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Di-μ-chloro-bis{bis[4-(2-pyridyl)benzaldehyde-κ^2C^2,N']iridium} dichloromethane sesquisolvate

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.011 Å
Disorder in solvent or counterion
R factor = 0.042
wR factor = 0.088
Data-to-parameter ratio = 16.5

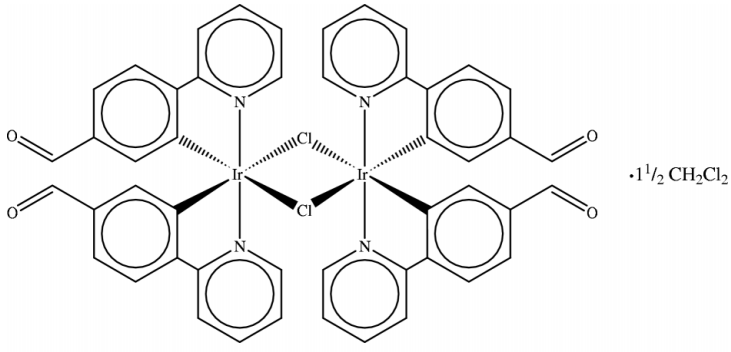
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $[Ir_2Cl_2(C_{12}H_8NO)_4]\cdot1.5CH_2Cl_2$ or $[Ir(fppy)_2Cl]_2\cdot1.5CH_2Cl_2$ [where fppy is 4-(2-pyridyl)benzaldehyde], is a dinuclear iridium(III) complex containing two six-coordinate iridium centres connected by two bridging chlorides, which has crystallized with the solvent dichloromethane.

Comment

Electrophosphorescent complexes that are capable of generating pure red, green and blue light are in high demand due to their potential use as dopants in full-colour organic light-emitting displays. Triply *ortho*-metallated iridium(III) complexes containing cyclometalating ligands, such as 2-phenylpyridine, have already been exploited in these kinds of devices with a great deal of success (Baldo *et al.*, 1999; Adachi *et al.*, 2000; Beeby *et al.*, 2003). These monomeric cyclometallated iridium(III) complexes may be synthesized by a variety of synthetic pathways, which include those that utilize dichloro-bridged species as precursors (Dedeian *et al.*, 1991; Grushin *et al.*, 2001; Lamansky *et al.*, 2001; Tamayo *et al.*, 2003). These dinuclear species are generally produced in high yield from the reactions of iridium(III) chloride and the corresponding cyclometallating ligand (Sprouse *et al.*, 1984).

A number of novel dichloro-bridged species of this nature have been reported, where they have primarily been used as precursors for the preparation of monomeric *ortho*-metallated iridium(III) and rhodium(III) complexes (Garces *et al.*, 1988; Tamayo *et al.*, 2003). Despite this, they have received little or no detailed structural attention.



(I)

The title compound, (I) (Fig. 1), consists of two octahedral iridium(III) centres, each ligated by two 4-(2-pyridyl)benzaldehyde (fppy) and two bridging chloride ions, together with one and a half molecules of disordered dichloromethane solvent per asymmetric unit. The chloride ligands reside in the

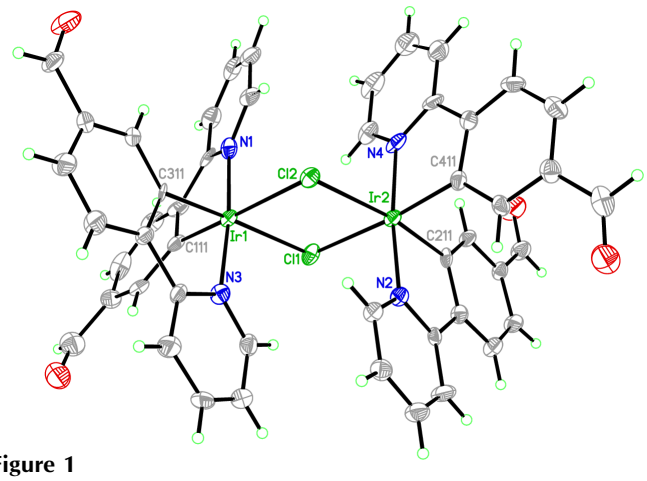


Figure 1
View of (I), with selected atoms labelled. Displacement ellipsoids for the non-H atoms are drawn at the 50% probability level. The solvent has been omitted.

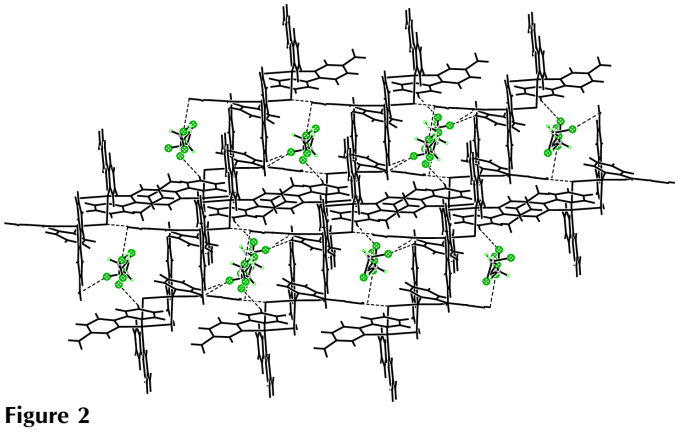


Figure 2
The crystal packing in the title compound, viewed down the channels occupied by the disordered dichloromethane, with selected C—H···Cl hydrogen bonds shown as dashed lines. The $[Ir(fppy)_2Cl]_2$ molecules are depicted in black for clarity.

equatorial plane *trans* to the fppy C atoms and the fppy N atoms occupy the apical sites with *trans* geometry. This is consistent with other dinuclear iridium(III) and rhodium(III) complexes of this type (Fronczek *et al.*, 1982; Steel, 1991; Garces *et al.*, 1993; Ghisdavu *et al.*, 1999). However, the Ir—Cl bond lengths fall into two groups, differing by approximately 0.1 Å, with both Ir—Cl1 bonds shorter than the Ir—Cl2 bonds (Table 1). This effect is also seen in the Ir—Cl—Ir angle, which is larger for Cl1 than Cl2. Some degree of asymmetry is seen in the other examples of chloride-bridged iridium(III) or rhodium(III) dimers, but in most cases pairs of Ir—Cl distances are constrained by crystal symmetry.

The disordered dichloromethane occupies channels within the structure (Fig. 2), with weak C—H···Cl interactions between the iridium dimer and the solvent, which limits the disorder to three components (see below).

