

# Crystal structure of bis[2-*tert*-butoxy-6-fluoro-3-(pyridin-2-yl- $\kappa$ N)pyridin-4-yl- $\kappa$ C<sup>4</sup>](pentane-2,4-dionato- $\kappa^2$ O, $O'$ )iridium(III)

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**Keywords:** crystal structure; iridium(III); C<sub>2</sub>N<sub>2</sub>O<sub>2</sub> coordination set

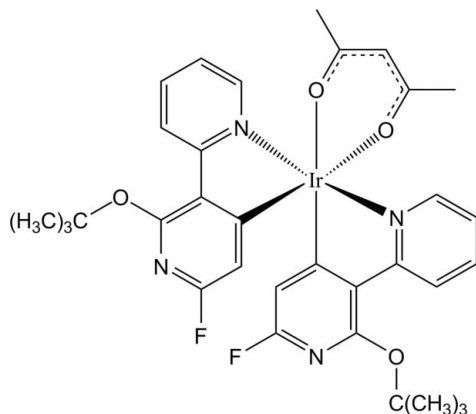
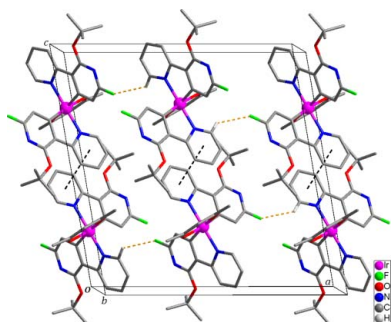
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The title molecule, [Ir(C<sub>14</sub>H<sub>14</sub>FN<sub>2</sub>O)<sub>2</sub>(C<sub>5</sub>H<sub>7</sub>O<sub>2</sub>)], is located on a twofold rotation axis, which passes through the Ir<sup>III</sup> atom and the central C atom of the pentane-2,4-dionate anion. The Ir<sup>III</sup> atom adopts a distorted octahedral coordination geometry, being *C,N*-chelated by two 2-*tert*-butoxy-6-fluoro-3-(pyridin-2-yl)pyridin-4-yl ligands and *O,O'*-chelated by the pentane-2,4-dionato ligand. The bipyridinate ligands, which are perpendicular to each other [dihedral angle between the two least-squares planes = 89.95 (5)°], are arranged in a *cis-C,C'* and *trans-N,N'* fashion relative to the central metal cation. Intramolecular C—H···O and C—H···N hydrogen bonds and intermolecular C—H···F hydrogen bonds as well as  $\pi$ – $\pi$  interactions between neighbouring pyridine rings [centroid–centroid distance 3.680 (1) Å] contribute to the stabilization of the molecular and crystal structure, respectively.

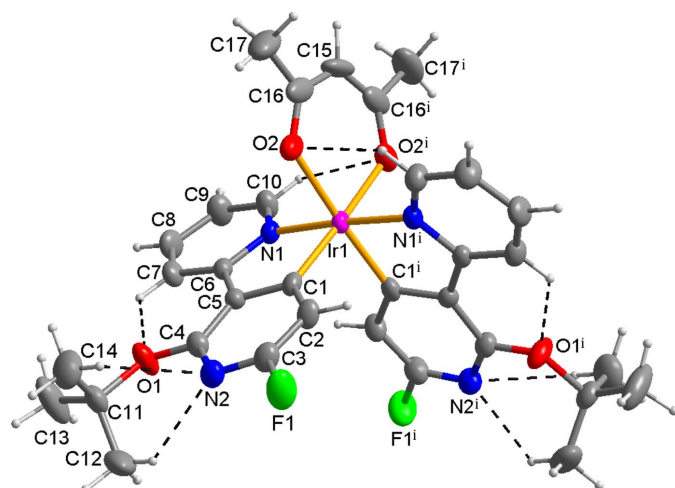
## 1. Chemical context

Iridium(III) compounds with fluorinated main dipyridyl ligands have attracted much attention due to their colour purity and high external quantum efficiency in organic light-emitting diodes (Lee *et al.*, 2009; Park *et al.*, 2013). In particular, heteroleptic Ir<sup>III</sup> compounds have many advantages such as easy tuning of emission energies and photophysical properties by modification of the ancillary ligands (Oh *et al.*, 2013). Herein, we report the results of the crystal-structure determination of an iridium(III) compound, [Ir(C<sub>14</sub>H<sub>14</sub>FN<sub>2</sub>O)<sub>2</sub>(C<sub>5</sub>H<sub>7</sub>O<sub>2</sub>)], with acetylacetonate (acac, *O,O'*) as an ancillary ligand.



