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X-Ray Structural Analysis of $Rh(CO)Cl[P(C_6H_5)_2OCH_2CH_2\text{-}n\text{-}C_6F_{13}]_2$.

A crystalline fragment of $Rh(CO)Cl[P(C_6H_5)_2OCH_2CH_2\text{-}n\text{-}C_6F_{13}]_2$ was sealed in a capillary tube and then optically aligned on the goniostat of a Siemens P4 automated X-ray diffractometer.[1] The reflections that were used for the determination of the monoclinic unit cell parameters were located and indexed by the automatic peak search routine XSCANS.[2] The corresponding lattice parameters and orientation matrix were provided from a nonlinear least-squares fit of the orientation angles of 40 centered reflections ($10° < 2\theta < 25°$) at 22 °C. The refined lattice parameters and other pertinent crystallographic information are summarized in Table 1.

Intensity data were measured with graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å) and variable ω scans (4.0-10.0°/min). Background counts were measured at the beginning and at the end of each scan with the crystal and counter kept stationary. The intensities of three standard reflections were measured after every 100 reflections and their combined intensity did not decreased by 2% during data collection. The data were corrected for Lorentz-polarization and the symmetry-equivalent reflections were averaged. No absorption correction was applied.

The initial coordinates for all of the non-hydrogen atoms were determined with a combination of direct methods and difference Fourier calculations performed with algorithms provided by SHELXTL IRIS operating on a Silicon Graphics IRIS Indigo

workstation. Idealized positions for the methylene and phenyl hydrogen atoms were included as fixed contributions using a riding model with isotropic temperature factors set at 1.2 times that of the adjacent carbon. Full-matrix least-squares refinement, based upon the minimization of $\sum w_i|F_o^2 - F_c^2|^2$, with $w_i^{-1} = [\sigma^2(F_o^2) + (0.0976\ P)^2 + 1.37\ P]$ where $P = (\mathrm{Max}(F_o^2,0) + 2\ F_c^2)/3$, was performed with SHELXL-93.[3] After convergence, the final discrepancy indices[4] were R1 = 0.0625, wR2 = 0.1539 for 5045 reflections with $I > 2\ \sigma(I)$ and the overall GOF value was 1.049. Although the molecular structure of $Rh(CO)Cl[P(C_6H_5)_2OCH_2CH_2\text{-}n\text{-}C_6F_{13}]_2$ is reasonably well-behaved, carbons C(40) and C(41) and fluorines F(22), F(23), F(24), F(25), and F(26) display large thermal displacements. However, attempts to refine this C_2F_5 fragment as a static two-site disorder were unsuccessful.

The refined positional parameters for $Rh(CO)Cl[P(C_6H_5)_2OCH_2CH_2\text{-}n\text{-}C_6F_{13}]_2$ with equivalent isotropic displacement parameters are provided in Table 2, Interatomic distances and bond angles are listed in Table 3, anisotropic displacement parameters are tabulated in Table 4, and idealized hydrogen atom coordinates are given in Table 5.

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[2]XSCANS (version 2.0) is a diffractometer control system developed by Siemens Analytical X-ray Instruments, Madison, WI.

[3]SHELXL-93 is a FORTRAN-77 program (Professor G.. Sheldrick, Institut fur Anorganische Chemie, University of Gottingen, D-37077, Gottingen, Germany) for single crystal X-ray structural analyses.

[4]The R-factors were calculated from the expressions $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ and $wR2 = [\Sigma(w_i(F_o^2 - F_c^2)^2)/ \Sigma(w_i(F_o^2)^2)]^{1/2}$ and the standard deviation of an observation of unit weight (GOF) is equal to $[\Sigma(w_i(F_o^2 - F_c^2)^2)/(n - p)]^{1/2}$, where n is the number of reflections and p is the number of parameters varied during the last refinement cycle.

Table 1. Crystal data and structure refinement for $Rh(CO)Cl[PPh_2OCH_2CH_2\text{-}n\text{-}C_6F_{13}]_2$.

