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[(1,2,5,6-η)-Cycloocta-1,5-diene]bis(1-methyl-3-propylimidazol-2-ylidene-κC)iridium(I) tetrafluoridoborate

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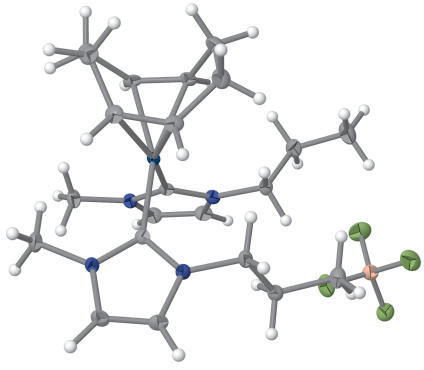
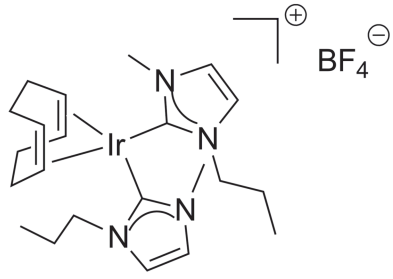
In the title complex $[Ir(C_8H_{12})(C_7H_{12}N_2)_2]BF_4$, the central Ir^I atom of the cationic complex has a distorted square-planar coordination environment, formed by a bidentate cycloocta-1,5-diene (COD) ligand, and two N-heterocyclic carbene ligands. Non-classical hydrogen-bonding interactions between the $[BF_4]^-$ anion and the N-heterocyclic carbenes on three distinct cationic iridium(I) complexes serve to establish the orientation of the $[BF_4]^-$ anion in the extended structure.

3D view



Chemical scheme



Structure description

N-heterocyclic carbenes (NHCs) have emerged as excellent alternative ligands for phosphines to synthesize active metal complexes in homogeneous catalysis (Cazin, 2013; de Frémont *et al.*, 2009; Diez-González *et al.*, 2009; Rovis & Nolan, 2013; Ruff *et al.*, 2016; Zuo *et al.*, 2014). The use of these complexes as catalysts for the transfer hydrogenation of several unsaturated substrates has also been studied and reported (Albrecht *et al.*, 2002; Gnanamgari *et al.*, 2007; Hillier *et al.*, 2001). The NHC ligands can be tuned sterically and electronically by having different substituents (wing tips) on the nitrogen atoms (Gusev, 2009). Though many imidazole-based NHC iridium complexes have been synthesized and structurally characterized (Herrmann *et al.*, 2006; Wang & Lin 1998; Chianese *et al.*, 2004), fewer structures of complexes with smaller wing-tip substituents have been reported. We continue to synthesize new imidazole and triazole-based NHC complexes of rhodium and iridium to study the effect of different substituents on the NHCs and the other ligands coordinating to the metal in transfer hydrogenation reactions (Nichol *et al.*, 2009, 2010, 2011, 2012; Idrees *et al.*, 2017*a*,*b*; Rood *et al.*, 2021; Rushlow *et al.*, 2021; Newman *et al.*, 2021; Castaldi *et al.*, 2021; Maynard *et al.*, 2023; Lerch *et al.*, 2024, 2025).

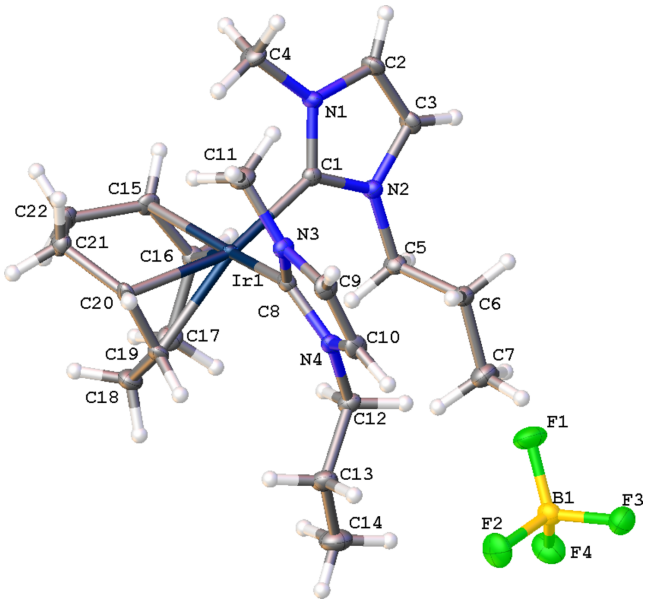


Figure 1
Molecular structure of the title compound (**3**) with displacement ellipsoids drawn at the 50% probability level.

Here we report the structure of an iridium complex with two identical imidazole-based monodentate carbene ligands.

