

ORGANOMETALLICS

Organometallics, 1998, 17(1), 10-12, DOI:[10.1021/om970784y](https://doi.org/10.1021/om970784y)

Terms & Conditions

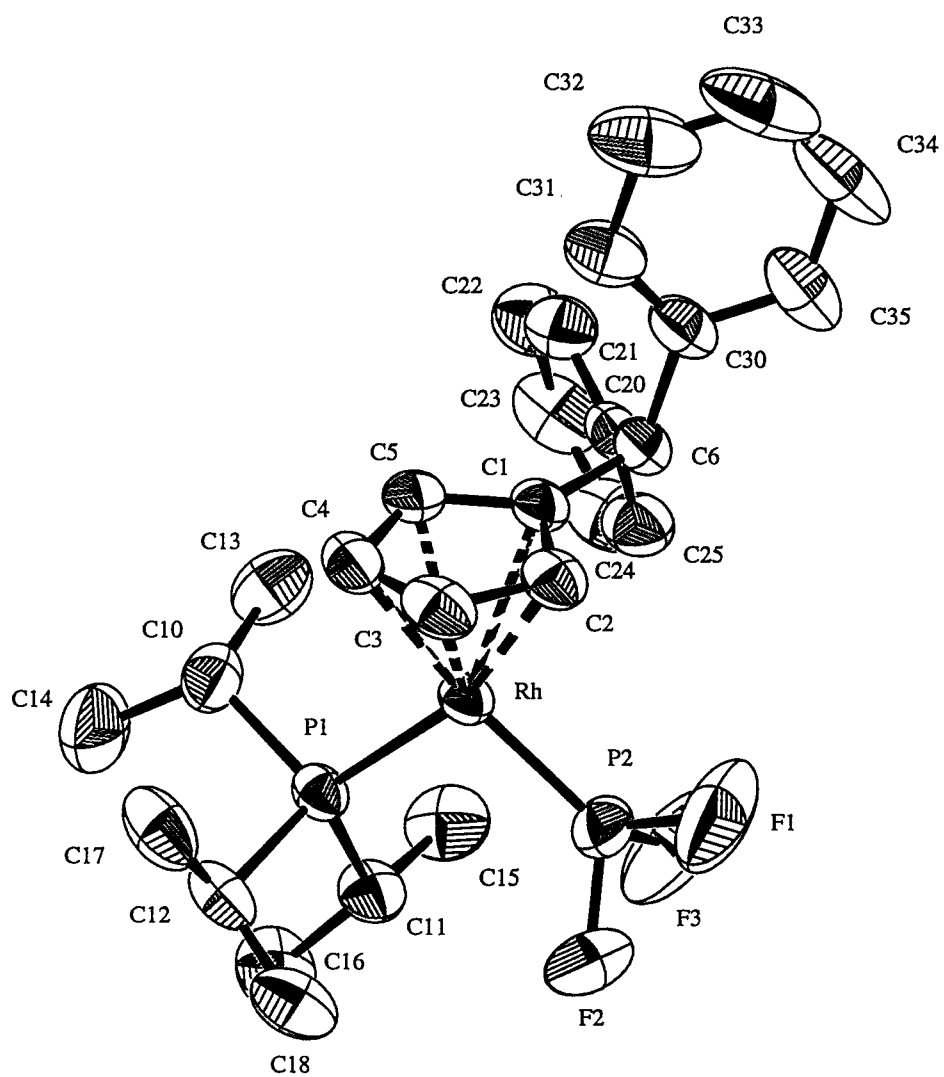
Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1998 American Chemical Society



ORTEP drawing of 5

Table 1. Crystal data and structure refinement for 5a)b).

formula	C ₂₇ H ₃₆ F ₃ P ₂ Rh
fw	582.41
crystal size, mm ³	0.55 x 0.30 x 0.25
crystal system	Monoclinic
space group	C 2/c (No.15)
cell dimensions determin	25 reflcns, 2° < Θ < 20°
a, Å	34.48(9)
b, Å	8.96(2)
c, Å	17.67(3)
β , deg	96.82(9)
V, Å ³	5427(3)
Z	8
d _{calc} , gcm ⁻³	1.426
diffractometer	CAD4 (Enraf-Nonius)
radiation	Mo-K α (0.70930 Å), graphite mono- chromator, Zr filter (factor 16.4)
temp, K	293(2)
μ , mm ⁻¹	0.781
scan method	ω/Θ
2 Θ (max), deg	48
tot. no. of rflcns scanned	4548
no. of unique rflcns	4162 [R(int) = 0.0136]
no. of data	4162
no. of obsd rflcns [I>2 σ (I)]	3736
correct. appl.	LP, emp. abs. corr. (Ψ -scans, min. transm. 80.0%)
structure solution	Patterson (SHELXS-86)
param	408 (full-matrix least-squares on F ² (SHELXL-93))
reflex/param ratio	10.2
final R indices [I>2 σ (I)]	R1 = 0.0364, wR2 = 0.0922
R indices (all data)	R1 = 0.0420, wR2 = 0.0972
resid electron density, eÅ ⁻³	1.058 / -0.425

a) Crystals grown from pentane

b) The positions of all hydrogen atoms were found in a final difference fourier synthesis and were refined anisotropically with fixed U_{eq}. except for H6 which was found and refined without restrictions.

