Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

cis-Dibromidobis(2-phenylpyridine-κN)-platinum(II)

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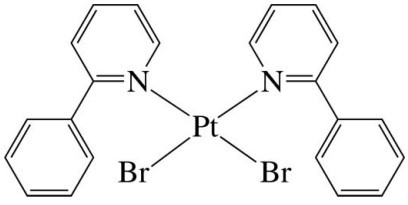
Received 28 July 2012; accepted 5 August 2012

Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.015 Å; R factor = 0.028; wR factor = 0.068; data-to-parameter ratio = 12.0.

In the title complex, $[PtBr_2(C_{11}H_9N)_2]$, the Pt^{II} ion has a distorted *cis*-Br_2N_2 square-planar coordination geometry defined by two N atoms from two 2-phenylpyridine (ppy) ligands and two Br^- anions. The ppy ligands are not planar, the dihedral angles between the pyridine and benzene rings being 49.0 (3) and 47.3 (3)°. In the crystal, the complex molecules are stacked in columns along the *a* axis. In the columns, there are numerous intra- and intermolecular π–π interactions between the six-membered rings, the shortest ring centroid–centroid distance being 3.774 (6) Å.

Related literature

For the crystal structures of the related Pt^{II} and Pd^{II} complexes, *cis*-$[PtCl_2(ppy)_2]$ and *trans*-$[PdX_2(ppy)_2]$ (X = Cl or I), see: Yoshinari *et al.* (2010); Ha (2011, 2012).



Experimental

Crystal data

$[PtBr_2(C_{11}H_9N)_2]$
M_r = 665.29
Monoclinic, *Cc*
a = 7.6268 (9) Å
b = 18.277 (2) Å
c = 15.1626 (18) Å
β = 96.948 (2)°
V = 2098.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 10.51 mm^{-1}
T = 200 K
0.24 × 0.20 × 0.14 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.729, T_{max} = 1.000
6126 measured reflections
2931 independent reflections
2645 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.068
S = 1.04
2931 reflections
244 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.93 e Å^{-3}
Absolute structure: Flack (1983), 856 Friedel pairs
Flack parameter: −0.037 (13)

Table 1
Selected bond lengths (Å).

Pt1—N1	2.075 (8)	Pt1—Br1	2.4216 (11)
Pt1—N2	2.074 (10)	Pt1—Br2	2.4258 (15)

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Priority Research Centers Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2011–0030747).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5600).

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supporting information

Acta Cryst. (2012). E**68**, m1169 [doi:10.1107/S160053681203471X]

cis-Dibromidobis(2-phenylpyridine-κN)platinum(II)

Kwang Ha

S1. Comment

Crystal structures of the related Pt^{II} and Pd^{II} complexes, such as *cis*-[$PtCl_2(ppy)_2$] (ppy = 2-phenylpyridine, $C_{11}H_9N$) (Yoshinari *et al.*, 2010) and *trans*-[$PdX_2(ppy)_2$] (*X* = Cl or I) (Ha, 2011; Ha, 2012), have been investigated previously.

The Pt^{II} ion in the title complex, [$PtBr_2(ppy)_2$], has a distorted *cis*-Br_2N_2 square-planar coordination geometry defined by two N atoms from two ppy ligands and two Br^- anions (Fig. 1). The Pt—N and Pt—Br bond lengths are nearly equivalent, respectively (Table 1). In the crystal, the two pyridine rings are inclined to the least-squares plane of the $PtBr_2N_2$ unit [maximum deviation = 0.092 (4) Å], making dihedral angles of 61.6 (2)° and 64.0 (2)°. The ppy ligands are not planar, the dihedral angles between the pyridine and benzene rings being 49.0 (3)° and 47.3 (3)°. The complex molecules are stacked in columns along the *a* axis. In the columns, numerous intra- and intermolecular π-π interactions between the six-membered rings are present, the shortest ring centroid-centroid distance being 3.774 (6) Å (Fig. 2).

S2. Experimental

To a solution of K_2PtBr_4 (0.2391 g, 0.403 mmol) in H_2O (20 ml)/MeOH (100 ml) was added 2-phenylpyridine (0.1810 g, 1.166 mmol) and stirred for 7 h at room temperature. The formed brown precipitate was removed by filtration and the solvent of the filtrate was evaporated. The residue was washed with H_2O and dried at 323 K, to give a yellow powder (0.1672 g). Crystals suitable for X-ray analysis were obtained by slow evaporation from a CH_3CN solution at room temperature.