The molecular structure of the title complex, $[Ir(C_8H_{12})(C_7H_{12}N_2)][BF_4]$, (**3**), comprises an Ir^I cation complex and a tetrafluoridoborate counter-anion, illustrated in Fig. 1. No solvent molecules are present in the crystal structure. The coordination environment of the central Ir^I atom of the cationic complex is distorted square-planar, defined by a bidentate cycloocta-1,5-diene (COD) ligand, and two NHC ligands. The carbene atoms, C1 and C8, deviate from the expected sp^2 hybridization in that the N1—C1—N2 and the N4—C8—N3 bond angles in the imidazole-based carbenes are 103.9 (2) and 104.1 (2)°, respectively. Other selected bond lengths and angles in the structure are: Ir1—C1(NHC) 2.052 (2) Å, Ir1—C8(NHC) 2.052 (2) Å, and C1—Ir1—C8 is 94.62 (9)°. Non-classical C—H···F hydrogen-bonding interactions between the NHCs of the iridium cation and the tetrafluoridoborate anion are summarized in Table 1. Notably, each $[BF_4]^-$ anion interacts with three separate cations as shown in Fig. 2. The crystal packing diagram of the complex is shown in Fig. 3, with the stabilizing H···F interactions shown as dotted orange lines. Two of the hydrogen-bonding interactions are with C—H groups of the NHC ring with the third interaction occurring with the propyl wing tip of the NHC.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···F4^{i}	0.95	2.53 (1)	3.380 (3)	150 (1)
C3—H3···F3^{ii}	0.95	2.53 (1)	3.336 (3)	143 (1)
C12—H12b···F1	0.99	2.51 (1)	3.354 (3)	144 (1)

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

Synthesis and crystallization

The synthesis scheme is shown in Fig. 4. All compounds used in the syntheses were obtained from Sigma-Aldrich and Strem and used as received; all syntheses were performed under a nitrogen atmosphere. NMR spectra were recorded at room temperature in $CDCl_3$ on a 400 MHz (operating at 100 MHz for ^{13}C) Varian spectrometer and referenced to the residual solvent peak (δ in p.p.m.).

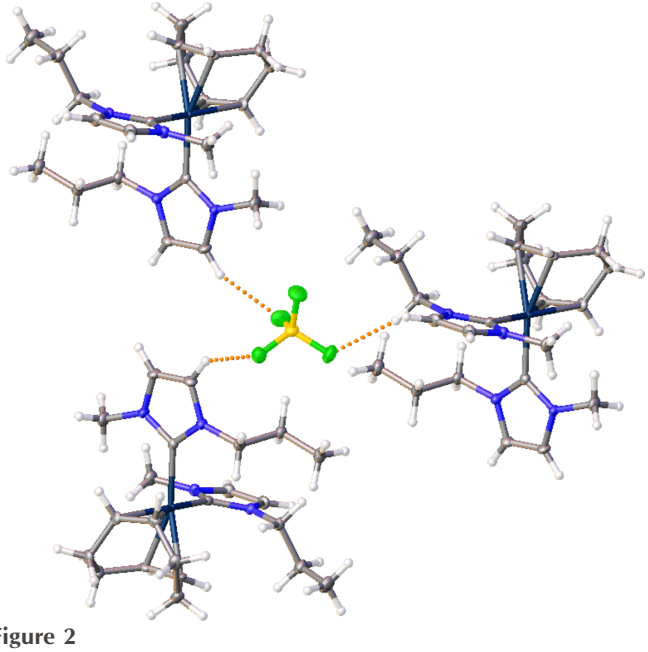


Figure 2
The title compound (**3**) showing the C—H···F hydrogen bonds (dotted orange lines) accepted by one $[BF_4]^-$ anion and the NHCs of three distinct iridium cations.

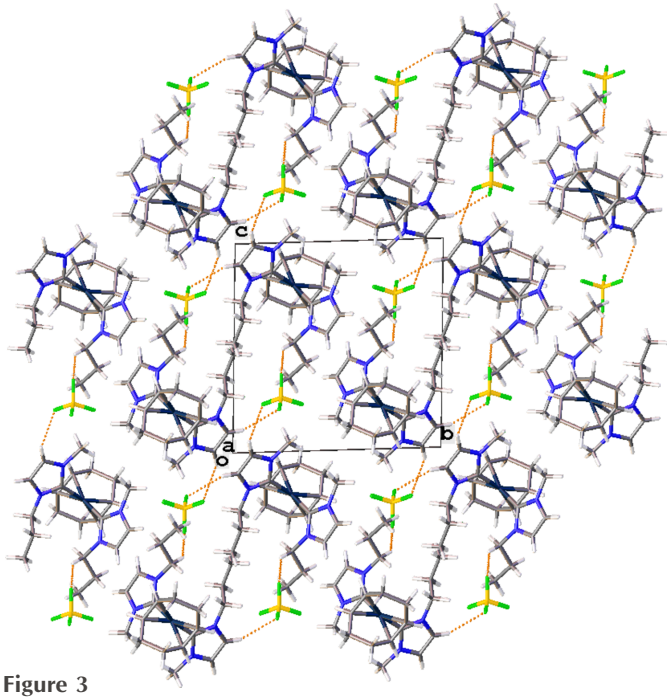


Figure 3
Packing diagram of the title compound shown along [100] with hydrogen-bonding interactions shown as dotted orange lines.