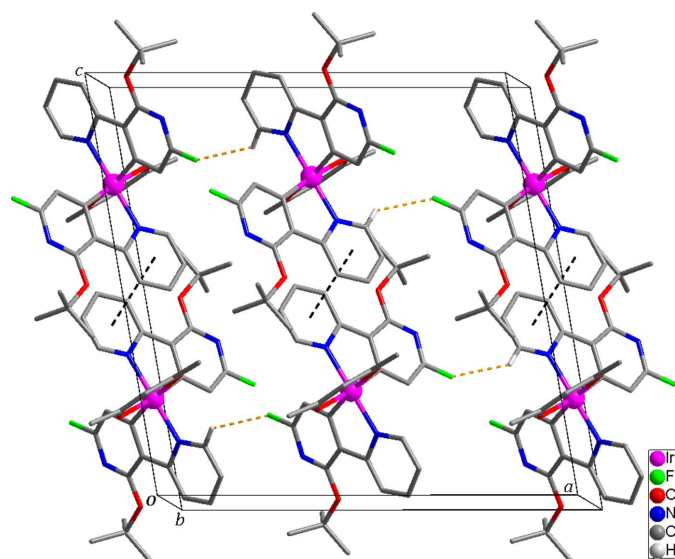
## 2. Structural commentary

The molecular structure of the title compound, Fig. 1, is generated by twofold rotation symmetry. The twofold rotation


**Figure 1**

View of the molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level; dashed lines represent intramolecular C—H...O and C—H...N hydrogen bonds [Symmetry code: (i)  $-x, y, \frac{3}{2}-z$ ].

axis passes through the Ir<sup>III</sup> atom and the central C atom (C15) of the acetylacetonate ligand. Therefore, the asymmetric unit consists of one Ir(III) atom on Wyckoff position 4e, one half of the acetylacetonate anion and one 2-*tert*-butoxy-6-fluoro-3-(pyridin-2-yl)pyridin-4-yl ligand. The Ir<sup>III</sup> atom is six-coordinated by the two main *C,N*-bidentate ligands and one ancillary *O,O'*-bidentate ligand, forming a distorted octahedral coordination sphere due to the narrow ligand bite angles, which range from 80.36 (7) to 88.65 (8)°. The *C,N*-bidentate ligands, which are perpendicular to each other [dihedral angle between the least-squares planes = 89.95 (5)°], are arranged in


**Figure 2**

Packing plot of the molecular components in the title compound. Yellow and black dashed lines represent intermolecular C—H...F and  $\pi$ – $\pi$  stacking interactions, respectively. H atoms not involved in intermolecular interactions have been omitted for clarity.

**Table 1**

Selected bond lengths (Å).

Ir1—C1	1.9760 (19)	Ir1—O2	2.1393 (15)
Ir1—N1	2.0344 (16)		

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C7—H7...O1	0.95	2.27	2.870 (2)	120
C10—H10...O2 <sup>i</sup>	0.95	2.48	3.089 (2)	122
C10—H10...F1 <sup>ii</sup>	0.95	2.41	3.055 (2)	125
C12—H12C...N2	0.98	2.29	2.927 (3)	122
C14—H14B...N2	0.98	2.59	3.153 (3)	116

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

a *cis-C,C'* and *trans-N,N'* fashion. The Ir—C bond length of 1.9760 (19) Å is shorter than the Ir—N bond length of 2.0344 (16) Å due to the electronegative fluorine substituent (Table 1). The Ir—C, Ir—N, and Ir—O bond lengths are in normal ranges as reported for similar Ir<sup>III</sup> compounds, *e.g.* [Ir(dfppy)<sub>2</sub>(acac)]; dfppy is a difluorinated bipyridine] (Kang *et al.*, 2013) or Ir(2',6'-bis(2-methoxyethoxy)-2,3'-bipyridinato-*N,C'*)(picolinate) (Frey *et al.*, 2014). Within the *C,N*-bidentate ligand of the title compound, the two pyridine rings are approximately co-planar, with a dihedral angle between the rings of 5.77 (9)°.

