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Tris(tribenzylammonium) hexachloridoplatinate(IV) chloride

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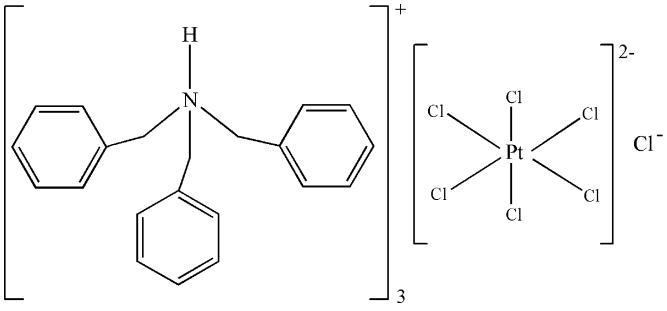
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.007 Å; R factor = 0.050; wR factor = 0.139; data-to-parameter ratio = 23.4.

In the title compound, $(C_{21}H_{22}N)_3[PtCl_6]Cl$, the Pt atom has an octahedral coordination. Intermolecular N—H···Cl hydrogen bonds help to stabilize the structure. The angles between the phenyl rings in the three cations are 66.86 (4)/70.02 (4)/54.31 (3), 78.72 (5)/32.93 (4)/55.77 (4) and 71.76 (5)/79.32 (5)/59.50 (5)°.

Related literature

For related literature, see: Yousefi, Amani & Khavasi (2007); Yousefi, Teimouri *et al.* (2007); Zeng *et al.* (1994); Jarvinen *et al.* (1988); Zordan & Brammer (2004); Hasan *et al.* (2001); Juan *et al.* (1998); Li & Liu (2003); Hu *et al.* (2003); Terzis & Mentzafos (1983); Bencini *et al.* (1992); Ciccarese *et al.* (1998); Delafontaine *et al.* (1987); Bokach *et al.* (2003); Zordan *et al.* (2005);



Experimental

Crystal data

$(C_{21}H_{22}N)_3[PtCl_6]Cl$
M_r = 1308.42
Monoclinic, $P2_1/c$
a = 10.3739 (3) Å
b = 16.4326 (5) Å
c = 34.9438 (8) Å
β = 98.313 (2)°
V = 5894.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.74 mm^{-1}
T = 120 (2) K
0.50 × 0.30 × 0.15 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: numerical [shape of crystal determined optically (*X-RED*; Stoe & Cie, 2005)]
T_{min} = 0.383, T_{max} = 0.665
70527 measured reflections
15914 independent reflections
14651 reflections with $I > 2\sigma(I)$
R_{int} = 0.100

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.139
S = 1.08
15914 reflections
680 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 2.37 e Å^{-3}
$\Delta\rho_{min}$ = −2.96 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pt1—Cl1	2.3032 (9)	Pt1—Cl4	2.3136 (10)
Pt1—Cl2	2.3286 (9)	Pt1—Cl5	2.3209 (9)
Pt1—Cl3	2.3307 (9)	Pt1—Cl6	2.3266 (9)
Cl1—Pt1—Cl2	89.91 (4)	Cl4—Pt1—Cl5	89.55 (4)
Cl1—Pt1—Cl3	177.97 (3)	Cl4—Pt1—Cl6	88.97 (4)
Cl1—Pt1—Cl4	90.00 (4)	Cl5—Pt1—Cl2	90.21 (3)
Cl1—Pt1—Cl5	90.47 (4)	Cl5—Pt1—Cl3	91.46 (3)
Cl1—Pt1—Cl6	89.48 (3)	Cl5—Pt1—Cl6	178.52 (3)
Cl2—Pt1—Cl3	89.45 (4)	Cl6—Pt1—Cl2	91.27 (3)
Cl2—Pt1—Cl4	179.75 (4)	Cl6—Pt1—Cl3	88.60 (3)
Cl4—Pt1—Cl3	90.64 (4)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*C*···Cl3	0.89 (5)	2.41 (5)	3.255 (3)	159 (4)
N2—H2···Cl7	0.86 (5)	2.37 (5)	3.132 (3)	149 (4)
N3—H3*B*···Cl7	0.93 (5)	2.17 (5)	3.095 (3)	177 (5)

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2340).

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supplementary materials

Acta Cryst. (2007). E**63**, m2748-m2749 [**doi:10.1107/S1600536807049689**]

Tris(tribenzylammonium) hexachloridoplatinate(IV) chloride

Y. Mohammad, S. Teimouri, V. Amani and H. R. Khavasi

Comment

We reported the synthesis and crystal structures of [(H_2DA18C6)Cl_2], (II), (Yousefi, Amani & Khavasi, 2007) and [H_2DA18C6][$PtCl_6$]·2H_2O, (III), (Yousefi, Teimouri *et al.*, 2007) [where H_2DA18C6 is 1,10-Diazonia-18-crown-6], recently. Several proton transfer systems using tribenzylamine, with proton donor molecules, such as {(TBA)(DBA)[$CuCl_4$]}, (IV), (Zeng *et al.*, 1994) and (TBA)[DCHSTO], (V), (Jarvinen *et al.*, 1988) [where TBA is tribenzylammonium, DBA is dibenzylammonium and DCHSTO is 1,1,1,1,2,2,2,3,3,3-decacarbonyl-2,3-(μ -hydrido)-2,3-(μ-sulfonyl)-*triangulo*-tri-osmium] have been synthesized and characterized by single-crystal X-ray diffraction methods.

There are also several proton transfer systems using H_2[$PtCl_6$]with proton acceptor molecules, such as [HpyBr-3]$_2$[$PtCl_6$]·2H_2O, (VI), and [HpyI-3]$_2$[$PtCl_6$]·2H_2O, (VII),(Zordan & Brammer, 2004), [BMIM]$_2$[$PtCl_6$], (VIII), and [EMIM]$_2$[$PtCl_6$], (IX), (Hasan *et al.*, 2001), {(DABCO)H_2[$PtCl_6$]}, (*X*), (Juan *et al.*, 1998), {*p*-C_6H_4(CH_2ImMe)$_2$[$PtCl_6$]}, (XI), (Li & Liu, 2003), [het][$PtCl_6$]·2H_2O, (XII), (Hu *et al.*, 2003), [9-MeGuaH]$_2$[$PtCl_6$]·2H_2O, (XIII), (Terzis & Mentzafos, 1983), [H_{10}[30]aneN_{10}][$PtCl_6$]$_2$$Cl_6$·2$H_2O$, (XIV), (Bencini *et al.*, 1992), [$H_2$$Me_2$ppz][$PtCl_6$], (XV) (Ciccarese *et al.*, 1998),[PA]$_2$[$PtCl_6$]Cl, (XVI), (Delafontaine *et al.*, 1987), [DEA]$_2$[$PtCl_6$], (XVII), (Bokach *et al.*, 2003) and [HpyCl-3]$_3$[$PtCl_6$]Cl, (XVIII), (Zordan *et al.*, 2005)[where hpy is halopyridinium, BMI*M*$^+$ is 1-*n*-butyl-3-methyl- imidazolium, EMI*M*$^+$ is 1-ethyl-3-methylimidazolium, DABCO is 1,4-diazabicyclo- octane, Im is imidazolium, het is 2-(α-hydroxyethyl)thiamine, 9-MeGuaH is 9-methylguaninium, [H_{10}[30]aneN_{10}] is [$C_{20}H_{60}N_{10}$]$_{10+}$ cation, $H_2$$Me_2$ppz is *N*,*N*'-dimethylpiperazinium, PA is pentane-1,5-diammonium and DEA is diethylammonium] have been synthesized and characterized by single-crystal X-ray diffraction methods. We report herein the synthesis and crystal structure of the title compound, (I).

