

# Serendipitous preparation of *fac*-(acetonitrile- $\kappa N$ )trichlorido[(1,2,5,6- $\eta$ )-cycloocta-1,5-diene]-iridium(III)

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A reaction between  $[(\text{COD})\text{IrCl}]_2$  (COD is cycloocta-1,5-diene), HCl and indene failed to provide the hoped for chloridoindenyliridium dimer, but instead produced the title compound,  $[\text{IrCl}_3(\text{CH}_3\text{CN})(\text{C}_8\text{H}_{12})]$ , which is an octahedral complex of iridium(III) with a chelating cycloocta-1,5-diene ligand, three chloride ligands in a *fac* arrangement, and one acetonitrile ligand. Attempts to devise a rational synthesis for the title compound were unsuccessful.

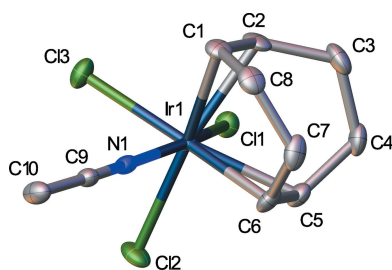
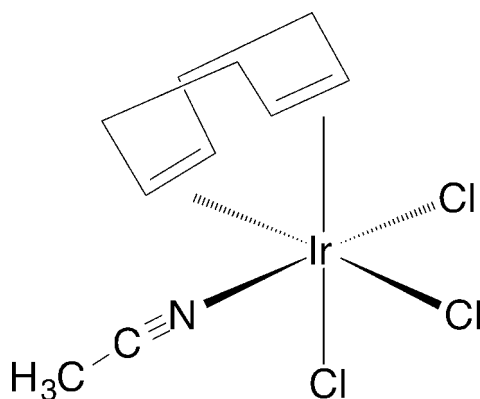
**Keywords:** crystal structure; iridium; cycloocta-diene; acetonitrile

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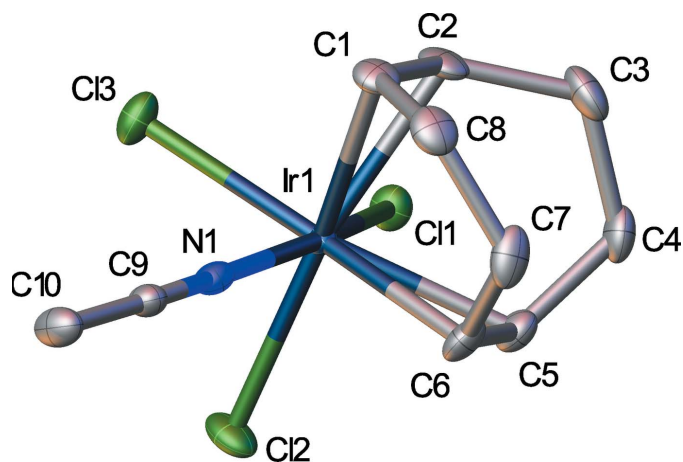
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## 1. Chemical context

We have published recently on the synthesis of a series of tetramethylalkylcyclopentadienyliridium complexes by the direct reaction between tetramethylalkylcyclopentadiene and iridium chloride, giving the  $[\text{Cp}^*\text{IrCl}_2]_2$  dimer (Morris *et al.*, 2014). From the dimer, a variety of other compounds can be made, such as amino acid complexes, that have shown significant anti-mycobacterial activity (Karpin *et al.*, 2013). Some of the reactions produced low yields of the chlorido-bridged dimer, thus limiting the number of products that could be made and tested.



An alternate route to Cp\*-type chlorido iridium dimers was reported using  $[(\text{COD})\text{IrCl}]_2$  as the starting material (El Amouri *et al.*, 1994) and, in our hands, this route does have promise for providing higher yields for many of the compounds. However, in the case of indene, there was no indication that an indenyl iridium complex had been prepared. Instead, a yellow–brown intractable solid was formed. Several attempts to dissolve the solid and to separate products through fractional crystallization all failed. During the course of this work-up, one of the solvents used was acetonitrile. At some point, the product mixture was allowed to stand in solution, and after about 24 hours several very nicely shaped



**Figure 1**  
The asymmetric unit of the title compound. Displacement ellipsoids are shown at the 50% probability level.

rectangular prisms had formed in the sample. These crystals were examined by X-ray crystallography and the results of that structure determination are reported here.

