



An iridium complex with an unsupported Ir—Zn bond: diiodido(η^5 -pentamethylcyclopentadienyl)-bis(trimethylphosphane)iridiumzinc(Ir—Zn) benzene hemisolvate

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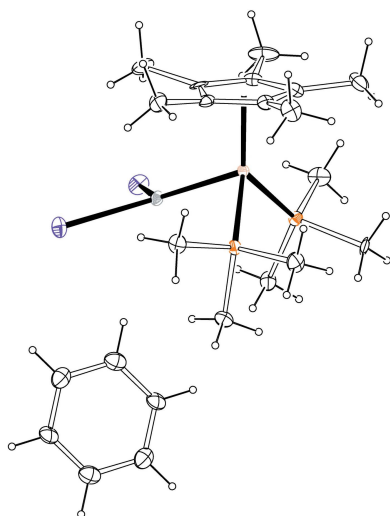
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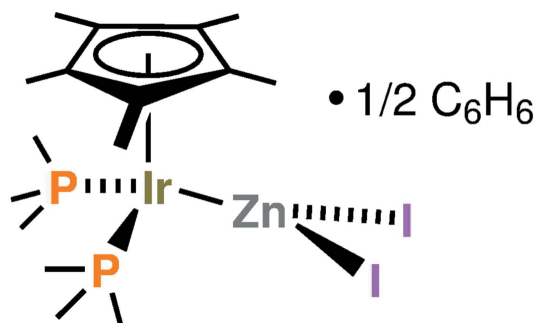
The title compound, [IrZnI₂(C₁₀H₁₅)(C₃H₉P)₂].0.5C₆H₆ or [Cp*(PMe₃)₂Ir]-[ZnI₂] (Cp* = *cyclo*-C₅Me₅) was obtained and characterized as its benzene solvate [Cp*(PMe₃)₂Ir]-[ZnI₂].0.5C₆H₆. The bimetallic complex in this structure contains the Lewis-acidic fragment ZnI₂ bonded to the Lewis-basic fragment Cp*(PMe₃)₂Ir, with an Ir—Zn bond distance of 2.452 (1) Å. The compound was obtained by reacting [Cp*(PMe₃)₂IrI₂] with 2-Ad₂Zn (2-Ad = 2-adamantyl), resulting in the reduction of the Ir^{III} complex and formation of the Ir^I-Zn^{II} adduct. The crystal studied was a twin by non-merohedry with a refined BASF parameter of 0.223 (1).

1. Chemical context

An intuitive way to create metal–metal bonds is by linking a Lewis-basic metal center to a Lewis-acidic metal center. Lewis acid/base adducts of the type [Cp^R(L)(L')Ir]-[ZnX₂] (Cp^R = either Cp, cyclopentadienyl, or Cp*, pentamethylcyclopentadienyl; L and L' = neutral ligand; X = halogen) have been known for a long time. Regarding the Lewis-basic fragment, it has been noted that electron-rich half-sandwich complexes can be considered 'metal bases *par excellence*' (Werner, 1983), and zinc dihalides are among the most well-known Lewis acids. The bimetallic complex [Cp(PPh₃)(CO)Ir]-[ZnBr₂] was isolated and spectroscopically characterized 49 years ago (Oliver & Graham, 1970). However, crystallographic characterization of such complexes having iridium–zinc bonds is elusive. While a related complex [Cp*(CO)₂Ir]-[ZnCl₂] was later prepared in a different group, it too was not structurally characterized, instead an adduct with mercury(II) chloride was crystallographically characterized (Einstein *et al.*, 1992). A cobalt complex [Cp(PMe₃)₂Co]-[ZnCl₂PMe₃] is known as well; it too is lacking crystallographic characterization (Dey & Werner, 1977). In fact, while complexes are known where a zinc dihalide acts as a bridge between metals (iridium: Kimura *et al.*, 2012) or where aggregation occurs to form multi-zinc clusters (rhodium and zinc: Molon *et al.*, 2010), a search of the Cambridge Crystallographic Database (Groom *et al.*, 2016) revealed no example of a structurally characterized complex [Cp^R(L)(L')M]-[ZnX₂] (M = either Co, Rh, or Ir) with a terminal (non-bridging) zinc dihalide. For iridium, it appears, in fact, that regardless of the ligand coordination sphere there is no single example of an unsupported iridium–zinc bond. The



scarcity of examples for iridium contrasts with the situation of rhodium, for which a couple of examples of unsupported Rh–Zn X_2 structures exist with a PNP ‘pincer’ providing the coordination environment at rhodium (Gair *et al.*, 2019). Additionally, several Rh–Zn structures exist with Zn–Cp* and Zn–C environments (Cadenbach *et al.*, 2009). In this contribution, we provide crystallographic characterization for [Cp*(PMe₃)₂Ir]-[ZnI₂] (benzene solvate). The bimetallic complex in this structure is the formal adduct of the Lewis base Cp*(PMe₃)₂Ir^I and the Lewis acid Zn^{II}I₂, providing the first structural characterization within the large class of metal–metal-bonded compounds [Cp^R(L)(L')M]-[ZnX₂] (M = Co, Rh, or Ir, X = halide, L, L' = neutral ligand). We did not synthesize the title compound from iridium(I). Rather, it was obtained through the reduction of iridium(III) with di-(2-adamantyl)zinc, as described under ‘Synthesis and crystallization’.



