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Table 1s. Crystal Data, Data Collection Conditions, and Solution and Refinement Details for $Ru(NC_4H_4)(PPh_3)_2Cl$

Crystal Data

formula	$C_{41}\ H_{36}\ N\ P_2\ Cl_3\ Ru$
color; habit	orange rhombic prism
crystal dimensions	0.73 0.61 0.55 mm
space group[a]	$P\bar{1}$
crystal system	triclinic
unit cell dimensions[b,c]	$\underline{a}$ = 9.924(2) Å
	$\underline{b}$ = 13.951(3) Å
	$\underline{c}$ = 14.370(3) Å
	α = 100.950(10)°
	β = 105.370(10)°
	γ = 99.240(10)°
volume	1836.1(7) $Å^3$
formula units / cell	Z = 2
formula weight	812.1 amu
density(calc.)	1.469 g/cm^3
absorption coefficient	0.754 mm^{-1}
F(000)	828 e^-

Data Collection

diffractometer used	Siemens P3/F
radiation	Mo-K_α (λ = 0.71073 Å)
temperature	24-26°C
monochromator	highly oriented graphite crystal
mosaic character[d]	0.20°
2θ range	3.0 to 50.0°
scan type	θ-2θ
scan speed	variable; 4.00 to 30.00°/min.
scan range	from 0.90° below 2θ for $K_{\alpha1}$ to 0.90° above 2θ for $K_{\alpha2}$
background measurement	stationary crystal and stationary counter at beginning and end of scan, each for 50% of total scan time
standard reflections	3 measured every 97 reflections
index ranges	$-11 \leq h \leq 1$, $-16 \leq k \leq 16$, $-16 \leq l \leq 17$
reflections collected	7061
unique reflections[e]	6456 (R_{int} = 1.93%)
observed reflections	5306 ($F > 4.0\sigma(F)$)

Solution and Refinement

system used[f]	Siemens SHELXTL PLUS (MicroVAX II)
solution	Patterson techniques
refinement method[g]	full-matrix least-squares
scattering factors	neutral atoms[h]
hydrogen atoms	riding model, fixed isotropic U
weighting scheme	$w = 1.0 / [\sigma^2(F) + 0.0010F^2]$
final residuals (obs. data)	R = 3.27%, wR = 4.30%
residuals (all data)	R = 4.30%, wR = 4.62%
goodness-of-fit	1.00
largest and mean Δ/σ	0.001, 0.000
data-to-parameter ratio	12.3:1
largest difference peak	0.63 $e^-/Å^3$
largest difference hole	-0.41 $e^-/Å^3$

(a) "International Tables for X-ray Crystallography", Vol. A., D. Reidel Publishing, Dordrecht, Holland/ Boston, U.S.A , 1983.

(b) Cell dimensions were determined by least-squares fit of the setting angles for 25 reflections with 2θ in the range 22.0 - 34.0°. Angle tolerances for centering, 2θ, ω and, χ; 0.02, 0.01 and, 0.04 .

(c) Estimated standard deviations in the least significant figure(s) are given in parentheses in this and all subsequent tables.

(d) Crystal mosaic character was determined from the width at half height of ω scans.

(e) $R_{int} = [\Sigma N(\Sigma w(F_{mean} - F)^2)/\Sigma(N-1)\Sigma wF^2]^{1/2}$

(f) G. M. Sheldrick, SHELXTL-PLUS, A Program For Crystal Structure Determination, Version 4.1, 1990, Siemens Analytical X-ray Instruments, Madison, Wisconsin.

(g) The quantity minimized in the least-squares procedures is:

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

$$R = R_1 = \Sigma||F_o|-|F_c|| \; / \; \Sigma|F_o|$$

$$wR = R_2 = [\Sigma w(|F_o|-|F_c|)^2 \; / \; \Sigma w(F_o)^2]^{1/2}$$

(h) "International Tables for X-ray Crystallography", Vol. 4., Kynoch Press, Birmingham, England, 1974.