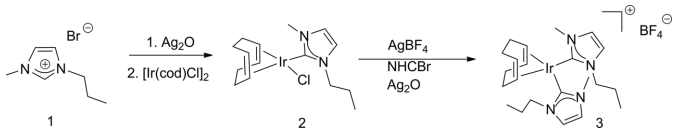


Figure 4
Reaction scheme for the synthesis of the title compound (**3**).

1-Methyl-3-propylimidazolium bromide (**1**) was synthesized by refluxing 1-methyl imidazole and 1-bromopropane in toluene for 48 h under nitrogen.

[(1,2,5,6-η)-Cycloocta-1,5-diene](1-methyl-3-propylimidazol-2-ylidene)chloridoiridium (2): Imidazolium bromide (**1**) (0.061 g, 0.298 mmol) and Ag_2O (0.034 g, 0.149 mmol) were stirred at room temperature in the dark for 1 h in CH_2Cl_2 (10 ml). The mixture was then filtered through Celite into $[Ir(cod)Cl]_2$ (0.100 g, 0.149 mmol), and stirred again in the dark for 1.5 h. The resulting solution was filtered through Celite and the solvent was removed under reduced pressure in a rotary evaporator. The yellow solid product (**2**) was dried under vacuum. Yield: 0.130 g (95%). ^{1}H NMR: δ 6.82 (*s*, 1H, N—C_4H), 6.80 (*s*, 1 H, N—C_5H), 4.57 (*s*, 3H, N—CH_3), 4.37 (*m*, 2 H, CH of COD), 4.29 (*m*, 2H, CH of COD), 4.09 (*t*, 2H, N—CH_2 of propyl), 1.97 (*m*, 2 H, CH_2 of propyl), 1.85–1.60 (*m*, 8H, CH_2 of COD), 1.01 (*t*, 3H, CH_3 of propyl). ^{13}C NMR: δ 180.11 (Ir—C), 121.59 (N—C_4H), 119.84 (N—C_5H), 84.16, 84.06 (CH of COD), 51.16 (N—CH_3), 37.46 (N—CH_2 of Pr), 33.76,33.39,29.76,29.40 (CH_2 of COD), 24.25 (CH_2 of propyl), 11.40 (CH_3 of propyl).

[(1,2,5,6-η)-Cycloocta-1,5-diene]bis(1-methyl-3-propylimidazol-2-ylidene)iridium(I) tetrafluoridoborate (3): Imidazolium bromide (**1**) (0.055 g, 0.269 mmol) and Ag_2O (0.031 g, 0.135 mmol) were stirred at room temperature in the dark for 1 h in CH_2Cl_2 (10 ml). The mixture was then filtered through Celite into a flask containing 0.124 g (0.269 mmol) of (**2**), in 10 ml of CH_2Cl_2. The solution was stirred in the dark for 1.5 h. The resulting mixture was filtered through Celite and the solvent was removed under reduced pressure. The rust-orange solid product (**3**) was dried under vacuum. Compound (**3**) was crystallized in the form of orange blocks suitable for data collection by slow diffusion of pentane into a CH_2Cl_2 solution. Yield: 0.170 g (99%). ^{1}H NMR: δ 7.10–7.00 (*m*, 4H, N—C_4H, N—C_5H), 4.39, 4.37 (*m*, 6H, N—CH_3), 4.22–4.15 (*m*, 4H, CH of COD), 3.96 (*m*, 4H, N—CH_2 of propyl), 3.82 (*m*, 2 H, CH_2 of COD), 3.76 (2.04 (*m*, 4H, CH_2 of propyl), 1.94–1.87 (*m*, 8H, CH_2 of COD), 1.02 (*m*, 6H, CH_3 of propyl). ^{13}C NMR: δ 176.19, 176.16 (Ir—C), 123.56, 123.34 (N—C_4H), 120.78, 120.39 (N—C_5H), 76.09, 75.27, 74.45 (CH of COD), 52.05,51.37 (N—CH_3), 38.12, 37.98 (N—CH_2 of propyl), 32.99, 31.40, 31.31, 29.69 (CH_2 of COD), 23.72, 23.50 (CH_2 of propyl), 11.38, 11.29 (CH_3 of propyl).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Ir(C_8H_{12})(C_7H_{12}N_2)_2]BF_4$
M_r	635.59
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	8.0252 (2), 12.1221 (3), 12.2566 (3)
α, β, γ (°)	87.486 (2), 83.233 (2), 87.913 (2)
V (Å^3)	1182.32 (5)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	5.71
Crystal size (mm)	0.13 × 0.08 × 0.03
Data collection	
Diffractometer	Rigaku XtaLAB Synergy-S
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2025)
T_{min}, T_{max}	0.582, 1.000
No. of measured, independent and observed [$I \geq 2u(I)$] reflections	36081, 5869, 5452
R_{int}	0.050
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.020, 0.042, 1.02
No. of reflections	5869
No. of parameters	293
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.32, −0.89