**Table 3**

Experimental details.

Crystal data	
Chemical formula	[Ir(C <sub>14</sub> H <sub>14</sub> FN <sub>2</sub> O) <sub>2</sub> (C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>2</sub> ]
<i>M<sub>r</sub></i>	781.85
Crystal system, space group	Monoclinic, <i>C2/c</i>
Temperature (K)	173
<i>a, b, c</i> (Å)	16.9404 (12), 10.7783 (7), 17.2561 (11)
$\beta$ (°)	100.001 (1)
<i>V</i> (Å <sup>3</sup> )	3102.9 (4)
<i>Z</i>	4
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	4.36
Crystal size (mm)	0.16 × 0.12 × 0.09
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Sheldrick, 1996)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.537, 0.687
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	15125, 3881, 3717
<i>R<sub>int</sub></i>	0.024
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.668
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>	0.017, 0.039, 1.01
No. of reflections	3881
No. of parameters	200
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	0.48, -0.59

Computer programs: *APEX2* and *SAINT* (Bruker, 2006), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008), *DIAMOND* (Brandenburg, 2005) and *publCIF* (Westrip, 2010).

### 3. Supramolecular features

The molecular structure is stabilized by weak intramolecular C—H···O and C—H···N hydrogen bonds (Table 2). Intermolecular C—H···F hydrogen bonds and  $\pi$ — $\pi$  interactions [ $Cg1 - Cg1^{iii} = 3.680(1) \text{ \AA}$ ,  $Cg1$  is the centroid of the N1, C6—C10 ring, symmetry code: (iii)  $-x, 1 - y, 2 - z$ ] contribute to the stabilization of the crystal structure (Fig. 2).

### 4. Synthesis and crystallization

The title compound was synthesized according to a previous report (Oh *et al.*, 2013). Yellow single crystals were obtained by slow evaporation from a dichloromethane/hexane solution.

### 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  $d(C-H) = 0.95 \text{ \AA}$ ,  $U_{iso}(H) = 1.2U_{eq}(C)$  for  $Csp^2$  H atoms, and  $0.98 \text{ \AA}$ ,  $U_{iso}(H) = 1.5U_{eq}(C)$  for methyl protons.

### Acknowledgements

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## supporting information

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## Crystal structure of bis[2-*tert*-butoxy-6-fluoro-3-(pyridin-2-yl- $\kappa$ N)pyridin-4-yl- $\kappa$ C<sup>4</sup>](pentane-2,4-dionato- $\kappa^2$ O, $O'$ )iridium(III)

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### Computing details

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2* (Bruker, 2006); data reduction: *S SAINT* (Bruker, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

### Bis[2-*tert*-butoxy-6-fluoro-3-(pyridin-2-yl- $\kappa$ N)pyridin-4-yl- $\kappa$ C<sup>4</sup>](pentane-2,4-dionato- $\kappa^2$ O, $O'$ )iridium(III)

#### Crystal data

[Ir(C<sub>14</sub>H<sub>14</sub>FN<sub>2</sub>O)<sub>2</sub>(C<sub>5</sub>H<sub>7</sub>O<sub>2</sub>)]

$M_r = 781.85$

Monoclinic, *C2/c*

Hall symbol: -C 2yc

$a = 16.9404$  (12) Å

$b = 10.7783$  (7) Å

$c = 17.2561$  (11) Å

$\beta = 100.001$  (1)°

$V = 3102.9$  (4) Å<sup>3</sup>

$Z = 4$

$F(000) = 1552$

$D_x = 1.674$  Mg m<sup>-3</sup>

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

Cell parameters from 3721 reflections

$\theta = 2.3$ – $28.3$ °

$\mu = 4.36$  mm<sup>-1</sup>

$T = 173$  K

Block, yellow

$0.16 \times 0.12 \times 0.09$  mm

#### Data collection

Bruker APEXII CCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.537$ ,  $T_{\max} = 0.687$

15125 measured reflections

3881 independent reflections

3717 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 28.3$ °,  $\theta_{\min} = 2.3$ °

