

# Crystal structure of chlorido( $\eta^2$ -phenyl isothiocyanate- $\kappa^2C,S$ )-*mer*-tris(trimethylphosphane- $\kappa P$ )-iridium(I)

Joseph S. Merola\* and Arthur W. Grieb

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Department of Chemistry 0212, Virginia Tech, Blacksburg, VA 24061, USA. \*Correspondence e-mail: jmerola@vt.edu

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The molecule of the title compound,  $[\text{IrCl}(\text{C}_7\text{H}_5\text{NS})(\text{C}_3\text{H}_9\text{P})_3]$ , is a distorted octahedral iridium complex with three  $\text{PMe}_3$  ligands arranged in a meridional geometry, a chloride ion *cis* to all three  $\text{PMe}_3$  groups and the phenyl isothiocyanate ligand bonded in an  $\eta^2$ -fashion through the C and S atoms. The C atom is *trans* to the chloride ion and the S atom is responsible for a significant deviation from an ideal octahedral geometry. The geometric parameters for the metal-complexing phenyl isothiocyanate group are compared with other metal-complexed phenyl isothiocyanates, as well as with examples of uncomplexed aryl isothiocyanates.

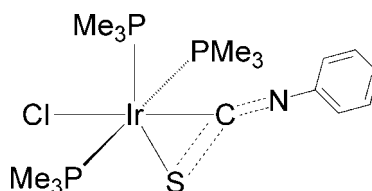
**Keywords:** crystal structure; iridium complex; phenyl isothiocyanate

CCDC reference: 1027097

**Supporting information:** this article has supporting information at journals.iucr.org/e

## 1. Chemical context

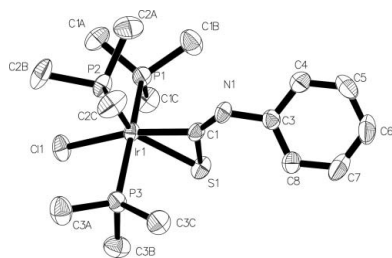
Various phenyl isothiocyanate complexes of metals have been characterized, all showing the effect of complexation of lengthening of N—C and C—S bonds and the bending of the N—C—S angle away from linearity. Complexation of an aryl isothiocyanate to a metal has a similar effect across a wide range of metal systems with the N—C bond length averaging about 1.26 Å, the C—S distance averaging about 1.74 Å and the N—C—S bond angle ranging from 137 to 142°.



## 2. Structural commentary

The molecule of the title iridium compound has a distorted octahedral coordination sphere with three  $\text{PMe}_3$  ligands arranged in a meridional geometry, a chloride ion *cis* to all three  $\text{PMe}_3$  groups and the phenyl isothiocyanate bonded in an  $\eta^2$  fashion to the C and S atoms (Fig. 1). The C atom is *trans* to the chloride ion and the S atom is significantly off from an ideal octahedral geometry [the P2—Ir1—S1 angle is 144.51 (5)° instead of the expected angle near 180°].

Upon complexation to the iridium cation in the title compound, the N—C bond in phenyl isothiocyanate lengthens to 1.256 (7) Å, the C—S bond lengthens to 1.757 (6) Å and the N—C—S bond angle bends to 137.2 (4)°. These significant changes in geometry reflect the normal consequences of  $\pi$ -bonding of the C—S  $\pi$ -electrons to the metal and  $\pi$ -back-bonding from the metal to the  $\pi^*$ -orbitals of the ligand.



**Table 1**

 Comparison of bond lengths and angles ( $\text{\AA}$ ,  $^\circ$ ) for the SCN moiety of isothiocyanate complexes.

