Table 1. Crystal data and structure refinement for 5.

Empirical formula	$C_{32}H_{24}Cl_2N_3O_3PPd$	
Formula weight	706.81	
Crystal colour and habit	yellow block	
Crystal size (mm)	0.11 x 0.09 x 0.09	
Temperature (K)	150(2)	
Wavelength (Å)	1.54184	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 8.0871(3) Å	α = 90°
	b = 13.8105(5) Å	β = 100.325(3)°
	c = 13.5808(4) Å	γ = 90°
Volume (Å^3)	1492.24(9)	
Z	2	
Calculated density (Mg/m^3)	1.573	
Absorption coefficient (mm^{-1})	7.490	
F(000)	712	
θ-range for data collection (°)	4.60/62.83	
Index ranges	$-9 \le h \le 9$, $-15 \le k \le 13$, $-15 \le l \le 15$	
Reflections collected	16618	
Independent reflections	4115 (R_{int} = 0.0495)	
Completeness to θ = 62.83°	99.4 %	
Absorption correction	Semi-empirical from equivalents (Multiscan)	
Max. and min. transmission	1.00000 and 0.58696	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	4115/1/381	
Goodness-of-fit on F^2	1.022	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0224, wR_2 = 0.0538	
R indices (all data)	R_1 = 0.0235, wR_2 = 0.0541	
Absolute structure parameter	-0.006(5)	
Largest diff. Peak and hole (e·Å^{-3})	0.251/-0.415	

Definitions:

$$R_1 = \frac{\sum \left| |F_o| - |F_c| \right|}{\sum |F_o|} \qquad wR_2 = \sqrt{\frac{\sum \left[w\left(F_o^2 - F_c^2\right)^2 \right]}{\sum \left[w\left(F_o^2\right)^2 \right]}}$$

$$GooF = \sqrt{\frac{\sum \left[w\left(F_o^2 - F_c^2\right) \right]}{(n-p)}}$$ n = number of reflections; p = number of parameters

Notes on the refinement of 5.

All hydrogen atom positions were calculated in deal positions (riding model).

Table 2. Atomic coordinates [x10^4] and equivalent isotropic displacement parameters [Å^{2}x10^3] for 5.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	1471(5)	8804(3)	6970(3)	36(1)
C(2)	715(5)	7916(3)	6962(3)	36(1)
C(3)	1562(3)	7318(4)	6386(2)	25(1)
C(4)	3710(5)	9542(3)	6161(3)	37(1)
C(5)	1322(4)	6294(3)	6153(2)	25(1)
C(6)	1375(4)	5902(3)	5217(2)	25(1)
C(7)	1199(5)	4923(3)	5019(3)	36(1)
C(8)	883(5)	4304(3)	5767(3)	42(1)
C(9)	752(5)	4677(3)	6697(3)	39(1)
C(10)	978(5)	5661(3)	6890(3)	32(1)
C(11)	2690(4)	6237(3)	2453(3)	25(1)
C(12)	2299(4)	6984(3)	1797(2)	25(1)
C(13)	1034(4)	6793(3)	914(2)	26(1)
C(14)	405(5)	5830(3)	738(3)	29(1)
C(15)	981(5)	5099(3)	1428(3)	31(1)
C(16)	2084(4)	5286(3)	2287(2)	28(1)
C(17)	341(4)	7539(3)	255(2)	31(1)
C(18)	-885(4)	7336(4)	-560(2)	36(1)
C(19)	-1459(5)	6383(3)	-757(3)	40(1)
C(20)	-844(5)	5655(3)	-125(3)	36(1)
C(21)	3019(4)	8401(3)	2901(3)	25(1)
C(22)	3075(4)	7956(3)	2004(2)	24(1)
C(23)	3955(4)	8446(3)	1319(3)	30(1)
C(24)	4635(5)	9385(3)	1571(3)	36(1)
C(25)	4453(5)	9811(3)	2491(3)	36(1)
C(26)	3671(5)	9329(3)	3160(3)	32(1)
C(27)	4223(5)	8009(3)	409(3)	38(1)
C(28)	5057(5)	8517(4)	-226(3)	50(1)
C(29)	5689(5)	9449(4)	17(4)	54(1)
C(30)	5493(5)	9866(4)	888(3)	45(1)
N(1)	2688(4)	8752(2)	6432(2)	27(1)
N(2)	2770(3)	7848(2)	6073(2)	23(1)
O(1)	1462(3)	6519(2)	4395(2)	27(1)
O(2)	3809(3)	6404(2)	3369(2)	25(1)
O(3)	2198(3)	7935(2)	3589(2)	24(1)
P(1)	3127(1)	7027(1)	4198(1)	22(1)
Cl(1)	6393(1)	7713(1)	7163(1)	33(1)
Cl(2)	7155(1)	6823(1)	5003(1)	36(1)
Pd(1)	4852(1)	7354(1)	5582(1)	20(1)
C(31)	7803(5)	7430(5)	2382(3)	49(1)
C(32)	7121(5)	6501(4)	2036(3)	41(1)
N(3)	6572(6)	5772(3)	1771(3)	60(1)

Table 3. Bond lengths [Å] and angles [°] for 5.

C(1)-N(1)	1.329(5)	C(30)-H(30)	0.9500
C(1)-C(2)	1.369(6)	N(1)-N(2)	1.346(4)
C(1)-H(1)	0.9500	N(2)-Pd(1)	2.037(3)
C(2)-C(3)	1.397(5)	O(1)-P(1)	1.583(2)
C(2)-H(2)	0.9500	O(2)-P(1)	1.592(2)
C(3)-N(2)	1.349(5)	O(3)-P(1)	1.612(2)
C(3)-C(5)	1.456(6)	P(1)-Pd(1)	2.1776(8)
C(4)-N(1)	1.455(5)	Cl(1)-Pd(1)	2.3347(8)
C(4)-H(4A)	0.9800	Cl(2)-Pd(1)	2.2693(9)
C(4)-H(4B)	0.9800	C(31)-C(32)	1.442(7)
C(4)-H(4C)	0.9800	C(31)-H(31A)	0.9800
C(5)-C(6)	1.390(5)	C(31)-H(31B)	0.9800
C(5)-C(10)	1.394(5)	C(31)-H(31C)	0.9800
C(6)-C(7)	1.380(6)	C(32)-N(3)	1.132(6)
C(6)-O(1)	1.416(4)		
C(7)-C(8)	1.386(6)	N(1)-C(1)-C(2)	108.7(4)
C(7)-H(7)	0.9500	N(1)-C(1)-H(1)	125.6
C(8)-C(9)	1.385(6)	C(2)-C(1)-H(1)	125.6
C(8)-H(8)	0.9500	C(1)-C(2)-C(3)	105.7(3)
C(9)-C(10)	1.390(6)	C(1)-C(2)-H(2)	127.2
C(9)-H(9)	0.9500	C(3)-C(2)-H(2)	127.2
C(10)-H(10)	0.9500	N(2)-C(3)-C(2)	108.2(4)
C(11)-C(12)	1.363(5)	N(2)-C(3)-C(5)	122.3(3)
C(11)-C(16)	1.407(5)	C(2)-C(3)-C(5)	129.5(3)
C(11)-O(2)	1.419(4)	N(1)-C(4)-H(4A)	109.5
C(12)-C(13)	1.454(5)	N(1)-C(4)-H(4B)	109.5
C(12)-C(22)	1.486(5)	H(4A)-C(4)-H(4B)	109.5
C(13)-C(17)	1.413(5)	N(1)-C(4)-H(4C)	109.5
C(13)-C(14)	1.429(5)	H(4A)-C(4)-H(4C)	109.5
C(14)-C(15)	1.399(5)	H(4B)-C(4)-H(4C)	109.5
C(14)-C(20)	1.424(5)	C(6)-C(5)-C(10)	117.1(4)
C(15)-C(16)	1.360(5)	C(6)-C(5)-C(3)	123.6(3)
C(15)-H(15)	0.9500	C(10)-C(5)-C(3)	119.3(3)
C(16)-H(16)	0.9500	C(7)-C(6)-C(5)	122.7(3)
C(17)-C(18)	1.377(5)	C(7)-C(6)-O(1)	117.0(3)
C(17)-H(17)	0.9500	C(5)-C(6)-O(1)	120.0(3)
C(18)-C(19)	1.404(7)	C(6)-C(7)-C(8)	119.2(4)
C(18)-H(18)	0.9500	C(6)-C(7)-H(7)	120.4
C(19)-C(20)	1.357(6)	C(8)-C(7)-H(7)	120.4
C(19)-H(19)	0.9500	C(9)-C(8)-C(7)	119.5(4)
C(20)-H(20)	0.9500	C(9)-C(8)-H(8)	120.2
C(21)-C(22)	1.372(5)	C(7)-C(8)-H(8)	120.2
C(21)-O(3)	1.397(4)	C(8)-C(9)-C(10)	120.5(4)
C(21)-C(26)	1.406(6)	C(8)-C(9)-H(9)	119.8
C(22)-C(23)	1.439(5)	C(10)-C(9)-H(9)	119.8
C(23)-C(24)	1.425(6)	C(9)-C(10)-C(5)	120.9(4)
C(23)-C(27)	1.426(5)	C(9)-C(10)-H(10)	119.5
C(24)-C(25)	1.413(6)	C(5)-C(10)-H(10)	119.5
C(24)-C(30)	1.419(5)	C(12)-C(11)-C(16)	124.6(3)
C(25)-C(26)	1.369(5)	C(12)-C(11)-O(2)	119.1(3)
C(25)-H(25)	0.9500	C(16)-C(11)-O(2)	116.2(3)
C(26)-H(26)	0.9500	C(11)-C(12)-C(13)	116.6(3)
C(27)-C(28)	1.379(6)	C(11)-C(12)-C(22)	121.3(3)
C(27)-H(27)	0.9500	C(13)-C(12)-C(22)	122.1(3)
C(28)-C(29)	1.402(7)	C(17)-C(13)-C(14)	119.0(3)
C(28)-H(28)	0.9500	C(17)-C(13)-C(12)	122.0(3)
C(29)-C(30)	1.351(7)	C(14)-C(13)-C(12)	118.9(3)
C(29)-H(29)	0.9500	C(15)-C(14)-C(20)	122.1(4)

