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# Crystal structure of [2,6-difluoro-3-(pyridin-2-yl- $\kappa N$ )pyridin-4-yl- $\kappa C^4$ ](pentane-2,4-dionato- $\kappa^2 O,O'$ )-platinum(II)

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The asymmetric unit of the title compound,  $[Pt(C_{10}H_5F_2N_2)(C_5H_7O_2)]$ , comprises one  $Pt^{II}$  atom, one 2,6-difluoro-2,3-bipyridine ligand and one acetylacetonate anion. The  $Pt^{II}$  atom adopts a distorted square-planar coordination geometry, being *C*,*N*-chelated by the 2,6-difluoro-3-(pyridin-2-yl)pyridin-4-yl ligand and *O*,*O'*-chelated by the pentane-2,4-dionate ligand. The two pyridine rings of the bipyridine ligand are approximately coplanar, making a dihedral angle of 1.2 (2)°. A variety of intra- and intermolecular C–H···O and C–H···F hydrogen bonds, as well as  $\pi$ - $\pi$  interactions [centroid–centroid distances = 4.337 (3) and 3.774 (3) Å] contribute to the stabilization of the molecular and crystal structures, and result in the formation of a threedimensional supramolecular framework.

### 1. Chemical context

Cyclometalated platinum(II) compounds with *C*,*N*-chelating ligands have been considered as an attractive research area due to their wide applications, such as biological imaging, non-linear optics, oxygen sensing and organic light-emitting diodes (OLEDs) (Hudson *et al.*, 2012). In particular, phenylpyridine (ppy) based platinum(II)  $\beta$ -diketonate compounds have been widely studied because of their excellent stability and high quantum efficiency in OLEDs (Rao *et al.*, 2012). However, examples of platinum(II) compounds with *C*,*N*-chelating bipyridine ligands are scarce. Herein, we report the result of our investigation on the crystal structure of a novel platinum(II) compound with fluorinated bipyridine and acetylacetonate (acac, *O*,*O*) ligands.





### 2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The asymmetric unit consists of one  $Pt^{II}$  atom, one 2,6-difluoro-2,3-bipyridine ligand and one acetylacetonate anion. The  $Pt^{II}$  atom is four-coordinated by the *C*,*N*-chelating 2',6'-difluoro-2,3'-bipyridinato ligand and by the *O*,*O*'-chelating



Figure 1

View of the molecular structure of the title compound, with the atomnumbering scheme. Displacement ellipsoids are drawn at the 50% probability level; dashed lines represent intramolecular  $C-H\cdots O$  and  $C-H\cdots F$  hydrogen bonds.

pentane-2,4-dionato ligand, forming a distorted square-planar coordination sphere due to narrow ligand bite angles, which range from 81.28 (17) to 93.25 (13)°. The Pt–C bond length of 1.951 (4) Å is shorter than the Pt–N bond length of 1.995 (4) Å due to the more electronegative fluorine substituent on the C-bound pyridine ring. The Pt–C, Pt–N and Pt–O bond lengths (Table 1) are in normal ranges as reported for similar Pt<sup>II</sup> compounds, *e.g.* [Pt(Bppy)(acac)] (Bppy is a boron-functionalized phenylpyridine; Rao *et al.*, 2012). Within



Figure 2

The two-dimensional supramolecular network formed through  $C-H\cdots F$  interactions (yellow dashed lines). H atoms not involved in intermolecular interactions have been omitted for clarity.

| Table 1                    |  |
|----------------------------|--|
| Selected bond lengths (Å). |  |

| Pt1-C1 | 1.951 (4) | Pt1-O1 | 2.074 (3) |
|--------|-----------|--------|-----------|
| Pt1-N2 | 1.995 (4) | Pt1-O2 | 2.001 (3) |

 Table 2

 Hydrogen-bond geometry (Å, °).

|                          | •    | ·                       |              |                             |
|--------------------------|------|-------------------------|--------------|-----------------------------|
| $D - H \cdots A$         | D-H  | $H \cdot \cdot \cdot A$ | $D \cdots A$ | $D - H \cdot \cdot \cdot A$ |
| C2-H2···O2               | 0.95 | 2.57                    | 3.040 (5)    | 111                         |
| $C7-H7\cdots F2$         | 0.95 | 2.31                    | 2.917 (6)    | 121                         |
| $C10-H10\cdots F1^{i}$   | 0.95 | 2.32                    | 3.180 (5)    | 150                         |
| C10-H10···O1             | 0.95 | 2.41                    | 3.006 (5)    | 120                         |
| $C12-H12\cdots F2^{ii}$  | 0.95 | 2.44                    | 3.361 (5)    | 163                         |
| $C15{-}H15A{\cdots}F1^i$ | 0.98 | 2.54                    | 3.481 (6)    | 161                         |

