Supporting Information
of

C–C and C–H Bonds Activation of Dialkylmethylenecyclopropane Promoted by Rh and Ir Complexes. Preparation and Structures of $M(\eta^1,\eta^2\text{-}CH_2CR_2CH{=}CH_2)(CO)(PPh_3)_2$ and *trans*-$M(CH{=}CHCMeR_2)(CO)(PPh_3)_2$ (M = Rh and Ir, R = CH_2CH_2Ph)

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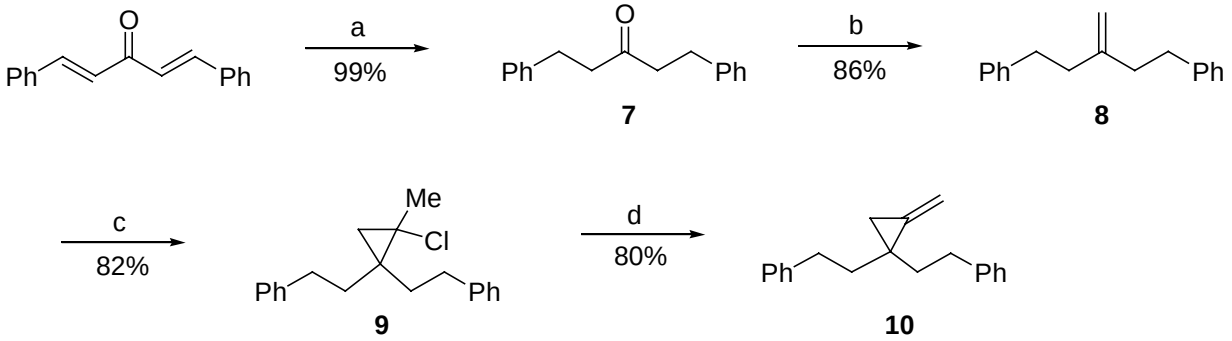
Preparation of Organic Compounds.

Scheme S-1 Preparation of 2,2-bis(2-phenylethyl)-1-methylenecyclopropane



Reagents: (a) H_2, Pd/C, THF/AcOEt, rt, 18 h. (b) ^{t}BuOK, $MePPh_3Br$, THF, rt, 18 h. (c) ^{n}BuLi, $CHCl_2CH_3$, -45 °C, 6 h, then rt, overnight (d) ^{t}BuOK, DMSO, rt, 12 h.

Preparation of 7. To a solution of 1,5-diphenyl-1,4-pentadien-3-one (11.8 g, 50.4 mmol) in THF (100 mL) and ethyl acetate (100 mL) was added 1 g of Pd/C (10%). Hydrogen gas was introduced into the reaction mixture with a balloon at ambient temperature. After 18 h the resulting mixture was filtered off thorough a Celite pad and washed with 15 mL of hexane (3 times). Evaporation of volatiles afforded 1,5-diphenyl-3-pentanone (**7**) (11.9 g, 50 mmol, 99%) as a colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 2.67 (t, J = 7.8 Hz, 4H, $PhCH_2CH_2$), 2.88 (t, J = 7.8 Hz, 4H, $PhCH_2CH_2$), 7.13-7.29 (m, 10H, Ph). ^{13}C{^{1}H} NMR ($CDCl_3$, 75.3 MHz): δ 29.65 ($PhCH_2CH_2$), 44.44 ($PhCH_2CH_2$), 126.06 (Ph-*para*), 128.25 (Ph-*ortho*), 128.44 (Ph-*meta*), 140.94 (Ph-*ipso*), 209.09 (*C*O).

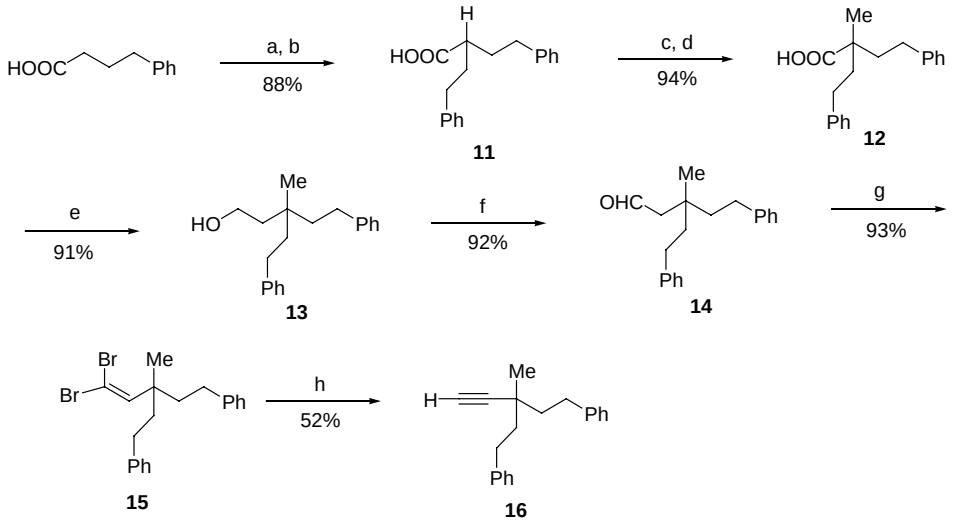
Preparation 8. To a solution of methyltriphenylphosphonium bromide (53.6 g, 150 mmol) in 250 mL of THF was added *tert*-BuOK (17.4 g, 155.0 mmol) at room temperature and the mixture was stirred for 1 h. To the resulting yellow suspension was added 1,5-diphenyl-3-pentanone (11.9 g, 50 mmol) with stirring for 18 h at room temperature. Resulting mixture was extracted with hexane (150 mL) and separated organic layer was washed with $NaHCO_3$ aq. (300 mL) and brine (200 mL), and dried over magnesium sulfate. Filtration and evaporation yielded pale yellow oil, which was subjected to column chromatography (silica gel, hexane, R_f = 0.25) to give 2-phenethyl-4-phenyl-1-butene (**8**) (10.2 g, 43.2 mmol, 86%) as a colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 2.33-2.39 (m, 4H, $PhCH_2CH_2$), 2.73-2.79 (m, 4H, $PhCH_2CH_2$), 4.81 (s, 2H, $C=CH_2$), 7.15-7.20 (m, 6H, Ph), 7.25-7.31 (m, 4H, Ph). ^{13}C{^{1}H} NMR ($CDCl_3$, 75.3 MHz): δ 34.35 ($PhCH_2CH_2$), 38.09 ($PhCH_2CH_2$), 109.63 ($C=CH_2$), 125.79 (Ph-*para*), 128.31 (Ph-*ortho* and *meta*), 142.11 (Ph-*ipso*), 148.63 ($C=CH_2$).

Preparation of 9. To a solution of **8** (11.7 g, 50 mmol) and 1,1-dichloroethane (42ml, 500 mmol) in 150 mL of diethyl ether was added dropwise *n*-BuLi (1.6 M solution in hexane, 600 mL, 960 mmol) over 6 h at –45 °C. After addition was completed, the mixture was slowly warmed up to room temperature and stirred overnight. The resulting mixture was washed with $NaHCO_3$ aq. (400 mL) and brine (300 mL), and dried over $MgSO_4$. Filtration and evaporation gave pale yellow oil, which was purified by column chromatography (silica gel, hexane, R_f = 0.14) to furnish 1-chloro-1-methyl-2,2-diphenethylcyclopropane (**9**) (12.3 g, 41.2 mmol, 82%) as a colorless oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 0.61 (d, J = 6.3 Hz, 1H), 0.85 (d, J = 6.3 Hz, 1H), 1.70 (s, 3H, CH_3), 1.75 (m, 2H, $PhCH_2CH_2$), 2.02 (m, 2H, $PhCH_2CH_2$), 2.73 (m, 2H, $PhCH_2CH_2$), 2.77 (m, 2H, $PhCH_2CH_2$), 7.16-7.32 (m, 10H, Ph). ^{13}C{^{1}H} NMR ($CDCl_3$, 75.3 MHz): δ 24.78 (CH_3), 27.98 (CH_2), 29.84 ($C(CH_3)Cl$), 33.00 ($PhCH_2CH_2$, 2 carbons), 33.88 ($PhCH_2CH_2$), 35.81 ($PhCH_2CH_2$), 50.50 ($C(CH_2CH_2Ph)_2$), 125.80 (Ph-*para*), 125.95 (Ph-*para*), 128.22 (Ph), 128.33

(Ph), 128.36 (Ph), 128.45 (Ph), 142.03 (Ph-*ipso*), 142.40 (Ph-*ipso*). Anal. Calcd for $C_{20}H_{23}Cl$: C, 80.38; H, 7.76. Found: C, 80.24; H, 7.90.

Preparation of 10. To a solution of 1-chloro-1-methyl-2,2-diphenethyl- cyclopropane (9.0 g, 30 mmol) in DMSO (100 mL) was added *tert*-BuOK (9.5 g, 85 mmol) at room temperature. During the mixture being stirred for 12 h, color of the solution changed immediately from colorless into black. The resulting suspension was diluted with hexane (100 mL) and washed with $NaHCO_3$ aq. (200 mL), 150 mL of H_2O (4 times), 150 mL of brine (2 times), and dried over $MgSO_4$. Filtration and evaporation afforded an orange oil, which was purified by column chromatography (silica gel, hexane, R_f = 0.25) to give 2,2-diphenethyl-1-methylenecyclopropane (**10**) (6.3 g, 24 mmol, 80%) as a pale yellow oil. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 0.97 (dd, *J* = 1.8, 2.4 Hz, 2H, C*H*$_2$), 1.77 (m, 4H, PhCH$_2$C*H*$_2$), 2.68 (m, 4H, PhC*H*$_2$CH$_2$), 5.23 (dt, *J* = 1.2, 2.4 Hz, 1H, C=C*H*$_2$), 5.27 (m, 1H, C=C*H*$_2$), 7.15-7.20 (m, 6H, Ph), 7.24-7.30 (m, 4H, Ph). ^{13}C{^{1}H} NMR ($CDCl_3$, 75.3 MHz): δ 15.78 (*C*H$_2$), 23.85 (*C*(CH$_2$CH$_2$Ph)$_2$), 32.97 (PhCH$_2$CH$_2$), 36.78 (PhCH$_2$*C*H$_2$), 102.02 (C=*C*H$_2$), 125.71 (Ph-*para*), 128.31 (Ph-*ortho*), 128.33 (Ph-*meta*), 141.52 (*C*=CH$_2$), 142.33 (Ph-*ipso*).

Scheme S-2



Reagents: (a) LDA, THF, 0 °C, 30 min. (b) HMPA, (2-bromoethyl)benzene , 0 °C to rt,12 h. (c) LDA, THF, 0 °C, 30 min. (d) HMPA, MeI , 40 °C,1 h. (e) $LiAlH_4$, THF, 50 °C, 10 h. (f) $(COCl)_2$, DMSO, CH_2Cl_2, –60 °C, 1 h. (g) CBr_4, PPh_3, CH_2Cl_2, 0 °C, 30 min. (h) ^{n}BuLi, THF, –78 °C, 1 h.

Preparation of 11. To a solution of diisopropylamine (13.7 mL, 98 mmol) in freshly distilled THF (65 mL) in 200 mL of Schlenk tube were added dropwise *n*-BuLi (61 mL, 98 mmol, 1.6 M in hexane solution) at –20 °C. The reaction mixture was stirred for 30 min at 0 °C to complete and 4-phenylbutanoic acid (7.23 g, 44 mmol) was added portionwise to give pale yellow suspension. HMPA (9 mL, 50 mmol) was added and the mixture was stirred for 30 min at room temperature to give dark yellow solution. To the resulting solution was added (2-bromoethyl)benzene (6 mL, 44 mmol) at 0 °C in one portion and the mixture was stirred overnight at ambient temperature. The pale yellow solution was quenched with 150 mL of 3 M HCl and extracted with hexane (50 mL x 4). The combined layer was washed with 3 M HCl (100 mL x 3), H_2O (100 mL x 2), brine (50 mL x 2), and dried over Na_2SO_4. Filtration and evaporation afforded a pale yellow oil. Bulb to bulb distillation (200-210 °C/ 3 Torr) gave

α-(2-phenylethyl)benzenebutanoic acid (**11**) (10.4 g, 38.9 mmol, 88% yield) a pale yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.90-2.01 (m, 2H, CH_2), 2.10-2.23 (m, 2H, CH_2), 2.60 (m, 1H, CH), 2.69-2.87 (m, 4H, CH_2Ph), 7.28-7.42 (m, 10H, Ph). $^{13}C\{^1H\}$ NMR (75.3 MHz, $CDCl_3$): δ 33.42, 33.74, 125.96, 128.36, 128.38, 141.30, 182.80.

Preparation of 12. To a solution of diisopropylamine (13.7 mL, 98 mmol) in freshly distilled THF (65 mL) in 200 mL of Schlenk tube were added dropwise *n*-BuLi (61 mL, 98 mmol, 1.6 M in hexane solution) at –20 °C. The reaction mixture was stirred for 30 min at 0 °C to complete and synthesized α-(2-phenethyl)benzenebutanoic acid (10.73 g, 40 mmol) was added portionwise at –20 °C to give dark yellow suspension. HMPA (9 mL, 50 mmol) was added and the mixture was stirred for 30 min at –20 °C and successively heated at 50 °C to give dark reddish orange suspension. To the resulting solution was added MeI (6.23 mL, 100 mmol) at –20 °C in one portion and the mixture was heated at 40 °C for 1 h. The white precipitates-containing yellow solution was quenched with 150 mL of 3 M HCl and extracted with hexane (50 mL x 4). The combined layer was washed with 3 M HCl (100 mL x 3), H_2O (100 mL x 2), brine (50 mL x 2), and dried over Na_2SO_4. Filtration and evaporation afforded a brown oil. Bulb to bulb distillation (210-220 °C/ 3 Torr) gave 2-methyl-2-phenethyl-4-phenylbutanoic acid (**12**) (10.7 g, 37.7 mmol, 94% yield) a colorless oil, which gradually solidified at room temperature. ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.47 (s, 3H, CH_3), 1.91-2.01 (m, 2H, CH_2), 2.11-2.22 (m, 2H, CH_2), 2.69-2.82 (m, 4H, CH_2Ph), 7.26-7.41 (m, 10H, Ph). $^{13}C\{^1H\}$ NMR (75.3 MHz, $CDCl_3$): δ 21.21, 31.01, 40.94, 45.90, 125.89, 128.31, 128.38, 141.88, 184.09.

Preparation of 13. To a suspension of $LiAlH_4$ (2.28 g, 60 mmol) in THF (50 mL) placed in a 100 mL of Schlenk tube equipped with a magnetic stirring bar was added dropwise THF (30 mL) solution of 2-methyl-2-phenethyl-4-phenylbutanoic acid (10.7 g, 37.7 mmol) at 0 °C. The reaction mixture was warmed to room temperature and heated at 50 °C for 10 h to give gray suspension, which was cooled to 0 °C and diluted with 50 mL of diethyl ether. Water (3 mL) was carefully added dropwise and successively 15% NaOH (3 mL) was added to the mixture. The mixture was stirred for 30 min at ambient temperature and the aqueous layer was separated and extracted with 20 mL of diethyl ether. The combined ethereal layer was washed with brine and dried over $MgSO_4$. Filtration and evaporation gave a pale yellow oil. Bulb to bulb distillation (210 to 220 °C/ 5 Torr) gave 2-methy-4-pheyl-2-(2-phenylethyl)-1-butanol (**13**) (9.2 g, 34.3 mmol) in 91% yield as a colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.05 (s, 3H, CH_3), 1.62-1.73 (m, 4H, CH_2), 2.61-2.68 (m, 4H, CH_2), 3.50 (s, 2H, CH_2O), 7.20-7.36 (m, 10H, Ph). $^{13}C\{^1H\}$ NMR (75.3 MHz, $CDCl_3$): δ 21.84, 30.10, 37.80, 38.64, 69.44, 125.70, 128.26, 128.38, 142.98. Calcd for $C_{19}H_{24}O$: C, 85.03; H, 9.01. Found: C, 85.26; H, 9.11.

Preparation of 14. To a solution of oxalyl chloride (4.63 mL, 53 mmol) in CH_2Cl_2 (75 mL) was added dropwise a mixture of dimethylsulfoxide (3.76 mL, 53 mmol) and CH_2Cl_2 (15 mL) at –50 °C. Within 5 min a mixture of 2-methy-4-pheyl-2-(2-phenylethyl)-1-butanol (6.1 g, 22.9 mmol) and CH_2Cl_2 (20 mL) was added to the above mixture. The reaction mixture was stirred for 15 min at –60 °C to give a pink suspension. To the resulting suspension was added NEt_3 (21 mL, 150 mmol) at –60 °C and the reaction mixture was stirred at room temperature for 1 h. Dichloromethane layer was washed with water (50 mL x 10) to remove DMSO, and with brine, and dried over $MgSO_4$. Filtration and evaporation gave a dark brown oil, which was bulb-to-bulb distilled (200-210 °C/5 Torr) to give α-methyl-α-(2-phenylethyl)benzenebutanal (**14**) (5.62 g, 21.1 mmol, 92% yield) as a pale yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.27 (s, 3H, CH_3), 1.88-1.96 (m, 4H, CH_2), 2.57-2.65 (m, 4H, CH_2), 7.23-7.39 (m, 10H, Ph), 9.58 (s, 1H, CHO). $^{13}C\{^1H\}$ NMR (75.3 MHz, $CDCl_3$): δ 18.31, 30.36, 37.31, 49.10, 125.98, 128.18, 128.42, 141.72, 205.63.

Preparation of 15. To a solution of carbon tetrabromide (27.9 g, 84 mmol) in dichloromethane (60 mL) was added dropwise a solution of triphenylphosphine (44.1 g, 168 mmol) in dichloromethane (60 mL) at 0 °C. The reaction mixture was stirred for 5 min at 0 °C to give a yellow suspension. To the resulting mixture was added dropwise a solution of α-methyl-α-(2-phenylethyl)benzenebutanal (5.62 g, 21.1 mmol) in dichloromethane (60 mL) at

0 °C and the mixture was stirred for 20 min at 0 °C and carefully quenched with 60 mL of water at 0 °C, and then extracted with dichloromethane (150 mL). The combined ethereal layer was washed with $NaHCO_3$ aq. (50 mL) and brine (50 mL), and dried over $MgSO_4$. Filtration and evaporation provided brown oily substances. Column chromatography (silica gel, hexane, R_f = 0.41) and successive bulb to bulb distillation (210 to 220 °C/ 2 Torr) gave 1,1-dibromo-3-methyl-3-phenethyl-5-phenyl-1-pentene (**15**) (8.30 g, 19.65 mmol, 93% yield) of as a pale yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.41 (s, 3H, C*H*$_3$), 1.82-1.94 (m, 2H, CH_2), 2.03-2.13 (m, 2H, CH_2), 2.61-2.75 (m, 4H, CH_2), 6.68 (s, 1H, =CH), 7.24-7.42 (m, 10H, Ph). ^{13}C{^{1}H} NMR (75.3 MHz, $CDCl_3$): δ 24.50, 30.90, 42.11, 42.43, 85.99, 125.81, 128.31, 128.40, 142.33, 144.73 (=CBr_2). Calcd for $C_{20}H_{22}Br_2$: C, 56.90; H, 5.25; Br, 37.85. Found: C, 57.16; H, 5.17; Br, 38.28.

Preparation of 16. To a solution of synthesized 1,1-dibromo-3-methyl-3-phenethyl-5-phenyl-1-pentene (3.75 g, 8.88 mmol) in THF (20 mL) was added dropwise *n*-BuLi (11.6 mL, 18.6 mmol, 1.6 M solution in hexane) at –78 °C. The reaction mixture was stirred for 1 h at –78 °C to give a yellow suspension. The mixture was carefully quenched with 50 mL of 1M HCl, and then extracted with diethyl ether (50 mL x 2). The combined ethereal layer was washed with $NaHCO_3$ aq. (50 mL) and brine (50 mL), and dried over $MgSO_4$. Filtration and evaporation provided a pale yellow oil. Column chromatography (silica gel, hexane, R_f = 0.31) and successive bulb to bulb distillation (180 to 190 °C/ 2 Torr) gave 3-methyl-1,5-diphenyl-3-ethynylpentane (**16**) (1.20 g, 4.5 mmol, 52% yield) of as a colorless oil, which gradually solidified at room temperature as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.40 (s, 3H, C*H*$_3$), 1.74-1.98 (m, 4H, CH_2), 2.31 (s, 1H, CH), 2.84-2.91 (m, 4H, CH_2), 7.23-7.39 (m, 10H, Ph). ^{13}C{^{1}H} NMR (75.3 MHz, $CDCl_3$): δ 26.32, 31.39, 35.07, 43.60, 69.89, 89.87, 125.76, 128.36, 128.36, 142.44. Calcd for $C_{20}H_{22}$: C, 91.55; H, 8.45. Found: C, 91.39; H, 8.12.