Identification code	snolan12
Empirical formula	$C_{41}H_{28}ClF_{26}O_3P_2Rh$
Formula weight	1262.93
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 20.430(4) Å α = 90° b = 10.652(1) Å β = 113.24(1)° c = 24.300(2) Å γ = 90°
Volume	4859.3(10) $Å^3$
Z	4
Density (calculated)	1.726 g/cm^3
Absorption coefficient	6.10 cm^{-1}
F(000)	2496
Crystal size	0.20 x 0.20 x 0.30 mm
θ range for data collection	2.12 to 25.00°
Index ranges	$0 \le h \le 22$, $0 \le k \le 12$, $-28 \le \ell \le 26$
Reflections collected	8494
Independent reflections	8243 (R_{int} = 0.0265)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7161 / 14 / 667
Goodness-of-fit on F^2	1.049
Final R indices [I>2σ(I)]	R1 = 0.0625, wR2 = 0.1539
R indices (all data)	R1 = 0.1163, wR2 = 0.1874
Largest diff. peak and hole	0.731 and -0.561 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for $Rh(CO)Cl[PPh_2OCH_2CH_2\text{-}n\text{-}C_6F_{13}]_2$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Rh	3516(1)	4452(1)	705(1)	43(1)
Cl	4719(1)	5071(1)	1159(1)	60(1)
P(1)	3261(1)	5517(1)	1419(1)	44(1)
P(2)	3737(1)	3207(1)	22(1)	43(1)
F(1)	1147(2)	7263(6)	-424(2)	182(2)
F(2)	1084(3)	8557(4)	181(3)	204(3)
F(3)	-93(2)	7474(7)	173(2)	195(3)
F(4)	-29(2)	6069(4)	-400(2)	168(2)
F(5)	-65(3)	9213(4)	-707(3)	199(3)
F(6)	-190(2)	7615(7)	-1256(2)	179(3)
F(7)	-1261(2)	8680(6)	-533(2)	159(2)
F(8)	-1344(2)	6920(4)	-976(2)	136(2)
F(9)	-1235(3)	9682(5)	-1631(3)	225(3)
F(10)	-1597(3)	7868(8)	-1980(2)	203(3)
F(11)	-2689(3)	9235(5)	-2193(2)	177(3)
F(12)	-2316(3)	10049(5)	-1355(3)	216(3)
F(13)	-2628(2)	8145(5)	-1458(3)	169(2)
F(14)	2712(2)	6814(6)	-799(2)	158(2)
F(15)	2358(2)	5098(4)	-1286(2)	163(2)
F(16)	2613(2)	8040(4)	-1701(2)	149(2)
F(17)	2491(2)	6531(5)	-2253(2)	144(2)
F(18)	1352(2)	7261(5)	-1577(2)	127(2)
F(19)	1245(2)	5892(4)	-2255(2)	139(2)
F(20)	1371(3)	9082(5)	-2310(3)	183(3)
F(21)	1393(2)	7806(5)	-2957(2)	160(2)
F(22)	59(3)	7640(10)	-2470(3)	318(4)
F(23)	188(5)	6949(8)	-3240(4)	319(6)
F(24)	-709(3)	8739(9)	-3453(4)	276(4)
F(25)	91(7)	9682(10)	-2793(6)	550(9)
F(26)	198(4)	9061(9)	-3628(3)	304(4)
O(1)	1990(2)	3839(4)	77(2)	100(2)
O(2)	2426(2)	5853(3)	1239(1)	55(1)
O(3)	3698(2)	3898(3)	-582(1)	49(1)
C(1)	2573(3)	4047(5)	324(2)	62(2)
C(2)	3411(2)	4588(4)	2079(2)	50(1)
C(3)	2970(3)	4669(5)	2392(2)	70(2)
C(4)	3099(3)	3904(7)	2887(2)	94(2)
C(5)	3665(3)	3083(6)	3079(2)	86(2)
C(6)	4097(3)	3009(6)	2773(2)	79(2)
C(7)	3968(3)	3747(5)	2269(2)	66(2)
C(8)	3692(2)	7023(4)	1682(2)	46(1)