$h = -22 \rightarrow 21$

$k = -14 \rightarrow 14$

$l = -15 \rightarrow 23$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.017$

$wR(F^2) = 0.039$

$S = 1.01$

3881 reflections

200 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

$$w = 1/[\sigma^2(F_o^2) + (0.0163P)^2 + 5.6671P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.48 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.59 \text{ e } \text{\AA}^{-3}$$

*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>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ir1	0.0000	0.424606 (10)	0.7500	0.01166 (4)
F1	0.22407 (8)	0.06652 (13)	0.79551 (8)	0.0273 (3)
O1	0.08930 (9)	0.14456 (15)	0.99685 (8)	0.0214 (3)
N1	-0.04307 (9)	0.41821 (15)	0.85288 (10)	0.0135 (3)
N2	0.15918 (10)	0.10711 (16)	0.89537 (10)	0.0180 (4)
C1	0.06958 (11)	0.29314 (18)	0.80481 (11)	0.0126 (4)
C2	0.12693 (11)	0.2228 (2)	0.77450 (12)	0.0169 (4)
H2	0.1371	0.2354	0.7226	0.020*
C3	0.16737 (11)	0.1357 (2)	0.82308 (12)	0.0180 (4)
C4	0.10416 (11)	0.17160 (19)	0.92486 (12)	0.0162 (4)
C5	0.05807 (10)	0.26689 (18)	0.88253 (11)	0.0127 (4)
C6	-0.00488 (11)	0.33982 (18)	0.90962 (11)	0.0129 (4)
C7	-0.02889 (12)	0.33774 (19)	0.98317 (11)	0.0160 (4)
H7	-0.0015	0.2861	1.0237	0.019*
C8	-0.09224 (12)	0.41045 (19)	0.99727 (12)	0.0190 (4)
H8	-0.1080	0.4099	1.0475	0.023*
C9	-0.13243 (12)	0.4840 (2)	0.93726 (12)	0.0205 (4)
H9	-0.1776	0.5317	0.9449	0.025*
C10	-0.10572 (12)	0.4864 (2)	0.86643 (12)	0.0179 (4)
H10	-0.1325	0.5382	0.8256	0.021*
C11	0.13969 (13)	0.06280 (19)	1.05388 (12)	0.0189 (4)
C12	0.14509 (17)	-0.0675 (2)	1.02218 (16)	0.0335 (6)
H12A	0.0912	-0.1032	1.0093	0.050*
H12B	0.1781	-0.1189	1.0621	0.050*
H12C	0.1695	-0.0647	0.9747	0.050*
C13	0.09314 (16)	0.0622 (3)	1.12145 (15)	0.0358 (6)
H13A	0.0397	0.0271	1.1035	0.054*
H13B	0.0879	0.1474	1.1398	0.054*
H13C	0.1217	0.0118	1.1647	0.054*
C14	0.22125 (14)	0.1217 (3)	1.07830 (14)	0.0307 (5)
H14A	0.2148	0.2057	1.0979	0.046*
H14B	0.2487	0.1256	1.0329	0.046*

