Reversible alkoxycarbene formation by C-H activation of ethers via discrete, isolable intermediates

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Supporting Information

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I. General Information

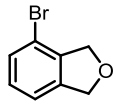
General Considerations. All manipulations were carried out using standard vacuum, Schlenk, cannula, or glovebox techniques. The following chemicals were purchased from commercial vendors and used as received: $IrCl_3 \cdot 3H_2O$, $ClPPh_2$, n-butyllithium, Di-μ-chlorotetrakis (1,5-cyclooctadiene)diiridium ($[(coe)_2IrCl]_2$)[1], and sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate ($NaBAr^F{}_4$)[2] were prepared by published procedures. Tetrahydrofuran, dichloromethane, acetonitrile, pentane, and diethyl ether were degassed with argon and dried over activated alumina using a solvent purification system. Benzene was degassed with nitrogen and stored over activated 4Å molecular sieves. ESI+MS were collected on a Thermo Scientific MSQ Plus mass spectrometer. Expected and observed masses for isotopomers are listed in order of decreasing intensity.

Spectroscopy. ^1H, ^{13}C and ^{31}P NMR spectra were recorded on Bruker NMR spectrometers at ambient temperature unless otherwise noted. ^1H and ^{13}C chemical shifts are referenced to residual solvent signals; ^{31}P chemical shifts are referenced to an external H_3PO_4 standard. ^{13}C assignments were made with the assistance of {^1H-^{13}C} HSQC experiments.

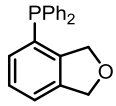
X-ray Crystallography. X-ray crystallographic data were collected on a Rigaku Oxford Diffraction Supernova diffractometer. Crystal samples were handled under immersion oil and quickly transferred to a cold nitrogen stream.

Elemental Analysis. Elemental analyses of complexes **1**, **2**, **3**, **4**, and **6** are of the bulk samples for which yields are reported. Elemental analyses were performed at the University of Rochester CENTC Elemental Analysis Facility or Robertson Microlit Laboratory in Ledgewood, NJ.

II. Synthesis and Characterization



4-bromo-1,3-dihydroisobenzofuran. The title compound is commercially available but was prepared by adaptation of a published procedure.[3]

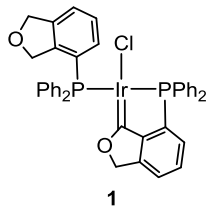


Preparation of (1,3-dihydroisobenzofuran-4-yl)diphenylphosphine (L1). In a 100 ml Schlenk flask, 1.54 g (7.78 mmol) of 4-bromo-1,3-dihydroisobenzofuran and 20 ml of tetrahydrofuran was added. The solution was cooled in a dry ice/acetone bath to -78 °C. Under nitrogen atmosphere a slight excess of n-butyllithium solution (5.0 ml, 2.5 M in hexane, 12.5 mmol) was added dropwise over a period of 30 minutes causing a color change from light yellow to orange. The resulting mixture was stirred for another 1 hour at -78 °C. Then, PPh_2Cl (1.40 ml, 7.78 mmol) was added dropwise at -78 °C. The solution was allowed to come to room temperature. After three hours at room temperature, the solution was placed in an ice bath and 30 mL degassed water was added. The solution was diluted with diethyl ether and the organic layer decanted by cannula transfer under nitrogen to Schlenk flask containing anhydrous Na_2SO_4. The aqueous layer was washed with two additional portions of degassed diethyl ether. The combined organic extracts were decanted from the Na_2SO_4 under nitrogen and evaporated to dryness under vacuum. The crude product was purified by silica gel flash chromatography (100% CH_2Cl_2) in a nitrogen glove box. Recrystallization from THF gave the product as an off-white solid. (2.02 g, 85%)

^{1}H NMR (300 MHz, C_6D_6): δ 4.87 (s, 2H, OC*H*$_2$), 5.16 (s, 2H, OC*H*$_2$), 6.76 (d, 7.36 Hz, 1H, C_6H_3), 6.91 (t, 7.48 Hz, 1H, C_6H_3), 7.02 (m, 7H, Ar), 7.34 (m, 4H, Ar).

^{31}P {^{1}H} NMR (121 MHz, C_6D_6): δ -12.78 (s).

^{13}C {^{1}H} NMR (151 MHz, C_6D_6): δ 73.52 (OCH_2), 73.61 (OCH_2), 121.57 (CH_{Ar}), 127.97 (CH_{Ar}), 128.97 (CH_{Ar}), 129.16 (CH_{Ar}), 131.49 (C_{Ar}), 131.56 (CH_{Ar}), 134.21 (CH_{Ar}), 136.17 (CH_{Ar}), 139.89 (CH_{Ar}), 144.48 (C_{Ar}).



1

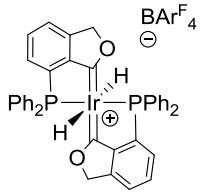
Preparation of complex 1. A heavy wall flask was charged with $[(coe)_2IrCl]_2$ (0.150 g, 0.167 mmol) **L1**, (0.206 g, 0.677 mmol, 4.05 equiv.), and 10 ml of benzene. The mixture was stirred for 3 hours at room temperature, then was heated to 60 °C for 10 hours. A color change from yellow-orange

to dark green was observed.[4] After cooling, the benzene solution was transferred to a 20 ml vial and concentrated to about 2 ml. On standing overnight at room temperature, dark green crystals appropriate for X-ray diffraction studies deposit from solution. The supernatant was removed with a pipette and concentrated to give a second portion of crystalline product. The resulting crystals were washed with 0.5 ml benzene and dried under vacuum to give the benzene solvate of **1** as a green crystalline solid (0.086 g, 28%). Anal. Calcd. for $C_{40}H_{32}ClIrO_2P_2 \cdot C_6D_6$: C, 60.55%; H, 4.20%. Found: 61.06%; H, 4.39%. ESI+MS calc. for [**1**+H]$^+$: 835.13, 833.12, 836.13. Found: 835.49, 833.49, 836.34.

^{1}H NMR (600 MHz, CD_2Cl_2): δ 2.97 (s, 2H, OCH_2), 4.73 (s, 2H, OCH_2), 4.97 (s, 2H, OCH_2), 7.13 (m, 1H, Ar), 7.24 (m, 3H, Ar), 7.35-7.48 (m, 14H, Ar), 7.53 (m, 1H, Ar), 7.85 (m, 3H, Ar), 7.98-8.04 (m, 4H, Ar).

^{31}P{^{1}H} NMR (121 MHz, CD_2Cl_2): δ 26.35 (d, 397.4 Hz), 49.98 (d, 397.4 Hz).

^{13}C{^{1}H} NMR (151 MHz, CD_2Cl_2): δ 73.36 (OCH_2), 74.95 (OCH_2), 83.88 (OCH_2), 122.30 (CH_{Ar}), 125.58 (CH_{Ar}), 127.01 (CH_{Ar}), 128.17 (CH_{Ar}), 128.91 (CH_{Ar}), 129.32 (C_{Ar}), 129.63 (C_{Ar}), 130.25 (CH_{Ar}), 130.82 (CH_{Ar}), 131.68 (CH_{Ar}), 132.01 (CH_{Ar}), 132.40 (CH_{Ar}), 132.75 (C_{Ar}), 133.07 (C_{Ar}), 134.29 (CH_{Ar}), 136.09 (CH_{Ar}), 138.72 (C_{Ar}), 139.88 (C_{Ar}), 144.02 (C_{Ar}), 169.98 (C_{Ar}), 210.12 (dd, 1.20, 10.32 Hz, Ir=*C*).



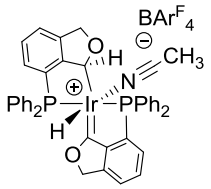
2

Preparation of complex 2. Complex **1** (0.100 g, 0.119 mmol) was taken up in 3 ml of dichloromethane and 1 equivalent of sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (0.106 g, 0.119 mmol) was added. The solution was stirred for 30 minutes during which the color changed from green to pale red-yellow. The resulting precipitate was removed by filtration through a PTFE syringe filter (0.45 μm pore size) and the solution was evaporated to dryness under vacuum. The solid was washed with a 1:1 mixture of diethyl ether and pentane to obtain **2** as an off-white solid. (0.163 g, 82%). Anal. Calcd. for $C_{72}H_{44}BF_{24}IrO_2P_2$: C, 52.03%; H, 2.67%. Found: C, 52.18%; H, 2.44%. ESI+MS calc. for [**2**-BAr$^F_4$]$^+$: 799.15, 797.15, 800.15. Found: 799.51, 797.51, 800.54.

^{1}H NMR (600 MHz, CD_2Cl_2): δ -6.09 (t, 15.3 Hz, 2H, Ir-*H*), 5.84 (s, 4H, OCH_2), 7.45-7.55 (m, 16H, Ar), 7.65 (m, 2H, Ar), 7.72 (m, 8H, Ar), 7.85-7.96 (m, 12H, Ar).

^{31}P {^{1}H} NMR (121 MHz, CD_2Cl_2): δ 33.36 (s).

^{13}C {^{1}H} NMR (151 MHz, CD_2Cl_2): δ 92.13 (OCH_2), 117.88 (CH_{Ar}), 124.10 (C_{Ar}), 124.80 (CH_{Ar}), 125.90 (C_{Ar}), 129.28 (CH_{Ar}), 129.36 (C_{Ar}), 131.78 (CH_{Ar}), 132.10 (CH_{Ar}), 133.59 (CH_{Ar}), 135.20 (CH_{Ar}), 137.29 (CH_{Ar}), 140.20 (C_{Ar}), 141.45 (C_{Ar}), 162.15 (q, 49.75 Hz, CF_3), 163.07 (C_{Ar}), 272.40 (t, 4.18 Hz, Ir=*C*).



3

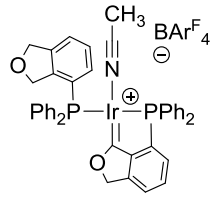
Preparation of complex 3. Complex **2** (0.100 g, 0.060 mmol) was dissolved in 1 ml of acetonitrile resulting in an immediate color change to yellow. The solution was then concentrated to dryness under vacuum, during which time yellow crystals suitable for X-ray diffraction deposited. After removal of the solvent, the residue was washed with pentane to give the product **4** as a yellow crystalline solid (100 mg, 98%). Single crystals of **4** can also be obtained from a saturated benzene solution by slow evaporation at room temperature. **4** is stable in acetonitrile for days, but will slowly convert to **5** in other solvents including benzene and diethyl ether. Anal. Calcd. For $C_{74}H_{47}BF_{24}IrNO_2P_2$: C, 52.19%; H, 2.78%. Found: C, 52.34%; H, 2.54.

^{1}H NMR (600 MHz, CD_3CN): δ –16.97 (t, 13.25 Hz, 1H, Ir-*H*), 1.24 (s, 3H, NCC*H*$_3$), (*Note*: this resonance corresponding to bound protio-MeCN is only observable immediately after dissolution in MeCN-d$_3$.), 4.76 (d, 12.39 Hz, 1H, OC*H*$_2$), 5.02 (d, 12.27 Hz, 1H, OC*H*$_2$), 5.69 (d, 18.10 Hz, 1H, OC*H*$_2$), 5.86 (d, 18.10 Hz, 1H, OC*H*$_2$), 6.38 (s, 1H, OC*H*), 7.06 (m, 1H, Ar), 7.12 (t, 7.72 Hz, 1H, Ar), 7.22 (m, 1H, Ar), 7.42-7.47 (m, 4H, Ar), 7.49-7.51 (m, 8H, Ar), 7.62 (m, 2H, Ar), 7.66 (s, 4H, Ar), 7.70-7.74 (m, 12H, Ar), 7.79 (m, 1H, Ar), 7.95 (m, 2H, Ar), 7.99 (m, 1H, Ar), 8.04 (m, 1H, Ar).

^{1}H NMR (600 MHz, C_6D_6): δ –16.58 (t, 12.92 Hz, 1H, Ir-*H*), 0.10 (s, 3H, NCC*H*$_3$), 4.36 (d, 17.93 Hz, 1H, OC*H*$_2$), 4.54 (d, 17.96 Hz, 1H, OC*H*$_2$), 4.80 (d, 12.37 Hz, 1H, OC*H*$_2$), 5.09 (d, 12.34 Hz, 1H, OC*H*$_2$), 6.35 (dd, 1.75, 7.50 Hz, 1H, OC*H*), 6.47 (s, 1H, Ar), 6.76 (m, 1H, Ar), 6.82 (m, 1H, Ar), 6.91 (t, 7.71 Hz, 1H, Ar), 6.99-7.13 (m, 14H, Ar), 7.28 (t, 7.08 Hz, 1H, Ar), 7.49 (m, 2H, Ar), 7.57 (s, 4H, Ar), 7.62 (m, 3H, Ar), 7.89-7.93 (m, 2H, Ar), 8.35 (s, 8H, Ar). ESI+MS calc. for [**3**-BAr$^F_4$]$^+$: 840.18, 838.17, 841.18. Found: 840.37, 838.57, 841.56.

^{31}P {^{1}H} NMR (121 MHz, CD_3CN): δ 29.05 (d, 364.8 Hz), 38.02 (d, 364.8 Hz).

^{13}C {^{1}H} NMR (151 MHz, CD_3CN): δ 1.28 (*C*H$_3$CN), 74.34 (OCH$_2$), 74.39 (OCH), 92.99 (OCH$_2$), 118.30 (CH$_3$CN), 118.70 (*C*H$_{Ar}$), 123.78 (*C*H$_{Ar}$), 124.17 (*C*H$_{Ar}$), 125.58 (*C*$_{Ar}$), 126.03 (*C*H$_{Ar}$), 126.35 (*C*H$_{Ar}$), 127.84 (*C*H$_{Ar}$), 128.18 (*C*H$_{Ar}$), 129.40 (*C*H$_{Ar}$), 129.64 (*C*H$_{Ar}$), 129.80 (*C*H$_{Ar}$), 130.06 (*C*$_{Ar}$), 130.24 (*C*$_{Ar}$), 130.72 (*C*$_{Ar}$), 131.10 (*C*$_{Ar}$), 131.66 (*C*$_{Ar}$), 131.97 (*C*H$_{Ar}$), 132.38 (*C*H$_{Ar}$), 132.55 (*C*$_{Ar}$), 132.68 (*C*H$_{Ar}$), 132.86 (*C*H$_{Ar}$), 133.15 (*C*H$_{Ar}$), 133.38 (*C*H$_{Ar}$), 134.95 (*C*H$_{Ar}$), 135.27 (*C*H$_{Ar}$), 135.67 (*C*H$_{Ar}$), 137.98 (*C*$_{Ar}$), 140.00 (*C*$_{Ar}$), 140.16 (*C*$_{Ar}$), 143.23 (*C*$_{Ar}$), 162.63 (q, 49.62 Hz, *C*F$_3$), 163.06 (*C*$_{Ar}$), 171.32 (*C*H$_{Ar}$), 263.14 (dd, 2.59, 7.89 Hz, Ir-*C*).



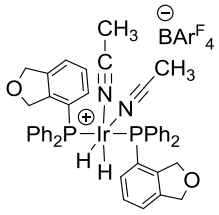
4

Preparation of complex 4. Complex **3** (0.100 g, 0.060 mmol) was dissolved in 2 mL diethyl ether and allowed to stand at room temperature for 18 hours, during which time the color changed from yellow to dark green. The solvent was removed under vacuum and the material was dissolved in a minimum of benzene. Green crystals of **4** were grown from a concentrated benzene solution by slow evaporation at room temperature (isolated as the benzene solvate **4**·C_6H_6; 0.100g, 96%). Anal. Calcd. For $C_{74}H_{47}BF_{24}IrNO_2P_2$·$C_6H_6$: C, 53.94%; H, 3.00%; N, 0.79%; Found: C, 54.12%; H, 3.02%; N, 0.69%. ESI+MS calc. for [**4**-BAr^F_4]$^+$: 840.18, 838.17, 841.18. Found: 840.56, 838.57, 841.57.

^{1}H NMR (600 MHz, C_6D_6): δ 0.60 (s, 3H, NCC*H*$_3$), 2.74 (s, 2H, OC*H*$_2$), 4.62 (s, 2H, OC*H*$_2$), 4.77 (s, 2H, OC*H*$_2$), 6.16 (m, 1H, Ar), 6.79 (d, 7.44 Hz, 1H, Ar), 6.95 (t, 7.44Hz, 1H, Ar), 7.02-7.11 (m, 14H, Ar), 7.20 (m, 1H, Ar), 7.25 (m, 1H, Ar), 7.60 (s, 4H, Ar), 7.62-7.65 (m, 3H, Ar), 7.68-7.72 (m, 4H, Ar), 8.40 (s, 8H, Ar).

^{31}P {^{1}H} NMR (121 MHz, C_6D_6): δ 21.72 (d, 336.5 Hz), 52.88 (d, 336.5 Hz).

^{13}C {^{1}H} NMR (151 MHz, C_6D_6): δ 0.17 (*C*H$_3$CN), 72.75 (OCH$_2$), 74.35 (OCH$_2$), 85.73 (OCH$_2$), 117.85 (*C*H$_{Ar}$), 122.50(CH$_3$*C*N), 123.15 (*C*H$_{Ar}$), 124.31 (*C*$_{Ar}$), 125.33 (*C*H$_{Ar}$), 126.12 (*C*$_{Ar}$), 127.90 (*C*H$_{Ar}$), 128.21 (*C*H$_{Ar}$), 128.81 (*C*H$_{Ar}$), 129.59 (*C*H$_{Ar}$), 129.82 (*C*$_{Ar}$), 130.03 (*C*$_{Ar}$), 130.30 (*C*$_{Ar}$), 130.56 (*C*$_{Ar}$), 130.93 (*C*$_{Ar}$), 131.30 (*C*H$_{Ar}$), 131.70 (*C*H$_{Ar}$), 132.01 (*C*H$_{Ar}$), 133.29 (*C*H$_{Ar}$), 134.74 (*C*$_{Ar}$), 135.30 (*C*H$_{Ar}$), 135.42 (*C*H$_{Ar}$), 139.43 (*C*$_{Ar}$), 140.63 (*C*$_{Ar}$), 143.29 (*C*$_{Ar}$), 162.80 (q, 49.66 Hz, *C*F$_3$), 227.78 (dd, 3.67, 12.62 Hz, Ir-*C*).



6

Preparation of ((1,3-dihydroisobenzofuran-4-yl)PPh$_2$)$_2$IrH$_2$(NCMe)$_2$BAr$^F_4$ (6). A 100 ml heavy-wall glass reaction vessel was charged with complex **2** (0.050 g, 0.030 mmol) and 1 ml of tetrahydrofuran. The solution was frozen solid in liquid nitrogen and the vessel evacuated under vacuum. The solution was allowed to thaw under static vacuum, after which the evacuated flask was charged with 1 atmosphere of hydrogen gas. The reaction was allowed to stir for 20 mins, at which point 0.5 ml of acetonitrile was added. The solution was then evaporated to dryness to give the product **7** (0.052g, 100%). Anal. Calcd. For $C_{76}H_{54}BF_{24}IrNO_2P_2$: C, 52.22%; H, 3.11%. Found: C, 52.32%; H, 2.68%. ESI+MS calc. for [**6**-BAr^F_4]$^+$: 840.18, 838.17, 841.18. Found: 840.56, 838.57, 841.57.

^{1}H NMR (600 MHz, C_6D_6): δ -20.43 (t, 15.60 Hz, 2H, Ir-*H*), 0.55 (s, 6H, NCC*H*$_3$), 4.59 (s, 4H, OC*H*$_2$), 4.66 (s, 4H, OC*H*$_2$), 6.78 (d, 7.57 Hz, 2H, Ar), 6.92 (t, 7.57 Hz, 2H, Ar), 6.97-6.99 (m, 12H, Ar), 7.23 (m, 2H, Ar), 7.50 (m, 8H, Ar), 7.66 (s, 4H, Ar), 8.39 (s, 8H, Ar).

^{31}P {^{1}H} NMR (121 MHz, C_6D_6): δ 13.76 (s).

^{13}C {^{1}H} NMR (151 MHz, C_6D_6): δ 0.27 (*C*H$_3$CN), 72.56 (OCH$_2$), 72.96 (OCH$_2$), 118.13 (*C*H$_{Ar}$), 119.14 (CH$_3$CN), 124.02 (*C*H$_{Ar}$), 126.14 (*C*$_{Ar}$), 126.56 (*C*$_{Ar}$), 127.85 (*C*H$_{Ar}$), 128.84 (*C*H$_{Ar}$), 129.91 (*C*$_{Ar}$), 130.60 (*C*$_{Ar}$), 131.39 (*C*H$_{Ar}$), 132.37 (*C*H$_{Ar}$), 134.09 (*C*H$_{Ar}$), 135.44 (*C*H$_{Ar}$), 141.42 (*C*$_{Ar}$), 143.12 (*C*$_{Ar}$), 162.68 (q, 49.63 Hz, *C*F$_3$).

III. NMR Experiments

Observation of complex 5 in solutions of 2 in THF. An NMR tube was charged with complex **2** (0.010 g, 0.006 mmol) and 0.5 ml of THF-d_8, giving a yellow solution that rapidly underwent a color change from yellow to green. The $^{31}P\{^1H\}$ NMR spectrum is consistent with two species, including a broad singlet assigned to complex **2**. The other observed species appears as a pair of doublets assigned as complex **5**. The relative intensity of the signals resulting from the two species is consistent with a molar ratio of 1/0.6 for complexes **5** and **2** respectively at room temperature in THF. Removal of the solvent and replacement by C_6D_6 returns a spectrum consistent with complete conversion back to complex **2**. Attempts to crystallize complex **5** gave crystals of **2** exclusively.

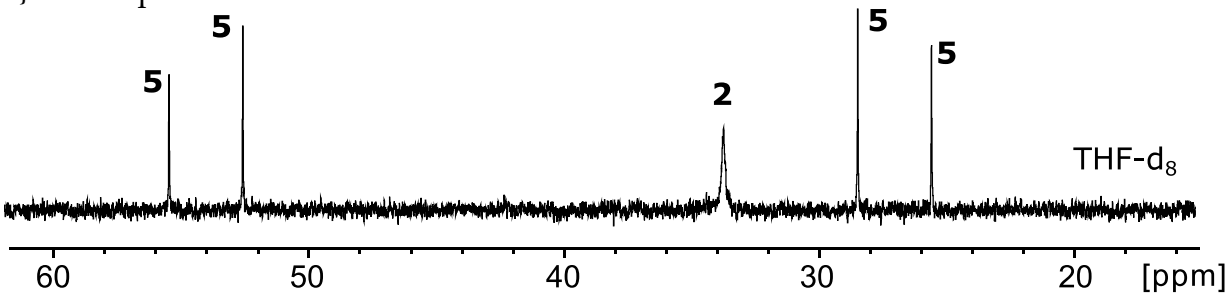
Partial assignment of a set of ^1H resonances associated with complex **5** was accomplished with assistance from ^1H-^{13}C HSQC.

