

Supporting Information for *J. Am. Chem. Soc.*, **1992**, 114(10), 3974-3975, DOI: [10.1021/ja00036a053](https://doi.org/10.1021/ja00036a053)

NGUYEN 3974-3975

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Experimental:

General Considerations. All manipulations were performed using standard Schlenk techniques. Argon was purified by passage through columns of BASF R3-11 catalyst (Chemalog) and 4 Å molecular sieves (Linde). Solid organometallic compounds were transferred and stored in a nitrogen-filled Vacuum Atmospheres drybox. NMR spectra were recorded with either a JEOL FX-90Q (89.60 MHz ^1H ; 22.53 MHz ^{13}C) or a QE-300 Plus (300.10 MHz ^1H ; 75.49 MHz ^{13}C) spectrometer.

Materials. Benzene and tetrahydrofuran were distilled or vacuum-transferred from sodium-benzophenone ketyl. Pentane was stirred over concentrated H_2SO_4 , dried over MgSO_4 and CaH_2 , and then transferred onto sodium-benzophenone ketyl solubilized with tetraglyme. Benzene- d_6 and THF- d_8 were dried over sodium-benzophenone ketyl. Methylene chloride- d_2 was dried over CaH_2 , vacuum-transferred, and then degassed by three continuous freeze-pump-thaw cycles. Deuterium oxide was degassed by bubbling a stream of argon through the solvent for 15 minutes. Ethanol- d_6 was dried over activated neutral alumina, vacuum-transferred and degassed by three continuous freeze-pump-thaw cycles. $\text{RuCl}_2(\text{PPh}_3)_3$,^{1a} $\text{RuCl}_2(\text{PPh}_3)_4$,^{1a} and $\text{OsCl}_2(\text{PPh}_3)_3$ ^{1b} were synthesized according to literature procedures. 3,3-Diphenylcyclopropene was prepared following a modification of a procedure described by Moore.²

(Ph_3P)₂ $\text{Cl}_2\text{Ru=CH-CH=CPh}_2$ 1. In a typical reaction, a 200 mL Schlenk flask equipped with a magnetic stirbar was charged with $\text{RuCl}_2(\text{PPh}_3)_4$ (6.00 g, 4.91 mmol) inside a nitrogen-filled drybox. Methylene chloride (40 mL) was added to dissolve the complex followed by 100 mL of benzene to dilute the solution. 3,3-Diphenylcyclopropene (954 mg, 1.01 equiv) was then added to the solution via pipet. The reaction flask was capped with a stopper, removed from the box, attached to a reflux condenser under argon and heated at 53 °C for 11 h. After allowing the solution to cool to RT, all the solvent was removed in vacuo to give a dark yellow-brown solid. Benzene (10 mL) was added to the solid and subsequent swirling of the mixture broke the solid into a fine powder. Pentane (80 mL) was then slowly added to the mixture via cannula while stirring vigorously. The mixture was stirred at RT for 1 h and allowed to settle before the supernatant was removed via cannula filtration. This washing procedure was repeated two more times to ensure the complete removal of all phosphine by-products. The resulting solid was then dried under vacuum overnight to afford 4.28 g (98%) of **1** as a yellow powder with a slight green tint. ^1H NMR (C_6D_6): δ 17.94 (pseudo-quartet = two overlapping triplets, 1 H, Ru=CH, J_{HH} = 10.2 Hz, J_{PH} = 9.7 Hz), 8.33 (d, 1 H, CH=CPh₂, J_{HH} = 10.2 Hz); ^{31}P NMR (C_6D_6): δ 28.2 (s); ^{13}C NMR (CD_2Cl_2): δ 288.9 (t, M=C, J_{CP} = 10.4 Hz), 149.9 (t, CH=CPh₂, J_{CP} = 11.58 Hz).

J-3975-m2

On the Stability of 1. Complex **1** showed no detectable decomposition in a 2:3 CD₂Cl₂/C₆D₆ solvent mixture after 2 weeks, was stable in the presence of 3 equiv of 1N HCl in diethylether for more than 3 days, and did not react with excess (> 5 equiv) acetone or propionaldehyde after several days at RT.

Other Derivatives of 1. A new complex showing a pseudo-quartet at 19.23 ppm and a doublet at 8.07 ppm characteristic of the vinylcarbene moiety was generated when **1** was treated with two equivalents of silver trifluoroacetate in a 1:2:2 THF-*d*₈/CD₂Cl₂/C₆D₆ solvent mixture. In addition, a new complex showing a pseudo-quartet at 18.77 ppm and a doublet at 8.40 ppm characteristic of the vinylcarbene moiety was generated when **1** was treated with one equivalent of silver trifluoroacetate in a 1:2:2 THF-*d*₈/CD₂Cl₂/C₆D₆ solvent mixture. Studies with alkoxides, other anionic ligands and counterions are currently in progress.

References:

1. (a) Stephenson, T. A.; Wilkinson, G. *J. Inorg. Nuclear Chem.* **1966**, *28*, 945-950. (b)
Hoffman, P. R.; Caulton, K. G. *J. Am. Chem. Soc.* **1975**, *97*, 4221-4228.
2. Moore, J. S.; Grubbs, R. H., unpublished results.