The asymmetric unit of (I), (Fig. 1), contains three independent protonated tribenzylamine cations, besides of $PtCl^{2-}_6$ and Cl^- anions. The Pt ion has an octahedral coordination (Table 1). In cations, the bond lengths and angles are in good agreement with the corresponding values in (IV) and (V). In $PtCl^{2-}_6$ anion, the Pt—Cl bond lengths and Cl—Pt—Cl bond angles (Table 1) are also within normal ranges, as in (III) and (XIV).

The intramolecular N—H···Cl hydrogen bonds (Table 2) seem to be effective in the stabilization of the structure (Fig. 2).

Experimental

For the preparation of the title compound, (I), a solution of tribenzylamine (220 mg, 0.74 mmol) in methanol (15 ml) was added to a solution of H_2PtCl_6·2H_2O (200 mg, 0.37 mmol) in acetonitrile (15 ml) and the resulting yellow solution was stirred for 30 min at 313 K. Then, it was left to evaporate slowly at room temperature. After two weeks, yellow prismatic crystals of (I) were isolated (yield; 200 mg, 82.6%, m.p. 470–472 K).

Refinement

H atoms (for NH) were located in difference syntheses and refined isotropically [N—H = 0.86 (4)–0.92 (5) Å and U_{iso}(H) = 0.044 (12)–0.053 (12) Å^2]. The remaining H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å, for aromatic and methylene H atoms and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

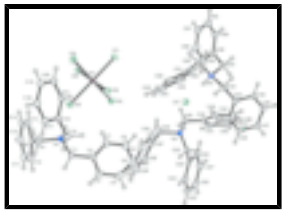


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level

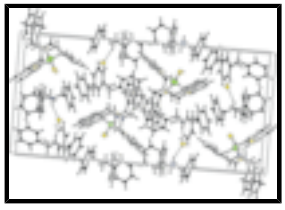


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

Tris(tribenzylammonium) hexachloridoplatinate(IV) chloride

Crystal data

$(C_{21}H_{22}N)_3[PtCl_6]Cl$	$Z = 4$
$M_r = 1308.42$	$F_{000} = 2648$
Monoclinic, $P2_1/c$	$D_x = 1.474$ Mg m^{-3}
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.3739$ (3) Å	Cell parameters from 2500 reflections
$b = 16.4326$ (5) Å	$\mu = 2.74$ mm^{-1}
$c = 34.9438$ (8) Å	$T = 120$ (2) K
$\beta = 98.313$ (2)°	Block, yellow
$V = 5894.3$ (3) Å^3	0.50 × 0.30 × 0.15 mm

Data collection

Stoe IPDSII diffractometer	15914 independent reflections
Radiation source: fine-focus sealed tube	14651 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.100$
Detector resolution: 0.15 mm pixels mm^{-1}	$\theta_{max} = 29.3°$
$T = 120(2)$ K	$\theta_{min} = 1.7°$
ω rotation scans	$h = -14 \rightarrow 14$

Absorption correction: numerical
[shape of crystal determined optically (X-RED; Stoe & Cie, 2005)]
T_{min} = 0.383, T_{max} = 0.665
70527 measured reflections

k = −22→22

l = −47→47

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.050

$wR(F^2)$ = 0.139

S = 1.08

15914 reflections

680 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0833P)^2 + 6.8082P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.019

$\Delta\rho_{max}$ = 2.37 e Å^{-3}

$\Delta\rho_{min}$ = −2.96 e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0050 (2)

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.564759 (12)	0.801342 (8)	0.114732 (4)	0.02524 (7)
Cl1	0.41445 (9)	0.71862 (6)	0.13797 (3)	0.03619 (19)
Cl2	0.59771 (10)	0.87062 (6)	0.17347 (3)	0.03488 (19)
Cl3	0.71158 (9)	0.88884 (6)	0.09110 (3)	0.03548 (19)
Cl4	0.53245 (10)	0.73201 (7)	0.05651 (3)	0.0402 (2)
Cl5	0.73046 (9)	0.71115 (6)	0.13744 (3)	0.03347 (19)
Cl6	0.39773 (8)	0.88988 (6)	0.09047 (3)	0.03364 (18)
Cl7	0.49267 (13)	0.80593 (6)	0.32782 (4)	0.0447 (3)
N1	1.0228 (3)	0.8698 (2)	0.08909 (9)	0.0290 (6)
H1C	0.939 (5)	0.861 (3)	0.0907 (14)	0.053 (12)*
N2	0.5637 (3)	0.9793 (2)	0.36167 (9)	0.0292 (6)

