Table V. Bond Lengths (Å) and Angles (deg) for 2

Bond Distances			
Al–O	1.800 (3)	Al–C(1)	1.968 (5)
O–C(2)	1.359 (5)	C(2)–C(3)	1.384 (6)
C(2)–C(7)	1.389 (6)	C(3)–C(4)	1.372 (6)
C(4)–C(5)	1.376 (7)	C(5)–C(6)	1.379 (7)
C(6)–C(7)	1.394 (6)		
Bond Angles			
O–Al–C(1)	108.7 (2)	Al–O–C(2)	125.0 (3)
O–Al–O	96.8 (2)	C(1)–Al–C(1)	119.4 (3)
O–C(2)–C(3)	120.9 (4)	O–C(2)–C(7)	119.6 (4)
C(3)–C(2)–C(7)	119.5 (4)	C(2)–C(3)–C(4)	120.3 (5)
C(3)–C(4)–C(5)	121.2 (5)	C(4)–C(5)–C(6)	118.8 (6)
C(5)–C(6)–C(7)	121.0 (5)	C(2)–C(7)–C(6)	119.2 (5)

and the anomalous dispersion corrections applied were those of Cromer and Liberman.[23]

Full-matrix least-squares refinement of all non-hydrogen atoms using anisotropic thermal parameters led to final values of $R = \sum||F_o| - |F_c||/\sum|F_o| = 0.088$ and $R_w = [\sum w(F_o - F_c)^2/\sum w(F_o)^2]^{1/2} = 0.093$. No hydrogen atoms were locatable on the final difference Fourier map, and no correction for absorption was applied (μ = 2.5 cm^{-1}). The final values of the fractional coordinates are listed in Table II, and thermal parameters are supplied as supplementary material.[24] Bond distances and angles are given in Table III.

X-ray Data Collection, Structure Determination, and Refinement for 2. Data collection procedures were the same as for 1, and pertinent parameters are given alongside those for 1 in Table I. The structure was solved via MULTAN and refined by using the SHELX program package. The aluminum and potassium atoms were shown to lie on twofold positions in the space group *Pbcn*. With all non-hydrogen atoms refined with anisotropic thermal parameters and hydrogen atoms fixed in positions located from a difference Fourier, final values of R = 0.031 and R_w = 0.031 were obtained. No correction for absorption was applied (μ = 4.0 cm^{-1}). Final fractional coordinates are given in Table IV, and bond distances and angles are presented in Table V. Thermal parameters are supplied as supplementary material. Scattering factors for H were taken from ref 25.

Acknowledgment. We are grateful to the National Science Foundation for support of this work.

Registry No. 1, 91711-78-3; 2, 91711-79-4.

Supplementary Material Available: Tables of bond lengths and angles and observed and calculated structure factors for 1 and 2, thermal parameters for 1, and hydrogen atom coordinates for 2 (18 pages). Ordering information is given on any current masthead page.

---

[22] Cromer, D. T.; Waber, J. T. *Acta Crystallogr.* **1965**, *18*, 104.

[23] Cromer, D. T.; Libermann, D. M. *J. Chem. Phys.* **1970**, *53*, 1891.

[24] See paragraph at the end of paper regarding supplementary material.

[25] "International tables for X-ray Crystallography"; Kynoch Press: Birmingham, England, 1974; Vol. IV, p 72.

Synthesis and Crystal and Molecular Structure of an η-Cyclopropene Complex of Molybdenum

Russel P. Hughes,*[1a,2] John W. Reisch,[1a] and Arnold L. Rheingold*[1b]

Departments of Chemistry, Dartmouth College, Hanover, New Hampshire 03755, and University of Delaware, Newark, Delaware 19711