H14C	0.2530	0.0718	1.1199	0.046*
O2	0.08159 (9)	0.56660 (14)	0.79971 (9)	0.0209 (3)
C15	0.0000	0.7398 (3)	0.7500	0.0318 (8)
H15	0.0000	0.8280	0.7500	0.038*
C16	0.06984 (15)	0.6828 (2)	0.78927 (13)	0.0244 (5)
C17	0.14050 (18)	0.7636 (3)	0.82222 (15)	0.0390 (6)
H17A	0.1846	0.7114	0.8482	0.059*
H17B	0.1248	0.8218	0.8605	0.059*
H17C	0.1579	0.8100	0.7794	0.059*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ir1	0.01340 (5)	0.01297 (5)	0.00844 (5)	0.000	0.00137 (4)	0.000
F1	0.0230 (6)	0.0369 (8)	0.0223 (7)	0.0164 (6)	0.0047 (5)	-0.0021 (6)
O1	0.0240 (7)	0.0250 (8)	0.0158 (7)	0.0097 (6)	0.0052 (6)	0.0096 (6)
N1	0.0140 (7)	0.0146 (8)	0.0117 (8)	-0.0011 (6)	0.0017 (6)	-0.0012 (6)
N2	0.0173 (8)	0.0188 (9)	0.0170 (9)	0.0019 (7)	0.0003 (7)	-0.0005 (7)
C1	0.0107 (8)	0.0140 (9)	0.0120 (9)	-0.0023 (7)	-0.0014 (7)	-0.0026 (7)
C2	0.0151 (9)	0.0228 (10)	0.0126 (9)	0.0011 (8)	0.0019 (7)	-0.0020 (8)
C3	0.0133 (9)	0.0212 (11)	0.0188 (10)	0.0029 (8)	0.0009 (7)	-0.0048 (8)
C4	0.0159 (9)	0.0172 (10)	0.0146 (10)	-0.0018 (8)	0.0003 (7)	0.0007 (8)
C5	0.0118 (8)	0.0147 (9)	0.0112 (9)	-0.0015 (7)	0.0007 (7)	-0.0005 (7)
C6	0.0138 (8)	0.0123 (9)	0.0119 (9)	-0.0018 (7)	0.0001 (7)	-0.0003 (7)
C7	0.0190 (9)	0.0161 (10)	0.0128 (10)	-0.0001 (8)	0.0028 (7)	0.0020 (8)
C8	0.0219 (10)	0.0219 (11)	0.0147 (10)	-0.0009 (8)	0.0072 (8)	-0.0003 (8)
C9	0.0199 (10)	0.0243 (11)	0.0188 (10)	0.0061 (9)	0.0072 (8)	-0.0002 (9)
C10	0.0183 (9)	0.0204 (10)	0.0151 (10)	0.0046 (8)	0.0033 (8)	0.0023 (8)
C11	0.0226 (10)	0.0180 (10)	0.0143 (10)	0.0030 (8)	-0.0018 (8)	0.0062 (8)
C12	0.0483 (15)	0.0170 (11)	0.0309 (14)	-0.0015 (11)	-0.0051 (11)	0.0037 (10)
C13	0.0379 (14)	0.0486 (17)	0.0223 (12)	0.0122 (12)	0.0091 (10)	0.0177 (11)
C14	0.0304 (12)	0.0350 (13)	0.0236 (12)	-0.0092 (11)	-0.0041 (10)	-0.0018 (10)
O2	0.0287 (8)	0.0202 (8)	0.0137 (7)	-0.0078 (6)	0.0034 (6)	-0.0029 (6)
C15	0.055 (2)	0.0143 (15)	0.0311 (19)	0.000	0.0203 (16)	0.000
C16	0.0433 (13)	0.0193 (11)	0.0147 (10)	-0.0088 (10)	0.0161 (9)	-0.0042 (8)
C17	0.0612 (17)	0.0295 (14)	0.0271 (14)	-0.0228 (13)	0.0095 (12)	-0.0064 (11)

*Geometric parameters (Å, °)*

Ir1—C1 <sup>i</sup>	1.9760 (19)	C9—C10	1.375 (3)
Ir1—C1	1.9760 (19)	C9—H9	0.9500
Ir1—N1 <sup>i</sup>	2.0344 (16)	C10—H10	0.9500
Ir1—N1	2.0344 (16)	C11—C14	1.512 (3)
Ir1—O2	2.1393 (15)	C11—C12	1.516 (3)
Ir1—O2 <sup>i</sup>	2.1393 (14)	C11—C13	1.517 (3)
F1—C3	1.365 (2)	C12—H12A	0.9800
O1—C4	1.342 (2)	C12—H12B	0.9800
O1—C11	1.477 (2)	C12—H12C	0.9800