J-3975-m3

X-Ray Diffraction Data for $C_{51}H_{42}P_2Cl_2Ru$: The crystals belong to the monoclinic system with unit cell parameters at 178 K: $a = 13.466(5)$, $b = 14.188(6)$, $c = 22.62(2) \text{ \AA}$, $\beta = 104.50(6)^\circ$, and $V = 4183(4) \text{ \AA}^3$. The space group is C2/c with $Z = 4$ formula units/unit cell and $D(\text{calc.}) = 1.41 \text{ Mg/m}^3$. Intensity data (2769 total) were collected on a Siemens R3m/V diffractometer system using monochromatized MoK α radiation ($\bar{\lambda} = 0.710730 \text{ \AA}$) via a θ - 2θ scan technique¹. Those 2482 reflections with $|F_o| > 3.0\sigma (|F_o|)$ were considered observed.

The structure was solved by direct methods and refined by full-matrix least-squares techniques². Hydrogen atoms were included using a riding model with $d(\text{C-H}) = 0.96 \text{ \AA}$ and $U(\text{iso}) = 0.08 \text{ \AA}^2$. At convergence, $R_F = 4.5\%$, $R_{wF} = 5.9\%$ and GOF = 1.43 for 246 variables. A final difference-Fourier map was featureless.

References.

1. Churchill, M. R.; Lashewycz, R. A.; Rotella, F. J. Inorg. Chem 1977, 16, 265-271.
- 2a. UCLA Crystallographic Computing Package, University of California, Los Angeles, 1981, C. Strouse, personal communication.
- 2b. SHELXTL PLUS Program set; Siemens Analytical X-Ray Instruments, Inc.; Madison, WI 1990.

Supplementary Material. Description of the X-ray diffraction experiment, tables of experimental data, atomic coordinates, thermal parameters, distances and angles (13 pages) and structure factor amplitudes (6 pages).

Acknowledgement. Funds for the purchase of the Siemens R3m/V diffractometer system were made available from the National Science Foundation under Grant CHE-85-14495.

The ORTEP plot is shown at the 50% probability level.

Collection of X-ray Diffraction Data. A dark red crystal of approximate dimensions $0.20 \times 0.23 \times 0.33$ mm was oil-mounted on a glass fiber and transferred to the Syntex P2₁ diffractometer which is equipped with a modified LT-1 low temperature system. Determination of Laue symmetry, crystal class, unit cell parameters and the crystal's orientation matrix were carried out by previously described techniques similar to those of Churchill¹. Low temperature (178 K) intensity data were collected via a θ - 2θ scan technique with MoK α radiation under the conditions given in Table 1.

All 2769 data were corrected for absorption and for Lorentz and polarization effects and placed on an approximately absolute scale. Any reflection with $I(\text{net}) < 0$ was assigned the value $|F_o| = 0$. The systematic extinctions observed were hkl for $h+k = 2n+1$ and $h0l$ for $l = 2n+1$; the diffraction symmetry was $2/m$. The two possible monoclinic space groups are Cc [C_s^4 ; No. 9] or C2/c [C_{2h}^6 ; No. 15]. The centrosymmetric space was chosen and later shown to be the correct choice.

Solution and Refinement of the Crystal Structure. All crystallographic calculations were carried out using either the UCI modified version of the UCLA Crystallographic Computing Package² or the SHELXTL PLUS program set³. The analytical scattering factors for neutral atoms were used throughout the analysis^{4a}; both the real ($\Delta f'$) and imaginary ($i\Delta f''$) components of anomalous dispersion^{4b} were included. The quantity minimized during least-squares analysis was $\sum w(|F_o|-|F_c|)^2$ where $w^{-1} = \sigma^2(|F_o|) + 0.001(|F_o|)^2$.

The structure was solved by direct methods (SHELXTL PLUS); and refined by full-matrix least-squares techniques.