2. Structural commentary

An anisotropic displacement plot showing [Cp*(PMe₃)₂Ir]-[ZnI₂] and its benzene solvate molecule is shown in Fig. 1. The Ir1–Zn1 distance is 2.452 (1) Å, which is within the expected distance range when compared to other examples of M–Zn bonds, specifically those of unsupported Rh–Zn bonds, which were determined to be 2.4224 (6) Å for Rh–ZnCl₂ and 2.4147 (5) Å for Rh–ZnBr₂ (Gair *et al.*, 2019). The only crystallographically characterized Ir–Zn bonds are those of a structure that contains a bridging zinc dihalide, which leads to expected longer M–Zn bond distances of 2.563 (1) and 2.566 (1) Å (Kimura *et al.*, 2012). Bond angles around the iridium center in [Cp*(PMe₃)₂Ir]-[ZnI₂] match those of a three-legged piano stool, with roughly 90° angles. The Zn1–Ir1–P1 angle was found to be 88.74 (7)°, the Zn1–Ir1–P2 angle 91.35 (7)°, and the P1–Ir1–P2 angle 93.81 (9)°. The ZnI₂ fragment is close to planar, with Zn1 being displaced from the I1–I2–Ir1 plane by only 0.1427 (11) Å. The Zn1–I1 distance is 2.588 (1) Å and the Zn1–I2 distance is 2.582 (1) Å. The angles about Zn are 127.19 (5)° for Ir1–Zn–I1, 126.73 (5)° for Ir1–Zn–I2, and 105.11 (4)° for I1–Zn–I2. The larger Ir–Zn–X angles and the comparably small X–Zn–X angle are consistent with what has been observed for the ZnBr₂ and ZnCl₂ fragments in the existing Rh–Zn complexes (Gair *et al.*, 2019). These complexes had Rh1–Zn1–X1 (where X = Br or Cl) angles of 130.14 (2) and 130.26 (4)°, Rh1–Zn1–X2 angles of 120.42 (2) and

120.31 (11)°, and X1–Zn1–X2 angles of 109.43 (2) and 109.41 (4)°. In [Cp*(PMe₃)₂Ir]-[ZnI₂], there is a relatively short intramolecular C–H···I interaction between H14B (on the C14 methyl group) and I1, with an H···I contact distance of 3.06 Å (this reported distance is based on the calculated position of H14B, which is placed at 0.98 Å from C14 and at an angle C14–H14B···I1 of 157°); the C14···I1 distance is 3.977 (12) Å.

3. Supramolecular features

The packing of [Cp*(PMe₃)₂Ir]-[ZnI₂].0.5C₆H₆ is shown in Fig. 2. Molecules of [Cp*(PMe₃)₂Ir]-[ZnI₂] and the C₆H₆ solvent pack through contacting van der Waals surfaces, without any particular short contacts. There are no intermolecular hydrogen bonds in the structure. A possible intramolecular C–H···I hydrogen bond is discussed above under *Structural commentary*.

4. Database survey

The Cambridge Crystallographic Database (version 5.40, including updates up to May 2019; Groom *et al.*, 2016) was