C(15)-C(14)-C(13)	119.6(3)
C(20)-C(14)-C(13)	118.3(3)
C(16)-C(15)-C(14)	121.7(4)
C(16)-C(15)-H(15)	119.1
C(14)-C(15)-H(15)	119.1
C(15)-C(16)-C(11)	118.1(3)
C(15)-C(16)-H(16)	120.9
C(11)-C(16)-H(16)	120.9
C(18)-C(17)-C(13)	120.5(4)
C(18)-C(17)-H(17)	119.8
C(13)-C(17)-H(17)	119.8
C(17)-C(18)-C(19)	120.7(4)
C(17)-C(18)-H(18)	119.7
C(19)-C(18)-H(18)	119.7
C(20)-C(19)-C(18)	120.1(3)
C(20)-C(19)-H(19)	119.9
C(18)-C(19)-H(19)	119.9
C(19)-C(20)-C(14)	121.4(4)
C(19)-C(20)-H(20)	119.3
C(14)-C(20)-H(20)	119.3
C(22)-C(21)-O(3)	118.9(3)
C(22)-C(21)-C(26)	124.0(3)
O(3)-C(21)-C(26)	117.0(3)
C(21)-C(22)-C(23)	117.5(3)
C(21)-C(22)-C(12)	119.5(3)
C(23)-C(22)-C(12)	122.9(3)
C(24)-C(23)-C(27)	118.8(3)
C(24)-C(23)-C(22)	119.2(3)
C(27)-C(23)-C(22)	122.0(4)
C(25)-C(24)-C(30)	121.5(4)
C(25)-C(24)-C(23)	119.6(3)
C(30)-C(24)-C(23)	118.8(4)
C(26)-C(25)-C(24)	121.2(4)
C(26)-C(25)-H(25)	119.4
C(24)-C(25)-H(25)	119.4
C(25)-C(26)-C(21)	118.3(4)
C(25)-C(26)-H(26)	120.8
C(21)-C(26)-H(26)	120.8
C(28)-C(27)-C(23)	119.6(4)
C(28)-C(27)-H(27)	120.2
C(23)-C(27)-H(27)	120.2
C(27)-C(28)-C(29)	121.2(4)
C(27)-C(28)-H(28)	119.4
C(29)-C(28)-H(28)	119.4
C(30)-C(29)-C(28)	120.2(4)
C(30)-C(29)-H(29)	119.9
C(28)-C(29)-H(29)	119.9
C(29)-C(30)-C(24)	121.3(4)
C(29)-C(30)-H(30)	119.3
C(24)-C(30)-H(30)	119.3
C(1)-N(1)-N(2)	109.8(3)
C(1)-N(1)-C(4)	127.5(3)
N(2)-N(1)-C(4)	122.4(3)
N(1)-N(2)-C(3)	107.6(3)
N(1)-N(2)-Pd(1)	121.8(2)
C(3)-N(2)-Pd(1)	127.6(3)
C(6)-O(1)-P(1)	124.3(2)
C(11)-O(2)-P(1)	117.4(2)
C(21)-O(3)-P(1)	117.9(2)
O(1)-P(1)-O(2)	107.01(13)
O(1)-P(1)-O(3)	95.71(13)
O(2)-P(1)-O(3)	104.25(12)
O(1)-P(1)-Pd(1)	112.27(9)
O(2)-P(1)-Pd(1)	118.23(9)
O(3)-P(1)-Pd(1)	116.68(9)
N(2)-Pd(1)-P(1)	84.98(8)
N(2)-Pd(1)-Cl(2)	178.71(9)
P(1)-Pd(1)-Cl(2)	94.16(3)
N(2)-Pd(1)-Cl(1)	87.96(8)
P(1)-Pd(1)-Cl(1)	172.57(3)
Cl(2)-Pd(1)-Cl(1)	92.93(3)
C(32)-C(31)-H(31A)	109.5
C(32)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(32)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
N(3)-C(32)-C(31)	179.2(5)

Table 4. Anisotropic displacement parameters [Å^{2}x10^3] for 5.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[(ha^*)^2U_{11}+...+2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	30(2)	39(3)	42(2)	-7(2)	14(2)	4(2)
C(2)	28(2)	45(3)	38(2)	-4(2)	16(2)	0(2)
C(3)	19(1)	34(2)	22(1)	0(2)	3(1)	-1(2)
C(4)	41(2)	30(2)	44(2)	-1(2)	15(2)	0(2)
C(5)	15(2)	30(2)	29(2)	4(2)	2(1)	-3(1)
C(6)	20(2)	31(2)	25(2)	4(2)	2(1)	-5(2)
C(7)	36(2)	35(2)	35(2)	-5(2)	3(2)	-7(2)
C(8)	42(2)	26(2)	59(3)	3(2)	11(2)	-9(2)
C(9)	40(2)	38(2)	40(2)	15(2)	9(2)	-8(2)
C(10)	28(2)	43(3)	25(2)	5(2)	6(2)	-5(2)
C(11)	21(2)	34(2)	22(2)	-5(2)	8(2)	5(2)
C(12)	27(2)	29(2)	19(2)	0(1)	7(1)	3(1)
C(13)	28(2)	32(2)	20(2)	0(2)	6(1)	1(2)
C(14)	30(2)	36(2)	22(2)	0(2)	7(1)	4(2)
C(15)	36(2)	27(2)	31(2)	-4(2)	10(2)	0(2)
C(16)	30(2)	30(2)	24(2)	1(2)	7(2)	9(2)
C(17)	34(2)	34(3)	24(2)	5(2)	4(1)	-3(2)
C(18)	38(2)	40(2)	27(2)	9(2)	-3(1)	0(2)
C(19)	40(2)	49(3)	25(2)	1(2)	-9(2)	-7(2)
C(20)	42(2)	35(2)	30(2)	-6(2)	3(2)	-6(2)
C(21)	23(2)	29(2)	22(2)	6(2)	1(2)	2(2)
C(22)	20(2)	31(2)	21(2)	4(2)	2(1)	2(2)
C(23)	22(2)	38(2)	27(2)	9(2)	1(1)	1(2)
C(24)	24(2)	43(3)	38(2)	15(2)	1(2)	-2(2)
C(25)	32(2)	32(2)	41(2)	8(2)	-4(2)	-6(2)
C(26)	34(2)	32(2)	28(2)	2(2)	-1(2)	2(2)
C(27)	32(2)	59(3)	23(2)	5(2)	7(2)	-2(2)
C(28)	38(2)	83(4)	31(2)	12(2)	12(2)	1(2)
C(29)	37(2)	76(4)	50(3)	31(3)	12(2)	-5(2)
C(30)	34(2)	52(3)	45(3)	21(2)	1(2)	-8(2)
N(1)	26(2)	27(2)	29(1)	-3(1)	9(1)	0(1)
N(2)	21(1)	26(2)	23(1)	0(1)	5(1)	-2(1)
O(1)	25(1)	32(1)	23(1)	2(1)	1(1)	-5(1)
O(2)	26(1)	30(1)	20(1)	-1(1)	2(1)	9(1)
O(3)	24(1)	29(1)	21(1)	3(1)	6(1)	5(1)
P(1)	21(1)	26(1)	18(1)	1(1)	2(1)	1(1)
Cl(1)	28(1)	45(1)	23(1)	-2(1)	-1(1)	-1(1)
Cl(2)	23(1)	47(1)	38(1)	-13(1)	7(1)	3(1)
Pd(1)	19(1)	25(1)	18(1)	0(1)	3(1)	-1(1)
C(31)	37(2)	59(3)	49(2)	-7(3)	4(2)	1(3)
C(32)	43(2)	50(3)	30(2)	5(2)	8(2)	2(2)
N(3)	76(3)	57(3)	48(2)	-3(2)	14(2)	-3(2)

Table 5. Hydrogen coordinates [x10^4] and isotropic displacement parameters [Å^{2}x10^3] for 5.

	x	y	z	U(eq)
H(1)	1174	9364	7305	43
H(2)	-196	7742	7281	43
H(4A)	3016	9961	5670	56
H(4B)	4640	9277	5871	56
H(4C)	4161	9919	6760	56
H(7)	1293	4677	4378	43
H(8)	757	3629	5643	51
H(9)	505	4258	7206	47
H(10)	897	5906	7533	38
H(15)	591	4455	1293	37
H(16)	2436	4788	2760	34
H(17)	725	8186	376	37
H(18)	-1349	7845	-994	43
H(19)	-2280	6248	-1334	48
H(20)	-1256	5016	-261	43
H(25)	4881	10444	2648	43
H(26)	3572	9614	3783	39
H(27)	3829	7371	242	45
H(28)	5207	8230	-840	60
H(29)	6256	9788	-433	65
H(30)	5939	10495	1048	53
H(31A)	7200	7679	2893	73
H(31B)	7675	7884	1818	73
H(31C)	8998	7360	2669	73

Table 1. Crystal data and structure refinement for 6.

Empirical formula	$C_{49}H_{47}Cl_2N_2O_{3.5}PRu$	
Formula weight	922.83	
Crystal colour and habit	red prism	
Crystal size (mm)	0.30 x 0.30 x 0.21	
Temperature (K)	150(2)	
Wavelength (Å)	1.54184	
Crystal system	Tetragonal	
Space group	$P4_32_12$	
Unit cell dimensions	a = 15.80010(10) Å	$\alpha = 90^o$
	b = 15.80010(10) Å	$\beta = 90^o$
	c = 35.7434(4) Å	$\gamma = 90^o$
Volume (Å^3)	8923.10(13)	
Z	8	
Calculated density (Mg/m^3)	1.374	
Absorption coefficient (mm^{-1})	4.636	
F(000)	3808	
θ-range for data collection (^{o})	3.73/62.59	
Index ranges	$-17 \le h \le 18$, $-16 \le k \le 16$, $-33 \le l \le 40$	
Reflections collected	27147	
Independent reflections	6661 (R_{int} = 0.0396)	
Completeness to $\theta = 62.59^o$	95.6 %	
Absorption correction	Semi-empirical from equivalents (Multiscan)	
Max. and min. transmission	1.00000 and 0.51880	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	6661/321/622	
Goodness-of-fit on F^2	1.104	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0405, wR_2 = 0.0989	
R indices (all data)	R_1 = 0.0452, wR_2 = 0.1005	
Absolute structure parameter	0.033(11)	
Largest diff. Peak and hole (e·Å^{-3})	0.550/-0.507	

Definitions:

$$R_1 = \frac{\sum \left| |F_o| - |F_c| \right|}{\sum |F_o|} \qquad wR_2 = \sqrt{\frac{\sum \left[w\left(F_o^2 - F_c^2\right)^2 \right]}{\sum \left[w\left(F_o^2\right)^2 \right]}}$$

$$GooF = \sqrt{\frac{\sum \left[w\left(F_o^2 - F_c^2\right) \right]}{(n-p)}}$$ n = number of reflections; p = number of parameters

Notes on the refinement of 6.