N1—C10	1.345 (3)	C13—H13A	0.9800
N1—C6	1.368 (2)	C13—H13B	0.9800
N2—C3	1.315 (3)	C13—H13C	0.9800
N2—C4	1.333 (3)	C14—H14A	0.9800
C1—C2	1.403 (3)	C14—H14B	0.9800
C1—C5	1.417 (3)	C14—H14C	0.9800
C2—C3	1.362 (3)	O2—C16	1.276 (3)
C2—H2	0.9500	C15—C16	1.400 (3)
C4—C5	1.414 (3)	C15—C16 <sup>i</sup>	1.400 (3)
C5—C6	1.465 (3)	C15—H15	0.9500
C6—C7	1.399 (3)	C16—C17	1.509 (3)
C7—C8	1.384 (3)	C17—H17A	0.9800
C7—H7	0.9500	C17—H17B	0.9800
C8—C9	1.385 (3)	C17—H17C	0.9800
C8—H8	0.9500		
C1 <sup>i</sup> —Ir1—C1	88.37 (10)	C10—C9—C8	118.72 (19)
C1 <sup>i</sup> —Ir1—N1 <sup>i</sup>	80.36 (7)	C10—C9—H9	120.6
C1—Ir1—N1 <sup>i</sup>	96.83 (7)	C8—C9—H9	120.6
C1 <sup>i</sup> —Ir1—N1	96.83 (7)	N1—C10—C9	122.37 (19)
C1—Ir1—N1	80.36 (7)	N1—C10—H10	118.8
N1 <sup>i</sup> —Ir1—N1	176.12 (9)	C9—C10—H10	118.8
C1 <sup>i</sup> —Ir1—O2	174.32 (7)	O1—C11—C14	109.26 (17)
C1—Ir1—O2	91.77 (7)	O1—C11—C12	112.12 (18)
N1 <sup>i</sup> —Ir1—O2	93.98 (6)	C14—C11—C12	112.3 (2)
N1—Ir1—O2	88.80 (6)	O1—C11—C13	101.36 (17)
C1 <sup>i</sup> —Ir1—O2 <sup>i</sup>	91.77 (7)	C14—C11—C13	111.1 (2)
C1—Ir1—O2 <sup>i</sup>	174.32 (7)	C12—C11—C13	110.2 (2)
N1 <sup>i</sup> —Ir1—O2 <sup>i</sup>	88.80 (6)	C11—C12—H12A	109.5
N1—Ir1—O2 <sup>i</sup>	93.98 (6)	C11—C12—H12B	109.5
O2—Ir1—O2 <sup>i</sup>	88.65 (8)	H12A—C12—H12B	109.5
C4—O1—C11	124.52 (16)	C11—C12—H12C	109.5
C10—N1—C6	120.19 (17)	H12A—C12—H12C	109.5
C10—N1—Ir1	123.15 (14)	H12B—C12—H12C	109.5
C6—N1—Ir1	116.67 (12)	C11—C13—H13A	109.5
C3—N2—C4	115.84 (18)	C11—C13—H13B	109.5
C2—C1—C5	117.59 (18)	H13A—C13—H13B	109.5
C2—C1—Ir1	127.09 (15)	C11—C13—H13C	109.5
C5—C1—Ir1	115.31 (13)	H13A—C13—H13C	109.5
C3—C2—C1	116.74 (18)	H13B—C13—H13C	109.5
C3—C2—H2	121.6	C11—C14—H14A	109.5
C1—C2—H2	121.6	C11—C14—H14B	109.5
N2—C3—C2	128.36 (19)	H14A—C14—H14B	109.5
N2—C3—F1	113.52 (18)	C11—C14—H14C	109.5
C2—C3—F1	118.12 (18)	H14A—C14—H14C	109.5
N2—C4—O1	119.76 (18)	H14B—C14—H14C	109.5
N2—C4—C5	122.80 (18)	C16—O2—Ir1	124.86 (15)
O1—C4—C5	117.42 (17)	C16—C15—C16 <sup>i</sup>	127.9 (3)