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

the *C*,*N*-bidentate ligand of the title compound, the two pyridine rings are approximately co-planar, making a dihedral angle of 1.2 (2)°, indicating that an effective  $\pi$  conjugation of the two pyridine rings occurs in the title compound. The molecular structure is stabilized by weak intramolecular C–H···O and C–H···F hydrogen bonds (Table 2).

#### 3. Supramolecular features

Intermolecular C-H···F hydrogen bonds between neighboring molecules lead to the formation of a two-dimensional supramolecular network extending parallel to the ( $\overline{1}10$ ) plane (Fig. 2, Table 2). These networks are interlinked by  $\pi$ - $\pi$  interactions [Cg1- $Cg2^{i}$  = 4.337 (3) Å and Cg1- $Cg2^{ii}$  = 3.774 (3) Å, where Cg1 and Cg2 are the centroids of the N1, C1-C5 and the N2, C6-C10 rings, respectively; symmetry codes: (i) -x + 1, -y + 2, -z + 2; (ii) -x + 2, -y + 2, -z + 2], resulting in the formation of an overall three-dimensional supramolecular framework (Fig. 3).



Figure 3

The three-dimensional supramolecular network formed through  $\pi$ - $\pi$  stacking interactions (black dashed lines). Yellow dashed lines indicate the C-H···F interactions. H atoms not involved in intermolecular interactions have been omitted for clarity.

### research communications

Table 3Experimental details.

| Crystal data   |                                     |
|--|-------------------------------------|
| Chemical formula   | $[Pt(C_{10}H_5F_2N_2)(C_5H_7O_2)]$  |
| $M_{\rm r}$  | 485.36                              |
| Crystal system, space group  | Triclinic, $P\overline{1}$          |
| Temperature (K)  | 180                                 |
| a, b, c (Å)  | 8.0442 (6), 9.8711 (7), 10.1458 (7) |
| $\alpha, \beta, \gamma$ (°)  | 97.683 (1), 112.320 (1), 99.410 (1) |
| $V(Å^3)$   | 718.12 (9)                          |
| Ζ  | 2                                   |
| Radiation type   | Μο Κα                               |
| $\mu (\text{mm}^{-1})$   | 9.80                                |
| Crystal size (mm)  | $0.27 \times 0.24 \times 0.12$      |
| Data collection  |                                     |
| Diffractometer   | Bruker APEXII CCD area              |
|  | detector                            |
| Absorption correction  | Multi-scan (SADABS; Bruker,         |
|  | 2006)                               |
| $T_{\min}, T_{\max}$   | 0.177, 0.386                        |
| No. of measured, independent and   | 7062, 2810, 2773                    |
| observed $[I > 2\sigma(I)]$ reflections                                      |                                     |
| R <sub>int</sub>   | 0.023                               |
| $(\sin \theta / \lambda)_{\max} ( \text{\AA}^{-1} )$                         | 0.617                               |
| Refinement   |                                     |
| $R[F^2 > 2\sigma(F^2)], wR(F^2), S$  | 0.017, 0.053, 1.07                  |
| No. of reflections   | 2810                                |
| No. of parameters  | 199                                 |
| H-atom treatment   | H-atom parameters constrained       |
| $\Delta \rho_{\rm max},  \Delta \rho_{\rm min} \ ({\rm e} \ {\rm \AA}^{-3})$ | 0.51, -1.27                         |

Computer programs: APEX2 and SAINT (Bruker, 2006), SHELXS97, SHELXL97 and SHELXTL (Sheldrick, 2008) and DIAMOND (Brandenburg, 2005).

### 4. Synthesis and crystallization

The title compound was synthesized according to a previous report (Rao *et al.*, 2012). Slow evaporation from a dichloro-

methane/hexane solution afforded yellow crystals suitable for X-ray crystallography analysis.