All hydrogen atom positions were calculated in deal positions (riding model). The target molecule was crystallized with 1 molecule of toluene and 0.5 molecule of THF, both of which were disordered.

Table 2. Atomic coordinates [x10^4] and equivalent isotropic displacement parameters [Å^{2}x10^3] for 6.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	6077(4)	1670(5)	4739(2)	57(2)
C(2)	5555(4)	1270(4)	4491(2)	43(1)
C(3)	5171(3)	1922(3)	4286(1)	36(1)
C(4)	6457(5)	3211(5)	4859(2)	78(2)
C(5)	4534(4)	1878(3)	3984(2)	39(1)
C(6)	4612(3)	1348(3)	3676(1)	30(1)
C(7)	4016(4)	1335(4)	3392(2)	40(1)
C(8)	3324(4)	1861(4)	3415(2)	47(1)
C(9)	3229(4)	2384(4)	3716(2)	52(2)
C(10)	3823(4)	2410(4)	3997(2)	50(2)
C(11)	6029(3)	-862(3)	3702(1)	27(1)
C(12)	5642(3)	-1461(3)	3481(1)	29(1)
C(13)	5121(3)	-2073(3)	3660(1)	31(1)
C(14)	5079(3)	-2079(3)	4055(2)	33(1)
C(15)	5558(3)	-1494(3)	4270(1)	29(1)
C(16)	6017(3)	-892(3)	4090(1)	28(1)
C(17)	4605(4)	-2645(3)	3458(2)	38(1)
C(18)	4072(4)	-3193(4)	3640(2)	51(2)
C(19)	4038(4)	-3198(4)	4034(2)	52(2)
C(20)	4523(4)	-2658(4)	4237(2)	42(1)
C(21)	5509(3)	-692(3)	2879(1)	28(1)
C(22)	5732(3)	-1418(3)	3062(1)	28(1)
C(23)	6062(3)	-2103(3)	2849(1)	32(1)
C(24)	6098(3)	-2025(4)	2450(1)	37(1)
C(25)	5802(4)	-1283(4)	2279(2)	39(1)
C(26)	5526(3)	-613(3)	2489(1)	34(1)
C(27)	6400(4)	-2841(4)	3016(2)	43(1)
C(28)	6746(4)	-3475(4)	2802(2)	50(2)
C(29)	6772(4)	-3398(4)	2411(2)	53(2)
C(30)	6449(4)	-2702(4)	2241(2)	48(2)
C(31)	6645(4)	2937(4)	3239(2)	49(2)
C(32)	7382(4)	2812(4)	2999(2)	49(2)
C(33)	7969(4)	2212(4)	3074(2)	45(2)
C(34)	7917(4)	1662(5)	3392(2)	57(2)
C(35)	7220(4)	1821(4)	3637(2)	53(2)
C(36)	6607(5)	2453(4)	3561(2)	52(2)
C(37)	5998(5)	3613(4)	3137(2)	63(2)
C(38)	5166(5)	3555(5)	3340(2)	74(2)
C(39)	6403(7)	4491(5)	3185(3)	130(5)
C(40)	8543(5)	990(5)	3459(2)	66(2)
N(1)	6003(4)	2506(4)	4678(1)	54(1)
N(2)	5449(3)	2681(3)	4400(1)	48(1)
O(1)	5298(2)	781(2)	3678(1)	28(1)
O(2)	6464(2)	-177(2)	3534(1)	26(1)
O(3)	5244(2)	5(2)	3083(1)	28(1)
P(1)	5905(1)	543(1)	3337(1)	26(1)
Cl(1)	7291(1)	459(1)	2708(1)	39(1)
Cl(2)	5624(1)	1777(1)	2623(1)	40(1)
Ru(1)	6715(1)	1558(1)	3089(1)	34(1)
C(41A)	4054(9)	6894(9)	2315(4)	138(6)
C(42A)	3225(10)	7338(9)	2377(4)	183(8)
O(4A)	3969(8)	6031(8)	2500	158(6)
C(41B)	4600(30)	5890(40)	2186(8)	146(12)
C(42B)	3940(50)	6550(40)	2341(18)	141(12)

O(4B)	4660(30)	5340(30)	2500	146(13)
C(43A)	3512(19)	4595(17)	4387(7)	107(7)
C(44A)	3171(14)	4636(15)	4035(7)	96(7)
C(45A)	2325(13)	4501(12)	4026(7)	85(5)
C(46A)	1953(18)	4370(20)	4361(7)	105(7)
C(47A)	2262(17)	4266(18)	4701(7)	136(8)
C(48A)	3088(16)	4451(13)	4706(7)	109(6)
C(49A)	4460(20)	4780(30)	4421(12)	227(17)
C(43B)	3347(14)	4560(13)	4233(5)	98(5)
C(44B)	3190(9)	4727(11)	3865(4)	84(5)
C(45B)	2371(9)	4657(8)	3709(4)	90(4)
C(46B)	1705(10)	4402(9)	3918(5)	100(5)
C(47B)	1879(15)	4218(19)	4302(6)	120(6)
C(48B)	2681(12)	4323(11)	4472(5)	111(5)
C(49B)	4159(16)	4647(13)	4388(7)	159(8)

Table 3. Bond lengths [Å] and angles [°] for 6.

C(1)-N(1)	1.343(9)	C(30)-H(30)	0.9500
C(1)-C(2)	1.366(8)	C(31)-C(36)	1.383(8)
C(1)-H(1)	0.9500	C(31)-C(32)	1.460(9)
C(2)-C(3)	1.400(8)	C(31)-C(37)	1.522(9)
C(2)-H(2)	0.9500	C(31)-Ru(1)	2.247(6)
C(3)-N(2)	1.340(7)	C(32)-C(33)	1.353(9)
C(3)-C(5)	1.480(8)	C(32)-Ru(1)	2.266(6)
C(4)-N(1)	1.474(8)	C(32)-H(32)	0.9500
C(4)-H(4A)	0.9800	C(33)-C(34)	1.431(8)
C(4)-H(4B)	0.9800	C(33)-Ru(1)	2.235(5)
C(4)-H(4C)	0.9800	C(33)-H(33)	0.9500
C(5)-C(6)	1.387(7)	C(34)-C(35)	1.430(9)
C(5)-C(10)	1.403(8)	C(34)-C(40)	1.472(10)
C(6)-C(7)	1.385(7)	C(34)-Ru(1)	2.191(6)
C(6)-O(1)	1.406(6)	C(35)-C(36)	1.418(10)
C(7)-C(8)	1.376(8)	C(35)-Ru(1)	2.156(5)
C(7)-H(7)	0.9500	C(35)-H(35)	0.9500
C(8)-C(9)	1.366(8)	C(36)-Ru(1)	2.208(6)
C(8)-H(8)	0.9500	C(36)-H(36)	0.9500
C(9)-C(10)	1.375(9)	C(37)-C(38)	1.504(10)
C(9)-H(9)	0.9500	C(37)-C(39)	1.538(9)
C(10)-H(10)	0.9500	C(37)-H(37)	1.0000
C(11)-C(12)	1.376(7)	C(38)-H(38A)	0.9800
C(11)-C(16)	1.386(6)	C(38)-H(38B)	0.9800
C(11)-O(2)	1.416(6)	C(38)-H(38C)	0.9800
C(12)-C(13)	1.423(7)	C(39)-H(39A)	0.9800
C(12)-C(22)	1.503(7)	C(39)-H(39B)	0.9800
C(13)-C(14)	1.414(7)	C(39)-H(39C)	0.9800
C(13)-C(17)	1.416(7)	C(40)-H(40A)	0.9800
C(14)-C(15)	1.419(7)	C(40)-H(40B)	0.9800
C(14)-C(20)	1.426(8)	C(40)-H(40C)	0.9800
C(15)-C(16)	1.359(7)	N(1)-N(2)	1.353(7)
C(15)-H(15)	0.9500	O(1)-P(1)	1.598(3)
C(16)-H(16)	0.9500	O(2)-P(1)	1.605(3)
C(17)-C(18)	1.370(8)	O(3)-P(1)	1.623(3)
C(17)-H(17)	0.9500	P(1)-Ru(1)	2.2351(13)
C(18)-C(19)	1.412(8)	Cl(1)-Ru(1)	2.3876(15)
C(18)-H(18)	0.9500	Cl(2)-Ru(1)	2.4211(14)
C(19)-C(20)	1.356(8)	C(41A)-C(42A)	1.502(15)
C(19)-H(19)	0.9500	C(41A)-O(4A)	1.521(13)
C(20)-H(20)	0.9500	C(41A)-H(41A)	0.9900
C(21)-C(22)	1.368(7)	C(41A)-H(41B)	0.9900
C(21)-O(3)	1.386(6)	C(42A)-C(42A)#1	1.535(18)
C(21)-C(26)	1.398(7)	C(42A)-H(42A)	0.9900
C(22)-C(23)	1.424(7)	C(42A)-H(42B)	0.9900
C(23)-C(27)	1.415(7)	O(4A)-C(41A)#1	1.521(13)
C(23)-C(24)	1.430(7)	C(41B)-O(4B)	1.430(19)
C(24)-C(25)	1.403(8)	C(41B)-C(42B)	1.57(2)
C(24)-C(30)	1.418(8)	C(41B)-H(41C)	0.9900
C(25)-C(26)	1.369(8)	C(41B)-H(41D)	0.9900
C(25)-H(25)	0.9500	C(42B)-C(42B)#1	1.57(2)
C(26)-H(26)	0.9500	C(42B)-H(42C)	0.9900
C(27)-C(28)	1.376(8)	C(42B)-H(42D)	0.9900
C(27)-H(27)	0.9500	O(4B)-C(41B)#1	1.430(19)
C(28)-C(29)	1.404(8)	C(43A)-C(48A)	1.341(17)
C(28)-H(28)	0.9500	C(43A)-C(44A)	1.368(16)
C(29)-C(30)	1.354(9)	C(43A)-C(49A)	1.54(4)
C(29)-H(29)	0.9500	C(44A)-C(45A)	1.354(17)