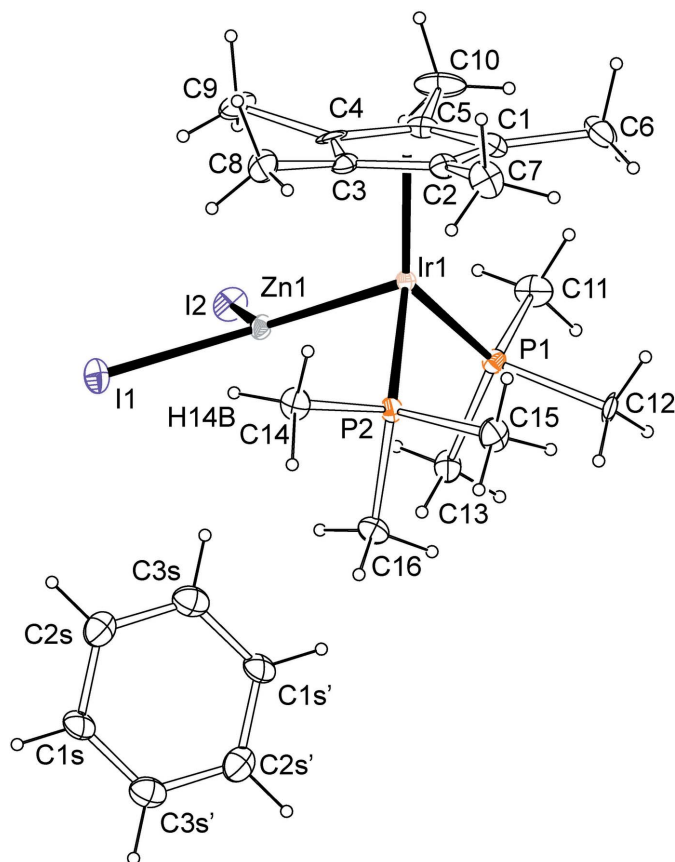


Figure 1
A view of the molecular structure of [Cp*(PMe₃)₂Ir]-[ZnI₂] and its benzene solvate molecule. Anisotropic displacement ellipsoids in this plot, generated with ORTEP-3 for Windows (Farrugia, 2012), are shown at the 30% level. The benzene molecule lies on a crystallographic twofold axis – atoms bearing primed labels are generated by symmetry.

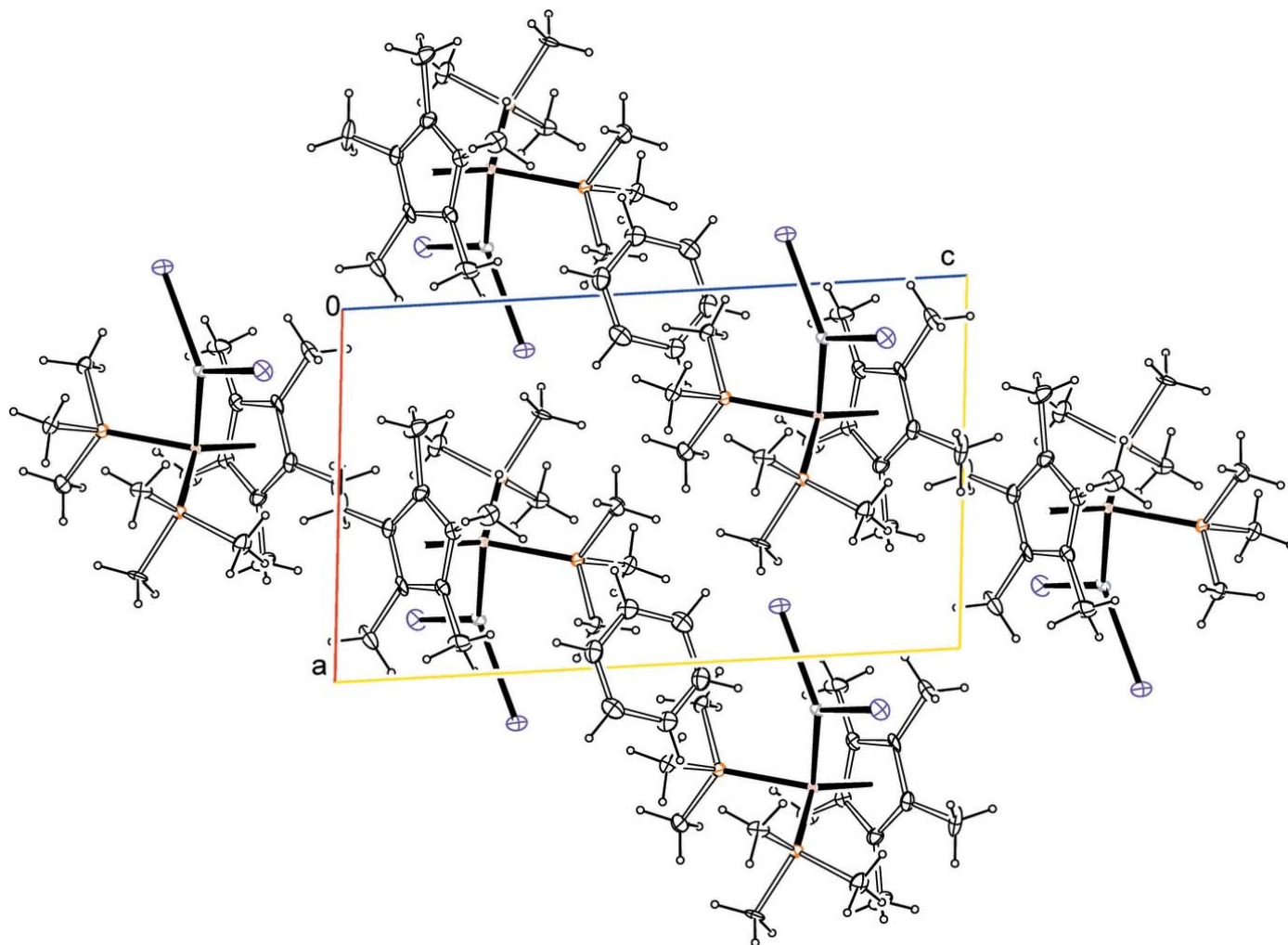


Figure 2
Packing of molecules of $[\text{Cp}^*(\text{PMe}_3)_2\text{Ir}]\text{-}[\text{ZnI}_2]$ and benzene solvate molecules, viewed along the b axis.

searched. No example of an unsupported iridium–zinc bond was found, using the substructure Ir–Zn (any bond). Only one structure was found, namely a structure that contains a bridging zinc dihalide, as discussed under *Chemical context* (Kimura *et al.*, 2012).

