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INTRODUCTION

This work was begun in 1971 in response to an invitation from the Editor of the Annual Reports on NMR spectroscopy to prepare a brief review on "NMR Spectroscopy of Organic-metal Carbonyl Complexes". The most recent review in the field available at that time, *Applications of Nuclear Magnetic Resonance to the Study of Organometallic Compounds* by M. L. Maddox, S. L. Stafford and H. D. Kaesz [*Advan. in Organometallic Chem.*, 1966, 3, 1] had already covered the literature up to 1964 and therefore we decided to begin our literature survey from the year 1965 onward. By the time we completed the literature search, we had collected material from over 2300 references. Even after deciding to include only Transition-Metal Carbonyl compounds in which the additional ligands formed direct metal-carbon bonds, the number of references was cut down to about 1100 and the number of compounds involved was in the region of 3000. In view of this "staggering" (to us) collection of data we decided to abandon the attempt of preparing a "brief" critical review of NMR properties of organic-metal carbonyl complexes. Instead, we sought and obtained the Editor's approval to publish a compilation of the collected information in the form of tables which in addition to presenting NMR spectroscopic data for each compound, would provide a rather useful comprehensive index of the organo-metal carbonyl compounds prepared during the seven year period 1965-1971: the period of explosive expansion in the field.

The Tables are numbered I-XIII according to the transition metal atom (or periodic group of atoms) and are subdivided, corresponding to the ligands, into monohapto, dihapto, trihapto, etc. A further division is according to the number of carbonyl groups attached to the metal (monocarbonyl, dicarbonyl, etc.), or arranged in order of increasing number of carbonyl groups. Compounds containing two or more carbon-bonded ligands of differing hapto order are sub-grouped as "Mixed Ligands" and arranged in order of increasing hapto number (i.e. h^1/h^2 , h^1/h^5 , h^3/h^4 , etc.).

In cases of possible ambiguity, the position at which a ligand is attached to a metal, or a substituent to a ligand, is indicated by an arrow. NMR chemical shifts for ^1H and ^{13}C are relative to Me_4Si , downfield shifts having positive values and upfield shifts negative values.

NMR chemical shifts for ^{19}F are relative to CFCl_3 at 56.4 MHz, unless otherwise indicated. In many cases authors failed to mention if shifts relative to the standard were upfield or downfield. Consequently, the ^{19}F data are reported as given in the original papers without conversion to the currently accepted convention.

Hopefully, this volume will prove sufficiently useful to induce the necessary daring required in undertaking the mission of updating this collection of NMR data.

**NMR DATA ON
ORGANIC-METAL
CARBONYL COMPLEXES
(1965–1971)**

by

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TABLE I

Titanium, vanadium, niobium, and tantalum complexes

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)		Remarks	References
(1) PENTAHAPTO LIGANDS								
$C_6H_5N_2O_3V$	1	$(h^5-C_5H_5)V(NO)_2(CO)$	$(CD_2)_2CO$	H 5.69	—	—		2
$C_{11}H_{11}NbO$	2	$(h^5-C_5H_5)_2Nb(H)(CO)$	$C_6D_5CD_3$	H -6.39	—	—		11
$C_{11}H_{11}OTa$	3	$(h^5-C_5H_5)_2Ta(H)(CO)$	—	H -6.80	—	—		11
$C_{22}H_{30}TiO_2$	4	$[h^5-C_5(CH_3)_5]_2Ti(CO)_2$	—	H 1.69	—	—		1
$C_{27}H_{35}O_2P_2V$	5	$(h^5-C_5H_5)V[P(CH_2CH_2^H)_2C_6H_5^H]_2(CO)_2$	C_6D_6	H 4.50t	$J_{PH} 2$	—		3
				H' 2.50	—			4
				H'' 1.20	—			
				H''' 7.33	—			
$C_{31}H_{59}O_2P_2V$	6	$(h^5-C_5H_5)V\{P[(CH_2)_3CH_2^H]_2(CO)_2\}$	C_6D_6	H 4.80t	$J_{PH} 2 (1.0)^*$	—		4
				H' ~1.60	—			3
				H'' 1.00	—			
				(0.81)*	—			
$[C_9H_5N_2O_2V]^{2-}$	7	$[(h^5-C_5H_5)V(CN)_2(CO)_2]^{2-}$	DMS	H 4.59s	—	Isolated as the disodium salt		3
$C_{41}H_{38}O_2P_3V$	8	$(h^5-C_5H_5)V\{[P(C_6H_5)_2CH_2^HCH_2^H]_2(C_6H_5)_2P\}(CO)_2$	$CDCl_3$	H 3.98s	—	100 MHz		5
				H' ~7.3	—			
				H'' ~2	—			
$C_{44}H_{37}NbO_2P_2$	9	$(h^5-C_5H_4-CH_3)Nb[P(C_6H_5)_3]_2(CO)_2$	CS_2	H 4.25m	—	—		933
				H' 1.95s	—			
				H'' 7.18m	—			

TABLE 1—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_4H_3O_2P_2Ta$	10	$(h^5-C_5H_5)Ta[P(C_6H_5)_3]_2(CO)_2$	CS_2	H 4.53	—	—	936
$[C_9H_5NO_3V]^-$	11	$[(h^5-C_5H_5)V(CN)(CO)_3]^-$	DMS	H 4.90s	—	Isolated as the sodium salt	3
$C_{26}H_{20}AsO_3V$	12	$(h^5-C_5H_5)V[As(C_6H_5)_3](CO)_3$	C_6D_6	H 4.62s H' 7.32	— —	—	3
$C_8H_8O_3PV$	13	$(h^5-C_5H_5)V(PH_3)(CO)_3$	C_6D_6	H 4.28d H' 3.69d (3.19)*	$J_{PH} 1.5$ $J_{PH} 324$	—	3 *6 *932
$C_{17}H_{26}O_3PV$	14	$(h^5-C_5H_5)V[P(CH'(CH''_3)_2)_3](CO)_3$	C_6D_6	H 4.73s H' 1.94 H'' 0.90	— — —	—	3
$C_{20}H_{32}O_3PV$	15	$(h^5-C_5H_5)V[P((CH'_2)_3CH''_3)_3](CO)_3$	C_6D_6	H 4.63d H' 1.40 H'' 0.85	$J_{PH} 1.0$ — —	—	3 4
$C_{18}H_{20}O_3PV$	16	$(h^5-C_5H_5)V[CH_2CH'_3)_2C_6H_5''']_-(CO)_3$	C_6D_6	H 4.60d H' 1.90 H'' 1.00 H''' 7.30	$J_{PH} 1$ — — —	—	4 3
$C_{26}H_{20}O_3PV$	17	$(h^5-C_5H_5)V[P(C_6H_5)_3](CO)_3$	C_6D_6	H 4.50d H' 7.30 (6.97)*	$J_{PH} 1$ —	—	3 *4
$C_{32}H_{25}O_3P_2V$	18	$(h^5-C_5H_5)V[P_2(C_6H_5)_4](CO)_3$	C_6H_6	H 4.13d H' 6.74	$J_{PH} 1$	—	3

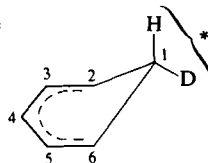
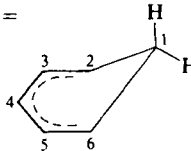
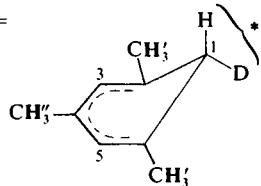
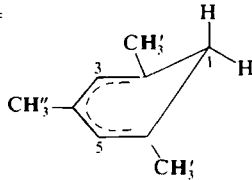
$C_{26}H_{20}O_3SbV$	19	$(h^5-C_5H_5)V[Sb(C_6H_5)_3](CO)_3$	C_6D_6	H	4.62s	—	—	3
				H'	7.28	—	—	
$C_{26}H_{20}O_3PTa$	20	$(h^5-C_5H_5)Ta[P(C_6H_5)_3](CO)_3$	CS_2	H	5.15	—	—	936
$C_9H_5O_4V$	21	$(h^5-C_5H_5)V(CO)_4$	CS_2	H	5.08	—	T 32°	7
			C_6D_6	H	4.30s	—	—	4
								3
								933
$C_{11}H_7O_5V$	22	$(h^5-C_5H_4 \cdot COCH_3)V(CO)_4$	—	H	5.57	—	T 32°	7
					5.17	—		
				H'	2.30	—		
$C_{32}H_{25}AsO_4V_2$	23	$(h^5-C_5H_5)_2V_2[As(C_6H_5)_3](CO)_4$	C_6D_6	H	4.71s	—	—	3
					4.12s	—		
				H'	7.19	—		
$C_{10}H_6DO_4V$	24	$(h^5-C_6H_6D)V(CO)_4$	$(CD_3)_2CO$	H_{-2}, H_{-6}	3.70	—	$C_6H_6D =$	8
				$H_{-3}, H_{-5} \sim$	4.68b	—		
				H_{-4}	6.48t	—		
				H_{-1}	2.57b	—		
							*Stereochemistry not known	
$C_{10}H_7O_4V$	25	$(h^5-C_6H_7)V(CO)_4$	C_6H_6	H_{-2}, H_{-6}	2.83t	—	$C_6H_7 =$	8
				H_{-3}, H_{-5}	3.65b	—		
				H_{-4}	5.45t	—		
				H_{-1}	2.17-1.47	—		
					comp	—		

TABLE 1—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References	
			(CD ₃) ₂ CO	H ₋₂ , H ₋₆ H ₋₃ , H ₋₅ H ₋₄ H ₋₁	3.67t 4.62b 6.42t 2.75–2.37 2.18–2.1	— — — — —		
C ₁₃ H ₁₂ DO ₄ V	26	(<i>h</i> ⁵ -C ₉ H ₁₂ D)V(CO) ₄	(CD ₃) ₂ CO	H ₋₁ H ₋₃ , H ₋₅ H' H''	2.39b 4.52s 1.74 2.60s	— — — —	C ₉ H ₁₂ D = 	8
						*Stereochemistry not known		
C ₁₃ H ₁₃ O ₄ V	27	(<i>h</i> ⁵ -C ₉ H ₁₃)V(CO) ₄	C ₆ D ₆	H ₋₁ H ₋₃ , H ₋₅ H' H''	1.97s 3.69s 1.43s 2.15	— — — —	C ₉ H ₁₃ = 	8
			(CD ₃) ₂ CO	H ₋₁ H ₋₃ , H ₋₅ H' H''	2.42s 4.52s 1.74s 2.61s	— — — —		

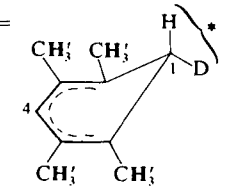
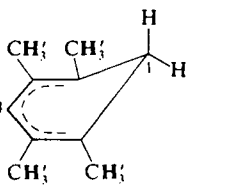
$C_{14}H_{14}DO_4V$	28	$(h^5-C_{10}H_{14}D)V(CO)_4$	$(CD_3)_2CO$	H_{-1} H_{-4} H'	2.48b 6.11b 1.73s	— — —	$C_{10}H_{14}D =$		8
							*Stereochemistry not known		
$C_{14}H_{15}O_4V$	29	$(h^5-C_{10}H_{15})V(CO)_4$	$(CD_3)_2CO$	H_{-1} H_{-4} H'	2.54s 6.22b 1.73s	— — —	$C_{10}H_{15} =$		8
							*Bridging CO		
$C_{32}H_{25}O_4PV_2$	30	$(h^5-C_5H_5)V(CO)_2[(CO)*[h^5-C_5H_5]-C_6D_6VP(C_6H_5)_3(CO)]$		H H'	4.62d 4.02s 7.15	J_{PH}^2 —			4 3
$C_9H_5NbO_4$	31	$(h^5-C_5H_5)Nb(CO)_4$	CS_2	H	5.50bd	—	—		933
$C_{10}H_7NbO_4$	32	$(h^5-C_5H_4 \cdot CH_3)Nb(CO)_4$	CS_2	H H'	5.44m 2.05bd	—	—		933
$C_9H_5O_4Ta$	33	$(h^5-C_5H_5)Ta(CO)_4$	CS_2	H	5.62s	—	—		933
$C_{10}H_7O_4Ta$	34	$(h^5-C_5H_4 \cdot CH_3)Ta(CO)_4$	CS_2	H H'	5.52t 5.37t 2.12s	— — —	—		933
$C_{15}H_{10}O_5V_2$	35	$[(h^5-C_5H_5)V(CO)_2]_2(CO)*$	C_6D_6	H H	4.57s 4.59s	—	*Bridging CO		4 3

TABLE 1—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
(2) <i>HEXAHAPTO LIGANDS</i>							
$[\text{C}_{12}\text{H}_{12}\text{O}_3\text{V}]^-$	36	$\{[h^6\text{-}1,3,5\text{-C}_6\text{H}_3(\text{CH}_3)_3]\text{V}(\text{CO})_3\}^-$	CD_3NO_2	H 6.82 H' 2.25	—	Isolated as the tetra- <i>n</i> -butyl ammonium salt	9
$\text{C}_{12}\text{H}_{12}\text{IO}_3\text{V}$	37	$[h^6\text{-}1,3,5\text{-C}_6\text{H}_3(\text{CH}_3)_3]\text{V}(\text{I})(\text{CO})_3$	CDCl_3	H 6.76 H' 2.27	— —	—	9
$\text{C}_{12}\text{H}_{13}\text{O}_3\text{V}$	38	$[h^6\text{-}1,3,5\text{-C}_6\text{H}_3(\text{CH}_3)_3]\text{V}(\text{H}'')(\text{CO})_3$	$\text{C}_6\text{D}_5\text{CD}_3$	H 4.43 H' 1.55 H'' -5.8	— — —	—	9
(3) <i>HEPTAHAPTO LIGANDS</i>							
$\text{C}_{10}\text{H}_7\text{O}_3\text{V}$	39	$(h^7\text{-C}_7\text{H}_7)\text{V}(\text{CO})_3$	$\text{C}_6\text{D}_5\text{CD}_3$	H 4.22bd H 4.7s	$J(^{51}\text{V}-\text{H}) \sim 2.0$	T 30° T -79°	10
(4) <i>MIXED LIGANDS</i>							
$\text{C}_{38}\text{H}_{30}\text{OPV}$	40	$(h^5\text{-C}_5\text{H}_5)\text{V}(h^2\text{-C}_6\text{H}_5\text{C}\equiv\text{CC}_6\text{H}_5)\text{-}[\text{P}(\text{C}_6\text{H}_5)_3](\text{CO})$	CS_2	H 5.00d H' 7.15m	$J_{\text{PH}1}$ —	—	934
$\text{C}_{34}\text{H}_{25}\text{NbO}$	41	$(h^5\text{-C}_5\text{H}_5)\text{Nb}(\text{C}_6\text{H}_5\text{C}\equiv\text{CC}_6\text{H}_5)_2\text{-}(\text{CO})$	CS_2	H 5.70 H' 7.20	— —	—	12 937

$C_{35}H_{27}NbO$	42	$(h^5-C_5H_4 \cdot CH_3)Nb(h^2-C_6H_5C \equiv CC_6H_5)_2(CO)$	—	H	5.50t 5.75t	—	—	933
				H'	1.5s	—		
				H''	7.18m			
$C_{48}H_{35}NbO$	43	$(h^5-C_5H_5)Nb[h^4-C_4(C_6H_5)_4]-(C_6H_5C \equiv CC_6H_5)(CO)$	—	H	5.1s	—	$C_4(C_6H_5)_4 =$ tetraphenylcyclobutadiene	938
				H'	7.2m			
$C_{48}H_{35}NbO$	44	$(h^5-C_5H_5)Nb[1,4-h^2-C_4(C_6H_5)_4]-(h^2-C_6H_5C \equiv CC_6H_5)(CO)$	—	H	5.15s	—	$C_4(C_6H_5)_4 =$ tetraphenylbutadiene	937
				H'	7.10			
$C_{34}H_{25}OTa$	45	$(h^5-C_5H_5)Ta(h^2-C_6H_5C \equiv CC_6H_5)(CO)$	CS ₂	H	5.65s	—	—	936
				H'	7.10m			
$C_{36}H_{25}O_3V$	46	$(h^5-C_5H_5)V[h^4-C_5O(C_6H_5)_4](CO)_2$	CS ₂	H	4.40s	—	$C_5O(C_6H_5)_4 =$ tetraphenylcyclopentadienone	934
				H'	7.10m			
$C_{21}H_{15}NbO_2$	47	$(h^5-C_5H_5)Nb(C_6H_5C \equiv CC_6H_5)(CO)_2$	CS ₂	H	4.80s	—	Hexamethyldisiloxane reference	13
				H'	3.00 2.90			
$C_{12}H_{10}NbO_2$	48	$(h^5-C_5H_5)Nb(h^1-C_5H_5)(CO)_2$	—	H	5.00	—	—	14
				H'	5.05 3.00 2.35	— — —		
$C_{40}H_{30}Nb_2O_2$	49	$[(h^5-C_5H_5)Nb(CO)]_2(PhC \equiv CPh)_2^*$	—	H	5.83	—	*Bridging $PhC \equiv CPh$ ligands	15

TABLE II
Chromium complexes

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)		Remarks	References		
(1) MONOHAPTO LIGANDS											
(a) Tetracarbonyl derivatives											
$C_{25}H_{22}CrNO_4P$	1	$Cr[C(CH_3)NH''CH_3][P(C_6H_5)_3](CO)_4$	$CHCl_3$	H	2.40	—	—	$J_{H'H''} \sim 5$	947		
				H'	2.69	—	—				
			C_6H_6	H	2.09	—	—				
				H'	1.68	—	—				
$C_{13}H_{21}CrO_5P$	2	$Cr[C(CH_3)OCH_3][P(C_2H_5)_3(CO)_4]$	C_6D_6	H	2.60	—	—		1019		
				H'	3.77	—	—				
$C_{19}H_{33}CrO_5P$	3	$Cr[C(CH_3)OCH_3][P(n-C_4H_9)_3](CO)_4$	C_6D_6	H	2.61	—	—		1019		
				H'	3.76	—	—				
$C_{25}H_{39}CrO_5P$	4	$Cr[C(CH_3)OCH_3][P(C_6H_{11})_3](CO)_4$	C_6D_6	H	2.84	—	—		1019		
				H'	4.07	—	—				
$C_{17}H_{21}CrO_5P$	5	$Cr[C(CH_3)OCH_3][P(C_2H_5)_2C_6H_5](CO)_4$	C_6D_6	H	2.21	—	—		1019		
				H'	5.45	—	—				
$C_{30}H_{41}CrO_5P$	6	$Cr[C(C_6H_5)OCH_3][P(C_6H_{11})_3](CO)_4$	C_6D_6	H	7.15	—	—		1019		
				H'	3.81	—	—				
$C_{25}H_{21}CrO_5P$	7	$Cr[C(CH_3)OCH_3][P(C_6H_5)_3](CO)_4$	C_6D_6	H	2.46s	—	—		945 17		
				H'	3.70s	—	—				
				H''	7.34m	—	—				