Compound	CCDC refcode	N—C	C—S	N—C—S	Reference
<b>Not complexing to a metal</b>					
Average of 16 compounds		1.16	1.57	176	Groom & Allen (2014)
C <sub>29</sub> H <sub>16</sub> N <sub>4</sub> S <sub>4</sub>	221549	1.152 (5)	1.566 (4)	175.7 (3)	Laliberté <i>et al.</i> (2004)
C <sub>21</sub> H <sub>23</sub> N <sub>1</sub> O <sub>2</sub> S <sub>1</sub>	673469	1.174 (3)	1.584 (3)	177.6 (3)	Majewska <i>et al.</i> (2008)
C <sub>24</sub> H <sub>37</sub> N <sub>1</sub> S <sub>1</sub>	637960	1.134 (7)	1.543 (6)	176.1 (5)	Biswas <i>et al.</i> (2007)
C <sub>21</sub> H <sub>21</sub> N <sub>1</sub> O <sub>1</sub> S <sub>1</sub>	646594	1.167 (4)	1.587 (4)	178.8 (3)	Majewska <i>et al.</i> (2007)
<b>Complexing to a metal</b>					
C <sub>48</sub> H <sub>44</sub> N <sub>1</sub> Ni <sub>1</sub> P <sub>3</sub> S	555280	1.26 (3)	1.68 (3)	142 (2)	Bianchini <i>et al.</i> (1984)
C <sub>49</sub> H <sub>47</sub> Co <sub>1</sub> N <sub>2</sub> P <sub>3</sub> S	555508	1.27 (2)	1.72 (1)	141 (1)	Bianchini <i>et al.</i> (1984)
C <sub>27</sub> H <sub>35</sub> N <sub>1</sub> S <sub>1</sub> V <sub>1</sub>	557730	1.265 (9)	1.745 (7)	138.6 (6)	Gambarotta <i>et al.</i> (1984)
C <sub>70</sub> H <sub>63</sub> Mo <sub>1</sub> N <sub>3</sub> P <sub>4</sub> S <sub>2</sub>	257394	1.256 (7)	1.737 (5)	134.9 (4)	Ohnishi <i>et al.</i> (2005)
C <sub>25</sub> H <sub>47</sub> ClN <sub>2</sub> O <sub>1</sub> Os <sub>1</sub> P <sub>2</sub> S <sub>1</sub>	661980	1.253 (7)	1.764 (6)	141.2 (4)	Flügel <i>et al.</i> (1996)
C <sub>16</sub> H <sub>32</sub> N <sub>1</sub> Ni <sub>1</sub> P <sub>3</sub> S	850129	1.253 (3)	1.707 (2)	142.2 (2)	Huang <i>et al.</i> (2013)
C <sub>16</sub> H <sub>32</sub> Cl <sub>1</sub> Ir <sub>1</sub> N <sub>1</sub> P <sub>3</sub> S <sub>1</sub>	1027097	1.256 (7)	1.757 (6)	137.2 (4)	This work

### 3. Database survey

A search of the Cambridge Crystallographic Database (Groom & Allen, 2014) on 28 January 2014 found 16 aryl isothiocyanates in which the SCN group is not disordered on coordinating to a metal. All of those structures display a nearly linear N—C—S geometry (ranging from 174–179° with an average of 176°). The multiply bonded nature of both the C—S and C—N bonds is seen in the bond lengths. For C—N, the distances range from 1.14 to 1.17  $\text{\AA}$  with an average of 1.16  $\text{\AA}$  and the C—S distances range from 1.54 to 1.59  $\text{\AA}$  with an average of 1.57  $\text{\AA}$ . Of those 16, four structures of good precision with no disorder, ionic interactions or other complex interactions that could affect the geometry of the N—C—S group were chosen for comparison to contrast ‘free’ *versus* ‘complexed’ isothiocyanates. The first entry in Table 1 shows the average values for all 16 structures, the next four entries are the specific non-complexed aryl isothiocyanates, the next six entries are other examples from the CCDC in which phenyl isothiocyanate is complexed to a metal and the last entry is the data from the title compound. For the structures of several uncomplexed aryl isothiocyanates, see: Majewska *et al.* (2007, 2008); Laliberté *et al.* (2004); Biswas *et al.* (2007). For the

structures of a cobalt and a nickel complex of phenyl isothiocyanate, see: Bianchini *et al.* (1984). For the structure of a vanadium complex of phenyl isothiocyanate see: Gambarotta *et al.* (1984). For a phenyl isothiocyanate complex of molybdenum, see: Ohnishi *et al.* (2005). For a phenyl isothiocyanate complex of osmium, see: Flügel *et al.* (1996). For a tris-trimethylphosphine nickel complex of phenyl isothiocyanate, see: Huang *et al.* (2013).