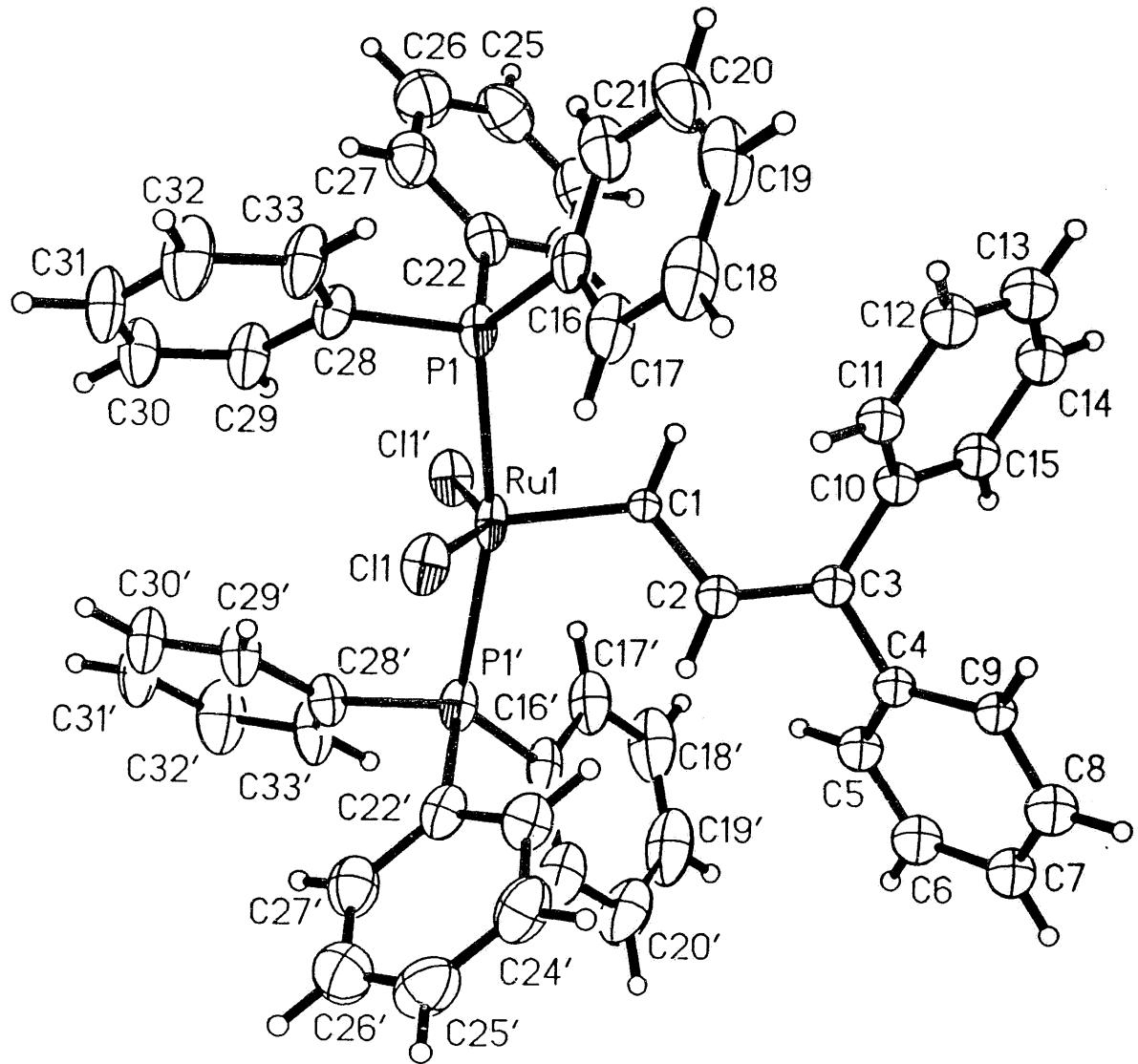
The molecule is located about a two-fold rotation axis at $1/2, y, 1/4$. The ruthenium atom lies on the two-fold axis and was assigned a site-occupancy-factor of $1/2$. The carbene portion of the molecule is disordered about the symmetry axis resulting in the observed partial orientations shown in the ORTEP diagrams (Figures 1-3). Carbon atoms labelled C(1) through C(15), and

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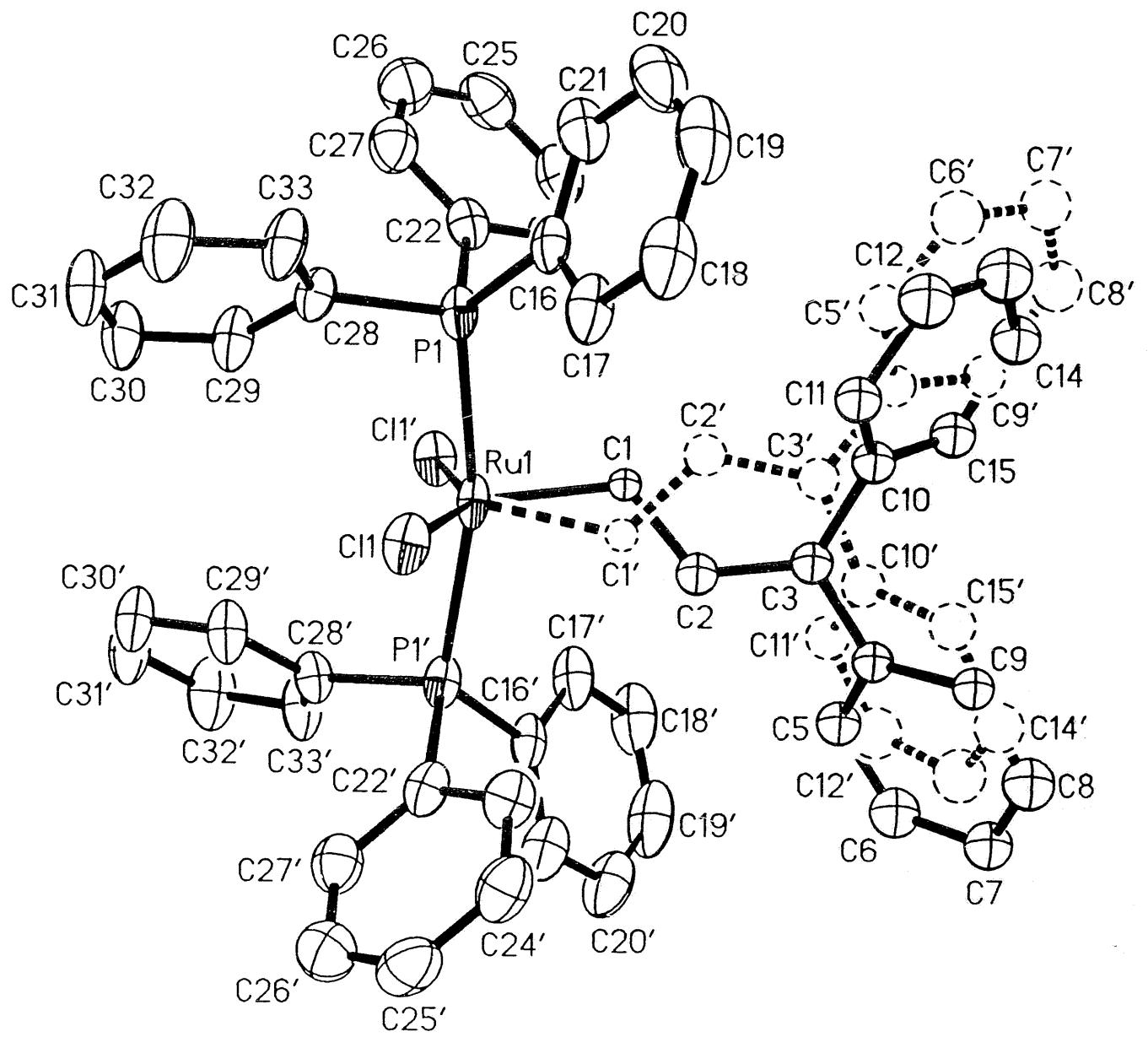
their associated hydrogen atoms, were included in the refinement with site-occupancy-factors of 1/2. The carbene moiety was refined using isotropic temperature factors. Other disorder models were tried but proved less satisfactory resulting in larger discrepancies in interatomic distances and angles. (Other models tried were (a) C(1) and C(3) fixed on the two-fold axis, C(4)-C(9) included as the sole phenyl component with site-occupancies = 1.0, (b) C(1) fixed on the two-fold, C(2) and C(3) with s.o.f = 1/2 and C(4)-C(9) at full site-occupancy.) The non-centrosymmetric space group Cc was tried but, it was decided that the molecule was best described as presented.