Table 2s. Atomic Coordinates[a] ($x10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 x10^3$)

for $Ru(NC_4H_4)(PPh_3)_2Cl$

	x/a	y/b	z/c	U(eq)[b]
Ru	1032(1)	2426(1)	2023(1)	30(1)*
Cl1	1292(1)	3888(1)	3335(1)	43(1)*
P1	1903(1)	1604(1)	3242(1)	33(1)*
P2	3091(1)	3158(1)	1741(1)	31(1)*
C1	-1070(4)	2573(3)	1124(3)	50(1)*
C2	-272(4)	2391(3)	494(3)	47(1)*
C3	48(3)	1441(3)	530(2)	44(1)*
C4	-619(4)	1104(3)	1193(3)	47(1)*
N	-1330(3)	1785(3)	1565(2)	53(1)*
C5	350(3)	1019(3)	3568(2)	42(1)*
C6	4(4)	10(3)	3531(3)	58(2)*
C7	-1199(6)	-384(4)	3753(3)	82(2)*
C8	-2076(6)	201(5)	4005(3)	88(3)*
C9	-1763(5)	1200(5)	4052(4)	87(3)*
C10	-545(4)	1617(4)	3829(3)	65(2)*
C11	2671(3)	521(2)	2926(2)	37(1)*
C12	2462(4)	60(3)	1944(3)	51(1)*
C13	2990(5)	-793(3)	1692(3)	68(2)*
C14	3699(5)	-1189(3)	2430(3)	70(2)*
C15	3899(5)	-751(3)	3404(3)	64(2)*
C16	3399(4)	101(3)	3657(3)	53(2)*
C17	3197(3)	2251(2)	4461(2)	36(1)*
C18	4649(4)	2446(3)	4558(3)	47(1)*
C19	5656(4)	2920(3)	5471(3)	57(2)*
C20	5226(5)	3196(3)	6299(3)	63(2)*
C21	3798(5)	3005(3)	6215(3)	64(2)*
C22	2788(5)	2546(3)	5308(3)	52(2)*
C23	3303(3)	2401(2)	618(2)	39(1)*
C24	3749(4)	1508(3)	639(3)	56(2)*
C25	3711(5)	862(3)	-240(4)	76(2)*
C26	3248(5)	1105(4)	-1138(4)	75(2)*
C27	2786(5)	1970(3)	-1165(3)	68(2)*
C28	2818(4)	2615(3)	-298(3)	53(2)*

C29	3038(3)	4366(2)	1402(2)	35(1)*
C30	1844(4)	4776(3)	1305(3)	45(1)*
C31	1824(5)	5671(3)	1005(3)	59(2)*
C32	3004(5)	6148(3)	806(3)	57(2)*
C33	4198(5)	5752(3)	913(3)	55(2)*
C34	4229(4)	4866(3)	1209(3)	47(1)*
C35	4880(3)	3529(2)	2657(2)	36(1)*
C36	5048(4)	4262(3)	3505(3)	45(1)*
C37	6364(4)	4644(3)	4214(3)	52(1)*
C38	7523(4)	4295(3)	4088(3)	63(2)*
C39	7395(4)	3575(4)	3257(3)	67(2)*
C40	6072(4)	3188(3)	2530(3)	51(1)*
Cl2	1651(2)	4558(1)	8261(1)	99(1)*
Cl3	-338(2)	2860(1)	6801(2)	156(1)*
C41	492(7)	4091(4)	7060(5)	105(3)*

(a) Atoms have occupancies of 1.0.

(b) For atoms marked with *, the equivalent isotropic U is defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 3s. Bond Lengths (Å)
for $Ru(NC_4H_4)(PPh_3)_2Cl$

Ru-Cl1	2.427 (1)	Ru-P1	2.327 (1)
Ru-P2	2.304 (1)	Ru-C1	2.208 (4)
Ru-C2	2.222 (3)	Ru-C3	2.187 (3)
Ru-C4	2.161 (3)	Ru-N	2.239 (3)
P1-C5	1.839 (4)	P1-C11	1.835 (4)
P1-C17	1.835 (3)	P2-C23	1.835 (4)
P2-C29	1.844 (4)	P2-C35	1.833 (3)
C1-C2	1.368 (6)	C1-N	1.393 (6)
C2-C3	1.419 (6)	C3-C4	1.404 (6)
C4-N	1.382 (5)	C5-C6	1.381 (6)
C5-C10	1.386 (6)	C6-C7	1.373 (7)
C7-C8	1.356 (9)	C8-C9	1.364 (10)
C9-C10	1.397 (8)	C11-C12	1.380 (5)
C11-C16	1.391 (5)	C12-C13	1.399 (6)
C13-C14	1.370 (7)	C14-C15	1.364 (7)
C15-C16	1.384 (6)	C17-C18	1.386 (5)
C17-C22	1.394 (6)	C18-C19	1.386 (5)
C19-C20	1.375 (7)	C20-C21	1.367 (7)
C21-C22	1.378 (5)	C23-C24	1.390 (6)
C23-C28	1.384 (5)	C24-C25	1.393 (7)
C25-C26	1.376 (8)	C26-C27	1.362 (8)
C27-C28	1.381 (6)	C29-C30	1.383 (5)
C29-C34	1.394 (5)	C30-C31	1.398 (6)
C31-C32	1.377 (7)	C32-C33	1.371 (7)
C33-C34	1.383 (6)	C35-C36	1.387 (5)
C35-C40	1.385 (5)	C36-C37	1.376 (4)
C37-C38	1.360 (6)	C38-C39	1.368 (6)
C39-C40	1.392 (5)	Cl2-C41	1.734 (6)
Cl3-C41	1.705 (6)		

