$$Fe^{2+} < Ru^{2+} < Os^{2+} \text{ for } O_h$$
$$Ni^{2+} < Pd^{2+} < Pt^{2+} \text{ for } D_{4h}$$
$$Ag^+ < Au^+ \text{ and } Hg^{2+} < Ag^+ \text{ for } D_{\infty h}$$
$$Cd^{2+} < Hg^{2+} < Zn^{2+} \text{ and } Zn^{2+} < Cu^+ \text{ for } T_d$$

The ^{15}N chemical shifts show the following trends: (i) For isoelectronic complexes of the $D_{\infty h}$ and T_d geometries, a substantial shift to lower field is observed as the metal oxidation number is increased. This trend is in contrast to that of ^{13}C chemical shifts. (ii) For the complexes of each periodic family, a shift to higher field is observed in going down the periodic table except for those of the zinc family.

The results listed in Table I show that the J_{C-N} values for all the complexes are larger than that for the free CN^- and that the J_{C-N} values for complexs of each symmetry are of the following orders:

$$Fe^{2+} < Ru^{2+} < Os^{2+} \text{ for } O_h$$
$$Pd^{2+} < Ni^{2+} < Pt^{2+} \text{ for } D_{4h}$$
$$Ag^+ < Au^+ \text{ and } Hg^{2+} < Au^+ \text{ for } D_{\infty h}$$
$$Hg^{2+} < Cd^{2+} < Zn^{2+} \text{ and } Cu^+ < Zn^{2+} \text{ for } T_d$$

As to the relationship between J_{C-N} values and ^{13}C or ^{15}N chemical shifts, J_{C-N} is in most cases found to increase with the increase in the ^{13}C and/or the ^{15}N shifts to higher field (or with decreasing δ values).

The C-N force constants of the cyanide complexes are known to be in the following orders:

$$Os^{2+} < Fe^{2+} < Ru^{2+} \text{ for } O_h \qquad Ni^{2+} < Pt^{2+} \text{ for } D_{4h}$$
$$Ag^+ < Au^+ \text{ and } Au^+ < Hg^{2+} \text{ for } D_{\infty h}$$
$$Hg^{2+} < Cd^{2+} < Zn^{2+} \text{ and } Cu^+ < Zn^{2+} \text{ for } T_d$$

A correlation between the ^{15}N shift or J_{C-N} value and the C-N force constants is observed in each family except for a few cases. This relation is also found for ^{13}C chemical shifts as noted by Pesek and Mason.[7]

However, the ^{15}N shifts and the C-N force constants show the reversed trend for the isoelectronic pairs. This reversal may be correlated with the large difference in the nitrogen charge between the complexes of the isoelectronic structures with different oxidation states.

Acknowledgment. We thank Mr. Y. Masuda and Miss M. Suzuki for their help in recording the ^{13}C and ^{15}N NMR spectra.

Registry No. $[Fe(CN)_6]^{4-}$, 13408-63-4; $[Ru(CN)_6]^{4-}$, 21029-33-4; $[Os(CN)_6]^{4-}$, 19356-45-7; $[Ni(CN)_4]^{2-}$, 45042-08-6; $[Pd(CN)_4]^{2-}$, 15004-87-2; $[Pt(CN)_4]^{2-}$, 15004-88-3; $[Ag(CN)_2]^-$, 15391-88-5; $[Au(CN)_2]^-$, 14950-87-9; $Hg(CN)_2$, 592-04-1; $[Cu(CN)_4]^{3-}$, 19441-11-3; $[Zn(CN)_4]^{2-}$, 19440-55-2; $[Cd(CN)_4]^{2-}$, 16041-14-8; $[Hg(CN)_4]^{2-}$, 19426-03-0; CN^-, 57-12-5.

