

cis-Bis[(1-adamantylmethyl)amine- κ N]-dichloridoplatinum(II) *N,N*-dimethylformamide solvate

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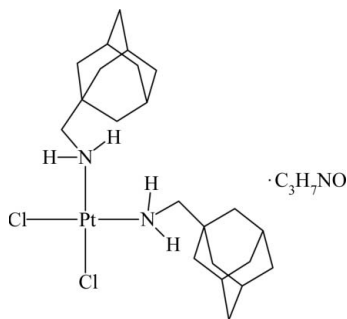
Received 18 August 2009; accepted 19 September 2009

 Key indicators: single-crystal X-ray study; $T = 200$ K; mean $\sigma(\text{C}-\text{C}) = 0.018$ Å; R factor = 0.059; wR factor = 0.152; data-to-parameter ratio = 16.0.

The asymmetric unit of the title compound {systematic name: *cis*-dichloridobis[(3,7-dimethylbicyclo[3.3.1]non-1-ylmethyl)amine- κ N]platinum(II) *N,N*-dimethylformamide solvate}, [PtCl₂(C₁₁H₁₉N)₂] \cdot C₃H₇NO, consists of two metrically similar Pt complexes and two dimethylformamide solvent molecules. Each Pt^{II} center is coordinated by the amine groups of two (1-adamantylmethyl)amine ligands and two Cl atoms in a *cis*-square-planar arrangement. The Pt^{II} centers lie slightly outside [0.031 (4) and 0.038 (4) Å] the coordination planes. The N–Pt–N and Cl–Pt–Cl angles [92.1 (4)–92.30 (11)°] are slightly more open than the N–Pt–Cl angles [87.3 (3)–88.3 (3)°]. N–H \cdots O and N–H \cdots Cl intermolecular hydrogen bonds are observed, forming two discrete pairs of complexes and solvent molecules.

Related literature

For the antiviral and antitumor activity of Pt complexes with polycyclic cages such as adamantamine, see: Hay *et al.* (1985); Ho *et al.* (1972); Widell *et al.* (1986). The synthesis and spectroscopic characterization of the title compound is described by Rochon *et al.* (1993).



Experimental

Crystal data

 [PtCl₂(C₁₁H₁₉N)₂] \cdot C₃H₇NO

 $M_r = 669.63$

 Triclinic, $P\bar{1}$
 $a = 12.299$ (3) Å

 $b = 14.035$ (4) Å

 $c = 15.644$ (4) Å

 $\alpha = 81.137$ (3)°

 $\beta = 82.323$ (3)°

 $\gamma = 89.292$ (3)°

 $V = 2644.3$ (12) Å³
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 5.53$ mm⁻¹
 $T = 200$ K

 $0.35 \times 0.29 \times 0.23$ mm

Data collection

Bruker SMART APEXII CCD diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 2001)

 $T_{\min} = 0.151$, $T_{\max} = 0.281$

26513 measured reflections

9285 independent reflections

 5724 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.099$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.059$
 $wR(F^2) = 0.152$
 $S = 0.97$

9285 reflections

581 parameters

H-atom parameters constrained

 $\Delta\rho_{\max} = 7.80$ e Å⁻³
 $\Delta\rho_{\min} = -2.82$ e Å⁻³
Table 1

Selected bond lengths (Å).

| | | | |
|----------|-----------|----------|-----------|
| Pt1–N11 | 2.040 (9) | Pt2–N21 | 2.048 (8) |
| Pt1–N12 | 2.026 (9) | Pt2–N22 | 2.056 (9) |
| Pt1–Cl11 | 2.304 (3) | Pt2–Cl21 | 2.307 (3) |
| Pt1–Cl12 | 2.312 (3) | Pt2–Cl22 | 2.306 (3) |

Table 2

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------------------------|-------|-------------|-------------|---------------|
| N11–H11A \cdots O2 | 0.92 | 1.95 | 2.863 (13) | 170 |
| N11–H11B \cdots Cl12 ⁱ | 0.92 | 2.64 | 3.409 (10) | 141 |
| N12–H12A \cdots Cl11 ⁱ | 0.92 | 2.63 | 3.299 (9) | 131 |
| N12–H12B \cdots O2 | 0.92 | 1.93 | 2.843 (11) | 175 |
| N21–H21A \cdots Cl22 ⁱⁱ | 0.92 | 2.55 | 3.238 (10) | 132 |
| N21–H21B \cdots O1 | 0.92 | 1.91 | 2.821 (12) | 173 |
| N22–H22A \cdots O1 | 0.92 | 1.94 | 2.843 (11) | 165 |
| N22–H22B \cdots Cl21 ⁱⁱ | 0.92 | 2.64 | 3.354 (10) | 136 |

 Symmetry codes: (i) $-x + 2, -y, -z + 2$; (ii) $-x + 1, -y + 1, -z + 2$.

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL and publCIF (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2221).

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supporting information

Acta Cryst. (2009). E65, m1297–m1298 [https://doi.org/10.1107/S1600536809037982]

cis-Bis[(1-adamantylmethyl)amine- κ N]dichloridoplatinum(II) *N,N*-dimethylformamide solvate

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S1. Comment

Cisplatin [*cis*-Pt(NH₃)₂Cl₂] is now a well known antitumor drug, but it has numerous side effects and resistance to the drug is an important problem. Replacement of the NH₃ ligand by an amine more compatible to the human system might possibly surmount some of these problems. One such amine is the polycyclic cage molecule adamantanamine, which has been demonstrated to exhibit both antiviral (Hay *et al.*, 1985; Widell *et al.*, 1986) and antitumor activity (Ho *et al.*, 1972). The synthesis and the spectroscopic study of Pt^{II} compounds with adamantanamine derivatives have been reported (Rochon *et al.*, 1993).

In the title compound (one of the Pt complex is shown in Fig. 1), the Pt metal center exhibits a *cis* square-planar geometry formed by two amine groups from (1-adamantylmethyl)amine and two Cl atoms. The Pt centers are slightly outside [0.031 (4) and 0.038 (4) Å] the N₂Cl₂ planes. The bulky adamantane cycles slightly open the N—Pt—N angles [92.1 (4)°] compared to the N—Pt—Cl angles [87.3 (3)–88.3 (3)°]. However, the Cl—Pt—Cl angles are also opened to the same extent [92.17 (11)–92.30 (11)°]. The Pt—N [2.026 (9)–2.056 (9) Å] and Pt—Cl [2.304 (3)–2.312 (3) Å] are normal as well as all other bond distances and angles.

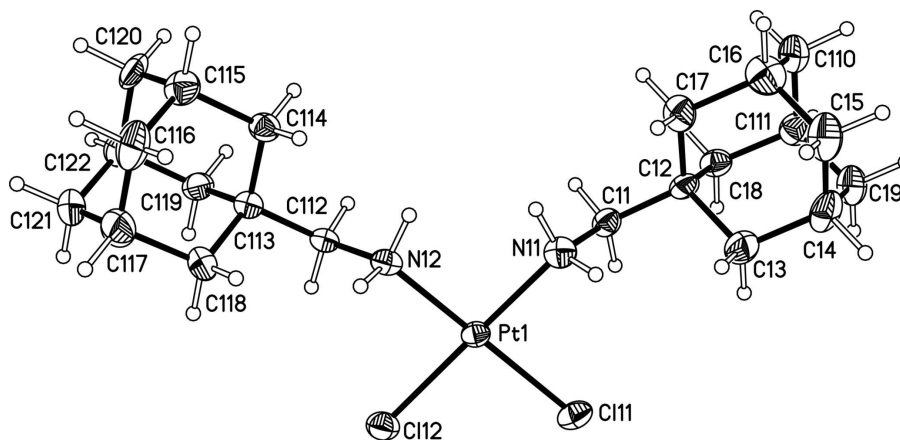
The asymmetric unit of the title compound is described as two crystallographically independent Pt complexes and two dimethylformamide (DMF) solvent molecules linked by N—H···O hydrogen bonds (Fig. 2) between the amine groups and the O atoms from the DMF molecules. N—H···Cl hydrogen bonds between the amine groups and Cl atoms from symmetry equivalent complexes are also observed, forming discrete pairs of complexes and solvent molecules (Fig. 3).

