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# Crystal structure of *trans*-dichlorido(4-nitroaniline- $\kappa N^1$ )(piperidine- $\kappa N$ )platinum(II)

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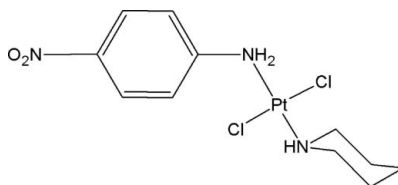
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In the title complex, [PtCl<sub>2</sub>(C<sub>5</sub>H<sub>11</sub>N)(C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>)], the Pt<sup>II</sup> metal atom displays a slightly distorted *trans*-PtN<sub>2</sub>Cl<sub>2</sub> square-planar coordination geometry. The dihedral angle between the mean plane of the benzene and piperidine rings is 89.03 (3)°. In the crystal structure, inversion dimers are formed *via* N–H···Cl hydrogen-bond interactions, resulting in chains parallel to the [001] direction. The benzene rings within the chains show  $\pi$ – $\pi$  stacking interactions [centroid-to-centroid distances of 3.801 (3) Å] and neighbouring chains interact *via* N–H···O hydrogen bonds.

## 1. Chemical context

The title compound is one of many complexes which have been synthesized for the purpose of potential medical applications (Klein & Hambley, 2009; Wilson & Lippard, 2014; Peng *et al.*, 2014). It is notable that according to the procedure used for the synthesis of complexes of the type *cis*-[PtCl<sub>2</sub>(piperidine)(another amine)] (piperidine hereafter denoted Pip) (Dinh & Da, 2003; Nguyen Thi Thanh *et al.*, 2014), the reaction between K[PtCl<sub>3</sub>(Pip)] and *p*-nitroaniline under appropriate conditions gave no *cis* complex, as expected, but instead gave the *trans*-[PtCl<sub>2</sub>(*p*-nitroaniline)(Pip)] derivative, (I).

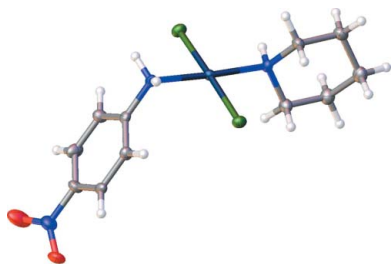


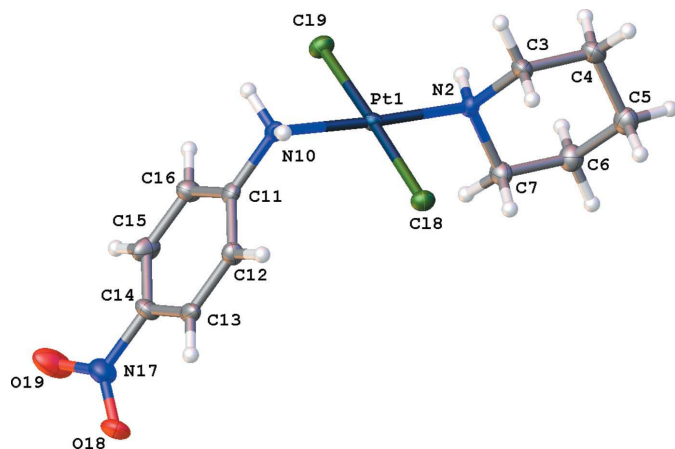
To explain this we suppose that *p*-nitroaniline first coordinates with Pt<sup>II</sup> *via* the N atom of the amino group to form *cis*-[PtCl<sub>2</sub>(*p*-nitroaniline)(Pip)] based on the *trans* effect. Then, in the reaction solution, the *cis* complex converts into the *trans* complex and the thermodynamics of this conversion are currently under investigation by us.

The anticancer activity of the title compound was tested according to the method described by Skehan *et al.* (1990) against four human cancer cell lines (HepG2, RD, MCF7 and FI). The IC<sub>50</sub> values calculated based on OD values taken on an Elisa instrument at 515–540 nm are >10, 4.86, >10 and 8.25  $\mu\text{g ml}^{-1}$ , respectively.