5. Synthesis and crystallization

The synthesis was performed using air-free conditions, solvents were dried over Na/benzophenone, $[\text{Cp}^*\text{IrI}_2]_2$ was purchased from Sigma Aldrich, 2-Ad₂Zn was synthesized according to literature (Armstrong *et al.*, 2017). $[\text{Cp}^*(\text{PMe}_3)_2\text{Ir}]\text{-}[\text{ZnI}_2]$ was obtained *via* reduction of $\text{Cp}^*(\text{PMe}_3)_2\text{IrI}_2$ with 2-Ad₂Zn. $\text{Cp}^*(\text{PMe}_3)_2\text{IrI}_2$ was generated *in situ* *via* reaction of 50 mg of $[\text{Cp}^*\text{IrI}_2]_2$ (0.04 mmol) with two equivalents of PMe_3 (added as a 1 M PMe_3 solution in THF, 100 μL , 0.1 mmol) over 1 h of stirring at room temperature. Next, 30 mg (0.08 mmol) of 2-Ad₂Zn were added to the reaction mixture, and the reaction was allowed to proceed overnight with stirring at room temperature, resulting in a

yellow solution and yellow precipitate. The solution layer was decanted into a round-bottom flask, and dried *in vacuo* to yield a yellow solid, which was extracted with C_6H_6 forming a colorless solution, with some precipitate forming over time. The colorless crystals of $[\text{Cp}^*(\text{PMe}_3)_2\text{Ir}]\text{-}[\text{ZnI}_2]$ grew out of the benzene solution *via* slow evaporation at room temperature.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The crystal studied was a twin by non-merohedry with a twin transformation matrix of 1.00 0.00 0.00, $-0.90 - 1.00$ 0.00, 0.06 0.00 $- 1.00$ and a refined BASF parameter of 0.223 (1). The *TWINABS* (Bruker, 2012) function in *APEX2* (Bruker, 2014) was used to de-twin the data. U^{ij} components of ADPs for atoms C1 through C5 were restrained to be similar to each other (SIMU 0.01 command of *SHELXL*).

Table 1
Experimental details.

Crystal data	
Chemical formula	[IrZnI ₂ (C ₁₀ H ₁₅)(C ₃ H ₉ P) ₂]-0.5C ₆ H ₆
<i>M_r</i>	837.79
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.5353 (7), 10.1962 (8), 14.6331 (10)
α , β , γ (°)	95.975 (2), 91.255 (2), 114.847 (2)
<i>V</i> (Å ³)	1280.58 (16)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	8.67
Crystal size (mm)	0.22 × 0.03 × 0.02
Data collection	
Diffractometer	Bruker Kappa <i>APEX</i> DUO CCD
Absorption correction	Multi-scan (<i>TWINABS</i> ; Bruker, 2012)
<i>T</i> _{min} , <i>T</i> _{max}	0.560, 0.746
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	56694, 5865, 4967
<i>R</i> _{int}	0.056
(sin θ /λ) _{max} (Å ⁻¹)	0.651
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.040, 0.116, 1.13
No. of reflections	5865
No. of parameters	238
No. of restraints	30
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	1.81, -1.66

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT* (Sheldrick, 2015a), *SHELXL2016* (Sheldrick, 2015b), *PLATON* (Spek, 2009) and *SHELXTL* (Sheldrick, 2008).

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Acta Cryst. (2019). E75, 1824-1827 [https://doi.org/10.1107/S2056989019014622]

An iridium complex with an unsupported Ir—Zn bond: diiodido(η^5 -pentamethylcyclopentadienyl)bis(trimethylphosphane)iridiumzinc(Ir—Zn) benzene hemisolvate

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Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *APEX2* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015b); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Diiodido(η^5 -pentamethylcyclopentadienyl)bis(trimethylphosphane)\ iridiumzinc(Ir—Zn) benzene hemisolvate

Crystal data

$[\text{IrZnI}_2(\text{C}_{10}\text{H}_{15})(\text{C}_3\text{H}_9\text{P})_2] \cdot 0.5\text{C}_6\text{H}_6$

$M_r = 837.79$

Triclinic, $P\bar{1}$

$a = 9.5353$ (7) Å

$b = 10.1962$ (8) Å

$c = 14.6331$ (10) Å

$\alpha = 95.975$ (2)°

$\beta = 91.255$ (2)°

$\gamma = 114.847$ (2)°

$V = 1280.58$ (16) Å³

$Z = 2$

$F(000) = 786$

$D_x = 2.173$ Mg m⁻³

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

Cell parameters from 9876 reflections

$\theta = 2.2$ – 27.5 °

$\mu = 8.66$ mm⁻¹

$T = 150$ K

Needle, colourless

$0.22 \times 0.03 \times 0.02$ mm

Data collection

Bruker Kappa APEX DUO CCD
diffractometer

Radiation source: sealed tube with Bruker
Triumph monochromator

φ and ω scans

Absorption correction: multi-scan
(*TWINABS*; Bruker, 2012)

