

Synthesis, crystal structure and photophysical properties of chlorido[2-(2',6'-difluoro-2,3'-bipyridin-6-yl- κN^1)-6-(pyridin-2-yloxy- κN)phenyl- κC^1]-platinum(II)

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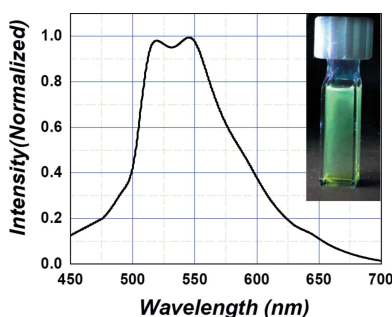
Keywords: crystal structure; 2,3'-bipyridine; platinum compound; luminescence; OLED.**CCDC reference:** 2053861**Supporting information:** this article has supporting information at journals.iucr.org/e

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The title compound, [Pt(C₂₁H₁₂F₂N₃O)Cl], crystallizes with two crystallographically independent molecules (*A* and *B*) in the asymmetric unit, which adopt similar conformations. The Pt^{II} atoms in both molecules adopt distorted square-planar geometries, coordinated by one C and two N atoms from the tridentate 2',6'-difluoro-6-[3-(pyridin-2-yloxy)phenyl]-2,3'-bipyridine ligand and a chloride anion: the C and Cl atoms are *trans*. In the crystal, C—H \cdots Cl/F hydrogen bonds, F \cdots π and weak π – π stacking interactions between adjacent *A* and *B* molecules and between pairs of inversion-related *B* molecules lead to the formation of a two-dimensional supramolecular network lying parallel to the *ab* plane. The sheets are stacked along the *c*-axis direction and linked by F \cdots π and weak π – π stacking interactions between pairs of inversion-related *A* molecules, forming a three-dimensional supramolecular network. The photoluminescence quantum efficiency of the title compound in the blue–green region of the visible region ($\lambda_{\max} = 517$ and 544 nm) is estimated to be ~ 0.2 – 0.3 , indicating that the title compound could be a suitable candidate as the emitting material in organic light-emitting diode (OLED) applications.

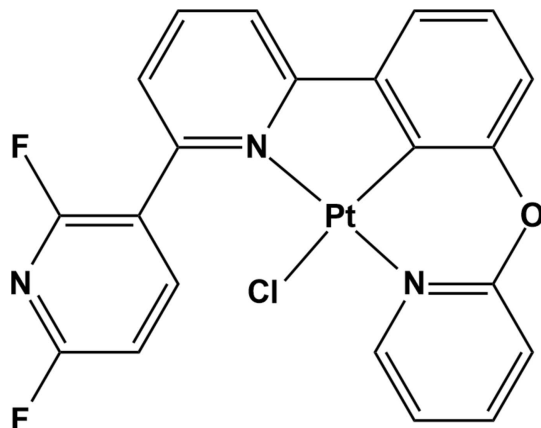
1. Chemical context

The C,N-chelating 2,3'-bipyridine-based transition-metal compounds have attracted much interest because of their wide applications as biological labels, photosensitizers in water reduction, sensors and organic light-emitting diodes (OLEDs) (Zaen *et al.*, 2019*a,b*). Especially, highly efficient phosphorescent metal complexes containing Ir^{III} and Pt^{II} can be synthesized by using 2,3'-bipyridine as ligand, which feature a high triplet-state energy (Lee *et al.*, 2018). In terms of the efficiency and stability of OLEDs, tetradentate ligand-based Pt^{II} complexes are known to be very good candidates as triplet emitters (Wang & Wang, 2019). The design of tetradentate ligands is focused on making appropriate coordination modes in order to form five or six-membered metallacycles. To achieve blue emission in Pt-based triplet emitters, two strategies have been employed as follows: (i) incorporation of a high-triplet-energy moiety into the ligand framework; (ii) the breakage of π -conjugation in the ligand to increase the energy gap (Fleetham *et al.*, 2016; Kang *et al.*, 2020). With these in mind, we have recently synthesized 2',6'-difluoro-6-[3-(pyridin-2-yloxy)phenyl]-2,3'-bipyridine as a ligand with high triplet energy (Park *et al.*, 2020). By using this ligand, we have



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synthesized its coordination metal complex containing Pt^{II} and determined its crystal structure: herein, we report the structural and photophysical characteristics of chlorido[2',6'-difluoro-6-[3-(pyridin-2-yloxy)phenyl]-2,3'-bipyridine-κ³N,C,N']-platinum(II).



2. Structural commentary

The asymmetric unit of the title compound, Pt(C₂₁H₁₂F₂N₃O)Cl, contains two crystallographically independent molecules (*A* and *B* denote the Pt1- and Pt2-containing molecules, respectively), which adopt similar conformations (Fig. 1 and Table 1). The coordination sphere of the Pt^{II} atoms in both molecules is a distorted square-planar geometry, with the respective coordination sites occupied by one C and two N atoms from the 2',6'-difluoro-6-[3-(pyridin-2-yloxy)phenyl]-2,3'-bipyridine ligand together with a chloride anion. The average length [1.949 (4) Å] of the Pt—C bonds is

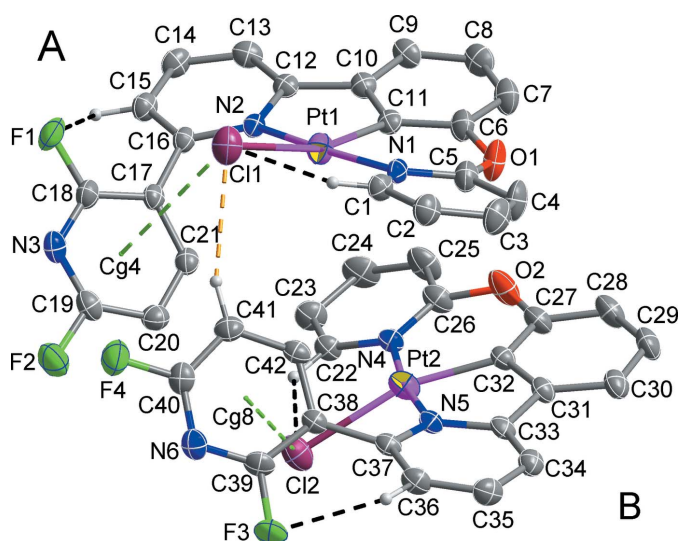


Figure 1

The molecular structure of the title compound, showing the atom numbering scheme and displacement ellipsoids at the 50% probability level. Black and green dashed lines represent intramolecular C—H...Cl/F and Cl... π interactions, respectively, and yellow dashed line represents intermolecular C—H...Cl interaction. H atoms not involved in intra- and intermolecular interactions are not shown for clarity.

Table 1
Selected geometric parameters (Å, °).