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Synthesis and X-ray Structural Characterization of an Ortho-Metalated Ruthenium Complex of Acetophenone

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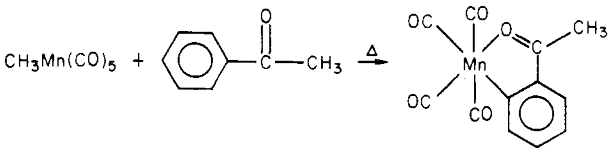
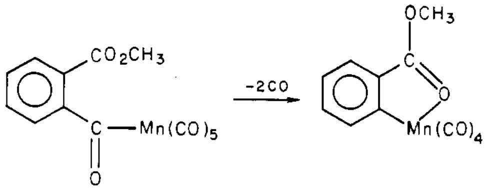
Received December 4, 1981

The directing effects of oxygen functional groups in the ortho metalation of aromatic rings by transition-metal complexes are now well established.[1-4] Kaesz prepared a large number of manganese compounds such as $CH_3C(\overline{O)C_6H_4}$-$\overline{Mn}(CO)_4$ by reacting $CH_3Mn(CO)_5$ with an aryl ketone (eq 1).[4] Several other compounds that contain a chelating carbonyl group, prepared via other routes, are also known.[5-10] For example, Casey prepared an ortho-metalated ester according to eq 2.[8,9]

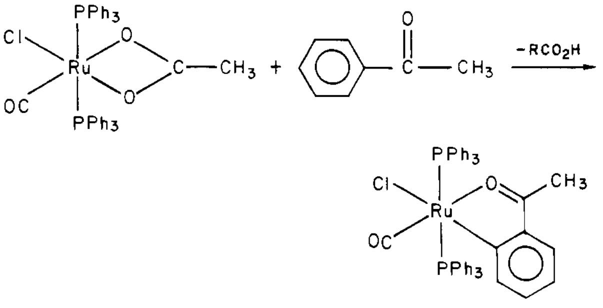


(1)



(2)

During the course of our investigation into the decarbonylation of aromatic aldehydes using Rh and Ru complexes,[11-13] we became interested in the possible existence of ortho-metalated aromatic aldehydes. As a model, we initially investigated the reaction of one of the catalysts with acetophenone. The reaction of $Ru[O_2C(CH_3)]Cl(CO)(PPh_3)_2$[14] with acetophenone at elevated temperatures resulted in the quantitative formation of $CH_3C(\overline{O)C_6H_4Ru}Cl(CO)(PPh_3)_2$ (**1**) according to eq 3. This new complex was characterized by ^1H and ^{31}P NMR, IR, and single-crystal X-ray diffraction. Its exchange reaction with benzoic acid has been investigated.



(3)

1

Experimental Section

Reactions and Solvents. Ruthenium trichloride hydrate was obtained from Engelhard Industries. All solvents were reagent grade. Triphenylphosphine was recrystallized from ethanol. Acetophenone was

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Table I. Summary of Crystal Data and Intensity Collection

Crystal Parameters			
cryst syst	monoclinic	Z	2
space group	$P2_1$	calcd density	1.431 g/cm^3
cell parameters		measd density (flotation)	1.42 g/cm^3
a	9.760 (4) Å		
b	15.509 (6) Å	temp	23 °C
c	12.455 (7) Å	abs coeff	6.03 cm^{-1}
β	95.61 (2)°	formula	$C_{45}H_{37}ClO_2P_2Ru$
V	1876 (3) Å^3	fw	808

Measurement of Intensity Data	
diffractometer	CAD4
radiation	Mo K$\bar{\alpha}$ (λ = 0.710 69 Å), graphite monochromatized
scan range, 2θ	0–50°
unique reflctns measd (quadrant)	3643 ($+h, +k, \pm l$)
obsd reflctns	2336 [$F_o^2 \geqslant 1.5\sigma(F_o^2)$]
refinement by full-matrix least squares	
no. of parameters	224
R^b	0.075
$R_w{}^b$	0.071
GOF^b	1.47
p^a	0.04

^{a} The intensity data were processed as described in: "CAD4 and SDP Users Manual"; Enraf-Nonius: Delft, Holland, 1978. The net intensity I is given as $I = [K/(\mathrm{NPI})](C - 2B)$, where K = 20.1166 times the attenuator factor, NPI = ratio of fastest possible scan rate to scan rate for the measurement, C = total count, and B = total background count. The standard deviation in the net intensity is given by $\sigma^2(I) = [\mathrm{K}/(\mathrm{NPI})]^2[C + 4B + (pI)^2]$, where p is a factor used to downweight intense reflections. The observed structure amplitude F_o is given by $F_o = (I/Lp)^{1/2}$, where Lp = Lorentz and polarization factors. The $\sigma(I)$'s were converted to the estimated errors in the relative structure factors $\sigma(F_o)$ by $\sigma(F_o) = {}^1/_2[\sigma(I)/I]F_o$. ^{b} The function minimized was $\Sigma w(|F_o| - |F_c|)^2$, where $w = 1/\sigma^2(F_o)$. The unweighted and weighted residuals are defined as follows: $R = (\Sigma ||F_o| - |F_c||)/\Sigma |F_o|$; $R_w = [(\Sigma w(|F_o| - |F_c|))^2/(\Sigma w|F_o|)^2]^{1/2}$. The error in an observation of unit weight (GOF) is $[\Sigma w(|F_o| - |F_c|)^2/(\mathrm{NO} - \mathrm{NV})]^{1/2}$, where NO and NV are the numbers of observations and variables, respectively.