Experimental

$IrCl_3·3H_2O$ (0.35 g, 1.0 mmol), 4-(2-pyridyl)benzaldehyde (0.92 g, 5.0 mmol), 2-ethoxyethanol (15 ml) and water (7 ml) were placed in a reaction vessel and heated to 383 K for 8 h with continuous stirring. The initial dark-brown solution became lighter in colour and an orange precipitate formed. The solution was cooled to room temperature and was filtered. The resulting solid was washed with ethanol (2 × 10 ml) and acetone (2 × 10 ml). The product was dissolved in dichloromethane and column chromatography (silica gel, dichloromethane) yielded a bright-orange solid (0.44 g, 73%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.53 (4H, *s*), 9.27 (4H, *d*, J = 4.8 Hz), 8.07 (4H, *d*, J = 7.8 Hz), 7.94 (4H, *td*, J = 8.0 Hz), 7.68 (4H, *d*, J = 8.4 Hz), 7.32 (4H, *dd*, J = 1.5 Hz), 6.91 (4H, *td*, J = 6.0 Hz), 6.29 (4H, *d*, J = 1.5 Hz). MS (EI$^+$): m/z 1184 (M^+), 592 [$(M - IrC_{24}H_{16}N_2O_2 - Cl)^+$], 557 [$(M - IrC_{24}H_{16}N_2O_2 - Cl_2)^+$]. Crystals of (I) were grown from dichloromethane.

Crystal data

$[Ir_2Cl_2(C_{12}H_8NO)_4]·1.5CH_2Cl_2$	Z = 2
M_r = 1311.46	D_x = 1.96 Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
a = 10.577 (2) Å	Cell parameters from 999 reflections
b = 12.779 (2) Å	θ = 3.1–27.4°
c = 17.924 (3) Å	μ = 6.34 mm^{-1}
α = 75.562 (4)°	T = 120 (2) K
β = 88.993 (3)°	Block, clear intense orange
γ = 71.629 (3)°	0.15 × 0.10 × 0.10 mm
V = 2221.7 (7) Å^3	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	10 151 independent reflections
ω scans	7329 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)	R_{int} = 0.052
T_{min} = 0.419, T_{max} = 0.531	θ_{max} = 27.5°
23 666 measured reflections	$h = -13 \rightarrow 13$
	$k = -16 \rightarrow 16$
	$l = -22 \rightarrow 23$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.042	$w = 1/[\sigma^2(F_o^2) + (0.0321P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.088	$(\Delta/\sigma)_{max}$ = 0.002
S = 1.03	$\Delta\rho_{max}$ = 1.83 e Å^{-3}
10 151 reflections	$\Delta\rho_{min}$ = −2.60 e Å^{-3}
614 parameters	

Table 1
Selected geometric parameters (Å, °).

Ir1—C111	1.976 (7)	Ir2—C411	1.974 (7)
Ir1—C311	1.990 (6)	Ir2—C211	2.000 (6)
Ir1—N1	2.034 (6)	Ir2—N2	2.040 (6)
Ir1—N3	2.046 (6)	Ir2—N4	2.040 (6)
Ir1—Cl1	2.5020 (17)	Ir2—Cl1	2.5075 (19)
Ir1—Cl2	2.5187 (18)	Ir2—Cl2	2.5260 (16)
C111—Ir1—C311	92.9 (3)	C411—Ir2—N2	93.5 (3)
C111—Ir1—N1	80.8 (3)	C211—Ir2—N2	81.2 (2)
C311—Ir1—N1	96.6 (2)	C411—Ir2—N4	80.5 (3)
C111—Ir1—N3	94.7 (3)	C211—Ir2—N4	95.4 (2)
C311—Ir1—N3	80.5 (2)	N2—Ir2—N4	173.1 (2)
N1—Ir1—N3	174.5 (2)	C411—Ir2—Cl1	174.7 (2)
C111—Ir1—Cl1	92.0 (2)	C211—Ir2—Cl1	91.39 (19)
C311—Ir1—Cl1	172.9 (2)	N2—Ir2—Cl1	91.22 (17)
N1—Ir1—Cl1	89.34 (16)	N4—Ir2—Cl1	94.88 (19)
N3—Ir1—Cl1	93.94 (16)	C411—Ir2—Cl2	95.29 (19)
C111—Ir1—Cl2	171.5 (2)	C211—Ir2—Cl2	171.86 (19)
C311—Ir1—Cl2	93.32 (19)	N2—Ir2—Cl2	93.90 (16)
N1—Ir1—Cl2	92.77 (17)	N4—Ir2—Cl2	90.17 (16)
N3—Ir1—Cl2	92.00 (17)	Cl1—Ir2—Cl2	82.17 (5)
Cl1—Ir1—Cl2	82.43 (5)	Ir1—Cl1—Ir2	98.16 (6)
C411—Ir2—C211	91.5 (3)	Ir1—Cl2—Ir2	97.24 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14A···Cl52	0.93	2.89	3.715 (10)	148
C33—H33A···Cl71^{i}	0.93	2.78	3.557 (10)	142
C43—H43A···Cl72^{ii}	0.93	2.56	3.205 (11)	127

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

All H atoms were positioned geometrically (C—H = 0.93 or 0.97 Å) and refined using a riding model, with U_{iso} = 1.2 or 1.5 times U_{eq}(parent C atom). The solvent, dichloromethane, was modelled as disordered in three components, all partially occupied. One molecule of dichloromethane is rotationally disordered about the central C atom and the partial occupancies of the two components were refined (0.57/0.43) and then fixed. The remaining solvent molecule is located close to an inversion centre and was assigned 50% occupancy. Anisotropic displacement parameters were refined for all non-H atoms (including the solvent). Although there is a small amount of electron density unaccounted for in this disordered solvent model, all peaks larger than 1 e Å are within 1 Å of an Ir atom. The deepest hole is located 1.37 Å from atom H17*A*.

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SMART-NT*; data reduction: *SAINT-NT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Crystal data

$[Ir_2Cl_2(C_{12}H_8NO)_4]\cdot 1.5CH_2Cl_2$
$M_r = 1311.46$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.577\ (2)$ Å
$b = 12.779\ (2)$ Å
$c = 17.924\ (3)$ Å
$\alpha = 75.562\ (4)°$
$\beta = 88.993\ (3)°$
$\gamma = 71.629\ (3)°$
$V = 2221.7\ (7)$ Å^3
$Z = 2$
$F(000) = 1262$
$D_x = 1.96$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 999 reflections
$\theta = 3.1–27.4°$
$\mu = 6.34$ mm^{-1}
$T = 120$ K
Block, clear_intense_orange
0.15 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD 1K area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 1998)
$T_{min} = 0.419$, $T_{max} = 0.531$
23666 measured reflections
10151 independent reflections
7329 reflections with $I > 2\sigma(I)'$
$R_{int} = 0.052$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.2°$
$h = -13\rightarrow13$
$k = -16\rightarrow16$
$l = -22\rightarrow23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.088$
$S = 1.03$
10151 reflections
614 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
$w = 1/[\sigma^2(F_o^2) + (0.0321P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.83$ e Å^{-3}
$\Delta\rho_{min} = -2.60$ e Å^{-3}

Special details

Experimental. The data collection nominally covered full sphere of reciprocal Space, by a combination of 5 sets of ω scans each set at different φ and/or 2θ angles and each scan (16 s exposure) covering 0.3° in ω. Crystal to detector distance 4.51 cm.