S2. Experimental

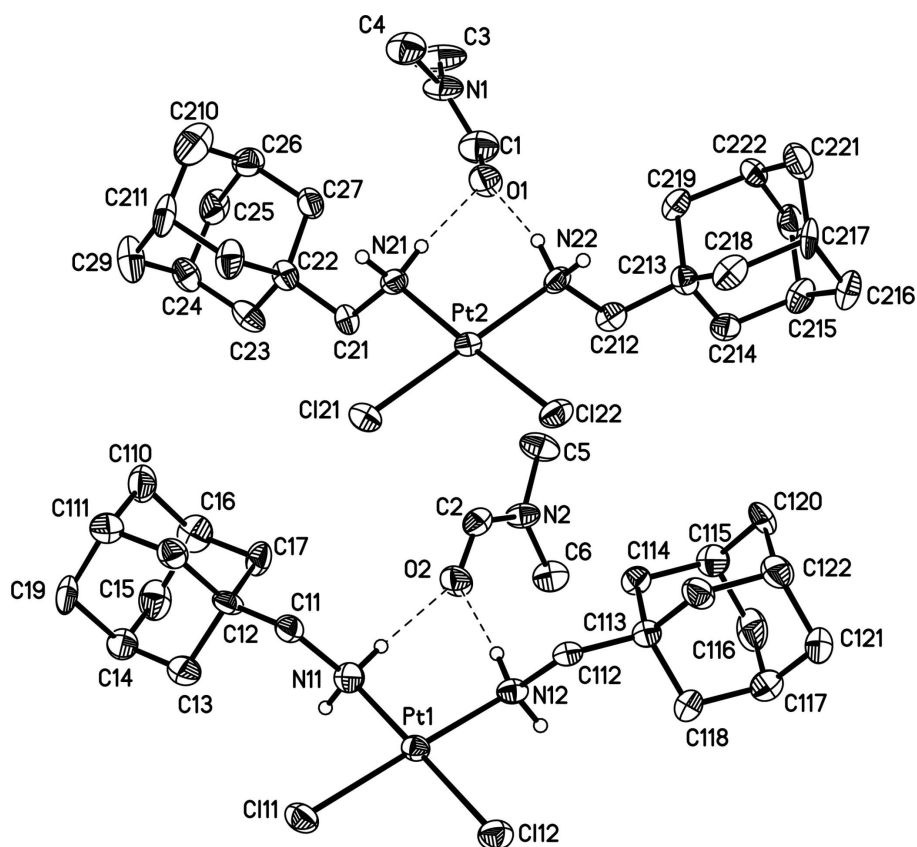
One mmol of K₂[PtCl₄] and 2 mmol of (1-adamantylmethyl)amine were heated in a DMF solution at 80°C for 3 h. The solution was concentrated, cooled to 0°C and the KCl was filtered off. The mixture was evaporated to dryness and the residue washed with ether, acetone and then with water. After drying, the residue was washed with ether and dried. Yield 68%, dec. 195–225°C, ν (Pt—Cl) IR 341, 325, Raman 334, 325 cm⁻¹, ¹⁹⁵Pt NMR -2213 p.p.m. The crystals were recrystallized in DMF for crystallographic studies.

S3. Refinement

H atoms were placed at calculated positions (C—H = 0.95–1.00 Å, N—H = 0.92 Å) and were allowed to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ for the CH, CH₂ and NH₂ groups and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for the CH₃ groups. The highest residual electron density was found 1.0 Å from Pt2.

**Figure 1**

A view of one of the crystallographically independent molecules of the title compound. Displacement ellipsoids are shown at the 50% probability level.

**Figure 2**

A view of the asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms not participating in hydrogen bonds have been omitted for clarity.

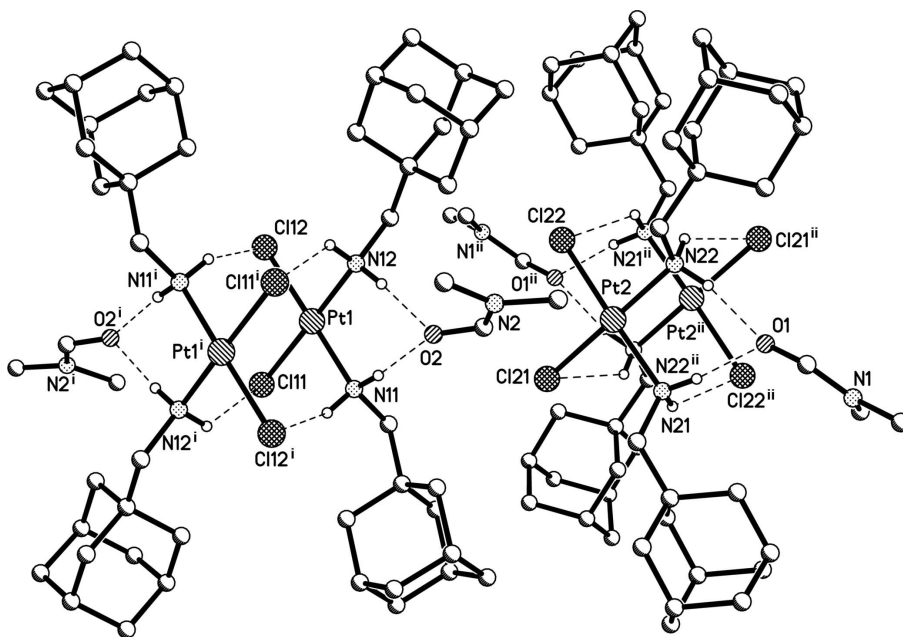


Figure 3

The hydrogen bonding pattern in the title compound. H atoms not participating in hydrogen bonds have been omitted for clarity. [Symmetry codes: (i) $-x+2, -y, -z+2$; (ii) $-x+1, -y+1, -z+2$.]

cis-dichloridobis[(3,7-dimethyl-bicyclo[3.3.1]non-1-ylmethyl)amine- κN]platinum(II) *N,N*-dimethylformamide solvate}

Crystal data

$[\text{PtCl}_2(\text{C}_{11}\text{H}_{19}\text{N})_2] \cdot \text{C}_3\text{H}_7\text{NO}$

$M_r = 669.63$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 12.299\ (3)\ \text{\AA}$

$b = 14.035\ (4)\ \text{\AA}$

$c = 15.644\ (4)\ \text{\AA}$

$\alpha = 81.137\ (3)^\circ$

$\beta = 82.323\ (3)^\circ$

$\gamma = 89.292\ (3)^\circ$

$V = 2644.3\ (12)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1344$

$D_x = 1.682\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 6035 reflections

$\theta = 2.2\text{--}26.3^\circ$

$\mu = 5.53\ \text{mm}^{-1}$

$T = 200\ \text{K}$

Block, yellow

$0.35 \times 0.29 \times 0.23\ \text{mm}$

Data collection

Bruker SMART APEXII CCD
diffractometer

Radiation source: normal-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2001)

$T_{\min} = 0.151, T_{\max} = 0.281$

26513 measured reflections

9285 independent reflections

5724 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.099$

$\theta_{\max} = 25.0^\circ, \theta_{\min} = 1.5^\circ$

$h = -14 \rightarrow 14$

$k = -16 \rightarrow 16$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.059$

$wR(F^2) = 0.152$

$S = 0.97$

9285 reflections

581 parameters

0 restraints

0 constraints

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

$w = 1/[\sigma^2(F_o^2) + (0.0732P)^2]$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 7.80 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -2.82 \text{ e } \text{\AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|-------------|--------------|-------------|----------------------------------|
| Pt1 | 1.00670 (3) | 0.12043 (3) | 0.99942 (3) | 0.02177 (15) |
| Pt2 | 0.50836 (3) | 0.38164 (3) | 0.99668 (3) | 0.02119 (15) |
| Cl11 | 1.1120 (2) | 0.0882 (2) | 1.1116 (2) | 0.0311 (7) |
| Cl12 | 1.1596 (2) | 0.1589 (2) | 0.8970 (2) | 0.0313 (7) |
| Cl21 | 0.6257 (2) | 0.3401 (2) | 1.0995 (2) | 0.0306 (7) |
| Cl22 | 0.6520 (2) | 0.4151 (2) | 0.8854 (2) | 0.0308 (7) |
| N11 | 0.8725 (7) | 0.0841 (7) | 1.0899 (6) | 0.028 (2) |
| H11A | 0.8125 | 0.0835 | 1.0606 | 0.034* |
| H11B | 0.8818 | 0.0220 | 1.1168 | 0.034* |
| N12 | 0.9139 (7) | 0.1428 (6) | 0.9006 (6) | 0.024 (2) |
| H12A | 0.9334 | 0.0971 | 0.8651 | 0.029* |
| H12B | 0.8421 | 0.1302 | 0.9247 | 0.029* |
| N21 | 0.3800 (7) | 0.3594 (7) | 1.0955 (6) | 0.025 (2) |
| H21A | 0.3861 | 0.4046 | 1.1315 | 0.030* |
| H21B | 0.3165 | 0.3728 | 1.0710 | 0.030* |
| N22 | 0.4049 (7) | 0.4215 (7) | 0.9047 (6) | 0.025 (2) |
| H22A | 0.3353 | 0.4261 | 0.9336 | 0.030* |
| H22B | 0.4255 | 0.4822 | 0.8764 | 0.030* |
| C11 | 0.8455 (9) | 0.1455 (8) | 1.1597 (8) | 0.026 (3) |
| H11C | 0.8083 | 0.2042 | 1.1347 | 0.031* |
| H11D | 0.9151 | 0.1664 | 1.1767 | 0.031* |
| C12 | 0.7745 (8) | 0.0994 (8) | 1.2407 (8) | 0.027 (3) |
| C13 | 0.8333 (10) | 0.0124 (9) | 1.2863 (9) | 0.037 (3) |
| H13A | 0.8459 | -0.0371 | 1.2474 | 0.044* |
| H13B | 0.9056 | 0.0332 | 1.2985 | 0.044* |
| C14 | 0.7644 (11) | -0.0307 (9) | 1.3717 (9) | 0.040 (3) |
| H14 | 0.8035 | -0.0870 | 1.4008 | 0.048* |
| C15 | 0.6534 (11) | -0.0633 (10) | 1.3540 (10) | 0.046 (4) |
| H15A | 0.6093 | -0.0920 | 1.4095 | 0.055* |
| H15B | 0.6633 | -0.1130 | 1.3151 | 0.055* |
| C16 | 0.5936 (10) | 0.0243 (10) | 1.3106 (9) | 0.042 (4) |
| H16 | 0.5208 | 0.0030 | 1.2983 | 0.050* |
| C17 | 0.6638 (9) | 0.0671 (9) | 1.2227 (8) | 0.033 (3) |