Table 4s. Bond Angles (°)
for $Ru(NC_4H_4)(PPh_3)_2Cl$

Cl1-Ru-P1	88.7(1)	Cl1-Ru-P2	90.7(1)
P1-Ru-P2	102.6(1)	Cl1-Ru-C1	93.5(1)
P1-Ru-C1	137.7(1)	P2-Ru-C1	119.6(1)
Cl1-Ru-C2	117.4(1)	P1-Ru-C2	150.6(1)
P2-Ru-C2	91.1(1)	C1-Ru-C2	36.0(2)
Cl1-Ru-C3	153.8(1)	P1-Ru-C3	114.1(1)
P2-Ru-C3	96.3(1)	C1-Ru-C3	61.2(1)
C2-Ru-C3	37.5(1)	Cl1-Ru-C4	136.4(1)
P1-Ru-C4	90.5(1)	P2-Ru-C4	131.8(1)
C1-Ru-C4	59.9(1)	C2-Ru-C4	61.5(1)
C3-Ru-C4	37.7(1)	Cl1-Ru-N	101.4(1)
P1-Ru-N	101.8(1)	P2-Ru-N	153.0(1)
C1-Ru-N	36.5(1)	C2-Ru-N	61.9(1)
C3-Ru-N	62.9(1)	C4-Ru-N	36.5(1)
Ru-P1-C5	106.8(1)	Ru-P1-C11	119.5(1)
C5-P1-C11	101.0(2)	Ru-P1-C17	123.2(1)
C5-P1-C17	103.0(2)	C11-P1-C17	100.2(1)
Ru-P2-C23	110.0(1)	Ru-P2-C29	114.3(1)
C23-P2-C29	101.1(2)	Ru-P2-C35	125.0(1)
C23-P2-C35	105.6(2)	C29-P2-C35	97.9(1)
Ru-C1-C2	72.6(2)	Ru-C1-N	73.0(2)
C2-C1-N	112.3(4)	Ru-C2-C1	71.5(2)
Ru-C2-C3	69.9(2)	C1-C2-C3	106.8(4)
Ru-C3-C2	72.5(2)	Ru-C3-C4	70.2(2)
C2-C3-C4	105.1(3)	Ru-C4-C3	72.2(2)
Ru-C4-N	74.8(2)	C3-C4-N	112.0(3)
Ru-N-C1	70.5(2)	Ru-N-C4	68.6(2)
C1-N-C4	103.7(3)	P1-C5-C6	123.4(3)
P1-C5-C10	118.1(3)	C6-C5-C10	118.4(4)
C5-C6-C7	120.4(5)	C6-C7-C8	121.1(5)
C7-C8-C9	120.0(5)	C8-C9-C10	119.8(6)
C5-C10-C9	120.2(5)	P1-C11-C12	120.4(3)
P1-C11-C16	121.4(3)	C12-C11-C16	118.0(3)
C11-C12-C13	120.9(4)	C12-C13-C14	119.6(4)
C13-C14-C15	120.3(4)	C14-C15-C16	120.4(4)

C11-C16-C15	120.8(4)	P1-C17-C18	119.3(3)
P1-C17-C22	122.8(3)	C18-C17-C22	117.9(3)
C17-C18-C19	120.8(4)	C18-C19-C20	120.2(4)
C19-C20-C21	119.6(3)	C20-C21-C22	120.6(4)
C17-C22-C21	120.8(4)	P2-C23-C24	120.4(3)
P2-C23-C28	121.0(3)	C24-C23-C28	117.8(3)
C23-C24-C25	120.4(4)	C24-C25-C26	120.5(5)
C25-C26-C27	119.4(5)	C26-C27-C28	120.6(4)
C23-C28-C27	121.3(4)	P2-C29-C30	122.3(3)
P2-C29-C34	118.8(3)	C30-C29-C34	118.9(3)
C29-C30-C31	120.5(4)	C30-C31-C32	119.7(4)
C31-C32-C33	120.1(4)	C32-C33-C34	120.7(4)
C29-C34-C33	120.1(4)	P2-C35-C36	116.0(3)
P2-C35-C40	125.1(2)	C36-C35-C40	118.7(3)
C35-C36-C37	121.1(4)	C36-C37-C38	119.7(3)
C37-C38-C39	120.6(3)	C38-C39-C40	120.3(4)
C35-C40-C39	119.6(4)	Cl2-C41-Cl3	114.1(4)