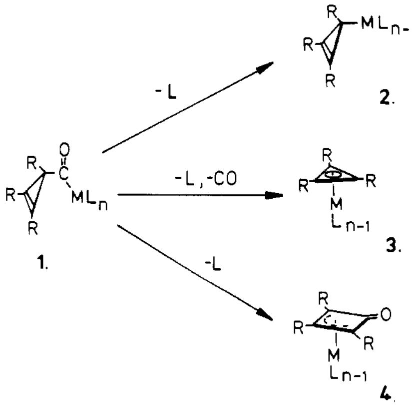
Received June 19, 1984

The 16-electron cation $[Mo(C_5Me_5)(CO)_3]^+$ (6) reacts with sodium 2,3-diphenyl-2-cyclopropene-1-carboxylate with displacement of CO and formation of the chelate complex 9, containing the first example of a molybdenum–cyclopropene bond. Complex 9 has been completely characterized spectroscopically and by a single-crystal X-ray diffraction study. Crystals of 9 are monoclinic of space group $P2_1/c$ (No. 14, C_{2h}^5) with a = 16.638 (5) Å, b = 11.526 (3) Å, c = 15.892 (5) Å, β = 114.54 (2)°, V = 2772.4 (13) Å^3, Z = 4, R_F = 0.0493, R_{wF} = 0.0509, and GOF = 1.235. ^{13}C NMR studies indicate that the solid-state structure of 9 is maintained in solution.

Introduction

Although the transition-metal chemistry of cyclopropenes has been investigated extensively, simple η^2-cyclopropene complexes are rare and have only been characterized chemically and spectroscopically for niobium[3] and crystallographically for platinum.[4,5] The two most common modes of reactivity involve cyclo-oligomerization reactions[6,7] and ring-opening reactions to give η-allyl[8,9] or vinylketene[10-12] complexes. We have been particularly interested in the chemistry of (2-cyclopropene-1-carbonyl)transition metal compounds[13] 1 and

Scheme I



---

[1] (a) Dartmouth College. (b) University of Delaware.

[2] Alfred P. Sloan Research Fellow, 1980–1984.

[3] Fredericks, S.; Thomas, J. L. *J. Am. Chem. Soc.* **1978**, *100*, 350–351.

[4] Visser, J. P.; Schipperijn, A. J.; Lukas, *J. Organomet. Chem.* **1973**, *47*, 433–438.

[5] DeBoer, J. J.; Bright, D. *J. Chem. Soc., Dalton Trans.* **1975**, 662–665.

[6] Binger, P.; Doyle, M. J.; McMeeking, J.; Kruger, C. *J. Organomet. Chem.* **1977**, *135*, 405–414.

[7] Binger, P.; Doyle, M. J. *J. Organomet. Chem.* **1978**, *162*, 195–207.

[8] Fiato, R.; Mushak, P.; Battiste, M. A. *J. Chem. Soc., Chem. Commun.* **1975**, 869–871.

[9] Mushak, P.; Battiste, M. A. *J. Organomet. Chem.* **1969**, *17*, P46–P48.

[10] Dettlaf, G.; Behrens, U.; Weiss, E. *Chem. Ber.* **1978**, *111*, 3019–3028.

Table I. Selected Bond Angles and Distances for $[(\eta^5\text{-}C_5Me_5)Mo(CO)_2(C_{16}H_{11}O_2)]$ (9)

Bond Distances (Å)

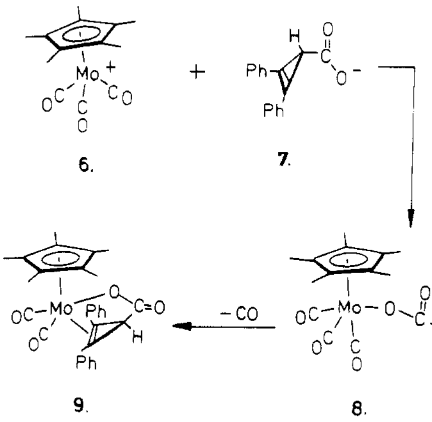
Mo-C(1)	2.025 (5)	Mo-CENT[a]	2.004 (5)	C(3)-C(4)	1.490 (9)
Mo-C(2)	1.990 (6)	C(1)-O(1)	1.124 (6)	C(4)-C(5)	1.511 (6)
Mo-C(5)	2.248 (6)	C(2)-O(2)	1.150 (7)	C(4)-C(6)	1.507 (7)
Mo-C(6)	2.333 (4)	C(3)-O(3)	1.300 (7)	C(5)-C(6)	1.408 (7)
Mo-O(3)	2.123 (3)	C(3)-O(4)	1.228 (7)	C(5)-C(16)	1.480 (8)
				C(6)-C(26)	1.456 (7)