## 2. Structural commentary

The molecular structure of the title compound is illustrated in Fig. 1 and surprisingly shows a *trans* arrangement of the two Cl





**Figure 1**  
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

atoms [ $\text{Cl8}-\text{Pt1}-\text{Cl9} = 177.84(4)^\circ$ ]. The piperidine ring adopts the usual chair conformation, with the  $\text{N2}-\text{Pt1}$  bond in the equatorial position. The piperidine ring is oriented nearly perpendicular to the coordination plane of the  $\text{Pt}^{\text{II}}$  atom, thereby reducing the van der Waals repulsion; the dihedral angle between the least-squares mean planes through the piperidine ring and the four atoms coordinated to the Pt atom is  $89.6(2)^\circ$ . One short intramolecular contact is observed, *i.e.*  $\text{H7B}\cdots\text{Cl8} = 2.83 \text{ \AA}$ . The mean planes through the piperidine ring and the benzene ring make a dihedral angle of  $89.0(3)^\circ$ .

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H2}\cdots\text{O18}^{\text{i}}$	0.93	2.27	3.182 (6)	165
$\text{N10}-\text{H10A}\cdots\text{Cl8}^{\text{ii}}$	0.92	2.32	3.198 (4)	158
$\text{N10}-\text{H10B}\cdots\text{Cl9}^{\text{iii}}$	0.92	2.37	3.255 (4)	161

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

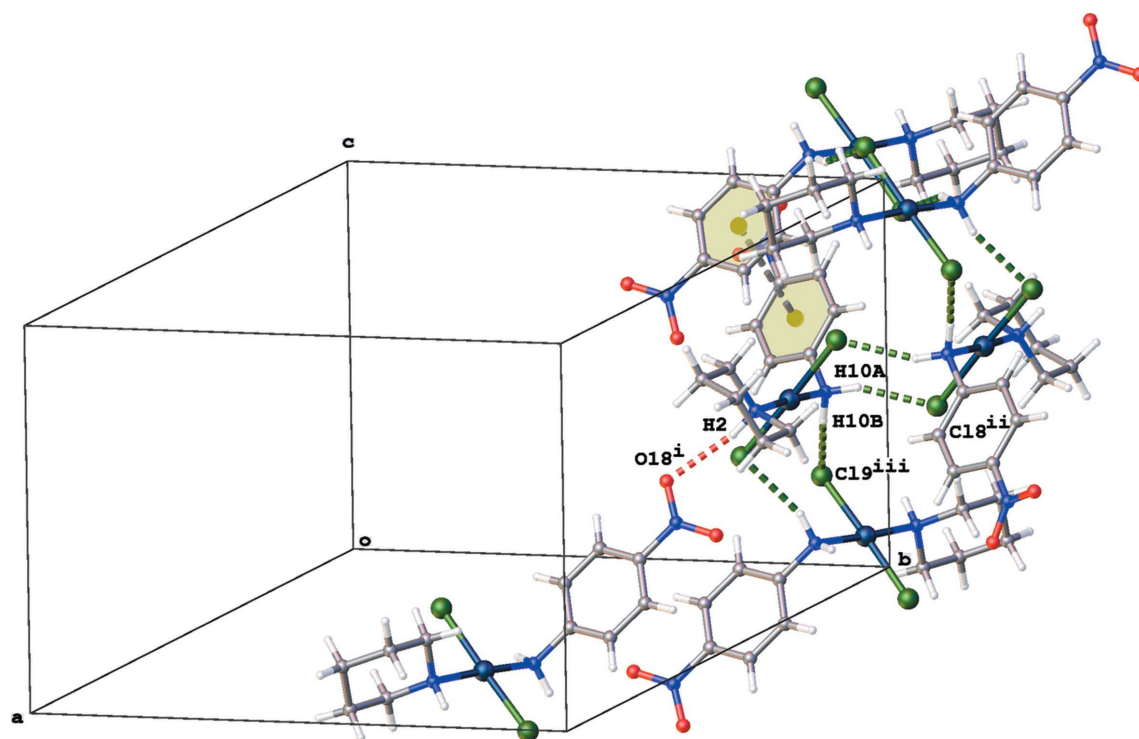
The dihedral angle between the mean planes of the nitro substituent and the benzene ring is  $16.6(3)^\circ$ .