### 4. Synthesis and crystallization

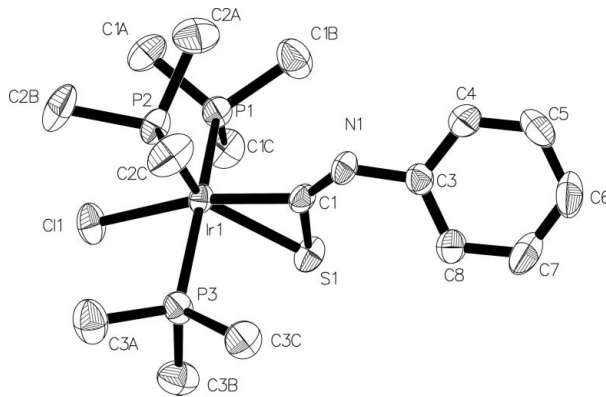
The crystal used in this experiment was obtained from a reaction between  $[\text{Ir}(\text{COD})(\text{PMe}_3)_3]\text{Cl}$  (COD = 1,5-cyclo-

**Table 2**

Experimental details.

Crystal data	
Chemical formula	$[\text{IrCl}(\text{C}_7\text{H}_5\text{NS})(\text{C}_3\text{H}_9\text{P})_3]$
$M_r$	591.05
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
$a, b, c$ ( $\text{\AA}$ )	8.964 (2), 27.074 (7), 9.721 (2)
$\beta$ ( $^\circ$ )	102.054 (19)
$V$ ( $\text{\AA}^3$ )	2307.3 (10)
$Z$	4
Radiation type	Mo $K\alpha$
$\mu$ ( $\text{mm}^{-1}$ )	6.20
Crystal size (mm)	0.3 $\times$ 0.2 $\times$ 0.2
Data collection	
Diffractometer	Siemens P4
Absorption correction	$\psi$ scan (North <i>et al.</i> , 1968)
$T_{\text{min}}, T_{\text{max}}$	0.757, 0.891
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	5294, 5294, 4133
$(\sin \theta/\lambda)_{\text{max}}$ ( $\text{\AA}^{-1}$ )	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.031, 0.080, 0.93
No. of reflections	5294
No. of parameters	218
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ ( $\text{e \AA}^{-3}$ )	1.00, -1.19

Computer programs: XSCANS (Siemens, 1994), SHELXTL and SHELXS97 (Sheldrick, 2008), SHELXL97 (Sheldrick, 2008), and OLEX2 (Dolomanov *et al.*, 2009).


**Figure 1**

Displacement ellipsoid drawing of the title compound. Ellipsoids are drawn at the 50% probability level and hydrogen atoms are omitted for clarity.

octadiene) and phenyl isothiocyanate in toluene solution. Suitable single crystals were grown from dichloromethane by the layering of diethyl ether.

### 5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were placed at calculated positions and refined using a model in which the hydrogen rides on the atom to which it is attached. For methyl hydrogen atoms  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  and for the phenyl hydrogen atoms,  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

### Acknowledgements

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## supporting information

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## Crystal structure of chlorido( $\eta^2$ -phenyl isothiocyanate- $\kappa^2C,S$ )-*mer*-tris(trimethylphosphane- $\kappa P$ )iridium(I)

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### Computing details

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS* (Siemens, 1994); data reduction: *SHELXTL* (Sheldrick, 2008); 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).