Computer programs: *CrysAlis PRO* (Rigaku OD, 2025), *SHELXT* (Sheldrick, 2015), *OLEX2.refine* (Bourhis *et al.*, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2026). **11**, x260189 [https://doi.org/10.1107/S2414314626001896]

[(1,2,5,6-η)-Cycloocta-1,5-diene]bis(1-methyl-3-propylimidazol-2-ylidene-κC)iridium(I) tetrafluoridoborate

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[(1,2,5,6-η)-Cycloocta-1,5-diene]bis(1-methyl-3-propylimidazol-2-ylidene-κC)iridium(I) tetrafluoridoborate

Crystal data

$[Ir(C_8H_{12})(C_7H_{12}N_2)_2]\cdot BF_4$
M_r = 635.59
Triclinic, $P\overline{1}$
a = 8.0252 (2) Å
b = 12.1221 (3) Å
c = 12.2566 (3) Å
α = 87.486 (2)°
β = 83.233 (2)°
γ = 87.913 (2)°
V = 1182.32 (5) Å^3
Z = 2
$F(000)$ = 626.581
D_x = 1.785 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 26079 reflections
θ = 3.6–28.3°
μ = 5.71 mm^{-1}
T = 100 K
Plate, orange
0.13 × 0.08 × 0.03 mm

Data collection

Rigaku XtaLAB Synergy-S diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.0 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2025)
T_{min} = 0.582, T_{max} = 1.000
36081 measured reflections
5869 independent reflections
5452 reflections with $I \geq 2u(I)$
R_{int} = 0.050
θ_{max} = 28.3°, θ_{min} = 3.2°
h = −10→10
k = −16→16
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.042
S = 1.02
5869 reflections
293 parameters
0 restraints
56 constraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.016P)^2 + 0.6194P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.0004
$\Delta\rho_{max}$ = 1.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.89 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Ir1	0.549050 (11)	0.715665 (7)	0.205112 (7)	0.01026 (3)
N1	0.3239 (3)	0.81530 (16)	0.03638 (17)	0.0141 (4)

N2	0.3191 (3)	0.92069 (16)	0.17287 (17)	0.0137 (4)
N3	0.2859 (3)	0.53777 (16)	0.26516 (17)	0.0144 (4)
N4	0.3082 (3)	0.63481 (16)	0.40447 (17)	0.0138 (4)
C1	0.3824 (3)	0.82161 (19)	0.1357 (2)	0.0124 (5)
C2	0.2255 (3)	0.9081 (2)	0.0126 (2)	0.0174 (5)
H2	0.1709 (3)	0.9222 (2)	−0.0515 (2)	0.0209 (6)*
C3	0.2230 (3)	0.9741 (2)	0.0983 (2)	0.0165 (5)
H3	0.1663 (3)	1.0440 (2)	0.1062 (2)	0.0198 (6)*
C4	0.3724 (4)	0.7291 (2)	−0.0423 (2)	0.0209 (6)
H4a	0.442 (2)	0.7607 (4)	−0.1062 (7)	0.0313 (8)*
H4b	0.436 (2)	0.6698 (8)	−0.0072 (5)	0.0313 (8)*
H4c	0.2714 (4)	0.6993 (11)	−0.0662 (12)	0.0313 (8)*
C5	0.3494 (3)	0.9661 (2)	0.2778 (2)	0.0165 (5)
H5a	0.4475 (3)	0.9267 (2)	0.3050 (2)	0.0197 (6)*
H5b	0.3764 (3)	1.0451 (2)	0.2655 (2)	0.0197 (6)*
C6	0.1984 (3)	0.9556 (2)	0.3646 (2)	0.0175 (5)
H6a	0.1013 (3)	0.9977 (2)	0.3391 (2)	0.0210 (6)*
H6b	0.1683 (3)	0.8770 (2)	0.3750 (2)	0.0210 (6)*
C7	0.2352 (4)	0.9989 (2)	0.4742 (2)	0.0234 (6)
H7a	0.242 (2)	1.0795 (3)	0.4679 (5)	0.0351 (9)*
H7b	0.1450 (13)	0.9784 (14)	0.5318 (4)	0.0351 (9)*
H7c	0.3422 (12)	0.9666 (12)	0.4932 (8)	0.0351 (9)*
C8	0.3667 (3)	0.62583 (19)	0.2968 (2)	0.0139 (5)
C9	0.1781 (3)	0.4938 (2)	0.3517 (2)	0.0188 (5)
H9	0.1081 (3)	0.4326 (2)	0.3498 (2)	0.0225 (6)*
C10	0.1919 (3)	0.5546 (2)	0.4383 (2)	0.0177 (5)
H10	0.1330 (3)	0.5448 (2)	0.5098 (2)	0.0213 (6)*
C11	0.3069 (3)	0.4958 (2)	0.1546 (2)	0.0204 (5)
H11a	0.2387 (18)	0.5413 (10)	0.1076 (4)	0.0306 (8)*
H11b	0.4254 (5)	0.4985 (14)	0.1243 (6)	0.0306 (8)*
H11c	0.271 (2)	0.4192 (5)	0.1575 (3)	0.0306 (8)*
C12	0.3632 (3)	0.71348 (19)	0.4791 (2)	0.0157 (5)
H12a	0.4511 (3)	0.75974 (19)	0.4386 (2)	0.0188 (6)*
H12b	0.2672 (3)	0.76281 (19)	0.5054 (2)	0.0188 (6)*
C13	0.4323 (4)	0.6551 (2)	0.5773 (2)	0.0217 (6)
H13a	0.3412 (4)	0.6151 (2)	0.6222 (2)	0.0260 (7)*
H13b	0.5206 (4)	0.6002 (2)	0.5510 (2)	0.0260 (7)*
C14	0.5052 (4)	0.7364 (3)	0.6477 (2)	0.0307 (7)
H14a	0.6003 (17)	0.7725 (13)	0.6047 (6)	0.0461 (10)*
H14b	0.4189 (9)	0.7923 (10)	0.6717 (15)	0.0461 (10)*
H14c	0.544 (2)	0.6971 (4)	0.7122 (9)	0.0461 (10)*
C15	0.7544 (3)	0.7682 (2)	0.0800 (2)	0.0160 (5)
H15	0.7161 (3)	0.8000 (2)	0.0101 (2)	0.0192 (6)*
C16	0.7361 (3)	0.8405 (2)	0.1663 (2)	0.0167 (5)
H16	0.6881 (3)	0.9150 (2)	0.1465 (2)	0.0200 (6)*
C17	0.8466 (3)	0.8414 (2)	0.2566 (2)	0.0218 (6)
H17a	0.9543 (3)	0.8748 (2)	0.2271 (2)	0.0261 (7)*
H17b	0.7922 (3)	0.8889 (2)	0.3151 (2)	0.0261 (7)*