Bond Angles (deg)

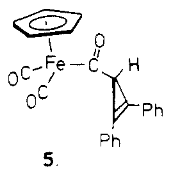
CENT-Mo-C(1)	118.0 (2)	O(3)-Mo-MENE	79.4 (2)	C(3)-C(4)-C(6)	119.3 (5)
CENT-Mo-C(2)	102.6 (2)	Mo-C(1)-O(1)	176.0 (4)	C(4)-C(5)-C(6)	62.1 (3)
CENT-Mo-O(3)	103.0 (2)	Mo-C(2)-O(2)	175.6 (5)	C(5)-C(6)-C(4)	62.3 (3)
CENT-Mo-MENE[a]	141.1 (2)	Mo-O(3)-C(3)	116.0 (4)	C(5)-C(4)-C(6)	55.6 (3)
C(1)-Mo-C(2)	82.4 (2)	O(3)-C(3)-O(4)	123.3 (6)	C(4)-C(5)-C(16)	126.0 (4)
C(1)-Mo-O(3)	84.3 (2)	C(4)-C(3)-O(4)	123.8 (5)	C(4)-C(6)-C(26)	129.0 (3)
C(1)-Mo-MENE	100.9 (2)	O(3)-C(3)-C(4)	112.8 (4)	C(5)-C(6)-C(26)	138.1 (5)
C(2)-Mo-O(3)	154.4 (2)	C(3)-C(4)-C(5)	117.6 (4)	C(6)-C(5)-C(16)	137.4 (5)
C(2)-Mo-MENE	81.8 (2)				

[a] CENT = centroid of Cp ring; MENE = midpoint of alkene bond.

Scheme II



their reactions to afford η^1-[13] and η^3-cyclopropenyl[14] or η^3-oxocyclobutenyl[14,15] compounds 2–4 (Scheme I). A key step in all these reactions has been proposed to involve coordination of the cyclopropene double bond in a (2-cyclopropene-1-carbonyl)metal complex prior to cyclopropenyl migration or ring expansion.[15] A stable (2-cyclopropene-1-carbonyl)iron complex, 5, in which the cyclopropene double bond remains uncoordinated has been characterized.[13a]



5

Results and Discussion

With a view to testing the generality of such coordination induced ring expansion reactions we attempted to generate a complex in which the cyclopropene olefin was part of a larger chelate ring. The system we chose involved reaction of the 16-electron, coordinatively unsaturated cation 6[16] with the 2,3-diphenyl-2-cyclopropene-1-carboxylate anion 7 (Scheme II). The anticipated initial tricarbonyl adduct 8 was not isolated, however, and the reaction proceeded with loss of carbon monoxide to afford the chelated complex 9, containing the first example of a molybdenum–cyclopropene bond. Indeed 9 appears to be the first reported example of a transition-metal complex containing both an unopened coordinated cyclopropene ring and CO ligands (vide supra).

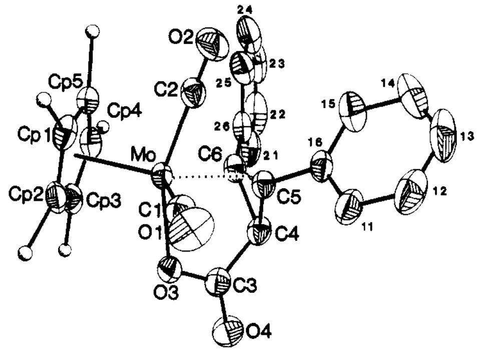


Figure 1. Molecular structure and labeling diagram for 9. Ring methyl groups are reduced in size, and hydrogen atoms have been removed for greater clarity.

Complex 9 has been completely characterized by a single-crystal X-ray diffraction study. The molecular structure and labeling scheme for 9 is shown in Figure 1, and a stereoview is provided in Figure 2. Selected bond angles and distances are provided in Table I. The coordination geometry about Mo is best described as distorted tetragonal pyramidal (a "four-legged piano stool", $MoCp(CO)_2LL'$ complex) with the Mo atom substantially raised above the basal plane. If the η-C_5Me_5 ring is treated as occupying three coordination sites, the complex is electronically seven-coordinate.[17] The cis-carbonyl arrangement is required to accommodate the chelating cyclopropenecarboxylate ligand;[18] however, $MoCp(CO)_2LL'$

---

[11] Binger, P.; Cetinkaya, B.; Kruger, C. *J. Organomet. Chem.* **1978**, *159*, 63–72.