^1H NMR (600 MHz, THF-d_8): δ 3.66 (s, 2H, OCH_2), 4.61 (s, 2H, OCH_2), 4.92 (s, 2H, OCH_2), no metal hydride resonance is observed in either protio-THF or THF-d_8, consistent with the formulation of **5** as the THF analogue of complex **4**. ^1H NMR resonances of complex **2** in THF can be detected in the same sample at δ -6.10 (br, 2H, Ir-*H*), 5.97 (br, 4H, OCH_2).

$^{31}P\{^1H\}$ NMR of **5** (243 MHz, THF-d_8): δ 26.66 (d, 351.29 Hz), 53.65 (d, 351.29 Hz).

$^{31}P\{^1H\}$ NMR of **2** (243 MHz, THF-d_8): δ 33.36 (br).

$^{31}P\{^1H\}$ NMR spectra of **2** in THF-d_8



Observation of complex 4 as a product of dehydrogenation of complex 6. A J. Young NMR tube was charged with complex **6** (0.050 mg, 0.003 mmol), 2,2-dimethylbutene (1.8 μL, 0.015 mmol, 5 equivalents), 0.5 ml of benzene-d_6, and a capillary of triphenylphosphine in benzene-d_6 as an integration standard and sealed under nitrogen. The sample was heated at 80 °C and monitored by $^{31}P\{^1H\}$ NMR spectroscopy. Complex **6** was observed to slowly convert to complex **4** over 24 hours, causing a color change from light yellow to green. The NMR yield of complex **4** is estimated to be 62%. In a control experiment, a benzene solution of complex **4** was found to slowly decompose at 80 °C over a similar timeframe.

IV. X-Ray Crystallographic Data

Complex **1**. A suitable crystal of **1**·(C_6H_6) was selected for analysis and mounted in a polyimide loop. All measurements were made on a Rigaku Oxford Diffraction Supernova Eos CCD with filtered Cu-Kα radiation at a temperature of 100 K. Using Olex2,[5] the structure was solved with the ShelXT structure solution program using Direct Methods and refined with the ShelXL refinement package[6] using Least Squares minimization.

Table 1. Crystal data and structure refinement for complex **1**.

Empirical formula	$C_{40}H_{32}ClIrO_2P_2$·(C_6H_6)	
Formula weight	912.35	
Temperature	100 K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 8.41924(8) Å	α = 90°
	b = 18.7237(2) Å	β = 97.6709(9)°
	c = 24.1937(2) Å	γ = 90°
Volume	3779.75(7) $Å^3$	
Z	4	
Density (calculated)	1.603 Mg/m^3	
Absorption coefficient	8.590 mm^{-1}	
F(000)	1816	
Crystal size	0.089 x 0.039 x 0.01 mm^3	
Theta range for data collection	3.687 to 73.416°.	
Index ranges	-9<=h<=10, -22<=k<=18, -30<=l<=29	
Reflections collected	36409	
Independent reflections	7488 [R(int) = 0.0439]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.58334	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7488 / 0 / 469	
Goodness-of-fit on F^2	1.059	
Final R indices [I>2sigma(I)]	R1 = 0.0301, wR2 = 0.0748	
R indices (all data)	R1 = 0.0329, wR2 = 0.0766	
Largest diff. peak and hole	1.594 and -1.395 e/$Å^{-3}$	

Table 2. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^4) for complex **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	74900(2)	28145(2)	28213(2)	160(1)
Cl(1)	77912(10)	15647(4)	29997(3)	237(2)
P(1)	58232(10)	25979(5)	19937(3)	174(2)
P(2)	91021(10)	31755(4)	36081(3)	168(2)
O(1)	75540(30)	43903(13)	28980(9)	226(5)
O(2)	76920(50)	13373(17)	47854(14)	534(9)
C(1)	70930(40)	37780(17)	26262(13)	186(6)
C(2)	69320(40)	50217(18)	25806(13)	218(7)
C(3)	60650(40)	39865(18)	21181(13)	184(6)
C(4)	58950(40)	47136(19)	20814(13)	216(7)
C(5)	48760(40)	50025(19)	16380(14)	249(7)
C(6)	40840(40)	45240(20)	12535(14)	264(7)
C(7)	42940(40)	37840(19)	12937(13)	229(7)
C(8)	53100(40)	35019(18)	17377(13)	199(6)
C(9)	65290(40)	21147(18)	14180(13)	202(7)
C(10)	70210(40)	24590(20)	9603(13)	235(7)
C(11)	75700(40)	20590(20)	5403(14)	271(8)
C(12)	76450(40)	13240(20)	5709(14)	285(8)
C(13)	71490(40)	9750(20)	10279(15)	274(8)
C(14)	65860(40)	13682(19)	14451(14)	243(7)
C(15)	38930(40)	21763(17)	20254(15)	212(7)
C(16)	28330(40)	20580(20)	15386(16)	272(8)
C(17)	12980(40)	17990(20)	15695(17)	318(8)
C(18)	8320(40)	16580(20)	20850(18)	324(8)
C(19)	18820(50)	17500(20)	25641(17)	333(9)
C(20)	34170(40)	20110(20)	25388(15)	259(7)
C(21)	102310(40)	24701(19)	40078(13)	208(7)
C(22)	94460(50)	19690(20)	42987(13)	256(7)
C(23)	77320(50)	19290(20)	44096(16)	341(9)
C(24)	90750(60)	9060(20)	47734(17)	460(11)
C(25)	102460(50)	13680(20)	45330(15)	337(9)
C(26)	118470(50)	12590(20)	45028(16)	389(10)
C(27)	126690(50)	17600(20)	42358(17)	388(10)
C(28)	118780(50)	23610(20)	39877(15)	289(8)
C(29)	106430(40)	38039(18)	34555(13)	204(7)
C(30)	109250(40)	44685(19)	37153(14)	240(7)
C(31)	120290(40)	49350(20)	35385(15)	294(8)
C(32)	128750(50)	47500(20)	31110(17)	355(9)
C(33)	126310(50)	40910(30)	28569(17)	386(10)
C(34)	115090(50)	36270(20)	30227(16)	302(8)
C(35)	80990(40)	36116(18)	41396(13)	202(7)

C(36)	64810(40)	37940(20)	40331(14)	238(7)
C(37)	57140(40)	40980(20)	44452(15)	317(9)
C(38)	65420(50)	42280(20)	49711(15)	345(9)
C(39)	81490(50)	40470(20)	50848(14)	299(8)
C(40)	89260(40)	37440(20)	46720(14)	253(7)
C(41)	100810(60)	37700(30)	15160(20)	474(11)
C(42)	97940(60)	44260(30)	17440(20)	501(12)
C(43)	95470(60)	50250(30)	14030(30)	614(15)
C(44)	96310(60)	49600(40)	8510(30)	689(18)
C(45)	99540(60)	43130(40)	6210(20)	630(16)
C(46)	101740(50)	37180(30)	9550(20)	508(12)

Table 3. Bond lengths [Å] and angles [°] for complex **1**.

Ir(1)-Cl(1)	2.3869(8)	C(17)-C(18)	1.382(6)
Ir(1)-P(1)	2.3222(8)	C(18)-H(18)	0.9500
Ir(1)-P(2)	2.2876(8)	C(18)-C(19)	1.372(6)
Ir(1)-C(1)	1.883(3)	C(19)-H(19)	0.9500
P(1)-C(8)	1.834(3)	C(19)-C(20)	1.390(5)
P(1)-C(9)	1.826(3)	C(20)-H(20)	0.9500
P(1)-C(15)	1.817(4)	C(21)-C(22)	1.392(5)
P(2)-C(21)	1.827(3)	C(21)-C(28)	1.409(5)
P(2)-C(29)	1.825(3)	C(22)-C(23)	1.504(5)
P(2)-C(35)	1.823(3)	C(22)-C(25)	1.393(5)
O(1)-C(1)	1.353(4)	C(23)-H(23A)	0.9900
O(1)-C(2)	1.468(4)	C(23)-H(23B)	0.9900
O(2)-C(23)	1.437(5)	C(24)-H(24A)	0.9900
O(2)-C(24)	1.420(6)	C(24)-H(24B)	0.9900
C(1)-C(3)	1.459(4)	C(24)-C(25)	1.487(6)
C(2)-H(2A)	0.9900	C(25)-C(26)	1.375(6)
C(2)-H(2B)	0.9900	C(26)-H(26)	0.9500
C(2)-C(4)	1.507(4)	C(26)-C(27)	1.378(6)
C(3)-C(4)	1.370(5)	C(27)-H(27)	0.9500
C(3)-C(8)	1.385(5)	C(27)-C(28)	1.400(6)
C(4)-C(5)	1.390(5)	C(28)-H(28)	0.9500
C(5)-H(5)	0.9500	C(29)-C(30)	1.400(5)
C(5)-C(6)	1.395(5)	C(29)-C(34)	1.393(5)
C(6)-H(6)	0.9500	C(30)-H(30)	0.9500
C(6)-C(7)	1.399(5)	C(30)-C(31)	1.385(5)
C(7)-H(7)	0.9500	C(31)-H(31)	0.9500
C(7)-C(8)	1.385(5)	C(31)-C(32)	1.376(5)
C(9)-C(10)	1.391(5)	C(32)-H(32)	0.9500
C(9)-C(14)	1.400(5)	C(32)-C(33)	1.382(6)
C(10)-H(10)	0.9500	C(33)-H(33)	0.9500
C(10)-C(11)	1.390(5)	C(33)-C(34)	1.382(5)
C(11)-H(11)	0.9500	C(34)-H(34)	0.9500
C(11)-C(12)	1.380(5)	C(35)-C(36)	1.394(5)
C(12)-H(12)	0.9500	C(35)-C(40)	1.402(4)
C(12)-C(13)	1.395(5)	C(36)-H(36)	0.9500
C(13)-H(13)	0.9500	C(36)-C(37)	1.381(5)
C(13)-C(14)	1.383(5)	C(37)-H(37)	0.9500
C(14)-H(14)	0.9500	C(37)-C(38)	1.388(5)
C(15)-C(16)	1.397(5)	C(38)-H(38)	0.9500
C(15)-C(20)	1.390(5)	C(38)-C(39)	1.386(5)
C(16)-H(16)	0.9500	C(39)-H(39)	0.9500
C(16)-C(17)	1.392(5)	C(39)-C(40)	1.386(5)
C(17)-H(17)	0.9500	C(40)-H(40)	0.9500

C(41)-H(41)	0.9500
C(41)-C(42)	1.381(7)
C(41)-C(46)	1.372(7)
C(42)-H(42)	0.9500
C(42)-C(43)	1.390(7)
C(43)-H(43)	0.9500
C(43)-C(44)	1.353(8)
C(44)-H(44)	0.9500
C(44)-C(45)	1.376(9)
C(45)-H(45)	0.9500
C(45)-C(46)	1.375(8)
C(46)-H(46)	0.9500

P(1)-Ir(1)-Cl(1)	91.27(3)
P(2)-Ir(1)-Cl(1)	95.87(3)
P(2)-Ir(1)-P(1)	172.85(3)
C(1)-Ir(1)-Cl(1)	174.53(10)
C(1)-Ir(1)-P(1)	83.38(10)
C(1)-Ir(1)-P(2)	89.49(10)
C(8)-P(1)-Ir(1)	102.60(11)
C(9)-P(1)-Ir(1)	121.57(11)
C(9)-P(1)-C(8)	106.61(15)
C(15)-P(1)-Ir(1)	118.70(12)
C(15)-P(1)-C(8)	104.09(15)
C(15)-P(1)-C(9)	101.59(15)
C(21)-P(2)-Ir(1)	115.84(11)
C(29)-P(2)-Ir(1)	112.39(10)
C(29)-P(2)-C(21)	103.85(15)
C(35)-P(2)-Ir(1)	116.10(11)
C(35)-P(2)-C(21)	102.00(15)
C(35)-P(2)-C(29)	105.23(15)
C(1)-O(1)-C(2)	111.7(2)
C(24)-O(2)-C(23)	109.7(3)
O(1)-C(1)-Ir(1)	131.3(2)
O(1)-C(1)-C(3)	106.4(3)
C(3)-C(1)-Ir(1)	122.2(2)
O(1)-C(2)-H(2A)	111.0
O(1)-C(2)-H(2B)	111.0
O(1)-C(2)-C(4)	103.8(3)
H(2A)-C(2)-H(2B)	109.0
C(4)-C(2)-H(2A)	111.0
C(4)-C(2)-H(2B)	111.0
C(4)-C(3)-C(1)	111.4(3)
C(4)-C(3)-C(8)	125.0(3)
C(8)-C(3)-C(1)	123.5(3)
C(3)-C(4)-C(2)	106.5(3)
C(3)-C(4)-C(5)	119.0(3)
C(5)-C(4)-C(2)	134.5(3)
C(4)-C(5)-H(5)	121.4
C(4)-C(5)-C(6)	117.1(3)
C(6)-C(5)-H(5)	121.4
C(5)-C(6)-H(6)	118.5
C(5)-C(6)-C(7)	123.0(3)
C(7)-C(6)-H(6)	118.5
C(6)-C(7)-H(7)	120.3
C(8)-C(7)-C(6)	119.4(3)
C(8)-C(7)-H(7)	120.3
C(3)-C(8)-P(1)	108.3(2)
C(3)-C(8)-C(7)	116.5(3)
C(7)-C(8)-P(1)	135.0(3)
C(10)-C(9)-P(1)	122.7(3)
C(10)-C(9)-C(14)	119.2(3)
C(14)-C(9)-P(1)	118.1(3)
C(9)-C(10)-H(10)	120.1
C(11)-C(10)-C(9)	119.7(4)
C(11)-C(10)-H(10)	120.1
C(10)-C(11)-H(11)	119.5
C(12)-C(11)-C(10)	121.0(3)
C(12)-C(11)-H(11)	119.5
C(11)-C(12)-H(12)	120.2
C(11)-C(12)-C(13)	119.5(3)
C(13)-C(12)-H(12)	120.2
C(12)-C(13)-H(13)	120.1
C(14)-C(13)-C(12)	119.8(3)
C(14)-C(13)-H(13)	120.1
C(9)-C(14)-H(14)	119.7
C(13)-C(14)-C(9)	120.7(3)
C(13)-C(14)-H(14)	119.7
C(16)-C(15)-P(1)	120.5(3)
C(20)-C(15)-P(1)	120.0(3)
C(20)-C(15)-C(16)	119.3(3)
C(15)-C(16)-H(16)	119.9
C(17)-C(16)-C(15)	120.2(4)
C(17)-C(16)-H(16)	119.9
C(16)-C(17)-H(17)	120.2
C(18)-C(17)-C(16)	119.5(4)

C(18)-C(17)-H(17)	120.2	C(29)-C(30)-H(30)	119.9
C(17)-C(18)-H(18)	119.7	C(31)-C(30)-C(29)	120.2(3)
C(19)-C(18)-C(17)	120.6(3)	C(31)-C(30)-H(30)	119.9
C(19)-C(18)-H(18)	119.7	C(30)-C(31)-H(31)	119.7
C(18)-C(19)-H(19)	119.8	C(32)-C(31)-C(30)	120.6(4)
C(18)-C(19)-C(20)	120.3(4)	C(32)-C(31)-H(31)	119.7
C(20)-C(19)-H(19)	119.8	C(31)-C(32)-H(32)	120.1
C(15)-C(20)-C(19)	119.9(3)	C(31)-C(32)-C(33)	119.9(4)
C(15)-C(20)-H(20)	120.1	C(33)-C(32)-H(32)	120.1
C(19)-C(20)-H(20)	120.1	C(32)-C(33)-H(33)	120.0
C(22)-C(21)-P(2)	120.4(3)	C(34)-C(33)-C(32)	120.0(3)
C(22)-C(21)-C(28)	117.1(3)	C(34)-C(33)-H(33)	120.0
C(28)-C(21)-P(2)	122.1(3)	C(29)-C(34)-H(34)	119.5
C(21)-C(22)-C(23)	130.9(3)	C(33)-C(34)-C(29)	121.0(4)
C(21)-C(22)-C(25)	121.0(4)	C(33)-C(34)-H(34)	119.5
C(25)-C(22)-C(23)	108.1(3)	C(36)-C(35)-P(2)	120.8(2)
O(2)-C(23)-C(22)	104.8(3)	C(36)-C(35)-C(40)	118.6(3)
O(2)-C(23)-H(23A)	110.8	C(40)-C(35)-P(2)	120.5(3)
O(2)-C(23)-H(23B)	110.8	C(35)-C(36)-H(36)	119.8
C(22)-C(23)-H(23A)	110.8	C(37)-C(36)-C(35)	120.5(3)
C(22)-C(23)-H(23B)	110.8	C(37)-C(36)-H(36)	119.8
H(23A)-C(23)-H(23B)	108.9	C(36)-C(37)-H(37)	119.8
O(2)-C(24)-H(24A)	110.7	C(36)-C(37)-C(38)	120.5(3)
O(2)-C(24)-H(24B)	110.7	C(38)-C(37)-H(37)	119.8
O(2)-C(24)-C(25)	105.4(3)	C(37)-C(38)-H(38)	120.1
H(24A)-C(24)-H(24B)	108.8	C(39)-C(38)-C(37)	119.8(3)
C(25)-C(24)-H(24A)	110.7	C(39)-C(38)-H(38)	120.1
C(25)-C(24)-H(24B)	110.7	C(38)-C(39)-H(39)	120.0
C(22)-C(25)-C(24)	108.6(4)	C(40)-C(39)-C(38)	119.9(3)
C(26)-C(25)-C(22)	121.5(4)	C(40)-C(39)-H(39)	120.0
C(26)-C(25)-C(24)	129.8(4)	C(35)-C(40)-H(40)	119.7
C(25)-C(26)-H(26)	120.6	C(39)-C(40)-C(35)	120.7(3)
C(25)-C(26)-C(27)	118.8(4)	C(39)-C(40)-H(40)	119.7
C(27)-C(26)-H(26)	120.6	C(42)-C(41)-H(41)	120.2
C(26)-C(27)-H(27)	119.7	C(46)-C(41)-H(41)	120.2
C(26)-C(27)-C(28)	120.6(4)	C(46)-C(41)-C(42)	119.6(5)
C(28)-C(27)-H(27)	119.7	C(41)-C(42)-H(42)	120.0
C(21)-C(28)-H(28)	119.5	C(41)-C(42)-C(43)	120.1(5)
C(27)-C(28)-C(21)	121.1(4)	C(43)-C(42)-H(42)	120.0
C(27)-C(28)-H(28)	119.5	C(42)-C(43)-H(43)	120.3
C(30)-C(29)-P(2)	124.4(3)	C(44)-C(43)-C(42)	119.3(6)
C(34)-C(29)-P(2)	117.1(3)	C(44)-C(43)-H(43)	120.3
C(34)-C(29)-C(30)	118.3(3)	C(43)-C(44)-H(44)	119.4

C(43)-C(44)-C(45)	121.2(5)	C(46)-C(45)-H(45)	120.2
C(45)-C(44)-H(44)	119.4	C(41)-C(46)-C(45)	120.3(5)
C(44)-C(45)-H(45)	120.2	C(41)-C(46)-H(46)	119.9
C(46)-C(45)-C(44)	119.6(5)	C(45)-C(46)-H(46)	119.9

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for complex **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	186(1)	145(1)	151(1)	-1(1)	29(1)	-10(1)
Cl(1)	305(4)	172(4)	228(3)	6(3)	20(3)	5(3)
P(1)	198(4)	155(4)	170(3)	-10(3)	30(3)	-6(3)
P(2)	180(4)	170(4)	159(3)	-5(3)	41(3)	2(3)
O(1)	294(13)	153(12)	226(11)	10(9)	22(10)	3(10)
O(2)	820(30)	304(17)	562(19)	129(15)	391(19)	-20(16)
C(1)	232(16)	138(16)	193(14)	3(12)	42(12)	-33(13)
C(2)	283(17)	129(15)	237(15)	8(12)	15(13)	18(13)
C(3)	187(15)	190(16)	184(14)	41(12)	58(12)	31(13)
C(4)	225(16)	220(17)	213(15)	-15(13)	63(13)	-21(14)
C(5)	260(17)	214(18)	274(17)	26(14)	43(14)	8(14)
C(6)	294(18)	258(19)	231(16)	39(14)	4(14)	11(15)
C(7)	216(16)	253(18)	213(15)	-11(13)	9(13)	-6(14)
C(8)	221(16)	186(17)	204(14)	-7(13)	80(12)	-11(13)
C(9)	187(16)	230(18)	184(15)	-50(12)	8(12)	4(13)
C(10)	235(17)	263(19)	206(15)	-18(14)	23(13)	-6(14)
C(11)	232(17)	390(20)	203(16)	-18(15)	63(13)	3(15)
C(12)	214(17)	400(20)	233(16)	-110(15)	-9(13)	68(15)
C(13)	283(18)	231(18)	295(17)	-63(14)	-7(14)	47(15)
C(14)	229(17)	254(19)	240(16)	-8(14)	15(13)	22(14)
C(15)	219(17)	162(17)	259(16)	-15(12)	48(14)	3(13)
C(16)	235(18)	259(19)	312(18)	0(15)	3(15)	-19(15)
C(17)	239(18)	250(20)	440(20)	-15(16)	-43(16)	-29(15)
C(18)	219(17)	229(19)	540(20)	-60(17)	99(16)	-52(15)
C(19)	380(20)	270(20)	380(20)	-66(16)	162(17)	-76(17)
C(20)	276(18)	236(18)	282(17)	-37(14)	97(14)	-48(15)
C(21)	239(17)	195(17)	181(14)	-47(13)	-6(12)	26(14)
C(22)	350(20)	246(18)	173(14)	-29(14)	43(13)	35(16)
C(23)	460(20)	270(20)	323(19)	53(16)	168(17)	-25(18)
C(24)	810(30)	290(20)	300(20)	61(17)	150(20)	40(20)
C(25)	540(30)	240(20)	215(16)	-5(14)	0(16)	11(18)
C(26)	530(30)	280(20)	311(19)	-9(16)	-113(18)	131(19)
C(27)	310(20)	420(30)	390(20)	-130(19)	-102(17)	135(18)
C(28)	263(18)	300(20)	282(17)	-55(16)	-27(14)	28(16)
C(29)	177(15)	225(17)	208(14)	2(13)	25(12)	-9(13)
C(30)	236(17)	236(18)	260(16)	-42(14)	73(13)	-35(14)
C(31)	300(19)	235(19)	352(19)	-59(15)	64(15)	-64(15)
C(32)	330(20)	330(20)	420(20)	-30(18)	128(17)	-112(17)
C(33)	370(20)	420(30)	430(20)	-117(18)	259(19)	-105(18)

C(34)	314(19)	280(20)	347(19)	-88(16)	182(16)	-64(16)
C(35)	210(16)	218(17)	187(14)	12(13)	52(12)	-2(13)
C(36)	200(16)	295(19)	218(15)	2(14)	31(13)	15(14)
C(37)	245(18)	450(20)	273(17)	-18(17)	96(14)	96(17)
C(38)	350(20)	440(20)	265(17)	-51(17)	121(16)	91(18)
C(39)	325(19)	370(20)	202(15)	-72(15)	50(14)	43(17)
C(40)	255(17)	299(19)	207(16)	-36(14)	43(13)	27(15)
C(41)	410(20)	450(30)	590(30)	50(20)	150(20)	20(20)
C(42)	490(30)	540(30)	530(30)	110(20)	250(20)	120(20)
C(43)	540(30)	490(30)	890(40)	160(30)	390(30)	140(30)
C(44)	450(30)	860(50)	780(40)	420(40)	190(30)	150(30)
C(45)	360(30)	1070(50)	460(30)	100(30)	30(20)	-70(30)
C(46)	320(20)	610(30)	580(30)	-90(30)	20(20)	-90(20)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for complex **1**.

	x	y	z	U(eq)
H(2A)	7816	5310	2464	26
H(2B)	6294	5325	2804	26
H(5)	4727	5504	1599	30
H(6)	3368	4710	951	32
H(7)	3746	3478	1019	28
H(10)	6983	2965	935	28
H(11)	7898	2296	227	33
H(12)	8032	1057	283	34
H(13)	7197	469	1052	33
H(14)	6235	1129	1753	29
H(16)	3161	2155	1185	33
H(17)	576	1720	1239	38
H(18)	-226	1495	2108	39
H(19)	1559	1636	2915	40
H(20)	4139	2076	2872	31
H(23A)	7412	2377	4583	41
H(23B)	7003	1846	4059	41
H(24A)	8815	478	4538	55
H(24B)	9511	750	5154	55
H(26)	12377	845	4663	47
H(27)	13782	1698	4220	47
H(28)	12461	2700	3803	35
H(30)	10357	4600	4014	29
H(31)	12204	5388	3714	35
H(32)	13626	5075	2991	43
H(33)	13234	3957	2568	46
H(34)	11325	3180	2839	36
H(36)	5903	3709	3674	29
H(37)	4611	4220	4368	38
H(38)	6009	4440	5252	41
H(39)	8718	4131	5445	36
H(40)	10030	3625	4751	30
H(41)	10213	3357	1745	57
H(42)	9765	4469	2133	60
H(43)	9322	5475	1557	74
H(44)	9464	5369	618	83
H(45)	10025	4278	233	76
H(46)	10390	3270	798	61

Complex **2**. A suitable crystal of **2**·0.5(Et_2O) was selected for analysis and mounted in a polyimide loop. All measurements were made on a Rigaku Oxford Diffraction Supernova Eos CCD with filtered Mo-Kα radiation at a temperature of 100 K. Using Olex2,[5] the structure was solved with the ShelXT structure solution program using Direct Methods and refined with the ShelXL refinement package[6] using Least Squares minimization. Two-site disorder in the ether solvent was modeled with an occupancy constraint. The metal hydrides were located in the difference map and refined without restraint.