C18	0.8840 (3)	0.7260 (2)	0.3081 (2)	0.0217 (6)
H18a	0.9871 (3)	0.6938 (2)	0.2677 (2)	0.0261 (7)*
H18b	0.9050 (3)	0.7337 (2)	0.3853 (2)	0.0261 (7)*
C19	0.7406 (3)	0.6479 (2)	0.3053 (2)	0.0158 (5)
H19	0.6938 (3)	0.6179 (2)	0.3795 (2)	0.0189 (6)*
C20	0.7253 (3)	0.5773 (2)	0.2198 (2)	0.0152 (5)
H20	0.6704 (3)	0.5065 (2)	0.2450 (2)	0.0183 (6)*
C21	0.8430 (3)	0.5686 (2)	0.1151 (2)	0.0177 (5)
H21a	0.9445 (3)	0.5247 (2)	0.1308 (2)	0.0213 (6)*
H21b	0.7874 (3)	0.5285 (2)	0.0614 (2)	0.0213 (6)*
C22	0.8961 (3)	0.6809 (2)	0.0635 (2)	0.0187 (5)
H22a	0.9303 (3)	0.6735 (2)	−0.0162 (2)	0.0224 (6)*
H22b	0.9943 (3)	0.7052 (2)	0.0970 (2)	0.0224 (6)*
F1	−0.0053 (2)	0.77004 (14)	0.62832 (14)	0.0317 (4)
F2	0.0743 (2)	0.66988 (13)	0.77507 (15)	0.0325 (4)
F3	−0.1646 (2)	0.77746 (13)	0.79418 (14)	0.0270 (4)
F4	0.0893 (2)	0.85740 (13)	0.76949 (15)	0.0312 (4)
B1	−0.0009 (4)	0.7694 (2)	0.7411 (3)	0.0189 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ir1	0.01091 (5)	0.01099 (5)	0.00872 (5)	−0.00063 (3)	−0.00122 (3)	0.00178 (3)
N1	0.0173 (10)	0.0140 (10)	0.0115 (10)	0.0022 (8)	−0.0040 (8)	−0.0007 (8)
N2	0.0163 (10)	0.0121 (9)	0.0128 (10)	0.0013 (8)	−0.0026 (8)	0.0003 (8)
N3	0.0131 (10)	0.0158 (10)	0.0142 (11)	−0.0031 (8)	−0.0006 (8)	−0.0003 (8)
N4	0.0135 (10)	0.0154 (10)	0.0123 (10)	−0.0015 (8)	−0.0009 (8)	0.0030 (8)
C1	0.0128 (11)	0.0122 (11)	0.0117 (12)	−0.0021 (9)	0.0003 (9)	0.0016 (9)
C2	0.0201 (13)	0.0170 (12)	0.0153 (13)	0.0021 (10)	−0.0059 (10)	0.0045 (9)
C3	0.0177 (12)	0.0127 (11)	0.0187 (13)	0.0022 (10)	−0.0030 (10)	0.0047 (9)
C4	0.0283 (14)	0.0195 (12)	0.0156 (13)	0.0017 (11)	−0.0045 (11)	−0.0061 (10)
C5	0.0188 (12)	0.0158 (12)	0.0154 (13)	−0.0004 (10)	−0.0039 (10)	−0.0036 (9)
C6	0.0170 (12)	0.0210 (12)	0.0146 (13)	0.0009 (10)	−0.0021 (10)	−0.0018 (10)
C7	0.0271 (15)	0.0263 (14)	0.0165 (14)	−0.0004 (12)	0.0001 (11)	−0.0040 (11)
C8	0.0125 (11)	0.0145 (11)	0.0150 (12)	0.0013 (9)	−0.0030 (9)	0.0003 (9)
C9	0.0144 (12)	0.0202 (12)	0.0212 (14)	−0.0061 (10)	0.0011 (10)	0.0013 (10)
C10	0.0125 (12)	0.0216 (12)	0.0179 (13)	−0.0047 (10)	0.0026 (10)	0.0049 (10)
C11	0.0235 (14)	0.0205 (13)	0.0182 (14)	−0.0037 (11)	−0.0039 (11)	−0.0054 (10)
C12	0.0199 (13)	0.0145 (11)	0.0127 (12)	−0.0017 (10)	−0.0015 (10)	−0.0004 (9)
C13	0.0267 (14)	0.0240 (13)	0.0143 (13)	0.0012 (11)	−0.0032 (11)	0.0012 (10)
C14	0.0352 (17)	0.0383 (17)	0.0205 (15)	−0.0042 (14)	−0.0089 (13)	−0.0038 (12)
C15	0.0164 (12)	0.0173 (12)	0.0129 (12)	−0.0044 (10)	0.0031 (9)	0.0047 (9)
C16	0.0141 (12)	0.0145 (11)	0.0210 (14)	−0.0036 (10)	−0.0002 (10)	0.0028 (10)
C17	0.0189 (13)	0.0240 (13)	0.0230 (15)	−0.0072 (11)	−0.0020 (11)	−0.0039 (11)
C18	0.0171 (13)	0.0306 (14)	0.0185 (14)	−0.0003 (11)	−0.0061 (10)	−0.0009 (11)
C19	0.0151 (12)	0.0197 (12)	0.0125 (12)	0.0025 (10)	−0.0041 (9)	0.0039 (9)
C20	0.0134 (11)	0.0140 (11)	0.0173 (13)	0.0037 (9)	−0.0010 (9)	0.0056 (9)
C21	0.0210 (13)	0.0154 (12)	0.0160 (13)	0.0032 (10)	0.0000 (10)	−0.0003 (9)