*Crystallographic Data and Details of Structure Refinement of **6***

Experimental

Data Collection

A colorless prismatic crystal of $C_{57}OP_2IrH_{53}$ having approximate dimensions of 0.40 x 0.30 x 0.08 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC5R diffractometer with graphite monochromated Mo-Kα radiation and a rotating anode generator.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 20 carefully centered reflections in the range $18.76 < 2\theta < 21.35^o$ corresponded to a primitive monoclinic cell with dimensions:

a = 10.750(2) Å
b = 28.200(3) Å β = 99.44(1)^o
c = 15.413(2) Å
V = 4609(1) Å^3

For Z = 4 and F.W. = 1008.21, the calculated density is 1.45 g/cm^3. The systematic absences of:

h0l: h+l ± 2n
0k0: k ± 2n

uniquely determine the space group to be:

$P2_1/n$ (No. 14)

The data were collected at a temperature of 23 ± 1^{o}C using the ω-2θ scan technique to a maximum 2θ value of 55.0^o. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.28^o with a take-off angle of 6.0^o. Scans of $(0.75 + 0.30 \tan \theta)^o$ were made at a speed of 4.0^o/min (in ω). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 3 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm, the crystal to detector distance was 258 mm, and the detector aperture was 6.0 x 6.0 mm (horizontal x vertical).

Data Reduction

Of the 11344 reflections which were collected, 10788 were unique (R_{int} = 0.030); equivalent reflections were merged. The intensities of three representative reflections were measured after every 150 reflections. No decay correction was applied.

The linear absorption coefficient, μ, for Mo-Kα radiation is 30.1 cm^{-1}. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.70 to 1.00. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by heavy-atom Patterson methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[3] on F was based on 6205 observed reflections ($I > 3.00\sigma(I)$) and 550 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.037$$

$$R_W = [\, \Sigma \, w \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, w \, Fo^2]^{1/2} = 0.029$$

The standard deviation of an observation of unit weight[4] was 1.17. The weighting scheme was based on counting statistics and included a factor (p = 0.004) to downweight the intense reflections. Plots of $\Sigma \, w \, (|Fo| - |Fc|)^2$ versus |Fo|, reflection order in data collection, $\sin \theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.63 and -0.89 e$^-$/Å^3, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) PATTY: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(2) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized:

$\Sigma w(|F_o|-|F_c|)^2$ where

$w = 1/[\sigma^2(Fo)] = [\sigma^2_c(Fo) + p^2Fo^2/4]^{-1}$

$\sigma_c(Fo)$ = e.s.d. based on counting statistics

p = p-factor

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations

N_v = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) teXsan for Windows: Crystal Structure Analysis Package, Molecular Structure Corporation (1997).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{57}H_{53}OP_2Ir$
Formula Weight	1008.21
Crystal Color, Habit	colorless, prismatic
Crystal Dimensions	0.40 X 0.30 X 0.08 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	20 (18.8 - 21.4°)
Omega Scan Peak Width at Half-height	0.28°
Lattice Parameters	a = 10.750(2) Å b = 28.200(3) Å c = 15.413(2) Å β = 99.44(1) ° V = 4609(1) Å ^{3}
Space Group	$P2_1/n$ (No. 14)
Z value	4
D_{calc}	1.453 g/cm^3
F_{000}	2040.00
μ(MoKα)	30.14 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC5R
Radiation	MoKα (λ = 0.71069 Å)

	graphite monochromated
Attenuator	Zr foil (factors = 1.00, 3.64, 12.10, 44.80)
Take-off Angle	6.0^{o}
Detector Aperture	6.0 mm horizontal
	6.0 mm vertical
Crystal to Detector Distance	258 mm
Voltage, Current	50kV, 180mA
Temperature	23.0^{o}C
Scan Type	ω-2θ
Scan Rate	4.0^{o}/min (in ω) (up to 3 scans)
Scan Width	$(0.75 + 0.30 \tan \theta)^{o}$
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 11344
	Unique: 10788 (R_{int} = 0.030)
Corrections	Lorentz-polarization
	Absorption
	(trans. factors: 0.7043 - 0.9997)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF92 PATTY)
Refinement	Full-matrix least-squares on F
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	$1/\sigma^2(Fo) = 4Fo^2/\sigma^2(Fo^2)$
π-factor	0.0043
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	6205
No. Variables	550
Reflection/Parameter Ratio	11.28
Residuals: R; Rw	0.037 ; 0.029
Goodness of Fit Indicator	1.17
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.63 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.89 $e^-/Å^3$

Table S1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ir()	0.16338(2)	0.136356(9)	0.31935(1)	2.754(4)
P(1)	0.1828(1)	0.06442(5)	0.24251(9)	2.81(3)
P(2)	-0.0554(1)	0.14140(6)	0.31781(8)	2.94(3)
O(1)	0.1651(5)	0.2082(2)	0.1737(3)	6.1(1)
C(1)	0.1646(6)	0.1804(2)	0.2279(4)	3.9(2)
C(2)	0.3648(5)	0.1439(2)	0.3589(4)	3.6(1)
C(3)	0.3591(5)	0.1777(2)	0.4361(4)	3.4(1)
C(4)	0.2213(5)	0.1699(2)	0.4434(4)	3.5(1)
C(5)	0.1831(6)	0.1220(2)	0.4584(4)	3.9(2)
C(6)	0.3812(6)	0.2288(2)	0.4097(4)	3.8(1)
C(7)	0.5173(6)	0.2410(3)	0.4036(5)	5.8(2)
C(8)	0.5410(6)	0.2878(3)	0.3636(5)	4.4(2)
C(9)	0.5141(7)	0.2946(3)	0.2763(5)	6.1(2)
C(10)	0.5428(9)	0.3357(4)	0.2359(5)	7.3(3)
C(11)	0.5989(8)	0.3719(3)	0.2875(6)	7.2(3)
C(12)	0.6248(8)	0.3669(3)	0.3753(6)	6.8(2)

C(13)	0.5951(7)	0.3255(3)	0.4134(5)	5.5(2)
C(14)	0.4468(6)	0.1638(2)	0.5222(4)	4.4(2)
C(15)	0.4290(7)	0.1924(3)	0.6026(4)	5.3(2)
C(16)	0.4854(7)	0.1684(3)	0.6872(4)	4.6(2)
C(17)	0.4222(8)	0.1336(4)	0.7238(6)	7.9(3)
C(18)	0.470(1)	0.1111(4)	0.8011(7)	9.7(4)
C(19)	0.587(1)	0.1234(3)	0.8424(5)	7.4(3)
C(20)	0.6522(8)	0.1579(3)	0.8091(5)	6.6(2)
C(21)	0.6000(7)	0.1803(3)	0.7311(4)	5.2(2)
C(22)	0.2157(5)	0.0093(2)	0.3048(4)	3.3(1)
C(23)	0.3037(7)	0.0115(2)	0.3810(4)	4.8(2)
C(24)	0.3436(7)	-0.0286(3)	0.4277(5)	5.9(2)
C(25)	0.2973(8)	-0.0719(3)	0.4002(6)	6.2(2)
C(26)	0.2111(7)	-0.0749(3)	0.3243(6)	6.6(2)
C(27)	0.1723(7)	-0.0344(3)	0.2770(5)	5.2(2)
C(28)	0.3161(5)	0.0642(2)	0.1802(4)	3.0(1)
C(29)	0.3772(6)	0.0235(2)	0.1628(4)	4.1(2)
C(30)	0.4720(7)	0.0239(3)	0.1130(5)	5.3(2)
C(31)	0.5083(7)	0.0656(3)	0.0787(5)	5.4(2)
C(32)	0.4496(7)	0.1060(3)	0.0946(5)	5.6(2)
C(33)	0.3554(6)	0.1065(2)	0.1454(4)	4.4(2)
C(34)	0.0524(5)	0.0485(2)	0.1545(4)	3.2(1)
C(35)	-0.0550(6)	0.0264(2)	0.1725(4)	4.1(2)
C(36)	-0.1588(6)	0.0191(3)	0.1069(5)	5.0(2)
C(37)	-0.1545(7)	0.0346(3)	0.0234(5)	5.5(2)
C(38)	-0.0502(7)	0.0576(2)	0.0037(4)	4.8(2)
C(39)	0.0540(6)	0.0635(2)	0.0685(4)	4.1(2)
C(40)	-0.1538(5)	0.1650(2)	0.2179(3)	3.1(1)
C(41)	-0.1218(6)	0.1524(2)	0.1378(4)	3.9(2)
C(42)	-0.1933(6)	0.1679(2)	0.0606(4)	4.3(2)
C(43)	-0.2951(6)	0.1969(2)	0.0620(4)	4.4(2)
C(44)	-0.3252(6)	0.2102(3)	0.1402(4)	5.1(2)
C(45)	-0.2566(6)	0.1947(3)	0.2181(4)	4.8(2)
C(46)	-0.1393(5)	0.0875(2)	0.3408(3)	3.3(1)
C(47)	-0.2685(6)	0.0823(3)	0.3121(4)	5.2(2)
C(48)	-0.3265(8)	0.0401(3)	0.3277(5)	6.6(2)
C(49)	-0.2622(9)	0.0028(3)	0.3700(5)	7.1(3)
C(50)	-0.1336(8)	0.0080(3)	0.3984(4)	5.5(2)
C(51)	-0.0731(7)	0.0501(2)	0.3847(4)	4.5(2)
C(52)	-0.0933(5)	0.1831(2)	0.4005(3)	3.0(1)
C(53)	-0.0696(6)	0.2306(2)	0.3897(4)	3.9(2)
C(54)	-0.0995(6)	0.2639(3)	0.4488(5)	5.0(2)
C(55)	-0.1473(6)	0.2495(3)	0.5219(5)	5.2(2)
C(56)	-0.1682(7)	0.2025(3)	0.5356(4)	5.2(2)
C(57)	-0.1419(6)	0.1695(2)	0.4748(4)	4.3(2)
H(1)	0.4051	0.1147	0.3770	4.371
H(2)	0.4044	0.1578	0.3143	4.371
H(3)	0.1732	0.1956	0.4601	4.201
H(4)	0.1089	0.1174	0.4833	4.654
H(5)	0.2459	0.1000	0.4835	4.654
H(6)	0.3314	0.2344	0.3538	4.620
H(7)	0.3543	0.2492	0.4521	4.620

H(8)	0.5638	0.2405	0.4616	6.992
H(9)	0.5482	0.2170	0.3694	6.992
H(10)	0.4733	0.2698	0.2407	7.366
H(11)	0.5241	0.3390	0.1738	8.769
H(12)	0.6196	0.4006	0.2610	8.680
H(13)	0.6637	0.3920	0.4108	8.209
H(14)	0.6120	0.3225	0.4756	6.602
H(15)	0.4321	0.1314	0.5339	5.271
H(16)	0.5316	0.1677	0.5132	5.271
H(17)	0.4682	0.2224	0.5998	6.352
H(18)	0.3413	0.1967	0.6022	6.352
H(19)	0.3411	0.1245	0.6943	9.421
H(20)	0.4231	0.0874	0.8250	11.591
H(21)	0.6225	0.1077	0.8952	8.842
H(22)	0.7334	0.1667	0.8387	7.965
H(23)	0.6465	0.2047	0.7082	6.238
H(24)	0.3372	0.0414	0.4014	5.711
H(25)	0.4041	-0.0261	0.4799	7.041
H(26)	0.3243	-0.0996	0.4330	7.452
H(27)	0.1779	-0.1049	0.3041	7.901
H(28)	0.1140	-0.0371	0.2238	6.283
H(29)	0.3533	-0.0057	0.1857	4.939
H(30)	0.5128	-0.0049	0.1022	6.306
H(31)	0.5739	0.0659	0.0443	6.513
H(32)	0.4736	0.1349	0.0703	6.692
H(33)	0.3169	0.1356	0.1568	5.252
H(34)	-0.0583	0.0160	0.2307	4.863
H(35)	-0.2318	0.0036	0.1201	6.017
H(36)	-0.2248	0.0293	-0.0217	6.643
H(37)	-0.0495	0.0693	-0.0540	5.793
H(38)	0.1278	0.0780	0.0543	4.966
H(39)	-0.0501	0.1330	0.1359	4.674
H(40)	-0.1718	0.1583	0.0058	5.203
H(41)	-0.3440	0.2076	0.0086	5.259
H(42)	-0.3952	0.2306	0.1413	6.097
H(43)	-0.2795	0.2045	0.2724	5.702
H(44)	-0.3161	0.1074	0.2821	6.204
H(45)	-0.4146	0.0370	0.3082	7.890
H(46)	-0.3043	-0.0258	0.3798	8.467
H(47)	-0.0866	-0.0176	0.4275	6.573
H(48)	0.0147	0.0533	0.4056	5.395
H(49)	-0.0321	0.2406	0.3411	4.730
H(50)	-0.0870	0.2966	0.4389	5.977
H(51)	-0.1660	0.2724	0.5631	6.221
H(52)	-0.2006	0.1927	0.5864	6.231
H(53)	-0.1573	0.1368	0.4841	5.175

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir()	0.0352(1)	0.0350(1)	0.03367(9)	0.0020(2)	0.00319(7)	-0.0038(1)

P(1)	0.0379(8)	0.0333(8)	0.0348(8)	0.0015(7)	0.0037(6)	-0.0020(6)
P(2)	0.0373(7)	0.0429(9)	0.0306(7)	0.0016(8)	0.0033(6)	-0.0023(7)
O(1)	0.107(4)	0.053(3)	0.079(4)	0.007(3)	0.030(3)	0.027(3)
C(1)	0.055(4)	0.039(4)	0.056(4)	0.002(3)	0.013(3)	-0.005(3)
C(2)	0.045(3)	0.044(4)	0.048(3)	0.003(3)	0.006(3)	-0.006(3)
C(3)	0.042(3)	0.042(4)	0.042(3)	0.001(3)	-0.004(3)	-0.011(3)
C(4)	0.039(3)	0.054(4)	0.039(3)	0.006(3)	0.003(3)	-0.007(3)
C(5)	0.048(4)	0.057(4)	0.042(3)	0.006(3)	0.008(3)	-0.005(3)
C(6)	0.046(4)	0.045(4)	0.052(4)	0.008(3)	-0.002(3)	-0.004(3)
C(7)	0.053(5)	0.070(6)	0.096(6)	-0.002(4)	0.004(4)	0.012(5)
C(8)	0.048(4)	0.052(4)	0.067(5)	0.002(3)	0.005(3)	0.002(4)
C(9)	0.078(6)	0.073(6)	0.079(6)	-0.005(5)	0.007(5)	-0.017(5)
C(10)	0.101(8)	0.109(8)	0.070(6)	0.005(7)	0.022(5)	0.006(6)
C(11)	0.097(7)	0.073(7)	0.110(8)	0.006(5)	0.032(6)	0.026(6)
C(12)	0.089(6)	0.069(6)	0.103(7)	-0.022(6)	0.020(5)	-0.018(6)
C(13)	0.078(6)	0.068(5)	0.065(5)	-0.008(5)	0.018(4)	-0.004(4)
C(14)	0.050(4)	0.048(4)	0.065(4)	0.002(3)	-0.003(3)	-0.001(3)
C(15)	0.079(5)	0.064(5)	0.051(4)	0.006(4)	-0.011(4)	-0.005(4)
C(16)	0.063(5)	0.061(5)	0.048(4)	0.005(4)	-0.006(3)	-0.000(3)
C(17)	0.081(6)	0.112(8)	0.099(7)	-0.030(6)	-0.001(5)	0.024(6)
C(18)	0.108(8)	0.14(1)	0.117(9)	-0.022(8)	0.020(7)	0.060(8)
C(19)	0.135(9)	0.085(7)	0.060(5)	0.014(6)	0.014(5)	0.032(5)
C(20)	0.101(7)	0.089(6)	0.049(5)	0.001(6)	-0.026(4)	-0.010(4)
C(21)	0.079(5)	0.067(5)	0.046(4)	-0.016(4)	-0.005(4)	0.006(4)
C(22)	0.041(3)	0.039(4)	0.044(3)	0.005(3)	0.007(3)	0.002(3)
C(23)	0.074(5)	0.049(4)	0.054(4)	0.005(4)	-0.001(4)	0.014(3)
C(24)	0.086(6)	0.058(5)	0.075(5)	0.010(5)	0.004(4)	0.026(4)
C(25)	0.076(6)	0.056(5)	0.105(7)	0.019(4)	0.018(5)	0.034(5)
C(26)	0.079(6)	0.038(4)	0.126(7)	-0.005(4)	-0.005(5)	0.018(5)
C(27)	0.061(5)	0.047(4)	0.085(5)	-0.004(4)	-0.003(4)	0.007(4)
C(28)	0.036(3)	0.043(3)	0.033(3)	-0.001(3)	0.006(2)	-0.012(3)
C(29)	0.049(4)	0.048(4)	0.060(4)	0.009(3)	0.011(3)	-0.000(3)
C(30)	0.061(5)	0.073(6)	0.070(5)	0.018(4)	0.021(4)	-0.012(4)
C(31)	0.060(5)	0.093(6)	0.062(5)	0.007(5)	0.036(4)	-0.007(4)
C(32)	0.086(6)	0.061(5)	0.077(5)	0.000(4)	0.048(4)	0.010(4)
C(33)	0.075(5)	0.040(4)	0.061(4)	0.003(3)	0.036(4)	0.013(3)
C(34)	0.038(3)	0.037(3)	0.044(3)	0.003(3)	0.002(3)	-0.010(3)
C(35)	0.049(4)	0.053(4)	0.050(4)	0.000(3)	0.004(3)	-0.012(3)
C(36)	0.041(4)	0.066(5)	0.082(5)	0.002(4)	0.003(4)	-0.024(4)
C(37)	0.054(5)	0.083(6)	0.065(5)	0.015(4)	-0.016(4)	-0.037(4)
C(38)	0.073(5)	0.059(5)	0.044(4)	0.024(4)	-0.012(4)	-0.010(3)
C(39)	0.051(4)	0.057(4)	0.047(4)	0.013(3)	-0.002(3)	-0.012(3)
C(40)	0.036(3)	0.046(4)	0.036(3)	0.002(3)	0.005(2)	0.003(3)
C(41)	0.057(4)	0.053(4)	0.037(3)	0.015(3)	0.005(3)	0.002(3)
C(42)	0.066(5)	0.058(4)	0.039(3)	0.012(4)	0.005(3)	0.003(3)
C(43)	0.051(4)	0.060(5)	0.051(4)	0.006(4)	-0.005(3)	0.021(3)
C(44)	0.040(4)	0.089(6)	0.060(4)	0.028(4)	-0.004(3)	-0.001(4)
C(45)	0.045(4)	0.093(6)	0.043(4)	0.013(4)	0.007(3)	-0.007(4)
C(46)	0.044(3)	0.049(4)	0.032(3)	-0.005(3)	0.007(3)	-0.001(3)
C(47)	0.052(4)	0.085(6)	0.058(4)	-0.016(4)	0.004(3)	0.005(4)
C(48)	0.063(5)	0.118(8)	0.067(5)	-0.027(6)	0.003(4)	0.002(6)
C(49)	0.112(8)	0.092(7)	0.064(5)	-0.059(6)	0.015(5)	0.000(5)