| | | | | |
|------|-------------|-------------|------------|-----------|
| H17A | 0.6739 | 0.0177 | 1.1835 | 0.040* |
| H17B | 0.6254 | 0.1227 | 1.1934 | 0.040* |
| C18 | 0.7575 (9) | 0.1732 (9) | 1.3017 (8) | 0.029 (3) |
| H18A | 0.7190 | 0.2295 | 1.2737 | 0.035* |
| H18B | 0.8299 | 0.1957 | 1.3122 | 0.035* |
| C19 | 0.7469 (11) | 0.0470 (10) | 1.4320 (8) | 0.042 (3) |
| H19A | 0.7021 | 0.0198 | 1.4875 | 0.050* |
| H19B | 0.8188 | 0.0670 | 1.4455 | 0.050* |
| C110 | 0.5759 (10) | 0.1016 (10) | 1.3705 (9) | 0.042 (3) |
| H11E | 0.5299 | 0.0753 | 1.4257 | 0.051* |
| H11F | 0.5382 | 0.1579 | 1.3417 | 0.051* |
| C111 | 0.6906 (10) | 0.1326 (10) | 1.3894 (9) | 0.037 (3) |
| H111 | 0.6818 | 0.1832 | 1.4284 | 0.044* |
| C112 | 0.9164 (8) | 0.2395 (8) | 0.8425 (7) | 0.025 (3) |
| H11G | 0.9935 | 0.2625 | 0.8288 | 0.030* |
| H11H | 0.8749 | 0.2860 | 0.8755 | 0.030* |
| C113 | 0.8697 (9) | 0.2402 (8) | 0.7573 (8) | 0.028 (3) |
| C114 | 0.7502 (8) | 0.2058 (8) | 0.7745 (8) | 0.026 (3) |
| H11I | 0.7063 | 0.2472 | 0.8117 | 0.031* |
| H11J | 0.7457 | 0.1387 | 0.8057 | 0.031* |
| C115 | 0.7041 (10) | 0.2106 (9) | 0.6873 (9) | 0.033 (3) |
| H115 | 0.6259 | 0.1881 | 0.6991 | 0.040* |
| C116 | 0.7692 (11) | 0.1466 (10) | 0.6313 (9) | 0.046 (4) |
| H11K | 0.7388 | 0.1496 | 0.5755 | 0.055* |
| H11L | 0.7637 | 0.0791 | 0.6613 | 0.055* |
| C117 | 0.8906 (11) | 0.1789 (10) | 0.6129 (9) | 0.046 (4) |
| H117 | 0.9343 | 0.1358 | 0.5763 | 0.055* |
| C118 | 0.9350 (9) | 0.1754 (9) | 0.7006 (8) | 0.034 (3) |
| H11M | 0.9313 | 0.1082 | 0.7316 | 0.040* |
| H11N | 1.0129 | 0.1961 | 0.6898 | 0.040* |
| C119 | 0.8761 (9) | 0.3426 (9) | 0.7076 (8) | 0.033 (3) |
| H11O | 0.8344 | 0.3862 | 0.7438 | 0.040* |
| H11P | 0.9536 | 0.3647 | 0.6960 | 0.040* |
| C120 | 0.7092 (10) | 0.3150 (9) | 0.6396 (9) | 0.039 (3) |
| H12C | 0.6655 | 0.3573 | 0.6760 | 0.046* |
| H12D | 0.6785 | 0.3185 | 0.5838 | 0.046* |
| C121 | 0.8971 (10) | 0.2848 (10) | 0.5652 (9) | 0.042 (3) |
| H12E | 0.9745 | 0.3072 | 0.5535 | 0.051* |
| H12F | 0.8683 | 0.2886 | 0.5087 | 0.051* |
| C122 | 0.8302 (10) | 0.3481 (9) | 0.6220 (9) | 0.036 (3) |
| H122 | 0.8347 | 0.4163 | 0.5916 | 0.043* |
| C21 | 0.3643 (9) | 0.2604 (8) | 1.1537 (7) | 0.025 (3) |
| H21C | 0.3335 | 0.2147 | 1.1208 | 0.030* |
| H21D | 0.4369 | 0.2359 | 1.1672 | 0.030* |
| C22 | 0.2910 (9) | 0.2626 (8) | 1.2367 (8) | 0.027 (3) |
| C23 | 0.2776 (9) | 0.1592 (8) | 1.2867 (9) | 0.033 (3) |
| H23A | 0.2448 | 0.1177 | 1.2510 | 0.040* |
| H23B | 0.3506 | 0.1330 | 1.2973 | 0.040* |

| | | | | |
|------|-------------|-------------|-------------|-----------|
| C24 | 0.2043 (10) | 0.1579 (10) | 1.3739 (9) | 0.036 (3) |
| H24 | 0.1973 | 0.0902 | 1.4055 | 0.043* |
| C25 | 0.0903 (10) | 0.1947 (9) | 1.3549 (9) | 0.041 (3) |
| H25A | 0.0592 | 0.1529 | 1.3185 | 0.049* |
| H25B | 0.0403 | 0.1921 | 1.4103 | 0.049* |
| C26 | 0.0996 (10) | 0.2980 (9) | 1.3072 (9) | 0.036 (3) |
| H26 | 0.0254 | 0.3223 | 1.2955 | 0.044* |
| C27 | 0.1764 (9) | 0.3021 (9) | 1.2207 (8) | 0.034 (3) |
| H27A | 0.1837 | 0.3696 | 1.1908 | 0.041* |
| H27B | 0.1444 | 0.2634 | 1.1823 | 0.041* |
| C28 | 0.3380 (10) | 0.3259 (9) | 1.2930 (8) | 0.037 (3) |
| H28A | 0.3457 | 0.3928 | 1.2615 | 0.045* |
| H28B | 0.4119 | 0.3027 | 1.3040 | 0.045* |
| C29 | 0.2507 (12) | 0.2204 (10) | 1.4295 (9) | 0.050 (4) |
| H29A | 0.3228 | 0.1952 | 1.4437 | 0.059* |
| H29B | 0.2010 | 0.2195 | 1.4849 | 0.059* |
| C210 | 0.1496 (14) | 0.3623 (11) | 1.3623 (11) | 0.061 (5) |
| H21E | 0.1013 | 0.3623 | 1.4183 | 0.073* |
| H21F | 0.1558 | 0.4293 | 1.3311 | 0.073* |
| C211 | 0.2644 (12) | 0.3252 (10) | 1.3804 (8) | 0.042 (3) |
| H211 | 0.2971 | 0.3670 | 1.4168 | 0.050* |
| C212 | 0.3992 (9) | 0.3588 (9) | 0.8380 (8) | 0.031 (3) |
| H21G | 0.3533 | 0.3019 | 0.8650 | 0.037* |
| H21H | 0.4741 | 0.3354 | 0.8211 | 0.037* |
| C213 | 0.3545 (8) | 0.4031 (8) | 0.7564 (8) | 0.026 (3) |
| C214 | 0.3578 (9) | 0.3252 (9) | 0.6998 (8) | 0.031 (3) |
| H21I | 0.3122 | 0.2697 | 0.7310 | 0.037* |
| H21J | 0.4341 | 0.3028 | 0.6879 | 0.037* |
| C215 | 0.3149 (10) | 0.3628 (9) | 0.6132 (8) | 0.032 (3) |
| H215 | 0.3187 | 0.3102 | 0.5765 | 0.039* |
| C216 | 0.3852 (10) | 0.4487 (9) | 0.5644 (8) | 0.037 (3) |
| H21K | 0.4624 | 0.4286 | 0.5519 | 0.044* |
| H21L | 0.3582 | 0.4728 | 0.5082 | 0.044* |
| C217 | 0.3781 (10) | 0.5276 (9) | 0.6210 (8) | 0.035 (3) |
| H217 | 0.4234 | 0.5841 | 0.5896 | 0.042* |
| C218 | 0.4229 (9) | 0.4896 (9) | 0.7074 (8) | 0.032 (3) |
| H21M | 0.5004 | 0.4703 | 0.6949 | 0.038* |
| H21N | 0.4201 | 0.5413 | 0.7441 | 0.038* |
| C219 | 0.2345 (9) | 0.4343 (9) | 0.7761 (8) | 0.030 (3) |
| H21O | 0.2301 | 0.4862 | 0.8127 | 0.036* |
| H21P | 0.1894 | 0.3790 | 0.8085 | 0.036* |
| C220 | 0.1947 (9) | 0.3931 (10) | 0.6334 (8) | 0.037 (3) |
| H22C | 0.1645 | 0.4156 | 0.5783 | 0.045* |
| H22D | 0.1503 | 0.3372 | 0.6654 | 0.045* |
| C221 | 0.2589 (11) | 0.5595 (10) | 0.6414 (9) | 0.044 (4) |
| H22E | 0.2552 | 0.6098 | 0.6796 | 0.053* |
| H22F | 0.2302 | 0.5868 | 0.5867 | 0.053* |
| C222 | 0.1897 (10) | 0.4717 (10) | 0.6873 (8) | 0.036 (3) |