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ir1	0.60771 (3)	0.18730 (2)	0.23140 (2)	0.01512 (7)	
Ir2	0.72796 (3)	0.43026 (2)	0.24848 (2)	0.01583 (8)	
Cl1	0.51553 (17)	0.39773 (14)	0.21707 (10)	0.0217 (4)	
Cl2	0.82189 (16)	0.21749 (13)	0.26446 (9)	0.0188 (4)	
N1	0.5575 (6)	0.1602 (5)	0.3430 (3)	0.0202 (13)	
C11	0.6419 (7)	0.1311 (5)	0.4057 (4)	0.0213 (16)	
H11A	0.7327	0.1171	0.3996	0.026*	
C12	0.5957 (9)	0.1216 (6)	0.4789 (4)	0.0291 (18)	
H12A	0.6562	0.0986	0.5215	0.035*	
C13	0.4618 (8)	0.1458 (6)	0.4896 (4)	0.0292 (18)	
H13A	0.4298	0.1448	0.5383	0.035*	
C14	0.3761 (8)	0.1715 (6)	0.4258 (4)	0.0267 (17)	
H14A	0.2851	0.1860	0.4316	0.032*	
C15	0.4246 (7)	0.1760 (5)	0.3527 (4)	0.0203 (15)	
C16	0.3504 (7)	0.1838 (6)	0.2823 (4)	0.0209 (16)	
C17	0.2165 (7)	0.1924 (6)	0.2795 (4)	0.0276 (18)	
H17A	0.1663	0.2037	0.3216	0.033*	
C18	0.1587 (8)	0.1841 (6)	0.2142 (5)	0.035 (2)	
H18A	0.0684	0.1914	0.2117	0.041*	
C19	0.2350 (7)	0.1648 (6)	0.1512 (4)	0.0255 (17)	
C110	0.3682 (7)	0.1616 (5)	0.1535 (4)	0.0199 (15)	
H10A	0.4183	0.1489	0.1115	0.024*	
C111	0.4280 (7)	0.1767 (6)	0.2165 (4)	0.0187 (15)	
C112	0.1716 (9)	0.1479 (7)	0.0855 (5)	0.037 (2)	
H11B	0.0815	0.1546	0.0868	0.044*	
O1	0.2274 (6)	0.1261 (5)	0.0305 (3)	0.0430 (15)	
N2	0.7644 (6)	0.4695 (5)	0.1344 (3)	0.0181 (13)	
C21	0.8378 (7)	0.3960 (6)	0.0959 (4)	0.0203 (15)	
H21A	0.8742	0.3196	0.1222	0.024*	
C22	0.8614 (7)	0.4289 (6)	0.0196 (4)	0.0237 (16)	
H22A	0.9141	0.3757	−0.0048	0.028*	
C23	0.8068 (7)	0.5409 (6)	−0.0204 (4)	0.0254 (17)	
H23A	0.8196	0.5648	−0.0726	0.030*	

C24	0.7321 (8)	0.6172 (6)	0.0189 (4)	0.0263 (17)
H24A	0.6944	0.6937	−0.0071	0.032*
C25	0.7127 (6)	0.5814 (5)	0.0963 (4)	0.0149 (13)
C26	0.6395 (7)	0.6543 (6)	0.1446 (4)	0.0181 (14)
C27	0.5764 (7)	0.7716 (6)	0.1157 (4)	0.0226 (16)
H27A	0.5775	0.8061	0.0635	0.027*
C28	0.5124 (7)	0.8360 (6)	0.1652 (4)	0.0228 (16)
H28A	0.4739	0.9146	0.1472	0.027*
C29	0.5060 (7)	0.7821 (6)	0.2424 (4)	0.0187 (15)
C210	0.5690 (7)	0.6649 (5)	0.2709 (4)	0.0185 (15)
H21B	0.5649	0.6305	0.3227	0.022*
C211	0.6375 (7)	0.5990 (5)	0.2232 (4)	0.0160 (14)
C212	0.4364 (8)	0.8525 (6)	0.2935 (4)	0.0269 (17)
H21C	0.3988	0.9305	0.2718	0.032*
O2	0.4243 (6)	0.8170 (5)	0.3612 (3)	0.0420 (15)
N3	0.6483 (6)	0.2046 (5)	0.1178 (3)	0.0187 (13)
C31	0.6061 (7)	0.3023 (6)	0.0618 (4)	0.0227 (16)
H31A	0.5532	0.3681	0.0744	0.027*
C32	0.6387 (8)	0.3088 (6)	−0.0142 (4)	0.0286 (18)
H32A	0.6082	0.3776	−0.0518	0.034*
C33	0.7163 (8)	0.2123 (7)	−0.0327 (4)	0.0300 (18)
H33A	0.7427	0.2151	−0.0827	0.036*
C34	0.7553 (8)	0.1103 (7)	0.0238 (4)	0.0308 (18)
H34A	0.8064	0.0436	0.0116	0.037*
C35	0.7180 (7)	0.1077 (6)	0.0986 (4)	0.0196 (15)
C36	0.7468 (7)	0.0051 (5)	0.1627 (4)	0.0176 (14)
C37	0.8169 (8)	−0.1047 (6)	0.1556 (4)	0.0261 (17)
H37A	0.8484	−0.1155	0.1084	0.031*
C38	0.8388 (7)	−0.1970 (6)	0.2195 (4)	0.0264 (17)
H38A	0.8843	−0.2704	0.2155	0.032*
C39	0.7917 (7)	−0.1786 (6)	0.2902 (4)	0.0220 (16)
C310	0.7213 (7)	−0.0707 (5)	0.2980 (4)	0.0184 (15)
H31B	0.6898	−0.0610	0.3454	0.022*
C311	0.6976 (7)	0.0242 (5)	0.2338 (4)	0.0156 (14)
C312	0.8208 (7)	−0.2794 (6)	0.3567 (4)	0.0256 (17)
H31C	0.8671	−0.3499	0.3480	0.031*
O3	0.7888 (6)	−0.2776 (4)	0.4222 (3)	0.0382 (15)
N4	0.7043 (6)	0.4036 (5)	0.3642 (3)	0.0234 (14)
C41	0.5911 (8)	0.3957 (6)	0.3988 (4)	0.0259 (17)
H41A	0.5174	0.4025	0.3682	0.031*
C42	0.5815 (9)	0.3782 (6)	0.4766 (4)	0.034 (2)
H42A	0.5028	0.3731	0.4988	0.040*
C43	0.6931 (11)	0.3681 (7)	0.5222 (5)	0.040 (2)
H43A	0.6899	0.3537	0.5756	0.049*
C44	0.8067 (9)	0.3793 (6)	0.4885 (4)	0.0331 (19)
H44A	0.8798	0.3750	0.5186	0.040*
C45	0.8121 (8)	0.3972 (6)	0.4087 (4)	0.0232 (16)
C46	0.9218 (7)	0.4192 (5)	0.3639 (4)	0.0225 (16)