C(44A)-H(44A)	0.9500
C(45A)-C(46A)	1.347(16)
C(45A)-H(45A)	0.9500
C(46A)-C(47A)	1.320(16)
C(46A)-H(46A)	0.9500
C(47A)-C(48A)	1.337(17)
C(47A)-H(47A)	0.9500
C(48A)-H(48A)	0.9500
C(49A)-H(49A)	0.9800
C(49A)-H(49B)	0.9800
C(49A)-H(49C)	0.9800
C(43B)-C(44B)	1.363(13)
C(43B)-C(49B)	1.41(3)
C(43B)-C(48B)	1.407(15)
C(44B)-C(45B)	1.414(14)
C(44B)-H(44B)	0.9500
C(45B)-C(46B)	1.350(13)
C(45B)-H(45B)	0.9500
C(46B)-C(47B)	1.433(14)
C(46B)-H(46B)	0.9500
C(47B)-C(48B)	1.414(15)
C(47B)-H(47B)	0.9500
C(48B)-H(48B)	0.9500
C(49B)-H(49D)	0.9800
C(49B)-H(49E)	0.9800
C(49B)-H(49F)	0.9800

N(1)-C(1)-C(2)	107.3(6)
N(1)-C(1)-H(1)	126.3
C(2)-C(1)-H(1)	126.3
C(1)-C(2)-C(3)	105.1(5)
C(1)-C(2)-H(2)	127.5
C(3)-C(2)-H(2)	127.5
N(2)-C(3)-C(2)	111.0(5)
N(2)-C(3)-C(5)	119.1(5)
C(2)-C(3)-C(5)	129.9(5)
N(1)-C(4)-H(4A)	109.5
N(1)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
N(1)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(6)-C(5)-C(10)	117.4(5)
C(6)-C(5)-C(3)	123.2(5)
C(10)-C(5)-C(3)	119.5(5)
C(7)-C(6)-C(5)	121.9(5)
C(7)-C(6)-O(1)	121.3(5)
C(5)-C(6)-O(1)	116.7(5)
C(8)-C(7)-C(6)	119.3(5)
C(8)-C(7)-H(7)	120.4
C(6)-C(7)-H(7)	120.4
C(9)-C(8)-C(7)	119.9(6)
C(9)-C(8)-H(8)	120.0
C(7)-C(8)-H(8)	120.0
C(8)-C(9)-C(10)	121.2(6)
C(8)-C(9)-H(9)	119.4
C(10)-C(9)-H(9)	119.4
C(9)-C(10)-C(5)	120.3(6)
C(9)-C(10)-H(10)	119.9
C(5)-C(10)-H(10)	119.9
C(12)-C(11)-C(16)	123.0(5)
C(12)-C(11)-O(2)	119.9(4)
C(16)-C(11)-O(2)	117.1(4)
C(11)-C(12)-C(13)	117.8(4)
C(11)-C(12)-C(22)	120.0(4)
C(13)-C(12)-C(22)	122.1(4)
C(14)-C(13)-C(17)	118.6(5)
C(14)-C(13)-C(12)	118.7(5)
C(17)-C(13)-C(12)	122.6(5)
C(13)-C(14)-C(15)	120.7(5)
C(13)-C(14)-C(20)	119.3(5)
C(15)-C(14)-C(20)	119.9(5)
C(16)-C(15)-C(14)	119.0(4)
C(16)-C(15)-H(15)	120.5
C(14)-C(15)-H(15)	120.5
C(15)-C(16)-C(11)	120.3(5)
C(15)-C(16)-H(16)	119.9
C(11)-C(16)-H(16)	119.9
C(18)-C(17)-C(13)	121.0(5)
C(18)-C(17)-H(17)	119.5
C(13)-C(17)-H(17)	119.5
C(17)-C(18)-C(19)	120.1(6)
C(17)-C(18)-H(18)	120.0
C(19)-C(18)-H(18)	120.0
C(20)-C(19)-C(18)	120.5(6)
C(20)-C(19)-H(19)	119.7
C(18)-C(19)-H(19)	119.7
C(19)-C(20)-C(14)	120.5(5)
C(19)-C(20)-H(20)	119.7
C(14)-C(20)-H(20)	119.7
C(22)-C(21)-O(3)	119.4(4)
C(22)-C(21)-C(26)	123.2(5)
O(3)-C(21)-C(26)	117.4(4)
C(21)-C(22)-C(23)	118.3(4)
C(21)-C(22)-C(12)	119.4(4)
C(23)-C(22)-C(12)	122.3(4)
C(27)-C(23)-C(22)	122.5(5)
C(27)-C(23)-C(24)	118.5(5)
C(22)-C(23)-C(24)	118.9(5)
C(25)-C(24)-C(30)	122.0(5)
C(25)-C(24)-C(23)	119.6(5)
C(30)-C(24)-C(23)	118.4(5)
C(26)-C(25)-C(24)	120.8(5)
C(26)-C(25)-H(25)	119.6
C(24)-C(25)-H(25)	119.6
C(25)-C(26)-C(21)	119.0(5)
C(25)-C(26)-H(26)	120.5
C(21)-C(26)-H(26)	120.5
C(28)-C(27)-C(23)	120.9(5)
C(28)-C(27)-H(27)	119.5
C(23)-C(27)-H(27)	119.5
C(27)-C(28)-C(29)	120.2(6)
C(27)-C(28)-H(28)	119.9
C(29)-C(28)-H(28)	119.9
C(30)-C(29)-C(28)	120.3(6)
C(30)-C(29)-H(29)	119.8
C(28)-C(29)-H(29)	119.8
C(29)-C(30)-C(24)	121.6(5)
C(29)-C(30)-H(30)	119.2
C(24)-C(30)-H(30)	119.2
C(36)-C(31)-C(32)	116.7(7)
C(36)-C(31)-C(37)	123.9(6)
C(32)-C(31)-C(37)	119.3(5)
C(36)-C(31)-Ru(1)	70.4(3)

C(32)-C(31)-Ru(1)	71.9(3)
C(37)-C(31)-Ru(1)	130.9(4)
C(33)-C(32)-C(31)	121.7(6)
C(33)-C(32)-Ru(1)	71.2(4)
C(31)-C(32)-Ru(1)	70.4(3)
C(33)-C(32)-H(32)	119.1
C(31)-C(32)-H(32)	119.1
Ru(1)-C(32)-H(32)	132.4
C(32)-C(33)-C(34)	122.8(6)
C(32)-C(33)-Ru(1)	73.8(4)
C(34)-C(33)-Ru(1)	69.5(3)
C(32)-C(33)-H(33)	118.6
C(34)-C(33)-H(33)	118.6
Ru(1)-C(33)-H(33)	131.1
C(35)-C(34)-C(33)	115.2(7)
C(35)-C(34)-C(40)	122.9(6)
C(33)-C(34)-C(40)	121.9(6)
C(35)-C(34)-Ru(1)	69.5(3)
C(33)-C(34)-Ru(1)	72.8(3)
C(40)-C(34)-Ru(1)	127.6(5)
C(36)-C(35)-C(34)	122.1(6)
C(36)-C(35)-Ru(1)	73.0(3)
C(34)-C(35)-Ru(1)	72.1(3)
C(36)-C(35)-H(35)	118.9
C(34)-C(35)-H(35)	118.9
Ru(1)-C(35)-H(35)	128.2
C(31)-C(36)-C(35)	121.3(6)
C(31)-C(36)-Ru(1)	73.5(3)
C(35)-C(36)-Ru(1)	69.1(3)
C(31)-C(36)-H(36)	119.4
C(35)-C(36)-H(36)	119.4
Ru(1)-C(36)-H(36)	130.9
C(38)-C(37)-C(31)	115.4(6)
C(38)-C(37)-C(39)	111.4(6)
C(31)-C(37)-C(39)	109.1(7)
C(38)-C(37)-H(37)	106.8
C(31)-C(37)-H(37)	106.8
C(39)-C(37)-H(37)	106.8
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(34)-C(40)-H(40A)	109.5
C(34)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(34)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(1)-N(1)-N(2)	112.1(5)
C(1)-N(1)-C(4)	129.0(6)
N(2)-N(1)-C(4)	118.9(5)
C(3)-N(2)-N(1)	104.6(5)
C(6)-O(1)-P(1)	127.5(3)
C(11)-O(2)-P(1)	117.4(3)
C(21)-O(3)-P(1)	121.0(3)
O(1)-P(1)-O(2)	99.26(18)
O(1)-P(1)-O(3)	99.43(17)
O(2)-P(1)-O(3)	103.23(17)
O(1)-P(1)-Ru(1)	118.48(13)
O(2)-P(1)-Ru(1)	111.59(13)
O(3)-P(1)-Ru(1)	121.59(12)
C(35)-Ru(1)-C(34)	38.4(2)
C(35)-Ru(1)-C(36)	37.9(3)
C(34)-Ru(1)-C(36)	69.0(3)
C(35)-Ru(1)-C(33)	66.7(2)
C(34)-Ru(1)-C(33)	37.7(2)
C(36)-Ru(1)-C(33)	78.0(2)
C(35)-Ru(1)-P(1)	89.44(15)
C(34)-Ru(1)-P(1)	110.77(17)
C(36)-Ru(1)-P(1)	96.46(16)
C(33)-Ru(1)-P(1)	148.08(17)
C(35)-Ru(1)-C(31)	67.3(3)
C(34)-Ru(1)-C(31)	81.5(3)
C(36)-Ru(1)-C(31)	36.2(2)
C(33)-Ru(1)-C(31)	66.5(2)
P(1)-Ru(1)-C(31)	124.99(16)
C(35)-Ru(1)-C(32)	77.8(2)
C(34)-Ru(1)-C(32)	66.5(3)
C(36)-Ru(1)-C(32)	65.5(2)
C(33)-Ru(1)-C(32)	35.0(2)
P(1)-Ru(1)-C(32)	161.75(16)
C(31)-Ru(1)-C(32)	37.7(2)
C(35)-Ru(1)-Cl(1)	121.1(2)
C(34)-Ru(1)-Cl(1)	90.4(2)
C(36)-Ru(1)-Cl(1)	158.6(2)
C(33)-Ru(1)-Cl(1)	89.13(17)
P(1)-Ru(1)-Cl(1)	85.50(5)
C(31)-Ru(1)-Cl(1)	149.41(16)
C(32)-Ru(1)-Cl(1)	112.22(17)
C(35)-Ru(1)-Cl(2)	149.4(2)
C(34)-Ru(1)-Cl(2)	161.02(17)
C(36)-Ru(1)-Cl(2)	112.3(2)
C(33)-Ru(1)-Cl(2)	123.30(16)
P(1)-Ru(1)-Cl(2)	88.09(5)
C(31)-Ru(1)-Cl(2)	89.50(18)
C(32)-Ru(1)-Cl(2)	96.28(18)
Cl(1)-Ru(1)-Cl(2)	89.02(5)
C(42A)-C(41A)-O(4A)	106.2(12)
C(42A)-C(41A)-H(41A)	110.5
O(4A)-C(41A)-H(41A)	110.5
C(42A)-C(41A)-H(41B)	110.5
O(4A)-C(41A)-H(41B)	110.5
H(41A)-C(41A)-H(41B)	108.7
C(41A)-C(42A)-C(42A)#1	108.6(6)
C(41A)-C(42A)-H(42A)	110.0
C(42A)#1-C(42A)-H(42A)	110.0
C(41A)-C(42A)-H(42B)	110.0
C(42A)#1-C(42A)-H(42B)	110.0
H(42A)-C(42A)-H(42B)	108.4
C(41A)#1-O(4A)-C(41A)	110.3(16)
O(4B)-C(41B)-C(42B)	100(2)
O(4B)-C(41B)-H(41C)	111.7
C(42B)-C(41B)-H(41C)	111.7
O(4B)-C(41B)-H(41D)	111.7
C(42B)-C(41B)-H(41D)	111.7
H(41C)-C(41B)-H(41D)	109.5