C(9)	3807(3)	7502(5)	2246(2)	64(2)
C(10)	4083(3)	8703(5)	2399(2)	77(2)
C(11)	4233(3)	9432(5)	1997(3)	81(2)
C(12)	4119(3)	8957(5)	1441(3)	76(2)
C(13)	3851(3)	7755(5)	1275(2)	59(1)
C(14)	2102(3)	6701(5)	756(2)	69(2)
C(15)	1306(3)	6509(6)	511(2)	71(2)
C(16)	926(3)	7355(6)	10(3)	78(2)
C(17)	121(3)	7260(7)	-261(3)	83(2)
C(18)	-306(4)	8040(6)	-798(3)	93(2)
C(19)	-1103(4)	8110(7)	-960(3)	101(3)
C(20)	-1571(5)	8677(7)	-1541(4)	124(3)
C(21)	-2322(4)	8998(7)	-1626(4)	133(4)
C(22)	3078(2)	1959(4)	-301(2)	51(1)
C(23)	3053(3)	966(5)	52(3)	85(2)
C(24)	2531(4)	101(6)	-151(3)	107(3)
C(25)	2031(4)	180(6)	-721(3)	105(2)
C(26)	2034(3)	1162(6)	-1080(3)	94(2)
C(27)	2573(3)	2052(5)	-880(2)	69(2)
C(28)	4578(2)	2367(4)	289(2)	45(1)
C(29)	4950(3)	2141(5)	-69(2)	60(1)
C(30)	5559(3)	1426(5)	128(2)	69(2)
C(31)	5804(3)	912(5)	690(2)	68(2)
C(32)	5449(3)	1115(5)	1061(2)	66(2)
C(33)	4841(3)	1854(4)	861(2)	58(1)
C(34)	3907(3)	5190(4)	-565(2)	54(1)
C(35)	3484(3)	5802(5)	-1160(2)	63(2)
C(36)	2732(3)	6090(6)	-1269(2)	72(2)
C(37)	2322(3)	6866(6)	-1814(2)	77(2)
C(38)	1531(3)	7046(6)	-2034(3)	85(2)
C(39)	1147(4)	7925(7)	-2536(3)	94(2)
C(40)	330(5)	7952(12)	-2844(4)	175(5)
C(41)	-25(5)	9054(15)	-3240(4)	254(7)

Table 3. Interatomic distances [Å] and bond angles [°] for $Rh(CO)Cl[PPh_2OCH_2CH_2\text{-}n\text{-}C_6F_{13}]_2$.

Rh-C(1)	1.829(5)	Rh-P(1)	2.3000(13)
Rh-P(2)	2.3036(12)	Rh-Cl	2.3565(13)
P(1)-O(2)	1.624(3)	P(1)-C(2)	1.804(5)
P(1)-C(8)	1.821(5)	P(2)-O(3)	1.616(3)
P(2)-C(28)	1.814(4)	P(2)-C(22)	1.834(5)
F(1)-C(16)	1.305(8)	F(2)-C(16)	1.345(7)
F(3)-C(17)	1.311(8)	F(4)-C(17)	1.317(8)
F(5)-C(18)	1.329(8)	F(6)-C(18)	1.307(9)
F(7)-C(19)	1.347(9)	F(8)-C(19)	1.354(8)
F(9)-C(20)	1.335(10)	F(10)-C(20)	1.355(10)
F(11)-C(21)	1.308(9)	F(12)-C(21)	1.296(9)
F(13)-C(21)	1.257(9)	F(14)-C(36)	1.393(7)
F(15)-C(36)	1.295(7)	F(16)-C(37)	1.365(7)
F(17)-C(37)	1.295(7)	F(18)-C(38)	1.318(8)
F(19)-C(38)	1.376(7)	F(20)-C(39)	1.354(8)
F(21)-C(39)	1.313(8)	F(22)-C(40)	1.280(12)
F(23)-C(40)	1.390(12)	F(24)-C(41)	1.327(12)
F(25)-C(41)	1.22(2)	F(26)-C(41)	1.199(12)
O(1)-C(1)	1.123(6)	O(2)-C(14)	1.422(6)
O(3)-C(34)	1.436(5)	C(2)-C(7)	1.377(7)
C(2)-C(3)	1.390(7)	C(3)-C(4)	1.391(8)
C(4)-C(5)	1.377(9)	C(5)-C(6)	1.362(9)
C(6)-C(7)	1.390(7)	C(8)-C(9)	1.392(6)
C(8)-C(13)	1.396(7)	C(9)-C(10)	1.388(7)
C(10)-C(11)	1.375(9)	C(11)-C(12)	1.375(8)
C(12)-C(13)	1.389(7)	C(14)-C(15)	1.509(7)
C(15)-C(16)	1.466(7)	C(16)-C(17)	1.515(8)
C(17)-C(18)	1.503(8)	C(18)-C(19)	1.518(10)
C(19)-C(20)	1.486(10)	C(20)-C(21)	1.506(12)
C(22)-C(23)	1.376(7)	C(22)-C(27)	1.383(6)
C(23)-C(24)	1.346(8)	C(24)-C(25)	1.361(9)
C(25)-C(26)	1.364(9)	C(26)-C(27)	1.388(8)
C(28)-C(29)	1.384(7)	C(28)-C(33)	1.389(6)