### 5. Refinement

Crystal data, data collection and crystal structure refinement details are summarized in Table 3. All H atoms were positioned geometrically and refined using a riding model, with d(C-H) = 0.95 Å,  $U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$  for  $Csp^2$ -H, and 0.98 Å,  $U_{\rm iso}(H) = 1.5U_{\rm eq}(C)$  for methyl protons.

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### supporting information

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Crystal structure of [2,6-difluoro-3-(pyridin-2-yl- $\kappa N$ )pyridin-4-yl- $\kappa C^4$ ] (pentane-2,4-dionato- $\kappa^2 O, O'$ )platinum(II)

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**Computing details** 

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT* (Bruker, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

 $[2,6-Difluoro-3-(pyridin-2-yl-\kappa N)pyridin-4-yl-\kappa C^{4}]$  (pentane-2,4-dionato- $\kappa^{2}O,O'$ ) platinum(II)

### Crystal data

[Pt(C<sub>10</sub>H<sub>5</sub>F<sub>2</sub>N<sub>2</sub>)(C<sub>5</sub>H<sub>7</sub>O<sub>2</sub>)]  $M_r = 485.36$ Triclinic, *P*1 Hall symbol: -P 1 a = 8.0442 (6) Å b = 9.8711 (7) Å c = 10.1458 (7) Å a = 97.683 (1)°  $\beta = 112.320$  (1)°  $\gamma = 99.410$  (1)° V = 718.12 (9) Å<sup>3</sup>

Data collection

Bruker APEXII CCD area-detector diffractometer Radiation source: fine-focus sealed tube Graphite monochromator  $\varphi$  and  $\omega$  scans Absorption correction: multi-scan (*SADABS*; Bruker, 2006)  $T_{\min} = 0.177, T_{\max} = 0.386$ 

### Refinement

Refinement on  $F^2$ Least-squares matrix: full  $R[F^2 > 2\sigma(F^2)] = 0.017$  $wR(F^2) = 0.053$ S = 1.072810 reflections 199 parameters 0 restraints Z = 2 F(000) = 456  $D_x = 2.245 \text{ Mg m}^{-3}$ Mo K $\alpha$  radiation,  $\lambda = 0.71073 \text{ Å}$ Cell parameters from 2773 reflections  $\theta = 2.1-26.0^{\circ}$   $\mu = 9.80 \text{ mm}^{-1}$  T = 180 KBlock, yellow  $0.27 \times 0.24 \times 0.12 \text{ mm}$ 

7062 measured reflections 2810 independent reflections 2773 reflections with  $I > 2\sigma(I)$  $R_{int} = 0.023$  $\theta_{max} = 26.0^{\circ}, \ \theta_{min} = 2.1^{\circ}$  $h = -9 \rightarrow 9$  $k = -12 \rightarrow 12$  $l = -12 \rightarrow 12$ 

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  $w = 1/[\sigma^2(F_o^2) + (0.0295P)^2 + 1.5655P]$ Δ Δ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\rm max} = 0.002$ 

$$\Delta \rho_{\rm max} = 0.51 \text{ e } \text{\AA}^{-3}$$
  
 $\Delta \rho_{\rm min} = -1.27 \text{ e } \text{\AA}^{-3}$ 

### 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 coordin | ates and isotropic of | or equivalent isotropic | displacement | parameters ( | $(Å^2)$ |
|---------------------------|-----------------------|-------------------------|--------------|--------------|---------|
|                           |                       |                         |              | r            | /       |