$T_{\min} = 0.560$, $T_{\max} = 0.746$

56694 measured reflections

5865 independent reflections

4967 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.056$

$\theta_{\max} = 27.6$ °, $\theta_{\min} = 1.4$ °

$h = -12 \rightarrow 12$

$k = -13 \rightarrow 13$

$l = 0 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.116$

$S = 1.13$

5865 reflections

238 parameters

30 restraints

Primary atom site location: structure-invariant
direct methods

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2 + 11.6185P]$$

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

$$\Delta\rho_{\max} = 1.81 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -1.66 \text{ e } \text{\AA}^{-3}$$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refined as a 2-component twin

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ir1	0.64620 (4)	0.30438 (4)	0.23280 (2)	0.01416 (10)
Zn1	0.85316 (12)	0.54793 (12)	0.22619 (7)	0.0182 (2)
I1	1.13849 (8)	0.64673 (8)	0.29085 (5)	0.03107 (17)
I2	0.84656 (9)	0.74030 (8)	0.12668 (5)	0.03387 (18)
P1	0.4792 (3)	0.4076 (3)	0.25762 (17)	0.0184 (5)
P2	0.7072 (3)	0.3167 (3)	0.38389 (16)	0.0184 (5)
C1	0.5046 (12)	0.1007 (11)	0.1315 (7)	0.028 (2)
C2	0.6108 (11)	0.0698 (10)	0.1844 (7)	0.0216 (18)
C3	0.7631 (12)	0.1679 (11)	0.1690 (7)	0.0224 (18)
C4	0.7521 (13)	0.2568 (12)	0.1035 (7)	0.027 (2)
C5	0.5942 (13)	0.2200 (11)	0.0809 (6)	0.0260 (19)
C6	0.3309 (13)	0.0135 (13)	0.1213 (9)	0.039 (3)
H6A	0.302415	-0.058383	0.066236	0.059*
H6B	0.280848	0.079058	0.115315	0.059*
H6C	0.296607	-0.036785	0.175766	0.059*
C7	0.5730 (14)	-0.0549 (12)	0.2404 (9)	0.036 (3)
H7A	0.587149	-0.134379	0.204256	0.054*
H7B	0.465243	-0.089402	0.256554	0.054*
H7C	0.642101	-0.022047	0.296775	0.054*
C8	0.9134 (13)	0.1610 (14)	0.1988 (9)	0.038 (3)
H8A	0.951864	0.122296	0.145845	0.056*
H8B	0.894569	0.097313	0.247218	0.056*
H8C	0.990738	0.259090	0.222445	0.056*
C9	0.8854 (16)	0.3580 (13)	0.0514 (8)	0.042 (3)
H9A	0.891465	0.304718	-0.007005	0.064*
H9B	0.983291	0.391807	0.088981	0.064*
H9C	0.866425	0.442011	0.038967	0.064*
C10	0.5338 (18)	0.2725 (17)	0.0030 (8)	0.049 (4)
H10A	0.561866	0.237987	-0.055749	0.074*
H10B	0.579434	0.379230	0.011319	0.074*
H10C	0.420718	0.234441	0.002733	0.074*
C11	0.3809 (14)	0.4250 (14)	0.1551 (8)	0.035 (3)
H11A	0.305145	0.462747	0.173110	0.053*
H11B	0.327569	0.329362	0.118423	0.053*
H11C	0.457013	0.492346	0.118469	0.053*