[12] Newton, M. G.; Pantaleo, N. S.; King, R. B.; Chu, C.-K. *J. Chem. Soc., Chem. Commun.* **1979**, 10–12.

[13] (a) DeSimone, D. M.; Desrosiers, P. J.; Hughes, R. P. *J. Am. Chem. Soc.* **1982**, *104*, 4842–4846. (b) Gommper, R.; Bartmann, E. *Angew. Chem., Int. Ed. Engl.* **1978**, *17*, 456–457. (c) Gommper, R.; Bartmann, E.; Noth, H. *Chem. Ber.* **1979**, *112*, 218–233.

[14] Hughes, R. P.; Lambert, J. M. J.; Reisch, J. W.; Smith, W. L. *Organometallics* **1982**, *1*, 1403–1405.

[15] Donaldson, W. A.; Hughes, R. P. *J. Am. Chem. Soc.* **1982**, *104*, 4846–4859.

[16] Barnes, S. G.; Green, M. *J. Chem. Soc., Chem. Commun.* **1980**, 267–268.

[17] Kubacek, P.; Hoffmann, R.; Havlas, Z. *Organometallics* **1982**, *1*, 180–188. This reference provides citations for numerous crystal structures of compounds of the type $Mo(C_5H_5)(CO)_2LL'$.

[18] Bernal, I.; LaPlaca, S. J.; Korp, J.; Brunner, H.; Herrmann, W. A. *Inorg. Chem.* **1978**, *17*, 382–388. Reisner, M. G.; Bernal, I.; Brunner, H.; Wachter, J. *J. Organomet. Chem.* **1977**, *137*, 329–347. Beck, W.; Danzer, W.; Liu, A. T.; Huttner, G. *Angew. Chem., Int. Ed. Engl.* **1976**, *15*, 495–496. Botherton, P. D.; Raston, C. L.; White, A. M.; Wild, S. B. *J. Chem. Soc., Dalton Trans.* **1976**, 1193–1195.

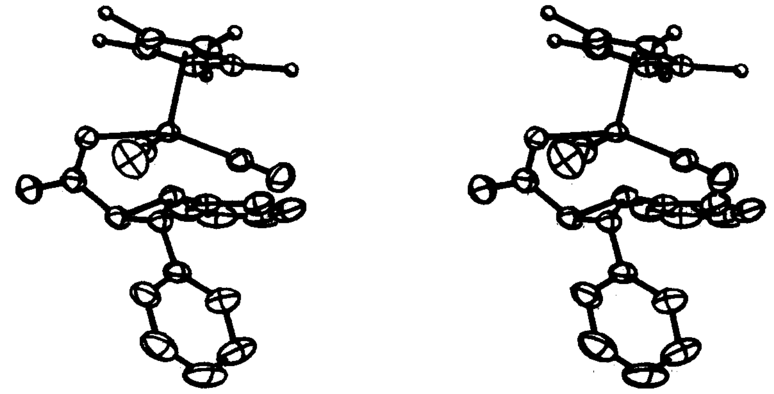
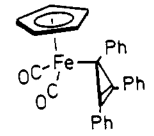


Figure 2. A stereoview of the molecular structure of **9**.

complexes in which L and L′ are not chelating generally adopt trans-CO arrangements, with only one known exception.[19] The distortions of the typical "four-legged piano stool" structures found in **9** may also be attributed to the constraints imposed by a chelating ligand in the basal plane.