Pt1—C11	1.949 (4)	Pt2—C32	1.948 (4)
Pt1—N1	2.035 (3)	Pt2—N4	2.042 (3)
Pt1—N2	2.040 (3)	Pt2—N5	2.049 (3)
Pt1—Cl1	2.4193 (8)	Pt2—Cl2	2.4154 (8)
C11—Pt1—N1	90.92 (14)	C32—Pt2—N4	90.87 (14)
C11—Pt1—N2	80.86 (14)	C32—Pt2—N5	80.98 (13)
N1—Pt1—N2	171.61 (12)	N4—Pt2—N5	171.56 (11)
C11—Pt1—Cl1	163.28 (11)	C32—Pt2—Cl2	163.13 (11)
N1—Pt1—Cl1	94.81 (9)	N4—Pt2—Cl2	94.78 (9)
N2—Pt1—Cl1	93.56 (9)	N5—Pt2—Cl2	93.65 (8)

slightly shorter than that [2.042 (3) Å] of the Pt—N bonds because of back bonding between the metal and the anionic C atom of the ligand. The Cl1 and Cl2 atoms deviate from the mean plane consisting of the Pt and coordinated N/C atoms [r.m.s. deviations = 0.013 (1) (*A*) and 0.017 (1) Å (*B*)] with deviations of 0.700 (6) Å for *A* and 0.720 (6) Å for *B*.

In each molecule, there are intramolecular C—H...Cl/F interactions, contributing to the stabilization of the molecular structure (Table 2 and black dashed lines in Fig. 1). Moreover, an intramolecular Cl... π interaction [Cl1...Cg4 = 3.4537 (19) Å, Cl2...Cg8 = 3.455 (2) Å; green dashed lines in Fig. 1; Cg4 and Cg8 are the centroids of the N3/C17—C21 and N6/C38—C42 rings, respectively] between the coordinated chloride ion and the pyridine ring with fluorine substituents are also observed. Molecules *A* and *B* are interlinked by a C—H...Cl interaction (Table 2 and yellow dashed line in Fig. 1). In the 6-phenyl-2,3'-bipyridine system in both molecules, the phenylpyridine moieties are approximately coplanar with the dihedral angles between the pyridine ring and the attached phenyl rings being 10.01 (11)° for *A* and 9.64 (11)° for *B*. However, the terminal difluoro-pyridine ring is tilted by 46.08 (9)° for *A* and 46.96 (8)° for *B* with respect to phenylpyridine ring plane. This distortion may be caused by the intramolecular Cl... π interaction described above. The pyridine ring of the pyridine-2-yloxy group is slightly tilted by 22.09 (13)° for *A* and 19.70 (13)° for *B* relative to the phenylpyridine ring plane.

3. Supramolecular features

In the crystal structure, intermolecular C—H...Cl/F hydrogen bonds (Table 2, yellow dashed lines in Figs. 1 and 2) between adjacent *A* and *B* molecules and between pairs of inversion-related *B* molecules lead to the formation of a two-dimensional supramolecular network lying parallel to the *ab* plane. In addition, this network is consolidated by halogen... π and weak π — π stacking interactions [red and black dashed lines in Fig. 2, respectively; F2...Cg5ⁱ = 3.819 (3); Cg6...Cg7ⁱⁱ = 4.022 (2) Å; Cg5, Cg6 and Cg7 are the centroids of the N4/C22—C26, C27—C32 and N5/C33—C37 rings, respectively; symmetry codes: (i) $-x + 2, -y + 1, -z$; (ii) $-x + 2, -y + 2, -z$] between pairs of inversion-related *B* molecules. These sheets are stacked along the *c*-axis direction and connected by F... π and weak π — π stacking interactions [sky-blue and green

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

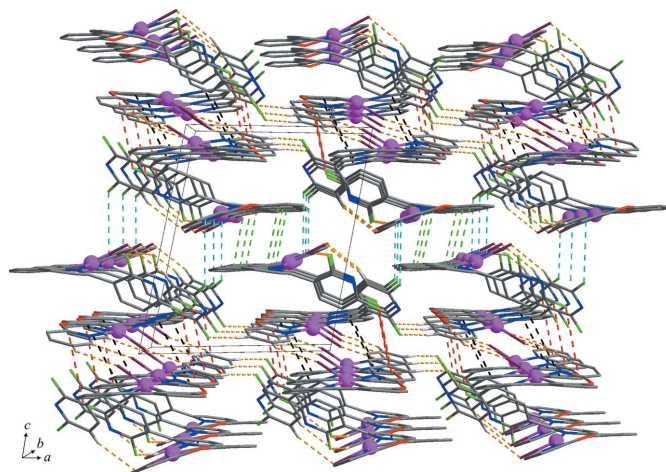
$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1–H1 \cdots C11	0.95	2.46	3.175 (4)	132
C3–H3 \cdots F1 ⁱ	0.95	2.53	3.474 (5)	172
C15–H15 \cdots F1	0.95	2.56	2.989 (5)	108
C22–H22 \cdots Cl2	0.95	2.45	3.170 (4)	132
C23–H23 \cdots Cl2 ⁱⁱ	0.95	2.82	3.540 (5)	133
C24–H24 \cdots F3 ⁱⁱⁱ	0.95	2.50	3.443 (5)	172
C36–H36 \cdots F3	0.95	2.55	2.975 (5)	108
C41–H41 \cdots Cl1	0.95	2.79	3.684 (4)	158

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

dashed lines in Fig. 3, respectively; $F4\cdots Cg1^{iii} = 3.834 (3) \text{ \AA}$; $Cg2\cdots Cg3^{iv} = 4.073 (2) \text{ \AA}$; $Cg1, Cg2$ and $Cg3$ are the centroids of the N1/C1–C5, C6–C11 and N2/C12–C16 rings, respectively; symmetry code: (iii) $-x + 2, -y + 1, -z + 1$; (iv) $-x + 1, -y + 1, -z + 1$] between pairs of inversion-related A molecules, resulting in the formation of a three-dimensional supramolecular network.

4. Luminescent property

The bright blueish-green emission of the title compound in solution is dominated by phosphorescence as supported by an excited-state lifetime of more than 1 ms. Emission maxima appear at 517 and 544 nm at room temperature, as shown in Fig. 4. The emission observed in the title compound is attributable to an intra-ligand charge transfer (ILCT) transition mixed with a metal-to-ligand charge-transfer (MLCT) transition based on previous reports (Wang & Wang, 2019). Contrary to our expectations, the title compound shows green emission. It may be that the chloride ion bound directly to the platinum ion causes this effect because 2',6'-difluoro-2,3'-bipyridine (dfppy)-based platinum complexes without chloride ions often exhibit blue emission at room temperature. The photoluminescence quantum efficiency of the title compound

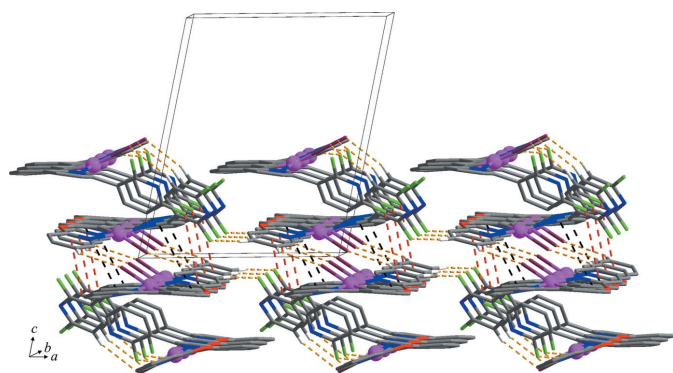

Figure 3

The three-dimensional supramolecular network formed through $F\cdots\pi$ and $\pi\cdots\pi$ stacking interactions (sky-blue and green dashed lines) between the two-dimensional networks stacked along the c -axis direction. H atoms not involved in the intermolecular interactions have been omitted for clarity. Colour codes: violet = platinum, plum = chloride, green = fluorine, red = oxygen, blue = nitrogen, grey = carbon and white = hydrogen.