C47	1.0382 (8)	0.4203 (6)	0.3973 (4)	0.0251 (17)	
H47A	1.0550	0.3954	0.4506	0.030*	
C48	1.1300 (7)	0.4586 (6)	0.3512 (4)	0.0259 (17)	
H48A	1.2080	0.4604	0.3733	0.031*	
C49	1.1029 (7)	0.4946 (6)	0.2709 (4)	0.0238 (16)	
C410	0.9888 (7)	0.4865 (5)	0.2380 (4)	0.0193 (15)	
H41B	0.9742	0.5085	0.1846	0.023*	
C411	0.8956 (7)	0.4464 (5)	0.2827 (4)	0.0181 (15)	
C412	1.1893 (7)	0.5493 (6)	0.2235 (5)	0.0286 (18)	
H41C	1.2638	0.5529	0.2482	0.034*	
O4	1.1710 (6)	0.5907 (5)	0.1540 (3)	0.0365 (14)	
C51	−0.053 (3)	0.0908 (19)	0.5027 (17)	0.086 (8)	0.50
H51A	−0.0594	0.0966	0.4478	0.104*	0.50
H51B	−0.1330	0.1447	0.5146	0.104*	0.50
Cl51	−0.0460 (6)	−0.0511 (5)	0.5549 (3)	0.0727 (17)	0.50
Cl52	0.0758 (6)	0.1275 (5)	0.5215 (4)	0.0708 (17)	0.50
C61	−0.0708 (12)	0.0781 (10)	0.7248 (6)	0.068 (3)	0.57
H61A	−0.1088	0.0174	0.7440	0.082*	0.57
H61B	0.0179	0.0541	0.7500	0.082*	0.57
Cl61	−0.0560 (6)	0.0979 (5)	0.6200 (3)	0.0866 (18)	0.57
Cl62	−0.1623 (6)	0.1921 (6)	0.7485 (4)	0.096 (2)	0.57
C71	−0.0708 (12)	0.0781 (10)	0.7248 (6)	0.068 (3)	0.43
H71A	0.0250	0.0436	0.7243	0.082*	0.43
H71B	−0.1156	0.0381	0.7009	0.082*	0.43
Cl71	−0.1217 (6)	0.0763 (5)	0.8249 (4)	0.0558 (15)	0.43
Cl72	−0.1220 (7)	0.2259 (7)	0.6771 (4)	0.082 (2)	0.43

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ir1	0.01611 (15)	0.01162 (14)	0.01596 (14)	−0.00359 (11)	0.00360 (11)	−0.00185 (10)
Ir2	0.01949 (15)	0.01215 (14)	0.01470 (14)	−0.00415 (11)	0.00349 (11)	−0.00274 (10)
Cl1	0.0197 (9)	0.0141 (8)	0.0289 (9)	−0.0041 (7)	0.0036 (7)	−0.0032 (7)
Cl2	0.0176 (8)	0.0142 (8)	0.0219 (8)	−0.0021 (7)	0.0027 (7)	−0.0040 (7)
N1	0.020 (3)	0.013 (3)	0.028 (3)	−0.003 (2)	0.003 (3)	−0.009 (2)
C11	0.025 (4)	0.009 (3)	0.023 (4)	0.002 (3)	0.002 (3)	−0.004 (3)
C12	0.049 (5)	0.016 (4)	0.019 (4)	−0.009 (3)	0.005 (4)	−0.001 (3)
C13	0.046 (5)	0.017 (4)	0.028 (4)	−0.014 (4)	0.017 (4)	−0.009 (3)
C14	0.029 (4)	0.024 (4)	0.029 (4)	−0.011 (3)	0.014 (3)	−0.007 (3)
C15	0.027 (4)	0.011 (3)	0.022 (4)	−0.012 (3)	0.009 (3)	0.002 (3)
C16	0.025 (4)	0.018 (3)	0.014 (3)	−0.004 (3)	0.010 (3)	0.001 (3)
C17	0.025 (4)	0.021 (4)	0.030 (4)	−0.003 (3)	0.013 (3)	−0.003 (3)
C18	0.012 (4)	0.019 (4)	0.065 (6)	−0.002 (3)	0.005 (4)	−0.004 (4)
C19	0.024 (4)	0.023 (4)	0.026 (4)	−0.004 (3)	−0.005 (3)	−0.003 (3)
C110	0.021 (4)	0.015 (3)	0.018 (3)	−0.004 (3)	0.002 (3)	0.003 (3)
C111	0.021 (4)	0.015 (3)	0.018 (3)	−0.008 (3)	0.002 (3)	0.003 (3)
C112	0.032 (5)	0.037 (5)	0.038 (5)	−0.007 (4)	−0.003 (4)	−0.008 (4)
O1	0.049 (4)	0.047 (4)	0.039 (4)	−0.021 (3)	0.002 (3)	−0.015 (3)