S3. Refinement

H atoms were positioned geometrically and allowed to ride on their respective parent atoms: C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C). The highest peak (1.73 e Å^{-3}) and the deepest hole (-0.93 e Å^{-3}) in the difference Fourier map are located 1.31 Å and 0.88 Å, respectively, from the atoms H11 and Pt1.

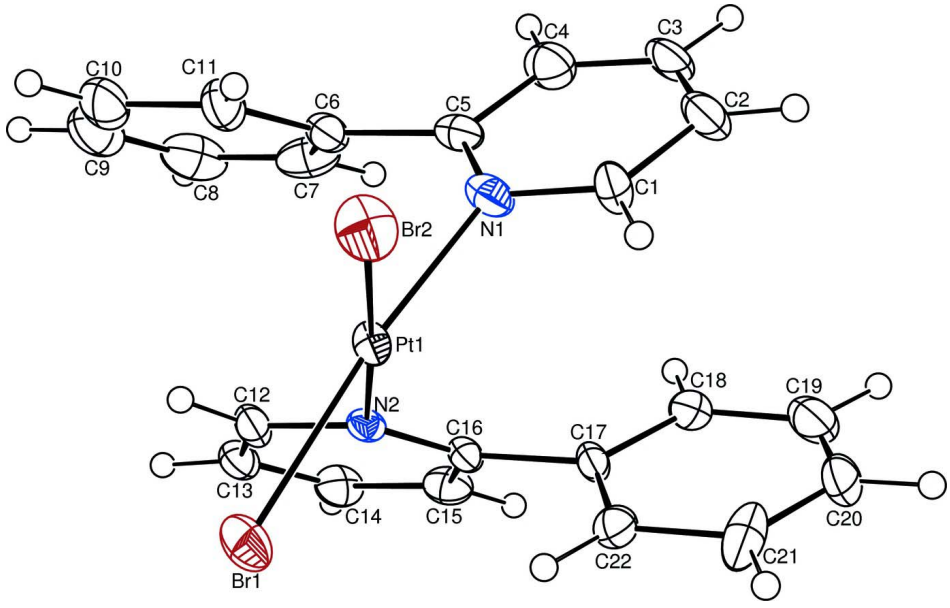

Figure 1

A view of the molecular structure of the title complex, with displacement ellipsoids drawn at the 40% probability level and the atom numbering.