C(42B)#1-C(42B)-C(41B)	105.0(19)
C(42B)#1-C(42B)-H(42C)	110.7
C(41B)-C(42B)-H(42C)	110.7
C(42B)#1-C(42B)-H(42D)	110.7
C(41B)-C(42B)-H(42D)	110.7
H(42C)-C(42B)-H(42D)	108.8
C(41B)-O(4B)-C(41B)#1	122(3)
C(48A)-C(43A)-C(44A)	126(2)
C(48A)-C(43A)-C(49A)	116.9(15)
C(44A)-C(43A)-C(49A)	116.8(15)
C(45A)-C(44A)-C(43A)	113.7(14)
C(45A)-C(44A)-H(44A)	123.1
C(43A)-C(44A)-H(44A)	123.1
C(46A)-C(45A)-C(44A)	115.7(14)
C(46A)-C(45A)-H(45A)	122.2
C(44A)-C(45A)-H(45A)	122.2
C(47A)-C(46A)-C(45A)	132(2)
C(47A)-C(46A)-H(46A)	113.8
C(45A)-C(46A)-H(46A)	113.8
C(46A)-C(47A)-C(48A)	110(2)
C(46A)-C(47A)-H(47A)	124.9
C(48A)-C(47A)-H(47A)	124.9
C(47A)-C(48A)-C(43A)	121(2)
C(47A)-C(48A)-H(48A)	119.6
C(43A)-C(48A)-H(48A)	119.6
C(44B)-C(43B)-C(49B)	121.9(13)
C(44B)-C(43B)-C(48B)	120.1(16)
C(49B)-C(43B)-C(48B)	118.0(13)
C(43B)-C(44B)-C(45B)	122.1(11)
C(43B)-C(44B)-H(44B)	118.9
C(45B)-C(44B)-H(44B)	118.9
C(46B)-C(45B)-C(44B)	121.2(11)
C(46B)-C(45B)-H(45B)	119.4
C(44B)-C(45B)-H(45B)	119.4
C(45B)-C(46B)-C(47B)	116.1(16)
C(45B)-C(46B)-H(46B)	121.9
C(47B)-C(46B)-H(46B)	121.9
C(48B)-C(47B)-C(46B)	124.1(17)
C(48B)-C(47B)-H(47B)	118.0
C(46B)-C(47B)-H(47B)	118.0
C(43B)-C(48B)-C(47B)	116.1(16)
C(43B)-C(48B)-H(48B)	122.0
C(47B)-C(48B)-H(48B)	122.0
C(43B)-C(49B)-H(49D)	109.5
C(43B)-C(49B)-H(49E)	109.5
H(49D)-C(49B)-H(49E)	109.5
C(43B)-C(49B)-H(49F)	109.5
H(49D)-C(49B)-H(49F)	109.5
H(49E)-C(49B)-H(49F)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 -y+1,-x+1,-z+1/2

Table 4. Anisotropic displacement parameters [Å^{2}x10^3] for 6.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[(ha^*)^2U_{11}+...+2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	70(5)	63(5)	37(3)	6(3)	-1(3)	16(4)
C(2)	60(4)	34(3)	34(3)	4(2)	-4(3)	-1(3)
C(3)	37(3)	37(3)	35(3)	-2(2)	5(2)	0(3)
C(4)	78(5)	74(5)	83(5)	-30(4)	-38(4)	11(5)
C(5)	46(4)	34(3)	36(3)	4(2)	3(3)	3(3)
C(6)	31(3)	28(3)	31(3)	8(2)	2(2)	-5(2)
C(7)	44(3)	38(3)	37(3)	0(2)	1(3)	-5(3)
C(8)	42(4)	51(4)	47(3)	5(3)	-4(3)	11(3)
C(9)	43(4)	43(4)	70(4)	-2(3)	6(3)	10(3)
C(10)	49(4)	48(4)	53(4)	-9(3)	7(3)	10(3)
C(11)	23(3)	27(3)	31(3)	6(2)	2(2)	1(2)
C(12)	29(3)	26(3)	31(3)	5(2)	-1(2)	2(2)
C(13)	29(3)	30(3)	33(3)	1(2)	3(2)	2(2)
C(14)	30(3)	33(3)	37(3)	4(2)	6(2)	5(2)
C(15)	32(3)	33(3)	23(2)	0(2)	2(2)	10(2)
C(16)	31(3)	27(3)	25(2)	-2(2)	-1(2)	3(2)
C(17)	41(4)	31(3)	41(3)	-1(2)	-1(3)	-7(3)
C(18)	53(4)	42(4)	56(4)	4(3)	1(3)	-11(3)
C(19)	47(4)	50(4)	58(4)	13(3)	9(3)	-14(3)
C(20)	47(4)	35(3)	43(3)	10(3)	7(3)	-3(3)
C(21)	26(3)	30(3)	27(3)	-1(2)	-8(2)	-8(2)
C(22)	26(3)	35(3)	25(3)	-1(2)	2(2)	-5(2)
C(23)	35(3)	26(3)	33(3)	-1(2)	-2(2)	-2(2)
C(24)	34(3)	46(4)	31(3)	-6(3)	-1(2)	-6(3)
C(25)	41(3)	52(4)	25(3)	1(3)	-3(2)	-10(3)
C(26)	36(3)	40(3)	26(3)	5(2)	-7(2)	-3(2)
C(27)	48(4)	39(3)	41(3)	0(3)	2(3)	4(3)
C(28)	61(4)	35(3)	55(4)	-7(3)	0(3)	8(3)
C(29)	65(4)	46(4)	48(3)	-15(3)	3(3)	9(4)
C(30)	51(4)	58(4)	35(3)	-18(3)	-1(3)	-3(3)
C(31)	59(4)	39(3)	49(4)	-7(3)	10(3)	-24(3)
C(32)	67(5)	44(4)	37(3)	1(3)	8(3)	-33(3)
C(33)	50(4)	51(4)	35(3)	-3(3)	-1(3)	-29(3)
C(34)	61(4)	70(5)	41(4)	8(3)	-16(3)	-40(4)
C(35)	73(5)	65(5)	21(3)	-3(3)	-4(3)	-47(4)
C(36)	65(5)	50(4)	40(3)	-11(3)	9(3)	-28(4)
C(37)	86(5)	34(4)	69(5)	-10(3)	18(4)	-19(4)
C(38)	86(6)	59(5)	78(5)	12(4)	2(4)	-13(4)
C(39)	122(9)	45(5)	224(12)	-29(6)	64(9)	-32(5)
C(40)	55(5)	72(5)	72(5)	15(4)	-20(4)	-25(4)
N(1)	64(4)	61(4)	37(3)	-12(3)	-7(3)	14(3)
N(2)	59(3)	46(3)	38(3)	-5(2)	-5(3)	7(2)
O(1)	35(2)	25(2)	24(2)	1(1)	1(1)	0(2)
O(2)	24(2)	26(2)	29(2)	4(1)	0(1)	-1(2)
O(3)	27(2)	30(2)	28(2)	0(2)	-6(2)	-3(1)
P(1)	29(1)	27(1)	23(1)	3(1)	-1(1)	-6(1)
Cl(1)	39(1)	45(1)	31(1)	1(1)	0(1)	-4(1)
Cl(2)	43(1)	38(1)	37(1)	8(1)	1(1)	-4(1)
Ru(1)	43(1)	35(1)	24(1)	1(1)	2(1)	-17(1)
C(41A)	162(11)	176(11)	77(8)	-26(8)	3(8)	-147(9)
C(42A)	310(20)	124(12)	118(14)	8(10)	-61(14)	2(14)
O(4A)	155(8)	155(8)	163(15)	-24(7)	-24(7)	-21(11)
C(41B)	130(20)	190(20)	130(30)	-25(18)	-20(20)	-50(20)

C(42B)	180(20)	140(20)	100(20)	0(20)	-10(20)	-40(20)
O(4B)	133(17)	133(17)	170(30)	-16(17)	-16(17)	-40(20)
C(43A)	91(12)	52(12)	178(15)	-22(16)	-15(10)	1(13)
C(44A)	105(11)	49(12)	134(14)	19(16)	21(12)	4(12)
C(45A)	98(10)	42(9)	115(11)	-22(10)	3(10)	16(10)
C(46A)	86(11)	70(15)	159(12)	-11(14)	30(9)	32(12)
C(47A)	179(15)	105(15)	125(12)	-5(15)	43(13)	-8(16)
C(48A)	172(15)	46(11)	110(13)	-43(11)	-26(11)	17(13)
C(49A)	85(15)	200(40)	390(40)	0(40)	-52(16)	10(20)
C(43B)	109(9)	45(9)	141(11)	-3(11)	-2(9)	4(10)
C(44B)	83(7)	67(11)	102(9)	-41(9)	37(7)	-9(8)
C(45B)	100(9)	57(9)	112(10)	-49(8)	18(7)	1(7)
C(46B)	63(8)	44(7)	193(12)	-16(9)	13(8)	6(7)
C(47B)	128(10)	53(11)	180(11)	-15(11)	49(10)	-11(10)
C(48B)	163(11)	56(9)	113(11)	11(10)	26(8)	-3(10)
C(49B)	129(12)	35(10)	310(20)	-2(14)	-87(15)	24(12)

