Resisting B-H Oxidative Addition: The Divergent Reactivity of the *o*-Carborane and Carba-*closo*-dodecaborate Ligand Substituents

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ABSTRACT

Here, we report a study of two isoelectronic Ir(I) complexes supported by different carboranyl phosphines, bearing either *o*-carborane or carba-*closo*-dodecaborate ligand substituents. The neutral Ir(I) complex containing the *o*-carboranyl phosphine ligand is not isolable and undergoes spontaneous B-H cyclometalation to afford an Ir(III) hydride. In contrast, the anionic Ir(I) complex supported by a phosphine with a carba-*closo*-dodecaborate ligand R-group is stable towards B-H activation. This divergent reactivity has important implications for the design of carborane containing ligands for catalysis. Both compounds are fully characterized by multinuclear NMR spectroscopy, HRMS spectrometry, and single crystal x-ray diffraction studies.

Keywords: carborane anion, carborane ligand, cyclometalation, carboranyl phosphine, boron cluster

Introduction

The proliferation of contemporary homogenous catalytic methods is largely due to the availability of a diverse array of ligand architectures. Due to their shape and 3-dimensional aromaticity, icosahedral carboranes [1] are an interesting alternative to classical alkyl and aryl ligand substituents. Soon after the discovery of *o*-carborane [2] **1** (Fig 1, left) in 1963 a carboranyl phosphine ligand [3] and complex [4] were reported by Smith. Kumada [5] was the

first to implement such ligands in homogenous catalysis, but these and all subsequent systems containing *o*-carborane **1**

fragments have not yielded

catalysts [6] that surpass the activity of systems supported by ubiquitous trialkyl or triaryl phosphines. Perhaps this non-competitive catalytic behavior is due to the decomposition of the cluster via well-known B-vertex extrusion [1b, 7] and B-H cyclometalation reactions. Hawthorne [8] was the first to observe intramolecular B-H oxidative addition of an *o*-carboranyl phosphine, as well as analogous intermolecular reactions with unsubstituted dicarbaborane icosahedra at an Ir(I) center.

In contrast to *o*-carborane **1**, the isoelectronic and weakly coordinating carba-*closo*-dodecaborate anion [1e] **2** (Fig 1, center) is not susceptible to B-vertex extrusion reactions and is renowned for its inert properties, particularly when polyhalogenated [1h, 9]. We recently reported the first utilization of the carba-*closo*-dodecaborate as a ligand substituent for a

Fig 1. *o*-Carborane **1**, carba-*closo*-dodecaborate anion **2**, and zwitterionic Ir complex **3**. Unlabeled vertices = B-H

transition metal-based catalyst [10]. Notably, this zwitterionic Au(I) complex, featuring an anionic carboranyl phosphine, is far more active than all known systems for the hydroamination of alkynes. In addition, we reported an unusually stable pseudo-low coordinate zwitterionic Ir(I) compound **3** (Fig 1, right) that does not undergo spontaneous intramolecular B-H oxidative addition [11]. Although not identical, **3** is reminiscent of Hawthorne's unstable Ir(I) complexes [8] and its behavior suggests that ligands bearing a carba-*closo*-dodecaborate substituent [12] are inherently more resistant to B-H activation. Given our interest in catalyst design we are seeking stronger evidence that the carba-*closo*-dodecaborate ligand substituent has enhanced chemical stability towards B-H oxidative addition. Here, we report such a study by the preparation and analysis of two isoelectronic iridium (I) complexes containing phosphines with *o*-carborane and carba-*closo*-dodecaborate moieties, respectively. Where the former *o*-carborane containing complex is not isolable and spontaneously undergoes cyclometalation at one of the B-H vertices, the carba-*closo*-dodecaborate analogue is stable.

Results and Discussion

Reacting the known [13] *o*-carborane phosphine **4** with $\frac{1}{2}$ an equivalent of $(\text{ClIr}(\text{COD}))_2$ in hexane solvent results in a color change from light orange to red orange and subsequent formation of a precipitate (Fig 2, next page). Based on Hawthorne's prior observations [8], it was predicted that the ensuing Ir(I) complex **5** would be unstable towards cyclometalation and produce the corresponding Ir(III) complex **6**. Indeed, analysis of the precipitate by ^1H NMR spectroscopy shows clean formation of an iridium hydride at -16.42 ppm (d, $^2J_{\text{P-H}} = 13.1$ Hz), suggesting cyclometalation of the *o*-carborane cluster. The coupling constant is consistent with an iridium (III) hydride disposed *cis* to a phosphine (range $^2J_{\text{P-H}}$ from 10-20 Hz) [8]. In addition

Fig 2. Synthesis of the cyclometalated Ir complexes **6**. Solid-state structure of diastereomer **6''**. Color code: Grey = C, white = H, violet = P, red = Ir, brown = B, green = chlorine. Unlabeled vertices = B-H. Notable bond lengths (Å): Ir-P = 2.320(5); Ir-B = 2.094(2); Ir-Cl = 2.498(5); C1-C2 = 1.384(3); C3-C4 = 1.362(3). Selected bond angles (°): B-Ir-P = 72.1; P-Ir-Cl = 90.2.

to the expected ^1H signals for the phosphine *i*Pr-groups and COD protons, two carborane C-H resonances appear in a 4:1 ratio. The presence of two carborane C-H signals suggests the formation of a diastereomeric mixture (**6'**, **6''**), resulting from competitive B-H oxidative addition at the B3 and B6 positions (Fig 2). Such competitive cyclometalations have been observed previously [14] with other metals, and occur preferentially at B3/B6 positions rather than at B4/B5, since the B3/B6 boron atoms are more activated (attached to 2-carbon atoms). All other ligand ^1H resonances from the two diastereomers **6'** and **6''** are superimposed by coincidence. Analysis of the ^{31}P NMR spectra also shows a 4:1 mixture of compounds and is in agreement with our assignment. The ^{11}B NMR spectrum is uninformative due to the multitude of broad overlapping resonances, which cannot be resolved. However, the solution and solid-state

infrared spectra of complexes **6** show bands typical for B-H stretches of *o*-carborane (2460-2625 cm^{-1}), as well as the presence of an Ir-H absorbance at 2223 cm^{-1} [8].

A single-crystal X-ray diffraction study of one of the diastereomers **6''** confirms that cyclometalation occurs adjacent to the two carborane carbon atoms (Figure 2, bottom right). Compound **6''** adopts a distorted octahedral geometry with the hydride, which was located from the difference electron density map, *cis* to the phosphine ligand. The Ir-P, Ir-B and Ir-Cl bond lengths are 2.320(5), 2.094(2) and 2.498(5) Å, respectively. The cyclooctadiene C-C double bond lengths *trans* to the phosphine (C1-C2 = 1.384(3) Å) and metalated B-vertex (C3-C4 = 1.362(3) Å) are in the typical range (1.35-1.44) for olefins coordinated to Ir [15].

We next turned our attention to preparing a complex bearing a phosphine with a carba-*closo*-dodecaborate substituent, which is isoelectronic with the unstable complex **5**. We predicted that treating the previously reported [11] zwitterion **3** with a nucleophilic chloride source should produce the anionic isoelectronic complex **7** (Fig 3). Thus,

Fig 3. Synthesis of anionic Ir(I) complex **7**. Solid-state structure of **7** (note: most hydrogens and NMe_4^+ counteranion omitted for clarity). Color code: grey = C, white = H, violet = P, red = Ir, brown = B, green = Cl. Unlabeled vertices = B-H. Notable bond lengths (Å): Ir-P = 2.371(7); Ir-Cl = 2.394(8); C1-C2 = 1.401(5); C3-C4 = 1.422(5). Selected bond angle ($^\circ$): P-Ir-Cl = 91.4.

treatment of solution of **3** dissolved in C₆H₅F with five equivalents of NMe₄Cl resulted in the formation of an orange precipitate **7**. Analysis of the precipitate by ³¹P NMR shows the formation of a single new product **7** (s, 32.95 ppm). Importantly, the ¹H NMR spectrum of **7** shows no Ir-H resonance, suggesting that the carba-*closo*-dodecaborate substituent is not cyclometalated. Moreover, as indicated by ¹¹B NMR spectroscopy (three resonances 1:5:5 ratio; 5:5 overlapping) the local C_{5v} symmetry of the cluster is retained, confirming that cyclometalation has not occurred. In addition, solution I.R. shows no Ir-H absorbance, ruling out the possibility of a rapid reversible cyclometalation process faster than the NMR time scale.

A single-crystal X-ray diffraction structure confirms the identity of the square planar Ir (I) complex **7** (Fig 3, previous page). While the Ir-P bond length (2.371(7) Å) is similar to complex **6**, the Ir-Cl (2.394(8) Å) and olefin bond lengths (C1-C2 = 1.401(5) Å, C3-C4 = 1.422(5) Å) are comparatively contracted and elongated, respectively. These observations can be explained by the decrease in coordination number and oxidation state, which allows for stronger M-L σ and π interactions. The closest B-H approach to the Ir center is 2.83 (Ir-H1) which is outside the range of typical Ir B-H agostic interactions. For comparison, the zwitterionic precursor **3** displays two strong agostic interactions with the metal center (Ir-H distances = 1.93(4) and 1.92(4) Å) [11].

Summary and Conclusion

The study above provides strong evidence that the carba-*closo*-dodecaborate ligand substituent is far less susceptible to intramolecular B-H oxidative addition reactions compared to its neutral cousin, *o*-carborane. This observation is important since it supports the notion that *o*-carborane may not be a suitable ligand substituent for catalysts that mediate reactions involving

oxidative addition/reductive elimination sequences. In addition, the ability of the carba-*closo*-dodecaborate ligand R-group to resist intramolecular B-H oxidative addition suggests that ligands containing this group should be useful for a variety of catalytic processes.

Experimental

Unless otherwise stated, all manipulations were carried out using standard Schlenk or glovebox techniques (O_2 , H_2O < 1ppm) under an argon or dinitrogen atmosphere. The iridium complex **3** and 1-diisopropylphosphino-1,2-dicarba-*closo*-dodecaborane ligand **4** were prepared according to literature [11, 13]. Solvents were dried on NaK, K, or CaH_2 and distilled under argon before use. Reagents were purchased from commercial vendors and used without further purification. NMR spectra were recorded on Bruker Avance 300MHz, Varian Inova 300MHz, Varian Inova 400MHz, or Varian Inova 500MHz spectrometers. Standard Varian pulse sequences, gCOSY and gHSQC were used for the COSY and HSQC experiments. Both are standard Varian pulse sequences that accompany the VnmrJ 2.2D software. ^1H NMR and ^{13}C NMR chemical shifts were referenced to residual solvent. ^{11}B NMR chemical shifts were externally referenced to BF_3OEt_2 . ^{31}P NMR chemical shifts were externally referenced to 80% H_3PO_4 in H_2O . HRMS was recorded on Agilent Technologies 6210 (time of flight LC/MS) using ESI technique. IR spectra were recorded on Attenuated Reflectance (ATR) and were run on ABB MB3000 spectrometer in the $525\text{--}4000\text{ cm}^{-1}$ frequency range using a diamond crystal.

Synthesis of complexes 6 $\text{Ir}(\text{COD})\text{Cl}[P(\text{iPr})_2\text{C}_2\text{B}_{10}\text{H}_{11}]$ (mixture of two diastereomers)

A solution of $[\text{Ir}(\text{COD})\text{Cl}]_2$ (30 mg, 0.089 mmol) in hexane (6 mL) was added to a hexane solution of 1-diisopropylphosphino-1,2-dicarba-*closo*-dodecaborane **4** (23.2 mg, 0.089 mmol) and allowed to stir overnight. The resulting precipitate was filtered and washed with hexane (3 x 1mL) to afford **6** as a vermilion solid in 95% yield (50.5 mg, 0.084 mmol). ^1H NMR (300 MHz,

C_6D_6 , 25 °C): δ =5.87 (bs, 1H, C-H_{carborane} minor isomer), 5.75 (bs, 1H, C-H_{carborane} major isomer), 5.15 (m, 1H, CH_{COD}), 5.03(m, 1H, CH_{COD}), 4.86 (m, 1H, CH_{COD}), 4.55 (m, 1H, CH_{COD}), 2.95 (m, 1H, CH₂), 2.59 (m, 1H, CH), 2.53 (m, 1H, CH₂), 2.26 (m, 1H, CH), 2.08 (m, 1H, CH₂), 1.89 (m, 2H, CH₂), 1.81 (m, 1H, CH₂), 1.73 (m, 1H, CH₂), 1.63 (m, 1H, CH₂), 0.99 (dd, $^3\text{J}(\text{P-H})$ = 15.7, $^3\text{J}(\text{H-H})$ = 7.5 Hz, 3H, CH₃), 0.94 (dd, $^3\text{J}(\text{P-H})$ = 19.5, $^3\text{J}(\text{H-H})$ = 7.4 Hz, 3H, CH₃), 0.85 (dd, $^3\text{J}(\text{P-H})$ = 16.9, $^3\text{J}(\text{H-H})$ = 7.5 Hz, 3H, CH₃), 0.75 (dd, $^3\text{J}(\text{P-H})$ = 12.0, $^3\text{J}(\text{H-H})$ = 7.3 Hz, 3H, CH₃), -16.42 (d, $^2\text{J}(\text{P-H})$ = 13.1 Hz, 1H, Ir-H); $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, C_6D_6 , 25 °C): δ = 104.7 (CH_{COD}), 94.6 (CH_{COD}), 86.9 (d, $^2\text{J}(\text{P-C})$ = 17.4 Hz, CH_{COD}), 82.0 (CH_{COD}), 64.7 (CH_{carborane}) 32.8 (CH₂), 32.2 (d, $^1\text{J}(\text{P-C})$ = 19.8 Hz, CH), 32.1 (CH₂), 31.3 (CH₂), 27.7 (CH₂), 24.3 (d, $^1\text{J}(\text{P-C})$ = 12.9 Hz, PCH), 21.6 (CH₃), 20.2 (CH₃), 18.4 (d, $^2\text{J}(\text{P-C})$ = 6.2 Hz, CH₃), 18.4 (d, $^2\text{J}(\text{P-C})$ = 7.3 Hz, CH₃); $^{31}\text{P}\{^1\text{H}\}$ NMR (162 MHz, C_6D_6 , 25 °C): δ = 43.0, 20.9 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (96 MHz, C_6D_6 , 25 °C): δ = 2.8, 0.0, -3.1, -4.3, -5.7, -6.6, -7.8, -9.6, -18.0 (B-Ir) ppm. HRMS: calculated [M-] {C₁₆H₃₇B₁₀ClIrP}: 596.2949 *m/z*; Found [M-] {C₁₆H₃₇B₁₀ClIrP}: 596.2915 *m/z*. (**Note:** the resonance for the carborane carbon attached to P is not observable in the ^{13}C NMR spectrum.)

Synthesis of complex 7 Ir(COD)Cl[P(iPr)₂CB₁₁H₁₁][N(CH₃)₄]

Complex **3** (50 mg, 0.089 mmol) was dissolved in a solution of fluorobenzene and tetramethylammonium chloride (48.95 mg, 0.45 mmol) was added to the solution and stirred overnight. The resulting precipitate was filtered and washed with fluorobenzene (2 x 1mL), and hexane (2 x 1mL) to afford **7** as a light red solid in 95% yield (50.5 mg, 0.085). Crystals suitable for a single crystal x-ray diffraction study were obtained by layering a tetrahydrofuran solution with hexanes. ^1H NMR (500 MHz, THF-*d*₈, 25 °C): δ = 4.55 (bs, 2H, CH_{COD}), 4.09 (bs, 2H, CH_{COD}), 3.27 (s, 12H, N(CH₃)₄⁺), 2.86 (m, 2H, CH), 2.15 (bm, 4H, CH₂), 2.03 (bm, 4H, CH₂), 1.48 (dd, $^3\text{J}(\text{P-H})$ = 15.7, $^3\text{J}(\text{H-H})$ = 6.9 Hz, 6H, CH₃), 1.33 (dd, $^3\text{J}(\text{P-H})$ = 12.9, $^3\text{J}(\text{H-H})$ = 6.9 Hz,

6H, CH₃) ppm; ³¹P{¹H} NMR (300 MHz, THF-*d*₈, 25 °C): δ= 32.9 ppm; ¹¹B{¹H} NMR (300 MHz, THF-*d*₈, 25 °C): δ= 0.8, -9.0, -9.7 ppm. HRMS: calculated [M-] {C₁₅H₃₇B₁₁ClIrP}: 595.3047 *m/z*; Found [M-] {C₁₅H₃₇B₁₁ClIrP}: 595.3061 *m/z*.

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Author Contributions

The manuscript was written through contributions of all authors. All authors have given approval to the final version of the manuscript. These authors contributed equally.

Notes

The authors declare no competing financial interests.

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TOC Artwork

The neutral Ir(I) complex containing the *o*-carboranyl phosphine ligand is not isolable and undergoes spontaneous B-H cyclometalation to afford an Ir(III) hydride. In contrast, the anionic Ir(I) complex supported by a phosphine with a carba-*closo*-dodecaborate ligand R-group is stable towards B-H activation.

X-Ray Structure Data, Complex 6''

A colorless prism fragment (0.173 x 0.102 x 0.077 mm³) was used for the single crystal x-ray diffraction study of [C₂H₁₀B₁₀][C₃H₇]₂PC₈H₁₂ClIrH (sample vL67_0m). The crystal was coated with paratone oil and mounted on to a cryo-loop glass fiber. X-ray intensity data were collected at 100(2) K on a Bruker APEX2³ platform-CCD x-ray diffractometer system (fine focus Mo-radiation, $\lambda = 0.71073$ Å, 50KV/35mA power). The CCD detector was placed at a distance of 5.0800 cm from the crystal.

A total of 3600 frames were collected for a sphere of reflections (with scan width of 0.3° in ω and ϕ , starting ω and 2θ angles of -30° , and ϕ angles of 0° , 90° , 120° , 180° , 240° , and 270° for every 600 frames, 10 sec/frame exposure time). The frames were integrated using the Bruker SAINT software package⁴ and using a narrow-frame integration algorithm. Based on a monoclinic crystal system, the integrated frames yielded a total of 50645 reflections at a maximum 2θ angle of 59.148° (0.72 Å resolution), of which 6585 were independent reflections ($R_{\text{int}} = 0.0330$, $R_{\text{sig}} = 0.0183$, redundancy = 7.7, completeness = 99.9%) and 6018 (91.4%) reflections were greater than $2\sigma(I)$. The unit cell parameters were, $\mathbf{a} = 13.5940(5)$ Å, $\mathbf{b} = 10.8808(4)$ Å, $\mathbf{c} = 17.2450(6)$ Å, $\beta = 112.7908(5)^\circ$, $V = 2351.62(15)$ Å³, $Z = 4$, calculated density $D_c = 1.684$ g/cm³. Absorption corrections were applied (absorption coefficient $\mu = 5.862$ mm⁻¹; min/max transmission = 0.430/0.661) to the raw intensity data using the SADABS program⁵.

The Bruker SHELXTL software package⁶ was used for phase determination and structure refinement. The distribution of intensities ($E^2 - 1 = 0.862$) and systematic absent reflections indicated one possible space group, P2(1)/n. The space group P2(1)/n (#14) was later determined to be correct. Direct methods of phase determination followed by two Fourier cycles of refinement led to an electron density map from which most of the non-hydrogen atoms were identified in the asymmetric unit of the unit cell. With subsequent isotropic refinement, all of the non-hydrogen atoms were identified. There was one molecule of [C₂H₁₀B₁₀][C₃H₇]₂PC₈H₁₂ClIrH present in the asymmetric unit of the unit cell.

