metal-organic compounds

Di-μ-iodido-bis[(η^4-cycloocta-1,5-diene)-iridium(I)]

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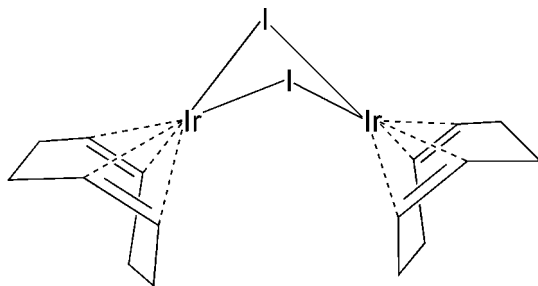Correspondence e-mail: tyama@chem.es.osaka-u.ac.jp

The molecular structure of the title compound, $[Ir_2I_2(C_8H_{12})_2]$, has C_2 symmetry. The dinuclear structure features two bridging I atoms and a bent geometry for the $Ir_2(\mu\text{-}I)_2$ core, with a hinge angle of 95.26 (1)°.

Related literature

For related literature, see: Aullón *et al.* (1998); Cotton *et al.* (1986, 1999); Dorta *et al.* (1997); Pettinari *et al.* (2002); De Ridder & Imhoff (1994); Tani *et al.* (1995); Yamagata *et al.* (1997, 2007).

Experimental

Crystal data

$[Ir_2I_2(C_8H_{12})_2]$
$M_r = 854.56$
Monoclinic, $C2/c$
$a = 12.3438$ (4) Å
$b = 11.8161$ (4) Å
$c = 11.9435$ (3) Å
$\beta = 96.6568$ (14)°

$V = 1730.28$ (10) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 18.92$ mm^{-1}
$T = 100$ (1) K
$0.39 \times 0.28 \times 0.22$ mm

Data collection

Rigaku R-AXIS RAPID imaging-plate diffractometer
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
$T_{min} = 0.018$, $T_{max} = 0.200$
27799 measured reflections

2909 independent reflections
2909 reflections with $I > 2\sigma(I)$
$R_{int} = 0.095$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.102$
$S = 1.19$
2909 reflections
91 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 5.91$ e Å^{-3}
$\Delta\rho_{min} = -5.04$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ir—C1	2.116 (8)	Ir—I	2.6901 (5)
Ir—C2	2.112 (7)	Ir—I^i	2.6991 (6)
Ir—C5	2.122 (8)	Ir$\cdots$Ir^i	2.9228 (6)
Ir—C6	2.113 (8)		
I—Ir—I^i	85.54 (2)	Ir—I—Ir^i	65.687 (15)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *TEXSAN* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97*; molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

References

Aullón, G., Ujaque, G., Lledós, A., Alvaez, S. & Alemany, P. (1998). *Inorg. Chem.* **37**, 804–813.
Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). *J. Appl. Cryst.* **38**, 381–388.
Cotton, F. A., Lahuerta, P., Sanau, M. & Schwotzer, W. (1986). *Inorg. Chim. Acta*, **120**, 153–157.
Cotton, F. A., Wilkinson, G., Murillo, C. A. & Bochmann, M. (1999). *Advanced Inorganic Chemistry*, 6th ed. New York: John Wiley & Sons Inc.
De Ridder, D. J. A. & Imhoff, P. (1994). *Acta Cryst.* C**50**, 1569–1572.
Dorta, R., Egli, P., Zücher, E. & Togni, A. (1997). *J. Am. Chem. Soc.* **119**, 10857–10858.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Higashi, T. (1999). *NUMABS*. Rigaku Corporation, Tokyo, Japan.
Pettinari, C., Marchetti, F., Cingolani, A., Bianchini, G., Drozdov, A., Vertlib, V. & Troyanov, S. (2002). *J. Organomet. Chem.* **651**, 5–14.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2004). *TEXSAN*. Version 2.0. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Tani, K., Onouchi, J., Yamagata, T. & Kataoka, Y. (1995). *Chem. Lett.* pp. 955–956.
Yamagata, T., Iseki, A. & Tani, K. (1997). *Chem. Lett.* pp. 1255–1256.
Yamagata, T., Nagata, M., Mashima, K. & Tani, K. (2007). *Acta Cryst.* E**63**, m1498.