### Chlorido( $\eta^2$ -phenyl isothiocyanate- $\kappa^2C,S$ )-*mer*-tris(trimethylphosphane- $\kappa P$ )iridium(I)

#### Crystal data

[IrCl(C<sub>7</sub>H<sub>5</sub>NS)(C<sub>3</sub>H<sub>9</sub>P)<sub>3</sub>]

$M_r = 591.05$

Monoclinic,  $P2_1/n$

$a = 8.964$  (2) Å

$b = 27.074$  (7) Å

$c = 9.721$  (2) Å

$\beta = 102.054$  (19)°

$V = 2307.3$  (10) Å<sup>3</sup>

$Z = 4$

$F(000) = 1160$

$D_x = 1.701$  Mg m<sup>-3</sup>

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

Cell parameters from 45 reflections

$\theta = 2-22^\circ$

$\mu = 6.20$  mm<sup>-1</sup>

$T = 293$  K

Prism, yellow

$0.3 \times 0.2 \times 0.2$  mm

#### Data collection

Siemens P4

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega$  scans

Absorption correction:  $\psi$  scan

(North *et al.*, 1968)

$T_{\min} = 0.757$ ,  $T_{\max} = 0.891$

5294 measured reflections

5294 independent reflections

4133 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.0000$

$\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 2.3^\circ$

$h = -11 \rightarrow 11$

$k = 0 \rightarrow 35$

$l = 0 \rightarrow 12$

2 standard reflections every 400 reflections

intensity decay: 0.0 (1)

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.080$

$S = 0.93$

5294 reflections

218 parameters

0 restraints

Primary atom site location: heavy-atom method

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 1.00$  e Å<sup>-3</sup>

$$\Delta\rho_{\min} = -1.19 \text{ e } \text{\AA}^{-3}$$

Extinction correction: *SHELXL97* (Sheldrick, 2008),  $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.00040 (9)

### 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.

**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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ir1	0.43752 (2)	0.345208 (7)	0.04153 (2)	0.02506 (7)
Cl1	0.46057 (19)	0.27098 (5)	-0.10524 (16)	0.0442 (4)
P1	0.39424 (18)	0.28837 (5)	0.20883 (16)	0.0331 (3)
P2	0.68593 (17)	0.35657 (5)	0.13576 (17)	0.0352 (3)
P3	0.43328 (19)	0.38958 (5)	-0.16484 (16)	0.0355 (3)
S1	0.17603 (16)	0.37728 (5)	0.03289 (17)	0.0377 (3)
C1A	0.5316 (8)	0.2394 (2)	0.2543 (7)	0.0543 (17)
H1AA	0.5381	0.2210	0.1713	0.082*
H1AB	0.5002	0.2178	0.3213	0.082*
H1AC	0.6296	0.2532	0.2946	0.082*
C1B	0.3641 (9)	0.3133 (2)	0.3741 (7)	0.0578 (19)
H1BA	0.4540	0.3305	0.4207	0.087*
H1BB	0.3430	0.2868	0.4328	0.087*
H1BC	0.2792	0.3357	0.3562	0.087*
C1C	0.2226 (7)	0.2537 (2)	0.1451 (7)	0.0500 (16)
H1CA	0.1409	0.2759	0.1075	0.075*
H1CB	0.1968	0.2352	0.2211	0.075*
H1CC	0.2385	0.2314	0.0727	0.075*
C2A	0.7354 (8)	0.3558 (3)	0.3284 (7)	0.060 (2)
H2AA	0.6775	0.3806	0.3646	0.091*
H2AB	0.8423	0.3624	0.3596	0.091*
H2AC	0.7122	0.3239	0.3618	0.091*
C2B	0.8222 (8)	0.3143 (3)	0.0871 (9)	0.065 (2)
H2BA	0.8001	0.2813	0.1129	0.097*
H2BB	0.9233	0.3232	0.1352	0.097*
H2BC	0.8156	0.3159	-0.0127	0.097*
C2C	0.7610 (8)	0.4167 (2)	0.1038 (8)	0.0579 (19)
H2CA	0.7478	0.4219	0.0043	0.087*
H2CB	0.8676	0.4181	0.1466	0.087*
H2CC	0.7074	0.4418	0.1435	0.087*
C3A	0.5891 (9)	0.3812 (3)	-0.2562 (8)	0.0586 (19)
H3AA	0.6814	0.3943	-0.1998	0.088*