### 3. Supramolecular features

In the crystal, inversion dimers are formed *via*  $\text{N}-\text{H}\cdots\text{Cl}$  interactions between the aniline N atom and both Cl atoms, resulting in chains of molecules along the [001] direction (Fig. 2 and Table 1). Within these chains,  $\pi-\pi$  interactions occur between the aromatic rings [ $\text{Cg}\cdots\text{Cg}^{\text{iv}} = 3.801(3) \text{ \AA}$ ;  $\text{Cg}$  is the centroid of the C11–C16 ring; symmetry code: (iv)  $-x, y, -z + \frac{3}{2}$ ; Fig. 2]. Neighbouring chains are linked *via*  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds between the piperidine N atom and a nitro O atom (Fig. 2 and Table 1).

### 4. Database survey

A search of the Cambridge Structural Database (Version 5.36; last update February 2015; Groom & Allen, 2014) for Pt complexes with Pt coordinated to exactly two Cl atoms and



**Figure 2**  
Partial packing diagram of the title compound, showing a chain of molecules formed parallel to the [001] direction *via*  $\text{N}-\text{H}\cdots\text{Cl}$  interactions (green dotted lines) and  $\pi-\pi$  interactions (grey dotted line). Neighbouring chains interact *via*  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds (red dotted line).

**Table 2**  
 Experimental details.

Crystal data	
Chemical formula	[PtCl <sub>2</sub> (C <sub>5</sub> H <sub>11</sub> N)(C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> )]
<i>M<sub>r</sub></i>	489.27
Crystal system, space group	Monoclinic, <i>C2/c</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	15.8763 (11), 18.5394 (11), 10.8707 (6)
$\beta$ (°)	103.119 (7)
<i>V</i> (Å <sup>3</sup> )	3116.1 (3)
<i>Z</i>	8
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	9.35
Crystal size (mm)	0.35 × 0.15 × 0.1
Data collection	
Diffraction	Agilent SuperNova (single source at offset, Eos detector)
Absorption correction	Multi-scan ( <i>CrysAlis PRO</i> ; Agilent, 2012)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.538, 1.000
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	8156, 3109, 2713
<i>R<sub>int</sub></i>	0.044
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.625
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.032, 0.072, 1.10
No. of reflections	3109
No. of parameters	172
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$ , $\Delta\rho_{min}$ (e Å <sup>-3</sup> )	2.75, -1.82

Computer programs: *CrysAlis PRO* (Agilent, 2012), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

two N atoms gave 713 hits. The majority of these Pt complexes display a *cis* coordination of the Cl atoms (474 structures), with the remaining 239 structures showing a *trans* coordination. There is no difference in the Pt–Cl distances between both configurations. The average Pt–Cl distances are 2.300 (15) and 2.299 (12) Å for the *cis* and *trans* arrangements, respectively, and correspond to the observed distances of 2.3039 (11) and 2.2917 (12) Å for Pt1–Cl8 and Pt1–Cl9, respectively.

## 5. Synthesis and crystallization

The starting complex K[PtCl<sub>3</sub>(piperidine)] (0.425 g, 1 mmol), prepared according to the synthetic procedure of Da *et al.* (2001) with slight modifications, was dissolved in water (10 ml) and filtered to afford a clear solution. To this solution, *p*-nitroaniline (1 mmol) in ethanol (10 ml) was added gradually while stirring at 413–318 K. After 1 h, a brown powder appeared and the reaction mixture was then stirred further for 24 h until all the precipitate was completely dissolved. The solvent was removed *in vacuo* to give a brown–yellow product.