Hydrogen atoms were included using a riding model with $d(C-H) = 0.96\text{\AA}$ and $U(\text{iso}) = 0.08\text{\AA}^2$. Refinement of positional and thermal parameters (isotropic for carbon atoms C(1) to C(15)) led to convergence with $R_F = 4.5\%$, $R_{wF} = 5.9\%$ and GOF = 1.43 for 246 variables refined against those 2482 data with $|F_O| > 3.0\sigma(|F_O|)$. A final difference-Fourier map was devoid of significant features. $\rho(\text{max}) = 0.85 \text{ e\AA}^{-3}$.

J-3975-m4



$\lambda - 3975 \text{ nm}$



J-3975-m8

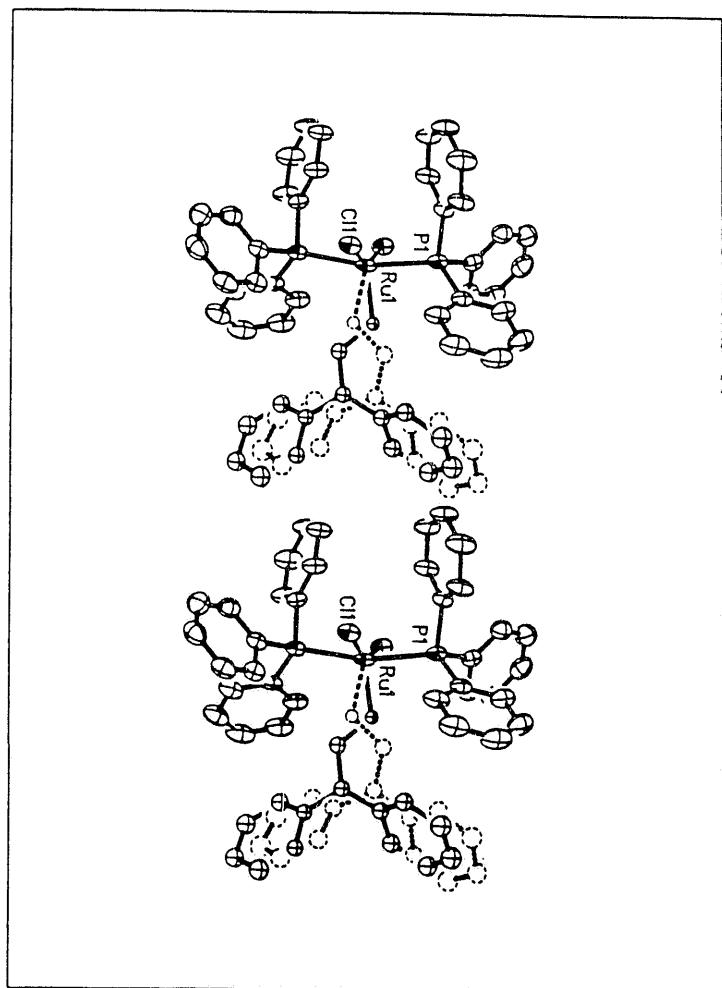


Table 1. Experimental Data for the X-ray Diffraction Study

Formula: $C_{51}H_{42}P_2Cl_2Ru$

J-3975-m19

Fw: 888.8

Temperature (K): 178

Crystal System: Monoclinic

Space Group: C2/c

a = 13.466(5) Å

b = 14.188(6) Å

c = 22.62(2) Å

β = 104.50(6) $^{\circ}$

V = 4183(4) Å³

Z = 4

D_{calcd}, Mg/m³ = 1.411

Diffractometer: Syntex P2₁ (Siemens R3m/V System)

Radiation: MoK α ($\bar{\lambda}$ = 0.710730 Å)

Monochromator: Highly oriented graphite

Data Collected: + h , + k , ± l

Scan Type: θ -2 θ

Scan Range: 1.20 $^{\circ}$ plus K α -separation

Scan Speed: 4.0 deg min⁻¹ (in ω)