c) weighting scheme : $w = 1/[\sigma^2(F_o^2) + (0.0634 \cdot P)^2 + 6.3885 \cdot P]$ where
 $P = (F_o^2 + 2F_c^2)/3$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Rh	4117(1)	1698(1)	4995(1)	38(1)
P(1)	4159(1)	2625(1)	3810(1)	41(1)
P(2)	4582(1)	2898(1)	5558(1)	56(1)
F(1)	4723(1)	2463(5)	6379(2)	143(2)
F(2)	4986(1)	3023(6)	5310(2)	151(2)
F(3)	4577(1)	4577(4)	5730(3)	139(2)
C(1)	3638(1)	1139(4)	5757(2)	44(1)
C(2)	3976(1)	208(4)	5926(2)	51(1)
C(3)	4015(1)	-745(4)	5306(2)	57(1)
C(4)	3731(1)	-314(5)	4728(2)	58(1)
C(5)	3489(1)	824(4)	5005(2)	49(1)
C(6)	3478(1)	2192(4)	6316(2)	48(1)
C(10)	3670(1)	2551(5)	3229(2)	56(1)
C(11)	4364(1)	4541(4)	3736(2)	52(1)
C(12)	4474(1)	1479(5)	3251(2)	58(1)
C(13)	3365(2)	3531(6)	3554(3)	73(1)
C(14)	3666(2)	2827(9)	2378(3)	94(2)
C(15)	4129(2)	5715(5)	4101(3)	72(1)
C(16)	4453(2)	5052(7)	2948(3)	91(2)
C(17)	4330(2)	-132(5)	3177(3)	75(1)
C(18)	4900(2)	1532(7)	3600(4)	83(2)
C(20)	3276(1)	3537(4)	5925(2)	48(1)
C(21)	2878(1)	3566(5)	5680(2)	60(1)
C(22)	2710(2)	4794(6)	5306(3)	74(1)
C(23)	2925(2)	6024(6)	5173(3)	79(1)
C(24)	3317(2)	6020(5)	5422(3)	77(1)
C(25)	3490(1)	4790(5)	5787(3)	62(1)
C(30)	3220(1)	1388(5)	6829(2)	56(1)
C(31)	3004(2)	153(7)	6595(3)	79(1)
C(32)	2752(2)	-510(8)	7068(5)	111(2)
C(33)	2722(2)	47(11)	7764(5)	116(3)
C(34)	2947(2)	1235(11)	8022(4)	107(2)
C(35)	3193(2)	1921(7)	7553(3)	82(2)

Table 3. Bond lengths [$\text{\AA}$] for **5**.

Rh-P(2)	2.082(4)
Rh-C(2)	2.220(5)
Rh-C(4)	2.258(5)
Rh-P(1)	2.275(3)
Rh-C(3)	2.294(6)
Rh-C(5)	2.304(6)
Rh-C(1)	2.307(5)
P(1)-C(12)	1.862(5)
P(1)-C(11)	1.867(5)
P(1)-C(10)	1.870(6)
P(2)-F(2)	1.512(5)
P(2)-F(1)	1.527(4)
P(2)-F(3)	1.535(5)
C(1)-C(5)	1.398(5)
C(1)-C(2)	1.434(6)
C(1)-C(6)	1.518(5)
C(2)-C(3)	1.410(6)
C(3)-C(4)	1.385(7)

C(4)-C(5)	1.438(6)
C(6)-C(20)	1.517(6)
C(6)-C(30)	1.526(6)
C(10)-C(14)	1.525(7)
C(10)-C(13)	1.532(7)
C(11)-C(15)	1.519(7)
C(11)-C(16)	1.532(6)
C(12)-C(17)	1.526(7)
C(12)-C(18)	1.526(8)
C(20)-C(25)	1.380(6)
C(20)-C(21)	1.390(7)
C(21)-C(22)	1.376(7)
C(22)-C(23)	1.364(8)
C(23)-C(24)	1.370(8)
C(24)-C(25)	1.376(7)
C(30)-C(31)	1.369(7)
C(30)-C(35)	1.381(7)
C(31)-C(32)	1.409(7)
C(32)-C(33)	1.34(1)
C(33)-C(34)	1.36(1)
C(34)-C(35)	1.399(9)

Table 4. Bond angles [deg] for **5**.