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supplementary materials

Di-μ-iodido-bis[(η⁴-cycloocta-1,5-diene)iridium(I)]

T. Yamagata, M. Nagata, K. Mashima and K. Tani

Comment

Crystal data for binuclear complexes of d^8 transition metals of the type $[L_2M(\mu\text{-}X)]_2$ (M= Rh or Ir; X = halide) and their theoretical analyses have been reported (Aullón *et al.*, 1998; Cotton, *et al.*, 1999). However, their iodide analogues are fairly rare. Among the known complexes, cyclooctadiene derivatives of the Group 8 transition metals, *i.e.* $[M(\mu\text{-}Cl)(COD)]_2$ (M = Ir^I or Rh^I; cod = *cis,cis*-1,5-cyclooctadiene), have been used as key starting materials for the preparation of various kinds of Ir^I or Rh^I complexes, that are efficient catalyst precursors. For example, the molecular structure of $[Ir(\mu\text{-}Cl)\{(R)\text{-binap}\}]_2$ has been reported (Yamagata *et al.*, 1997), which was prepared from the reaction of $[Ir(\mu\text{-}Cl)(cod)]_2$ with two equivalents of (*R*)-binap, where (*R*)-binap is (*R*)-(+)-2,2'-bis(diphenylphosphanyl)-1,1'-binaphthyl, as well as its use as an efficient catalyst for the asymmetric hydrogenation of prochiral imines (Tani *et al.*, 1995).

The catalytic asymmetric olefin hydroamination with $[Ir(\mu\text{-}Cl)(diphosphine)]_2$ and the structure of $[Ir(\mu\text{-}Cl)\{(R)\text{-}binap\}]_2$ have also been investigated by Togni and co-workers (Dorta *et al.*, 1997). Although $[Rh(\mu\text{-}Cl)(cod)]_2$ (De Ridder & Imhoff, 1994) has an almost planar structure (the hinge angle is 169.1 (3)°), $[Ir(\mu\text{-}Br)(cod)]_2$ (Yamagata *et al.*, 2007), $[Ir(\mu\text{-}Cl)(cod)]_2$ (Cotton *et al.*, 1986), and $[Rh(\mu\text{-}Br)(cod)]_2$ (Pettinari *et al.*, 2002) show bent structures; with hinge angles of 101.58 (3)°, 109.4 (3)°, and 148.7 (3)°, respectively. Thus, it was thought of interest to examine the structure of $[Ir(\mu\text{-}I)(cod)]_2$, (I), Fig. 1 & Table 1. The structure of (I) resembles those of the aforementioned $[M(\mu\text{-}X)(cod)]_2$ structures, indeed the structures are isomorphous. In (I), the $Ir_2(\mu\text{-}I)_2$ core shows a bent geometry with the hinge angle of 95.26 (1)°. The $M\cdots M$ distances in (I), $[Ir(\mu\text{-}Br)(cod)]_2$, $[Ir(\mu\text{-}Cl)(cod)]_2$, and $[Rh(\mu\text{-}Br)(cod)]_2$ are 2.9228 (6), 2.9034 (5), 2.910 (1), and 3.565 Å, respectively. The degree of bending is Ir > Rh and I > Br > Cl. These tendencies can be explained by the differences in diffuseness of the metal's d orbitals and by analyzing the $<p_z^2/d_z^2>$ and $<d_z^2/d_z^2>$ overlap integrals between the Slater orbitals (EH calculations) (Aullón *et al.*, 1998).

