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cis-Dichlorido(*N*-cyclohexylpropane-1,3-diamine-κ^2N,N')platinum(II)

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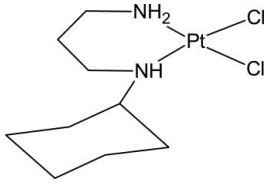
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.010 Å; R factor = 0.035; wR factor = 0.090; data-to-parameter ratio = 23.8.

The reaction of *N*-cyclohexylpropane-1,3-diamine with potassium tetrachloroplatinate(II) produced the monomeric title complex, $[PtCl_2(C_9H_{18}N_2)]$. In the asymmetric unit there are two crystallographically independent Pt^{II} complexes, where each Pt^{II} ion is tetracoordinate in a distorted square-planar geometry. N—H···Cl hydrogen bonds between the complexes form a three-dimensional network in the crystal structure.

Related literature

For related literature, see: Allen (2002); Davies *et al.* (2002); Jakuper *et al.* (2003); Melanson *et al.* (1987).



Experimental

Crystal data

$[PtCl_2(C_9H_{18}N_2)]$
M_r = 422.26
Monoclinic, $P2_1/c$
a = 18.6553 (17) Å
b = 12.2229 (11) Å
c = 11.7912 (10) Å
β = 105.620 (1)°
V = 2589.4 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 11.22 mm^{-1}
T = 293 (2) K
0.27 × 0.25 × 0.18 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.068, T_{max} = 0.133
16372 measured reflections
6027 independent reflections
4679 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.090
S = 1.00
6027 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.68 e Å^{-3}
$\Delta\rho_{min}$ = −1.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···Cl3^{i}	0.90	2.68	3.377 (6)	135
N3—H3A···Cl1^{ii}	0.90	2.66	3.374 (6)	137
N2—H2A···Cl4^{i}	0.91	2.81	3.622 (6)	150
N1—H1B···Cl3^{iii}	0.90	2.66	3.439 (6)	146
N1—H1A···Cl2^{iv}	0.90	2.75	3.605 (6)	160

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (iv) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *APEXII* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2159).

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supplementary materials

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cis-Dichlorido(*N*-cyclohexylpropane-1,3-diamine-κ^2N,N')platinum(II)

M.-J. Xie, X.-Z. Chen, W.-P. Liu, S.-Q. Hou and Q.-S. Ye

Comment

Cisplatin is commonly used for the treatment of testicular and overian cancer as well as cervical, bladder, head and neck tumors. The application of cisplatin in therapy is limited by the dose-dependent nephrotoxicity and other side effects (Jakuper *et al.*, 2003). Therefore, the search for the new potent platinum complexes possessing high antitumor activity and lack of cross-resistance is continuing. The title compound, (I), is a new soluble cisplatin analogue containing an asymmetric chelating diamine *N*-cyclohexylpropane-1,3-diamine and its carrier and anticancer tests are in progress.

The Pt^{II} ion has a square planar geometry formed by an *N*-cyclohexylpropane-1,3-diamine ligand and two Cl atoms (Fig. 1). The crystal structures of a large number of square-planar dichloroplatinum(II) complexes with amine ligands have been reported, as found in the Cambridge Structural Database, Version 5.27 (Allen 2002). Among them, several Pt^{II} complexes contain the chelating ligand 1,2-diaminoethane as well as its N-substituted derivatives, such as, *N*,*N*-dimethylethane-1,2-diamine (Melanson *et al.*, 1987) and *N*-(2-hydroxyethyl)ethane-1,2-diamine (Davies *et al.*, 2002). The chelating nature of the 1,2-diaminoethane portion of these ligands ensures a *cis* configuration; in the present study, the *N*-cyclohexylpropane-1,3-diamine ligand also ensures such a geometry. In the crystal structure, he N—H···Cl hydrogen bonds (Table 1) form a three-dimensional network.

Experimental

Potassium tetrachloroplatinate (5 g, 12 mmol) was dissolved in water (50 ml) and treated with KI (12 g, 72 mmol). After standing in dark for 30 min at room temperature, an aqueous solution (50 ml) of *N*-cyclohexylpropane-1,3-diamine (1.8 g, 12 mmol) was added dropwise. The mixture was stirred for 4 h and the yellow precipitate was filtrated off. Then to a suspension of di(*N*-cyclohexylpropane-1,3-diamine)PtI_2 (2.5 g, 0.044 mmol) in 100 ml water was added silver nitrate (1.26 g, 7.40 mmol), and the reaction mixture was stirred at 313 K for 8 h. After that the AgI formed was filtrated off, potassium chloride (1.1 g, 14.7 mmol) was added to the filtrate and then a yellow crystalline product precipitated. Single crystals suitable for X-ray diffraction were obtained from aqueous solution.