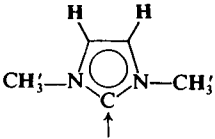
$C_{14}H_{16}CrN_4O_4$	8	$Cr(C_3H_8N_2)_2(CO)_4$	$(CD_3)_2CO$	H H'	7.07s 3.52s	—	$C_3H_8N_2 =$	18
								
<i>(b) Pentacarbonyl derivatives</i>								
$C_8H_3CrO_5$	9	$Cr(C\equiv CCH_3)(CO)_5$	CH_2Cl_2	H	1.57	—	—	19
$C_7H_5CrNO_5$	10	$Cr[C(CH_3) \cdots NH_2](CO)_5$	$CDCl_3$	H	2.77	—	Carbene complex	20
				H'	8.10	—		
			C_6D_6	H	1.87	—		
				H'	6.8	—		
			$(CD_3)_2CO$	H	2.76	—		
				H'	10.60	—		
$C_8H_7CrNO_5$	11	$Cr[C(CH_3) \cdots NH'CH_3''](CO)_5$	$(CD_3)_2CO$	H	2.84s	—	—	21
				H'	10.25t	—		
				H''	—	—		
			$CDCl_3$	H	2.55	—	Carbene complex	20
				H'	8.23	—		
				H''	3.10	—		
			C_6D_6	H	1.89	—		
				H'	7.8	—		
				H''	1.67	—		
			$(CD_3)_2CO$	H	2.50	—		
				H'	10.20	—		
				H''	3.40	—		
			$CHCl_3$	H	2.69m	$J_{HH''} \sim 0.3$	<i>cis</i> -isomer, viz.: $(CO)_5Cr \begin{array}{c} \diagup \\ C \equiv N \end{array} \begin{array}{c} H \\ \diagdown \end{array}$ $H_3C \diagup C \equiv N \diagdown CH_3$	22
				H'	8.35m	$J_{H'H''} 5$		23
				H''	3.20m	—		947

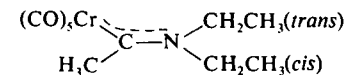
TABLE II—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	Refer- ences
$C_9H_9CrNO_5$	12	$Cr[C(CH_3)_2 \cdots NH'CH''CH_3'''] \cdot (CO)_5$	C_6H_6	H	2.05	—	<i>trans</i> -isomer	23
				H''	1.80	—		
			$CHCl_3$	H	2.81	$J_{HH''} 0.85$		23 947
				H'	~ 8.8	$J_{H'H''} 4.9$		
				H''	3.65	—		
			C_6H_6	H	2.15	—	Carbene complex	20
				H''	2.80	—		
			$CDCl_3$	H	2.67	—		
				H'	8.68	—		
				H''	3.43	—		
				H'''	1.37	—		
			C_6D_6	H	2.10	—		
				H'	8.2	—		
				H''	2.20	—		
				H'''	0.47	—		
			$(CD_3)_2CO$	H	2.63	—		
				H'	10.37	—		
				H''	3.57	—		
				H'''	1.27	—		
$C_{10}H_{11}CrNO_5$	13	$Cr[C(CH_3)_2 \cdots NH'CH''(CH_3'')_2] \cdot (CO)_5$	$CDCl_3$	H	2.77	—	Carbene complex	20
				H'	8.67	—		
				H''	4.0	—		
				H'''	1.37	—		

			C ₆ D ₆	H	2.56	—		
				H'	8.25	—		
				H''	3.18	—		
				H'''	0.60	—		
			(CD ₃) ₂ CO	H	2.80	—		
				H'	10.50	—		
				H''	4.19	—		
				H'''	1.47	—		
C ₁₁ H ₁₃ CrNO ₅	14	Cr[C(CH ₃) ₃ —NH'C(CH ₃) ₃]- (CO) ₅	CDCl ₃	H	2.90	—	Carbene complex	20
				H'	9.10	—		
				H''	1.50	—		
			C ₆ D ₆	H	2.53	—		
				H'	8.90	—		
				H''	0.83	—		
			(CD ₃) ₂ CO	H	2.97	—		
				H'	10.70	—		
				H''	1.57	—		
			CHCl ₃	H	2.79d	J _{HH'} 1.15	cis-isomer	22
				H''	1.40s	—		
C ₁₃ H ₁₅ CrNO ₅	15	Cr[C(CH ₃) ₃ —NH'C ₆ H ₁₁](CO) ₅	CDCl ₃	H	2.77	—	Carbene complex	20
				H'	8.67	—		
				H''	3.77*	—	*Methine proton of cyclohexyl group	
				H''	1.58†	—	†Methylene protons of cyclohexyl group	
			C ₆ D ₆	H	2.17	—		
				H''	2.99*	—		
				H''	1.10†	—		

TABLE II—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_9H_9CrNO_5$	16	$Cr[C(CH_3)_2 \rightleftharpoons N(CH_2)_2](CO)_5$	$(CD_3)_2CO$	H	2.75	—	*Methine proton of cyclohexyl group	23 22
				H'	10.58	—	†Methylene protons of cyclohexyl group	
				H''	4.0*	—		
				H''	1.75†	—		
			$CHCl_3$	H	2.69m	$J_{HH'} 0.85^*$	‡CH ₃ ' <i>trans</i> to CCH ₃	
				H'	3.87q‡	$J_{HH'} 0.3^\dagger$	§CH ₃ ' <i>cis</i> to CCH ₃	
					3.30m§		<i>to CCH₃</i>	
				H	2.20			
				H'	3.22*			
					2.08†			
$C_{11}H_{13}CrNO_5$	17	$Cr[C(CH_3)_2 \rightleftharpoons N(CH_2CH_3)_2](CO)_5$	$CDCl_3$	H	2.78	—	Carbene complex, viz.:	20
				H' _{cis}	3.70	—		
				H' _{trans}	4.23	—		
				H'' _{cis}	1.25	—		
				H'' _{trans}	1.42	—		
			C_6D_6	H	2.33	—		
				H' _{cis}	2.70	—		
				H' _{trans}	3.70	—		
				H'' _{cis}	0.49	—		
				H'' _{trans}	0.88	—		
			$(CD_3)_2CO$	H	2.83	—		
				H' _{cis}	4.78	—		
				H' _{trans}	4.30	—		
				H'' _{cis}	1.27	—		
				H'' _{trans}	1.47	—		



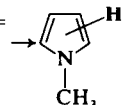
$C_{14}H_{11}CrNO_5$	18	$Cr[C(CH_3)_3 \cdots NH'C_6H_5''']-(CO)_5$	$CDCl_3$	H	2.47	—	Carbene complex	20
				H''	4.10	—		
				H'''	7.30	—		
			C_6D_6	H	2.07	—		
				H''	3.37	—		
				H'''	7.16	—		
			$(CD_3)_2CO$	H	2.70	—		
				H'	10.43	—		
				H''	4.83	—		
				H'''	7.33	—		
$C_{14}H_9CrNO_5$	19	$Cr[C(CH_3)N=CH'C_6H_5']-(CO)_5$	$(CD_3)_2CO$	H	2.68d	J 2.5	Carbene complex	24
				H'	7.63q	J 2.5		
				H''	7.51m	—		
$C_{15}H_{11}CrNO_5$	20	$Cr[C(CH_3)N=C(CH_3)C_6H_5']-(CO)_5$	$(CD_3)_2CO$	H	2.66s, 2.56s	—	Carbene complex	24
				H'	7.55m	—		
$C_{20}H_{13}CrNO_5$	21	$Cr[C(CH_3)N=C(C_6H_5)_2](CO)_5$	$(CD_3)_2CO$	H	2.84s	—	Carbene complex	24
				H'	7.60s	—		
$C_{13}H_9CrNO_5$	22	$Cr[C(CH_3)_3 \cdots NH'C_6H_5']-(CO)_5$	$CDCl_3$	H	2.70	—	Carbene complex	20
				H'	10.43	—		
				H''	7.33	—		
			C_6D_6	H	2.18	—		
				H''	6.46	—		
			$(CD_3)_2CO$	H	2.65	—		
				H'	12.96	—		
				H''	7.24	—		
				H'''	7.24	—		
$C_{14}H_{11}CrNO_5$	23	$Cr[C(CH_3)_3 \cdots NH'-p-C_6H_4CH_3''']-(CO)_5$	$CDCl_3$	H	2.67	—	Carbene complex	20
				H'	9.97	—		
				H''	7.18	—		
				H'''	2.44	—		
				H'''	2.44	—		

TABLE II—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References			
$C_{14}H_8F_3CrNO_3$	24	$Cr[C(CH_3)_3 \cdots NH'-p-C_6H_4CF_3]-(CO)_5$	C_6D_6	H	2.15	—	Carbene complex	20			
				H''	6.31	—					
				H'''	1.92	—					
			$(CD_3)_2CO$	H	2.67	—					
				H'	12.01	—					
				H''	7.20	—					
			$CDCl_3$	H	2.79	—			—		
					H'	10.53				—	
					H''	7.68				—	
			$(CD_3)_2CO$	H	2.67	—					
				H'	12.13	—					
				H''	7.60	—					
$C_{13}H_8ClCrNO_3$	25	$Cr[C(CH_3)_3 \cdots NH'-p-C_6H_4Cl]-(CO)_5$	$CHCl_3$	H	2.53d	$J_{HH'} 0.9$	<i>cis</i> -isomer	22			
			$CDCl_3$	H	2.68	—	Carbene complex	20			
				H'	10.37	—					
				H''	7.28	—					
			$(CD_3)_2CO$	H	2.67	—					
				H'	12.09	—					
				H''	7.40	—					
			$C_{13}H_{10}CrN_2O_5$	26	$Cr[C(CH_3)_3 \cdots NH'-p-C_6H_4-NH_2'']-(CO)_5$	$(CD_3)_2CO$	H	2.57	—	Carbene complex	20
							H'	11.83	—		
							H''	6.73	—		
							H'''	4.80	—		

C ₁₄ H ₁₁ CrNO ₆	27	Cr[C(CH ₃) ₃ NH'-p-C ₆ H ₄ -OCH ₃ '''] ₂ (CO) ₅	CDCl ₃	H	2.65	—	Carbene complex	20
				H'	10.40	—		
				H''	7.03	—		
				H'''	3.83	—		
			C ₆ D ₆	H	2.23	—		
				H''	6.30	—		
				H'''	2.24	—		
			(CD ₃) ₂ CO	H	2.63	—		
				H'	11.98	—		
				H''	7.09	—		
				H'''	3.80	—		
			CHCl ₃	H	2.62d	J _{HH'} 1.0		
				H'	3.83s	—		22
C ₁₃ H ₈ CrO ₃ S	28	Cr[C(CH ₃) ₃ SC ₆ H ₅](CO) ₅	C ₆ D ₆	H	2.92	—	Carbene complex	21
				H'	6.90, 6.55	—		
C ₁₂ H ₇ CrNO ₅	29	Cr[C(NH ₂)C ₆ H ₅](CO) ₅	(CD ₃) ₂ CO	H	7.28	—	Carbene complex	25
				H'	10.37	—		
C ₁₃ H ₉ CrNO ₅	30	Cr[C(NH ₂)p-C ₆ H ₄ CH ₃ '''] ₂ (CO) ₅	(CD ₃) ₂ CO	H	6.62	—	Carbene complex	25
				H'	9.34	—		
				H''	1.79	—		
C ₁₂ H ₆ BrCrNO ₅	31	Cr[C(NH ₂)p-C ₆ H ₄ Br](CO) ₅	(CD ₃) ₂ CO	H	7.49, 7.07	—	Carbene complex	25
				H'	10.20	—		
C ₁₂ H ₆ ClCrNO ₅	32	Cr[C(NH ₂)m-C ₆ H ₄ Cl](CO) ₅	(CD ₃) ₂ CO	H	7.17	—	Carbene complex	25
				H'	10.23	—		
C ₁₂ H ₆ ClCrNO ₅	33	Cr[C(NH ₂)p-C ₆ H ₄ Cl](CO) ₅	(CD ₃) ₂ CO	H	7.40, 7.07	—	Carbene complex	25
				H'	10.10	—		
C ₁₄ H ₁₂ CrN ₂ O ₅	34	Cr[C(NH ₂)p-C ₆ H ₄ N(CH ₃) ₂](CO) ₅	(CD ₃) ₂ CO	H	7.48, 6.68	—	Carbene complex	25
				H'	9.67	—		
				H''	2.97	—		

TABLE II—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{13}H_9CrNO_6$	35	$Cr[C(NH_2')m-C_6H_4OCH_3'']_3(CO)_5$	$(CD_3)_2CO$	H	7.13, 6.70	Carbene complex	25
				H'	10.0		
				H''	3.68		
$C_{13}H_9CrNO_6$	36	$Cr[C(NH_2'')p-C_6H_4OCH_3']_3(CO)_5$	$(CD_3)_2CO$	H	7.35, 6.92	Carbene complex	25
				H'	9.97		
				H''	3.75		
$C_{11}H_8CrN_2O_5$	37	$Cr[C(NH_2)\alpha-C_5H_6N](CO)_5$	$(CD_3)_2CO$	H	-72* Hz	Carbene complex $C_5H_6N = $ 	26
						*Relative to <i>N</i> -methylpyrrole	
$C_{10}H_5CrNO_6$	38	$Cr[C(NH_2)\alpha-C_4H_3O](CO)_5$	$(CD_3)_2CO$	H	-112* Hz	Carbene complex $C_4H_3O = $ 	26
						*Relative to free furan	
$C_{10}H_5CrNO_5S$	39	$Cr[C(NH_2)\alpha-C_4H_3S](CO)_5$	$(CD_3)_2CO$	H	-63 Hz*	Carbene complex $C_4H_3S = $ 	26
						*Relative to free thiophene	

$C_{14}H_9CrNO_5$	40	$Cr\{C(N=CHCH_3)C_6H_5\}(CO)_5$	$(CD_3)_2CO$	H H' H''	7.34q 2.27d 7.56	$J = 6$ $J = 6$	Carbene complex	27
$C_{18}H_{15}CrFeNO_5$	41	$Cr\{C[N(CH_3)_2]Fc\}(CO)_5$	$CDCl_3$	H H' H''	-36 Hz* -22 Hz* -5 Hz*	— — —	Fc = ferrocene moiety H = proton α -carbene substituent H' = proton β -carbene substituent H'' = protons of unsubstituted ring *Relative to ferrocene	26
$C_{20}H_{17}CrFeNO_5$	42	$Cr\{C(NC_4H_9)Fc\}(CO)_5$	$CDCl_3$	H H' H''	-32 Hz* -32 Hz* -2 Hz*	— — —	*Relative to ferrocene (See above)	26
$C_{24}H_{17}CrNO_5$	43	$Cr\{C[NHCH(CH_3)C_6H_5][C_{10}H_7]\}(CO)_5$	CD_3OD $CDCl_3$	H H' H H'	4.45 1.62 4.28 1.34	— — — —	<i>cis</i> -isomer; exists in two atrop- isomeric forms owing to barrier to free rotation about carbene- naphthyl bond:	29

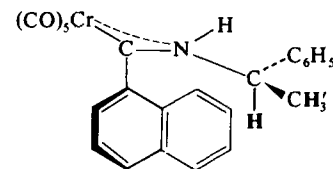
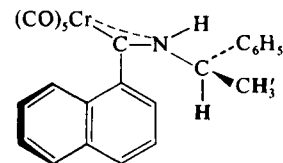
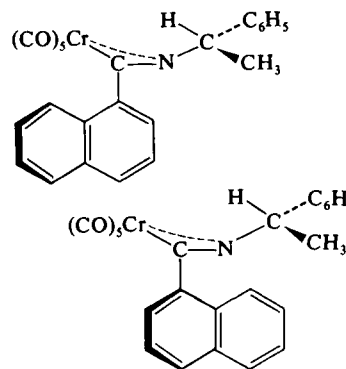
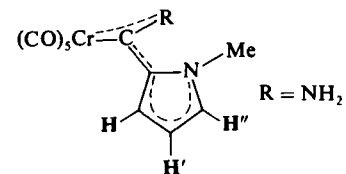
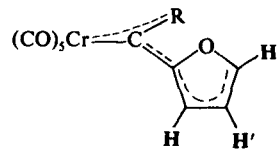


TABLE II—*cont.*

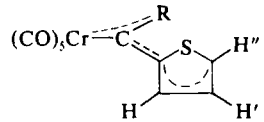
Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
			CD ₃ OD	H 5.92 H' 1.95	— —	<i>trans</i> -isomer, which also exhibits atropisomerism:	29
			CDCl ₃	H 5.80 H' 1.72	— —		
C ₁₁ H ₈ CrN ₂ O ₅	44	Cr[C(NH ₂)C ₅ H ₆ N](CO) ₅	(CD ₃) ₂ CO	H -70° H' 0 H'' -25	— — —	Structure:  R = NH ₂	30

100 MHz

$C_{13}H_{11}CrNO_6$	45	$Cr[C(OCH_2CH_3)C_5H_6N](CO)_5$	$(CD_3)_2CO$	H	-159*	—	Structure analogous to that above ($R = OCH_2CH_3$) 100 MHz	30
				H'	-15	—		
				H''	-55	—		
$C_{15}H_{18}CrN_2O_6$	46	$Cr[C(O-N^+Me_4)C_5H_6N](CO)_5$	$(CD_3)_2CO$	H	-75*	—	Structure analogous to that above ($R = O-N^+Me_4$) 100 MHz	30
				H'	+26	—		
				H''	+26	—		
$C_{10}H_5CrNO_6$	47	$Cr[C(NH_2)C_4H_3O](CO)_5$	$(CD_3)_2CO$	H	-112*	—	Structure:	31
				H'	-31	—		30
				H''	-29	—		
							 $R = NH_2$	
							100 MHz	
							The chemical shifts for free furan (in Hz) relative to TMS are: H -641, H' -641, and H'' -753	
$C_{14}H_{11}CrNO_6$	48	$Cr[C(NC_4H_9)C_4H_3O](CO)_5$	$(CD_3)_2CO$	H	-18*	—	Structure analogous to that above 100 MHz ($R = N$ in a pyrrolidine ring)	31
				H'	-18	—		
				H''	-22	—		
$C_{11}H_6CrO_7$	49	$Cr[C(OCH_3)C_4H_3O](CO)_5$	$(CD_3)_2CO$	H	-78*	—	Structure analogous to that above ($R = OCH_3$) 100 MHz	31
				H'	-37	—		
				H''	-67	—		
$C_{12}H_8CrO_7$	50	$Cr[C(OCH_2CH_3)C_4H_3O](CO)_5$	$(CD_3)_2CO$	H	-78*	—	Structure analogous to that above ($R = OCH_2CH_3$) 100 MHz	31
				H'	-37	—		
				H''	-66	—		