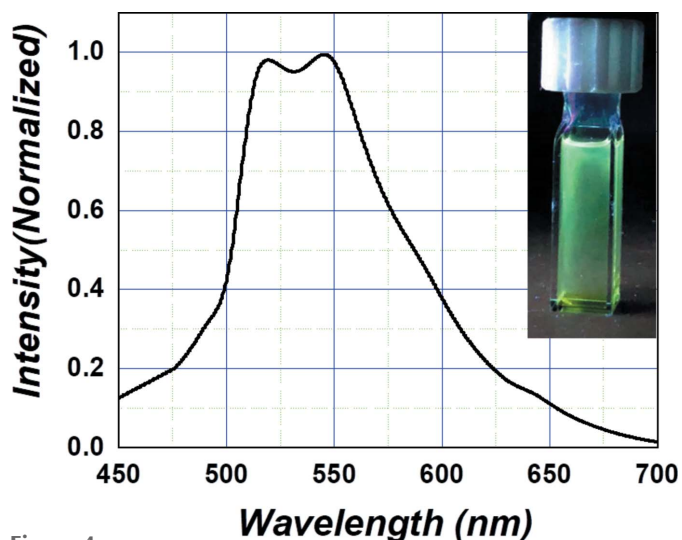
was estimated to be $\sim 0.2\text{--}0.3$ (Fig. 4, inset). Such efficiency is enough to use the title compound as the emitting material in organic light-emitting diode (OLED) applications.

5. Database survey

A survey of *SciFinder* (SciFinder, 2020) for 6-[3-(pyridin-2-yloxy)phenyl]-2,3'-bipyridine (*i.e.*, the title ligand without specifying the fluorine substituents), gave two hits. These are the reports of the crystal structures and photophysical properties of the free ligands for 2',6'-difluoro-6-[3-(pyridin-2-yloxy)phenyl]-2,3'-bipyridine and 2',6'-dimethoxy-6-[3-(pyridin-2-yloxy)phenyl]-2,3'-bipyridine (Park *et al.*, 2020). The survey revealed no exact matches for the reported structure of the


Figure 2

The two-dimensional supramolecular network formed through intermolecular $C-H\cdots Cl/F$ hydrogen bonds (yellow dashed lines), $F\cdots\pi$ (red dashed lines) and $\pi\cdots\pi$ stacking (black dashed lines) interactions between aromatic rings of inversion-related B molecules. For clarity, H atoms not involved in the intermolecular interactions have been omitted. Colour codes: violet = platinum, plum = chloride, green = fluorine, red = oxygen, blue = nitrogen, grey = carbon and white = hydrogen.


Figure 4

Emission spectrum of the title compound in solution at room temperature (Inset: Emission photo).

Table 3
Experimental details.

Crystal data	
Chemical formula	[Pt(C ₂₁ H ₁₂ F ₂ N ₃ O)Cl]
<i>M</i> _r	590.88
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	173
<i>a</i> , <i>b</i> , <i>c</i> (Å)	12.4924 (9), 12.5008 (9), 14.1163 (11)
α , β , γ (°)	74.498 (3), 73.401 (3), 61.954 (3)
<i>V</i> (Å ³)	1841.3 (2)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	7.80
Crystal size (mm)	0.46 × 0.32 × 0.24
Data collection	
Diffraction	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2014)
<i>T</i> _{min} , <i>T</i> _{max}	0.233, 0.746
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	34679, 9126, 7667
<i>R</i> _{int}	0.045
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.667
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.028, 0.067, 1.03
No. of reflections	9126
No. of parameters	523
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	1.64, -1.21

Computer programs: *APEX2* (Bruker, 2014), *SAINT* (Bruker, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2010), *SHELXTL* (Sheldrick, 2008) and *pubCIF* (Westrip, 2010).

title ligand: to the best of our knowledge, this is the first crystal structure reported for a platinum complex with the title ligand.

6. Synthesis and crystallization

All experiments were performed under a dry N₂ atmosphere using standard Schlenk techniques. All solvents used in this study were freshly distilled over appropriate drying reagents prior to use. All starting materials were commercially purchased and used without further purification. The ¹H NMR spectrum was recorded on a JEOL 400 MHz spectrometer. The ligand, 2',3'-difluoro-6-[3-(pyridin-2-yloxy)phenyl]-2,3'-bipyridine (Park *et al.*, 2018, 2020) and starting material, PtCl₂(PhCN)₂, (Uchiyama *et al.*, 1980) were synthesized according to previous reports.

The title compound was synthesized as follows: A mixture of the ligand (0.36 g, 1.0 mmol), PtCl₂(PhCN)₂ (0.47 g, 1.0 mmol) and xylene (10 ml) was refluxed (433 K) for 48 h under an N₂ flow. The xylene was removed by distillation and the crude product was purified by silica gel column chromatography (CH₂Cl₂:hexane = 1:1, *v/v*) to give the title

compound as a yellow solid in 40% yield. Orange–red crystals suitable for X-ray crystallography analysis were obtained from a CH₂Cl₂/hexane solution by slow evaporation. ¹H NMR (400 MHz, CDCl₃) δ 9.91 (*dd*, *J* = 6.0, 2.0 Hz, 1H), 8.20 (*m*, 1H), 7.97 (*t*, *J* = 8.0 Hz, ¹H), 7.90–7.84 (*m*, 2H), 7.50–7.42 (*m*, 2H), 7.30–7.22 (*m*, 2H), 7.06 (*d*, *J* = 7.6 Hz, 1H), 6.97–6.91 (*m*, 2H). ¹³C NMR (100 MHz, CDCl₃) δ 206.5, 167.3, 156.4, 155.9, 151.0, 148.1, 146.6, 146.5, 140.1, 139.0, 125.7, 125.0, 121.0, 118.4, 118.3, 117.6, 115.9, 106.0, 105.9, 105.7, 105.6. Analysis calculated for C₂₁H₁₂ClF₂N₃O: C 42.69; H 2.05; N 7.11%; found: C 42.70, H 2.06, N 7.09%.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were positioned geometrically and refined using a riding model: C–H = 0.95 Å with *U*_{iso}(H) = 1.2*U*_{eq}(C).

