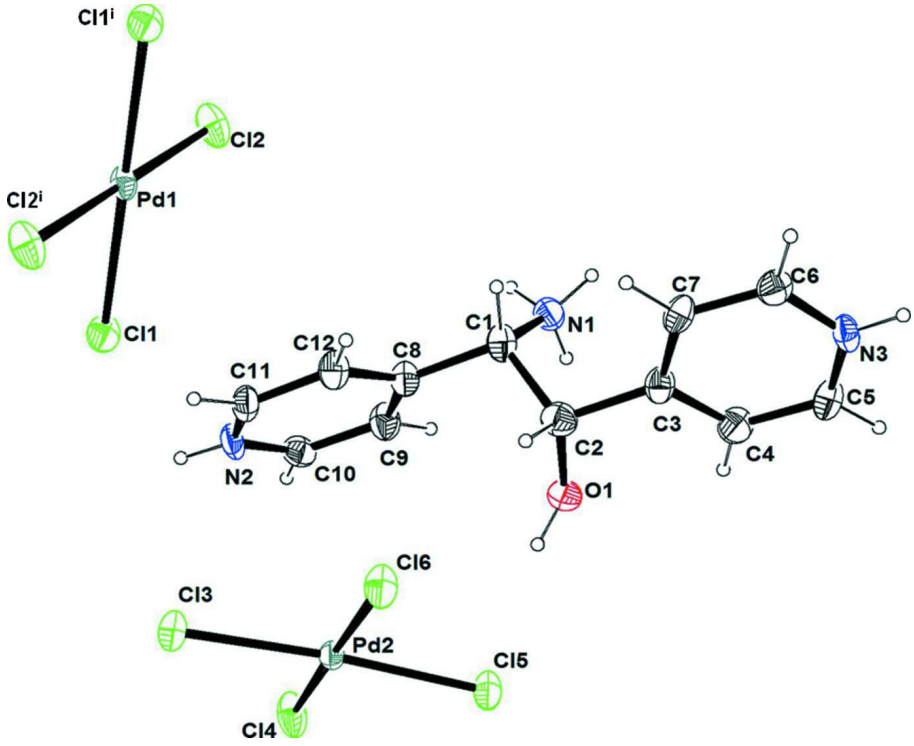

Figure 1

The molecular structure of the asymmetric unit of the title compound, with the atom-labelling. Displacement ellipsoids are drawn at the 50% probability level. [symmetry code: (i) -*x* + 1, -*y* + 2, -*z* + 1].