C(50)	0.095(6)	0.054(5)	0.056(5)	-0.012(5)	0.006(4)	0.010(4)
C(51)	0.071(5)	0.055(5)	0.043(4)	-0.015(4)	0.005(3)	0.007(3)
C(52)	0.027(3)	0.047(4)	0.039(3)	0.006(3)	0.003(2)	-0.005(3)
C(53)	0.045(4)	0.053(4)	0.053(4)	0.003(3)	0.012(3)	-0.006(3)
C(54)	0.055(4)	0.056(5)	0.076(5)	0.002(4)	0.005(4)	-0.022(4)
C(55)	0.049(4)	0.082(6)	0.064(5)	0.014(4)	0.003(3)	-0.033(4)
C(56)	0.063(5)	0.101(7)	0.035(4)	-0.000(5)	0.014(3)	-0.014(4)
C(57)	0.046(4)	0.076(5)	0.041(4)	0.002(4)	0.006(3)	-0.007(3)

The general temperature factor expression:

$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Ir(1)	P(1)	2.375(2)	Ir(1)	P(2)	2.353(2)
Ir(1)	C(1)	1.881(7)	Ir(1)	C(2)	2.162(6)
Ir(1)	C(4)	2.132(6)	Ir(1)	C(5)	2.157(6)
P(1)	C(22)	1.831(6)	P(1)	C(28)	1.851(6)
P(1)	C(34)	1.839(6)	P(2)	C(40)	1.844(6)
P(2)	C(46)	1.832(7)	P(2)	C(52)	1.829(6)
O(1)	C(1)	1.146(7)	C(2)	C(3)	1.534(8)
C(3)	C(4)	1.520(8)	C(3)	C(6)	1.527(9)
C(3)	C(14)	1.546(8)	C(4)	C(5)	1.441(9)
C(6)	C(7)	1.521(9)	C(7)	C(8)	1.50(1)
C(8)	C(9)	1.34(1)	C(8)	C(13)	1.38(1)
C(9)	C(10)	1.38(1)	C(10)	C(11)	1.37(1)
C(11)	C(12)	1.34(1)	C(12)	C(13)	1.37(1)
C(14)	C(15)	1.517(9)	C(15)	C(16)	1.506(9)
C(16)	C(17)	1.37(1)	C(16)	C(21)	1.347(9)
C(17)	C(18)	1.37(1)	C(18)	C(19)	1.35(1)
C(19)	C(20)	1.35(1)	C(20)	C(21)	1.393(9)
C(22)	C(23)	1.383(8)	C(22)	C(27)	1.361(9)
C(23)	C(24)	1.371(9)	C(24)	C(25)	1.36(1)
C(25)	C(26)	1.37(1)	C(26)	C(27)	1.383(9)
C(28)	C(29)	1.369(8)	C(28)	C(33)	1.402(8)
C(29)	C(30)	1.373(9)	C(30)	C(31)	1.37(1)
C(31)	C(32)	1.34(1)	C(32)	C(33)	1.377(9)
C(34)	C(35)	1.380(8)	C(34)	C(39)	1.394(8)
C(35)	C(36)	1.392(9)	C(36)	C(37)	1.37(1)
C(37)	C(38)	1.37(1)	C(38)	C(39)	1.384(8)
C(40)	C(41)	1.382(7)	C(40)	C(45)	1.388(8)
C(41)	C(42)	1.377(8)	C(42)	C(43)	1.370(9)
C(43)	C(44)	1.351(9)	C(44)	C(45)	1.373(9)
C(46)	C(47)	1.395(8)	C(46)	C(51)	1.385(9)
C(47)	C(48)	1.38(1)	C(48)	C(49)	1.36(1)
C(49)	C(50)	1.39(1)	C(50)	C(51)	1.386(9)
C(52)	C(53)	1.378(9)	C(52)	C(57)	1.389(8)
C(53)	C(54)	1.381(9)	C(54)	C(55)	1.37(1)
C(55)	C(56)	1.37(1)	C(56)	C(57)	1.383(9)

Table S4. Bond Angles(^{o})

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	Ir(1)	P(2)	102.49(6)	P(1)	Ir(1)	C(1)	100.3(2)

P(1)	Ir(1)	C(2)	93.4(2)	P(1)	Ir(1)	C(4)	142.1(2)
P(1)	Ir(1)	C(5)	109.4(2)	P(2)	Ir(1)	C(1)	94.7(2)
P(2)	Ir(1)	C(2)	161.9(2)	P(2)	Ir(1)	C(4)	97.3(2)
P(2)	Ir(1)	C(5)	87.5(2)	C(1)	Ir(1)	C(2)	90.9(3)
C(1)	Ir(1)	C(4)	110.0(3)	C(1)	Ir(1)	C(5)	149.0(3)
C(2)	Ir(1)	C(4)	64.6(2)	C(2)	Ir(1)	C(5)	78.9(2)
C(4)	Ir(1)	C(5)	39.3(2)	Ir(1)	P(1)	C(22)	119.3(2)
Ir(1)	P(1)	C(28)	113.6(2)	Ir(1)	P(1)	C(34)	117.2(2)
C(22)	P(1)	C(28)	99.8(3)	C(22)	P(1)	C(34)	103.7(3)
C(28)	P(1)	C(34)	100.3(3)	Ir(1)	P(2)	C(40)	117.8(2)
Ir(1)	P(2)	C(46)	118.1(2)	Ir(1)	P(2)	C(52)	111.6(2)
C(40)	P(2)	C(46)	103.2(3)	C(40)	P(2)	C(52)	100.8(3)
C(46)	P(2)	C(52)	103.1(3)	Ir(1)	C(1)	O(1)	178.2(6)
Ir(1)	C(2)	C(3)	96.6(4)	C(2)	C(3)	C(4)	97.5(5)
C(2)	C(3)	C(6)	110.6(5)	C(2)	C(3)	C(14)	114.3(5)
C(4)	C(3)	C(6)	110.6(6)	C(4)	C(3)	C(14)	111.4(6)
C(6)	C(3)	C(14)	111.7(5)	Ir(1)	C(4)	C(3)	98.2(4)
Ir(1)	C(4)	C(5)	71.3(4)	C(3)	C(4)	C(5)	117.0(6)
Ir(1)	C(5)	C(4)	69.4(4)	C(3)	C(6)	C(7)	115.0(6)
C(6)	C(7)	C(8)	117.1(7)	C(7)	C(8)	C(9)	121.0(8)
C(7)	C(8)	C(13)	122.3(8)	C(9)	C(8)	C(13)	116.7(8)
C(8)	C(9)	C(10)	123.1(9)	C(9)	C(10)	C(11)	118.4(9)
C(10)	C(11)	C(12)	120(1)	C(11)	C(12)	C(13)	119.8(9)
C(8)	C(13)	C(12)	121.6(8)	C(3)	C(14)	C(15)	115.1(6)
C(14)	C(15)	C(16)	112.4(6)	C(15)	C(16)	C(17)	121.6(8)
C(15)	C(16)	C(21)	121.9(8)	C(17)	C(16)	C(21)	116.5(7)
C(16)	C(17)	C(18)	123.2(9)	C(17)	C(18)	C(19)	119(1)
C(18)	C(19)	C(20)	120.4(9)	C(19)	C(20)	C(21)	119.6(8)
C(16)	C(21)	C(20)	121.7(8)	P(1)	C(22)	C(23)	117.0(5)
P(1)	C(22)	C(27)	125.2(5)	C(23)	C(22)	C(27)	117.3(6)
C(22)	C(23)	C(24)	121.4(7)	C(23)	C(24)	C(25)	120.6(8)
C(24)	C(25)	C(26)	119.0(7)	C(25)	C(26)	C(27)	120.1(8)
C(22)	C(27)	C(26)	121.6(7)	P(1)	C(28)	C(29)	122.8(5)
P(1)	C(28)	C(33)	120.2(5)	C(29)	C(28)	C(33)	116.9(6)
C(28)	C(29)	C(30)	121.8(7)	C(29)	C(30)	C(31)	120.4(7)
C(30)	C(31)	C(32)	119.0(7)	C(31)	C(32)	C(33)	121.6(7)
C(28)	C(33)	C(32)	120.3(7)	P(1)	C(34)	C(35)	121.6(5)
P(1)	C(34)	C(39)	120.0(5)	C(35)	C(34)	C(39)	118.0(6)
C(34)	C(35)	C(36)	121.2(7)	C(35)	C(36)	C(37)	119.4(7)
C(36)	C(37)	C(38)	120.9(7)	C(37)	C(38)	C(39)	119.4(7)
C(34)	C(39)	C(38)	121.0(7)	P(2)	C(40)	C(41)	117.5(5)
P(2)	C(40)	C(45)	124.3(5)	C(41)	C(40)	C(45)	118.2(6)
C(40)	C(41)	C(42)	120.3(6)	C(41)	C(42)	C(43)	120.6(6)
C(42)	C(43)	C(44)	119.3(6)	C(43)	C(44)	C(45)	121.3(7)
C(40)	C(45)	C(44)	120.2(6)	P(2)	C(46)	C(47)	121.5(6)
P(2)	C(46)	C(51)	119.8(5)	C(47)	C(46)	C(51)	118.7(7)
C(46)	C(47)	C(48)	119.4(8)	C(47)	C(48)	C(49)	122.6(8)
C(48)	C(49)	C(50)	118.0(8)	C(49)	C(50)	C(51)	120.7(8)
C(46)	C(51)	C(50)	120.7(7)	P(2)	C(52)	C(53)	118.4(5)
P(2)	C(52)	C(57)	123.5(5)	C(53)	C(52)	C(57)	118.1(6)
C(52)	C(53)	C(54)	120.8(7)	C(53)	C(54)	C(55)	120.0(7)
C(54)	C(55)	C(56)	120.4(7)	C(55)	C(56)	C(57)	119.5(7)

C(52) C(57) C(56) 121.2(7)

*Crystallographic Data and Details of Structure Refinement of **7***

Experimental

Data Collection

A yellow prismatic crystal of $C_{57}H_{53}OP_2Rh$ having approximate dimensions of 0.50 x 0.50 x 0.25 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC5R diffractometer with graphite monochromated Mo-Kα radiation and a rotating anode generator.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 20 carefully centered reflections in the range $6.76 < 2\theta < 13.67^o$ corresponded to a primitive triclinic cell with dimensions:

a = 12.275(3) Å α = 102.78(2)^o
b = 21.191(6) Å β = 113.40(2)^o
c = 10.029(3) Å γ = 91.96(3)^o
V = 2313(1) Å^3

For Z = 2 and F.W. = 918.90, the calculated density is 1.32 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P-1 (No. 2)

The data were collected at a temperature of 23 $\pm$ 1^{o}C using the ω-2θ scan technique to a maximum 2θ value of 50.0^o. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.27^o with a take-off angle of 6.0^o. Scans of $(0.79 + 0.30 \tan \theta)^o$ were made at speeds ranging from 8.0 to 4.0^o/min (in ω). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 3 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm, the crystal to detector distance was 258 mm, and the detector aperture was 6.0 x 6.0 mm (horizontal x vertical).

Data Reduction

Of the 8654 reflections which were collected, 8145 were unique (R_{int} = 0.096); equivalent reflections were merged. The intensities of three representative reflections were measured after every 150 reflections. No decay correction was applied.

The linear absorption coefficient, μ, for Mo-Kα radiation is 4.8 cm^{-1}. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.93 to 1.00. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by heavy-atom Patterson methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[3] on F was based on 3086 observed reflections ($I > 3.00\sigma(I)$) and 550 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.051$$

$$R_W = [\, \Sigma \, w \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, w \, Fo^2]^{1/2} = 0.052$$

The standard deviation of an observation of unit weight[4] was 1.20. The weighting scheme was based on counting statistics and included a factor (p = 0.029) to downweight the intense reflections. Plots of $\Sigma \, w \, (|Fo| - |Fc|)^2$ versus |Fo|, reflection order in data collection, $\sin\theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.42 and -0.36 e$^-$/Å^3, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) PATTY: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(2) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized:

$\Sigma w(|F_o|-|F_c|)^2$ where

$w = 1/[\sigma^2(Fo)] = [\sigma^2_c(Fo) + p^2Fo^2/4]^{-1}$

$\sigma_c(Fo)$ = e.s.d. based on counting statistics

p = p-factor

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations

N_v = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) teXsan for Windows: Crystal Structure Analysis Package, Molecular Structure Corporation (1997).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{57}H_{53}OP_2Rh$
Formula Weight	918.90
Crystal Color, Habit	yellow, prismatic
Crystal Dimensions	0.50 X 0.50 X 0.25 mm
Crystal System	triclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	20 (6.8 - 13.7°)
Omega Scan Peak Width at Half-height	0.27°
Lattice Parameters	a = 12.275(3) Å b = 21.191(6) Å c = 10.029(3) Å α = 102.78(2) ° β = 113.40(2) ° γ = 91.96(3) ° V = 2313(1) Å^3
Space Group	P-1 (No. 2)
Z value	2
D_{calc}	1.319 g/cm^3
F_{000}	956.00
μ(MoKα)	4.77 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC5R
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Attenuator	Zr foil (factors = 1.00, 3.64, 12.10, 44.80)
Take-off Angle	6.0^o
Detector Aperture	6.0 mm horizontal 6.0 mm vertical
Crystal to Detector Distance	258 mm
Voltage, Current	50 kV, 180 mA
Temperature	23.0^{o}C
Scan Type	ω-2θ
Scan Rate	8.0 - 4.0^o/min (in ω) (up to 3 scans)
Scan Width	(0.79 + 0.30 tan θ)^o
$2\theta_{max}$	50.0^o
No. of Reflections Measured	Total: 8654 Unique: 8145 (R_{int} = 0.096)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.9336 - 0.9993)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF92 PATTY)
Refinement	Full-matrix least-squares on F
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	$1/\sigma^2(Fo) = 4Fo^2/\sigma^2(Fo^2)$
p-factor	0.0290
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	3086
No. Variables	550
Reflection/Parameter Ratio	5.61
Residuals: R; Rw	0.051 ; 0.052
Goodness of Fit Indicator	1.20
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.42 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.36 e$^-$/Å^3

Table S5. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Rh(1)	0.02000(7)	0.17399(4)	0.29879(9)	3.12(2)
P(1)	-0.1580(2)	0.1347(1)	0.3023(3)	3.42(7)
P(2)	0.2122(2)	0.1989(1)	0.3209(3)	3.10(7)
O(1)	-0.0467(6)	0.0935(4)	-0.0119(8)	6.9(2)
C(1)	-0.0216(9)	0.1188(5)	0.106(1)	4.8(3)
C(2)	0.0603(7)	0.2436(5)	0.5014(9)	3.1(2)
C(3)	0.0479(8)	0.3053(5)	0.538(1)	4.4(3)
C(4)	-0.0037(8)	0.3519(5)	0.438(1)	4.6(3)
C(5)	0.0984(9)	0.3875(5)	0.421(1)	5.9(3)
C(6)	-0.0540(9)	0.4044(5)	0.521(1)	5.1(3)
C(7)	-0.153(1)	0.3817(5)	0.562(1)	6.0(3)
C(8)	-0.0977(9)	0.3140(5)	0.286(1)	5.4(3)
C(9)	-0.155(1)	0.3504(6)	0.159(1)	6.4(4)
C(10)	-0.189(1)	0.4336(6)	0.654(1)	5.4(4)

C(11)	-0.140(1)	0.4450(9)	0.805(2)	11.7(6)
C(12)	-0.170(2)	0.498(1)	0.889(2)	15.8(9)
C(13)	-0.250(2)	0.536(1)	0.832(3)	11.5(7)
C(14)	-0.302(1)	0.5209(8)	0.683(2)	9.6(6)
C(15)	-0.274(1)	0.4706(7)	0.593(1)	7.0(4)
C(16)	-0.255(1)	0.3877(7)	0.168(1)	5.9(4)
C(17)	-0.243(1)	0.4554(7)	0.182(1)	8.0(4)
C(18)	-0.338(2)	0.4890(8)	0.179(2)	9.7(5)
C(19)	-0.444(1)	0.4593(9)	0.165(2)	9.9(5)
C(20)	-0.453(1)	0.3924(8)	0.156(2)	8.9(5)
C(21)	-0.362(1)	0.3583(6)	0.152(1)	6.3(3)
C(22)	-0.2038(8)	0.1780(5)	0.445(1)	3.6(2)
C(23)	-0.1365(8)	0.1786(5)	0.596(1)	5.2(3)
C(24)	-0.168(1)	0.2121(7)	0.711(1)	6.8(4)
C(25)	-0.260(1)	0.2458(7)	0.678(2)	6.9(4)
C(26)	-0.326(1)	0.2474(5)	0.533(2)	5.9(3)
C(27)	-0.2977(9)	0.2131(5)	0.418(1)	4.5(3)
C(28)	-0.2937(7)	0.1284(4)	0.131(1)	3.3(2)
C(29)	-0.2915(8)	0.1631(5)	0.030(1)	4.0(3)
C(30)	-0.395(1)	0.1603(5)	-0.099(1)	5.0(3)
C(31)	-0.5007(9)	0.1248(6)	-0.128(1)	5.1(3)
C(32)	-0.5031(8)	0.0913(5)	-0.027(1)	4.9(3)
C(33)	-0.4040(8)	0.0926(5)	0.100(1)	4.2(3)
C(34)	-0.1620(7)	0.0498(5)	0.320(1)	3.9(3)
C(35)	-0.2023(9)	0.0285(5)	0.413(1)	5.5(3)
C(36)	-0.198(1)	-0.0356(7)	0.421(1)	6.4(4)
C(37)	-0.160(1)	-0.0787(6)	0.338(2)	6.0(4)
C(38)	-0.122(1)	-0.0593(7)	0.241(2)	7.6(4)
C(39)	-0.123(1)	0.0059(6)	0.236(1)	6.1(4)
C(40)	0.2990(8)	0.1300(5)	0.330(1)	3.3(2)
C(41)	0.2480(9)	0.0687(6)	0.237(1)	5.8(3)
C(42)	0.312(1)	0.0182(6)	0.235(1)	7.0(4)
C(43)	0.430(1)	0.0244(6)	0.328(1)	5.9(4)
C(44)	0.4821(9)	0.0848(6)	0.423(1)	5.8(3)
C(45)	0.4185(8)	0.1353(5)	0.424(1)	4.4(3)
C(46)	0.2173(7)	0.2245(4)	0.1595(9)	2.9(2)
C(47)	0.3104(9)	0.2127(5)	0.114(1)	4.8(3)
C(48)	0.316(1)	0.2372(6)	0.001(1)	6.1(4)
C(49)	0.230(1)	0.2713(6)	-0.071(1)	5.4(3)
C(50)	0.1379(9)	0.2822(6)	-0.030(1)	5.5(3)
C(51)	0.1317(8)	0.2582(5)	0.084(1)	4.8(3)
C(52)	0.3185(7)	0.2629(4)	0.480(1)	3.1(2)
C(53)	0.3506(8)	0.2550(5)	0.623(1)	4.3(3)
C(54)	0.4337(9)	0.3003(6)	0.748(1)	5.1(3)
C(55)	0.4875(9)	0.3538(6)	0.729(1)	5.6(3)
C(56)	0.4550(9)	0.3641(5)	0.589(1)	4.9(3)
C(57)	0.3725(8)	0.3170(5)	0.465(1)	4.0(3)
H(1)	0.0957	0.2265	0.5866	3.761
H(2)	0.0755	0.3243	0.6423	5.291
H(3)	0.0687	0.4197	0.3679	7.031
H(4)	0.1594	0.4080	0.5174	7.031
H(5)	0.1305	0.3571	0.3665	7.031