purified by vacuum distillation and storage under nitrogen. All other reagents were used without further purification unless otherwise noted.

Physical Measurements. ^{1}H NMR spectra were recorded at 300 MHz with a Nicolet NT300 spectrometer equipped with a Nicolet 1180E data system. Chemical shifts are referenced to internal standard tetramethylsilane and are reported as δ values (negative values are upfield from Me_4Si). ^{31}P NMR spectra were recorded at 40.5 MHz by using a Varian Associates XL-100 FT instrument; chemical shifts were referenced to external standard H_3PO_4. Infrared spectra were recorded on a Perkin-Elmer Model 237 spectrometer and are accurate within ±5 cm^{-1}.

Synthesis of $CH_3C(O)C_6H_4RuCl(CO)(PPh_3)_2$ (1). All manipulations were carried out by using standard Schlenk-tube techniques under a purified nitrogen atmosphere unless otherwise noted.

$Ru(O_2CMe)Cl(CO)(PPh_3)_2$[14] (0.3 g, 0.37 mmol) was added to 10 mL of neat acetophenone. The solution was heated to 120 °C for 30 min, and then the acetophenone was removed with heating under vacuum. The resultant yellow solid was washed with Et_2O and dried to give a 90% yield of product. Recrystallization of the product from CH_2Cl_2/heptane can be used for further purification. Crystals suitable for X-ray analysis were obtained by slow evaporation from a toluene solution in air. All of the crystals were small rectangular plates. Anal. Calcd for $RuP_2ClO_2C_{45}H_{37}$: C, 66.87; H, 4.58. Found: C, 66.76; H, 4.75. IR (KBr disk): ν(CO) 1924 (s) cm^{-1}; ν in 1600–1380 cm^{-1} region 1585 (sh), 1570 (m), 1525 (w), 1480 (m), 1430 (m) cm^{-1}. ^{1}H NMR recorded at ambient temperature with $CDCl_3$ solvent: methyl group δ 1.81 (singlet, 3); aromatic region δ 6.25 (t, 1), 6.40 (d, 1), 6.52 (t, 1), 7.05 (d, 1).

Catalytic decarbonylation reactions and the measurement of activities with Ru catalysts were carried out with procedures identical with those that have been published in detail for rhodium diphosphine catalysts.[11-13]

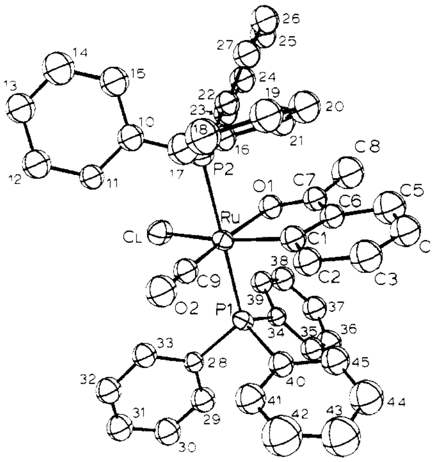

Figure 1. ORTEP drawing of the molecular structure of $CH_3C(O)C_6HRuCl(CO)(PPh_3)_2$ showing the labeling scheme.

Collection and Reduction of X-ray Data. A summary of crystal data is presented in Table I. A crystal of **1** was secured to the end of a glass fiber with 5-min epoxy resin. The crystal was found to belong to the monoclinic crystal class by the Enraf-Nonius CAD 4-SDP peak search, centering, and indexing programs. A higher order symmetry was not indicated by a Delaunay reduction calculation (program TRACER).[15] After data collection (vide infra) the only systematic absence noted was $0k0$, $k = 2n + 1$, which indicates the space group to be $P2_1$ (noncentric) or $P2_1/m$ (centric). The space group $P2_1$ was verified by successful solution and refinement and by examination of the resulting crystal structure (vide infra).