H3AB	0.5660	0.3983	-0.3447	0.088*
H3AC	0.6022	0.3466	-0.2723	0.088*
C3B	0.2699 (8)	0.3716 (2)	-0.2991 (7)	0.0528 (17)
H3BA	0.2793	0.3375	-0.3228	0.079*
H3BB	0.2656	0.3916	-0.3813	0.079*
H3BC	0.1783	0.3761	-0.2642	0.079*
C3C	0.4144 (9)	0.4560 (2)	-0.1565 (7)	0.0536 (18)
H3CA	0.3149	0.4641	-0.1412	0.080*
H3CB	0.4276	0.4704	-0.2435	0.080*
H3CC	0.4907	0.4688	-0.0805	0.080*
C1	0.3493 (6)	0.39985 (18)	0.1318 (6)	0.0295 (11)
N1	0.3916 (5)	0.43280 (15)	0.2224 (5)	0.0330 (10)
C3	0.2897 (6)	0.4657 (2)	0.2672 (6)	0.0336 (12)
C4	0.3135 (9)	0.4781 (2)	0.4081 (7)	0.0576 (19)
H4	0.3936	0.4634	0.4710	0.069*
C5	0.2239 (12)	0.5111 (3)	0.4568 (7)	0.086 (3)
H5	0.2426	0.5181	0.5525	0.103*
C6	0.1056 (10)	0.5344 (3)	0.3676 (8)	0.068 (2)
H6	0.0451	0.5573	0.4018	0.081*
C7	0.0792 (8)	0.5232 (2)	0.2275 (8)	0.0567 (19)
H7	-0.0013	0.5382	0.1658	0.068*
C8	0.1712 (7)	0.4895 (2)	0.1760 (7)	0.0448 (15)
H8	0.1535	0.4829	0.0801	0.054*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ir1	0.02846 (11)	0.01590 (10)	0.03174 (11)	-0.00011 (9)	0.00841 (7)	-0.00018 (8)
Cl1	0.0563 (9)	0.0274 (7)	0.0530 (9)	-0.0037 (6)	0.0206 (7)	-0.0132 (6)
P1	0.0430 (8)	0.0220 (7)	0.0358 (8)	0.0002 (6)	0.0115 (6)	0.0035 (6)
P2	0.0300 (7)	0.0232 (7)	0.0522 (9)	-0.0020 (5)	0.0081 (7)	-0.0023 (6)
P3	0.0502 (9)	0.0229 (7)	0.0355 (8)	-0.0011 (6)	0.0140 (7)	0.0003 (6)
S1	0.0295 (7)	0.0297 (7)	0.0525 (9)	0.0006 (6)	0.0055 (6)	-0.0032 (6)
C1A	0.062 (4)	0.033 (3)	0.066 (4)	0.012 (3)	0.009 (4)	0.014 (3)
C1B	0.093 (6)	0.040 (4)	0.048 (4)	0.004 (4)	0.032 (4)	0.002 (3)
C1C	0.045 (4)	0.043 (4)	0.063 (4)	-0.008 (3)	0.015 (3)	0.006 (3)
C2A	0.053 (4)	0.064 (5)	0.055 (4)	-0.011 (4)	-0.011 (3)	-0.002 (4)
C2B	0.042 (4)	0.058 (5)	0.099 (6)	0.022 (3)	0.025 (4)	0.010 (4)
C2C	0.048 (4)	0.028 (3)	0.090 (5)	-0.012 (3)	-0.003 (4)	0.006 (3)
C3A	0.073 (5)	0.046 (4)	0.067 (5)	-0.001 (4)	0.039 (4)	0.002 (3)
C3B	0.068 (5)	0.043 (4)	0.044 (4)	-0.005 (3)	0.003 (3)	0.003 (3)
C3C	0.083 (5)	0.026 (3)	0.055 (4)	0.004 (3)	0.021 (4)	0.008 (3)
C1	0.033 (3)	0.021 (2)	0.035 (3)	0.006 (2)	0.007 (2)	0.003 (2)
N1	0.033 (2)	0.021 (2)	0.044 (3)	0.0041 (19)	0.007 (2)	-0.0039 (19)
C3	0.040 (3)	0.028 (3)	0.034 (3)	0.002 (2)	0.010 (2)	-0.001 (2)
C4	0.079 (5)	0.049 (4)	0.043 (4)	0.027 (4)	0.008 (4)	0.003 (3)
C5	0.138 (9)	0.090 (6)	0.034 (4)	0.049 (6)	0.029 (5)	-0.001 (4)
C6	0.084 (6)	0.055 (5)	0.073 (5)	0.028 (4)	0.036 (5)	-0.008 (4)