*Compound Nos. 44-58, chemical shifts in Hz relative to the corresponding signal of the free heterocycle (viz., *N*-methylpyrrolidine, furan, or thiophen). The chemical shifts for the free *N*-methyl pyrrolidine (in Hz) relative to TMS are: H -616, H' -616, H'' -616

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{14}H_{15}CrNO_7$	51	$Cr[C(O^-N^+Me_4)C_4H_3O](CO)_5$	$(CD_3)_2CO$	H	-29*	Structure analogous to that above (R = $O^-N^+Me_4$) 100 MHz	30
				H'	+4		
				H''	+13		
$C_{16}H_8CrO_7$	52	$Cr[C(OPh)C_4H_3O](CO)_5$	$(CD_3)_2CO$	H	-97*	Structure analogous to that above (R = OPh) 100 MHz	31
				H'	-50		
				H''	-83		
$C_{12}H_6CrO_8$	53	$Cr[C(OCOCH_3)C_4H_3O](CO)_5$	$(CD_3)_2CO$	H	-90*	Structure analogous to that above (R = $OCOCH_3$) 100 MHz	31
				H'	-50		
				H''	-87		
$C_{10}H_5CrNO_5S$	54	$Cr[C(NH_2)C_4H_3S](CO)_5$	$(CD_3)_2CO$	H	-63*	Structure:  R = NH_2 100 MHz The chemical shifts for free thio-phen (in Hz) relative to TMS are: H -708, H' -708, H'' -738	30
				H'	-14		
				H''	-50		
$C_{14}H_{15}CrNO_6S$	55	$Cr[C(O^-N^+Me_4)C_4H_3S](CO)_5$	$(CD_3)_2CO$	H	-66*	Structure analogous to that above (R = $O^-N^+Me_4$) 100 MHz	30
				H'	+3		
				H''	+5		
$C_{12}H_8CrO_6S$	56	$Cr[C(OCH_2CH_3)C_4H_3S](CO)_5$	$(CD_3)_2CO$	H	-129*	Structure analogous to that above (R = OCH_2CH_3) 100 MHz	30
				H'	-29		
				H''	-65		

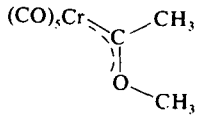
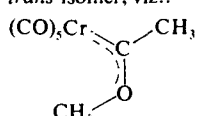
$C_{12}H_8CrO_6S$	57	$Cr[C(SCH_2CH_3)C_4H_9O](CO)_5$	$(CD_3)_2CO$	H	-128*	—	Structure analogous to that above (R = SCH_2CH_3) 100 MHz	31
				H'	-63	—		
				H''	-87	—		
$C_{16}H_8CrO_6S$	58	$Cr[C(SPh)C_4H_9O](CO)_5$	$(CD_3)_2CO$	H	+8*	—	Structure analogous to that above (R = SPh) 100 MHz	31
				H'	-29	—		
				H''	-77	—		
$C_8H_6CrO_6$	59	$Cr[C(OC'H_3)C''H_3](C'''O)_5$	$CHCl_3$	^{13}C	362.3	—		32
				$^{13}C'$	67.2	—		
				$^{13}C''$	49.1	—		
				$^{13}C'''$	217.6	—	<i>cis</i> -isomer	
					223.6	—	<i>trans</i> -isomer	
$C_8H_6CrO_6$	60	$Cr[C(CH_3)OCH_3](CO)_5$	$CDCl_3$	H	3.01	—	<i>cis</i> -isomer, viz.: 	966
				H'	4.31	—		
				H	2.97	—	<i>trans</i> -isomer, viz.: 	966
				H'	4.81	—		17
			$(CD_3)_2CO$	H	3.17	—	<i>cis</i> -isomer	T -40°
				H'	4.39	—		966
				H	3.00	—	<i>trans</i> -isomer	T -40°
				H'	4.89	—		
				H	3.03s	—	<i>trans</i> -isomer	T +40°
				H	4.68s	—		

TABLE II—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References		
$C_{13}H_{12}CrO_7$	61	$Cr[C(OCH_3)CH'=CH''CH'''=C(OCH_3^{IV})CH_3^V](CO)_5$	CD_3OD	H	3.05	— } <i>cis</i> -isomer	T -40° 966		
				H'	4.34			— }	
				H	2.97	— } <i>trans</i> -isomer			T -40°
				H'	4.83			— }	
			C_6H_5Cl	H	2.24	— } <i>cis</i> -isomer	T -40° 966		
				H'	3.22			— }	
				H	2.51	— } <i>trans</i> -isomer			T -40°
				H'	4.17			— }	
			C_6H_5F	H	2.31	— } <i>cis</i> -isomer	T -40° 966		
				H'	3.30			— }	
				H	2.56	— } <i>trans</i> -isomer			T -40°
				H'	4.23			— }	
			C_6D_6	H	2.33	—	—		
				H'	3.72				
			H	3.95s	—	*in acetone- d_6 Carbene complex	34		
			H'	7.21d*	J 14				
			H''	7.58dd	J 11				
			H'''	4.96bd	J 9.5				
			H^{IV}	2.92s	—				
			H^V	1.70s	—				
$C_{13}H_8CrO_6$	62	$Cr[C(OCH_3)C_6H_5](CO)_5$	C_6H_6	H	3.78	—	1019 33 35 36 37		
			C_6D_6	H'	6.95			—	

			(CD ₃) ₂ CO	H	4.22	—	<i>cis</i> -isomer	T -26.5°	38
				H	5.12	—	<i>trans</i> -isomer		
C ₁₄ H ₁₀ CrO ₆	63	Cr[C(OCH ₃) <i>p</i> -C ₆ H ₄ CH ₃](CO) ₅	(CD ₃) ₂ CO	H	4.24	—	<i>cis</i> -isomer	T -37°	38
				H'	7.41, 7.06	—			
				H	5.07	—	<i>trans</i> -isomer		
				H'	7.74, 7.41	—			
C ₁₄ H ₇ CrF ₃ O ₆	64	Cr[C(OCH ₃) <i>p</i> -C ₆ H ₄ CF ₃](CO) ₅	(CD ₃) ₂ CO	H	4.25	—	<i>cis</i> -isomer	T +4°	38
				H	5.15	—	<i>trans</i> -isomer		
C ₁₄ H ₇ CrF ₃ O ₆	65	Cr[C(OCH ₃) <i>m</i> -C ₆ H ₄ CF ₃](CO) ₅	(CD ₃) ₂ CO	H	4.29	—	<i>cis</i> -isomer	T -26°	38
				H	5.16	—	<i>trans</i> -isomer		
C ₁₄ H ₇ CrF ₃ O ₆	66	Cr[C(OCH ₃) <i>p</i> -C ₆ H ₄ CF ₃](CO) ₅	(CD ₃) ₂ CO	H	4.31	—	<i>cis</i> -isomer	T -21°	38
				H'	8.09, 7.46	—			
				H	5.19	—	<i>trans</i> -isomer		
				H'	8.00, 7.72	—			
C ₁₃ H ₇ BrCrO ₆	67	Cr[C(OCH ₃) <i>p</i> -C ₆ H ₄ Br](CO) ₅	(CD ₃) ₂ CO	H	4.27	—	<i>cis</i> -isomer	T -29°	38
				H'	7.83, 7.20	—			
				H	5.12	—	<i>trans</i> -isomer		
				H'	7.83, 7.64	—			
C ₁₃ H ₇ ClCrO ₆	68	Cr[C(OCH ₃) <i>m</i> -C ₆ H ₄ Cl](CO) ₅	(CD ₃) ₂ CO	H	4.29	—	<i>cis</i> -isomer		38
				H'	—	—	T -27°		
				H	5.15	—	<i>trans</i> -isomer		
				H'	—	—	T -27°		
C ₁₃ H ₇ ClCrO ₆	69	[Cr[C(OCH ₃) <i>p</i> -C ₆ H ₄ Cl](CO) ₅	(CD ₃) ₂ CO	H	4.28	—	<i>cis</i> -isomer, viz.:		38
				H'	7.67, 7.27	—	T -50°		

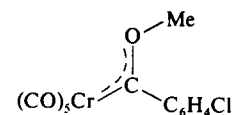
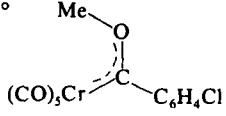


TABLE II—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
				H	5.12	—	<i>trans</i> -isomer, viz.:	
				H'	7.67	—	T -50°	
								
C ₁₃ H ₇ CrFO ₆	70	Cr[C(OCH ₃) ₃] <i>p</i> -C ₆ H ₄ F(CO) ₅	(CD ₃) ₂ CO	H	4.28	—	<i>cis</i> -isomer (see above) T -35.5°	38
				H	5.12	—	<i>trans</i> -isomer	
C ₁₄ H ₁₀ CrO ₇	71	Cr[C(OCH ₃) ₃] <i>o</i> -C ₆ H ₄ OCH ₃ (CO) ₅	(CD ₃) ₂ CO	H	4.17	—	<i>cis</i> -isomer (see above) T -15°	38
				H	5.05	—	<i>trans</i> -isomer	
C ₁₄ H ₁₀ CrO ₇	72	Cr[C(OCH ₃) ₃] <i>m</i> -C ₆ H ₄ OCH ₃ (CO) ₅	(CD ₃) ₂ CO	H	4.24	—	<i>cis</i> -isomer (see above) T -28°	38
				H	5.09	—	<i>trans</i> -isomer	
C ₁₅ H ₁₃ CrNO ₆	73	Cr[C(OCH ₃) ₃] <i>m</i> -C ₆ H ₄ N(CH ₃) ₂ (CO) ₅	(CD ₃) ₂ CO	H	4.25	—	<i>cis</i> -isomer (see above) T -32°	38
				H	5.08	—	<i>trans</i> -isomer	
C ₁₇ H ₁₂ CrFeO ₆	74	Cr[C(OCH ₃)Fc](CO) ₅	CDCl ₃	H	-84 Hz*	—	Fc = ferrocene moiety	26
				H'	-63 Hz*	—	H = proton α - to Carbene Substituent	
				H''	-9 Hz*	—	H' = proton β - to Carbene Substituent	
							H'' = protons of unsubstituted ring	
							*Relative to ferrocene	
C ₁₈ H ₁₄ CrFeO ₆	75	Cr[C(OEt)Fc](CO) ₅	CDCl ₃	H	-83 Hz*	—	*Relative to ferrocene	26
				H'	-60 Hz*	—	(see above)	
				H''	-6 Hz*	—		

$C_9H_8CrO_6$	76	$Cr[C(OCH_2CH_3)CH_3^{\eta}](CO)_5$	$CDCl_3$	H H' H''	4.90q 1.64t 2.90s	—	Carbene complex	39
$C_9H_8CrO_6$	77	$Cr[C(OCH_2CH_3)CH_3^{\eta}](CO)_5$	C_6H_6	H H' H''	4.52q 1.25t 2.61s	—	Carbene complex	40
$C_{12}H_{14}CrO_6$	78	$Cr[C(OCH_2CH_3)CH_2^{\eta}(CH_2''')_2-CH_3^{IV}](CO)_5$	$CDCl_3$	H H' H'' H''' H^{IV}	4.90q 1.62t 3.12t 1.41m 0.92t	—	Carbene complex	39
$C_{12}H_{16}CrO_6Si$	79	$Cr[C(OEt)CH_2Si(CH_3)_3](CO)_5$	CCl_4	H	—358 Hz	—	Carbene complex	41
$C_{14}H_{10}CrO_6$	80	$Cr[C(OCH_2CH_3)C_6H_5^{\eta}](CO)_5$	$CDCl_3$	H H' H''	5.09q 1.75t 7.52m	—	Carbene complex	39
$C_{10}H_{11}CrNO_6$	81	$Cr[C(OCH_2CH_3)N(CH_3)_2](CO)_5$	C_6D_6	H H' H''	4.32q 0.93t 2.15s, 2.88s	—	Carbene complex	42
			$CDCl_3$	H H' H''	4.62q 1.42t 3.06s, 3.57s	—		
$C_{12}H_{15}CrNO_6$	82	$Cr[C(OCH_2CH_3)N(CH_2CH_3)_2](CO)_5$	C_6H_6	H H' H''	4.51q 3.71q, 2.90q 1.04t, 0.93t, 0.75t	—	Carbene complex	43
$C_{13}H_{11}CrNO_6$	83	$Cr[C(OEt)C_5H_5N](CO)_5$	$(CD_3)_2CO$	H	—159* Hz	—	*Relative to free <i>N</i> -methyl pyrrole	26
$C_{12}H_8CrO_7$	84	$Cr[C(OEt)C_4H_3O](CO)_5$	$(CD_3)_2CO$	H	—78* Hz	—	*Relative to free furan	26
$C_{12}H_8CrO_6S$	85	$Cr[C(OEt)C_4H_3S](CO)_5$	$(CD_3)_2CO$	H	—129* Hz	—	*Relative to free thiophen	26

TABLE II—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{14}H_{20}CrLiNO_7$	86	$Cr\{C[OLiO(C_2H_5)_2]N[CH_2-CH_3]_2\}(CO)_5$	$(CD_3)_2CO$	H	2.55q	—	Carbene complex	43
				H'	1.00t	—		
				H''	3.4q	—		
					1.1t	—		
$C_{10}H_{12}CrO_6Si$	87	$Cr\{C[OSi(CH_3)_3]CH_3\}(CO)_5$	C_6H_6	H	10.0	—	Carbene complex	44
				H'	2.52	—		
$C_{15}H_{17}CrNO_6$	88	$Cr\{C[C(OCH_3)=CH_2]NH''-C_6H_{11}''\}(CO)_5$	C_6H_6	H	3.15	—	— *Methine proton	45
				H'	4.35, 3.90	J 3.5		
				H''	9.20	—		
				H'''	4.17*	—		
$C_{15}H_{17}CrNO_6$	89	$Cr\{C[C(OCH_3)=CH_2]NH''-C_6H_{11}''\}(CO)_5$	C_6D_6	H	3.15	—	—	46
				H'	4.35, 3.90	J 3.5		
				H''	9.50	—		
				H'''	4.17, 2.0— 0.58	—		
$C_{16}H_{21}CrNO_7$	90	$Cr\{C[C(OCH_3)_2CH_3]NH''C_6H_{11}''\}-C_6D_6$ (CO) ₅	C_6D_6	H	2.88	—	—	46
				H'	1.07	—		
				H''	0.13	—		
				H'''	4.40, 1.92— 0.58	—		
$C_{15}H_{17}CrNO_6$	91	$Cr\{C(OCH_3)(CH_3)CNC_6H_{11}''\}-$ (CO) ₅	C_6D_6	H	3.20	—	—	46
				H'	1.77	—		
				H''	3.16, 2.16— 0.58	—		

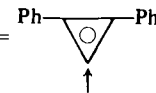
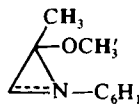
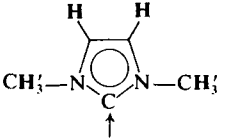
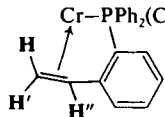
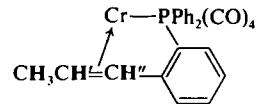
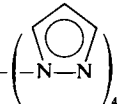
C_6HCrNO_5	92	$Cr(C=NH)(CO)_5$	$(CH_3)_2CO$	H	4.59	—	—	1017
$C_9H_9CrNO_5Sn$	93	$Cr(C=NSn(CH_3)_3)(CO)_5$	C_6H_6	H	0.11	$J(^{119}Sn-H) = 60$ $J(^{117}Sn-H) = 57$	—	1017
$[C_7H_3CrO_6]^-$	94	$[Cr(COCH_3)(CO)_5]^-$	CH_2Cl	H	2.32	—	Isolated as tetramethyl-ammonium salt	33
$C_{14}H_{15}CrNO_6$	95	$Cr[C(COCH_3)NH'C_6H_{11}](CO)_5$	C_6H_6	H H' H''	1.93 9.50 4.05*	— — —	— *Methine proton	45
			C_6D_6	H H' H''	1.93 9.20 4.05, 2.08– 0.58	— — —	—	46
$[C_{10}H_{11}CrO_6Si]^-$	96	$\{Cr[COCH_2Si(CH_3)_3](CO)_5\}^-$	$(CD_3)_2CO$	H	–275 Hz	—	Isolated as the tetramethyl-ammonium salt	41
$[C_{12}H_5CrO_6]^-$	97	$[Cr(COC_6H_5)(CO)_5]^-$	CH_2Cl_2	H	7.26	—	Isolated as the tetramethyl-ammonium salt	33
$C_{20}H_{10}CrO_5$	98	$Cr[C_3(C_6H_5)_2](CO)_5$	$CDCl_3$	H	8.32m 7.74m	— —	$C_3(C_6H_5)_2 =$ 	48
$C_{15}H_{17}CrNO_6$	99	$Cr(C_{10}H_{17}NO)(CO)_5$	C_6H_6	H H'	1.77 3.20	— —	$C_{10}H_{17}NO =$  (a carbene complex)	45

TABLE II—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{10}H_8CrN_2O_5$	100	$Cr(C_5H_8N_2)(CO)_5$	$(CD_3)_2CO$	H 7.24s H' 3.87s H 6.88 H' 3.87	— — — —	$C_5H_8N_2 =$ 	49 18
(2) DIHAPTO DERIVATIVES							
$C_{24}H_{17}CrO_4P$	101		$CDCl_3$	H 3.08 H' 3.64 H'' 5.63	$J_{HH'} 5.0^*$ $J_{H'H''} 9.0$ $J_{HH''} 13.5$	*Incorrect assignment (see below)	50
			C_6D_6	H 2.86dd H' 3.25dd H'' 5.06 hept.	$J_{HH'} 0$ $J_{H'H''} 9.0$ $J_{HH''} 13.0$	$J_{PH'} = J_{PH} = 5.0^\dagger$ $J_{PH''} \sim 2$ † Confirmed by ^{31}P decoupling	51
$C_{25}H_{19}CrO_4P$	102		$CDCl_3$	H 1.84 H' 4.58 H'' 5.56	$J_{HH'} 6.2$ $J_{H'H''} 10$	—	52
(3) TRIHAPTO DERIVATIVES							
$C_{17}H_{17}BCrN_8O_2$	103	$(h^3-C_3H_3)Cr[B(Pz)_4](CO)_2$	C_6D_6	H 4.3, 1.6	—	TMS external	53
						$B(Pz)_4 = B-$ 	