H2	0.573 (4)	0.928 (3)	0.3583 (12)	0.048 (9)*
N3	0.4371 (3)	0.6229 (2)	0.33856 (9)	0.0283 (6)
H3B	0.453 (5)	0.678 (3)	0.3361 (15)	0.044 (12)*
C1	1.0744 (4)	0.9222 (2)	0.12397 (11)	0.0312 (7)
H1A	1.1571	0.9458	0.1199	0.057*
H1B	1.0140	0.9666	0.1259	0.057*
C2	1.0934 (4)	0.8757 (2)	0.16170 (11)	0.0314 (7)
C3	1.2213 (4)	0.8609 (3)	0.17931 (12)	0.0380 (8)
H3A	1.2916	0.8797	0.1681	0.046*
C4	1.2412 (6)	0.8179 (3)	0.21358 (15)	0.0527 (13)
H4	1.3259	0.8092	0.2257	0.063*
C5	1.1392 (7)	0.7878 (3)	0.23004 (15)	0.0570 (14)
H5	1.1547	0.7583	0.2529	0.068*
C6	1.0112 (7)	0.8018 (3)	0.21211 (17)	0.0519 (13)
H6	0.9416	0.7809	0.2230	0.062*
C7	0.9882 (4)	0.8464 (3)	0.17828 (13)	0.0397 (9)
H7	0.9033	0.8568	0.1667	0.048*
C8	1.0397 (4)	0.9147 (2)	0.05201 (11)	0.0321 (7)
H8A	1.1317	0.9252	0.0519	0.048*
H8B	1.0096	0.8801	0.0301	0.048*
C9	0.9668 (4)	0.9941 (2)	0.04744 (10)	0.0295 (7)
C10	1.0259 (5)	1.0668 (3)	0.06002 (13)	0.0434 (10)
H10	1.1125	1.0671	0.0716	0.052*
C11	0.9565 (7)	1.1389 (3)	0.05543 (16)	0.0578 (14)
H11	0.9960	1.1875	0.0643	0.069*
C12	0.8279 (6)	1.1389 (4)	0.03756 (18)	0.0628 (16)
H12	0.7810	1.1874	0.0347	0.075*
C13	0.7698 (5)	1.0670 (4)	0.02402 (16)	0.0524 (13)
H13	0.6841	1.0670	0.0117	0.063*
C14	0.8389 (4)	0.9951 (3)	0.02877 (13)	0.0398 (9)
H14	0.7995	0.9468	0.0194	0.048*
C15	1.0873 (4)	0.7869 (2)	0.09061 (12)	0.0324 (7)
H15A	1.1800	0.7939	0.0903	0.039*
H15B	1.0761	0.7604	0.1147	0.039*
C16	1.0328 (4)	0.7331 (2)	0.05745 (10)	0.0292 (7)
C17	1.1151 (4)	0.7034 (3)	0.03247 (13)	0.0376 (9)
H17	1.2017	0.7199	0.0354	0.045*
C18	1.0676 (4)	0.6487 (3)	0.00304 (13)	0.0416 (9)
H18	1.1227	0.6285	−0.0134	0.050*
C19	0.9379 (4)	0.6247 (3)	−0.00148 (12)	0.0385 (8)
H19	0.9063	0.5879	−0.0208	0.046*
C20	0.8559 (4)	0.6555 (3)	0.02276 (12)	0.0360 (8)
H20	0.7686	0.6404	0.0193	0.043*
C21	0.9027 (4)	0.7089 (2)	0.05230 (12)	0.0302 (7)
H21	0.8470	0.7286	0.0687	0.056*
C22	0.6665 (4)	1.0129 (2)	0.39266 (11)	0.0314 (7)
H22A	0.6725	1.0713	0.3891	0.048*
H22B	0.6391	1.0037	0.4177	0.048*
C23	0.7999 (3)	0.9761 (2)	0.39287 (10)	0.0293 (7)

C24	0.9080 (4)	1.0262 (3)	0.39871 (14)	0.0431 (10)
H24	0.8971	1.0822	0.4004	0.052*
C25	1.0333 (4)	0.9936 (4)	0.40211 (17)	0.0540 (13)
H25	1.1052	1.0280	0.4063	0.065*
C26	1.0512 (4)	0.9109 (3)	0.39923 (14)	0.0464 (11)
H26	1.1347	0.8892	0.4012	0.056*
C27	0.9432 (4)	0.8604 (3)	0.39334 (14)	0.0432 (10)
H27	0.9543	0.8044	0.3916	0.052*
C28	0.8178 (4)	0.8931 (3)	0.38997 (13)	0.0375 (8)
H28	0.7459	0.8588	0.3858	0.045*
C29	0.4278 (3)	0.9918 (3)	0.37210 (12)	0.0332 (7)
H29A	0.4087	1.0496	0.3719	0.040*
H29B	0.3649	0.9661	0.3526	0.040*
C30	0.4123 (3)	0.9574 (2)	0.41130 (12)	0.0333 (8)
C31	0.3746 (4)	1.0075 (3)	0.43907 (12)	0.0354 (8)
H31	0.3597	1.0624	0.4337	0.043*
C32	0.3584 (4)	0.9767 (3)	0.47537 (14)	0.0438 (10)
H32	0.3310	1.0109	0.4938	0.053*
C33	0.3827 (4)	0.8962 (3)	0.48390 (14)	0.0452 (10)
H33	0.3735	0.8762	0.5083	0.054*
C34	0.4212 (4)	0.8442 (3)	0.45618 (16)	0.0470 (11)
H34	0.4378	0.7896	0.4620	0.056*
C35	0.4346 (4)	0.8743 (3)	0.41959 (14)	0.0418 (9)
H35	0.4582	0.8396	0.4008	0.050*
C36	0.5658 (4)	1.0173 (2)	0.32189 (11)	0.0320 (7)
H36A	0.4971	0.9925	0.3039	0.048*
H36B	0.5453	1.0747	0.3235	0.048*
C37	0.6916 (4)	1.0095 (2)	0.30549 (10)	0.0326 (7)
C38	0.7758 (5)	1.0745 (3)	0.30585 (14)	0.0438 (9)
H38	0.7569	1.1233	0.3174	0.053*
C39	0.8885 (5)	1.0675 (4)	0.28909 (17)	0.0557 (13)
H39	0.9454	1.1114	0.2896	0.067*
C40	0.9163 (6)	0.9958 (4)	0.27173 (17)	0.0605 (15)
H40	0.9926	0.9910	0.2608	0.073*
C41	0.8313 (7)	0.9309 (4)	0.27043 (19)	0.0665 (17)
H41	0.8492	0.8829	0.2581	0.080*
C42	0.7188 (5)	0.9376 (3)	0.28755 (14)	0.0471 (10)
H42	0.6618	0.8938	0.2870	0.057*
C43	0.5588 (4)	0.5842 (2)	0.36070 (11)	0.0325 (7)
H43A	0.5443	0.5263	0.3631	0.059*
H43B	0.6307	0.5915	0.3461	0.059*
C44	0.5955 (4)	0.6204 (2)	0.40085 (11)	0.0301 (7)
C45	0.6793 (4)	0.6872 (3)	0.40602 (12)	0.0336 (8)
H45	0.7101	0.7105	0.3848	0.040*
C46	0.7164 (4)	0.7190 (3)	0.44272 (12)	0.0378 (8)
H46	0.7732	0.7630	0.4461	0.045*
C47	0.6694 (4)	0.6855 (3)	0.47461 (12)	0.0344 (8)
H47	0.6932	0.7076	0.4991	0.041*
C48	0.5867 (4)	0.6187 (3)	0.46948 (11)	0.0351 (8)