H(6)	0.0108	0.4277	0.6112	6.073
H(7)	-0.0848	0.4332	0.4580	6.073
H(8)	-0.1260	0.3497	0.6160	7.168
H(9)	-0.2217	0.3626	0.4712	7.168
H(10)	-0.1614	0.2957	0.3027	6.421
H(11)	-0.0615	0.2799	0.2476	6.421
H(12)	-0.0938	0.3803	0.1631	7.728
H(13)	-0.1864	0.3187	0.0648	7.728
H(14)	-0.0858	0.4178	0.8534	14.081
H(15)	-0.1308	0.5070	0.9956	18.919
H(16)	-0.2675	0.5719	0.8931	13.833
H(17)	-0.3628	0.5455	0.6358	11.481
H(18)	-0.3147	0.4620	0.4870	8.426
H(19)	-0.1706	0.4779	0.1936	9.633
H(20)	-0.3299	0.5345	0.1868	11.598
H(21)	-0.5083	0.4832	0.1621	11.882
H(22)	-0.5238	0.3707	0.1532	10.632
H(23)	-0.3733	0.3123	0.1379	7.520
H(24)	-0.0687	0.1559	0.6211	6.225
H(25)	-0.1230	0.2106	0.8121	8.131
H(26)	-0.2795	0.2691	0.7555	8.261
H(27)	-0.3913	0.2719	0.5102	7.099
H(28)	-0.3456	0.2141	0.3179	5.448
H(29)	-0.2195	0.1887	0.0480	4.810
H(30)	-0.3922	0.1836	-0.1690	5.949
H(31)	-0.5708	0.1235	-0.2157	6.180
H(32)	-0.5760	0.0664	-0.0464	5.829
H(33)	-0.4092	0.0693	0.1689	4.994
H(34)	-0.2331	0.0575	0.4719	6.543
H(35)	-0.2235	-0.0494	0.4888	7.686
H(36)	-0.1597	-0.1226	0.3454	7.203
H(37)	-0.0947	-0.0894	0.1797	9.138
H(38)	-0.0946	0.0199	0.1699	7.327
H(39)	0.1651	0.0618	0.1714	6.916
H(40)	0.2731	-0.0229	0.1666	8.368
H(41)	0.4743	-0.0114	0.3267	7.045
H(42)	0.5645	0.0911	0.4904	6.926
H(43)	0.4577	0.1763	0.4924	5.328
H(44)	0.3698	0.1877	0.1618	5.762
H(45)	0.3807	0.2303	-0.0273	7.364
H(46)	0.2336	0.2875	-0.1505	6.435
H(47)	0.0778	0.3063	-0.0805	6.626
H(48)	0.0662	0.2655	0.1109	5.802
H(49)	0.3150	0.2177	0.6366	5.151
H(50)	0.4536	0.2947	0.8457	6.141
H(51)	0.5477	0.3837	0.8139	6.744
H(52)	0.4878	0.4026	0.5773	5.897
H(53)	0.3534	0.3227	0.3669	4.744

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S6. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rh(1)	0.0293(4)	0.0473(6)	0.0413(5)	-0.0015(4)	0.0170(4)	0.0070(4)
P(1)	0.032(1)	0.052(2)	0.048(2)	0.006(1)	0.018(1)	0.016(1)
P(2)	0.035(1)	0.048(2)	0.039(2)	0.005(1)	0.019(1)	0.014(1)
O(1)	0.067(5)	0.112(8)	0.065(6)	-0.015(5)	0.034(5)	-0.024(5)
C(1)	0.048(7)	0.051(8)	0.087(9)	-0.007(5)	0.043(7)	-0.005(7)
C(2)	0.039(5)	0.050(7)	0.038(6)	0.013(5)	0.023(5)	0.014(5)
C(3)	0.042(6)	0.068(8)	0.048(6)	0.012(6)	0.014(5)	0.004(6)
C(4)	0.049(6)	0.062(8)	0.067(8)	0.012(6)	0.027(6)	0.015(6)
C(5)	0.062(7)	0.087(9)	0.087(8)	0.013(6)	0.041(7)	0.028(7)
C(6)	0.067(7)	0.065(8)	0.059(7)	0.004(6)	0.027(6)	0.011(6)
C(7)	0.072(8)	0.069(9)	0.098(9)	0.018(6)	0.052(7)	0.014(7)
C(8)	0.066(7)	0.078(9)	0.054(7)	-0.002(6)	0.027(6)	0.006(6)
C(9)	0.078(8)	0.078(9)	0.09(1)	0.016(7)	0.033(7)	0.031(8)
C(10)	0.076(8)	0.062(9)	0.09(1)	0.026(7)	0.052(8)	0.022(8)
C(11)	0.16(2)	0.20(2)	0.09(1)	0.09(1)	0.06(1)	0.03(1)
C(12)	0.21(2)	0.25(3)	0.13(2)	0.10(2)	0.09(2)	-0.01(2)
C(13)	0.17(2)	0.15(2)	0.15(2)	0.03(1)	0.12(2)	-0.02(1)
C(14)	0.15(2)	0.09(1)	0.17(2)	0.03(1)	0.11(1)	0.03(1)
C(15)	0.10(1)	0.07(1)	0.11(1)	0.012(8)	0.068(9)	0.010(9)
C(16)	0.08(1)	0.07(1)	0.063(8)	0.026(8)	0.022(7)	0.025(7)
C(17)	0.09(1)	0.09(1)	0.09(1)	0.018(9)	-0.006(8)	0.049(9)
C(18)	0.10(1)	0.11(1)	0.12(1)	0.06(1)	-0.00(1)	0.03(1)
C(19)	0.09(1)	0.14(2)	0.09(1)	0.08(1)	-0.01(1)	0.01(1)
C(20)	0.066(9)	0.13(1)	0.11(1)	0.05(1)	0.023(8)	-0.01(1)
C(21)	0.078(9)	0.066(9)	0.061(8)	-0.001(7)	0.006(7)	-0.003(6)
C(22)	0.033(5)	0.056(7)	0.053(6)	0.001(5)	0.026(5)	0.008(5)
C(23)	0.039(6)	0.089(9)	0.066(8)	0.003(6)	0.018(6)	0.020(7)
C(24)	0.078(9)	0.12(1)	0.059(8)	-0.015(8)	0.035(7)	0.006(8)
C(25)	0.09(1)	0.09(1)	0.10(1)	-0.008(8)	0.063(9)	0.006(9)
C(26)	0.061(8)	0.046(8)	0.12(1)	0.001(6)	0.055(8)	0.002(8)
C(27)	0.059(7)	0.048(7)	0.066(7)	0.001(6)	0.036(6)	-0.002(6)
C(28)	0.037(5)	0.045(6)	0.047(6)	0.007(4)	0.022(5)	0.012(5)
C(29)	0.040(6)	0.050(7)	0.054(7)	0.002(5)	0.020(5)	-0.002(6)
C(30)	0.066(8)	0.073(8)	0.064(7)	0.023(6)	0.031(6)	0.037(6)
C(31)	0.050(7)	0.076(9)	0.057(7)	0.006(6)	0.012(6)	0.013(6)
C(32)	0.024(5)	0.065(8)	0.076(8)	-0.002(5)	0.011(5)	-0.000(6)
C(33)	0.045(6)	0.059(7)	0.056(7)	0.008(5)	0.022(5)	0.015(6)
C(34)	0.029(5)	0.058(7)	0.057(7)	0.002(5)	0.014(5)	0.015(6)
C(35)	0.080(8)	0.060(8)	0.083(8)	0.005(6)	0.046(7)	0.026(7)
C(36)	0.094(9)	0.07(1)	0.10(1)	0.003(8)	0.045(8)	0.046(8)
C(37)	0.061(8)	0.051(9)	0.10(1)	0.002(6)	0.010(7)	0.034(8)
C(38)	0.11(1)	0.07(1)	0.14(1)	0.025(8)	0.07(1)	0.030(9)
C(39)	0.097(9)	0.066(9)	0.10(1)	0.019(7)	0.065(8)	0.032(8)
C(40)	0.043(6)	0.048(7)	0.047(6)	0.009(5)	0.026(5)	0.019(5)
C(41)	0.058(7)	0.066(9)	0.071(8)	0.014(7)	0.011(6)	0.002(7)
C(42)	0.09(1)	0.061(9)	0.09(1)	0.025(8)	0.025(8)	-0.015(7)
C(43)	0.10(1)	0.054(9)	0.082(9)	0.037(8)	0.048(8)	0.022(7)
C(44)	0.060(7)	0.068(9)	0.10(1)	0.029(7)	0.033(7)	0.032(8)
C(45)	0.035(6)	0.049(7)	0.089(8)	0.006(5)	0.027(6)	0.022(6)
C(46)	0.038(5)	0.033(6)	0.043(6)	0.002(4)	0.022(5)	0.005(5)
C(47)	0.073(7)	0.059(7)	0.072(8)	0.023(6)	0.050(6)	0.019(6)

C(48)	0.098(9)	0.10(1)	0.079(9)	0.017(8)	0.071(8)	0.033(8)
C(49)	0.079(8)	0.084(9)	0.049(7)	0.011(7)	0.028(6)	0.031(6)
C(50)	0.061(7)	0.089(9)	0.063(8)	0.003(6)	0.018(6)	0.042(7)
C(51)	0.049(6)	0.087(9)	0.060(7)	0.012(6)	0.028(6)	0.029(7)
C(52)	0.028(5)	0.037(6)	0.052(6)	0.014(4)	0.016(4)	0.010(5)
C(53)	0.047(6)	0.076(8)	0.039(6)	0.002(5)	0.017(5)	0.016(6)
C(54)	0.055(7)	0.09(1)	0.043(6)	-0.008(6)	0.021(5)	0.014(6)
C(55)	0.044(6)	0.084(9)	0.057(8)	-0.007(6)	0.003(6)	-0.002(7)
C(56)	0.067(7)	0.036(7)	0.074(8)	-0.012(5)	0.027(6)	0.003(6)
C(57)	0.052(6)	0.056(7)	0.044(6)	0.011(5)	0.020(5)	0.014(5)

The general temperature factor expression:

$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S7. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Rh(1)	P(1)	2.328(3)	Rh(1)	P(2)	2.311(3)
Rh(1)	C(1)	1.88(1)	Rh(1)	C(2)	2.09(1)
P(1)	C(22)	1.82(1)	P(1)	C(28)	1.831(9)
P(1)	C(34)	1.85(1)	P(2)	C(40)	1.84(1)
P(2)	C(46)	1.839(9)	P(2)	C(52)	1.832(9)
O(1)	C(1)	1.10(1)	C(2)	C(3)	1.31(1)
C(3)	C(4)	1.53(1)	C(4)	C(5)	1.53(1)
C(4)	C(6)	1.53(1)	C(4)	C(8)	1.52(1)
C(6)	C(7)	1.53(1)	C(7)	C(10)	1.47(1)
C(8)	C(9)	1.57(2)	C(9)	C(16)	1.50(2)
C(10)	C(11)	1.35(2)	C(10)	C(15)	1.35(2)
C(11)	C(12)	1.40(2)	C(12)	C(13)	1.32(3)
C(13)	C(14)	1.33(2)	C(14)	C(15)	1.39(2)
C(16)	C(17)	1.41(2)	C(16)	C(21)	1.37(2)
C(17)	C(18)	1.38(2)	C(18)	C(19)	1.36(2)
C(19)	C(20)	1.40(2)	C(20)	C(21)	1.36(2)
C(22)	C(23)	1.40(1)	C(22)	C(27)	1.36(1)
C(23)	C(24)	1.41(2)	C(24)	C(25)	1.32(2)
C(25)	C(26)	1.36(2)	C(26)	C(27)	1.39(1)
C(28)	C(29)	1.39(1)	C(28)	C(33)	1.41(1)
C(29)	C(30)	1.40(1)	C(30)	C(31)	1.37(1)
C(31)	C(32)	1.36(1)	C(32)	C(33)	1.36(1)
C(34)	C(35)	1.36(1)	C(34)	C(39)	1.35(1)
C(35)	C(36)	1.38(2)	C(36)	C(37)	1.32(2)
C(37)	C(38)	1.36(2)	C(38)	C(39)	1.40(2)
C(40)	C(41)	1.38(1)	C(40)	C(45)	1.38(1)
C(41)	C(42)	1.35(2)	C(42)	C(43)	1.36(2)
C(43)	C(44)	1.37(1)	C(44)	C(45)	1.35(1)
C(46)	C(47)	1.40(1)	C(46)	C(51)	1.36(1)
C(47)	C(48)	1.37(1)	C(48)	C(49)	1.36(2)
C(49)	C(50)	1.35(1)	C(50)	C(51)	1.38(1)
C(52)	C(53)	1.38(1)	C(52)	C(57)	1.37(1)
C(53)	C(54)	1.38(1)	C(54)	C(55)	1.38(1)
C(55)	C(56)	1.37(1)	C(56)	C(57)	1.40(1)

Table S8. Bond Angles(^{o})

atom	atom	atom	angle	atom	atom	atom	angle

P(1)	Rh(1)	P(2)	169.2(1)	P(1)	Rh(1)	C(1)	91.3(3)
P(1)	Rh(1)	C(2)	89.9(3)	P(2)	Rh(1)	C(1)	90.1(3)
P(2)	Rh(1)	C(2)	89.8(3)	C(1)	Rh(1)	C(2)	173.7(5)
Rh(1)	P(1)	C(22)	119.4(3)	Rh(1)	P(1)	C(28)	115.7(3)
Rh(1)	P(1)	C(34)	113.0(3)	C(22)	P(1)	C(28)	101.2(5)
C(22)	P(1)	C(34)	103.7(5)	C(28)	P(1)	C(34)	101.7(4)
Rh(1)	P(2)	C(40)	114.3(3)	Rh(1)	P(2)	C(46)	113.6(3)
Rh(1)	P(2)	C(52)	120.6(3)	C(40)	P(2)	C(46)	102.6(4)
C(40)	P(2)	C(52)	101.4(4)	C(46)	P(2)	C(52)	102.0(4)
Rh(1)	C(1)	O(1)	171(1)	Rh(1)	C(2)	C(3)	134.6(8)
C(2)	C(3)	C(4)	130(1)	C(3)	C(4)	C(5)	108.8(9)
C(3)	C(4)	C(6)	108.5(9)	C(3)	C(4)	C(8)	110.1(9)
C(5)	C(4)	C(6)	106.3(9)	C(5)	C(4)	C(8)	110.5(9)
C(6)	C(4)	C(8)	112.5(9)	C(4)	C(6)	C(7)	117(1)
C(6)	C(7)	C(10)	115(1)	C(4)	C(8)	C(9)	120(1)
C(8)	C(9)	C(16)	116(1)	C(7)	C(10)	C(11)	120(1)
C(7)	C(10)	C(15)	123(1)	C(11)	C(10)	C(15)	117(1)
C(10)	C(11)	C(12)	119(2)	C(11)	C(12)	C(13)	125(2)
C(12)	C(13)	C(14)	114(2)	C(13)	C(14)	C(15)	123(2)
C(10)	C(15)	C(14)	121(2)	C(9)	C(16)	C(17)	120(1)
C(9)	C(16)	C(21)	123(1)	C(17)	C(16)	C(21)	117(1)
C(16)	C(17)	C(18)	120(2)	C(17)	C(18)	C(19)	122(2)
C(18)	C(19)	C(20)	118(2)	C(19)	C(20)	C(21)	120(2)
C(16)	C(21)	C(20)	123(1)	P(1)	C(22)	C(23)	119.2(8)
P(1)	C(22)	C(27)	124.7(8)	C(23)	C(22)	C(27)	116.1(9)
C(22)	C(23)	C(24)	121(1)	C(23)	C(24)	C(25)	120(1)
C(24)	C(25)	C(26)	121(1)	C(25)	C(26)	C(27)	120(1)
C(22)	C(27)	C(26)	122(1)	P(1)	C(28)	C(29)	119.2(7)
P(1)	C(28)	C(33)	123.0(8)	C(29)	C(28)	C(33)	117.7(9)
C(28)	C(29)	C(30)	120.0(9)	C(29)	C(30)	C(31)	121(1)
C(30)	C(31)	C(32)	119(1)	C(31)	C(32)	C(33)	122(1)
C(28)	C(33)	C(32)	120(1)	P(1)	C(34)	C(35)	124.3(9)
P(1)	C(34)	C(39)	118.1(9)	C(35)	C(34)	C(39)	118(1)
C(34)	C(35)	C(36)	119(1)	C(35)	C(36)	C(37)	123(1)
C(36)	C(37)	C(38)	119(1)	C(37)	C(38)	C(39)	118(1)
C(34)	C(39)	C(38)	122(1)	P(2)	C(40)	C(41)	121.0(8)
P(2)	C(40)	C(45)	123.7(8)	C(41)	C(40)	C(45)	115(1)
C(40)	C(41)	C(42)	122(1)	C(41)	C(42)	C(43)	122(1)
C(42)	C(43)	C(44)	117(1)	C(43)	C(44)	C(45)	121(1)
C(40)	C(45)	C(44)	123(1)	P(2)	C(46)	C(47)	122.0(8)
P(2)	C(46)	C(51)	120.1(7)	C(47)	C(46)	C(51)	117.9(9)
C(46)	C(47)	C(48)	120(1)	C(47)	C(48)	C(49)	121(1)
C(48)	C(49)	C(50)	120(1)	C(49)	C(50)	C(51)	120(1)
C(46)	C(51)	C(50)	121(1)	P(2)	C(52)	C(53)	118.3(8)
P(2)	C(52)	C(57)	123.7(8)	C(53)	C(52)	C(57)	117.9(9)
C(52)	C(53)	C(54)	121(1)	C(53)	C(54)	C(55)	120(1)
C(54)	C(55)	C(56)	121(1)	C(55)	C(56)	C(57)	119(1)
C(52)	C(57)	C(56)	121.7(9)				

*Crystallographic Data and Details of Structure Refinement of **8***

Experimental

Data Collection

A pale yellow prismatic crystal of $C_{57}H_{53}OP_2Ir$ having approximate dimensions of 0.30 x 0.30 x 0.20 mm was mounted in a glass capillary. All measurements were made on a Rigaku AFC5R diffractometer with graphite monochromated Mo-Kα radiation and a rotating anode generator.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 20 carefully centered reflections in the range $6.88 < 2\theta < 9.52^o$ corresponded to a primitive monoclinic cell with dimensions:

a = 10.837(5) Å
b = 24.909(4) Å $\beta = 103.76(3)^o$
c = 18.244(5) Å
V = 4783(2) $Å^3$

For Z = 4 and F.W. = 1008.21, the calculated density is 1.40 g/cm^3. The systematic absences of:

h0l: l ± 2n
0k0: k ± 2n

uniquely determine the space group to be:

$P2_1/c$ (No. 14)

The data were collected at a temperature of 23 ± 1°C using the ω-2θ scan technique to a maximum 2θ value of 55.0^o. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.31^o with a take-off angle of 6.0^o. Scans of $(0.79 + 0.30 \tan \theta)^o$ were made at a speed of 16.0^o/min (in ω). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 5 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm, the crystal to detector distance was 250 mm, and the detector aperture was 6.0 x 6.0 mm (horizontal x vertical).

Data Reduction

Of the 11824 reflections which were collected, 11248 were unique ($R_{int} = 0.068$); equivalent reflections were merged. The intensities of three representative reflections were measured after every 150 reflections. No decay correction was applied.