Atomic coordinates, isotropic and anisotropic displacement parameters of all the non-hydrogen atoms were refined by means of a full matrix least-squares procedure on F^2 . The H-atoms were

included in the refinement in calculated positions riding on the atoms to which they were attached, except the hydride atom and four of the H-atoms of the C₈H₁₂-group were refined unrestrained. The refinement converged at R1 = 0.0164, wR2 = 0.0349, with intensity I > 2σ (I). The largest peak/hole in the final difference map was 0.927/-0.782 e/Å³.

Full crystallographic data for 6'' can be found at the Cambridge crystallographic database under reference # CCDC 1057296

Table 1. Crystal data and structure refinement for vL67_0m.

Identification code	vL67_0m	
Empirical formula	C16 H37 B10 Cl Ir P	
Formula weight	596.17	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n (#14)	
Unit cell dimensions	a = 13.5940(5) Å	$\alpha = 90^\circ$.
	b = 10.8808(4) Å	$\beta = 112.7908(5)^\circ$.
	c = 17.2450(6) Å	$\gamma = 90^\circ$.
Volume	2351.62(15) Å ³	
Z	4	
Density (calculated)	1.684 Mg/m ³	
Absorption coefficient	5.862 mm ⁻¹	
F(000)	1168	
Crystal size	0.173 x 0.102 x 0.077 mm ³	
Theta range for data collection	2.268 to 29.574°.	
Index ranges	-18 ≤ h ≤ 18, -15 ≤ k ≤ 15, -23 ≤ l ≤ 23	
Reflections collected	50645	
Independent reflections	6585 [R(int) = 0.0330]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6585 / 0 / 288	
Goodness-of-fit on F ²	1.051	
Final R indices [I > 2sigma(I)]	R1 = 0.0164, wR2 = 0.0349	
R indices (all data)	R1 = 0.0198, wR2 = 0.0362	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.927 and -0.782 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for vL67_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	2448(1)	1910(1)	70(1)	8(1)
Cl(1)	595(1)	1723(1)	26(1)	15(1)
C(1C)	2471(2)	3511(2)	999(1)	18(1)
C(2C)	3496(2)	3323(2)	1077(1)	20(1)
C(3C)	4104(3)	4082(3)	689(2)	49(1)
C(4C)	3604(2)	4243(2)	-254(2)	32(1)
C(5C)	2734(2)	3345(2)	-751(1)	18(1)
C(6C)	1686(2)	3438(2)	-822(1)	18(1)
C(7C)	1252(2)	4421(2)	-428(2)	30(1)
C(8C)	1803(3)	4578(3)	506(2)	47(1)
C(1)	2513(1)	-842(2)	-242(1)	10(1)
C(2)	1252(2)	-602(2)	-816(1)	10(1)
B(3)	2159(2)	529(2)	-837(1)	10(1)
B(4)	3266(2)	-454(2)	-790(1)	12(1)
B(5)	2981(2)	-2025(2)	-666(1)	14(1)
B(6)	1689(2)	-2091(2)	-645(1)	12(1)
B(7)	769(2)	-1561(2)	-1643(1)	13(1)
B(8)	1060(2)	24(2)	-1760(1)	13(1)
B(9)	2354(2)	98(2)	-1776(1)	14(1)
B(10)	2864(2)	-1446(2)	-1665(1)	14(1)
B(11)	1876(2)	-2471(2)	-1579(1)	14(1)
B(12)	1494(2)	-1159(2)	-2269(1)	14(1)
P(1)	2894(1)	39(1)	765(1)	9(1)
C(3)	4340(2)	-187(2)	1374(1)	13(1)
C(4)	2098(2)	-633(2)	1315(1)	12(1)
C(5)	4650(2)	264(2)	2285(1)	19(1)
C(6)	4796(2)	-1472(2)	1367(1)	18(1)
C(7)	2424(2)	-1939(2)	1657(1)	18(1)
C(8)	2031(2)	237(2)	1994(1)	17(1)

Table 3. Bond lengths [Å] and angles [°] for vL67_0m.

Ir(1)-B(3)	2.094(2)	C(2)-B(7)	1.683(3)
Ir(1)-C(6C)	2.230(2)	C(2)-B(8)	1.689(3)
Ir(1)-C(5C)	2.242(2)	C(2)-B(6)	1.712(3)
Ir(1)-P(1)	2.3203(5)	C(2)-B(3)	1.752(3)
Ir(1)-C(2C)	2.344(2)	C(2)-H(2)	0.93(2)
Ir(1)-C(1C)	2.359(2)	B(3)-B(8)	1.796(3)
Ir(1)-Cl(1)	2.4976(5)	B(3)-B(9)	1.801(3)
Ir(1)-H(1)	1.45(2)	B(3)-B(4)	1.822(3)
C(1C)-C(2C)	1.362(3)	B(4)-B(10)	1.761(3)
C(1C)-C(8C)	1.515(3)	B(4)-B(9)	1.775(3)
C(1C)-H(1C)	0.93(3)	B(4)-B(5)	1.784(3)
C(2C)-C(3C)	1.498(3)	B(4)-H(4)	1.1200
C(2C)-H(2C)	0.98(3)	B(5)-B(11)	1.771(3)
C(3C)-C(4C)	1.510(4)	B(5)-B(6)	1.771(3)
C(3C)-H(3B)	0.9900	B(5)-B(10)	1.783(3)
C(3C)-H(3C)	0.9900	B(5)-H(5)	1.1200
C(4C)-C(5C)	1.517(3)	B(6)-B(11)	1.773(3)
C(4C)-H(4B)	0.9900	B(6)-B(7)	1.786(3)
C(4C)-H(4C)	0.9900	B(6)-H(6)	1.1200
C(5C)-C(6C)	1.384(3)	B(7)-B(11)	1.769(3)
C(5C)-H(5D)	1.00(3)	B(7)-B(12)	1.775(3)
C(6C)-C(7C)	1.506(3)	B(7)-B(8)	1.798(3)
C(6C)-H(6D)	0.96(3)	B(7)-H(7)	1.1200
C(7C)-C(8C)	1.499(4)	B(8)-B(9)	1.773(3)
C(7C)-H(7D)	0.9900	B(8)-B(12)	1.782(3)
C(7C)-H(7E)	0.9900	B(8)-H(8)	1.1200
C(8C)-H(8D)	0.9900	B(9)-B(12)	1.787(3)
C(8C)-H(8E)	0.9900	B(9)-B(10)	1.799(3)
C(1)-C(2)	1.634(3)	B(9)-H(9)	1.1200
C(1)-B(4)	1.694(3)	B(10)-B(12)	1.774(3)
C(1)-B(5)	1.720(3)	B(10)-B(11)	1.795(3)
C(1)-B(6)	1.727(3)	B(10)-H(10)	1.1200
C(1)-B(3)	1.768(3)	B(11)-B(12)	1.801(3)
C(1)-P(1)	1.8728(19)	B(11)-H(11)	1.1200

B(12)-H(12)	1.1200	C(2C)-Ir(1)-C(1C)	33.66(8)
P(1)-C(4)	1.8441(18)	B(3)-Ir(1)-Cl(1)	91.36(6)
P(1)-C(3)	1.851(2)	C(6C)-Ir(1)-Cl(1)	81.17(6)
C(3)-C(6)	1.532(3)	C(5C)-Ir(1)-Cl(1)	117.17(6)
C(3)-C(5)	1.539(3)	P(1)-Ir(1)-Cl(1)	90.218(16)
C(3)-H(3A)	1.0000	C(2C)-Ir(1)-Cl(1)	113.12(6)
C(4)-C(8)	1.536(3)	C(1C)-Ir(1)-Cl(1)	80.18(6)
C(4)-C(7)	1.537(3)	B(3)-Ir(1)-H(1)	82.0(9)
C(4)-H(4A)	1.0000	C(6C)-Ir(1)-H(1)	105.3(9)
C(5)-H(5A)	0.9800	C(5C)-Ir(1)-H(1)	69.3(9)
C(5)-H(5B)	0.9800	P(1)-Ir(1)-H(1)	82.2(9)
C(5)-H(5C)	0.9800	C(2C)-Ir(1)-H(1)	73.4(9)
C(6)-H(6A)	0.9800	C(1C)-Ir(1)-H(1)	106.8(9)
C(6)-H(6B)	0.9800	Cl(1)-Ir(1)-H(1)	171.1(9)
C(6)-H(6C)	0.9800	C(2C)-C(1C)-C(8C)	122.5(2)
C(7)-H(7A)	0.9800	C(2C)-C(1C)-Ir(1)	72.55(12)
C(7)-H(7B)	0.9800	C(8C)-C(1C)-Ir(1)	109.69(15)
C(7)-H(7C)	0.9800	C(2C)-C(1C)-H(1C)	118.0(17)
C(8)-H(8A)	0.9800	C(8C)-C(1C)-H(1C)	117.1(17)
C(8)-H(8B)	0.9800	Ir(1)-C(1C)-H(1C)	102.5(16)
C(8)-H(8C)	0.9800	C(1C)-C(2C)-C(3C)	126.4(3)
		C(1C)-C(2C)-Ir(1)	73.79(13)
B(3)-Ir(1)-C(6C)	96.69(8)	C(3C)-C(2C)-Ir(1)	108.25(15)
B(3)-Ir(1)-C(5C)	93.20(8)	C(1C)-C(2C)-H(2C)	117.4(16)
C(6C)-Ir(1)-C(5C)	36.07(8)	C(3C)-C(2C)-H(2C)	114.2(16)
B(3)-Ir(1)-P(1)	72.09(6)	Ir(1)-C(2C)-H(2C)	102.6(16)
C(6C)-Ir(1)-P(1)	165.78(6)	C(2C)-C(3C)-C(4C)	116.7(2)
C(5C)-Ir(1)-P(1)	149.65(6)	C(2C)-C(3C)-H(3B)	108.1
B(3)-Ir(1)-C(2C)	155.32(8)	C(4C)-C(3C)-H(3B)	108.1
C(6C)-Ir(1)-C(2C)	90.48(9)	C(2C)-C(3C)-H(3C)	108.1
C(5C)-Ir(1)-C(2C)	78.83(8)	C(4C)-C(3C)-H(3C)	108.1
P(1)-Ir(1)-C(2C)	103.35(6)	H(3B)-C(3C)-H(3C)	107.3
B(3)-Ir(1)-C(1C)	170.73(8)	C(3C)-C(4C)-C(5C)	117.4(2)
C(6C)-Ir(1)-C(1C)	78.37(8)	C(3C)-C(4C)-H(4B)	107.9
C(5C)-Ir(1)-C(1C)	87.37(8)	C(5C)-C(4C)-H(4B)	107.9
P(1)-Ir(1)-C(1C)	111.44(6)	C(3C)-C(4C)-H(4C)	107.9

C(5C)-C(4C)-H(4C)	107.9	C(2)-C(1)-P(1)	109.18(12)
H(4B)-C(4C)-H(4C)	107.2	B(4)-C(1)-P(1)	112.33(13)
C(6C)-C(5C)-C(4C)	123.6(2)	B(5)-C(1)-P(1)	139.66(14)
C(6C)-C(5C)-Ir(1)	71.49(12)	B(6)-C(1)-P(1)	132.85(13)
C(4C)-C(5C)-Ir(1)	112.35(15)	B(3)-C(1)-P(1)	91.26(11)
C(6C)-C(5C)-H(5D)	117.3(16)	C(1)-C(2)-B(7)	112.80(15)
C(4C)-C(5C)-H(5D)	115.3(16)	C(1)-C(2)-B(8)	112.48(14)
Ir(1)-C(5C)-H(5D)	105.2(15)	B(7)-C(2)-B(8)	64.46(13)
C(5C)-C(6C)-C(7C)	125.5(2)	C(1)-C(2)-B(6)	62.09(12)
C(5C)-C(6C)-Ir(1)	72.44(12)	B(7)-C(2)-B(6)	63.48(13)
C(7C)-C(6C)-Ir(1)	112.11(14)	B(8)-C(2)-B(6)	117.43(15)
C(5C)-C(6C)-H(6D)	117.5(16)	C(1)-C(2)-B(3)	62.84(12)
C(7C)-C(6C)-H(6D)	113.7(16)	B(7)-C(2)-B(3)	117.68(14)
Ir(1)-C(6C)-H(6D)	103.9(16)	B(8)-C(2)-B(3)	62.87(12)
C(8C)-C(7C)-C(6C)	116.4(2)	B(6)-C(2)-B(3)	117.90(15)
C(8C)-C(7C)-H(7D)	108.2	C(1)-C(2)-H(2)	116.0(14)
C(6C)-C(7C)-H(7D)	108.2	B(7)-C(2)-H(2)	121.2(14)
C(8C)-C(7C)-H(7E)	108.2	B(8)-C(2)-H(2)	119.9(14)
C(6C)-C(7C)-H(7E)	108.2	B(6)-C(2)-H(2)	115.5(14)
H(7D)-C(7C)-H(7E)	107.3	B(3)-C(2)-H(2)	112.6(14)
C(7C)-C(8C)-C(1C)	117.2(2)	C(2)-B(3)-C(1)	55.31(11)
C(7C)-C(8C)-H(8D)	108.0	C(2)-B(3)-B(8)	56.85(11)
C(1C)-C(8C)-H(8D)	108.0	C(1)-B(3)-B(8)	101.65(14)
C(7C)-C(8C)-H(8E)	108.0	C(2)-B(3)-B(9)	100.74(14)
C(1C)-C(8C)-H(8E)	108.0	C(1)-B(3)-B(9)	101.56(14)
H(8D)-C(8C)-H(8E)	107.2	B(8)-B(3)-B(9)	59.07(12)
C(2)-C(1)-B(4)	109.94(14)	C(2)-B(3)-B(4)	99.37(14)
C(2)-C(1)-B(5)	109.66(15)	C(1)-B(3)-B(4)	56.29(11)
B(4)-C(1)-B(5)	63.02(12)	B(8)-B(3)-B(4)	104.43(15)
C(2)-C(1)-B(6)	61.18(12)	B(9)-B(3)-B(4)	58.68(12)
B(4)-C(1)-B(6)	114.14(15)	C(2)-B(3)-Ir(1)	114.69(12)
B(5)-C(1)-B(6)	61.85(12)	C(1)-B(3)-Ir(1)	103.96(11)
C(2)-C(1)-B(3)	61.85(12)	B(8)-B(3)-Ir(1)	137.10(14)
B(4)-C(1)-B(3)	63.45(12)	B(9)-B(3)-Ir(1)	143.92(14)
B(5)-C(1)-B(3)	116.55(14)	B(4)-B(3)-Ir(1)	118.39(13)
B(6)-C(1)-B(3)	116.25(14)	C(1)-B(4)-B(10)	105.73(15)

C(1)-B(4)-B(9)	105.68(15)	C(1)-B(6)-B(7)	103.69(15)
B(10)-B(4)-B(9)	61.15(13)	B(5)-B(6)-B(7)	107.31(15)
C(1)-B(4)-B(5)	59.20(12)	B(11)-B(6)-B(7)	59.60(12)
B(10)-B(4)-B(5)	60.37(13)	C(2)-B(6)-H(6)	125.7
B(9)-B(4)-B(5)	109.62(16)	C(1)-B(6)-H(6)	124.6
C(1)-B(4)-B(3)	60.26(11)	B(5)-B(6)-H(6)	122.2
B(10)-B(4)-B(3)	110.18(16)	B(11)-B(6)-H(6)	123.4
B(9)-B(4)-B(3)	60.07(12)	B(7)-B(6)-H(6)	122.9
B(5)-B(4)-B(3)	110.73(15)	C(2)-B(7)-B(11)	104.54(15)
C(1)-B(4)-H(4)	124.2	C(2)-B(7)-B(12)	103.65(15)
B(10)-B(4)-H(4)	121.4	B(11)-B(7)-B(12)	61.09(13)
B(9)-B(4)-H(4)	121.8	C(2)-B(7)-B(6)	59.06(12)
B(5)-B(4)-H(4)	120.3	B(11)-B(7)-B(6)	59.84(12)
B(3)-B(4)-H(4)	119.8	B(12)-B(7)-B(6)	108.56(16)
C(1)-B(5)-B(11)	104.87(15)	C(2)-B(7)-B(8)	57.95(12)
C(1)-B(5)-B(6)	59.26(12)	B(11)-B(7)-B(8)	108.97(16)
B(11)-B(5)-B(6)	60.06(12)	B(12)-B(7)-B(8)	59.83(13)
C(1)-B(5)-B(10)	103.69(16)	B(6)-B(7)-B(8)	108.37(15)
B(11)-B(5)-B(10)	60.67(13)	C(2)-B(7)-H(7)	125.6
B(6)-B(5)-B(10)	108.38(16)	B(11)-B(7)-H(7)	121.8
C(1)-B(5)-B(4)	57.78(11)	B(12)-B(7)-H(7)	122.3
B(11)-B(5)-B(4)	107.71(16)	B(6)-B(7)-H(7)	121.1
B(6)-B(5)-B(4)	107.70(15)	B(8)-B(7)-H(7)	121.3
B(10)-B(5)-B(4)	59.17(13)	C(2)-B(8)-B(9)	104.44(15)
C(1)-B(5)-H(5)	125.1	C(2)-B(8)-B(12)	103.09(16)
B(11)-B(5)-H(5)	122.0	B(9)-B(8)-B(12)	60.35(13)
B(6)-B(5)-H(5)	121.1	C(2)-B(8)-B(3)	60.28(12)
B(10)-B(5)-H(5)	122.6	B(9)-B(8)-B(3)	60.61(12)
B(4)-B(5)-H(5)	122.2	B(12)-B(8)-B(3)	109.68(16)
C(2)-B(6)-C(1)	56.74(11)	C(2)-B(8)-B(7)	57.59(12)
C(2)-B(6)-B(5)	103.84(15)	B(9)-B(8)-B(7)	107.95(16)
C(1)-B(6)-B(5)	58.89(12)	B(12)-B(8)-B(7)	59.44(12)
C(2)-B(6)-B(11)	103.13(15)	B(3)-B(8)-B(7)	109.75(15)
C(1)-B(6)-B(11)	104.52(15)	C(2)-B(8)-H(8)	125.6
B(5)-B(6)-B(11)	59.97(12)	B(9)-B(8)-H(8)	122.3
C(2)-B(6)-B(7)	57.46(12)	B(12)-B(8)-H(8)	122.6