2 θ Range: 4.0 to 45.0 $^{\circ}$

μ (MoK α), mm⁻¹ = 0.605

Reflections Collected: 2769

Reflections with |F_o| > 3.0 σ (|F_o|): 2482

No. of Variables: 246

R_F = 4.5%, R_{wF} = 5.9%

Goodness of Fit: 1.43

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement coefficients ($\text{\AA}^2 \times 10^4$)

J-3975-m10

	x	y	z	U(eq)	SOF
Ru(1)	5000	3537(1)	2500	273(2)	0.50
C1(1)	6386(1)	3089(1)	2115(1)	345(4)	1.00
P(1)	6107(1)	3339(1)	3496(1)	296(4)	1.00
C(1)	5083(7)	4848(5)	2644(3)	171(19)	0.50
C(2)	4670(7)	5530(6)	2173(4)	277(20)	0.50
C(3)	4769(7)	6517(7)	2268(4)	270(21)	0.50
C(4)	4206(7)	7109(6)	1750(4)	255(20)	0.50
C(5)	3186(9)	6905(9)	1432(5)	325(29)	0.50
C(6)	2699(8)	7467(7)	943(5)	417(25)	0.50
C(7)	3151(8)	8262(7)	772(5)	382(24)	0.50
C(8)	4126(9)	8490(8)	1105(5)	422(26)	0.50
C(9)	4688(9)	7938(8)	1604(6)	269(27)	0.50
C(10)	5389(7)	6977(7)	2832(4)	289(22)	0.50
C(11)	6385(7)	6752(6)	3083(4)	309(21)	0.50
C(12)	6940(10)	7250(10)	3605(6)	445(36)	0.50
C(13)	6493(9)	7960(8)	3847(5)	462(27)	0.50
C(14)	5511(10)	8186(10)	3599(7)	383(33)	0.50
C(15)	4929(8)	7708(7)	3073(5)	335(23)	0.50
C(16)	7227(3)	4110(3)	3773(2)	356(17)	1.00
C(17)	7712(4)	4476(3)	3343(3)	450(20)	1.00
C(18)	8546(4)	5077(4)	3534(3)	595(25)	1.00
C(19)	8908(4)	5298(4)	4141(4)	646(27)	1.00
C(20)	8443(5)	4921(4)	4564(3)	621(24)	1.00
C(21)	7594(4)	4323(4)	4389(3)	495(21)	1.00
C(22)	5510(4)	3316(3)	4136(2)	347(17)	1.00
C(23)	4843(4)	4040(3)	4185(2)	404(18)	1.00
C(24)	4384(4)	4065(4)	4666(3)	478(21)	1.00
C(25)	4568(5)	3345(4)	5099(3)	548(23)	1.00
C(26)	5217(5)	2623(4)	5050(3)	558(23)	1.00
C(27)	5704(4)	2605(4)	4576(2)	461(20)	1.00
C(28)	6633(3)	2157(3)	3488(2)	306(16)	1.00
C(29)	5953(4)	1413(3)	3286(3)	411(19)	1.00
C(30)	6319(4)	3(3)	3222(3)	492(21)	1.00
C(31)	7354(4)	351(.)	3356(3)	515(23)	1.00
C(32)	8032(4)	1073(4)	3557(3)	587(24)	1.00

0(33) 1683(4) 1976(3) 3622(3) 458(20) 1.00

* Equivalent isotropic U defined as one third of the
trace of the orthogonalized U_{ij} tensor

J-3975-m11

Table 3. Interatomic Distances (\AA) with Esd's

J-3975-m12

Ru(1)-Cl(1)	2.338(2)	Ru(1)-P(1)	2.387(2)
Ru(1)-C(1)	1.887(7)	P(1)-C(16)	1.841(5)
P(1)-C(22)	1.824(6)	P(1)-C(28)	1.823(5)
C(1)-C(2)	1.444(11)	C(2)-C(3)	1.419(13)
C(3)-C(4)	1.485(12)	C(3)-C(10)	1.489(12)
C(4)-C(5)	1.412(13)	C(4)-C(9)	1.421(15)
C(5)-C(6)	1.388(15)	C(6)-C(7)	1.383(15)
C(7)-C(8)	1.379(14)	C(8)-C(9)	1.425(16)
C(10)-C(11)	1.357(13)	C(10)-C(15)	1.387(15)
C(11)-C(12)	1.418(15)	C(12)-C(13)	1.357(19)
C(13)-C(14)	1.340(16)	C(14)-C(15)	1.423(17)
C(16)-C(17)	1.400(8)	C(16)-C(21)	1.389(8)
C(17)-C(18)	1.391(7)	C(18)-C(19)	1.372(10)
C(19)-C(20)	1.376(11)	C(20)-C(21)	1.400(8)
C(22)-C(23)	1.388(7)	C(22)-C(27)	1.395(7)
C(23)-C(24)	1.380(9)	C(24)-C(25)	1.394(8)
C(25)-C(26)	1.369(9)	C(26)-C(27)	1.389(9)
C(28)-C(29)	1.397(6)	C(28)-C(33)	1.393(7)
C(29)-C(30)	1.375(7)	C(30)-C(31)	1.371(8)
C(31)-C(32)	1.372(8)	C(32)-C(33)	1.386(8)