| | | | | |
|------|--------------|-------------|-------------|-----------|
| H222 | 0.1116 | 0.4919 | 0.6998 | 0.044* |
| O1 | 0.1953 (6) | 0.4012 (6) | 1.0075 (6) | 0.038 (2) |
| N1 | 0.0234 (8) | 0.4174 (7) | 1.0768 (8) | 0.039 (3) |
| C1 | 0.0970 (10) | 0.3779 (10) | 1.0247 (10) | 0.045 (4) |
| H1 | 0.0729 | 0.3271 | 0.9978 | 0.054* |
| C3 | -0.0896 (10) | 0.3810 (10) | 1.0928 (12) | 0.059 (5) |
| H3A | -0.0946 | 0.3247 | 1.0633 | 0.088* |
| H3B | -0.1385 | 0.4315 | 1.0701 | 0.088* |
| H3C | -0.1112 | 0.3622 | 1.1557 | 0.088* |
| C4 | 0.0489 (10) | 0.4994 (9) | 1.1196 (10) | 0.043 (3) |
| H4A | 0.1243 | 0.5217 | 1.0982 | 0.064* |
| H4B | 0.0416 | 0.4789 | 1.1829 | 0.064* |
| H4C | -0.0021 | 0.5521 | 1.1062 | 0.064* |
| O2 | 0.6969 (6) | 0.1013 (6) | 0.9856 (6) | 0.035 (2) |
| N2 | 0.5460 (7) | 0.0836 (7) | 0.9195 (7) | 0.030 (2) |
| C2 | 0.6048 (9) | 0.1270 (9) | 0.9700 (8) | 0.029 (3) |
| H2 | 0.5732 | 0.1803 | 0.9948 | 0.035* |
| C5 | 0.4361 (9) | 0.1158 (9) | 0.9092 (10) | 0.041 (4) |
| H5A | 0.4165 | 0.1666 | 0.9448 | 0.061* |
| H5B | 0.3847 | 0.0615 | 0.9281 | 0.061* |
| H5C | 0.4323 | 0.1412 | 0.8477 | 0.061* |
| C6 | 0.5893 (9) | 0.0038 (8) | 0.8775 (9) | 0.036 (3) |
| H6A | 0.6606 | -0.0147 | 0.8962 | 0.055* |
| H6B | 0.5984 | 0.0231 | 0.8141 | 0.055* |
| H6C | 0.5384 | -0.0511 | 0.8939 | 0.055* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|------|-------------|-------------|-------------|--------------|---------------|--------------|
| Pt1 | 0.0202 (2) | 0.0212 (3) | 0.0250 (3) | 0.00066 (18) | -0.00497 (19) | -0.0053 (2) |
| Pt2 | 0.0207 (2) | 0.0200 (3) | 0.0230 (3) | 0.00236 (18) | -0.00192 (19) | -0.0046 (2) |
| Cl11 | 0.0281 (15) | 0.0326 (18) | 0.0365 (19) | 0.0051 (12) | -0.0141 (13) | -0.0093 (15) |
| Cl12 | 0.0241 (14) | 0.0338 (18) | 0.0350 (19) | 0.0010 (12) | -0.0014 (12) | -0.0045 (14) |
| Cl21 | 0.0255 (14) | 0.0323 (18) | 0.0346 (19) | 0.0047 (12) | -0.0092 (13) | -0.0031 (14) |
| Cl22 | 0.0259 (14) | 0.0320 (18) | 0.0324 (18) | 0.0024 (12) | 0.0055 (12) | -0.0066 (14) |
| N11 | 0.028 (5) | 0.028 (6) | 0.030 (6) | -0.001 (4) | -0.006 (4) | -0.008 (5) |
| N12 | 0.019 (5) | 0.021 (5) | 0.031 (6) | 0.000 (4) | 0.000 (4) | -0.003 (4) |
| N21 | 0.026 (5) | 0.024 (6) | 0.024 (6) | 0.004 (4) | 0.001 (4) | -0.002 (4) |
| N22 | 0.022 (5) | 0.032 (6) | 0.022 (6) | 0.002 (4) | 0.003 (4) | -0.007 (5) |
| C11 | 0.028 (6) | 0.024 (7) | 0.026 (7) | 0.004 (5) | -0.006 (5) | -0.003 (5) |
| C12 | 0.024 (6) | 0.023 (7) | 0.032 (8) | 0.008 (5) | -0.005 (5) | 0.003 (5) |
| C13 | 0.039 (7) | 0.034 (8) | 0.037 (8) | 0.010 (6) | -0.006 (6) | -0.002 (6) |
| C14 | 0.063 (9) | 0.023 (7) | 0.033 (8) | 0.019 (6) | -0.009 (7) | -0.003 (6) |
| C15 | 0.064 (10) | 0.036 (9) | 0.036 (9) | -0.005 (7) | -0.005 (7) | -0.001 (7) |
| C16 | 0.041 (8) | 0.040 (9) | 0.046 (9) | -0.010 (6) | -0.006 (7) | -0.011 (7) |
| C17 | 0.038 (7) | 0.040 (8) | 0.024 (7) | -0.003 (6) | -0.006 (6) | -0.014 (6) |
| C18 | 0.025 (6) | 0.033 (7) | 0.032 (8) | 0.000 (5) | -0.008 (5) | -0.007 (6) |
| C19 | 0.050 (8) | 0.060 (10) | 0.016 (7) | 0.003 (7) | -0.005 (6) | -0.011 (7) |