B(3)-B(8)-H(8)	119.4	B(5)-B(11)-B(10)	59.98(13)
B(7)-B(8)-H(8)	121.6	B(6)-B(11)-B(10)	107.76(15)
B(8)-B(9)-B(4)	107.37(15)	B(7)-B(11)-B(12)	59.63(13)
B(8)-B(9)-B(12)	60.09(13)	B(5)-B(11)-B(12)	107.35(16)
B(4)-B(9)-B(12)	106.38(16)	B(6)-B(11)-B(12)	107.98(16)
B(8)-B(9)-B(10)	107.41(16)	B(10)-B(11)-B(12)	59.10(13)
B(4)-B(9)-B(10)	59.05(13)	B(7)-B(11)-H(11)	121.8
B(12)-B(9)-B(10)	59.29(13)	B(5)-B(11)-H(11)	121.8
B(8)-B(9)-B(3)	60.32(12)	B(6)-B(11)-H(11)	121.4
B(4)-B(9)-B(3)	61.25(12)	B(10)-B(11)-H(11)	122.4
B(12)-B(9)-B(3)	109.23(15)	B(12)-B(11)-H(11)	122.3
B(10)-B(9)-B(3)	109.43(15)	B(10)-B(12)-B(7)	107.69(16)
B(8)-B(9)-H(9)	122.1	B(10)-B(12)-B(8)	108.11(16)
B(4)-B(9)-H(9)	122.5	B(7)-B(12)-B(8)	60.73(12)
B(12)-B(9)-H(9)	122.1	B(10)-B(12)-B(9)	60.69(13)
B(10)-B(9)-H(9)	122.0	B(7)-B(12)-B(9)	108.36(15)
B(3)-B(9)-H(9)	120.0	B(8)-B(12)-B(9)	59.57(13)
B(4)-B(10)-B(12)	107.55(16)	B(10)-B(12)-B(11)	60.28(13)
B(4)-B(10)-B(5)	60.46(12)	B(7)-B(12)-B(11)	59.28(12)
B(12)-B(10)-B(5)	108.05(15)	B(8)-B(12)-B(11)	108.25(15)
B(4)-B(10)-B(11)	107.69(15)	B(9)-B(12)-B(11)	108.93(16)
B(12)-B(10)-B(11)	60.61(13)	B(10)-B(12)-H(12)	121.6
B(5)-B(10)-B(11)	59.35(13)	B(7)-B(12)-H(12)	121.8
B(4)-B(10)-B(9)	59.80(13)	B(8)-B(12)-H(12)	121.6
B(12)-B(10)-B(9)	60.01(13)	B(9)-B(12)-H(12)	121.2
B(5)-B(10)-B(9)	108.62(15)	B(11)-B(12)-H(12)	121.5
B(11)-B(10)-B(9)	108.65(16)	C(4)-P(1)-C(3)	111.18(9)
B(4)-B(10)-H(10)	122.0	C(4)-P(1)-C(1)	105.50(9)
B(12)-B(10)-H(10)	121.7	C(3)-P(1)-C(1)	108.09(9)
B(5)-B(10)-H(10)	121.6	C(4)-P(1)-Ir(1)	121.64(7)
B(11)-B(10)-H(10)	121.7	C(3)-P(1)-Ir(1)	114.68(7)
B(9)-B(10)-H(10)	121.3	C(1)-P(1)-Ir(1)	92.68(6)
B(7)-B(11)-B(5)	108.08(15)	C(6)-C(3)-C(5)	110.35(17)
B(7)-B(11)-B(6)	60.57(12)	C(6)-C(3)-P(1)	117.42(14)
B(5)-B(11)-B(6)	59.97(12)	C(5)-C(3)-P(1)	110.36(14)
B(7)-B(11)-B(10)	107.02(16)	C(6)-C(3)-H(3A)	106.0

C(5)-C(3)-H(3A)	106.0	H(6A)-C(6)-H(6B)	109.5
P(1)-C(3)-H(3A)	106.0	C(3)-C(6)-H(6C)	109.5
C(8)-C(4)-C(7)	111.76(16)	H(6A)-C(6)-H(6C)	109.5
C(8)-C(4)-P(1)	111.57(14)	H(6B)-C(6)-H(6C)	109.5
C(7)-C(4)-P(1)	115.10(14)	C(4)-C(7)-H(7A)	109.5
C(8)-C(4)-H(4A)	105.9	C(4)-C(7)-H(7B)	109.5
C(7)-C(4)-H(4A)	105.9	H(7A)-C(7)-H(7B)	109.5
P(1)-C(4)-H(4A)	105.9	C(4)-C(7)-H(7C)	109.5
C(3)-C(5)-H(5A)	109.5	H(7A)-C(7)-H(7C)	109.5
C(3)-C(5)-H(5B)	109.5	H(7B)-C(7)-H(7C)	109.5
H(5A)-C(5)-H(5B)	109.5	C(4)-C(8)-H(8A)	109.5
C(3)-C(5)-H(5C)	109.5	C(4)-C(8)-H(8B)	109.5
H(5A)-C(5)-H(5C)	109.5	H(8A)-C(8)-H(8B)	109.5
H(5B)-C(5)-H(5C)	109.5	C(4)-C(8)-H(8C)	109.5
C(3)-C(6)-H(6A)	109.5	H(8A)-C(8)-H(8C)	109.5
C(3)-C(6)-H(6B)	109.5	H(8B)-C(8)-H(8C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for vL67_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Ir(1)	10(1)	7(1)	9(1)	0(1)	4(1)	-1(1)
Cl(1)	12(1)	13(1)	20(1)	0(1)	9(1)	0(1)
C(1C)	25(1)	16(1)	15(1)	-6(1)	7(1)	-2(1)
C(2C)	23(1)	18(1)	17(1)	-7(1)	6(1)	-9(1)
C(3C)	60(2)	59(2)	36(2)	-26(1)	30(2)	-47(2)
C(4C)	31(1)	29(1)	33(1)	9(1)	8(1)	-14(1)
C(5C)	27(1)	12(1)	17(1)	3(1)	12(1)	-4(1)
C(6C)	24(1)	12(1)	14(1)	5(1)	4(1)	-1(1)
C(7C)	42(2)	21(1)	31(1)	10(1)	19(1)	13(1)
C(8C)	54(2)	35(2)	31(1)	-14(1)	-6(1)	27(1)
C(1)	10(1)	10(1)	10(1)	0(1)	3(1)	0(1)
C(2)	10(1)	10(1)	10(1)	0(1)	4(1)	-1(1)
B(3)	12(1)	10(1)	10(1)	1(1)	6(1)	-1(1)
B(4)	12(1)	13(1)	13(1)	-2(1)	7(1)	-2(1)
B(5)	16(1)	14(1)	15(1)	-2(1)	7(1)	1(1)
B(6)	15(1)	10(1)	14(1)	-1(1)	6(1)	-2(1)
B(7)	13(1)	13(1)	11(1)	-3(1)	3(1)	-3(1)
B(8)	15(1)	15(1)	10(1)	0(1)	4(1)	-3(1)
B(9)	16(1)	16(1)	12(1)	-1(1)	7(1)	-3(1)
B(10)	15(1)	18(1)	12(1)	-4(1)	7(1)	-2(1)
B(11)	16(1)	15(1)	12(1)	-4(1)	7(1)	-3(1)
B(12)	15(1)	17(1)	12(1)	-4(1)	6(1)	-4(1)
P(1)	9(1)	9(1)	8(1)	0(1)	3(1)	-1(1)
C(3)	11(1)	15(1)	12(1)	1(1)	2(1)	1(1)
C(4)	14(1)	13(1)	10(1)	2(1)	5(1)	-1(1)
C(5)	15(1)	25(1)	13(1)	-3(1)	1(1)	-2(1)
C(6)	14(1)	20(1)	19(1)	2(1)	3(1)	3(1)
C(7)	23(1)	14(1)	17(1)	4(1)	9(1)	-1(1)
C(8)	23(1)	18(1)	15(1)	0(1)	12(1)	1(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for vL67_0m.

	x	y	z	U(eq)
H(1)	3518(18)	1810(20)	90(14)	10
H(1C)	2240(20)	3120(20)	1376(17)	23(7)
H(2C)	3940(20)	2790(20)	1536(17)	24(7)
H(3B)	4816	3703	835	58
H(3C)	4218	4907	950	58
H(4B)	4178	4194	-472	38
H(4C)	3302	5083	-373	38
H(5D)	2870(20)	2880(20)	-1200(17)	27(7)
H(6D)	1150(20)	3040(20)	-1291(17)	24(7)
H(7D)	1283	5215	-698	36
H(7E)	491	4239	-559	36
H(8D)	1253	4758	734	56
H(8E)	2271	5309	613	56
H(2)	833(18)	-350(20)	-526(14)	12
H(4)	4103	-100	-497	15
H(5)	3618	-2692	-297	17
H(6)	1472	-2782	-257	15
H(7)	-67	-1924	-1923	15
H(8)	415	692	-2113	16
H(9)	2578	812	-2146	17
H(10)	3423	-1739	-1966	17
H(11)	1779	-3436	-1822	17
H(12)	1145	-1266	-2969	17
H(3A)	4712	372	1116	15
H(4A)	1354	-703	883	14
H(5A)	4419	-340	2601	29
H(5B)	4302	1054	2282	29
H(5C)	5426	366	2551	29
H(6A)	5553	-1485	1739	28
H(6B)	4717	-1680	793	28

H(6C)	4408	-2074	1564	28
H(7A)	3095	-1905	2153	27
H(7B)	2520	-2448	1223	27
H(7C)	1865	-2296	1813	27
H(8A)	1494	-68	2195	26
H(8B)	1830	1061	1756	26
H(8C)	2727	274	2465	26

Table 6. Torsion angles [°] for vL67_0m.

C(8C)-C(1C)-C(2C)-C(3C)	-1.6(4)
Ir(1)-C(1C)-C(2C)-C(3C)	101.0(2)
C(8C)-C(1C)-C(2C)-Ir(1)	-102.6(2)
C(1C)-C(2C)-C(3C)-C(4C)	-55.5(4)
Ir(1)-C(2C)-C(3C)-C(4C)	27.5(3)
C(2C)-C(3C)-C(4C)-C(5C)	-18.1(4)
C(3C)-C(4C)-C(5C)-C(6C)	79.7(3)
C(3C)-C(4C)-C(5C)-Ir(1)	-2.3(3)
C(4C)-C(5C)-C(6C)-C(7C)	0.0(3)
Ir(1)-C(5C)-C(6C)-C(7C)	105.0(2)
C(4C)-C(5C)-C(6C)-Ir(1)	-105.0(2)
C(5C)-C(6C)-C(7C)-C(8C)	-55.3(3)
Ir(1)-C(6C)-C(7C)-C(8C)	28.4(3)
C(6C)-C(7C)-C(8C)-C(1C)	-19.9(4)
C(2C)-C(1C)-C(8C)-C(7C)	83.0(4)
Ir(1)-C(1C)-C(8C)-C(7C)	1.6(4)
B(4)-C(1)-C(2)-B(7)	67.70(19)
B(5)-C(1)-C(2)-B(7)	0.2(2)
B(6)-C(1)-C(2)-B(7)	-39.58(15)
B(3)-C(1)-C(2)-B(7)	110.53(16)
P(1)-C(1)-C(2)-B(7)	-168.66(12)
B(4)-C(1)-C(2)-B(8)	-2.9(2)
B(5)-C(1)-C(2)-B(8)	-70.39(19)
B(6)-C(1)-C(2)-B(8)	-110.18(17)
B(3)-C(1)-C(2)-B(8)	39.93(15)
P(1)-C(1)-C(2)-B(8)	120.74(14)
B(4)-C(1)-C(2)-B(6)	107.28(16)
B(5)-C(1)-C(2)-B(6)	39.79(14)
B(3)-C(1)-C(2)-B(6)	150.10(15)
P(1)-C(1)-C(2)-B(6)	-129.08(14)
B(4)-C(1)-C(2)-B(3)	-42.83(14)
B(5)-C(1)-C(2)-B(3)	-110.32(16)
B(6)-C(1)-C(2)-B(3)	-150.10(15)
P(1)-C(1)-C(2)-B(3)	80.82(12)

B(7)-C(2)-B(3)-C(1)	-102.87(17)
B(8)-C(2)-B(3)-C(1)	-138.21(15)
B(6)-C(2)-B(3)-C(1)	-29.89(15)
C(1)-C(2)-B(3)-B(8)	138.21(15)
B(7)-C(2)-B(3)-B(8)	35.35(16)
B(6)-C(2)-B(3)-B(8)	108.32(18)
C(1)-C(2)-B(3)-B(9)	96.71(15)
B(7)-C(2)-B(3)-B(9)	-6.2(2)
B(8)-C(2)-B(3)-B(9)	-41.51(14)
B(6)-C(2)-B(3)-B(9)	66.82(19)
C(1)-C(2)-B(3)-B(4)	37.04(12)
B(7)-C(2)-B(3)-B(4)	-65.83(19)
B(8)-C(2)-B(3)-B(4)	-101.18(15)
B(6)-C(2)-B(3)-B(4)	7.15(19)
C(1)-C(2)-B(3)-Ir(1)	-90.28(14)
B(7)-C(2)-B(3)-Ir(1)	166.85(13)
B(8)-C(2)-B(3)-Ir(1)	131.51(16)
B(6)-C(2)-B(3)-Ir(1)	-120.17(15)
B(4)-C(1)-B(3)-C(2)	134.41(15)
B(5)-C(1)-B(3)-C(2)	99.16(17)
B(6)-C(1)-B(3)-C(2)	29.14(14)
P(1)-C(1)-B(3)-C(2)	-111.15(11)
C(2)-C(1)-B(3)-B(8)	-34.72(13)
B(4)-C(1)-B(3)-B(8)	99.68(15)
B(5)-C(1)-B(3)-B(8)	64.44(18)
B(6)-C(1)-B(3)-B(8)	-5.59(19)
P(1)-C(1)-B(3)-B(8)	-145.88(12)
C(2)-C(1)-B(3)-B(9)	-95.15(15)
B(4)-C(1)-B(3)-B(9)	39.26(14)
B(5)-C(1)-B(3)-B(9)	4.0(2)
B(6)-C(1)-B(3)-B(9)	-66.01(18)
P(1)-C(1)-B(3)-B(9)	153.70(12)
C(2)-C(1)-B(3)-B(4)	-134.41(15)
B(5)-C(1)-B(3)-B(4)	-35.25(15)
B(6)-C(1)-B(3)-B(4)	-105.27(17)
P(1)-C(1)-B(3)-B(4)	114.44(12)

C(2)-C(1)-B(3)-Ir(1)	110.57(12)
B(4)-C(1)-B(3)-Ir(1)	-115.03(13)
B(5)-C(1)-B(3)-Ir(1)	-150.27(13)
B(6)-C(1)-B(3)-Ir(1)	139.70(13)
P(1)-C(1)-B(3)-Ir(1)	-0.59(11)
C(2)-C(1)-B(4)-B(10)	-62.51(19)
B(5)-C(1)-B(4)-B(10)	40.02(15)
B(6)-C(1)-B(4)-B(10)	3.9(2)
B(3)-C(1)-B(4)-B(10)	-104.58(17)
P(1)-C(1)-B(4)-B(10)	175.70(13)
C(2)-C(1)-B(4)-B(9)	1.3(2)
B(5)-C(1)-B(4)-B(9)	103.81(17)
B(6)-C(1)-B(4)-B(9)	67.74(19)
B(3)-C(1)-B(4)-B(9)	-40.79(14)
P(1)-C(1)-B(4)-B(9)	-120.50(14)
C(2)-C(1)-B(4)-B(5)	-102.53(16)
B(6)-C(1)-B(4)-B(5)	-36.07(16)
B(3)-C(1)-B(4)-B(5)	-144.60(16)
P(1)-C(1)-B(4)-B(5)	135.69(15)
C(2)-C(1)-B(4)-B(3)	42.07(14)
B(5)-C(1)-B(4)-B(3)	144.60(16)
B(6)-C(1)-B(4)-B(3)	108.53(16)
P(1)-C(1)-B(4)-B(3)	-79.71(13)
C(2)-B(3)-B(4)-C(1)	-36.54(12)
B(8)-B(3)-B(4)-C(1)	-94.54(15)
B(9)-B(3)-B(4)-C(1)	-133.47(16)
Ir(1)-B(3)-B(4)-C(1)	88.24(14)
C(2)-B(3)-B(4)-B(10)	60.51(17)
C(1)-B(3)-B(4)-B(10)	97.05(16)
B(8)-B(3)-B(4)-B(10)	2.51(19)
B(9)-B(3)-B(4)-B(10)	-36.42(15)
Ir(1)-B(3)-B(4)-B(10)	-174.72(13)
C(2)-B(3)-B(4)-B(9)	96.94(15)
C(1)-B(3)-B(4)-B(9)	133.47(16)
B(8)-B(3)-B(4)-B(9)	38.93(14)
Ir(1)-B(3)-B(4)-B(9)	-138.29(16)

C(2)-B(3)-B(4)-B(5)	-4.39(18)
C(1)-B(3)-B(4)-B(5)	32.14(14)
B(8)-B(3)-B(4)-B(5)	-62.39(18)
B(9)-B(3)-B(4)-B(5)	-101.33(17)
Ir(1)-B(3)-B(4)-B(5)	120.38(15)
C(2)-C(1)-B(5)-B(11)	1.16(19)
B(4)-C(1)-B(5)-B(11)	-101.81(16)
B(6)-C(1)-B(5)-B(11)	40.65(14)
B(3)-C(1)-B(5)-B(11)	-66.41(19)
P(1)-C(1)-B(5)-B(11)	164.80(17)
C(2)-C(1)-B(5)-B(6)	-39.49(14)
B(4)-C(1)-B(5)-B(6)	-142.46(16)
B(3)-C(1)-B(5)-B(6)	-107.06(17)
P(1)-C(1)-B(5)-B(6)	124.2(2)
C(2)-C(1)-B(5)-B(10)	63.97(18)
B(4)-C(1)-B(5)-B(10)	-39.00(14)
B(6)-C(1)-B(5)-B(10)	103.46(16)
B(3)-C(1)-B(5)-B(10)	-3.6(2)
P(1)-C(1)-B(5)-B(10)	-132.39(19)
C(2)-C(1)-B(5)-B(4)	102.97(16)
B(6)-C(1)-B(5)-B(4)	142.46(16)
B(3)-C(1)-B(5)-B(4)	35.40(16)
P(1)-C(1)-B(5)-B(4)	-93.4(2)
B(10)-B(4)-B(5)-C(1)	-134.60(16)
B(9)-B(4)-B(5)-C(1)	-96.98(16)
B(3)-B(4)-B(5)-C(1)	-32.53(14)
C(1)-B(4)-B(5)-B(11)	96.73(16)
B(10)-B(4)-B(5)-B(11)	-37.87(15)
B(9)-B(4)-B(5)-B(11)	-0.2(2)
B(3)-B(4)-B(5)-B(11)	64.20(19)
C(1)-B(4)-B(5)-B(6)	33.35(14)
B(10)-B(4)-B(5)-B(6)	-101.25(17)
B(9)-B(4)-B(5)-B(6)	-63.63(19)
B(3)-B(4)-B(5)-B(6)	0.8(2)
C(1)-B(4)-B(5)-B(10)	134.60(16)
B(9)-B(4)-B(5)-B(10)	37.62(15)