P(2)-Rh-C(2)	100.4(2)
P(2)-Rh-C(4)	156.0(1)
C(2)-Rh-C(4)	60.0(2)
P(2)-Rh-P(1)	97.0(1)
C(2)-Rh-P(1)	161.3(1)
C(4)-Rh-P(1)	101.5(2)
P(2)-Rh-C(3)	120.6(2)
C(2)-Rh-C(3)	36.3(2)
C(4)-Rh-C(3)	35.4(2)
P(1)-Rh-C(3)	126.7(1)
P(2)-Rh-C(5)	147.4(1)
C(2)-Rh-C(5)	60.0(2)
C(4)-Rh-C(5)	36.7(2)
P(1)-Rh-C(5)	107.1(1)
C(3)-Rh-C(5)	60.1(2)
P(2)-Rh-C(1)	113.3(2)
C(2)-Rh-C(1)	36.9(3)
C(4)-Rh-C(1)	60.3(2)
P(1)-Rh-C(1)	138.3(1)
C(3)-Rh-C(1)	60.8(2)
C(5)-Rh-C(1)	35.3(2)
C(12)-P(1)-C(11)	102.7(2)
C(12)-P(1)-C(10)	103.5(2)
C(11)-P(1)-C(10)	108.6(2)
C(12)-P(1)-Rh	113.2(2)
C(11)-P(1)-Rh	117.8(1)
C(10)-P(1)-Rh	110.0(2)
F(2)-P(2)-F(1)	95.4(3)
F(2)-P(2)-F(3)	90.9(3)
F(1)-P(2)-F(3)	94.1(3)
F(2)-P(2)-Rh	125.6(2)
F(1)-P(2)-Rh	117.6(2)
F(3)-P(2)-Rh	125.1(2)
C(5)-C(1)-C(2)	106.2(3)
C(5)-C(1)-C(6)	128.6(4)
C(2)-C(1)-C(6)	125.1(3)
C(5)-C(1)-Rh	72.2(2)
C(2)-C(1)-Rh	68.3(2)
C(6)-C(1)-Rh	126.0(3)
C(3)-C(2)-C(1)	109.8(4)
C(3)-C(2)-Rh	74.7(3)

C(1)-C(2)-Rh	74.9(2)
C(4)-C(3)-C(2)	106.4(4)
C(4)-C(3)-Rh	70.9(2)
C(2)-C(3)-Rh	68.9(2)
C(3)-C(4)-C(5)	109.4(4)
C(3)-C(4)-Rh	73.7(3)
C(5)-C(4)-Rh	73.4(3)
C(1)-C(5)-C(4)	107.8(4)
C(1)-C(5)-Rh	72.5(2)
C(4)-C(5)-Rh	69.9(3)
C(20)-C(6)-C(1)	112.3(3)
C(20)-C(6)-C(30)	112.3(3)
C(1)-C(6)-C(30)	112.2(4)
C(14)-C(10)-C(13)	110.6(5)
C(14)-C(10)-P(1)	116.0(4)
C(13)-C(10)-P(1)	112.8(3)
C(15)-C(11)-C(16)	110.7(4)
C(15)-C(11)-P(1)	112.4(3)
C(16)-C(11)-P(1)	117.2(3)
C(17)-C(12)-C(18)	110.5(4)
C(17)-C(12)-P(1)	111.3(3)
C(18)-C(12)-P(1)	111.2(4)
C(25)-C(20)-C(21)	117.2(4)
C(25)-C(20)-C(6)	120.2(4)
C(21)-C(20)-C(6)	122.6(4)
C(22)-C(21)-C(20)	120.5(4)
C(23)-C(22)-C(21)	121.5(5)
C(22)-C(23)-C(24)	118.5(5)
C(23)-C(24)-C(25)	120.6(5)
C(24)-C(25)-C(20)	121.6(5)
C(31)-C(30)-C(35)	117.9(4)
C(31)-C(30)-C(6)	122.3(4)
C(35)-C(30)-C(6)	119.8(4)
C(30)-C(31)-C(32)	120.7(6)
C(33)-C(32)-C(31)	120.6(7)
C(32)-C(33)-C(34)	119.6(6)
C(33)-C(34)-C(35)	120.4(6)
C(30)-C(35)-C(34)	120.7(7)