Table 6. Crystal data and structure refinement for complex **2**.

Empirical formula	$C_{72}H_{44}BF_{24}IrO_2P_2$·0.5($C_4H_{10}O$)	
Formula weight	1699.08	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.2902(2) Å	α = 88.6800(14)°
	b = 16.0229(3) Å	β = 89.2622(14)°
	c = 16.6282(3) Å	γ = 78.5165(14)°
Volume	3469.02(10) $Å^3$	
Z	2	
Density (calculated)	1.627 Mg/m^3	
Absorption coefficient	2.083 mm^{-1}	
F(000)	1682	
Crystal size	0.239 x 0.048 x 0.044 mm^3	
Theta range for data collection	2.984 to 30.303°.	
Index ranges	-18<=h<=18, -21<=k<=21, -23<=l<=22	
Reflections collected	83918	
Independent reflections	18625 [R(int) = 0.0414]	
Completeness to theta = 26.000°	99.8 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.958 and 0.807	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18625 / 0 / 961	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0325, wR2 = 0.0695	
R indices (all data)	R1 = 0.0388, wR2 = 0.0719	
Largest diff. peak and hole	1.793 and -1.177 e/$Å^{-3}$	

Table 7. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^4) for complex **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	1099(2)	98492(2)	24343(2)	109(1)
P(1)	10462(5)	107618(4)	18337(4)	128(1)
P(2)	-8848(5)	89708(4)	30285(4)	121(1)
O(1)	4285(15)	83784(12)	12575(11)	180(4)
O(2)	-1379(15)	113093(12)	36153(11)	175(4)
C(1)	5817(19)	91271(15)	14846(15)	131(5)
C(2)	9330(20)	81342(18)	4716(16)	213(6)
C(3)	14200(20)	88718(17)	2463(15)	182(5)
C(4)	19890(20)	90801(19)	-4079(17)	241(6)
C(5)	23050(30)	98590(20)	-3945(17)	276(7)
C(6)	20870(20)	104244(19)	2468(16)	237(6)
C(7)	15180(20)	102134(17)	9019(15)	160(5)
C(8)	12000(20)	94411(16)	8684(15)	152(5)
C(9)	21660(20)	109241(17)	23792(15)	164(5)
C(10)	29950(20)	102460(20)	24799(18)	278(6)
C(11)	38020(20)	103310(30)	29719(19)	369(8)
C(12)	37990(30)	110930(30)	33530(20)	375(9)
C(13)	29730(30)	117560(20)	32610(20)	401(9)
C(14)	21550(30)	116780(20)	27772(19)	295(7)
C(15)	4020(20)	118287(16)	15250(15)	166(5)
C(16)	-6290(20)	121116(17)	17125(15)	185(5)
C(17)	-11300(20)	129286(18)	14792(17)	239(6)
C(18)	-5970(30)	134579(18)	10532(17)	257(6)
C(19)	4260(30)	131823(18)	8626(17)	270(7)
C(20)	9360(20)	123748(18)	11021(17)	217(6)
C(21)	-3399(19)	105753(16)	33815(15)	138(5)
C(22)	-6430(20)	115741(18)	43963(15)	196(5)
C(23)	-11920(20)	108670(17)	46092(15)	173(5)
C(24)	-17920(20)	106831(19)	52543(16)	235(6)
C(25)	-21610(20)	99290(20)	52296(17)	276(7)
C(26)	-19700(20)	93621(19)	45855(16)	229(6)
C(27)	-13690(20)	95482(16)	39384(14)	144(5)
C(28)	-9989(19)	103000(16)	39861(14)	136(5)
C(29)	-3130(20)	79099(16)	33926(15)	158(5)
C(30)	7490(20)	76596(17)	34351(16)	186(5)
C(31)	11840(20)	68613(19)	37501(17)	240(6)
C(32)	5650(30)	63079(18)	40173(17)	265(6)
C(33)	-4850(30)	65460(20)	39713(19)	303(7)
C(34)	-9320(20)	73458(18)	36607(18)	238(6)

C(35)	-19850(20)	87919(16)	24683(15)	145(5)
C(36)	-18290(20)	81506(18)	18966(17)	210(6)
C(37)	-26290(20)	80310(20)	14110(18)	269(6)
C(38)	-35860(20)	85520(20)	14831(18)	294(7)
C(39)	-37500(20)	91880(20)	20494(18)	297(7)
C(40)	-29550(20)	93095(19)	25454(17)	222(6)
F(1)	40591(19)	81501(13)	19910(20)	821(11)
F(2)	32171(17)	78260(13)	30155(14)	451(5)
F(3)	26917(18)	76496(14)	18500(14)	504(6)
F(4)	70068(15)	59636(13)	11335(12)	396(5)
F(5)	74382(15)	57708(18)	23604(14)	547(6)
F(6)	72183(16)	47181(13)	16669(17)	544(7)
F(7)	73237(15)	23206(13)	31684(14)	416(5)
F(8)	64832(15)	13656(13)	35577(12)	399(5)
F(9)	73062(14)	12444(12)	24351(12)	334(4)
F(10)	33880(20)	26188(19)	3662(14)	697(8)
F(11)	49250(20)	20080(30)	1244(15)	924(12)
F(12)	39300(30)	13770(20)	7819(18)	875(11)
F(13)	35900(20)	21548(14)	52900(13)	568(7)
F(14)	50021(18)	24005(16)	57119(19)	714(9)
F(15)	36320(20)	27807(13)	63882(12)	499(6)
F(16)	37395(14)	64757(11)	53673(11)	279(4)
F(17)	31903(15)	58436(11)	63941(10)	293(4)
F(18)	21833(13)	63066(11)	54131(10)	268(4)
F(19)	10290(40)	54010(30)	5115(18)	1510(20)
F(20)	6240(40)	64361(19)	12140(20)	1286(19)
F(21)	-3770(30)	56350(20)	9980(20)	1127(16)
F(22)	5270(20)	31807(15)	39409(19)	761(9)
F(23)	-7320(20)	37260(30)	32405(15)	1082(15)
F(24)	-2480(20)	44084(14)	42037(13)	533(6)
C(41)	42360(20)	51657(17)	25619(15)	154(5)
C(42)	37100(20)	60164(17)	25395(15)	169(5)
C(43)	41740(20)	66872(17)	22835(17)	192(5)
C(44)	51910(20)	65345(18)	20377(17)	211(6)
C(45)	57310(20)	57001(17)	20476(16)	186(5)
C(46)	52620(20)	50324(17)	23006(15)	161(5)
C(47)	35520(20)	75719(19)	22790(20)	306(7)
C(48)	68380(20)	55314(19)	18005(19)	255(6)
C(49)	43130(20)	34898(16)	25164(15)	150(5)
C(50)	52250(20)	30249(17)	28394(15)	164(5)
C(51)	57790(20)	22891(17)	24934(16)	189(5)
C(52)	54490(20)	19823(19)	17941(17)	233(6)
C(53)	45540(20)	24410(20)	14471(17)	237(6)

C(54)	39930(20)	31719(18)	18000(16)	198(5)
C(55)	67160(20)	18111(19)	29084(18)	251(6)
C(56)	42110(30)	21210(30)	6850(20)	364(8)
C(57)	37747(19)	43421(16)	39042(15)	144(5)
C(58)	39000(20)	35843(17)	43631(15)	165(5)
C(59)	38260(20)	35727(17)	52005(15)	169(5)
C(60)	35940(20)	43218(17)	56204(16)	181(5)
C(61)	34580(20)	50854(17)	51784(15)	161(5)
C(62)	35650(19)	50903(17)	43464(15)	159(5)
C(63)	40220(20)	27304(19)	56450(17)	242(6)
C(64)	31500(20)	59181(18)	55900(16)	190(5)
C(65)	24770(20)	45277(16)	26994(15)	153(5)
C(66)	20380(20)	49953(17)	20242(16)	188(5)
C(67)	9880(20)	51269(18)	18752(17)	224(6)
C(68)	3300(20)	47832(19)	23714(18)	243(6)
C(69)	7540(20)	42940(19)	30269(17)	217(6)
C(70)	17920(20)	41794(17)	31896(15)	179(5)
C(71)	5700(30)	56660(20)	11630(20)	375(8)
C(72)	610(20)	39200(20)	35883(19)	311(7)
B(1)	37080(20)	43780(18)	29112(17)	141(5)
O(3)	50000	50000	0	1140(20)
C(74)	64120(60)	36900(50)	-190(50)	1200(30)
C(73)	54160(80)	41600(70)	1540(50)	560(30)
C(73A)	59470(80)	45380(70)	-1930(50)	570(30)

Table 8. Bond lengths [Å] and angles [°] for complex **2**.

Ir(1)-H	1.49(4)	C(15)-C(20)	1.404(3)
Ir(1)-HA	1.55(4)	C(16)-H(16)	0.9500
Ir(1)-P(1)	2.3042(6)	C(16)-C(17)	1.394(4)
Ir(1)-P(2)	2.3125(6)	C(17)-H(17)	0.9500
Ir(1)-C(1)	1.999(2)	C(17)-C(18)	1.387(4)
Ir(1)-C(21)	1.994(3)	C(18)-H(18)	0.9500
P(1)-C(7)	1.840(3)	C(18)-C(19)	1.378(5)
P(1)-C(9)	1.818(3)	C(19)-H(19)	0.9500
P(1)-C(15)	1.819(3)	C(19)-C(20)	1.388(4)
P(2)-C(27)	1.834(3)	C(20)-H(20)	0.9500
P(2)-C(29)	1.812(3)	C(21)-C(28)	1.443(3)
P(2)-C(35)	1.817(3)	C(22)-H(22A)	0.9900
O(1)-C(1)	1.320(3)	C(22)-H(22B)	0.9900
O(1)-C(2)	1.485(3)	C(22)-C(23)	1.498(4)
O(2)-C(21)	1.325(3)	C(23)-C(24)	1.389(4)
O(2)-C(22)	1.486(3)	C(23)-C(28)	1.381(4)
C(1)-C(8)	1.448(3)	C(24)-H(24)	0.9500
C(2)-H(2A)	0.9900	C(24)-C(25)	1.393(4)
C(2)-H(2B)	0.9900	C(25)-H(25)	0.9500
C(2)-C(3)	1.495(4)	C(25)-C(26)	1.408(4)
C(3)-C(4)	1.389(4)	C(26)-H(26)	0.9500
C(3)-C(8)	1.385(4)	C(26)-C(27)	1.394(3)
C(4)-H(4)	0.9500	C(27)-C(28)	1.393(3)
C(4)-C(5)	1.395(4)	C(29)-C(30)	1.390(4)
C(5)-H(5)	0.9500	C(29)-C(34)	1.401(4)
C(5)-C(6)	1.405(4)	C(30)-H(30)	0.9500
C(6)-H(6)	0.9500	C(30)-C(31)	1.388(4)
C(6)-C(7)	1.391(4)	C(31)-H(31)	0.9500
C(7)-C(8)	1.388(3)	C(31)-C(32)	1.387(4)
C(9)-C(10)	1.393(4)	C(32)-H(32)	0.9500
C(9)-C(14)	1.388(4)	C(32)-C(33)	1.374(5)
C(10)-H(10)	0.9500	C(33)-H(33)	0.9500
C(10)-C(11)	1.388(4)	C(33)-C(34)	1.392(4)
C(11)-H(11)	0.9500	C(34)-H(34)	0.9500
C(11)-C(12)	1.388(5)	C(35)-C(36)	1.399(4)
C(12)-H(12)	0.9500	C(35)-C(40)	1.394(4)
C(12)-C(13)	1.375(5)	C(36)-H(36)	0.9500
C(13)-H(13)	0.9500	C(36)-C(37)	1.388(4)
C(13)-C(14)	1.387(4)	C(37)-H(37)	0.9500
C(14)-H(14)	0.9500	C(37)-C(38)	1.381(5)
C(15)-C(16)	1.389(4)	C(38)-H(38)	0.9500

C(38)-C(39)	1.387(5)	C(50)-H(50)	0.9500
C(39)-H(39)	0.9500	C(50)-C(51)	1.392(4)
C(39)-C(40)	1.394(4)	C(51)-C(52)	1.382(4)
C(40)-H(40)	0.9500	C(51)-C(55)	1.494(4)
F(1)-C(47)	1.328(3)	C(52)-H(52)	0.9500
F(2)-C(47)	1.342(4)	C(52)-C(53)	1.392(4)
F(3)-C(47)	1.338(4)	C(53)-C(54)	1.395(4)
F(4)-C(48)	1.334(3)	C(53)-C(56)	1.488(4)
F(5)-C(48)	1.344(4)	C(54)-H(54)	0.9500
F(6)-C(48)	1.323(4)	C(57)-C(58)	1.402(3)
F(7)-C(55)	1.340(4)	C(57)-C(62)	1.399(4)
F(8)-C(55)	1.347(4)	C(57)-B(1)	1.654(4)
F(9)-C(55)	1.339(3)	C(58)-H(58)	0.9500
F(10)-C(56)	1.326(4)	C(58)-C(59)	1.395(4)
F(11)-C(56)	1.311(4)	C(59)-C(60)	1.382(4)
F(12)-C(56)	1.324(5)	C(59)-C(63)	1.501(4)
F(13)-C(63)	1.331(3)	C(60)-H(60)	0.9500
F(14)-C(63)	1.310(4)	C(60)-C(61)	1.394(4)
F(15)-C(63)	1.332(3)	C(61)-C(62)	1.389(4)
F(16)-C(64)	1.344(3)	C(61)-C(64)	1.495(4)
F(17)-C(64)	1.341(3)	C(62)-H(62)	0.9500
F(18)-C(64)	1.344(3)	C(65)-C(66)	1.402(4)
F(19)-C(71)	1.275(5)	C(65)-C(70)	1.403(3)
F(20)-C(71)	1.256(4)	C(65)-B(1)	1.647(4)
F(21)-C(71)	1.302(4)	C(66)-H(66)	0.9500
F(22)-C(72)	1.348(4)	C(66)-C(67)	1.394(4)
F(23)-C(72)	1.303(4)	C(67)-C(68)	1.379(4)
F(24)-C(72)	1.313(4)	C(67)-C(71)	1.495(4)
C(41)-C(42)	1.402(4)	C(68)-H(68)	0.9500
C(41)-C(46)	1.404(4)	C(68)-C(69)	1.386(4)
C(41)-B(1)	1.652(4)	C(69)-C(70)	1.384(4)
C(42)-H(42)	0.9500	C(69)-C(72)	1.500(4)
C(42)-C(43)	1.397(4)	C(70)-H(70)	0.9500
C(43)-C(44)	1.383(4)	O(3)-C(73)#1	1.369(11)
C(43)-C(47)	1.492(4)	O(3)-C(73)	1.369(11)
C(44)-H(44)	0.9500	O(3)-C(73A)#1	1.365(11)
C(44)-C(45)	1.386(4)	O(3)-C(73A)	1.365(11)
C(45)-C(46)	1.395(4)	C(74)-H(74A)	0.9800
C(45)-C(48)	1.497(4)	C(74)-H(74B)	0.9800
C(46)-H(46)	0.9500	C(74)-H(74C)	0.9800
C(49)-C(50)	1.397(4)	C(74)-H(74D)	0.9800
C(49)-C(54)	1.409(4)	C(74)-H(74E)	0.9800
C(49)-B(1)	1.636(4)	C(74)-H(74F)	0.9800

C(74)-C(73)	1.416(12)
C(74)-C(73A)	1.402(12)
C(73)-H(73A)	0.9900
C(73)-H(73B)	0.9900
C(73A)-H(73C)	0.9900
C(73A)-H(73D)	0.9900

H-Ir(1)-HA	178(2)
P(1)-Ir(1)-H	90.0(15)
P(1)-Ir(1)-HA	90.6(15)
P(1)-Ir(1)-P(2)	177.87(2)
P(2)-Ir(1)-H	88.1(16)
P(2)-Ir(1)-HA	91.4(15)
C(1)-Ir(1)-H	89.9(16)
C(1)-Ir(1)-HA	88.8(15)
C(1)-Ir(1)-P(1)	83.75(7)
C(1)-Ir(1)-P(2)	97.11(7)
C(21)-Ir(1)-H	90.6(16)
C(21)-Ir(1)-HA	90.7(15)
C(21)-Ir(1)-P(1)	95.53(7)
C(21)-Ir(1)-P(2)	83.63(7)
C(21)-Ir(1)-C(1)	179.11(10)
C(7)-P(1)-Ir(1)	102.85(8)
C(9)-P(1)-Ir(1)	116.11(8)
C(9)-P(1)-C(7)	107.03(12)
C(9)-P(1)-C(15)	104.37(12)
C(15)-P(1)-Ir(1)	119.55(9)
C(15)-P(1)-C(7)	105.93(12)
C(27)-P(2)-Ir(1)	102.52(8)
C(29)-P(2)-Ir(1)	121.04(9)
C(29)-P(2)-C(27)	104.38(12)
C(29)-P(2)-C(35)	102.72(12)
C(35)-P(2)-Ir(1)	117.22(8)
C(35)-P(2)-C(27)	107.75(12)
C(1)-O(1)-C(2)	111.60(19)
C(21)-O(2)-C(22)	111.73(19)
O(1)-C(1)-Ir(1)	133.26(18)
O(1)-C(1)-C(8)	107.6(2)
C(8)-C(1)-Ir(1)	119.12(18)
O(1)-C(2)-H(2A)	111.0
O(1)-C(2)-H(2B)	111.0
O(1)-C(2)-C(3)	103.6(2)
H(2A)-C(2)-H(2B)	109.0
C(3)-C(2)-H(2A)	111.0
C(3)-C(2)-H(2B)	111.0
C(4)-C(3)-C(2)	135.0(3)
C(8)-C(3)-C(2)	106.3(2)
C(8)-C(3)-C(4)	118.8(2)
C(3)-C(4)-H(4)	121.3
C(3)-C(4)-C(5)	117.3(3)
C(5)-C(4)-H(4)	121.3
C(4)-C(5)-H(5)	118.4
C(4)-C(5)-C(6)	123.2(3)
C(6)-C(5)-H(5)	118.4
C(5)-C(6)-H(6)	120.3
C(7)-C(6)-C(5)	119.3(3)
C(7)-C(6)-H(6)	120.3
C(6)-C(7)-P(1)	133.5(2)
C(8)-C(7)-P(1)	110.20(18)
C(8)-C(7)-C(6)	116.3(2)
C(3)-C(8)-C(1)	110.9(2)
C(3)-C(8)-C(7)	125.0(2)
C(7)-C(8)-C(1)	124.0(2)
C(10)-C(9)-P(1)	119.3(2)
C(14)-C(9)-P(1)	120.8(2)
C(14)-C(9)-C(10)	119.5(3)
C(9)-C(10)-H(10)	120.1
C(11)-C(10)-C(9)	119.9(3)
C(11)-C(10)-H(10)	120.1
C(10)-C(11)-H(11)	119.8
C(10)-C(11)-C(12)	120.4(3)
C(12)-C(11)-H(11)	119.8
C(11)-C(12)-H(12)	120.2
C(13)-C(12)-C(11)	119.5(3)
C(13)-C(12)-H(12)	120.2
C(12)-C(13)-H(13)	119.6
C(12)-C(13)-C(14)	120.7(3)
C(14)-C(13)-H(13)	119.6
C(9)-C(14)-H(14)	120.0
C(13)-C(14)-C(9)	120.0(3)
C(13)-C(14)-H(14)	120.0
C(16)-C(15)-P(1)	119.85(19)
C(16)-C(15)-C(20)	119.4(2)
C(20)-C(15)-P(1)	120.8(2)
C(15)-C(16)-H(16)	119.8
C(15)-C(16)-C(17)	120.3(3)

