from the carbonyls to the chromium.[59] There is a fourth allowed transition predicted at higher energies which does not involve the chromium orbitals at all, although if the chromium 4p orbitals had been included, they would have been involved in the $1t_{1u}$ MO to some extent.

A feature of the spectrum which the present treatment does not properly represent is the d–d transition $t_{2g}(\pi) \rightarrow e_g(\sigma^*)$. The calculated t_{2g}–e_g splitting is far too large. This is caused, in part, by the large charge dependence of the chromium 3d Coulomb integrals and also by the fact that the e_g chromium 3d orbitals were given the same Coulomb integrals as the t_{2g} orbitals, causing them to interact too strongly with the carbonyl groups. A smaller (less negative) H_{ii} would have been preferable for the e_g 3d orbitals, but, in order to preserve the rotational invariance of the results, all of the 3d orbitals had to be assigned identical H_{ii} values.

For our purposes the spectrum of $C_6H_6Cr(CO)_3$ can be divided into three regions.

(i) In the region below 34,500 cm^{-1} there is a peak at 31,220 cm^{-1} and a shoulder at 26,620 cm^{-1}. The two transitions calculated to occur at 32,750 cm^{-1} are assigned to this region. They both involve charge transfer from the chromium to the ring and, to a lesser extent, to the carbonyl groups. The transition polarized along the z direction is predicted to be much stronger than that polarized in the xy plane.[21]

(ii) The next transition (38,480 cm^{-1}) is clearly seen in the spectrum of the benzene complex, although it is not so well resolved in the other arene complexes. It is predicted to be a charge-transfer band from the chromium to the carbonyls.

(iii) In the region above 41,500 cm^{-1} there is a peak at 45,410 cm^{-1}. This transition involves charge-transfer transitions from the ring and the chromium to the carbonyls.

The spectrum of the aniline complex is very similar to that of the benzene complex except for a somewhat greater intensity at the peak in region (iii) and a considerably greater intensity at about 40,500 cm^{-1}. The calculations on the aniline complex allow the molecule only C_s symmetry. However, with free rotation of the ring it should have effective C_{3v} symmetry so that the broadening of the bands due to the splitting of the doubly degenerate transitions would not be as great as Table VIII suggests. All of the bands predicted to occur in the aniline complex can be correlated with those in the benzene complex and suggest the same assignments as given there, except for the one band calculated to occur at 35,970 cm^{-1}. This band involves charge transfer from the nitrogen of the amino group to the carbonyls and may account for the increased intensity at the longer wavelength portion of region (iii) seen in the experimental spectrum. It is also seen that the three transitions which make up the intense portion of region (iii) are predicted to be more intense in the aniline complex than in the benzene complex; this agrees with experiment.

Acknowledgments.—We wish to thank Professor L. C. Cusachs for the use of his program for calculating molecular transition moments and Dr. B. B. Townsend and the staff of the LSU computer research center for their help.

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(59) It should be pointed out, however, that the inclusion of electron repulsion might well alter this picture. In the first two transitions involving electron transfer from orbitals localized on the chromium to orbitals delocalized over the carbonyls energy would be released, thereby lowering the calculated transition energies. This would increase the likelihood that the assignments given here for these bands are correct. However, for the third transition the opposite effect would hold and the change in electron repulsion on going from a delocalized orbital to one localized on the chromium would increase the calculated transition energy, possibly moving it completely out of the range of interest. The fourth predicted band would not be affected in this manner since both of the MO's involved are delocalized on the carbonyls; thus, it might well be better to associate the shoulder at 51,280 cm^{-1} with this transition. None of the assignments given for the half-sandwich complexes involves transitions from a delocalized to a strongly localized MO and they should not suffer from the above restrictions.

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Pentacarbonyls of Ruthenium and Osmium. III. Triphenylphosphine-Substituted Carbonyls of Ruthenium and Osmium and Their Reactions with Molecular Hydrogen

BY F. L'EPLATTENIER AND F. CALDERAZZO

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The preparation and characterization of $Ru(CO)_4P(C_6H_5)_3$ and $Os(CO)_4P(C_6H_5)_3$ have been accomplished and a new route to the already known disubstituted $Ru(CO)_3(P(C_6H_5)_3)_2$ and $Os(CO)_3(P(C_6H_5)_3)_2$ has been found. Reaction with molecular hydrogen on some of these triphenylphosphine-substituted carbonyls has led to $OsH_2(CO)_3P(C_6H_5)_3$, $RuH_2(CO)_2(P(C_6H_5)_3)_2$, and $OsH_2(CO)_2(P(C_6H_5)_3)_2$. For the latter two compounds, the nuclear magnetic resonance and infrared spectra indicate an octahedral structure with both hydrogens in a *cis* position and the triphenylphosphine substituents in *trans* positions.