Refinement

The H atoms were placed at calculated positions (C—H = 0.97 or 0.98 Å, N—H = 0.90 or 0.91 Å) and were refined as riding, with U_{iso}(H) = 1.2U_{eq}(C,*N*). The highest peak and deepest hole in the final difference Fourier map are located 1.91 and 0.62 Å, respectively, from atoms Cl3 and Pt2.

Figures

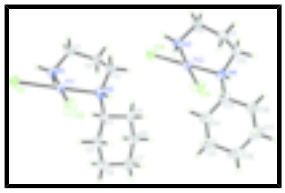


Fig. 1. The asymmetric unit of (I), shown with 30% probability displacement ellipsoids.

cis-Dichlorido(*N*-cyclohexylpropane-1,3-diamine-κ^2N,N')platinum(II)

Crystal data

$[PtCl_2(C_9H_{18}N_2)]$	F_{000} = 1600
M_r = 422.26	D_x = 2.166 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4537 reflections
a = 18.6553 (17) Å	θ = 2.3–27.4º
b = 12.2229 (11) Å	μ = 11.22 mm^{-1}
c = 11.7912 (10) Å	T = 293 (2) K
β = 105.620 (1)º	BLOCK, yellow
V = 2589.4 (4) Å^3	0.27 × 0.25 × 0.18 mm
Z = 8	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	6027 independent reflections
Radiation source: fine-focus sealed tube	4679 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.034
T = 293(2) K	θ_{max} = 28.3º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)	h = −23→24
T_{min} = 0.068, T_{max} = 0.133	k = −14→15
16372 measured reflections	l = −8→15

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.035	$w = 1/[\sigma^2(F_o^2) + (0.0458P)^2 + 1.8205P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.090	$(\Delta/\sigma)_{max}$ = 0.002
S = 1.00	$\Delta\rho_{max}$ = 2.68 e Å^{-3}

6027 reflections	$\Delta\rho_{min} = -1.16$ e Å^{-3}
253 parameters	Extinction correction: SHELXL97
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00297 (8)
Secondary atom site location: difference Fourier map	

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}
Pt1	0.602854 (15)	0.33059 (2)	0.54069 (2)	0.03545 (9)
Pt2	0.723992 (16)	0.86089 (2)	0.35584 (2)	0.03850 (9)
Cl1	0.52757 (11)	0.18859 (15)	0.56509 (17)	0.0517 (5)
Cl2	0.66417 (14)	0.32878 (19)	0.73912 (17)	0.0716 (7)
Cl3	0.63984 (11)	0.75890 (16)	0.21861 (15)	0.0524 (5)
Cl4	0.79928 (14)	0.8797 (2)	0.2320 (2)	0.0754 (7)
N1	0.5448 (3)	0.3328 (4)	0.3681 (5)	0.0397 (13)
H1A	0.5748	0.3091	0.3249	0.048*
H1B	0.5068	0.2852	0.3576	0.048*
N2	0.6684 (3)	0.4588 (4)	0.5132 (5)	0.0414 (14)
H2A	0.6920	0.4840	0.5863	0.050*
N3	0.6554 (3)	0.8520 (4)	0.4639 (5)	0.0370 (13)
H3A	0.6129	0.8186	0.4248	0.044*
H3B	0.6772	0.8098	0.5262	0.044*
N4	0.7996 (3)	0.9567 (5)	0.4747 (5)	0.0456 (15)
H4B	0.8251	0.9909	0.4291	0.055*
C1	0.5145 (4)	0.4410 (6)	0.3228 (7)	0.0481 (18)
H1D	0.4819	0.4670	0.3687	0.058*
H1C	0.4850	0.4332	0.2419	0.058*
C2	0.5749 (4)	0.5249 (6)	0.3282 (6)	0.0457 (18)
H2B	0.5521	0.5916	0.2905	0.055*
H2C	0.6080	0.4978	0.2837	0.055*
C3	0.6210 (4)	0.5524 (5)	0.4530 (6)	0.0450 (17)
H3C	0.6529	0.6144	0.4496	0.054*
H3D	0.5877	0.5740	0.4996	0.054*
C4	0.7300 (4)	0.4255 (6)	0.4594 (6)	0.0404 (16)
H4A	0.7075	0.3853	0.3866	0.049*
C5	0.7835 (5)	0.3490 (6)	0.5422 (8)	0.059 (2)