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References

- Brandenburg, K. (2010). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Bruker (2014). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Fleetham, T., Li, G. & Li, J. (2016). *Adv. Mater.* **29**, 1601861.
- Kang, J., Zaen, R., Park, K.-M., Lee, K. H., Lee, J. Y. & Kang, Y. (2020). *Cryst. Growth Des.* **20**, 6129–6138.
- Lee, C., Zaen, R., Park, K.-M., Lee, K. H., Lee, J. Y. & Kang, Y. (2018). *Organometallics*, **37**, 4639–4647.
- Park, K.-M., Moon, S.-H. & Kang, Y. (2018). *Acta Cryst.* **E74**, 1475–1479.
- Park, K.-M., Yang, K., Moon, S.-H. & Kang, Y. (2020). *Acta Cryst.* **C79**, 381–388.
- SciFinder (2020). Chemical Abstracts Service: Columbus, OH, 2010; RN 58-08-2 (accessed December 31, 2020).
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Uchiyama, Y., Nakamura, Y., Miwa, T., Kawaguchi, S. & Okeya, S. (1980). *Chem. Lett.* **3**, 337–338.
- Wang, X. & Wang, S. (2019). *Chem. Rec.* **19**, 1693–1709.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
- Zaen, R., Kim, M., Park, K.-M., Lee, K. H., Lee, J. Y. & Kang, Y. (2019a). *Dalton Trans.* **48**, 9734–9743.
- Zaen, R., Park, K.-M., Lee, K. H., Lee, J. Y. & Kang, Y. (2019b). *Adv. Optical Mater.* **7**, 1901387.

supporting information

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Synthesis, crystal structure and photophysical properties of chlorido[2-(2',6'-difluoro-2,3'-bipyridin-6-yl- κ N¹)-6-(pyridin-2-yloxy- κ N)phenyl- κ C¹]platinum(II)

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Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINTE* (Bruker, 2014); data reduction: *SAINTE* (Bruker, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *pubCIF* (Westrip, 2010).

Chlorido[2-(2',6'-difluoro-2,3'-bipyridin-6-yl- κ N¹)-6-(pyridin-2-yloxy- κ N)phenyl- κ C¹]platinum(II)

Crystal data

[Pt(C₂₁H₁₂F₂N₃O)Cl]
M_r = 590.88
 Triclinic, *P* $\bar{1}$
a = 12.4924 (9) Å
b = 12.5008 (9) Å
c = 14.1163 (11) Å
 α = 74.498 (3)°
 β = 73.401 (3)°
 γ = 61.954 (3)°
V = 1841.3 (2) Å³

Z = 4
F(000) = 1120
D_x = 2.131 Mg m⁻³
 Mo *K* α radiation, λ = 0.71073 Å
 Cell parameters from 9258 reflections
 θ = 2.6–28.3°
 μ = 7.80 mm⁻¹
T = 173 K
 Block, yellow
 0.46 × 0.32 × 0.24 mm

Data collection

Bruker APEXII CCD
 diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2014)
T_{min} = 0.233, *T_{max}* = 0.746
 34679 measured reflections

9126 independent reflections
 7667 reflections with *I* > 2 σ (*I*)
R_{int} = 0.045
 θ_{\max} = 28.3°, θ_{\min} = 1.5°
h = -16→16
k = -15→16
l = -18→18

Refinement

Refinement on *F*²
 Least-squares matrix: full
R[*F*² > 2 σ (*F*²)] = 0.028
wR(*F*²) = 0.067
S = 1.03
 9126 reflections
 523 parameters
 0 restraints

Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0327P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.64 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -1.21 \text{ e } \text{Å}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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	0.69646 (2)	0.61157 (2)	0.39509 (2)	0.03247 (5)
Pt2	0.88563 (2)	0.80611 (2)	0.10492 (2)	0.03240 (5)
Cl1	0.86494 (8)	0.44909 (8)	0.47237 (7)	0.0410 (2)
Cl2	1.05014 (8)	0.63393 (8)	0.02853 (7)	0.0413 (2)
F1	0.8999 (2)	0.1430 (2)	0.4219 (2)	0.0689 (7)
F2	1.2132 (2)	0.1920 (3)	0.1978 (2)	0.0730 (8)
F3	1.3562 (2)	0.6034 (2)	0.0774 (2)	0.0685 (7)
F4	1.3006 (3)	0.2977 (2)	0.3009 (2)	0.0711 (7)
O1	0.5471 (3)	0.9163 (2)	0.3614 (3)	0.0668 (9)
O2	0.5792 (2)	0.9597 (3)	0.1333 (3)	0.0674 (9)
N1	0.7262 (3)	0.7497 (3)	0.4159 (2)	0.0358 (7)
N2	0.6446 (3)	0.4930 (3)	0.3661 (2)	0.0340 (7)
N3	1.0540 (3)	0.1720 (3)	0.3099 (3)	0.0504 (9)
N4	0.7472 (3)	0.7748 (3)	0.0861 (2)	0.0358 (7)
N5	1.0042 (3)	0.8593 (3)	0.1331 (2)	0.0340 (7)
N6	1.3250 (3)	0.4527 (3)	0.1888 (3)	0.0479 (8)
C1	0.8297 (4)	0.7229 (4)	0.4491 (3)	0.0421 (9)
H1	0.8809	0.6389	0.4688	0.050*
C2	0.8652 (5)	0.8078 (4)	0.4562 (4)	0.0550 (11)
H2	0.9387	0.7833	0.4797	0.066*
C3	0.7916 (5)	0.9306 (4)	0.4283 (4)	0.0661 (13)
H3	0.8138	0.9921	0.4322	0.079*
C4	0.6870 (5)	0.9618 (4)	0.3953 (4)	0.0657 (13)
H4	0.6358	1.0455	0.3748	0.079*
C5	0.6559 (4)	0.8701 (4)	0.3920 (3)	0.0511 (11)
C6	0.4800 (4)	0.8536 (4)	0.3637 (3)	0.0505 (10)
C7	0.3573 (4)	0.9249 (4)	0.3571 (3)	0.0586 (12)
H7	0.3244	1.0117	0.3499	0.070*
C8	0.2835 (4)	0.8706 (4)	0.3610 (3)	0.0587 (12)
H8	0.1985	0.9199	0.3585	0.070*
C9	0.3308 (4)	0.7440 (4)	0.3685 (3)	0.0490 (10)
H9	0.2791	0.7059	0.3720	0.059*
C10	0.4556 (4)	0.6748 (4)	0.3706 (3)	0.0416 (9)
C11	0.5324 (4)	0.7272 (3)	0.3681 (3)	0.0393 (8)
C12	0.5184 (3)	0.5402 (3)	0.3718 (3)	0.0375 (8)
C13	0.4631 (4)	0.4677 (4)	0.3732 (3)	0.0459 (10)
H13	0.3762	0.5021	0.3785	0.055*
C14	0.5330 (4)	0.3454 (4)	0.3668 (3)	0.0498 (10)
H14	0.4949	0.2933	0.3719	0.060*