In a previous paper of this series[1] we reported the synthesis of dihydridotetracarbonylosmium, $OsH_2(CO)_4$, by the reaction of pentacarbonylosmium with molecular hydrogen at elevated temperature and pressure. We did not succeed in preparing the unstable

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(1) F. L'Eplattenier and F. Calderazzo, *Inorg. Chem.*, **6**, 2092 (1967).

TABLE I

ANALYTICAL AND NMR DATA OF TRIPHENYLPHOSPHINE-SUBSTITUTED CARBONYL COMPOUNDS OF RUTHENIUM AND OSMIUM

Compound[a]	% C		% H		% P		Nmr[b]		
	Calcd	Found	Calcd	Found	Calcd	Found	Chem shift[c]	Multiplicity	*J*, cps
$Ru(CO)_4P(C_6H_5)_3$ (I)	55.58	55.72	3.18	3.30	6.51	6.31			
$Ru(CO)_3(P(C_6H_5)_3)_2$[d] (II)	66.01	65.38	4.26	4.39					
$RuH_2(CO)_2(P(C_6H_5)_3)_2$ (III)	66.76	66.53	4.72	4.84	9.06	8.84	16.90	Triplet	23
$Os(CO)_4P(C_6H_5)_3$ (IV)	46.81	47.03	2.68	2.87	5.49	5.26			
$Os(CO)_3(P(C_6H_5)_3)_2$[d] (V)	58.64	58.88	3.79	3.96	7.75	7.52			
$OsH_2(CO)_2(P(C_6H_5)_3)_2$[e] (VI)	59.06	59.01[f]	4.17	4.35[f]	8.02	8.14[f]	17.65	Triplet	23
		59.23[g]		4.01[g]		7.88[g]			

[a] All compounds are colorless except I and V which are light yellow. [b] In tetrahydrofuran solutions. [c] In ppm from tetramethylsilane (τ 10) as internal standard. [d] Collmann and Roper[3] obtained these compounds by a different route, namely, by zinc reduction of halogen complexes of ruthenium(II) and osmium(II) of formula $MX_2(CO)_2(P(C_6H_5)_3)_2$ in the presence of carbon monoxide. [e] Molecular weight: calcd, 772.8; found, 792. [f] From $Os(CO)_3(P(C_6H_5)_3)_2$ and hydrogen. [g] From $OsH_2(CO)_4$ and excess triphenylphosphine.

TABLE II

INFRARED DATA OF TRIPHENYLPHOSPHINE-SUBSTITUTED CARBONYL COMPOUNDS OF RUTHENIUM AND OSMIUM

Compound	ν_{C-O}, cm^{-1}	ν_{M-H}, cm^{-1}	ν_{M-D}, cm^{-1}	Medium
$Ru(CO)_4P(C_6H_5)_3$	2060 vs, 1986 m, 1953 vs			Heptane
$Ru(CO)_3(P(C_6H_5)_3)_2$	1900			THF[a]
$RuH_2(CO)_2(P(C_6H_5)_3)_2$	2011 vs, 1974 vs	1878 m, 1823 m		Halocarbon
$RuD_2(CO)_2(P(C_6H_5)_3)_2$[b]	2004, 1950		1360, 1321	Halocarbon
$Os(CO)_4P(C_6H_5)_3$	2060 s, 1980 m, 1943 vs			Heptane
$Os(CO)_3(P(C_6H_5)_3)_2$	1890			THF
$OsH_2(CO)_3P(C_6H_5)_3$	2079 vs, 2027 vs, 2018 vs	1959 w, 1922 w		Heptane
	2075 vs, 2029 s, 2005 vs	1955 m, 1923 m		Halocarbon
$OsH_2(CO)_2(P(C_6H_5)_3)_2$	2014 vs, 1990 vs	1928 m, 1873 m		Halocarbon

[a] THF = tetrahydrofuran. [b] Not isolated in a pure state. The bands due to small amounts of $Ru(CO)_3(P(C_6H_5)_3)_2$ (see text) have been subtracted.

dihydridotetracarbonylruthenium, $RuH_2(CO)_4$,[2] by allowing pentacarbonylruthenium to react with molecular hydrogen under similar conditions. The known stabilizing influence of triphenylphosphine on metal–hydrogen bonds prompted us to investigate similar hydrogenation reactions of triphenylphosphine-substituted carbonyls of ruthenium and osmium. For this purpose, we have prepared the new compounds $Ru(CO)_4P(C_6H_5)_3$ and $Os(CO)_4P(C_6H_5)_3$ and found a new convenient route to the already known[3] disubstituted compounds $Ru(CO)_3(P(C_6H_5)_3)_2$ and $Os(CO)_3(P(C_6H_5)_3)_2$.