The linear absorption coefficient, μ, for Mo-Kα radiation is 29.0 cm^{-1}. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.85 to 1.00. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[3] on F was based on 4680 observed reflections ($I > 3.00\sigma(I)$) and 550 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.043$$

$$R_w = [\, \Sigma \, w \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, w \, Fo^2]^{1/2} = 0.039$$

The standard deviation of an observation of unit weight[4] was 1.33. The weighting scheme was based on counting statistics and included a factor (p = 0.010) to downweight the intense reflections. Plots of $\Sigma \, w \, (|Fo| - |Fc|)^2$ versus |Fo|, reflection order in data collection, $\sin\theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.89 and -0.91 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

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Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.
(2) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.
(3) Least Squares function minimized:

$\Sigma w(|F_o|-|F_c|)^2$ where

$w = 1/[\sigma^2(Fo)] = [\sigma^2_c(Fo) + p^2Fo^2/4]^{-1}$

$\sigma_c(Fo)$ = e.s.d. based on counting statistics

p = p-factor

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations

N_v = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).
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EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{57}H_{53}OP_2Ir$
Formula Weight	1008.21
Crystal Color, Habit	pale yellow, prismatic
Crystal Dimensions	0.30 X 0.30 X 0.20 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	20 (6.9 - 9.5°)
Omega Scan Peak Width at Half-height	0.31°
Lattice Parameters	a = 10.837(5) Å b = 24.909(4) Å c = 18.244(5) Å β = 103.76(3) ° V = 4783(2) Å^3
Space Group	$P2_1/c$ (No. 14)
Z value	4
D_{calc}	1.400 g/cm^3
F_{000}	2040.00
μ(MoKα)	29.04 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC5R
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Attenuator	Zr foil (factors = 1.00, 3.64, 12.10, 44.80)
Take-off Angle	6.0°

Detector Aperture	6.0 mm horizontal 6.0 mm vertical
Crystal to Detector Distance	250 mm
Voltage, Current	50kV, 180mA
Temperature	23.0°C
Scan Type	ω-2θ
Scan Rate	16.0°/min (in ω) (up to 5 scans)
Scan Width	$(0.79 + 0.30 \tan \theta)^{o}$
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 11824 Unique: 11248 (R_{int} = 0.068)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.8493 - 0.9997)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	$1/\sigma^2(Fo) = 4Fo^2/\sigma^2(Fo^2)$
p-factor	0.0100
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	4680
No. Variables	550
Reflection/Parameter Ratio	8.51
Residuals: R; Rw	0.043 ; 0.039
Goodness of Fit Indicator	1.33
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.89 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.91 $e^-/Å^3$

Table S9. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ir(1)	0.03085(3)	0.21569(1)	0.24651(2)	3.450(7)
P(1)	0.1543(2)	0.14025(9)	0.2569(1)	3.65(5)
P(2)	-0.0457(2)	0.30166(9)	0.2457(1)	3.71(5)
O(1)	-0.1267(7)	0.1681(3)	0.3462(4)	8.6(3)
C(1)	-0.0652(8)	0.1864(4)	0.3111(5)	4.8(2)
C(2)	0.1117(7)	0.2412(3)	0.1581(4)	3.6(2)
C(3)	0.2253(7)	0.2528(3)	0.1509(4)	3.6(2)
C(4)	0.2656(7)	0.2697(3)	0.0789(4)	4.0(2)
C(5)	0.1600(8)	0.2590(4)	0.0082(4)	5.5(3)
C(6)	0.3884(8)	0.2382(4)	0.0754(5)	5.0(2)
C(7)	0.3714(9)	0.1791(4)	0.0609(5)	5.6(3)
C(8)	0.4921(9)	0.1464(4)	0.0711(5)	4.8(3)
C(9)	0.487(1)	0.0934(5)	0.0535(7)	8.8(4)
C(10)	0.595(1)	0.0619(5)	0.0618(9)	12.7(5)
C(11)	0.712(1)	0.0839(6)	0.0916(8)	9.7(5)
C(12)	0.720(1)	0.1357(5)	0.1082(6)	6.9(3)
C(13)	0.610(1)	0.1677(4)	0.0966(6)	7.2(3)
C(14)	0.2958(8)	0.3297(4)	0.0828(5)	4.7(2)
C(15)	0.3913(9)	0.3506(4)	0.1516(5)	5.7(3)

C(16)	0.418(1)	0.4095(4)	0.1468(5)	5.6(3)
C(17)	0.512(1)	0.4270(5)	0.1127(7)	7.5(4)
C(18)	0.531(1)	0.4806(7)	0.1064(8)	9.5(5)
C(19)	0.460(2)	0.5173(6)	0.1336(9)	10.1(6)
C(20)	0.370(2)	0.5017(7)	0.1684(9)	11.2(6)
C(21)	0.348(1)	0.4475(6)	0.1748(7)	7.7(4)
C(22)	0.1363(8)	0.0915(3)	0.3286(5)	3.8(2)
C(23)	0.029(1)	0.0604(5)	0.3137(6)	7.7(4)
C(24)	0.011(1)	0.0228(6)	0.3663(8)	9.0(5)
C(25)	0.098(1)	0.0184(4)	0.4333(7)	8.0(4)
C(26)	0.202(1)	0.0507(5)	0.4507(6)	6.8(3)
C(27)	0.2205(9)	0.0866(4)	0.3973(6)	5.8(3)
C(28)	0.1479(8)	0.0961(4)	0.1761(5)	4.2(2)
C(29)	0.2058(9)	0.0467(4)	0.1842(5)	6.1(3)
C(30)	0.202(1)	0.0137(4)	0.1219(8)	7.7(4)
C(31)	0.140(1)	0.0302(6)	0.0515(7)	8.3(4)
C(32)	0.080(1)	0.0793(5)	0.0428(6)	6.8(3)
C(33)	0.0825(8)	0.1120(4)	0.1044(5)	4.9(2)
C(34)	0.3214(7)	0.1606(3)	0.2874(4)	3.6(2)
C(35)	0.4170(9)	0.1414(4)	0.2570(5)	4.9(2)
C(36)	0.5404(8)	0.1638(4)	0.2806(5)	5.6(3)
C(37)	0.5621(9)	0.2052(4)	0.3305(5)	5.9(3)
C(38)	0.4679(8)	0.2246(4)	0.3627(5)	5.2(2)
C(39)	0.3482(7)	0.2015(3)	0.3409(4)	4.0(2)
C(40)	0.0771(8)	0.3516(4)	0.2866(4)	4.2(2)
C(41)	0.2005(8)	0.3358(4)	0.3138(5)	4.7(2)
C(42)	0.2905(9)	0.3743(5)	0.3499(6)	6.8(3)
C(43)	0.256(1)	0.4251(5)	0.3557(6)	7.8(4)
C(44)	0.130(1)	0.4421(4)	0.3288(6)	7.4(4)
C(45)	0.0432(9)	0.4055(4)	0.2942(5)	6.1(3)
C(46)	-0.1195(7)	0.3266(3)	0.1509(4)	3.6(2)
C(47)	-0.0574(9)	0.3605(4)	0.1120(5)	5.6(3)
C(48)	-0.108(1)	0.3734(4)	0.0368(6)	7.1(3)
C(49)	-0.225(1)	0.3514(5)	0.0015(5)	6.3(3)
C(50)	-0.2862(9)	0.3171(5)	0.0390(5)	7.1(3)
C(51)	-0.2325(8)	0.3042(4)	0.1126(5)	5.8(3)
C(52)	-0.1601(7)	0.3168(4)	0.3026(4)	4.1(2)
C(53)	-0.2665(8)	0.3500(4)	0.2766(5)	5.1(3)
C(54)	-0.3425(9)	0.3639(4)	0.3260(6)	5.9(3)
C(55)	-0.3112(9)	0.3467(5)	0.4002(5)	6.1(3)
C(56)	-0.2049(9)	0.3156(4)	0.4256(5)	5.8(3)
C(57)	-0.1317(8)	0.3007(4)	0.3765(5)	5.2(3)
H(1)	0.0496	0.2453	0.1120	4.283
H(2)	0.2915	0.2506	0.1956	4.332
H(3)	0.0827	0.2519	0.0224	6.621
H(4)	0.1496	0.2897	-0.0237	6.621
H(5)	0.1821	0.2289	-0.0180	6.621
H(6)	0.4212	0.2533	0.0361	5.979
H(7)	0.4483	0.2429	0.1223	5.979
H(8)	0.3244	0.1653	0.0946	6.694
H(9)	0.3239	0.1745	0.0104	6.694
H(10)	0.4058	0.0772	0.0348	10.594

H(11)	0.5873	0.0253	0.0470	15.205
H(12)	0.7861	0.0622	0.1002	11.623
H(13)	0.8011	0.1514	0.1280	8.315
H(14)	0.6181	0.2051	0.1070	8.633
H(15)	0.3272	0.3384	0.0399	5.656
H(16)	0.2182	0.3483	0.0801	5.656
H(17)	0.3589	0.3444	0.1949	6.857
H(18)	0.4686	0.3315	0.1565	6.857
H(19)	0.5634	0.4018	0.0940	8.966
H(20)	0.5951	0.4927	0.0826	11.416
H(21)	0.4748	0.5545	0.1279	12.166
H(22)	0.3226	0.5275	0.1882	13.491
H(23)	0.2841	0.4362	0.1990	9.246
H(24)	-0.0332	0.0647	0.2675	9.184
H(25)	-0.0619	0.0002	0.3556	10.830
H(26)	0.0857	-0.0078	0.4687	9.568
H(27)	0.2596	0.0484	0.4987	8.168
H(28)	0.2941	0.1087	0.4083	6.928
H(29)	0.2494	0.0348	0.2330	7.285
H(30)	0.2424	-0.0203	0.1285	9.210
H(31)	0.1380	0.0080	0.0089	9.951
H(32)	0.0358	0.0908	-0.0061	8.151
H(33)	0.0395	0.1456	0.0977	5.829
H(34)	0.4006	0.1135	0.2205	5.934
H(35)	0.6080	0.1498	0.2614	6.717
H(36)	0.6441	0.2211	0.3435	7.119
H(37)	0.4845	0.2528	0.3987	6.240
H(38)	0.2826	0.2140	0.3631	4.825
H(39)	0.2253	0.2997	0.3086	5.591
H(40)	0.3762	0.3639	0.3700	8.126
H(41)	0.3180	0.4506	0.3789	9.357
H(42)	0.1065	0.4783	0.3345	8.911
H(43)	-0.0423	0.4164	0.2748	7.276
H(44)	0.0220	0.3755	0.1372	6.750
H(45)	-0.0644	0.3965	0.0102	8.483
H(46)	-0.2630	0.3604	-0.0495	7.599
H(47)	-0.3659	0.3022	0.0142	8.547
H(48)	-0.2742	0.2792	0.1378	7.010
H(49)	-0.2866	0.3628	0.2261	6.116
H(50)	-0.4162	0.3853	0.3084	7.109
H(51)	-0.3629	0.3564	0.4335	7.278
H(52)	-0.1818	0.3043	0.4768	6.990
H(53)	-0.0595	0.2785	0.3946	6.267

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S10. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	0.0358(1)	0.0524(2)	0.0445(2)	-0.0027(2)	0.0128(1)	-0.0006(2)
P(1)	0.042(1)	0.048(1)	0.050(1)	-0.003(1)	0.014(1)	-0.003(1)
P(2)	0.043(1)	0.054(1)	0.044(1)	-0.001(1)	0.008(1)	-0.003(1)
O(1)	0.109(6)	0.108(6)	0.143(7)	-0.003(5)	0.090(6)	0.039(5)

C(1)	0.048(5)	0.052(6)	0.083(7)	0.006(5)	0.018(5)	0.014(5)
C(2)	0.053(5)	0.045(5)	0.044(5)	-0.007(4)	0.023(4)	0.006(4)
C(3)	0.041(5)	0.058(6)	0.038(5)	-0.001(4)	0.008(4)	0.002(4)
C(4)	0.041(5)	0.065(7)	0.043(5)	-0.011(4)	0.006(4)	0.012(4)
C(5)	0.065(6)	0.115(9)	0.031(5)	-0.010(6)	0.014(4)	0.010(5)
C(6)	0.059(6)	0.079(7)	0.052(6)	-0.009(5)	0.016(5)	0.006(5)
C(7)	0.061(6)	0.085(8)	0.067(7)	-0.010(6)	0.017(5)	-0.012(6)
C(8)	0.057(6)	0.072(7)	0.053(6)	-0.010(5)	0.014(5)	-0.002(5)
C(9)	0.089(9)	0.066(9)	0.16(1)	-0.014(7)	-0.018(8)	-0.005(9)
C(10)	0.13(1)	0.08(1)	0.23(2)	0.03(1)	-0.04(1)	-0.00(1)
C(11)	0.12(1)	0.09(1)	0.13(1)	0.013(9)	-0.023(9)	0.01(1)
C(12)	0.074(8)	0.11(1)	0.082(8)	0.006(8)	0.030(6)	0.003(8)
C(13)	0.071(7)	0.095(9)	0.12(1)	-0.015(7)	0.043(7)	-0.030(7)
C(14)	0.055(6)	0.076(7)	0.045(5)	-0.013(5)	0.007(4)	0.005(5)
C(15)	0.069(7)	0.084(8)	0.059(6)	-0.012(6)	0.004(5)	0.004(6)
C(16)	0.066(7)	0.073(8)	0.065(7)	-0.010(6)	0.002(5)	-0.001(6)
C(17)	0.091(9)	0.078(9)	0.12(1)	-0.021(7)	0.032(8)	0.014(7)
C(18)	0.10(1)	0.13(1)	0.14(1)	-0.04(1)	0.035(9)	0.02(1)
C(19)	0.18(2)	0.06(1)	0.13(1)	-0.03(1)	0.01(1)	0.008(9)
C(20)	0.18(2)	0.10(1)	0.16(1)	0.01(1)	0.06(1)	-0.02(1)
C(21)	0.091(9)	0.10(1)	0.11(1)	-0.002(8)	0.030(7)	-0.004(9)
C(22)	0.053(5)	0.043(5)	0.053(5)	0.004(4)	0.022(4)	0.010(5)
C(23)	0.080(8)	0.10(1)	0.11(1)	-0.024(7)	0.023(7)	0.031(8)
C(24)	0.11(1)	0.11(1)	0.13(1)	-0.041(9)	0.037(9)	-0.00(1)
C(25)	0.15(1)	0.054(8)	0.13(1)	-0.019(8)	0.09(1)	0.026(8)
C(26)	0.12(1)	0.077(8)	0.070(7)	0.005(7)	0.042(7)	0.018(6)
C(27)	0.073(7)	0.066(7)	0.089(8)	0.006(6)	0.034(6)	0.014(6)
C(28)	0.049(5)	0.052(6)	0.057(6)	-0.009(4)	0.013(4)	-0.017(5)
C(29)	0.092(8)	0.061(8)	0.077(7)	0.002(6)	0.020(6)	-0.020(6)
C(30)	0.092(9)	0.073(8)	0.13(1)	-0.007(7)	0.032(8)	-0.042(9)
C(31)	0.086(9)	0.12(1)	0.11(1)	-0.039(8)	0.028(8)	-0.07(1)
C(32)	0.088(8)	0.10(1)	0.074(7)	-0.011(7)	0.019(6)	-0.035(7)
C(33)	0.048(5)	0.065(7)	0.073(7)	-0.011(5)	0.019(5)	-0.012(6)
C(34)	0.044(5)	0.049(6)	0.050(5)	0.016(4)	0.019(4)	0.010(4)
C(35)	0.055(5)	0.068(7)	0.066(6)	0.004(5)	0.015(5)	0.002(5)
C(36)	0.050(6)	0.092(9)	0.077(7)	0.007(6)	0.028(5)	0.018(6)
C(37)	0.057(6)	0.095(9)	0.067(6)	-0.008(6)	0.001(5)	0.005(6)
C(38)	0.054(5)	0.082(8)	0.058(6)	-0.009(6)	0.007(4)	-0.005(6)
C(39)	0.051(5)	0.058(7)	0.043(5)	-0.004(4)	0.010(4)	0.004(4)
C(40)	0.059(6)	0.067(7)	0.034(5)	-0.016(5)	0.010(4)	-0.013(5)
C(41)	0.049(5)	0.072(7)	0.050(6)	-0.013(5)	0.001(4)	-0.004(5)
C(42)	0.067(7)	0.10(1)	0.079(8)	-0.029(7)	0.000(6)	-0.005(7)
C(43)	0.11(1)	0.09(1)	0.083(9)	-0.045(9)	0.005(7)	-0.023(8)
C(44)	0.12(1)	0.069(8)	0.094(9)	-0.023(8)	0.022(8)	-0.033(7)
C(45)	0.085(8)	0.064(7)	0.079(7)	-0.014(6)	0.016(6)	-0.022(6)
C(46)	0.047(5)	0.047(5)	0.040(5)	-0.002(4)	0.009(4)	-0.004(4)
C(47)	0.076(7)	0.076(8)	0.057(6)	-0.012(6)	0.007(5)	0.006(6)
C(48)	0.13(1)	0.086(9)	0.055(7)	-0.010(8)	0.024(7)	0.013(6)
C(49)	0.087(8)	0.10(1)	0.045(6)	0.017(7)	0.008(6)	-0.005(6)
C(50)	0.078(8)	0.14(1)	0.048(6)	-0.022(7)	0.003(6)	-0.014(7)
C(51)	0.058(6)	0.110(9)	0.054(6)	-0.021(6)	0.014(5)	-0.013(6)
C(52)	0.038(5)	0.069(6)	0.048(5)	-0.000(4)	0.008(4)	-0.013(5)

C(53)	0.058(6)	0.083(7)	0.053(6)	0.012(5)	0.014(5)	-0.004(5)
C(54)	0.062(7)	0.085(8)	0.081(7)	0.020(6)	0.021(6)	-0.011(7)
C(55)	0.051(6)	0.12(1)	0.065(7)	0.000(6)	0.033(5)	-0.029(7)
C(56)	0.062(6)	0.109(9)	0.056(6)	-0.008(6)	0.026(5)	-0.004(6)
C(57)	0.052(5)	0.095(9)	0.053(6)	0.004(5)	0.014(5)	-0.003(5)

The general temperature factor expression:

$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S11. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Ir(1)	P(1)	2.288(3)	Ir(1)	P(2)	2.295(2)
Ir(1)	C(1)	1.89(1)	Ir(1)	C(2)	2.108(8)
P(1)	C(22)	1.829(9)	P(1)	C(28)	1.828(9)
P(1)	C(34)	1.836(9)	P(2)	C(40)	1.844(9)
P(2)	C(46)	1.833(9)	P(2)	C(52)	1.835(9)
O(1)	C(1)	1.12(1)	C(2)	C(3)	1.30(1)
C(3)	C(4)	1.54(1)	C(4)	C(5)	1.53(1)
C(4)	C(6)	1.56(1)	C(4)	C(14)	1.53(1)
C(6)	C(7)	1.50(1)	C(7)	C(8)	1.51(1)
C(8)	C(9)	1.36(1)	C(8)	C(13)	1.36(1)
C(9)	C(10)	1.39(2)	C(10)	C(11)	1.37(2)
C(11)	C(12)	1.32(2)	C(12)	C(13)	1.41(2)
C(14)	C(15)	1.52(1)	C(15)	C(16)	1.50(1)
C(16)	C(17)	1.39(1)	C(16)	C(21)	1.38(2)
C(17)	C(18)	1.36(2)	C(18)	C(19)	1.36(2)
C(19)	C(20)	1.34(2)	C(20)	C(21)	1.38(2)
C(22)	C(23)	1.37(1)	C(22)	C(27)	1.37(1)
C(23)	C(24)	1.39(2)	C(24)	C(25)	1.36(2)
C(25)	C(26)	1.36(2)	C(26)	C(27)	1.37(1)
C(28)	C(29)	1.37(1)	C(28)	C(33)	1.39(1)
C(29)	C(30)	1.39(1)	C(30)	C(31)	1.36(2)
C(31)	C(32)	1.38(2)	C(32)	C(33)	1.38(1)
C(34)	C(35)	1.37(1)	C(34)	C(39)	1.39(1)
C(35)	C(36)	1.42(1)	C(36)	C(37)	1.36(1)
C(37)	C(38)	1.38(1)	C(38)	C(39)	1.39(1)
C(40)	C(41)	1.37(1)	C(40)	C(45)	1.41(1)
C(41)	C(42)	1.41(1)	C(42)	C(43)	1.33(2)
C(43)	C(44)	1.40(2)	C(44)	C(45)	1.35(1)
C(46)	C(47)	1.38(1)	C(46)	C(51)	1.38(1)
C(47)	C(48)	1.39(1)	C(48)	C(49)	1.39(1)
C(49)	C(50)	1.36(1)	C(50)	C(51)	1.37(1)
C(52)	C(53)	1.41(1)	C(52)	C(57)	1.37(1)
C(53)	C(54)	1.40(1)	C(54)	C(55)	1.38(1)
C(55)	C(56)	1.38(1)	C(56)	C(57)	1.38(1)

Table S12. Bond Angles(^{o})

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	Ir(1)	P(2)	165.94(8)	P(1)	Ir(1)	C(1)	91.6(3)
P(1)	Ir(1)	C(2)	88.3(3)	P(2)	Ir(1)	C(1)	96.4(3)
P(2)	Ir(1)	C(2)	85.9(3)	C(1)	Ir(1)	C(2)	169.1(4)
Ir(1)	P(1)	C(22)	116.4(3)	Ir(1)	P(1)	C(28)	121.2(4)
Ir(1)	P(1)	C(34)	108.3(3)	C(22)	P(1)	C(28)	100.8(5)