(4) TETRAHAPTO DERIVATIVES

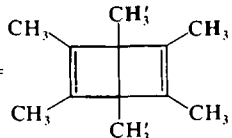
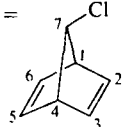
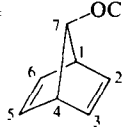
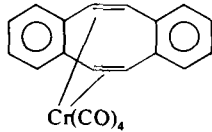
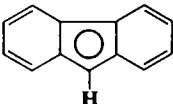
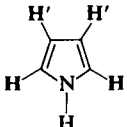
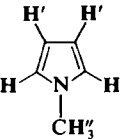
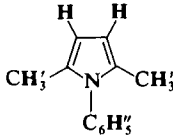
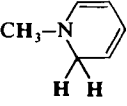
$C_{11}H_{12}CrO_3$	104	$(h^4-C_4(CH_3)_4)Cr(CO)_3$	—	H	1.85	—	$C_4(CH_3)_4$ = tetramethylcyclobutadiene	54
$C_8H_6CrO_4$	105	$(h^4-C_4H_6)Cr(CO)_4$	—	H	1.58s	—	C_4H_6 = 	55
$C_8H_4CrO_4$	106	$(h^4-C_4H_4)Cr(CO)_4$	—	H	3.88s	—	C_4H_4 = cyclobutadiene	55
$C_{12}H_6CrO_4$	107	$(h^4-C_8H_6)Cr(CO)_4$	—	H	4.35s, 6.92m (ratio 1:2)	—	C_8H_6 = benzocyclobutadiene	55
$C_{16}H_{18}CrO_4$	108	$[1,2,4,5-h^4-C_6(CH_3)_6]Cr(CO)_4$	$CDCl_3$	H H'	1.74s 0.90s	—	$C_6(CH_3)_6$ = 	56 57 1028
$C_{11}H_8CrO_4$	109	$(h^4-C_7H_8)Cr(CO)_4$	$CDCl_3$	H_{-1}, H_{-4} $H_{-2}, H_{-3},$ H_{-5}, H_{-6} H_{-7}	3.67 4.47 1.34	—	C_7H_8 = norbornadiene	58
$C_{11}H_7ClCrO_4$	110	$(h^4-C_7H_7Cl)Cr(CO)_4$	$CDCl_3$	H_{-1}, H_{-4} H_{-2}, H_{-3} H_{-5}, H_{-6} H_{-7}	3.77 4.22 4.37 3.62	—	C_7H_7Cl = 	58
$C_{18}H_{12}CrO_6$	111	$(h^4-C_{14}H_{12}O_2)Cr(CO)_4$	$CDCl_3$	H_{-1}, H_{-4} H_{-2}, H_{-3} H_{-5}, H_{-6} H_{-7}	3.97 4.30 4.42 4.49	—	$C_{14}H_{12}O_2$ = 	58

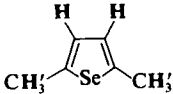
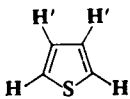
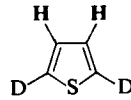
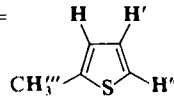
TABLE II—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{20}H_{12}CrO_4$	112	$(h^4-C_{16}H_{12})Cr(CO)_4$	—	H H'	5.30 7.12	— —	Structure: 	962
(5) PENTAHAPTO DERIVATIVES								
$C_{24}H_{20}CrNO_2P$	113	$(h^5-C_5H_5)Cr(NO)(PPh_3)(CO)$	$CDCl_3$ C_6D_6	H H	4.70d 4.39	J 1.3 J_{PH} 2.0	—	59 946
$C_7H_5CrNO_3$	114	$(h^5-C_5H_5)Cr(NO)(CO)_2$	$CDCl_3$ $(CD_3)_2CO$ $(CD_3)_2CO$	H H H	5.06s 5.23s 5.38 5.08	— — — —	— — T 35° T 32°	59 60 61 7
$C_9H_7CrNO_4$	115	$(h^5-C_5H_4COCH_3)Cr(NO)(CO)_2$	—	H	5.70, 5.15	—	T 32°	7
$C_{26}H_{20}AuCrO_3P$	116	$(h^5-C_5H_5)Cr[AuP(C_6H_5)_3](CO)_3$	$CDCl_3$	H	4.79	—	—	62
$C_{11}H_{14}CrGeO_3$	117	$(h^5-C_5H_5)Cr[Ge(CH_3)_3](CO)_3$	$CDCl_3$	H H'	4.75 0.69	— —	—	63 64
$C_{26}H_{20}CrGeO_3$	118	$(h^5-C_5H_5)Cr[Ge(C_6H_5)_3](CO)_3$	$CDCl_3$	H H'	4.90 7.49b	— —	60 and 100 MHz	65
$C_8H_6CrO_3$	119	$(h^5-C_5H_5)Cr(H')(CO)_3$	THF	H'	-5.46	—	—	67

			Hexane	H	4.78	—	—	66
				H'	-5.46	—	—	
			CF ₃ CO ₂ H	H	4.78	—	—	66
				H'	-5.46	—	—	67
C ₂₆ H ₂₀ CrO ₃ Pb	120	(<i>h</i> ⁵ -C ₅ H ₅)Cr[Pb(C ₆ H ₅) ₃](CO) ₃	THF	H	5.05	—	—	65
				H'	7.5m	—	—	
C ₈ H ₈ CrO ₃ Si	121	(<i>h</i> ⁵ -C ₅ H ₅)Cr(SiH ₃)(CO) ₃	Et ₂ O	H	4.89s	—	—	68
				H'	4.12s	—	—	
C ₁₁ H ₁₄ CrO ₃ Sn	122	(<i>h</i> ⁵ -C ₅ H ₅)Cr[Sn(CH ₃) ₃](CO) ₃	CDCl ₃	H	4.75	—	—	63
				H'	0.52	<i>J</i> (¹¹⁷ Sn-H') = 46.0 <i>J</i> (¹¹⁹ Sn-H') = 48.1	—	64
C ₂₆ H ₂₀ CrO ₃ Sn	123	(<i>h</i> ⁵ -C ₅ H ₅)Cr[Sn(C ₆ H ₅) ₃](CO) ₃	CDCl ₃	H	4.84	—	—	65
				H'	7.43m	—	—	
[C ₂₁ H ₁₅ CrO ₃] ⁻	124	{[<i>h</i> ⁵ -C ₅ H ₄ ·CH'(C ₆ H ₅) ₂]Cr(CO) ₃ } ⁻ (CD ₃) ₂ CO		H	4.73t	—	Isolated as the TI ⁺ salt	69
					4.45t	—		
				H'	5.30s	—		
				H''	7.49bs	—		
C ₂₁ H ₁₄ CrO ₃	125	[<i>h</i> ⁵ -C ₅ H ₄ (=C(C ₆ H ₅) ₂)]Cr(CO) ₃	(CD ₃) ₂ CO	H	5.72t, 4.77t	—	—	69
				H'	7.68 comp.	—		
					7.37 comp.	—		
C ₂₆ H ₁₉ CrO ₃ P	126	[<i>h</i> ⁵ -C ₅ H ₄ P(C ₆ H ₅) ₃]Cr(CO) ₃	CHCl ₃	H	4.92m, 4.65m	<i>J</i> ~ 2.5	—	66
				H'	~ 7.85	—		
[C ₂₆ H ₂₀ CrO ₃ P] ⁺	127	{[<i>h</i> ⁵ -C ₅ H ₄ P(C ₆ H ₅) ₃]Cr(H'')(CO) ₃ } ⁺ CF ₃ CO ₂ H		H	5.42, 5.20	<i>J</i> 2.5	—	66
				H'	~ 7.85			
				H''	-5.09			

TABLE II—cont.

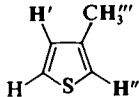
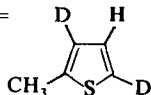
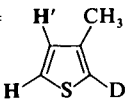
Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{16}H_9CrO_3$	128	$(h^5-C_{13}H_9)Cr(CO)_3$	—	H	4.1	—	$C_{13}H_9 =$ 	70
$C_7H_5CrNO_3$	129	$(h^5-C_4H_5N)Cr(CO)_3$	$(CD_3)_2CO$	H H'	6.40t 5.30t	— —	$C_4H_5N =$ 	71
$C_8H_7CrNO_3$	130	$(h^5-C_5H_7N)Cr(CO)_3$	$(CD_3)_2CO$	H H' H''	6.50t 5.12t* 3.48s	—	$C_5H_7N =$ 	71
$C_{15}H_{13}CrNO_3$	131	$(h^5-C_{12}H_{13}N)Cr(CO)_3$	$(CD_3)_2CO$	H H' H''	5.40 2.08s 7.65m	— — —	$C_{12}H_{13}N =$ 	71
$C_9H_9CrNO_3$	132	$(h^5-C_6H_9N)Cr(CO)_3^+$	C_6D_6	H	1.48	—	$C_6H_9N =$  Other signals at δ 5.46, 4.78, 3.12, 2.34 in the ratio 1:2:1:2	72

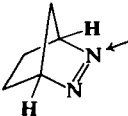
$C_7H_4CrO_3Se$	133	$(h^5-C_4H_4Se)Cr(CO)_3$	$CDCl_3$	H	5.9	—	C_4H_4Se = Selenophene	73
$C_9H_8CrO_3Se$	134	$(h^5-C_6H_8Se)Cr(CO)_3$	$CDCl_3$	H H'	5.4 2.31	—	C_6H_8Se = 	74
$C_7H_4CrO_3S$	135	$(h^5-C_4H_4S)Cr(CO)_3$	$CDCl_3$	H H'	5.37 5.61	J 2.8, 1.2, 0.9 J 2.8, 2.2, 1.2	C_4H_4S = 	74
			$(CD_3)_2CO$	H H'	5.93 5.93	— —		
$C_7H_2D_2CrO_3S$	136	$(h^5-C_4H_2D_2S)Cr(CO)_3$	$CDCl_3$	H	5.59	—	$C_4H_2D_2S$ = 	74
$C_8H_6CrO_3S$	137	$(h^5-C_5H_6S)Cr(CO)_3$	$CDCl_3$	H H' H'' H'''	5.36 5.53 5.22 2.28	— — — —	C_5H_6S = 	74
			$(CD_3)_2CO$	H H' H'' H'''	5.76 5.76 5.76 2.30	— — — —		

*The only appreciable change in the chemical shifts compared to the uncomplexed ligand is at the β -position (N -methylpyrrole $\delta \beta-H = 5.95$)

†A bonding interaction between the metal and the nitrogen lone pair of electrons is indicated, in addition to the interaction with the diene system

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References		
$C_8H_6CrO_3S$	138	$(h^5-C_5H_6S)Cr(CO)_3$	$CDCl_3$	H	5.40	—	$C_5H_6S =$ 	74		
				H'	5.56	—				
				H''	5.12	—				
				H'''	2.27	—				
			$(CD_3)_2CO$	H	5.92	—				
				H'	5.76	—				
$C_8H_4D_2CrO_3S$	139	$(h^5-C_5H_4D_2S)Cr(CO)_3$	$CDCl_3$	H	5.53	—	$C_5H_4D_2S =$ 	74		
$C_8H_5DCrO_3S$	140	$(h^5-C_5H_5DS)Cr(CO)_3$	$CDCl_3$	H	5.40	—	$C_5H_5DS =$ 	74		
					H'	5.56				
(6) HEXAHAPTO LIGANDS										
(a) Dicarbonyl derivatives										
$C_8H_7Cl_3CrO_2Si$	141	$(h^6-C_6H_6)Cr(SiCl_3)(H')(CO)_2$	CH_3CN	H	6.00	—	—	402		
				H'	−10.53	—	—	401		
$C_{27}H_{22}As_2CrO_2$	142	$[h^6-C_6H_5As(C_6H_5'')CH_2^tAs-(C_6H_5')_2]Cr(CO)_2$	$(CD_3)_2CO$	H	5.0s	—	A non-fluxional π -arene complex, the second arsenic atom being coordinated to the metal	709		
				H'	3.4	—		144		
				H''	7.4	—				

$C_{16}H_{26}CrN_2O_2$	143	$[h^6-1,3,5-C_6H_3(CH_3)_3](C_5H_8N_2)-Cr(CO)_2$	C_6D_6	H	4.67 4.27	—	$C_5H_8N_2 =$ 	710
$C_{15}H_{13}CrNO_6$	144	$[h^6-1,4-C_6H_4(CO_2CH_3)_2]Cr(NC-CH=CH_2)(CO)_2$	$(CD_3)_2CO$	H	5.4–6.0	—	σ -bonded acrylonitrile Compared to free and π -bonded acrylonitrile (δ 5.0–6.0 and 0.8–1.0 respectively)	75
$C_{38}H_{27}CrO_2P$	145	$(h^6-C_{18}H_{12})Cr(PPh_3)(CO)_2$	—	—	—	—	$C_{18}H_{12}$ = Triphenylene	76
$C_{38}H_{27}AsCrO_2$	146	$(h^6-C_{18}H_{12})Cr(AsPh_3)(CO)_2$	—	—	—	—	$C_{18}H_{12}$ = Triphenylene	76
$C_{29}H_{19}CrO_2N$	147	$(h^6-C_{18}H_{12})Cr(quinoline)(CO)_2$	—	—	—	—	$C_{18}H_{12}$ = Triphenylene	76
$C_{26}H_{17}CrO_2N$	148	$(h^6-C_{18}H_{12})Cr(pyridine)(CO)_2$	—	—	—	—	$C_{18}H_{12}$ = Triphenylene	76
<i>(b) Tricarbonyl derivatives</i>								
$C_9H_6CrO_3$	149	$(h^6-C_6H_6)Cr(CO)_3$	$CDCl_3$	H	5.37	—	—	711
			$CDCl_3$	H	5.303*	—	T 30° 100 MHz $J(^{13}C-H) = 173 \pm 1^\dagger$	712
			CCl_4	H	5.23	—	—	16
			$(CH_3)_2CO$	H	5.63	—		
			CH_2Cl_2	^{13}CH	93.7	—		
				^{13}CO	2 23.8	—		32

*The upfield shift relative to benzene (δ 7.347) is attributed to the magnetic anisotropy of the chromium tricarbonyl moiety and the ring-metal bond. Reduction of the π -electron density in the complex, which would produce a downfield shift of ~ -2 ppm, is compensated for by reduction in the ring current, thus producing an upfield shift of 1.7 to 2.7 ppm.

† Increase in J_{CH} relative to benzene (J_{CH} 159.2) is attributed to the effect of withdrawal of π -electrons from the ring in the complex (~ 0.35 electron from each carbon p_z orbital).

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{10}H_8CrO_3$	150	$(h^6-C_6H_3 \cdot CH_3)Cr(CO)_3$	CCl_4	H_{ortho}	5.08	—	—	16
				H_{meta}	5.32	—		
				H_{para}	5.08	—		
			$(CH_3)_2CO$	H_{ortho}	5.49	—		
				H_{meta}	5.69	—		
				H_{para}	5.49	—		
			CCl_4	H'	2.18	—	—	713
			$CDCl_3$	H_{ortho}	5.140*	—	T 30° 100 MHz	712
				H_{meta}	5.386*	—	J_{ortho} 6.2, 6.4; J_{meta} 1.0; J_{para} 0.0	
				H_{para}	5.102*	—		
				H'	2.183*	—	*To higher field than corresponding values for the uncomplexed arene	
$C_{11}H_{10}CrO_3$	151	$[h^6-1,2-C_6H_4(CH_3)_2]Cr(CO)_3$	$CDCl_3$	H_{-3}, H_{-6}	5.212*	$J_{3,4}$ 6.2	T 30° 100 MHz	712
				H_{-4}, H_{-5}	5.272*	$J_{4,5}$ 6.4	*To higher field than corresponding values for the uncomplexed arene	1009
				H'	2.163*	—		
$C_{11}H_{10}CrO_3$	152	$[h^6-1,3-C_6H_4(CH_3)_2]Cr(CO)_3$	$CDCl_3$	H_{-2}	5.013	$J_{2,4}$ 1.2	T 30° 100 MHz	712
				H_{-4}, H_{-6}	4.983	$J_{4,5}$ 6.0	δ values, particularly for the aromatic protons, are greater for the uncomplexed arene	1009
				H_{-5}	5.431	$J_{2,5}$ 0.5		
				H'	2.193	—		
$C_{11}H_{10}CrO_3$	153	$[h^6-1,4-C_6H_4(CH_3)_2]Cr(CO)_3$	$CDCl_3$	H	5.231	$J_{2,3}$ 6.1	T 30° 100 MHz	712
						$J_{2,6}$ 1.0	Ring J_{CH} 172. Methyl J_{CH}	
				H'	2.123	—	127.5 δ and J_{HH} greater, J_{CH} less, for the uncomplexed arene	

$C_{12}H_{12}CrO_3$	154	$[h^6-1,2,3-C_6H_3(CH_3)_3]Cr(CO)_3$	$CDCl_3$	H	5.26	—	T 33°	147
				H'	2.19	—	Free ligand δ 6.94 and 2.25	
			CCl_4	H	5.16	—	—	16
				H'	2.14	—		
			$(CH_3)_2CO$	H	5.56	—		
			$CDCl_3$	H₋₄, H₋₆	5.115	$J_{4,5}$ 6.2	T 30° 100 MHz	712
$C_{12}H_{12}CrO_3$	155	$[h^6-1,2,4-C_6H_3(CH_3)_3]Cr(CO)_3$	$CDCl_3$	H₋₅	5.256	—	Aromatic and, to a lesser extent, the methyl signals are to higher field than corresponding signal for free arene. Partial three-point bonding of the $M(CO)_3$ moiety to the ring has been postulated to occur most strongly at the positions bearing methyl groups. Degree of upfield shift is $Cr > W > Mo$	1009
				H'₋₁, H'₋₃	2.219	—		
				H'₋₂	2.131	—		
				H₋₃	5.136	$J_{3,5}$ 0.5	T 30° 100 MHz	712
				H₋₅	5.069	$J_{3,6}$ 6.2	δ and J values are greater for the uncomplexed arene	1009
				H₋₆	5.358	—		
$C_{12}H_{12}CrO_3$	156	$[h^5-1,3,5-C_6H_3(CH_3)_3]Cr(CO)_3$	CH_2Cl_2	H'₋₁	2.214	—		
				H'₋₂	2.214	—		
				H'₋₄	2.274	—		
				$^{13}CH_3$	21.0	—	22.62 MHz	148
				^{13}CH	92.4	—		1009
				$^{13}C-CH_3$	111.5	—		
$C_{12}H_{12}CrO_3$			$CDCl_3$	^{13}CO	235.5	—		
				H	4.884	—	T 30° 100 MHz	712
				H'	2.194	—	Ring $J_{^{13}CH}$ 172. Methyl $J_{^{13}CH}$ 129 Corresponding δ values greater and $J_{^{13}CH}$ are less for the uncomplexed arene	