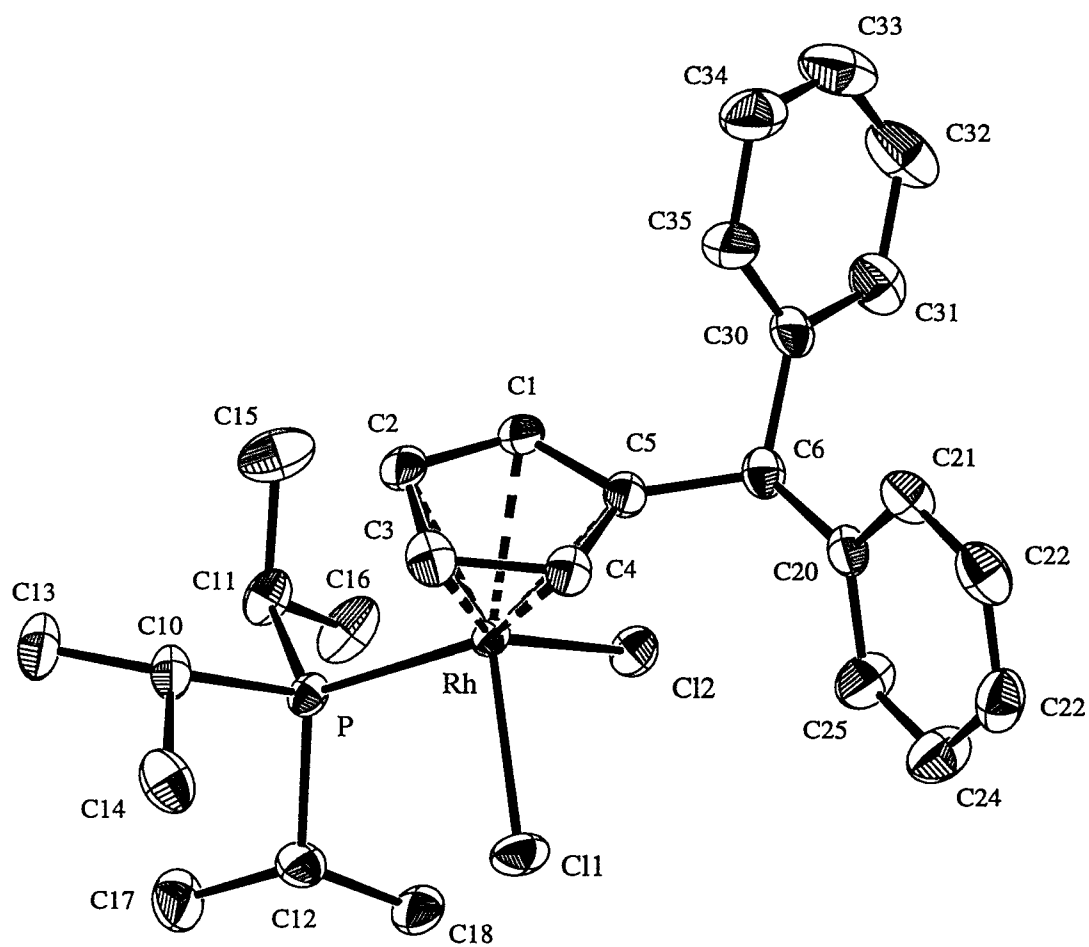
Table 5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 5.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Rh	44(1)	35(1)	37(1)	-1(1)	13(1)	-7(1)
P(1)	50(1)	36(1)	40(1)	0(1)	14(1)	-4(1)
P(2)	57(1)	61(1)	50(1)	0(1)	4(1)	-19(1)
F(1)	173(4)	160(4)	78(2)	35(2)	-50(2)	-90(3)
F(2)	69(2)	244(5)	144(3)	-77(3)	28(2)	-71(3)
F(3)	126(3)	73(2)	200(4)	-34(2)	-50(3)	-27(2)
C(1)	48(2)	44(2)	42(2)	0(2)	16(1)	-11(2)
C(2)	59(2)	47(2)	48(2)	11(2)	15(2)	-5(2)
C(3)	71(3)	40(2)	65(2)	7(2)	27(2)	-4(2)
C(4)	74(3)	50(2)	54(2)	-15(2)	28(2)	-25(2)
C(5)	46(2)	52(2)	50(2)	-3(2)	15(2)	-15(2)
C(6)	51(2)	54(2)	41(2)	-3(2)	14(2)	-6(2)
C(10)	62(2)	54(2)	50(2)	-1(2)	-1(2)	-11(2)
C(11)	64(2)	41(2)	53(2)	7(2)	15(2)	-11(2)
C(12)	76(3)	55(2)	48(2)	0(2)	30(2)	6(2)
C(13)	55(3)	69(3)	91(4)	4(3)	-8(2)	6(2)