| | | | | | | |
|------|------------|------------|------------|------------|------------|------------|
| C110 | 0.044 (8) | 0.056 (10) | 0.026 (8) | 0.000 (7) | -0.004 (6) | -0.003 (7) |
| C111 | 0.038 (7) | 0.035 (8) | 0.038 (9) | 0.008 (6) | -0.007 (6) | -0.008 (6) |
| C112 | 0.019 (5) | 0.030 (7) | 0.026 (7) | 0.006 (5) | 0.000 (5) | -0.005 (5) |
| C113 | 0.023 (6) | 0.033 (7) | 0.026 (7) | 0.004 (5) | -0.001 (5) | -0.003 (6) |
| C114 | 0.022 (6) | 0.029 (7) | 0.028 (7) | -0.002 (5) | -0.002 (5) | -0.007 (5) |
| C115 | 0.034 (7) | 0.034 (8) | 0.035 (8) | 0.000 (5) | -0.009 (6) | -0.012 (6) |
| C116 | 0.066 (10) | 0.046 (9) | 0.031 (9) | -0.002 (7) | -0.018 (7) | -0.013 (7) |
| C117 | 0.051 (8) | 0.054 (10) | 0.033 (9) | 0.021 (7) | -0.003 (6) | -0.012 (7) |
| C118 | 0.033 (7) | 0.041 (8) | 0.025 (7) | 0.004 (6) | 0.002 (5) | -0.003 (6) |
| C119 | 0.023 (6) | 0.038 (8) | 0.033 (8) | 0.001 (5) | -0.003 (5) | 0.007 (6) |
| C120 | 0.044 (8) | 0.049 (9) | 0.026 (8) | 0.016 (6) | -0.018 (6) | -0.002 (6) |
| C121 | 0.042 (7) | 0.059 (10) | 0.023 (8) | 0.009 (6) | -0.002 (6) | 0.000 (7) |
| C122 | 0.038 (7) | 0.030 (8) | 0.035 (8) | 0.005 (6) | -0.003 (6) | 0.005 (6) |
| C21 | 0.028 (6) | 0.026 (7) | 0.022 (7) | -0.003 (5) | -0.008 (5) | -0.001 (5) |
| C22 | 0.030 (6) | 0.024 (7) | 0.027 (7) | -0.004 (5) | -0.009 (5) | -0.002 (5) |
| C23 | 0.031 (6) | 0.024 (7) | 0.046 (9) | -0.005 (5) | -0.020 (6) | 0.001 (6) |
| C24 | 0.038 (7) | 0.035 (8) | 0.032 (8) | -0.005 (6) | -0.008 (6) | 0.008 (6) |
| C25 | 0.048 (8) | 0.039 (8) | 0.028 (8) | -0.006 (6) | 0.010 (6) | 0.004 (6) |
| C26 | 0.039 (7) | 0.032 (8) | 0.036 (8) | 0.004 (6) | 0.002 (6) | -0.002 (6) |
| C27 | 0.032 (7) | 0.043 (8) | 0.025 (7) | 0.004 (6) | -0.005 (5) | 0.001 (6) |
| C28 | 0.053 (8) | 0.032 (8) | 0.029 (8) | -0.011 (6) | -0.010 (6) | -0.009 (6) |
| C29 | 0.072 (10) | 0.047 (9) | 0.030 (9) | -0.017 (8) | -0.017 (7) | 0.002 (7) |
| C210 | 0.100 (13) | 0.033 (9) | 0.043 (10) | -0.003 (8) | 0.015 (9) | -0.003 (8) |
| C211 | 0.067 (9) | 0.042 (9) | 0.017 (7) | -0.010 (7) | -0.003 (6) | -0.008 (6) |
| C212 | 0.029 (6) | 0.032 (7) | 0.031 (8) | 0.001 (5) | -0.002 (5) | -0.009 (6) |
| C213 | 0.022 (6) | 0.031 (7) | 0.027 (7) | -0.003 (5) | -0.006 (5) | -0.002 (6) |
| C214 | 0.019 (6) | 0.042 (8) | 0.032 (8) | 0.003 (5) | -0.004 (5) | -0.006 (6) |
| C215 | 0.039 (7) | 0.033 (8) | 0.028 (8) | -0.011 (6) | -0.001 (6) | -0.015 (6) |
| C216 | 0.038 (7) | 0.051 (9) | 0.020 (7) | -0.010 (6) | 0.003 (5) | -0.006 (6) |
| C217 | 0.047 (8) | 0.044 (8) | 0.010 (7) | -0.009 (6) | 0.003 (5) | 0.004 (6) |
| C218 | 0.031 (6) | 0.030 (7) | 0.037 (8) | -0.012 (5) | 0.001 (5) | -0.016 (6) |
| C219 | 0.025 (6) | 0.042 (8) | 0.026 (7) | -0.003 (5) | 0.001 (5) | -0.013 (6) |
| C220 | 0.032 (7) | 0.055 (9) | 0.025 (8) | -0.002 (6) | -0.009 (5) | -0.001 (7) |
| C221 | 0.063 (9) | 0.039 (9) | 0.031 (8) | 0.009 (7) | -0.015 (7) | 0.001 (7) |
| C222 | 0.032 (7) | 0.050 (9) | 0.027 (8) | 0.015 (6) | -0.010 (6) | -0.001 (7) |
| O1 | 0.022 (4) | 0.051 (6) | 0.038 (6) | 0.001 (4) | -0.001 (4) | 0.002 (4) |
| N1 | 0.037 (6) | 0.023 (6) | 0.060 (8) | 0.007 (5) | -0.009 (5) | -0.015 (6) |
| C1 | 0.042 (8) | 0.035 (8) | 0.060 (11) | 0.000 (6) | -0.009 (7) | -0.015 (7) |
| C3 | 0.024 (7) | 0.040 (9) | 0.113 (15) | 0.002 (6) | 0.002 (8) | -0.026 (9) |
| C4 | 0.045 (8) | 0.031 (8) | 0.057 (10) | 0.000 (6) | -0.012 (7) | -0.017 (7) |
| O2 | 0.021 (4) | 0.047 (6) | 0.037 (6) | -0.001 (4) | -0.007 (4) | -0.002 (4) |
| N2 | 0.022 (5) | 0.026 (6) | 0.044 (7) | 0.001 (4) | -0.004 (4) | -0.013 (5) |
| C2 | 0.031 (7) | 0.028 (7) | 0.029 (8) | 0.001 (5) | 0.001 (5) | -0.008 (6) |
| C5 | 0.024 (6) | 0.035 (8) | 0.062 (10) | 0.000 (5) | -0.010 (6) | -0.002 (7) |
| C6 | 0.036 (7) | 0.026 (7) | 0.048 (9) | -0.004 (5) | -0.004 (6) | -0.010 (6) |

Geometric parameters (Å, °)

| | | | |
|----------|------------|-----------|------------|
| Pt1—N11 | 2.040 (9) | C21—H21C | 0.9900 |
| Pt1—N12 | 2.026 (9) | C21—H21D | 0.9900 |
| Pt1—C111 | 2.304 (3) | C22—C28 | 1.512 (16) |
| Pt1—C112 | 2.312 (3) | C22—C23 | 1.539 (16) |
| Pt2—N21 | 2.048 (8) | C22—C27 | 1.545 (15) |
| Pt2—N22 | 2.056 (9) | C23—C24 | 1.529 (17) |
| Pt2—C121 | 2.307 (3) | C23—H23A | 0.9900 |
| Pt2—C122 | 2.306 (3) | C23—H23B | 0.9900 |
| N11—C11 | 1.493 (14) | C24—C29 | 1.494 (18) |
| N11—H11A | 0.9200 | C24—C25 | 1.539 (17) |
| N11—H11B | 0.9200 | C24—H24 | 1.0000 |
| N12—C112 | 1.511 (14) | C25—C26 | 1.524 (17) |
| N12—H12A | 0.9200 | C25—H25A | 0.9900 |
| N12—H12B | 0.9200 | C25—H25B | 0.9900 |
| N21—C21 | 1.538 (14) | C26—C210 | 1.53 (2) |
| N21—H21A | 0.9200 | C26—C27 | 1.537 (16) |
| N21—H21B | 0.9200 | C26—H26 | 1.0000 |
| N22—C212 | 1.474 (15) | C27—H27A | 0.9900 |
| N22—H22A | 0.9200 | C27—H27B | 0.9900 |
| N22—H22B | 0.9200 | C28—C211 | 1.535 (17) |
| C11—C12 | 1.501 (15) | C28—H28A | 0.9900 |
| C11—H11C | 0.9900 | C28—H28B | 0.9900 |
| C11—H11D | 0.9900 | C29—C211 | 1.551 (18) |
| C12—C18 | 1.509 (16) | C29—H29A | 0.9900 |
| C12—C17 | 1.515 (15) | C29—H29B | 0.9900 |
| C12—C13 | 1.540 (16) | C210—C211 | 1.55 (2) |
| C13—C14 | 1.526 (17) | C210—H21E | 0.9900 |
| C13—H13A | 0.9900 | C210—H21F | 0.9900 |
| C13—H13B | 0.9900 | C211—H211 | 1.0000 |
| C14—C15 | 1.518 (18) | C212—C213 | 1.501 (16) |
| C14—C19 | 1.544 (17) | C212—H21G | 0.9900 |
| C14—H14 | 1.0000 | C212—H21H | 0.9900 |
| C15—C16 | 1.540 (19) | C213—C214 | 1.506 (16) |
| C15—H15A | 0.9900 | C213—C218 | 1.528 (15) |
| C15—H15B | 0.9900 | C213—C219 | 1.540 (14) |
| C16—C110 | 1.534 (18) | C214—C215 | 1.535 (17) |
| C16—C17 | 1.561 (17) | C214—H21I | 0.9900 |
| C16—H16 | 1.0000 | C214—H21J | 0.9900 |
| C17—H17A | 0.9900 | C215—C216 | 1.534 (16) |
| C17—H17B | 0.9900 | C215—C220 | 1.538 (16) |
| C18—C111 | 1.535 (17) | C215—H215 | 1.0000 |
| C18—H18A | 0.9900 | C216—C217 | 1.515 (17) |
| C18—H18B | 0.9900 | C216—H21K | 0.9900 |
| C19—C111 | 1.491 (18) | C216—H21L | 0.9900 |
| C19—H19A | 0.9900 | C217—C221 | 1.534 (17) |
| C19—H19B | 0.9900 | C217—C218 | 1.545 (17) |