N2	0.019 (3)	0.016 (3)	0.019 (3)	−0.005 (2)	0.002 (2)	−0.004 (2)
C21	0.022 (4)	0.018 (4)	0.020 (4)	−0.007 (3)	0.001 (3)	−0.002 (3)
C22	0.028 (4)	0.027 (4)	0.020 (4)	−0.012 (3)	0.005 (3)	−0.009 (3)
C23	0.030 (4)	0.027 (4)	0.018 (4)	−0.009 (3)	0.004 (3)	−0.003 (3)
C24	0.037 (5)	0.023 (4)	0.015 (3)	−0.008 (3)	0.001 (3)	0.000 (3)
C25	0.018 (3)	0.013 (3)	0.017 (3)	−0.007 (3)	0.003 (3)	−0.007 (3)
C26	0.018 (4)	0.015 (3)	0.021 (3)	−0.004 (3)	0.001 (3)	−0.006 (3)
C27	0.026 (4)	0.017 (4)	0.023 (4)	−0.007 (3)	0.004 (3)	−0.002 (3)
C28	0.028 (4)	0.012 (3)	0.023 (4)	−0.002 (3)	−0.002 (3)	−0.002 (3)
C29	0.024 (4)	0.017 (3)	0.019 (3)	−0.009 (3)	0.007 (3)	−0.007 (3)
C210	0.023 (4)	0.012 (3)	0.019 (3)	−0.004 (3)	0.001 (3)	−0.002 (3)
C211	0.017 (3)	0.010 (3)	0.024 (4)	−0.005 (3)	0.001 (3)	−0.008 (3)
C212	0.035 (5)	0.024 (4)	0.022 (4)	−0.011 (3)	0.008 (3)	−0.006 (3)
O2	0.061 (4)	0.034 (3)	0.031 (3)	−0.012 (3)	0.017 (3)	−0.014 (3)
N3	0.017 (3)	0.014 (3)	0.022 (3)	−0.001 (2)	0.003 (2)	−0.006 (2)
C31	0.024 (4)	0.016 (3)	0.028 (4)	−0.005 (3)	−0.003 (3)	−0.005 (3)
C32	0.039 (5)	0.026 (4)	0.022 (4)	−0.014 (4)	−0.003 (3)	−0.002 (3)
C33	0.047 (5)	0.037 (5)	0.012 (3)	−0.023 (4)	0.003 (3)	−0.004 (3)
C34	0.046 (5)	0.027 (4)	0.021 (4)	−0.014 (4)	0.004 (4)	−0.007 (3)
C35	0.029 (4)	0.015 (3)	0.017 (3)	−0.011 (3)	0.005 (3)	−0.003 (3)
C36	0.025 (4)	0.013 (3)	0.014 (3)	−0.005 (3)	0.004 (3)	−0.004 (3)
C37	0.033 (4)	0.021 (4)	0.024 (4)	−0.006 (3)	0.008 (3)	−0.010 (3)
C38	0.028 (4)	0.018 (4)	0.027 (4)	0.003 (3)	−0.001 (3)	−0.006 (3)
C39	0.027 (4)	0.020 (4)	0.023 (4)	−0.011 (3)	−0.003 (3)	−0.006 (3)
C310	0.023 (4)	0.016 (3)	0.019 (3)	−0.009 (3)	0.000 (3)	−0.005 (3)
C311	0.025 (4)	0.006 (3)	0.019 (3)	−0.009 (3)	−0.001 (3)	−0.002 (2)
C312	0.028 (4)	0.014 (3)	0.028 (4)	−0.002 (3)	−0.003 (3)	0.002 (3)
O3	0.052 (4)	0.022 (3)	0.027 (3)	0.000 (3)	0.006 (3)	0.002 (2)
N4	0.036 (4)	0.011 (3)	0.020 (3)	−0.006 (3)	0.009 (3)	−0.001 (2)
C41	0.033 (4)	0.015 (4)	0.029 (4)	−0.005 (3)	0.013 (3)	−0.009 (3)
C42	0.052 (6)	0.022 (4)	0.029 (4)	−0.012 (4)	0.028 (4)	−0.013 (3)
C43	0.076 (7)	0.030 (5)	0.020 (4)	−0.021 (4)	0.011 (4)	−0.010 (3)
C44	0.053 (5)	0.029 (4)	0.023 (4)	−0.021 (4)	0.004 (4)	−0.006 (3)
C45	0.036 (4)	0.016 (3)	0.014 (3)	−0.008 (3)	0.003 (3)	0.003 (3)
C46	0.034 (4)	0.006 (3)	0.025 (4)	−0.002 (3)	−0.007 (3)	−0.006 (3)
C47	0.037 (4)	0.020 (4)	0.013 (3)	−0.004 (3)	−0.002 (3)	−0.002 (3)
C48	0.023 (4)	0.017 (4)	0.034 (4)	0.004 (3)	−0.012 (3)	−0.010 (3)
C49	0.026 (4)	0.024 (4)	0.025 (4)	−0.009 (3)	0.004 (3)	−0.011 (3)
C410	0.022 (4)	0.016 (3)	0.021 (4)	−0.005 (3)	−0.002 (3)	−0.009 (3)
C411	0.018 (4)	0.014 (3)	0.023 (4)	−0.006 (3)	0.000 (3)	−0.005 (3)
C412	0.018 (4)	0.024 (4)	0.045 (5)	−0.002 (3)	0.000 (3)	−0.018 (4)
O4	0.035 (3)	0.050 (4)	0.032 (3)	−0.019 (3)	0.011 (3)	−0.017 (3)
C51	0.076 (18)	0.057 (16)	0.12 (2)	−0.023 (14)	0.028 (17)	−0.015 (15)
Cl51	0.062 (4)	0.082 (4)	0.065 (4)	−0.029 (3)	0.005 (3)	0.004 (3)
Cl52	0.058 (4)	0.053 (3)	0.087 (4)	−0.010 (3)	−0.015 (3)	−0.003 (3)
C61	0.065 (8)	0.064 (8)	0.067 (8)	−0.017 (6)	0.011 (6)	−0.007 (6)
Cl61	0.073 (4)	0.086 (4)	0.077 (4)	0.001 (3)	−0.020 (3)	−0.012 (3)
Cl62	0.052 (3)	0.123 (5)	0.139 (6)	−0.020 (3)	0.000 (4)	−0.089 (5)

C71	0.065 (8)	0.064 (8)	0.067 (8)	−0.017 (6)	0.011 (6)	−0.007 (6)
Cl71	0.058 (4)	0.064 (4)	0.060 (4)	−0.032 (3)	0.025 (3)	−0.027 (3)
Cl72	0.050 (4)	0.113 (6)	0.062 (4)	−0.023 (4)	−0.003 (3)	0.014 (4)

Geometric parameters (Å, º)

Ir1—C111	1.976 (7)	N3—C31	1.344 (8)
Ir1—C311	1.990 (6)	N3—C35	1.351 (8)
Ir1—N1	2.034 (6)	C31—C32	1.387 (10)
Ir1—N3	2.046 (6)	C31—H31A	0.9300
Ir1—Cl1	2.5020 (17)	C32—C33	1.364 (11)
Ir1—Cl2	2.5187 (18)	C32—H32A	0.9300
Ir2—C411	1.974 (7)	C33—C34	1.382 (10)
Ir2—C211	2.000 (6)	C33—H33A	0.9300
Ir2—N2	2.040 (6)	C34—C35	1.386 (10)
Ir2—N4	2.040 (6)	C34—H34A	0.9300
Ir2—Cl1	2.5075 (19)	C35—C36	1.464 (9)
Ir2—Cl2	2.5260 (16)	C36—C37	1.401 (9)
N1—C11	1.347 (9)	C36—C311	1.416 (9)
N1—C15	1.370 (9)	C37—C38	1.386 (10)
C11—C12	1.383 (10)	C37—H37A	0.9300
C11—H11A	0.9300	C38—C39	1.400 (10)
C12—C13	1.372 (11)	C38—H38A	0.9300
C12—H12A	0.9300	C39—C310	1.386 (9)
C13—C14	1.378 (11)	C39—C312	1.474 (9)
C13—H13A	0.9300	C310—C311	1.406 (9)
C14—C15	1.393 (10)	C310—H31B	0.9300
C14—H14A	0.9300	C312—O3	1.220 (9)
C15—C16	1.463 (10)	C312—H31C	0.9300
C16—C17	1.386 (10)	N4—C41	1.358 (9)
C16—C111	1.430 (9)	N4—C45	1.373 (10)
C17—C18	1.373 (11)	C41—C42	1.363 (10)
C17—H17A	0.9300	C41—H41A	0.9300
C18—C19	1.404 (11)	C42—C43	1.402 (12)
C18—H18A	0.9300	C42—H42A	0.9300
C19—C110	1.397 (10)	C43—C44	1.367 (12)
C19—C112	1.458 (11)	C43—H43A	0.9300
C110—C111	1.387 (10)	C44—C45	1.395 (10)
C110—H10A	0.9300	C44—H44A	0.9300
C112—O1	1.188 (10)	C45—C46	1.459 (10)
C112—H11B	0.9300	C46—C47	1.384 (10)
N2—C21	1.344 (9)	C46—C411	1.421 (9)
N2—C25	1.358 (8)	C47—C48	1.391 (11)
C21—C22	1.369 (9)	C47—H47A	0.9300
C21—H21A	0.9300	C48—C49	1.403 (10)
C22—C23	1.371 (9)	C48—H48A	0.9300
C22—H22A	0.9300	C49—C410	1.395 (10)
C23—C24	1.382 (10)	C49—C412	1.458 (11)