C7	0.043 (4)	0.042 (4)	0.080 (5)	0.016 (3)	0.002 (4)	-0.007 (4)
C8	0.057 (4)	0.033 (3)	0.042 (3)	0.010 (3)	0.006 (3)	-0.007 (3)

*Geometric parameters (Å, °)*

Ir1—C11	2.4982 (14)	C2B—H2BA	0.9600
Ir1—P1	2.3297 (15)	C2B—H2BB	0.9600
Ir1—P2	2.2450 (16)	C2B—H2BC	0.9600
Ir1—P3	2.3319 (15)	C2C—H2CA	0.9600
Ir1—S1	2.4846 (15)	C2C—H2CB	0.9600
Ir1—C1	1.968 (5)	C2C—H2CC	0.9600
P1—C1A	1.801 (6)	C3A—H3AA	0.9600
P1—C1B	1.814 (6)	C3A—H3AB	0.9600
P1—C1C	1.799 (6)	C3A—H3AC	0.9600
P2—C2A	1.832 (7)	C3B—H3BA	0.9600
P2—C2B	1.808 (6)	C3B—H3BB	0.9600
P2—C2C	1.813 (6)	C3B—H3BC	0.9600
P3—C3A	1.819 (6)	C3C—H3CA	0.9600
P3—C3B	1.813 (7)	C3C—H3CB	0.9600
P3—C3C	1.810 (6)	C3C—H3CC	0.9600
S1—C1	1.757 (6)	C1—N1	1.256 (7)
C1A—H1AA	0.9600	N1—C3	1.408 (6)
C1A—H1AB	0.9600	C3—C4	1.383 (8)
C1A—H1AC	0.9600	C3—C8	1.391 (8)
C1B—H1BA	0.9600	C4—H4	0.9300
C1B—H1BB	0.9600	C4—C5	1.351 (9)
C1B—H1BC	0.9600	C5—H5	0.9300
C1C—H1CA	0.9600	C5—C6	1.375 (10)
C1C—H1CB	0.9600	C6—H6	0.9300
C1C—H1CC	0.9600	C6—C7	1.368 (10)
C2A—H2AA	0.9600	C7—H7	0.9300
C2A—H2AB	0.9600	C7—C8	1.391 (8)
C2A—H2AC	0.9600	C8—H8	0.9300
P1—Ir1—C11	85.01 (6)	H2AA—C2A—H2AB	109.5
P1—Ir1—P3	164.96 (6)	H2AA—C2A—H2AC	109.5
P1—Ir1—S1	87.77 (5)	H2AB—C2A—H2AC	109.5
P2—Ir1—C11	98.62 (5)	P2—C2B—H2BA	109.5
P2—Ir1—P1	95.81 (6)	P2—C2B—H2BB	109.5
P2—Ir1—P3	96.72 (6)	P2—C2B—H2BC	109.5
P2—Ir1—S1	144.51 (5)	H2BA—C2B—H2BB	109.5
P3—Ir1—C11	84.92 (5)	H2BA—C2B—H2BC	109.5
P3—Ir1—S1	86.85 (6)	H2BB—C2B—H2BC	109.5
S1—Ir1—C11	116.86 (5)	P2—C2C—H2CA	109.5
C1—Ir1—C11	161.48 (16)	P2—C2C—H2CB	109.5
C1—Ir1—P1	92.54 (16)	P2—C2C—H2CC	109.5
C1—Ir1—P2	99.88 (16)	H2CA—C2C—H2CB	109.5
C1—Ir1—P3	93.46 (15)	H2CA—C2C—H2CC	109.5