The product was washed consecutively with a 0.1 M HCl solution (2 × 2 ml), warm water (2 × 2 ml) and diethyl ether (2 × 2 ml). The yield was 80%. Single crystals suitable for X-ray determination were obtained by slow evaporation within 12 h from an acetone solution at room temperature. IR (KBr, cm<sup>-1</sup>): 3199, 3113 ( $\nu_{\text{NH}}$ ); 3070, 2927, 2862 ( $\nu_{\text{CH}}$ ); 1596, 1525, 1479 ( $\nu_{\text{C}=\text{C}}$  arom); 1342, 1325 ( $\nu_{\text{NO}}$ ); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz):  $\delta$  8.21 (2H, *d*, <sup>3</sup>*J* = 9.0 Hz, Ar-*H*), 7.47 (2H, *d*, <sup>3</sup>*J* = 9.0 Hz, Ar-*H*), 5.49 (2H, *br*, O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub>), 3.66 (1H, *br*, C<sub>5</sub>H<sub>10</sub>NH), 3.26 (2H <sub>$\alpha$</sub> , *d*, <sup>2</sup>*J*<sub>ae</sub> = 13.0 Hz, C<sub>5</sub>H<sub>10</sub>NH), 2.99 (2H <sub>$\alpha$</sub> , *q*, <sup>2</sup>*J*<sub>ae</sub>, <sup>3</sup>*J*<sub>aa</sub>, <sup>3</sup>*J*<sub>aa(NH)</sub> = 13.0 Hz, C<sub>5</sub>H<sub>10</sub>NH), 1.69–1.43 (4H <sub>$\beta$</sub> , 2H <sub>$\gamma$</sub> , *ov*, C<sub>5</sub>H<sub>10</sub>NH). <sup>13</sup>C{<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  149.6, 125.1, 124.2 (O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub>), 54.0, 27.2, 24.3 (C<sub>5</sub>H<sub>10</sub>NH).

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were placed at idealized positions and refined in riding mode, with *U*<sub>iso</sub>(H) values assigned as 1.2*U*<sub>eq</sub> of the parent atoms, with C–H distances of 0.95 (aromatic) and 0.99 Å (methylene), and N–H distances of 0.93 (NH) and 0.92 Å (NH<sub>2</sub>).

## Acknowledgements

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## References

- Agilent (2012). *CrysAlis PRO*. Agilent Technologies, Yarnton, Oxfordshire, England.
- Da, T. T., Vu, D. B. & Dinh, N. H. (2001). *J. Pharm. Sci. (Vietnam)*, **6**, 6–8.
- Dinh, N. H. & Da, T. T. (2003). *J. Coord. Chem.* **41**, 683–689.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Groom, C. R. & Allen, F. H. (2014). *Angew. Chem. Int. Ed.* **53**, 662–671.
- Klein, A. V. & Hambley, T. W. (2009). *Chem. Rev.* **109**, 4911–4920.
- Nguyen Thi Thanh, C., Nguyen Bich, N. & Van Meervelt, L. (2014). *Acta Cryst. C* **70**, 297–301.
- Peng, Y., Zhong, H., Chen, Z.-F., Liu, Y.-C., Zhang, G.-H., Qin, Q.-P. & Liang, H. (2014). *Chem. Pharm. Bull.* **62**, 221–228.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Skehan, P., Storeng, R., Scudiero, D., Monks, A., McMahon, J., Vistica, D., Warren, J. T., Bokesch, H., Kenney, S. & Boyd, M. R. (1990). *J. Natl. Cancer Inst.* **82**, 1107–1112.
- Wilson, J. J. & Lippard, S. J. (2014). *Chem. Rev.* **114**, 4470–4495.

## supporting information

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### Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis PRO* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

### *trans*-Dichlorido(4-nitroaniline- $\kappa N^1$ )(piperidine- $\kappa N$ )platinum(II)

#### Crystal data

[PtCl<sub>2</sub>(C<sub>5</sub>H<sub>11</sub>N)(C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>)]

$M_r = 489.27$

Monoclinic, *C2/c*

$a = 15.8763$  (11) Å

$b = 18.5394$  (11) Å

$c = 10.8707$  (6) Å

$\beta = 103.119$  (7)°

$V = 3116.1$  (3) Å<sup>3</sup>

$Z = 8$

$F(000) = 1856$

$D_x = 2.086$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 3549 reflections

$\theta = 3.4$ – $28.8^\circ$

$\mu = 9.35$  mm<sup>-1</sup>

$T = 100$  K

, brown

$0.35 \times 0.15 \times 0.1$  mm

#### Data collection

Agilent SuperNova (single source at offset, Eos detector) diffractometer

Radiation source: SuperNova (Mo) X-ray Source

Mirror monochromator

Detector resolution: 15.9631 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)