The Mo distances to the cyclopropene ring carbon atoms (see Figure 1 and Table I) clearly reveal the η^2-olefin bonding. The short C(5)–C(6) distance 1.408 (7) Å (compared to the C(4)–C(5) and C(5)–C(6) distances of 1.511 (6) and 1.507 (7) Å suggests a relatively small π-acceptor character in this formally d^4 metal–olefin bond. In contrast, the coordinated olefin bond length in the d^{10} Pt(O)–cyclopropene complex $Pt(PPh_3)_2(\eta^2\text{-cyclopropene})$ is 1.585 (2) Å, indicating that the Pt–olefin bond has a more "metallacyclopropane" character.[5] These C–C distances may be compared to those found for the uncomplexed cyclopropene molecule (C—C = 1.515 Å and C=C = 1.300 Å) by microwave spectroscopy[20] and the η^1-triphenylcyclopropenyl ligand in **10** (mean C—C = 1.512 Å and C=C = 1.292 Å).[13c] The phenyl groups are displaced from the plane of the cyclopropene ring, away from the metal, the "bend-back" angles for the ipso-carbon atoms (calculated as the angle between the exocyclic C–C bond and the C(4)–C(5)–C(6) plane) being 39.7° (C(5)–C(16)) and 36.9° (C(6)–C(26)). The corresponding angle at the saturated cyclopropene carbon atom is 57.4° (C(4)–C(3)).



10.

The solid-state structure of **9** apparently is maintained in solution, with two Mo–CO and two cyclopropene olefinic carbon resonances being observed in the ^{13}C NMR spectrum at ambient temperature. No evidence of any further ring opening reactions of **9** have been observed, indicating that (2-cyclopropene-1-carbonyl)metal complexes may have an enhanced reactivity toward ring expansion. Further experiments to test this hypothesis are currently in progress in our laboratories.

Experimental Section

General Data. All reactions were run and worked up in oven dried glassware, using conventional Schlenck techniques under an atmosphere of dinitrogen that was deoxygenated over BASF catalyst and dried over P_4O_{10}. Hydrocarbon and ether solvents were dried by distillation from Na/K alloy; dichloromethane was dried by distillation from P_4O_{10}. All solvents were stored and transferred under purified dinitrogen.

Table II. Crystal and Refinement Data for $[(\eta^5\text{-}C_5Me_5)Mo(CO)_2(C_{16}H_{11}O_2)]\cdot CH_2Cl_2$ (9)

formula	$C_{28}H_{26}MoO_4\cdot CH_2Cl_2$
fwt	607.35
cryst system	monoclinic
space group	$P2_1/c$ [No. 14, C^5_{2h}]
a, Å	16.638 (5)
b, Å	11.526 (3)
c, Å	15.892 (5)
β, deg	114.54 (2)
V, Å^3	2772.4 (13)
Z	4
ρ(calcd), g cm^{-3}	1.455
temp, °C	23
cryst dimens, mm	0.22 × 0.30 × 0.32
radiatn	graphite-monochromated Mo Kα (λ = 0.71073 Å)
diffractometer	Nicolet R3
abs coeff, cm^{-1}	6.86
scan speed, deg/min	var 3.5–20
2θ scan range, deg	$3 \leq 2\theta \leq 50$
scan technique	θ/2θ
data collected	$\pm h, \pm k, +l$
scan width, deg	$1.8 + \Delta(\alpha_1 - \alpha_2)$
ignorance factor	0.001
unique data	4770 rflns (4993 collected)
unique data with $(F_o)^2 > 3\sigma(F_o)^2$	3996
std rflns	3/147 (18% decay obs)
R_F, %	4.93
R_{wF}, %	5.09
GOF	1.235

^1H and $^{13}C\{^1H\}$ NMR spectra were run on a Varian Associates XL-300 FT spectrometer; chemical shifts are quoted in parts per million downfield from internal tetramethylsilane. IR spectra were run on a Perkin-Elmer 599 instrument and calibrated by using the 1601 cm^{-1} peak of polystyrene.

2,3-Diphenyl-2-cyclopropene-1-carboxylic acid[21] and bis(η-pentamethylcyclopentadienyl)hexacarbonyldimolybdenum[22] were prepared by literature methods.

Sodium 2,3-Diphenyl-2-cyclopropene-1-carboxylate. Sodium hydride (0.085 g of a 1:1 oil dispersion, 1.77 mmol of NaH) was washed with hexane (5 × 6 mL), dried under vacuum, and slurried in THF (10 mL). A solution of 2,3-diphenyl-2-cyclopropene-1-carboxylic acid (0.380 g, 1.61 mmol) in THF (20 mL) was added, with magnetic stirring. Vigorous evolution of H_2 was observed and the product precipitated as a white solid. The

---

(19) Reisner, G. M.; Bernal, I.; Brunner, H.; Muschiol, M.; Siebrecht, B. *J. Chem. Soc., Chem. Commun.* **1978**, 691–692.