C(17)-C(16)-H(16)	119.8	C(29)-C(30)-H(30)	120.0
C(16)-C(17)-H(17)	120.1	C(31)-C(30)-C(29)	120.0(3)
C(18)-C(17)-C(16)	119.7(3)	C(31)-C(30)-H(30)	120.0
C(18)-C(17)-H(17)	120.1	C(30)-C(31)-H(31)	119.8
C(17)-C(18)-H(18)	119.8	C(32)-C(31)-C(30)	120.3(3)
C(19)-C(18)-C(17)	120.4(3)	C(32)-C(31)-H(31)	119.8
C(19)-C(18)-H(18)	119.8	C(31)-C(32)-H(32)	119.9
C(18)-C(19)-H(19)	119.8	C(33)-C(32)-C(31)	120.2(3)
C(18)-C(19)-C(20)	120.4(3)	C(33)-C(32)-H(32)	119.9
C(20)-C(19)-H(19)	119.8	C(32)-C(33)-H(33)	120.0
C(15)-C(20)-H(20)	120.1	C(32)-C(33)-C(34)	120.1(3)
C(19)-C(20)-C(15)	119.8(3)	C(34)-C(33)-H(33)	120.0
C(19)-C(20)-H(20)	120.1	C(29)-C(34)-H(34)	120.0
O(2)-C(21)-Ir(1)	132.88(18)	C(33)-C(34)-C(29)	120.1(3)
O(2)-C(21)-C(28)	107.3(2)	C(33)-C(34)-H(34)	120.0
C(28)-C(21)-Ir(1)	119.77(18)	C(36)-C(35)-P(2)	118.4(2)
O(2)-C(22)-H(22A)	111.1	C(40)-C(35)-P(2)	122.4(2)
O(2)-C(22)-H(22B)	111.1	C(40)-C(35)-C(36)	119.1(2)
O(2)-C(22)-C(23)	103.3(2)	C(35)-C(36)-H(36)	119.7
H(22A)-C(22)-H(22B)	109.1	C(37)-C(36)-C(35)	120.6(3)
C(23)-C(22)-H(22A)	111.1	C(37)-C(36)-H(36)	119.7
C(23)-C(22)-H(22B)	111.1	C(36)-C(37)-H(37)	119.9
C(24)-C(23)-C(22)	135.1(3)	C(38)-C(37)-C(36)	120.1(3)
C(28)-C(23)-C(22)	106.3(2)	C(38)-C(37)-H(37)	119.9
C(28)-C(23)-C(24)	118.6(2)	C(37)-C(38)-H(38)	120.1
C(23)-C(24)-H(24)	121.3	C(37)-C(38)-C(39)	119.8(3)
C(23)-C(24)-C(25)	117.3(3)	C(39)-C(38)-H(38)	120.1
C(25)-C(24)-H(24)	121.3	C(38)-C(39)-H(39)	119.7
C(24)-C(25)-H(25)	118.3	C(38)-C(39)-C(40)	120.6(3)
C(24)-C(25)-C(26)	123.5(3)	C(40)-C(39)-H(39)	119.7
C(26)-C(25)-H(25)	118.3	C(35)-C(40)-C(39)	119.8(3)
C(25)-C(26)-H(26)	120.4	C(35)-C(40)-H(40)	120.1
C(27)-C(26)-C(25)	119.1(3)	C(39)-C(40)-H(40)	120.1
C(27)-C(26)-H(26)	120.4	C(42)-C(41)-C(46)	115.2(2)
C(26)-C(27)-P(2)	133.1(2)	C(42)-C(41)-B(1)	122.7(2)
C(28)-C(27)-P(2)	110.78(18)	C(46)-C(41)-B(1)	122.0(2)
C(28)-C(27)-C(26)	116.0(2)	C(41)-C(42)-H(42)	118.7
C(23)-C(28)-C(21)	111.3(2)	C(43)-C(42)-C(41)	122.7(2)
C(23)-C(28)-C(27)	125.4(2)	C(43)-C(42)-H(42)	118.7
C(27)-C(28)-C(21)	123.3(2)	C(42)-C(43)-C(47)	118.8(3)
C(30)-C(29)-P(2)	120.08(19)	C(44)-C(43)-C(42)	120.7(3)
C(30)-C(29)-C(34)	119.4(2)	C(44)-C(43)-C(47)	120.6(2)
C(34)-C(29)-P(2)	120.5(2)	C(43)-C(44)-H(44)	120.9

C(43)-C(44)-C(45)	118.2(2)	F(9)-C(55)-C(51)	112.9(3)
C(45)-C(44)-H(44)	120.9	F(10)-C(56)-C(53)	114.1(3)
C(44)-C(45)-C(46)	120.9(2)	F(11)-C(56)-F(10)	106.9(3)
C(44)-C(45)-C(48)	118.5(2)	F(11)-C(56)-F(12)	105.6(3)
C(46)-C(45)-C(48)	120.5(2)	F(11)-C(56)-C(53)	113.1(3)
C(41)-C(46)-H(46)	118.8	F(12)-C(56)-F(10)	103.5(3)
C(45)-C(46)-C(41)	122.4(2)	F(12)-C(56)-C(53)	112.7(3)
C(45)-C(46)-H(46)	118.8	C(58)-C(57)-B(1)	123.5(2)
F(1)-C(47)-F(2)	106.4(3)	C(62)-C(57)-C(58)	115.2(2)
F(1)-C(47)-F(3)	107.1(3)	C(62)-C(57)-B(1)	120.8(2)
F(1)-C(47)-C(43)	113.4(3)	C(57)-C(58)-H(58)	118.7
F(2)-C(47)-C(43)	112.6(3)	C(59)-C(58)-C(57)	122.7(2)
F(3)-C(47)-F(2)	104.0(3)	C(59)-C(58)-H(58)	118.7
F(3)-C(47)-C(43)	112.6(3)	C(58)-C(59)-C(63)	119.0(2)
F(4)-C(48)-F(5)	105.0(2)	C(60)-C(59)-C(58)	120.9(2)
F(4)-C(48)-C(45)	112.6(2)	C(60)-C(59)-C(63)	120.1(2)
F(5)-C(48)-C(45)	112.2(3)	C(59)-C(60)-H(60)	121.2
F(6)-C(48)-F(4)	106.8(3)	C(59)-C(60)-C(61)	117.6(2)
F(6)-C(48)-F(5)	106.3(3)	C(61)-C(60)-H(60)	121.2
F(6)-C(48)-C(45)	113.3(2)	C(60)-C(61)-C(64)	120.4(2)
C(50)-C(49)-C(54)	115.3(2)	C(62)-C(61)-C(60)	121.0(2)
C(50)-C(49)-B(1)	121.9(2)	C(62)-C(61)-C(64)	118.5(2)
C(54)-C(49)-B(1)	122.6(2)	C(57)-C(62)-H(62)	118.7
C(49)-C(50)-H(50)	118.5	C(61)-C(62)-C(57)	122.6(2)
C(51)-C(50)-C(49)	123.0(2)	C(61)-C(62)-H(62)	118.7
C(51)-C(50)-H(50)	118.5	F(13)-C(63)-F(15)	104.8(2)
C(50)-C(51)-C(55)	118.9(2)	F(13)-C(63)-C(59)	112.4(2)
C(52)-C(51)-C(50)	120.9(3)	F(14)-C(63)-F(13)	107.0(3)
C(52)-C(51)-C(55)	120.1(3)	F(14)-C(63)-F(15)	106.6(3)
C(51)-C(52)-H(52)	121.2	F(14)-C(63)-C(59)	112.7(2)
C(51)-C(52)-C(53)	117.6(3)	F(15)-C(63)-C(59)	112.8(3)
C(53)-C(52)-H(52)	121.2	F(16)-C(64)-F(18)	105.5(2)
C(52)-C(53)-C(54)	121.5(3)	F(16)-C(64)-C(61)	112.4(2)
C(52)-C(53)-C(56)	117.6(3)	F(17)-C(64)-F(16)	107.0(2)
C(54)-C(53)-C(56)	120.9(3)	F(17)-C(64)-F(18)	106.2(2)
C(49)-C(54)-H(54)	119.2	F(17)-C(64)-C(61)	113.2(2)
C(53)-C(54)-C(49)	121.7(3)	F(18)-C(64)-C(61)	112.1(2)
C(53)-C(54)-H(54)	119.2	C(66)-C(65)-C(70)	115.2(2)
F(7)-C(55)-F(8)	106.4(3)	C(66)-C(65)-B(1)	123.4(2)
F(7)-C(55)-C(51)	112.9(2)	C(70)-C(65)-B(1)	121.4(2)
F(8)-C(55)-C(51)	112.2(2)	C(65)-C(66)-H(66)	119.1
F(9)-C(55)-F(7)	106.0(2)	C(67)-C(66)-C(65)	121.8(2)
F(9)-C(55)-F(8)	105.9(2)	C(67)-C(66)-H(66)	119.1

C(66)-C(67)-C(71)	118.7(3)	C(65)-B(1)-C(41)	112.0(2)
C(68)-C(67)-C(66)	121.8(3)	C(65)-B(1)-C(57)	105.8(2)
C(68)-C(67)-C(71)	119.5(3)	C(73)-O(3)-C(73)#1	180.0
C(67)-C(68)-H(68)	121.3	C(73A)#1-O(3)-C(73A)	180.0(5)
C(67)-C(68)-C(69)	117.4(3)	H(74A)-C(74)-H(74B)	109.5
C(69)-C(68)-H(68)	121.3	H(74A)-C(74)-H(74C)	109.5
C(68)-C(69)-C(72)	119.0(3)	H(74B)-C(74)-H(74C)	109.5
C(70)-C(69)-C(68)	121.1(3)	H(74D)-C(74)-H(74E)	109.5
C(70)-C(69)-C(72)	119.8(3)	H(74D)-C(74)-H(74F)	109.5
C(65)-C(70)-H(70)	118.6	H(74E)-C(74)-H(74F)	109.5
C(69)-C(70)-C(65)	122.7(3)	C(73)-C(74)-H(74A)	109.5
C(69)-C(70)-H(70)	118.6	C(73)-C(74)-H(74B)	109.5
F(19)-C(71)-F(21)	101.5(4)	C(73)-C(74)-H(74C)	109.5
F(19)-C(71)-C(67)	112.1(3)	C(73A)-C(74)-H(74D)	109.5
F(20)-C(71)-F(19)	106.6(4)	C(73A)-C(74)-H(74E)	109.5
F(20)-C(71)-F(21)	107.6(4)	C(73A)-C(74)-H(74F)	109.5
F(20)-C(71)-C(67)	114.1(3)	O(3)-C(73)-C(74)	129.8(8)
F(21)-C(71)-C(67)	114.0(3)	O(3)-C(73)-H(73A)	104.8
F(22)-C(72)-C(69)	113.2(3)	O(3)-C(73)-H(73B)	104.8
F(23)-C(72)-F(22)	103.6(3)	C(74)-C(73)-H(73A)	104.8
F(23)-C(72)-F(24)	109.5(3)	C(74)-C(73)-H(73B)	104.8
F(23)-C(72)-C(69)	114.0(3)	H(73A)-C(73)-H(73B)	105.8
F(24)-C(72)-F(22)	103.0(3)	O(3)-C(73A)-C(74)	131.4(9)
F(24)-C(72)-C(69)	112.6(3)	O(3)-C(73A)-H(73C)	104.4
C(41)-B(1)-C(57)	109.1(2)	O(3)-C(73A)-H(73D)	104.4
C(49)-B(1)-C(41)	108.6(2)	C(74)-C(73A)-H(73C)	104.4
C(49)-B(1)-C(57)	111.7(2)	C(74)-C(73A)-H(73D)	104.4
C(49)-B(1)-C(65)	109.6(2)	H(73C)-C(73A)-H(73D)	105.6

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z

Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for complex **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	129(1)	96(1)	107(1)	-3(1)	10(1)	-37(1)
P(1)	153(3)	110(3)	130(3)	-11(2)	12(2)	-51(2)
P(2)	132(3)	109(3)	126(3)	-1(2)	13(2)	-36(2)
O(1)	253(10)	141(9)	159(9)	-36(7)	50(7)	-74(8)
O(2)	232(10)	148(9)	157(9)	-49(7)	31(7)	-65(8)
C(1)	149(12)	98(11)	149(11)	-12(9)	2(9)	-29(9)
C(2)	323(16)	177(13)	161(12)	-72(10)	61(11)	-95(12)
C(3)	235(14)	175(13)	146(12)	-6(10)	5(10)	-65(11)
C(4)	315(16)	273(15)	156(13)	-56(11)	56(11)	-109(13)
C(5)	363(17)	335(17)	176(13)	-29(12)	107(12)	-181(14)
C(6)	329(16)	253(15)	178(13)	-21(11)	60(11)	-176(13)
C(7)	203(13)	171(13)	117(11)	-12(9)	1(10)	-65(10)
C(8)	185(13)	156(12)	127(11)	-4(9)	-4(9)	-59(10)
C(9)	164(12)	204(13)	143(11)	9(10)	21(10)	-83(10)
C(10)	233(15)	376(18)	203(14)	-79(12)	28(11)	0(13)
C(11)	156(14)	650(20)	254(16)	-3(16)	16(12)	24(15)
C(12)	275(17)	660(30)	272(16)	73(16)	-79(13)	-299(18)
C(13)	560(20)	307(18)	415(19)	44(15)	-221(17)	-269(17)
C(14)	385(18)	207(15)	327(16)	13(12)	-149(14)	-131(13)
C(15)	233(13)	140(12)	144(11)	1(9)	-12(10)	-84(10)
C(16)	269(14)	140(12)	156(12)	1(9)	-13(10)	-63(11)
C(17)	310(16)	169(14)	215(14)	-10(11)	0(12)	10(12)
C(18)	438(19)	123(13)	199(13)	2(10)	-40(13)	-23(12)
C(19)	458(19)	166(14)	219(14)	41(11)	-6(13)	-146(13)
C(20)	260(15)	192(14)	220(13)	32(11)	0(11)	-98(11)
C(21)	155(12)	110(11)	147(11)	16(9)	-33(9)	-20(9)
C(22)	259(14)	201(13)	138(12)	-69(10)	32(10)	-62(11)
C(23)	176(13)	201(13)	136(12)	-14(10)	-17(10)	-21(10)
C(24)	269(15)	285(15)	155(12)	-69(11)	46(11)	-63(12)
C(25)	317(16)	361(17)	177(13)	-26(12)	105(12)	-139(14)
C(26)	281(15)	249(15)	189(13)	-6(11)	51(11)	-135(12)
C(27)	157(12)	167(12)	115(11)	-5(9)	3(9)	-52(10)
C(28)	140(12)	143(12)	122(11)	-3(9)	-11(9)	-23(9)
C(29)	204(13)	127(12)	148(11)	-1(9)	14(10)	-44(10)
C(30)	213(13)	176(13)	165(12)	-1(10)	32(10)	-32(11)
C(31)	254(15)	230(15)	194(13)	31(11)	39(11)	51(12)
C(32)	407(18)	149(14)	206(14)	39(10)	12(12)	17(12)
C(33)	426(19)	215(15)	288(16)	95(12)	-9(14)	-120(14)
C(34)	247(15)	200(14)	277(15)	68(11)	-10(12)	-78(12)

C(35)	158(12)	139(12)	154(11)	15(9)	-3(9)	-71(10)
C(36)	239(14)	187(14)	221(13)	-27(10)	5(11)	-81(11)
C(37)	349(17)	278(16)	225(14)	-24(12)	-34(12)	-168(13)
C(38)	262(15)	480(20)	198(14)	39(13)	-51(12)	-224(15)
C(39)	154(14)	480(20)	255(15)	12(14)	6(11)	-73(14)
C(40)	185(13)	284(15)	202(13)	-12(11)	23(11)	-59(12)
F(1)	482(15)	160(10)	1760(30)	212(14)	574(17)	20(10)
F(2)	435(13)	317(11)	542(13)	-174(10)	16(10)	83(9)
F(3)	492(14)	338(12)	587(14)	12(10)	-202(11)	155(10)
F(4)	304(10)	433(12)	435(11)	136(9)	170(9)	-60(9)
F(5)	205(10)	990(20)	459(13)	-121(13)	1(9)	-153(12)
F(6)	321(11)	236(10)	1030(20)	26(11)	345(12)	23(9)
F(7)	255(10)	302(11)	673(14)	-121(10)	-156(10)	11(8)
F(8)	327(11)	457(12)	336(10)	116(9)	58(8)	89(9)
F(9)	268(10)	275(10)	414(11)	-81(8)	101(8)	61(8)
F(10)	687(18)	950(20)	389(13)	-360(13)	-258(12)	50(15)
F(11)	484(15)	2000(40)	421(14)	-745(19)	218(12)	-500(20)
F(12)	1340(30)	800(20)	697(19)	-253(16)	-255(19)	-690(20)
F(13)	1110(20)	339(12)	378(12)	104(9)	-239(13)	-435(13)
F(14)	354(13)	555(16)	1150(20)	567(16)	25(14)	38(11)
F(15)	931(19)	363(12)	224(10)	77(8)	83(11)	-190(12)
F(16)	296(10)	260(9)	317(9)	-104(7)	55(7)	-134(8)
F(17)	439(11)	288(10)	141(8)	-66(7)	-21(7)	-36(8)
F(18)	185(8)	297(9)	297(9)	-94(7)	-17(7)	22(7)
F(19)	1660(40)	2030(50)	314(15)	500(20)	0(20)	820(30)
F(20)	2280(50)	478(18)	1300(30)	614(19)	-1230(30)	-750(20)
F(21)	910(20)	1120(30)	1520(30)	970(20)	-960(20)	-660(20)
F(22)	788(19)	367(14)	1130(20)	144(14)	562(17)	-176(13)
F(23)	830(20)	2470(50)	321(13)	13(19)	33(13)	-1240(30)
F(24)	889(19)	405(12)	339(11)	-78(9)	342(12)	-223(12)
C(41)	170(12)	180(13)	119(11)	-12(9)	-11(9)	-48(10)
C(42)	156(12)	179(13)	179(12)	-11(10)	10(10)	-49(10)
C(43)	184(13)	153(13)	236(13)	5(10)	3(10)	-24(10)
C(44)	204(14)	185(14)	253(14)	23(11)	24(11)	-65(11)
C(45)	159(13)	188(13)	212(13)	-6(10)	37(10)	-41(10)
C(46)	165(12)	152(12)	160(12)	7(9)	-6(10)	-17(10)
C(47)	227(15)	179(15)	510(20)	32(13)	85(14)	-32(12)
C(48)	221(15)	212(15)	325(16)	31(12)	64(12)	-32(12)
C(49)	165(12)	159(12)	142(11)	-10(9)	28(9)	-69(10)
C(50)	194(13)	157(12)	156(12)	-12(9)	10(10)	-70(10)
C(51)	170(13)	175(13)	226(13)	-34(10)	42(10)	-44(10)
C(52)	204(14)	253(15)	259(14)	-116(11)	87(11)	-79(12)
C(53)	228(14)	324(16)	193(13)	-97(11)	42(11)	-126(12)

C(54)	191(13)	261(15)	163(12)	-20(10)	-2(10)	-92(11)
C(55)	243(15)	194(14)	299(15)	-60(11)	59(12)	1(12)
C(56)	282(17)	550(20)	300(17)	-226(16)	41(13)	-156(16)
C(57)	112(11)	162(12)	160(12)	-11(9)	-4(9)	-32(9)
C(58)	167(12)	168(13)	171(12)	-23(10)	-14(10)	-59(10)
C(59)	165(12)	190(13)	168(12)	22(10)	-25(10)	-72(10)
C(60)	179(13)	226(14)	152(12)	-10(10)	3(10)	-75(11)
C(61)	134(12)	190(13)	163(12)	-35(10)	-5(9)	-41(10)
C(62)	130(12)	176(13)	173(12)	-3(10)	-14(9)	-31(10)
C(63)	317(16)	251(15)	185(13)	42(11)	-21(11)	-122(13)
C(64)	182(13)	233(14)	157(12)	-35(10)	-15(10)	-40(11)
C(65)	174(12)	134(12)	158(12)	-20(9)	2(10)	-40(10)
C(66)	204(13)	177(13)	196(13)	16(10)	-28(10)	-70(11)
C(67)	243(14)	188(14)	242(14)	-2(11)	-102(11)	-42(11)
C(68)	164(13)	286(16)	285(15)	-85(12)	-50(11)	-46(12)
C(69)	204(14)	279(15)	202(13)	-92(11)	40(11)	-120(12)
C(70)	197(13)	203(13)	148(12)	-25(10)	-3(10)	-69(11)
C(71)	400(20)	370(20)	387(19)	140(15)	-227(16)	-155(16)
C(72)	240(15)	480(20)	269(15)	-91(14)	54(12)	-192(15)
B(1)	160(13)	144(13)	123(12)	-3(10)	1(10)	-38(11)
O(3)	1230(70)	1370(70)	720(40)	-440(40)	-290(40)	50(50)
C(74)	1180(70)	1290(70)	1020(50)	-520(50)	-330(50)	70(50)
C(73)	750(70)	690(70)	300(40)	-30(40)	80(40)	-290(60)
C(73A)	610(70)	760(80)	360(50)	-60(40)	20(40)	-180(60)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for complex **2**.

	x	y	z	U(eq)
H	-820(30)	10280(30)	1980(20)	53(12)
HA	1070(30)	9380(30)	2890(20)	49(12)
H(2A)	422	8055	66	26
H(2B)	1455	7602	525	26
H(4)	2156	8707	-847	29
H(5)	2687	10015	-841	33
H(6)	2325	10946	233	28
H(10)	3007	9727	2212	33
H(11)	4361	9864	3049	44
H(12)	4363	11157	3675	45
H(13)	2962	12274	3531	48
H(14)	1588	12140	2719	35
H(16)	-995	11747	2001	22
H(17)	-1834	13122	1612	29
H(18)	-938	14014	892	31
H(19)	784	13547	566	32
H(20)	1645	12192	980	26
H(22A)	-1133	12125	4339	24
H(22B)	-130	11626	4809	24
H(24)	-1944	11056	5694	28
H(25)	-2562	9790	5671	33
H(26)	-2248	8859	4592	27
H(30)	1176	8035	3249	22
H(31)	1910	6693	3783	29
H(32)	867	5763	4233	32
H(33)	-907	6164	4152	36
H(34)	-1659	7509	3630	29
H(36)	-1171	7794	1840	25
H(37)	-2517	7591	1028	32
H(38)	-4130	8475	1146	35
H(39)	-4409	9544	2100	36
H(40)	-3075	9744	2935	27
H(42)	3010	6142	2705	20
H(44)	5511	6989	1867	25
H(46)	5653	4467	2296	19
H(50)	5479	3220	3317	20
H(52)	5820	1477	1559	28
H(54)	3379	3463	1551	24
H(58)	4042	3057	4093	20

H(60)	3530	4317	6190	22
H(62)	3493	5622	4067	19
H(66)	2469	5229	1658	23
H(68)	-386	4878	2268	29
H(70)	2050	3851	3652	21
H(74A)	6465	3099	170	180
H(74B)	6536	3702	-601	180
H(74C)	6923	3944	255	180
H(74D)	7104	3568	-253	180
H(74E)	6453	3599	565	180
H(74F)	6002	3309	-247	180
H(73A)	4944	3842	-104	67
H(73B)	5325	4081	740	67
H(73C)	6433	4875	14	68
H(73D)	5988	4590	-786	68

Complex **3**. A suitable crystal of **3** was selected for analysis and mounted in a polyimide loop. All measurements were made on a Rigaku Oxford Diffraction Supernova Eos CCD with filtered Mo-Kα radiation at a temperature of 100 K. Using Olex2,[5] the structure was solved with the ShelXT structure solution program using Direct Methods and refined with the ShelXL refinement package[6] using Least Squares minimization. Site disorder in the alkoxyalkyl/alkoxycarbene ligand was refined with a similarity restraint to a refined occupancy of 0.50(4), consistent with the symmetrical nature of the disorder. The metal hydride was located in the difference map and refined with a restraint placed on the Ir-H bond length. Disorder in the trifluoromethyl groups of the anion was modeled with appropriate similarity restraints.