C22	0.0171 (12)	0.0223 (13)	0.0152 (13)	−0.0021 (10)	0.0041 (10)	0.0010 (10)
F1	0.0382 (10)	0.0414 (10)	0.0159 (9)	−0.0028 (8)	−0.0038 (7)	−0.0016 (7)
F2	0.0374 (10)	0.0181 (8)	0.0413 (11)	0.0067 (7)	−0.0056 (8)	0.0030 (7)
F3	0.0254 (9)	0.0300 (8)	0.0252 (9)	0.0002 (7)	−0.0009 (7)	−0.0036 (7)
F4	0.0335 (9)	0.0217 (8)	0.0412 (11)	−0.0053 (7)	−0.0136 (8)	−0.0047 (7)
B1	0.0215 (15)	0.0158 (13)	0.0195 (16)	0.0017 (12)	−0.0041 (12)	0.0010 (11)

Geometric parameters (Å, º)

Ir1—C1	2.052 (2)	C11—H11a	0.9800
Ir1—C8	2.052 (2)	C11—H11b	0.9800
Ir1—C15	2.207 (2)	C11—H11c	0.9800
Ir1—C16	2.169 (2)	C12—H12a	0.9900
Ir1—C19	2.193 (2)	C12—H12b	0.9900
Ir1—C20	2.170 (2)	C12—C13	1.520 (4)
N1—C1	1.361 (3)	C13—H13a	0.9900
N1—C2	1.392 (3)	C13—H13b	0.9900
N1—C4	1.464 (3)	C13—C14	1.515 (4)
N2—C1	1.363 (3)	C14—H14a	0.9800
N2—C3	1.388 (3)	C14—H14b	0.9800
N2—C5	1.470 (3)	C14—H14c	0.9800
N3—C8	1.362 (3)	C15—H15	1.0000
N3—C9	1.387 (3)	C15—C16	1.395 (4)
N3—C11	1.458 (3)	C15—C22	1.527 (3)
N4—C8	1.356 (3)	C16—H16	1.0000
N4—C10	1.388 (3)	C16—C17	1.498 (4)
N4—C12	1.464 (3)	C17—H17a	0.9900
C2—H2	0.9500	C17—H17b	0.9900
C2—C3	1.346 (4)	C17—C18	1.543 (4)
C3—H3	0.9500	C18—H18a	0.9900
C4—H4a	0.9800	C18—H18b	0.9900
C4—H4b	0.9800	C18—C19	1.521 (4)
C4—H4c	0.9800	C19—H19	1.0000
C5—H5a	0.9900	C19—C20	1.401 (4)
C5—H5b	0.9900	C20—H20	1.0000
C5—C6	1.520 (3)	C20—C21	1.506 (3)
C6—H6a	0.9900	C21—H21a	0.9900
C6—H6b	0.9900	C21—H21b	0.9900
C6—C7	1.528 (4)	C21—C22	1.529 (3)
C7—H7a	0.9800	C22—H22a	0.9900
C7—H7b	0.9800	C22—H22b	0.9900
C7—H7c	0.9800	F1—B1	1.387 (4)
C9—H9	0.9500	F2—B1	1.398 (3)
C9—C10	1.336 (4)	F3—B1	1.398 (3)
C10—H10	0.9500	F4—B1	1.389 (3)
C8—Ir1—C1	94.62 (9)	H11c—C11—H11b	109.5
C15—Ir1—C1	90.86 (9)	H12a—C12—N4	109.28 (12)