|      | x             | у             | Z             | $U_{ m iso}$ */ $U_{ m eq}$ |  |
|------|---------------|---------------|---------------|-----------------------------|--|
| Pt1  | 0.541428 (18) | 0.778516 (13) | 0.974446 (14) | 0.01645 (7)                 |  |
| F1   | 0.6043 (5)    | 0.8519 (4)    | 0.4799 (3)    | 0.0462 (8)                  |  |
| F2   | 0.9252 (4)    | 1.1982 (3)    | 0.8748 (3)    | 0.0362 (6)                  |  |
| 01   | 0.4622 (4)    | 0.7037 (3)    | 1.1284 (3)    | 0.0240 (6)                  |  |
| O2   | 0.3730 (4)    | 0.6133 (3)    | 0.8158 (3)    | 0.0231 (6)                  |  |
| N1   | 0.7621 (5)    | 1.0252 (4)    | 0.6783 (4)    | 0.0294 (8)                  |  |
| N2   | 0.7143 (5)    | 0.9517 (4)    | 1.1169 (4)    | 0.0197 (7)                  |  |
| C1   | 0.6273 (6)    | 0.8664 (4)    | 0.8434 (5)    | 0.0209 (8)                  |  |
| C2   | 0.5731 (6)    | 0.8150 (5)    | 0.6931 (5)    | 0.0251 (8)                  |  |
| H2   | 0.4892        | 0.7267        | 0.6431        | 0.030*                      |  |
| C3   | 0.6477 (6)    | 0.8990 (5)    | 0.6230 (5)    | 0.0290 (9)                  |  |
| C4   | 0.8076 (6)    | 1.0704 (4)    | 0.8184 (5)    | 0.0245 (8)                  |  |
| C5   | 0.7490 (5)    | 0.9996 (4)    | 0.9079 (4)    | 0.0205 (8)                  |  |
| C6   | 0.7995 (6)    | 1.0466 (4)    | 1.0634 (5)    | 0.0210 (8)                  |  |
| C7   | 0.9196 (6)    | 1.1711 (4)    | 1.1559 (5)    | 0.0263 (9)                  |  |
| H7   | 0.9801        | 1.2372        | 1.1190        | 0.032*                      |  |
| C8   | 0.9507 (6)    | 1.1986 (5)    | 1.3023 (5)    | 0.0295 (9)                  |  |
| H8   | 1.0316        | 1.2836        | 1.3659        | 0.035*                      |  |
| C9   | 0.8626 (6)    | 1.1006 (5)    | 1.3545 (5)    | 0.0279 (9)                  |  |
| H9   | 0.8829        | 1.1168        | 1.4544        | 0.034*                      |  |
| C10  | 0.7447 (6)    | 0.9790 (5)    | 1.2585 (5)    | 0.0249 (8)                  |  |
| H10  | 0.6829        | 0.9121        | 1.2937        | 0.030*                      |  |
| C11  | 0.3374 (6)    | 0.5912 (4)    | 1.0981 (5)    | 0.0219 (8)                  |  |
| C12  | 0.2383 (6)    | 0.5027 (4)    | 0.9600 (5)    | 0.0247 (9)                  |  |
| H12  | 0.1450        | 0.4256        | 0.9525        | 0.030*                      |  |
| C13  | 0.2611 (6)    | 0.5149 (4)    | 0.8326 (5)    | 0.0230 (8)                  |  |
| C14  | 0.1488 (7)    | 0.4045 (5)    | 0.6953 (5)    | 0.0328 (10)                 |  |
| H14A | 0.1816        | 0.4288        | 0.6163        | 0.049*                      |  |
| H14B | 0.0170        | 0.3996        | 0.6684        | 0.049*                      |  |
| H14C | 0.1746        | 0.3131        | 0.7117        | 0.049*                      |  |
| C15  | 0.3027 (7)    | 0.5529 (5)    | 1.2257 (5)    | 0.0305 (10)                 |  |
| H15A | 0.3822        | 0.6245        | 1.3142        | 0.046*                      |  |

## supporting information

| H15B | 0.3306 | 0.4613 | 1.2389 | 0.046* |
|------|--------|--------|--------|--------|
| H15C | 0.1728 | 0.5479 | 1.2072 | 0.046* |