C(14)	99(4)	124(5)	56(3)	6(3)	-12(3)	-16(4)
C(15)	79(3)	41(2)	97(4)	-1(2)	15(3)	-6(2)
C(16)	132(5)	74(4)	69(3)	19(3)	26(3)	-38(4)
C(17)	109(4)	53(3)	69(3)	-12(2)	39(3)	10(3)
C(18)	73(3)	92(4)	89(4)	0(3)	37(3)	18(3)
C(20)	57(2)	47(2)	44(2)	-9(2)	21(2)	-5(2)
C(21)	59(3)	59(3)	65(3)	4(2)	16(2)	-5(2)
C(22)	67(3)	79(3)	78(3)	8(3)	15(2)	7(3)
C(23)	100(4)	57(3)	87(3)	11(2)	39(3)	15(3)
C(24)	93(4)	47(3)	99(4)	3(2)	41(3)	-6(2)
C(25)	64(2)	54(3)	73(3)	-8(2)	22(2)	-11(2)
C(30)	56(2)	70(3)	45(2)	12(2)	18(2)	9(2)
C(31)	83(3)	88(4)	71(3)	16(3)	30(3)	-23(3)
C(32)	101(4)	109(5)	131(6)	43(4)	52(4)	-23(4)
C(33)	95(4)	151(7)	114(6)	75(6)	62(4)	31(5)
C(34)	117(5)	153(6)	62(3)	37(4)	54(3)	64(5)
C(35)	97(4)	101(4)	53(3)	5(3)	31(3)	24(3)

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**.

	x	y	z	U(eq)
H(2)	4132(12)	235(46)	6375(25)	61
H(3)	4227(13)	-1433(51)	5309(25)	68
H(4)	3685(13)	-608(52)	4291(26)	69
H(5)	3265(12)	1306(47)	4754(23)	58
H(6)	3712(12)	2606(47)	6684(23)	62(11)
H(10)	3607(13)	1614(49)	3326(26)	67
H(11)	4623(12)	4411(46)	4074(23)	62
H(12)	4470(12)	1970(49)	2746(27)	70
H(13A)	3409(18)	3503(63)	4153(39)	110
H(13B)	3136(19)	3255(65)	3374(37)	110
H(13C)	3398(17)	4539(73)	3402(34)	110
H(14A)	3879(21)	2307(91)	2148(42)	142
H(14B)	3733(21)	3867(87)	2271(41)	142
H(14C)	3426(22)	2636(84)	2174(44)	142
H(15A)	4107(17)	5484(72)	4570(36)	108
H(15B)	3902(18)	5965(69)	3806(34)	108
H(15C)	4314(17)	6723(65)	4212(32)	108
H(16A)	4608(21)	4369(84)	2702(41)	136
H(16B)	4591(20)	6004(92)	3016(39)	136
H(16C)	4214(22)	5191(77)	2626(40)	136
H(17A)	4058(19)	-170(67)	2977(35)	112
H(17B)	4362(16)	-575(67)	3691(35)	112
H(17C)	4512(16)	-673(70)	2849(34)	112
H(18A)	4952(18)	1137(78)	4111(40)	124
H(18B)	5010(19)	2470(83)	3638(39)	124
H(18C)	5044(19)	922(77)	3354(38)	124
H(21)	2728(13)	2772(55)	5791(25)	72
H(22)	2449(16)	4724(57)	5123(29)	89
H(23)	2790(15)	6871(59)	4816(31)	95
H(24)	3440(16)	6782(59)	5286(33)	93
H(25)	3755(14)	4776(52)	5964(25)	75
H(31)	3020(16)	-296(65)	6210(31)	95
H(32)	2625(21)	-1426(80)	6831(40)	133
H(33)	2569(20)	-334(78)	8126(39)	139
H(34)	2929(20)	1632(69)	8503(43)	129
H(35)	3316(17)	2711(64)	7654(36)	98



ORTEP drawing of 7a

Table 1. Crystal data and structure refinement for **7a**^{a)b)}.

formula	C ₂₇ H ₃₆ Cl ₂ P Rh
fw	565.34
crystal size, mm ³	0.40 x 0.25 x 0.08
crystal system	Monoclinic
space group	Cc (no. 9)
cell dimensions determin	25 reflcns, 10 < Θ < 25
a, Å	8.865(2)
b, Å	23.214(2)
c, Å	13.172(3)
β , deg	106.85(1)
V, Å ³	2594(1)
Z	4
dcalc, gcm ⁻³	1.447
diffractometer	CAD4 (Enraf-Nonius)
radiation	Mo-K α (0.71073 Å), graphite mono-chromator, Zr filter (factor 16.4)
temp, K	173(2)
μ , mm ⁻¹	0.931
scan method	Ω/Θ -scan
2 Θ (max), deg	58
tot. no. of reflcns scanned	3624
no. of unique rflcns	3624 [R(int) = 0.0000]
no. of data	3624
no. of obsd rflcns [I > 2 σ (I)]	3488
correct. appl.	LP- and empirical abs.-corr. (Ψ -scans, min. transm. 89.48%)
structure solution	SHELXS-86
param	290 (full-matrix least-squares on F ² (SHELXL-93))
reflex/param ratio	12.5
final R indices [I > 2 σ (I)]	R ₁ = 0.0284, wR ₂ = 0.0675 ^{c)}
R indices (all data)	R ₁ = 0.0308, wR ₂ = 0.0698 ^{c)}
resid electron density, eÅ ⁻³	0.673 / -0.813