Table 5. Hydrogen coordinates [x10^4] and isotropic displacement parameters [Å^{2}x10^3] for 6.

	x	y	z	U(eq)
H(1)	6427	1407	4921	68
H(2)	5471	678	4462	51
H(4A)	6473	3117	5130	117
H(4B)	6163	3743	4806	117
H(4C)	7036	3239	4762	117
H(7)	4083	966	3184	48
H(8)	2913	1861	3220	56
H(9)	2743	2736	3732	62
H(10)	3753	2790	4200	60
H(15)	5557	-1524	4535	35
H(16)	6332	-490	4230	33
H(17)	4628	-2650	3192	45
H(18)	3726	-3569	3500	61
H(19)	3672	-3583	4159	62
H(20)	4492	-2666	4502	50
H(25)	5792	-1245	2014	47
H(26)	5348	-103	2372	41
H(27)	6387	-2899	3281	51
H(28)	6968	-3968	2918	60
H(29)	7018	-3835	2264	63
H(30)	6458	-2667	1976	57
H(32)	7452	3161	2785	59
H(33)	8436	2152	2909	55
H(35)	7167	1492	3859	64
H(36)	6161	2545	3735	62
H(37)	5873	3543	2865	76
H(38A)	4959	2970	3331	112
H(38B)	4754	3930	3220	112
H(38C)	5243	3726	3601	112
H(39A)	6041	4920	3068	196
H(39B)	6961	4497	3065	196
H(39C)	6466	4617	3452	196
H(40A)	9018	1221	3603	100
H(40B)	8751	773	3220	100
H(40C)	8278	529	3601	100
H(41A)	4523	7218	2430	166
H(41B)	4168	6830	2044	166
H(42A)	2944	7444	2134	220
H(42B)	3322	7889	2501	220
H(41C)	4382	5596	1961	175
H(41D)	5145	6165	2127	175
H(42C)	4226	7053	2443	170
H(42D)	3541	6727	2142	170
H(44A)	3497	4748	3818	116
H(45A)	2013	4496	3799	102
H(46A)	1352	4358	4350	126
H(47A)	1944	4083	4911	164
H(48A)	3378	4481	4938	131
H(49A)	4573	5093	4652	340
H(49B)	4652	5113	4206	340
H(49C)	4777	4241	4427	340
H(44B)	3646	4896	3709	101
H(45B)	2287	4792	3453	107
H(46B)	1153	4347	3815	120
H(47B)	1428	4013	4453	144

H(48B)	2764	4239	4733	133
H(49D)	4484	4128	4345	238
H(49E)	4111	4748	4658	238
H(49F)	4449	5126	4271	238

Table 1. Crystal data and structure refinement for 7.

Empirical formula	$C_{41}H_{36}Cl_5N_2O_7PRu$	
Formula weight	978.01	
Crystal colour and habit	yellow block	
Crystal size (mm)	0.10 x 0.12 x 0.14	
Temperature (K)	150(2)	
Wavelength (Å)	0.71073	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 11.4579(2) Å	α = 90°
	b = 15.0138(2) Å	β = 100.677(2)°
	c = 12.2822(2) Å	γ = 90°
Volume (Å^3)	2076.29(6)	
Z	2	
Calculated density (Mg/m^3)	1.564	
Absorption coefficient (mm^{-1})	0.790	
F(000)	992	
θ-range for data collection (°)	3.02/32.51	
Index ranges	$-16 \le h \le 16$, $-21 \le k \le 22$, $-18 \le l \le 17$	
Reflections collected	30506	
Independent reflections	12948 (R_{int} = 0.0488)	
Completeness to θ = 32.51°	92.0 %	
Absorption correction	Semi-empirical from equivalents (Multiscan)	
Max. and min. transmission	1.00000 and 0.93125	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	12948/1/518	
Goodness-of-fit on F^2	0.923	
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0459, wR_2 = 0.0979	
R indices (all data)	R_1 = 0.0698, wR_2 = 0.1046	
Absolute structure parameter	-0.04(2)	
Largest diff. Peak and hole (e·Å^{-3})	1.026/-0.932	

Definitions:

$$R_1 = \frac{\sum \left| |F_o| - |F_c| \right|}{\sum |F_o|} \qquad wR_2 = \sqrt{\frac{\sum \left[w\left(F_o^2 - F_c^2\right)^2 \right]}{\sum \left[w\left(F_o^2\right)^2 \right]}}$$

$$GooF = \sqrt{\frac{\sum \left[w\left(F_o^2 - F_c^2\right) \right]}{(n-p)}}$$ n = number of reflections; p = number of parameters

Notes on the refinement of 7.

All hydrogen atom positions were calculated in deal positions (riding model). The target molecule was co-crystallized with one $CHCl_3$.

Table 2. Atomic coordinates [x10^4] and equivalent isotropic displacement parameters [Å^{2}x10^3] for 7.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	5431(4)	5385(3)	3800(3)	35(1)
C(2)	4289(4)	5103(3)	3451(3)	35(1)
C(3)	3642(3)	5861(3)	3071(3)	30(1)
C(4)	6553(4)	6786(3)	3765(4)	41(1)
C(5)	2417(4)	5892(3)	2440(4)	32(1)
C(6)	1504(3)	6411(3)	2733(3)	31(1)
C(7)	411(4)	6466(3)	2052(4)	40(1)
C(8)	188(4)	5983(3)	1060(4)	47(1)
C(9)	1069(4)	5435(3)	791(4)	48(1)
C(10)	2171(4)	5398(3)	1475(4)	36(1)
C(11)	966(3)	8407(2)	4959(3)	25(1)
C(12)	1297(3)	8331(2)	6084(3)	24(1)
C(13)	350(3)	8220(2)	6712(3)	27(1)
C(14)	-845(3)	8254(3)	6144(4)	32(1)
C(15)	-1098(3)	8376(3)	4977(4)	34(1)
C(16)	-213(3)	8438(3)	4386(3)	33(1)
C(17)	573(3)	8026(3)	7859(3)	33(1)
C(18)	-338(3)	7921(4)	8425(3)	41(1)
C(19)	-1528(3)	8005(4)	7856(4)	41(1)
C(20)	-1776(3)	8155(3)	6751(4)	36(1)
C(21)	3360(3)	7774(2)	6263(3)	28(1)
C(22)	2568(3)	8327(2)	6621(3)	24(1)
C(23)	3005(3)	8900(3)	7546(3)	28(1)
C(24)	4168(3)	8771(3)	8164(3)	33(1)
C(25)	4896(3)	8109(3)	7808(3)	37(1)
C(26)	4530(3)	7643(3)	6873(4)	34(1)
C(27)	2340(4)	9637(3)	7836(4)	35(1)
C(28)	2788(4)	10180(3)	8723(4)	39(1)
C(29)	3925(4)	10004(3)	9347(4)	45(1)
C(30)	4587(4)	9339(3)	9076(4)	41(1)
C(31)	2962(3)	9175(2)	2109(3)	29(1)
C(32)	2359(3)	8385(3)	1623(3)	30(1)
C(33)	2955(3)	7726(2)	1171(3)	30(1)
C(34)	4204(3)	7790(3)	1161(3)	33(1)
C(35)	4812(4)	8542(3)	1663(3)	35(1)
C(36)	4186(3)	9208(3)	2129(3)	33(1)
C(37)	2283(5)	9931(3)	2506(4)	43(1)
C(38)	3017(7)	10547(4)	3316(6)	97(3)
C(39)	1651(5)	10441(3)	1502(4)	49(1)
C(40)	4829(5)	7048(3)	682(4)	48(1)
C(41)	2037(10)	5392(6)	7229(9)	121(3)
N(1)	5468(3)	6262(2)	3672(3)	29(1)
N(2)	4374(3)	6585(2)	3217(2)	25(1)
O(1)	1660(2)	6872(2)	3729(2)	33(1)
O(2)	1855(2)	8487(2)	4306(2)	26(1)
O(3)	3057(2)	7252(2)	5329(2)	27(1)
O(4)	7775(3)	8051(3)	2079(3)	61(1)
O(5)	9311(3)	8512(2)	1205(3)	55(1)
O(6)	7984(4)	7411(3)	405(4)	67(1)
O(7)	7348(3)	8871(3)	442(3)	62(1)
P(1)	2605(1)	7634(1)	4105(1)	24(1)
Cl(1)	5120(1)	8451(1)	4540(1)	33(1)
Cl(2)	8104(1)	8210(1)	1038(1)	37(1)
Cl(3)	3034(2)	5124(2)	6352(3)	143(1)
Cl(4)	2839(5)	6024(3)	8317(4)	192(2)

Cl(5)	786(3)	5862(2)	6509(4)	168(1)
Ru(1)	3835(1)	7930(1)	2911(1)	23(1)

Table 3. Bond lengths [Å] and angles [°] for 7.