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{13}H_{14}CrO_3$	157	$[h^6-1,2,3,5-C_6H_2(CH_3)_4]Cr(CO)_3$	$CDCl_3$	H	4.987	—	T 30° 100 MHz	712
				H'_{-1}	2.229	—	All signals to higher field than corresponding signal for free arene, the shift being greatest for the aromatic protons	
				H'_{-3}	2.070	—		
				H'_{-2}	2.117	—		
$C_{13}H_{14}CrO_3$	158	$[h^6-1,2,4,5-C_6H_2(CH_3)_4]Cr(CO)_3$	CH_2Cl_2	$^{13}CH_3$	18.6	—	22.62 MHz	148
				^{13}CH	99.0	—		
				$^{13}C-CH_3$	107.6	—		
				^{13}CO	235.5	—		
			$CDCl_3$	H	5.254	—	T 30° 100 MHz	712
				H'	2.110	—	δ greater for the free arene	
$C_{14}H_{16}CrO_3$	159	$[h^6-1,2,3,4,5-C_6H(CH_3)_5]Cr(CO)_3$	$CDCl_3$	H	5.116	—	T 30° 100 MHz	712 1009
				H'_{-1}, H'_{-5}	2.174	—	δ compared to δ free arene	
				H'_2, H'_{-4}	2.140	—		
				H'_{-3}	2.249	—		
$C_{15}H_{18}CrO_3$	160	$[h^6-C_6(CH_3)_6]Cr(CO)_3$	$CDCl_3$	H	2.220	—	T 30° 100 MHz	712 1028
$C_{11}H_{10}CrO_3$	161	$[h^6-C_6H_5(CH_2CH'_3)]Cr(CO)_3$	$CDCl_3$	H	5.28m	—	—	714
				H'	2.34q	J 7		
				H''	1.22t	J 7		
			CCl_4	H	5.17m	—	—	143
				H'	2.42q	—		
				H''	1.22t	—		

C ₁₂ H ₁₂ CrO ₃	162	[h ⁶ -C ₆ H ₅ CH(CH ₃) ₂]Cr(CO) ₃	CCl ₄	H	5.12s	—	—	715
				H'	1.21d	—		
			CCl ₄	H	5.18s*	—	T 30° *Multiplet at T -15°	716
C ₁₅ H ₁₈ CrO ₃	163	[h ⁶ -1,4-C ₆ H ₄ (CH(CH ₃) ₂) ₂]Cr(CO) ₃	CCl ₄	H	5.10m	—	—	715
				H'	1.20d	J 6.5		
C ₁₃ H ₁₄ CrO ₃	164	[h ⁶ -C ₆ H ₅ C(CF ₃) ₃]Cr(CO) ₃	CCl ₄	H	5.23m	—	—	143
				H'	1.32s	—		
			CCl ₄	H	5.45d, 5.24t, 5.12t	J 6.5	T +50° to -15°	716
C ₁₇ H ₂₂ CrO ₃	165	{h ⁶ -1,3-C ₆ H ₄ [C(CH ₃) ₃] ₂ }Cr(CO) ₃	—	H ₋₂	5.63s	—	—	963
				H ₋₄	5.15d	—		
				H ₋₅	5.01t	—		
				H ₋₆	5.51d	—		
				H'	1.37s	—		
C ₁₇ H ₂₂ CrO ₃	166	{h ⁶ -1,4-C ₆ H ₄ [C(CH ₃) ₃] ₂ }Cr(CO) ₃	CCl ₄	H	5.23s	—	—	717
				H'	1.30s	—		715
			(CD ₃) ₂ CO	n.a.		—	T +30° to -55°	963
The aromatic protons remain as sharp singlets over the temperature range shown. The variable temperature NMR spectra of other tricarbonyl (arene) chromium compounds are therefore explained in terms of varying conformer populations arising from thermodynamic rather than kinetic restriction of rotation								718

TABLE II—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{21}H_{30}CrO_3$	167	$\{h^6\text{-}1,3,5\text{-}C_6H_3[C(CH_3)_3]_3\}\text{-}Cr(CO)_3$	—	H	5.72s	—	—	963
				H'	1.32s	—		
$C_{11}H_7CrDO_3$	168	$(h^6\text{-}C_6H_5CD=CH_2)Cr(CO)_3$	$CDCl_3$	H	5.41m	—	—	719
				H'	5.67, 5.41	—		
$C_{11}H_8CrO_3$	169	$(h^6\text{-}C_6H_5CH'=CH_2)Cr(CO)_3$	$CDCl_3$	H, H''	5.77s, 5.40m	—	The aromatic protons of the complex are shifted ~ 1.9 ppm upfield relative to styrene and H' by ~ 0.4 ppm	714
				H'	6.32q			
$C_{17}H_{12}CrO_3$	170	$(h^6\text{-}C_6H_5'CH=CH'C_6H_5'')Cr(CO)_3$ — <i>cis</i>	—	H	$\sim 6.1d$	$J_{HH'}13$	Aromatic protons of complexed ring (C_6H_5') and α -olefinic proton (H) shifted to high field with respect to the free ligand [δ 7.21 (aromatic H) and 6.59 (olefinic H)]	720
				H'	$\sim 6.7d$	—		
				H''	5.23s	—		
				H'''	7.28s	—		
$C_{17}H_{12}CrO_3$	171	$(h^6\text{-}C_6H_5'CH=CH'C_6H_5'')Cr(CO)_3$ — <i>trans</i>	—	H	6.64d	$J_{HH'}15$	High field shift of H'' and H relative to free ligand (δ 7.37 and 7.02 respectively) is attributed to a diminution of the ring current effect on complexation	720
				H'	7.00d	—		
				H''	$\sim 5.45m$	—		
				H'''	~ 7.35	—		
$C_{17}H_{10}CrO_3$	172	$(h^6\text{-}p\text{-}C_6H_4ClCH=CHC_6H_4Cl)\text{-}Cr(CO)_3$ <i>trans</i>	—	H	5.56s	—	—	720
				H'	7.33, 7.24	—		

$C_{23}H_{16}CrO_3$	173	$\{h^6-C_6H_5[CH=C(C_6H_5)_2]Cr(CO)_3$	—	H	6.48s	—	—	720
				H'	5.35, 5.14	—	—	
					5.10	—	—	
				H''	7.30	—	—	
$C_{13}H_{12}CrO_3$	174	$\{h^6-C_6H_5[CH'(CH_3)CH''=CH_2^I]Cr(CO)_3$	CCl_4	H	5.10	—	—	721
				H''	3.10 comp.	—	—	
				H''	1.32d	J 6.7	—	
				H'''	5.80–4.70	—	—	
				H^{IV}	comp.	—	—	
$C_{14}H_{14}CrO_3$	175	$\{h^6-C_6H_5[CH'(CH_3)CH''=CH^{IV}CH_3^V]Cr(CO)_3$	CCl_4	H	5.13s	—	—	721
				H'	3.12–2.78	—	—	
					comp.	—	—	
				H''	1.31d	J 6.9	—	
				H'''	5.54–5.27	—	—	
				H^{IV}	comp. m.	—	—	
				H^V	1.71d	J 3.4	—	
$C_{13}H_{12}CrO_5$	176	$\{h^6-C_6H_5[CH(CH_3)CH_2CO_2H]Cr(CO)_3$	$CDCl_3$	H	1.34	—	—	749
$C_{13}H_{14}CrO_4$	177	$\{h^6-C_6H_5[CH'(CH_3)CH''(CH_3^{IV})OH]Cr(CO)_3$	$CDCl_3$	H	5.40bs	—	} <i>Erythro</i> -DL-isomer T 30–35°	721
				H'	2.62 oct.	$J_{H'H''}$ 3.7		
				H''	1.28d	$J_{H'H''}$ 6.4		
				H'''	4.03 oct.	$J_{H'''H^{IV}}$ 7		
				H^{IV}	1.32d	—		
				H	5.40s	—	} <i>Threo</i> -DL-isomer	
				H'	2.53 quint.	$J_{H'H''}$ 6.3		
				H''	1.37d	$J_{H'H''}$ 6.9		
				H'''	3.84 quint.	$J_{H'''H^{IV}}$ 6.2, 6.0		
				H^{IV}	1.31d	—		

TABLE II—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{15}H_{16}CrO_5$	178	$\{h^6-C_6H_5[CH'(CH_3'')CH'''(CH_3^{IV})-OCOCH_3^V]\}Cr(CO)_3$		H	5.39	—	Erythro-DL-isomer	721
				H'	2.77 oct.	$J_{H'H''} 4.1, 4.3$		
				H''	1.36d	$J_{H'H''} 7.0$		
				H'''	5.09 oct.	$J_{H'''H^{IV}} 6.4, 6.3$		
				H ^{IV}	1.27d	—		
				H ^V	2.12s	—		
				H	5.36s	—	Threo-DL-isomer	
				H'	2.71 quint.	$J_{H'H''} 6.8, 6.4$		
				H''	1.35d	$J_{H'H''} 7.3$		
				H'''	4.97 quint.	$J_{H'''H^{IV}} 6.4, 6.1$		
$C_{16}H_{18}CrO_5$	179	$\{h^6-C_6H_5[CH'(CH_3'')CH'''(CH_2^{IV}-CH_3^V)OCOCH_3^{VI}]\}Cr(CO)_3$	$CDCl_3$	H	5.33s	—	Erythro-DL-isomer	721
				H'	2.96–2.54	—		
					comp. m.	—		
				H''	1.38d	$J 7.3$		
				H'''	5.3–4.7	—		
					comp. m.	—		
				H ^{IV}	1.85–1.4	—		
					comp. m.	—		
				H ^V	1.00t	$J 7.0$		
				H ^{VI}	2.11s	—		
$C_{14}H_{16}CrO_6S$	180	$\{h^6-C_6H_5[C(CH_3)_2CH_2^?OSO_2-CH_3^?]\}Cr(CO)_3$	$CDCl_3$	H	5.68–5.10m	—	—	722
				H'	1.41s	—		
				H''	4.12s	—		
				H'''	2.99s	—		

C ₁₄ H ₁₆ CrO ₆ S	181	{h ⁶ -C ₆ H ₅ {CH'(CH ₃ ')CH'''(CH ₃ ^{IV})-OSO ₂ CH ₃ } }Cr(CO) ₃		H	5.35s	—	} <i>Erythro</i> -DL-isomer	721
				H'	2.80 oct.	J _{H'H'''} 3.8		
				H''	1.38d	J _{H'H''} 7.2		
				H'''	4.86 oct.	J _{H'''H^{IV}} 6.7		
				H ^{IV}	1.41d	—		
				H ^V	2.89s	—		
				H	5.33s	—	} <i>Threo</i> -DL-isomer	
				H'	2.73	J _{H'H'''} 6.6, 6.4		
				H''	1.35d	J _{H'H''} 6.9		
				H'''	4.74	J _{H'''H^{IV}} 6.4, 6.3		
H ^{IV}	1.43	—						
H ^V	2.91s	—						
C ₁₅ H ₁₈ CrO ₆ S	182	{h ⁶ -C ₆ H ₅ {CH'(CH ₃ ')CH'''(CH ₂ -CH ₃ ^V)OSO ₂ CH ₃ ^{VI} } }Cr(CO) ₃		H	5.38s	—	<i>Erythro</i> -DL-isomer	721
				H'	3.15–2.70b comp.	J _{H'H'''} 6.8		
				H''	1.41d	J _{H'H''} 7.1		
				H'''	4.73 sext.	J _{H'''H^{VI}} 1.5, 3.3		
				H ^{IV}	1.78 oct.	J _{H^{IV}H^V} 7.5, 6.7		
				H ^V	1.14t	—		
				H ^{VI}	2.98s	—		
C ₁₅ H ₁₈ CrO ₆ S	183	[h ⁶ -1,3-C ₆ H ₄ (CH ₃ ')(C(CH ₃ ') ₂ -CH ₂ ^{''} OSO ₂ CH ₃ ^{IV})]Cr(CO) ₃	CDCl ₃	H	5.34s	—	—	722
				H'	2.26s	—		
				H''	1.48s	—		
				H'''	4.13	—		
				H ^{IV}	3.02s	—		
C ₁₅ H ₁₈ CrO ₆ S	184	[(h ⁶ -1,4-C ₆ H ₄ (CH ₃ ')(C(CH ₃ ') ₂ -CH ₂ ^{''} OSO ₂ CH ₃ ^{IV})]Cr(CO) ₃	CDCl ₃	H	~5.74d, 5.25d	J 7	—	722
				H'	2.36s	—		
				H''	1.49s	—		
				H'''	4.22s	—		
				H ^{IV}	3.12s	—		

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_9H_5BrCrO_3$	185	$(h^6-C_6H_5Br)Cr(CO)_3$	$CDCl_3$	H 5.23	—	—	73
$C_{10}H_7BrCrO_3$	186	$[h^6-C_6H_4-1(Br)-4(CH_3)]Cr(CO)_3$	$CDCl_3$	H_{-2} 5.60 H_{-3} 5.20 H' 2.09	— — —	T 33° ($J + J' = 6.7, J_A + J_B = 3.6$) Free ligand δ 7.28, 6.95 and 2.24 respectively	147
$C_{10}H_7ClCrO_3$	187	$[h^6-C_6H_4-1(Cl)-4(CH_3)]Cr(CO)_3$	$CDCl_3$	H_{-2} 5.57 H_{-3} 5.28 H' 2.09	— — —	T 33° ($J + J' = 6.8, J_A + J_B = 3.6$) Free ligand δ 7.13, 7.0 and 2.26 respectively	147
$C_{10}H_7CrFO_3$	188	$[h^6-C_6H_4-1(F)-4(CH_3)]Cr(CO)_3$	$CDCl_3$	H 5.38 H' 2.06	— —	T 33° ($J + J' = 6.8, J_A + J_B = 3.9$) Free ligand δ 6.77, 7.1, 2.28	147
$C_9H_5CrIO_3$	189	$(h^6-C_6H_5I)Cr(CO)_3$	$CDCl_3$	H 5.58, 5.21	—	—	73
$C_{10}H_9CrO_4$	190	$[h^6-C_6H_4-1(OH)-4(CH_3)]Cr(CO)_3$	$CDCl_3$	H_{-2} 5.20 H_{-3} 5.53 H' 2.06	— — —	T 33° ($J + J' = 7.0, J_A + J_B = 4.3$) Free ligand δ 6.63, 6.87 and 2.19 respectively	147
$C_{10}H_9CrNO_3$	191	$[h^6-1,2-C_6H_4(NH_2)CH_3]Cr(CO)_3$	$CDCl_3$	H 5.48, 4.96 H' 3.59 H'' 2.11	— — —	—	723
$C_{10}H_9CrNO_3$	192	$[h^6-1,3-C_6H_4(NH_2)CH_3]Cr(CO)_3$	$CDCl_3$	H 5.59 4.80 H' 3.58 H'' 2.26	— — — —	—	723

C ₁₀ H ₉ CrNO ₃	193	[h ⁶ -C ₆ H ₄ -1(NH ₂) ² -4(CH ₃) ²]Cr(CO) ₃	CDCl ₃	H ₋₂	4.87	—	T 33° (<i>J</i> + <i>J'</i> = 7.0, <i>J</i> _A + <i>J</i> _B = 4.1) Free ligand δ 6.38, 6.83, 2.18 and 3.29 respectively	147
				H ₋₃	5.48	—		
				H'	2.04	—		
				H''	3.43	—		
C ₁₁ H ₁₁ CrNO ₃	194	[h ⁶ -C ₆ H ₅ ·N(CH ₃) ₂]Cr(CO) ₃	CCl ₄	H _{ortho}	4.72	—	—	16
				H _{meta}	5.46	—		
				H _{para}	4.66	—		
			(CH ₃) ₂ CO	H _{ortho}	5.03	—		
				H _{meta}	5.78	—		
				H _{para}	5.10	—		
C ₁₂ H ₁₃ CrNO ₃	195	{h ⁶ -C ₆ H ₄ -1[N(CH ₃) ₂]-4(CH ₃) ² }-Cr(CO) ₃	CCl ₄	H ₋₂	4.75	—	Free ligand: CCl ₄ : H ₋₂ 6.54; H ₋₃ 6.9, H' 2.21	16
				H ₋₃	5.37	—		
				H'	2.09	—		
			Acetone	H ₋₂	5.09	—	Acetone: H ₋₂ 6.68; H ₋₃ 7.01	
				H ₋₃	5.72	—		
			CDCl ₃	H ₋₂	4.83	—	T 33° Free ligand δ 6.53, 6.91, 2.21 and 2.78 respectively	147
				H ₋₃	5.50	—		
				H'	2.06	—		
				H''	2.82	—		
C ₁₂ H ₁₃ CrNO ₃	196	{h ⁶ -1,2-C ₆ H ₄ (NH ₂)CH''(CH ₃ '') ₂ }-Cr(CO) ₃	CDCl ₃	H	5.6, 4.85	—	—	724
				H'	3.67	—		
				H''	2.72	—		
				H'''	1.30t	<i>J</i> 6.4		
C ₁₄ H ₁₇ CrNO ₃	197	{h ⁶ -1,2-C ₆ H ₄ [N(CH ₃) ₂]-[CH''(CH ₃ '') ₂]}Cr(CO) ₃	—	H	5.7-4.9	—	—	724
				H'	2.70	—		
				H''	3.20	—		
				H'''	1.26t	<i>J</i> _{H''H'''} 6.6		

TABLE II—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)		Remarks	References
$C_{10}H_8CrO_4$	198	$(h^6-C_6H_5, OCH_3)Cr(CO)_3$	CCl_4	H_{ortho}	5.06	—	—		16
				H_{meta}	5.41	—			
				H_{para}	4.80	—			
			$(CH_3)_2CO$	H_{ortho}	5.45	—			
				H_{meta}	5.85	—			
				H_{para}	5.14				
			$CDCl_3$	H_{ortho}	5.14	$J_{2,3} = J_{5,6} = 7.2$	—		
				H_{meta}	5.58	$J_{3,4} = J_{4,5} = 5.7$			
				H_{para}	4.90	$J_{2,4} = J_{4,6} = 1.0$			
$C_{11}H_{10}CrO_4$	199	$[h^6-1,2-C_6H_4(OCH_3)CH_3]Cr(CO)_3$	$CDCl_3$	H	5.68, 5.57,	—	—	723	
					5.46	—			
					5.08, 5.98	—			
					4.83, 4.73	—			
				H'	3.70	—			
				H''	2.27	—			
				$C_{11}H_{10}CrO_4$	200	$[h^6-1,3-C_6H_4(OCH_3)CH_3]Cr(CO)_3$	$CDCl_3$		H
H'	3.76	—							
H''	2.18	—							
$C_{11}H_{10}CrO_4$	201	$[h^6-C_6H_4-1(OCH_3)-4(CH_3)]-Cr(CO)_3$	CCl_4	H_{-2}	5.30	—	—	16	
				H_{-3}	5.08	—			
				H'	2.09	—			
			$(CH_3)_2CO$	H_{-2}	5.74	—			
				H_{-3}	5.47	—			