B(3)-B(4)-B(5)-B(10)	102.06(17)
B(7)-C(2)-B(6)-C(1)	138.97(15)
B(8)-C(2)-B(6)-C(1)	102.27(17)
B(3)-C(2)-B(6)-C(1)	30.12(15)
C(1)-C(2)-B(6)-B(5)	-37.06(13)
B(7)-C(2)-B(6)-B(5)	101.91(16)
B(8)-C(2)-B(6)-B(5)	65.21(19)
B(3)-C(2)-B(6)-B(5)	-6.9(2)
C(1)-C(2)-B(6)-B(11)	-98.91(15)
B(7)-C(2)-B(6)-B(11)	40.06(14)
B(8)-C(2)-B(6)-B(11)	3.4(2)
B(3)-C(2)-B(6)-B(11)	-68.79(19)
C(1)-C(2)-B(6)-B(7)	-138.97(15)
B(8)-C(2)-B(6)-B(7)	-36.70(16)
B(3)-C(2)-B(6)-B(7)	-108.85(17)
B(4)-C(1)-B(6)-C(2)	-100.37(16)
B(5)-C(1)-B(6)-C(2)	-136.88(15)
B(3)-C(1)-B(6)-C(2)	-29.34(14)
P(1)-C(1)-B(6)-C(2)	90.06(18)
C(2)-C(1)-B(6)-B(5)	136.88(15)
B(4)-C(1)-B(6)-B(5)	36.52(16)
B(3)-C(1)-B(6)-B(5)	107.54(16)
P(1)-C(1)-B(6)-B(5)	-133.06(19)
C(2)-C(1)-B(6)-B(11)	96.36(16)
B(4)-C(1)-B(6)-B(11)	-4.0(2)
B(5)-C(1)-B(6)-B(11)	-40.52(15)
B(3)-C(1)-B(6)-B(11)	67.02(19)
P(1)-C(1)-B(6)-B(11)	-173.58(15)
C(2)-C(1)-B(6)-B(7)	34.72(13)
B(4)-C(1)-B(6)-B(7)	-65.65(19)
B(5)-C(1)-B(6)-B(7)	-102.17(16)
B(3)-C(1)-B(6)-B(7)	5.38(19)
P(1)-C(1)-B(6)-B(7)	124.77(16)
C(1)-B(5)-B(6)-C(2)	36.06(13)
B(11)-B(5)-B(6)-C(2)	-97.35(16)
B(10)-B(5)-B(6)-C(2)	-59.26(19)

B(4)-B(5)-B(6)-C(2)	3.30(19)
B(11)-B(5)-B(6)-C(1)	-133.41(16)
B(10)-B(5)-B(6)-C(1)	-95.31(17)
B(4)-B(5)-B(6)-C(1)	-32.76(14)
C(1)-B(5)-B(6)-B(11)	133.41(16)
B(10)-B(5)-B(6)-B(11)	38.09(15)
B(4)-B(5)-B(6)-B(11)	100.65(17)
C(1)-B(5)-B(6)-B(7)	95.82(16)
B(11)-B(5)-B(6)-B(7)	-37.58(15)
B(10)-B(5)-B(6)-B(7)	0.5(2)
B(4)-B(5)-B(6)-B(7)	63.07(19)
C(1)-C(2)-B(7)-B(11)	-1.5(2)
B(8)-C(2)-B(7)-B(11)	103.52(16)
B(6)-C(2)-B(7)-B(11)	-40.47(14)
B(3)-C(2)-B(7)-B(11)	68.7(2)
C(1)-C(2)-B(7)-B(12)	-64.68(19)
B(8)-C(2)-B(7)-B(12)	40.32(15)
B(6)-C(2)-B(7)-B(12)	-103.67(16)
B(3)-C(2)-B(7)-B(12)	5.5(2)
C(1)-C(2)-B(7)-B(6)	38.99(14)
B(8)-C(2)-B(7)-B(6)	143.99(15)
B(3)-C(2)-B(7)-B(6)	109.20(17)
C(1)-C(2)-B(7)-B(8)	-105.00(16)
B(6)-C(2)-B(7)-B(8)	-143.99(15)
B(3)-C(2)-B(7)-B(8)	-34.79(16)
C(1)-B(6)-B(7)-C(2)	-34.40(13)
B(5)-B(6)-B(7)-C(2)	-95.64(16)
B(11)-B(6)-B(7)-C(2)	-133.39(16)
C(2)-B(6)-B(7)-B(11)	133.39(16)
C(1)-B(6)-B(7)-B(11)	98.99(16)
B(5)-B(6)-B(7)-B(11)	37.75(15)
C(2)-B(6)-B(7)-B(12)	95.11(16)
C(1)-B(6)-B(7)-B(12)	60.71(18)
B(5)-B(6)-B(7)-B(12)	-0.5(2)
B(11)-B(6)-B(7)-B(12)	-38.28(15)
C(2)-B(6)-B(7)-B(8)	31.67(13)

C(1)-B(6)-B(7)-B(8)	-2.73(19)
B(5)-B(6)-B(7)-B(8)	-63.97(19)
B(11)-B(6)-B(7)-B(8)	-101.72(16)
C(1)-C(2)-B(8)-B(9)	3.2(2)
B(7)-C(2)-B(8)-B(9)	-102.33(16)
B(6)-C(2)-B(8)-B(9)	-66.0(2)
B(3)-C(2)-B(8)-B(9)	43.07(14)
C(1)-C(2)-B(8)-B(12)	65.47(18)
B(7)-C(2)-B(8)-B(12)	-40.02(14)
B(6)-C(2)-B(8)-B(12)	-3.7(2)
B(3)-C(2)-B(8)-B(12)	105.39(16)
C(1)-C(2)-B(8)-B(3)	-39.91(15)
B(7)-C(2)-B(8)-B(3)	-145.40(16)
B(6)-C(2)-B(8)-B(3)	-109.05(17)
C(1)-C(2)-B(8)-B(7)	105.49(17)
B(6)-C(2)-B(8)-B(7)	36.35(16)
B(3)-C(2)-B(8)-B(7)	145.40(16)
C(1)-B(3)-B(8)-C(2)	34.01(12)
B(9)-B(3)-B(8)-C(2)	130.62(16)
B(4)-B(3)-B(8)-C(2)	91.87(15)
Ir(1)-B(3)-B(8)-C(2)	-91.71(19)
C(2)-B(3)-B(8)-B(9)	-130.62(16)
C(1)-B(3)-B(8)-B(9)	-96.60(15)
B(4)-B(3)-B(8)-B(9)	-38.75(14)
Ir(1)-B(3)-B(8)-B(9)	137.7(2)
C(2)-B(3)-B(8)-B(12)	-94.17(16)
C(1)-B(3)-B(8)-B(12)	-60.16(17)
B(9)-B(3)-B(8)-B(12)	36.45(15)
B(4)-B(3)-B(8)-B(12)	-2.30(19)
Ir(1)-B(3)-B(8)-B(12)	174.12(15)
C(2)-B(3)-B(8)-B(7)	-30.62(14)
C(1)-B(3)-B(8)-B(7)	3.40(18)
B(9)-B(3)-B(8)-B(7)	100.00(17)
B(4)-B(3)-B(8)-B(7)	61.25(18)
Ir(1)-B(3)-B(8)-B(7)	-122.33(18)
B(11)-B(7)-B(8)-C(2)	-95.63(16)

B(12)-B(7)-B(8)-C(2)	-133.34(16)
B(6)-B(7)-B(8)-C(2)	-32.10(14)
C(2)-B(7)-B(8)-B(9)	96.02(16)
B(11)-B(7)-B(8)-B(9)	0.4(2)
B(12)-B(7)-B(8)-B(9)	-37.32(15)
B(6)-B(7)-B(8)-B(9)	63.92(18)
C(2)-B(7)-B(8)-B(12)	133.34(16)
B(11)-B(7)-B(8)-B(12)	37.71(15)
B(6)-B(7)-B(8)-B(12)	101.24(17)
C(2)-B(7)-B(8)-B(3)	31.60(14)
B(11)-B(7)-B(8)-B(3)	-64.03(19)
B(12)-B(7)-B(8)-B(3)	-101.74(17)
B(6)-B(7)-B(8)-B(3)	-0.5(2)
C(2)-B(8)-B(9)-B(4)	-2.2(2)
B(12)-B(8)-B(9)-B(4)	-99.26(17)
B(3)-B(8)-B(9)-B(4)	40.68(14)
B(7)-B(8)-B(9)-B(4)	-62.33(19)
C(2)-B(8)-B(9)-B(12)	97.03(16)
B(3)-B(8)-B(9)-B(12)	139.93(16)
B(7)-B(8)-B(9)-B(12)	36.92(15)
C(2)-B(8)-B(9)-B(10)	59.96(18)
B(12)-B(8)-B(9)-B(10)	-37.08(15)
B(3)-B(8)-B(9)-B(10)	102.86(16)
B(7)-B(8)-B(9)-B(10)	-0.2(2)
C(2)-B(8)-B(9)-B(3)	-42.90(14)
B(12)-B(8)-B(9)-B(3)	-139.93(16)
B(7)-B(8)-B(9)-B(3)	-103.01(16)
C(1)-B(4)-B(9)-B(8)	0.6(2)
B(10)-B(4)-B(9)-B(8)	100.25(17)
B(5)-B(4)-B(9)-B(8)	62.97(19)
B(3)-B(4)-B(9)-B(8)	-40.24(14)
C(1)-B(4)-B(9)-B(12)	-62.44(18)
B(10)-B(4)-B(9)-B(12)	37.17(14)
B(5)-B(4)-B(9)-B(12)	-0.12(19)
B(3)-B(4)-B(9)-B(12)	-103.32(16)
C(1)-B(4)-B(9)-B(10)	-99.61(16)

B(5)-B(4)-B(9)-B(10)	-37.28(14)
B(3)-B(4)-B(9)-B(10)	-140.48(16)
C(1)-B(4)-B(9)-B(3)	40.88(14)
B(10)-B(4)-B(9)-B(3)	140.48(16)
B(5)-B(4)-B(9)-B(3)	103.20(16)
C(2)-B(3)-B(9)-B(8)	40.30(14)
C(1)-B(3)-B(9)-B(8)	96.76(15)
B(4)-B(3)-B(9)-B(8)	134.80(16)
Ir(1)-B(3)-B(9)-B(8)	-128.9(3)
C(2)-B(3)-B(9)-B(4)	-94.50(15)
C(1)-B(3)-B(9)-B(4)	-38.04(13)
B(8)-B(3)-B(9)-B(4)	-134.80(16)
Ir(1)-B(3)-B(9)-B(4)	96.3(2)
C(2)-B(3)-B(9)-B(12)	4.08(19)
C(1)-B(3)-B(9)-B(12)	60.54(18)
B(8)-B(3)-B(9)-B(12)	-36.22(15)
B(4)-B(3)-B(9)-B(12)	98.58(17)
Ir(1)-B(3)-B(9)-B(12)	-165.10(19)
C(2)-B(3)-B(9)-B(10)	-59.15(18)
C(1)-B(3)-B(9)-B(10)	-2.69(19)
B(8)-B(3)-B(9)-B(10)	-99.45(17)
B(4)-B(3)-B(9)-B(10)	35.35(15)
Ir(1)-B(3)-B(9)-B(10)	131.7(2)
C(1)-B(4)-B(10)-B(12)	61.76(19)
B(9)-B(4)-B(10)-B(12)	-37.76(15)
B(5)-B(4)-B(10)-B(12)	101.21(17)
B(3)-B(4)-B(10)-B(12)	-1.8(2)
C(1)-B(4)-B(10)-B(5)	-39.45(14)
B(9)-B(4)-B(10)-B(5)	-138.97(16)
B(3)-B(4)-B(10)-B(5)	-102.99(16)
C(1)-B(4)-B(10)-B(11)	-2.2(2)
B(9)-B(4)-B(10)-B(11)	-101.70(17)
B(5)-B(4)-B(10)-B(11)	37.27(15)
B(3)-B(4)-B(10)-B(11)	-65.72(19)
C(1)-B(4)-B(10)-B(9)	99.52(16)
B(5)-B(4)-B(10)-B(9)	138.97(16)

B(3)-B(4)-B(10)-B(9)	35.98(14)
C(1)-B(5)-B(10)-B(4)	38.32(14)
B(11)-B(5)-B(10)-B(4)	137.88(16)
B(6)-B(5)-B(10)-B(4)	100.06(17)
C(1)-B(5)-B(10)-B(12)	-62.04(19)
B(11)-B(5)-B(10)-B(12)	37.52(15)
B(6)-B(5)-B(10)-B(12)	-0.3(2)
B(4)-B(5)-B(10)-B(12)	-100.36(17)
C(1)-B(5)-B(10)-B(11)	-99.56(16)
B(6)-B(5)-B(10)-B(11)	-37.82(15)
B(4)-B(5)-B(10)-B(11)	-137.88(16)
C(1)-B(5)-B(10)-B(9)	1.5(2)
B(11)-B(5)-B(10)-B(9)	101.10(17)
B(6)-B(5)-B(10)-B(9)	63.29(19)
B(4)-B(5)-B(10)-B(9)	-36.78(15)
B(8)-B(9)-B(10)-B(4)	-100.18(16)
B(12)-B(9)-B(10)-B(4)	-137.61(16)
B(3)-B(9)-B(10)-B(4)	-36.26(15)
B(8)-B(9)-B(10)-B(12)	37.43(14)
B(4)-B(9)-B(10)-B(12)	137.61(16)
B(3)-B(9)-B(10)-B(12)	101.35(17)
B(8)-B(9)-B(10)-B(5)	-63.12(19)
B(4)-B(9)-B(10)-B(5)	37.06(15)
B(12)-B(9)-B(10)-B(5)	-100.55(17)
B(3)-B(9)-B(10)-B(5)	0.8(2)
B(8)-B(9)-B(10)-B(11)	-0.1(2)
B(4)-B(9)-B(10)-B(11)	100.06(16)
B(12)-B(9)-B(10)-B(11)	-37.56(14)
B(3)-B(9)-B(10)-B(11)	63.79(19)
C(2)-B(7)-B(11)-B(5)	2.1(2)
B(12)-B(7)-B(11)-B(5)	99.92(17)
B(6)-B(7)-B(11)-B(5)	-37.94(15)
B(8)-B(7)-B(11)-B(5)	62.76(19)
C(2)-B(7)-B(11)-B(6)	40.09(14)
B(12)-B(7)-B(11)-B(6)	137.86(16)
B(8)-B(7)-B(11)-B(6)	100.70(16)

C(2)-B(7)-B(11)-B(10)	-61.08(18)
B(12)-B(7)-B(11)-B(10)	36.70(14)
B(6)-B(7)-B(11)-B(10)	-101.17(16)
B(8)-B(7)-B(11)-B(10)	-0.5(2)
C(2)-B(7)-B(11)-B(12)	-97.78(16)
B(6)-B(7)-B(11)-B(12)	-137.86(16)
B(8)-B(7)-B(11)-B(12)	-37.16(14)
C(1)-B(5)-B(11)-B(7)	-2.0(2)
B(6)-B(5)-B(11)-B(7)	38.21(15)
B(10)-B(5)-B(11)-B(7)	-99.61(17)
B(4)-B(5)-B(11)-B(7)	-62.41(19)
C(1)-B(5)-B(11)-B(6)	-40.25(14)
B(10)-B(5)-B(11)-B(6)	-137.82(17)
B(4)-B(5)-B(11)-B(6)	-100.62(16)
C(1)-B(5)-B(11)-B(10)	97.57(16)
B(6)-B(5)-B(11)-B(10)	137.82(17)
B(4)-B(5)-B(11)-B(10)	37.20(14)
C(1)-B(5)-B(11)-B(12)	60.88(18)
B(6)-B(5)-B(11)-B(12)	101.13(16)
B(10)-B(5)-B(11)-B(12)	-36.69(15)
B(4)-B(5)-B(11)-B(12)	0.51(19)
C(2)-B(6)-B(11)-B(7)	-38.98(14)
C(1)-B(6)-B(11)-B(7)	-97.56(16)
B(5)-B(6)-B(11)-B(7)	-137.54(16)
C(2)-B(6)-B(11)-B(5)	98.56(16)
C(1)-B(6)-B(11)-B(5)	39.98(14)
B(7)-B(6)-B(11)-B(5)	137.54(16)
C(2)-B(6)-B(11)-B(10)	60.93(19)
C(1)-B(6)-B(11)-B(10)	2.4(2)
B(5)-B(6)-B(11)-B(10)	-37.63(15)
B(7)-B(6)-B(11)-B(10)	99.91(17)
C(2)-B(6)-B(11)-B(12)	-1.49(19)
C(1)-B(6)-B(11)-B(12)	-60.07(18)
B(5)-B(6)-B(11)-B(12)	-100.05(17)
B(7)-B(6)-B(11)-B(12)	37.49(15)
B(4)-B(10)-B(11)-B(7)	63.65(19)

B(12)-B(10)-B(11)-B(7)	-36.93(14)
B(5)-B(10)-B(11)-B(7)	101.42(16)
B(9)-B(10)-B(11)-B(7)	0.4(2)
B(4)-B(10)-B(11)-B(5)	-37.77(15)
B(12)-B(10)-B(11)-B(5)	-138.35(16)
B(9)-B(10)-B(11)-B(5)	-101.05(17)
B(4)-B(10)-B(11)-B(6)	-0.1(2)
B(12)-B(10)-B(11)-B(6)	-100.73(17)
B(5)-B(10)-B(11)-B(6)	37.62(15)
B(9)-B(10)-B(11)-B(6)	-63.4(2)
B(4)-B(10)-B(11)-B(12)	100.58(17)
B(5)-B(10)-B(11)-B(12)	138.35(16)
B(9)-B(10)-B(11)-B(12)	37.30(15)
B(4)-B(10)-B(12)-B(7)	-63.9(2)
B(5)-B(10)-B(12)-B(7)	0.0(2)
B(11)-B(10)-B(12)-B(7)	36.93(15)
B(9)-B(10)-B(12)-B(7)	-101.55(17)
B(4)-B(10)-B(12)-B(8)	0.3(2)
B(5)-B(10)-B(12)-B(8)	64.1(2)
B(11)-B(10)-B(12)-B(8)	101.11(16)
B(9)-B(10)-B(12)-B(8)	-37.37(14)
B(4)-B(10)-B(12)-B(9)	37.67(15)
B(5)-B(10)-B(12)-B(9)	101.52(17)
B(11)-B(10)-B(12)-B(9)	138.48(15)
B(4)-B(10)-B(12)-B(11)	-100.81(16)
B(5)-B(10)-B(12)-B(11)	-36.97(15)
B(9)-B(10)-B(12)-B(11)	-138.48(15)
C(2)-B(7)-B(12)-B(10)	61.89(19)
B(11)-B(7)-B(12)-B(10)	-37.37(15)
B(6)-B(7)-B(12)-B(10)	0.4(2)
B(8)-B(7)-B(12)-B(10)	101.26(17)
C(2)-B(7)-B(12)-B(8)	-39.37(14)
B(11)-B(7)-B(12)-B(8)	-138.64(16)
B(6)-B(7)-B(12)-B(8)	-100.91(17)
C(2)-B(7)-B(12)-B(9)	-2.3(2)
B(11)-B(7)-B(12)-B(9)	-101.56(17)