| | | | |
|---------------|------------|---------------|------------|
| C110—C111 | 1.560 (17) | C217—H217 | 1.0000 |
| C110—H11E | 0.9900 | C218—H21M | 0.9900 |
| C110—H11F | 0.9900 | C218—H21N | 0.9900 |
| C111—H111 | 1.0000 | C219—C222 | 1.575 (16) |
| C112—C113 | 1.519 (16) | C219—H21O | 0.9900 |
| C112—H11G | 0.9900 | C219—H21P | 0.9900 |
| C112—H11H | 0.9900 | C220—C222 | 1.484 (18) |
| C113—C118 | 1.517 (16) | C220—H22C | 0.9900 |
| C113—C119 | 1.523 (16) | C220—H22D | 0.9900 |
| C113—C114 | 1.528 (14) | C221—C222 | 1.532 (17) |
| C114—C115 | 1.538 (16) | C221—H22E | 0.9900 |
| C114—H11I | 0.9900 | C221—H22F | 0.9900 |
| C114—H11J | 0.9900 | C222—H222 | 1.0000 |
| C115—C116 | 1.501 (17) | O1—C1 | 1.239 (14) |
| C115—C120 | 1.536 (17) | N1—C1 | 1.312 (16) |
| C115—H115 | 1.0000 | N1—C3 | 1.463 (15) |
| C116—C117 | 1.542 (18) | N1—C4 | 1.474 (15) |
| C116—H11K | 0.9900 | C1—H1 | 0.9500 |
| C116—H11L | 0.9900 | C3—H3A | 0.9800 |
| C117—C118 | 1.536 (18) | C3—H3B | 0.9800 |
| C117—C121 | 1.555 (19) | C3—H3C | 0.9800 |
| C117—H117 | 1.0000 | C4—H4A | 0.9800 |
| C118—H11M | 0.9900 | C4—H4B | 0.9800 |
| C118—H11N | 0.9900 | C4—H4C | 0.9800 |
| C119—C122 | 1.512 (18) | O2—C2 | 1.229 (13) |
| C119—H11O | 0.9900 | N2—C2 | 1.354 (14) |
| C119—H11P | 0.9900 | N2—C5 | 1.441 (14) |
| C120—C122 | 1.541 (16) | N2—C6 | 1.445 (14) |
| C120—H12C | 0.9900 | C2—H2 | 0.9500 |
| C120—H12D | 0.9900 | C5—H5A | 0.9800 |
| C121—C122 | 1.513 (17) | C5—H5B | 0.9800 |
| C121—H12E | 0.9900 | C5—H5C | 0.9800 |
| C121—H12F | 0.9900 | C6—H6A | 0.9800 |
| C122—H122 | 1.0000 | C6—H6B | 0.9800 |
| C21—C22 | 1.483 (15) | C6—H6C | 0.9800 |
| | | | |
| N12—Pt1—N11 | 92.1 (4) | C22—C21—N21 | 113.5 (9) |
| N12—Pt1—C111 | 177.6 (3) | C22—C21—H21C | 108.9 |
| N11—Pt1—C111 | 87.5 (3) | N21—C21—H21C | 108.9 |
| N12—Pt1—C112 | 88.2 (3) | C22—C21—H21D | 108.9 |
| N11—Pt1—C112 | 179.0 (3) | N21—C21—H21D | 108.9 |
| C111—Pt1—C112 | 92.17 (11) | H21C—C21—H21D | 107.7 |
| N21—Pt2—N22 | 92.1 (4) | C21—C22—C28 | 111.4 (9) |
| N21—Pt2—C122 | 177.0 (3) | C21—C22—C23 | 108.5 (10) |
| N22—Pt2—C122 | 87.3 (3) | C28—C22—C23 | 109.0 (10) |
| N21—Pt2—C121 | 88.3 (3) | C21—C22—C27 | 111.8 (10) |
| N22—Pt2—C121 | 178.8 (3) | C28—C22—C27 | 107.4 (10) |
| C122—Pt2—C121 | 92.30 (11) | C23—C22—C27 | 108.7 (9) |

| | | | |
|---------------|------------|----------------|------------|
| C11—N11—Pt1 | 118.1 (7) | C24—C23—C22 | 110.6 (10) |
| C11—N11—H11A | 107.8 | C24—C23—H23A | 109.5 |
| Pt1—N11—H11A | 107.8 | C22—C23—H23A | 109.5 |
| C11—N11—H11B | 107.8 | C24—C23—H23B | 109.5 |
| Pt1—N11—H11B | 107.8 | C22—C23—H23B | 109.5 |
| H11A—N11—H11B | 107.1 | H23A—C23—H23B | 108.1 |
| C112—N12—Pt1 | 120.2 (7) | C29—C24—C23 | 111.2 (10) |
| C112—N12—H12A | 107.3 | C29—C24—C25 | 109.7 (12) |
| Pt1—N12—H12A | 107.3 | C23—C24—C25 | 108.2 (10) |
| C112—N12—H12B | 107.3 | C29—C24—H24 | 109.2 |
| Pt1—N12—H12B | 107.3 | C23—C24—H24 | 109.2 |
| H12A—N12—H12B | 106.9 | C25—C24—H24 | 109.2 |
| C21—N21—Pt2 | 119.8 (7) | C26—C25—C24 | 109.8 (10) |
| C21—N21—H21A | 107.4 | C26—C25—H25A | 109.7 |
| Pt2—N21—H21A | 107.4 | C24—C25—H25A | 109.7 |
| C21—N21—H21B | 107.4 | C26—C25—H25B | 109.7 |
| Pt2—N21—H21B | 107.4 | C24—C25—H25B | 109.7 |
| H21A—N21—H21B | 106.9 | H25A—C25—H25B | 108.2 |
| C212—N22—Pt2 | 117.7 (7) | C25—C26—C210 | 109.8 (12) |
| C212—N22—H22A | 107.9 | C25—C26—C27 | 109.8 (10) |
| Pt2—N22—H22A | 107.9 | C210—C26—C27 | 107.5 (11) |
| C212—N22—H22B | 107.9 | C25—C26—H26 | 109.9 |
| Pt2—N22—H22B | 107.9 | C210—C26—H26 | 109.9 |
| H22A—N22—H22B | 107.2 | C27—C26—H26 | 109.9 |
| N11—C11—C12 | 116.0 (9) | C26—C27—C22 | 111.0 (10) |
| N11—C11—H11C | 108.3 | C26—C27—H27A | 109.4 |
| C12—C11—H11C | 108.3 | C22—C27—H27A | 109.4 |
| N11—C11—H11D | 108.3 | C26—C27—H27B | 109.4 |
| C12—C11—H11D | 108.3 | C22—C27—H27B | 109.4 |
| H11C—C11—H11D | 107.4 | H27A—C27—H27B | 108.0 |
| C11—C12—C18 | 107.2 (9) | C22—C28—C211 | 111.4 (10) |
| C11—C12—C17 | 112.9 (10) | C22—C28—H28A | 109.3 |
| C18—C12—C17 | 109.1 (9) | C211—C28—H28A | 109.3 |
| C11—C12—C13 | 110.3 (9) | C22—C28—H28B | 109.3 |
| C18—C12—C13 | 107.9 (10) | C211—C28—H28B | 109.3 |
| C17—C12—C13 | 109.3 (10) | H28A—C28—H28B | 108.0 |
| C14—C13—C12 | 110.3 (10) | C24—C29—C211 | 109.8 (11) |
| C14—C13—H13A | 109.6 | C24—C29—H29A | 109.7 |
| C12—C13—H13A | 109.6 | C211—C29—H29A | 109.7 |
| C14—C13—H13B | 109.6 | C24—C29—H29B | 109.7 |
| C12—C13—H13B | 109.6 | C211—C29—H29B | 109.7 |
| H13A—C13—H13B | 108.1 | H29A—C29—H29B | 108.2 |
| C15—C14—C13 | 110.2 (12) | C26—C210—C211 | 110.1 (12) |
| C15—C14—C19 | 109.0 (11) | C26—C210—H21E | 109.6 |
| C13—C14—C19 | 108.9 (11) | C211—C210—H21E | 109.6 |
| C15—C14—H14 | 109.6 | C26—C210—H21F | 109.6 |
| C13—C14—H14 | 109.6 | C211—C210—H21F | 109.6 |
| C19—C14—H14 | 109.6 | H21E—C210—H21F | 108.2 |