C(29)-C(30)	1.375(7)	C(30)-C(31)	1.369(7)
C(31)-C(32)	1.380(8)	C(32)-C(33)	1.385(7)
C(34)-C(35)	1.509(6)	C(35)-C(36)	1.485(8)
C(36)-C(37)	1.503(7)	C(37)-C(38)	1.502(9)
C(38)-C(39)	1.492(9)	C(39)-C(40)	1.536(11)
C(40)-C(41)	1.51(2)		

C(1)-Rh-P(1)	89.5(2)	C(1)-Rh-P(2)	88.1(2)
P(1)-Rh-P(2)	174.32(5)	C(1)-Rh-Cl	176.8(2)
P(1)-Rh-Cl	90.79(5)	P(2)-Rh-Cl	91.90(5)
O(2)-P(1)-C(2)	98.8(2)	O(2)-P(1)-C(8)	102.2(2)
C(2)-P(1)-C(8)	106.4(2)	O(2)-P(1)-Rh	115.57(12)
C(2)-P(1)-Rh	113.0(2)	C(8)-P(1)-Rh	118.5(2)
O(3)-P(2)-C(28)	104.5(2)	O(3)-P(2)-C(22)	100.2(2)
C(28)-P(2)-C(22)	103.1(2)	O(3)-P(2)-Rh	116.02(12)
C(28)-P(2)-Rh	116.98(14)	C(22)-P(2)-Rh	113.9(2)
C(14)-O(2)-P(1)	117.4(3)	C(34)-O(3)-P(2)	120.1(3)
O(1)-C(1)-Rh	177.3(5)	C(7)-C(2)-C(3)	119.0(5)
C(7)-C(2)-P(1)	118.9(4)	C(3)-C(2)-P(1)	122.1(4)
C(2)-C(3)-C(4)	119.7(5)	C(5)-C(4)-C(3)	120.7(6)
C(6)-C(5)-C(4)	119.4(5)	C(5)-C(6)-C(7)	120.6(6)
C(2)-C(7)-C(6)	120.5(6)	C(9)-C(8)-C(13)	119.8(4)
C(9)-C(8)-P(1)	122.6(4)	C(13)-C(8)-P(1)	117.4(3)
C(10)-C(9)-C(8)	119.7(5)	C(11)-C(10)-C(9)	120.7(5)
C(12)-C(11)-C(10)	119.5(5)	C(11)-C(12)-C(13)	121.3(6)
C(12)-C(13)-C(8)	119.0(5)	O(2)-C(14)-C(15)	108.5(4)
C(16)-C(15)-C(14)	112.2(5)	F(1)-C(16)-F(2)	101.8(6)
F(1)-C(16)-C(15)	112.7(5)	F(2)-C(16)-C(15)	110.2(5)
F(1)-C(16)-C(17)	107.8(5)	F(2)-C(16)-C(17)	106.5(5)
C(15)-C(16)-C(17)	116.6(5)	F(3)-C(17)-F(4)	104.9(7)
F(3)-C(17)-C(18)	109.8(6)	F(4)-C(17)-C(18)	108.2(5)
F(3)-C(17)-C(16)	106.7(5)	F(4)-C(17)-C(16)	106.1(5)
C(18)-C(17)-C(16)	120.0(6)	F(6)-C(18)-F(5)	106.7(7)
F(6)-C(18)-C(17)	108.0(6)	F(5)-C(18)-C(17)	109.0(5)
F(6)-C(18)-C(19)	109.5(6)	F(5)-C(18)-C(19)	106.7(6)
C(17)-C(18)-C(19)	116.6(6)	F(7)-C(19)-F(8)	104.5(7)
F(7)-C(19)-C(20)	106.8(7)	F(8)-C(19)-C(20)	105.3(6)
F(7)-C(19)-C(18)	112.4(6)	F(8)-C(19)-C(18)	107.6(6)
C(20)-C(19)-C(18)	119.2(7)	F(9)-C(20)-F(10)	104.2(8)