## 2. Structural commentary

While the total number of cycloocta-1,5-diene complexes structurally characterized is quite large, the number that are directly comparable to the title compound is small. The title compound is a pseudo-octahedral complex of iridium with three chloride ligands occupying one face of the octahedron and the alkenes of the COD and the acetonitrile ligand occupying the opposite face (Fig. 1). Considering the varying ligands about the central iridium, there is very little distortion from ideal octahedral angles, with the most significant distortion being the N1–Ir1–Cl2 distorted away from the COD group with an angle of 164.05 (11)°. All other angles, including those involving the alkene centroids, deviate by no more than 5° from the ideal. All three Ir–Cl bond lengths are similar [range 2.3603 (11) to 2.3670 (11) Å], which is in keeping with both types of *trans* ligands, alkene and acetonitrile, being expected to be strong *trans*-influence ligands and would have a similar magnitude of effect on the chloride *trans* to either ligand.

The facial Ir–Cl distances may be contrasted with the average distance of 2.441 (2) Å for *fac*-[(Me<sub>3</sub>P)<sub>3</sub>IrCl<sub>3</sub>] (CCDC: 896073) and related compounds (Merola *et al.*, 2013) that have somewhat longer Ir–Cl distances due to the effect of the *trans* PMe<sub>3</sub> groups.

Choudhury *et al.* (2005) reported on a COD complex of iridium with three chlorides and a SnCl<sub>3</sub> ligand completing the octahedral coordination about the central Ir atom (CCDC: 273475). In that case, though, the compound is a dinuclear one with Ir–Cl–Ir bridges. So, there are long Ir–Cl bonds (those involved in bridging) of 2.544 (4) Å and a shorter terminal Ir–Cl bond of 2.385 (6) Å. C=C bond lengths for the COD

**Table 1**  
Experimental details.

Crystal data	
Chemical formula	[IrCl <sub>3</sub> (C <sub>2</sub> H <sub>3</sub> N)(C <sub>8</sub> H <sub>12</sub> )]
<i>M<sub>r</sub></i>	447.78
Crystal system, space group	Orthorhombic, <i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.25131 (10), 11.85605 (14), 12.94150 (15)
<i>V</i> (Å <sup>3</sup> )	1266.04 (3)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
<i>μ</i> (mm <sup>-1</sup> )	11.15
Crystal size (mm)	0.22 × 0.15 × 0.11
Data collection	
Diffractometer	Agilent Xcalibur Eos Gemini ultra
Absorption correction	Analytical ( <i>SCALE3 ABSPACK</i> ; Clark & Reid, 1995)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.204, 0.396
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	27207, 4333, 4173
<i>R<sub>int</sub></i>	0.040
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.755
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.019, 0.038, 1.08
No. of reflections	4333
No. of parameters	137
H-atom treatment	H-atom parameters constrained
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	1.07, -0.74
Absolute structure	Flack <i>x</i> determined using 1715 quotients [( <i>I</i> <sup>+</sup> ) - ( <i>I</i> <sup>-</sup> )] / [( <i>I</i> <sup>+</sup> ) + ( <i>I</i> <sup>-</sup> )] (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	-0.011 (4)

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

ring are similar to the title compound at 1.38 (1) and 1.41 (2) Å.

## 3. Supramolecular features

Although there appear to be some close C–H⋯Cl intermolecular interactions, there are no important supramolecular features to speak of in this structure.

## 4. Database survey

A substructure search of the CCDC (Groom & Allen, 2014) for the 1,5-COD–Ir fragment resulted in over 850 hits. This is not a surprising result since [CODIrCl]<sub>2</sub> is a convenient, high-yield organometallic starting material made in one step from IrCl<sub>3</sub>·H<sub>2</sub>O and cycloocta-1,5-diene (Crabtree & Morris, 1977). From [CODIrCl]<sub>2</sub>, a wide variety of ligand addition, chloride replacement or bridge-splitting reactions can be carried out, leading to a wide variety of compounds containing the COD chelate. Using *Mercury* (Macrae *et al.*, 2008), an analysis of the COD–Ir search of the database for structures with an octahedral coordination around the metal showed that the C=C bonds of the COD ligands ranged from 1.184 to 1.508 Å with a mean of 1.394 Å. For the title compound, the values of 1.392 (7) and 1.389 (6) Å are pretty much right at the mean for COD C=C bonds.

An analysis of the CCDC database (Groom & Allen, 2014) for octahedral iridium complexes with acetonitrile ligands uncovered 99 hits with Ir–N distances measuring from a minimum of 1.897 Å to a maximum of 2.246 Å with a mean of 2.068 Å. For the title compound, the Ir–N distance of 2.023 (4) Å places it just below the mean.