			CDCl ₃	H ₋₂	5.18	—	T 33°	147
				H ₋₃	5.45	—	Free ligand δ 6.67, 6.96, 2.23	
				H'	2.06	—	and 3.65 respectively	
				H''	3.67	—		
C ₁₃ H ₁₄ CrO ₄	202	[h ⁶ -C ₆ H ₄ -1(OCH ₃) ₂ -2[CH''-(CH ₃ '') ₂]]Cr(CO) ₃	CDCl ₃	H	5.7-4.8	—	—	724
				H'	3.77s	—		
				H''	3.18	—		
				H'''	1.30—1.18	J _{H''H'''} 6.7		
C ₁₃ H ₁₄ CrO ₃	203	{h ⁶ -C ₆ H ₄ -1(OCH ₃) ₂ -4[CH''-(CH ₃ '') ₂]]Cr(CO) ₃	CDCl ₃	H ₋₂ , H ₋₆	5.11	J _{2,3} 7.3	T -46°	725
				H ₋₃ , H ₋₅	5.59	—		
				H'	3.77	—		
				H''	2.54	—		
				H'''	1.27	J = 6.7		
				H ₋₂ , H ₋₆	5.11	—	T 52°	
				H ₋₃ , H ₋₅	5.52	—		
				H'	3.73	—		
				H''	2.54	—		
				H'''	1.23	—		
C ₁₄ H ₁₆ CrO ₃	204	{h ⁶ -C ₆ H ₄ -1(OCH ₃) ₂ -4[C(CH ₃ '') ₃]]Cr(CO) ₃	CDCl ₃	H ₋₂ , H ₋₆	5.08	J _{2,3} 7.1	T -46°	725
				H ₋₃ , H ₋₅	5.76	—		
				H'	3.78	—		
				H''	1.29	—		
				H ₋₂ , H ₋₆	5.04	J _{2,3} 7.2	T 52°	
				H ₋₃ , H ₋₅	5.68	—		
				H'	3.73	—		
				H''	1.28	—		
C ₁₅ H ₁₈ CrO ₇ S	205	[h ⁶ -1,4-C ₆ H ₄ (OCH ₃) ₂ (C(CH ₃ '') ₂ -CH ₂ '')OSO ₂ CH ₃ ^{IV})]Cr(CO) ₃	CDCl ₃	H	5.67d, 5.06d	J 7.5	—	722
				H'	3.75s	—		
				H''	1.36s	—		
				H'''	4.08s	—		
				H ^{IV}	3.01s	—		

TABLE II—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{11}H_{10}CrO_5$	206	$[h^6-1,2-C_6H_4(OCH_3)_2]Cr(CO)_3$	$CDCl_3$	H_{-3}, H_{-6} 5.36 H_{-4}, H_{-5} 5.13 H' 3.81	$J_{3,4} = J_{5,6} = 6.9$ — $J_{4,5}$ 5.3 —		711
$C_{11}H_{10}CrO_5$	207	$[h^6-1,3-C_6H_4(OCH_3)_2]Cr(CO)_3$	$CDCl_3$	H_{-2} 5.22 H_{-4}, H_{-6} 4.88 H_{-5} 5.62	$J_{2,4}$ 1.8 —		711
$C_{11}H_{10}CrO_5$	208	$[h^6-1,4-C_6H_4(OCH_3)_2]Cr(CO)_3$	$CDCl_3$	H 5.32 H' 3.67	— —		711
$C_{19}H_{26}CrO_5$	209	$[h^6-C_6H_2-1,4(tBu)_2-2,5(OCH_3)_2]-Cr(CO)_3$	$(CD_3)_2CO$ CCl_2F_2	n.a.	—	T + 30° to -55° T + 30° to -75°	718
$C_{12}H_{12}CrO_2$	210	$[h^6-1,2,3-C_6H_3(OCH_3)_3]Cr(CO)_3$	$CDCl_3$	H_{-4}, H_{-6} 4.85 H_{-5} 5.50	$J_{4,5} = J_{5,6}$ 7.0 —		711
$C_{12}H_{12}CrO_6$	211	$[h^6-1,2,4-C_6H_3(OCH_3)_3]Cr(CO)_3$	$CDCl_3$	H_{-3} 5.32 H_{-5} 4.75 H_{-6} 5.55	$J_{3,5}$ 2.4 — $J_{5,6}$ 7.2		711
$C_{12}H_{12}CrO_6$	212	$[h^6-1,3,5-C_6H_3(OCH_3)_3]Cr(CO)_3$	$CDCl_3$	H 5.00 H' 3.81	— —		711
$C_{10}H_8CrO_3S$	213	$(h^6-C_6H_5 \cdot SCH_3)Cr(CO)_3$	CCl_4 $(CH_3)_2CO$	H 5.25 H 4.37	— —		16
$C_{11}H_{10}CrO_3S$	214	$(h^6-C_6H_4-1(SCH_3)-4(CH_3))-Cr(CO)_3$	CCl_4	H_{-2} 5.13 H_{-3} 5.36 H' 2.16	— — —		16

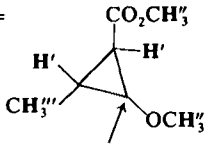
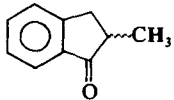
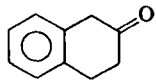
			(CH ₃) ₂ CO	H ₋₂	5.61	—		
				H ₋₃	5.79	—		
			CDCl ₃	H ₋₂	5.45	—	T 33°	147
				H ₋₃	5.26	—	Free ligand δ 7.07, 7.0, 2.25	
				H'	2.13	—	and 2.33 respectively	
				H''	2.42	—		
C ₁₆ H ₁₆ CrO ₅	215	[h ⁶ -C ₆ H ₅ (C ₇ H ₁₁ O ₃)]Cr(CO) ₃	C ₆ D ₆	H	5.28m, 4.52m	—	C ₇ H ₁₁ O ₃ =	726
				H'	1.90m	—		
				H''	3.27s, 3.33s	—		
				H'''	1.16d	J 5.5		
C ₂₀ H ₁₆ FeCrO ₃	216	[h ⁶ -C ₆ H ₅ (CH ₂ Fc)]Cr(CO) ₃	CCl ₄	H	5.15m	—	Hexamethyldisiloxane as reference	727
				H'	3.49s	—	Fc = Ferrocene moiety	
				H*	4.12m	—	*Ferrocenyl protons	
C ₁₉ H ₁₄ FeCrO ₃	217	[h ⁶ -C ₆ H ₅ (Fc)]Cr(CO) ₃	CCl ₄	H	5.33m	—	Hexamethyldisiloxane as reference	727
				H*	4.44t, 4.27t	—	Fc = Ferrocene moiety	
				H†	4.04s	—	*Substituted cyclopentadienyl ring †Unsubstituted cyclopentadienyl ring	
C ₁₅ H ₁₀ CrO ₃	218	[h ⁶ -C ₆ H ₅ (C ₆ H ₅)]Cr(CO) ₃	CDCl ₃	H	5.48m	—	—	728
				H'	7.42m	—		
C ₁₆ H ₁₂ CrO ₃	219	[h ⁶ -C ₆ H ₄ -1(CH ₃)-4(C ₆ H ₅)]Cr(CO) ₃	CDCl ₃	H	5.47m	—	—	728
				H'	2.38s, 2.20s	—		
				H''	7.33m	—		
C ₁₇ H ₁₄ CrO ₃	220	[h ⁶ -C ₆ H ₄ -1(CH ₃)-4(4-C ₆ H ₄ -CH ₃)]Cr(CO) ₃	CDCl	H	5.73, 5.27	—	—	728
				H'	7.37, 7.15	—		
				H''	2.37, 2.18	—		

TABLE II—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{15}H_9CrFO_3$	221	$[h^6-C_6H_5(m-C_6H_4F)]Cr(CO)_3$	C_6H_6	F	-0.66	—	Relative to C_6H_5F	729
			DMSO	F	-0.50	—	Free ligand: C_6H_6 : +0.05	
			Acetone	F	-0.72	—	DMSO -0.25	
$C_{15}H_9CrFO_3$	222	$[h^6-C_6H_5(p-C_6H_4F)]Cr(CO)_3$	C_6H_6	F	-0.55	—	Relative to C_6H_5F	729
			DMSO	F	-0.44	—	Free ligand: C_6H_6 : +2.97 DMSO: +2.50	
$C_{15}H_9FCrO_3$	223	$[h^6-C_6H_4-1(F)-4(C_6H_5)]Cr(CO)_3$	$CDCl_3$	H	5.78m	—	—	728
				H'	7.27m	—		
$C_{15}H_8F_2CrO_3$	224	$[h^6-C_6H_4-1(F)-2(2-C_6H_4F)]Cr(CO)_3$	$CDCl_3$	H	5.53, 4.82m	—	—	728
				H'	7.32m	—		
$C_{15}H_8F_2CrO_3$	225	$[h^6-C_6H_4-1(F)-4(4-C_6H_4F)]Cr(CO)_3$	$CDCl_3$	H	5.60	—	—	728
				H'	7.23	—		
$C_{14}H_{16}CrO_5$	226	$\{h^6-C_6H_5[CH'(OCH_2CH_3'')]_2\}Cr(CO)_3$	$CDCl_3$	H, H'	5.43m	—	—	714
				H''	3.65q	J 7		
				H'''	1.23t	J 7		
$C_{15}H_{18}CrO_5$	227	$\{h^6-1,4-C_6H_4(CH_3)[CH(OCH_2CH_3'')CH_3''']_2\}Cr(CO)_3$	$CDCl_3$	H	5.67, 5.18	—	T 33°	147
				H'	2.17	—		
				H''	3.65	—		
				H'''	1.23	—		
$C_{10}H_6CrO_4$	228	$(h^6-C_6H_5CH'=O)Cr(CO)_3$	$CDCl_3$	H	2.83m	—	—	714
				H'	4.75	—		

$C_{11}H_8CrO_4$	229	$[h^6-C_6H_4-1(CH''O)-4(CH_3)]-$ $Cr(CO)_3$	$CDCl_3$	H_{-2}	6.01	—	T 33° ($J + J' = 6.8$, $J_A + J_B = 3.2$) Free ligand δ 7.69, 7.26, 2.38 and 9.89 respectively	147
				H_{-3}	5.21	—		
				H'	2.33	—		
				H''	9.46	—		
$C_{11}H_8CrO_4$	230	$(h^6-C_6H_5COCH_3)Cr(CO)_3$	CCl_4	H_{ortho}	5.91	—	—	16 730
				H_{meta}	5.19	—		
				H_{para}	5.41	—		
			$(CH_3)_2CO$	H_{ortho}	6.35	—		
				H_{meta}	5.68	—		
				H_{para}	6.01	—		
$C_{12}H_{10}CrO_4$	231	$[h^6-C_6H_4-1(COCH_3)-2(CH_3)]-$ $Cr(CO)_3$	$CDCl_3$	H	~5.4 comp.	—	—	731
				H'	2.39, 2.45	—		
$C_{12}H_{10}CrO_4$	232	$[h^6-C_6H_4-1(COCH_3)-3(CH_3)]-$ $Cr(CO)_3$	$CDCl_3$	H	~5.5 comp.	—	—	731
				H'	2.28s, 2.41s	—		
$C_{12}H_{10}CrO_4$	233	$[h^6-C_6H_4-1(COCH_3)-4(CH_3)]-$ $Cr(CO)_3$	$CDCl_3$	H	~5.5 comp.	—	—	731 16
				H'	2.30, 2.39	—		
			CCl_4	H_{-2}	5.08	—		
				H_{-3}	6.03	—		
				H'	2.29	—		
			$(CH_3)_2CO$	H_{-2}	5.55	—		
				H_{-3}	6.39	—		
$C_{13}H_{12}CrO_4$	234	$[h^6-1,2-C_6H_4(CH_2CH_3)COCH_3]'-$ $Cr(CO)_3$	—	H	5-6	—	—	964
				H'	2.22, 3.0	—		
				H''	1.25t	J 7.5		
				H'''	2.46s	—		
$C_{13}H_{12}CrO_4$	235	$[h^6-1,3-C_6H_4(CH_2CH_3)COCH_3]'-$ $Cr(CO)_3$	—	H	2.50q	J 7.1	—	964
				H'	1.31t	—		
				H''	2.42s	—		

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{14}H_{14}CrO_4$	236	$\{h^6-1,2-C_6H_4[CH(CH_3)_2]-COCH_3\}Cr(CO)_3$	—	H 3.29 sept. H' 1.22, 1.25d H'' 2.46s	— J 6.6 —	—	964
$C_{14}H_{14}CrO_4$	237	$\{h^6-1,3-C_6H_4[CH(CH_3)_2]-COCH_3\}Cr(CO)_3$	—	H 2.70 sept. H' 4.30bd H'' 2.45s	— J 6.6 —	—	964
$C_{15}H_{16}CrO_4$	238	$\{h^6-1,3-C_6H_4[C(CH_3)_3]COCH_3\}Cr(CO)_3$	—	n.a.	—	Signals at δ 6.17s, 6.01d, 5.75d, 5.12t	964
$C_{13}H_{10}CrO_4$	239	$(h^6-C_{10}H_{10}O)Cr(CO)_3$	$CDCl_3$	H 1.26* 1.36†	— —	$C_{10}H_{10}O =$ 	967
			C_6H_6	H 0.93* 1.18†	— —	* <i>Exo</i> -isomer † <i>Endo</i> -isomer	965
$C_{13}H_{10}CrO_4$	240	$(h^6-C_{10}H_{10}O)Cr(CO)_3$	—	n.a.	—	$C_{10}H_{10}O =$  Signals at δ 5.5–5.1m, 3.45d, 3.2–2.6m	
$C_{11}H_8CrO_5$	241	$[h^6-C_6H_4-1(OH)-2(COCH_3)]Cr(CO)_3$	—	H 11.58 H' 2.55	— —	Aromatic protons gave signals at δ 5.08, 5.20 (1H), 5.73, 5.85, 5.96 (2H), 4.80, 4.90 (1H)	732
$C_{12}H_{10}CrO_5$	242	$[h^6-C_6H_3-1(CO_2H)-2,3(CH_3)_2]Cr(CO)_3$	CCl_4	H 6.5–5.0 H' 2.57, 2.24	— —	—	733

$C_{11}H_8CrO_6$	243	$[h^6-C_6H_4-1(CO_2H)-3(OCH_3)]-$ $Cr(CO)_3$	$(CD_3)_2CO$	H	5.97, 5.86, — 5.72, 5.62	—	723
				H'	3.85		
$C_{11}H_8CrO_5$	244	$(h^6-C_6H_5CO_2CH_3)Cr(CO)_3$	CCl_4	H_{ortho}	6.02 —	—	16
				H_{meta}	5.20 —		730
				H_{para}	5.42 —		717
			$(CH_3)_2CO$	H_{ortho}	6.26 —		
				H_{meta}	5.65 —		
				H_{para}	5.91 —		
				H'	3.88 —		
$C_{12}H_{10}CrO_5$	245	$[h^6-C_6H_4-1(CO_2CH_3)-2(CH_3)]-$ $Cr(CO)_3$	CCl_4	H	6.17, 6.07, — 5.61, 5.51, — 5.41	—	723 734
					5.17, 5.07, — 4.97		
				H'	3.88 —		
				H''	2.52 —		
			$(CD_3)_2CO$	H₋₃, H₋₅	5.48 —	—	717
				H₋₄	5.93 —		
				H₋₆	6.35 —		
				H'	3.87 —		
				H''	2.52 —		
			$CDCl_3$	H	6.16, 6.05 — 5.50, 5.05	—	713
$C_{12}H_{10}CrO_5$	246	$[h^6-C_6H_4-1(CO_2CH_3)-3(CH_3)]-$ $Cr(CO)_3$	CCl_4	H	5.82, 5.32, — 5.24	—	734
				H'	3.88 —		
				H''	2.25 —		

TABLE II—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)		Remarks	References
$C_{12}H_{10}CrO_5$	247	$[h^6-C_6H_4-1(CO_2CH_3)-4(CH_3)]-Cr(CO)_3$	$(CD_3)_2CO$	H_{-2}, H_{-6}	6.12	—	—	717
				H_{-4}, H_{-5}	5.80	—	—	
				H'	3.88	—	—	
				H''	2.28	—	—	
			$CDCl_3$	H	5.82m, 5.28m	—	—	713
				H'	2.39	—	—	
			$CDCl_3$	H_{-2}	6.18	—	T 33° Free ligand δ 7.86, 7.15, 2.34 and 3.81 respectively	147
				H_{-3}	5.16	—		713
				H'	3.87	—		
				H''	2.26	—		
			$(CD_3)_2CO$	H_{-2}	6.28–6.40	J_{ortho} 6.62	—	717
				H_{-3}	5.47–5.58	J_{meta} 1.50	—	
				H'	3.87	J_{para} 0.08	—	
				H''	2.30	—	—	
$C_{13}H_{12}CrO_5$	248	$[h^6-C_6H_3-1(CO_2CH_3)-2,5(CH_3)_2]-Cr(CO)_3$	CCl_4	H_{-2}	5.04	—	—	16
				H_{-3}	6.09	—	—	
				H''	2.26	—	—	
				H	5.99, 5.40	—	—	
			CCl_4	H'	5.10	—	—	733
				H''	3.90	—	—	
$C_{11}H_7ClCrO_5$	249	$[h^6-C_6H_4-1(CO_2CH_3)-3(Cl)]-Cr(CO)_3$	$(CD_3)_2CO$	H_{-2}	2.46, 2.20	—	—	717
				H_{-2}	6.33	—	—	