(20) Kasai, P. H.; Myers, R. J.; Eggers, D. F.; Wiberg, K. B. *J. Chem. Phys.* **1959**, *30*, 512–516.

(21) Breslow, R.; Winter, R.; Battiste, M. A. *J. Org. Chem.* **1959**, *24*, 415–416. See ref 15 for a modified version of this procedure.

(22) Birdwhistell, R.; Hackett, P.; Manning, A. R. *J. Organomet. Chem.* **1978**, *157*, 239–241.

Table III. Final Fractional Atomic Coordinates ($\times 10^4$) for $[(\eta^5\text{-}C_5Me_5)Mo(CO)_2)(C_{16}H_{11}O_2)]\cdot CH_2Cl_2$ (9)

atom	*x*	*y*	*z*
Mo	2351 (1)	4697 (1)	6474 (1)
O(1)	841 (3)	2829 (4)	5685 (3)
O(2)	687 (2)	6267 (4)	6048 (2)
O(3)	3195 (2)	3278 (3)	7120 (2)
O(4)	3902 (2)	2377 (3)	8467 (2)
Cp(1)	2110 (3)	5267 (5)	5000 (3)
Cp(2)	2749 (4)	4365 (4)	5267 (3)
Cp(3)	3529 (3)	4807 (4)	5991 (3)
Cp(4)	3381 (4)	5941 (6)	6200 (4)
Cp(5)	2495 (3)	6235 (4)	5581 (3)
Cm(1)	1234 (4)	5271 (6)	4171 (3)
Cm(2)	2686 (5)	3217 (5)	4798 (4)
Cm(3)	4392 (4)	4189 (6)	6425 (5)
Cm(4)	4055 (4)	6756 (7)	6850 (5)
Cm(5)	2140 (5)	7455 (6)	5450 (5)
C(1)	1398 (3)	3468 (5)	5992 (3)
C(2)	1318 (4)	5730 (5)	6218 (4)
C(3)	3431 (4)	3169 (6)	8005 (4)
C(4)	3032 (3)	4071 (4)	8385 (3)
C(5)	2122 (3)	4511 (4)	7764 (3)
C(6)	2844 (3)	5259 (4)	7948 (3)
C(11)	893 (4)	3434 (6)	7893 (4)
C(12)	182 (4)	3361 (8)	8125 (5)
C(13)	−87 (5)	4307 (9)	8453 (5)
C(14)	326 (4)	5336 (7)	8516 (5)
C(15)	1043 (4)	5437 (6)	8274 (4)
C(16)	1330 (3)	4466 (4)	7966 (3)
C(21)	2666 (4)	7390 (5)	8070 (4)
C(22)	2983 (5)	8460 (7)	8497 (5)
C(23)	3789 (5)	8502 (6)	9241 (4)
C(24)	4277 (5)	7527 (7)	9552 (4)
C(25)	3961 (3)	6470 (6)	9129 (3)
C(26)	3148 (3)	6385 (4)	8377 (3)
C_s[a]	3339 (5)	4510 (6)	1813 (6)
Cl(1)	3805 (2)	4839 (2)	1052 (2)
Cl(2)	2191	4513	1280
Cl(2′)	2168	4528	833
Cl(2″)	2223	4531	1790

[a] Italicized atoms form the disordered solvent molecule CH_2Cl_2 (see text).

resultant slurry was used in the following reaction.