Table 5s. Anisotropic Displacement Parameters[a] ($Å^2 x 10^3$) for $Ru(NC_4H_4)(PPh_3)_2Cl$

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru	25(1)	32(1)	32(1)	6(1)	5(1)	11(1)
Cl1	39(1)	42(1)	45(1)	13(1)	9(1)	4(1)
P1	33(1)	34(1)	32(1)	6(1)	9(1)	13(1)
P2	29(1)	32(1)	33(1)	8(1)	8(1)	13(1)
C1	33(2)	54(2)	54(2)	15(2)	-4(2)	13(2)
C2	39(2)	57(2)	35(2)	3(2)	-6(1)	19(2)
C3	34(2)	55(2)	33(2)	4(2)	0(1)	5(2)
C4	39(2)	42(2)	47(2)	-1(2)	-2(2)	11(2)
N	31(2)	63(2)	52(2)	1(1)	2(1)	12(2)
C5	36(2)	55(2)	35(2)	0(2)	9(1)	19(2)
C6	57(2)	60(2)	49(2)	-10(2)	10(2)	22(2)
C7	76(3)	96(4)	56(3)	-31(3)	13(2)	29(3)
C8	58(3)	139(5)	57(3)	-23(3)	17(2)	40(3)
C9	58(3)	142(5)	82(3)	28(3)	40(3)	43(4)
C10	51(2)	88(3)	69(3)	16(2)	29(2)	33(2)
C11	37(2)	35(2)	39(2)	8(1)	6(1)	14(1)
C12	55(2)	49(2)	46(2)	20(2)	5(2)	9(2)
C13	77(3)	56(3)	57(2)	30(2)	2(2)	-1(2)
C14	72(3)	41(2)	78(3)	29(2)	-5(2)	0(2)
C15	69(3)	42(2)	74(3)	21(2)	0(2)	24(2)
C16	64(2)	47(2)	47(2)	15(2)	8(2)	20(2)
C17	44(2)	31(2)	32(2)	7(1)	5(1)	15(1)
C18	43(2)	53(2)	42(2)	5(2)	6(2)	21(2)
C19	49(2)	56(2)	57(2)	1(2)	-2(2)	27(2)
C20	79(3)	46(2)	43(2)	5(2)	-9(2)	13(2)
C21	84(3)	60(3)	43(2)	20(2)	14(2)	4(2)
C22	62(2)	51(2)	42(2)	14(2)	14(2)	12(2)
C23	36(2)	37(2)	43(2)	4(1)	16(1)	11(1)
C24	52(2)	52(2)	60(2)	18(2)	13(2)	8(2)
C25	58(3)	60(3)	99(4)	27(2)	19(3)	-9(3)
C26	72(3)	86(3)	59(3)	13(3)	29(2)	-8(2)
C27	86(3)	64(3)	50(2)	0(2)	29(2)	5(2)
C28	66(3)	47(2)	43(2)	3(2)	19(2)	13(2)
C29	39(2)	33(2)	32(2)	6(1)	7(1)	10(1)

C30	44(2)	42(2)	53(2)	15(2)	11(2)	18(2)
C31	65(3)	45(2)	67(3)	21(2)	9(2)	24(2)
C32	84(3)	36(2)	48(2)	11(2)	8(2)	21(2)
C33	67(3)	44(2)	54(2)	-2(2)	22(2)	19(2)
C34	49(2)	45(2)	50(2)	6(2)	17(2)	19(2)
C35	30(2)	38(2)	42(2)	7(1)	8(1)	20(1)
C36	38(2)	47(2)	47(2)	9(2)	8(2)	13(2)
C37	44(2)	52(2)	49(2)	-2(2)	0(2)	15(2)
C38	36(2)	80(3)	60(3)	-5(2)	-3(2)	27(2)
C39	33(2)	94(3)	75(3)	21(2)	10(2)	28(3)
C40	34(2)	69(3)	48(2)	14(2)	9(2)	14(2)
C12	82(1)	99(1)	112(1)	19(1)	13(1)	37(1)
C13	125(2)	90(1)	200(2)	21(1)	-13(1)	3(1)
C41	124(5)	103(5)	103(4)	57(4)	26(4)	42(4)

(a)The anisotropic displacement exponent takes the form: $-2\pi^2(\underline{h}^2\underline{a}^{*2}U_{11} + \ldots + 2\underline{klb^*c^*}U_{23})$