H48	0.5556	0.5955	0.4907	0.042*
C49	0.5503 (4)	0.5865 (2)	0.43289 (11)	0.0318 (7)
H49	0.4950	0.5417	0.4297	0.048*
C50	0.4064 (4)	0.5867 (2)	0.29801 (10)	0.0305 (7)
H50A	0.3825	0.5300	0.3002	0.057*
H50B	0.3320	0.6150	0.2841	0.057*
C51	0.5184 (4)	0.5922 (2)	0.27511 (10)	0.0302 (7)
C52	0.5413 (4)	0.6634 (3)	0.25527 (11)	0.0356 (8)
H52	0.4890	0.7088	0.2570	0.043*
C53	0.6415 (4)	0.6669 (3)	0.23304 (12)	0.0406 (9)
H53	0.6562	0.7145	0.2199	0.049*
C54	0.7199 (4)	0.5994 (3)	0.23033 (12)	0.0407 (9)
H54	0.7869	0.6018	0.2153	0.049*
C55	0.6989 (4)	0.5283 (3)	0.24996 (11)	0.0363 (8)
H55	0.7522	0.4833	0.2484	0.044*
C56	0.5977 (4)	0.5249 (2)	0.27198 (11)	0.0320 (7)
H56	0.5828	0.4770	0.2848	0.058*
C57	0.3250 (4)	0.6107 (3)	0.36107 (11)	0.0343 (8)
H57A	0.3450	0.6386	0.3857	0.041*
H57B	0.3180	0.5531	0.3665	0.041*
C58	0.1944 (4)	0.6404 (3)	0.34116 (11)	0.0341 (8)
C59	0.1653 (4)	0.7231 (3)	0.33780 (14)	0.0436 (10)
H59	0.2287	0.7617	0.3461	0.052*
C60	0.0404 (5)	0.7475 (4)	0.32182 (15)	0.0537 (12)
H60	0.0205	0.8026	0.3194	0.064*
C61	−0.0549 (5)	0.6898 (4)	0.30954 (16)	0.0602 (16)
H61	−0.1384	0.7063	0.2992	0.072*
C62	−0.0256 (5)	0.6089 (4)	0.31270 (15)	0.0557 (13)
H62	−0.0896	0.5705	0.3046	0.067*
C63	0.0999 (4)	0.5832 (3)	0.32798 (13)	0.0435 (10)
H63	0.1199	0.5280	0.3293	0.052*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.02343 (9)	0.02670 (10)	0.02591 (9)	−0.00133 (4)	0.00464 (5)	−0.00017 (4)
Cl1	0.0323 (4)	0.0313 (4)	0.0467 (5)	−0.0034 (3)	0.0116 (4)	0.0038 (4)
Cl2	0.0392 (5)	0.0346 (4)	0.0304 (4)	0.0009 (3)	0.0037 (3)	−0.0053 (3)
Cl3	0.0269 (4)	0.0385 (5)	0.0421 (5)	−0.0010 (3)	0.0086 (3)	0.0089 (4)
Cl4	0.0428 (5)	0.0454 (5)	0.0316 (4)	0.0002 (4)	0.0030 (4)	−0.0090 (4)
Cl5	0.0308 (4)	0.0352 (4)	0.0349 (4)	0.0048 (3)	0.0068 (3)	0.0028 (3)
Cl6	0.0257 (4)	0.0337 (4)	0.0406 (5)	0.0006 (3)	0.0020 (3)	0.0041 (4)
Cl7	0.0578 (7)	0.0307 (5)	0.0428 (6)	−0.0071 (4)	−0.0015 (5)	−0.0014 (4)
N1	0.0228 (13)	0.0333 (15)	0.0302 (15)	0.0005 (11)	0.0015 (11)	0.0001 (12)
N2	0.0280 (14)	0.0293 (15)	0.0287 (14)	0.0043 (11)	−0.0012 (11)	0.0014 (12)
N3	0.0277 (14)	0.0299 (15)	0.0257 (14)	−0.0015 (11)	−0.0015 (11)	−0.0006 (11)
C1	0.0302 (17)	0.0339 (18)	0.0285 (16)	−0.0009 (13)	0.0007 (13)	−0.0018 (14)
C2	0.0332 (17)	0.0335 (18)	0.0268 (16)	0.0029 (14)	0.0020 (13)	−0.0047 (14)