Data collection was carried out on a CAD 4 Enraf-Nonius diffractometer. Background counts were measured at both ends of the scan range with the use of an ω–2θ scan, equal, at each side, to one-fourth of the scan range of the peak. In this manner, the total duration of background measurement is equal to half of the time required for the peak scan. The intensities of three standard reflections were measured every 1.5 h of X-ray exposure, and no decay with time was noted. The data were corrected for Lorentz, polarization, background, and absorption (μ = 6.03 cm^{-1}) effects.[15]

Solution and Refinement of the Structure. The structure was solved by conventional heavy-atom techniques. The Ru atom was located by Patterson synthesis. Full-matrix least-squares refinement and difference Fourier calculations were used to locate all remaining nonhydrogen atoms. The atomic scattering factors were taken from the usual tabulation,[16] and the effects of anomalous dispersion were included in F_c by using Cromer and Ibers'[17] values of $\Delta f'$ and $\Delta f''$ for all nonhydrogen atoms. A table of observed and calculated structure factor amplitudes is available.[18]

The Ru, P, and Cl atoms were refined by full-matrix least-squares methods with anisotropic thermal parameters while all other nonhydrogen atoms were refined isotropically. Hydrogen atom positions were not included. The largest peak in the final difference Fourier map was 1.6 e/Å^3 and was located within 1 Å of the Ru atom. No chemically significant peaks were observed in this map. The final positional and thermal parameters of the atoms appear in Table II. The labeling scheme and an ORTEP drawing of **1** are shown in Figure 1.

The selection and verification of the noncentric space group $P2_1$ was based on an examination of the molecular structure. Although the molecule possesses pseudomirror symmetry (Figure 1), the pseudo mirror plane of the molecule is not coplanar with the crystallographic

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(15) All calculations were carried out on PDP 8A and 11/34 computers with use of the Enraf-Nonius CAD 4-SDP programs. This crystallographic computing package is described in: Frenz, B. A. In "Computing in Crystallography"; Schenk, H., Olthof-Hazekamp, R., van Koningsveld, H., Bassi, G. C., Eds.; Delft University Press: Delft, Holland, 1978; pp 64–71. "CAD 4 and SDP Users Manual"; Enraf-Nonius: Delft, Holland, 1978.

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(18) Supplementary material.