H5A	0.7569	0.2838	0.5545	0.071*
H5B	0.8025	0.3847	0.6178	0.071*
C6	0.8496 (5)	0.3153 (8)	0.4940 (10)	0.083 (3)
H6A	0.8838	0.2699	0.5513	0.099*
H6B	0.8315	0.2731	0.4223	0.099*
C7	0.8893 (5)	0.4154 (9)	0.4688 (9)	0.076 (3)
H7A	0.9299	0.3938	0.4367	0.091*
H7B	0.9102	0.4551	0.5414	0.091*
C8	0.8363 (5)	0.4884 (8)	0.3822 (8)	0.069 (2)
H8A	0.8174	0.4494	0.3085	0.083*
H8B	0.8628	0.5525	0.3667	0.083*
C9	0.7717 (4)	0.5242 (6)	0.4281 (7)	0.0497 (18)
H9A	0.7376	0.5680	0.3687	0.060*
H9B	0.7901	0.5693	0.4975	0.060*
C10	0.6367 (4)	0.9577 (6)	0.5071 (6)	0.0434 (17)
H10A	0.6007	0.9469	0.5520	0.052*
H10B	0.6144	1.0047	0.4408	0.052*
C11	0.7055 (4)	1.0122 (6)	0.5841 (6)	0.0490 (18)
H11A	0.7300	0.9613	0.6454	0.059*
H11B	0.6901	1.0750	0.6221	0.059*
C12	0.7617 (4)	1.0502 (6)	0.5198 (7)	0.0522 (19)
H12A	0.7364	1.0959	0.4539	0.063*
H12B	0.7992	1.0946	0.5729	0.063*
C13	0.8599 (4)	0.9035 (7)	0.5691 (7)	0.057 (2)
H13A	0.8391	0.8861	0.6349	0.068*
C14	0.8847 (5)	0.7984 (8)	0.5265 (9)	0.079 (3)
H14A	0.9017	0.8126	0.4570	0.095*
H14B	0.8429	0.7484	0.5044	0.095*
C15	0.9478 (5)	0.7448 (10)	0.6214 (11)	0.103 (4)
H15A	0.9294	0.7242	0.6879	0.124*
H15B	0.9640	0.6789	0.5898	0.124*
C16	1.0129 (6)	0.8215 (10)	0.6624 (11)	0.100 (4)
H16A	1.0343	0.8371	0.5977	0.119*
H16B	1.0509	0.7873	0.7250	0.119*
C17	0.9875 (6)	0.9275 (11)	0.7069 (11)	0.117 (5)
H17A	0.9712	0.9124	0.7768	0.140*
H17B	1.0291	0.9779	0.7286	0.140*
C18	0.9242 (5)	0.9807 (8)	0.6145 (9)	0.085 (3)
H18A	0.9070	1.0445	0.6483	0.102*
H18B	0.9426	1.0051	0.5492	0.102*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.04393 (17)	0.03630 (14)	0.02848 (15)	−0.00389 (11)	0.01381 (11)	−0.00052 (10)
Pt2	0.04833 (18)	0.04223 (16)	0.02812 (15)	0.00332 (12)	0.01576 (12)	0.00176 (11)
Cl1	0.0504 (11)	0.0522 (11)	0.0551 (12)	−0.0103 (8)	0.0186 (9)	0.0089 (9)
Cl2	0.0905 (17)	0.0851 (16)	0.0325 (10)	−0.0331 (13)	0.0052 (10)	0.0066 (10)