$T_{\min} = 0.538$ ,  $T_{\max} = 1.000$

8156 measured reflections

3109 independent reflections

2713 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 26.4^\circ$ ,  $\theta_{\min} = 2.8^\circ$

$h = -19 \rightarrow 15$

$k = -17 \rightarrow 23$

$l = -13 \rightarrow 13$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.072$

$S = 1.10$

3109 reflections

172 parameters

0 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

$$w = 1/[\sigma^2(F_o^2) + (0.0296P)^2 + 0.5839P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.003$   
 $\Delta\rho_{\max} = 2.75 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -1.82 \text{ e } \text{\AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C3	0.2646 (4)	0.9772 (3)	0.4633 (5)	0.0233 (13)
H3A	0.2439	1.0130	0.5173	0.028*
H3B	0.2335	0.9859	0.3748	0.028*
C4	0.3620 (4)	0.9877 (3)	0.4750 (5)	0.0243 (13)
H4A	0.3815	0.9562	0.4132	0.029*
H4B	0.3734	1.0383	0.4551	0.029*
C5	0.4128 (4)	0.9694 (3)	0.6083 (5)	0.0267 (13)
H5A	0.4755	0.9727	0.6122	0.032*
H5B	0.3985	1.0045	0.6691	0.032*
C6	0.3905 (4)	0.8933 (3)	0.6443 (6)	0.0255 (14)
H6A	0.4109	0.8580	0.5892	0.031*
H6B	0.4210	0.8833	0.7326	0.031*
C7	0.2938 (4)	0.8839 (3)	0.6313 (5)	0.0220 (13)
H7A	0.2816	0.8332	0.6501	0.026*
H7B	0.2746	0.9151	0.6937	0.026*
C11	-0.0526 (3)	0.8256 (3)	0.5180 (4)	0.0175 (11)
C12	-0.0838 (4)	0.8538 (3)	0.6181 (5)	0.0193 (11)
H12	-0.0832	0.9044	0.6328	0.023*
C13	-0.1159 (3)	0.8069 (3)	0.6957 (5)	0.0205 (12)
H13	-0.1370	0.8248	0.7649	0.025*
C14	-0.1167 (4)	0.7338 (3)	0.6710 (5)	0.0225 (12)
C15	-0.0857 (4)	0.7057 (3)	0.5722 (5)	0.0266 (14)
H15	-0.0870	0.6552	0.5571	0.032*
C16	-0.0528 (4)	0.7522 (3)	0.4957 (5)	0.0218 (12)
H16	-0.0303	0.7339	0.4280	0.026*
C18	0.10439 (9)	0.97037 (6)	0.62798 (11)	0.0190 (3)
C19	0.12310 (9)	0.80109 (7)	0.32660 (11)	0.0212 (3)
N2	0.2441 (3)	0.9028 (2)	0.5016 (4)	0.0160 (9)
H2	0.2629	0.8713	0.4469	0.019*
N10	-0.0192 (3)	0.8739 (2)	0.4368 (4)	0.0157 (9)