C3	0.036 (2)	0.041 (2)	0.0352 (19)	0.0052 (16)	−0.0015 (15)	−0.0042 (16)
C4	0.060 (3)	0.055 (3)	0.038 (2)	0.019 (2)	−0.010 (2)	−0.001 (2)
C5	0.091 (4)	0.051 (3)	0.030 (2)	0.018 (3)	0.012 (2)	0.007 (2)
C6	0.071 (4)	0.045 (3)	0.045 (3)	0.004 (2)	0.026 (3)	0.0040 (19)
C7	0.042 (2)	0.042 (2)	0.037 (2)	0.0012 (17)	0.0123 (17)	−0.0035 (17)
C8	0.0322 (17)	0.0362 (19)	0.0281 (17)	0.0022 (14)	0.0054 (13)	−0.0002 (14)
C9	0.0300 (16)	0.0315 (17)	0.0273 (16)	−0.0013 (13)	0.0052 (13)	0.0018 (13)
C10	0.049 (2)	0.039 (2)	0.040 (2)	−0.0032 (18)	−0.0021 (18)	0.0007 (17)
C11	0.088 (4)	0.033 (2)	0.053 (3)	0.006 (2)	0.012 (3)	0.000 (2)
C12	0.076 (4)	0.058 (3)	0.061 (3)	0.034 (3)	0.035 (3)	0.021 (3)
C13	0.032 (2)	0.067 (3)	0.059 (3)	0.012 (2)	0.014 (2)	0.028 (3)
C14	0.0298 (18)	0.048 (2)	0.041 (2)	−0.0041 (16)	0.0033 (15)	0.0102 (18)
C15	0.0290 (17)	0.0325 (17)	0.0343 (19)	0.0044 (14)	−0.0002 (14)	−0.0016 (15)
C16	0.0287 (16)	0.0314 (17)	0.0269 (16)	0.0033 (13)	0.0023 (12)	0.0021 (13)
C17	0.0301 (19)	0.045 (2)	0.037 (2)	0.0038 (15)	0.0033 (16)	−0.0030 (16)
C18	0.038 (2)	0.051 (2)	0.035 (2)	0.0046 (18)	0.0060 (16)	−0.0099 (18)
C19	0.043 (2)	0.037 (2)	0.0339 (19)	0.0031 (16)	0.0003 (16)	−0.0051 (16)
C20	0.0337 (18)	0.0357 (19)	0.037 (2)	−0.0034 (15)	0.0010 (15)	−0.0009 (16)
C21	0.0281 (17)	0.0326 (17)	0.0311 (18)	0.0000 (13)	0.0082 (14)	0.0022 (14)
C22	0.0305 (17)	0.0337 (18)	0.0282 (16)	0.0014 (14)	−0.0017 (13)	−0.0034 (14)
C23	0.0277 (16)	0.0335 (17)	0.0247 (15)	0.0014 (13)	−0.0029 (12)	−0.0009 (13)
C24	0.0286 (18)	0.043 (2)	0.054 (3)	−0.0018 (16)	−0.0036 (17)	−0.013 (2)
C25	0.0265 (19)	0.067 (3)	0.066 (3)	−0.005 (2)	−0.0031 (19)	−0.017 (3)
C26	0.0293 (18)	0.067 (3)	0.041 (2)	0.0113 (19)	−0.0023 (16)	0.001 (2)
C27	0.036 (2)	0.047 (3)	0.045 (2)	0.0126 (17)	0.0041 (17)	0.007 (2)
C28	0.0315 (18)	0.038 (2)	0.042 (2)	0.0032 (15)	0.0034 (15)	0.0083 (17)
C29	0.0228 (15)	0.039 (2)	0.0372 (19)	0.0043 (13)	0.0018 (13)	0.0043 (16)
C30	0.0214 (15)	0.0375 (19)	0.0399 (19)	0.0014 (13)	0.0010 (13)	0.0069 (16)
C31	0.0260 (16)	0.039 (2)	0.042 (2)	0.0015 (14)	0.0054 (14)	0.0075 (16)
C32	0.038 (2)	0.053 (3)	0.040 (2)	0.0069 (18)	0.0053 (17)	0.0065 (19)
C33	0.0290 (18)	0.059 (3)	0.048 (2)	0.0027 (18)	0.0041 (16)	0.020 (2)
C34	0.036 (2)	0.041 (2)	0.064 (3)	0.0049 (17)	0.008 (2)	0.019 (2)
C35	0.034 (2)	0.042 (2)	0.050 (2)	0.0038 (16)	0.0077 (17)	0.0084 (19)
C36	0.0308 (17)	0.0352 (18)	0.0277 (16)	0.0053 (14)	−0.0037 (13)	0.0037 (14)
C37	0.0350 (18)	0.0384 (19)	0.0241 (15)	0.0074 (15)	0.0031 (13)	0.0031 (14)
C38	0.043 (2)	0.045 (2)	0.044 (2)	0.0000 (18)	0.0109 (18)	−0.0001 (19)
C39	0.043 (2)	0.068 (3)	0.059 (3)	0.000 (2)	0.015 (2)	0.010 (3)
C40	0.052 (3)	0.076 (4)	0.058 (3)	0.024 (3)	0.025 (2)	0.021 (3)
C41	0.087 (4)	0.056 (3)	0.064 (4)	0.024 (3)	0.038 (3)	0.006 (3)
C42	0.059 (3)	0.039 (2)	0.046 (2)	0.007 (2)	0.018 (2)	0.0028 (19)
C43	0.0337 (18)	0.0324 (18)	0.0295 (17)	0.0052 (14)	−0.0017 (14)	−0.0001 (14)
C44	0.0302 (16)	0.0294 (17)	0.0289 (16)	0.0017 (13)	−0.0023 (13)	0.0004 (13)
C45	0.0322 (18)	0.0385 (19)	0.0298 (18)	−0.0002 (15)	0.0037 (14)	−0.0002 (15)
C46	0.040 (2)	0.0365 (19)	0.034 (2)	−0.0030 (16)	−0.0022 (16)	−0.0015 (17)
C47	0.0351 (19)	0.0381 (19)	0.0278 (17)	0.0006 (15)	−0.0030 (14)	−0.0048 (15)
C48	0.0321 (18)	0.043 (2)	0.0286 (17)	0.0012 (15)	−0.0002 (14)	0.0010 (15)
C49	0.0285 (16)	0.0353 (18)	0.0293 (17)	−0.0013 (14)	−0.0033 (13)	−0.0010 (14)
C50	0.0306 (16)	0.0355 (18)	0.0239 (15)	−0.0026 (14)	−0.0009 (12)	−0.0009 (13)
C51	0.0293 (16)	0.0358 (18)	0.0237 (15)	−0.0022 (14)	−0.0026 (12)	0.0007 (13)

C52	0.0364 (19)	0.040 (2)	0.0280 (17)	−0.0009 (15)	−0.0040 (14)	0.0024 (15)
C53	0.038 (2)	0.051 (2)	0.0305 (18)	−0.0120 (18)	−0.0027 (15)	0.0076 (17)
C54	0.0322 (18)	0.060 (3)	0.0296 (18)	−0.0078 (18)	0.0024 (14)	0.0010 (18)
C55	0.0283 (17)	0.050 (2)	0.0285 (17)	0.0037 (15)	−0.0026 (13)	−0.0010 (16)
C56	0.0297 (16)	0.0380 (19)	0.0264 (16)	−0.0007 (14)	−0.0026 (13)	0.0030 (14)
C57	0.0305 (17)	0.044 (2)	0.0274 (17)	−0.0020 (15)	0.0016 (13)	0.0044 (15)
C58	0.0286 (17)	0.048 (2)	0.0256 (16)	−0.0009 (15)	0.0037 (13)	−0.0005 (15)
C59	0.035 (2)	0.055 (3)	0.039 (2)	0.0060 (19)	−0.0005 (17)	−0.002 (2)
C60	0.050 (3)	0.066 (3)	0.044 (2)	0.021 (2)	0.003 (2)	−0.001 (2)
C61	0.030 (2)	0.110 (5)	0.039 (3)	0.012 (2)	−0.0017 (18)	0.002 (3)
C62	0.036 (2)	0.089 (4)	0.040 (2)	−0.010 (2)	−0.0014 (18)	−0.004 (3)
C63	0.036 (2)	0.059 (3)	0.035 (2)	−0.0093 (19)	0.0022 (16)	−0.0040 (19)

Geometric parameters (Å, °)

Pt1—Cl1	2.3032 (9)	C29—H29B	0.9700
Pt1—Cl2	2.3286 (9)	C30—C31	1.373 (6)
Pt1—Cl3	2.3307 (9)	C30—C35	1.407 (6)
Pt1—Cl4	2.3136 (10)	C31—C32	1.398 (6)
Pt1—Cl5	2.3209 (9)	C31—H31	0.9300
Pt1—Cl6	2.3266 (9)	C32—C33	1.372 (7)
N1—H1C	0.89 (5)	C32—H32	0.9300
N2—H2	0.86 (4)	C33—C34	1.392 (8)
N3—H3B	0.92 (5)	C33—H33	0.9300
C1—C2	1.512 (5)	C34—C35	1.397 (7)
C1—N1	1.525 (5)	C34—H34	0.9300
C1—H1A	0.9700	C35—H35	0.9300
C1—H1B	0.9700	C36—C37	1.504 (6)
C2—C7	1.393 (6)	C36—N2	1.527 (5)
C2—C3	1.401 (5)	C36—H36A	0.9700
C3—C4	1.380 (7)	C36—H36B	0.9700
C3—H3A	0.9300	C37—C38	1.380 (6)
C4—C5	1.367 (9)	C37—C42	1.386 (6)
C4—H4	0.9300	C38—C39	1.386 (7)
C5—C6	1.403 (9)	C38—H38	0.9300
C5—H5	0.9300	C39—C40	1.375 (9)
C6—C7	1.382 (7)	C39—H39	0.9300
C6—H6	0.9300	C40—C41	1.380 (10)
C7—H7	0.9300	C40—H40	0.9300
C8—C9	1.505 (5)	C41—C42	1.391 (8)
C8—N1	1.523 (5)	C41—H41	0.9300
C8—H8A	0.9700	C42—H42	0.9300
C8—H8B	0.9700	C43—C44	1.520 (5)
C9—C10	1.385 (6)	C43—N3	1.521 (5)
C9—C14	1.392 (5)	C43—H43A	0.9700
C10—C11	1.384 (7)	C43—H43B	0.9700
C10—H10	0.9300	C44—C49	1.391 (6)
C11—C12	1.389 (9)	C44—C45	1.396 (5)
C11—H11	0.9300	C45—C46	1.387 (6)