Cl3	0.0640 (12)	0.0575 (11)	0.0339 (9)	0.0017 (9)	0.0103 (9)	−0.0100 (8)
Cl4	0.0845 (17)	0.1035 (18)	0.0551 (13)	0.0096 (14)	0.0477 (13)	0.0110 (12)
N1	0.040 (3)	0.046 (3)	0.035 (3)	−0.006 (3)	0.014 (3)	−0.007 (3)
N2	0.056 (4)	0.036 (3)	0.033 (3)	−0.009 (3)	0.014 (3)	−0.003 (2)
N3	0.041 (3)	0.043 (3)	0.028 (3)	−0.002 (2)	0.012 (2)	−0.003 (2)
N4	0.042 (3)	0.056 (4)	0.041 (3)	−0.014 (3)	0.015 (3)	0.005 (3)
C1	0.041 (4)	0.055 (5)	0.048 (5)	0.008 (3)	0.013 (3)	0.009 (4)
C2	0.053 (5)	0.041 (4)	0.047 (4)	0.005 (3)	0.020 (4)	0.014 (3)
C3	0.056 (5)	0.037 (4)	0.051 (5)	0.001 (3)	0.029 (4)	−0.003 (3)
C4	0.038 (4)	0.049 (4)	0.035 (4)	−0.003 (3)	0.011 (3)	−0.005 (3)
C5	0.061 (5)	0.050 (5)	0.071 (6)	−0.005 (4)	0.027 (5)	0.009 (4)
C6	0.064 (6)	0.073 (7)	0.111 (9)	0.021 (5)	0.025 (6)	0.013 (6)
C7	0.046 (5)	0.095 (7)	0.088 (7)	−0.008 (5)	0.022 (5)	0.013 (6)
C8	0.051 (5)	0.091 (7)	0.069 (6)	−0.007 (5)	0.022 (4)	0.011 (5)
C9	0.055 (5)	0.056 (5)	0.041 (4)	−0.007 (4)	0.019 (4)	0.000 (3)
C10	0.047 (4)	0.046 (4)	0.039 (4)	0.009 (3)	0.014 (3)	−0.012 (3)
C11	0.049 (5)	0.052 (4)	0.043 (4)	0.000 (4)	0.007 (3)	−0.008 (3)
C12	0.056 (5)	0.044 (4)	0.051 (5)	−0.005 (4)	0.006 (4)	0.000 (4)
C13	0.039 (4)	0.076 (6)	0.060 (5)	−0.001 (4)	0.021 (4)	0.001 (4)
C14	0.061 (6)	0.073 (6)	0.098 (8)	−0.005 (5)	0.014 (5)	0.003 (6)
C15	0.049 (6)	0.107 (9)	0.144 (11)	0.013 (6)	0.009 (7)	0.033 (8)
C16	0.043 (6)	0.142 (11)	0.112 (10)	0.021 (6)	0.017 (6)	0.006 (8)
C17	0.053 (7)	0.145 (12)	0.130 (11)	0.005 (7)	−0.012 (7)	−0.034 (9)
C18	0.055 (6)	0.090 (7)	0.100 (8)	−0.002 (5)	0.004 (5)	−0.037 (6)

Geometric parameters (Å, °)

Pt1—N1	2.031 (5)	C6—H6A	0.9700
Pt1—N2	2.067 (5)	C6—H6B	0.9700
Pt1—Cl1	2.2990 (18)	C7—C8	1.509 (12)
Pt1—Cl2	2.311 (2)	C7—H7A	0.9700
Pt2—N3	2.038 (5)	C7—H7B	0.9700
Pt2—N4	2.064 (6)	C8—C9	1.513 (11)
Pt2—Cl4	2.294 (2)	C8—H8A	0.9700
Pt2—Cl3	2.2954 (19)	C8—H8B	0.9700
N1—C1	1.481 (8)	C9—H9A	0.9700
N1—H1A	0.9000	C9—H9B	0.9700
N1—H1B	0.9000	C10—C11	1.512 (9)
N2—C3	1.503 (8)	C10—H10A	0.9700
N2—C4	1.509 (9)	C10—H10B	0.9700
N2—H2A	0.9100	C11—C12	1.521 (10)
N3—C10	1.465 (8)	C11—H11A	0.9700
N3—H3A	0.9000	C11—H11B	0.9700
N3—H3B	0.9000	C12—H12A	0.9700
N4—C13	1.501 (9)	C12—H12B	0.9700
N4—C12	1.514 (9)	C13—C14	1.498 (12)
N4—H4B	0.9100	C13—C18	1.507 (11)
C1—C2	1.512 (10)	C13—H13A	0.9800
C1—H1D	0.9700	C14—C15	1.535 (13)