C1—Ir1—S1	44.63 (16)	H2CB—C2C—H2CC	109.5
C1A—P1—Ir1	116.9 (2)	P3—C3A—H3AA	109.5
C1A—P1—C1B	106.1 (3)	P3—C3A—H3AB	109.5
C1B—P1—Ir1	116.8 (2)	P3—C3A—H3AC	109.5
C1C—P1—Ir1	111.1 (2)	H3AA—C3A—H3AB	109.5
C1C—P1—C1A	101.0 (3)	H3AA—C3A—H3AC	109.5
C1C—P1—C1B	103.0 (3)	H3AB—C3A—H3AC	109.5
C2A—P2—Ir1	115.0 (3)	P3—C3B—H3BA	109.5
C2B—P2—Ir1	118.2 (3)	P3—C3B—H3BB	109.5
C2B—P2—C2A	103.2 (4)	P3—C3B—H3BC	109.5
C2B—P2—C2C	103.2 (3)	H3BA—C3B—H3BB	109.5
C2C—P2—Ir1	115.2 (2)	H3BA—C3B—H3BC	109.5
C2C—P2—C2A	99.6 (3)	H3BB—C3B—H3BC	109.5
C3A—P3—Ir1	118.7 (2)	P3—C3C—H3CA	109.5
C3B—P3—Ir1	110.3 (2)	P3—C3C—H3CB	109.5
C3B—P3—C3A	101.7 (4)	P3—C3C—H3CC	109.5
C3C—P3—Ir1	117.3 (2)	H3CA—C3C—H3CB	109.5
C3C—P3—C3A	103.5 (3)	H3CA—C3C—H3CC	109.5
C3C—P3—C3B	103.3 (3)	H3CB—C3C—H3CC	109.5
C1—S1—Ir1	51.90 (17)	S1—C1—Ir1	83.5 (2)
P1—C1A—H1AA	109.5	N1—C1—Ir1	139.2 (4)
P1—C1A—H1AB	109.5	N1—C1—S1	137.2 (4)
P1—C1A—H1AC	109.5	C1—N1—C3	123.1 (5)
H1AA—C1A—H1AB	109.5	C4—C3—N1	119.0 (5)
H1AA—C1A—H1AC	109.5	C4—C3—C8	117.2 (5)
H1AB—C1A—H1AC	109.5	C8—C3—N1	123.7 (5)
P1—C1B—H1BA	109.5	C3—C4—H4	119.1
P1—C1B—H1BB	109.5	C5—C4—C3	121.9 (6)
P1—C1B—H1BC	109.5	C5—C4—H4	119.1
H1BA—C1B—H1BB	109.5	C4—C5—H5	119.4
H1BA—C1B—H1BC	109.5	C4—C5—C6	121.3 (7)
H1BB—C1B—H1BC	109.5	C6—C5—H5	119.4
P1—C1C—H1CA	109.5	C5—C6—H6	120.8
P1—C1C—H1CB	109.5	C7—C6—C5	118.4 (6)
P1—C1C—H1CC	109.5	C7—C6—H6	120.8
H1CA—C1C—H1CB	109.5	C6—C7—H7	119.6
H1CA—C1C—H1CC	109.5	C6—C7—C8	120.8 (6)
H1CB—C1C—H1CC	109.5	C8—C7—H7	119.6
P2—C2A—H2AA	109.5	C3—C8—H8	119.8
P2—C2A—H2AB	109.5	C7—C8—C3	120.4 (6)
P2—C2A—H2AC	109.5	C7—C8—H8	119.8
Ir1—S1—C1—N1	-175.8 (7)	P3—Ir1—P2—C2B	-85.8 (3)
Ir1—C1—N1—C3	-176.7 (4)	P3—Ir1—P2—C2C	36.8 (3)
Cl1—Ir1—P1—C1A	52.0 (3)	P3—Ir1—S1—C1	-98.1 (2)
Cl1—Ir1—P1—C1B	179.2 (3)	P3—Ir1—C1—S1	81.98 (17)
Cl1—Ir1—P1—C1C	-63.2 (2)	P3—Ir1—C1—N1	-102.4 (6)
Cl1—Ir1—P2—C2A	-122.4 (3)	S1—Ir1—P1—C1A	169.2 (3)