Table 6s. Hydrogen Atom Coordinates[a] ($x10^4$) and Isotropic Displacement Parameters ($Å^2x10^3$)

for $Ru(NC_4H_4)(PPh_3)_2Cl$

	x/a	y/b	z/c	U
H1A	-1440	3165	1237	80
H2A	-24	2809	78	80
H3A	515	1066	132	80
H4A	-635	462	1345	80
H6A	617	-408	3349	80
H7A	-1429	-1087	3723	80
H8A	-2917	-88	4152	80
H9A	-2369	1618	4248	80
H10A	-327	2316	3841	80
H12A	1946	331	1428	80
H13A	2857	-1100	1008	80
H14A	4050	-1781	2261	80
H15A	4394	-1038	3914	80
H16A	3553	409	4344	80
H18A	4955	2249	3984	80
H19A	6657	3057	5528	80
H20A	5924	3528	6930	80
H21A	3501	3188	6795	80
H22A	1787	2428	5254	80
H24A	4092	1343	1266	80
H25A	4010	244	-216	80
H26A	3239	663	-1741	80
H27A	2432	2130	-1793	80
H28A	2508	3230	-328	80
H30A	1024	4441	1444	80
H31A	993	5953	936	80
H32A	2994	6762	597	80
H33A	5020	6095	781	80
H34A	5069	4594	1280	80
H36A	4226	4504	3592	80
H37A	6461	5157	4792	80
H38A	8437	4551	4589	80
H39A	8215	3331	3170	80

H40A	5973	2690	1941	80
H41A	1031	4162	6603	80
H41B	-224	4479	6947	80

(a) Atoms have occupancies of 1.0.

Table 1. Crystal data for (Phpy)Ru(Cl)(PEt_3)$_2$.

Identification code	bc11msc
Empirical formula	C_{22} H_{38} Cl N P_2 Ru
Formula weight	514.99
Crystal size	0.35 x 0.10 x 0.10 mm
Crystal color, habit	orange needle
Crystal system	Orthorhombic
Space group	Fdd2
Unit cell dimensions	
a = 22.1440(10) Å	$\alpha = 90°$
b = 39.726(3) Å	$\beta = 90°$
c = 10.8680(7) Å	$\gamma = 90°$
Volume	9560.5(10) Å^3
Z	16
Density (calculated)	1.431 Mg$\cdot$m^{-3}
Absorption coefficient	0.909 mm^{-1}
F(000)	4288
Absorption correction	none applied
Max. and min. trans. coeff.	0.92 and 0.90

Table 2. Data collection for (Phpy)Ru(Cl)(PEt_3)$_2$.

Diffractometer	RAXIS
Temperature	123(2) K
Radiation source	Rigaku rotating anode, 12.5 kW
Wavelength	0.71073 A (MoKα)
Monochromator	graphite
Theta range, data coll'n	2.05 to 25.18deg
Scan type	Oscillation, 3.0°
Data images	30 exposures, 12.0 minutes each
Index ranges	-24 <= h <= 26, -47 <= k <= 42, -9 <= l <= 13
Reflections collected	7513
Independent reflections	3760 (R_{int} = 0.0494)
Standard reflections	0
Stability of standards	NA

Table 3. Solution and refinement of (Phpy)Ru(Cl)(PEt_3)$_2$.

System for solution	SHELXTL v.5[1,2]
Structure solution	direct
System for refinement	SHELXTL v. 5[1,2]
Hydrogen atoms	riding, isotropic riding U
Data/ restraints/ parameters	3760 / 1 / 251
Final R indices[3] [I>2σ(I)]	R1 = 0.0536, wR2 = 0.1342
Reflections observed	3439
R indices (all data)	R1 = 0.0556, wR2 = 0.1355
Goodness-of-fit[4] on F^2	1.063
Absolute structure parameter	0.00(5)
Extinction coefficient	0.0021(2)
Largest diff. peak and hole	1.821 and -1.165 e•Å^{-3}

1) G. M. Sheldrick, SHELXTL PLUS, *A Program for Crystal Structure Determination.* Version 5-β, 1995, Siemens Anayltical X-ray Instruments, Madison, Wisconsin.

2) Scattering factors (neutral atoms) are from "International Tables for Crystallography" Vol. C, D. Reidel Publishing Co.Boston, 1991.

3) $$R1 = \frac{\sum ||Fo| - |Fc||}{\sum |Fo|}; wR2 = \sqrt{\frac{\sum \left[w\left(Fo^2 - Fc^2\right)^2 \right]}{\sum \left[w\left(Fo^2\right)^2 \right]}}$$

4) $$Goodness - of - Fit = \sqrt{\frac{\sum \left[w\left(Fo^2 - Fc^2\right)^2 \right]}{(M - N)}}$$

where M is the number of reflections and N is the number of parameters refined.