F(9)-C(20)-C(19)	107.5(6)	F(10)-C(20)-C(19)	107.5(7)
F(9)-C(20)-C(21)	111.0(7)	F(10)-C(20)-C(21)	108.4(7)
C(19)-C(20)-C(21)	117.4(8)	F(13)-C(21)-F(12)	111.6(9)
F(13)-C(21)-F(11)	109.2(7)	F(12)-C(21)-F(11)	104.7(7)
F(13)-C(21)-C(20)	113.7(7)	F(12)-C(21)-C(20)	108.7(7)
F(11)-C(21)-C(20)	108.4(8)	C(23)-C(22)-C(27)	119.6(5)
C(23)-C(22)-P(2)	119.5(4)	C(27)-C(22)-P(2)	120.7(4)
C(24)-C(23)-C(22)	121.1(6)	C(23)-C(24)-C(25)	119.9(7)
C(24)-C(25)-C(26)	120.5(6)	C(25)-C(26)-C(27)	120.3(6)
C(22)-C(27)-C(26)	118.5(5)	C(29)-C(28)-C(33)	118.0(4)
C(29)-C(28)-P(2)	122.5(3)	C(33)-C(28)-P(2)	119.4(4)
C(30)-C(29)-C(28)	121.5(5)	C(31)-C(30)-C(29)	119.7(5)
C(30)-C(31)-C(32)	120.5(5)	C(31)-C(32)-C(33)	119.3(5)
C(32)-C(33)-C(28)	121.0(5)	O(3)-C(34)-C(35)	109.5(4)
C(36)-C(35)-C(34)	114.9(5)	F(15)-C(36)-F(14)	105.6(6)
F(15)-C(36)-C(35)	113.1(5)	F(14)-C(36)-C(35)	109.4(4)
F(15)-C(36)-C(37)	107.7(5)	F(14)-C(36)-C(37)	103.4(5)
C(35)-C(36)-C(37)	116.7(5)	F(17)-C(37)-F(16)	100.4(5)
F(17)-C(37)-C(38)	110.0(5)	F(16)-C(37)-C(38)	106.1(5)
F(17)-C(37)-C(36)	109.7(5)	F(16)-C(37)-C(36)	106.3(5)
C(38)-C(37)-C(36)	122.1(6)	F(18)-C(38)-F(19)	105.6(6)
F(18)-C(38)-C(39)	110.4(6)	F(19)-C(38)-C(39)	103.6(5)
F(18)-C(38)-C(37)	109.9(5)	F(19)-C(38)-C(37)	104.9(5)
C(39)-C(38)-C(37)	121.1(6)	F(21)-C(39)-F(20)	103.4(7)
F(21)-C(39)-C(38)	109.7(6)	F(20)-C(39)-C(38)	104.8(5)
F(21)-C(39)-C(40)	107.4(6)	F(20)-C(39)-C(40)	108.0(7)
C(38)-C(39)-C(40)	122.0(8)	F(22)-C(40)-F(23)	105.1(11)
F(22)-C(40)-C(41)	114.9(10)	F(23)-C(40)-C(41)	103.8(8)
F(22)-C(40)-C(39)	109.9(7)	F(23)-C(40)-C(39)	102.3(8)
C(41)-C(40)-C(39)	118.8(10)	F(26)-C(41)-F(25)	134(2)
F(26)-C(41)-F(24)	111.4(9)	F(25)-C(41)-F(24)	106.9(11)
F(26)-C(41)-C(40)	105.7(11)	F(25)-C(41)-C(40)	88.9(9)
F(24)-C(41)-C(40)	102.6(11)		

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for $Rh(CO)Cl[PPh_2OCH_2CH_2\text{-}n\text{-}C_6F_{13}]_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2U_{11} + \ldots + 2hka^*b^*U_{12}]$.