## 5. Synthesis and crystallization

The title complex was formed as a few isolated crystals from an attempted reaction between [(COD)IrCl]<sub>2</sub> and indene with HCl in an attempt to synthesize the [indenylIrCl<sub>2</sub>]<sub>2</sub> dimer, which would have been a useful starting material for our studies. Unfortunately, this did not provide the desired product. The reaction produced some very intractable solids. After multiple attempts to dissolve the solid in many different solvents, including acetonitrile, some well-shaped prisms formed on the side of the flask and these crystals were used in this investigation and were shown to be that of the title complex. Attempts to make this material in a rational fashion were not successful.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms were positioned geometrically and refined as riding with C–H = 0.96–0.98 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$ .

## Acknowledgements

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## supporting information

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## Serendipitous preparation of *fac*-(acetonitrile- $\kappa$ N)trichlorido[(1,2,5,6- $\eta$ )-cycloocta-1,5-diene]iridium(III)

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### Computing details

Data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO* (Agilent, 2014); data reduction: *CrysAlis PRO* (Agilent, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

### *fac*-(Acetonitrile- $\kappa$ N)trichlorido[(1,2,5,6- $\eta$ )-cycloocta-1,5-diene]iridium(III)

#### Crystal data

[IrCl<sub>3</sub>(C<sub>2</sub>H<sub>3</sub>N)(C<sub>8</sub>H<sub>12</sub>)]  
 $M_r = 447.78$   
 Orthorhombic,  $P2_12_12_1$   
 $a = 8.25131$  (10) Å  
 $b = 11.85605$  (14) Å  
 $c = 12.94150$  (15) Å  
 $V = 1266.04$  (3) Å<sup>3</sup>  
 $Z = 4$   
 $F(000) = 840$

$D_x = 2.349$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å  
 Cell parameters from 12030 reflections  
 $\theta = 4.0$ – $32.2^\circ$   
 $\mu = 11.15$  mm<sup>-1</sup>  
 $T = 100$  K  
 Prism, clear light orange  
 $0.22 \times 0.15 \times 0.11$  mm

#### Data collection

Agilent Xcalibur Eos Gemini ultra  
 diffractometer  
 Radiation source: Enhance (Mo) X-ray Source,  
 Agilent Gemini System  
 Graphite monochromator  
 Detector resolution: 16.0122 pixels mm<sup>-1</sup>  
 $\omega$  scans  
 Absorption correction: analytical  
 (SCALE3 ABSPACK; Clark & Reid, 1995)

$T_{\min} = 0.204$ ,  $T_{\max} = 0.396$   
 27207 measured reflections  
 4333 independent reflections  
 4173 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.040$   
 $\theta_{\max} = 32.4^\circ$ ,  $\theta_{\min} = 3.4^\circ$   
 $h = -11 \rightarrow 12$   
 $k = -17 \rightarrow 17$   
 $l = -19 \rightarrow 19$

#### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.019$   
 $wR(F^2) = 0.038$   
 $S = 1.08$   
 4333 reflections  
 137 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0124P)^2 + 1.2315P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.002$   
 $\Delta\rho_{\max} = 1.07$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.74$  e Å<sup>-3</sup>

Absolute structure: Flack  $x$  determined using  
1715 quotients  $[(F^+)-(F^-)]/[(F^+)+(F^-)]$  (Parsons *et al.*, 2013)  
Absolute structure parameter:  $-0.011$  (4)