Synthesis of Complex 9. Bis(*η*-pentamethylcyclopentadienyl)hexacarbonyldimolybdenum (0.514 g, 0.816 mmol) was dissolved in dichloromethane (30 mL), and silver hexafluorophosphate (0.413 g, 1.63 mmol) was added to give a black precipitate of metallic Ag and a solution of $[Mo(\eta\text{-}C_5Me_5)(CO)_3]^+BF_4^-$[16] This solution was filtered and added dropwise, at −80 °C, to the slurry prepared in the previous reaction. The mixture was stirred cold for 1 h, then allowed to warm to ambient temperature, and stirred overnight. Evaporation of the solution to dryness, followed by column chromatography of the residue on Florisil (2.5 × 25 cm), yielded a red-orange band on elution with acetone. Evaporation of the eluate and recrystallization of the residue from dichloromethane/hexane afforded the product **9** as orange crystals: 0.25 g, 25%; mp 124–129 °C dec; IR (CH_2Cl_2) ν_{CO} 2022, 1961, $\nu_{C=O}$ 1630 cm^{-1}; ^1H NMR ($CDCl_3$) δ 7.39 (m, 10 H, Ph), 1.98 (s, 1 H, CH), 1.67 (s, 15 H, C_5Me_2); $^{13}C\{^1H\}$ NMR ($CDCl_3$) δ 228.79 (MoCO), 222.24 (MoCO), 183.67 (C=O), 139.77–125.99 (Ph), 108.73 (C_5Me_5), 71.91 (CPh), 58.64 (CPh), 44.22 (CH), 10.04 (C_5*Me*$_5$). A single crystal was selected for X-ray diffraction.

X-ray Diffraction Study of 9. An orange crystal was mounted on a glass fiber with epoxy cement. Unit cell parameters are reported in Table II, along with the details of data collection and refinement, and were obtained from the angular settings of 25 well-centered refections (24° < 2θ < 30°) including Friedel relatives to check optical alignment. The data were corrected for L_p effects as well as for a linear 18% decay in reflection intensity. No correction for absorption was required: regular crystal shape, low absorption coefficient (μ = 6.9 cm^{-1}), and max/min transmission = 1.08/1.00.

The structure was solved by standard techniques that revealed the position of the Mo atom. All remaining non-hydrogen atoms were located by subsequent difference Fourier syntheses. Early in the refinement process a molecule of CH_2Cl_2 was located and found to be present in a 1:1 ratio with the Mo complex. While the solvent's C atom and one of the Cl atoms were well behaved, the second Cl atom was highly disordered, appearing to occupy a number of positions, the loci of which were defined by a circle swept out by rotation about the CS–Cl(1) axis. Although a fully satisfactory modeling of the disorder could not be achieved, several Cl(2) positions were located in difference maps and refined with fixed positional and occupancy parameters, the latter adjusted to maintain a total Cl(2) occupancy of 1.0. The partial success of this model is seen in the reasonable final residuals and the "clean" difference map (see below).

All non-hydrogen atoms were refined with anisotropic thermal parameters, and hydrogen atoms were fixed in idealized positions [d(C–H) = 0.96 Å, U = 1.2 × the isotropic equivalent for the carbon atom to which it was attached] by using a "riding" model. Convergence was obtained at the residuals shown in Table II. The final difference map showed a low, diffuse background (maximum peak = 0.4 e/A^3), and trends of F_o vs. F_c, sin θ, Miller index, and parity group showed no unusual features.

The programs used throughout data collection, refinement, and graphics preparation were those included in the Nicolet program packages P3, SHELXTL, and xP, and were processed on our in-house Data General Nova 4 computer.

Final positional parameters for the non-hydrogen atoms are provided in Table III. For other tables available as supplementary material see the paragraph following the Acknowledgment.

Acknowledgment. R.P.H. is grateful to the National Science Foundation, to the donors of the Petroleum Research Fund, administered by the American Chemical Society, and to the Alfred P. Sloan Foundation for generous financial support. The purchases of the University of Delaware diffractometer and the Dartmouth College XL-300 NMR spectrometer were supported by the National Science Foundation.

Registry No. 6·BF_4, 75593-04-3; 7·H, 17825-58-0; 7·Na, 63467-50-5; 9, 92366-02-4; 9·CH_2Cl_2, 92366-03-5; $[Mo(\eta\text{-}C_5Me_5)(CO)_3]_2$, 56200-14-7.

Supplementary Material Available: Table 4S, atom coordinates and temperature factors, Table 5S, bond lengths, Table 6S, bond angles, Table 7S, anisotropic temperature factors, Table 8S, and observed and calculated structure factors (29 pages). Ordering information is given on any current masthead page.