C15	0.6593 (4)	0.2998 (4)	0.3530 (3)	0.0463 (9)
H15	0.7091	0.2161	0.3457	0.056*
C16	0.7148 (4)	0.3742 (3)	0.3495 (3)	0.0370 (8)
C17	0.8482 (3)	0.3332 (3)	0.3148 (3)	0.0365 (8)
C18	0.9353 (4)	0.2176 (3)	0.3469 (3)	0.0461 (10)
C19	1.0912 (4)	0.2433 (4)	0.2383 (3)	0.0492 (10)
C20	1.0203 (4)	0.3602 (4)	0.1990 (3)	0.0475 (9)
H20	1.0544	0.4082	0.1473	0.057*
C21	0.8959 (4)	0.4040 (3)	0.2393 (3)	0.0426 (9)
H21	0.8418	0.4847	0.2146	0.051*
C22	0.7757 (3)	0.6672 (4)	0.0570 (3)	0.0408 (9)
H22	0.8606	0.6136	0.0403	0.049*
C23	0.6911 (4)	0.6315 (5)	0.0502 (4)	0.0566 (12)
H23	0.7162	0.5556	0.0294	0.068*
C24	0.5660 (4)	0.7100 (5)	0.0748 (4)	0.0658 (14)
H24	0.5042	0.6880	0.0715	0.079*
C25	0.5344 (4)	0.8173 (5)	0.1032 (4)	0.0655 (13)
H25	0.4499	0.8718	0.1202	0.079*
C26	0.6258 (4)	0.8477 (4)	0.1076 (3)	0.0500 (10)
C27	0.6426 (4)	1.0252 (4)	0.1338 (3)	0.0480 (10)
C28	0.5712 (4)	1.1484 (4)	0.1399 (3)	0.0576 (12)
H28	0.4841	1.1823	0.1463	0.069*
C29	0.6266 (4)	1.2206 (4)	0.1368 (3)	0.0589 (12)
H29	0.5775	1.3056	0.1394	0.071*
C30	0.7530 (4)	1.1732 (4)	0.1298 (3)	0.0507 (10)
H30	0.7910	1.2249	0.1261	0.061*
C31	0.8231 (4)	1.0476 (4)	0.1284 (3)	0.0398 (9)
C32	0.7694 (3)	0.9716 (3)	0.1304 (3)	0.0380 (8)
C33	0.9573 (4)	0.9852 (4)	0.1276 (3)	0.0398 (9)
C34	1.0291 (4)	1.0404 (4)	0.1256 (3)	0.0439 (9)
H34	0.9949	1.1272	0.1193	0.053*
C35	1.1513 (4)	0.9709 (4)	0.1327 (3)	0.0499 (10)
H35	1.2035	1.0087	0.1281	0.060*
C36	1.1962 (4)	0.8450 (4)	0.1465 (3)	0.0466 (9)
H36	1.2797	0.7955	0.1541	0.056*
C37	1.1221 (3)	0.7895 (4)	0.1496 (3)	0.0370 (8)
C38	1.1627 (3)	0.6569 (3)	0.1841 (3)	0.0349 (8)
C39	1.2793 (3)	0.5693 (4)	0.1529 (3)	0.0452 (10)
C40	1.2510 (4)	0.4174 (4)	0.2611 (3)	0.0494 (10)
C41	1.1313 (4)	0.4895 (4)	0.2994 (3)	0.0463 (9)
H41	1.0810	0.4570	0.3502	0.056*
C42	1.0885 (3)	0.6118 (4)	0.2596 (3)	0.0414 (9)
H42	1.0066	0.6665	0.2843	0.050*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.03777 (9)	0.02938 (8)	0.03200 (8)	-0.01344 (6)	-0.01039 (6)	-0.00506 (6)

Pt2	0.02768 (8)	0.03840 (9)	0.03250 (8)	-0.01276 (6)	-0.00509 (6)	-0.01087 (6)
Cl1	0.0438 (5)	0.0350 (4)	0.0486 (5)	-0.0142 (4)	-0.0198 (4)	-0.0065 (4)
Cl2	0.0340 (5)	0.0435 (5)	0.0498 (5)	-0.0123 (4)	-0.0076 (4)	-0.0212 (4)
F1	0.0752 (18)	0.0410 (13)	0.0822 (19)	-0.0289 (13)	-0.0188 (15)	0.0153 (13)
F2	0.0478 (15)	0.0675 (18)	0.093 (2)	-0.0155 (14)	-0.0027 (14)	-0.0253 (15)
F3	0.0387 (13)	0.0711 (17)	0.0841 (19)	-0.0261 (13)	0.0130 (12)	-0.0154 (14)
F4	0.0702 (18)	0.0477 (15)	0.0856 (19)	-0.0189 (14)	-0.0214 (15)	-0.0003 (14)
O1	0.071 (2)	0.0312 (15)	0.105 (3)	-0.0161 (15)	-0.047 (2)	0.0014 (16)
O2	0.0295 (15)	0.071 (2)	0.104 (3)	-0.0123 (15)	-0.0051 (15)	-0.0447 (19)
N1	0.0453 (18)	0.0280 (15)	0.0366 (16)	-0.0167 (14)	-0.0065 (13)	-0.0082 (12)
N2	0.0411 (17)	0.0318 (16)	0.0313 (16)	-0.0158 (14)	-0.0099 (13)	-0.0047 (12)
N3	0.050 (2)	0.0360 (18)	0.067 (2)	-0.0129 (17)	-0.0152 (18)	-0.0159 (17)
N4	0.0288 (15)	0.0432 (18)	0.0364 (16)	-0.0142 (14)	-0.0073 (12)	-0.0088 (14)
N5	0.0321 (16)	0.0387 (17)	0.0330 (16)	-0.0136 (14)	-0.0054 (12)	-0.0122 (13)
N6	0.0372 (18)	0.045 (2)	0.061 (2)	-0.0130 (16)	-0.0155 (17)	-0.0106 (17)
C1	0.048 (2)	0.042 (2)	0.045 (2)	-0.0228 (19)	-0.0103 (18)	-0.0106 (17)
C2	0.064 (3)	0.051 (3)	0.062 (3)	-0.030 (2)	-0.014 (2)	-0.015 (2)
C3	0.090 (4)	0.049 (3)	0.079 (3)	-0.040 (3)	-0.024 (3)	-0.012 (2)
C4	0.084 (3)	0.031 (2)	0.092 (4)	-0.022 (2)	-0.039 (3)	-0.006 (2)
C5	0.062 (3)	0.037 (2)	0.052 (3)	-0.015 (2)	-0.018 (2)	-0.0069 (19)
C6	0.056 (3)	0.037 (2)	0.053 (3)	-0.011 (2)	-0.021 (2)	-0.0040 (19)
C7	0.063 (3)	0.041 (2)	0.066 (3)	-0.006 (2)	-0.031 (2)	-0.008 (2)
C8	0.046 (2)	0.061 (3)	0.057 (3)	-0.008 (2)	-0.022 (2)	-0.006 (2)
C9	0.041 (2)	0.056 (3)	0.047 (2)	-0.011 (2)	-0.0166 (18)	-0.011 (2)
C10	0.045 (2)	0.045 (2)	0.034 (2)	-0.0149 (19)	-0.0134 (17)	-0.0064 (17)
C11	0.044 (2)	0.038 (2)	0.0312 (19)	-0.0135 (18)	-0.0126 (16)	-0.0006 (16)
C12	0.041 (2)	0.042 (2)	0.0297 (19)	-0.0163 (18)	-0.0118 (16)	-0.0026 (16)
C13	0.045 (2)	0.061 (3)	0.041 (2)	-0.025 (2)	-0.0128 (18)	-0.0124 (19)
C14	0.063 (3)	0.054 (3)	0.052 (2)	-0.038 (2)	-0.018 (2)	-0.007 (2)
C15	0.058 (3)	0.042 (2)	0.046 (2)	-0.025 (2)	-0.0131 (19)	-0.0092 (18)
C16	0.049 (2)	0.0316 (18)	0.0343 (19)	-0.0173 (17)	-0.0125 (16)	-0.0048 (15)
C17	0.045 (2)	0.0310 (18)	0.037 (2)	-0.0149 (17)	-0.0091 (16)	-0.0110 (16)
C18	0.055 (3)	0.034 (2)	0.053 (3)	-0.020 (2)	-0.012 (2)	-0.0076 (18)
C19	0.043 (2)	0.047 (2)	0.058 (3)	-0.013 (2)	-0.010 (2)	-0.022 (2)
C20	0.052 (2)	0.052 (2)	0.041 (2)	-0.026 (2)	-0.0040 (18)	-0.0090 (19)
C21	0.054 (2)	0.036 (2)	0.035 (2)	-0.0141 (18)	-0.0130 (17)	-0.0053 (16)
C22	0.0339 (19)	0.048 (2)	0.047 (2)	-0.0187 (18)	-0.0086 (16)	-0.0132 (18)
C23	0.051 (3)	0.067 (3)	0.065 (3)	-0.033 (2)	-0.011 (2)	-0.016 (2)
C24	0.042 (3)	0.094 (4)	0.081 (3)	-0.039 (3)	-0.010 (2)	-0.027 (3)
C25	0.032 (2)	0.081 (3)	0.091 (4)	-0.020 (2)	-0.008 (2)	-0.038 (3)
C26	0.036 (2)	0.064 (3)	0.052 (3)	-0.017 (2)	-0.0089 (18)	-0.020 (2)
C27	0.036 (2)	0.055 (3)	0.048 (2)	-0.011 (2)	-0.0038 (18)	-0.021 (2)
C28	0.039 (2)	0.063 (3)	0.064 (3)	-0.004 (2)	-0.011 (2)	-0.032 (2)
C29	0.055 (3)	0.045 (2)	0.060 (3)	-0.001 (2)	-0.010 (2)	-0.024 (2)
C30	0.058 (3)	0.044 (2)	0.045 (2)	-0.013 (2)	-0.008 (2)	-0.0184 (19)
C31	0.040 (2)	0.040 (2)	0.037 (2)	-0.0118 (18)	-0.0059 (16)	-0.0147 (17)
C32	0.035 (2)	0.042 (2)	0.0330 (19)	-0.0118 (17)	-0.0047 (15)	-0.0111 (16)
C33	0.042 (2)	0.043 (2)	0.033 (2)	-0.0153 (18)	0.0004 (16)	-0.0188 (17)