| | | | |
|----------------|------------|----------------|------------|
| C14—C15—C16 | 108.9 (11) | C28—C211—C210 | 108.8 (11) |
| C14—C15—H15A | 109.9 | C28—C211—C29 | 109.6 (11) |
| C16—C15—H15A | 109.9 | C210—C211—C29 | 107.8 (11) |
| C14—C15—H15B | 109.9 | C28—C211—H211 | 110.2 |
| C16—C15—H15B | 109.9 | C210—C211—H211 | 110.2 |
| H15A—C15—H15B | 108.3 | C29—C211—H211 | 110.2 |
| C110—C16—C15 | 110.8 (12) | N22—C212—C213 | 116.6 (10) |
| C110—C16—C17 | 109.7 (10) | N22—C212—H21G | 108.1 |
| C15—C16—C17 | 108.9 (11) | C213—C212—H21G | 108.1 |
| C110—C16—H16 | 109.1 | N22—C212—H21H | 108.1 |
| C15—C16—H16 | 109.1 | C213—C212—H21H | 108.1 |
| C17—C16—H16 | 109.1 | H21G—C212—H21H | 107.3 |
| C12—C17—C16 | 109.5 (10) | C212—C213—C214 | 106.1 (10) |
| C12—C17—H17A | 109.8 | C212—C213—C218 | 112.3 (9) |
| C16—C17—H17A | 109.8 | C214—C213—C218 | 109.4 (10) |
| C12—C17—H17B | 109.8 | C212—C213—C219 | 111.5 (10) |
| C16—C17—H17B | 109.8 | C214—C213—C219 | 108.3 (9) |
| H17A—C17—H17B | 108.2 | C218—C213—C219 | 109.2 (10) |
| C12—C18—C111 | 112.2 (10) | C213—C214—C215 | 110.8 (10) |
| C12—C18—H18A | 109.2 | C213—C214—H21I | 109.5 |
| C111—C18—H18A | 109.2 | C215—C214—H21I | 109.5 |
| C12—C18—H18B | 109.2 | C213—C214—H21J | 109.5 |
| C111—C18—H18B | 109.2 | C215—C214—H21J | 109.5 |
| H18A—C18—H18B | 107.9 | H21I—C214—H21J | 108.1 |
| C111—C19—C14 | 110.7 (11) | C216—C215—C214 | 109.8 (10) |
| C111—C19—H19A | 109.5 | C216—C215—C220 | 110.6 (11) |
| C14—C19—H19A | 109.5 | C214—C215—C220 | 108.4 (10) |
| C111—C19—H19B | 109.5 | C216—C215—H215 | 109.4 |
| C14—C19—H19B | 109.5 | C214—C215—H215 | 109.4 |
| H19A—C19—H19B | 108.1 | C220—C215—H215 | 109.4 |
| C16—C110—C111 | 108.0 (11) | C217—C216—C215 | 108.5 (10) |
| C16—C110—H11E | 110.1 | C217—C216—H21K | 110.0 |
| C111—C110—H11E | 110.1 | C215—C216—H21K | 110.0 |
| C16—C110—H11F | 110.1 | C217—C216—H21L | 110.0 |
| C111—C110—H11F | 110.1 | C215—C216—H21L | 110.0 |
| H11E—C110—H11F | 108.4 | H21K—C216—H21L | 108.4 |
| C19—C111—C18 | 109.8 (10) | C216—C217—C221 | 110.8 (11) |
| C19—C111—C110 | 109.5 (11) | C216—C217—C218 | 109.3 (11) |
| C18—C111—C110 | 107.6 (11) | C221—C217—C218 | 109.1 (10) |
| C19—C111—H111 | 110.0 | C216—C217—H217 | 109.2 |
| C18—C111—H111 | 110.0 | C221—C217—H217 | 109.2 |
| C110—C111—H111 | 110.0 | C218—C217—H217 | 109.2 |
| N12—C112—C113 | 115.3 (9) | C213—C218—C217 | 109.9 (9) |
| N12—C112—H11G | 108.5 | C213—C218—H21M | 109.7 |
| C113—C112—H11G | 108.5 | C217—C218—H21M | 109.7 |
| N12—C112—H11H | 108.5 | C213—C218—H21N | 109.7 |
| C113—C112—H11H | 108.5 | C217—C218—H21N | 109.7 |
| H11G—C112—H11H | 107.5 | H21M—C218—H21N | 108.2 |

| | | | |
|----------------|------------|----------------|------------|
| C118—C113—C112 | 111.1 (10) | C213—C219—C222 | 108.9 (9) |
| C118—C113—C119 | 108.2 (10) | C213—C219—H21O | 109.9 |
| C112—C113—C119 | 108.8 (10) | C222—C219—H21O | 109.9 |
| C118—C113—C114 | 108.6 (10) | C213—C219—H21P | 109.9 |
| C112—C113—C114 | 110.8 (9) | C222—C219—H21P | 109.9 |
| C119—C113—C114 | 109.4 (9) | H21O—C219—H21P | 108.3 |
| C113—C114—C115 | 109.6 (10) | C222—C220—C215 | 109.1 (10) |
| C113—C114—H11I | 109.8 | C222—C220—H22C | 109.9 |
| C115—C114—H11I | 109.8 | C215—C220—H22C | 109.9 |
| C113—C114—H11J | 109.8 | C222—C220—H22D | 109.9 |
| C115—C114—H11J | 109.8 | C215—C220—H22D | 109.9 |
| H11I—C114—H11J | 108.2 | H22C—C220—H22D | 108.3 |
| C116—C115—C120 | 109.7 (11) | C222—C221—C217 | 108.7 (11) |
| C116—C115—C114 | 109.9 (10) | C222—C221—H22E | 109.9 |
| C120—C115—C114 | 109.8 (10) | C217—C221—H22E | 109.9 |
| C116—C115—H115 | 109.1 | C222—C221—H22F | 109.9 |
| C120—C115—H115 | 109.1 | C217—C221—H22F | 109.9 |
| C114—C115—H115 | 109.1 | H22E—C221—H22F | 108.3 |
| C115—C116—C117 | 110.3 (11) | C220—C222—C221 | 112.0 (11) |
| C115—C116—H11K | 109.6 | C220—C222—C219 | 109.6 (10) |
| C117—C116—H11K | 109.6 | C221—C222—C219 | 108.0 (10) |
| C115—C116—H11L | 109.6 | C220—C222—H222 | 109.1 |
| C117—C116—H11L | 109.6 | C221—C222—H222 | 109.1 |
| H11K—C116—H11L | 108.1 | C219—C222—H222 | 109.1 |
| C118—C117—C116 | 108.5 (11) | C1—N1—C3 | 119.7 (11) |
| C118—C117—C121 | 108.7 (12) | C1—N1—C4 | 122.7 (11) |
| C116—C117—C121 | 108.6 (11) | C3—N1—C4 | 117.6 (11) |
| C118—C117—H117 | 110.3 | O1—C1—N1 | 125.5 (13) |
| C116—C117—H117 | 110.3 | O1—C1—H1 | 117.2 |
| C121—C117—H117 | 110.3 | N1—C1—H1 | 117.2 |
| C113—C118—C117 | 111.2 (10) | N1—C3—H3A | 109.5 |
| C113—C118—H11M | 109.4 | N1—C3—H3B | 109.5 |
| C117—C118—H11M | 109.4 | H3A—C3—H3B | 109.5 |
| C113—C118—H11N | 109.4 | N1—C3—H3C | 109.5 |
| C117—C118—H11N | 109.4 | H3A—C3—H3C | 109.5 |
| H11M—C118—H11N | 108.0 | H3B—C3—H3C | 109.5 |
| C122—C119—C113 | 111.3 (11) | N1—C4—H4A | 109.5 |
| C122—C119—H11O | 109.4 | N1—C4—H4B | 109.5 |
| C113—C119—H11O | 109.4 | H4A—C4—H4B | 109.5 |
| C122—C119—H11P | 109.4 | N1—C4—H4C | 109.5 |
| C113—C119—H11P | 109.4 | H4A—C4—H4C | 109.5 |
| H11O—C119—H11P | 108.0 | H4B—C4—H4C | 109.5 |
| C115—C120—C122 | 108.3 (10) | C2—N2—C5 | 119.3 (10) |
| C115—C120—H12C | 110.0 | C2—N2—C6 | 121.7 (10) |
| C122—C120—H12C | 110.0 | C5—N2—C6 | 119.0 (10) |
| C115—C120—H12D | 110.0 | O2—C2—N2 | 123.5 (11) |
| C122—C120—H12D | 110.0 | O2—C2—H2 | 118.2 |
| H12C—C120—H12D | 108.4 | N2—C2—H2 | 118.2 |