C1—H1C	0.9700	C14—H14A	0.9700
C2—C3	1.528 (10)	C14—H14B	0.9700
C2—H2B	0.9700	C15—C16	1.507 (15)
C2—H2C	0.9700	C15—H15A	0.9700
C3—H3C	0.9700	C15—H15B	0.9700
C3—H3D	0.9700	C16—C17	1.520 (15)
C4—C5	1.516 (10)	C16—H16A	0.9700
C4—C9	1.534 (9)	C16—H16B	0.9700
C4—H4A	0.9800	C17—C18	1.520 (14)
C5—C6	1.546 (12)	C17—H17A	0.9700
C5—H5A	0.9700	C17—H17B	0.9700
C5—H5B	0.9700	C18—H18A	0.9700
C6—C7	1.500 (13)	C18—H18B	0.9700
N1—Pt1—N2	90.6 (2)	C6—C7—C8	110.3 (7)
N1—Pt1—Cl1	87.50 (16)	C6—C7—H7A	109.6
N2—Pt1—Cl1	178.14 (16)	C8—C7—H7A	109.6
N1—Pt1—Cl2	177.55 (17)	C6—C7—H7B	109.6
N2—Pt1—Cl2	90.78 (16)	C8—C7—H7B	109.6
Cl1—Pt1—Cl2	91.06 (7)	H7A—C7—H7B	108.1
N3—Pt2—N4	92.0 (2)	C7—C8—C9	111.7 (7)
N3—Pt2—Cl4	177.16 (16)	C7—C8—H8A	109.3
N4—Pt2—Cl4	87.25 (17)	C9—C8—H8A	109.3
N3—Pt2—Cl3	89.21 (16)	C7—C8—H8B	109.3
N4—Pt2—Cl3	177.96 (17)	C9—C8—H8B	109.3
Cl4—Pt2—Cl3	91.46 (9)	H8A—C8—H8B	107.9
C1—N1—Pt1	115.0 (4)	C8—C9—C4	111.3 (7)
C1—N1—H1A	108.5	C8—C9—H9A	109.4
Pt1—N1—H1A	108.5	C4—C9—H9A	109.4
C1—N1—H1B	108.5	C8—C9—H9B	109.4
Pt1—N1—H1B	108.5	C4—C9—H9B	109.4
H1A—N1—H1B	107.5	H9A—C9—H9B	108.0
C3—N2—C4	115.2 (5)	N3—C10—C11	110.8 (6)
C3—N2—Pt1	110.7 (4)	N3—C10—H10A	109.5
C4—N2—Pt1	114.2 (4)	C11—C10—H10A	109.5
C3—N2—H2A	105.2	N3—C10—H10B	109.5
C4—N2—H2A	105.2	C11—C10—H10B	109.5
Pt1—N2—H2A	105.2	H10A—C10—H10B	108.1
C10—N3—Pt2	114.7 (4)	C10—C11—C12	115.0 (6)
C10—N3—H3A	108.6	C10—C11—H11A	108.5
Pt2—N3—H3A	108.6	C12—C11—H11A	108.5
C10—N3—H3B	108.6	C10—C11—H11B	108.5
Pt2—N3—H3B	108.6	C12—C11—H11B	108.5
H3A—N3—H3B	107.6	H11A—C11—H11B	107.5
C13—N4—C12	113.2 (6)	N4—C12—C11	113.2 (6)
C13—N4—Pt2	119.8 (5)	N4—C12—H12A	108.9
C12—N4—Pt2	111.6 (4)	C11—C12—H12A	108.9
C13—N4—H4B	103.3	N4—C12—H12B	108.9
C12—N4—H4B	103.3	C11—C12—H12B	108.9
Pt2—N4—H4B	103.3	H12A—C12—H12B	107.7