C(1)-N(1)	1.328(5)	C(31)-C(36)	1.400(6)
C(1)-C(2)	1.366(6)	C(31)-C(32)	1.443(6)
C(1)-H(1)	0.9500	C(31)-C(37)	1.507(6)
C(2)-C(3)	1.390(5)	C(31)-Ru(1)	2.258(4)
C(2)-H(2)	0.9500	C(32)-C(33)	1.377(5)
C(3)-N(2)	1.364(5)	C(32)-Ru(1)	2.200(4)
C(3)-C(5)	1.473(6)	C(32)-H(32)	0.9500
C(4)-N(1)	1.457(5)	C(33)-C(34)	1.437(5)
C(4)-H(4A)	0.9800	C(33)-Ru(1)	2.209(4)
C(4)-H(4B)	0.9800	C(33)-H(33)	0.9500
C(4)-H(4C)	0.9800	C(34)-C(35)	1.408(6)
C(5)-C(10)	1.382(6)	C(34)-C(40)	1.502(6)
C(5)-C(6)	1.403(6)	C(34)-Ru(1)	2.276(3)
C(6)-C(7)	1.374(6)	C(35)-C(36)	1.413(6)
C(6)-O(1)	1.388(5)	C(35)-Ru(1)	2.255(4)
C(7)-C(8)	1.400(7)	C(35)-H(35)	0.9500
C(7)-H(7)	0.9500	C(36)-Ru(1)	2.216(4)
C(8)-C(9)	1.389(6)	C(36)-H(36)	0.9500
C(8)-H(8)	0.9500	C(37)-C(38)	1.498(8)
C(9)-C(10)	1.382(7)	C(37)-C(39)	1.518(7)
C(9)-H(9)	0.9500	C(37)-H(37)	1.0000
C(10)-H(10)	0.9500	C(38)-H(38A)	0.9800
C(11)-C(12)	1.368(5)	C(38)-H(38B)	0.9800
C(11)-C(16)	1.404(5)	C(38)-H(38C)	0.9800
C(11)-O(2)	1.414(4)	C(39)-H(39A)	0.9800
C(12)-C(13)	1.452(5)	C(39)-H(39B)	0.9800
C(12)-C(22)	1.484(5)	C(39)-H(39C)	0.9800
C(13)-C(17)	1.415(6)	C(40)-H(40A)	0.9800
C(13)-C(14)	1.419(5)	C(40)-H(40B)	0.9800
C(14)-C(20)	1.418(5)	C(40)-H(40C)	0.9800
C(14)-C(15)	1.420(6)	C(41)-Cl(5)	1.692(11)
C(15)-C(16)	1.355(6)	C(41)-Cl(4)	1.754(11)
C(15)-H(15)	0.9500	C(41)-Cl(3)	1.755(11)
C(16)-H(16)	0.9500	C(41)-H(41)	1.0000
C(17)-C(18)	1.365(5)	N(1)-N(2)	1.363(4)
C(17)-H(17)	0.9500	N(2)-Ru(1)	2.125(3)
C(18)-C(19)	1.418(6)	O(1)-P(1)	1.584(3)
C(18)-H(18)	0.9500	O(2)-P(1)	1.587(3)
C(19)-C(20)	1.353(6)	O(3)-P(1)	1.603(3)
C(19)-H(19)	0.9500	O(4)-Cl(2)	1.420(3)
C(20)-H(20)	0.9500	O(5)-Cl(2)	1.434(3)
C(21)-C(22)	1.361(5)	O(6)-Cl(2)	1.422(4)
C(21)-O(3)	1.380(5)	O(7)-Cl(2)	1.426(3)
C(21)-C(26)	1.423(5)	P(1)-Ru(1)	2.2577(10)
C(22)-C(23)	1.439(5)	Cl(1)-Ru(1)	2.3853(9)
C(23)-C(24)	1.419(5)		
C(23)-C(27)	1.426(5)	N(1)-C(1)-C(2)	108.6(3)
C(24)-C(25)	1.417(6)	N(1)-C(1)-H(1)	125.7
C(24)-C(30)	1.418(6)	C(2)-C(1)-H(1)	125.7
C(25)-C(26)	1.344(6)	C(1)-C(2)-C(3)	105.8(3)
C(25)-H(25)	0.9500	C(1)-C(2)-H(2)	127.1
C(26)-H(26)	0.9500	C(3)-C(2)-H(2)	127.1
C(27)-C(28)	1.381(6)	N(2)-C(3)-C(2)	109.3(4)
C(27)-H(27)	0.9500	N(2)-C(3)-C(5)	123.2(3)
C(28)-C(29)	1.409(7)	C(2)-C(3)-C(5)	126.8(4)
C(28)-H(28)	0.9500	N(1)-C(4)-H(4A)	109.5
C(29)-C(30)	1.333(7)	N(1)-C(4)-H(4B)	109.5
C(29)-H(29)	0.9500	H(4A)-C(4)-H(4B)	109.5
C(30)-H(30)	0.9500	N(1)-C(4)-H(4C)	109.5

H(4A)-C(4)-H(4C)	109.5	C(26)-C(25)-C(24)	121.4(3)
H(4B)-C(4)-H(4C)	109.5	C(26)-C(25)-H(25)	119.3
C(10)-C(5)-C(6)	118.4(4)	C(24)-C(25)-H(25)	119.3
C(10)-C(5)-C(3)	117.2(4)	C(25)-C(26)-C(21)	119.5(4)
C(6)-C(5)-C(3)	124.4(4)	C(25)-C(26)-H(26)	120.3
C(7)-C(6)-O(1)	117.4(3)	C(21)-C(26)-H(26)	120.3
C(7)-C(6)-C(5)	121.0(4)	C(28)-C(27)-C(23)	121.2(4)
O(1)-C(6)-C(5)	121.5(4)	C(28)-C(27)-H(27)	119.4
C(6)-C(7)-C(8)	119.9(4)	C(23)-C(27)-H(27)	119.4
C(6)-C(7)-H(7)	120.1	C(27)-C(28)-C(29)	119.3(4)
C(8)-C(7)-H(7)	120.1	C(27)-C(28)-H(28)	120.3
C(9)-C(8)-C(7)	119.3(4)	C(29)-C(28)-H(28)	120.3
C(9)-C(8)-H(8)	120.3	C(30)-C(29)-C(28)	121.1(4)
C(7)-C(8)-H(8)	120.3	C(30)-C(29)-H(29)	119.5
C(10)-C(9)-C(8)	120.2(4)	C(28)-C(29)-H(29)	119.5
C(10)-C(9)-H(9)	119.9	C(29)-C(30)-C(24)	121.5(4)
C(8)-C(9)-H(9)	119.9	C(29)-C(30)-H(30)	119.3
C(9)-C(10)-C(5)	121.2(4)	C(24)-C(30)-H(30)	119.3
C(9)-C(10)-H(10)	119.4	C(36)-C(31)-C(32)	116.0(3)
C(5)-C(10)-H(10)	119.4	C(36)-C(31)-C(37)	122.9(4)
C(12)-C(11)-C(16)	124.8(3)	C(32)-C(31)-C(37)	121.1(4)
C(12)-C(11)-O(2)	119.1(3)	C(36)-C(31)-Ru(1)	70.2(2)
C(16)-C(11)-O(2)	116.1(3)	C(32)-C(31)-Ru(1)	68.9(2)
C(11)-C(12)-C(13)	116.8(3)	C(37)-C(31)-Ru(1)	134.1(3)
C(11)-C(12)-C(22)	121.0(3)	C(33)-C(32)-C(31)	121.5(3)
C(13)-C(12)-C(22)	122.1(3)	C(33)-C(32)-Ru(1)	72.2(2)
C(17)-C(13)-C(14)	118.5(3)	C(31)-C(32)-Ru(1)	73.3(2)
C(17)-C(13)-C(12)	122.6(3)	C(33)-C(32)-H(32)	119.3
C(14)-C(13)-C(12)	118.9(4)	C(31)-C(32)-H(32)	119.3
C(20)-C(14)-C(13)	119.3(4)	Ru(1)-C(32)-H(32)	127.4
C(20)-C(14)-C(15)	120.8(4)	C(32)-C(33)-C(34)	121.6(3)
C(13)-C(14)-C(15)	119.9(4)	C(32)-C(33)-Ru(1)	71.4(2)
C(16)-C(15)-C(14)	121.1(4)	C(34)-C(33)-Ru(1)	73.9(2)
C(16)-C(15)-H(15)	119.5	C(32)-C(33)-H(33)	119.2
C(14)-C(15)-H(15)	119.5	C(34)-C(33)-H(33)	119.2
C(15)-C(16)-C(11)	118.4(4)	Ru(1)-C(33)-H(33)	127.7
C(15)-C(16)-H(16)	120.8	C(35)-C(34)-C(33)	117.6(3)
C(11)-C(16)-H(16)	120.8	C(35)-C(34)-C(40)	122.2(4)
C(18)-C(17)-C(13)	121.1(4)	C(33)-C(34)-C(40)	120.1(4)
C(18)-C(17)-H(17)	119.4	C(35)-C(34)-Ru(1)	71.1(2)
C(13)-C(17)-H(17)	119.4	C(33)-C(34)-Ru(1)	68.8(2)
C(17)-C(18)-C(19)	119.7(4)	C(40)-C(34)-Ru(1)	128.6(3)
C(17)-C(18)-H(18)	120.2	C(34)-C(35)-C(36)	119.9(4)
C(19)-C(18)-H(18)	120.2	C(34)-C(35)-Ru(1)	72.7(2)
C(20)-C(19)-C(18)	120.8(3)	C(36)-C(35)-Ru(1)	70.1(2)
C(20)-C(19)-H(19)	119.6	C(34)-C(35)-H(35)	120.1
C(18)-C(19)-H(19)	119.6	C(36)-C(35)-H(35)	120.1
C(19)-C(20)-C(14)	120.5(4)	Ru(1)-C(35)-H(35)	129.5
C(19)-C(20)-H(20)	119.8	C(31)-C(36)-C(35)	123.4(4)
C(14)-C(20)-H(20)	119.8	C(31)-C(36)-Ru(1)	73.4(2)
C(22)-C(21)-O(3)	122.3(3)	C(35)-C(36)-Ru(1)	73.1(2)
C(22)-C(21)-C(26)	122.3(4)	C(31)-C(36)-H(36)	118.3
O(3)-C(21)-C(26)	115.3(3)	C(35)-C(36)-H(36)	118.3
C(21)-C(22)-C(23)	117.7(3)	Ru(1)-C(36)-H(36)	127.4
C(21)-C(22)-C(12)	121.2(3)	C(38)-C(37)-C(31)	114.9(5)
C(23)-C(22)-C(12)	121.2(3)	C(38)-C(37)-C(39)	110.6(4)
C(24)-C(23)-C(27)	117.7(4)	C(31)-C(37)-C(39)	108.3(4)
C(24)-C(23)-C(22)	119.7(3)	C(38)-C(37)-H(37)	107.6
C(27)-C(23)-C(22)	122.5(3)	C(31)-C(37)-H(37)	107.6
C(25)-C(24)-C(30)	122.2(4)	C(39)-C(37)-H(37)	107.6
C(25)-C(24)-C(23)	118.6(4)	C(37)-C(38)-H(38A)	109.5
C(30)-C(24)-C(23)	119.2(4)	C(37)-C(38)-H(38B)	109.5