				$\left. \begin{array}{l} \text{H}_{-4}, \text{H}_{-5} \\ \text{H}_{-6} \\ \text{H}' \end{array} \right\}$	6.02	—		
					3.93	—		
$\text{C}_{11}\text{H}_7\text{ClCrO}_5$	250	$[\text{h}^6\text{-C}_6\text{H}_4\text{-I}(\text{CO}_2\text{CH}_3)\text{-4(Cl)}]\text{-Cr}(\text{CO})_3$	$(\text{CD}_3)_2\text{CO}$	H_{-2}	6.41–6.52	—	—	717
				H_{-3}	5.83–5.95	—		
				H'	3.87	—		
$\text{C}_{11}\text{H}_9\text{CrNO}_5$	251	$[\text{h}^6\text{-C}_6\text{H}_4\text{-I}(\text{CO}_2\text{CH}_3)\text{-4}(\text{NH}_2')]\text{-Cr}(\text{CO})_3$	$(\text{CD}_3)_2\text{CO}$	H_{-2}	6.33–6.45	—	—	717
				H_{-3}	5.15–5.27	—		
				H'	3.80	—		
				H''	4.77	—		
$\text{C}_{12}\text{H}_{10}\text{CrO}_6$	252	$[\text{h}^6\text{-C}_6\text{H}_4\text{-I}(\text{CO}_2\text{CH}_3)\text{-2}(\text{OCH}_3')]\text{-Cr}(\text{CO})_3$	$(\text{CD}_3)_2\text{CO}$	H_{-3}	5.57	—	—	717
				H_{-4}	6.05	—		
				H_{-5}	5.18	—		
				H_{-6}	6.33	—		
				H'	3.85	—		
				H''	3.80	—		
$\text{C}_{12}\text{H}_{10}\text{CrO}_6$	253	$[\text{h}^6\text{-C}_6\text{H}_4\text{-I}(\text{CO}_2\text{CH}_3)\text{-4}(\text{OCH}_3')]\text{-Cr}(\text{CO})_3$	$(\text{CD}_3)_2\text{CO}$	H_{-2}	6.38–6.50	J_{ortho} 7.31	—	717
				H_{-3}	5.47–5.60	J_{meta} 2.05 J_{para} 0.01		
				H'	3.83	—		
				H''	3.83	—		
$\text{C}_{13}\text{H}_{10}\text{CrO}_7$	254	$[\text{h}^6\text{-1,3-C}_6\text{H}_4(\text{CO}_2\text{CH}_3)_2]\text{Cr}(\text{CO})_3$	$(\text{CD}_3)_2\text{CO}$	H_{-2}	6.85	—	—	717
				H_{-4}	6.57	—		
				H_{-5}	5.75	—		
				H_{-6}	6.57	—		
				H'	3.93	—		
$\text{C}_{13}\text{H}_{10}\text{CrO}_7$	255	$[\text{h}^6\text{-1,4-C}_6\text{H}_4(\text{CO}_2\text{CH}_3)_2]\text{Cr}(\text{CO})_3$	$(\text{CD}_3)_2\text{CO}$	H	6.28	—	—	717
				H'	3.90	—		
$\text{C}_{12}\text{H}_{14}\text{CrGeO}_3$	256	$[\text{h}^6\text{-C}_6\text{H}_5\text{Ge}(\text{CH}_3)_3]\text{Cr}(\text{CO})_3$	CCl_4	H	5.5–5.1m	—	—	715
				H'	0.42s	—		

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{24}H_{21}CrO_3P$	257	$\{h^6-1,2-C_6H_4(CH_3)[P(2-CH_3-C_6H_4)_2]Cr(CO)_3\}$	$CDCl_3$	H	5.6–4.8	—	149
				H'	2.81, 2.29, 2.22		
				H''	7.4–6.8		
$C_{12}H_{14}CrO_3Si$	258	$[h^6-C_6H_5Si(CH_3)_3]Cr(CO)_3$	CCl_4	H	5.23	—	143
				H'	0.30s		
$C_{13}H_{16}CrO_3Si$	259	$\{h^6-C_6H_4-1[Si(CH_3)_3]-4(CH_3)-Cr(CO)_3\}$	$CDCl_3$	H ₋₂	5.41	T 33° Free ligand δ 7.34, 7.07, 2.29 and 0.23 respectively	147
				H ₋₃	4.99		
				H'	2.19		
				H''	0.28		
$C_{14}H_{19}CrNO_3Si$	260	$\{h^6-C_6H_4-1[Si(CH_3)_3]-4[N-(CH_3)_2]Cr(CO)_3\}$	$CDCl_3$	H ₋₂	5.58	T 33° Free ligand δ 7.29, 6.61, 2.84 and 0.21 respectively	147
				H ₋₃	4.81		
				H'	2.89		
				H''	0.26		
$C_{15}H_{22}CrO_3Si_2$	261	$[h^6-1,4-C_6H_4(Si(CH_3)_3)_2]Cr(CO)_3$	CCl_4	H	5.19s	—	715
				H'	0.29s		
$C_{13}H_{16}CrO_3Sn$	262	$[h^6-C_6H_5CH_2Sn(CH_3)_3]Cr(CO)_3$	$CDCl_3$	H	5.13bm	p -Dioxane as internal reference	143
				H'	2.03		
				H''	0.13		

$$J(^{117}Sn-H') =$$

$$54.5$$

$$J(^{119}Sn-H') =$$

$$56.8$$

$$J(^{117}Sn-H) = 51.6$$

$$J(^{119}Sn-H) = 53.6$$

145

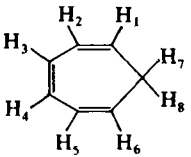
C ₁₂ H ₁₄ CrO ₃ Sn	263	[h ⁶ -C ₆ H ₅ Sn(CH ₃) ₃]Cr(CO) ₃	CCl ₄	H	5.2-5.0bs	—	—	715
			—	H'	0.32s	—	J(¹¹⁹ Sn-H) = 55.4	145
			CDCl ₃	H	5.28m	—	—	143
				H'	0.40s	—	J(¹¹⁷ Sn-H') = 53.0 J(¹¹⁹ Sn-H') = 55.4	
C ₁₅ H ₂₂ CrO ₃ Sn ₂	264	[h ⁶ -1,4-C ₆ H ₄ (Sn(CH ₃) ₃) ₂]-Cr(CO) ₃	CCl ₄	H	5.14m	—	—	143
				H'	0.40s	—	J(¹¹⁷ Sn-H') = 52.9 J(¹¹⁹ Sn-H') = 55.3	145
C ₁₇ H ₁₆ CrO ₃ Sn	265	{h ⁶ -C ₆ H ₅ [Sn(CH ₃) ₂ C ₆ H ₅]}-Cr(CO) ₃	CCl ₄	H	5.24m	—	—	143
				H'	0.65	—	J(¹¹⁷ Sn-H') = 53.8 J(¹¹⁹ Sn-H') = 56.1	145
				H''	7.39m	—	—	
C ₂₀ H ₁₆ Cr ₂ O ₆ Sn	266	[(h ⁶ -C ₆ H ₅) ₂ Sn(CH ₃) ₂][Cr(CO) ₃] ₂	CDCl ₃	H	5.33m	—	—	143
				H'	0.45	—	J(¹¹⁷ Sn-H') = 55.5 J(¹¹⁹ Sn-H') = 58.1	145
C ₁₀ H ₈ CrO ₃	267	(h ⁶ -C ₇ H ₈)Cr(CO) ₃	C ₆ D ₆	H ₋₁ , H ₋₆	2.671	J _{1,2} = J _{5,6} 8.2	C ₇ H ₈ = 	735
				H ₋₂ , H ₋₅	4.185	J _{2,3} = J _{4,5} 6.97		955
				H ₋₃ , H ₋₄	5.297	J _{3,4} 8.45		

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
				H_{-7} 1.082 H_{-8} 2.170	$J_{6,7} = J_{1,7}$ 3.17 $J_{6,8} = J_{1,8}$ 8.90 $J_{7,8}$ -14.05	$J_{1,5} = J_{2,6} \sim J_{1,6} < 0.5$ $J_{1,3} + J_{1,4} = J_{4,6} + J_{3,6} = 1.27$ $J_{2,4} = J_{3,5} = 0.73$ $J_{2,5} = 0.51$ $J_{2,7} = J_{5,7} = -1.07$ $J_{2,8} = J_{5,8} = 0.92$	
			CCl_4	H_{-7} <i>exo</i> 1.77 H_{-7} <i>endo</i> ~ 2.9			
			CH_2Cl_2	$^{13}CH_2$ 24.8 ^{13}CH 57.6, 99.0 101.9 ^{13}CO 232.7	— — —	22.62 MHz The average coordination shift relative to free cycloheptatriene is considerably greater than that for arenes, implying stronger metal-triene bonding than metal-arene bonding	148
$C_{11}H_{10}CrO_3$	268	$(h^6-C_7H_7 \cdot CH_3)Cr(CO)_3$	—	H 1.97	—	1-Methylcyclohepta-1,3,5-triene chromium tricarbonyl	736
$C_{11}H_{10}CrO_3$	269	$[1,2,3,4,5,6-h^6-7-C_7H_7(CH_3)]-Cr(CO)_3$	CS_2	$7-CH_{3exo}$ 0.1d H_{-7endo} ~ 3.0	— —	— —	955
			C_6D_6	$7-CH_{3exo}$ 0.36d	—		
$C_{13}H_{12}CrO_3$	270	$[1,2,3,4,5,6-h^6-7-exo-C_7H_7(CH_2-CH=CH_2)]Cr(CO)_3$	—	H 0.95dd	—	—	955
$C_{13}H_{10}CrO_3$	271	$(1,2,3,4,5,6-h^6-C_{10}H_{10})Cr(CO)_3$	—	$H_{-1}, H_{-6} \sim 3^*$ $H_{-2}, H_{-5} \sim 4.8^*$ $H_{-3}, H_{-4} \sim 5.9^*$	— — —	$C_{10}H_{10} = endo-7$ -propargyl-1,3,5-cycloheptatriene *Estimated from published spectra	737 955

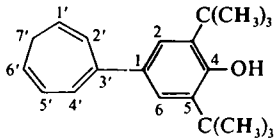
				H_{-7}	$\sim 2.0^*$	J 4		"Axial" H_{-7} shielded by triene system and gives signal at higher field than that for <i>exo</i> -isomer
				CH_2	~ 2.6	—		Signals from H_{-1} and H_{-6} are also to higher field than those of <i>exo</i> -isomer
				$\equiv CH$	$\sim 2.0^*$	—		$C_{10}H_{10}$ = <i>exo</i> -7-propargyl-1,3,5-cycloheptatriene
				H_{-1}, H_{-6}	$\sim 3.7^*$	—		"Axial" CH_2 of propargyl group is shielded by triene system and gives a signal to higher field than that for <i>endo</i> -isomer (above)
				H_{-2}, H_{-5}	$\sim 4.8^*$	—		
				H_{-3}, H_{-4}	$\sim 5.9^*$	—		
				H_{-7}	$\sim 3.0^*$	J 8		
				CH_2	$\sim 1.0^*$	—		
				$\equiv CH$	$\sim 1.7^*$	—		
$C_{14}H_{14}CrO_5$	272	$[1,2,3,4,5,6-h^6-7-exo-C_7H_7-(CH_2CO_2CH_2CH_3)]Cr(CO)_3$	CS_2	H_{-7endo}	3.7	—	—	955
				H'	1.18d	—	—	
$C_{14}H_{14}CrO_5$	273	$[1,2,3,4,5,6-h^6-7-endo-C_7H_7-(CH_2CO_2CH_2CH_3)]Cr(CO)_3$	CS_2	H_{-7exo}	2.0m	—	—	955
				H'	2.7d	—	—	
$C_{11}H_7CrNO_3$	274	$[1,2,3,4,5,6-h^6-7-exo-C_7H_7-(CN)]Cr(CO)_3$	$CDCl_3$	H_{-7endo}	3.5t	—	—	955
$C_{16}H_{12}CrO_3$	275	$[1,2,3,4,5,6-h^6-7-exo-C_7H_7-(C_6H_5)]Cr(CO)_3$		H_{-7endo}	~ 3.8	—	—	955
				H'	6.9m	—	—	
$C_{16}H_{12}CrO_3$	276	$[1,2,3,4,5,6-h^6-7-endo-C_7H_7-(C_6H_5)]Cr(CO)_3$	—	H_{-7exo}	2.43t	—	—	955
				H'	7.3s	—	—	
$C_{24}H_{28}CrO_4$	277	$(h^6-C_{21}H_{28}O)Cr(CO)_3$	$CDCl_3$	H_{-7endo}	2.9m	—	Structure:	738
				H_{-7exo}	1.85d	—		
				OH	4.68s	—	Other signals at 7.43s, 6.24bd, 5.0m, 3.4m, in ratio 2:1:2:2	
				CH_3	8.5s	—		

TABLE II—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{11}H_{10}CrO_4$	278	[1,2,3,4,5,6- <i>h</i> ⁶ -1- $C_7H_7(OCH_3)$]- $Cr(CO)_3$	$CDCl_3$	H_{-2}	5.2m	—	$C_7H_7(OCH_3) = 1$ -methoxy-1,3,5-cycloheptatriene	739
				H_{-3}, H_{-4}	5.7t	—		
				H_{-5}	4.05m	—		
				H_{-6}	3.3m	—		
				H_{-7endo}	2.8m	—		
				H_{-7exo}	2.1m	—		
				H'	3.6s	—		
$C_{11}H_{10}CrO_4$	279	(1,2,3,4,5,6- <i>h</i> ⁶ -2- $C_7H_7 \cdot OCH_3$)- $Cr(CO)_3$	$CDCl_3$	H_{-1}	4.7m	—	2- $C_7H_7OCH_3 = 2$ -methoxy-1,3,5-cycloheptatriene	740
				H_{-3}, H_{-4}	6.15m	—		
				H'	3.38s	—		
$C_{11}H_{10}CrO_4$	280	[1,2,3,4,5,6- <i>h</i> ⁶ -3- $C_7H_7(OCH_3)$]- $Cr(CO)_3$	$CDCl_3$	H_{-7exo}	~ 1.7	—	—	955
				H_{-7endo}	~ 2.8	—		
$C_{11}H_{10}CrO_4$	281	[1,2,3,4,5,6- <i>h</i> ⁶ -7- $C_7H_7(OCH_3)$]- $Cr(CO)_3$	$CDCl_3$	H_{-1}, H_{-6}	3.3m	—	$C_7H_7(OCH_3) = endo$ -7-methoxy-1,3,5-cycloheptatriene	739
				H_{-2}, H_{-5}	4.7m	—		
				H_{-3}, H_{-4}	6.0m	—		
				H_{-7exo}	3.3m	—		
				H'	3.33s	—		
				H_{-7endo}	~ 3.8	—	<i>Exo</i> -isomer	955
				H'	2.95	—		
$C_{12}H_{12}CrO_5$	282	[1,2,3,4,5,6- <i>h</i> ⁶ -7,7- $C_7H_6(OCH_3)_2$]- $Cr(CO)_3$	$(CD_3)_2CO$	H_{-1}, H_{-6}	3.88dt	$J_{1,2} 9.1$	7,7- $C_7H_6(OCH_3)_2 = 7,7$ -di-methoxy-1,3,5-cycloheptatriene	740
				H_{-2}, H_{-5}	5.2m	—		
				H_{-3}, H_{-4}	6.0m	—		
				H'	2.72s, 3.3s	—		

			CDCl ₃	H ₋₁ , H ₋₆ H ₋₂ H ₋₃ , H ₋₄ H'	3.82 5.05 5.8 2.75*, 3.31†	— — — —	*Exo-OCH ₃ †Endo-OCH ₃	955
C ₁₂ H ₁₂ CrO ₄	283	[1,2,3,4,5,6- <i>h</i> ⁶ -2-C ₇ H ₇ (OCH ₂ ⁺ -CH ₃ ⁻)]Cr(CO) ₃	CDCl ₃	H ₋₁ , H ₋₆ H ₋₃ , H ₋₄ H ₋₅ H _{-7endo} H _{-7exo} H' H''	3.9-2.6m 6.22 4.77m 3.9-2.6m 1.7m 3.9-2.6m 1.27t	— — — — — — —	—	739
C ₁₂ H ₁₂ CrO ₄	284	[1,2,3,4,5,6- <i>h</i> ⁶ -7-C ₇ H ₇ (OCH ₂ ⁺ -CH ₃ ⁻)]Cr(CO) ₃	CDCl ₃	H ₋₁ , H ₋₆ H ₋₂ , H ₋₅ H ₋₃ , H ₋₄ H' H''	3.35m 4.78m 6.05m 3.51q 1.22t	— — — — —	—	739
C ₁₇ H ₁₄ CrO ₄	285	[1,2,3,4,5,6- <i>h</i> ⁶ -C ₇ H ₆ -2(OCH ₃ ⁺ -1(C ₆ H ₅ ⁻))]Cr(CO) ₃	CDCl ₃	H ₋₁ , H ₋₆ H ₋₃ , H ₋₄ H ₋₅ H _{-7endo} H' H''	4.2m 6.07m 4.9m 3.78m 3.48s 7.2m, 6.82m	— — — — — —	C ₇ H ₆ = disubstituted-1,3,4-cycloheptatriene	740
C ₁₂ H ₁₀ CrO ₅	286	[1,2,3,4,5,6- <i>h</i> ⁶ -1-C ₇ H ₇ (CO ₂ CH ₃ ⁺)]Cr(CO) ₃	CDCl ₃	H ₋₂ , H ₋₃ , H ₋₄ H ₋₅ H ₋₆ , H _{-7endo} H _{-7exo}	6.2m — 5.0 3.65 1.45	— — — — —	C ₇ H ₇ = substituted-1,3,5-cycloheptatriene	741

TABLE II—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{12}H_{10}CrO_5$	287	[1,2,3,4,5,6- <i>h</i> ⁶ -3- $C_7H_7(CO_2CH_3)$] $Cr(CO)_3$	$CDCl_3$	$H_{-1}, H_{-6},$	4.1–2.7m	—	741
				H_{-7endo}	—	—	
				H_{-2}	5.65d	—	
				H_{-4}	7.1d	—	
				H_{-5}	4.97t	—	
				H_{-7exo}	1.85bd	—	
$C_{12}H_{10}CrO_5$	288	[1,2,3,4,5,6- <i>h</i> ⁶ -7- $C_7H_7(CO_2CH_3)$] $Cr(CO)_3$	$CDCl_3$	H_{-1}, H_{-6}	3.75bm	—	741
				H_{-2}, H_{-5}	5.05bd	—	
				H_{-3}, H_{-4}	6.0m	—	
				H_{-7exo}	1.58bs	—	
				H'	3.49s	—	
						C_7H_7 = substituted-1,3,5-cycloheptatriene	
$C_{13}H_9CrNO_5$	289	[1,2,3,4,5,6- <i>h</i> ⁶ - $C_7H_6-7(CN)-1(CO_2CH_3)$] $Cr(CO)_3$	—	$H_{-2}, H_{-3},$	6.35m	—	740
				H_{-4}	—	—	
				H_{-5}	5.14m	—	
				H_{-6}	3.77t	—	
				H_{-7endo}	5.02d	—	
				H'	3.92s	—	
$C_{13}H_{12}CrO_6$	290	[1,2,3,4,5,6- <i>h</i> ⁶ - $C_7H_6-7(OCH_3)-(CO_2CH_3)$] $Cr(CO)_3$	$(CD_3)_2CO$	$H_{-2}, H_{-3},$	6.34	—	740
				H_{-4}	—	—	
				H_{-5}	5.55	—	
				H_{-6}	4.45t	$J_{6,7} 8$	
				H_{-7endo}	5.02d	—	
				H'	2.92s	—	
				H''	3.88	—	