C12—C13	1.379 (9)	C45—H45	0.9300
C12—H12	0.9300	C46—C47	1.393 (6)
C13—C14	1.379 (7)	C46—H46	0.9300
C13—H13	0.9300	C47—C48	1.389 (6)
C14—H14	0.9300	C47—H47	0.9300
C15—C16	1.502 (5)	C48—C49	1.385 (5)
C15—N1	1.515 (5)	C48—H48	0.9300
C15—H15A	0.9700	C49—H49	0.9300
C15—H15B	0.9700	C50—C51	1.505 (5)
C16—C21	1.393 (5)	C50—N3	1.527 (5)
C16—C17	1.395 (6)	C50—H50A	0.9700
C17—C18	1.401 (6)	C50—H50B	0.9700
C17—H17	0.9300	C51—C56	1.393 (5)
C18—C19	1.389 (6)	C51—C52	1.398 (6)
C18—H18	0.9300	C52—C53	1.386 (6)
C19—C20	1.381 (6)	C52—H52	0.9300
C19—H19	0.9300	C53—C54	1.386 (7)
C20—C21	1.388 (6)	C53—H53	0.9300
C20—H20	0.9300	C54—C55	1.388 (6)
C21—H21	0.9300	C54—H54	0.9300
C22—C23	1.510 (5)	C55—C56	1.389 (6)
C22—N2	1.510 (5)	C55—H55	0.9300
C22—H22A	0.9700	C56—H56	0.9300
C22—H22B	0.9700	C57—N3	1.509 (5)
C23—C28	1.381 (6)	C57—C58	1.512 (5)
C23—C24	1.383 (5)	C57—H57A	0.9700
C24—C25	1.394 (6)	C57—H57B	0.9700
C24—H24	0.9300	C58—C63	1.389 (6)
C25—C26	1.378 (8)	C58—C59	1.393 (7)
C25—H25	0.9300	C59—C60	1.394 (6)
C26—C27	1.385 (7)	C59—H59	0.9300
C26—H26	0.9300	C60—C61	1.391 (9)
C27—C28	1.396 (6)	C60—H60	0.9300
C27—H27	0.9300	C61—C62	1.365 (9)
C28—H28	0.9300	C61—H61	0.9300
C29—C30	1.512 (6)	C62—C63	1.399 (7)
C29—N2	1.521 (5)	C62—H62	0.9300
C29—H29A	0.9700	C63—H63	0.9300
Cl1—Pt1—Cl2	89.91 (4)	C28—C27—H27	119.8
Cl1—Pt1—Cl3	177.97 (3)	C23—C28—C27	120.5 (4)
Cl1—Pt1—Cl4	90.00 (4)	C23—C28—H28	119.8
Cl1—Pt1—Cl5	90.47 (4)	C27—C28—H28	119.8
Cl1—Pt1—Cl6	89.48 (3)	C30—C29—N2	112.9 (3)
Cl2—Pt1—Cl3	89.45 (4)	C30—C29—H29A	109.0
Cl2—Pt1—Cl4	179.75 (4)	N2—C29—H29A	109.0
Cl4—Pt1—Cl3	90.64 (4)	C30—C29—H29B	109.0
Cl4—Pt1—Cl5	89.55 (4)	N2—C29—H29B	109.0
Cl4—Pt1—Cl6	88.97 (4)	H29A—C29—H29B	107.8
Cl5—Pt1—Cl2	90.21 (3)	C31—C30—C35	119.5 (4)

Cl5—Pt1—Cl3	91.46 (3)	C31—C30—C29	119.6 (4)
Cl5—Pt1—Cl6	178.52 (3)	C35—C30—C29	120.9 (4)
Cl6—Pt1—Cl2	91.27 (3)	C30—C31—C32	120.5 (4)
Cl6—Pt1—Cl3	88.60 (3)	C30—C31—H31	119.7
C15—N1—C8	111.1 (3)	C32—C31—H31	119.7
C15—N1—C1	112.2 (3)	C33—C32—C31	120.3 (5)
C8—N1—C1	109.6 (3)	C33—C32—H32	119.9
C15—N1—H1C	106 (3)	C31—C32—H32	119.9
C8—N1—H1C	112 (3)	C32—C33—C34	120.2 (4)
C1—N1—H1C	106 (3)	C32—C33—H33	119.9
C22—N2—C29	111.2 (3)	C34—C33—H33	119.9
C22—N2—C36	113.7 (3)	C33—C34—C35	119.8 (4)
C29—N2—C36	107.4 (3)	C33—C34—H34	120.1
C22—N2—H2	112 (3)	C35—C34—H34	120.1
C29—N2—H2	107 (3)	C34—C35—C30	119.8 (5)
C36—N2—H2	105 (3)	C34—C35—H35	120.1
C57—N3—C43	108.9 (3)	C30—C35—H35	120.1
C57—N3—C50	111.0 (3)	C37—C36—N2	116.1 (3)
C43—N3—C50	110.8 (3)	C37—C36—H36A	108.3
C57—N3—H3B	110 (3)	N2—C36—H36A	108.3
C43—N3—H3B	108 (3)	C37—C36—H36B	108.3
C50—N3—H3B	108 (3)	N2—C36—H36B	108.3
C2—C1—N1	113.4 (3)	H36A—C36—H36B	107.4
C2—C1—H1A	108.9	C38—C37—C42	119.7 (4)
N1—C1—H1A	108.9	C38—C37—C36	120.9 (4)
C2—C1—H1B	108.9	C42—C37—C36	119.3 (4)
N1—C1—H1B	108.9	C37—C38—C39	120.2 (5)
H1A—C1—H1B	107.7	C37—C38—H38	119.9
C7—C2—C3	120.4 (4)	C39—C38—H38	119.9
C7—C2—C1	121.8 (4)	C40—C39—C38	120.1 (5)
C3—C2—C1	117.8 (4)	C40—C39—H39	120.0
C4—C3—C2	118.9 (5)	C38—C39—H39	120.0
C4—C3—H3A	120.5	C39—C40—C41	120.2 (5)
C2—C3—H3A	120.5	C39—C40—H40	119.9
C5—C4—C3	121.5 (5)	C41—C40—H40	119.9
C5—C4—H4	119.3	C40—C41—C42	119.8 (5)
C3—C4—H4	119.3	C40—C41—H41	120.1
C4—C5—C6	119.5 (5)	C42—C41—H41	120.1
C4—C5—H5	120.2	C37—C42—C41	120.0 (5)
C6—C5—H5	120.2	C37—C42—H42	120.0
C7—C6—C5	120.3 (5)	C41—C42—H42	120.0
C7—C6—H6	119.9	C44—C43—N3	112.7 (3)
C5—C6—H6	119.9	C44—C43—H43A	109.1
C6—C7—C2	119.4 (5)	N3—C43—H43A	109.1
C6—C7—H7	120.3	C44—C43—H43B	109.1
C2—C7—H7	120.3	N3—C43—H43B	109.1
C9—C8—N1	113.1 (3)	H43A—C43—H43B	107.8
C9—C8—H8A	109.0	C49—C44—C45	119.1 (4)
N1—C8—H8A	109.0	C49—C44—C43	121.2 (3)