C12	0.3114 (11)	0.3065 (12)	0.3218 (8)	0.026 (2)
H12A	0.237710	0.350330	0.319995	0.040*
H12B	0.346343	0.310499	0.385961	0.040*
H12C	0.260818	0.204706	0.293688	0.040*
C13	0.5420 (12)	0.5912 (11)	0.3179 (8)	0.028 (2)
H13A	0.451169	0.609824	0.330705	0.042*
H13B	0.608472	0.662236	0.279284	0.042*
H13C	0.600217	0.600006	0.375988	0.042*
C14	0.8854 (12)	0.2999 (13)	0.4124 (7)	0.027 (2)
H14A	0.905137	0.313444	0.479545	0.041*
H14B	0.972012	0.374360	0.385704	0.041*
H14C	0.874887	0.203020	0.387452	0.041*
C15	0.5697 (13)	0.1720 (12)	0.4447 (7)	0.034 (3)
H15A	0.609739	0.184805	0.508784	0.051*
H15B	0.556651	0.076787	0.414398	0.051*
H15C	0.469393	0.177272	0.443155	0.051*
C16	0.7304 (13)	0.4736 (11)	0.4657 (7)	0.029 (2)
H16A	0.772321	0.465670	0.525593	0.043*
H16B	0.629520	0.476117	0.472535	0.043*
H16C	0.801849	0.563231	0.442954	0.043*
C1S	1.1540 (14)	1.0646 (12)	0.5329 (8)	0.033 (3)
H1S	1.259917	1.108754	0.555309	0.040*
C2S	1.1106 (14)	0.9857 (13)	0.4464 (9)	0.037 (3)
H2S	1.186666	0.975586	0.409107	0.045*
C3S	0.9552 (14)	0.9211 (13)	0.4139 (8)	0.037 (3)
H3S	0.925314	0.866769	0.354327	0.045*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ir1	0.01386 (16)	0.01348 (16)	0.01504 (16)	0.00549 (13)	0.00113 (12)	0.00274 (11)
Zn1	0.0172 (5)	0.0147 (5)	0.0226 (5)	0.0060 (4)	0.0056 (4)	0.0042 (4)
I1	0.0205 (3)	0.0307 (4)	0.0406 (4)	0.0092 (3)	0.0000 (3)	0.0061 (3)
I2	0.0403 (4)	0.0313 (4)	0.0366 (4)	0.0197 (3)	0.0079 (3)	0.0114 (3)
P1	0.0175 (12)	0.0213 (12)	0.0192 (12)	0.0108 (10)	0.0015 (9)	0.0038 (9)
P2	0.0168 (11)	0.0198 (12)	0.0172 (11)	0.0058 (9)	0.0004 (9)	0.0057 (9)
C1	0.025 (4)	0.025 (4)	0.026 (4)	0.007 (4)	-0.003 (4)	-0.007 (4)
C2	0.028 (4)	0.014 (4)	0.024 (4)	0.011 (3)	0.003 (3)	0.003 (3)
C3	0.030 (4)	0.018 (4)	0.021 (4)	0.012 (3)	0.007 (3)	-0.002 (3)
C4	0.036 (5)	0.028 (4)	0.015 (4)	0.015 (4)	0.012 (3)	-0.007 (3)
C5	0.035 (4)	0.027 (4)	0.017 (4)	0.016 (4)	-0.001 (3)	-0.003 (3)
C6	0.030 (6)	0.031 (6)	0.052 (8)	0.014 (5)	-0.012 (5)	-0.017 (5)
C7	0.042 (7)	0.022 (6)	0.046 (7)	0.013 (5)	0.000 (5)	0.013 (5)
C8	0.026 (6)	0.036 (7)	0.055 (8)	0.021 (5)	0.005 (5)	-0.007 (6)
C9	0.057 (8)	0.030 (6)	0.034 (7)	0.011 (6)	0.027 (6)	0.004 (5)
C10	0.086 (11)	0.061 (9)	0.016 (6)	0.049 (8)	-0.010 (6)	-0.004 (6)
C11	0.043 (7)	0.044 (7)	0.032 (6)	0.033 (6)	-0.007 (5)	0.003 (5)
C12	0.011 (4)	0.028 (6)	0.037 (6)	0.005 (4)	0.013 (4)	0.005 (4)

C13	0.024 (5)	0.017 (5)	0.045 (7)	0.011 (4)	0.005 (4)	0.003 (4)
C14	0.027 (5)	0.036 (6)	0.026 (5)	0.017 (5)	-0.003 (4)	0.012 (4)
C15	0.033 (6)	0.034 (6)	0.029 (5)	0.006 (5)	0.005 (4)	0.014 (5)
C16	0.031 (6)	0.030 (5)	0.023 (5)	0.012 (5)	-0.004 (4)	0.000 (4)
C1S	0.036 (6)	0.018 (5)	0.041 (7)	0.009 (5)	0.000 (5)	-0.006 (5)
C2S	0.040 (7)	0.026 (6)	0.047 (7)	0.014 (5)	0.015 (5)	0.010 (5)
C3S	0.048 (8)	0.031 (6)	0.030 (6)	0.015 (5)	0.000 (5)	0.004 (4)

Geometric parameters (Å, °)