Experimental

In a Schlenk flask with ether (50 ml) were added $[Ir(\mu\text{-}Cl)(cod)]_2$ (0.429 g, 0.639 mmol) and NaI (1.33 g, 8.86 mmol). The mixture was stirred at ambient temperature for 12 h. All volatiles were removed under reduced pressure and the residual washed with five portions of water (15 ml). The washings were monitored using aqueous silver nitrate. The resulting solid was washed with ethanol (10 ml) and dried *in vacuo* to yield $[Ir(\mu\text{-}I)(cod)]_2$ as a deep-red solid (0.441 g, 81%). Recrystallization from THF afforded an analytically pure product; m.pt. 522–527 K (dec.). ^{1}H NMR (CDCl$_3$, 308 K, 300 MHz, δ, p.p.m.): 4.43–4.44 (m, 8H, =C*H*), 2.10–2.14 (m, 8H, –C*H*H–), 1.13–1.36 (m, 8H, –CH*H*–). Analysis found: C 22.82, H 2.86%; $C_{16}H_{24}I_2Ir_2$ requires: C 22.49, H 2.83%.

supplementary materials

Refinement

All H-atoms were included in the riding model approximation with C—H distances in the range 0.95–0.99 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$ [or $1.5U_{eq}(C)$ for methyl groups]. The final difference Fourier map gave a maximum peak of 5.91 e Å^{-3} 2.58 Å from the Ir atom and 2.35 Å from the I atom. The minimum hole of -5.04 e Å^{-3} was 0.66 Å from the Ir atom.
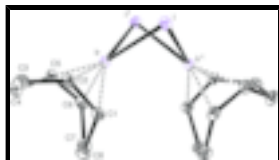
Figures

Fig. 1. The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level. The carbon-bound H-atoms have been omitted for clarity. Symmetry code: (i) $1 - x, y, 3/2 - z$.

Di-µ-iodido-bis[(η^4-cycloocta-1,5-diene)iridium(I)]

Crystal data

$[Ir_2I_2(C_8H_{12})_2]$	$F_{000} = 1520$
$M_r = 854.56$	$D_x = 3.280$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation $\lambda = 0.71075$ Å
Hall symbol: -C 2yc	Cell parameters from 41734 reflections
$a = 12.3438$ (4) Å	$\theta = 3.1–31.9º$
$b = 11.8161$ (4) Å	$\mu = 18.92$ mm^{-1}
$c = 11.9435$ (3) Å	$T = 100$ (1) K
$\beta = 96.6568$ (14)º	Platelet, red
$V = 1730.28$ (10) Å^3	$0.39 \times 0.28 \times 0.22$ mm
$Z = 4$	

Data collection

Rigaku R-AXIS RAPID imaging-plate diffractometer	2909 independent reflections
Radiation source: normal-focus sealed tube	2909 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.095$
Detector resolution: 10.00 pixels mm^{-1}	$\theta_{max} = 31.6º$
$T = 100(1)$ K	$\theta_{min} = 3.1º$
ω scans	$h = -18 \rightarrow 18$
Absorption correction: numerical (NUMABS; Higashi, 1999)	$k = -17 \rightarrow 17$
$T_{min} = 0.018$, $T_{max} = 0.200$	$l = -17 \rightarrow 17$
27799 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.102$	$w = 1/[\sigma^2(F_o^2) + (0.0244P)^2 + 97.8696P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.19$	$(\Delta/\sigma)_{max} = 0.001$
2909 reflections	$\Delta\rho_{max} = 5.91$ e Å^{-3}
91 parameters	$\Delta\rho_{min} = -5.04$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. Indexing was performed from 3 oscillations which were exposed for 2.0 minutes. The camera radius was 127.40 mm. Readout performed in the 0.100 mm pixel mode. #1 Phi=0.0, chi=55.0, omega=80.0 to 260.0 with 2.0deg step #2 Phi=180.0, chi=45.0, omega=0.0 to 180.0 with 2.0deg step #3 Phi=90.0, chi=20.0, omega=0.0 to 120.0 with 2.0deg step #4 Phi=180.0, chi= −5.0, omega=0.0 to 120.0 with 2.0deg step A total of 300 images, corresponding to 600.0 °. Osillation angles were collected with 4 different goniometer setting. Exposure time was 2.0 minutes per degree. The camera radius was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

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.

Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)

8.2950 (0.0021) *x* − 8.7297 (0.0018) *y* − 1.5346 (0.0022) *z* = 0.3948 (0.0020)

* 0.0000 (0.0000) Ir * 0.0000 (0.0000) I * 0.0000 (0.0000) I_$1

Rms deviation of fitted atoms = 0.0000

8.2950 (0.0021) *x* + 8.7297 (0.0019) *y* − 1.5346 (0.0022) *z* = 5.5983 (0.0018)

Angle to previous plane (with approximate e.s.d.) = 84.74 (0.01)

* 0.0000 (0.0000) Ir_$1 * 0.0000 (0.0000) I * 0.0000 (0.0000) I_$1

Rms deviation of fitted atoms = 0.0000

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}
Ir	0.38310 (2)	0.18522 (2)	0.75987 (2)	0.01168 (9)
I	0.52845 (4)	0.29804 (4)	0.90380 (4)	0.01538 (11)
C1	0.3674 (7)	0.0519 (7)	0.8752 (7)	0.0168 (13)
H1	0.4422	0.0649	0.9002	0.020*
C2	0.2902 (6)	0.1384 (7)	0.8903 (7)	0.0167 (13)
H2	0.3161	0.2062	0.9269	0.020*
C3	0.1697 (7)	0.1290 (8)	0.8517 (8)	0.0223 (16)
H3A	0.1338	0.2018	0.8654	0.027*
H3B	0.1375	0.0700	0.8966	0.027*
C4	0.1472 (7)	0.0988 (8)	0.7252 (7)	0.0214 (15)
H4A	0.1357	0.0161	0.7176	0.026*
H4B	0.0793	0.1368	0.6928	0.026*
C5	0.2387 (6)	0.1330 (7)	0.6594 (7)	0.0179 (14)
H5	0.2383	0.2069	0.6280	0.021*
C6	0.3252 (7)	0.0589 (7)	0.6427 (7)	0.0180 (14)
H6	0.3789	0.0844	0.5977	0.022*
C7	0.3372 (8)	−0.0590 (8)	0.6926 (8)	0.0255 (17)
H7A	0.4074	−0.0915	0.6758	0.031*
H7B	0.2779	−0.1074	0.6560	0.031*
C8	0.3333 (8)	−0.0612 (7)	0.8202 (8)	0.0223 (16)
H8A	0.2583	−0.0797	0.8358	0.027*
H8B	0.3825	−0.1214	0.8539	0.027*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ir	0.01187 (13)	0.01351 (13)	0.00961 (13)	−0.00130 (8)	0.00106 (9)	−0.00053 (8)
I	0.0146 (2)	0.0182 (2)	0.0131 (2)	−0.00157 (16)	0.00073 (16)	−0.00549 (16)
C1	0.017 (3)	0.016 (3)	0.018 (3)	−0.002 (3)	0.003 (3)	0.003 (3)
C2	0.015 (3)	0.019 (3)	0.018 (3)	−0.006 (3)	0.007 (3)	−0.003 (3)
C3	0.022 (4)	0.021 (4)	0.025 (4)	0.001 (3)	0.004 (3)	−0.004 (3)
C4	0.013 (3)	0.028 (4)	0.023 (4)	−0.005 (3)	0.004 (3)	−0.004 (3)
C5	0.012 (3)	0.023 (4)	0.018 (3)	0.000 (3)	−0.002 (3)	−0.003 (3)
C6	0.016 (3)	0.023 (4)	0.015 (3)	−0.004 (3)	0.002 (3)	−0.003 (3)
C7	0.024 (4)	0.022 (4)	0.032 (5)	−0.002 (3)	0.006 (3)	−0.011 (3)
C8	0.023 (4)	0.017 (3)	0.028 (4)	−0.003 (3)	0.006 (3)	0.000 (3)