a) Crystals grown from acetone

b) The positions of all hydrogen atoms were found in a final difference fourier synthesis and were refined isotropically with fixed U_{eq} except for H6 which was found and refined without restrictions.

c) weighting scheme : $w = 1/[\sigma^2(F_o^2) + (0.0351 \cdot P)^2 + 2.0436 \cdot P]$ where

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

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7a**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Rh	4383(1)	2563(1)	2212(1)	17(1)
P	5896(1)	3360(1)	2056(1)	20(1)
Cl(1)	2047(1)	3101(1)	1428(1)	33(1)
Cl(2)	4434(1)	2120(1)	575(1)	28(1)
C(1)	5665(5)	1866(2)	3159(3)	25(1)
C(2)	5827(6)	2366(2)	3806(3)	28(1)
C(3)	4292(6)	2535(2)	3813(3)	28(1)
C(4)	3192(5)	2102(2)	3257(3)	24(1)
C(5)	4020(5)	1687(2)	2863(3)	24(1)
C(6)	3412(5)	1148(2)	2249(4)	24(1)
C(10)	6297(5)	3761(2)	3337(3)	27(1)
C(11)	7856(5)	3215(2)	1888(3)	28(1)
C(12)	4905(6)	3885(2)	1008(4)	29(1)
C(13)	7781(6)	4135(2)	3663(4)	38(1)
C(14)	4832(7)	4091(2)	3386(4)	39(1)
C(15)	8758(6)	2768(3)	2675(4)	42(1)
C(16)	7787(6)	3035(3)	757(4)	39(1)
C(17)	5923(7)	4409(2)	932(4)	43(1)
C(18)	4207(6)	3617(2)	-91(3)	34(1)
C(20)	1636(5)	1087(2)	2049(3)	25(1)
C(21)	989(6)	728(2)	2655(4)	33(1)
C(22)	-657(7)	693(2)	2450(4)	37(1)
C(22)	-1631(6)	1011(2)	1652(4)	37(1)
C(24)	-994(6)	1380(3)	1065(4)	41(1)
C(25)	624(6)	1411(2)	1248(4)	38(1)
C(30)	4396(5)	635(2)	2761(4)	29(1)
C(31)	4778(6)	206(2)	2145(5)	36(1)
C(32)	5724(7)	-259(2)	2601(6)	51(2)
C(33)	6321(7)	-289(3)	3697(6)	53(2)
C(34)	5963(6)	130(2)	4327(5)	47(1)
C(35)	4999(6)	590(2)	3869(4)	39(1)

Table 3. Bond lengths [$\text{\AA}$] for **7a**.

Rh-C(3)	2.135(4)
Rh-C(1)	2.155(4)
Rh-C(2)	2.167(4)
Rh-C(4)	2.237(4)
Rh-C(5)	2.266(4)
Rh-P	2.328(1)
Rh-Cl(1)	2.382(1)
Rh-Cl(2)	2.400(1)
P-C(11)	1.844(4)
P-C(12)	1.860(4)
P-C(10)	1.870(4)
C(1)-C(2)	1.423(6)
C(1)-C(5)	1.457(6)
C(2)-C(3)	1.419(7)
C(3)-C(4)	1.444(6)
C(4)-C(5)	1.398(6)
C(5)-C(6)	1.504(6)
C(6)-C(30)	1.514(6)
C(6)-C(20)	1.526(6)
C(10)-C(14)	1.525(7)
C(10)-C(13)	1.529(6)

C(11)-C(15)	1.520(7)
C(11)-C(16)	1.531(6)
C(12)-C(18)	1.532(6)
C(12)-C(17)	1.535(6)
C(20)-C(21)	1.389(6)
C(20)-C(25)	1.391(6)
C(21)-C(22)	1.407(7)
C(22)-C(22)	1.367(8)
C(22)-C(24)	1.380(8)
C(24)-C(25)	1.386(7)
C(30)-C(31)	1.387(7)
C(30)-C(35)	1.405(7)
C(31)-C(32)	1.392(7)
C(32)-C(33)	1.39(1)
C(33)-C(34)	1.375(9)
C(34)-C(35)	1.392(7)

Table 4. Bond angles [deg] for **7a**.