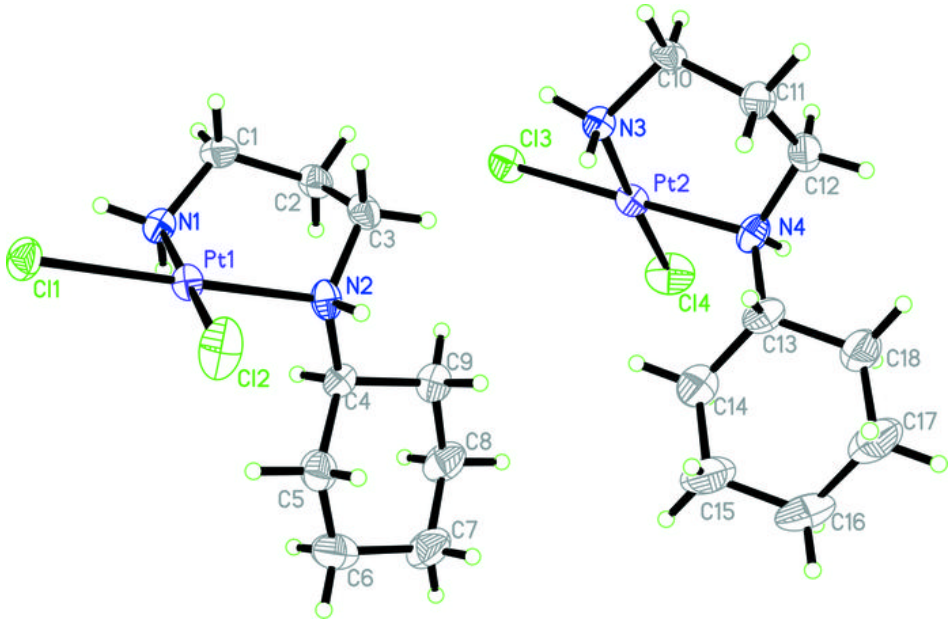
N1—C1—C2	112.5 (6)	C14—C13—N4	111.1 (7)
N1—C1—H1D	109.1	C14—C13—C18	111.6 (7)
C2—C1—H1D	109.1	N4—C13—C18	111.0 (7)
N1—C1—H1C	109.1	C14—C13—H13A	107.6
C2—C1—H1C	109.1	N4—C13—H13A	107.6
H1D—C1—H1C	107.8	C18—C13—H13A	107.6
C1—C2—C3	114.2 (6)	C13—C14—C15	111.5 (9)
C1—C2—H2B	108.7	C13—C14—H14A	109.3
C3—C2—H2B	108.7	C15—C14—H14A	109.3
C1—C2—H2C	108.7	C13—C14—H14B	109.3
C3—C2—H2C	108.7	C15—C14—H14B	109.3
H2B—C2—H2C	107.6	H14A—C14—H14B	108.0
N2—C3—C2	113.2 (5)	C16—C15—C14	111.2 (9)
N2—C3—H3C	108.9	C16—C15—H15A	109.4
C2—C3—H3C	108.9	C14—C15—H15A	109.4
N2—C3—H3D	108.9	C16—C15—H15B	109.4
C2—C3—H3D	108.9	C14—C15—H15B	109.4
H3C—C3—H3D	107.7	H15A—C15—H15B	108.0
N2—C4—C5	109.9 (6)	C15—C16—C17	110.0 (9)
N2—C4—C9	112.4 (6)	C15—C16—H16A	109.7
C5—C4—C9	110.6 (6)	C17—C16—H16A	109.7
N2—C4—H4A	107.9	C15—C16—H16B	109.7
C5—C4—H4A	107.9	C17—C16—H16B	109.7
C9—C4—H4A	107.9	H16A—C16—H16B	108.2
C4—C5—C6	112.3 (7)	C18—C17—C16	111.8 (9)
C4—C5—H5A	109.1	C18—C17—H17A	109.3
C6—C5—H5A	109.1	C16—C17—H17A	109.3
C4—C5—H5B	109.1	C18—C17—H17B	109.3
C6—C5—H5B	109.1	C16—C17—H17B	109.3
H5A—C5—H5B	107.9	H17A—C17—H17B	107.9
C7—C6—C5	110.0 (8)	C13—C18—C17	112.2 (9)
C7—C6—H6A	109.7	C13—C18—H18A	109.2
C5—C6—H6A	109.7	C17—C18—H18A	109.2
C7—C6—H6B	109.7	C13—C18—H18B	109.2
C5—C6—H6B	109.7	C17—C18—H18B	109.2
H6A—C6—H6B	108.2	H18A—C18—H18B	107.9

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3B···Cl3^{i}	0.90	2.68	3.377 (6)	135
N3—H3A···Cl1^{ii}	0.90	2.66	3.374 (6)	137
N2—H2A···Cl4^{i}	0.91	2.81	3.622 (6)	150
N1—H1B···Cl3^{iii}	0.90	2.66	3.439 (6)	146
N1—H1A···Cl2^{iv}	0.90	2.75	3.605 (6)	160

Symmetry codes: (i) *x*, −*y*+3/2, *z*+1/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+1, *y*−1/2, −*z*+1/2; (iv) *x*, −*y*+1/2, *z*−1/2.

Fig. 1


C1
C2
C3
N1
Pt1
N2
Cl1
Cl2
C4
C9
C8
C5
C7
C6
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C11
N3
Cl3
Pt2
C12
N4
Cl4
C13
C18
C14
C17
C15
C16