Table 11. Crystal data and structure refinement for complex **3**.

Empirical formula	$C_{74}H_{47}BF_{24}IrNO_2P_2$	
Formula weight	1703.07	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.2753(5) Å	α = 91.118(3)°
	b = 15.5619(3) Å	β = 110.507(4)°
	c = 16.6725(7) Å	γ = 100.549(3)°
Volume	3396.4(2) $Å^3$	
Z	2	
Density (calculated)	1.665 Mg/m^3	
Absorption coefficient	2.127 mm^{-1}	
F(000)	1684	
Crystal size	0.171 x 0.122 x 0.056 mm^3	
Theta range for data collection	2.980 to 29.445°.	
Index ranges	-18<=h<=19, -20<=k<=21, -22<=l<=22	
Reflections collected	67020	
Independent reflections	16594 [R(int) = 0.0600]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.904 and 0.763	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16594 / 55 / 1026	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.0433, wR2 = 0.0858	
R indices (all data)	R1 = 0.0625, wR2 = 0.0941	
Largest diff. peak and hole	1.399 and -1.029 $e.Å^{-3}$	

Table 12. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^4) for complex **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	95689(2)	34056(2)	71704(2)	243(1)
P(1)	96789(9)	20030(6)	67667(6)	314(2)
P(2)	96602(7)	48614(6)	75699(6)	217(2)
O(1)	107180(20)	35401(18)	91551(17)	366(7)
O(2)	87950(20)	33873(18)	51689(16)	327(6)
N(1)	81150(30)	30480(20)	72740(20)	404(9)
C(1)	104350(30)	16410(20)	77820(20)	343(10)
C(1A)	73860(40)	29620(30)	74110(30)	458(12)
C(2)	109140(30)	9290(30)	79630(30)	357(10)
C(2A)	64670(40)	28790(40)	76210(40)	731(19)
C(3)	115400(30)	8620(30)	88070(30)	393(10)
C(4)	117060(30)	14900(30)	94750(30)	379(10)
C(5)	112290(30)	21940(30)	92960(20)	313(9)
C(6)	106070(40)	22470(30)	84620(30)	385(11)
C(7)	112090(40)	29880(30)	98100(30)	416(11)
C(9)	84710(30)	12200(20)	63230(20)	338(10)
C(10)	82980(40)	4400(30)	66700(30)	382(10)
C(11)	73320(40)	-1030(30)	63640(30)	482(12)
C(12)	65510(40)	1370(30)	57230(30)	476(12)
C(13)	67150(40)	9100(30)	53600(30)	576(15)
C(14)	76770(40)	14580(30)	56610(30)	548(15)
C(15)	104050(40)	18430(30)	60890(30)	360(10)
C(16)	114260(40)	22760(30)	63620(30)	409(11)
C(17)	120340(40)	21230(30)	59090(30)	445(12)
C(18)	116300(40)	15450(30)	51740(30)	495(13)
C(19)	106310(40)	11250(30)	49000(30)	490(13)
C(20)	100100(40)	12680(30)	53470(30)	423(11)
C(21)	93630(30)	53480(20)	65450(20)	250(8)
C(22)	94430(30)	62190(30)	63520(30)	306(9)
C(23)	91960(30)	63960(30)	54950(30)	352(10)
C(24)	88700(30)	57400(30)	48210(30)	336(9)
C(25)	87840(30)	48770(30)	50150(20)	293(9)
C(26)	90260(30)	47060(30)	58690(20)	293(9)
C(27)	85090(30)	40000(30)	45080(20)	333(9)
C(29)	87030(30)	50490(20)	79990(30)	270(8)
C(30)	78300(30)	53240(30)	74900(30)	376(10)
C(31)	70600(40)	53730(40)	78020(30)	501(12)
C(32)	71530(40)	51480(40)	86160(30)	502(13)
C(33)	80210(40)	48770(30)	91320(30)	445(12)

C(34)	87980(30)	48270(30)	88240(30)	329(9)
C(35)	108550(30)	55410(20)	82860(20)	251(8)
C(36)	108500(40)	63130(30)	87260(30)	387(10)
C(37)	117770(40)	68610(30)	92120(30)	499(13)
C(38)	126830(40)	66490(30)	92650(30)	445(12)
C(39)	126940(30)	58840(30)	88440(30)	387(10)
C(40)	117810(30)	53270(30)	83530(30)	311(9)
C(8)	100100(200)	30300(80)	84380(80)	230(30)
C(28)	90700(200)	38200(180)	59540(180)	270(40)
C(8B)	103980(160)	30910(90)	83510(90)	240(30)
C(28B)	87600(200)	36830(170)	59470(190)	270(40)
F(1)	69060(20)	52029(16)	28026(18)	456(7)
F(2)	65230(20)	58040(16)	37727(17)	460(7)
F(3)	54550(20)	55730(17)	24872(19)	562(8)
F(7)	47590(30)	-10290(20)	34720(30)	1097(17)
F(8)	57260(20)	-15081(16)	29168(17)	462(6)
F(9)	63230(40)	-9760(20)	42055(19)	888(13)
F(13)	7270(20)	-10834(19)	4640(20)	643(9)
F(14)	20610(20)	-8870(16)	1481(18)	473(7)
F(15)	21150(30)	-13684(17)	13371(19)	675(9)
F(16)	-230(20)	15540(30)	14900(30)	1210(20)
F(17)	9120(30)	16540(30)	27730(20)	1042(16)
F(18)	11170(30)	26500(20)	20290(30)	998(15)
F(19)	33630(30)	41750(20)	-2002(19)	685(10)
F(20)	30380(20)	34750(20)	-14110(17)	592(8)
F(21)	44930(20)	42976(17)	-7686(19)	546(7)
F(22)	43990(20)	4768(18)	-12246(16)	507(7)
F(23)	56840(20)	14680(20)	-11808(18)	582(8)
F(24)	58320(20)	6144(17)	-1692(16)	427(6)
C(41)	49010(30)	28020(20)	27240(20)	196(7)
C(42)	53740(30)	36400(20)	26270(20)	212(7)
C(43)	56890(30)	43340(20)	32650(20)	221(7)
C(44)	55560(30)	42210(20)	40410(20)	282(9)
C(45)	51110(30)	33910(30)	41700(20)	303(9)
C(46)	47830(30)	27090(20)	35240(20)	273(8)
C(47)	61510(30)	52240(30)	30840(30)	312(9)
C(48)	49570(50)	32350(30)	49990(30)	544(15)
C(49)	54050(30)	13230(20)	24830(20)	203(7)
C(50)	64200(30)	16020(30)	25300(20)	271(8)
C(51)	71580(30)	11040(30)	28610(30)	338(9)
C(52)	69260(30)	3080(30)	31730(30)	354(10)
C(53)	59460(30)	250(30)	31530(20)	310(9)
C(54)	52010(30)	5260(20)	28210(20)	242(8)

C(55)	81990(40)	14300(40)	28520(40)	596(15)
C(56)	56740(40)	-8650(30)	34400(30)	469(12)
C(57)	33990(30)	14170(20)	18480(20)	204(7)
C(58)	26620(30)	18030(20)	20070(20)	227(8)
C(59)	16470(30)	13610(30)	17790(20)	267(8)
C(60)	13200(30)	5180(20)	13770(20)	253(8)
C(61)	20310(30)	1190(20)	12090(20)	228(8)
C(62)	30430(30)	5630(20)	14320(20)	206(7)
C(63)	9060(30)	17930(30)	20040(30)	369(10)
C(64)	17300(30)	-7990(30)	7900(30)	325(9)
C(65)	45930(30)	21520(20)	10860(20)	199(7)
C(66)	49180(30)	15910(20)	6200(20)	232(8)
C(67)	48530(30)	17000(20)	-2230(20)	253(8)
C(68)	44640(30)	23850(30)	-6370(20)	291(9)
C(69)	41390(30)	29600(30)	-1940(20)	269(8)
C(70)	41930(30)	28400(30)	6500(20)	250(8)
C(71)	37530(40)	37170(30)	-6380(30)	382(10)
C(72)	51920(40)	10680(30)	-6900(30)	357(10)
B(1)	45730(30)	19350(30)	20430(20)	187(8)
F(4)	52640(110)	39050(90)	55550(90)	630(30)
F(5)	40010(70)	29300(90)	49170(50)	980(30)
F(6)	54860(100)	26010(50)	54120(40)	840(30)
F(10A)	82610(80)	18800(200)	22390(110)	780(70)
F(11A)	88350(170)	8580(140)	30100(300)	690(60)
F(12A)	87190(90)	21170(80)	35840(90)	500(30)
F(4A)	56000(300)	38000(200)	56300(200)	960(80)
F(5A)	39710(180)	35140(150)	48480(130)	1100(60)
F(6A)	47000(200)	24970(80)	51170(100)	790(50)
F(10)	81150(80)	13300(140)	19550(100)	860(40)
F(11)	87850(150)	8790(150)	31800(200)	810(70)
F(12)	86100(110)	21690(100)	30900(200)	1160(90)

Table 13. Bond lengths [Å] and angles [°] for complex **3**.

Ir(1)-H	1.46(2)	C(10)-H(10)	0.9500
Ir(1)-P(1)	2.3204(10)	C(10)-C(11)	1.393(6)
Ir(1)-P(2)	2.3164(9)	C(11)-H(11)	0.9500
Ir(1)-N(1)	2.117(4)	C(11)-C(12)	1.363(7)
Ir(1)-C(8)	2.111(12)	C(12)-H(12)	0.9500
Ir(1)-C(28)	2.06(3)	C(12)-C(13)	1.375(7)
Ir(1)-C(8B)	2.033(13)	C(13)-H(13)	0.9500
Ir(1)-C(28B)	2.06(3)	C(13)-C(14)	1.392(7)
P(1)-C(1)	1.824(4)	C(14)-H(14)	0.9500
P(1)-C(9)	1.818(4)	C(15)-C(16)	1.396(6)
P(1)-C(15)	1.822(5)	C(15)-C(20)	1.390(6)
P(2)-C(21)	1.827(4)	C(16)-H(16)	0.9500
P(2)-C(29)	1.813(4)	C(16)-C(17)	1.381(7)
P(2)-C(35)	1.821(4)	C(17)-H(17)	0.9500
O(1)-C(7)	1.464(5)	C(17)-C(18)	1.385(6)
O(1)-C(8)	1.380(14)	C(18)-H(18)	0.9500
O(1)-C(8B)	1.382(14)	C(18)-C(19)	1.364(7)
O(2)-C(27)	1.470(4)	C(19)-H(19)	0.9500
O(2)-C(28)	1.35(3)	C(19)-C(20)	1.386(7)
O(2)-C(28B)	1.39(3)	C(20)-H(20)	0.9500
N(1)-C(1A)	1.126(6)	C(21)-C(22)	1.392(5)
C(1)-C(2)	1.390(6)	C(21)-C(26)	1.379(5)
C(1)-C(6)	1.384(6)	C(22)-H(22)	0.9500
C(1A)-C(2A)	1.457(7)	C(22)-C(23)	1.393(6)
C(2)-H(2)	0.9500	C(23)-H(23)	0.9500
C(2)-C(3)	1.396(6)	C(23)-C(24)	1.391(6)
C(2A)-H(2AA)	0.9800	C(24)-H(24)	0.9500
C(2A)-H(2AB)	0.9800	C(24)-C(25)	1.381(5)
C(2A)-H(2AC)	0.9800	C(25)-C(26)	1.385(5)
C(3)-H(3)	0.9500	C(25)-C(27)	1.502(6)
C(3)-C(4)	1.394(6)	C(26)-C(28)	1.40(3)
C(4)-H(4)	0.9500	C(26)-C(28B)	1.59(3)
C(4)-C(5)	1.377(6)	C(27)-H(27A)	0.9900
C(5)-C(6)	1.376(5)	C(27)-H(27B)	0.9900
C(5)-C(7)	1.500(6)	C(29)-C(30)	1.387(6)
C(6)-C(8)	1.603(19)	C(29)-C(34)	1.392(6)
C(6)-C(8B)	1.401(14)	C(30)-H(30)	0.9500
C(7)-H(7A)	0.9900	C(30)-C(31)	1.383(6)
C(7)-H(7B)	0.9900	C(31)-H(31)	0.9500
C(9)-C(10)	1.374(6)	C(31)-C(32)	1.376(7)
C(9)-C(14)	1.389(6)	C(32)-H(32)	0.9500

C(32)-C(33)	1.382(7)	C(44)-C(45)	1.387(5)
C(33)-H(33)	0.9500	C(45)-C(46)	1.387(5)
C(33)-C(34)	1.388(6)	C(45)-C(48)	1.492(6)
C(34)-H(34)	0.9500	C(46)-H(46)	0.9500
C(35)-C(36)	1.399(5)	C(48)-F(4)	1.284(13)
C(35)-C(40)	1.388(6)	C(48)-F(5)	1.318(10)
C(36)-H(36)	0.9500	C(48)-F(6)	1.397(8)
C(36)-C(37)	1.394(6)	C(48)-F(4A)	1.32(3)
C(37)-H(37)	0.9500	C(48)-F(5A)	1.49(2)
C(37)-C(38)	1.366(7)	C(48)-F(6A)	1.183(12)
C(38)-H(38)	0.9500	C(49)-C(50)	1.408(5)
C(38)-C(39)	1.375(6)	C(49)-C(54)	1.398(5)
C(39)-H(39)	0.9500	C(49)-B(1)	1.639(5)
C(39)-C(40)	1.389(6)	C(50)-H(50)	0.9500
C(40)-H(40)	0.9500	C(50)-C(51)	1.387(6)
C(8)-H(8)	1.0000	C(51)-C(52)	1.382(6)
C(28B)-H(28B)	1.0000	C(51)-C(55)	1.485(7)
F(1)-C(47)	1.323(5)	C(52)-H(52)	0.9500
F(2)-C(47)	1.330(4)	C(52)-C(53)	1.376(6)
F(3)-C(47)	1.340(5)	C(53)-C(54)	1.397(5)
F(7)-C(56)	1.305(6)	C(53)-C(56)	1.502(6)
F(8)-C(56)	1.344(5)	C(54)-H(54)	0.9500
F(9)-C(56)	1.326(6)	C(55)-F(10A)	1.266(12)
F(13)-C(64)	1.325(5)	C(55)-F(11A)	1.35(3)
F(14)-C(64)	1.326(5)	C(55)-F(12A)	1.486(16)
F(15)-C(64)	1.334(5)	C(55)-F(10)	1.460(16)
F(16)-C(63)	1.282(5)	C(55)-F(11)	1.30(2)
F(17)-C(63)	1.300(5)	C(55)-F(12)	1.182(13)
F(18)-C(63)	1.308(5)	C(57)-C(58)	1.400(5)
F(19)-C(71)	1.327(5)	C(57)-C(62)	1.405(5)
F(20)-C(71)	1.328(5)	C(57)-B(1)	1.636(5)
F(21)-C(71)	1.340(5)	C(58)-H(58)	0.9500
F(22)-C(72)	1.342(5)	C(58)-C(59)	1.398(5)
F(23)-C(72)	1.346(5)	C(59)-C(60)	1.383(5)
F(24)-C(72)	1.338(5)	C(59)-C(63)	1.497(6)
C(41)-C(42)	1.394(5)	C(60)-H(60)	0.9500
C(41)-C(46)	1.409(5)	C(60)-C(61)	1.384(5)
C(41)-B(1)	1.632(5)	C(61)-C(62)	1.396(5)
C(42)-H(42)	0.9500	C(61)-C(64)	1.496(5)
C(42)-C(43)	1.395(5)	C(62)-H(62)	0.9500
C(43)-C(44)	1.381(5)	C(65)-C(66)	1.399(5)
C(43)-C(47)	1.505(5)	C(65)-C(70)	1.402(5)
C(44)-H(44)	0.9500	C(65)-B(1)	1.645(5)

C(66)-H(66)	0.9500
C(66)-C(67)	1.391(5)
C(67)-C(68)	1.377(6)
C(67)-C(72)	1.490(6)
C(68)-H(68)	0.9500
C(68)-C(69)	1.388(6)
C(69)-C(70)	1.399(5)
C(69)-C(71)	1.492(6)
C(70)-H(70)	0.9500

P(1)-Ir(1)-H	80(2)
P(2)-Ir(1)-H	93(2)
P(2)-Ir(1)-P(1)	172.91(4)
N(1)-Ir(1)-H	175(2)
N(1)-Ir(1)-P(1)	96.30(10)
N(1)-Ir(1)-P(2)	90.78(10)
C(8)-Ir(1)-H	95(2)
C(8)-Ir(1)-P(1)	86.1(4)
C(8)-Ir(1)-P(2)	94.8(3)
C(8)-Ir(1)-N(1)	80.3(8)
C(28)-Ir(1)-H	88(2)
C(28)-Ir(1)-P(1)	97.1(8)
C(28)-Ir(1)-P(2)	82.4(8)
C(28)-Ir(1)-N(1)	96.9(8)
C(28)-Ir(1)-C(8)	176.0(9)
C(8B)-Ir(1)-H	79(2)
C(8B)-Ir(1)-P(1)	81.9(4)
C(8B)-Ir(1)-P(2)	97.0(4)
C(8B)-Ir(1)-N(1)	97.0(7)
C(8B)-Ir(1)-C(28B)	177.1(9)
C(28B)-Ir(1)-H	100(2)
C(28B)-Ir(1)-P(1)	95.6(8)
C(28B)-Ir(1)-P(2)	85.4(8)
C(28B)-Ir(1)-N(1)	84.6(7)
C(1)-P(1)-Ir(1)	102.75(13)
C(9)-P(1)-Ir(1)	115.54(14)
C(9)-P(1)-C(1)	108.10(19)
C(9)-P(1)-C(15)	106.5(2)
C(15)-P(1)-Ir(1)	120.45(14)
C(15)-P(1)-C(1)	102.0(2)
C(21)-P(2)-Ir(1)	102.61(12)
C(29)-P(2)-Ir(1)	114.93(13)
C(29)-P(2)-C(21)	106.16(18)
C(29)-P(2)-C(35)	105.35(17)
C(35)-P(2)-Ir(1)	120.80(12)
C(35)-P(2)-C(21)	105.73(17)
C(8)-O(1)-C(7)	110.6(5)
C(8B)-O(1)-C(7)	109.3(6)
C(28)-O(2)-C(27)	109.1(12)
C(28B)-O(2)-C(27)	112.3(12)
C(1A)-N(1)-Ir(1)	170.0(3)
C(2)-C(1)-P(1)	131.6(3)
C(6)-C(1)-P(1)	110.8(3)
C(6)-C(1)-C(2)	117.3(4)
N(1)-C(1A)-C(2A)	177.4(5)
C(1)-C(2)-H(2)	120.4
C(1)-C(2)-C(3)	119.2(4)
C(3)-C(2)-H(2)	120.4
C(1A)-C(2A)-H(2AA)	109.5
C(1A)-C(2A)-H(2AB)	109.5
C(1A)-C(2A)-H(2AC)	109.5
H(2AA)-C(2A)-H(2AB)	109.5
H(2AA)-C(2A)-H(2AC)	109.5
H(2AB)-C(2A)-H(2AC)	109.5
C(2)-C(3)-H(3)	119.0
C(4)-C(3)-C(2)	122.0(4)
C(4)-C(3)-H(3)	119.0
C(3)-C(4)-H(4)	120.6
C(5)-C(4)-C(3)	118.8(4)
C(5)-C(4)-H(4)	120.6
C(4)-C(5)-C(7)	135.2(4)
C(6)-C(5)-C(4)	118.5(4)
C(6)-C(5)-C(7)	106.3(4)
C(1)-C(6)-C(8)	126.0(5)
C(1)-C(6)-C(8B)	123.1(7)
C(5)-C(6)-C(1)	124.2(4)
C(5)-C(6)-C(8)	109.3(5)
C(5)-C(6)-C(8B)	110.7(6)
O(1)-C(7)-C(5)	103.7(3)
O(1)-C(7)-H(7A)	111.0
O(1)-C(7)-H(7B)	111.0
C(5)-C(7)-H(7A)	111.0
C(5)-C(7)-H(7B)	111.0
H(7A)-C(7)-H(7B)	109.0
C(10)-C(9)-P(1)	121.9(3)
C(10)-C(9)-C(14)	119.5(4)