Table II. Positional and Isotropic Thermal Parameters and Their Esd's for **1**

atom	*x*	*y*	*z*	*B*, Å^2	atom	*x*	*y*	*z*	*B*, Å^2
Ru	0.3643 (1)	0.2500 (0)	0.14384 (9)	*a*	C21	0.294 (2)	0.469 (1)	−0.053 (1)	3.8 (4)
Cl	0.4039 (5)	0.0967 (3)	0.0950 (3)	*a*	C22	0.477 (2)	0.300 (1)	−0.113 (1)	3.3 (3)
P1	0.4008 (4)	0.2127 (3)	0.3292 (3)	*a*	C23	0.583 (1)	0.241 (1)	−0.091 (1)	3.5 (3)
P2	0.3236 (4)	0.2883 (3)	−0.0417 (3)	*a*	C24	0.705 (2)	0.245 (2)	−0.143 (1)	4.2 (3)
O1	0.5791 (9)	0.2670 (7)	0.1360 (7)	3.3 (2)	C25	0.718 (2)	0.314 (1)	−0.216 (1)	4.2 (4)
O2	0.0659 (10)	0.2545 (10)	0.1570 (8)	4.5 (2)	C26	0.613 (2)	0.370 (1)	−0.242 (1)	4.7 (4)
C1	0.383 (2)	0.379 (1)	0.182 (1)	3.5 (4)	C27	0.490 (2)	0.366 (1)	−0.191 (1)	3.9 (4)
C2	0.282 (2)	0.435 (1)	0.213 (1)	3.8 (4)	C28	0.320 (2)	0.116 (1)	0.378 (1)	2.5 (3)
C3	0.322 (2)	0.522 (1)	0.238 (1)	4.8 (4)	C29	0.361 (2)	0.082 (1)	0.479 (1)	4.0 (4)
C4	0.455 (2)	0.552 (1)	0.237 (1)	4.5 (4)	C30	0.293 (2)	0.011 (1)	0.518 (1)	4.6 (4)
C5	0.559 (2)	0.501 (1)	0.203 (2)	5.6 (5)	C31	0.180 (2)	−0.028 (1)	0.454 (1)	4.4 (4)
C6	0.519 (2)	0.407 (1)	0.182 (1)	3.2 (3)	C32	0.141 (2)	0.007 (1)	0.355 (1)	4.0 (4)
C7	0.619 (2)	0.345 (1)	0.153 (1)	3.5 (4)	C33	0.209 (2)	0.077 (1)	0.312 (1)	3.5 (4)
C8	0.770 (2)	0.367 (2)	0.139 (2)	6.6 (5)	C34	0.582 (1)	0.197 (1)	0.381 (1)	2.4 (3)
C9	0.184 (1)	0.251 (2)	0.153 (1)	2.9 (3)	C35	0.636 (2)	0.223 (1)	0.487 (1)	3.6 (4)
C10	0.220 (2)	0.214 (1)	−0.130 (1)	3.6 (4)	C36	0.778 (2)	0.199 (1)	0.521 (1)	4.9 (4)
C11	0.144 (2)	0.148 (1)	−0.089 (1)	3.1 (3)	C37	0.856 (2)	0.160 (1)	0.450 (1)	4.6 (4)
C12	0.061 (2)	0.092 (1)	−0.156 (1)	4.3 (4)	C38	0.804 (2)	0.134 (1)	0.347 (1)	4.4 (4)
C13	0.061 (2)	0.102 (1)	−0.271 (1)	4.4 (4)	C39	0.663 (2)	0.152 (1)	0.314 (1)	3.3 (3)
C14	0.140 (2)	0.163 (1)	−0.313 (2)	5.4 (5)	C40	0.331 (2)	0.295 (1)	0.418 (1)	3.4 (4)
C15	0.221 (2)	0.221 (1)	−0.245 (1)	4.4 (4)	C41	0.193 (2)	0.282 (1)	0.436 (1)	4.5 (4)
C16	0.226 (2)	0.389 (1)	−0.064 (1)	2.9 (3)	C42	0.138 (2)	0.347 (2)	0.499 (2)	7.6 (6)
C17	0.081 (2)	0.383 (1)	−0.081 (1)	4.1 (4)	C43	0.209 (2)	0.419 (2)	0.540 (2)	7.0 (6)
C18	0.010 (2)	0.461 (1)	−0.093 (1)	4.7 (4)	C44	0.343 (2)	0.429 (1)	0.517 (2)	5.8 (5)
C19	0.078 (2)	0.541 (1)	−0.084 (1)	4.0 (4)	C45	0.406 (2)	0.368 (1)	0.452 (1)	4.3 (4)
C20	0.221 (2)	0.545 (1)	−0.067 (1)	4.0 (4)					

[a] Anisotropic thermal parameters are included as supplementary material.

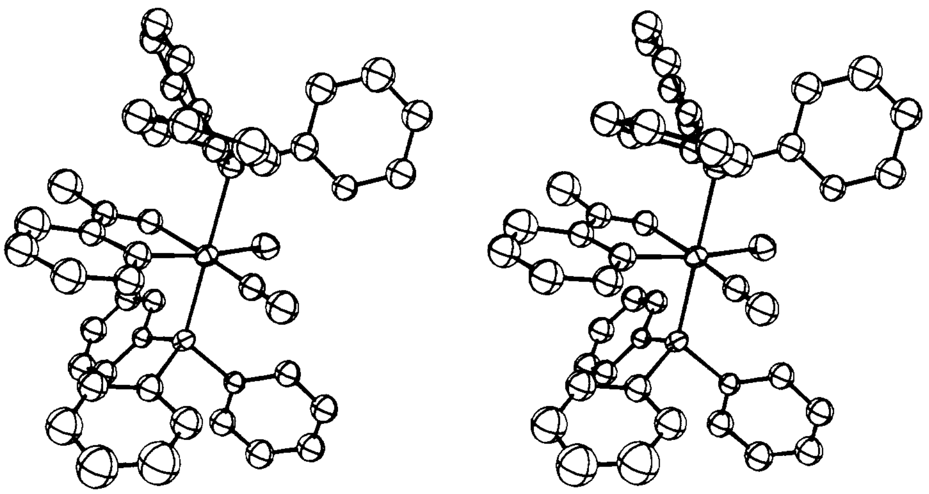

Figure 2. ORTEP stereoview of **1**.

mirror plane required by the $P2_1/m$ space group. Therefore, the centric $P2_1/m$ space group is clearly ruled out.