Notes on the solution and refinement of (Phpy)Ru(Cl)(PEt_3)$_2$.

The crystal used was selected from a sample under Paratone oil and mounted on the drawn tip of a glass capillary with a small quantity of silicone sealer. This assembly was then placed in the 123 K nitrogen stream of a Rigaku R-Axis II image plate diffractometer at Molecular Structure Corporation. Examination of the data frames from the image plate showed the presence of satellite peaks neighboring each indexed reflection. These satellites undoubtedly lead to the large disagreement observed for refinement against all data as collected on a Nicolet P3.

Data reduction was performed on a Silicon Graphics Indy workstation and a solution obtained from a preliminary dataset was applied to these structure factors. Final refinement was performed on a Silicon Graphics Indigo2 workstation using a β–release of SHELXTL v.5. The largest peaks in the final difference map were located near the heavy atoms and are likely to be absorption artifacts. All non–hydrogen atoms were refined with anisotropic thermal parameters. Hydrogen atoms were placed at calculated distances and allowed to ride on the position of the parent atom. Values for hydrogen thermal parameters were set to be 1.2 times the U_{eq} of the corresponding carbon atom.

Many thanks to Molecular Structure Corporation for data collection and processing, especially Dr. Catherine L. Day, Dr. Jan M. Troup, and Dr. Beverly R. Vincent.

Table 4. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for (Phpy)Ru(Cl)(PEt_3)$_2$.

U_{eq} is defined as one–third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ru	1785(1)	567(1)	7920(1)	40(1)
Cl	2534(1)	999(1)	8318(2)	45(1)
N	2053(2)	162(1)	9299(5)	46(1)
P(1)	1617(1)	797(1)	6021(2)	42(1)
P(2)	1083(1)	887(1)	8922(2)	42(1)
C(1)	2452(3)	141(2)	8282(6)	42(1)
C(2)	2145(3)	65(1)	7173(6)	44(1)
C(3)	1505(3)	39(1)	7491(7)	47(2)
C(4)	1486(3)	107(1)	8809(7)	47(2)
C(5)	3103(3)	184(2)	8443(7)	43(1)
C(6)	3489(3)	51(2)	7570(8)	55(2)
C(7)	4114(3)	82(2)	7714(9)	56(2)
C(8)	4340(3)	242(2)	8732(10)	63(2)
C(9)	3962(3)	383(2)	9595(8)	56(2)
C(10)	3341(3)	352(2)	9451(7)	48(2)
C(11)	1645(3)	1258(2)	5853(7)	47(1)
C(12)	1861(3)	1400(2)	4623(7)	47(2)
C(13)	2171(3)	641(2)	4914(7)	48(1)
C(14)	2821(3)	688(2)	5279(7)	53(2)
C(15)	889(3)	674(2)	5337(8)	52(2)
C(16)	737(3)	815(2)	4056(8)	51(2)
C(17)	1094(3)	793(2)	10581(7)	51(2)

C(18)	1727(3)	865(2)	11129(8)	57(2)
C(19)	1153(3)	1348(2)	8858(7)	49(1)
C(20)	831(3)	1549(2)	9868(8)	54(2)
C(21)	279(3)	842(2)	8588(7)	51(2)
C(22)	40(3)	471(2)	8504(9)	63(2)

Table 5. Bond lengths [Å] for (Phpy)Ru(Cl)(PEt_3)$_2$.

Ru-C(4)	2.172(6)	Ru-C(3)	2.238(6)
Ru-N	2.276(5)	Ru-C(1)	2.279(6)
Ru-P(2)	2.284(2)	Ru-P(1)	2.288(2)
Ru-C(2)	2.296(5)	Ru-Cl	2.4246(14)
N-C(4)	1.382(8)	N-C(1)	1.418(9)
P(1)-C(13)	1.827(7)	P(1)-C(15)	1.840(7)
P(1)-C(11)	1.844(6)	P(2)-C(21)	1.826(7)
P(2)-C(19)	1.838(6)	P(2)-C(17)	1.841(7)
C(1)-C(2)	1.417(9)	C(1)-C(5)	1.462(8)
C(2)-C(3)	1.462(10)	C(3)-C(4)	1.457(11)
C(5)-C(6)	1.381(10)	C(5)-C(10)	1.388(11)
C(6)-C(7)	1.399(9)	C(7)-C(8)	1.370(13)
C(8)-C(9)	1.375(12)	C(9)-C(10)	1.390(9)
C(11)-C(12)	1.527(10)	C(13)-C(14)	1.504(9)
C(15)-C(16)	1.538(11)	C(17)-C(18)	1.550(9)
C(19)-C(20)	1.534(9)	C(21)-C(22)	1.569(9)

Table 6. Bond angles [°] for (Phpy)Ru(Cl)(PEt_3)$_2$.