C(14)-C(9)-P(1)	118.4(3)	C(23)-C(24)-H(24)	120.9
C(9)-C(10)-H(10)	120.0	C(25)-C(24)-C(23)	118.2(4)
C(9)-C(10)-C(11)	120.0(4)	C(25)-C(24)-H(24)	120.9
C(11)-C(10)-H(10)	120.0	C(24)-C(25)-C(26)	118.6(4)
C(10)-C(11)-H(11)	119.8	C(24)-C(25)-C(27)	135.3(4)
C(12)-C(11)-C(10)	120.4(5)	C(26)-C(25)-C(27)	106.1(3)
C(12)-C(11)-H(11)	119.8	C(21)-C(26)-C(25)	123.9(4)
C(11)-C(12)-H(12)	119.9	C(21)-C(26)-C(28)	124.8(12)
C(11)-C(12)-C(13)	120.3(5)	C(21)-C(26)-C(28B)	125.1(11)
C(13)-C(12)-H(12)	119.9	C(25)-C(26)-C(28)	110.2(12)
C(12)-C(13)-H(13)	120.1	C(25)-C(26)-C(28B)	110.8(11)
C(12)-C(13)-C(14)	119.8(5)	O(2)-C(27)-C(25)	103.9(3)
C(14)-C(13)-H(13)	120.1	O(2)-C(27)-H(27A)	111.0
C(9)-C(14)-C(13)	120.0(5)	O(2)-C(27)-H(27B)	111.0
C(9)-C(14)-H(14)	120.0	C(25)-C(27)-H(27A)	111.0
C(13)-C(14)-H(14)	120.0	C(25)-C(27)-H(27B)	111.0
C(16)-C(15)-P(1)	118.0(3)	H(27A)-C(27)-H(27B)	109.0
C(20)-C(15)-P(1)	123.0(4)	C(30)-C(29)-P(2)	121.1(3)
C(20)-C(15)-C(16)	118.8(4)	C(30)-C(29)-C(34)	119.5(4)
C(15)-C(16)-H(16)	119.8	C(34)-C(29)-P(2)	119.1(3)
C(17)-C(16)-C(15)	120.3(4)	C(29)-C(30)-H(30)	120.0
C(17)-C(16)-H(16)	119.8	C(31)-C(30)-C(29)	120.0(4)
C(16)-C(17)-H(17)	119.9	C(31)-C(30)-H(30)	120.0
C(16)-C(17)-C(18)	120.2(5)	C(30)-C(31)-H(31)	119.8
C(18)-C(17)-H(17)	119.9	C(32)-C(31)-C(30)	120.3(5)
C(17)-C(18)-H(18)	120.1	C(32)-C(31)-H(31)	119.8
C(19)-C(18)-C(17)	119.7(5)	C(31)-C(32)-H(32)	119.9
C(19)-C(18)-H(18)	120.1	C(31)-C(32)-C(33)	120.2(4)
C(18)-C(19)-H(19)	119.5	C(33)-C(32)-H(32)	119.9
C(18)-C(19)-C(20)	121.0(4)	C(32)-C(33)-H(33)	120.1
C(20)-C(19)-H(19)	119.5	C(32)-C(33)-C(34)	119.8(4)
C(15)-C(20)-H(20)	120.0	C(34)-C(33)-H(33)	120.1
C(19)-C(20)-C(15)	120.0(5)	C(29)-C(34)-H(34)	120.0
C(19)-C(20)-H(20)	120.0	C(33)-C(34)-C(29)	120.1(4)
C(22)-C(21)-P(2)	131.6(3)	C(33)-C(34)-H(34)	120.0
C(26)-C(21)-P(2)	110.7(3)	C(36)-C(35)-P(2)	120.2(3)
C(26)-C(21)-C(22)	117.7(4)	C(40)-C(35)-P(2)	120.2(3)
C(21)-C(22)-H(22)	120.7	C(40)-C(35)-C(36)	119.5(4)
C(21)-C(22)-C(23)	118.7(4)	C(35)-C(36)-H(36)	120.5
C(23)-C(22)-H(22)	120.7	C(37)-C(36)-C(35)	119.1(4)
C(22)-C(23)-H(23)	118.6	C(37)-C(36)-H(36)	120.5
C(24)-C(23)-C(22)	122.9(4)	C(36)-C(37)-H(37)	119.6
C(24)-C(23)-H(23)	118.6	C(38)-C(37)-C(36)	120.9(4)

C(38)-C(37)-H(37)	119.6	C(41)-C(46)-H(46)	118.4
C(37)-C(38)-H(38)	119.9	C(45)-C(46)-C(41)	123.2(3)
C(37)-C(38)-C(39)	120.3(4)	C(45)-C(46)-H(46)	118.4
C(39)-C(38)-H(38)	119.9	F(1)-C(47)-F(2)	106.8(3)
C(38)-C(39)-H(39)	120.0	F(1)-C(47)-F(3)	106.9(3)
C(38)-C(39)-C(40)	120.1(4)	F(1)-C(47)-C(43)	112.8(3)
C(40)-C(39)-H(39)	120.0	F(2)-C(47)-F(3)	105.6(3)
C(35)-C(40)-C(39)	120.2(4)	F(2)-C(47)-C(43)	112.8(3)
C(35)-C(40)-H(40)	119.9	F(3)-C(47)-C(43)	111.5(3)
C(39)-C(40)-H(40)	119.9	F(4)-C(48)-C(45)	115.7(8)
Ir(1)-C(8)-H(8)	108.6	F(4)-C(48)-F(5)	105.2(9)
O(1)-C(8)-Ir(1)	125.3(11)	F(4)-C(48)-F(6)	105.3(8)
O(1)-C(8)-C(6)	97.8(12)	F(5)-C(48)-C(45)	114.3(5)
O(1)-C(8)-H(8)	108.6	F(5)-C(48)-F(6)	104.7(6)
C(6)-C(8)-Ir(1)	106.7(10)	F(6)-C(48)-C(45)	110.7(5)
C(6)-C(8)-H(8)	108.6	F(4A)-C(48)-C(45)	112.0(16)
O(2)-C(28)-Ir(1)	131.5(18)	F(4A)-C(48)-F(5A)	102.6(15)
O(2)-C(28)-C(26)	109.8(19)	F(5A)-C(48)-C(45)	102.0(8)
C(26)-C(28)-Ir(1)	118.7(16)	F(6A)-C(48)-C(45)	116.8(7)
O(1)-C(8B)-Ir(1)	130.9(9)	F(6A)-C(48)-F(4A)	121.1(17)
O(1)-C(8B)-C(6)	108.1(9)	F(6A)-C(48)-F(5A)	97.6(13)
C(6)-C(8B)-Ir(1)	120.4(8)	C(50)-C(49)-B(1)	118.9(3)
Ir(1)-C(28B)-H(28B)	106.0	C(54)-C(49)-C(50)	115.4(3)
O(2)-C(28B)-Ir(1)	128.9(19)	C(54)-C(49)-B(1)	125.7(3)
O(2)-C(28B)-C(26)	98.2(16)	C(49)-C(50)-H(50)	118.9
O(2)-C(28B)-H(28B)	106.0	C(51)-C(50)-C(49)	122.3(4)
C(26)-C(28B)-Ir(1)	109.8(14)	C(51)-C(50)-H(50)	118.9
C(26)-C(28B)-H(28B)	106.0	C(50)-C(51)-C(55)	118.7(4)
C(42)-C(41)-C(46)	114.6(3)	C(52)-C(51)-C(50)	120.9(4)
C(42)-C(41)-B(1)	126.3(3)	C(52)-C(51)-C(55)	120.4(4)
C(46)-C(41)-B(1)	118.9(3)	C(51)-C(52)-H(52)	120.9
C(41)-C(42)-H(42)	118.7	C(53)-C(52)-C(51)	118.3(4)
C(41)-C(42)-C(43)	122.7(3)	C(53)-C(52)-H(52)	120.9
C(43)-C(42)-H(42)	118.7	C(52)-C(53)-C(54)	121.0(4)
C(42)-C(43)-C(47)	118.7(3)	C(52)-C(53)-C(56)	118.4(4)
C(44)-C(43)-C(42)	121.2(3)	C(54)-C(53)-C(56)	120.5(4)
C(44)-C(43)-C(47)	120.1(3)	C(49)-C(54)-H(54)	119.0
C(43)-C(44)-H(44)	121.1	C(53)-C(54)-C(49)	122.1(4)
C(43)-C(44)-C(45)	117.9(3)	C(53)-C(54)-H(54)	119.0
C(45)-C(44)-H(44)	121.1	C(51)-C(55)-F(12A)	106.5(7)
C(44)-C(45)-C(48)	119.9(4)	F(10A)-C(55)-C(51)	116.8(6)
C(46)-C(45)-C(44)	120.5(3)	F(10A)-C(55)-F(11A)	111.0(18)
C(46)-C(45)-C(48)	119.6(4)	F(10A)-C(55)-F(12A)	99.8(13)

F(11A)-C(55)-C(51)	117.1(11)	F(13)-C(64)-C(61)	112.7(4)
F(11A)-C(55)-F(12A)	103.1(14)	F(14)-C(64)-F(15)	105.2(4)
F(10)-C(55)-C(51)	106.3(6)	F(14)-C(64)-C(61)	113.1(3)
F(11)-C(55)-C(51)	110.1(12)	F(15)-C(64)-C(61)	112.1(3)
F(11)-C(55)-F(10)	100.5(16)	C(66)-C(65)-C(70)	115.7(3)
F(12)-C(55)-C(51)	119.9(8)	C(66)-C(65)-B(1)	120.9(3)
F(12)-C(55)-F(10)	105.0(13)	C(70)-C(65)-B(1)	123.1(3)
F(12)-C(55)-F(11)	112.7(16)	C(65)-C(66)-H(66)	118.6
F(7)-C(56)-F(8)	107.5(5)	C(67)-C(66)-C(65)	122.8(4)
F(7)-C(56)-F(9)	107.6(5)	C(67)-C(66)-H(66)	118.6
F(7)-C(56)-C(53)	113.0(4)	C(66)-C(67)-C(72)	120.1(4)
F(8)-C(56)-C(53)	111.6(4)	C(68)-C(67)-C(66)	120.6(4)
F(9)-C(56)-F(8)	103.9(4)	C(68)-C(67)-C(72)	119.3(3)
F(9)-C(56)-C(53)	112.7(4)	C(67)-C(68)-H(68)	120.8
C(58)-C(57)-C(62)	115.3(3)	C(67)-C(68)-C(69)	118.4(3)
C(58)-C(57)-B(1)	123.6(3)	C(69)-C(68)-H(68)	120.8
C(62)-C(57)-B(1)	121.0(3)	C(68)-C(69)-C(70)	120.8(4)
C(57)-C(58)-H(58)	118.9	C(68)-C(69)-C(71)	117.9(3)
C(59)-C(58)-C(57)	122.1(3)	C(70)-C(69)-C(71)	121.2(4)
C(59)-C(58)-H(58)	118.9	C(65)-C(70)-H(70)	119.1
C(58)-C(59)-C(63)	119.5(4)	C(69)-C(70)-C(65)	121.8(4)
C(60)-C(59)-C(58)	121.3(3)	C(69)-C(70)-H(70)	119.1
C(60)-C(59)-C(63)	119.1(4)	F(19)-C(71)-F(20)	106.9(4)
C(59)-C(60)-H(60)	121.0	F(19)-C(71)-F(21)	105.4(4)
C(59)-C(60)-C(61)	117.9(3)	F(19)-C(71)-C(69)	113.5(3)
C(61)-C(60)-H(60)	121.0	F(20)-C(71)-F(21)	105.5(3)
C(60)-C(61)-C(62)	120.7(3)	F(20)-C(71)-C(69)	112.7(4)
C(60)-C(61)-C(64)	120.5(3)	F(21)-C(71)-C(69)	112.3(4)
C(62)-C(61)-C(64)	118.8(3)	F(22)-C(72)-F(23)	106.1(3)
C(57)-C(62)-H(62)	118.7	F(22)-C(72)-C(67)	111.8(4)
C(61)-C(62)-C(57)	122.7(3)	F(23)-C(72)-C(67)	112.3(4)
C(61)-C(62)-H(62)	118.7	F(24)-C(72)-F(22)	106.8(3)
F(16)-C(63)-F(17)	106.7(4)	F(24)-C(72)-F(23)	106.0(4)
F(16)-C(63)-F(18)	105.8(4)	F(24)-C(72)-C(67)	113.5(3)
F(16)-C(63)-C(59)	114.4(4)	C(41)-B(1)-C(49)	105.1(3)
F(17)-C(63)-F(18)	103.3(4)	C(41)-B(1)-C(57)	112.3(3)
F(17)-C(63)-C(59)	112.4(4)	C(41)-B(1)-C(65)	114.1(3)
F(18)-C(63)-C(59)	113.4(4)	C(49)-B(1)-C(65)	109.6(3)
F(13)-C(64)-F(14)	106.2(3)	C(57)-B(1)-C(49)	112.0(3)
F(13)-C(64)-F(15)	107.0(4)	C(57)-B(1)-C(65)	104.0(3)

Table 14. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for complex **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	388(1)	133(1)	197(1)	36(1)	98(1)	40(1)
P(1)	481(7)	162(5)	209(5)	10(4)	0(4)	92(4)
P(2)	267(5)	157(4)	240(5)	21(4)	112(4)	35(4)
O(1)	501(19)	289(15)	223(14)	20(11)	45(13)	39(13)
O(2)	467(18)	268(15)	224(13)	70(11)	72(12)	120(13)
N(1)	540(30)	236(18)	410(20)	-60(15)	247(19)	-144(17)
C(1)	460(20)	174(18)	255(19)	68(15)	-15(17)	7(17)
C(1A)	480(30)	400(30)	410(30)	-50(20)	200(20)	-200(20)
C(2)	490(30)	191(19)	350(20)	109(17)	96(19)	66(18)
C(2A)	530(30)	870(50)	700(40)	-50(30)	330(30)	-300(30)
C(3)	370(20)	340(20)	450(30)	200(20)	110(20)	83(19)
C(4)	310(20)	410(20)	320(20)	167(19)	18(18)	19(19)
C(5)	320(20)	280(20)	242(19)	82(16)	42(16)	-65(17)
C(6)	530(30)	200(20)	280(20)	40(16)	-4(19)	24(19)
C(7)	490(30)	390(20)	230(20)	63(18)	3(19)	-20(20)
C(9)	500(30)	175(19)	260(20)	-30(15)	61(18)	56(18)
C(10)	460(30)	410(30)	270(20)	88(18)	134(19)	70(20)
C(11)	500(30)	510(30)	410(30)	130(20)	180(20)	0(20)
C(12)	500(30)	500(30)	360(20)	-80(20)	150(20)	-30(20)
C(13)	610(30)	390(30)	450(30)	-60(20)	-150(20)	120(20)
C(14)	710(40)	230(20)	420(30)	-16(19)	-130(20)	60(20)
C(15)	530(30)	182(19)	340(20)	38(16)	80(20)	146(19)
C(16)	570(30)	260(20)	330(20)	-2(18)	30(20)	170(20)
C(17)	590(30)	320(20)	410(30)	40(20)	110(20)	200(20)
C(18)	730(40)	320(20)	490(30)	70(20)	230(30)	230(30)
C(19)	830(40)	280(20)	360(20)	-21(19)	200(30)	160(20)
C(20)	640(30)	200(20)	350(20)	-20(17)	90(20)	60(20)
C(21)	290(20)	194(18)	310(20)	68(15)	151(16)	67(15)
C(22)	300(20)	198(19)	460(20)	102(17)	165(18)	69(16)
C(23)	350(20)	250(20)	450(20)	156(18)	128(19)	65(18)
C(24)	310(20)	350(20)	370(20)	212(18)	113(18)	103(18)
C(25)	300(20)	340(20)	270(19)	114(17)	122(17)	111(17)
C(26)	410(20)	250(20)	290(20)	107(16)	167(18)	157(18)
C(27)	390(20)	400(20)	232(19)	152(17)	97(17)	165(19)
C(29)	260(20)	207(18)	350(20)	-48(16)	140(17)	4(15)
C(30)	350(20)	410(30)	420(20)	70(20)	180(20)	140(20)
C(31)	390(30)	600(30)	560(30)	60(30)	200(20)	140(20)
C(32)	390(30)	600(30)	580(30)	-70(30)	300(20)	30(20)
C(33)	470(30)	520(30)	340(20)	-50(20)	210(20)	-30(20)

C(34)	340(20)	350(20)	290(20)	-21(17)	140(18)	21(18)
C(35)	290(20)	154(17)	302(19)	23(15)	111(16)	23(15)
C(36)	400(30)	250(20)	470(30)	-53(19)	90(20)	93(18)
C(37)	510(30)	210(20)	620(30)	-90(20)	20(20)	40(20)
C(38)	360(30)	260(20)	540(30)	40(20)	30(20)	-86(19)
C(39)	290(20)	360(20)	510(30)	70(20)	170(20)	-15(18)
C(40)	320(20)	250(20)	380(20)	17(17)	164(18)	23(17)
C(8)	330(80)	200(40)	150(40)	20(30)	70(50)	70(50)
C(28)	430(120)	220(90)	200(50)	80(50)	180(80)	20(80)
C(8B)	190(70)	310(50)	210(40)	10(30)	80(40)	40(50)
C(28B)	410(110)	140(70)	300(50)	60(50)	210(90)	0(70)
F(1)	494(16)	343(14)	643(17)	-12(12)	414(14)	-59(12)
F(2)	607(18)	257(13)	536(16)	-100(11)	326(14)	-92(12)
F(3)	493(17)	361(15)	709(19)	311(14)	98(14)	-5(13)
F(7)	1210(30)	610(20)	2350(50)	960(30)	1440(40)	630(20)
F(8)	534(17)	324(14)	516(16)	32(12)	161(13)	117(12)
F(9)	1780(40)	550(20)	386(17)	220(15)	300(20)	530(20)
F(13)	325(15)	492(17)	990(20)	-307(17)	231(15)	-153(13)
F(14)	515(17)	320(14)	603(17)	-144(12)	301(14)	-51(12)
F(15)	1050(30)	229(14)	577(18)	91(13)	97(17)	118(15)
F(16)	343(19)	1660(40)	1420(40)	-900(30)	20(20)	390(20)
F(17)	1430(40)	1550(40)	900(30)	570(30)	890(30)	1140(30)
F(18)	940(30)	490(20)	2150(50)	340(30)	1140(30)	390(20)
F(19)	1130(30)	790(20)	534(17)	448(16)	514(19)	700(20)
F(20)	630(19)	573(18)	381(15)	228(13)	-40(13)	78(15)
F(21)	648(19)	349(15)	630(18)	182(13)	262(15)	-1(13)
F(22)	663(19)	483(16)	314(13)	-138(12)	133(13)	73(14)
F(23)	850(20)	631(19)	532(17)	139(15)	545(17)	208(17)
F(24)	523(16)	473(16)	406(14)	10(12)	271(12)	193(13)
C(41)	216(18)	186(17)	205(17)	33(13)	88(14)	62(14)
C(42)	219(18)	228(18)	227(17)	58(14)	124(15)	49(14)
C(43)	205(18)	215(18)	257(18)	37(14)	92(15)	58(14)
C(44)	430(20)	178(18)	264(19)	-14(15)	169(17)	54(17)
C(45)	480(30)	230(20)	265(19)	54(16)	221(18)	73(18)
C(46)	430(20)	153(17)	300(20)	53(15)	199(18)	55(16)
C(47)	320(20)	250(20)	360(20)	11(17)	144(18)	-1(17)
C(48)	1050(50)	290(30)	390(30)	20(20)	460(30)	-30(30)
C(49)	239(19)	206(17)	161(16)	-24(13)	72(14)	43(14)
C(50)	270(20)	270(20)	264(19)	0(15)	97(16)	30(16)
C(51)	250(20)	390(20)	330(20)	-67(18)	54(17)	62(18)
C(52)	350(20)	430(30)	280(20)	-21(18)	54(17)	210(20)
C(53)	450(30)	290(20)	226(19)	42(16)	118(17)	159(19)
C(54)	290(20)	223(18)	221(18)	31(14)	108(15)	52(15)

C(55)	300(30)	650(40)	850(40)	110(30)	180(30)	180(30)
C(56)	650(30)	400(30)	470(30)	130(20)	250(30)	280(20)
C(57)	240(19)	205(17)	187(16)	67(14)	98(14)	51(14)
C(58)	249(19)	189(17)	281(19)	70(14)	137(15)	47(15)
C(59)	280(20)	290(20)	320(20)	113(16)	188(17)	108(16)
C(60)	193(19)	280(20)	288(19)	104(16)	97(15)	27(15)
C(61)	230(19)	223(18)	236(18)	72(14)	95(15)	32(15)
C(62)	222(18)	205(17)	225(17)	50(14)	107(14)	70(14)
C(63)	310(20)	340(20)	530(30)	120(20)	230(20)	101(19)
C(64)	300(20)	280(20)	370(20)	0(17)	126(18)	-23(17)
C(65)	193(18)	198(17)	206(17)	7(14)	93(14)	-4(14)
C(66)	226(19)	236(18)	248(18)	21(15)	119(15)	10(15)
C(67)	260(20)	280(20)	229(18)	-22(15)	144(15)	-38(16)
C(68)	290(20)	360(20)	189(18)	20(16)	108(16)	-48(17)
C(69)	240(20)	300(20)	234(18)	65(16)	82(15)	-4(16)
C(70)	250(20)	290(20)	237(18)	33(15)	129(15)	28(16)
C(71)	430(30)	480(30)	270(20)	122(19)	147(19)	100(20)
C(72)	510(30)	350(20)	250(20)	10(17)	230(20)	10(20)
B(1)	210(20)	181(19)	210(19)	49(15)	114(16)	49(15)
F(4)	1370(90)	340(30)	390(50)	10(30)	560(60)	210(40)
F(5)	1010(50)	1400(80)	610(40)	90(60)	630(40)	-220(60)
F(6)	1740(90)	760(40)	390(30)	410(30)	560(50)	780(50)
F(10A)	350(50)	1420(190)	720(90)	490(100)	330(60)	220(80)
F(11A)	240(60)	480(70)	1400(180)	-190(70)	390(80)	10(50)
F(12A)	320(40)	290(40)	820(70)	-110(40)	150(50)	-10(30)
F(4A)	1700(200)	650(130)	230(60)	-20(80)	210(110)	-310(120)
F(5A)	1660(120)	1040(130)	1030(90)	-70(100)	1180(90)	-90(120)
F(6A)	1770(130)	370(60)	430(70)	160(50)	700(80)	100(80)
F(10)	410(40)	1140(100)	1140(80)	0(80)	480(50)	50(50)
F(11)	290(70)	1000(100)	1080(110)	-130(70)	60(70)	360(60)
F(12)	440(60)	830(70)	2100(300)	-780(120)	600(110)	-290(50)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for complex **3**.

	x	y	z	U(eq)
H	10600(20)	3580(40)	7150(40)	81(19)
H(2)	10816	493	7519	43
H(2AA)	5904	2995	7122	110
H(2AB)	6592	3304	8107	110
H(2AC)	6287	2283	7775	110
H(3)	11864	373	8930	47
H(4)	12139	1434	10044	45
H(7A)	10809	2826	10183	50
H(7B)	11910	3292	10172	50
H(10)	8838	271	7120	46
H(11)	7217	-644	6602	58
H(12)	5890	-230	5527	57
H(13)	6173	1068	4904	69
H(14)	7791	1994	5415	66
H(16)	11705	2679	6863	49
H(17)	12730	2414	6103	53
H(18)	12048	1442	4860	59
H(19)	10357	728	4395	59
H(20)	9315	973	5147	51
H(22)	9661	6683	6796	37
H(23)	9252	6991	5365	42
H(24)	8712	5882	4243	40
H(27A)	7769	3848	4164	40
H(27B)	8896	3998	4118	40
H(30)	7761	5479	6926	45
H(31)	6465	5564	7452	60
H(32)	6619	5178	8824	60
H(33)	8086	4725	9695	53
H(34)	9395	4642	9178	39
H(36)	10222	6463	8694	46
H(37)	11780	7388	9510	60
H(38)	13309	7031	9595	53
H(39)	13326	5736	8889	46
H(40)	11790	4799	8063	37
H(8)	9379	2799	8565	28
H(28B)	8026	3544	5884	32
H(42)	5486	3742	2105	25
H(44)	5764	4697	4473	34
H(46)	4464	2153	3627	33

H(50)	6606	2151	2329	33
H(52)	7430	-35	3396	42
H(54)	4534	317	2826	29
H(58)	2857	2384	2279	27
H(60)	629	221	1221	30
H(62)	3509	276	1297	25
H(66)	5194	1115	890	28
H(68)	4420	2462	-1212	35
H(70)	3953	3236	935	30

Complex **4**. A suitable crystal of **4** was selected for analysis and mounted in a polyimide loop. All measurements were made on a Rigaku Oxford Diffraction Supernova Eos CCD with filtered Cu-Kα radiation at a temperature of 100 K. Using Olex2,[5] the structure was solved with the ShelXT structure solution program using Direct Methods and refined with the ShelXL refinement package[6] using Least Squares minimization. Disorder in the acetonitrile ligand, a phenyl group of the of phosphine ligand, and in the trifluoromethyl groups of the anion were modeled with appropriate similarity restraints.