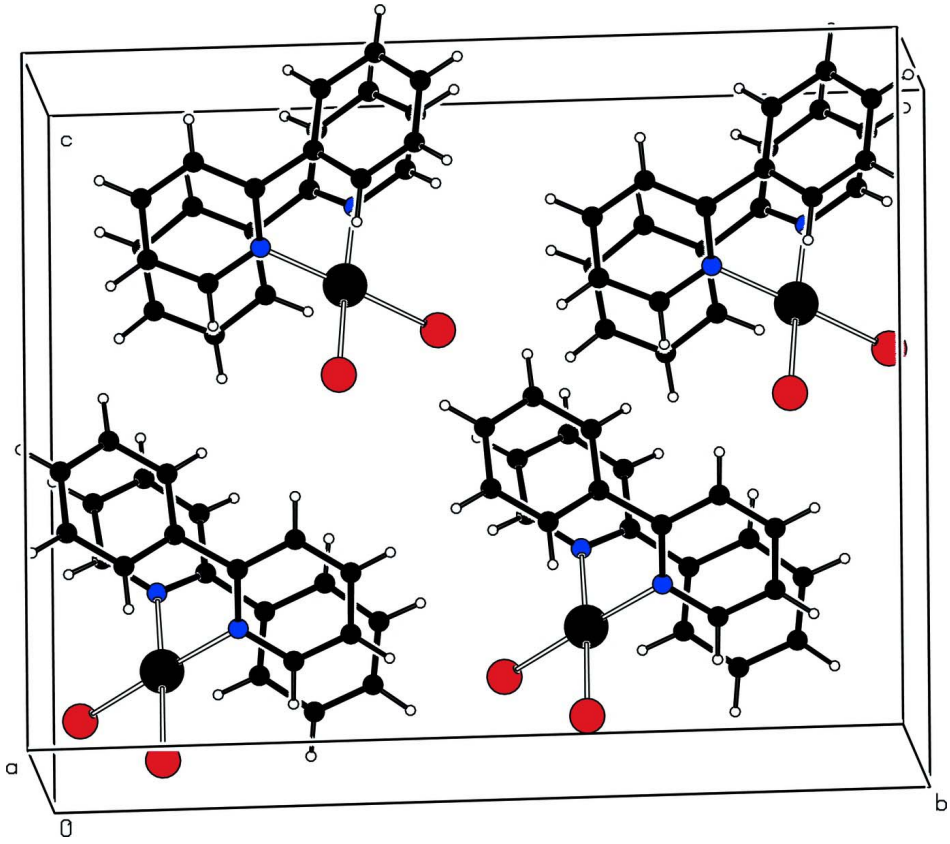

Figure 2

A view of the unit-cell contents of the title complex.

cis-Dibromidobis(2-phenylpyridine-κN)platinum(II)

Crystal data

$[PtBr_2(C_{11}H_9N)_2]$
M_r = 665.29
Monoclinic, *Cc*
Hall symbol: C -2yc
a = 7.6268 (9) Å
b = 18.277 (2) Å
c = 15.1626 (18) Å
β = 96.948 (2)°
V = 2098.1 (4) Å^3
Z = 4
F(000) = 1248
D_x = 2.106 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 4325 reflections
θ = 2.2–26.0°
μ = 10.51 mm^{-1}
T = 200 K
Stick, yellow
0.24 × 0.20 × 0.14 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.729, T_{max} = 1.000
6126 measured reflections
2931 independent reflections
2645 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 26.0°, θ_{min} = 2.6°
h = −9→8
k = −22→22
l = −18→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.068
S = 1.04
2931 reflections
244 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0286P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.93 e Å^{-3}
Absolute structure: Flack (1983), 856 Friedel pairs
Absolute structure parameter: −0.037 (13)