C34	0.052 (2)	0.042 (2)	0.040 (2)	-0.019 (2)	-0.0089 (18)	-0.0125 (17)
C35	0.053 (3)	0.060 (3)	0.055 (3)	-0.035 (2)	-0.0053 (19)	-0.019 (2)
C36	0.036 (2)	0.058 (3)	0.052 (2)	-0.021 (2)	-0.0093 (17)	-0.015 (2)
C37	0.036 (2)	0.047 (2)	0.0302 (19)	-0.0164 (18)	-0.0043 (15)	-0.0132 (16)
C38	0.0292 (18)	0.044 (2)	0.0349 (19)	-0.0143 (16)	-0.0083 (15)	-0.0107 (16)
C39	0.032 (2)	0.062 (3)	0.047 (2)	-0.025 (2)	-0.0054 (17)	-0.011 (2)
C40	0.050 (2)	0.045 (2)	0.058 (3)	-0.017 (2)	-0.022 (2)	-0.008 (2)
C41	0.050 (2)	0.055 (3)	0.035 (2)	-0.025 (2)	-0.0102 (18)	-0.0031 (18)
C42	0.035 (2)	0.053 (2)	0.034 (2)	-0.0157 (18)	-0.0054 (15)	-0.0114 (17)

Geometric parameters (Å, °)

Pt1—C11	1.949 (4)	C12—C13	1.368 (5)
Pt1—N1	2.035 (3)	C13—C14	1.370 (6)
Pt1—N2	2.040 (3)	C13—H13	0.9500
Pt1—C11	2.4193 (8)	C14—C15	1.375 (6)
Pt2—C32	1.948 (4)	C14—H14	0.9500
Pt2—N4	2.042 (3)	C15—C16	1.381 (5)
Pt2—N5	2.049 (3)	C15—H15	0.9500
Pt2—C12	2.4154 (8)	C16—C17	1.465 (5)
F1—C18	1.334 (5)	C17—C21	1.380 (5)
F2—C19	1.356 (5)	C17—C18	1.389 (5)
F3—C39	1.341 (4)	C19—C20	1.363 (6)
F4—C40	1.347 (5)	C20—C21	1.379 (5)
O1—C5	1.354 (5)	C20—H20	0.9500
O1—C6	1.380 (5)	C21—H21	0.9500
O2—C26	1.347 (5)	C22—C23	1.360 (6)
O2—C27	1.385 (5)	C22—H22	0.9500
N1—C5	1.344 (5)	C23—C24	1.398 (6)
N1—C1	1.364 (5)	C23—H23	0.9500
N2—C16	1.369 (5)	C24—C25	1.348 (7)
N2—C12	1.385 (5)	C24—H24	0.9500
N3—C19	1.292 (6)	C25—C26	1.382 (6)
N3—C18	1.311 (5)	C25—H25	0.9500
N4—C26	1.344 (5)	C27—C28	1.382 (6)
N4—C22	1.366 (5)	C27—C32	1.391 (5)
N5—C37	1.365 (5)	C28—C29	1.357 (7)
N5—C33	1.386 (5)	C28—H28	0.9500
N6—C40	1.301 (6)	C29—C30	1.384 (6)
N6—C39	1.302 (5)	C29—H29	0.9500
C1—C2	1.364 (6)	C30—C31	1.395 (5)
C1—H1	0.9500	C30—H30	0.9500
C2—C3	1.383 (6)	C31—C32	1.389 (5)
C2—H2	0.9500	C31—C33	1.477 (5)
C3—C4	1.359 (7)	C33—C34	1.355 (5)
C3—H3	0.9500	C34—C35	1.374 (6)
C4—C5	1.388 (6)	C34—H34	0.9500
C4—H4	0.9500	C35—C36	1.378 (6)