Results and Discussion

X-ray Structure. $CH_3C(\overline{O)C_6H_4Ru}Cl(CO)(PPh_3)_2$ (**1**) was structurally characterized by single-crystal X-ray diffraction. The crystal consists of discrete monomeric units. The ruthenium atom is six-coordinate with a distorted octahedral environment. The most important feature of the structure is the chelated ortho-metalated acetophenone ligand. The entire ortho-metalated acetophenone, the ruthenium and chlorine atoms, and the carbonyl ligand form a nearly planar arrangement (Table SI, supplementary material). The C–O bond in the ortho-metalated acetophenone (1.29 (2) Å) has been lengthened appreciably relative to that in the free ketone (1.216 (2) Å)[19] but is similar to the distances observed in other ortho-metalated aromatic ketones.[4] The Ru–O distance (2.125 (8) Å) is very similar to distances observed in ruthenium carboxylate complexes. For example, the Ru–O distance trans to CO in $Ru(O_2CMe)Cl(CO)(PPh_3)_2$[20] is 2.13 (1) Å while the Ru–O distance in $Ru(O_2CPh)(Cl)_2(PPh_3)_2$ is 2.118 (1) Å.[21] These results suggest some π-electron delocalization within the cyclo-metalated ring. Consistent with this is the C6–C7 distance of 1.44 (2) Å, which is significantly shorter than the comparable bond in free acetophenone (1.494 (2) Å)[19] through which less delocalization is expected. The Ru-C1 distance of 2.07 (2) Å is short in comparison to observed Ru^{II}–C(sp^2) distances of 2.16 (1) Å in a σ-naphthyl–ruthenium complex[22] and 2.128 (4) Å in a cationic ruthenium(II)–dimethylimidazolium complex.[23] Multiple-bond character has been ascribed to a ruthenium–carbene bond of length 2.045 Å;[24] however, Ru^{II}–C(sp^2) distances as short as 1.96 (1) Å have

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Table III. Selected Distances and Angles in $CH_3C(O)C_6H_4RuCl(CO)(PPh_3)_2$

		Distances (Å)			
Ru-P1	2.373 (4)	P1-Cl	3.430 (5)	P2-Cl	2.476 (6)
Ru-P2	2.381 (4)	P1-C9	2.95 (1)	P2-C9	2.96 (1)
Ru-Cl	2.494 (4)	P1-C1	3.16 (2)	P2-C1	3.13 (2)
Ru-C9	1.78 (1)	P1-O1	3.216 (9)	P2-O1	3.185 (9)
Ru-O1	2.125 (8)	Cl-C9	3.35 (2)	C1-C9	2.78 (2)
Ru-C1	2.07 (2)	Cl-O1	3.16 (1)	C1-O1	2.69 (2)
P1-C28	1.82 (1)	C9-O2	1.16 (1)	C3-C4	1.38 (2)
P1-C34	1.84 (1)	C7-O1	1.29 (2)	C4-C5	1.38 (2)
P1-C40	1.86 (2)	C7-C8	1.54 (2)	C5-C6	1.53 (2)
P2-C10	1.84 (2)	C7-C6	1.44 (2)		
P2-C16	1.84 (2)	C6-C1	1.39 (2)		
P2-C22	1.83 (1)	C1-C2	1.39 (2)		
		C2-C3	1.43 (2)		
		Angles (Deg)			
P1-Ru-Cl	89.6 (1)	P2-Ru-Cl	90.9 (1)	O1-C7-C6	118 (1)
P1-Ru-C9	89.6 (4)	P2-Ru-C9	89.5 (4)	C8-C7-C6	124 (1)
P1-Ru-C1	90.6 (4)	P2-Ru-C1	89.1 (4)	C7-C6-C1	117 (1)
P1-Ru-O1	91.1 (2)	P2-Ru-O1	89.8 (2)	C7-C6-C5	121 (1)
Cl-Ru-O1	86.0 (3)	C1-Ru-O1	79.8 (5)	C6-C1-C2	120 (1)
Cl-Ru-C9	101.8 (7)	C1-Ru-C9	92.4 (8)	C1-C2-C3	118 (1)
Ru-O1-C7	113.0 (9)	Ru-C1-C6	111 (1)	C2-C3-C4	123 (2)
Cl-Ru-C1	165.8 (4)	C4-C5-C6	114 (2)	C1-C6-C5	121 (1)
P1-Ru-P2	179.0 (2)	Ru-C9-O2	177 (2)	O1-C7-C8	118 (1)
C9-Ru-O1	172.2 (8)	C3-C4-C5	123 (2)		