	U11	U22	U33	U23	U13	U12
Rh	48(1)	43(1)	41(1)	-3(1)	21(1)	-2(1)
Cl	50(1)	66(1)	64(1)	-11(1)	21(1)	-5(1)
P(1)	45(1)	49(1)	40(1)	0(1)	19(1)	1(1)
P(2)	52(1)	39(1)	42(1)	-1(1)	21(1)	-3(1)
F(1)	93(2)	348(6)	120(2)	125(3)	57(2)	76(3)
F(2)	119(3)	70(3)	290(6)	27(4)	-63(4)	2(3)
F(3)	98(3)	384(8)	107(3)	80(4)	45(2)	94(4)
F(4)	116(3)	77(2)	214(5)	50(3)	-37(3)	-18(2)
F(5)	116(3)	95(3)	271(6)	86(3)	-46(4)	-29(3)
F(6)	126(3)	322(7)	86(2)	60(4)	38(2)	77(4)
F(7)	117(3)	223(5)	118(3)	-22(3)	27(3)	61(3)
F(8)	98(3)	97(3)	182(4)	44(3)	23(3)	-19(2)
F(9)	113(4)	212(4)	271(5)	178(4)	-8(4)	-33(3)
F(10)	168(5)	290(8)	128(4)	1(5)	33(4)	48(5)
F(11)	115(4)	179(5)	178(5)	49(4)	-4(3)	0(4)
F(12)	139(4)	132(4)	289(7)	-57(5)	-11(5)	40(4)
F(13)	93(3)	159(4)	213(5)	56(4)	16(3)	-18(3)
F(14)	136(3)	259(5)	80(2)	16(3)	43(2)	91(3)
F(15)	70(2)	125(3)	269(5)	119(3)	38(3)	-4(2)
F(16)	99(3)	92(3)	198(4)	43(3)	-2(3)	-21(2)
F(17)	135(3)	232(5)	72(2)	39(3)	49(2)	74(3)
F(18)	99(2)	202(4)	95(2)	21(3)	55(2)	35(3)
F(19)	112(3)	95(3)	175(4)	7(3)	19(3)	-23(2)
F(20)	172(5)	97(3)	221(6)	16(4)	14(4)	9(3)
F(21)	155(3)	235(5)	100(2)	72(3)	60(2)	90(3)
F(22)	144(3)	605(13)	244(5)	230(7)	118(3)	159(6)
F(23)	278(9)	208(7)	417(12)	-133(8)	81(9)	-62(7)
F(24)	130(5)	326(9)	293(8)	74(8)	1(5)	50(6)
F(25)	400(12)	342(10)	959(21)	-380(11)	324(13)	-38(10)
F(26)	286(7)	426(9)	221(6)	177(6)	124(5)	220(7)
O(1)	58(2)	123(3)	118(3)	-52(3)	33(2)	-20(2)
O(2)	52(2)	57(2)	58(2)	3(2)	23(1)	4(2)
O(3)	67(2)	44(2)	40(1)	2(1)	24(1)	-2(2)
C(1)	55(3)	71(3)	59(3)	-18(2)	23(2)	-6(3)
C(2)	60(2)	50(3)	42(2)	-6(2)	23(2)	-6(2)
C(3)	86(3)	70(4)	69(3)	5(3)	47(2)	0(3)
C(4)	111(4)	122(5)	64(3)	9(3)	50(3)	-26(4)
C(5)	100(4)	90(4)	48(3)	17(3)	9(3)	-36(4)
C(6)	79(4)	75(4)	64(3)	18(3)	8(3)	-3(3)
C(7)	62(3)	77(4)	55(3)	10(3)	20(2)	1(3)
C(8)	44(2)	50(3)	45(2)	-2(2)	18(2)	4(2)
C(9)	69(3)	71(3)	61(3)	-7(3)	35(2)	0(3)
C(10)	71(3)	76(4)	76(3)	-36(3)	22(3)	-11(3)