C9—C8—H8B	109.0	C45—C44—C43	119.7 (4)
N1—C8—H8B	109.0	C46—C45—C44	120.1 (4)
H8A—C8—H8B	107.8	C46—C45—H45	120.0
C10—C9—C14	119.1 (4)	C44—C45—H45	120.0
C10—C9—C8	121.4 (4)	C45—C46—C47	120.5 (4)
C14—C9—C8	119.4 (4)	C45—C46—H46	119.7
C11—C10—C9	120.2 (5)	C47—C46—H46	119.7
C11—C10—H10	119.9	C48—C47—C46	119.4 (4)
C9—C10—H10	119.9	C48—C47—H47	120.3
C10—C11—C12	120.1 (5)	C46—C47—H47	120.3
C10—C11—H11	119.9	C49—C48—C47	120.1 (4)
C12—C11—H11	119.9	C49—C48—H48	119.9
C13—C12—C11	119.9 (5)	C47—C48—H48	119.9
C13—C12—H12	120.1	C48—C49—C44	120.8 (4)
C11—C12—H12	120.1	C48—C49—H49	119.6
C14—C13—C12	119.9 (5)	C44—C49—H49	119.6
C14—C13—H13	120.0	C51—C50—N3	113.4 (3)
C12—C13—H13	120.0	C51—C50—H50A	108.9
C13—C14—C9	120.7 (4)	N3—C50—H50A	108.9
C13—C14—H14	119.6	C51—C50—H50B	108.9
C9—C14—H14	119.6	N3—C50—H50B	108.9
C16—C15—N1	112.8 (3)	H50A—C50—H50B	107.7
C16—C15—H15A	109.0	C56—C51—C52	118.8 (4)
N1—C15—H15A	109.0	C56—C51—C50	120.3 (3)
C16—C15—H15B	109.0	C52—C51—C50	120.9 (4)
N1—C15—H15B	109.0	C53—C52—C51	120.5 (4)
H15A—C15—H15B	107.8	C53—C52—H52	119.8
C21—C16—C17	119.2 (4)	C51—C52—H52	119.8
C21—C16—C15	121.2 (4)	C52—C53—C54	120.0 (4)
C17—C16—C15	119.5 (3)	C52—C53—H53	120.0
C16—C17—C18	120.1 (4)	C54—C53—H53	120.0
C16—C17—H17	119.9	C53—C54—C55	120.2 (4)
C18—C17—H17	119.9	C53—C54—H54	119.9
C19—C18—C17	119.9 (4)	C55—C54—H54	119.9
C19—C18—H18	120.1	C54—C55—C56	119.5 (4)
C17—C18—H18	120.1	C54—C55—H55	120.2
C20—C19—C18	119.9 (4)	C56—C55—H55	120.2
C20—C19—H19	120.0	C55—C56—C51	120.9 (4)
C18—C19—H19	120.0	C55—C56—H56	119.5
C19—C20—C21	120.5 (4)	C51—C56—H56	119.5
C19—C20—H20	119.8	N3—C57—C58	115.1 (3)
C21—C20—H20	119.8	N3—C57—H57A	108.5
C20—C21—C16	120.3 (4)	C58—C57—H57A	108.5
C20—C21—H21	119.8	N3—C57—H57B	108.5
C16—C21—H21	119.8	C58—C57—H57B	108.5
C23—C22—N2	114.1 (3)	H57A—C57—H57B	107.5
C23—C22—H22A	108.7	C63—C58—C59	119.9 (4)
N2—C22—H22A	108.7	C63—C58—C57	118.5 (4)
C23—C22—H22B	108.7	C59—C58—C57	121.5 (4)