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Cl1—Ir1—P2—C2B	0.0 (3)	S1—Ir1—P1—C1B	-63.6 (3)
Cl1—Ir1—P2—C2C	122.6 (3)	S1—Ir1—P1—C1C	54.0 (2)
Cl1—Ir1—P3—C3A	-55.1 (3)	S1—Ir1—P2—C2A	57.8 (3)
Cl1—Ir1—P3—C3B	61.5 (3)	S1—Ir1—P2—C2B	-179.8 (3)
Cl1—Ir1—P3—C3C	179.3 (3)	S1—Ir1—P2—C2C	-57.2 (3)
Cl1—Ir1—S1—C1	179.2 (2)	S1—Ir1—P3—C3A	-172.4 (3)
Cl1—Ir1—C1—S1	-2.4 (6)	S1—Ir1—P3—C3B	-55.8 (3)
Cl1—Ir1—C1—N1	173.2 (4)	S1—Ir1—P3—C3C	62.0 (3)
P1—Ir1—P2—C2A	-36.6 (3)	S1—Ir1—C1—N1	175.6 (8)
P1—Ir1—P2—C2B	85.8 (3)	S1—C1—N1—C3	-3.2 (9)
P1—Ir1—P2—C2C	-151.5 (3)	C1—Ir1—P1—C1A	-146.4 (3)
P1—Ir1—P3—C3A	-103.2 (3)	C1—Ir1—P1—C1B	-19.2 (3)
P1—Ir1—P3—C3B	13.3 (3)	C1—Ir1—P1—C1C	98.4 (3)
P1—Ir1—P3—C3C	131.2 (3)	C1—Ir1—P2—C2A	57.1 (3)
P1—Ir1—S1—C1	95.9 (2)	C1—Ir1—P2—C2B	179.5 (3)
P1—Ir1—C1—S1	-84.23 (17)	C1—Ir1—P2—C2C	-57.9 (3)
P1—Ir1—C1—N1	91.4 (6)	C1—Ir1—P3—C3A	143.4 (3)
P2—Ir1—P1—C1A	-46.2 (3)	C1—Ir1—P3—C3B	-100.0 (3)
P2—Ir1—P1—C1B	81.0 (3)	C1—Ir1—P3—C3C	17.8 (3)
P2—Ir1—P1—C1C	-161.4 (2)	C1—N1—C3—C4	140.5 (6)
P2—Ir1—P3—C3A	43.0 (3)	C1—N1—C3—C8	-44.4 (8)
P2—Ir1—P3—C3B	159.6 (3)	N1—C3—C4—C5	177.1 (7)
P2—Ir1—P3—C3C	-82.6 (3)	N1—C3—C8—C7	-177.1 (6)
P2—Ir1—S1—C1	-1.0 (2)	C3—C4—C5—C6	-1.0 (14)
P2—Ir1—C1—S1	179.42 (14)	C4—C3—C8—C7	-1.9 (9)
P2—Ir1—C1—N1	-5.0 (6)	C4—C5—C6—C7	0.7 (14)
P3—Ir1—P1—C1A	100.1 (3)	C5—C6—C7—C8	-1.0 (12)
P3—Ir1—P1—C1B	-132.7 (3)	C6—C7—C8—C3	1.7 (11)
P3—Ir1—P1—C1C	-15.1 (3)	C8—C3—C4—C5	1.6 (11)
P3—Ir1—P2—C2A	151.8 (3)		

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