Ir1—P2	2.251 (2)	C8—H8B	0.9800
Ir1—C5	2.264 (9)	C8—H8C	0.9800
Ir1—P1	2.265 (2)	C9—H9A	0.9800
Ir1—C3	2.265 (9)	C9—H9B	0.9800
Ir1—C4	2.267 (9)	C9—H9C	0.9800
Ir1—C1	2.291 (10)	C10—H10A	0.9800
Ir1—C2	2.301 (9)	C10—H10B	0.9800
Ir1—Zn1	2.4516 (11)	C10—H10C	0.9800
Zn1—I2	2.5819 (13)	C11—H11A	0.9800
Zn1—I1	2.5880 (13)	C11—H11B	0.9800
P1—C11	1.815 (11)	C11—H11C	0.9800
P1—C13	1.825 (11)	C12—H12A	0.9800
P1—C12	1.840 (10)	C12—H12B	0.9800
P2—C14	1.822 (10)	C12—H12C	0.9800
P2—C16	1.826 (10)	C13—H13A	0.9800
P2—C15	1.840 (10)	C13—H13B	0.9800
C1—C2	1.417 (14)	C13—H13C	0.9800
C1—C5	1.449 (15)	C14—H14A	0.9800
C1—C6	1.510 (15)	C14—H14B	0.9800
C2—C3	1.414 (14)	C14—H14C	0.9800
C2—C7	1.504 (14)	C15—H15A	0.9800
C3—C4	1.417 (15)	C15—H15B	0.9800
C3—C8	1.521 (15)	C15—H15C	0.9800
C4—C5	1.412 (15)	C16—H16A	0.9800
C4—C9	1.538 (15)	C16—H16B	0.9800
C5—C10	1.509 (15)	C16—H16C	0.9800
C6—H6A	0.9800	C1S—C3S ⁱ	1.360 (17)
C6—H6B	0.9800	C1S—C2S	1.381 (17)
C6—H6C	0.9800	C1S—H1S	0.9500
C7—H7A	0.9800	C2S—C3S	1.393 (18)
C7—H7B	0.9800	C2S—H2S	0.9500
C7—H7C	0.9800	C3S—H3S	0.9500
C8—H8A	0.9800		
P2—Ir1—C5	160.3 (3)	C1—C6—H6B	109.5
P2—Ir1—P1	93.81 (9)	H6A—C6—H6B	109.5
C5—Ir1—P1	102.1 (3)	C1—C6—H6C	109.5
P2—Ir1—C3	101.5 (3)	H6A—C6—H6C	109.5

C5—Ir1—C3	61.2 (4)	H6B—C6—H6C	109.5
P1—Ir1—C3	162.4 (3)	C2—C7—H7A	109.5
P2—Ir1—C4	133.0 (3)	C2—C7—H7B	109.5
C5—Ir1—C4	36.3 (4)	H7A—C7—H7B	109.5
P1—Ir1—C4	131.8 (3)	C2—C7—H7C	109.5
C3—Ir1—C4	36.4 (4)	H7A—C7—H7C	109.5
P2—Ir1—C1	127.8 (3)	H7B—C7—H7C	109.5
C5—Ir1—C1	37.1 (4)	C3—C8—H8A	109.5
P1—Ir1—C1	103.0 (3)	C3—C8—H8B	109.5
C3—Ir1—C1	60.6 (4)	H8A—C8—H8B	109.5
C4—Ir1—C1	60.6 (4)	C3—C8—H8C	109.5
P2—Ir1—C2	99.7 (3)	H8A—C8—H8C	109.5
C5—Ir1—C2	60.8 (4)	H8B—C8—H8C	109.5
P1—Ir1—C2	132.8 (3)	C4—C9—H9A	109.5
C3—Ir1—C2	36.1 (4)	C4—C9—H9B	109.5
C4—Ir1—C2	60.1 (4)	H9A—C9—H9B	109.5
C1—Ir1—C2	36.0 (4)	C4—C9—H9C	109.5
P2—Ir1—Zn1	91.35 (7)	H9A—C9—H9C	109.5
C5—Ir1—Zn1	100.5 (3)	H9B—C9—H9C	109.5
P1—Ir1—Zn1	88.74 (7)	C5—C10—H10A	109.5
C3—Ir1—Zn1	99.4 (3)	C5—C10—H10B	109.5
C4—Ir1—Zn1	80.8 (3)	H10A—C10—H10B	109.5
C1—Ir1—Zn1	137.2 (3)	C5—C10—H10C	109.5
C2—Ir1—Zn1	135.3 (2)	H10A—C10—H10C	109.5
Ir1—Zn1—I2	126.73 (5)	H10B—C10—H10C	109.5
Ir1—Zn1—I1	127.19 (5)	P1—C11—H11A	109.5
I2—Zn1—I1	105.11 (4)	P1—C11—H11B	109.5
C11—P1—C13	99.5 (5)	H11A—C11—H11B	109.5
C11—P1—C12	100.2 (6)	P1—C11—H11C	109.5
C13—P1—C12	100.5 (5)	H11A—C11—H11C	109.5
C11—P1—Ir1	115.7 (4)	H11B—C11—H11C	109.5
C13—P1—Ir1	121.9 (3)	P1—C12—H12A	109.5
C12—P1—Ir1	115.6 (4)	P1—C12—H12B	109.5
C14—P2—C16	100.7 (5)	H12A—C12—H12B	109.5
C14—P2—C15	100.1 (5)	P1—C12—H12C	109.5
C16—P2—C15	98.6 (5)	H12A—C12—H12C	109.5
C14—P2—Ir1	115.9 (4)	H12B—C12—H12C	109.5
C16—P2—Ir1	121.8 (3)	P1—C13—H13A	109.5
C15—P2—Ir1	116.2 (4)	P1—C13—H13B	109.5
C2—C1—C5	107.5 (9)	H13A—C13—H13B	109.5
C2—C1—C6	125.9 (10)	P1—C13—H13C	109.5
C5—C1—C6	126.3 (10)	H13A—C13—H13C	109.5
C2—C1—Ir1	72.4 (6)	H13B—C13—H13C	109.5
C5—C1—Ir1	70.4 (5)	P2—C14—H14A	109.5
C6—C1—Ir1	127.9 (8)	P2—C14—H14B	109.5
C3—C2—C1	108.6 (9)	H14A—C14—H14B	109.5
C3—C2—C7	124.2 (9)	P2—C14—H14C	109.5
C1—C2—C7	126.9 (10)	H14A—C14—H14C	109.5