C(22)	P(1)	C(34)	103.4(4)	C(28)	P(1)	C(34)	104.8(4)
Ir(1)	P(2)	C(40)	113.7(4)	Ir(1)	P(2)	C(46)	113.4(3)
Ir(1)	P(2)	C(52)	118.7(3)	C(40)	P(2)	C(46)	105.3(4)
C(40)	P(2)	C(52)	98.8(4)	C(46)	P(2)	C(52)	105.2(4)
Ir(1)	C(1)	O(1)	176(1)	Ir(1)	C(2)	C(3)	136.0(7)
C(2)	C(3)	C(4)	127.9(8)	C(3)	C(4)	C(5)	111.5(7)
C(3)	C(4)	C(6)	108.5(7)	C(3)	C(4)	C(14)	109.1(8)
C(5)	C(4)	C(6)	110.7(8)	C(5)	C(4)	C(14)	108.5(8)
C(6)	C(4)	C(14)	108.6(8)	C(4)	C(6)	C(7)	115.4(9)
C(6)	C(7)	C(8)	116(1)	C(7)	C(8)	C(9)	120(1)
C(7)	C(8)	C(13)	123(1)	C(9)	C(8)	C(13)	116(1)
C(8)	C(9)	C(10)	122(1)	C(9)	C(10)	C(11)	120(2)
C(10)	C(11)	C(12)	119(2)	C(11)	C(12)	C(13)	120(1)
C(8)	C(13)	C(12)	122(1)	C(4)	C(14)	C(15)	118.0(9)
C(14)	C(15)	C(16)	112.8(9)	C(15)	C(16)	C(17)	120(1)
C(15)	C(16)	C(21)	121(1)	C(17)	C(16)	C(21)	118(1)
C(16)	C(17)	C(18)	119(1)	C(17)	C(18)	C(19)	121(2)
C(18)	C(19)	C(20)	121(2)	C(19)	C(20)	C(21)	119(2)
C(16)	C(21)	C(20)	121(2)	P(1)	C(22)	C(23)	117.6(9)
P(1)	C(22)	C(27)	123.5(8)	C(23)	C(22)	C(27)	119(1)
C(22)	C(23)	C(24)	120(1)	C(23)	C(24)	C(25)	120(1)
C(24)	C(25)	C(26)	122(1)	C(25)	C(26)	C(27)	118(1)
C(22)	C(27)	C(26)	122(1)	P(1)	C(28)	C(29)	121.6(8)
P(1)	C(28)	C(33)	119.9(8)	C(29)	C(28)	C(33)	118(1)
C(28)	C(29)	C(30)	121(1)	C(29)	C(30)	C(31)	120(1)
C(30)	C(31)	C(32)	119(1)	C(31)	C(32)	C(33)	121(1)
C(28)	C(33)	C(32)	120(1)	P(1)	C(34)	C(35)	124.5(8)
P(1)	C(34)	C(39)	116.1(7)	C(35)	C(34)	C(39)	119.1(9)
C(34)	C(35)	C(36)	119(1)	C(35)	C(36)	C(37)	120(1)
C(36)	C(37)	C(38)	122(1)	C(37)	C(38)	C(39)	118(1)
C(34)	C(39)	C(38)	121.9(9)	P(2)	C(40)	C(41)	120.2(8)
P(2)	C(40)	C(45)	120.2(8)	C(41)	C(40)	C(45)	119.5(9)
C(40)	C(41)	C(42)	119(1)	C(41)	C(42)	C(43)	120(1)
C(42)	C(43)	C(44)	122(1)	C(43)	C(44)	C(45)	118(1)
C(40)	C(45)	C(44)	121(1)	P(2)	C(46)	C(47)	122.5(7)
P(2)	C(46)	C(51)	118.5(8)	C(47)	C(46)	C(51)	118.2(9)
C(46)	C(47)	C(48)	121(1)	C(47)	C(48)	C(49)	118(1)
C(48)	C(49)	C(50)	121(1)	C(49)	C(50)	C(51)	120(1)
C(46)	C(51)	C(50)	121(1)	P(2)	C(52)	C(53)	122.6(8)
P(2)	C(52)	C(57)	118.2(7)	C(53)	C(52)	C(57)	118.6(9)
C(52)	C(53)	C(54)	119(1)	C(53)	C(54)	C(55)	121(1)
C(54)	C(55)	C(56)	119.7(9)	C(55)	C(56)	C(57)	120(1)
C(52)	C(57)	C(56)	122(1)				

*Crystallographic Data and Details of Structure Refinement of **15***

Experimental

Data Collection

A dark yellow prismatic crystal of $C_{57}H_{51}OP_2Rh$ having approximate dimensions of 0.10 x 0.20 x 0.35 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC5R diffractometer with graphite monochromated Mo-Kα radiation and a rotating anode generator.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 20 carefully centered reflections in the range $14.09 < 2\theta < 16.34^{o}$

corresponded to a C-centered monoclinic cell with dimensions:

a = 48.726(5) Å
b = 9.180(6) Å β = 117.36(1)°
c = 23.832(8) Å
V = 9467(6) Å^3

For Z = 8 and F.W. = 916.88, the calculated density is 1.29 g/cm^3. Based on the systematic absences of:

hkl: h+k ± 2n
h0l: l ± 2n

packing considerations, a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

C2/c (No. 15)

The data were collected at a temperature of 23 ± 1°C using the ω-2θ scan technique to a maximum 2θ value of 55.0°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.32° with a take-off angle of 6.0°. Scans of (0.68 + 0.30 tan θ)° were made at speeds ranging from 8.0 to 4.0°/min (in ω). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 3 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm, the crystal to detector distance was 258 mm, and the detector aperture was 6.0 x 6.0 mm (horizontal x vertical).

Data Reduction

Of the 11603 reflections which were collected, 11471 were unique ($R_{int} = 0.046$); equivalent reflections were merged. The intensities of three representative reflections were measured after every 150 reflections. No decay correction was applied.

The linear absorption coefficient, μ, for Mo-Kα radiation is 4.7 cm^{-1}. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.96 to 1.00. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by heavy-atom Patterson methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[3] on F was based on 6134 observed reflections ($I > 3.00\sigma(I)$) and 550 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, | \, |Fo| - |Fc| \, | \, / \, \Sigma \, |Fo| = 0.044$$

$$R_w = [\, \Sigma \, w \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, w \, Fo^2]^{1/2} = 0.048$$

The standard deviation of an observation of unit weight[4] was 1.30. The weighting scheme was based on counting statistics and included a factor (p = 0.019) to downweight the intense reflections. Plots of $\Sigma \, w \, (|Fo| - |Fc|)^2$ versus |Fo|, reflection order in data collection, sin θ/λ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.75 and -0.37 e$^-$/Å ^{3}, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) PATTY: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.
(2) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and

Smits, J.M.M.(1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized:

$\Sigma w(|F_o| - |F_c|)^2$ where

$w = 1/[\sigma^2(F_o)] = [\sigma^2_c(F_o) + p^2F_o^2/4]^{-1}$

$\sigma_c(F_o)$ = e.s.d. based on counting statistics

p = p-factor

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(|F_o| - |F_c|)^2/(N_o - N_v)]^{1/2}$

where: N_o = number of observations

N_v = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) teXsan for Windows: Crystal Structure Analysis Package, Molecular Structure Corporation (1997).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{57}H_{51}OP_2Rh$
Formula Weight	916.88
Crystal Color, Habit	dark yellow, prismatic
Crystal Dimensions	0.10 X 0.20 X 0.35 mm
Crystal System	monoclinic
Lattice Type	C-centered
No. of Reflections Used for Unit Cell Determination (2θ range)	20 (14.1 - 16.3°)
Omega Scan Peak Width at Half-height	0.32°
Lattice Parameters	a = 48.726(5) Å b = 9.180(6) Å c = 23.832(8) Å β = 117.36(1)° V = 9467(6) Å^3
Space Group	C2/c (No. 15)
Z value	8
D_{calc}	1.286 g/cm^3
F_{000}	3808.00
μ(MoKα)	0.466 mm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC5R
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Attenuator	Zr foil (factors = 1.00, 3.52, 11.54, 41.93)
Take-off Angle	6.0°
Detector Aperture	6.0 mm horizontal 6.0 mm vertical
Crystal to Detector Distance	258 mm

Voltage, Current	50 kV, 180 mA
Temperature	23.0°C
Scan Type	ω-2θ
Scan Rate	8.0 - 4.0°/min (in ω) (up to 3 scans)
Scan Width	(0.68 + 0.30 tan θ)°
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 11603
	Unique: 11471 (R_{int} = 0.046)
Corrections	Lorentz-polarization
	Absorption
	(trans. factors: 0.9649 - 0.9989)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF92 PATTY)
Refinement	Full-matrix least-squares on F
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	$1/\sigma^2(Fo) = 4Fo^2/\sigma^2(Fo^2)$
p-factor	0.0195
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	6134
No. Variables	550
Reflection/Parameter Ratio	11.15
Residuals: R; Rw	0.044 ; 0.048
Goodness of Fit Indicator	1.30
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.75 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.37 $e^-/Å^3$

Table S13. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Rh(1)	0.167519(7)	0.19696(4)	0.36148(1)	2.811(6)
P(1)	0.15878(2)	0.2960(1)	0.26594(5)	2.94(2)
P(2)	0.17391(2)	0.1360(1)	0.46079(5)	2.87(2)
O(1)	0.22709(8)	0.0564(4)	0.3831(2)	6.1(1)
C(1)	0.20513(9)	0.1147(5)	0.3764(2)	3.7(1)
C(2)	0.12401(9)	0.2640(4)	0.3393(2)	3.29(9)
C(3)	0.09786(9)	0.2991(5)	0.3237(2)	3.67(9)
C(4)	0.06529(9)	0.3429(5)	0.3020(2)	3.9(1)
C(5)	0.0612(1)	0.5034(6)	0.2800(3)	6.8(2)
C(6)	0.0438(1)	0.2515(5)	0.2441(2)	4.7(1)
C(7)	0.0444(1)	0.0891(6)	0.2551(2)	5.5(1)
C(8)	0.0234(1)	-0.0032(6)	0.1982(2)	5.0(1)
C(9)	0.0227(1)	-0.1518(7)	0.2051(3)	7.8(2)
C(10)	0.0038(2)	-0.2409(7)	0.1556(3)	8.5(2)
C(11)	-0.0141(1)	-0.1855(8)	0.0976(3)	7.1(2)
C(12)	-0.0136(1)	-0.0364(8)	0.0896(3)	7.0(2)
C(13)	0.0049(1)	0.0512(6)	0.1390(3)	6.2(1)
C(14)	0.0561(1)	0.3222(6)	0.3552(2)	5.1(1)
C(15)	0.0710(1)	0.4255(6)	0.4115(3)	6.2(2)
C(16)	0.0646(1)	0.3810(6)	0.4656(3)	5.6(1)
C(17)	0.0877(1)	0.3282(7)	0.5219(4)	7.2(2)
C(18)	0.0819(2)	0.2887(8)	0.5706(3)	8.6(2)

C(19)	0.0525(2)	0.2961(8)	0.5637(4)	8.5(2)
C(20)	0.0290(1)	0.3479(7)	0.5084(3)	7.1(2)
C(21)	0.0353(1)	0.3914(6)	0.4604(3)	6.1(2)
C(22)	0.18722(9)	0.2485(4)	0.2391(2)	3.18(8)
C(23)	0.2167(1)	0.3093(5)	0.2690(2)	4.5(1)
C(24)	0.2393(1)	0.2714(6)	0.2516(2)	4.8(1)
C(25)	0.2331(1)	0.1696(6)	0.2057(2)	5.0(1)
C(26)	0.2048(1)	0.1068(6)	0.1766(2)	5.2(1)
C(27)	0.1818(1)	0.1456(5)	0.1928(2)	3.9(1)
C(28)	0.16022(9)	0.4977(4)	0.2667(2)	3.46(9)
C(29)	0.1683(1)	0.5744(6)	0.2264(3)	5.4(1)
C(30)	0.1702(1)	0.7245(6)	0.2292(3)	6.6(2)
C(31)	0.1638(1)	0.7978(6)	0.2718(3)	6.6(2)
C(32)	0.1559(1)	0.7253(6)	0.3110(3)	6.6(2)
C(33)	0.1540(1)	0.5720(5)	0.3093(2)	5.0(1)
C(34)	0.12186(9)	0.2507(5)	0.1983(2)	3.29(9)
C(35)	0.1068(1)	0.3416(5)	0.1474(2)	4.9(1)
C(36)	0.0789(1)	0.3018(7)	0.0974(2)	6.0(1)
C(37)	0.0661(1)	0.1697(7)	0.0976(2)	5.6(1)
C(38)	0.0806(1)	0.0765(6)	0.1473(3)	5.4(1)
C(39)	0.1084(1)	0.1173(5)	0.1978(2)	4.2(1)
C(40)	0.20784(8)	0.0248(4)	0.5090(2)	3.00(8)
C(41)	0.2056(1)	-0.1232(5)	0.5183(2)	4.1(1)
C(42)	0.2319(1)	-0.2064(5)	0.5512(2)	5.0(1)
C(43)	0.2607(1)	-0.1444(6)	0.5753(2)	5.1(1)
C(44)	0.2633(1)	0.0028(6)	0.5660(2)	4.8(1)
C(45)	0.23708(9)	0.0854(5)	0.5327(2)	3.9(1)
C(46)	0.17812(8)	0.2951(4)	0.5105(2)	3.12(8)
C(47)	0.1977(1)	0.3005(5)	0.5751(2)	4.4(1)
C(48)	0.1989(1)	0.4233(6)	0.6096(2)	5.3(1)
C(49)	0.1807(1)	0.5410(5)	0.5818(2)	5.1(1)
C(50)	0.1609(1)	0.5386(5)	0.5179(3)	5.1(1)
C(51)	0.1601(1)	0.4172(5)	0.4822(2)	4.1(1)
C(52)	0.14242(8)	0.0315(4)	0.4636(2)	3.18(9)
C(53)	0.1394(1)	0.0220(6)	0.5184(2)	4.8(1)
C(54)	0.1167(1)	-0.0645(7)	0.5203(3)	6.2(2)
C(55)	0.0976(1)	-0.1432(6)	0.4692(3)	6.1(2)
C(56)	0.0998(1)	-0.1324(6)	0.4140(3)	6.1(1)
C(57)	0.1225(1)	-0.0446(5)	0.4111(2)	4.5(1)
H(1)	0.0600	0.5636	0.3113	8.195
H(2)	0.0783	0.5323	0.2738	8.195
H(3)	0.0427	0.5130	0.2415	8.195
H(4)	0.0232	0.2845	0.2304	5.677
H(5)	0.0496	0.2679	0.2116	5.677
H(6)	0.0650	0.0565	0.2690	6.591
H(7)	0.0385	0.0730	0.2875	6.591
H(8)	0.0355	-0.1943	0.2451	9.307
H(9)	0.0035	-0.3427	0.1624	10.206
H(10)	-0.0267	-0.2470	0.0634	8.516
H(11)	-0.0262	0.0054	0.0494	8.439
H(12)	0.0050	0.1531	0.1321	7.457
H(13)	0.0343	0.3345	0.3373	6.084

H(14)	0.0614	0.2255	0.3707	6.084
H(15)	0.0927	0.4257	0.4260	7.490
H(16)	0.0631	0.5209	0.3983	7.490
H(17)	0.1081	0.3192	0.5268	8.692
H(18)	0.0983	0.2561	0.6094	10.334
H(19)	0.0483	0.2654	0.5971	10.205
H(20)	0.0085	0.3536	0.5034	8.481
H(21)	0.0190	0.4296	0.4227	7.313
H(22)	0.2214	0.3781	0.3020	5.405
H(23)	0.2591	0.3163	0.2717	5.767
H(24)	0.2486	0.1427	0.1940	6.056
H(25)	0.2007	0.0355	0.1448	6.215
H(26)	0.1621	0.1009	0.1717	4.707
H(27)	0.1725	0.5232	0.1967	6.424
H(28)	0.1759	0.7764	0.2016	7.918
H(29)	0.1651	0.9011	0.2736	7.957
H(30)	0.1515	0.7779	0.3402	7.954
H(31)	0.1484	0.5211	0.3372	6.001
H(32)	0.1157	0.4331	0.1465	5.869
H(33)	0.0686	0.3666	0.0629	7.216
H(34)	0.0470	0.1424	0.0630	6.690
H(35)	0.0718	-0.0157	0.1473	6.451
H(36)	0.1183	0.0528	0.2325	5.047
H(37)	0.1858	-0.1678	0.5020	4.880
H(38)	0.2300	-0.3074	0.5572	6.028
H(39)	0.2786	-0.2019	0.5981	6.116
H(40)	0.2832	0.0469	0.5825	5.791
H(41)	0.2391	0.1860	0.5259	4.658
H(42)	0.2104	0.2191	0.5956	5.320
H(43)	0.2126	0.4257	0.6535	6.379
H(44)	0.1816	0.6242	0.6063	6.116
H(45)	0.1479	0.6197	0.4982	6.074
H(46)	0.1470	0.4176	0.4379	4.972
H(47)	0.1530	0.0751	0.5548	5.783
H(48)	0.1144	-0.0688	0.5577	7.402
H(49)	0.0827	-0.2062	0.4716	7.351
H(50)	0.0858	-0.1847	0.3776	7.289
H(51)	0.1241	-0.0377	0.3730	5.352

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S14. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Rh(1)	0.0329(1)	0.0401(2)	0.0332(1)	0.0024(2)	0.0146(1)	0.0018(2)
P(1)	0.0390(5)	0.0364(5)	0.0348(5)	0.0018(5)	0.0155(4)	0.0004(5)
P(2)	0.0359(5)	0.0385(5)	0.0346(5)	-0.0000(4)	0.0162(4)	0.0002(5)
O(1)	0.060(2)	0.095(3)	0.083(3)	0.034(2)	0.039(2)	0.019(2)
C(1)	0.044(2)	0.054(3)	0.041(2)	0.001(2)	0.018(2)	0.004(2)
C(2)	0.042(2)	0.047(2)	0.036(2)	0.001(2)	0.017(2)	0.001(2)
C(3)	0.041(2)	0.048(2)	0.049(2)	-0.002(2)	0.019(2)	-0.003(2)
C(4)	0.038(2)	0.048(3)	0.056(3)	0.003(2)	0.015(2)	-0.001(2)
C(5)	0.064(3)	0.065(4)	0.115(5)	0.016(3)	0.028(3)	0.007(4)