C6—C7	1.380 (6)	C35—H35	0.9500
C6—C11	1.388 (5)	C36—C37	1.381 (5)
C7—C8	1.362 (7)	C36—H36	0.9500
C7—H7	0.9500	C37—C38	1.470 (5)
C8—C9	1.391 (6)	C38—C39	1.380 (5)
C8—H8	0.9500	C38—C42	1.386 (5)
C9—C10	1.387 (5)	C40—C41	1.369 (6)
C9—H9	0.9500	C41—C42	1.371 (5)
C10—C11	1.383 (6)	C41—H41	0.9500
C10—C12	1.482 (5)	C42—H42	0.9500
C11—Pt1—N1	90.92 (14)	C21—C17—C16	121.3 (3)
C11—Pt1—N2	80.86 (14)	C18—C17—C16	123.7 (4)
N1—Pt1—N2	171.61 (12)	N3—C18—F1	114.5 (4)
C11—Pt1—C11	163.28 (11)	N3—C18—C17	125.7 (4)
N1—Pt1—C11	94.81 (9)	F1—C18—C17	119.7 (4)
N2—Pt1—C11	93.56 (9)	N3—C19—F2	114.7 (4)
C32—Pt2—N4	90.87 (14)	N3—C19—C20	126.8 (4)
C32—Pt2—N5	80.98 (13)	F2—C19—C20	118.4 (4)
N4—Pt2—N5	171.56 (11)	C19—C20—C21	115.4 (4)
C32—Pt2—C12	163.13 (11)	C19—C20—H20	122.3
N4—Pt2—C12	94.78 (9)	C21—C20—H20	122.3
N5—Pt2—C12	93.65 (8)	C20—C21—C17	121.5 (4)
C5—O1—C6	127.3 (3)	C20—C21—H21	119.3
C26—O2—C27	128.0 (3)	C17—C21—H21	119.3
C5—N1—C1	114.8 (3)	C23—C22—N4	124.6 (4)
C5—N1—Pt1	125.2 (3)	C23—C22—H22	117.7
C1—N1—Pt1	119.8 (2)	N4—C22—H22	117.7
C16—N2—C12	117.5 (3)	C22—C23—C24	118.0 (4)
C16—N2—Pt1	129.2 (3)	C22—C23—H23	121.0
C12—N2—Pt1	113.1 (2)	C24—C23—H23	121.0
C19—N3—C18	115.8 (4)	C25—C24—C23	119.1 (4)
C26—N4—C22	115.1 (3)	C25—C24—H24	120.5
C26—N4—Pt2	125.5 (3)	C23—C24—H24	120.5
C22—N4—Pt2	119.2 (2)	C24—C25—C26	119.6 (4)
C37—N5—C33	117.7 (3)	C24—C25—H25	120.2
C37—N5—Pt2	129.0 (2)	C26—C25—H25	120.2
C33—N5—Pt2	113.1 (2)	N4—C26—O2	124.0 (4)
C40—N6—C39	115.3 (4)	N4—C26—C25	123.7 (4)
C2—C1—N1	124.8 (4)	O2—C26—C25	112.2 (4)
C2—C1—H1	117.6	C28—C27—O2	115.6 (4)
N1—C1—H1	117.6	C28—C27—C32	121.5 (4)
C1—C2—C3	118.4 (4)	O2—C27—C32	122.9 (4)
C1—C2—H2	120.8	C29—C28—C27	119.5 (4)
C3—C2—H2	120.8	C29—C28—H28	120.3
C4—C3—C2	118.9 (4)	C27—C28—H28	120.3
C4—C3—H3	120.5	C28—C29—C30	121.5 (4)
C2—C3—H3	120.5	C28—C29—H29	119.2

C3—C4—C5	119.3 (4)	C30—C29—H29	119.2
C3—C4—H4	120.4	C29—C30—C31	118.4 (4)
C5—C4—H4	120.4	C29—C30—H30	120.8
N1—C5—O1	124.2 (4)	C31—C30—H30	120.8
N1—C5—C4	123.8 (4)	C32—C31—C30	121.4 (4)
O1—C5—C4	112.0 (4)	C32—C31—C33	115.2 (3)
O1—C6—C7	115.9 (4)	C30—C31—C33	123.3 (4)
O1—C6—C11	122.8 (4)	C31—C32—C27	117.6 (4)
C7—C6—C11	121.3 (4)	C31—C32—Pt2	114.9 (3)
C8—C7—C6	119.9 (4)	C27—C32—Pt2	126.6 (3)
C8—C7—H7	120.1	C34—C33—N5	122.0 (4)
C6—C7—H7	120.1	C34—C33—C31	125.6 (4)
C7—C8—C9	120.9 (4)	N5—C33—C31	112.4 (3)
C7—C8—H8	119.5	C33—C34—C35	120.1 (4)
C9—C8—H8	119.5	C33—C34—H34	120.0
C10—C9—C8	118.0 (4)	C35—C34—H34	120.0
C10—C9—H9	121.0	C34—C35—C36	118.3 (4)
C8—C9—H9	121.0	C34—C35—H35	120.8
C11—C10—C9	122.3 (4)	C36—C35—H35	120.8
C11—C10—C12	114.5 (3)	C35—C36—C37	121.1 (4)
C9—C10—C12	123.1 (4)	C35—C36—H36	119.4
C10—C11—C6	117.4 (4)	C37—C36—H36	119.4
C10—C11—Pt1	115.3 (3)	N5—C37—C36	120.1 (4)
C6—C11—Pt1	126.4 (3)	N5—C37—C38	119.0 (3)
C13—C12—N2	121.7 (4)	C36—C37—C38	120.3 (3)
C13—C12—C10	125.7 (4)	C39—C38—C42	114.6 (3)
N2—C12—C10	112.5 (3)	C39—C38—C37	124.0 (3)
C12—C13—C14	120.2 (4)	C42—C38—C37	121.1 (3)
C12—C13—H13	119.9	N6—C39—F3	114.3 (4)
C14—C13—H13	119.9	N6—C39—C38	126.7 (4)
C13—C14—C15	118.6 (4)	F3—C39—C38	118.9 (4)
C13—C14—H14	120.7	N6—C40—F4	115.0 (4)
C15—C14—H14	120.7	N6—C40—C41	126.4 (4)
C14—C15—C16	120.9 (4)	F4—C40—C41	118.6 (4)
C14—C15—H15	119.6	C40—C41—C42	115.7 (4)
C16—C15—H15	119.6	C40—C41—H41	122.1
N2—C16—C15	120.5 (4)	C42—C41—H41	122.1
N2—C16—C17	118.4 (3)	C41—C42—C38	121.2 (4)
C15—C16—C17	120.5 (3)	C41—C42—H42	119.4
C21—C17—C18	114.7 (4)	C38—C42—H42	119.4
C5—N1—C1—C2	-1.9 (6)	C26—N4—C22—C23	-0.8 (6)
Pt1—N1—C1—C2	173.2 (3)	Pt2—N4—C22—C23	174.2 (3)
N1—C1—C2—C3	0.3 (7)	N4—C22—C23—C24	-0.1 (7)
C1—C2—C3—C4	0.2 (7)	C22—C23—C24—C25	0.5 (8)
C2—C3—C4—C5	1.0 (8)	C23—C24—C25—C26	0.0 (8)
C1—N1—C5—O1	-177.3 (4)	C22—N4—C26—O2	-176.9 (4)
Pt1—N1—C5—O1	8.0 (6)	Pt2—N4—C26—O2	8.5 (6)