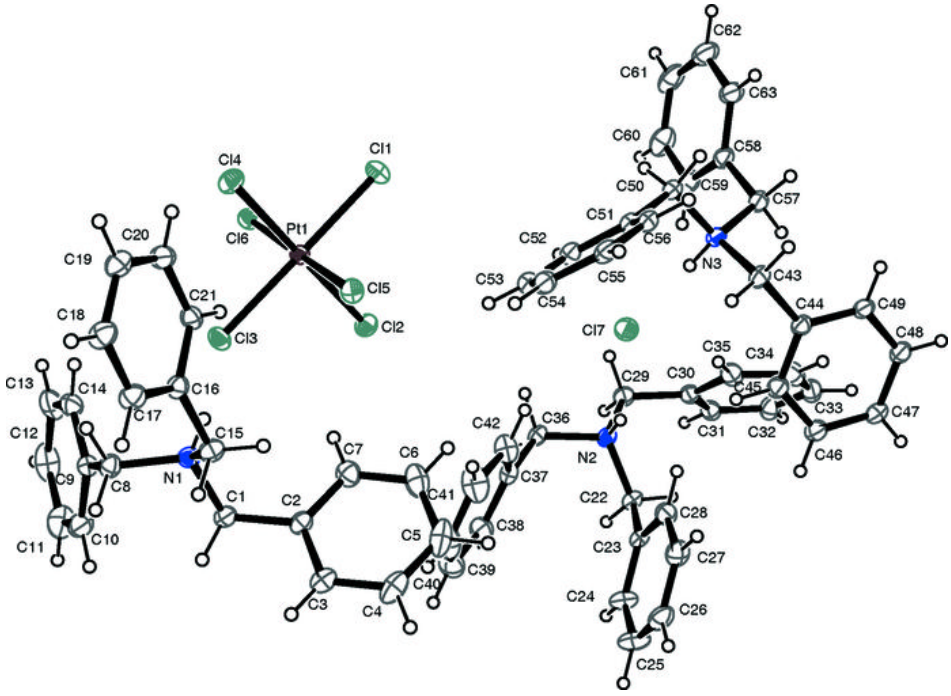
N2—C22—H22B	108.7	C58—C59—C60	119.4 (5)
H22A—C22—H22B	107.6	C58—C59—H59	120.3
C28—C23—C24	118.9 (4)	C60—C59—H59	120.3
C28—C23—C22	121.9 (3)	C61—C60—C59	120.4 (5)
C24—C23—C22	119.0 (4)	C61—C60—H60	119.8
C23—C24—C25	120.7 (4)	C59—C60—H60	119.8
C23—C24—H24	119.7	C62—C61—C60	119.9 (5)
C25—C24—H24	119.7	C62—C61—H61	120.0
C26—C25—C24	120.4 (4)	C60—C61—H61	120.0
C26—C25—H25	119.8	C61—C62—C63	120.6 (5)
C24—C25—H25	119.8	C61—C62—H62	119.7
C25—C26—C27	119.2 (4)	C63—C62—H62	119.7
C25—C26—H26	120.4	C58—C63—C62	119.7 (5)
C27—C26—H26	120.4	C58—C63—H63	120.2
C26—C27—C28	120.4 (5)	C62—C63—H63	120.2
C26—C27—H27	119.8		
N1—C1—C2—C7	−69.1 (5)	C37—C38—C39—C40	0.6 (8)
N1—C1—C2—C3	109.3 (4)	C38—C39—C40—C41	0.9 (9)
C7—C2—C3—C4	−0.9 (6)	C39—C40—C41—C42	−1.5 (9)
C1—C2—C3—C4	−179.4 (4)	C38—C37—C42—C41	0.7 (7)
C2—C3—C4—C5	1.8 (7)	C36—C37—C42—C41	176.6 (5)
C3—C4—C5—C6	−0.9 (8)	C40—C41—C42—C37	0.7 (9)
C4—C5—C6—C7	−0.7 (8)	N3—C43—C44—C49	91.8 (4)
C5—C6—C7—C2	1.5 (7)	N3—C43—C44—C45	−90.1 (4)
C3—C2—C7—C6	−0.7 (6)	C49—C44—C45—C46	0.1 (6)
C1—C2—C7—C6	177.7 (4)	C43—C44—C45—C46	−178.0 (4)
N1—C8—C9—C10	93.2 (4)	C44—C45—C46—C47	−0.9 (7)
N1—C8—C9—C14	−89.5 (4)	C45—C46—C47—C48	1.3 (7)
C14—C9—C10—C11	2.6 (7)	C46—C47—C48—C49	−0.8 (6)
C8—C9—C10—C11	180.0 (4)	C47—C48—C49—C44	−0.1 (6)
C9—C10—C11—C12	−1.2 (8)	C45—C44—C49—C48	0.4 (6)
C10—C11—C12—C13	−0.7 (9)	C43—C44—C49—C48	178.5 (4)
C11—C12—C13—C14	1.0 (8)	N3—C50—C51—C56	99.9 (4)
C12—C13—C14—C9	0.5 (7)	N3—C50—C51—C52	−82.9 (4)
C10—C9—C14—C13	−2.3 (7)	C56—C51—C52—C53	−0.2 (5)
C8—C9—C14—C13	−179.7 (4)	C50—C51—C52—C53	−177.5 (3)
N1—C15—C16—C21	−62.6 (5)	C51—C52—C53—C54	0.0 (6)
N1—C15—C16—C17	120.7 (4)	C52—C53—C54—C55	−0.3 (6)
C21—C16—C17—C18	−1.1 (6)	C53—C54—C55—C56	0.7 (6)
C15—C16—C17—C18	175.6 (4)	C54—C55—C56—C51	−1.0 (6)
C16—C17—C18—C19	0.6 (7)	C52—C51—C56—C55	0.7 (5)
C17—C18—C19—C20	0.7 (7)	C50—C51—C56—C55	178.0 (3)
C18—C19—C20—C21	−1.5 (7)	N3—C57—C58—C63	110.3 (4)
C19—C20—C21—C16	1.0 (6)	N3—C57—C58—C59	−73.3 (5)
C17—C16—C21—C20	0.3 (6)	C63—C58—C59—C60	1.2 (7)
C15—C16—C21—C20	−176.4 (4)	C57—C58—C59—C60	−175.2 (4)
N2—C22—C23—C28	−45.8 (5)	C58—C59—C60—C61	0.4 (8)
N2—C22—C23—C24	138.6 (4)	C59—C60—C61—C62	−0.8 (8)
C28—C23—C24—C25	−0.8 (7)	C60—C61—C62—C63	−0.4 (8)

C22—C23—C24—C25	175.0 (4)	C59—C58—C63—C62	−2.4 (7)
C23—C24—C25—C26	0.8 (8)	C57—C58—C63—C62	174.1 (4)
C24—C25—C26—C27	−0.7 (8)	C61—C62—C63—C58	2.0 (8)
C25—C26—C27—C28	0.6 (8)	C16—C15—N1—C8	−59.7 (4)
C24—C23—C28—C27	0.7 (6)	C16—C15—N1—C1	177.2 (3)
C22—C23—C28—C27	−174.9 (4)	C9—C8—N1—C15	174.7 (3)
C26—C27—C28—C23	−0.7 (7)	C9—C8—N1—C1	−60.8 (4)
N2—C29—C30—C31	122.2 (4)	C2—C1—N1—C15	−41.5 (4)
N2—C29—C30—C35	−58.5 (5)	C2—C1—N1—C8	−165.5 (3)
C35—C30—C31—C32	0.1 (6)	C23—C22—N2—C29	157.6 (3)
C29—C30—C31—C32	179.3 (4)	C23—C22—N2—C36	−81.1 (4)
C30—C31—C32—C33	1.4 (6)	C30—C29—N2—C22	−54.6 (4)
C31—C32—C33—C34	−1.3 (7)	C30—C29—N2—C36	−179.6 (3)
C32—C33—C34—C35	−0.2 (7)	C37—C36—N2—C22	58.2 (4)
C33—C34—C35—C30	1.6 (7)	C37—C36—N2—C29	−178.3 (3)
C31—C30—C35—C34	−1.5 (6)	C58—C57—N3—C43	−175.5 (3)
C29—C30—C35—C34	179.3 (4)	C58—C57—N3—C50	−53.2 (4)
N2—C36—C37—C38	−103.1 (4)	C44—C43—N3—C57	−59.4 (4)
N2—C36—C37—C42	81.1 (5)	C44—C43—N3—C50	178.2 (3)
C42—C37—C38—C39	−1.4 (7)	C51—C50—N3—C57	−176.2 (3)
C36—C37—C38—C39	−177.1 (4)	C51—C50—N3—C43	−54.9 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1C···Cl3	0.89 (5)	2.41 (5)	3.255 (3)	159 (4)
N2—H2···Cl7	0.86 (5)	2.37 (5)	3.132 (3)	149 (4)
N3—H3B···Cl7	0.93 (5)	2.17 (5)	3.095 (3)	177 (5)

Fig. 1


C62
C61
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Cl1
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Cl2

Fig. 2