B(6)-B(7)-B(12)-B(9)	-63.8(2)
B(8)-B(7)-B(12)-B(9)	37.08(15)
C(2)-B(7)-B(12)-B(11)	99.26(16)
B(6)-B(7)-B(12)-B(11)	37.72(15)
B(8)-B(7)-B(12)-B(11)	138.64(16)
C(2)-B(8)-B(12)-B(10)	-61.47(18)
B(9)-B(8)-B(12)-B(10)	37.87(15)
B(3)-B(8)-B(12)-B(10)	1.3(2)
B(7)-B(8)-B(12)-B(10)	-100.55(17)
C(2)-B(8)-B(12)-B(7)	39.08(14)
B(9)-B(8)-B(12)-B(7)	138.42(16)
B(3)-B(8)-B(12)-B(7)	101.86(16)
C(2)-B(8)-B(12)-B(9)	-99.34(16)
B(3)-B(8)-B(12)-B(9)	-36.56(15)
B(7)-B(8)-B(12)-B(9)	-138.42(16)
C(2)-B(8)-B(12)-B(11)	2.34(19)
B(9)-B(8)-B(12)-B(11)	101.68(17)
B(3)-B(8)-B(12)-B(11)	65.12(19)
B(7)-B(8)-B(12)-B(11)	-36.74(15)
B(8)-B(9)-B(12)-B(10)	-138.00(16)
B(4)-B(9)-B(12)-B(10)	-37.05(14)
B(3)-B(9)-B(12)-B(10)	-101.68(17)
B(8)-B(9)-B(12)-B(7)	-37.59(15)
B(4)-B(9)-B(12)-B(7)	63.36(19)
B(10)-B(9)-B(12)-B(7)	100.41(17)
B(3)-B(9)-B(12)-B(7)	-1.3(2)
B(4)-B(9)-B(12)-B(8)	100.95(16)
B(10)-B(9)-B(12)-B(8)	138.00(16)
B(3)-B(9)-B(12)-B(8)	36.32(15)
B(8)-B(9)-B(12)-B(11)	-100.52(16)
B(4)-B(9)-B(12)-B(11)	0.4(2)
B(10)-B(9)-B(12)-B(11)	37.49(14)
B(3)-B(9)-B(12)-B(11)	-64.2(2)
B(7)-B(11)-B(12)-B(10)	138.25(16)
B(5)-B(11)-B(12)-B(10)	37.08(14)
B(6)-B(11)-B(12)-B(10)	100.35(17)

B(5)-B(11)-B(12)-B(7)	-101.17(16)
B(6)-B(11)-B(12)-B(7)	-37.90(15)
B(10)-B(11)-B(12)-B(7)	-138.25(16)
B(7)-B(11)-B(12)-B(8)	37.37(15)
B(5)-B(11)-B(12)-B(8)	-63.80(19)
B(6)-B(11)-B(12)-B(8)	-0.5(2)
B(10)-B(11)-B(12)-B(8)	-100.87(17)
B(7)-B(11)-B(12)-B(9)	100.58(17)
B(5)-B(11)-B(12)-B(9)	-0.6(2)
B(6)-B(11)-B(12)-B(9)	62.68(19)
B(10)-B(11)-B(12)-B(9)	-37.67(15)
C(2)-C(1)-P(1)-C(4)	63.90(14)
B(4)-C(1)-P(1)-C(4)	-173.88(13)
B(5)-C(1)-P(1)-C(4)	-99.8(2)
B(6)-C(1)-P(1)-C(4)	-4.2(2)
B(3)-C(1)-P(1)-C(4)	124.43(11)
C(2)-C(1)-P(1)-C(3)	-177.09(12)
B(4)-C(1)-P(1)-C(3)	-54.87(15)
B(5)-C(1)-P(1)-C(3)	19.2(2)
B(6)-C(1)-P(1)-C(3)	114.85(18)
B(3)-C(1)-P(1)-C(3)	-116.56(11)
C(2)-C(1)-P(1)-Ir(1)	-60.02(11)
B(4)-C(1)-P(1)-Ir(1)	62.20(13)
B(5)-C(1)-P(1)-Ir(1)	136.3(2)
B(6)-C(1)-P(1)-Ir(1)	-128.08(17)
B(3)-C(1)-P(1)-Ir(1)	0.51(9)
C(4)-P(1)-C(3)-C(6)	75.75(17)
C(1)-P(1)-C(3)-C(6)	-39.59(17)
Ir(1)-P(1)-C(3)-C(6)	-141.38(13)
C(4)-P(1)-C(3)-C(5)	-51.86(17)
C(1)-P(1)-C(3)-C(5)	-167.21(14)
Ir(1)-P(1)-C(3)-C(5)	91.01(14)
C(3)-P(1)-C(4)-C(8)	81.99(16)
C(1)-P(1)-C(4)-C(8)	-161.07(14)
Ir(1)-P(1)-C(4)-C(8)	-57.90(15)
C(3)-P(1)-C(4)-C(7)	-46.71(17)

C(1)-P(1)-C(4)-C(7)	70.22(16)
Ir(1)-P(1)-C(4)-C(7)	173.39(12)

Symmetry transformations used to generate equivalent atoms:

X-Ray Structure Determination for Complex 7

A yellow prism fragment ($0.516 \times 0.193 \times 0.068 \text{ mm}^3$) was used for the single crystal x-ray diffraction study of $[[\text{CB}_{11}\text{H}_{11}]\text{P}[\text{C}_3\text{H}_7]_2\text{C}_8\text{H}_{12}\text{Ir}]^-\cdot\text{N}[\text{C}_4\text{H}_{12}]^+ \cdot [\text{C}_4\text{H}_8\text{O}]$ (sample vL147JE_0m). The crystal was coated with paratone oil and mounted on to a cryo-loop glass fiber. X-ray intensity data were collected at 100(2) K on a Bruker APEX2³ platform-CCD x-ray diffractometer system (fine focus Mo-radiation, $\lambda = 0.71073 \text{ \AA}$, 50KV/30mA power). The CCD detector was placed at a distance of 5.0600 cm from the crystal.

A total of 4800 frames were collected for a sphere of reflections (with scan width of 0.5° in ω and ϕ , starting ω and 2θ angles of -30° , and ϕ angles of 0° , 90° , 120° , 180° , 240° , and 270° , for every 360 frames, and 720 frames with ϕ -scan from 0 - 360° , 10 sec/frame exposure time). The frames were integrated using the Bruker SAINT software package⁴ and using a narrow-frame integration algorithm. Based on a monoclinic crystal system, the integrated frames yielded a total of 49431 reflections at a maximum 2θ angle of 61.012° ($0.70 \text{ \AA}$ resolution), of which 10323 were independent reflections ($R_{\text{int}} = 0.0221$, $R_{\text{sig}} = 0.0174$, redundancy = 4.8, completeness = 100%) and 9978 (96.7%) reflections were greater than $2\sigma(I)$. The unit cell parameters were, $\mathbf{a} = 10.3713(3) \text{ \AA}$, $\mathbf{b} = 11.0485(3) \text{ \AA}$, $\mathbf{c} = 14.7843(4) \text{ \AA}$, $\beta = 92.3520(5)^\circ$, $V = 1692.67(8) \text{ \AA}^3$, $Z = 2$, calculated density $D_c = 1.454 \text{ g/cm}^3$. Absorption corrections were applied (absorption coefficient $\mu = 4.090 \text{ mm}^{-1}$; min/max transmission = 0.227 / 0.768) to the raw intensity data using the SADABS program⁵.

The Bruker SHELXTL software package⁶ was used for phase determination and structure refinement. The distribution of intensities ($E^2-1 = 0.656$) and systematic absent reflections indicated two possible space groups, P2(1) and P2(1)/m. The space group P2(1) (#4) was later determined to be correct. Direct methods of phase determination followed by two Fourier cycles of refinement led to an electron density map from which most of the non-hydrogen atoms were identified in the asymmetric unit of the unit cell. With subsequent isotropic refinement, all of the non-hydrogen atoms were identified. There was one anion of $[\text{CB}_{11}\text{H}_{11}]\text{P}[\text{C}_3\text{H}_7]_2\text{C}_8\text{H}_{12}\text{Ir}]^-$, one cation of $\text{N}[\text{C}_4\text{H}_{12}]^+$, and one disordered THF solvent (disordered site occupancy ratios was 65%/35%) present in the asymmetric unit of the unit cell.

Atomic coordinates, isotropic and anisotropic displacement parameters of all the non-hydrogen atoms were refined by means of a full matrix least-squares procedure on F^2 . The H-atoms were included in the refinement in calculated positions riding on the atoms to which they were attached, except the H-atoms bonded to C1A, C2A, C5A, and C6A were refined unrestrained. The refinement converged at $R1 = 0.0201$, $wR2 = 0.0496$, with intensity $I > 2\sigma(I)$. The absolute structure Flack parameter, $x = -0.011(5)$. The largest peak/hole in the final difference map was $1.009/-0.738 \text{ e/\AA}^3$. The high residual electron density peak/hole is probably due to absorption correction errors and unresolved possible THF disorder.

Full crystallographic data for compound **7** can be found at the Cambridge crystallographic database under reference # CCDC 1057297

Table 7. Crystal data and structure refinement for vL147JE_0m.

Identification code	vL147JE_0m	
Empirical formula	C ₂₃ H ₅₇ B ₁₁ Cl Ir N O P	
Formula weight	741.22	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 10.3713(3) Å	α = 90°.
	b = 11.0485(3) Å	β = 92.3520(5)°.
	c = 14.7843(4) Å	γ = 90°.
Volume	1692.67(8) Å ³	
Z	2	
Density (calculated)	1.454 Mg/m ³	
Absorption coefficient	4.090 mm ⁻¹	
F(000)	748	
Crystal size	0.516 x 0.193 x 0.068 mm ³	
Theta range for data collection	1.965 to 30.506°.	
Index ranges	-14 ≤ h ≤ 14, -15 ≤ k ≤ 15, -21 ≤ l ≤ 21	
Reflections collected	49431	
Independent reflections	10323 [R(int) = 0.0221]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	10323 / 52 / 394	
Goodness-of-fit on F ²	1.056	
Final R indices [I > 2σ(I)]	R1 = 0.0201, wR2 = 0.0496	
R indices (all data)	R1 = 0.0211, wR2 = 0.0501	
Absolute structure parameter	-0.011(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.009 and -0.738 e.Å ⁻³	

Table 8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)

for vL147JE_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	5454(1)	2783(1)	3336(1)	10(1)
Cl(1)	5314(1)	1935(1)	1846(1)	17(1)
C(1A)	3458(4)	2196(4)	3462(3)	17(1)
C(2A)	3443(4)	3381(4)	3123(3)	16(1)
C(3A)	3136(3)	4488(4)	3680(3)	19(1)
C(4A)	4368(4)	5077(3)	4100(3)	20(1)
C(5A)	5436(3)	4171(3)	4299(2)	14(1)
C(6A)	5264(3)	3051(3)	4752(2)	16(1)
C(7A)	3964(3)	2662(6)	5113(2)	19(1)
C(8A)	3210(4)	1866(4)	4428(3)	21(1)
P(1)	7741(1)	2750(2)	3351(1)	10(1)
C(1)	8297(4)	4075(4)	2664(3)	11(1)
B(2)	7957(4)	4067(4)	1505(3)	17(1)
B(3)	7080(4)	5025(4)	2226(3)	15(1)
B(4)	8146(4)	5513(4)	3119(3)	15(1)
B(5)	9696(4)	4860(4)	2954(3)	16(1)
B(6)	9575(4)	3974(4)	1948(3)	17(1)
B(7)	9186(4)	4951(5)	1022(3)	22(1)
B(8)	7648(4)	5600(4)	1198(3)	20(1)
B(9)	7767(4)	6492(4)	2200(3)	20(1)
B(10)	9390(4)	6393(4)	2656(3)	20(1)
B(11)	10267(4)	5438(4)	1922(3)	20(1)
B(12)	9070(4)	6451(4)	1459(3)	23(1)
C(2)	8776(3)	2755(6)	4420(2)	14(1)
C(3)	8552(5)	1589(5)	4960(3)	19(1)
C(4)	8697(4)	3837(5)	5067(3)	17(1)
C(5)	8360(5)	1379(5)	2768(4)	19(1)
C(6)	7580(5)	234(3)	2962(3)	25(1)

C(7)	9812(5)	1106(5)	2915(4)	28(1)
N(1C)	6714(3)	9300(3)	9912(2)	17(1)
C(1C)	7471(4)	8323(4)	9475(3)	20(1)
C(2C)	7608(4)	10189(5)	10363(4)	40(1)
C(3C)	5898(4)	9931(4)	9206(3)	28(1)
C(4C)	5855(6)	8750(5)	10581(4)	39(1)
O(1S)	3448(15)	7529(16)	1419(13)	29(2)
C(1S)	3817(11)	7650(14)	2349(9)	50(2)
C(2S)	3576(12)	8948(9)	2582(6)	60(3)
C(3S)	2624(10)	9388(10)	1881(9)	61(2)
C(4S)	2485(14)	8413(13)	1204(12)	61(2)
O(1D)	3680(30)	7680(30)	1530(20)	34(5)
C(1D)	2590(30)	8210(20)	1079(14)	42(3)
C(2D)	2093(19)	9171(18)	1646(13)	61(2)
C(3D)	2611(18)	8927(15)	2540(10)	42(3)
C(4D)	3490(20)	7880(30)	2464(18)	50(2)

Table 9. Bond lengths [Å] and angles [°] for vL147JE_0m.

Ir(1)-C(5A)	2.093(3)	B(2)-B(7)	1.778(6)
Ir(1)-C(6A)	2.130(3)	B(2)-B(3)	1.779(6)
Ir(1)-C(1A)	2.184(4)	B(2)-B(8)	1.779(6)
Ir(1)-C(2A)	2.199(4)	B(2)-B(6)	1.779(6)
Ir(1)-P(1)	2.3709(7)	B(2)-H(2)	1.1200
Ir(1)-Cl(1)	2.3941(8)	B(3)-B(8)	1.770(6)
C(1A)-C(2A)	1.401(5)	B(3)-B(4)	1.771(6)
C(1A)-C(8A)	1.507(6)	B(3)-B(9)	1.771(6)
C(1A)-H(1A)	0.93(3)	B(3)-H(3)	1.1200
C(2A)-C(3A)	1.516(6)	B(4)-B(9)	1.768(6)
C(2A)-H(2A)	0.94(3)	B(4)-B(10)	1.775(6)
C(3A)-C(4A)	1.541(5)	B(4)-B(5)	1.788(6)
C(3A)-H(3A)	0.9900	B(4)-H(4)	1.1200
C(3A)-H(3B)	0.9900	B(5)-B(10)	1.776(6)
C(4A)-C(5A)	1.512(5)	B(5)-B(11)	1.778(6)
C(4A)-H(4A)	0.9900	B(5)-B(6)	1.781(7)
C(4A)-H(4B)	0.9900	B(5)-H(5)	1.1200
C(5A)-C(6A)	1.422(5)	B(6)-B(11)	1.771(6)
C(5A)-H(5A)	0.93(3)	B(6)-B(7)	1.776(6)
C(6A)-C(7A)	1.532(5)	B(6)-H(6)	1.1200
C(6A)-H(6A)	0.94(3)	B(7)-B(8)	1.778(7)
C(7A)-C(8A)	1.532(6)	B(7)-B(12)	1.785(7)
C(7A)-H(7A)	0.9900	B(7)-B(11)	1.787(6)
C(7A)-H(7B)	0.9900	B(7)-H(7)	1.1200
C(8A)-H(8A)	0.9900	B(8)-B(12)	1.778(6)
C(8A)-H(8B)	0.9900	B(8)-B(9)	1.779(7)
P(1)-C(5)	1.869(5)	B(8)-H(8)	1.1200
P(1)-C(2)	1.874(3)	B(9)-B(12)	1.775(7)
P(1)-C(1)	1.885(5)	B(9)-B(10)	1.791(6)
C(1)-B(5)	1.729(6)	B(9)-H(9)	1.1200
C(1)-B(6)	1.734(6)	B(10)-B(12)	1.788(6)
C(1)-B(2)	1.735(6)	B(10)-B(11)	1.789(7)
C(1)-B(4)	1.735(6)	B(10)-H(10)	1.1200
C(1)-B(3)	1.746(6)	B(11)-B(12)	1.786(6)

B(11)-H(11)	1.1200	O(1S)-C(1S)	1.418(19)
B(12)-H(12)	1.1200	O(1S)-C(4S)	1.423(18)
C(2)-C(4)	1.534(7)	C(1S)-C(2S)	1.498(15)
C(2)-C(3)	1.539(7)	C(1S)-H(1E)	0.9900
C(2)-H(2B)	1.0000	C(1S)-H(1F)	0.9900
C(3)-H(3C)	0.9800	C(2S)-C(3S)	1.483(13)
C(3)-H(3D)	0.9800	C(2S)-H(2F)	0.9900
C(3)-H(3E)	0.9800	C(2S)-H(2G)	0.9900
C(4)-H(4C)	0.9800	C(3S)-C(4S)	1.474(13)
C(4)-H(4D)	0.9800	C(3S)-H(3I)	0.9900
C(4)-H(4E)	0.9800	C(3S)-H(3J)	0.9900
C(5)-C(6)	1.535(7)	C(4S)-H(4I)	0.9900
C(5)-C(7)	1.543(7)	C(4S)-H(4J)	0.9900
C(5)-H(5B)	1.0000	O(1D)-C(1D)	1.42(3)
C(6)-H(6B)	0.9800	O(1D)-C(4D)	1.43(3)
C(6)-H(6C)	0.9800	C(1D)-C(2D)	1.456(16)
C(6)-H(6D)	0.9800	C(1D)-H(1G)	0.9900
C(7)-H(7C)	0.9800	C(1D)-H(1H)	0.9900
C(7)-H(7D)	0.9800	C(2D)-C(3D)	1.432(17)
C(7)-H(7E)	0.9800	C(2D)-H(2H)	0.9900
N(1C)-C(4C)	1.488(6)	C(2D)-H(2I)	0.9900
N(1C)-C(2C)	1.489(5)	C(3D)-C(4D)	1.477(18)
N(1C)-C(3C)	1.490(5)	C(3D)-H(3K)	0.9900
N(1C)-C(1C)	1.496(5)	C(3D)-H(3L)	0.9900
C(1C)-H(1B)	0.9800	C(4D)-H(4K)	0.9900
C(1C)-H(1C)	0.9800	C(4D)-H(4L)	0.9900
C(1C)-H(1D)	0.9800		
C(2C)-H(2C)	0.9800	C(5A)-Ir(1)-C(6A)	39.32(13)
C(2C)-H(2D)	0.9800	C(5A)-Ir(1)-C(1A)	97.17(15)
C(2C)-H(2E)	0.9800	C(6A)-Ir(1)-C(1A)	80.33(15)
C(3C)-H(3F)	0.9800	C(5A)-Ir(1)-C(2A)	80.93(14)
C(3C)-H(3G)	0.9800	C(6A)-Ir(1)-C(2A)	88.50(14)
C(3C)-H(3H)	0.9800	C(1A)-Ir(1)-C(2A)	37.28(13)
C(4C)-H(4F)	0.9800	C(5A)-Ir(1)-P(1)	92.42(10)
C(4C)-H(4G)	0.9800	C(6A)-Ir(1)-P(1)	97.24(9)
C(4C)-H(4H)	0.9800	C(1A)-Ir(1)-P(1)	161.05(12)