Table 4. Interatomic Angles (Deg.) with Esd's

J-3975-m/3

C1(1)-Ru(1)-P(1)	87.2(1)	C1(1)-Ru(1)-C(1)	108.3(3)
P(1)-Ru(1)-C(1)	87.5(2)	C1(1)-Ru(1)-Cl(1')	148.4(1)
P(1)-Ru(1)-Cl(1')	89.1(1)	C1(1)-Ru(1)-C(1')	102.8(3)
P(1)-Ru(1)-P(1')	166.5(1)	P(1)-Ru(1)-C(1A)	106.0(2)
Ru(1)-P(1)-C(16)	121.1(2)	Ru(1)-P(1)-C(22)	117.1(2)
C(16)-P(1)-C(22)	103.1(2)	Ru(1)-P(1)-C(28)	104.5(2)
C(16)-P(1)-C(28)	105.3(2)	C(22)-P(1)-C(28)	104.0(2)
Ru(1)-C(1)-C(2)	122.6(5)	C(1)-C(2)-C(3)	123.1(7)
C(2)-C(3)-C(4)	115.4(7)	C(2)-C(3)-C(10)	125.0(8)
C(4)-C(3)-C(10)	119.6(8)	C(3)-C(4)-C(5)	121.7(9)
C(3)-C(4)-C(9)	118.6(8)	C(5)-C(4)-C(9)	119.6(9)
C(4)-C(5)-C(6)	119.6(11)	C(5)-C(6)-C(7)	122.6(9)
C(6)-C(7)-C(8)	117.6(9)	C(7)-C(8)-C(9)	123.3(11)
C(4)-C(9)-C(8)	117.1(9)	C(3)-C(10)-C(11)	122.6(9)
C(3)-C(10)-C(15)	117.0(8)	C(11)-C(10)-C(15)	120.2(9)
C(10)-C(11)-C(12)	119.4(10)	C(11)-C(12)-C(13)	120.7(11)
C(12)-C(13)-C(14)	120.0(11)	C(13)-C(14)-C(15)	121.0(13)
C(10)-C(15)-C(14)	118.6(10)		
P(1)-C(16)-C(17)	117.9(4)	P(1)-C(16)-C(21)	121.7(4)
C(17)-C(16)-C(21)	120.3(4)	C(16)-C(17)-C(18)	119.5(5)
C(17)-C(18)-C(19)	120.5(6)	C(18)-C(19)-C(20)	119.9(5)
C(19)-C(20)-C(21)	121.3(6)	C(16)-C(21)-C(20)	118.4(6)
P(1)-C(22)-C(23)	118.2(4)	P(1)-C(22)-C(27)	122.6(4)
C(23)-C(22)-C(27)	119.2(5)	C(22)-C(23)-C(24)	120.5(5)
C(23)-C(24)-C(25)	120.0(5)	C(24)-C(25)-C(26)	119.8(6)
C(25)-C(26)-C(27)	120.7(5)	C(22)-C(27)-C(26)	119.8(5)
P(1)-C(28)-C(29)	118.3(3)	P(1)-C(28)-C(33)	122.8(3)
C(29)-C(28)-C(33)	118.7(4)	C(28)-C(29)-C(30)	120.2(5)
C(29)-C(30)-C(31)	120.9(5)	C(30)-C(31)-C(32)	119.7(5)
C(31)-C(32)-C(33)	120.7(5)	C(28)-C(33)-C(32)	120.0(4)

J. 3975-M14

Table 5. Anisotropic displacement coefficients ($\text{\AA}^2 \times 10^4$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru(1)	138(3)	156(3)	543(4)	0	118(2)	0
Cl(1)	201(6)	313(6)	554(8)	38(5)	158(6)	36(5)
P(1)	166(6)	217(6)	498(8)	11(5)	72(6)	-23(5)
C(16)	189(24)	212(24)	610(34)	27(20)	-6(24)	7(23)
C(17)	223(27)	301(27)	780(39)	-40(22)	41(26)	37(26)
C(18)	257(29)	404(32)	1055(55)	-71(25)	37(33)	57(33)
C(19)	290(33)	391(34)	1172(60)	-74(26)	23(38)	-71(36)
C(20)	392(33)	478(35)	838(46)	3(29)	-136(33)	-183(33)
C(21)	283(29)	380(30)	743(40)	12(23)	-18(28)	-89(27)
C(22)	231(26)	301(26)	494(30)	-15(20)	65(22)	-71(22)
C(23)	341(29)	383(28)	507(31)	7(24)	139(25)	-42(24)
C(24)	421(32)	423(31)	642(37)	-18(25)	229(29)	-132(27)
C(25)	624(40)	585(38)	507(34)	-106(31)	278(30)	-134(29)
C(26)	646(42)	520(36)	539(35)	-11(31)	206(32)	8(28)
C(27)	390(31)	391(30)	571(34)	-7(24)	64(27)	-18(26)
C(28)	220(25)	250(25)	465(28)	32(20)	117(21)	49(21)
C(29)	286(28)	262(27)	698(36)	5(21)	148(26)	34(24)
C(30)	490(36)	241(27)	748(39)	-50(24)	160(30)	-19(25)
C(31)	506(36)	252(27)	838(42)	111(25)	262(32)	-26(27)
C(32)	331(32)	405(32)	1048(50)	131(27)	212(33)	22(32)
C(33)	227(27)	279(27)	850(41)	63(22)	99(26)	76(26)

The anisotropic displacement exponent takes the form:

$$-2\pi^2(h^2a^2U_{11} + \dots + 2hka*b*U_{12})$$

Table 6. H-Atom coordinates ($\times 10^4$) and isotropic displacement coefficients ($\text{\AA}^2 \times 10^4$)