C23—H23A	0.9300	C410—C411	1.400 (10)
C24—C25	1.383 (9)	C410—H41B	0.9300
C24—H24A	0.9300	C412—O4	1.218 (9)
C25—C26	1.463 (9)	C412—H41C	0.9300
C26—C27	1.398 (9)	C51—Cl52	1.64 (3)
C26—C211	1.414 (9)	C51—Cl51	1.80 (2)
C27—C28	1.386 (10)	C51—H51A	0.9700
C27—H27A	0.9300	C51—H51B	0.9700
C28—C29	1.395 (9)	Cl51—C51^{i}	1.52 (3)
C28—H28A	0.9300	Cl51—Cl52^{i}	1.950 (9)
C29—C210	1.396 (9)	Cl51—Cl51^{i}	2.447 (11)
C29—C212	1.469 (10)	Cl52—Cl51^{i}	1.950 (9)
C210—C211	1.384 (9)	C61—Cl62	1.626 (13)
C210—H21B	0.9300	C61—Cl61	1.842 (13)
C212—O2	1.206 (8)	C61—H61A	0.9700
C212—H21C	0.9300	C61—H61B	0.9700

C111—Ir1—C311	92.9 (3)	C29—C210—H21B	119.5
C111—Ir1—N1	80.8 (3)	C210—C211—C26	117.6 (6)
C311—Ir1—N1	96.6 (2)	C210—C211—Ir2	128.7 (5)
C111—Ir1—N3	94.7 (3)	C26—C211—Ir2	113.5 (5)
C311—Ir1—N3	80.5 (2)	O2—C212—C29	125.0 (7)
N1—Ir1—N3	174.5 (2)	O2—C212—H21C	117.5
C111—Ir1—Cl1	92.0 (2)	C29—C212—H21C	117.5
C311—Ir1—Cl1	172.9 (2)	C31—N3—C35	118.8 (6)
N1—Ir1—Cl1	89.34 (16)	C31—N3—Ir1	125.2 (5)
N3—Ir1—Cl1	93.94 (16)	C35—N3—Ir1	115.9 (4)
C111—Ir1—Cl2	171.5 (2)	N3—C31—C32	122.4 (7)
C311—Ir1—Cl2	93.32 (19)	N3—C31—H31A	118.8
N1—Ir1—Cl2	92.77 (17)	C32—C31—H31A	118.8
N3—Ir1—Cl2	92.00 (17)	C33—C32—C31	118.7 (7)
Cl1—Ir1—Cl2	82.43 (5)	C33—C32—H32A	120.6
C411—Ir2—C211	91.5 (3)	C31—C32—H32A	120.6
C411—Ir2—N2	93.5 (3)	C32—C33—C34	119.3 (7)
C211—Ir2—N2	81.2 (2)	C32—C33—H33A	120.4
C411—Ir2—N4	80.5 (3)	C34—C33—H33A	120.4
C211—Ir2—N4	95.4 (2)	C33—C34—C35	119.8 (7)
N2—Ir2—N4	173.1 (2)	C33—C34—H34A	120.1
C411—Ir2—Cl1	174.7 (2)	C35—C34—H34A	120.1
C211—Ir2—Cl1	91.39 (19)	N3—C35—C34	120.7 (6)
N2—Ir2—Cl1	91.22 (17)	N3—C35—C36	113.9 (6)
N4—Ir2—Cl1	94.88 (19)	C34—C35—C36	125.4 (6)
C411—Ir2—Cl2	95.29 (19)	C37—C36—C311	121.6 (6)
C211—Ir2—Cl2	171.86 (19)	C37—C36—C35	123.5 (6)
N2—Ir2—Cl2	93.90 (16)	C311—C36—C35	115.0 (6)
N4—Ir2—Cl2	90.17 (16)	C38—C37—C36	119.4 (7)
Cl1—Ir2—Cl2	82.17 (5)	C38—C37—H37A	120.3
Ir1—Cl1—Ir2	98.16 (6)	C36—C37—H37A	120.3

Ir1—Cl2—Ir2	97.24 (5)	C37—C38—C39	119.3 (7)
C11—N1—C15	119.1 (6)	C37—C38—H38A	120.3
C11—N1—Ir1	125.9 (5)	C39—C38—H38A	120.3
C15—N1—Ir1	115.0 (4)	C310—C39—C38	121.9 (6)
N1—C11—C12	121.1 (7)	C310—C39—C312	121.0 (7)
N1—C11—H11A	119.4	C38—C39—C312	117.0 (6)
C12—C11—H11A	119.4	C39—C310—C311	119.7 (7)
C13—C12—C11	120.8 (7)	C39—C310—H31B	120.2
C13—C12—H12A	119.6	C311—C310—H31B	120.2
C11—C12—H12A	119.6	C310—C311—C36	118.1 (6)
C12—C13—C14	117.9 (7)	C310—C311—Ir1	127.2 (5)
C12—C13—H13A	121.0	C36—C311—Ir1	114.6 (4)
C14—C13—H13A	121.0	O3—C312—C39	125.1 (7)
C13—C14—C15	120.5 (7)	O3—C312—H31C	117.4
C13—C14—H14A	119.7	C39—C312—H31C	117.4
C15—C14—H14A	119.7	C41—N4—C45	119.0 (6)
N1—C15—C14	120.2 (7)	C41—N4—Ir2	125.4 (5)
N1—C15—C16	112.9 (6)	C45—N4—Ir2	115.5 (5)
C14—C15—C16	126.6 (7)	N4—C41—C42	122.6 (8)
C17—C16—C111	121.9 (7)	N4—C41—H41A	118.7
C17—C16—C15	123.1 (6)	C42—C41—H41A	118.7
C111—C16—C15	114.9 (6)	C41—C42—C43	118.3 (8)
C18—C17—C16	119.5 (7)	C41—C42—H42A	120.8
C18—C17—H17A	120.2	C43—C42—H42A	120.8
C16—C17—H17A	120.2	C44—C43—C42	120.2 (7)
C17—C18—C19	120.3 (7)	C44—C43—H43A	119.9
C17—C18—H18A	119.8	C42—C43—H43A	119.9
C19—C18—H18A	119.8	C43—C44—C45	119.5 (8)
C110—C19—C18	119.4 (7)	C43—C44—H44A	120.2
C110—C19—C112	122.4 (7)	C45—C44—H44A	120.2
C18—C19—C112	118.2 (7)	N4—C45—C44	120.3 (7)
C111—C110—C19	121.9 (7)	N4—C45—C46	113.6 (6)
C111—C110—H10A	119.0	C44—C45—C46	125.9 (7)
C19—C110—H10A	119.0	C47—C46—C411	122.7 (7)
C110—C111—C16	116.3 (6)	C47—C46—C45	123.0 (7)
C110—C111—Ir1	130.1 (5)	C411—C46—C45	114.2 (6)
C16—C111—Ir1	113.6 (5)	C46—C47—C48	120.1 (7)
O1—C112—C19	124.4 (8)	C46—C47—H47A	120.0
O1—C112—H11B	117.8	C48—C47—H47A	120.0
C19—C112—H11B	117.8	C47—C48—C49	118.8 (7)
C21—N2—C25	118.6 (6)	C47—C48—H48A	120.6
C21—N2—Ir2	125.9 (4)	C49—C48—H48A	120.6
C25—N2—Ir2	115.4 (4)	C410—C49—C48	120.2 (7)
N2—C21—C22	122.9 (6)	C410—C49—C412	120.8 (7)
N2—C21—H21A	118.6	C48—C49—C412	118.8 (7)
C22—C21—H21A	118.6	C49—C410—C411	122.4 (7)
C21—C22—C23	119.4 (7)	C49—C410—H41B	118.8
C21—C22—H22A	120.3	C411—C410—H41B	118.8