C(2A)-Ir(1)-P(1)	161.56(11)	C(5A)-C(6A)-C(7A)	122.5(3)
C(5A)-Ir(1)-Cl(1)	155.66(10)	C(5A)-C(6A)-Ir(1)	68.93(19)
C(6A)-Ir(1)-Cl(1)	162.58(9)	C(7A)-C(6A)-Ir(1)	114.9(2)
C(1A)-Ir(1)-Cl(1)	86.56(11)	C(5A)-C(6A)-H(6A)	115(4)
C(2A)-Ir(1)-Cl(1)	87.95(11)	C(7A)-C(6A)-H(6A)	113(3)
P(1)-Ir(1)-Cl(1)	91.43(3)	Ir(1)-C(6A)-H(6A)	115(3)
C(2A)-C(1A)-C(8A)	124.4(4)	C(6A)-C(7A)-C(8A)	111.3(3)
C(2A)-C(1A)-Ir(1)	71.9(3)	C(6A)-C(7A)-H(7A)	109.4
C(8A)-C(1A)-Ir(1)	110.6(3)	C(8A)-C(7A)-H(7A)	109.4
C(2A)-C(1A)-H(1A)	120(3)	C(6A)-C(7A)-H(7B)	109.4
C(8A)-C(1A)-H(1A)	112(3)	C(8A)-C(7A)-H(7B)	109.4
Ir(1)-C(1A)-H(1A)	108(3)	H(7A)-C(7A)-H(7B)	108.0
C(1A)-C(2A)-C(3A)	124.0(3)	C(1A)-C(8A)-C(7A)	112.7(3)
C(1A)-C(2A)-Ir(1)	70.8(3)	C(1A)-C(8A)-H(8A)	109.1
C(3A)-C(2A)-Ir(1)	112.6(3)	C(7A)-C(8A)-H(8A)	109.1
C(1A)-C(2A)-H(2A)	119(3)	C(1A)-C(8A)-H(8B)	109.1
C(3A)-C(2A)-H(2A)	113(3)	C(7A)-C(8A)-H(8B)	109.1
Ir(1)-C(2A)-H(2A)	105(3)	H(8A)-C(8A)-H(8B)	107.8
C(2A)-C(3A)-C(4A)	111.7(3)	C(5)-P(1)-C(2)	101.3(2)
C(2A)-C(3A)-H(3A)	109.3	C(5)-P(1)-C(1)	105.20(16)
C(4A)-C(3A)-H(3A)	109.3	C(2)-P(1)-C(1)	105.9(2)
C(2A)-C(3A)-H(3B)	109.3	C(5)-P(1)-Ir(1)	111.75(18)
C(4A)-C(3A)-H(3B)	109.3	C(2)-P(1)-Ir(1)	123.07(9)
H(3A)-C(3A)-H(3B)	107.9	C(1)-P(1)-Ir(1)	108.15(14)
C(5A)-C(4A)-C(3A)	112.8(3)	B(5)-C(1)-B(6)	61.9(3)
C(5A)-C(4A)-H(4A)	109.0	B(5)-C(1)-B(2)	112.5(3)
C(3A)-C(4A)-H(4A)	109.0	B(6)-C(1)-B(2)	61.7(3)
C(5A)-C(4A)-H(4B)	109.0	B(5)-C(1)-B(4)	62.1(3)
C(3A)-C(4A)-H(4B)	109.0	B(6)-C(1)-B(4)	112.3(3)
H(4A)-C(4A)-H(4B)	107.8	B(2)-C(1)-B(4)	111.7(3)
C(6A)-C(5A)-C(4A)	124.3(3)	B(5)-C(1)-B(3)	112.2(3)
C(6A)-C(5A)-Ir(1)	71.7(2)	B(6)-C(1)-B(3)	111.8(3)
C(4A)-C(5A)-Ir(1)	112.3(2)	B(2)-C(1)-B(3)	61.5(2)
C(6A)-C(5A)-H(5A)	118(3)	B(4)-C(1)-B(3)	61.2(2)
C(4A)-C(5A)-H(5A)	112(3)	B(5)-C(1)-P(1)	121.9(3)
Ir(1)-C(5A)-H(5A)	110(3)	B(6)-C(1)-P(1)	122.5(3)

B(2)-C(1)-P(1)	118.3(3)	C(1)-B(4)-B(10)	105.9(3)
B(4)-C(1)-P(1)	117.9(3)	B(9)-B(4)-B(10)	60.7(2)
B(3)-C(1)-P(1)	115.7(3)	B(3)-B(4)-B(10)	108.7(3)
C(1)-B(2)-B(7)	105.9(3)	C(1)-B(4)-B(5)	58.7(2)
C(1)-B(2)-B(3)	59.6(2)	B(9)-B(4)-B(5)	108.4(3)
B(7)-B(2)-B(3)	107.9(3)	B(3)-B(4)-B(5)	108.2(3)
C(1)-B(2)-B(8)	105.9(3)	B(10)-B(4)-B(5)	59.8(3)
B(7)-B(2)-B(8)	60.0(2)	C(1)-B(4)-H(4)	123.6
B(3)-B(2)-B(8)	59.7(2)	B(9)-B(4)-H(4)	121.6
C(1)-B(2)-B(6)	59.1(2)	B(3)-B(4)-H(4)	121.1
B(7)-B(2)-B(6)	59.9(2)	B(10)-B(4)-H(4)	121.8
B(3)-B(2)-B(6)	108.2(3)	B(5)-B(4)-H(4)	121.8
B(8)-B(2)-B(6)	107.8(3)	C(1)-B(5)-B(10)	106.1(3)
C(1)-B(2)-H(2)	123.5	C(1)-B(5)-B(11)	105.8(3)
B(7)-B(2)-H(2)	122.2	B(10)-B(5)-B(11)	60.4(3)
B(3)-B(2)-H(2)	121.5	C(1)-B(5)-B(6)	59.2(2)
B(8)-B(2)-H(2)	122.3	B(10)-B(5)-B(6)	108.2(3)
B(6)-B(2)-H(2)	121.6	B(11)-B(5)-B(6)	59.7(3)
C(1)-B(3)-B(8)	105.8(3)	C(1)-B(5)-B(4)	59.1(3)
C(1)-B(3)-B(4)	59.1(2)	B(10)-B(5)-B(4)	59.8(2)
B(8)-B(3)-B(4)	108.1(3)	B(11)-B(5)-B(4)	107.8(3)
C(1)-B(3)-B(9)	105.8(3)	B(6)-B(5)-B(4)	107.7(3)
B(8)-B(3)-B(9)	60.3(2)	C(1)-B(5)-H(5)	123.6
B(4)-B(3)-B(9)	59.9(2)	B(10)-B(5)-H(5)	121.8
C(1)-B(3)-B(2)	59.0(2)	B(11)-B(5)-H(5)	122.2
B(8)-B(3)-B(2)	60.2(2)	B(6)-B(5)-H(5)	121.7
B(4)-B(3)-B(2)	108.0(3)	B(4)-B(5)-H(5)	121.9
B(9)-B(3)-B(2)	108.4(3)	C(1)-B(6)-B(11)	105.9(3)
C(1)-B(3)-H(3)	123.9	C(1)-B(6)-B(7)	106.0(3)
B(8)-B(3)-H(3)	122.0	B(11)-B(6)-B(7)	60.5(2)
B(4)-B(3)-H(3)	121.6	C(1)-B(6)-B(2)	59.2(2)
B(9)-B(3)-H(3)	122.0	B(11)-B(6)-B(2)	108.4(3)
B(2)-B(3)-H(3)	121.4	B(7)-B(6)-B(2)	60.0(2)
C(1)-B(4)-B(9)	106.4(3)	C(1)-B(6)-B(5)	58.9(3)
C(1)-B(4)-B(3)	59.7(2)	B(11)-B(6)-B(5)	60.1(3)
B(9)-B(4)-B(3)	60.1(2)	B(7)-B(6)-B(5)	108.4(3)

B(2)-B(6)-B(5)	108.0(3)	B(4)-B(9)-B(3)	60.1(2)
C(1)-B(6)-H(6)	123.8	B(4)-B(9)-B(12)	107.9(3)
B(11)-B(6)-H(6)	121.8	B(3)-B(9)-B(12)	107.9(3)
B(7)-B(6)-H(6)	121.8	B(4)-B(9)-B(8)	107.8(3)
B(2)-B(6)-H(6)	121.5	B(3)-B(9)-B(8)	59.8(2)
B(5)-B(6)-H(6)	121.6	B(12)-B(9)-B(8)	60.0(3)
B(6)-B(7)-B(8)	108.0(3)	B(4)-B(9)-B(10)	59.8(2)
B(6)-B(7)-B(2)	60.1(2)	B(3)-B(9)-B(10)	108.0(3)
B(8)-B(7)-B(2)	60.0(2)	B(12)-B(9)-B(10)	60.2(2)
B(6)-B(7)-B(12)	107.6(3)	B(8)-B(9)-B(10)	108.1(3)
B(8)-B(7)-B(12)	59.9(3)	B(4)-B(9)-H(9)	121.8
B(2)-B(7)-B(12)	107.7(3)	B(3)-B(9)-H(9)	121.8
B(6)-B(7)-B(11)	59.6(2)	B(12)-B(9)-H(9)	121.7
B(8)-B(7)-B(11)	107.9(3)	B(8)-B(9)-H(9)	121.8
B(2)-B(7)-B(11)	107.7(3)	B(10)-B(9)-H(9)	121.6
B(12)-B(7)-B(11)	60.0(3)	B(4)-B(10)-B(5)	60.5(2)
B(6)-B(7)-H(7)	121.9	B(4)-B(10)-B(12)	107.0(3)
B(8)-B(7)-H(7)	121.7	B(5)-B(10)-B(12)	107.7(3)
B(2)-B(7)-H(7)	121.8	B(4)-B(10)-B(11)	107.8(3)
B(12)-B(7)-H(7)	121.9	B(5)-B(10)-B(11)	59.8(3)
B(11)-B(7)-H(7)	121.9	B(12)-B(10)-B(11)	59.9(3)
B(3)-B(8)-B(7)	108.3(3)	B(4)-B(10)-B(9)	59.4(2)
B(3)-B(8)-B(12)	107.8(3)	B(5)-B(10)-B(9)	107.9(3)
B(7)-B(8)-B(12)	60.3(3)	B(12)-B(10)-B(9)	59.5(3)
B(3)-B(8)-B(2)	60.2(2)	B(11)-B(10)-B(9)	107.5(3)
B(7)-B(8)-B(2)	60.0(2)	B(4)-B(10)-H(10)	122.0
B(12)-B(8)-B(2)	108.0(3)	B(5)-B(10)-H(10)	121.6
B(3)-B(8)-B(9)	59.9(2)	B(12)-B(10)-H(10)	122.3
B(7)-B(8)-B(9)	108.3(3)	B(11)-B(10)-H(10)	121.8
B(12)-B(8)-B(9)	59.9(3)	B(9)-B(10)-H(10)	122.2
B(2)-B(8)-B(9)	108.0(3)	B(6)-B(11)-B(5)	60.2(2)
B(3)-B(8)-H(8)	121.7	B(6)-B(11)-B(12)	107.8(3)
B(7)-B(8)-H(8)	121.4	B(5)-B(11)-B(12)	107.7(3)
B(12)-B(8)-H(8)	121.8	B(6)-B(11)-B(7)	59.9(2)
B(2)-B(8)-H(8)	121.7	B(5)-B(11)-B(7)	108.0(3)
B(9)-B(8)-H(8)	121.7	B(12)-B(11)-B(7)	59.9(3)

B(6)-B(11)-B(10)	108.0(3)	C(2)-C(4)-H(4C)	109.5
B(5)-B(11)-B(10)	59.7(3)	C(2)-C(4)-H(4D)	109.5
B(12)-B(11)-B(10)	60.0(3)	H(4C)-C(4)-H(4D)	109.5
B(7)-B(11)-B(10)	108.1(3)	C(2)-C(4)-H(4E)	109.5
B(6)-B(11)-H(11)	121.7	H(4C)-C(4)-H(4E)	109.5
B(5)-B(11)-H(11)	121.8	H(4D)-C(4)-H(4E)	109.5
B(12)-B(11)-H(11)	121.9	C(6)-C(5)-C(7)	109.3(4)
B(7)-B(11)-H(11)	121.7	C(6)-C(5)-P(1)	112.9(3)
B(10)-B(11)-H(11)	121.7	C(7)-C(5)-P(1)	116.4(4)
B(9)-B(12)-B(8)	60.1(3)	C(6)-C(5)-H(5B)	105.8
B(9)-B(12)-B(7)	108.1(3)	C(7)-C(5)-H(5B)	105.8
B(8)-B(12)-B(7)	59.8(3)	P(1)-C(5)-H(5B)	105.8
B(9)-B(12)-B(11)	108.3(3)	C(5)-C(6)-H(6B)	109.5
B(8)-B(12)-B(11)	108.0(3)	C(5)-C(6)-H(6C)	109.5
B(7)-B(12)-B(11)	60.1(3)	H(6B)-C(6)-H(6C)	109.5
B(9)-B(12)-B(10)	60.3(3)	C(5)-C(6)-H(6D)	109.5
B(8)-B(12)-B(10)	108.3(3)	H(6B)-C(6)-H(6D)	109.5
B(7)-B(12)-B(10)	108.2(3)	H(6C)-C(6)-H(6D)	109.5
B(11)-B(12)-B(10)	60.0(3)	C(5)-C(7)-H(7C)	109.5
B(9)-B(12)-H(12)	121.5	C(5)-C(7)-H(7D)	109.5
B(8)-B(12)-H(12)	121.7	H(7C)-C(7)-H(7D)	109.5
B(7)-B(12)-H(12)	121.7	C(5)-C(7)-H(7E)	109.5
B(11)-B(12)-H(12)	121.7	H(7C)-C(7)-H(7E)	109.5
B(10)-B(12)-H(12)	121.4	H(7D)-C(7)-H(7E)	109.5
C(4)-C(2)-C(3)	108.4(3)	C(4C)-N(1C)-C(2C)	110.4(4)
C(4)-C(2)-P(1)	119.0(3)	C(4C)-N(1C)-C(3C)	108.5(4)
C(3)-C(2)-P(1)	110.0(3)	C(2C)-N(1C)-C(3C)	109.3(4)
C(4)-C(2)-H(2B)	106.2	C(4C)-N(1C)-C(1C)	109.3(3)
C(3)-C(2)-H(2B)	106.2	C(2C)-N(1C)-C(1C)	110.0(3)
P(1)-C(2)-H(2B)	106.2	C(3C)-N(1C)-C(1C)	109.2(3)
C(2)-C(3)-H(3C)	109.5	N(1C)-C(1C)-H(1B)	109.5
C(2)-C(3)-H(3D)	109.5	N(1C)-C(1C)-H(1C)	109.5
H(3C)-C(3)-H(3D)	109.5	H(1B)-C(1C)-H(1C)	109.5
C(2)-C(3)-H(3E)	109.5	N(1C)-C(1C)-H(1D)	109.5
H(3C)-C(3)-H(3E)	109.5	H(1B)-C(1C)-H(1D)	109.5
H(3D)-C(3)-H(3E)	109.5	H(1C)-C(1C)-H(1D)	109.5

N(1C)-C(2C)-H(2C)	109.5	C(4S)-C(3S)-H(3J)	110.5
N(1C)-C(2C)-H(2D)	109.5	C(2S)-C(3S)-H(3J)	110.5
H(2C)-C(2C)-H(2D)	109.5	H(3I)-C(3S)-H(3J)	108.7
N(1C)-C(2C)-H(2E)	109.5	O(1S)-C(4S)-C(3S)	107.5(11)
H(2C)-C(2C)-H(2E)	109.5	O(1S)-C(4S)-H(4I)	110.2
H(2D)-C(2C)-H(2E)	109.5	C(3S)-C(4S)-H(4I)	110.2
N(1C)-C(3C)-H(3F)	109.5	O(1S)-C(4S)-H(4J)	110.2
N(1C)-C(3C)-H(3G)	109.5	C(3S)-C(4S)-H(4J)	110.2
H(3F)-C(3C)-H(3G)	109.5	H(4I)-C(4S)-H(4J)	108.5
N(1C)-C(3C)-H(3H)	109.5	C(1D)-O(1D)-C(4D)	104.0(17)
H(3F)-C(3C)-H(3H)	109.5	O(1D)-C(1D)-C(2D)	109.3(17)
H(3G)-C(3C)-H(3H)	109.5	O(1D)-C(1D)-H(1G)	109.8
N(1C)-C(4C)-H(4F)	109.5	C(2D)-C(1D)-H(1G)	109.8
N(1C)-C(4C)-H(4G)	109.5	O(1D)-C(1D)-H(1H)	109.8
H(4F)-C(4C)-H(4G)	109.5	C(2D)-C(1D)-H(1H)	109.8
N(1C)-C(4C)-H(4H)	109.5	H(1G)-C(1D)-H(1H)	108.3
H(4F)-C(4C)-H(4H)	109.5	C(3D)-C(2D)-C(1D)	105.5(15)
H(4G)-C(4C)-H(4H)	109.5	C(3D)-C(2D)-H(2H)	110.6
C(1S)-O(1S)-C(4S)	108.1(11)	C(1D)-C(2D)-H(2H)	110.6
O(1S)-C(1S)-C(2S)	105.8(11)	C(3D)-C(2D)-H(2I)	110.6
O(1S)-C(1S)-H(1E)	110.6	C(1D)-C(2D)-H(2I)	110.6
C(2S)-C(1S)-H(1E)	110.6	H(2H)-C(2D)-H(2I)	108.8
O(1S)-C(1S)-H(1F)	110.6	C(2D)-C(3D)-C(4D)	106.5(14)
C(2S)-C(1S)-H(1F)	110.6	C(2D)-C(3D)-H(3K)	110.4
H(1E)-C(1S)-H(1F)	108.7	C(4D)-C(3D)-H(3K)	110.4
C(3S)-C(2S)-C(1S)	105.3(9)	C(2D)-C(3D)-H(3L)	110.4
C(3S)-C(2S)-H(2F)	110.7	C(4D)-C(3D)-H(3L)	110.4
C(1S)-C(2S)-H(2F)	110.7	H(3K)-C(3D)-H(3L)	108.6
C(3S)-C(2S)-H(2G)	110.7	O(1D)-C(4D)-C(3D)	108.0(18)
C(1S)-C(2S)-H(2G)	110.7	O(1D)-C(4D)-H(4K)	110.1
H(2F)-C(2S)-H(2G)	108.8	C(3D)-C(4D)-H(4K)	110.1
C(4S)-C(3S)-C(2S)	106.2(9)	O(1D)-C(4D)-H(4L)	110.1
C(4S)-C(3S)-H(3I)	110.5	C(3D)-C(4D)-H(4L)	110.1
C(2S)-C(3S)-H(3I)	110.5	H(4K)-C(4D)-H(4L)	108.4

Symmetry transformations used to generate equivalent atoms:

Table 10. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for vL147JE_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U11	U22	U33	U23	U13	U12
Ir(1)	8(1)	11(1)	11(1)	0(1)	-1(1)	0(1)
Cl(1)	15(1)	19(1)	15(1)	-3(1)	-2(1)	-1(1)
C(1A)	9(2)	25(2)	17(2)	-1(2)	-2(1)	-5(1)
C(2A)	10(2)	22(2)	15(2)	1(2)	-2(1)	1(1)
C(3A)	13(2)	20(2)	24(2)	0(1)	0(1)	5(1)
C(4A)	15(2)	16(2)	30(2)	-3(1)	0(1)	3(1)
C(5A)	11(1)	17(2)	16(2)	-4(1)	0(1)	1(1)
C(6A)	11(1)	25(2)	13(1)	-1(1)	0(1)	1(1)
C(7A)	17(1)	27(2)	14(1)	4(2)	2(1)	1(2)
C(8A)	15(2)	26(2)	23(2)	6(2)	1(1)	-6(1)
P(1)	9(1)	10(1)	11(1)	1(1)	-1(1)	0(1)
C(1)	8(2)	13(2)	12(2)	1(1)	-1(1)	-1(1)
B(2)	16(2)	22(2)	11(2)	2(1)	-2(1)	-4(1)
B(3)	11(2)	17(2)	16(2)	4(1)	-5(1)	-1(1)
B(4)	16(2)	12(2)	18(2)	2(1)	-3(2)	-2(1)
B(5)	12(2)	19(2)	16(2)	5(2)	-3(1)	-3(2)
B(6)	11(2)	25(2)	16(2)	3(2)	1(1)	-2(1)
B(7)	16(2)	35(2)	14(2)	9(2)	0(1)	-7(2)
B(8)	14(2)	26(2)	19(2)	9(2)	-4(1)	-6(1)
B(9)	17(2)	17(2)	27(2)	10(2)	-6(2)	-4(1)
B(10)	18(2)	18(2)	22(2)	6(2)	-6(2)	-6(1)
B(11)	13(2)	29(2)	18(2)	10(2)	-4(1)	-6(2)
B(12)	17(2)	28(2)	24(2)	12(2)	-8(2)	-9(2)
C(2)	10(1)	17(1)	14(1)	2(2)	-3(1)	2(2)
C(3)	22(2)	19(2)	17(2)	9(2)	-3(2)	-1(2)
C(4)	15(2)	19(2)	17(2)	1(1)	-5(2)	-1(1)
C(5)	22(2)	16(2)	19(2)	-1(2)	1(2)	7(2)
C(6)	32(2)	12(2)	31(2)	-1(1)	-8(2)	2(2)
C(7)	22(2)	29(3)	33(2)	0(2)	6(2)	15(2)
N(1C)	14(1)	22(2)	16(1)	1(1)	2(1)	3(1)

C(1C)	19(2)	24(2)	18(2)	-1(1)	-1(1)	6(1)
C(2C)	22(2)	56(3)	41(3)	-31(2)	-2(2)	-2(2)
C(3C)	26(2)	26(2)	32(2)	8(2)	-5(2)	7(2)
C(4C)	44(3)	39(3)	34(3)	14(2)	22(2)	9(2)
O(1S)	27(5)	17(4)	44(5)	-6(3)	5(4)	-3(4)
C(1S)	37(7)	72(6)	41(4)	12(5)	8(4)	0(4)
C(2S)	94(9)	59(6)	29(4)	-13(4)	30(4)	-43(5)
C(3S)	33(4)	47(4)	100(6)	-24(4)	-13(4)	14(3)
C(4S)	33(4)	47(4)	100(6)	-24(4)	-13(4)	14(3)
O(1D)	34(10)	19(9)	49(9)	-15(7)	11(8)	-2(10)
C(1D)	49(8)	40(6)	38(5)	-8(4)	12(5)	-3(5)
C(2D)	33(4)	47(4)	100(6)	-24(4)	-13(4)	14(3)
C(3D)	49(8)	40(6)	38(5)	-8(4)	12(5)	-3(5)
C(4D)	37(7)	72(6)	41(4)	12(5)	8(4)	0(4)

Table 11. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for vL147JE_0m.

	x	y	z	U(eq)
H(1A)	3300(50)	1550(40)	3070(30)	20
H(2A)	3340(50)	3510(50)	2500(20)	19
H(3A)	2563	4252	4170	23
H(3B)	2669	5086	3290	23
H(4A)	4680	5698	3678	25
H(4B)	4155	5490	4669	25
H(5A)	6240(30)	4540(40)	4350(30)	17
H(6A)	5970(30)	2800(70)	5120(20)	20
H(7A)	3448	3390	5245	23
H(7B)	4113	2208	5685	23
H(8A)	3452	1009	4532	26
H(8B)	2275	1946	4528	26
H(2)	7482	3291	1136	20
H(3)	6027	4880	2329	18
H(4)	7792	5691	3812	18
H(5)	10365	4606	3537	19
H(6)	10168	3137	1866	21
H(7)	9524	4767	325	26
H(8)	6973	5844	617	24
H(9)	7171	7327	2282	25
H(10)	9866	7157	3040	24
H(11)	11320	5576	1819	24
H(12)	9335	7262	1051	28
H(2B)	9689	2722	4230	17
H(3C)	7676	1593	5184	29
H(3D)	9179	1545	5473	29
H(3E)	8658	885	4566	29
H(4C)	7811	3920	5264	26
H(4D)	8950	4576	4754	26
H(4E)	9281	3703	5595	26
H(5B)	8222	1538	2105	23

H(6B)	7845	-421	2563	38
H(6C)	6659	399	2852	38
H(6D)	7739	-7	3595	38
H(7C)	9970	742	3514	42
H(7D)	10304	1860	2876	42
H(7E)	10085	542	2448	42
H(1B)	8034	8683	9032	30
H(1C)	6877	7751	9169	30
H(1D)	7997	7895	9939	30
H(2C)	8168	10540	9915	59
H(2D)	8137	9778	10834	59
H(2E)	7105	10833	10638	59
H(3F)	5383	10558	9491	43
H(3G)	5321	9345	8899	43
H(3H)	6452	10306	8763	43
H(4F)	6379	8323	11046	58
H(4G)	5265	8178	10272	58
H(4H)	5356	9389	10865	58
H(1E)	4740	7446	2453	60
H(1F)	3296	7108	2722	60
H(2F)	3224	9015	3193	72
H(2G)	4385	9423	2570	72
H(3I)	1786	9558	2152	73
H(3J)	2937	10139	1598	73
H(4I)	1615	8047	1221	73
H(4J)	2600	8740	589	73
H(1G)	1916	7593	962	51
H(1H)	2835	8555	491	51
H(2H)	2379	9974	1436	73
H(2I)	1138	9154	1632	73
H(3K)	1909	8736	2951	51
H(3L)	3091	9639	2783	51
H(4K)	4319	8047	2790	60
H(4L)	3097	7153	2734	60

Table 12. Torsion angles [°] for vL147JE_0m.

C(8A)-C(1A)-C(2A)-C(3A)	-1.8(7)
Ir(1)-C(1A)-C(2A)-C(3A)	-104.8(4)
C(8A)-C(1A)-C(2A)-Ir(1)	103.0(4)
C(1A)-C(2A)-C(3A)-C(4A)	93.5(5)
Ir(1)-C(2A)-C(3A)-C(4A)	12.0(4)
C(2A)-C(3A)-C(4A)-C(5A)	-30.3(5)
C(3A)-C(4A)-C(5A)-C(6A)	-47.5(5)
C(3A)-C(4A)-C(5A)-Ir(1)	34.9(4)
C(4A)-C(5A)-C(6A)-C(7A)	-1.9(5)
Ir(1)-C(5A)-C(6A)-C(7A)	-106.9(3)
C(4A)-C(5A)-C(6A)-Ir(1)	104.9(3)
C(5A)-C(6A)-C(7A)-C(8A)	94.7(5)
Ir(1)-C(6A)-C(7A)-C(8A)	14.7(5)
C(2A)-C(1A)-C(8A)-C(7A)	-47.0(6)
Ir(1)-C(1A)-C(8A)-C(7A)	34.7(4)
C(6A)-C(7A)-C(8A)-C(1A)	-32.4(5)
C(5)-P(1)-C(1)-B(5)	-95.7(4)
C(2)-P(1)-C(1)-B(5)	11.0(4)
Ir(1)-P(1)-C(1)-B(5)	144.7(3)
C(5)-P(1)-C(1)-B(6)	-20.9(3)
C(2)-P(1)-C(1)-B(6)	85.9(3)
Ir(1)-P(1)-C(1)-B(6)	-140.4(3)
C(5)-P(1)-C(1)-B(2)	52.0(3)
C(2)-P(1)-C(1)-B(2)	158.7(3)
Ir(1)-P(1)-C(1)-B(2)	-67.6(3)
C(5)-P(1)-C(1)-B(4)	-168.6(3)
C(2)-P(1)-C(1)-B(4)	-61.9(3)
Ir(1)-P(1)-C(1)-B(4)	71.8(3)
C(5)-P(1)-C(1)-B(3)	121.9(3)
C(2)-P(1)-C(1)-B(3)	-131.3(3)
Ir(1)-P(1)-C(1)-B(3)	2.3(3)
B(5)-C(1)-B(2)-B(7)	-2.2(4)
B(6)-C(1)-B(2)-B(7)	-38.9(3)
B(4)-C(1)-B(2)-B(7)	65.5(4)

B(3)-C(1)-B(2)-B(7)	101.7(3)
P(1)-C(1)-B(2)-B(7)	-152.7(3)
B(5)-C(1)-B(2)-B(3)	-103.9(3)
B(6)-C(1)-B(2)-B(3)	-140.6(3)
B(4)-C(1)-B(2)-B(3)	-36.2(3)
P(1)-C(1)-B(2)-B(3)	105.6(3)
B(5)-C(1)-B(2)-B(8)	-64.8(4)
B(6)-C(1)-B(2)-B(8)	-101.6(3)
B(4)-C(1)-B(2)-B(8)	2.9(4)
B(3)-C(1)-B(2)-B(8)	39.1(3)
P(1)-C(1)-B(2)-B(8)	144.7(3)
B(5)-C(1)-B(2)-B(6)	36.8(3)
B(4)-C(1)-B(2)-B(6)	104.5(3)
B(3)-C(1)-B(2)-B(6)	140.6(3)
P(1)-C(1)-B(2)-B(6)	-113.8(3)
B(5)-C(1)-B(3)-B(8)	65.1(4)
B(6)-C(1)-B(3)-B(8)	-2.3(4)
B(2)-C(1)-B(3)-B(8)	-39.3(3)
B(4)-C(1)-B(3)-B(8)	101.9(3)
P(1)-C(1)-B(3)-B(8)	-149.0(3)
B(5)-C(1)-B(3)-B(4)	-36.9(3)
B(6)-C(1)-B(3)-B(4)	-104.2(3)
B(2)-C(1)-B(3)-B(4)	-141.2(3)
P(1)-C(1)-B(3)-B(4)	109.1(3)
B(5)-C(1)-B(3)-B(9)	2.1(4)
B(6)-C(1)-B(3)-B(9)	-65.3(4)
B(2)-C(1)-B(3)-B(9)	-102.3(3)
B(4)-C(1)-B(3)-B(9)	39.0(3)
P(1)-C(1)-B(3)-B(9)	148.1(3)
B(5)-C(1)-B(3)-B(2)	104.4(4)
B(6)-C(1)-B(3)-B(2)	37.0(3)
B(4)-C(1)-B(3)-B(2)	141.2(3)
P(1)-C(1)-B(3)-B(2)	-109.7(3)
B(7)-B(2)-B(3)-C(1)	-98.3(3)
B(8)-B(2)-B(3)-C(1)	-135.4(3)
B(6)-B(2)-B(3)-C(1)	-34.9(3)

C(1)-B(2)-B(3)-B(8)	135.4(3)
B(7)-B(2)-B(3)-B(8)	37.1(3)
B(6)-B(2)-B(3)-B(8)	100.4(3)
C(1)-B(2)-B(3)-B(4)	34.4(3)
B(7)-B(2)-B(3)-B(4)	-63.9(3)
B(8)-B(2)-B(3)-B(4)	-101.0(3)
B(6)-B(2)-B(3)-B(4)	-0.5(4)
C(1)-B(2)-B(3)-B(9)	97.8(3)
B(7)-B(2)-B(3)-B(9)	-0.5(4)
B(8)-B(2)-B(3)-B(9)	-37.6(3)
B(6)-B(2)-B(3)-B(9)	62.8(3)
B(5)-C(1)-B(4)-B(9)	101.8(3)
B(6)-C(1)-B(4)-B(9)	64.2(4)
B(2)-C(1)-B(4)-B(9)	-2.9(4)
B(3)-C(1)-B(4)-B(9)	-39.2(3)
P(1)-C(1)-B(4)-B(9)	-144.8(3)
B(5)-C(1)-B(4)-B(3)	141.1(3)
B(6)-C(1)-B(4)-B(3)	103.5(3)
B(2)-C(1)-B(4)-B(3)	36.3(3)
P(1)-C(1)-B(4)-B(3)	-105.6(3)
B(5)-C(1)-B(4)-B(10)	38.3(3)
B(6)-C(1)-B(4)-B(10)	0.7(4)
B(2)-C(1)-B(4)-B(10)	-66.4(4)
B(3)-C(1)-B(4)-B(10)	-102.7(3)
P(1)-C(1)-B(4)-B(10)	151.7(3)
B(6)-C(1)-B(4)-B(5)	-37.6(3)
B(2)-C(1)-B(4)-B(5)	-104.8(3)
B(3)-C(1)-B(4)-B(5)	-141.1(3)
P(1)-C(1)-B(4)-B(5)	113.3(3)
B(8)-B(3)-B(4)-C(1)	-98.0(3)
B(9)-B(3)-B(4)-C(1)	-135.6(3)
B(2)-B(3)-B(4)-C(1)	-34.3(3)
C(1)-B(3)-B(4)-B(9)	135.6(3)
B(8)-B(3)-B(4)-B(9)	37.6(3)
B(2)-B(3)-B(4)-B(9)	101.2(3)
C(1)-B(3)-B(4)-B(10)	97.8(3)

B(8)-B(3)-B(4)-B(10)	-0.1(4)
B(9)-B(3)-B(4)-B(10)	-37.8(3)
B(2)-B(3)-B(4)-B(10)	63.5(3)
C(1)-B(3)-B(4)-B(5)	34.4(3)
B(8)-B(3)-B(4)-B(5)	-63.5(4)
B(9)-B(3)-B(4)-B(5)	-101.1(3)
B(2)-B(3)-B(4)-B(5)	0.1(4)
B(6)-C(1)-B(5)-B(10)	101.9(3)
B(2)-C(1)-B(5)-B(10)	65.2(4)
B(4)-C(1)-B(5)-B(10)	-38.4(3)
B(3)-C(1)-B(5)-B(10)	-1.9(4)
P(1)-C(1)-B(5)-B(10)	-145.5(3)
B(6)-C(1)-B(5)-B(11)	38.7(3)
B(2)-C(1)-B(5)-B(11)	2.0(4)
B(4)-C(1)-B(5)-B(11)	-101.5(3)
B(3)-C(1)-B(5)-B(11)	-65.0(4)
P(1)-C(1)-B(5)-B(11)	151.4(3)
B(2)-C(1)-B(5)-B(6)	-36.7(3)
B(4)-C(1)-B(5)-B(6)	-140.2(3)
B(3)-C(1)-B(5)-B(6)	-103.8(4)
P(1)-C(1)-B(5)-B(6)	112.7(4)
B(6)-C(1)-B(5)-B(4)	140.2(3)
B(2)-C(1)-B(5)-B(4)	103.5(3)
B(3)-C(1)-B(5)-B(4)	36.5(3)
P(1)-C(1)-B(5)-B(4)	-107.1(4)
B(9)-B(4)-B(5)-C(1)	-98.5(3)
B(3)-B(4)-B(5)-C(1)	-34.8(3)
B(10)-B(4)-B(5)-C(1)	-136.3(3)
C(1)-B(4)-B(5)-B(10)	136.3(3)
B(9)-B(4)-B(5)-B(10)	37.9(3)
B(3)-B(4)-B(5)-B(10)	101.5(3)
C(1)-B(4)-B(5)-B(11)	98.2(3)
B(9)-B(4)-B(5)-B(11)	-0.3(4)
B(3)-B(4)-B(5)-B(11)	63.4(4)
B(10)-B(4)-B(5)-B(11)	-38.2(3)
C(1)-B(4)-B(5)-B(6)	35.2(3)

B(9)-B(4)-B(5)-B(6)	-63.3(4)
B(3)-B(4)-B(5)-B(6)	0.4(4)
B(10)-B(4)-B(5)-B(6)	-101.1(3)
B(5)-C(1)-B(6)-B(11)	-38.9(3)
B(2)-C(1)-B(6)-B(11)	102.3(3)
B(4)-C(1)-B(6)-B(11)	-1.2(4)
B(3)-C(1)-B(6)-B(11)	65.4(4)
P(1)-C(1)-B(6)-B(11)	-150.6(3)
B(5)-C(1)-B(6)-B(7)	-102.1(3)
B(2)-C(1)-B(6)-B(7)	39.0(3)
B(4)-C(1)-B(6)-B(7)	-64.4(4)
B(3)-C(1)-B(6)-B(7)	2.1(4)
P(1)-C(1)-B(6)-B(7)	146.2(3)
B(5)-C(1)-B(6)-B(2)	-141.2(3)
B(4)-C(1)-B(6)-B(2)	-103.5(3)
B(3)-C(1)-B(6)-B(2)	-36.9(3)
P(1)-C(1)-B(6)-B(2)	107.2(3)
B(2)-C(1)-B(6)-B(5)	141.2(3)
B(4)-C(1)-B(6)-B(5)	37.7(3)
B(3)-C(1)-B(6)-B(5)	104.3(3)
P(1)-C(1)-B(6)-B(5)	-111.7(4)
B(7)-B(2)-B(6)-C(1)	135.7(3)
B(3)-B(2)-B(6)-C(1)	35.1(3)
B(8)-B(2)-B(6)-C(1)	98.2(3)
C(1)-B(2)-B(6)-B(11)	-98.0(3)
B(7)-B(2)-B(6)-B(11)	37.7(3)
B(3)-B(2)-B(6)-B(11)	-62.8(4)
B(8)-B(2)-B(6)-B(11)	0.3(4)
C(1)-B(2)-B(6)-B(7)	-135.7(3)
B(3)-B(2)-B(6)-B(7)	-100.5(3)
B(8)-B(2)-B(6)-B(7)	-37.5(3)
C(1)-B(2)-B(6)-B(5)	-34.4(3)
B(7)-B(2)-B(6)-B(5)	101.3(3)
B(3)-B(2)-B(6)-B(5)	0.8(4)
B(8)-B(2)-B(6)-B(5)	63.8(4)
B(10)-B(5)-B(6)-C(1)	-98.3(3)

B(11)-B(5)-B(6)-C(1)	-135.8(3)
B(4)-B(5)-B(6)-C(1)	-35.2(3)
C(1)-B(5)-B(6)-B(11)	135.8(3)
B(10)-B(5)-B(6)-B(11)	37.5(3)
B(4)-B(5)-B(6)-B(11)	100.6(3)
C(1)-B(5)-B(6)-B(7)	98.0(3)
B(10)-B(5)-B(6)-B(7)	-0.3(4)
B(11)-B(5)-B(6)-B(7)	-37.8(3)
B(4)-B(5)-B(6)-B(7)	62.8(4)
C(1)-B(5)-B(6)-B(2)	34.5(3)
B(10)-B(5)-B(6)-B(2)	-63.8(4)
B(11)-B(5)-B(6)-B(2)	-101.3(3)
B(4)-B(5)-B(6)-B(2)	-0.7(4)
C(1)-B(6)-B(7)-B(8)	-1.1(4)
B(11)-B(6)-B(7)-B(8)	-100.7(4)
B(2)-B(6)-B(7)-B(8)	37.5(3)
B(5)-B(6)-B(7)-B(8)	-63.0(4)
C(1)-B(6)-B(7)-B(2)	-38.6(3)
B(11)-B(6)-B(7)-B(2)	-138.2(3)
B(5)-B(6)-B(7)-B(2)	-100.6(3)
C(1)-B(6)-B(7)-B(12)	62.1(4)
B(11)-B(6)-B(7)-B(12)	-37.5(3)
B(2)-B(6)-B(7)-B(12)	100.7(3)
B(5)-B(6)-B(7)-B(12)	0.2(4)
C(1)-B(6)-B(7)-B(11)	99.5(3)
B(2)-B(6)-B(7)-B(11)	138.2(3)
B(5)-B(6)-B(7)-B(11)	37.6(3)
C(1)-B(2)-B(7)-B(6)	38.6(3)
B(3)-B(2)-B(7)-B(6)	101.1(3)
B(8)-B(2)-B(7)-B(6)	138.0(3)
C(1)-B(2)-B(7)-B(8)	-99.5(3)
B(3)-B(2)-B(7)-B(8)	-37.0(3)
B(6)-B(2)-B(7)-B(8)	-138.0(3)
C(1)-B(2)-B(7)-B(12)	-61.9(4)
B(3)-B(2)-B(7)-B(12)	0.6(4)
B(8)-B(2)-B(7)-B(12)	37.6(3)