Experimental Section

Infrared and nmr spectra were measured with Perkin-Elmer Model 521 and Varian DP A-60 instruments, respectively. Microanalyses were done by Dr. A. Bernhardt, Mülheim, Germany. The analytical and nmr results are reported in Table I. The infrared data are in Table II.

The starting solutions of pentacarbonylruthenium and pentacarbonylosmium were prepared as previously described.[4] Although the compounds reported in this paper are rather stable to air, all of the preparations were carried out in an atmosphere of prepurified nitrogen.

Tetracarbonyltriphenylphosphineruthenium and -osmium.—The tetracarbonyltriphenylphosphine derivatives, $Ru(CO)_4P(C_6H_5)_3$ (I) and $Os(CO)_4P(C_6H_5)_3$ (IV), were prepared by treating the corresponding pentacarbonyls with 1 equiv of triphenylphosphine at room temperature in tetrahydrofuran under ultraviolet irradiation. The conversion of $Ru(CO)_5$ was practically complete after 3 hr. Small amounts of $Ru(CO)_3(P(C_6H_5)_3)_2$ were present in the reaction mixture.

In the case of osmium, the reaction was much slower, and after 12-hr irradiation a conversion of about 50% was obtained. Here, too, small amounts of $Os(CO)_3(P(C_6H_5)_3)_2$ were found. The unreacted pentacarbonyl was eliminated by distillation.

The crude products were then purified by chromatography on silica gel. Elution with heptane–tetrahydrofuran (10:1), under nitrogen and exclusion of light, yielded colorless crystals of the monosubstituted products. Both compounds are slightly soluble in heptane and well soluble in tetrahydrofuran. In solution these substances are sensitive to daylight and rapidly become yellow. I decomposes at 130°; IV melts with decomposition at 186°.

Tricarbonylbis(triphenylphosphine)ruthenium and -osmium.—The disubstituted compounds, $Ru(CO)_3(P(C_6H_5)_3)_2$ (II) and $Os(CO)_3(P(C_6H_5)_3)_2$ (V), were prepared by treating the pentacarbonyls with 2 equiv of triphenylphosphine in an autoclave at about 130° in tetrahydrofuran under an atmosphere of nitrogen. After 3 hr the infrared spectrum was substantially that of the pure disubstituted derivatives. The crude products were recrystallized from heptane–tetrahydrofuran (1:1). Both compounds are pale yellow, practically insoluble in heptane, and soluble in tetrahydrofuran.

Dihydridotricarbonyltriphenylphosphineosmium.—A solution of $Os(CO)_4P(C_6H_5)_3$ in tetrahydrofuran was treated with hydrogen at 120 atm and 130°. After 3 hr no starting material was detectable in the infrared spectrum of the reaction mixture. After evaporation of the solvent the crude material was recrystallized from heptane–tetrahydrofuran (1:1). The properties of $OsH_2(CO)_3P(C_6H_5)_3$ so obtained are identical with those already reported for the same compound obtained from $OsH_2(CO)_4$ and triphenylphosphine.[1]

We did not succeed in preparing $RuH_2(CO)_3P(C_6H_5)_3$ by a similar procedure, probably because of decomposition of $Ru(CO)_4P(C_6H_5)_3$ under the reaction conditions.

Dihydridodicarbonylbis(triphenylphosphine)ruthenium and -osmium.—The dihydrido derivatives $RuH_2(CO)_2(P(C_6H_5)_3)_2$ and $OsH_2(CO)_2(P(C_6H_5)_3)_2$ were obtained by treatment of the disubstituted products $M(CO)_3(P(C_6H_5)_3)_2$ (M = Ru and Os) with hydrogen at 120 atm and 130° in tetrahydrofuran. After

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[2] Professor F. G. A. Stone has obtained the thermally unstable $RuH_2(CO)_4$ by acidification of tetracarbonylruthenate solutions: Abstracts of Papers, 3rd International Symposium on Organometallic Chemistry, Munich, Aug 28–Sept 1, 1967, p 8.