C23—C22—H22A	120.3	C410—C411—C46	115.5 (6)
C22—C23—C24	118.1 (7)	C410—C411—Ir2	128.9 (5)
C22—C23—H23A	120.9	C46—C411—Ir2	115.4 (5)
C24—C23—H23A	120.9	O4—C412—C49	124.9 (7)
C23—C24—C25	120.9 (6)	O4—C412—H41C	117.6
C23—C24—H24A	119.6	C49—C412—H41C	117.6
C25—C24—H24A	119.6	Cl52—C51—Cl51	114.6 (15)
N2—C25—C24	120.1 (6)	Cl52—C51—H51A	108.6
N2—C25—C26	114.0 (6)	Cl51—C51—H51A	108.6
C24—C25—C26	125.9 (6)	Cl52—C51—H51B	108.6
C27—C26—C211	121.6 (6)	Cl51—C51—H51B	108.6
C27—C26—C25	122.6 (6)	H51A—C51—H51B	107.6
C211—C26—C25	115.8 (6)	C51^{i}—Cl51—C51	85.4 (13)
C28—C27—C26	119.5 (6)	C51^{i}—Cl51—Cl52^{i}	54.6 (11)
C28—C27—H27A	120.3	C51—Cl51—Cl52^{i}	106.7 (10)
C26—C27—H27A	120.3	Cl52^{i}—Cl51—Cl51^{i}	81.5 (4)
C27—C28—C29	119.5 (6)	C51—Cl52—Cl51^{i}	49.1 (10)
C27—C28—H28A	120.2	Cl62—C61—Cl61	113.8 (7)
C29—C28—H28A	120.2	Cl62—C61—H61A	108.8
C28—C29—C210	120.6 (6)	Cl61—C61—H61A	108.8
C28—C29—C212	118.3 (6)	Cl62—C61—H61B	108.8
C210—C29—C212	121.1 (6)	Cl61—C61—H61B	108.8
C211—C210—C29	121.1 (6)	H61A—C61—H61B	107.7
C211—C210—H21B	119.5		

C111—Ir1—Cl1—Ir2	174.2 (2)	N2—Ir2—C211—C26	2.5 (5)
N1—Ir1—Cl1—Ir2	93.43 (17)	N4—Ir2—C211—C26	176.5 (5)
N3—Ir1—Cl1—Ir2	−90.96 (17)	Cl1—Ir2—C211—C26	−88.5 (5)
Cl2—Ir1—Cl1—Ir2	0.54 (6)	C28—C29—C212—O2	−179.6 (8)
C211—Ir2—Cl1—Ir1	174.5 (2)	C210—C29—C212—O2	−2.1 (12)
N2—Ir2—Cl1—Ir1	93.23 (16)	C111—Ir1—N3—C31	81.2 (6)
N4—Ir2—Cl1—Ir1	−90.04 (16)	C311—Ir1—N3—C31	173.4 (6)
Cl2—Ir2—Cl1—Ir1	−0.54 (6)	Cl1—Ir1—N3—C31	−11.1 (6)
C311—Ir1—Cl2—Ir2	173.77 (19)	Cl2—Ir1—N3—C31	−93.6 (6)
N1—Ir1—Cl2—Ir2	−89.50 (16)	C111—Ir1—N3—C35	−95.6 (5)
N3—Ir1—Cl2—Ir2	93.17 (16)	C311—Ir1—N3—C35	−3.5 (5)
Cl1—Ir1—Cl2—Ir2	−0.54 (6)	Cl1—Ir1—N3—C35	172.1 (5)
C411—Ir2—Cl2—Ir1	175.9 (2)	Cl2—Ir1—N3—C35	89.6 (5)
N2—Ir2—Cl2—Ir1	−90.16 (17)	C35—N3—C31—C32	−4.2 (10)
N4—Ir2—Cl2—Ir1	95.44 (19)	Ir1—N3—C31—C32	179.1 (5)
Cl1—Ir2—Cl2—Ir1	0.54 (6)	N3—C31—C32—C33	0.0 (12)
C111—Ir1—N1—C11	166.2 (6)	C31—C32—C33—C34	2.8 (12)
C311—Ir1—N1—C11	74.3 (6)	C32—C33—C34—C35	−1.5 (12)
Cl1—Ir1—N1—C11	−101.8 (5)	C31—N3—C35—C34	5.4 (11)
Cl2—Ir1—N1—C11	−19.4 (5)	Ir1—N3—C35—C34	−177.5 (6)
C111—Ir1—N1—C15	−15.2 (5)	C31—N3—C35—C36	−174.1 (6)
C311—Ir1—N1—C15	−107.1 (5)	Ir1—N3—C35—C36	2.9 (8)
Cl1—Ir1—N1—C15	76.9 (5)	C33—C34—C35—N3	−2.6 (12)