C1—N1—C5—C4	3.2 (6)	C22—N4—C26—C25	1.3 (6)
Pt1—N1—C5—C4	-171.6 (4)	Pt2—N4—C26—C25	-173.3 (4)
C6—O1—C5—N1	10.8 (7)	C27—O2—C26—N4	6.4 (7)
C6—O1—C5—C4	-169.6 (4)	C27—O2—C26—C25	-172.0 (4)
C3—C4—C5—N1	-2.9 (8)	C24—C25—C26—N4	-0.9 (8)
C3—C4—C5—O1	177.5 (5)	C24—C25—C26—O2	177.5 (5)
C5—O1—C6—C7	161.3 (4)	C26—O2—C27—C28	165.0 (4)
C5—O1—C6—C11	-21.3 (7)	C26—O2—C27—C32	-16.3 (7)
O1—C6—C7—C8	-178.6 (4)	O2—C27—C28—C29	-177.4 (4)
C11—C6—C7—C8	4.0 (7)	C32—C27—C28—C29	3.9 (7)
C6—C7—C8—C9	-2.0 (7)	C27—C28—C29—C30	-1.5 (7)
C7—C8—C9—C10	-0.8 (7)	C28—C29—C30—C31	-1.5 (7)
C8—C9—C10—C11	1.7 (6)	C29—C30—C31—C32	2.1 (6)
C8—C9—C10—C12	-176.0 (4)	C29—C30—C31—C33	-176.0 (4)
C9—C10—C11—C6	0.2 (6)	C30—C31—C32—C27	0.1 (6)
C12—C10—C11—C6	178.1 (3)	C33—C31—C32—C27	178.4 (3)
C9—C10—C11—Pt1	169.8 (3)	C30—C31—C32—Pt2	169.9 (3)
C12—C10—C11—Pt1	-12.4 (4)	C33—C31—C32—Pt2	-11.8 (4)
O1—C6—C11—C10	179.7 (4)	C28—C27—C32—C31	-3.2 (6)
C7—C6—C11—C10	-3.1 (6)	O2—C27—C32—C31	178.2 (4)
O1—C6—C11—Pt1	11.4 (6)	C28—C27—C32—Pt2	-171.7 (3)
C7—C6—C11—Pt1	-171.3 (3)	O2—C27—C32—Pt2	9.7 (6)
C16—N2—C12—C13	7.8 (5)	C37—N5—C33—C34	8.4 (5)
Pt1—N2—C12—C13	-167.8 (3)	Pt2—N5—C33—C34	-167.7 (3)
C16—N2—C12—C10	-169.1 (3)	C37—N5—C33—C31	-169.4 (3)
Pt1—N2—C12—C10	15.3 (4)	Pt2—N5—C33—C31	14.5 (4)
C11—C10—C12—C13	-179.3 (4)	C32—C31—C33—C34	179.9 (4)
C9—C10—C12—C13	-1.5 (6)	C30—C31—C33—C34	-1.8 (6)
C11—C10—C12—N2	-2.5 (5)	C32—C31—C33—N5	-2.3 (5)
C9—C10—C12—N2	175.3 (3)	C30—C31—C33—N5	175.9 (3)
N2—C12—C13—C14	-1.3 (6)	N5—C33—C34—C35	-2.4 (6)
C10—C12—C13—C14	175.2 (4)	C31—C33—C34—C35	175.1 (4)
C12—C13—C14—C15	-4.0 (6)	C33—C34—C35—C36	-3.1 (6)
C13—C14—C15—C16	2.6 (6)	C34—C35—C36—C37	2.4 (6)
C12—N2—C16—C15	-9.2 (5)	C33—N5—C37—C36	-8.9 (5)
Pt1—N2—C16—C15	165.6 (3)	Pt2—N5—C37—C36	166.4 (3)
C12—N2—C16—C17	162.7 (3)	C33—N5—C37—C38	162.7 (3)
Pt1—N2—C16—C17	-22.5 (5)	Pt2—N5—C37—C38	-21.9 (5)
C14—C15—C16—N2	4.2 (6)	C35—C36—C37—N5	3.8 (6)
C14—C15—C16—C17	-167.5 (4)	C35—C36—C37—C38	-167.8 (4)
N2—C16—C17—C21	-45.1 (5)	N5—C37—C38—C39	142.1 (4)
C15—C16—C17—C21	126.7 (4)	C36—C37—C38—C39	-46.3 (5)
N2—C16—C17—C18	141.4 (4)	N5—C37—C38—C42	-44.8 (5)
C15—C16—C17—C18	-46.8 (5)	C36—C37—C38—C42	126.8 (4)
C19—N3—C18—F1	-178.8 (4)	C40—N6—C39—F3	-178.8 (3)
C19—N3—C18—C17	1.0 (6)	C40—N6—C39—C38	0.3 (6)
C21—C17—C18—N3	-2.0 (6)	C42—C38—C39—N6	-1.7 (6)
C16—C17—C18—N3	171.9 (4)	C37—C38—C39—N6	171.7 (4)

C21—C17—C18—F1	177.7 (3)	C42—C38—C39—F3	177.4 (3)
C16—C17—C18—F1	-8.4 (6)	C37—C38—C39—F3	-9.2 (5)
C18—N3—C19—F2	-176.8 (3)	C39—N6—C40—F4	-177.1 (3)
C18—N3—C19—C20	1.0 (6)	C39—N6—C40—C41	2.3 (6)
N3—C19—C20—C21	-1.7 (6)	N6—C40—C41—C42	-3.1 (6)
F2—C19—C20—C21	176.1 (3)	F4—C40—C41—C42	176.4 (3)
C19—C20—C21—C17	0.4 (5)	C40—C41—C42—C38	1.3 (5)
C18—C17—C21—C20	1.2 (5)	C39—C38—C42—C41	0.8 (5)
C16—C17—C21—C20	-172.8 (3)	C37—C38—C42—C41	-172.9 (3)

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C1—H1...C11	0.95	2.46	3.175 (4)	132
C3—H3...F1 ⁱ	0.95	2.53	3.474 (5)	172
C15—H15...F1	0.95	2.56	2.989 (5)	108
C22—H22...C12	0.95	2.45	3.170 (4)	132
C23—H23...C12 ⁱⁱ	0.95	2.82	3.540 (5)	133
C24—H24...F3 ⁱⁱⁱ	0.95	2.50	3.443 (5)	172
C36—H36...F3	0.95	2.55	2.975 (5)	108
C41—H41...C11	0.95	2.79	3.684 (4)	158

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