[3] J. P. Collmann and W. R. Roper, *J. Am. Chem. Soc.*, **87**, 4008 (1965); **88**, 3504 (1966).

[4] F. Calderazzo and F. L'Eplattenier, *Inorg. Chem.*, **6**, 1220 (1967).

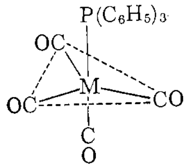
12 hr about 50% of the starting materials were converted to the dihydrido derivatives, which were purified by fractional recrystallization in heptane–tetrahydrofuran. Both compounds are colorless, insoluble in heptane, and slightly soluble in tetrahydrofuran. The osmium dihydrido compound was also obtained by allowing $OsH_2(CO)_4$[1] to react with 3 equiv of triphenylphosphine in tetrahydrofuran at reflux temperature for 12 hr (see Table I). The crude product was recrystallized from heptane–tetrahydrofuran.

Reactions of $M(CO)_3(P(C_6H_5)_3)_2$ with Deuterium.—Treating $Ru(CO)_3(P(C_6H_5)_3)_2$ with 99% deuterium (80 atm) at 140° for 12 hr in tetrahydrofuran and recrystallizing the reaction mixture from heptane–tetrahydrofuran resulted in the formation of $RuD_2(CO)_2(P(C_6H_5)_3)_2$. Since the latter was contaminated by some starting material, no elemental analysis was attempted. The compound was identified by its infrared spectrum in the carbonyl and metal–deuterium stretching regions (see Table II and Results and Discussion).

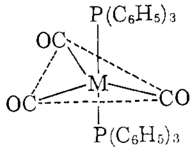
On the other hand, the reaction of $Os(CO)_3(P(C_6H_5)_3)_2$ with deuterium (60 atm) at 140° in tetrahydrofuran as solvent resulted in the formation of a crystalline solid which had a very complicated infrared spectrum but analyzed almost correctly for $OsD_2(CO)_2(P(C_6H_5)_3)_2$. *Anal.* Calcd for $C_{38}H_{30}D_2O_2P_2Os$: C, 58.98; H + D, 4.42; P, 7.99. Found: C, 57.08; H + D, 4.34; P, 8.13.

Results and Discussion

The infrared spectra (Table II) of the monosubstituted products $M(CO)_4P(C_6H_5)_3$ of ruthenium and osmium reported in this paper suggest a trigonal-bipyramidal structure with the triphenylphosphine group in the axial position as indicated in **1**. The symmetry C_{3v} of this molecule requires three infrared-active C–O stretching vibrations ($2\,A_1 + E$) in agreement with the experiment. No evidence was found for the presence of other isomeric species, with the triphenylphosphine group in an equatorial position (C_{2v} symmetry) or with a tetragonal-pyramidal structure (C_{4v} symmetry).



1



2

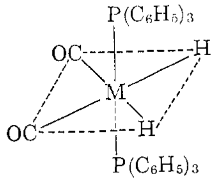
The disubstituted species $M(CO)_3(P(C_6H_5)_3)_2$ have been previously reported by Collman and Roper,[3] who obtained them by zinc reduction of halogen complexes of ruthenium(II) and osmium(II) of formula $MX_2(CO)_2(P(C_6H_5)_3)_2$ in the presence of carbon monoxide. Our spectral data (Table II) agree with those obtained by these authors and suggest a *trans*-trigonal-bipyramidal structure (2) of symmetry D_{3h} for which only one infrared-active C–O stretching vibration is expected.

We have previously obtained[1] nmr evidence that, in the course of the reaction of $OsH_2(CO)_4$ with a large excess of the liquid tri-*n*-butylphosphine, a disubstitution product was formed. We have now isolated and completely characterized the disubstitution products with triphenylphosphine of formula $MH_2(CO)_2(P(C_6H_5)_3)_2$ for both ruthenium and osmium. The best way to prepare them is the direct reaction of $M(CO)_3(P(C_6H_5)_3)_2$ with molecular hydrogen at high temperature and pressure, but in the case of osmium we could also obtain the same product by substitution of two carbonyl groups of $OsH_2(CO)_4$ by two triphenylphosphine molecules

$$M(CO)_3(P(C_6H_5)_3)_2 + H_2 \longrightarrow MH_2(CO)_2(P(C_6H_5)_3)_2 + CO \quad (1)$$

$$OsH_2(CO)_4 + 2P(C_6H_5)_3 \longrightarrow OsH_2(CO)_2(P(C_6H_5)_3)_2 + 2CO \quad (2)$$