C(4)-Ru-C(3)	38.6(3)	C(4)-Ru-N	36.1(2)
C(3)-Ru-N	63.1(2)	C(4)-Ru-C(1)	59.7(2)
C(3)-Ru-C(1)	61.3(2)	N-Ru-C(1)	36.3(2)
C(4)-Ru-P(2)	92.8(2)	C(3)-Ru-P(2)	115.6(2)
N-Ru-P(2)	104.9(2)	C(1)-Ru-P(2)	140.5(2)
C(4)-Ru-P(1)	133.4(2)	C(3)-Ru-P(1)	98.1(2)
N-Ru-P(1)	156.7(2)	C(1)-Ru-P(1)	123.9(2)
P(2)-Ru-P(1)	95.56(6)	C(4)-Ru-C(2)	62.0(2)
C(3)-Ru-C(2)	37.6(2)	N-Ru-C(2)	61.9(2)
C(1)-Ru-C(2)	36.1(2)	P(2)-Ru-C(2)	152.6(2)
P(1)-Ru-C(2)	94.8(2)	C(4)-Ru-Cl	136.5(2)
C(3)-Ru-Cl	153.0(2)	N-Ru-Cl	101.8(2)
C(1)-Ru-Cl	92.9(2)	P(2)-Ru-Cl	89.22(5)
P(1)-Ru-Cl	89.44(6)	C(2)-Ru-Cl	116.2(2)
C(4)-N-C(1)	104.8(6)	C(4)-N-Ru	67.8(3)
C(1)-N-Ru	72.0(3)	C(13)-P(1)-C(15)	103.4(3)
C(13)-P(1)-C(11)	104.5(3)	C(15)-P(1)-C(11)	104.7(3)
C(13)-P(1)-Ru	110.4(2)	C(15)-P(1)-Ru	113.7(2)
C(11)-P(1)-Ru	118.7(2)	C(21)-P(2)-C(19)	99.9(3)
C(21)-P(2)-C(17)	100.8(3)	C(19)-P(2)-C(17)	103.8(4)
C(21)-P(2)-Ru	121.0(2)	C(19)-P(2)-Ru	118.6(2)
C(17)-P(2)-Ru	110.1(2)	C(2)-C(1)-N	112.1(5)
C(2)-C(1)-C(5)	126.9(6)	N-C(1)-C(5)	121.0(6)
C(2)-C(1)-Ru	72.6(3)	N-C(1)-Ru	71.7(3)
C(5)-C(1)-Ru	125.1(4)	C(1)-C(2)-C(3)	106.2(6)
C(1)-C(2)-Ru	71.3(3)	C(3)-C(2)-Ru	69.0(3)
C(4)-C(3)-C(2)	104.3(6)	C(4)-C(3)-Ru	68.3(3)
C(2)-C(3)-Ru	73.4(3)	N-C(4)-C(3)	112.5(6)
N-C(4)-Ru	76.1(3)	C(3)-C(4)-Ru	73.2(4)
C(6)-C(5)-C(10)	119.5(6)	C(6)-C(5)-C(1)	118.9(7)
C(10)-C(5)-C(1)	121.6(6)	C(5)-C(6)-C(7)	120.1(8)
C(8)-C(7)-C(6)	119.5(7)	C(7)-C(8)-C(9)	121.1(6)
C(8)-C(9)-C(10)	119.3(8)	C(5)-C(10)-C(9)	120.4(7)
C(12)-C(11)-P(1)	117.5(5)	C(14)-C(13)-P(1)	115.2(5)
C(16)-C(15)-P(1)	117.4(5)	C(18)-C(17)-P(2)	110.5(5)
C(20)-C(19)-P(2)	116.9(5)	C(22)-C(21)-P(2)	115.6(4)