C(6)	0.040(2)	0.064(3)	0.066(3)	0.007(2)	0.016(2)	-0.004(3)
C(7)	0.059(3)	0.069(4)	0.063(3)	-0.007(3)	0.013(3)	-0.006(3)
C(8)	0.048(3)	0.071(4)	0.067(3)	-0.001(3)	0.024(3)	-0.008(3)
C(9)	0.100(5)	0.074(4)	0.079(4)	-0.016(4)	0.005(4)	-0.004(4)
C(10)	0.114(6)	0.074(4)	0.092(5)	-0.023(4)	0.011(4)	-0.018(4)
C(11)	0.064(3)	0.094(5)	0.088(4)	-0.009(4)	0.015(3)	-0.027(4)
C(12)	0.065(4)	0.098(5)	0.070(4)	0.009(4)	0.001(3)	-0.008(4)
C(13)	0.060(3)	0.074(4)	0.076(4)	0.002(3)	0.009(3)	-0.005(3)
C(14)	0.042(2)	0.078(4)	0.074(3)	-0.001(3)	0.028(2)	-0.022(3)
C(15)	0.073(4)	0.085(4)	0.087(4)	-0.011(3)	0.043(3)	-0.025(3)
C(16)	0.070(3)	0.066(4)	0.085(4)	-0.010(3)	0.044(3)	-0.021(3)
C(17)	0.079(4)	0.081(5)	0.120(6)	0.014(4)	0.050(4)	0.005(4)
C(18)	0.113(6)	0.095(5)	0.112(6)	0.009(5)	0.045(5)	0.023(5)
C(19)	0.120(6)	0.098(5)	0.131(6)	0.003(5)	0.080(5)	0.026(5)
C(20)	0.089(4)	0.085(5)	0.112(5)	0.001(4)	0.060(4)	-0.007(4)
C(21)	0.073(4)	0.078(4)	0.087(4)	-0.004(3)	0.043(3)	-0.010(3)
C(22)	0.047(2)	0.038(2)	0.036(2)	0.005(2)	0.019(2)	0.005(2)
C(23)	0.056(3)	0.063(3)	0.058(3)	-0.001(3)	0.031(2)	-0.007(3)
C(24)	0.049(3)	0.078(4)	0.062(3)	0.004(2)	0.030(2)	0.005(3)
C(25)	0.065(3)	0.068(4)	0.073(3)	0.025(3)	0.043(3)	0.013(3)
C(26)	0.085(4)	0.060(3)	0.062(3)	0.017(3)	0.043(3)	-0.006(3)
C(27)	0.056(3)	0.048(2)	0.047(2)	-0.002(2)	0.026(2)	-0.004(2)
C(28)	0.042(2)	0.038(2)	0.048(2)	0.002(2)	0.017(2)	-0.002(2)
C(29)	0.083(4)	0.051(3)	0.083(4)	-0.002(3)	0.050(3)	0.004(3)
C(30)	0.090(4)	0.042(4)	0.120(5)	-0.006(3)	0.050(4)	0.019(3)
C(31)	0.079(4)	0.035(3)	0.117(5)	0.008(3)	0.027(4)	0.006(4)
C(32)	0.101(5)	0.051(4)	0.098(5)	0.018(3)	0.044(4)	-0.015(3)
C(33)	0.076(3)	0.052(3)	0.067(3)	0.010(3)	0.037(3)	-0.002(3)
C(34)	0.040(2)	0.048(2)	0.036(2)	0.003(2)	0.017(2)	-0.004(2)
C(35)	0.066(3)	0.057(3)	0.050(3)	-0.001(2)	0.015(2)	0.010(2)
C(36)	0.064(3)	0.092(4)	0.049(3)	0.012(3)	0.006(2)	0.009(3)
C(37)	0.052(3)	0.097(5)	0.045(3)	-0.004(3)	0.008(2)	-0.021(3)
C(38)	0.057(3)	0.068(4)	0.080(4)	-0.019(3)	0.032(3)	-0.029(3)
C(39)	0.048(3)	0.055(3)	0.053(3)	-0.003(2)	0.019(2)	-0.004(2)
C(40)	0.035(2)	0.046(2)	0.034(2)	0.004(2)	0.017(2)	0.003(2)
C(41)	0.046(2)	0.052(3)	0.056(3)	0.007(2)	0.024(2)	0.003(2)
C(42)	0.067(3)	0.053(3)	0.076(3)	0.016(3)	0.037(3)	0.014(3)
C(43)	0.052(3)	0.081(4)	0.058(3)	0.030(3)	0.024(2)	0.016(3)
C(44)	0.042(2)	0.079(4)	0.053(3)	0.005(2)	0.014(2)	0.001(3)
C(45)	0.040(2)	0.054(3)	0.047(2)	0.002(2)	0.014(2)	0.006(2)
C(46)	0.042(2)	0.037(2)	0.043(2)	0.001(2)	0.022(2)	0.001(2)
C(47)	0.063(3)	0.057(3)	0.042(2)	0.011(3)	0.019(2)	-0.002(2)
C(48)	0.077(4)	0.072(4)	0.048(3)	0.000(3)	0.024(3)	-0.016(3)
C(49)	0.076(3)	0.053(3)	0.065(3)	-0.002(3)	0.033(3)	-0.018(3)
C(50)	0.068(3)	0.047(3)	0.074(3)	0.005(2)	0.030(3)	-0.006(3)
C(51)	0.058(3)	0.045(3)	0.047(3)	-0.001(2)	0.018(2)	-0.004(2)
C(52)	0.035(2)	0.039(2)	0.046(2)	0.003(2)	0.018(2)	0.003(2)
C(53)	0.056(3)	0.079(4)	0.054(3)	-0.014(3)	0.031(2)	-0.000(3)
C(54)	0.073(4)	0.094(5)	0.082(4)	-0.021(3)	0.047(3)	0.001(3)
C(55)	0.052(3)	0.079(4)	0.102(5)	-0.010(3)	0.036(3)	0.022(4)
C(56)	0.066(3)	0.067(4)	0.080(4)	-0.033(3)	0.019(3)	-0.006(3)
C(57)	0.057(3)	0.056(3)	0.055(3)	-0.007(2)	0.024(2)	0.001(2)

The general temperature factor expression:
$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S15. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Rh(1)	P(1)	2.302(1)	Rh(1)	P(2)	2.310(1)
Rh(1)	C(1)	1.859(5)	Rh(1)	C(2)	2.031(4)
P(1)	C(22)	1.826(4)	P(1)	C(28)	1.852(5)
P(1)	C(34)	1.828(4)	P(2)	C(40)	1.831(4)
P(2)	C(46)	1.831(5)	P(2)	C(52)	1.836(4)
O(1)	C(1)	1.141(5)	C(2)	C(3)	1.196(6)
C(3)	C(4)	1.481(6)	C(4)	C(5)	1.546(8)
C(4)	C(6)	1.543(7)	C(4)	C(14)	1.539(7)
C(6)	C(7)	1.511(8)	C(7)	C(8)	1.527(7)
C(8)	C(9)	1.376(8)	C(8)	C(13)	1.372(8)
C(9)	C(10)	1.382(9)	C(10)	C(11)	1.349(9)
C(11)	C(12)	1.383(9)	C(12)	C(13)	1.367(8)
C(14)	C(15)	1.528(7)	C(15)	C(16)	1.515(8)
C(16)	C(17)	1.382(9)	C(16)	C(21)	1.382(8)
C(17)	C(18)	1.366(9)	C(18)	C(19)	1.37(1)
C(19)	C(20)	1.37(1)	C(20)	C(21)	1.374(9)
C(22)	C(23)	1.392(6)	C(22)	C(27)	1.384(6)
C(23)	C(24)	1.392(6)	C(24)	C(25)	1.363(7)
C(25)	C(26)	1.355(7)	C(26)	C(27)	1.389(7)
C(28)	C(29)	1.384(7)	C(28)	C(33)	1.369(7)
C(29)	C(30)	1.381(7)	C(30)	C(31)	1.367(9)
C(31)	C(32)	1.340(9)	C(32)	C(33)	1.410(8)
C(34)	C(35)	1.375(6)	C(34)	C(39)	1.387(7)
C(35)	C(36)	1.383(7)	C(36)	C(37)	1.365(9)
C(37)	C(38)	1.366(8)	C(38)	C(39)	1.385(7)
C(40)	C(41)	1.388(7)	C(40)	C(45)	1.385(6)
C(41)	C(42)	1.385(7)	C(42)	C(43)	1.371(8)
C(43)	C(44)	1.385(8)	C(44)	C(45)	1.382(7)
C(46)	C(47)	1.391(6)	C(46)	C(51)	1.392(6)
C(47)	C(48)	1.381(7)	C(48)	C(49)	1.361(7)
C(49)	C(50)	1.378(7)	C(50)	C(51)	1.391(7)
C(52)	C(53)	1.383(6)	C(52)	C(57)	1.370(6)
C(53)	C(54)	1.381(7)	C(54)	C(55)	1.351(8)
C(55)	C(56)	1.372(8)	C(56)	C(57)	1.396(7)

Table S16. Bond Angles(º)

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	Rh(1)	P(2)	170.27(4)	P(1)	Rh(1)	C(1)	93.9(1)
P(1)	Rh(1)	C(2)	85.8(1)	P(2)	Rh(1)	C(1)	92.8(1)
P(2)	Rh(1)	C(2)	88.4(1)	C(1)	Rh(1)	C(2)	173.0(2)
Rh(1)	P(1)	C(22)	115.3(1)	Rh(1)	P(1)	C(28)	113.4(2)
Rh(1)	P(1)	C(34)	116.2(2)	C(22)	P(1)	C(28)	102.1(2)
C(22)	P(1)	C(34)	103.6(2)	C(28)	P(1)	C(34)	104.7(2)
Rh(1)	P(2)	C(40)	115.8(1)	Rh(1)	P(2)	C(46)	113.0(2)
Rh(1)	P(2)	C(52)	116.2(2)	C(40)	P(2)	C(46)	103.8(2)
C(40)	P(2)	C(52)	102.4(2)	C(46)	P(2)	C(52)	103.9(2)

Rh(1)	C(1)	O(1)	175.3(5)	Rh(1)	C(2)	C(3)	176.7(4)
C(2)	C(3)	C(4)	177.9(5)	C(3)	C(4)	C(5)	109.1(4)
C(3)	C(4)	C(6)	110.1(4)	C(3)	C(4)	C(14)	110.5(4)
C(5)	C(4)	C(6)	106.6(5)	C(5)	C(4)	C(14)	110.8(5)
C(6)	C(4)	C(14)	109.5(4)	C(4)	C(6)	C(7)	115.4(5)
C(6)	C(7)	C(8)	116.2(5)	C(7)	C(8)	C(9)	119.1(6)
C(7)	C(8)	C(13)	124.5(6)	C(9)	C(8)	C(13)	116.3(6)
C(8)	C(9)	C(10)	121.8(7)	C(9)	C(10)	C(11)	121.0(7)
C(10)	C(11)	C(12)	118.0(7)	C(11)	C(12)	C(13)	120.7(6)
C(8)	C(13)	C(12)	122.1(6)	C(4)	C(14)	C(15)	116.4(5)
C(14)	C(15)	C(16)	112.2(5)	C(15)	C(16)	C(17)	121.8(6)
C(15)	C(16)	C(21)	120.9(6)	C(17)	C(16)	C(21)	117.3(6)
C(16)	C(17)	C(18)	121.6(7)	C(17)	C(18)	C(19)	120.0(8)
C(18)	C(19)	C(20)	120.0(7)	C(19)	C(20)	C(21)	119.5(7)
C(16)	C(21)	C(20)	121.6(7)	P(1)	C(22)	C(23)	119.6(4)
P(1)	C(22)	C(27)	123.1(4)	C(23)	C(22)	C(27)	117.1(4)
C(22)	C(23)	C(24)	121.3(5)	C(23)	C(24)	C(25)	119.8(5)
C(24)	C(25)	C(26)	120.0(5)	C(25)	C(26)	C(27)	120.7(5)
C(22)	C(27)	C(26)	121.0(5)	P(1)	C(28)	C(29)	121.6(4)
P(1)	C(28)	C(33)	119.0(4)	C(29)	C(28)	C(33)	119.4(5)
C(28)	C(29)	C(30)	120.6(6)	C(29)	C(30)	C(31)	119.5(6)
C(30)	C(31)	C(32)	120.6(6)	C(31)	C(32)	C(33)	120.8(6)
C(28)	C(33)	C(32)	119.0(6)	P(1)	C(34)	C(35)	123.4(4)
P(1)	C(34)	C(39)	118.6(4)	C(35)	C(34)	C(39)	118.0(5)
C(34)	C(35)	C(36)	121.0(5)	C(35)	C(36)	C(37)	120.1(5)
C(36)	C(37)	C(38)	120.2(5)	C(37)	C(38)	C(39)	119.7(5)
C(34)	C(39)	C(38)	121.0(5)	P(2)	C(40)	C(41)	122.1(4)
P(2)	C(40)	C(45)	119.6(4)	C(41)	C(40)	C(45)	118.0(4)
C(40)	C(41)	C(42)	120.6(5)	C(41)	C(42)	C(43)	120.7(5)
C(42)	C(43)	C(44)	119.4(5)	C(43)	C(44)	C(45)	119.9(5)
C(40)	C(45)	C(44)	121.4(5)	P(2)	C(46)	C(47)	124.1(4)
P(2)	C(46)	C(51)	118.1(3)	C(47)	C(46)	C(51)	117.8(4)
C(46)	C(47)	C(48)	120.5(5)	C(47)	C(48)	C(49)	121.3(5)
C(48)	C(49)	C(50)	119.5(5)	C(49)	C(50)	C(51)	119.9(5)
C(46)	C(51)	C(50)	121.0(5)	P(2)	C(52)	C(53)	121.4(4)
P(2)	C(52)	C(57)	119.2(4)	C(53)	C(52)	C(57)	119.4(4)
C(52)	C(53)	C(54)	120.2(5)	C(53)	C(54)	C(55)	120.5(6)
C(54)	C(55)	C(56)	120.2(5)	C(55)	C(56)	C(57)	120.0(5)
C(52)	C(57)	C(56)	119.7(5)				

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Experimental

Data Collection

A yellow prismatic crystal of $C_{57}H_{51}OP_2Ir$ having approximate dimensions of 0.15 x 0.20 x 0.35 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC5R diffractometer with graphite monochromated Mo-Kα radiation and a rotating anode generator.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 20 carefully centered reflections in the range $19.26 < 2\theta < 21.21^{o}$ corresponded to a C-centered monoclinic cell with dimensions:

a = 48.811(4) Å
b = 9.156(3) Å β = 117.337(8)°
c = 23.799(3) Å

$V = 9448(3)$ Å^3

For Z = 8 and F.W. = 1006.20, the calculated density is 1.41 g/cm^3. Based on the systematic absences of:

hkl: h+k ± 2n

h0l: l ± 2n

packing considerations, a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

C2/c (No. 15)

The data were collected at a temperature of 23 ± 1°C using the ω-2θ scan technique to a maximum 2θ value of 55.0°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.31° with a take-off angle of 6.0°. Scans of (0.68 + 0.30 tan θ)° were made at a speed of 4.0°/min (in ω). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 3 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm, the crystal to detector distance was 258 mm, and the detector aperture was 9.0 x 13.0 mm (horizontal x vertical).

Data Reduction

Of the 11652 reflections which were collected, 11518 were unique ($R_{int} = 0.032$); equivalent reflections were merged. The intensities of three representative reflections were measured after every 150 reflections. No decay correction was applied.

The linear absorption coefficient, μ, for Mo-Kα radiation is 29.4 cm^{-1}. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.96 to 1.00. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by heavy-atom Patterson methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[3] on F was based on 7599 observed reflections ($I > 3.00\sigma(I)$) and 550 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, | \, |Fo| - |Fc| \, | \, / \Sigma \, |Fo| = 0.036$$

$$R_w = [\Sigma \, w \, (|Fo| - |Fc|)^2 / \Sigma \, w \, Fo^2]^{1/2} = 0.035$$

The standard deviation of an observation of unit weight[4] was 1.35. The weighting scheme was based on counting statistics and included a factor (p = 0.012) to downweight the intense reflections. Plots of $\Sigma \, w \, (|Fo| - |Fc|)^2$ versus $|Fo|$, reflection order in data collection, $\sin\theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.32 and -1.13 e$^-$/Å^3, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) PATTY: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(2) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized:

$$\Sigma w(|F_o| - |F_c|)^2 \text{ where}$$

$$w = 1/[\sigma^2(Fo)] = [\sigma^2_c(Fo) + p^2Fo^2/4]^{-1}$$

$\sigma_c(F_o)$ = e.s.d. based on counting statistics
p = p-factor

(4) Standard deviation of an observation of unit weight:
$[\Sigma w(|F_o| - |F_c|)^2/(N_o - N_v)]^{1/2}$
where: N_o = number of observations
N_v = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).
(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).
(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).
(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).
(9) teXsan for Windows: Crystal Structure Analysis Package, Molecular Structure Corporation (1997).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{57}H_{51}OP_2Ir$
Formula Weight	1006.20
Crystal Color, Habit	yellow, prismatic
Crystal Dimensions	0.15 X 0.20 X 0.35 mm
Crystal System	monoclinic
Lattice Type	C-centered
No. of Reflections Used for Unit Cell Determination (2θ range)	20 (19.3 - 21.2°)
Omega Scan Peak Width at Half-height	0.31°
Lattice Parameters	a = 48.811(4) Å b = 9.156(3) Å c = 23.799(3) Å β = 117.337(8) Å V = 9448(3) Å^3
Space Group	C2/c (No. 15)
Z value	8
D_{calc}	1.415 g/cm^3
F_{000}	4064.00
μ(MoKα)	2.941 mm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC5R
Radiation	MoKα (λ = 0.71069 ≈) graphite monochromated
Attenuator	Zr foil (factors = 1.00, 3.52, 11.54, 41.93)
Take-off Angle	6.0°
Detector Aperture	9.0 mm horizontal 13.0 mm vertical
Crystal to Detector Distance	258 mm
Voltage, Current	50 kV, 180 mA
Temperature	23.0°C
Scan Type	ω-2θ
Scan Rate	4.0°/min (in ω) (up to 3 scans)
Scan Width	(0.68 + 0.30 tan θ)°
$2\theta_{max}$	55.0°

No. of Reflections Measured	Total: 11652 Unique: 11518 (R_{int} = 0.032)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.9587 - 0.9997)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF92 PATTY)
Refinement	Full-matrix least-squares on F
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	$1/\sigma^2(Fo) = 4Fo^2/\sigma^2(Fo^2)$
p-factor	0.0122
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	7599
No. Variables	550
Reflection/Parameter Ratio	13.82
Residuals: R; Rw	0.036 ; 0.035
Goodness of Fit Indicator	1.35
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	1.32 $e^-/Å^3$
Minimum peak in Final Diff. Map	-1.13 $e^-/Å^3$

Table S17. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ir(1)	0.167286(4)	0.19721(2)	0.361703(7)	2.857(3)
P(1)	0.15888(2)	0.2963(1)	0.26602(5)	3.05(2)
P(2)	0.17392(2)	0.1355(1)	0.46120(5)	2.95(2)
O(1)	0.22700(8)	0.0579(5)	0.3836(2)	6.0(1)
C(1)	0.2046(1)	0.1163(6)	0.3766(2)	3.9(1)
C(2)	0.1239(1)	0.2631(5)	0.3395(2)	3.4(1)
C(3)	0.0975(1)	0.2984(5)	0.3235(2)	3.6(1)
C(4)	0.0649(1)	0.3427(6)	0.3021(2)	4.3(1)
C(5)	0.0608(1)	0.5028(7)	0.2798(3)	6.8(2)
C(6)	0.0437(1)	0.2519(6)	0.2441(3)	5.1(1)
C(7)	0.0444(1)	0.0885(7)	0.2550(2)	5.7(1)
C(8)	0.0233(1)	-0.0045(7)	0.1981(3)	5.0(1)
C(9)	0.0227(2)	-0.1531(8)	0.2051(3)	7.4(2)
C(10)	0.0037(2)	-0.2423(8)	0.1557(4)	8.4(2)
C(11)	-0.0143(1)	-0.1867(9)	0.0980(3)	7.1(2)
C(12)	-0.0139(1)	-0.0388(9)	0.0894(3)	7.2(2)
C(13)	0.0048(1)	0.0502(7)	0.1391(3)	6.2(2)
C(14)	0.0557(1)	0.3223(6)	0.3557(3)	5.4(1)
C(15)	0.0711(1)	0.4236(7)	0.4113(3)	6.3(2)
C(16)	0.0647(1)	0.3811(7)	0.4658(3)	5.6(2)
C(17)	0.0876(2)	0.3290(8)	0.5219(4)	7.3(2)
C(18)	0.0821(2)	0.2874(9)	0.5717(4)	9.0(3)
C(19)	0.0526(2)	0.2959(9)	0.5648(4)	8.6(3)
C(20)	0.0294(2)	0.3482(8)	0.5096(4)	7.2(2)
C(21)	0.0351(1)	0.3913(7)	0.4607(3)	6.3(2)
C(22)	0.1874(1)	0.2472(5)	0.2394(2)	3.3(1)
C(23)	0.1818(1)	0.1442(5)	0.1928(2)	4.0(1)