H10A	-0.0439	0.9185	0.4409	0.019*
H10B	-0.0373	0.8576	0.3552	0.019*
N17	-0.1522 (3)	0.6855 (3)	0.7523 (4)	0.0294 (12)
O18	-0.1616 (3)	0.7083 (2)	0.8546 (3)	0.0316 (10)
O19	-0.1721 (4)	0.6237 (2)	0.7150 (4)	0.0464 (14)
Pt1	0.113556 (13)	0.887195 (10)	0.474086 (16)	0.01473 (9)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C3	0.021 (3)	0.032 (3)	0.019 (3)	-0.008 (2)	0.007 (2)	0.001 (2)
C4	0.024 (4)	0.030 (3)	0.022 (3)	-0.003 (2)	0.010 (2)	0.000 (2)
C5	0.021 (3)	0.031 (3)	0.029 (3)	-0.001 (3)	0.007 (3)	-0.003 (3)
C6	0.022 (4)	0.026 (3)	0.028 (3)	0.000 (2)	0.005 (3)	0.000 (2)
C7	0.018 (3)	0.026 (3)	0.022 (3)	-0.001 (2)	0.003 (2)	0.003 (2)
C11	0.013 (3)	0.022 (3)	0.016 (2)	-0.002 (2)	0.000 (2)	0.000 (2)
C12	0.019 (3)	0.019 (3)	0.020 (3)	-0.001 (2)	0.006 (2)	-0.004 (2)
C13	0.013 (3)	0.034 (3)	0.014 (2)	-0.003 (2)	0.004 (2)	-0.002 (2)
C14	0.025 (3)	0.024 (3)	0.021 (3)	-0.004 (2)	0.010 (2)	0.005 (2)
C15	0.040 (4)	0.017 (3)	0.021 (3)	-0.001 (3)	0.004 (3)	-0.002 (2)
C16	0.025 (3)	0.021 (3)	0.020 (3)	-0.001 (2)	0.008 (2)	0.001 (2)
C18	0.0217 (8)	0.0195 (6)	0.0164 (6)	0.0017 (5)	0.0054 (5)	-0.0009 (5)
C19	0.0220 (8)	0.0239 (6)	0.0174 (6)	0.0023 (6)	0.0039 (5)	-0.0042 (5)
N2	0.012 (3)	0.020 (2)	0.016 (2)	-0.0003 (18)	0.0033 (18)	-0.0026 (18)
N10	0.013 (3)	0.019 (2)	0.015 (2)	0.0011 (18)	0.0022 (19)	-0.0009 (18)
N17	0.031 (3)	0.030 (3)	0.028 (3)	-0.003 (2)	0.009 (2)	0.006 (2)
O18	0.035 (3)	0.044 (2)	0.021 (2)	-0.007 (2)	0.0163 (18)	0.0022 (19)
O19	0.077 (4)	0.026 (2)	0.046 (3)	-0.006 (2)	0.034 (3)	0.003 (2)
Pt1	0.01469 (15)	0.01670 (13)	0.01350 (12)	0.00081 (7)	0.00464 (9)	0.00004 (7)

*Geometric parameters (Å, °)*

C3—H3A	0.9900	C12—H12	0.9500
C3—H3B	0.9900	C12—C13	1.387 (7)
C3—C4	1.535 (8)	C13—H13	0.9500
C3—N2	1.497 (6)	C13—C14	1.381 (7)
C4—H4A	0.9900	C14—C15	1.382 (7)
C4—H4B	0.9900	C14—N17	1.458 (7)
C4—C5	1.528 (8)	C15—H15	0.9500
C5—H5A	0.9900	C15—C16	1.380 (7)
C5—H5B	0.9900	C16—H16	0.9500
C5—C6	1.526 (7)	C18—Pt1	2.3039 (11)
C6—H6A	0.9900	C19—Pt1	2.2917 (12)
C6—H6B	0.9900	N2—H2	0.9300
C6—C7	1.520 (8)	N2—Pt1	2.046 (4)
C7—H7A	0.9900	N10—H10A	0.9200
C7—H7B	0.9900	N10—H10B	0.9200
C7—N2	1.492 (7)	N10—Pt1	2.068 (4)