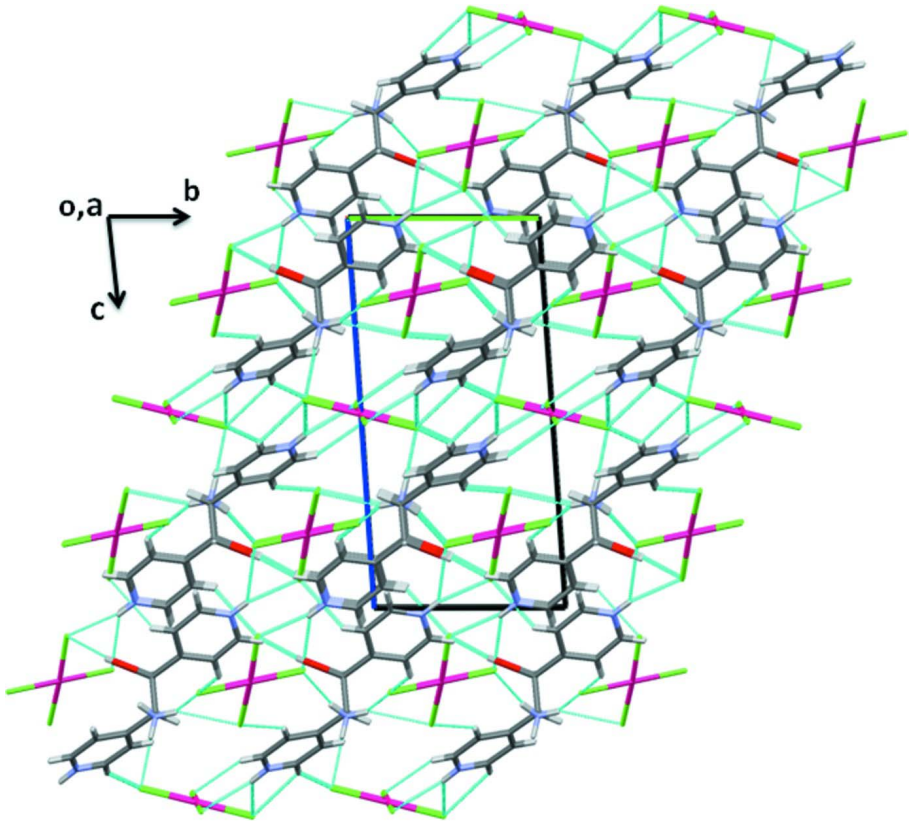

Figure 2

A view along the a axis of the crystal packing of the title compound, with the hydrogen bonds shown as dashed lines (see Table 1 for details).

Bis[(1*RS*,2*RS*)-4,4′-(1-azaniumyl-2-hydroxyethane-1,2- diyl)dipyridinium] tris[tetrachloridopalladate(II)]

Crystal data

$(C_{12}H_{16}N_3O)_2[PdCl_4]_3$
M_r = 1181.16
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.6970 (7) Å
b = 7.7339 (7) Å
c = 15.7254 (13) Å
α = 84.541 (2)°
β = 81.314 (2)°
γ = 78.717 (1)°
V = 905.40 (14) Å^3
Z = 1
$F(000)$ = 576
D_x = 2.166 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3544 reflections
θ = 2.7–28.2°
μ = 2.40 mm^{-1}
T = 100 K
Rectangular prism, red
0.29 × 0.22 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.543, T_{max} = 0.686
5043 measured reflections
3143 independent reflections
2927 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 25.0°, θ_{min} = 1.3°
h = −9→7
k = −9→9
l = −16→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.077$
$S = 1.07$
3143 reflections
232 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0322P)^2 + 2.1607P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.23$ e Å^{-3}
$\Delta\rho_{min} = -0.48$ e Å^{-3}

Special details

Experimental. Spectroscopic and TGA data for the title compound: IR(KBr, cm^{-1}): 3440, 3211, 3064, 2937, 2888, 1669, 1630, 1509, 1421, 1358, 1294, 999, 832. TGA: Calcd. for HCl: 3.08. Found: 3.26% (303–448 K); Calcd. for $PdCl_2$: 15.49. Found: 15.85% (448–523 K).

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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}
O1	−0.0806 (4)	0.6561 (4)	0.14345 (19)	0.0254 (10)
N1	−0.3332 (5)	0.8197 (5)	0.2757 (2)	0.0243 (12)
N2	0.1298 (5)	0.3847 (5)	0.4127 (2)	0.0229 (11)
N3	−0.2750 (5)	1.2478 (5)	0.0153 (2)	0.0209 (11)
C1	−0.1380 (6)	0.8184 (6)	0.2689 (3)	0.0240 (12)
C2	−0.0541 (6)	0.8136 (6)	0.1750 (3)	0.0255 (12)
C3	−0.1379 (6)	0.9732 (6)	0.1205 (3)	0.0221 (12)
C4	−0.2352 (6)	0.9472 (6)	0.0571 (3)	0.0269 (14)
C5	−0.3016 (6)	1.0887 (6)	0.0040 (3)	0.0250 (12)
C6	−0.1864 (6)	1.2805 (6)	0.0775 (3)	0.0239 (12)
C7	−0.1160 (6)	1.1430 (6)	0.1307 (3)	0.0219 (12)
C8	−0.0458 (6)	0.6609 (6)	0.3204 (3)	0.0229 (12)
C9	−0.1047 (6)	0.5003 (6)	0.3334 (3)	0.0259 (12)
C10	−0.0142 (6)	0.3628 (6)	0.3807 (3)	0.0233 (12)
C11	0.1937 (6)	0.5346 (6)	0.4001 (3)	0.0226 (12)
C12	0.1067 (6)	0.6767 (6)	0.3539 (3)	0.0234 (12)
Pd1	0.50000	1.00000	0.50000	0.0165 (1)
Cl1	0.53138 (14)	0.71363 (13)	0.46422 (7)	0.0220 (3)
Cl2	0.19678 (14)	1.02190 (13)	0.52122 (7)	0.0250 (3)
Pd2	0.39126 (4)	0.32273 (4)	0.19078 (2)	0.0158 (1)
Cl3	0.56147 (14)	0.25575 (14)	0.30002 (7)	0.0247 (3)
Cl4	0.30607 (16)	0.05224 (14)	0.21810 (8)	0.0300 (3)