Atomic displacement parameters  $(Å^2)$ 

|     | $U^{11}$     | $U^{22}$    | $U^{33}$    | $U^{12}$     | $U^{13}$    | $U^{23}$     |
|-----|--------------|-------------|-------------|--------------|-------------|--------------|
| Pt1 | 0.01828 (10) | 0.01327 (9) | 0.01850 (9) | 0.00005 (6)  | 0.00925 (7) | 0.00501 (6)  |
| F1  | 0.062 (2)    | 0.0564 (19) | 0.0253 (14) | 0.0043 (16)  | 0.0257 (14) | 0.0124 (13)  |
| F2  | 0.0389 (15)  | 0.0238 (13) | 0.0495 (17) | -0.0032 (11) | 0.0244 (13) | 0.0138 (12)  |
| 01  | 0.0251 (15)  | 0.0198 (14) | 0.0209 (14) | -0.0073 (12) | 0.0087 (12) | 0.0017 (11)  |
| O2  | 0.0242 (14)  | 0.0179 (14) | 0.0241 (14) | -0.0014 (11) | 0.0095 (12) | 0.0034 (11)  |
| N1  | 0.031 (2)    | 0.033 (2)   | 0.034 (2)   | 0.0088 (16)  | 0.0200 (17) | 0.0187 (17)  |
| N2  | 0.0176 (16)  | 0.0169 (16) | 0.0235 (17) | 0.0015 (13)  | 0.0083 (14) | 0.0045 (13)  |
| C1  | 0.029 (2)    | 0.0176 (19) | 0.025 (2)   | 0.0086 (16)  | 0.0169 (18) | 0.0103 (16)  |
| C2  | 0.027 (2)    | 0.025 (2)   | 0.022 (2)   | 0.0021 (17)  | 0.0101 (17) | 0.0073 (16)  |
| C3  | 0.032 (2)    | 0.037 (2)   | 0.021 (2)   | 0.0097 (19)  | 0.0124 (18) | 0.0108 (18)  |
| C4  | 0.023 (2)    | 0.021 (2)   | 0.035 (2)   | 0.0044 (16)  | 0.0161 (18) | 0.0130 (17)  |
| C5  | 0.0191 (18)  | 0.0190 (19) | 0.025 (2)   | 0.0043 (15)  | 0.0102 (16) | 0.0065 (16)  |
| C6  | 0.0198 (18)  | 0.0182 (19) | 0.028 (2)   | 0.0041 (15)  | 0.0119 (17) | 0.0077 (16)  |
| C7  | 0.023 (2)    | 0.0170 (19) | 0.037 (2)   | 0.0004 (16)  | 0.0115 (18) | 0.0070 (17)  |
| C8  | 0.025 (2)    | 0.021 (2)   | 0.031 (2)   | -0.0002 (17) | 0.0042 (18) | -0.0021 (17) |
| C9  | 0.029 (2)    | 0.027 (2)   | 0.022 (2)   | 0.0038 (18)  | 0.0074 (17) | -0.0002 (17) |
| C10 | 0.028 (2)    | 0.024 (2)   | 0.023 (2)   | 0.0032 (17)  | 0.0120 (17) | 0.0037 (16)  |
| C11 | 0.023 (2)    | 0.020(2)    | 0.028 (2)   | 0.0037 (16)  | 0.0136 (17) | 0.0129 (16)  |
| C12 | 0.021 (2)    | 0.0175 (19) | 0.034 (2)   | -0.0024 (16) | 0.0119 (18) | 0.0086 (17)  |
| C13 | 0.0207 (19)  | 0.0160 (19) | 0.027 (2)   | -0.0004 (15) | 0.0065 (17) | 0.0040 (16)  |
| C14 | 0.031 (2)    | 0.025 (2)   | 0.029 (2)   | -0.0074 (18) | 0.0057 (19) | -0.0023 (18) |
| C15 | 0.030 (2)    | 0.032 (2)   | 0.032 (2)   | 0.0008 (19)  | 0.016 (2)   | 0.0124 (19)  |
|     |              |             |             |              |             |              |

Geometric parameters (Å, °)

| Pt1—C1 | 1.951 (4) | С7—С8    | 1.389 (7) |
|--------|-----------|----------|-----------|
| Pt1—N2 | 1.995 (4) | С7—Н7    | 0.9500    |
| Pt1—O1 | 2.074 (3) | C8—C9    | 1.384 (7) |
| Pt1—O2 | 2.001 (3) | C8—H8    | 0.9500    |
| F1—C3  | 1.352 (5) | C9—C10   | 1.379 (6) |
| F2—C4  | 1.349 (5) | С9—Н9    | 0.9500    |
| 01—C11 | 1.282 (5) | C10—H10  | 0.9500    |
| O2—C13 | 1.288 (5) | C11—C12  | 1.399 (6) |
| N1C4   | 1.316 (6) | C11—C15  | 1.506 (6) |
| N1—C3  | 1.327 (6) | C12—C13  | 1.391 (6) |
| N2-C10 | 1.343 (5) | C12—H12  | 0.9500    |
| N2C6   | 1.361 (5) | C13—C14  | 1.504 (6) |
| C1—C5  | 1.406 (6) | C14—H14A | 0.9800    |
| C1—C2  | 1.410 (6) | C14—H14B | 0.9800    |
| С2—С3  | 1.368 (6) | C14—H14C | 0.9800    |
| С2—Н2  | 0.9500    | C15—H15A | 0.9800    |
| C4—C5  | 1.387 (6) | C15—H15B | 0.9800    |
|        |           |          |           |