Geometric parameters (Å, °)

Ir—C1	2.116 (8)	C3—H3A	0.9900
Ir—C2	2.112 (7)	C3—H3B	0.9900
Ir—C5	2.122 (8)	C4—C5	1.504 (12)
Ir—C6	2.113 (8)	C4—H4A	0.9900
Ir—I	2.6901 (5)	C4—H4B	0.9900

Ir—I[i]	2.6991 (6)	C5—C6	1.413 (12)
Ir—Ir[i]	2.9228 (6)	C5—H5	0.9500
I—Ir[i]	2.6991 (5)	C6—C7	1.516 (13)
C1—C2	1.422 (11)	C6—H6	0.9500
C1—C8	1.527 (12)	C7—C8	1.529 (14)
C1—H1	0.9500	C7—H7A	0.9900
C2—C3	1.511 (12)	C7—H7B	0.9900
C2—H2	0.9500	C8—H8A	0.9900
C3—C4	1.545 (12)	C8—H8B	0.9900
C2—Ir—C6	97.6 (3)	C2—C3—H3A	109.2
C2—Ir—C1	39.3 (3)	C4—C3—H3A	109.2
C6—Ir—C1	81.7 (3)	C2—C3—H3B	109.2
C2—Ir—C5	81.3 (3)	C4—C3—H3B	109.2
C6—Ir—C5	39.0 (3)	H3A—C3—H3B	107.9
C1—Ir—C5	91.0 (3)	C5—C4—C3	112.9 (7)
C2—Ir—I	92.1 (2)	C5—C4—H4A	109.0
C6—Ir—I	157.3 (2)	C3—C4—H4A	109.0
C1—Ir—I	93.3 (2)	C5—C4—H4B	109.0
C5—Ir—I	163.7 (2)	C3—C4—H4B	109.0
C2—Ir—I[i]	164.4 (2)	H4A—C4—H4B	107.8
C6—Ir—I[i]	90.2 (2)	C6—C5—C4	122.1 (8)
C1—Ir—I[i]	156.1 (2)	C6—C5—Ir	70.2 (4)
C5—Ir—I[i]	96.8 (2)	C4—C5—Ir	114.5 (5)
I—Ir—I[i]	85.54 (2)	C6—C5—H5	118.9
C2—Ir—Ir[i]	133.2 (2)	C4—C5—H5	118.9
C6—Ir—Ir[i]	102.0 (2)	Ir—C5—H5	85.5
C1—Ir—Ir[i]	102.6 (2)	C5—C6—C7	123.7 (8)
C5—Ir—Ir[i]	136.6 (2)	C5—C6—Ir	70.9 (5)
I—Ir—Ir[i]	57.305 (13)	C7—C6—Ir	112.3 (6)
I[i]—Ir—Ir[i]	57.008 (13)	C5—C6—H6	118.1
Ir—I—Ir[i]	65.687 (15)	C7—C6—H6	118.1
C2—C1—C8	121.9 (7)	Ir—C6—H6	86.9
C2—C1—Ir	70.2 (4)	C6—C7—C8	113.2 (7)
C8—C1—Ir	114.3 (6)	C6—C7—H7A	108.9
C2—C1—H1	119.0	C8—C7—H7A	108.9
C8—C1—H1	119.0	C6—C7—H7B	108.9
Ir—C1—H1	85.7	C8—C7—H7B	108.9
C1—C2—C3	124.0 (7)	H7A—C7—H7B	107.7
C1—C2—Ir	70.5 (4)	C1—C8—C7	112.1 (7)
C3—C2—Ir	113.2 (6)	C1—C8—H8A	109.2
C1—C2—H2	118.0	C7—C8—H8A	109.2
C3—C2—H2	118.0	C1—C8—H8B	109.2
Ir—C2—H2	86.3	C7—C8—H8B	109.2
C2—C3—C4	112.0 (7)	H8A—C8—H8B	107.9
C2—Ir—I—Ir[i]	142.2 (2)	C3—C4—C5—C6	91.6 (10)