*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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Ir1	0.70199 (2)	0.47821 (2)	0.68347 (2)	0.01178 (4)
Cl1	0.68059 (17)	0.64680 (9)	0.78048 (9)	0.0238 (2)
Cl2	0.85370 (14)	0.58778 (9)	0.56587 (9)	0.0202 (2)
Cl3	0.47576 (13)	0.52459 (13)	0.57940 (9)	0.0275 (2)
N1	0.5308 (5)	0.4220 (3)	0.7828 (3)	0.0153 (7)
C1	0.7775 (6)	0.3484 (4)	0.5677 (3)	0.0210 (9)
H1	0.7227	0.3540	0.5008	0.025*
C2	0.6888 (7)	0.2940 (4)	0.6442 (3)	0.0210 (9)
H2	0.5813	0.2686	0.6219	0.025*
C3	0.7669 (7)	0.2197 (4)	0.7247 (4)	0.0268 (12)
H3A	0.8639	0.1863	0.6953	0.032*
H3B	0.6930	0.1587	0.7413	0.032*
C4	0.8132 (6)	0.2806 (4)	0.8253 (4)	0.0245 (9)
H4A	0.7241	0.2736	0.8737	0.029*
H4B	0.9063	0.2430	0.8553	0.029*
C5	0.8528 (5)	0.4040 (4)	0.8121 (4)	0.0202 (9)
H5	0.8518	0.4477	0.8764	0.024*
C6	0.9554 (6)	0.4463 (4)	0.7360 (4)	0.0229 (10)
H6	1.0132	0.5148	0.7568	0.028*
C7	1.0494 (6)	0.3734 (5)	0.6606 (4)	0.0289 (12)
H7A	1.0816	0.3048	0.6959	0.035*
H7B	1.1476	0.4132	0.6414	0.035*
C8	0.9592 (6)	0.3407 (4)	0.5616 (4)	0.0254 (11)
H8A	0.9963	0.3892	0.5061	0.030*
H8B	0.9885	0.2640	0.5437	0.030*
C9	0.4307 (5)	0.3980 (4)	0.8376 (3)	0.0174 (9)
C10	0.3017 (7)	0.3700 (4)	0.9097 (3)	0.0246 (9)
H10A	0.2025	0.4047	0.8874	0.037*
H10B	0.3294	0.3972	0.9773	0.037*
H10C	0.2879	0.2896	0.9120	0.037*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ir1	0.01257 (6)	0.01427 (6)	0.00849 (6)	0.00042 (6)	0.00024 (6)	0.00067 (6)

C11	0.0356 (7)	0.0166 (5)	0.0193 (5)	-0.0010 (5)	0.0073 (5)	-0.0029 (4)
C12	0.0229 (5)	0.0206 (5)	0.0170 (5)	-0.0021 (4)	0.0046 (4)	0.0034 (4)
C13	0.0177 (5)	0.0456 (7)	0.0191 (5)	0.0062 (5)	-0.0037 (4)	0.0099 (6)
N1	0.0216 (19)	0.0134 (17)	0.0110 (16)	-0.0012 (14)	-0.0036 (14)	0.0013 (13)
C1	0.027 (3)	0.022 (2)	0.014 (2)	-0.002 (2)	0.0019 (19)	-0.0038 (16)
C2	0.031 (2)	0.0162 (19)	0.0162 (19)	-0.006 (2)	0.002 (2)	-0.0054 (15)
C3	0.041 (3)	0.016 (2)	0.024 (2)	0.007 (2)	0.012 (2)	0.0051 (18)
C4	0.026 (2)	0.027 (2)	0.020 (2)	0.0060 (19)	-0.001 (2)	0.0097 (19)
C5	0.0196 (19)	0.028 (2)	0.0133 (19)	0.0018 (16)	-0.0060 (19)	0.006 (2)
C6	0.015 (2)	0.036 (3)	0.018 (2)	0.0004 (18)	-0.0079 (17)	0.0053 (19)
C7	0.016 (2)	0.040 (3)	0.030 (3)	0.010 (2)	0.0045 (19)	0.009 (2)
C8	0.030 (3)	0.024 (2)	0.022 (2)	0.008 (2)	0.011 (2)	-0.002 (2)
C9	0.0157 (19)	0.021 (2)	0.015 (2)	-0.0023 (16)	-0.0014 (15)	-0.0035 (16)
C10	0.020 (2)	0.037 (3)	0.017 (2)	-0.007 (2)	0.003 (2)	-0.0031 (18)