Table 7. Anisotropic displacement parameters [$Å^2$ x 10^3] for (Phpy)Ru(Cl)(PEt_3)$_2$.
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}
Ru	49(1)	33(1)	39(1)	1(1)	1(1)	0(1)
Cl	52(1)	37(1)	47(1)	0(1)	-2(1)	-4(1)
N	61(3)	37(3)	41(3)	9(2)	-3(2)	3(2)
P(1)	52(1)	36(1)	38(1)	1(1)	0(1)	0(1)
P(2)	49(1)	36(1)	41(1)	1(1)	2(1)	1(1)
C(1)	52(3)	37(3)	37(3)	8(2)	3(2)	3(2)
C(2)	62(3)	26(3)	44(4)	-11(2)	-2(3)	7(3)
C(3)	64(3)	20(2)	56(4)	-4(2)	-2(3)	-4(2)
C(4)	43(3)	27(3)	71(5)	8(3)	-1(3)	-3(2)
C(5)	55(3)	31(3)	44(4)	5(2)	2(3)	5(2)
C(6)	56(3)	47(3)	61(5)	2(3)	6(3)	4(3)
C(7)	52(3)	44(3)	71(6)	0(3)	2(3)	3(3)
C(8)	52(3)	48(4)	88(7)	13(4)	-2(3)	8(3)
C(9)	60(3)	36(3)	72(6)	-1(3)	-10(3)	3(3)
C(10)	50(3)	43(3)	52(4)	1(3)	-4(3)	-2(2)
C(11)	53(3)	42(3)	45(4)	-5(3)	-1(3)	0(2)
C(12)	68(3)	38(3)	35(4)	3(3)	0(3)	-3(3)
C(13)	63(3)	31(3)	50(4)	-4(3)	2(3)	7(3)
C(14)	61(3)	46(3)	52(5)	5(3)	11(3)	4(3)
C(15)	65(3)	43(3)	48(4)	4(3)	-3(3)	-6(3)
C(16)	59(4)	43(4)	49(5)	3(3)	-11(3)	-2(3)
C(17)	54(3)	65(4)	34(4)	15(3)	5(3)	0(3)
C(18)	60(4)	62(4)	50(5)	-1(4)	2(3)	0(3)
C(19)	56(3)	48(3)	42(4)	-2(3)	7(3)	-6(3)
C(20)	81(4)	35(3)	46(4)	-7(3)	12(3)	5(3)
C(21)	58(3)	45(3)	49(4)	5(3)	4(3)	4(3)
C(22)	51(3)	55(4)	83(6)	-1(4)	0(4)	-6(3)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for (Phpy)Ru(Cl)(PEt_3)$_2$.

	x	y	z	U(eq)
H(2)	2319(3)	36(1)	6381(6)	53
H(3)	1176(3)	-11(1)	6960(7)	56
H(4)	1124(3)	112(1)	9278(7)	56
H(6)	3329(3)	-62(2)	6871(8)	66
H(7)	4380(3)	-7(2)	7111(9)	67
H(8)	4765(3)	256(2)	8843(10)	75
H(9)	4124(3)	499(2)	10283(8)	67
H(10)	3077(3)	448(2)	10045(7)	58
H(11A)	1234(3)	1347(2)	6011(7)	56
H(11B)	1912(3)	1348(2)	6506(7)	56
H(12A)	1826(18)	1645(2)	4632(16)	57
H(12B)	1611(13)	1308(9)	3957(8)	57
H(12C)	2283(7)	1336(9)	4490(20)	57
H(13A)	2098(3)	397(2)	4782(7)	57
H(13B)	2103(3)	756(2)	4118(7)	57
H(14A)	2882(6)	602(12)	6114(19)	64
H(14B)	2922(7)	928(2)	5256(48)	64
H(14C)	3081(3)	565(11)	4705(29)	64
H(15A)	878(3)	425(2)	5287(8)	62
H(15B)	564(3)	743(2)	5910(8)	62
H(16A)	344(9)	728(9)	3791(19)	61
H(16B)	1048(11)	745(9)	3468(11)	61
H(16C)	723(19)	1061(2)	4093(11)	61
H(17A)	789(3)	933(2)	11006(7)	61
H(17B)	989(3)	553(2)	10713(7)	61
H(18A)	1751(9)	771(12)	11961(20)	69
H(18B)	1794(10)	1109(2)	11161(48)	69
H(18C)	2037(3)	761(12)	10610(28)	69
H(19A)	1588(3)	1405(2)	8887(7)	58
H(19B)	997(3)	1424(2)	8052(7)	58
H(20A)	1007(15)	1493(9)	10670(9)	65
H(20B)	400(5)	1492(10)	9869(31)	65
H(20C)	879(19)	1790(2)	9710(26)	65
H(21A)	48(3)	961(2)	9236(7)	61
H(21B)	193(3)	956(2)	7798(7)	61
H(22A)	-383(8)	473(2)	8238(50)	75
H(22B)	69(23)	364(5)	9314(14)	75
H(22C)	283(16)	345(4)	7909(37)	75