B(6)-B(2)-B(7)-B(12)	-100.5(3)
C(1)-B(2)-B(7)-B(11)	1.4(4)
B(3)-B(2)-B(7)-B(11)	63.9(4)
B(8)-B(2)-B(7)-B(11)	100.9(4)
B(6)-B(2)-B(7)-B(11)	-37.1(3)
C(1)-B(3)-B(8)-B(7)	1.5(4)
B(4)-B(3)-B(8)-B(7)	63.6(4)
B(9)-B(3)-B(8)-B(7)	101.0(3)
B(2)-B(3)-B(8)-B(7)	-37.2(3)
C(1)-B(3)-B(8)-B(12)	-62.2(4)
B(4)-B(3)-B(8)-B(12)	-0.2(4)
B(9)-B(3)-B(8)-B(12)	37.2(3)
B(2)-B(3)-B(8)-B(12)	-101.0(3)
C(1)-B(3)-B(8)-B(2)	38.7(3)
B(4)-B(3)-B(8)-B(2)	100.8(3)
B(9)-B(3)-B(8)-B(2)	138.2(3)
C(1)-B(3)-B(8)-B(9)	-99.5(3)
B(4)-B(3)-B(8)-B(9)	-37.4(3)
B(2)-B(3)-B(8)-B(9)	-138.2(3)
B(6)-B(7)-B(8)-B(3)	-0.3(4)
B(2)-B(7)-B(8)-B(3)	37.3(3)
B(12)-B(7)-B(8)-B(3)	-100.5(3)
B(11)-B(7)-B(8)-B(3)	-63.2(4)
B(6)-B(7)-B(8)-B(12)	100.3(3)
B(2)-B(7)-B(8)-B(12)	137.8(3)
B(11)-B(7)-B(8)-B(12)	37.3(3)
B(6)-B(7)-B(8)-B(2)	-37.5(3)
B(12)-B(7)-B(8)-B(2)	-137.8(3)
B(11)-B(7)-B(8)-B(2)	-100.5(3)
B(6)-B(7)-B(8)-B(9)	63.2(4)
B(2)-B(7)-B(8)-B(9)	100.7(3)
B(12)-B(7)-B(8)-B(9)	-37.1(3)
B(11)-B(7)-B(8)-B(9)	0.2(4)
C(1)-B(2)-B(8)-B(3)	-39.0(3)
B(7)-B(2)-B(8)-B(3)	-138.5(3)
B(6)-B(2)-B(8)-B(3)	-101.0(3)

C(1)-B(2)-B(8)-B(7)	99.4(3)
B(3)-B(2)-B(8)-B(7)	138.5(3)
B(6)-B(2)-B(8)-B(7)	37.4(3)
C(1)-B(2)-B(8)-B(12)	61.6(4)
B(7)-B(2)-B(8)-B(12)	-37.8(3)
B(3)-B(2)-B(8)-B(12)	100.6(3)
B(6)-B(2)-B(8)-B(12)	-0.4(4)
C(1)-B(2)-B(8)-B(9)	-1.7(4)
B(7)-B(2)-B(8)-B(9)	-101.2(3)
B(3)-B(2)-B(8)-B(9)	37.3(3)
B(6)-B(2)-B(8)-B(9)	-63.7(4)
C(1)-B(4)-B(9)-B(3)	39.0(3)
B(10)-B(4)-B(9)-B(3)	138.3(3)
B(5)-B(4)-B(9)-B(3)	100.9(3)
C(1)-B(4)-B(9)-B(12)	-61.7(4)
B(3)-B(4)-B(9)-B(12)	-100.7(3)
B(10)-B(4)-B(9)-B(12)	37.6(3)
B(5)-B(4)-B(9)-B(12)	0.2(4)
C(1)-B(4)-B(9)-B(8)	1.7(4)
B(3)-B(4)-B(9)-B(8)	-37.3(3)
B(10)-B(4)-B(9)-B(8)	101.0(3)
B(5)-B(4)-B(9)-B(8)	63.6(4)
C(1)-B(4)-B(9)-B(10)	-99.3(3)
B(3)-B(4)-B(9)-B(10)	-138.3(3)
B(5)-B(4)-B(9)-B(10)	-37.5(3)
C(1)-B(3)-B(9)-B(4)	-38.6(3)
B(8)-B(3)-B(9)-B(4)	-138.1(3)
B(2)-B(3)-B(9)-B(4)	-100.6(3)
C(1)-B(3)-B(9)-B(12)	62.2(4)
B(8)-B(3)-B(9)-B(12)	-37.3(3)
B(4)-B(3)-B(9)-B(12)	100.8(3)
B(2)-B(3)-B(9)-B(12)	0.2(4)
C(1)-B(3)-B(9)-B(8)	99.5(3)
B(4)-B(3)-B(9)-B(8)	138.1(3)
B(2)-B(3)-B(9)-B(8)	37.5(3)
C(1)-B(3)-B(9)-B(10)	-1.5(4)

B(8)-B(3)-B(9)-B(10)	-100.9(3)
B(4)-B(3)-B(9)-B(10)	37.2(3)
B(2)-B(3)-B(9)-B(10)	-63.4(4)
B(3)-B(8)-B(9)-B(4)	37.4(3)
B(7)-B(8)-B(9)-B(4)	-63.5(4)
B(12)-B(8)-B(9)-B(4)	-100.8(3)
B(2)-B(8)-B(9)-B(4)	0.0(4)
B(7)-B(8)-B(9)-B(3)	-100.9(3)
B(12)-B(8)-B(9)-B(3)	-138.2(3)
B(2)-B(8)-B(9)-B(3)	-37.4(3)
B(3)-B(8)-B(9)-B(12)	138.2(3)
B(7)-B(8)-B(9)-B(12)	37.3(3)
B(2)-B(8)-B(9)-B(12)	100.8(3)
B(3)-B(8)-B(9)-B(10)	100.7(3)
B(7)-B(8)-B(9)-B(10)	-0.3(4)
B(12)-B(8)-B(9)-B(10)	-37.5(3)
B(2)-B(8)-B(9)-B(10)	63.3(4)
C(1)-B(4)-B(10)-B(5)	-37.8(3)
B(9)-B(4)-B(10)-B(5)	-138.1(3)
B(3)-B(4)-B(10)-B(5)	-100.6(3)
C(1)-B(4)-B(10)-B(12)	63.2(4)
B(9)-B(4)-B(10)-B(12)	-37.1(3)
B(3)-B(4)-B(10)-B(12)	0.4(4)
B(5)-B(4)-B(10)-B(12)	101.0(4)
C(1)-B(4)-B(10)-B(11)	0.1(4)
B(9)-B(4)-B(10)-B(11)	-100.2(3)
B(3)-B(4)-B(10)-B(11)	-62.7(3)
B(5)-B(4)-B(10)-B(11)	37.9(3)
C(1)-B(4)-B(10)-B(9)	100.2(3)
B(3)-B(4)-B(10)-B(9)	37.5(3)
B(5)-B(4)-B(10)-B(9)	138.1(3)
C(1)-B(5)-B(10)-B(4)	38.1(3)
B(11)-B(5)-B(10)-B(4)	137.4(3)
B(6)-B(5)-B(10)-B(4)	100.3(3)
C(1)-B(5)-B(10)-B(12)	-61.9(4)
B(11)-B(5)-B(10)-B(12)	37.5(3)

B(6)-B(5)-B(10)-B(12)	0.3(4)
B(4)-B(5)-B(10)-B(12)	-99.9(3)
C(1)-B(5)-B(10)-B(11)	-99.4(3)
B(6)-B(5)-B(10)-B(11)	-37.2(3)
B(4)-B(5)-B(10)-B(11)	-137.4(3)
C(1)-B(5)-B(10)-B(9)	0.9(4)
B(11)-B(5)-B(10)-B(9)	100.3(3)
B(6)-B(5)-B(10)-B(9)	63.1(4)
B(4)-B(5)-B(10)-B(9)	-37.2(3)
B(3)-B(9)-B(10)-B(4)	-37.3(3)
B(12)-B(9)-B(10)-B(4)	-138.0(3)
B(8)-B(9)-B(10)-B(4)	-100.5(3)
B(4)-B(9)-B(10)-B(5)	37.6(3)
B(3)-B(9)-B(10)-B(5)	0.4(4)
B(12)-B(9)-B(10)-B(5)	-100.4(4)
B(8)-B(9)-B(10)-B(5)	-62.9(4)
B(4)-B(9)-B(10)-B(12)	138.0(3)
B(3)-B(9)-B(10)-B(12)	100.7(4)
B(8)-B(9)-B(10)-B(12)	37.5(3)
B(4)-B(9)-B(10)-B(11)	100.8(3)
B(3)-B(9)-B(10)-B(11)	63.5(4)
B(12)-B(9)-B(10)-B(11)	-37.2(3)
B(8)-B(9)-B(10)-B(11)	0.2(4)
C(1)-B(6)-B(11)-B(5)	38.4(3)
B(7)-B(6)-B(11)-B(5)	138.1(3)
B(2)-B(6)-B(11)-B(5)	100.6(3)
C(1)-B(6)-B(11)-B(12)	-62.2(4)
B(7)-B(6)-B(11)-B(12)	37.5(3)
B(2)-B(6)-B(11)-B(12)	0.0(4)
B(5)-B(6)-B(11)-B(12)	-100.6(4)
C(1)-B(6)-B(11)-B(7)	-99.7(3)
B(2)-B(6)-B(11)-B(7)	-37.5(3)
B(5)-B(6)-B(11)-B(7)	-138.1(3)
C(1)-B(6)-B(11)-B(10)	1.2(4)
B(7)-B(6)-B(11)-B(10)	100.9(3)
B(2)-B(6)-B(11)-B(10)	63.4(4)

B(5)-B(6)-B(11)-B(10)	-37.2(3)
C(1)-B(5)-B(11)-B(6)	-38.5(3)
B(10)-B(5)-B(11)-B(6)	-138.3(3)
B(4)-B(5)-B(11)-B(6)	-100.5(3)
C(1)-B(5)-B(11)-B(12)	62.3(4)
B(10)-B(5)-B(11)-B(12)	-37.6(3)
B(6)-B(5)-B(11)-B(12)	100.8(3)
B(4)-B(5)-B(11)-B(12)	0.3(4)
C(1)-B(5)-B(11)-B(7)	-1.0(4)
B(10)-B(5)-B(11)-B(7)	-100.9(3)
B(6)-B(5)-B(11)-B(7)	37.5(3)
B(4)-B(5)-B(11)-B(7)	-63.0(4)
C(1)-B(5)-B(11)-B(10)	99.8(3)
B(6)-B(5)-B(11)-B(10)	138.3(3)
B(4)-B(5)-B(11)-B(10)	37.9(3)
B(8)-B(7)-B(11)-B(6)	100.7(3)
B(2)-B(7)-B(11)-B(6)	37.3(3)
B(12)-B(7)-B(11)-B(6)	138.0(3)
B(6)-B(7)-B(11)-B(5)	-37.6(3)
B(8)-B(7)-B(11)-B(5)	63.1(4)
B(2)-B(7)-B(11)-B(5)	-0.3(4)
B(12)-B(7)-B(11)-B(5)	100.4(3)
B(6)-B(7)-B(11)-B(12)	-138.0(3)
B(8)-B(7)-B(11)-B(12)	-37.2(3)
B(2)-B(7)-B(11)-B(12)	-100.6(4)
B(6)-B(7)-B(11)-B(10)	-100.8(3)
B(8)-B(7)-B(11)-B(10)	0.0(4)
B(2)-B(7)-B(11)-B(10)	-63.4(4)
B(12)-B(7)-B(11)-B(10)	37.2(3)
B(4)-B(10)-B(11)-B(6)	-0.8(4)
B(5)-B(10)-B(11)-B(6)	37.4(3)
B(12)-B(10)-B(11)-B(6)	-100.5(3)
B(9)-B(10)-B(11)-B(6)	-63.5(3)
B(4)-B(10)-B(11)-B(5)	-38.2(3)
B(12)-B(10)-B(11)-B(5)	-137.9(3)
B(9)-B(10)-B(11)-B(5)	-100.9(3)

B(4)-B(10)-B(11)-B(12)	99.7(3)
B(5)-B(10)-B(11)-B(12)	137.9(3)
B(9)-B(10)-B(11)-B(12)	37.0(3)
B(4)-B(10)-B(11)-B(7)	62.6(4)
B(5)-B(10)-B(11)-B(7)	100.7(3)
B(12)-B(10)-B(11)-B(7)	-37.2(3)
B(9)-B(10)-B(11)-B(7)	-0.1(4)
B(4)-B(9)-B(12)-B(8)	100.7(3)
B(3)-B(9)-B(12)-B(8)	37.2(3)
B(10)-B(9)-B(12)-B(8)	138.1(3)
B(4)-B(9)-B(12)-B(7)	63.6(4)
B(3)-B(9)-B(12)-B(7)	0.2(4)
B(8)-B(9)-B(12)-B(7)	-37.1(3)
B(10)-B(9)-B(12)-B(7)	101.1(3)
B(4)-B(9)-B(12)-B(11)	0.0(4)
B(3)-B(9)-B(12)-B(11)	-63.4(4)
B(8)-B(9)-B(12)-B(11)	-100.6(3)
B(10)-B(9)-B(12)-B(11)	37.5(3)
B(4)-B(9)-B(12)-B(10)	-37.5(3)
B(3)-B(9)-B(12)-B(10)	-100.9(3)
B(8)-B(9)-B(12)-B(10)	-138.1(3)
B(3)-B(8)-B(12)-B(9)	-37.2(3)
B(7)-B(8)-B(12)-B(9)	-138.5(3)
B(2)-B(8)-B(12)-B(9)	-100.8(3)
B(3)-B(8)-B(12)-B(7)	101.3(3)
B(2)-B(8)-B(12)-B(7)	37.7(3)
B(9)-B(8)-B(12)-B(7)	138.5(3)
B(3)-B(8)-B(12)-B(11)	64.0(4)
B(7)-B(8)-B(12)-B(11)	-37.3(3)
B(2)-B(8)-B(12)-B(11)	0.4(4)
B(9)-B(8)-B(12)-B(11)	101.2(3)
B(3)-B(8)-B(12)-B(10)	0.4(4)
B(7)-B(8)-B(12)-B(10)	-100.9(3)
B(2)-B(8)-B(12)-B(10)	-63.2(4)
B(9)-B(8)-B(12)-B(10)	37.7(3)
B(6)-B(7)-B(12)-B(9)	-63.8(4)

B(8)-B(7)-B(12)-B(9)	37.2(3)
B(2)-B(7)-B(12)-B(9)	-0.5(4)
B(11)-B(7)-B(12)-B(9)	-101.1(3)
B(6)-B(7)-B(12)-B(8)	-101.0(3)
B(2)-B(7)-B(12)-B(8)	-37.6(3)
B(11)-B(7)-B(12)-B(8)	-138.3(3)
B(6)-B(7)-B(12)-B(11)	37.3(3)
B(8)-B(7)-B(12)-B(11)	138.3(3)
B(2)-B(7)-B(12)-B(11)	100.6(3)
B(6)-B(7)-B(12)-B(10)	0.0(4)
B(8)-B(7)-B(12)-B(10)	101.0(3)
B(2)-B(7)-B(12)-B(10)	63.4(4)
B(11)-B(7)-B(12)-B(10)	-37.2(3)
B(6)-B(11)-B(12)-B(9)	63.4(4)
B(5)-B(11)-B(12)-B(9)	-0.2(4)
B(7)-B(11)-B(12)-B(9)	100.8(3)
B(10)-B(11)-B(12)-B(9)	-37.6(3)
B(6)-B(11)-B(12)-B(8)	-0.2(4)
B(5)-B(11)-B(12)-B(8)	-63.8(4)
B(7)-B(11)-B(12)-B(8)	37.2(3)
B(10)-B(11)-B(12)-B(8)	-101.2(3)
B(6)-B(11)-B(12)-B(7)	-37.5(3)
B(5)-B(11)-B(12)-B(7)	-101.0(3)
B(10)-B(11)-B(12)-B(7)	-138.5(3)
B(6)-B(11)-B(12)-B(10)	101.0(3)
B(5)-B(11)-B(12)-B(10)	37.4(3)
B(7)-B(11)-B(12)-B(10)	138.5(3)
B(4)-B(10)-B(12)-B(9)	37.0(3)
B(5)-B(10)-B(12)-B(9)	100.7(3)
B(11)-B(10)-B(12)-B(9)	138.2(3)
B(4)-B(10)-B(12)-B(8)	-0.5(4)
B(5)-B(10)-B(12)-B(8)	63.1(4)
B(11)-B(10)-B(12)-B(8)	100.6(4)
B(9)-B(10)-B(12)-B(8)	-37.6(3)
B(4)-B(10)-B(12)-B(7)	-63.9(4)
B(5)-B(10)-B(12)-B(7)	-0.2(4)

B(11)-B(10)-B(12)-B(7)	37.2(3)
B(9)-B(10)-B(12)-B(7)	-100.9(3)
B(4)-B(10)-B(12)-B(11)	-101.1(3)
B(5)-B(10)-B(12)-B(11)	-37.5(3)
B(9)-B(10)-B(12)-B(11)	-138.2(3)
C(5)-P(1)-C(2)-C(4)	173.0(3)
C(1)-P(1)-C(2)-C(4)	63.4(3)
Ir(1)-P(1)-C(2)-C(4)	-61.5(4)
C(5)-P(1)-C(2)-C(3)	-61.2(3)
C(1)-P(1)-C(2)-C(3)	-170.8(3)
Ir(1)-P(1)-C(2)-C(3)	64.3(4)
C(2)-P(1)-C(5)-C(6)	93.6(4)
C(1)-P(1)-C(5)-C(6)	-156.3(4)
Ir(1)-P(1)-C(5)-C(6)	-39.1(4)
C(2)-P(1)-C(5)-C(7)	-34.0(4)
C(1)-P(1)-C(5)-C(7)	76.1(4)
Ir(1)-P(1)-C(5)-C(7)	-166.8(3)
C(4S)-O(1S)-C(1S)-C(2S)	-27.4(18)
O(1S)-C(1S)-C(2S)-C(3S)	21.3(13)
C(1S)-C(2S)-C(3S)-C(4S)	-7.8(14)
C(1S)-O(1S)-C(4S)-C(3S)	23(2)
C(2S)-C(3S)-C(4S)-O(1S)	-8.5(19)
C(4D)-O(1D)-C(1D)-C(2D)	26(3)
O(1D)-C(1D)-C(2D)-C(3D)	-19(3)
C(1D)-C(2D)-C(3D)-C(4D)	4(2)
C(1D)-O(1D)-C(4D)-C(3D)	-23(3)
C(2D)-C(3D)-C(4D)-O(1D)	12(3)

Symmetry transformations used to generate equivalent atoms:

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