Cl5	0.23446 (15)	0.37787 (13)	0.07476 (7)	0.0241 (3)
Cl6	0.46316 (15)	0.60016 (13)	0.16265 (7)	0.0261 (3)
H1	−0.12040	0.92890	0.29190	0.0290*
H1′	0.014 (4)	0.584 (5)	0.130 (3)	0.0380*
H1A	−0.391 (6)	0.924 (3)	0.265 (3)	0.0360*
H1B	−0.361 (7)	0.742 (5)	0.247 (3)	0.0360*
H1C	−0.374 (7)	0.788 (7)	0.3275 (12)	0.0360*
H2	0.07710	0.81200	0.17130	0.0300*
H2′	0.175 (6)	0.299 (4)	0.444 (3)	0.0350*
H3′	−0.309 (6)	1.338 (4)	−0.016 (3)	0.0310*
H4	−0.25600	0.83250	0.05030	0.0320*
H5	−0.36640	1.07190	−0.04050	0.0300*
H6	−0.17290	1.39760	0.08450	0.0290*
H7	−0.05210	1.16390	0.17470	0.0260*
H9	−0.20700	0.48570	0.30960	0.0310*
H10	−0.05410	0.25300	0.39050	0.0280*
H11	0.29880	0.54330	0.42300	0.0280*
H12	0.15060	0.78450	0.34500	0.0280*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0310 (18)	0.0191 (15)	0.0257 (17)	−0.0019 (13)	−0.0048 (14)	−0.0037 (13)
N1	0.023 (2)	0.025 (2)	0.022 (2)	0.0003 (16)	−0.0014 (16)	0.0011 (16)
N2	0.022 (2)	0.0226 (19)	0.0203 (19)	0.0029 (15)	−0.0056 (15)	0.0074 (15)
N3	0.0170 (18)	0.0227 (19)	0.0197 (19)	−0.0009 (15)	−0.0016 (15)	0.0078 (15)
C1	0.022 (2)	0.026 (2)	0.025 (2)	−0.0060 (18)	−0.0078 (18)	0.0033 (19)
C2	0.022 (2)	0.026 (2)	0.028 (2)	−0.0038 (18)	−0.0023 (19)	−0.0030 (19)
C3	0.022 (2)	0.025 (2)	0.019 (2)	−0.0064 (18)	−0.0026 (18)	0.0042 (18)
C4	0.036 (3)	0.021 (2)	0.025 (2)	−0.009 (2)	−0.005 (2)	0.0004 (18)
C5	0.026 (2)	0.032 (2)	0.020 (2)	−0.011 (2)	−0.0088 (19)	0.0037 (19)
C6	0.029 (2)	0.022 (2)	0.021 (2)	−0.0080 (19)	−0.0011 (19)	0.0007 (18)
C7	0.022 (2)	0.029 (2)	0.018 (2)	−0.0110 (18)	−0.0060 (17)	0.0006 (18)
C8	0.024 (2)	0.023 (2)	0.022 (2)	−0.0039 (18)	−0.0070 (18)	0.0019 (18)
C9	0.029 (2)	0.023 (2)	0.028 (2)	−0.0077 (19)	−0.010 (2)	0.0029 (19)
C10	0.025 (2)	0.018 (2)	0.026 (2)	−0.0040 (18)	−0.0014 (19)	−0.0009 (18)
C11	0.018 (2)	0.030 (2)	0.019 (2)	−0.0020 (18)	−0.0055 (18)	0.0026 (18)
C12	0.022 (2)	0.026 (2)	0.023 (2)	−0.0082 (18)	−0.0049 (18)	0.0052 (18)
Pd1	0.0180 (2)	0.0144 (2)	0.0185 (2)	−0.0050 (2)	−0.0073 (2)	0.0038 (2)
Cl1	0.0290 (6)	0.0162 (5)	0.0224 (5)	−0.0075 (4)	−0.0071 (4)	0.0026 (4)
Cl2	0.0193 (5)	0.0206 (5)	0.0357 (6)	−0.0063 (4)	−0.0081 (4)	0.0079 (4)
Pd2	0.0177 (2)	0.0147 (2)	0.0151 (2)	−0.0023 (1)	−0.0044 (1)	0.0000 (1)
Cl3	0.0261 (6)	0.0283 (5)	0.0216 (5)	−0.0071 (4)	−0.0102 (4)	0.0034 (4)
Cl4	0.0375 (6)	0.0182 (5)	0.0389 (7)	−0.0095 (5)	−0.0204 (5)	0.0085 (5)
Cl5	0.0303 (6)	0.0203 (5)	0.0245 (5)	−0.0067 (4)	−0.0132 (4)	0.0031 (4)
Cl6	0.0338 (6)	0.0204 (5)	0.0286 (6)	−0.0114 (4)	−0.0137 (5)	0.0039 (4)