C15—Ir1—C8	163.45 (9)	H12b—C12—N4	109.28 (13)
C16—Ir1—C1	87.71 (9)	H12b—C12—H12a	107.9
C16—Ir1—C8	158.51 (10)	C13—C12—N4	111.7 (2)
C16—Ir1—C15	37.16 (9)	C13—C12—H12a	109.28 (14)
C19—Ir1—C1	162.51 (9)	C13—C12—H12b	109.28 (14)
C19—Ir1—C8	91.27 (9)	H13a—C13—C12	109.38 (14)
C19—Ir1—C15	88.08 (9)	H13b—C13—C12	109.38 (14)
C19—Ir1—C16	80.93 (9)	H13b—C13—H13a	108.0
C20—Ir1—C1	158.75 (10)	C14—C13—C12	111.3 (2)
C20—Ir1—C8	89.27 (9)	C14—C13—H13a	109.38 (16)
C20—Ir1—C15	80.19 (9)	C14—C13—H13b	109.38 (16)
C20—Ir1—C16	96.27 (9)	H14a—C14—C13	109.5
C20—Ir1—C19	37.46 (10)	H14b—C14—C13	109.5
C2—N1—C1	111.5 (2)	H14b—C14—H14a	109.5
C4—N1—C1	125.1 (2)	H14c—C14—C13	109.5
C4—N1—C2	123.1 (2)	H14c—C14—H14a	109.5
C3—N2—C1	111.2 (2)	H14c—C14—H14b	109.5
C5—N2—C1	124.7 (2)	H15—C15—Ir1	114.29 (7)
C5—N2—C3	124.1 (2)	C16—C15—Ir1	69.96 (13)
C9—N3—C8	111.2 (2)	C16—C15—H15	114.29 (15)
C11—N3—C8	124.8 (2)	C22—C15—Ir1	112.56 (15)
C11—N3—C9	124.1 (2)	C22—C15—H15	114.29 (14)
C10—N4—C8	110.9 (2)	C22—C15—C16	123.6 (2)
C12—N4—C8	126.0 (2)	C15—C16—Ir1	72.87 (14)
C12—N4—C10	123.1 (2)	H16—C16—Ir1	113.77 (7)
N1—C1—Ir1	128.01 (17)	H16—C16—C15	113.77 (15)
N2—C1—Ir1	127.76 (18)	C17—C16—Ir1	109.60 (17)
N2—C1—N1	103.9 (2)	C17—C16—C15	125.5 (2)
H2—C2—N1	126.78 (14)	C17—C16—H16	113.77 (14)
C3—C2—N1	106.4 (2)	H17a—C17—C16	108.74 (14)
C3—C2—H2	126.78 (15)	H17b—C17—C16	108.74 (14)
C2—C3—N2	107.0 (2)	H17b—C17—H17a	107.6
H3—C3—N2	126.50 (13)	C18—C17—C16	114.0 (2)
H3—C3—C2	126.50 (15)	C18—C17—H17a	108.74 (14)
H4a—C4—N1	109.5	C18—C17—H17b	108.74 (15)
H4b—C4—N1	109.5	H18a—C18—C17	109.11 (14)
H4b—C4—H4a	109.5	H18b—C18—C17	109.11 (15)
H4c—C4—N1	109.5	H18b—C18—H18a	107.8
H4c—C4—H4a	109.5	C19—C18—C17	112.5 (2)
H4c—C4—H4b	109.5	C19—C18—H18a	109.11 (14)
H5a—C5—N2	109.17 (12)	C19—C18—H18b	109.11 (14)
H5b—C5—N2	109.17 (12)	C18—C19—Ir1	112.43 (16)
H5b—C5—H5a	107.9	H19—C19—Ir1	113.86 (6)
C6—C5—N2	112.2 (2)	H19—C19—C18	113.86 (14)
C6—C5—H5a	109.17 (14)	C20—C19—Ir1	70.35 (14)
C6—C5—H5b	109.17 (13)	C20—C19—C18	124.7 (2)
H6a—C6—C5	109.38 (14)	C20—C19—H19	113.86 (14)
H6b—C6—C5	109.38 (13)	C19—C20—Ir1	72.20 (14)