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}
Pt1	0.39565 (2)	0.136006 (14)	0.162689 (18)	0.02282 (10)
Br1	0.19970 (16)	0.03626 (5)	0.11234 (8)	0.0369 (3)
Br2	0.5217 (2)	0.14016 (7)	0.02336 (11)	0.0415 (4)
N1	0.5395 (11)	0.2278 (4)	0.2077 (6)	0.030 (2)
N2	0.2978 (14)	0.1281 (4)	0.2842 (7)	0.021 (2)
C1	0.4929 (14)	0.2895 (5)	0.1628 (8)	0.035 (3)
H1	0.4181	0.2865	0.1081	0.042*
C2	0.5505 (16)	0.3567 (5)	0.1939 (10)	0.042 (3)
H2	0.5197	0.3997	0.1605	0.051*
C3	0.6514 (16)	0.3604 (5)	0.2727 (10)	0.044 (3)
H3	0.6870	0.4068	0.2970	0.052*
C4	0.7031 (14)	0.2986 (5)	0.3180 (8)	0.040 (3)
H4	0.7776	0.3013	0.3728	0.048*
C5	0.6453 (13)	0.2306 (5)	0.2829 (7)	0.029 (2)
C6	0.7103 (13)	0.1613 (5)	0.3294 (7)	0.029 (2)
C7	0.7024 (15)	0.1529 (7)	0.4178 (8)	0.043 (3)
H7	0.6555	0.1912	0.4503	0.052*
C8	0.7627 (16)	0.0885 (7)	0.4618 (9)	0.052 (3)
H8	0.7560	0.0824	0.5235	0.063*
C9	0.8311 (17)	0.0349 (7)	0.4137 (10)	0.056 (4)
H9	0.8734	−0.0087	0.4429	0.067*
C10	0.8406 (15)	0.0420 (6)	0.3247 (9)	0.046 (3)
H10	0.8896	0.0036	0.2931	0.055*
C11	0.7788 (14)	0.1051 (5)	0.2802 (8)	0.036 (3)
H11	0.7827	0.1102	0.2181	0.043*
C12	0.3481 (13)	0.0673 (4)	0.3308 (7)	0.027 (2)
H12	0.4130	0.0310	0.3039	0.032*
C13	0.3097 (13)	0.0563 (5)	0.4142 (7)	0.029 (2)
H13	0.3388	0.0115	0.4441	0.035*
C14	0.2264 (13)	0.1122 (5)	0.4554 (7)	0.033 (2)
H14	0.2045	0.1079	0.5156	0.040*
C15	0.1768 (13)	0.1735 (6)	0.4071 (7)	0.031 (2)
H15	0.1160	0.2115	0.4335	0.037*
C16	0.2145 (12)	0.1813 (5)	0.3183 (6)	0.023 (2)
C17	0.1496 (12)	0.2463 (4)	0.2664 (7)	0.024 (2)
C18	0.1739 (13)	0.3160 (5)	0.3025 (8)	0.035 (3)
H18	0.2335	0.3229	0.3606	0.042*
C19	0.1086 (17)	0.3755 (6)	0.2510 (11)	0.052 (4)
H19	0.1232	0.4236	0.2745	0.062*
C20	0.0250 (16)	0.3656 (6)	0.1683 (10)	0.046 (3)
H20	−0.0162	0.4068	0.1337	0.055*
C21	−0.0010 (15)	0.2976 (6)	0.1341 (8)	0.045 (3)
H21	−0.0622	0.2914	0.0762	0.054*
C22	0.0612 (12)	0.2370 (5)	0.1830 (7)	0.028 (2)
H22	0.0426	0.1892	0.1589	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.02761 (18)	0.01791 (14)	0.02340 (18)	−0.0005 (2)	0.00489 (12)	0.0005 (2)
Br1	0.0466 (7)	0.0262 (5)	0.0378 (6)	−0.0076 (5)	0.0053 (5)	−0.0108 (5)
Br2	0.0546 (10)	0.0435 (8)	0.0291 (8)	−0.0010 (6)	0.0162 (7)	0.0022 (6)
N1	0.032 (5)	0.026 (4)	0.035 (5)	−0.008 (4)	0.012 (4)	−0.002 (4)
N2	0.018 (5)	0.022 (4)	0.021 (6)	−0.005 (3)	−0.003 (4)	0.006 (4)
C1	0.040 (6)	0.019 (4)	0.048 (7)	0.001 (4)	0.009 (5)	0.008 (5)
C2	0.044 (7)	0.024 (5)	0.062 (9)	−0.010 (5)	0.019 (7)	0.001 (5)
C3	0.039 (7)	0.020 (5)	0.075 (10)	−0.013 (5)	0.020 (7)	−0.010 (6)
C4	0.038 (7)	0.035 (6)	0.047 (7)	−0.006 (5)	0.008 (5)	−0.009 (5)
C5	0.024 (5)	0.031 (5)	0.033 (6)	−0.008 (4)	0.005 (4)	−0.005 (5)
C6	0.027 (6)	0.025 (4)	0.033 (6)	−0.006 (4)	0.003 (4)	0.003 (4)
C7	0.026 (6)	0.067 (8)	0.034 (7)	−0.008 (6)	−0.003 (5)	−0.011 (6)
C8	0.046 (7)	0.067 (8)	0.042 (7)	−0.020 (7)	−0.002 (6)	0.008 (7)
C9	0.046 (8)	0.046 (7)	0.071 (10)	−0.009 (6)	−0.011 (7)	0.026 (7)
C10	0.040 (7)	0.032 (6)	0.061 (9)	−0.007 (5)	−0.012 (6)	−0.002 (6)
C11	0.040 (6)	0.028 (5)	0.039 (7)	−0.001 (5)	0.002 (5)	0.008 (5)
C12	0.032 (5)	0.017 (4)	0.031 (6)	−0.004 (4)	0.000 (4)	0.001 (4)
C13	0.029 (6)	0.025 (5)	0.033 (6)	−0.005 (4)	0.001 (5)	0.007 (4)
C14	0.033 (6)	0.041 (5)	0.026 (6)	−0.006 (5)	0.005 (5)	0.013 (5)
C15	0.027 (6)	0.037 (5)	0.029 (6)	−0.007 (4)	0.010 (4)	−0.007 (5)
C16	0.022 (5)	0.018 (4)	0.027 (5)	−0.004 (4)	0.001 (4)	0.004 (4)
C17	0.026 (5)	0.014 (4)	0.034 (6)	0.000 (4)	0.013 (4)	0.002 (4)
C18	0.026 (5)	0.026 (5)	0.053 (7)	−0.002 (4)	0.005 (5)	−0.002 (5)
C19	0.039 (7)	0.026 (5)	0.095 (12)	−0.005 (5)	0.026 (8)	−0.006 (7)
C20	0.038 (7)	0.027 (6)	0.076 (10)	0.003 (5)	0.018 (7)	0.021 (6)
C21	0.049 (7)	0.044 (7)	0.044 (7)	0.023 (6)	0.012 (6)	0.013 (6)
C22	0.024 (5)	0.029 (5)	0.030 (6)	0.002 (4)	0.005 (4)	0.001 (4)