J-3975-n/15

	x	y	z	U	SOF
H(1A)	5412	5070	3046	800	0.50
H(2A)	4310	5304	1777	800	0.50
H(5A)	2832	6380	1553	800	0.50
H(6A)	2021	7296	715	800	0.50
H(7A)	2799	8642	433	800	0.50
H(8A)	4441	9048	997	800	0.50
H(9A)	5363	8118	1831	800	0.50
H(11A)	6710	6260	2908	800	0.50
H(12A)	7640	7084	3789	800	0.50
H(13A)	6880	8300	4196	800	0.50
H(14A)	5195	8679	3779	800	0.50
H(15A)	4233	7887	2888	800	0.50
H(17A)	7470	4313	2920	800	1.00
H(18A)	8872	5340	3239	800	1.00
H(19A)	9483	5715	4269	800	1.00
H(20A)	8707	5072	4988	800	1.00
H(21A)	7274	4065	4687	800	1.00
H(23A)	4700	4529	3882	800	1.00
H(24A)	3938	4578	4703	800	1.00
H(25A)	4240	3355	5430	800	1.00
H(26A)	5337	2123	5346	800	1.00
H(27A)	6173	2106	4552	800	1.00
H(29A)	5226	1523	3191	800	1.00
H(30A)	5845	18	3083	800	1.00
H(31A)	7601	-271	3308	800	1.00
H(32A)	8756	951	3653	800	1.00
H(33A)	8164	2477	3761	800	1.00

STRUCTURE DETERMINATION SUMMARY

J-3975-m14

Crystal Data

Empirical Formula	C ₅₁ H ₄₂ P ₂ Cl ₂ Ru
Color; Habit	Dark red cube
Crystal Size (mm)	0.20 x 0.23 x 0.33
Crystal System	Monoclinic
Space Group	C2/c
Unit Cell Dimensions	$a = 13.466(5) \text{ \AA}$ $b = 14.188(6) \text{ \AA}$ $c = 22.62(2) \text{ \AA}$ $\beta = 104.50(6)^\circ$
Volume	4183(4) \AA^3
Z	4
Formula weight	888.8
Density(calc.)	1.411 Mg/m ³
Absorption Coefficient	0.605 mm ⁻¹
F(000)	1824

J-3975-1117

Data Collection

Diffractometer System	Siemens R3m/V
Radiation	MoK α ($\lambda = 0.71073 \text{ \AA}$)
Temperature (K)	178
Monochromator	Highly oriented graphite crystal
2 θ Range	4.0 to 45.0 $^{\circ}$
Scan Type	θ -2 θ
Scan Speed	Fixed; 4.00 $^{\circ}$ /min. in ω
Scan Range (ω)	1.20 $^{\circ}$ plus K α -separation
Background Measurement	Estimated from 96 step profile
Standard Reflections	1 measured every 99 reflections
Index Ranges	$0 \leq h \leq 14, 0 \leq k \leq 15$ $-24 \leq l \leq 23$
Reflections Collected	2769
Independent Reflections	2639 ($R_{\text{int}} = 1.4\%$); ($ F_o > 0$)
Observed Reflections	2482 ($ F_o > 3.0\sigma(F_o)$)
Absorption Correction	Semi-empirical (ψ -scan method)
Min./Max. Transmission	0.4871 / 0.7596

J-3975-m18

Solution and Refinement

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F_o) + 0.0010(F_o)^2$
Final R Indices (obs. data)	$R_F = 4.5\%$, $R_{wF} = 5.9\%$
R Indices (all data)	$R_F = 4.8\%$, $R_{wF} = 6.0\%$
Goodness-of-Fit	1.43
Number of Variables	246
Data-to-Parameter Ratio	10.1:1
Largest and Mean Δ/σ	0.001, < 0.001
Largest Difference Peak	$0.85 \text{ e}\text{\AA}^{-3}$
Largest Difference Hole	$-0.90 \text{ e}\text{\AA}^{-3}$

References.

J-3975-m19

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* The ORTEP plot is shown at the 50% probability level.

Acknowledgement. Funds for the purchase of the Siemens R3m/V diffractometer system were made available to UCI from the National Science Foundation under Grant CHE-85-14495.