In both compounds, the presence of an upfield triplet in the nmr spectrum suggests the presence of two equivalent hydrogens split by the two phosphorus nuclei of spin $I = {}^1/_2$. This, together with the observation of two equally intense CO stretching vibrations and of two metal–hydrogen stretching vibrations (see Table II) indicates that the most probable structure is



3

In the case of $RuH_2(CO)_2(P(C_6H_5)_3)_2$, the two carbonyl stretching vibrations were observed at 2011 and 1974 cm^{-1}, whereas the two metal–hydrogen stretching vibrations were unambiguously identified at 1878 and 1823 cm^{-1}. The former bands are shifted to 2004 and 1950 cm^{-1}, respectively, in the corresponding deuterated product. This is probably due to resonance interaction between the C–O and metal–hydrogen stretching vibrations.[1] The two metal–deuterium vibrations were detected at 1360 and 1321 cm^{-1}, with isotopic frequency ratios (1.381 and 1.380) slightly lower than expected but still in the range of the isotopic shifts observed for interacting vibrational states.[5] The assignment of the bands at 1928 and 1873 cm^{-1} in the spectrum of $OsH_2(CO)_2(P(C_6H_5)_3)_2$ as metal–hydrogen stretching vibrations is fairly sure, since only four bands were observed in the region 2200–1700 cm^{-1} and the bands at 2014 and 1990 cm^{-1} are easily assigned as C–O stretching vibrations on intensity grounds. The corresponding deuterated compound had an infrared spectrum too complicated for an unequivocal band assignment. Two new bands at 1410 and 1374 cm^{-1} with isotopic frequency ratios of 1.367 and 1.363 could however be attributed to metal–deuterium stretching vibrations and would support the above band assignment.

The higher wave numbers observed for the metal–hydrogen stretching vibrations in the osmium derivative compared to the ruthenium dihydride would suggest a higher metal–hydrogen bond strength for osmium than for ruthenium. This is in agreement with the exceptional thermal stability of $OsH_2(CO)_4$[1] compared to $RuH_2(CO)_4$.[2]

Reaction 1 represents a further example of an oxidative addition. The considerable stabilization of the metal–hydrogen bond induced by triphenylphosphine is experimentally verified in the case of ruthenium, since a relatively stable $RuH_2(CO)_2(P(C_6H_5)_3)_2$ could be isolated, whereas $RuH_2(CO)_4$ and $RuH_2(CO)_3P$-

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(5) L. Vaska, *J. Am. Chem. Soc.*, **88**, 4100 (1966).

$(C_6H_5)_3$ could not be obtained by similar hydrogenation reactions on $Ru(CO)_5$ and $Ru(CO)_4P(C_6H_5)_3$. The strong metal–hydrogen bond in the case of osmium makes it possible to synthesize the whole series of compounds, $OsH_2(CO)_4$,[1] $OsH_2(CO)_3P(C_6H_5)_3$,[1] and $OsH_2(CO)_2(P(C_6H_5)_3)_2$.

By the same principle, the still unknown dihydride compound of iron, $FeH_2(CO)_2(P(C_6H_5)_3)_2$, may be isolated by making use of a reaction similar to (1). Here, however, a lower thermal stability for the metal–hydrogen bond is to be expected. Attempts in this direction are now being made.

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Mössbauer Spectroscopy of Organometallic Compounds. Isomerism in $[(\pi\text{-}C_5H_5)Fe(CO)_2]_2SnCl_2$ and Related Molecules

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The Mössbauer spectra of a number of organotin compounds derived from $[\pi\text{-}C_5H_5Fe(CO)_2]_2$ have been examined at liquid nitrogen temperature, using both the 14.4-keV resonance γ radiation of ^{57}Fe and the 23.8-keV resonance γ radiation of ^{119}Sn. These measurements show that for $(\pi\text{-}C_5H_5)Fe(CO)_2SnCl_3$ and $(\pi\text{-}C_5H_5)Fe(CO)_2Sn(C_6H_5)_3$ there are no observable conformational changes on dissolution of the crystalline solids in solvents which set to a glassy matrix at low temperatures. The ^{57}Fe Mössbauer parameters in $[(\pi\text{-}C_5H_5)Fe(CO)_2]_2SnCl_2$ and $[(\pi\text{-}C_5H_5)Fe(CO)_2]_2GeCl_2$ are found to be invariant with respect to dissolution, and from these data it is concluded that the anomalous bond distances and bond angles, derived from the X-ray diffraction data for these compounds, arise from the specific bonding interactions within the molecule, and not from stacking forces between molecules in the crystalline state. The ^{119}Sn Mössbauer spectra and infrared data for $[(\pi\text{-}C_5H_5)Fe(CO)_2]_2SnCl_2$, moreover, show the existence of two structural forms in solution, and these are identified with the two possible rotational isomers obtained by rotation of the metal–metal bond. On the basis of isomer shift systematics, an assignment of the parameters to the two forms can be made.