C(3)-Rh-C(1)	64.5(2)
C(3)-Rh-C(2)	38.5(2)
C(1)-Rh-C(2)	38.4(2)
C(3)-Rh-C(4)	38.5(2)
C(1)-Rh-C(4)	63.1(2)
C(2)-Rh-C(4)	63.5(2)
C(3)-Rh-C(5)	63.2(2)
C(1)-Rh-C(5)	38.4(2)
C(2)-Rh-C(5)	63.4(2)
C(4)-Rh-C(5)	36.2(2)
C(3)-Rh-P	107.4(1)
C(1)-Rh-P	115.3(1)
C(2)-Rh-P	93.4(1)
C(4)-Rh-P	145.3(1)
C(5)-Rh-P	153.5(1)
C(3)-Rh-Cl(1)	99.6(1)
C(1)-Rh-Cl(1)	153(1)
C(2)-Rh-Cl(1)	136.5(1)
C(4)-Rh-Cl(1)	90.7(1)
C(5)-Rh-Cl(1)	115.7(1)
P-Rh-Cl(1)	89.79(4)
C(3)-Rh-Cl(2)	152.9(1)
C(1)-Rh-Cl(2)	93.1(1)
C(2)-Rh-Cl(2)	128.4(1)
C(4)-Rh-Cl(2)	118.9(1)
C(5)-Rh-Cl(2)	89.9(1)
P-Rh-Cl(2)	95.72(4)
Cl(1)-Rh-Cl(2)	94.30(4)
C(11)-P-C(12)	106.8(2)
C(11)-P-C(10)	105.0(2)
C(12)-P-C(10)	105.6(2)
C(11)-P-Rh	116.9(2)
C(12)-P-Rh	115.2(2)
C(10)-P-Rh	106.3(1)
C(2)-C(1)-C(5)	108.2(4)
C(2)-C(1)-Rh	71.2(2)
C(5)-C(1)-Rh	74.9(2)
C(3)-C(2)-C(1)	107.4(4)
C(3)-C(2)-Rh	69.5(2)
C(1)-C(2)-Rh	70.3(2)
C(2)-C(3)-C(4)	108.2(4)
C(2)-C(3)-Rh	72.0(3)
C(4)-C(3)-Rh	74.6(2)
C(5)-C(4)-C(3)	108.5(4)
C(5)-C(4)-Rh	73.0(2)
C(3)-C(4)-Rh	66.9(2)

C(4)-C(5)-C(1)	107.3(4)
C(4)-C(5)-C(6)	128.9(4)
C(1)-C(5)-C(6)	123.8(4)
C(4)-C(5)-Rh	70.8(2)
C(1)-C(5)-Rh	66.7(2)
C(6)-C(5)-Rh	127.7(3)
C(5)-C(6)-C(30)	110.2(4)
C(5)-C(6)-C(20)	111.1(4)
C(30)-C(6)-C(20)	115.9(4)
C(14)-C(10)-C(13)	112.1(4)
C(14)-C(10)-P	110.3(3)
C(13)-C(10)-P	117.3(3)
C(15)-C(11)-C(16)	109.9(4)
C(15)-C(11)-P	111.7(3)
C(16)-C(11)-P	113.1(3)
C(18)-C(12)-C(17)	110.1(4)
C(18)-C(12)-P	114.2(3)
C(17)-C(12)-P	114.1(3)
C(21)-C(20)-C(25)	118.6(4)
C(21)-C(20)-C(6)	122.2(4)
C(25)-C(20)-C(6)	119.2(4)
C(20)-C(21)-C(22)	120.1(5)
C(22)-C(21)-C(21)	120.4(5)
C(22)-C(22)-C(24)	119.7(5)
C(22)-C(24)-C(25)	120.4(5)
C(24)-C(25)-C(20)	120.7(5)
C(31)-C(30)-C(35)	118.1(5)
C(31)-C(30)-C(6)	120.7(4)
C(35)-C(30)-C(6)	121.2(4)
C(30)-C(31)-C(32)	121.5(5)
C(33)-C(32)-C(31)	119.2(6)
C(34)-C(33)-C(32)	120.5(5)
C(33)-C(34)-C(35)	120.1(6)
C(34)-C(35)-C(30)	120.5(5)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7a**.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Rh	14(1)	20(1)	17(1)	1(1)	3(1)	-1(1)
P	17(1)	24(1)	19(1)	1(1)	5(1)	-4(1)
Cl(1)	17(1)	36(1)	42(1)	11(1)	5(1)	4(1)
Cl(2)	32(1)	31(1)	18(1)	-2(1)	5(1)	-1(1)
C(1)	22(2)	23(2)	26(2)	5(2)	1(2)	0(2)
C(2)	32(2)	28(2)	19(2)	7(2)	-2(2)	-4(2)
C(3)	39(2)	28(2)	20(2)	1(2)	14(2)	-5(2)
C(4)	28(2)	26(2)	20(2)	2(2)	9(2)	-5(2)
C(5)	29(2)	22(2)	20(2)	4(1)	4(2)	-5(2)
C(6)	26(2)	23(2)	26(2)	0(2)	10(2)	-6(2)
C(10)	31(2)	25(2)	24(2)	-4(2)	7(2)	-9(2)
C(11)	19(2)	39(2)	26(2)	-4(2)	9(2)	-6(2)
C(12)	28(2)	25(2)	32(2)	9(2)	6(2)	-3(2)
C(13)	42(3)	39(3)	29(2)	-8(2)	6(2)	-17(2)
C(14)	50(3)	30(2)	41(3)	-9(2)	20(2)	0(2)
C(15)	27(2)	66(4)	37(3)	12(3)	14(2)	12(2)
C(16)	24(2)	67(4)	28(2)	-8(2)	10(2)	-2(2)
C(17)	55(3)	34(3)	34(2)	8(2)	4(2)	-17(2)