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s		
2	0	0	2177	1976	4	-11	1	1	465	489	17	11	7	1	110	-60	-40	5	1	2	934	-863	8		
4	0	0	946	865	8	-9	1	1	1052	990	11	-12	8	1	797	794	16	7	1	2	1694	-1607	9		
6	0	0	1042	986	9	-7	1	1	1303	1210	9	-10	8	1	812	799	13	9	1	2	480	-508	15		
8	0	0	2343	2210	10	-5	1	1	324	-240	11	-6	8	1	496	494	14	11	1	2	333	-314	15		
10	0	0	408	401	15	-3	1	1	244	-189	15	-4	8	1	226	253	17	13	1	2	313	-306	18		
12	0	0	319	342	19	-1	1	1	2453	2423	3	-2	8	1	881	862	10	-14	2	2	286	293	22		
14	0	0	585	638	17	-1	1	1	1370	1391	4	-2	8	1	1138	1210	9	-12	2	2	385	390	16		
1	1	0	2003	1942	3	3	1	1	110	-12	25	-2	8	1	1138	1210	9	-10	2	2	192	-183	23		
3	1	0	2614	2413	5	5	1	1	909	-791	9	2	8	1	972	971	6	-8	2	2	769	712	11		
5	1	0	1533	1350	7	7	1	1	2422	2270	9	4	8	1	264	305	13	-6	2	2	780	693	9		
7	1	0	566	575	11	9	1	1	1168	1110	11	6	8	1	1005	1013	10	-4	2	2	747	676	8		
9	1	0	681	649	12	11	1	1	237	214	22	8	8	1	512	486	13	-2	2	2	2182	2122	5		
11	1	0	473	469	15	13	1	1	296	278	22	10	8	1	909	891	13	0	2	2	914	911	3		
13	1	0	55	53	61	-14	2	1	528	528	19	-11	9	1	849	818	14	2	2	2	2212	-2192	5		
0	2	0	2249-2283	4	-12	2	1	652	656	14	-9	9	1	767	766	13	4	2	2	1220	-1125	2			
2	2	0	1846-1775	5	-10	2	1	804	799	12	-7	9	1	620	572	13	6	2	2	680	608	10			
4	2	0	315	286	11	-8	2	1	1136	1118	10	-5	9	1	746	754	12	8	2	2	664	618	12		
6	2	0	755	-688	10	-6	2	1	903	853	9	-3	9	1	1691	1700	9	10	2	2	188	190	23		
8	2	0	99	-2	-34	-4	2	1	635	587	8	-1	9	1	873	863	9	-12	2	2	179	-157	32		
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11	3	0	3923-4059	4	0	2	2	1	2316	2376	3	3	9	1	614	620	10	-11	3	2	787	800	13		
13	3	0	875	780	7	2	2	1	1541	1502	5	5	9	1	833	858	11	-9	3	2	898	858	11		
5	3	0	352	-373	11	-4	2	1	1272	1177	7	7	9	1	201	-105	23	-7	3	2	1246	1174	9		
7	3	0	1609-1546	9	6	2	1	1093	1089	9	9	9	1	629	603	14	-5	3	2	1336	1266	8			
9	3	0	1425-1392	11	8	2	2	1	2131	2013	10	11	9	1	850	881	14	-3	3	2	70	21	-31		
11	3	0	187	214	28	10	2	2	613	600	14	-8	10	1	177	154	27	-1	3	2	452	446	7		
13	3	0	435	-425	17	12	2	2	178	158	26	-6	10	1	517	494	15	2045	2121	5					
0	4	0	392	-399	8	-13	3	1	116	157	-41	-4	10	1	824	853	11	3	3	2	463	-425	8		
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6	4	0	353	-351	12	-7	3	1	350	-303	13	2	10	1	619	656	11	9	3	2	1456	1386	11		
8	4	0	565	-566	13	-5	3	1	332	314	13	4	10	1	673	677	12	11	3	2	90	-187	-47		
10	4	0	1210-1170	12	-3	3	1	699	-618	8	6	10	1	372	353	15	13	3	2	483	446	17			
12	4	0	320	-304	18	-1	3	1	2177	2166	5	8	10	1	233	-215	18	-12	4	2	687	698	14		
1	5	0	104	32	19	1	3	1	276	275	9	10	10	1	128	134	-55	-10	4	2	1235	1222	12		
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h k l 10Fo 10Fc 10s										h k l 10Fo 10Fc 10s										h k l 10Fo 10Fc 10s										h k l 10Fo 10Fc 10s																																																																																																																																																																																																																																																																																																																																																																																																																									
-13 3 3 128 63 36	-2 10 3 142 153 20	5 3 4 1240 1244 9	-3 11 4 399 367 13	7 5 5 1161 1132 10	-11 3 3 690 -728 16	0 10 3 745 -746 9	7 3 4 1610 1557 10	-1 11 4 716 -729 12	9 5 5 663 -628 13	-9 3 3 203 -189 19	2 10 3 626 -634 11	9 3 4 336 -300 16	1 11 4 833 -812 11	11 5 5 334 -329 20	-7 3 3 126 -103 22	4 10 3 776 -780 11	11 3 4 96 -99 40	1 11 4 676 -719 12	12 6 5 212 -212 30	-5 3 3 693 -671 9	6 10 3 107 -97 36	13 3 4 369 -375 20	5 11 4 632 -632 13	10 6 5 1310 -1325 12	-3 3 3 1337 -1254 6	8 10 3 263 -228 19	12 4 4 764 -741 14	7 11 4 166 -79 25	-8 6 6 5 699 -703 12	-1 3 3 1436 -1424 5	10 10 3 413 -400 20	10 4 4 460 -418 15	8 12 4 314 -318 20	-6 6 6 5 806 -783 9	-1 3 3 1621 -1644 5	-9 11 3 522 -557 16	8 4 4 501 -474 12	4 12 4 165 -119 24	-4 6 6 5 2412 -2365 7	-1 3 3 78 -53 26	-7 11 3 112 -95 32	-6 4 4 803 -767 10	4 12 4 308 -311 14	-2 6 6 5 159 -174 25	3 3 3 263 -226 13	-5 11 3 165 -147 22	-4 4 4 1749 -1657 7	4 12 4 110 -55 33	-0 6 6 5 483 -461 10	7 3 3 257 -228 20	-3 11 3 1323 -1316 11	-2 4 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3	17	17	803	-880	13	6	0	18	455	-488	16	-2	2	19	913	-947	11	-1	5	20	335	-369	20
5	17	17	457	-472	16	-9	1	18	527	-531	15	0	2	19	666	-658	26	1	5	20	248	-302	16
-12	2	17	234	-267	30	-7	1	18	345	-302	18	2	2	19	705	-762	14	3	5	20	131	-230	37
-10	2	17	528	-540	16	-5	1	18	481	-486	13	4	2	19	317	-374	22	-8	6	20	740	-692	15
-8	2	17	783	-787	13	-1	1</																