C3—C2—Ir1	70.6 (5)	H14B—C14—H14C	109.5
C1—C2—Ir1	71.7 (6)	P2—C15—H15A	109.5
C7—C2—Ir1	128.4 (8)	P2—C15—H15B	109.5
C2—C3—C4	107.8 (9)	H15A—C15—H15B	109.5
C2—C3—C8	127.2 (10)	P2—C15—H15C	109.5
C4—C3—C8	123.8 (10)	H15A—C15—H15C	109.5
C2—C3—Ir1	73.3 (5)	H15B—C15—H15C	109.5
C4—C3—Ir1	71.9 (5)	P2—C16—H16A	109.5
C8—C3—Ir1	130.4 (7)	P2—C16—H16B	109.5
C5—C4—C3	109.0 (9)	H16A—C16—H16B	109.5
C5—C4—C9	123.7 (11)	P2—C16—H16C	109.5
C3—C4—C9	126.4 (10)	H16A—C16—H16C	109.5
C5—C4—Ir1	71.7 (5)	H16B—C16—H16C	109.5
C3—C4—Ir1	71.7 (5)	C3S ⁱ —C1S—C2S	119.9 (11)
C9—C4—Ir1	130.9 (7)	C3S ⁱ —C1S—H1S	120.0
C4—C5—C1	107.0 (9)	C2S—C1S—H1S	120.0
C4—C5—C10	125.0 (11)	C1S—C2S—C3S	119.9 (11)
C1—C5—C10	126.6 (11)	C1S—C2S—H2S	120.1
C4—C5—Ir1	72.0 (5)	C3S—C2S—H2S	120.1
C1—C5—Ir1	72.5 (5)	C1S ⁱ —C3S—C2S	120.2 (11)
C10—C5—Ir1	131.1 (8)	C1S ⁱ —C3S—H3S	119.9
C1—C6—H6A	109.5	C2S—C3S—H3S	119.9
C5—C1—C2—C3	0.8 (11)	Ir1—C3—C4—C9	127.8 (10)
C6—C1—C2—C3	174.3 (10)	C2—C3—C4—Ir1	65.0 (7)
Ir1—C1—C2—C3	-61.2 (7)	C8—C3—C4—Ir1	-127.0 (10)
C5—C1—C2—C7	-173.2 (10)	C3—C4—C5—C1	-2.1 (10)
C6—C1—C2—C7	0.3 (17)	C9—C4—C5—C1	168.1 (10)
Ir1—C1—C2—C7	124.7 (11)	Ir1—C4—C5—C1	-64.5 (7)
C5—C1—C2—Ir1	62.1 (7)	C3—C4—C5—C10	-169.6 (10)
C6—C1—C2—Ir1	-124.5 (11)	C9—C4—C5—C10	0.6 (15)
C1—C2—C3—C4	-2.1 (11)	Ir1—C4—C5—C10	128.0 (10)
C7—C2—C3—C4	172.1 (10)	C3—C4—C5—Ir1	62.4 (6)
Ir1—C2—C3—C4	-64.1 (7)	C9—C4—C5—Ir1	-127.4 (10)
C1—C2—C3—C8	-169.6 (10)	C2—C1—C5—C4	0.8 (11)
C7—C2—C3—C8	4.6 (16)	C6—C1—C5—C4	-172.6 (10)
Ir1—C2—C3—C8	128.5 (10)	Ir1—C1—C5—C4	64.2 (6)
C1—C2—C3—Ir1	61.9 (7)	C2—C1—C5—C10	168.1 (10)
C7—C2—C3—Ir1	-123.9 (10)	C6—C1—C5—C10	-5.4 (17)
C2—C3—C4—C5	2.7 (11)	Ir1—C1—C5—C10	-128.6 (11)
C8—C3—C4—C5	170.7 (9)	C2—C1—C5—Ir1	-63.4 (7)
Ir1—C3—C4—C5	-62.4 (6)	C6—C1—C5—Ir1	123.2 (11)
C2—C3—C4—C9	-167.2 (10)	C3S ⁱ —C1S—C2S—C3S	0 (2)
C8—C3—C4—C9	0.8 (16)	C1S—C2S—C3S—C1S ⁱ	0 (2)

Symmetry code: (i) $-x+2, -y+2, -z+1$.