C6—Ir—I—Ir[i]	26.6 (6)	C3—C4—C5—Ir	10.4 (10)
C1—Ir—I—Ir[i]	102.9 (2)	C2—Ir—C5—C6	−113.7 (5)
C5—Ir—I—Ir[i]	−152.1 (8)	C1—Ir—C5—C6	−75.5 (5)
I[i]—Ir—I—Ir[i]	−53.207 (18)	I—Ir—C5—C6	179.2 (6)
C6—Ir—C1—C2	−112.9 (5)	I[i]—Ir—C5—C6	81.9 (5)
C5—Ir—C1—C2	−74.9 (5)	Ir[i]—Ir—C5—C6	34.2 (6)
I—Ir—C1—C2	89.3 (4)	C2—Ir—C5—C4	3.5 (6)
I[i]—Ir—C1—C2	175.8 (4)	C6—Ir—C5—C4	117.2 (9)
Ir[i]—Ir—C1—C2	146.5 (4)	C1—Ir—C5—C4	41.7 (7)
C2—Ir—C1—C8	117.0 (8)	I—Ir—C5—C4	−63.6 (12)
C6—Ir—C1—C8	4.1 (6)	I[i]—Ir—C5—C4	−160.9 (6)
C5—Ir—C1—C8	42.0 (6)	Ir[i]—Ir—C5—C4	151.4 (5)
I—Ir—C1—C8	−153.7 (6)	C4—C5—C6—C7	−2.6 (12)
I[i]—Ir—C1—C8	−67.3 (9)	Ir—C5—C6—C7	104.5 (8)
Ir[i]—Ir—C1—C8	−96.5 (6)	C4—C5—C6—Ir	−107.1 (7)
C8—C1—C2—C3	−1.6 (12)	C2—Ir—C6—C5	66.0 (5)
Ir—C1—C2—C3	105.4 (8)	C1—Ir—C6—C5	102.0 (5)
C8—C1—C2—Ir	−107.0 (7)	I—Ir—C6—C5	−179.4 (5)
C6—Ir—C2—C1	66.9 (5)	I[i]—Ir—C6—C5	−100.5 (5)
C5—Ir—C2—C1	102.4 (5)	Ir[i]—Ir—C6—C5	−156.7 (4)
I—Ir—C2—C1	−92.6 (4)	C2—Ir—C6—C7	−53.6 (6)
I[i]—Ir—C2—C1	−173.6 (6)	C1—Ir—C6—C7	−17.5 (6)
Ir[i]—Ir—C2—C1	−47.6 (5)	C5—Ir—C6—C7	−119.5 (8)
C6—Ir—C2—C3	−52.7 (6)	I—Ir—C6—C7	61.1 (9)
C1—Ir—C2—C3	−119.5 (8)	I[i]—Ir—C6—C7	139.9 (6)
C5—Ir—C2—C3	−17.1 (6)	Ir[i]—Ir—C6—C7	83.7 (6)
I—Ir—C2—C3	147.9 (6)	C5—C6—C7—C8	−53.0 (11)
I[i]—Ir—C2—C3	66.9 (11)	Ir—C6—C7—C8	28.2 (9)
Ir[i]—Ir—C2—C3	−167.1 (4)	C2—C1—C8—C7	91.0 (10)
C1—C2—C3—C4	−54.0 (11)	Ir—C1—C8—C7	10.0 (9)
Ir—C2—C3—C4	27.4 (9)	C6—C7—C8—C1	−24.7 (11)
C2—C3—C4—C5	−24.4 (11)		

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2.

Fig. 1