Table 16. Crystal data and structure refinement for complex **4**.

Empirical formula	$C_{74}H_{47}BF_{24}IrNO_2P_2$	
Formula weight	1703.07	
Temperature	100 K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.26025(19) Å	α = 90.9277(10)°
	b = 15.46771(19) Å	β = 110.5820(12)°
	c = 17.3328(2) Å	γ = 103.1837(11)°
Volume	3465.25(8) Å^3	
Z	2	
Density (calculated)	1.632 Mg/m^3	
Absorption coefficient	5.172 mm^{-1}	
F(000)	1684	
Crystal size	0.149 x 0.082 x 0.055 mm^3	
Theta range for data collection	3.419 to 73.403°.	
Index ranges	-13<=h<=17, -19<=k<=19, -21<=l<=20	
Reflections collected	65797	
Independent reflections	13690 [R(int) = 0.0345]	
Completeness to theta = 67.684°	99.8 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.856 and 0.635	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13690 / 63 / 1040	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0393, wR2 = 0.0969	
R indices (all data)	R1 = 0.0430, wR2 = 0.0997	
Largest diff. peak and hole	2.511 and -1.439 e/Å^{-3}	

Table 17. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^4) for complex **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	96312(2)	82054(2)	21461(2)	314(1)
P(1)	98635(8)	68293(6)	18381(7)	416(3)
P(2)	94391(7)	95162(6)	26144(6)	315(2)
O(1)	105240(20)	84500(20)	39902(17)	466(7)
O(2)	101090(30)	109590(20)	4450(20)	517(8)
N(1)	88680(30)	83240(20)	9064(19)	351(7)
C(1)	102910(30)	79770(30)	32640(30)	429(10)
C(2)	110590(40)	79980(30)	46890(30)	552(13)
C(3)	111870(30)	72010(30)	42930(30)	505(12)
C(4)	116900(30)	65290(40)	45670(40)	611(16)
C(5)	116400(30)	58830(40)	39740(40)	625(17)
C(6)	111080(30)	58780(30)	31250(30)	522(13)
C(7)	106060(30)	65510(30)	28510(30)	470(11)
C(8)	106830(30)	71890(30)	34480(30)	429(11)
C(9)	106270(30)	67220(20)	12160(30)	418(10)
C(10)	116680(30)	71910(30)	15250(30)	498(12)
C(11)	122960(40)	71340(30)	10880(30)	556(13)
C(12)	118970(40)	66220(30)	3290(30)	559(13)
C(13)	108580(40)	61740(30)	120(30)	539(12)
C(14)	102270(40)	62160(30)	4500(30)	470(11)
C(15)	86750(40)	59460(30)	14230(30)	516(12)
C(21)	87310(30)	101380(30)	18320(20)	354(8)
C(22)	77470(30)	102260(30)	17670(30)	488(11)
C(23)	72250(40)	107130(40)	11630(30)	583(13)
C(24)	76590(40)	111070(30)	6200(30)	536(12)
C(25)	86280(30)	110160(30)	6780(30)	419(9)
C(26)	91510(30)	105250(30)	12790(20)	348(8)
C(27)	101740(30)	105760(30)	12030(30)	405(9)
C(28)	92620(40)	113770(30)	1960(30)	481(11)
C(29)	106460(30)	103600(30)	31450(20)	327(8)
C(30)	106350(30)	112320(30)	33490(30)	419(9)
C(31)	115540(40)	118820(30)	36960(30)	497(11)
C(32)	124880(40)	116780(30)	38270(30)	484(11)
C(33)	125120(30)	108190(30)	36250(30)	418(9)
C(34)	115970(30)	101630(30)	32840(20)	354(8)
C(35)	86930(30)	93160(30)	32910(30)	455(10)
C(36)	89160(40)	98290(30)	40130(30)	487(11)
C(37)	82710(40)	96390(40)	44670(30)	641(15)
C(38)	73960(50)	89410(50)	41880(30)	771(19)

C(39)	71620(50)	84170(50)	34560(40)	830(20)
C(40)	78160(40)	85850(40)	30240(30)	656(16)
C(16A)	85080(170)	52400(130)	16920(120)	380(40)
C(17A)	75000(170)	46180(140)	13600(140)	530(50)
C(18)	67600(150)	47770(130)	6520(100)	420(40)
C(19A)	70030(70)	55170(60)	2700(60)	480(20)
C(20A)	79620(70)	61120(60)	5860(60)	510(30)
C(16)	86320(180)	50260(110)	15600(110)	360(30)
C(17)	77210(170)	43920(120)	12690(120)	450(40)
C(18A)	68120(170)	46190(140)	9230(100)	490(40)
C(19)	67810(70)	54930(70)	8890(70)	580(30)
C(20)	76970(70)	61480(60)	11950(70)	500(20)
C(41A)	86300(300)	84100(300)	2250(110)	430(50)
C(42A)	80200(500)	86500(200)	-5670(170)	1150(160)
C(41)	83490(90)	83170(120)	2420(50)	380(20)
C(42)	77180(60)	82860(160)	-6280(50)	1010(60)
F(1)	27600(50)	-3360(30)	16760(40)	1530(20)
F(2)	39920(50)	-3720(20)	26650(20)	1470(30)
F(3)	38370(50)	-8660(20)	14730(30)	1350(20)
F(4)	42270(30)	22130(30)	-3690(18)	753(10)
F(5)	49240(30)	11212(18)	-3396(16)	588(8)
F(6)	58590(20)	24180(18)	1790(16)	526(7)
F(7)	92750(30)	25490(20)	35620(20)	764(11)
F(8)	88100(20)	28930(20)	23293(18)	704(9)
F(9)	100820(20)	37380(20)	32730(20)	719(10)
F(10)	84530(30)	64900(18)	37650(20)	698(9)
F(11)	94678(18)	60549(17)	48211(17)	509(6)
F(12)	79399(19)	60318(18)	47490(20)	593(8)
F(13)	43730(40)	34490(20)	61420(30)	1199(19)
F(14)	56070(30)	45120(20)	61162(17)	666(8)
F(15)	41210(20)	42950(20)	51650(20)	624(8)
F(16)	55000(20)	6816(17)	56869(16)	502(6)
F(17)	65000(20)	7696(18)	49958(17)	519(6)
F(18)	70320(20)	15394(19)	61880(16)	582(8)
F(19)	14330(20)	30370(30)	16890(40)	1360(20)
F(20)	18430(30)	38790(30)	28020(30)	1003(15)
F(21)	13380(20)	43880(20)	16310(20)	663(9)
F(23)	58240(20)	63857(19)	21100(20)	679(8)
C(43)	50740(20)	22580(20)	23050(20)	229(6)
C(44)	45900(30)	13950(20)	23970(20)	281(7)
C(45)	42920(30)	6820(20)	17860(20)	344(8)
C(46)	44300(30)	8090(30)	10420(20)	359(8)
C(47)	48730(30)	16680(20)	9210(20)	311(8)

C(48)	51940(30)	23670(20)	15400(20)	274(7)
C(49)	37970(50)	-2250(30)	19300(30)	629(16)
C(50)	49650(40)	18520(30)	970(30)	406(9)
C(51)	66660(20)	36330(20)	32098(19)	212(6)
C(52)	73790(30)	32440(20)	30480(20)	243(7)
C(53)	84250(30)	36940(20)	32890(20)	281(7)
C(54)	87980(30)	45470(20)	36930(20)	288(7)
C(55)	81060(30)	49450(20)	38680(20)	257(7)
C(56)	70740(20)	44940(20)	36430(20)	228(6)
C(57)	91380(30)	32190(30)	31060(30)	353(8)
C(58)	84800(30)	58760(30)	42960(30)	353(8)
C(59)	53880(20)	28840(20)	38890(20)	220(6)
C(60)	50660(30)	34140(20)	43580(20)	271(7)
C(61)	51170(30)	32520(30)	51560(20)	350(8)
C(62)	54830(30)	25520(30)	55210(20)	363(9)
C(63)	58110(30)	20110(30)	50790(20)	298(7)
C(64)	57760(20)	21840(20)	42800(20)	255(7)
C(65)	47970(50)	38740(30)	56430(30)	530(13)
C(66)	62100(30)	12550(30)	54780(20)	412(9)
C(67)	47030(20)	37980(20)	25631(19)	231(6)
C(68)	50420(30)	45960(30)	22710(20)	331(8)
C(69)	44010(30)	51560(30)	19330(30)	461(11)
C(70)	33690(30)	49230(30)	18430(20)	374(9)
C(71)	30020(30)	41220(30)	21020(20)	314(8)
C(72)	36540(30)	35710(20)	24570(20)	300(7)
C(73)	19050(30)	38500(40)	20370(40)	602(14)
B(1)	54450(30)	31290(20)	29900(20)	215(7)
F(22A)	50550(60)	57080(50)	8450(40)	720(20)
F(24A)	42180(80)	64230(80)	12520(90)	1170(60)
C(74A)	48660(70)	59170(60)	15170(60)	420(20)
F(22)	45230(40)	67520(30)	22140(40)	592(18)
F(24)	45250(80)	62590(60)	10730(40)	750(30)
C(74)	48310(60)	61700(60)	18800(50)	440(20)

Table 18. Bond lengths [Å] and angles [°] for complex **4**.

Ir(1)-P(1)	2.3097(10)	C(15)-C(20A)	1.516(10)
Ir(1)-P(2)	2.2805(10)	C(15)-C(16)	1.437(18)
Ir(1)-N(1)	2.072(3)	C(15)-C(20)	1.420(10)
Ir(1)-C(1)	1.912(4)	C(21)-C(22)	1.406(6)
P(1)-C(7)	1.821(4)	C(21)-C(26)	1.376(6)
P(1)-C(9)	1.810(5)	C(22)-H(22)	0.9300
P(1)-C(15)	1.819(5)	C(22)-C(23)	1.397(7)
P(2)-C(21)	1.819(4)	C(23)-H(23)	0.9300
P(2)-C(29)	1.826(4)	C(23)-C(24)	1.377(7)
P(2)-C(35)	1.828(4)	C(24)-H(24)	0.9300
O(1)-C(1)	1.340(5)	C(24)-C(25)	1.389(7)
O(1)-C(2)	1.470(5)	C(25)-C(26)	1.399(6)
O(2)-C(27)	1.430(5)	C(25)-C(28)	1.464(7)
O(2)-C(28)	1.436(5)	C(26)-C(27)	1.495(6)
N(1)-C(41A)	1.126(15)	C(27)-H(27A)	0.9700
N(1)-C(41)	1.127(7)	C(27)-H(27B)	0.9700
C(1)-C(8)	1.448(6)	C(28)-H(28A)	0.9700
C(2)-H(2A)	0.9700	C(28)-H(28B)	0.9700
C(2)-H(2B)	0.9700	C(29)-C(30)	1.394(5)
C(2)-C(3)	1.479(8)	C(29)-C(34)	1.397(5)
C(3)-C(4)	1.392(7)	C(30)-H(30)	0.9300
C(3)-C(8)	1.385(6)	C(30)-C(31)	1.383(6)
C(4)-H(4)	0.9300	C(31)-H(31)	0.9300
C(4)-C(5)	1.393(9)	C(31)-C(32)	1.382(7)
C(5)-H(5)	0.9300	C(32)-H(32)	0.9300
C(5)-C(6)	1.398(7)	C(32)-C(33)	1.379(7)
C(6)-H(6)	0.9300	C(33)-H(33)	0.9300
C(6)-C(7)	1.391(6)	C(33)-C(34)	1.384(6)
C(7)-C(8)	1.376(7)	C(34)-H(34)	0.9300
C(9)-C(10)	1.398(6)	C(35)-C(36)	1.368(6)
C(9)-C(14)	1.389(6)	C(35)-C(40)	1.411(7)
C(10)-H(10)	0.9300	C(36)-H(36)	0.9300
C(10)-C(11)	1.376(8)	C(36)-C(37)	1.393(7)
C(11)-H(11)	0.9300	C(37)-H(37)	0.9300
C(11)-C(12)	1.384(7)	C(37)-C(38)	1.379(8)
C(12)-H(12)	0.9300	C(38)-H(38)	0.9300
C(12)-C(13)	1.387(7)	C(38)-C(39)	1.387(8)
C(13)-H(13)	0.9300	C(39)-H(39)	0.9300
C(13)-C(14)	1.377(7)	C(39)-C(40)	1.372(7)
C(14)-H(14)	0.9300	C(40)-H(40)	0.9300
C(15)-C(16A)	1.20(2)	C(16A)-H(16A)	0.9300

C(16A)-C(17A)	1.45(3)	F(19)-C(73)	1.305(7)
C(17A)-H(17A)	0.9300	F(20)-C(73)	1.360(7)
C(17A)-C(18)	1.38(3)	F(21)-C(73)	1.330(5)
C(18)-H(18)	0.9300	F(23)-C(74A)	1.408(9)
C(18)-C(19A)	1.37(2)	F(23)-C(74)	1.288(9)
C(19A)-H(19A)	0.9300	C(43)-C(44)	1.396(5)
C(19A)-C(20A)	1.378(13)	C(43)-C(48)	1.404(5)
C(20A)-H(20A)	0.9300	C(43)-B(1)	1.638(5)
C(16)-H(16)	0.9300	C(44)-H(44)	0.9300
C(16)-C(17)	1.36(3)	C(44)-C(45)	1.397(5)
C(17)-H(17)	0.9300	C(45)-C(46)	1.381(5)
C(17)-C(18A)	1.35(3)	C(45)-C(49)	1.487(6)
C(18A)-H(18A)	0.9300	C(46)-H(46)	0.9300
C(18A)-C(19)	1.36(2)	C(46)-C(47)	1.389(5)
C(19)-H(19)	0.9300	C(47)-C(48)	1.386(5)
C(19)-C(20)	1.381(12)	C(47)-C(50)	1.505(5)
C(20)-H(20)	0.9300	C(48)-H(48)	0.9300
C(41A)-C(42A)	1.458(17)	C(51)-C(52)	1.396(4)
C(42A)-H(42A)	0.9600	C(51)-C(56)	1.408(5)
C(42A)-H(42B)	0.9600	C(51)-B(1)	1.640(5)
C(42A)-H(42C)	0.9600	C(52)-H(52)	0.9300
C(41)-C(42)	1.452(9)	C(52)-C(53)	1.401(5)
C(42)-H(42D)	0.9600	C(53)-C(54)	1.378(5)
C(42)-H(42E)	0.9600	C(53)-C(57)	1.495(5)
C(42)-H(42F)	0.9600	C(54)-H(54)	0.9300
F(1)-C(49)	1.355(9)	C(54)-C(55)	1.389(5)
F(2)-C(49)	1.241(6)	C(55)-C(56)	1.387(5)
F(3)-C(49)	1.282(6)	C(55)-C(58)	1.498(5)
F(4)-C(50)	1.325(5)	C(56)-H(56)	0.9300
F(5)-C(50)	1.329(5)	C(59)-C(60)	1.398(5)
F(6)-C(50)	1.331(5)	C(59)-C(64)	1.404(5)
F(7)-C(57)	1.321(5)	C(59)-B(1)	1.636(5)
F(8)-C(57)	1.309(5)	C(60)-H(60)	0.9300
F(9)-C(57)	1.329(5)	C(60)-C(61)	1.390(5)
F(10)-C(58)	1.329(5)	C(61)-C(62)	1.375(6)
F(11)-C(58)	1.343(4)	C(61)-C(65)	1.513(6)
F(12)-C(58)	1.331(5)	C(62)-H(62)	0.9300
F(13)-C(65)	1.323(5)	C(62)-C(63)	1.385(6)
F(14)-C(65)	1.330(6)	C(63)-C(64)	1.400(5)
F(15)-C(65)	1.335(6)	C(63)-C(66)	1.490(6)
F(16)-C(66)	1.342(5)	C(64)-H(64)	0.9300
F(17)-C(66)	1.341(5)	C(67)-C(68)	1.391(5)
F(18)-C(66)	1.348(5)	C(67)-C(72)	1.400(5)

C(67)-B(1)	1.646(5)
C(68)-H(68)	0.9300
C(68)-C(69)	1.389(5)
C(69)-C(70)	1.384(6)
C(69)-C(74A)	1.535(9)
C(69)-C(74)	1.566(10)
C(70)-H(70)	0.9300
C(70)-C(71)	1.377(6)
C(71)-C(72)	1.395(5)
C(71)-C(73)	1.487(6)
C(72)-H(72)	0.9300
F(22A)-C(74A)	1.335(10)
F(24A)-C(74A)	1.311(10)
F(22)-C(74)	1.295(10)
F(24)-C(74)	1.331(9)

P(2)-Ir(1)-P(1)	172.84(4)
N(1)-Ir(1)-P(1)	92.05(9)
N(1)-Ir(1)-P(2)	94.71(9)
C(1)-Ir(1)-P(1)	83.16(14)
C(1)-Ir(1)-P(2)	89.98(14)
C(1)-Ir(1)-N(1)	174.61(15)
C(7)-P(1)-Ir(1)	102.75(17)
C(9)-P(1)-Ir(1)	120.50(13)
C(9)-P(1)-C(7)	104.0(2)
C(9)-P(1)-C(15)	106.9(2)
C(15)-P(1)-Ir(1)	114.49(16)
C(15)-P(1)-C(7)	106.8(2)
C(21)-P(2)-Ir(1)	116.36(13)
C(21)-P(2)-C(29)	101.23(18)
C(21)-P(2)-C(35)	103.4(2)
C(29)-P(2)-Ir(1)	114.95(13)
C(29)-P(2)-C(35)	109.32(19)
C(35)-P(2)-Ir(1)	110.66(17)
C(1)-O(1)-C(2)	111.2(4)
C(27)-O(2)-C(28)	109.5(3)
C(41A)-N(1)-Ir(1)	167(2)
C(41)-N(1)-Ir(1)	171.3(8)
O(1)-C(1)-Ir(1)	131.7(3)
O(1)-C(1)-C(8)	107.1(4)
C(8)-C(1)-Ir(1)	121.2(3)
O(1)-C(2)-H(2A)	110.9
O(1)-C(2)-H(2B)	110.9
O(1)-C(2)-C(3)	104.3(4)
H(2A)-C(2)-H(2B)	108.9
C(3)-C(2)-H(2A)	110.9
C(3)-C(2)-H(2B)	110.9
C(4)-C(3)-C(2)	135.7(5)
C(8)-C(3)-C(2)	106.6(4)
C(8)-C(3)-C(4)	117.7(5)
C(3)-C(4)-H(4)	121.1
C(3)-C(4)-C(5)	117.9(5)
C(5)-C(4)-H(4)	121.1
C(4)-C(5)-H(5)	118.4
C(4)-C(5)-C(6)	123.2(5)
C(6)-C(5)-H(5)	118.4
C(5)-C(6)-H(6)	120.5
C(7)-C(6)-C(5)	119.0(5)
C(7)-C(6)-H(6)	120.5
C(6)-C(7)-P(1)	134.5(4)
C(8)-C(7)-P(1)	108.7(3)
C(8)-C(7)-C(6)	116.7(4)
C(3)-C(8)-C(1)	110.6(4)
C(7)-C(8)-C(1)	123.8(4)
C(7)-C(8)-C(3)	125.5(4)
C(10)-C(9)-P(1)	117.4(3)
C(14)-C(9)-P(1)	123.5(4)
C(14)-C(9)-C(10)	119.1(5)
C(9)-C(10)-H(10)	119.7
C(11)-C(10)-C(9)	120.6(4)
C(11)-C(10)-H(10)	119.7
C(10)-C(11)-H(11)	119.9
C(10)-C(11)-C(12)	120.2(5)
C(12)-C(11)-H(11)	119.9
C(11)-C(12)-H(12)	120.3
C(11)-C(12)-C(13)	119.3(5)
C(13)-C(12)-H(12)	120.3
C(12)-C(13)-H(13)	119.5
C(14)-C(13)-C(12)	120.9(5)
C(14)-C(13)-H(13)	119.5
C(9)-C(14)-H(14)	120.0
C(13)-C(14)-C(9)	119.9(4)
C(13)-C(14)-H(14)	120.0
C(16A)-C(15)-P(1)	125.8(11)
C(16A)-C(15)-C(20A)	120.9(11)
C(20A)-C(15)-P(1)	112.3(5)