Geometric parameters (Å, º)

Pt1—N1	2.075 (8)	C9—H9	0.9500
Pt1—N2	2.074 (10)	C10—C11	1.390 (14)
Pt1—Br1	2.4216 (11)	C10—H10	0.9500
Pt1—Br2	2.4258 (15)	C11—H11	0.9500
N1—C5	1.316 (13)	C12—C13	1.347 (14)
N1—C1	1.343 (12)	C12—H12	0.9500
N2—C16	1.303 (12)	C13—C14	1.391 (14)
N2—C12	1.346 (12)	C13—H13	0.9500
C1—C2	1.368 (14)	C14—C15	1.366 (14)
C1—H1	0.9500	C14—H14	0.9500
C2—C3	1.343 (19)	C15—C16	1.418 (13)
C2—H2	0.9500	C15—H15	0.9500
C3—C4	1.356 (16)	C16—C17	1.477 (12)
C3—H3	0.9500	C17—C22	1.370 (14)
C4—C5	1.400 (13)	C17—C18	1.389 (13)

C4—H4	0.9500	C18—C19	1.396 (17)
C5—C6	1.505 (13)	C18—H18	0.9500
C6—C7	1.358 (16)	C19—C20	1.348 (19)
C6—C11	1.406 (14)	C19—H19	0.9500
C7—C8	1.402 (17)	C20—C21	1.351 (16)
C7—H7	0.9500	C20—H20	0.9500
C8—C9	1.363 (17)	C21—C22	1.385 (13)
C8—H8	0.9500	C21—H21	0.9500
C9—C10	1.366 (18)	C22—H22	0.9500

N2—Pt1—N1	89.8 (3)	C9—C10—C11	120.1 (12)
N2—Pt1—Br1	87.3 (3)	C9—C10—H10	119.9
N1—Pt1—Br1	173.9 (2)	C11—C10—H10	119.9
N2—Pt1—Br2	176.9 (3)	C10—C11—C6	118.4 (10)
N1—Pt1—Br2	90.7 (2)	C10—C11—H11	120.8
Br1—Pt1—Br2	92.50 (5)	C6—C11—H11	120.8
C5—N1—C1	120.2 (9)	N2—C12—C13	122.4 (10)
C5—N1—Pt1	124.1 (7)	N2—C12—H12	118.8
C1—N1—Pt1	114.5 (7)	C13—C12—H12	118.8
C16—N2—C12	121.9 (10)	C12—C13—C14	118.4 (9)
C16—N2—Pt1	123.1 (7)	C12—C13—H13	120.8
C12—N2—Pt1	114.4 (7)	C14—C13—H13	120.8
N1—C1—C2	121.6 (12)	C15—C14—C13	118.2 (9)
N1—C1—H1	119.2	C15—C14—H14	120.9
C2—C1—H1	119.2	C13—C14—H14	120.9
C3—C2—C1	118.6 (11)	C14—C15—C16	121.1 (9)
C3—C2—H2	120.7	C14—C15—H15	119.4
C1—C2—H2	120.7	C16—C15—H15	119.4
C2—C3—C4	120.5 (10)	N2—C16—C15	117.8 (9)
C2—C3—H3	119.7	N2—C16—C17	122.5 (9)
C4—C3—H3	119.7	C15—C16—C17	119.5 (8)
C3—C4—C5	119.2 (11)	C22—C17—C18	120.3 (9)
C3—C4—H4	120.4	C22—C17—C16	119.1 (8)
C5—C4—H4	120.4	C18—C17—C16	120.5 (9)
N1—C5—C4	119.7 (10)	C17—C18—C19	118.2 (11)
N1—C5—C6	120.4 (9)	C17—C18—H18	120.9
C4—C5—C6	119.9 (9)	C19—C18—H18	120.9
C7—C6—C11	120.4 (10)	C20—C19—C18	120.8 (11)
C7—C6—C5	120.3 (9)	C20—C19—H19	119.6
C11—C6—C5	119.3 (9)	C18—C19—H19	119.6
C6—C7—C8	120.8 (11)	C19—C20—C21	120.7 (11)
C6—C7—H7	119.6	C19—C20—H20	119.6
C8—C7—H7	119.6	C21—C20—H20	119.6
C9—C8—C7	118.3 (12)	C20—C21—C22	120.4 (12)
C9—C8—H8	120.9	C20—C21—H21	119.8
C7—C8—H8	120.9	C22—C21—H21	119.8
C8—C9—C10	122.0 (12)	C17—C22—C21	119.5 (9)
C8—C9—H9	119.0	C17—C22—H22	120.3