*Geometric parameters (Å, °)*

Ir1—C11	2.3670 (11)	C4—H4A	0.9700
Ir1—C12	2.3603 (11)	C4—H4B	0.9700
Ir1—C13	2.3666 (10)	C4—C5	1.509 (6)
Ir1—N1	2.023 (4)	C5—H5	0.9800
Ir1—C1	2.236 (4)	C5—C6	1.392 (7)
Ir1—C2	2.245 (4)	C6—H6	0.9800
Ir1—C5	2.257 (5)	C6—C7	1.517 (7)
Ir1—C6	2.231 (4)	C7—H7A	0.9700
N1—C9	1.125 (6)	C7—H7B	0.9700
C1—H1	0.9800	C7—C8	1.531 (8)
C1—C2	1.389 (6)	C8—H8A	0.9700
C1—C8	1.504 (7)	C8—H8B	0.9700
C2—H2	0.9800	C9—C10	1.454 (6)
C2—C3	1.510 (7)	C10—H10A	0.9600
C3—H3A	0.9700	C10—H10B	0.9600
C3—H3B	0.9700	C10—H10C	0.9600
C3—C4	1.537 (7)		
C12—Ir1—C11	85.23 (4)	C2—C3—H3B	108.6
C12—Ir1—C13	85.61 (4)	C2—C3—C4	114.6 (4)
C13—Ir1—C11	92.68 (5)	H3A—C3—H3B	107.6
N1—Ir1—C11	83.63 (11)	C4—C3—H3A	108.6
N1—Ir1—C12	164.05 (11)	C4—C3—H3B	108.6
N1—Ir1—C13	83.55 (11)	C3—C4—H4A	108.6
N1—Ir1—C1	113.18 (16)	C3—C4—H4B	108.6
N1—Ir1—C2	77.86 (16)	H4A—C4—H4B	107.6
N1—Ir1—C5	77.73 (16)	C5—C4—C3	114.5 (4)
N1—Ir1—C6	113.88 (16)	C5—C4—H4A	108.6
C1—Ir1—C11	163.18 (12)	C5—C4—H4B	108.6
C1—Ir1—C12	78.41 (12)	Ir1—C5—H5	114.5
C1—Ir1—C13	89.92 (14)	C4—C5—Ir1	110.0 (3)

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C1—Ir1—C2	36.12 (16)	C4—C5—H5	114.5
C1—Ir1—C5	94.14 (18)	C6—C5—Ir1	70.9 (3)
C2—Ir1—C11	159.73 (12)	C6—C5—C4	124.1 (5)
C2—Ir1—C12	114.52 (12)	C6—C5—H5	114.5
C2—Ir1—C13	93.37 (14)	Ir1—C6—H6	113.6
C2—Ir1—C5	79.33 (18)	C5—C6—Ir1	73.0 (3)
C5—Ir1—C11	88.79 (13)	C5—C6—H6	113.6
C5—Ir1—C12	113.44 (12)	C5—C6—C7	124.2 (5)
C5—Ir1—C13	160.95 (12)	C7—C6—Ir1	112.4 (3)
C6—Ir1—C11	92.97 (14)	C7—C6—H6	113.6
C6—Ir1—C12	78.03 (13)	C6—C7—H7A	108.4
C6—Ir1—C13	162.18 (12)	C6—C7—H7B	108.4
C6—Ir1—C1	79.97 (19)	C6—C7—C8	115.7 (4)
C6—Ir1—C2	87.1 (2)	H7A—C7—H7B	107.4
C6—Ir1—C5	36.15 (17)	C8—C7—H7A	108.4
C9—N1—Ir1	175.1 (4)	C8—C7—H7B	108.4
Ir1—C1—H1	114.7	C1—C8—C7	115.2 (4)
C2—C1—Ir1	72.3 (3)	C1—C8—H8A	108.5
C2—C1—H1	114.7	C1—C8—H8B	108.5
C2—C1—C8	122.3 (5)	C7—C8—H8A	108.5
C8—C1—Ir1	110.8 (3)	C7—C8—H8B	108.5
C8—C1—H1	114.7	H8A—C8—H8B	107.5
Ir1—C2—H2	114.2	N1—C9—C10	178.4 (5)
C1—C2—Ir1	71.6 (3)	C9—C10—H10A	109.5
C1—C2—H2	114.2	C9—C10—H10B	109.5
C1—C2—C3	122.5 (5)	C9—C10—H10C	109.5
C3—C2—Ir1	113.0 (3)	H10A—C10—H10B	109.5
C3—C2—H2	114.2	H10A—C10—H10C	109.5
C2—C3—H3A	108.6	H10B—C10—H10C	109.5
Ir1—C1—C2—C3	-106.1 (4)	C3—C4—C5—Ir1	32.7 (5)
Ir1—C1—C8—C7	27.6 (5)	C3—C4—C5—C6	-47.3 (6)
Ir1—C2—C3—C4	10.1 (6)	C4—C5—C6—Ir1	101.7 (4)
Ir1—C5—C6—C7	-105.8 (4)	C4—C5—C6—C7	-4.2 (7)
Ir1—C6—C7—C8	3.1 (6)	C5—C6—C7—C8	87.1 (6)
C1—C2—C3—C4	92.3 (5)	C6—C7—C8—C1	-20.8 (7)
C2—C1—C8—C7	-54.0 (6)	C8—C1—C2—Ir1	103.8 (4)
C2—C3—C4—C5	-29.0 (6)	C8—C1—C2—C3	-2.3 (7)

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