C4—C5—C1	118.65 (17)	C16—C15—H15	116.1
C4—C5—C6	126.30 (17)	C16 <sup>i</sup> —C15—H15	116.1
C1—C5—C6	114.98 (17)	O2—C16—C15	126.7 (2)
N1—C6—C7	118.92 (17)	O2—C16—C17	114.8 (2)
N1—C6—C5	112.52 (16)	C15—C16—C17	118.5 (2)
C7—C6—C5	128.56 (17)	C16—C17—H17A	109.5
C8—C7—C6	120.46 (18)	C16—C17—H17B	109.5
C8—C7—H7	119.8	H17A—C17—H17B	109.5
C6—C7—H7	119.8	C16—C17—H17C	109.5
C7—C8—C9	119.21 (19)	H17A—C17—H17C	109.5
C7—C8—H8	120.4	H17B—C17—H17C	109.5
C9—C8—H8	120.4		
C1 <sup>i</sup> —Ir1—N1—C10	-89.11 (17)	C2—C1—C5—C4	-0.4 (3)
C1—Ir1—N1—C10	-176.28 (17)	Ir1—C1—C5—C4	178.33 (14)
O2—Ir1—N1—C10	91.72 (16)	C2—C1—C5—C6	-177.59 (17)
O2 <sup>i</sup> —Ir1—N1—C10	3.15 (16)	Ir1—C1—C5—C6	1.2 (2)
C1 <sup>i</sup> —Ir1—N1—C6	90.96 (14)	C10—N1—C6—C7	-3.9 (3)
C1—Ir1—N1—C6	3.79 (14)	Ir1—N1—C6—C7	176.01 (14)
O2—Ir1—N1—C6	-88.21 (14)	C10—N1—C6—C5	175.95 (17)
O2 <sup>i</sup> —Ir1—N1—C6	-176.77 (14)	Ir1—N1—C6—C5	-4.1 (2)
C1 <sup>i</sup> —Ir1—C1—C2	78.83 (17)	C4—C5—C6—N1	-175.00 (18)
N1 <sup>i</sup> —Ir1—C1—C2	-1.26 (18)	C1—C5—C6—N1	1.9 (2)
N1—Ir1—C1—C2	176.04 (18)	C4—C5—C6—C7	4.9 (3)
O2—Ir1—C1—C2	-95.48 (17)	C1—C5—C6—C7	-178.21 (19)
C1 <sup>i</sup> —Ir1—C1—C5	-99.77 (15)	N1—C6—C7—C8	2.4 (3)
N1 <sup>i</sup> —Ir1—C1—C5	-179.86 (14)	C5—C6—C7—C8	-177.44 (19)
N1—Ir1—C1—C5	-2.56 (13)	C6—C7—C8—C9	1.0 (3)
O2—Ir1—C1—C5	85.92 (14)	C7—C8—C9—C10	-2.8 (3)
C5—C1—C2—C3	-0.6 (3)	C6—N1—C10—C9	2.1 (3)
Ir1—C1—C2—C3	-179.21 (15)	Ir1—N1—C10—C9	-177.85 (16)
C4—N2—C3—C2	0.1 (3)	C8—C9—C10—N1	1.4 (3)
C4—N2—C3—F1	-179.61 (17)	C4—O1—C11—C14	65.0 (3)
C1—C2—C3—N2	0.9 (3)	C4—O1—C11—C12	-60.2 (3)
C1—C2—C3—F1	-179.45 (17)	C4—O1—C11—C13	-177.8 (2)
C3—N2—C4—O1	176.95 (18)	C1—Ir1—O2—C16	-177.15 (16)
C3—N2—C4—C5	-1.3 (3)	N1 <sup>i</sup> —Ir1—O2—C16	85.88 (16)
C11—O1—C4—N2	11.9 (3)	N1—Ir1—O2—C16	-96.84 (16)
C11—O1—C4—C5	-169.79 (18)	O2 <sup>i</sup> —Ir1—O2—C16	-2.82 (13)
N2—C4—C5—C1	1.4 (3)	Ir1—O2—C16—C15	6.0 (3)
O1—C4—C5—C1	-176.82 (17)	Ir1—O2—C16—C17	-172.81 (14)
N2—C4—C5—C6	178.27 (18)	C16 <sup>i</sup> —C15—C16—O2	-3.43 (16)
O1—C4—C5—C6	0.0 (3)	C16 <sup>i</sup> —C15—C16—C17	175.3 (2)

Symmetry code: (i)  $-x, y, -z+3/2$ .



*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>
C7—H7 $\cdots$ O1	0.95	2.27	2.870 (2)	120
C10—H10 $\cdots$ O2 <sup>i</sup>	0.95	2.48	3.089 (2)	122
C10—H10 $\cdots$ F1 <sup>ii</sup>	0.95	2.41	3.055 (2)	125
C12—H12C $\cdots$ N2	0.98	2.29	2.927 (3)	122
C14—H14B $\cdots$ N2	0.98	2.59	3.153 (3)	116

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