Geometric parameters (Å, º)

Pd1—Cl2	2.2821 (11)	C1—C8	1.514 (7)
Pd1—Cl1^{i}	2.2950 (10)	C2—C3	1.526 (7)
Pd1—Cl1	2.2950 (10)	C3—C4	1.385 (7)
Pd1—Cl2^{i}	2.2821 (11)	C3—C7	1.383 (6)
Pd2—Cl4	2.2960 (12)	C4—C5	1.376 (7)
Pd2—Cl5	2.2985 (12)	C6—C7	1.366 (7)
Pd2—Cl3	2.2760 (12)	C8—C9	1.391 (7)
Pd2—Cl6	2.3056 (11)	C8—C12	1.388 (7)
O1—C2	1.419 (6)	C9—C10	1.373 (7)
O1—H1′	0.84 (4)	C11—C12	1.375 (7)
N1—C1	1.488 (6)	C1—H1	1.0000
N2—C10	1.330 (6)	C2—H2	1.0000
N2—C11	1.332 (6)	C4—H4	0.9500
N3—C5	1.319 (6)	C5—H5	0.9500
N3—C6	1.342 (6)	C6—H6	0.9500
N1—H1C	0.86 (2)	C7—H7	0.9500
N1—H1A	0.86 (3)	C9—H9	0.9500
N1—H1B	0.86 (4)	C10—H10	0.9500
N2—H2′	0.84 (4)	C11—H11	0.9500
N3—H3′	0.84 (4)	C12—H12	0.9500
C1—C2	1.521 (7)		
Cl1^{i}—Pd1—Cl2^{i}	89.74 (4)	C3—C4—C5	119.5 (4)
Cl1—Pd1—Cl2^{i}	90.26 (4)	N3—C5—C4	119.6 (4)
Cl1—Pd1—Cl2	89.74 (4)	N3—C6—C7	119.1 (4)
Cl1—Pd1—Cl1^{i}	180.00	C3—C7—C6	120.0 (4)
Cl1^{i}—Pd1—Cl2	90.26 (4)	C1—C8—C9	122.8 (4)
Cl2—Pd1—Cl2^{i}	180.00	C9—C8—C12	118.9 (4)
Cl4—Pd2—Cl5	89.59 (4)	C1—C8—C12	118.3 (4)
Cl3—Pd2—Cl6	92.45 (4)	C8—C9—C10	119.6 (4)
Cl3—Pd2—Cl4	89.51 (4)	N2—C10—C9	119.4 (4)
Cl4—Pd2—Cl6	177.33 (4)	N2—C11—C12	119.7 (4)
Cl5—Pd2—Cl6	88.58 (4)	C8—C12—C11	119.3 (4)
Cl3—Pd2—Cl5	176.06 (4)	C8—C1—H1	109.00
C2—O1—H1′	114 (3)	N1—C1—H1	109.00
C10—N2—C11	123.0 (4)	C2—C1—H1	109.00
C5—N3—C6	123.1 (4)	C3—C2—H2	109.00
C1—N1—H1C	110 (4)	C1—C2—H2	109.00
C1—N1—H1A	111 (3)	O1—C2—H2	109.00
H1A—N1—H1B	113 (4)	C3—C4—H4	120.00
C1—N1—H1B	115 (4)	C5—C4—H4	120.00
H1B—N1—H1C	102 (5)	N3—C5—H5	120.00
H1A—N1—H1C	106 (5)	C4—C5—H5	120.00
C10—N2—H2′	115 (3)	C7—C6—H6	120.00
C11—N2—H2′	122 (3)	N3—C6—H6	121.00
C6—N3—H3′	113 (3)	C3—C7—H7	120.00