Cl2—Ir1—N1—C15	159.3 (4)	C33—C34—C35—C36	176.8 (7)
C15—N1—C11—C12	−2.7 (10)	N3—C35—C36—C37	179.5 (7)
Ir1—N1—C11—C12	175.9 (5)	C34—C35—C36—C37	0.0 (12)
N1—C11—C12—C13	−2.4 (11)	N3—C35—C36—C311	−0.2 (9)
C11—C12—C13—C14	4.6 (11)	C34—C35—C36—C311	−179.7 (7)
C12—C13—C14—C15	−1.9 (11)	C311—C36—C37—C38	0.0 (11)
C11—N1—C15—C14	5.4 (9)	C35—C36—C37—C38	−179.6 (7)
Ir1—N1—C15—C14	−173.3 (5)	C36—C37—C38—C39	−0.7 (11)
C11—N1—C15—C16	−168.1 (6)	C37—C38—C39—C310	1.3 (11)
Ir1—N1—C15—C16	13.1 (7)	C37—C38—C39—C312	−178.5 (7)
C13—C14—C15—N1	−3.1 (10)	C38—C39—C310—C311	−1.1 (11)
C13—C14—C15—C16	169.4 (7)	C312—C39—C310—C311	178.7 (6)
N1—C15—C16—C17	175.7 (6)	C39—C310—C311—C36	0.3 (10)
C14—C15—C16—C17	2.7 (11)	C39—C310—C311—Ir1	−176.7 (5)
N1—C15—C16—C111	−1.6 (8)	C37—C36—C311—C310	0.2 (10)
C14—C15—C16—C111	−174.6 (7)	C35—C36—C311—C310	179.8 (6)
C111—C16—C17—C18	5.7 (11)	C37—C36—C311—Ir1	177.6 (6)
C15—C16—C17—C18	−171.4 (7)	C35—C36—C311—Ir1	−2.7 (8)
C16—C17—C18—C19	1.3 (11)	C111—Ir1—C311—C310	−85.3 (6)
C17—C18—C19—C110	−4.2 (11)	N1—Ir1—C311—C310	−4.2 (6)
C17—C18—C19—C112	175.3 (7)	N3—Ir1—C311—C310	−179.6 (6)
C18—C19—C110—C111	0.1 (10)	Cl2—Ir1—C311—C310	89.0 (6)
C112—C19—C110—C111	−179.4 (7)	C111—Ir1—C311—C36	97.5 (5)
C19—C110—C111—C16	6.4 (10)	N1—Ir1—C311—C36	178.6 (5)
C19—C110—C111—Ir1	−175.0 (5)	N3—Ir1—C311—C36	3.3 (5)
C17—C16—C111—C110	−9.4 (10)	Cl2—Ir1—C311—C36	−88.2 (5)
C15—C16—C111—C110	167.9 (6)	C310—C39—C312—O3	−1.0 (12)
C17—C16—C111—Ir1	171.7 (5)	C38—C39—C312—O3	178.8 (8)
C15—C16—C111—Ir1	−10.9 (7)	C411—Ir2—N4—C41	171.4 (6)
C311—Ir1—C111—C110	−68.7 (6)	C211—Ir2—N4—C41	80.7 (6)
N1—Ir1—C111—C110	−164.9 (7)	Cl1—Ir2—N4—C41	−11.1 (5)
N3—Ir1—C111—C110	12.0 (6)	Cl2—Ir2—N4—C41	−93.3 (5)
C311—Ir1—C111—C16	109.9 (5)	C411—Ir2—N4—C45	−6.4 (5)
N1—Ir1—C111—C16	13.7 (5)	C211—Ir2—N4—C45	−97.0 (5)
N3—Ir1—C111—C16	−169.4 (5)	Cl1—Ir2—N4—C45	171.1 (5)
C110—C19—C112—O1	2.9 (13)	Cl2—Ir2—N4—C45	89.0 (5)
C18—C19—C112—O1	−176.7 (8)	C45—N4—C41—C42	−2.0 (10)
C411—Ir2—N2—C21	84.9 (6)	Ir2—N4—C41—C42	−179.7 (5)
C211—Ir2—N2—C21	175.9 (6)	N4—C41—C42—C43	0.0 (11)
Cl1—Ir2—N2—C21	−92.9 (6)	C41—C42—C43—C44	2.0 (12)
Cl2—Ir2—N2—C21	−10.7 (6)	C42—C43—C44—C45	−2.0 (12)
C411—Ir2—N2—C25	−92.4 (5)	C41—N4—C45—C44	2.0 (10)
C211—Ir2—N2—C25	−1.4 (5)	Ir2—N4—C45—C44	180.0 (5)
Cl1—Ir2—N2—C25	89.8 (5)	C41—N4—C45—C46	−173.7 (6)
Cl2—Ir2—N2—C25	172.1 (4)	Ir2—N4—C45—C46	4.2 (7)
C25—N2—C21—C22	−0.9 (10)	C43—C44—C45—N4	0.0 (11)
Ir2—N2—C21—C22	−178.1 (5)	C43—C44—C45—C46	175.1 (7)
N2—C21—C22—C23	−1.1 (11)	N4—C45—C46—C47	178.1 (6)

C21—C22—C23—C24	1.6 (11)	C44—C45—C46—C47	2.6 (11)
C22—C23—C24—C25	−0.2 (11)	N4—C45—C46—C411	1.7 (8)
C21—N2—C25—C24	2.3 (10)	C44—C45—C46—C411	−173.7 (7)
Ir2—N2—C25—C24	179.7 (5)	C411—C46—C47—C48	5.8 (10)
C21—N2—C25—C26	−177.5 (6)	C45—C46—C47—C48	−170.2 (6)
Ir2—N2—C25—C26	0.0 (7)	C46—C47—C48—C49	−0.7 (10)
C23—C24—C25—N2	−1.7 (11)	C47—C48—C49—C410	−3.1 (10)
C23—C24—C25—C26	178.0 (7)	C47—C48—C49—C412	171.6 (6)
N2—C25—C26—C27	−178.5 (6)	C48—C49—C410—C411	2.0 (10)
C24—C25—C26—C27	1.7 (11)	C412—C49—C410—C411	−172.6 (6)
N2—C25—C26—C211	2.2 (9)	C49—C410—C411—C46	2.7 (10)
C24—C25—C26—C211	−177.6 (7)	C49—C410—C411—Ir2	179.0 (5)
C211—C26—C27—C28	1.2 (11)	C47—C46—C411—C410	−6.6 (10)
C25—C26—C27—C28	−178.0 (7)	C45—C46—C411—C410	169.7 (6)
C26—C27—C28—C29	−3.2 (11)	C47—C46—C411—Ir2	176.5 (5)
C27—C28—C29—C210	3.1 (11)	C45—C46—C411—Ir2	−7.1 (7)
C27—C28—C29—C212	−179.5 (7)	C211—Ir2—C411—C410	−73.9 (6)
C28—C29—C210—C211	−1.0 (11)	N2—Ir2—C411—C410	7.4 (6)
C212—C29—C210—C211	−178.3 (7)	N4—Ir2—C411—C410	−169.1 (7)
C29—C210—C211—C26	−1.0 (10)	Cl2—Ir2—C411—C410	101.6 (6)
C29—C210—C211—Ir2	−176.9 (5)	C211—Ir2—C411—C46	102.4 (5)
C27—C26—C211—C210	0.8 (10)	N2—Ir2—C411—C46	−176.3 (5)
C25—C26—C211—C210	−179.9 (6)	N4—Ir2—C411—C46	7.2 (5)
C27—C26—C211—Ir2	177.4 (5)	Cl2—Ir2—C411—C46	−82.0 (5)
C25—C26—C211—Ir2	−3.3 (8)	C410—C49—C412—O4	−0.3 (12)
C411—Ir2—C211—C210	−88.0 (7)	C48—C49—C412—O4	−175.0 (7)
N2—Ir2—C211—C210	178.6 (7)	Cl52—C51—Cl51—C51^{i}	−77.1 (16)
N4—Ir2—C211—C210	−7.5 (7)	Cl52—C51—Cl51—Cl52^{i}	−127.9 (14)
Cl1—Ir2—C211—C210	87.6 (6)	Cl52—C51—Cl51—Cl51^{i}	−77.1 (16)
C411—Ir2—C211—C26	95.9 (5)	Cl51—C51—Cl52—Cl51^{i}	88.8 (16)

Symmetry code: (i) −*x*, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14*A*···Cl52	0.93	2.89	3.715 (10)	148
C33—H33*A*···Cl71^{ii}	0.93	2.78	3.557 (10)	142
C43—H43*A*···Cl72^{iii}	0.93	2.56	3.205 (11)	127

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