C11—C12	1.396 (7)	N17—O18	1.231 (5)
C11—C16	1.382 (7)	N17—O19	1.232 (6)
C11—N10	1.440 (6)		
H3A—C3—H3B	107.9	C13—C12—H12	120.5
C4—C3—H3A	109.3	C12—C13—H13	120.5
C4—C3—H3B	109.3	C14—C13—C12	119.0 (5)
N2—C3—H3A	109.3	C14—C13—H13	120.5
N2—C3—H3B	109.3	C13—C14—C15	122.2 (5)
N2—C3—C4	111.8 (4)	C13—C14—N17	118.2 (5)
C3—C4—H4A	109.5	C15—C14—N17	119.6 (5)
C3—C4—H4B	109.5	C14—C15—H15	120.6
H4A—C4—H4B	108.1	C16—C15—C14	118.9 (5)
C5—C4—C3	110.8 (4)	C16—C15—H15	120.6
C5—C4—H4A	109.5	C11—C16—H16	120.1
C5—C4—H4B	109.5	C15—C16—C11	119.7 (5)
C4—C5—H5A	109.6	C15—C16—H16	120.1
C4—C5—H5B	109.6	C3—N2—H2	106.2
H5A—C5—H5B	108.1	C3—N2—Pt1	111.5 (3)
C6—C5—C4	110.2 (5)	C7—N2—C3	112.2 (4)
C6—C5—H5A	109.6	C7—N2—H2	106.2
C6—C5—H5B	109.6	C7—N2—Pt1	113.9 (3)
C5—C6—H6A	109.3	Pt1—N2—H2	106.2
C5—C6—H6B	109.3	C11—N10—H10A	108.0
H6A—C6—H6B	107.9	C11—N10—H10B	108.0
C7—C6—C5	111.7 (5)	C11—N10—Pt1	117.0 (3)
C7—C6—H6A	109.3	H10A—N10—H10B	107.3
C7—C6—H6B	109.3	Pt1—N10—H10A	108.0
C6—C7—H7A	109.3	Pt1—N10—H10B	108.0
C6—C7—H7B	109.3	O18—N17—C14	118.7 (4)
H7A—C7—H7B	108.0	O18—N17—O19	122.8 (5)
N2—C7—C6	111.5 (4)	O19—N17—C14	118.5 (5)
N2—C7—H7A	109.3	C19—Pt1—C18	177.84 (4)
N2—C7—H7B	109.3	N2—Pt1—C18	91.59 (12)
C12—C11—N10	119.4 (4)	N2—Pt1—C19	88.59 (12)
C16—C11—C12	121.2 (5)	N2—Pt1—N10	176.94 (15)
C16—C11—N10	119.4 (4)	N10—Pt1—C18	89.56 (12)
C11—C12—H12	120.5	N10—Pt1—C19	90.37 (12)
C13—C12—C11	119.0 (5)		
C3—C4—C5—C6	54.8 (6)	C12—C11—N10—Pt1	97.9 (5)
C3—N2—Pt1—C18	-66.5 (3)	C12—C13—C14—C15	0.7 (9)
C3—N2—Pt1—C19	115.7 (3)	C12—C13—C14—N17	-178.9 (5)
C4—C3—N2—C7	54.8 (6)	C13—C14—C15—C16	0.0 (9)
C4—C3—N2—Pt1	-176.0 (3)	C13—C14—N17—O18	-16.4 (8)
C4—C5—C6—C7	-55.5 (6)	C13—C14—N17—O19	163.1 (6)
C5—C6—C7—N2	55.4 (6)	C14—C15—C16—C11	-0.9 (8)
C6—C7—N2—C3	-54.8 (6)	C15—C14—N17—O18	164.0 (5)



C6—C7—N2—Pt1	177.4 (3)	C15—C14—N17—O19	-16.5 (8)
C7—N2—Pt1—C18	61.7 (3)	C16—C11—C12—C13	-0.3 (8)
C7—N2—Pt1—C19	-116.1 (3)	C16—C11—N10—Pt1	-81.8 (5)
C11—C12—C13—C14	-0.6 (8)	N2—C3—C4—C5	-54.9 (6)
C11—N10—Pt1—C18	-82.4 (3)	N10—C11—C12—C13	180.0 (5)
C11—N10—Pt1—C19	95.5 (3)	N10—C11—C16—C15	-179.2 (5)
C12—C11—C16—C15	1.1 (8)	N17—C14—C15—C16	179.6 (5)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N2—H2 $\cdots$ O18 <sup>i</sup>	0.93	2.27	3.182 (6)	165
N10—H10A $\cdots$ C18 <sup>ii</sup>	0.92	2.32	3.198 (4)	158
N10—H10B $\cdots$ C19 <sup>iii</sup>	0.92	2.37	3.255 (4)	161

Symmetry codes: (i)  $x+1/2, -y+3/2, z-1/2$ ; (ii)  $-x, -y+2, -z+1$ ; (iii)  $-x, y, -z+1/2$ .