been observed.[25] It is therefore risky to use the Ru–C1 distance to support multiple-bonding arguments. Indeed, a Ru–C single bond is expected to be 2.06 Å, based on the covalent radii of Ru[26] and C(sp^2).[27]

The Ru–C9 distance (1.78 (1) Å) is somewhat short for a ruthenium–carbonyl bond. Ru–C(carbonyl) distances generally range from 1.82 to 1.87 Å,[28] and the shortness observed here could be due to the lack of a significant trans influence from the weakly coordinated ketone oxygen atom.

The phosphine atoms are mutually trans ($\angle$P1–Ru–P2 = 179.0 (2)°), and the Ru–P distances (Ru–P1 = 2.373 (4) Å; Ru–P2 = 2.381(4) Å) are in the range found for other ruthenium complexes with trans-triphenylphosphine ligands.[20,21,29,30] The Ru–Cl distance in **1** (2.494 (4) Å) is long compared with the distance observed in $Ru(O_2CPh)Cl(CO)(PPh_3)_2$ (2.397 (5) Å)[20] but is comparable to the distance of 2.452 (2) Å found in $RuCl[CN(C_6H_4\text{-}4\text{-}Me)(CH_2)_2N(C_6H_4\text{-}4\text{-}Me)](PEt_3)_2$.[31] These differences can be attributed to the trans influence such that the longer Ru–Cl bonds are trans to Ru–C(sp^2) bonds while the shorter bond is trans to a weakly coordinated benzoate oxygen atom. Other distances and angles in the structure are normal.

Exchange Reactions. $CH_3C(O)C_6H_4RuCl(CO)(PPh_3)_2$ (**1**) was found to undergo exchange reactions with carboxylic acids. Complex **1** was refluxed in toluene solution with a large excess of benzoic acid, and the known benzoate complex $Ru(O_2CPh)Cl(CO)(PPh_3)_2$[20] was obtained in quantitative yield.

This result demonstrates the reversible nature of reaction 3 and suggests a general scheme for the synthesis of numerous carboxylate and ortho-metalated complexes. Although the mechanism of this exchange reaction has not been examined in detail, it probably involves initial dissociation of the ketone oxygen atom followed by protonation of ruthenium and reductive elimination of acetophenone. Experiments in progress are directed at understanding these exchange reactions.

The ruthenium carboxylate complexes and complex **1** were found to catalytically decarbonylate benzaldehyde with an identical activity (10 molar turnovers/h).[32] Since the above exchange reaction is facile, and since an aromatic aldehyde should be capable of functioning as an ortho-directing group, it seems plausible that an ortho-metalated benzaldehyde may be important in the decarbonylation reactions. At the present time, attempts to isolate an ortho-metalated aldehyde via the above exchange reaction have not been successful. However, work is continuing in this area.

Acknowledgment. Support of this research through a grant from the National Science Foundattion is gratefully acknowledged (NSF No. CHE 78-21840). We also thank the NSF for partial support of our X-ray diffraction and structure-solving equipment (NSF No. CHE 77-28505). Engelhard Industries is gratefully acknowledged for a generous loan of $RuCl_3$.

Registry No. **1**, 815434-77-2; $Ru(O_2CMe)Cl(CO)(PPh_3)_2$, 50661-66-0; acetophenone, 98-86-2.

Supplementary Material Available: Listings of weighted least-squares planes, anisotropic thermal parameters, and observed and calculated structure factor amplitudes (13 pages). Ordering information is given on any current masthead page.

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[32] This activity may be compared with a value of 1.1 × 10^3 turnovers/h with $[Rh(dppp)_2]BF_4$ as a catalyst (dppp = 1,3-bis(diphenylphosphino)propane).[11-13]