C(18)	36(3)	35(2)	25(2)	10(2)	-1(2)	-6(2)
C(20)	30(2)	20(2)	25(2)	-2(2)	8(2)	-6(2)
C(21)	37(3)	24(2)	41(3)	2(2)	15(2)	1(2)
C(22)	44(3)	27(2)	48(3)	-1(2)	25(3)	-4(2)
C(22)	26(2)	40(3)	46(3)	-12(2)	11(2)	-6(2)
C(24)	29(2)	53(3)	38(3)	9(2)	5(2)	-3(2)
C(25)	31(2)	47(3)	33(2)	10(2)	6(2)	-7(2)
C(30)	26(2)	21(2)	39(2)	3(2)	9(2)	-7(2)
C(31)	34(3)	31(2)	50(3)	0(2)	22(2)	-4(2)
C(32)	40(3)	31(3)	97(5)	6(3)	42(3)	6(2)
C(33)	33(3)	41(3)	88(5)	27(3)	24(3)	10(2)
C(34)	32(3)	47(3)	56(3)	23(3)	5(2)	-2(2)
C(35)	37(3)	31(2)	42(3)	10(2)	1(2)	1(2)

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7a**.

	x	y	z	U(eq)
H(1)	6488(5)	1681(2)	2956(3)	30
H(2)	6786(6)	2553(2)	4166(3)	34
H(3)	4032(6)	2875(2)	4128(3)	34
H(4)	2091(5)	2098(2)	3174(3)	29
H(6)	3460(56)	1185(21)	1609(38)	20(12)
H(10)	6459(5)	3458(2)	3898(3)	32
H(11)	8469(5)	3582(2)	2042(3)	33
H(12)	3989(6)	4040(2)	1222(4)	35
H(13A)	7690(21)	4446(10)	3146(18)	56
H(13B)	8705(8)	3898(4)	3684(30)	56
H(13C)	7898(26)	4300(14)	4366(14)	56
H(14A)	3907(10)	3841(6)	3150(31)	58
H(14B)	4690(28)	4429(10)	2921(25)	58
H(14C)	4959(21)	4216(15)	4116(7)	58
H(15A)	8740(44)	2873(10)	3391(6)	64
H(15B)	9852(14)	2752(13)	2651(25)	64
H(15C)	8265(31)	2390(4)	2489(21)	64
H(16A)	7420(46)	3360(6)	274(6)	59
H(16B)	7057(37)	2711(12)	538(12)	59
H(16C)	8840(11)	2918(17)	736(8)	59
H(17A)	6898(23)	4279(2)	796(33)	65
H(17B)	6181(42)	4624(10)	1601(13)	65
H(17C)	5340(20)	4659(9)	351(22)	65
H(18A)	3651(38)	3261(9)	-24(5)	51
H(18B)	5058(7)	3530(15)	-405(13)	51
H(18C)	3467(34)	3889(7)	-547(10)	51
H(21)	1659(6)	505(2)	3210(4)	40
H(22)	-1094(7)	447(2)	2868(4)	45
H(22A)	-2742(6)	978(2)	1503(4)	45
H(24)	-1669(6)	1613(3)	531(4)	50
H(25)	1047(6)	1657(2)	822(4)	45
H(31)	4385(6)	230(2)	1394(5)	43
H(32)	5957(7)	-553(2)	2167(6)	61
H(33)	6983(7)	-602(3)	4013(6)	63
H(34)	6374(6)	106(2)	5077(5)	56
H(35)	4747(6)	877(2)	4309(4)	47