H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(34)-C(40)-H(40A)	109.5
C(34)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(34)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
Cl(5)-C(41)-Cl(4)	116.5(6)
Cl(5)-C(41)-Cl(3)	111.1(6)
Cl(4)-C(41)-Cl(3)	106.4(6)
Cl(5)-C(41)-H(41)	107.5
Cl(4)-C(41)-H(41)	107.5
Cl(3)-C(41)-H(41)	107.5
C(1)-N(1)-N(2)	110.7(3)
C(1)-N(1)-C(4)	124.9(3)
N(2)-N(1)-C(4)	123.1(3)
N(1)-N(2)-C(3)	105.5(3)
N(1)-N(2)-Ru(1)	128.7(2)
C(3)-N(2)-Ru(1)	125.6(2)
C(6)-O(1)-P(1)	125.9(2)
C(11)-O(2)-P(1)	119.1(2)
C(21)-O(3)-P(1)	124.4(2)
O(1)-P(1)-O(2)	105.49(14)
O(1)-P(1)-O(3)	95.69(14)
O(2)-P(1)-O(3)	103.48(14)
O(1)-P(1)-Ru(1)	115.37(11)
O(2)-P(1)-Ru(1)	111.31(10)
O(3)-P(1)-Ru(1)	123.19(10)
O(4)-Cl(2)-O(6)	109.6(3)
O(4)-Cl(2)-O(7)	110.0(2)
O(6)-Cl(2)-O(7)	108.5(3)
O(4)-Cl(2)-O(5)	109.5(2)
O(6)-Cl(2)-O(5)	109.7(2)
O(7)-Cl(2)-O(5)	109.4(2)
N(2)-Ru(1)-C(32)	125.60(13)
N(2)-Ru(1)-C(33)	96.01(12)
C(32)-Ru(1)-C(33)	36.39(14)
N(2)-Ru(1)-C(36)	146.05(13)
C(32)-Ru(1)-C(36)	66.17(14)
C(33)-Ru(1)-C(36)	77.74(14)
N(2)-Ru(1)-C(35)	110.04(13)
C(32)-Ru(1)-C(35)	78.26(14)
C(33)-Ru(1)-C(35)	66.03(15)
C(36)-Ru(1)-C(35)	36.82(15)
N(2)-Ru(1)-P(1)	83.93(8)
C(32)-Ru(1)-P(1)	92.22(10)
C(33)-Ru(1)-P(1)	111.88(11)
C(36)-Ru(1)-P(1)	129.58(11)
C(35)-Ru(1)-P(1)	165.90(11)
N(2)-Ru(1)-C(31)	162.64(12)
C(32)-Ru(1)-C(31)	37.76(14)
C(33)-Ru(1)-C(31)	66.84(13)
C(36)-Ru(1)-C(31)	36.44(14)
C(35)-Ru(1)-C(31)	66.53(14)
P(1)-Ru(1)-C(31)	99.59(10)
N(2)-Ru(1)-C(34)	88.87(13)
C(32)-Ru(1)-C(34)	66.54(14)
C(33)-Ru(1)-C(34)	37.32(14)
C(36)-Ru(1)-C(34)	65.80(15)
C(35)-Ru(1)-C(34)	36.19(15)
P(1)-Ru(1)-C(34)	147.38(11)
C(31)-Ru(1)-C(34)	79.00(14)
N(2)-Ru(1)-Cl(1)	92.85(9)
C(32)-Ru(1)-Cl(1)	140.70(11)
C(33)-Ru(1)-Cl(1)	163.15(10)
C(36)-Ru(1)-Cl(1)	86.91(11)
C(35)-Ru(1)-Cl(1)	97.45(11)
P(1)-Ru(1)-Cl(1)	83.26(3)
C(31)-Ru(1)-Cl(1)	104.43(10)
C(34)-Ru(1)-Cl(1)	128.96(10)

Table 4. Anisotropic displacement parameters [Å^{2}x10^3] for 7.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[(ha^*)^2U_{11}+...+2hka^*b^*U_{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	41(2)	35(2)	27(2)	2(2)	4(2)	14(2)
C(2)	46(2)	25(2)	34(2)	3(2)	6(2)	3(2)
C(3)	37(2)	28(2)	26(2)	-1(1)	10(2)	3(2)
C(4)	27(2)	44(2)	50(3)	2(2)	3(2)	3(2)
C(5)	31(2)	30(2)	35(2)	-1(2)	6(2)	-7(2)
C(6)	34(2)	29(2)	32(2)	-6(2)	12(2)	-4(2)
C(7)	29(2)	38(2)	53(3)	-12(2)	8(2)	2(2)
C(8)	28(2)	60(3)	51(3)	-18(2)	1(2)	-8(2)
C(9)	43(3)	50(3)	52(3)	-27(2)	12(2)	-8(2)
C(10)	31(2)	33(2)	46(3)	-14(2)	8(2)	-4(2)
C(11)	23(2)	24(2)	28(2)	-2(1)	5(1)	0(1)
C(12)	23(2)	21(2)	28(2)	0(1)	7(2)	-1(1)
C(13)	20(2)	27(2)	35(2)	-2(1)	4(2)	1(1)
C(14)	24(2)	30(2)	42(2)	-8(2)	6(2)	1(1)
C(15)	24(2)	33(2)	43(2)	-5(2)	-2(2)	2(2)
C(16)	32(2)	35(2)	29(2)	1(2)	-4(2)	2(2)
C(17)	26(2)	39(2)	34(2)	-1(2)	7(1)	-5(2)
C(18)	39(2)	43(2)	44(2)	-2(3)	15(2)	-2(3)
C(19)	30(2)	44(3)	57(2)	-9(3)	22(2)	-7(2)
C(20)	23(2)	42(3)	47(2)	-4(2)	13(2)	-3(1)
C(21)	28(2)	31(3)	25(2)	11(1)	7(1)	4(1)
C(22)	19(2)	30(2)	24(2)	4(1)	6(1)	1(1)
C(23)	26(2)	39(2)	19(2)	7(1)	8(1)	-7(1)
C(24)	25(2)	51(2)	22(2)	11(2)	6(2)	-3(2)
C(25)	21(2)	61(3)	26(2)	16(2)	1(1)	3(2)
C(26)	25(2)	44(2)	36(2)	14(2)	11(2)	10(2)
C(27)	35(2)	34(2)	40(2)	1(2)	19(2)	-2(2)
C(28)	43(2)	44(3)	34(2)	-3(2)	14(2)	-9(2)
C(29)	54(3)	58(3)	25(2)	-8(2)	10(2)	-29(2)
C(30)	34(2)	60(3)	26(2)	7(2)	1(2)	-16(2)
C(31)	37(2)	25(2)	24(2)	6(1)	5(2)	1(2)
C(32)	28(2)	37(2)	25(2)	8(2)	3(2)	3(2)
C(33)	39(2)	23(2)	25(2)	1(1)	1(2)	-3(1)
C(34)	41(2)	39(3)	21(2)	4(2)	11(2)	7(2)
C(35)	34(2)	38(2)	35(2)	8(2)	12(2)	-1(2)
C(36)	37(2)	28(2)	32(2)	8(2)	2(2)	-5(2)
C(37)	69(4)	31(3)	32(3)	9(2)	14(2)	15(2)
C(38)	139(7)	64(4)	66(4)	-32(3)	-37(4)	48(4)
C(39)	68(3)	35(2)	42(3)	7(2)	4(3)	25(2)
C(40)	62(3)	47(3)	39(3)	5(2)	20(2)	11(2)
C(41)	154(9)	74(5)	141(9)	0(5)	40(7)	-2(5)
N(1)	28(2)	35(2)	25(2)	2(1)	6(1)	5(1)
N(2)	24(2)	32(2)	20(1)	1(1)	6(1)	2(1)
O(1)	33(1)	34(1)	36(2)	-9(1)	14(1)	-9(1)
O(2)	29(1)	29(1)	21(1)	0(1)	5(1)	7(1)
O(3)	33(1)	25(1)	26(1)	4(1)	9(1)	5(1)
O(4)	44(2)	108(3)	32(2)	4(2)	12(1)	-12(2)
O(5)	27(2)	67(2)	72(2)	12(2)	12(2)	-4(1)
O(6)	67(3)	62(2)	76(3)	-6(2)	26(2)	-6(2)
O(7)	40(2)	71(2)	72(3)	22(2)	1(2)	14(2)
P(1)	28(1)	22(1)	23(1)	0(1)	7(1)	1(1)
Cl(1)	36(1)	36(1)	26(1)	-1(1)	1(1)	-7(1)
Cl(2)	25(1)	49(1)	38(1)	9(1)	9(1)	1(1)
Cl(3)	106(2)	132(2)	188(3)	-19(2)	23(2)	6(2)

Cl(4)	280(5)	154(3)	149(3)	2(2)	56(3)	-68(3)
Cl(5)	153(2)	98(2)	268(4)	-18(2)	78(3)	23(2)
Ru(1)	24(1)	23(1)	22(1)	1(1)	5(1)	0(1)

Table 5. Hydrogen coordinates [x10^4] and isotropic displacement parameters [Å^{2}x10^3] for 7.

	x	y	z	U(eq)
H(1)	6088	5014	4088	41
H(2)	3997	4512	3464	42
H(4A)	6890	6883	4549	62
H(4B)	6370	7361	3397	62
H(4C)	7128	6465	3412	62
H(7)	-192	6831	2253	48
H(8)	-559	6029	576	57
H(9)	915	5086	136	58
H(10)	2770	5025	1279	44
H(15)	-1901	8414	4605	41
H(16)	-387	8501	3603	40
H(17)	1369	7969	8243	39
H(18)	-175	7791	9195	49
H(19)	-2159	7957	8257	50
H(20)	-2579	8194	6380	44
H(25)	5658	7993	8240	44
H(26)	5048	7229	6622	41
H(27)	1576	9757	7411	42
H(28)	2334	10667	8910	47
H(29)	4225	10365	9971	55
H(30)	5357	9243	9502	49
H(32)	1533	8320	1615	36
H(33)	2530	7216	859	36
H(35)	5642	8601	1688	42
H(36)	4619	9705	2473	39
H(37)	1662	9664	2880	52
H(38A)	3479	10200	3923	145
H(38B)	2494	10960	3616	145
H(38C)	3558	10885	2941	145
H(39A)	2239	10706	1113	74
H(39B)	1165	10913	1742	74
H(39C)	1140	10033	1002	74
H(40A)	5689	7113	923	72
H(40B)	4632	7072	-129	72
H(40C)	4574	6474	939	72
H(41)	1803	4822	7552	146