## supporting information

| C5—C6                   | 1.457 (6)            | C15—H15C                           | 0.9800               |
|-------------------------|----------------------|------------------------------------|----------------------|
| C6—C7                   | 1.393 (6)            |                                    |                      |
|                         |                      |                                    |                      |
| C1—Pt1—N2               | 81.28 (17)           | С6—С7—Н7                           | 120.0                |
| C1—Pt1—O2               | 92.90 (16)           | C9—C8—C7                           | 119.3 (4)            |
| N2—Pt1—O2               | 174.15 (12)          | С9—С8—Н8                           | 120.4                |
| C1—Pt1—O1               | 174.40 (14)          | С7—С8—Н8                           | 120.4                |
| N2—Pt1—O1               | 93.25 (13)           | С10—С9—С8                          | 118.6 (4)            |
| O2—Pt1—O1               | 92.55 (12)           | С10—С9—Н9                          | 120.7                |
| C11—O1—Pt1              | 123.4 (3)            | С8—С9—Н9                           | 120.7                |
| C13—O2—Pt1              | 123.9 (3)            | N2-C10-C9                          | 122.4 (4)            |
| C4-N1-C3                | 113.8 (4)            | N2-C10-H10                         | 118.8                |
| $C10 - N^2 - C6$        | 1199(4)              | C9-C10-H10                         | 118.8                |
| C10 - N2 - Pt1          | 1234(3)              | 01-C11-C12                         | 125.5(4)             |
| C6-N2-Pt1               | 1167(3)              | 01 - C11 - C15                     | 125.5(1)<br>115.4(4) |
| $C_{5}$ $C_{1}$ $C_{2}$ | 117.9(4)             | $C_{12}$ $C_{11}$ $C_{15}$         | 119.4 (4)            |
| $C_{5}$ $C_{1}$ $P_{1}$ | 114 5 (3)            | $C_{12} = C_{11} = C_{12}$         | 117.1(4)<br>127.3(4) |
| $C_2 = C_1 = P_1$       | 114.5(3)<br>127 A(3) | $C_{13} = C_{12} = C_{11}$         | 127.5 (+)            |
| $C_2 = C_1 = C_1$       | 127.4(3)<br>116.6(4) | $C_{13} - C_{12} - H_{12}$         | 116.4                |
| $C_3 = C_2 = C_1$       | 110.0 (4)            | C11 - C12 - 1112<br>O2 - C12 - C12 | 110.4<br>127.1(4)    |
| $C_3 = C_2 = H_2$       | 121.7                | 02 - C13 - C12                     | 127.1(4)<br>1120(4)  |
| C1 - C2 - H2            | 121.7                | 02-013-014                         | 113.0(4)             |
| $NI = C_2 = C_2$        | 115.5 (4)            | C12 - C13 - C14                    | 119.9 (4)            |
| $NI = C_2 = C_2$        | 127.9 (4)            | C13 - C14 - H14A                   | 109.5                |
| F1 - C3 - C2            | 118.6 (4)            | CI3-CI4-HI4B                       | 109.5                |
| NI - C4 - F2            | 113.7 (4)            | H14A - C14 - H14B                  | 109.5                |
| NI-C4-C5                | 126.6 (4)            | С13—С14—Н14С                       | 109.5                |
| F2—C4—C5                | 119.7 (4)            | H14A—C14—H14C                      | 109.5                |
| C4—C5—C1                | 117.2 (4)            | H14B—C14—H14C                      | 109.5                |
| C4—C5—C6                | 127.6 (4)            | C11—C15—H15A                       | 109.5                |
| C1—C5—C6                | 115.3 (4)            | C11—C15—H15B                       | 109.5                |
| N2—C6—C7                | 119.9 (4)            | H15A—C15—H15B                      | 109.5                |
| N2—C6—C5                | 112.2 (4)            | C11—C15—H15C                       | 109.5                |
| C7—C6—C5                | 128.0 (4)            | H15A—C15—H15C                      | 109.5                |
| C8—C7—C6                | 119.9 (4)            | H15B—C15—H15C                      | 109.5                |
| С8—С7—Н7                | 120.0                |                                    |                      |
|                         |                      |                                    |                      |
| N2—Pt1—O1—C11           | 176.1 (3)            | C2—C1—C5—C6                        | 180.0 (4)            |
| O2-Pt1-O1-C11           | -3.1 (3)             | Pt1-C1-C5-C6                       | 3.4 (5)              |
| C1—Pt1—O2—C13           | -175.2 (3)           | C10—N2—C6—C7                       | 0.7 (6)              |
| O1—Pt1—O2—C13           | 3.5 (3)              | Pt1-N2-C6-C7                       | 178.9 (3)            |
| C1-Pt1-N2-C10           | -179.3 (4)           | C10—N2—C6—C5                       | -179.6 (4)           |
| O1-Pt1-N2-C10           | 1.9 (3)              | Pt1-N2-C6-C5                       | -1.4 (4)             |
| C1—Pt1—N2—C6            | 2.6 (3)              | C4—C5—C6—N2                        | 179.1 (4)            |
| O1—Pt1—N2—C6            | -176.2 (3)           | C1—C5—C6—N2                        | -1.3 (5)             |
| N2—Pt1—C1—C5            | -3.2 (3)             | C4—C5—C6—C7                        | -1.2 (7)             |
| O2-Pt1-C1-C5            | 176.2 (3)            | C1—C5—C6—C7                        | 178.4 (4)            |
| N2—Pt1—C1—C2            | -179.4 (4)           | N2-C6-C7-C8                        | -0.6 (6)             |
| O2—Pt1—C1—C2            | 0.0 (4)              | C5—C6—C7—C8                        | 179.8 (4)            |