C(24)	0.2049(1)	0.1056(6)	0.1767(2)	5.1(1)
C(25)	0.2331(1)	0.1673(7)	0.2059(3)	5.3(2)
C(26)	0.2393(1)	0.2711(7)	0.2520(3)	5.1(1)
C(27)	0.2168(1)	0.3085(6)	0.2697(2)	4.5(1)
C(28)	0.1603(1)	0.4963(5)	0.2668(2)	3.4(1)
C(29)	0.1685(1)	0.5733(6)	0.2268(3)	5.4(2)
C(30)	0.1705(1)	0.7246(6)	0.2295(3)	6.5(2)
C(31)	0.1649(1)	0.7989(7)	0.2727(3)	6.5(2)
C(32)	0.1563(2)	0.7258(6)	0.3120(3)	6.4(2)
C(33)	0.1544(1)	0.5741(6)	0.3096(2)	4.9(1)
C(34)	0.1222(1)	0.2509(5)	0.1989(2)	3.5(1)
C(35)	0.1066(1)	0.3424(6)	0.1479(2)	4.8(1)
C(36)	0.0786(1)	0.3026(8)	0.0978(2)	6.0(2)
C(37)	0.0661(1)	0.1692(8)	0.0983(3)	6.0(2)
C(38)	0.0810(1)	0.0764(7)	0.1479(3)	5.4(1)
C(39)	0.1088(1)	0.1176(6)	0.1985(2)	4.3(1)
C(40)	0.2078(1)	0.0232(5)	0.5087(2)	3.2(1)
C(41)	0.2052(1)	-0.1237(6)	0.5182(2)	4.1(1)
C(42)	0.2316(1)	-0.2085(6)	0.5511(2)	4.9(1)
C(43)	0.2601(1)	-0.1456(7)	0.5746(3)	5.3(1)
C(44)	0.2630(1)	0.0005(7)	0.5651(2)	4.8(1)
C(45)	0.2369(1)	0.0846(6)	0.5326(2)	4.1(1)
C(46)	0.1781(1)	0.2958(5)	0.5108(2)	3.4(1)
C(47)	0.1981(1)	0.3021(6)	0.5751(2)	4.3(1)
C(48)	0.1993(1)	0.4256(7)	0.6100(2)	5.2(1)
C(49)	0.1806(1)	0.5426(6)	0.5825(3)	5.0(1)
C(50)	0.1608(1)	0.5385(6)	0.5186(3)	5.1(1)
C(51)	0.1599(1)	0.4172(6)	0.4829(2)	4.1(1)
C(52)	0.14262(9)	0.0324(5)	0.4644(2)	3.3(1)
C(53)	0.1391(1)	0.0241(6)	0.5187(2)	5.0(1)
C(54)	0.1169(1)	-0.0634(7)	0.5217(3)	6.1(2)
C(55)	0.0978(1)	-0.1415(7)	0.4705(3)	6.2(2)
C(56)	0.1000(1)	-0.1339(6)	0.4149(3)	5.8(2)
C(57)	0.1225(1)	-0.0457(5)	0.4119(2)	4.3(1)
H(1)	0.0779	0.5315	0.2735	8.160
H(2)	0.0596	0.5636	0.3109	8.160
H(3)	0.0424	0.5121	0.2411	8.160
H(4)	0.0497	0.2687	0.2119	6.071
H(5)	0.0232	0.2850	0.2301	6.071
H(6)	0.0385	0.0723	0.2876	6.842
H(7)	0.0649	0.0559	0.2688	6.842
H(8)	0.0357	-0.1957	0.2450	8.919
H(9)	0.0034	-0.3443	0.1625	10.028
H(10)	-0.0270	-0.2487	0.0639	8.532
H(11)	-0.0265	0.0026	0.0490	8.676
H(12)	0.0048	0.1524	0.1321	7.437
H(13)	0.0341	0.3363	0.3382	6.496
H(14)	0.0607	0.2251	0.3709	6.496
H(15)	0.0927	0.4213	0.4255	7.557
H(16)	0.0636	0.5199	0.3981	7.557
H(17)	0.1080	0.3212	0.5266	8.790
H(18)	0.0984	0.2534	0.6101	10.777

H(19)	0.0483	0.2657	0.5982	10.282
H(20)	0.0090	0.3547	0.5050	8.660
H(21)	0.0187	0.4285	0.4229	7.585
H(22)	0.1621	0.0996	0.1717	4.763
H(23)	0.2007	0.0346	0.1447	6.105
H(24)	0.2487	0.1391	0.1947	6.325
H(25)	0.2589	0.3171	0.2716	6.095
H(26)	0.2214	0.3768	0.3029	5.434
H(27)	0.1729	0.5220	0.1971	6.473
H(28)	0.1759	0.7763	0.2013	7.802
H(29)	0.1669	0.9022	0.2754	7.776
H(30)	0.1517	0.7783	0.3409	7.629
H(31)	0.1490	0.5236	0.3379	5.898
H(32)	0.1153	0.4347	0.1470	5.747
H(33)	0.0681	0.3677	0.0634	7.207
H(34)	0.0470	0.1412	0.0639	7.212
H(35)	0.0723	-0.0165	0.1479	6.438
H(36)	0.1188	0.0531	0.2334	5.121
H(37)	0.1854	-0.1674	0.5022	4.926
H(38)	0.2297	-0.3098	0.5572	5.939
H(39)	0.2780	-0.2031	0.5976	6.381
H(40)	0.2829	0.0434	0.5808	5.760
H(41)	0.2390	0.1858	0.5265	4.979
H(42)	0.2111	0.2212	0.5954	5.150
H(43)	0.2133	0.4286	0.6538	6.288
H(44)	0.1813	0.6256	0.6070	5.999
H(45)	0.1476	0.6193	0.4988	6.147
H(46)	0.1467	0.4173	0.4386	4.970
H(47)	0.1522	0.0800	0.5547	5.973
H(48)	0.1151	-0.0690	0.5597	7.339
H(49)	0.0826	-0.2025	0.4729	7.412
H(50)	0.0863	-0.1883	0.3789	6.963
H(51)	0.1240	-0.0391	0.3736	5.138

B_{eq} = 8/3 $\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S18. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	0.03453(8)	0.04284(9)	0.03252(8)	0.00143(9)	0.01656(6)	0.00084(9)
P(1)	0.0413(6)	0.0407(6)	0.0356(5)	0.0005(6)	0.0189(5)	-0.0003(5)
P(2)	0.0378(6)	0.0418(7)	0.0347(6)	-0.0005(5)	0.0185(5)	0.0012(5)
O(1)	0.055(2)	0.105(3)	0.077(3)	0.031(2)	0.038(2)	0.019(2)
C(1)	0.045(3)	0.066(4)	0.038(2)	-0.004(3)	0.020(2)	0.009(2)
C(2)	0.038(2)	0.056(3)	0.033(2)	-0.004(2)	0.014(2)	0.000(2)
C(3)	0.041(2)	0.051(3)	0.043(2)	0.001(2)	0.017(2)	-0.001(2)
C(4)	0.038(2)	0.055(3)	0.062(3)	0.002(2)	0.017(2)	-0.004(3)
C(5)	0.070(4)	0.067(4)	0.107(5)	0.017(3)	0.028(4)	0.004(4)
C(6)	0.040(3)	0.066(4)	0.077(4)	0.004(3)	0.018(3)	-0.006(3)
C(7)	0.060(3)	0.085(5)	0.057(3)	-0.005(3)	0.015(3)	-0.003(3)
C(8)	0.054(3)	0.075(4)	0.056(3)	0.002(3)	0.018(3)	-0.003(3)
C(9)	0.100(5)	0.066(5)	0.080(5)	-0.004(4)	0.009(4)	-0.002(4)
C(10)	0.105(6)	0.084(5)	0.091(5)	-0.014(5)	0.014(4)	-0.006(4)

C(11)	0.063(4)	0.107(6)	0.082(5)	-0.015(4)	0.017(3)	-0.035(5)
C(12)	0.065(4)	0.106(6)	0.071(4)	-0.001(4)	0.003(3)	-0.017(4)
C(13)	0.066(4)	0.086(5)	0.068(4)	-0.001(3)	0.017(3)	-0.011(4)
C(14)	0.045(3)	0.078(4)	0.086(4)	-0.005(3)	0.033(3)	-0.022(3)
C(15)	0.068(4)	0.095(5)	0.090(4)	-0.015(4)	0.049(4)	-0.027(4)
C(16)	0.068(4)	0.065(4)	0.087(4)	-0.009(3)	0.041(4)	-0.023(4)
C(17)	0.087(5)	0.088(6)	0.119(6)	0.015(4)	0.061(5)	0.008(5)
C(18)	0.107(6)	0.101(6)	0.133(7)	0.023(5)	0.055(6)	0.038(5)
C(19)	0.126(7)	0.097(6)	0.130(7)	0.009(6)	0.082(6)	0.024(5)
C(20)	0.091(5)	0.090(6)	0.118(6)	-0.006(4)	0.071(5)	-0.006(5)
C(21)	0.061(4)	0.095(5)	0.090(5)	-0.003(4)	0.040(3)	-0.014(4)
C(22)	0.052(3)	0.043(2)	0.035(2)	0.003(2)	0.023(2)	0.004(2)
C(23)	0.059(3)	0.044(3)	0.052(3)	0.000(2)	0.030(2)	0.000(2)
C(24)	0.079(4)	0.068(4)	0.059(3)	0.016(3)	0.042(3)	-0.002(3)
C(25)	0.067(4)	0.084(5)	0.064(3)	0.023(3)	0.042(3)	0.013(3)
C(26)	0.049(3)	0.082(4)	0.065(3)	-0.000(3)	0.029(3)	0.002(3)
C(27)	0.053(3)	0.068(4)	0.051(3)	-0.000(3)	0.025(2)	-0.010(3)
C(28)	0.044(2)	0.037(3)	0.048(3)	0.001(2)	0.019(2)	0.002(2)
C(29)	0.084(4)	0.048(3)	0.084(4)	-0.001(3)	0.047(3)	0.001(3)
C(30)	0.093(5)	0.046(4)	0.114(6)	-0.003(3)	0.052(4)	0.021(4)
C(31)	0.074(4)	0.042(3)	0.109(5)	0.000(3)	0.024(4)	-0.002(4)
C(32)	0.098(5)	0.047(4)	0.101(5)	0.018(3)	0.050(4)	-0.012(3)
C(33)	0.070(4)	0.056(4)	0.067(3)	0.009(3)	0.037(3)	-0.003(3)
C(34)	0.043(2)	0.056(3)	0.036(2)	-0.000(2)	0.019(2)	-0.004(2)
C(35)	0.060(3)	0.064(4)	0.044(3)	-0.003(3)	0.011(2)	0.008(3)
C(36)	0.069(4)	0.090(5)	0.044(3)	0.013(4)	0.004(3)	0.003(3)
C(37)	0.053(3)	0.112(6)	0.051(3)	-0.001(4)	0.014(3)	-0.020(4)
C(38)	0.061(3)	0.075(4)	0.068(4)	-0.022(3)	0.029(3)	-0.026(3)
C(39)	0.049(3)	0.061(4)	0.049(3)	-0.002(3)	0.020(2)	-0.011(3)
C(40)	0.040(2)	0.050(3)	0.034(2)	0.001(2)	0.020(2)	-0.003(2)
C(41)	0.050(3)	0.056(3)	0.057(3)	0.006(2)	0.030(2)	0.008(3)
C(42)	0.071(4)	0.056(3)	0.067(3)	0.020(3)	0.037(3)	0.015(3)
C(43)	0.056(3)	0.090(5)	0.058(3)	0.026(3)	0.028(3)	0.012(3)
C(44)	0.042(3)	0.083(4)	0.053(3)	0.000(3)	0.018(2)	-0.003(3)
C(45)	0.042(3)	0.065(3)	0.051(3)	-0.002(3)	0.021(2)	0.003(3)
C(46)	0.046(2)	0.049(3)	0.040(2)	-0.002(2)	0.026(2)	-0.002(2)
C(47)	0.064(3)	0.058(3)	0.042(2)	0.005(3)	0.025(2)	-0.001(3)
C(48)	0.072(4)	0.080(4)	0.043(3)	-0.002(3)	0.023(3)	-0.018(3)
C(49)	0.079(4)	0.057(4)	0.060(3)	-0.002(3)	0.038(3)	-0.017(3)
C(50)	0.074(4)	0.044(3)	0.073(4)	0.004(3)	0.031(3)	-0.005(3)
C(51)	0.053(3)	0.054(3)	0.047(3)	0.003(3)	0.020(2)	0.001(2)
C(52)	0.037(2)	0.040(3)	0.049(3)	0.003(2)	0.022(2)	0.004(2)
C(53)	0.055(3)	0.086(4)	0.055(3)	-0.018(3)	0.032(3)	-0.000(3)
C(54)	0.066(4)	0.104(5)	0.076(4)	-0.019(4)	0.044(3)	0.011(4)
C(55)	0.049(3)	0.088(5)	0.098(5)	-0.008(3)	0.035(3)	0.020(4)
C(56)	0.062(4)	0.060(4)	0.080(4)	-0.020(3)	0.018(3)	-0.001(3)
C(57)	0.059(3)	0.049(3)	0.053(3)	-0.005(3)	0.024(3)	-0.000(2)

The general temperature factor expression:
$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S19. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance

Ir(1)	P(1)	2.306(1)	Ir(1)	P(2)	2.308(1)
Ir(1)	C(1)	1.844(6)	Ir(1)	C(2)	2.027(5)
P(1)	C(22)	1.831(5)	P(1)	C(28)	1.832(5)
P(1)	C(34)	1.817(5)	P(2)	C(40)	1.831(5)
P(2)	C(46)	1.835(5)	P(2)	C(52)	1.827(5)
O(1)	C(1)	1.158(6)	C(2)	C(3)	1.206(6)
C(3)	C(4)	1.488(7)	C(4)	C(5)	1.540(9)
C(4)	C(6)	1.534(8)	C(4)	C(14)	1.545(8)
C(6)	C(7)	1.517(9)	C(7)	C(8)	1.530(8)
C(8)	C(9)	1.373(9)	C(8)	C(13)	1.369(8)
C(9)	C(10)	1.38(1)	C(10)	C(11)	1.34(1)
C(11)	C(12)	1.37(1)	C(12)	C(13)	1.380(9)
C(14)	C(15)	1.504(8)	C(15)	C(16)	1.516(9)
C(16)	C(17)	1.38(1)	C(16)	C(21)	1.395(8)
C(17)	C(18)	1.38(1)	C(18)	C(19)	1.37(1)
C(19)	C(20)	1.37(1)	C(20)	C(21)	1.373(9)
C(22)	C(23)	1.383(7)	C(22)	C(27)	1.392(7)
C(23)	C(24)	1.393(7)	C(24)	C(25)	1.350(8)
C(25)	C(26)	1.376(8)	C(26)	C(27)	1.390(7)
C(28)	C(29)	1.385(7)	C(28)	C(33)	1.378(7)
C(29)	C(30)	1.388(8)	C(30)	C(31)	1.36(1)
C(31)	C(32)	1.361(9)	C(32)	C(33)	1.391(9)
C(34)	C(35)	1.380(7)	C(34)	C(39)	1.383(7)
C(35)	C(36)	1.389(8)	C(36)	C(37)	1.37(1)
C(37)	C(38)	1.362(9)	C(38)	C(39)	1.391(7)
C(40)	C(41)	1.378(7)	C(40)	C(45)	1.387(7)
C(41)	C(42)	1.395(7)	C(42)	C(43)	1.368(9)
C(43)	C(44)	1.375(9)	C(44)	C(45)	1.381(7)
C(46)	C(47)	1.388(7)	C(46)	C(51)	1.386(7)
C(47)	C(48)	1.388(8)	C(48)	C(49)	1.362(8)
C(49)	C(50)	1.379(8)	C(50)	C(51)	1.387(8)
C(52)	C(53)	1.383(7)	C(52)	C(57)	1.382(7)
C(53)	C(54)	1.373(8)	C(54)	C(55)	1.349(9)
C(55)	C(56)	1.378(9)	C(56)	C(57)	1.392(8)

Table S20. Bond Angles(º)

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	Ir(1)	P(2)	170.70(5)	P(1)	Ir(1)	C(1)	93.4(2)
P(1)	Ir(1)	C(2)	86.3(1)	P(2)	Ir(1)	C(1)	92.5(2)
P(2)	Ir(1)	C(2)	88.7(1)	C(1)	Ir(1)	C(2)	172.9(2)
Ir(1)	P(1)	C(22)	115.2(2)	Ir(1)	P(1)	C(28)	113.2(2)
Ir(1)	P(1)	C(34)	115.8(2)	C(22)	P(1)	C(28)	102.6(2)
C(22)	P(1)	C(34)	103.8(2)	C(28)	P(1)	C(34)	104.7(3)
Ir(1)	P(2)	C(40)	115.7(2)	Ir(1)	P(2)	C(46)	112.7(2)
Ir(1)	P(2)	C(52)	116.3(2)	C(40)	P(2)	C(46)	104.5(2)
C(40)	P(2)	C(52)	102.6(2)	C(46)	P(2)	C(52)	103.5(2)
Ir(1)	C(1)	O(1)	175.6(6)	Ir(1)	C(2)	C(3)	176.7(5)
C(2)	C(3)	C(4)	178.5(6)	C(3)	C(4)	C(5)	109.0(5)
C(3)	C(4)	C(6)	109.5(5)	C(3)	C(4)	C(14)	110.7(5)
C(5)	C(4)	C(6)	106.2(5)	C(5)	C(4)	C(14)	111.0(5)
C(6)	C(4)	C(14)	110.3(5)	C(4)	C(6)	C(7)	115.3(5)
C(6)	C(7)	C(8)	116.4(6)	C(7)	C(8)	C(9)	119.1(7)

C(7)	C(8)	C(13)	124.4(7)	C(9)	C(8)	C(13)	116.5(7)
C(8)	C(9)	C(10)	121.7(7)	C(9)	C(10)	C(11)	120.9(8)
C(10)	C(11)	C(12)	118.7(8)	C(11)	C(12)	C(13)	120.3(8)
C(8)	C(13)	C(12)	121.9(7)	C(4)	C(14)	C(15)	115.9(5)
C(14)	C(15)	C(16)	112.3(6)	C(15)	C(16)	C(17)	121.5(7)
C(15)	C(16)	C(21)	121.3(7)	C(17)	C(16)	C(21)	117.2(7)
C(16)	C(17)	C(18)	122.2(8)	C(17)	C(18)	C(19)	119.2(9)
C(18)	C(19)	C(20)	119.6(8)	C(19)	C(20)	C(21)	120.9(8)
C(16)	C(21)	C(20)	120.8(7)	P(1)	C(22)	C(23)	122.8(4)
P(1)	C(22)	C(27)	119.2(4)	C(23)	C(22)	C(27)	117.9(5)
C(22)	C(23)	C(24)	120.4(5)	C(23)	C(24)	C(25)	121.1(6)
C(24)	C(25)	C(26)	119.9(6)	C(25)	C(26)	C(27)	119.8(6)
C(22)	C(27)	C(26)	120.9(5)	P(1)	C(28)	C(29)	121.6(4)
P(1)	C(28)	C(33)	120.3(4)	C(29)	C(28)	C(33)	118.1(6)
C(28)	C(29)	C(30)	120.8(6)	C(29)	C(30)	C(31)	120.0(7)
C(30)	C(31)	C(32)	120.3(7)	C(31)	C(32)	C(33)	119.9(7)
C(28)	C(33)	C(32)	120.9(6)	P(1)	C(34)	C(35)	123.8(5)
P(1)	C(34)	C(39)	118.6(4)	C(35)	C(34)	C(39)	117.5(5)
C(34)	C(35)	C(36)	121.5(6)	C(35)	C(36)	C(37)	119.7(6)
C(36)	C(37)	C(38)	120.2(6)	C(37)	C(38)	C(39)	120.0(6)
C(34)	C(39)	C(38)	121.0(6)	P(2)	C(40)	C(41)	121.7(4)
P(2)	C(40)	C(45)	119.4(4)	C(41)	C(40)	C(45)	118.8(5)
C(40)	C(41)	C(42)	120.4(6)	C(41)	C(42)	C(43)	119.9(6)
C(42)	C(43)	C(44)	120.3(6)	C(43)	C(44)	C(45)	119.8(6)
C(40)	C(45)	C(44)	120.8(6)	P(2)	C(46)	C(47)	123.8(5)
P(2)	C(46)	C(51)	118.4(4)	C(47)	C(46)	C(51)	117.8(5)
C(46)	C(47)	C(48)	120.5(6)	C(47)	C(48)	C(49)	121.2(5)
C(48)	C(49)	C(50)	119.0(6)	C(49)	C(50)	C(51)	120.3(6)
C(46)	C(51)	C(50)	121.1(5)	P(2)	C(52)	C(53)	122.2(4)
P(2)	C(52)	C(57)	119.4(4)	C(53)	C(52)	C(57)	118.3(5)
C(52)	C(53)	C(54)	121.4(6)	C(53)	C(54)	C(55)	119.8(6)
C(54)	C(55)	C(56)	120.9(6)	C(55)	C(56)	C(57)	119.3(6)
C(52)	C(57)	C(56)	120.2(5)				