H6b—C6—H6a	108.0	H20—C20—Ir1	113.57 (6)
C7—C6—C5	111.3 (2)	H20—C20—C19	113.57 (14)
C7—C6—H6a	109.38 (14)	C21—C20—Ir1	110.01 (16)
C7—C6—H6b	109.38 (14)	C21—C20—C19	126.2 (2)
H7a—C7—C6	109.5	C21—C20—H20	113.57 (13)
H7b—C7—C6	109.5	H21a—C21—C20	108.94 (13)
H7b—C7—H7a	109.5	H21b—C21—C20	108.94 (14)
H7c—C7—C6	109.5	H21b—C21—H21a	107.8
H7c—C7—H7a	109.5	C22—C21—C20	113.2 (2)
H7c—C7—H7b	109.5	C22—C21—H21a	108.94 (14)
N3—C8—Ir1	127.60 (18)	C22—C21—H21b	108.94 (15)
N4—C8—Ir1	128.11 (18)	C21—C22—C15	111.8 (2)
N4—C8—N3	104.1 (2)	H22a—C22—C15	109.26 (14)
H9—C9—N3	126.73 (14)	H22a—C22—C21	109.26 (14)
C10—C9—N3	106.5 (2)	H22b—C22—C15	109.26 (14)
C10—C9—H9	126.73 (15)	H22b—C22—C21	109.26 (15)
C9—C10—N4	107.3 (2)	H22b—C22—H22a	107.9
H10—C10—N4	126.35 (14)	F2—B1—F1	109.0 (2)
H10—C10—C9	126.35 (15)	F3—B1—F1	109.5 (2)
H11a—C11—N3	109.5	F3—B1—F2	108.8 (2)
H11b—C11—N3	109.5	F4—B1—F1	110.8 (2)
H11b—C11—H11a	109.5	F4—B1—F2	109.6 (2)
H11c—C11—N3	109.5	F4—B1—F3	109.1 (2)
H11c—C11—H11a	109.5		

Ir1—C1—N1—C2	−174.0 (2)	N3—C9—C10—N4	−0.2 (2)
Ir1—C1—N1—C4	−0.6 (3)	N4—C8—N3—C9	0.6 (2)
Ir1—C1—N2—C3	173.9 (2)	N4—C8—N3—C11	179.58 (18)
Ir1—C1—N2—C5	−5.6 (2)	N4—C12—C13—C14	174.2 (2)
Ir1—C8—N3—C9	176.1 (2)	C1—N1—C2—C3	0.3 (2)
Ir1—C8—N3—C11	−4.9 (3)	C1—N2—C3—C2	−0.1 (2)
Ir1—C8—N4—C10	−176.2 (2)	C1—N2—C5—C6	−103.8 (2)
Ir1—C8—N4—C12	0.8 (3)	C2—C3—N2—C5	179.42 (19)
Ir1—C15—C16—C17	102.20 (15)	C3—N2—C5—C6	76.8 (2)
Ir1—C15—C22—C21	14.39 (19)	C3—C2—N1—C4	−173.1 (2)
Ir1—C16—C15—C22	−104.36 (13)	C8—N3—C9—C10	−0.2 (2)
Ir1—C16—C17—C18	36.38 (18)	C8—N4—C10—C9	0.6 (2)
Ir1—C19—C18—C17	9.70 (19)	C8—N4—C12—C13	−121.2 (3)
Ir1—C19—C20—C21	102.15 (14)	C9—C10—N4—C12	−176.5 (2)
Ir1—C20—C19—C18	−104.21 (14)	C10—N4—C12—C13	55.5 (2)
Ir1—C20—C21—C22	38.70 (19)	C10—C9—N3—C11	−179.2 (2)
N1—C1—N2—C3	0.3 (2)	C15—C16—C17—C18	−46.2 (3)
N1—C1—N2—C5	−179.22 (17)	C15—C22—C21—C20	−35.1 (3)
N1—C2—C3—N2	−0.2 (2)	C16—C15—C22—C21	94.6 (3)
N2—C1—N1—C2	−0.4 (2)	C16—C17—C18—C19	−30.8 (2)
N2—C1—N1—C4	172.96 (18)	C17—C16—C15—C22	−2.2 (3)
N2—C5—C6—C7	177.7 (2)	C17—C18—C19—C20	90.7 (2)
N3—C8—N4—C10	−0.7 (2)	C18—C19—C20—C21	−2.1 (3)

N3—C8—N4—C12	176.34 (17)	C19—C20—C21—C22	−43.4 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···F4^{i}	0.95	2.53 (1)	3.380 (3)	150 (1)
C3—H3···F3^{ii}	0.95	2.53 (1)	3.336 (3)	143 (1)
C12—H12*b*···F1	0.99	2.51 (1)	3.354 (3)	144 (1)

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