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|-------------------|-------------|---------------------|-------------|
| C122—C121—C117 | 109.1 (10) | N2—C5—H5A | 109.5 |
| C122—C121—H12E | 109.9 | N2—C5—H5B | 109.5 |
| C117—C121—H12E | 109.9 | H5A—C5—H5B | 109.5 |
| C122—C121—H12F | 109.9 | N2—C5—H5C | 109.5 |
| C117—C121—H12F | 109.9 | H5A—C5—H5C | 109.5 |
| H12E—C121—H12F | 108.3 | H5B—C5—H5C | 109.5 |
| C119—C122—C121 | 109.3 (11) | N2—C6—H6A | 109.5 |
| C119—C122—C120 | 109.6 (10) | N2—C6—H6B | 109.5 |
| C121—C122—C120 | 110.4 (11) | H6A—C6—H6B | 109.5 |
| C119—C122—H122 | 109.2 | N2—C6—H6C | 109.5 |
| C121—C122—H122 | 109.2 | H6A—C6—H6C | 109.5 |
| C120—C122—H122 | 109.2 | H6B—C6—H6C | 109.5 |
| | | | |
| N12—Pt1—N11—C11 | -118.0 (8) | C115—C120—C122—C119 | -59.8 (14) |
| C111—Pt1—N11—C11 | 64.4 (8) | C115—C120—C122—C121 | 60.7 (14) |
| N11—Pt1—N12—C112 | 122.5 (8) | Pt2—N21—C21—C22 | 162.7 (7) |
| C112—Pt1—N12—C112 | -58.5 (7) | N21—C21—C22—C28 | -62.7 (13) |
| N22—Pt2—N21—C21 | 123.0 (8) | N21—C21—C22—C23 | 177.4 (9) |
| C121—Pt2—N21—C21 | -58.1 (8) | N21—C21—C22—C27 | 57.5 (12) |
| N21—Pt2—N22—C212 | -114.7 (8) | C21—C22—C23—C24 | 178.9 (10) |
| C122—Pt2—N22—C212 | 68.2 (7) | C28—C22—C23—C24 | 57.5 (12) |
| Pt1—N11—C11—C12 | -159.0 (8) | C27—C22—C23—C24 | -59.3 (13) |
| N11—C11—C12—C18 | -179.9 (9) | C22—C23—C24—C29 | -58.8 (14) |
| N11—C11—C12—C17 | -59.8 (13) | C22—C23—C24—C25 | 61.7 (13) |
| N11—C11—C12—C13 | 62.8 (13) | C29—C24—C25—C26 | 59.9 (14) |
| C11—C12—C13—C14 | 176.4 (11) | C23—C24—C25—C26 | -61.6 (14) |
| C18—C12—C13—C14 | 59.6 (13) | C24—C25—C26—C210 | -58.2 (14) |
| C17—C12—C13—C14 | -58.9 (14) | C24—C25—C26—C27 | 59.8 (14) |
| C12—C13—C14—C15 | 59.4 (14) | C25—C26—C27—C22 | -57.7 (14) |
| C12—C13—C14—C19 | -60.0 (14) | C210—C26—C27—C22 | 61.8 (14) |
| C13—C14—C15—C16 | -60.2 (14) | C21—C22—C27—C26 | 176.5 (10) |
| C19—C14—C15—C16 | 59.2 (14) | C28—C22—C27—C26 | -61.0 (13) |
| C14—C15—C16—C110 | -60.4 (14) | C23—C22—C27—C26 | 56.8 (13) |
| C14—C15—C16—C17 | 60.4 (14) | C21—C22—C28—C211 | -177.8 (11) |
| C11—C12—C17—C16 | -177.5 (10) | C23—C22—C28—C211 | -58.1 (14) |
| C18—C12—C17—C16 | -58.4 (13) | C27—C22—C28—C211 | 59.4 (13) |
| C13—C12—C17—C16 | 59.4 (13) | C23—C24—C29—C211 | 58.1 (15) |
| C110—C16—C17—C12 | 60.7 (14) | C25—C24—C29—C211 | -61.5 (14) |
| C15—C16—C17—C12 | -60.7 (13) | C25—C26—C210—C211 | 59.1 (14) |
| C11—C12—C18—C111 | -177.0 (10) | C27—C26—C210—C211 | -60.3 (14) |
| C17—C12—C18—C111 | 60.4 (13) | C22—C28—C211—C210 | -59.5 (14) |
| C13—C12—C18—C111 | -58.2 (12) | C22—C28—C211—C29 | 58.2 (15) |
| C15—C14—C19—C111 | -61.1 (14) | C26—C210—C211—C28 | 59.4 (14) |
| C13—C14—C19—C111 | 59.1 (14) | C26—C210—C211—C29 | -59.4 (14) |
| C15—C16—C110—C111 | 59.1 (14) | C24—C29—C211—C28 | -57.2 (15) |
| C17—C16—C110—C111 | -61.2 (14) | C24—C29—C211—C210 | 61.1 (15) |
| C14—C19—C111—C18 | -57.2 (14) | Pt2—N22—C212—C213 | -160.5 (7) |
| C14—C19—C111—C110 | 60.8 (14) | N22—C212—C213—C214 | 179.9 (9) |

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| C12—C18—C111—C19 | 58.2 (14) | N22—C212—C213—C218 | 60.4 (13) |
| C12—C18—C111—C110 | -60.9 (13) | N22—C212—C213—C219 | -62.5 (13) |
| C16—C110—C111—C19 | -59.2 (14) | C212—C213—C214—C215 | -179.3 (9) |
| C16—C110—C111—C18 | 60.1 (14) | C218—C213—C214—C215 | -58.0 (12) |
| Pt1—N12—C112—C113 | 163.9 (7) | C219—C213—C214—C215 | 60.9 (12) |
| N12—C112—C113—C118 | -62.2 (12) | C213—C214—C215—C216 | 59.3 (12) |
| N12—C112—C113—C119 | 178.8 (8) | C213—C214—C215—C220 | -61.6 (12) |
| N12—C112—C113—C114 | 58.6 (12) | C214—C215—C216—C217 | -60.1 (13) |
| C118—C113—C114—C115 | -59.7 (12) | C220—C215—C216—C217 | 59.4 (13) |
| C112—C113—C114—C115 | 178.1 (10) | C215—C216—C217—C221 | -59.4 (14) |
| C119—C113—C114—C115 | 58.2 (13) | C215—C216—C217—C218 | 60.9 (13) |
| C113—C114—C115—C116 | 60.4 (13) | C212—C213—C218—C217 | 176.0 (10) |
| C113—C114—C115—C120 | -60.4 (13) | C214—C213—C218—C217 | 58.5 (12) |
| C120—C115—C116—C117 | 61.2 (14) | C219—C213—C218—C217 | -59.8 (12) |
| C114—C115—C116—C117 | -59.7 (14) | C216—C217—C218—C213 | -60.7 (12) |
| C115—C116—C117—C118 | 58.3 (15) | C221—C217—C218—C213 | 60.6 (13) |
| C115—C116—C117—C121 | -59.7 (15) | C212—C213—C219—C222 | -175.1 (10) |
| C112—C113—C118—C117 | -177.8 (10) | C214—C213—C219—C222 | -58.8 (12) |
| C119—C113—C118—C117 | -58.5 (13) | C218—C213—C219—C222 | 60.2 (12) |
| C114—C113—C118—C117 | 60.1 (13) | C216—C215—C220—C222 | -59.0 (14) |
| C116—C117—C118—C113 | -58.9 (14) | C214—C215—C220—C222 | 61.3 (13) |
| C121—C117—C118—C113 | 59.0 (13) | C216—C217—C221—C222 | 58.2 (14) |
| C118—C113—C119—C122 | 59.5 (12) | C218—C217—C221—C222 | -62.2 (13) |
| C112—C113—C119—C122 | -179.7 (9) | C215—C220—C222—C221 | 58.5 (14) |
| C114—C113—C119—C122 | -58.6 (13) | C215—C220—C222—C219 | -61.3 (13) |
| C116—C115—C120—C122 | -60.4 (13) | C217—C221—C222—C220 | -58.2 (14) |
| C114—C115—C120—C122 | 60.5 (13) | C217—C221—C222—C219 | 62.6 (13) |
| C118—C117—C121—C122 | -59.1 (13) | C213—C219—C222—C220 | 60.5 (13) |
| C116—C117—C121—C122 | 58.8 (15) | C213—C219—C222—C221 | -61.8 (13) |
| C113—C119—C122—C121 | -61.4 (13) | C3—N1—C1—O1 | -178.5 (14) |
| C113—C119—C122—C120 | 59.7 (13) | C4—N1—C1—O1 | 3 (2) |
| C117—C121—C122—C119 | 60.3 (14) | C5—N2—C2—O2 | 176.5 (11) |
| C117—C121—C122—C120 | -60.4 (14) | C6—N2—C2—O2 | -1.7 (18) |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------------------------|-------|-------------|-------------|---------------|
| N11—H11A \cdots O2 | 0.92 | 1.95 | 2.863 (13) | 170 |
| N11—H11B \cdots C112 ⁱ | 0.92 | 2.64 | 3.409 (10) | 141 |
| N12—H12A \cdots C111 ⁱ | 0.92 | 2.63 | 3.299 (9) | 131 |
| N12—H12B \cdots O2 | 0.92 | 1.93 | 2.843 (11) | 175 |
| N21—H21A \cdots C122 ⁱⁱ | 0.92 | 2.55 | 3.238 (10) | 132 |
| N21—H21B \cdots O1 | 0.92 | 1.91 | 2.821 (12) | 173 |
| N22—H22A \cdots O1 | 0.92 | 1.94 | 2.843 (11) | 165 |
| N22—H22B \cdots C121 ⁱⁱ | 0.92 | 2.64 | 3.354 (10) | 136 |

Symmetry codes: (i) $-x+2, -y, -z+2$; (ii) $-x+1, -y+1, -z+2$.