| C5-C1-C2-C3  | 1.4 (6)    | C6—C7—C8—C9     | 0.5 (6)    |
|--------------|------------|-----------------|------------|
| Pt1—C1—C2—C3 | 177.4 (3)  | C7—C8—C9—C10    | -0.6 (7)   |
| C4—N1—C3—F1  | -178.8 (4) | C6—N2—C10—C9    | -0.8 (6)   |
| C4—N1—C3—C2  | 0.9 (7)    | Pt1-N2-C10-C9   | -178.9 (3) |
| C1-C2-C3-N1  | -1.8 (7)   | C8—C9—C10—N2    | 0.8 (7)    |
| C1—C2—C3—F1  | 177.9 (4)  | Pt1-01-C11-C12  | 0.5 (6)    |
| C3—N1—C4—F2  | 179.4 (4)  | Pt1-01-C11-C15  | 178.7 (3)  |
| C3—N1—C4—C5  | 0.3 (6)    | O1—C11—C12—C13  | 3.4 (7)    |
| N1—C4—C5—C1  | -0.6 (6)   | C15-C11-C12-C13 | -174.8 (4) |
| F2—C4—C5—C1  | -179.6 (4) | Pt1-02-C13-C12  | -1.3 (6)   |
| N1-C4-C5-C6  | 179.1 (4)  | Pt1             | 179.2 (3)  |
| F2C4C5C6     | 0.0 (6)    | C11—C12—C13—O2  | -3.0 (7)   |
| C2-C1-C5-C4  | -0.3 (6)   | C11—C12—C13—C14 | 176.4 (4)  |
| Pt1-C1-C5-C4 | -176.9 (3) |                 |            |
|              |            |                 |            |

### Hydrogen-bond geometry (Å, °)

| D—H···A                        | D—H  | $H \cdots A$ | $D \cdots A$ | D—H···A |
|--------------------------------|------|--------------|--------------|---------|
| С2—Н2…О2                       | 0.95 | 2.57         | 3.040 (5)    | 111     |
| C7—H7…F2                       | 0.95 | 2.31         | 2.917 (6)    | 121     |
| C10— $H10$ ···F1 <sup>i</sup>  | 0.95 | 2.32         | 3.180 (5)    | 150     |
| C10—H10…O1                     | 0.95 | 2.41         | 3.006 (5)    | 120     |
| C12—H12…F2 <sup>ii</sup>       | 0.95 | 2.44         | 3.361 (5)    | 163     |
| C15—H15 $A$ ···F1 <sup>i</sup> | 0.98 | 2.54         | 3.481 (6)    | 161     |
|                                |      |              |              |         |

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