C10—C9—H9	119.0	C21—C22—H22	120.3
N2—Pt1—N1—C5	51.4 (8)	C8—C9—C10—C11	−0.3 (19)
Br2—Pt1—N1—C5	−125.5 (7)	C9—C10—C11—C6	1.2 (16)
N2—Pt1—N1—C1	−116.7 (7)	C7—C6—C11—C10	−1.2 (15)
Br2—Pt1—N1—C1	66.4 (7)	C5—C6—C11—C10	179.0 (9)
N1—Pt1—N2—C16	55.9 (9)	C16—N2—C12—C13	2.7 (16)
Br1—Pt1—N2—C16	−118.6 (9)	Pt1—N2—C12—C13	174.1 (8)
N1—Pt1—N2—C12	−115.3 (8)	N2—C12—C13—C14	−4.8 (15)
Br1—Pt1—N2—C12	70.1 (8)	C12—C13—C14—C15	4.4 (15)
C5—N1—C1—C2	−1.1 (15)	C13—C14—C15—C16	−2.2 (14)
Pt1—N1—C1—C2	167.5 (8)	C12—N2—C16—C15	−0.2 (15)
N1—C1—C2—C3	−2.1 (16)	Pt1—N2—C16—C15	−170.9 (7)
C1—C2—C3—C4	3.6 (17)	C12—N2—C16—C17	−176.5 (9)
C2—C3—C4—C5	−2.0 (16)	Pt1—N2—C16—C17	12.9 (14)
C1—N1—C5—C4	2.7 (14)	C14—C15—C16—N2	0.1 (14)
Pt1—N1—C5—C4	−164.7 (7)	C14—C15—C16—C17	176.4 (9)
C1—N1—C5—C6	−174.7 (8)	N2—C16—C17—C22	45.9 (13)
Pt1—N1—C5—C6	17.9 (12)	C15—C16—C17—C22	−130.2 (9)
C3—C4—C5—N1	−1.2 (15)	N2—C16—C17—C18	−135.6 (10)
C3—C4—C5—C6	176.2 (9)	C15—C16—C17—C18	48.2 (13)
N1—C5—C6—C7	−132.2 (11)	C22—C17—C18—C19	−1.0 (14)
C4—C5—C6—C7	50.3 (13)	C16—C17—C18—C19	−179.4 (9)
N1—C5—C6—C11	47.6 (13)	C17—C18—C19—C20	−0.4 (16)
C4—C5—C6—C11	−129.9 (10)	C18—C19—C20—C21	1.5 (18)
C11—C6—C7—C8	0.2 (16)	C19—C20—C21—C22	−1.3 (17)
C5—C6—C7—C8	−180.0 (9)	C18—C17—C22—C21	1.2 (14)
C6—C7—C8—C9	0.7 (17)	C16—C17—C22—C21	179.7 (8)
C7—C8—C9—C10	−0.7 (18)	C20—C21—C22—C17	−0.1 (15)