I. Introduction

Early in the development of the technique of recoilless emission and absorption of γ radiation (Mössbauer effect) it was recognized that this spectroscopic tool could be used to elucidate the structure and bonding of organometallic compounds, especially those containing iron and/or tin.[2] It was not recognized until recently however, that Mössbauer spectroscopy could be exploited in a unique manner to resolve some of the discrepancies which have been reported regarding the structural information obtained from X-ray diffraction methods, on the one hand, and that inferred from nuclear magnetic resonance and infrared investigations, on the other. This uniqueness derives from the fact that it is possible to extract a number of Mössbauer parameters not only from samples of the neat solid in question, but also from frozen solutions of the same material in structureless (glassy) matrices. A recent application of this technique—in conjunction with low-temperature nmr and infrared studies—has been in the elucidation of the conformation of $\pi\text{-}C_8H_8Fe(CO)_3$ and related molecules in solution at low temperatures.[3] In the present study, the Mössbauer spectra of $[(\pi\text{-}C_5H_5)Fe(CO)_2]_2SnCl_2$, $(\pi\text{-}C_5H_5)Fe(CO)_2SnCl_3$, and a number of related molecules have been studied both in the neat solid and in frozen solutions in order to clarify some of the conformational features of these organometallic compounds. Of particular interest in this group of compounds is the fact that the Mössbauer parameters of both the ^{57}Fe and ^{119}Sn resonances can be obtained from the same sample prepared from natural abundance precursors, and the information derived from the two "probe" atoms can be used to derive structural information pertaining to only a portion of the whole molecule. Such structural information is particularly pertinent with respect to the existence of rotational isomers[4] in these compounds.

II. Experimental Section

A number of the absorbers used in this study were prepared from commercially available samples of the requisite starting materials. $[(\pi\text{-}C_5H_5)Fe(CO)_2]_2SnCl_2$ (I), $\pi\text{-}C_5H_5Fe(CO)_2SnCl_3$ (II), and $(\pi\text{-}C_5H_5)Fe(CO)_2Sn(C_6H_5)_3$ (III) were synthesized using the method of Bonati and Wilkinson.[5] A sample of $[(\pi\text{-}C_5H_5)Fe(CO)_2]GeCl_2$ (IV) was generously made available to us by Dr. P. Woodward. The dimer, $[(\pi\text{-}C_5H_5)Fe(CO)_2]_2$ (V), was obtained from Alfa Inorganics, Inc.

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[1] On leave from Universite Libre de Bruxelles, Brussels, Belgium.

[2] See for example: Proceedings of the Panel on the Application of the Mössbauer Effect in Chemistry and Solid State Physics, International Atomic Energy Agency, Vienna, 1966; V. I. Gol'danskii, *At. Energy Rev.*, **1**, 3 (1962); V. I. Gol'danskii, "The Mössbauer Effect and Its Applications in Chemistry," Consultants Bureau, New York, N. Y., 1964; R. H. Herber, *Ann. Rev. Phys. Chem.*, **17**, 261 (1966).

[3] R. Grubbs, R. Breslow, R. H. Herber, and S. J. Lippard, Jr., *J. Am. Chem. Soc.*, **89**, 6864 (1967).

[4] The term "conformers" has been suggested for configurationally distinguishable species in equilibrium with each other by A. Davison and W. C. Rode, *Inorg. Chem.*, **6**, 2124 (1967), in conjunction with their nmr studies of $\pi\text{-}C_5H_5Mo(CO)_2$ allyl complexes. The term "isomers" has been retained in the present discussion for the sake of clarity, although the same type of rotational change is involved here as that discussed by these authors.

[5] F. Bonati and G. Wilkinson, *J. Chem. Soc.*, 179 (1964). The authors are indebted to A. Hoffman of this laboratory for carrying out these syntheses.