C(16)-C(15)-P(1)	123.0(10)
C(20)-C(15)-P(1)	120.5(5)
C(20)-C(15)-C(16)	113.2(11)
C(22)-C(21)-P(2)	121.5(3)
C(26)-C(21)-P(2)	120.0(3)
C(26)-C(21)-C(22)	118.5(4)
C(21)-C(22)-H(22)	119.9
C(23)-C(22)-C(21)	120.2(4)
C(23)-C(22)-H(22)	119.9
C(22)-C(23)-H(23)	119.6
C(24)-C(23)-C(22)	120.7(4)
C(24)-C(23)-H(23)	119.6
C(23)-C(24)-H(24)	120.4
C(23)-C(24)-C(25)	119.2(4)
C(25)-C(24)-H(24)	120.4
C(24)-C(25)-C(26)	120.2(4)
C(24)-C(25)-C(28)	130.1(4)
C(26)-C(25)-C(28)	109.7(4)
C(21)-C(26)-C(25)	121.1(4)
C(21)-C(26)-C(27)	131.4(4)
C(25)-C(26)-C(27)	107.4(4)
O(2)-C(27)-C(26)	105.3(3)
O(2)-C(27)-H(27A)	110.7
O(2)-C(27)-H(27B)	110.7
C(26)-C(27)-H(27A)	110.7
C(26)-C(27)-H(27B)	110.7
H(27A)-C(27)-H(27B)	108.8
O(2)-C(28)-C(25)	105.3(3)
O(2)-C(28)-H(28A)	110.7
O(2)-C(28)-H(28B)	110.7
C(25)-C(28)-H(28A)	110.7
C(25)-C(28)-H(28B)	110.7
H(28A)-C(28)-H(28B)	108.8
C(30)-C(29)-P(2)	120.7(3)
C(30)-C(29)-C(34)	118.7(4)
C(34)-C(29)-P(2)	120.3(3)
C(29)-C(30)-H(30)	119.9
C(31)-C(30)-C(29)	120.2(4)
C(31)-C(30)-H(30)	119.9
C(30)-C(31)-H(31)	119.8
C(32)-C(31)-C(30)	120.4(4)
C(32)-C(31)-H(31)	119.8
C(31)-C(32)-H(32)	119.9
C(33)-C(32)-C(31)	120.1(4)
C(33)-C(32)-H(32)	119.9
C(32)-C(33)-H(33)	120.0
C(32)-C(33)-C(34)	119.9(4)
C(34)-C(33)-H(33)	120.0
C(29)-C(34)-H(34)	119.7
C(33)-C(34)-C(29)	120.6(4)
C(33)-C(34)-H(34)	119.7
C(36)-C(35)-P(2)	124.9(4)
C(36)-C(35)-C(40)	118.9(4)
C(40)-C(35)-P(2)	116.2(4)
C(35)-C(36)-H(36)	119.9
C(35)-C(36)-C(37)	120.2(5)
C(37)-C(36)-H(36)	119.9
C(36)-C(37)-H(37)	119.7
C(38)-C(37)-C(36)	120.5(5)
C(38)-C(37)-H(37)	119.7
C(37)-C(38)-H(38)	120.1
C(37)-C(38)-C(39)	119.7(5)
C(39)-C(38)-H(38)	120.1
C(38)-C(39)-H(39)	120.1
C(40)-C(39)-C(38)	119.8(5)
C(40)-C(39)-H(39)	120.1
C(35)-C(40)-H(40)	119.7
C(39)-C(40)-C(35)	120.7(5)
C(39)-C(40)-H(40)	119.7
C(15)-C(16A)-H(16A)	119.4
C(15)-C(16A)-C(17A)	121.2(19)
C(17A)-C(16A)-H(16A)	119.4
C(16A)-C(17A)-H(17A)	120.2
C(18)-C(17A)-C(16A)	120(2)
C(18)-C(17A)-H(17A)	120.2
C(17A)-C(18)-H(18)	120.5
C(19A)-C(18)-C(17A)	119.0(18)
C(19A)-C(18)-H(18)	120.5
C(18)-C(19A)-H(19A)	119.2
C(18)-C(19A)-C(20A)	121.5(11)
C(20A)-C(19A)-H(19A)	119.2
C(15)-C(20A)-H(20A)	122.2
C(19A)-C(20A)-C(15)	115.6(8)
C(19A)-C(20A)-H(20A)	122.2
C(15)-C(16)-H(16)	119.4
C(17)-C(16)-C(15)	121.2(18)

C(17)-C(16)-H(16)	119.4
C(16)-C(17)-H(17)	119.5
C(18A)-C(17)-C(16)	120.9(17)
C(18A)-C(17)-H(17)	119.5
C(17)-C(18A)-H(18A)	119.6
C(17)-C(18A)-C(19)	120.9(19)
C(19)-C(18A)-H(18A)	119.6
C(18A)-C(19)-H(19)	120.5
C(18A)-C(19)-C(20)	119.0(13)
C(20)-C(19)-H(19)	120.5
C(15)-C(20)-H(20)	119.0
C(19)-C(20)-C(15)	122.0(8)
C(19)-C(20)-H(20)	119.0
N(1)-C(41A)-C(42A)	156(4)
C(41A)-C(42A)-H(42A)	109.5
C(41A)-C(42A)-H(42B)	109.5
C(41A)-C(42A)-H(42C)	109.5
H(42A)-C(42A)-H(42B)	109.5
H(42A)-C(42A)-H(42C)	109.5
H(42B)-C(42A)-H(42C)	109.5
N(1)-C(41)-C(42)	176.8(14)
C(41)-C(42)-H(42D)	109.5
C(41)-C(42)-H(42E)	109.5
C(41)-C(42)-H(42F)	109.5
H(42D)-C(42)-H(42E)	109.5
H(42D)-C(42)-H(42F)	109.5
H(42E)-C(42)-H(42F)	109.5
C(44)-C(43)-C(48)	115.2(3)
C(44)-C(43)-B(1)	125.3(3)
C(48)-C(43)-B(1)	119.4(3)
C(43)-C(44)-H(44)	118.9
C(43)-C(44)-C(45)	122.3(3)
C(45)-C(44)-H(44)	118.9
C(44)-C(45)-C(49)	119.5(3)
C(46)-C(45)-C(44)	121.0(3)
C(46)-C(45)-C(49)	119.5(3)
C(45)-C(46)-H(46)	121.0
C(45)-C(46)-C(47)	117.9(3)
C(47)-C(46)-H(46)	121.0
C(46)-C(47)-C(50)	119.8(3)
C(48)-C(47)-C(46)	120.7(3)
C(48)-C(47)-C(50)	119.5(3)
C(43)-C(48)-H(48)	118.6
C(47)-C(48)-C(43)	122.8(3)
C(47)-C(48)-H(48)	118.6
F(1)-C(49)-C(45)	109.9(5)
F(2)-C(49)-F(1)	100.0(6)
F(2)-C(49)-F(3)	113.3(5)
F(2)-C(49)-C(45)	116.2(4)
F(3)-C(49)-F(1)	100.3(5)
F(3)-C(49)-C(45)	114.7(4)
F(4)-C(50)-F(5)	107.4(4)
F(4)-C(50)-F(6)	106.3(4)
F(4)-C(50)-C(47)	112.2(3)
F(5)-C(50)-F(6)	105.6(3)
F(5)-C(50)-C(47)	112.7(3)
F(6)-C(50)-C(47)	112.2(3)
C(52)-C(51)-C(56)	115.5(3)
C(52)-C(51)-B(1)	124.5(3)
C(56)-C(51)-B(1)	119.9(3)
C(51)-C(52)-H(52)	119.1
C(51)-C(52)-C(53)	121.8(3)
C(53)-C(52)-H(52)	119.1
C(52)-C(53)-C(57)	118.1(3)
C(54)-C(53)-C(52)	121.5(3)
C(54)-C(53)-C(57)	120.4(3)
C(53)-C(54)-H(54)	121.1
C(53)-C(54)-C(55)	117.9(3)
C(55)-C(54)-H(54)	121.1
C(54)-C(55)-C(58)	119.4(3)
C(56)-C(55)-C(54)	120.7(3)
C(56)-C(55)-C(58)	119.9(3)
C(51)-C(56)-H(56)	118.7
C(55)-C(56)-C(51)	122.7(3)
C(55)-C(56)-H(56)	118.7
F(7)-C(57)-F(9)	105.1(4)
F(7)-C(57)-C(53)	111.6(3)
F(8)-C(57)-F(7)	107.3(4)
F(8)-C(57)-F(9)	106.0(3)
F(8)-C(57)-C(53)	113.3(3)
F(9)-C(57)-C(53)	113.1(3)
F(10)-C(58)-F(11)	105.4(3)
F(10)-C(58)-F(12)	107.8(4)
F(10)-C(58)-C(55)	112.3(3)
F(11)-C(58)-C(55)	112.4(3)
F(12)-C(58)-F(11)	105.6(3)

F(12)-C(58)-C(55)	112.8(3)	C(68)-C(69)-C(74)	122.6(4)
C(60)-C(59)-C(64)	115.7(3)	C(70)-C(69)-C(68)	120.9(4)
C(60)-C(59)-B(1)	122.5(3)	C(70)-C(69)-C(74A)	123.6(4)
C(64)-C(59)-B(1)	121.4(3)	C(70)-C(69)-C(74)	114.1(4)
C(59)-C(60)-H(60)	118.9	C(69)-C(70)-H(70)	121.1
C(61)-C(60)-C(59)	122.1(3)	C(71)-C(70)-C(69)	117.9(3)
C(61)-C(60)-H(60)	118.9	C(71)-C(70)-H(70)	121.1
C(60)-C(61)-C(65)	119.5(4)	C(70)-C(71)-C(72)	121.1(3)
C(62)-C(61)-C(60)	121.1(3)	C(70)-C(71)-C(73)	120.0(4)
C(62)-C(61)-C(65)	119.4(4)	C(72)-C(71)-C(73)	118.9(4)
C(61)-C(62)-H(62)	120.7	C(67)-C(72)-H(72)	119.0
C(61)-C(62)-C(63)	118.7(3)	C(71)-C(72)-C(67)	122.1(3)
C(63)-C(62)-H(62)	120.7	C(71)-C(72)-H(72)	119.0
C(62)-C(63)-C(64)	120.1(3)	F(19)-C(73)-F(20)	106.1(5)
C(62)-C(63)-C(66)	118.4(3)	F(19)-C(73)-F(21)	107.6(5)
C(64)-C(63)-C(66)	121.4(4)	F(19)-C(73)-C(71)	113.5(4)
C(59)-C(64)-H(64)	118.9	F(20)-C(73)-C(71)	110.6(4)
C(63)-C(64)-C(59)	122.2(3)	F(21)-C(73)-F(20)	104.8(4)
C(63)-C(64)-H(64)	118.9	F(21)-C(73)-C(71)	113.6(4)
F(13)-C(65)-F(14)	106.9(4)	C(43)-B(1)-C(51)	111.3(3)
F(13)-C(65)-F(15)	107.0(5)	C(43)-B(1)-C(67)	105.7(3)
F(13)-C(65)-C(61)	112.0(4)	C(51)-B(1)-C(67)	110.4(3)
F(14)-C(65)-F(15)	105.9(4)	C(59)-B(1)-C(43)	113.9(3)
F(14)-C(65)-C(61)	111.2(4)	C(59)-B(1)-C(51)	103.7(2)
F(15)-C(65)-C(61)	113.5(4)	C(59)-B(1)-C(67)	111.9(3)
F(16)-C(66)-F(18)	105.7(3)	F(23)-C(74A)-C(69)	107.1(6)
F(16)-C(66)-C(63)	112.0(3)	F(22A)-C(74A)-F(23)	106.3(7)
F(17)-C(66)-F(16)	106.2(4)	F(22A)-C(74A)-C(69)	118.4(7)
F(17)-C(66)-F(18)	107.0(4)	F(24A)-C(74A)-F(23)	112.7(10)
F(17)-C(66)-C(63)	113.7(3)	F(24A)-C(74A)-C(69)	109.2(7)
F(18)-C(66)-C(63)	111.8(4)	F(24A)-C(74A)-F(22A)	103.3(9)
C(68)-C(67)-C(72)	115.5(3)	F(23)-C(74)-C(69)	111.9(6)
C(68)-C(67)-B(1)	124.2(3)	F(23)-C(74)-F(22)	110.5(7)
C(72)-C(67)-B(1)	120.4(3)	F(23)-C(74)-F(24)	102.6(8)
C(67)-C(68)-H(68)	118.7	F(22)-C(74)-C(69)	118.5(7)
C(69)-C(68)-C(67)	122.6(4)	F(22)-C(74)-F(24)	106.8(8)
C(69)-C(68)-H(68)	118.7	F(24)-C(74)-C(69)	104.9(7)
C(68)-C(69)-C(74A)	114.3(4)		

Table 19. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for complex **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	393(1)	238(1)	215(1)	39(1)	25(1)	33(1)
P(1)	419(5)	192(4)	422(6)	25(4)	-79(4)	35(4)
P(2)	359(5)	311(5)	253(4)	-5(4)	105(4)	57(4)
O(1)	549(18)	463(17)	220(13)	106(12)	33(12)	-24(14)
O(2)	650(20)	570(20)	471(18)	273(15)	298(16)	271(17)
N(1)	396(17)	402(18)	257(17)	2(13)	70(14)	184(15)
C(1)	450(20)	330(20)	330(20)	68(17)	39(18)	-81(17)
C(2)	500(30)	620(30)	280(20)	210(20)	-25(19)	-100(20)
C(3)	330(20)	550(30)	440(20)	260(20)	18(18)	-89(19)
C(4)	300(20)	710(40)	600(30)	440(30)	-10(20)	-40(20)
C(5)	330(20)	580(30)	910(40)	570(30)	130(20)	110(20)
C(6)	360(20)	360(20)	730(30)	300(20)	70(20)	65(18)
C(7)	390(20)	320(20)	500(30)	187(19)	-16(19)	-36(17)
C(8)	370(20)	330(20)	380(20)	229(18)	-42(17)	-48(16)
C(9)	410(20)	202(18)	450(20)	40(16)	-70(18)	86(16)
C(10)	410(20)	320(20)	570(30)	-65(19)	-70(20)	136(18)
C(11)	380(20)	350(20)	780(40)	-20(20)	-10(20)	156(19)
C(12)	560(30)	310(20)	720(30)	50(20)	90(20)	180(20)
C(13)	680(30)	300(20)	470(30)	32(19)	30(20)	90(20)
C(14)	500(20)	270(20)	430(20)	59(17)	-50(20)	18(18)
C(15)	430(20)	260(20)	640(30)	-70(20)	-20(20)	24(18)
C(21)	390(20)	340(20)	320(19)	8(15)	90(16)	132(17)
C(22)	390(20)	650(30)	430(20)	30(20)	151(19)	140(20)
C(23)	430(20)	810(40)	540(30)	60(30)	120(20)	280(30)
C(24)	520(30)	550(30)	500(30)	100(20)	50(20)	270(20)
C(25)	480(20)	330(20)	380(20)	13(17)	82(18)	93(18)
C(26)	349(19)	340(20)	327(19)	4(15)	94(16)	80(16)
C(27)	470(20)	420(20)	380(20)	147(18)	190(19)	152(19)
C(28)	570(30)	440(20)	410(20)	156(19)	100(20)	200(20)
C(29)	380(20)	294(19)	282(18)	19(14)	88(15)	86(16)
C(30)	450(20)	350(20)	430(20)	-41(17)	102(19)	129(18)
C(31)	600(30)	310(20)	510(30)	-38(19)	140(20)	90(20)
C(32)	480(20)	410(20)	430(20)	65(19)	100(20)	-54(19)
C(33)	430(20)	440(20)	390(20)	118(18)	160(18)	102(19)
C(34)	400(20)	340(20)	330(20)	60(16)	131(16)	99(17)
C(35)	420(20)	590(30)	320(20)	49(19)	150(18)	50(20)
C(36)	440(20)	620(30)	370(20)	-20(20)	139(19)	90(20)
C(37)	580(30)	970(40)	380(30)	-30(30)	230(20)	130(30)
C(38)	580(30)	1270(60)	430(30)	120(30)	300(30)	0(30)

C(39)	700(40)	1090(50)	540(30)	-30(30)	360(30)	-270(40)
C(40)	680(30)	740(40)	410(30)	-30(20)	270(20)	-200(30)
C(16A)	420(60)	370(100)	230(70)	-10(60)	50(50)	-10(60)
C(17A)	500(90)	670(130)	310(80)	50(80)	170(60)	-120(80)
C(18)	310(50)	530(100)	350(90)	-150(60)	90(60)	30(60)
C(19A)	410(50)	430(50)	470(50)	-20(40)	30(40)	70(40)
C(20A)	470(50)	350(50)	480(50)	20(40)	-30(40)	0(40)
C(16)	590(80)	170(70)	200(60)	0(40)	70(50)	0(50)
C(17)	680(110)	320(70)	230(60)	60(50)	160(60)	-100(60)
C(18A)	520(80)	460(70)	320(90)	0(60)	110(80)	-150(50)
C(19)	340(50)	590(60)	690(70)	-10(50)	120(50)	0(40)
C(20)	370(40)	340(50)	680(60)	-70(40)	120(40)	20(40)
C(41A)	260(110)	800(90)	190(60)	60(60)	10(60)	140(110)
C(42A)	2000(400)	550(180)	590(170)	120(120)	-200(200)	700(200)
C(41)	160(40)	780(60)	240(30)	0(30)	80(20)	200(50)
C(42)	250(40)	2490(180)	210(40)	120(60)	0(30)	310(60)
F(1)	1400(50)	770(30)	2060(60)	380(30)	620(40)	-440(30)
F(2)	3060(70)	428(19)	490(20)	108(16)	650(30)	-410(30)
F(3)	3030(70)	249(15)	1150(30)	9(17)	1460(40)	20(30)
F(4)	860(20)	1250(30)	415(16)	422(18)	323(16)	590(20)
F(5)	980(20)	445(15)	398(14)	-82(11)	431(15)	12(14)
F(6)	714(18)	495(15)	416(14)	30(11)	372(13)	-26(13)
F(7)	990(20)	840(20)	1060(30)	590(20)	770(20)	720(20)
F(8)	648(18)	1090(30)	515(17)	-138(16)	214(14)	504(19)
F(9)	389(14)	700(20)	1200(30)	-127(19)	475(17)	100(13)
F(10)	900(20)	289(14)	675(19)	144(13)	60(17)	60(14)
F(11)	289(11)	459(14)	622(17)	-113(12)	49(11)	-8(10)
F(12)	399(13)	433(15)	910(20)	-314(14)	317(14)	-57(11)
F(13)	2410(50)	660(20)	1390(40)	280(20)	1720(40)	390(30)
F(14)	940(20)	545(17)	423(15)	-170(13)	142(15)	203(16)
F(15)	593(17)	720(20)	706(19)	-134(16)	395(15)	209(15)
F(16)	555(15)	434(14)	438(14)	166(11)	186(12)	-42(12)
F(17)	612(16)	553(16)	513(15)	276(13)	244(13)	297(13)
F(18)	506(15)	583(17)	399(14)	233(12)	-70(12)	3(13)
F(19)	270(15)	580(20)	2790(70)	-80(30)	130(30)	-25(15)
F(20)	600(20)	1590(40)	1290(30)	900(30)	660(20)	640(20)
F(21)	322(13)	850(20)	850(20)	282(17)	123(14)	330(14)
F(23)	667(19)	454(16)	850(20)	268(15)	255(17)	24(14)
C(43)	228(15)	263(17)	208(15)	23(13)	85(12)	75(13)
C(44)	383(19)	257(17)	213(16)	37(13)	127(14)	73(15)
C(45)	540(20)	234(18)	255(18)	28(14)	183(17)	33(16)
C(46)	560(20)	250(18)	278(19)	-17(14)	198(18)	61(17)
C(47)	420(20)	299(18)	244(17)	20(14)	186(16)	56(16)

C(48)	329(18)	254(17)	240(17)	33(13)	129(14)	35(14)
C(49)	1140(50)	290(20)	340(20)	-59(18)	350(30)	-170(30)
C(50)	560(30)	370(20)	310(20)	-1(16)	213(19)	72(19)
C(51)	222(15)	252(16)	178(14)	60(12)	85(12)	69(13)
C(52)	288(16)	255(17)	230(16)	59(13)	126(13)	96(14)
C(53)	275(17)	360(19)	284(17)	99(15)	150(14)	145(15)
C(54)	214(15)	359(19)	313(18)	106(15)	119(14)	70(14)
C(55)	243(16)	260(17)	263(17)	77(13)	91(13)	54(13)
C(56)	217(15)	253(16)	233(16)	52(13)	84(13)	92(13)
C(57)	314(18)	430(20)	430(20)	111(17)	219(17)	166(17)
C(58)	260(17)	285(19)	460(20)	36(16)	94(16)	19(15)
C(59)	184(14)	242(16)	207(15)	-10(12)	71(12)	3(12)
C(60)	292(17)	268(17)	257(17)	-10(13)	146(14)	8(14)
C(61)	430(20)	340(20)	308(19)	-28(15)	243(17)	-21(16)
C(62)	430(20)	400(20)	216(17)	9(15)	165(16)	-57(17)
C(63)	269(17)	343(19)	223(17)	68(14)	71(14)	-11(14)
C(64)	217(15)	328(18)	206(16)	29(13)	76(13)	41(13)
C(65)	870(40)	420(20)	440(30)	10(20)	470(30)	70(20)
C(66)	400(20)	480(20)	290(20)	159(18)	97(17)	38(18)
C(67)	229(15)	281(17)	167(15)	-27(12)	52(12)	65(13)
C(68)	284(17)	390(20)	337(19)	150(16)	118(15)	115(16)
C(69)	360(20)	490(30)	530(30)	280(20)	111(19)	169(19)
C(70)	331(19)	420(20)	340(20)	52(17)	28(16)	187(17)
C(71)	242(17)	370(20)	294(18)	-18(15)	36(14)	113(15)
C(72)	241(16)	291(18)	334(19)	15(15)	77(14)	48(14)
C(73)	300(20)	660(30)	880(40)	260(30)	190(20)	220(20)
B(1)	205(16)	234(18)	201(17)	5(14)	74(14)	45(14)
F(22A)	920(50)	760(50)	680(40)	260(30)	520(40)	220(40)
F(24A)	1100(70)	1090(70)	2180(140)	1300(90)	1190(90)	890(60)
C(74A)	570(60)	430(50)	420(60)	280(50)	250(50)	290(50)
F(22)	520(30)	340(30)	840(50)	170(30)	120(30)	170(20)
F(24)	880(60)	670(50)	370(30)	280(30)	-10(40)	-70(50)
C(74)	510(50)	560(60)	290(50)	160(40)	120(40)	240(50)

Table 20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for complex **4**.

	x	y	z	U(eq)
H(2A)	10647	7827	5030	66
H(2B)	11725	8381	5031	66
H(4)	12049	6511	5128	73
H(5)	11976	5433	4152	75
H(6)	11089	5433	2749	63
H(10)	11939	7543	2030	60
H(11)	12990	7441	1302	67
H(12)	12321	6579	35	67
H(13)	10584	5841	-504	65
H(14)	9534	5906	234	56
H(22)	7443	9960	2127	59
H(23)	6576	10772	1127	70
H(24)	7308	11430	218	64
H(27A)	10730	10950	1669	49
H(27B)	10296	9986	1181	49
H(28A)	8866	11234	-393	58
H(28B)	9512	12021	317	58
H(30)	10009	11378	3252	50
H(31)	11543	12460	3841	60
H(32)	13102	12120	4051	58
H(33)	13141	10680	3719	50
H(34)	11616	9585	3146	43
H(36)	9499	10306	4203	58
H(37)	8432	9985	4961	77
H(38)	6964	8821	4490	93
H(39)	6564	7954	3258	99
H(40)	7679	8212	2550	79
H(16A)	9035	5090	2122	46
H(17A)	7352	4114	1623	63
H(18)	6105	4387	437	51
H(19A)	6509	5621	-213	58
H(20A)	8159	6583	304	61
H(16)	9238	4862	1852	43
H(17)	7723	3793	1309	54
H(18A)	6200	4173	705	59
H(19)	6153	5645	663	70
H(20)	7673	6741	1254	60
H(42A)	8172	8401	-1004	172
H(42B)	8180	9293	-556	172

H(42C)	7296	8433	-663	172
H(42D)	7987	7986	-960	152
H(42E)	7732	8883	-775	152
H(42F)	7019	7968	-723	152
H(44)	4462	1291	2882	34
H(46)	4231	334	635	43
H(48)	5503	2932	1445	33
H(52)	7154	2671	2773	29
H(54)	9491	4846	3842	35
H(56)	6634	4771	3784	27
H(60)	4810	3890	4128	33
H(62)	5509	2445	6053	44
H(64)	6018	1823	3999	31
H(68)	5725	4762	2303	40
H(70)	2937	5295	1615	45
H(72)	3383	3037	2629	36

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