C5—N3—H3′	124 (3)	C6—C7—H7	120.00
N1—C1—C8	111.3 (4)	C8—C9—H9	120.00
C2—C1—C8	109.4 (4)	C10—C9—H9	120.00
N1—C1—C2	110.0 (4)	N2—C10—H10	120.00
O1—C2—C3	109.6 (4)	C9—C10—H10	120.00
O1—C2—C1	107.9 (4)	N2—C11—H11	120.00
C1—C2—C3	111.6 (4)	C12—C11—H11	120.00
C2—C3—C7	122.2 (4)	C11—C12—H12	120.00
C4—C3—C7	118.7 (4)	C8—C12—H12	120.00
C2—C3—C4	119.1 (4)		

C11—N2—C10—C9	−1.0 (7)	C1—C2—C3—C4	−114.2 (5)
C10—N2—C11—C12	1.7 (7)	C1—C2—C3—C7	67.6 (6)
C6—N3—C5—C4	−0.7 (7)	C2—C3—C4—C5	−175.9 (4)
C5—N3—C6—C7	1.7 (7)	C7—C3—C4—C5	2.4 (7)
N1—C1—C2—O1	−61.0 (5)	C2—C3—C7—C6	176.8 (4)
N1—C1—C2—C3	59.5 (5)	C4—C3—C7—C6	−1.4 (7)
C8—C1—C2—O1	61.5 (5)	C3—C4—C5—N3	−1.4 (7)
C8—C1—C2—C3	−178.1 (4)	N3—C6—C7—C3	−0.6 (7)
N1—C1—C8—C9	30.7 (6)	C1—C8—C9—C10	179.9 (4)
N1—C1—C8—C12	−151.1 (4)	C12—C8—C9—C10	1.7 (7)
C2—C1—C8—C9	−91.0 (5)	C1—C8—C12—C11	−179.3 (4)
C2—C1—C8—C12	87.2 (5)	C9—C8—C12—C11	−1.0 (7)
O1—C2—C3—C4	5.3 (6)	C8—C9—C10—N2	−0.7 (7)
O1—C2—C3—C7	−172.9 (4)	N2—C11—C12—C8	−0.6 (7)

Symmetry code: (i) −*x*+1, −*y*+2, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1′···Cl5	0.84 (4)	2.22 (4)	3.047 (3)	168 (4)
N1—H1*A*···Cl3^{ii}	0.86 (3)	2.62 (2)	3.355 (4)	145 (4)
N1—H1*A*···Cl4^{ii}	0.86 (3)	2.54 (4)	3.203 (4)	135 (4)
N1—H1*B*···Cl6^{iii}	0.86 (4)	2.49 (5)	3.310 (4)	160 (4)
N1—H1*C*···Cl1^{iii}	0.86 (2)	2.22 (2)	3.080 (3)	177 (6)
N2—H2′···Cl2^{iv}	0.84 (4)	2.35 (4)	3.137 (4)	157 (4)
N3—H3′···Cl5^{v}	0.84 (4)	2.44 (4)	3.150 (4)	143 (4)
N3—H3′···Cl6^{v}	0.84 (4)	2.71 (5)	3.353 (4)	135 (3)
C4—H4···Cl5^{vi}	0.95	2.64	3.406 (5)	139
C6—H6···O1^{vii}	0.95	2.54	3.454 (6)	161
C9—H9···Cl3^{iii}	0.95	2.78	3.599 (5)	145
C10—H10···Cl2^{viii}	0.95	2.75	3.649 (5)	159
C11—H11···Cl1	0.95	2.61	3.486 (5)	154
C11—H11···Cl1^{ix}	0.95	2.80	3.422 (5)	124

Symmetry codes: (ii) *x*−1, *y*+1, *z*; (iii) *x*−1, *y*, *z*; (iv) *x*, *y*−1, *z*; (v) −*x*, −*y*+2, −*z*; (vi) −*x*, −*y*+1, −*z*; (vii) *x*, *y*+1, *z*; (viii) −*x*, −*y*+1, −*z*+1; (ix) −*x*+1, −*y*+1, −*z*+1.