C(11)	83(3)	47(3)	113(4)	-18(3)	40(3)	-10(3)
C(12)	85(4)	55(3)	83(4)	9(3)	29(3)	-7(3)
C(13)	71(3)	49(3)	57(3)	-5(2)	26(2)	-4(2)
C(14)	58(3)	58(3)	83(3)	8(3)	19(3)	6(3)
C(15)	55(3)	86(4)	68(3)	17(3)	18(2)	8(3)
C(16)	66(3)	66(4)	92(4)	15(3)	22(3)	8(3)
C(17)	71(4)	90(5)	77(4)	10(3)	17(3)	5(3)
C(18)	78(4)	79(4)	96(5)	21(4)	5(4)	3(4)
C(19)	87(4)	88(5)	104(5)	18(4)	14(4)	6(4)
C(20)	129(6)	87(5)	116(6)	19(5)	5(5)	2(5)
C(21)	73(5)	91(5)	179(8)	31(6)	-9(5)	18(4)
C(22)	60(2)	42(3)	59(2)	-7(2)	33(2)	-3(2)
C(23)	85(4)	65(3)	91(4)	13(3)	19(3)	-30(3)
C(24)	108(4)	68(4)	148(6)	9(4)	55(4)	-34(4)
C(25)	106(4)	79(4)	138(5)	-37(4)	58(4)	-50(4)
C(26)	93(4)	96(5)	86(4)	-22(4)	28(3)	-34(4)
C(27)	75(3)	70(3)	62(3)	-10(3)	27(3)	-20(3)
C(28)	50(2)	33(2)	51(2)	-6(2)	21(2)	-9(2)
C(29)	65(3)	63(3)	54(3)	-5(2)	24(2)	-9(3)
C(30)	53(3)	74(4)	85(3)	-12(3)	33(2)	4(3)
C(31)	56(3)	53(3)	88(4)	-10(3)	20(3)	7(2)
C(32)	77(3)	43(3)	69(3)	3(2)	18(3)	-4(3)
C(33)	71(3)	46(3)	58(3)	0(2)	27(2)	2(2)
C(34)	63(3)	46(3)	54(2)	3(2)	24(2)	-16(2)
C(35)	71(3)	58(3)	66(3)	8(2)	34(2)	-3(3)
C(36)	84(3)	67(3)	68(3)	12(3)	33(3)	-2(3)
C(37)	96(4)	72(4)	69(3)	-4(3)	39(3)	-14(3)
C(38)	89(4)	83(4)	77(4)	7(3)	25(3)	4(4)
C(39)	101(4)	98(5)	75(4)	-5(4)	25(3)	22(4)
C(40)	120(7)	244(12)	129(7)	-21(8)	16(6)	52(8)
C(41)	145(7)	506(20)	99(6)	124(9)	35(6)	174(10)

Table 5. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $Rh(CO)Cl[PPh_2OCH_2CH_2\text{-}n\text{-}C_6F_{13}]_2$.

	x	y	z	U(eq)
H(3A)	2592(3)	5232(5)	2270(2)	84
H(4A)	2799(3)	3948(7)	3092(2)	113
H(5A)	3751(3)	2582(6)	3414(2)	103
H(6A)	4482(3)	2461(6)	2903(2)	95
H(7A)	4260(3)	3672(5)	2059(2)	79
H(9A)	3701(3)	7019(5)	2519(2)	77
H(10A)	4167(3)	9017(5)	2778(2)	92
H(11A)	4410(3)	10241(5)	2101(3)	97
H(12A)	4224(3)	9450(5)	1170(3)	91
H(13A)	3779(3)	7442(5)	898(2)	70
H(14A)	2277(3)	6547(5)	444(2)	83
H(14B)	2218(3)	7559(5)	894(2)	83
H(15A)	1198(3)	5647(6)	378(2)	86
H(15B)	1139(3)	6650(6)	828(2)	86
H(23A)	3402(3)	891(5)	438(3)	102
H(24A)	2513(4)	-549(6)	98(3)	128
H(25A)	1685(4)	-441(6)	-866(3)	126
H(26A)	1673(3)	1235(6)	-1460(3)	112
H(27A)	2594(3)	2697(5)	-1131(2)	83
H(29A)	4783(3)	2481(5)	-453(2)	72
H(30A)	5804(3)	1294(5)	-118(2)	83
H(31A)	6214(3)	420(5)	822(2)	82
H(32A)	5615(3)	760(5)	1441(2)	79
H(33A)	4607(3)	2008(4)	1113(2)	69
H(34A)	4412(3)	5242(4)	-479(2)	65
H(34B)	3821(3)	5626(4)	-249(2)	65
H(35A)	3720(3)	6576(5)	-1186(2)	76
H(35B)	3490(3)	5252(5)	-1476(2)	76