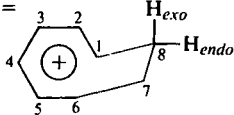
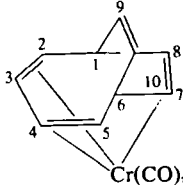
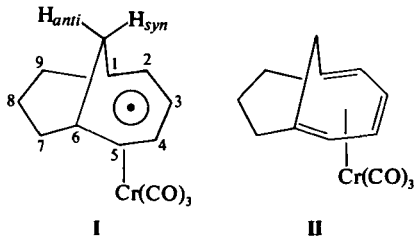
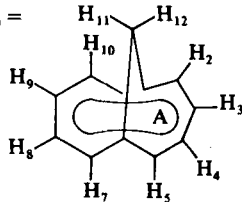
$C_{18}H_{20}CrO_8$	291	{1,2,3,4,5,6- <i>h</i> ⁶ -7,7- $C_7H_6(OCH_3)_2$ - $[CH(CO_2Et)_2]Cr(CO)_3$ }	CS_2	H	3.33	—	C_7H_6 = disubstituted-1,3,5-cycloheptatriene	740
$C_{20}H_{14}Cr_2O_6S_2$	292	(1,2,3,4,5,6- <i>h</i> ⁶ -7- <i>exo</i> - $C_7H_7S)_2-Cr(CO)_3I_2$	$CDCl_3$	H _{-7endo}	3.8-3.7	—	—	955
$C_{11}H_8CrO_3$	293	(1,2,3,4,5,6- <i>h</i> ⁶ - C_8H_8) $Cr(CO)_3$	$CDCl_3$	H ₋₁ , H ₋₆ H ₋₂ , H ₋₅ H ₋₃ , H ₋₄ H ₋₇ , H ₋₈	4.62 5.18 6.26 4.92	— — — —	C_8H_8 = cyclooctatetraene T -40°	911 1020
$[C_{11}H_9CrO_3]^+$	294	$[(h^6-C_8H_9)Cr(CO)_3]^+$	SO_2	H ₋₁ , H ₋₇	4.37	$J_{12} = J_{6,7}$ 8	C_8H_9 = 	155
				H ₋₂ , H ₋₆ H ₋₃ , H ₋₅ H ₋₄	6.53 6.62 5.68	$J_{2,3} = J_{5,6}$ 7.5 $J_{3,4} = J_{4,5}$ 10.0 $J_{1,8endo} = J_{7,8endo}$ 8.5		
				H _{-8endo}	3.40	$J_{1,8exo} = J_{7,8exo}$ 10.0		
				H ₋₈	-1.05	$J_{8endo,8exo}$ 7		
$C_{13}H_{10}CrO_3$	295	$(h^6-C_{10}H_{10})Cr(CO)_3$	C_6D_6	H ₋₁ , H ₋₆ H ₋₂ , H ₋₅ H ₋₃ , H ₋₄ H ₋₇ , H ₋₈ H ₋₉ , H ₋₁₀	2.74 3.44 4.35 3.29 5.19	— — — — —	Structure: 	94

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{13}H_{12}CrO_3$	296	$(h^6-C_{10}H_{12})Cr(CO)_3$	C_6D_6	H_{-2}, H_{-5} 5.71 H_{-3}, H_{-4} 4.49 H_{-7}, H_{-8}, H_{-9} 1.8–0.3m H_{anti} –0.82 H_{syn} –2.43	$J_{2,3} = J_{4,5}$ 6.73 $J_{3,4} = 6.18$ $J_{2,4} = J_{3,5}$ 0.69 $J_{2,5}$ 1.09 $J_{syn, anti}$ 3.4 $J(^{13}C-H_{syn}) = 164$	Complex obtained from (4,3,1,0 ^{1,6}) deca-2,4-diene Homoaromatic structure (I) favoured over the cycloheptatriene structure (II). <i>Syn</i> and <i>anti</i> bridge protons shifted upfield by resultant diamagnetic ring current	742 1034
							
$C_{14}H_{10}CrO_3$	297	$(h^6-C_{11}H_{10})Cr(CO)_3$	C_6D_6	H_{-2}, H_{-5} 6.201	$J_{2,3} = J_{4,5}$ 7.05	$C_{11}H_{10} =$ 	721

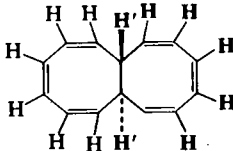
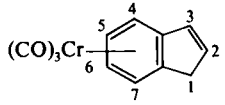
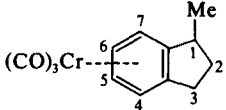
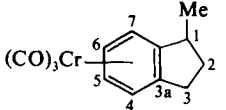
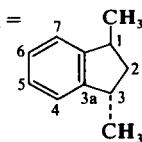
						H_{-3}, H_{-4} 4.329 H_{-7}, H_{-10} 6.768 H_{-8}, H_{-9} 6.416 H_{-11} -1.769 H_{-12} -1.138	$J_{3,4}$ 7.31 $J_{7,8} = J_{9,10}$ 8.16 $J_{8,9}$ 9.22 $J_{11,12}$ -8.90	743 744
$C_{20}H_{14}Cr_2O_6$	298	(1,2,3,4,5,6- h^6 : 7,8,9,10,11,12- h^6 - $C_{14}H_{14}$)[Cr(CO) ₃] ₂	CDCl ₃	H	6.25-5.7	—	Cr complexed to half ring A $J_{2,4} = J_{7,5} = 0.37$; $J_{2,5} = 1.18$ $J_{7,9} = J_{8,10} = 0.24$; $J_{7,10} = 1.56$ $J_{2,11} = J_{5,11} = 0.91$ $J_{7,12} = J_{10,12} = 1.08$ $J_{2,12} = J_{5,12} < 0.4$ $J_{7,11} = J_{10,11} < 0.3$; $J_{2,7} = J_{5,10} \sim 0$ $J_{5,7} = J_{2,10} = 0.49$	745
					5.3-5.05	—	$C_{14}H_{14} =$ 	
					4.95-4.7	—	100MHz	
					4.55-4.3	—		
				H'	3.7-3.2	—		
$C_{12}H_8CrO_3$	299	(h^6 -C ₉ H ₈)Cr(CO) ₃	CDCl ₃	H ₋₁	3.48s	—	Structure:	746
								
				H_{-2}, H_{-3}	6.88s	—		
				H_{-4}, H_{-7}	5.78m	—		
				H_{-5}, H_{-6}	5.25	—		

TABLE II—cont.

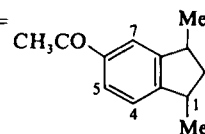
Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{13}H_{12}CrO_3$	300	$(h^6-C_{10}H_{12})Cr(CO)_3$	—	H_{-7} H_{-6} H_{-5} H_{-4}	 	$C_{10}H_{12}$ = 1-methylindane <i>trans</i> -tricarbonylchromium complex, viz.: 	153
				H_{-7} H_{-6} H_{-5} H_{-4}	 	 	
						100 MHz <i>cis</i> -tricarbonylchromium complex, viz.: 	
						100 MHz The aromatic protons of the <i>cis</i> -complex show alternating δ -values due to the complex having a preferred conformation in which the metal-CO bonds are directed over positions C_{3a} , C_5 , and C_7 . This property was used to assign the <i>cis</i> -structure to other complexes showing this effect (see below):	

$C_{14}H_{14}CrO_3$	301	$(h^6-C_{11}H_{14})Cr(CO)_3$	—	H_{-7} 5.43d* H_{-6} 5.0t H_{-5} 5.36t* H_{-4} 5.12d CH_3 1.24, 1.17	—
$C_{16}H_{16}CrO_4$	302	$(h^6-C_{13}H_{16}O_4)Cr(CO)_3$	—	H_{-7} 6.12s* H_{-5} 6.08d* H_{-4} 5.12d	—
$C_{16}H_{16}CrO_4$	303	$(h^6-C_{13}H_{16}O)Cr(CO)_3$	—	H_{-7} 5.38d* H_{-6} 5.73d† H_{-4} 5.88s†	—
$C_{15}H_{16}CrO_3$	304	$(h^6-C_{12}H_{16})Cr(CO)_3$	—	H^* 5.44m, 5.26m	—

$C_{11}H_{14}$ = 747
153

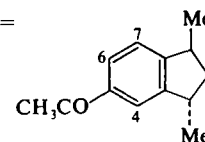


$C_{13}H_{16}O$ = 747



*Deshielded by superimposed metal-carbonyl bond and *ortho*-acetyl group

$C_{13}H_{16}O$ = 747



*Deshielded by metal-carbonyl bond

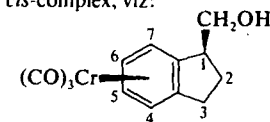
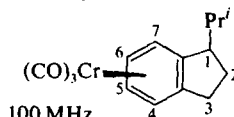
†Deshielded by *ortho*-acetyl group

$C_{12}H_{16}$ = 1-isopropylindane 153
trans-tricarbonylchromium complex.
 100 MHz
 *Aromatic protons

*Protons lying under superimposed metal-carbonyl bonds are deshielded relative to adjacent unc eclipsed protons, suggesting that the preferred conformation is that in which the metal-CO bonds are directed over C_{3a} , C_5 , and C_7 in order to minimize nonbonded interactions with the *cis*-methyl group at C_1

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{13}H_{12}CrO_4$	305	$(h^6-C_{10}H_{12}O)Cr(CO)_3$	—	H_{-7}	5.61d	—	<i>cis</i> -complex, viz:
				H_{-6}	4.95t	—	
				H_{-5}	5.34t	—	
				H_{-4}	5.11d	—	
				H^*	5.59d, 5.44d 5.27m (in ratio 1:1:2)	—	100 MHz $C_{10}H_{12}O$ = 1-hydroxymethylindane <i>trans</i> -tricarbonylchromium complex *Aromatic protons <i>cis</i> -complex, viz:
				H_{-7}	5.92d	—	
				H_{-6}	5.03t	—	
				H_{-5}	5.48t	—	
				H_{-4}	5.21d	—	
$C_{14}H_{11}CrNO_3$	306	$(h^6-C_{11}H_{11}N)Cr(CO)_3$	—	H^*	5.61d, 5.46d 5.32m (in ratio 1:1:2)	—	100 MHz $C_{11}H_{11}N$ = 1-cyanomethylindane <i>trans</i> -tricarbonylchromium complex *Aromatic protons <i>cis</i> -complex, viz.:
				H_{-7}	5.73d	—	
				H_{-6}	5.11t	—	
				H_{-5}	5.53t	—	
				H_{-4}	5.28d	—	
							100 MHz



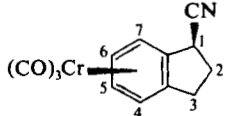
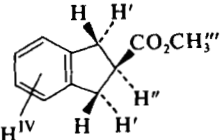
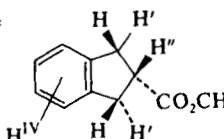
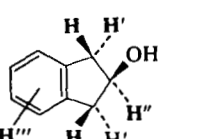
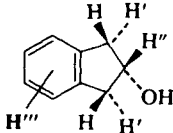
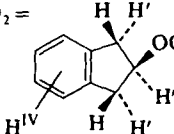
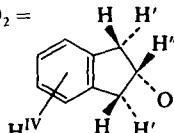
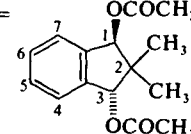
$C_{13}H_9CrNO_3$	307	$(h^6-C_{10}H_9N)Cr(CO)_3$	—	$H^{\bullet}$ H_{-7} H_{-6} H_{-5} H_{-4}	5.58d, 5.45d 5.32m (in ratio 1:1:2) 5.71d 5.16t 5.38t 5.25d	— — — —	$C_{10}H_9N = 1$ -cyanoindane <i>trans</i> -tricarbonylchromium complex *Aromatic protons <i>cis</i> -complex, viz.:	153
								100MHz
$C_{14}H_{12}CrO_5$	308	$(h^6-C_{11}H_{12}O_2)Cr(CO)_3$	$CDCl_3$	H, H' H'' H''' H^{IV}	3.0–3.6m 3.80s ~5.50	— — —	$C_{11}H_{12}O_2 =$ 	748
							40 and 100 MHz	
$C_{14}H_{12}CrO_5$	309	$(h^6-C_{11}H_{12}O_2)Cr(CO)_3$	$CDCl_3$	H, H' H'' H''' H^{IV}	3.03–3.6m 3.76s ~5.45	— — —	$C_{11}H_{12}O_2 =$ 	748
							40 and 100 MHz	
$C_{12}H_{10}CrO_4$	310	$(h^6-C_9H_{10}O)Cr(CO)_3$	$CDCl_3$	H H' H'' H''' OH	3.20q 2.85q ~4.60m ~5.40m 2.32	J 6, 17 J 1.3, 17 — — —	$C_9H_{10}O =$ 	748
							40 and 100 MHz	

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{12}H_{10}CrO_4$	311	$(h^6-C_9H_{10}O)Cr(CO)_3$	$CDCl_3$	H	2.82q	J 6.5, 14.8	$C_9H_{10}O =$  40 and 100 MHz	748
				H'	3.05q	J 6.5, 14.8		
				H''	$\sim 4.80m$	—		
				H'''	$\sim 5.40m$	—		
				OH	1.93	—		
$C_{14}H_{12}CrO_5$	312	$(h^6-C_{11}H_{12}O_2)Cr(CO)_3$	$CDCl_3$	H	3.21q	J 6, 17	$C_{11}H_{12}O_2 =$  40 and 100 MHz	748
				H'	2.90q	J 2, 17		
				H''	$\sim 5.30m$	—		
				H'''	2.09s	—		
				H ^{IV}	$\sim 5.30m$	—		
$C_{14}H_{12}CrO_5$	313	$(h^6-C_{11}H_{12}O_2)Cr(CO)_3$	$CDCl_3$	H	2.86q	J 6.75, 16	$C_{11}H_{12}O_2 =$  40 and 100 MHz	748
				H'	3.20q	J 7.2, 16		
				H''	$\sim 5.30m$	—		
				H'''	2.05s	—		
				H ^{IV}	$\sim 5.30m$	—		
$C_{18}H_{18}CrO_7$	314	$(h^6-C_{15}H_{18}O_4)Cr(CO)_3$	—	H ₋₇	5.50d	—	$C_{15}H_{18}O_4 =$  100 MHz	153
				H ₋₆	5.20	—		
				H ₋₅	5.36	—		
				H ₋₄	5.36	—		

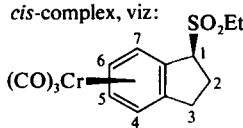
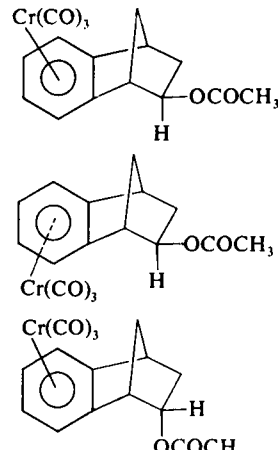
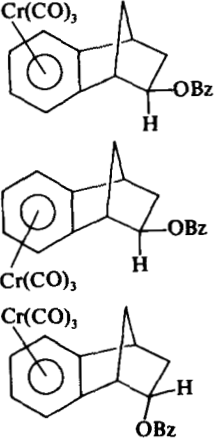
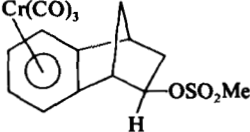
$C_{13}H_{10}CrO_4$	315	$(\eta^6-C_{10}H_{10}O)Cr(CO)_3$	$CDCl_3$	CH_3^* $CH_3^\dagger$	1.5 1.38	—	$C_{10}H_{10}O = 3\text{-methylindane-1-one}$ * <i>cis</i> - to coordinated $Cr(CO)_3$ group † <i>trans</i> - to coordinated $Cr(CO)_3$ group	749
$C_{14}H_{14}CrO_5S$	316	$(\eta^6-C_{11}H_{14}O_2S)Cr(CO)_3$	—	H^* H_{-7} H_{-6} H_{-5} H_{-4}	5.95d, 5.45d, 5.30m (in ratio 1:2:1). 6.21d 4.97t 5.56t 5.10d	— — — —	$C_{11}H_{14}O_2S = 1\text{-ethylsulphonyl-}$ indane. <i>trans</i> -tricarbonyl- chromium complex *Aromatic protons <i>cis</i> -complex, viz:	153
$C_{16}H_{14}CrO_5$	317	$(\eta^6-C_{13}H_{14}O_2)Cr(CO)_3$	—	n.m.	—	—	 Structures: 	750

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{20}H_{15}BrCrO_6S$	318	$(h^6-C_{17}H_{15}BrO_3S)Cr(CO)_3$	—	n.m.	—	Structures: 	751
$C_{15}H_{14}CrO_6$	319	$(h^6-C_{12}H_{14}O_3S)Cr(CO)_3$	—	n.m.	—	(Bz = p -SO ₂ C ₆ H ₄ Br) Structures: 	750

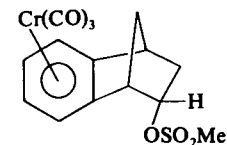
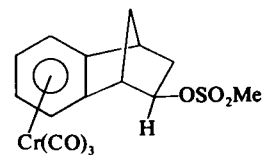
$C_{23}H_{14}CrO_3$ 320 ($h^6-C_{20}H_{14}$)Cr(CO)₃

CDCl₃

H 5.40m
H' 5.18s
H'' 7.28m

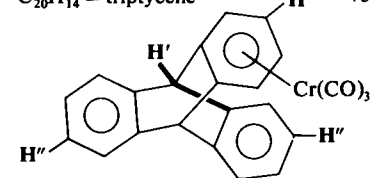
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—



$C_{20}H_{14}$ = triptycene

752



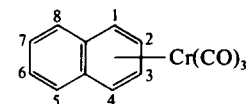
$C_{13}H_8CrO_3$ 321 ($h^6-C_{10}H_8$)Cr(CO)₃

CDCl₃

H₋₁, H₋₄ 6.09
H₋₂, H₋₃ 5.48
H₋₅, H₋₈ 7.53
H₋₆, H₋₇ 7.37

$J_{1,3}$ 1.05 $J_{1,4}$ 0.2
 $J_{2,3}$ 5.5
 $J_{5,6}$ 8.55 $J_{5,7}$ 1.25
 $J_{5,8}$ 0.3
 $J_{6,7}$ 6.0

Structure:



753

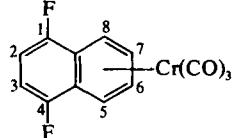
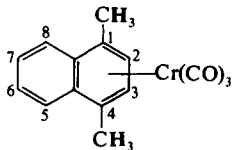
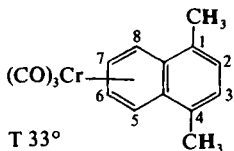
754

70

T 33°

Values of J and δ decreased in complexed ring relative to uncomplexed ring and free ligand

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{13}H_6CrF_2O_3$	322	$(h^6-C_{10}H_6F_2)Cr(CO)_3$	CCl_4	H_{-2}, H_{-3} 6.92 H_{-5}, H_{-8} 6.26 H_{-6}, H_{-7} 5.52	$J_{2,3}$ 5.8 $J_{5,8}$ 0.2 $J_{6,7}$ 5.8 $J_{5,6}$ 6.6 $J_{5,7}$ 1.07	Structure:  T 33° Values of δ and J of complexed ring decreased relative to free ligand	754
$C_{15}H_{12}CrO_3$	323	$(h^6-C_{12}H_{12})Cr(CO)_3$	$CDCl_3$	H_{-2}, H_{-3} 5.42 H_{-5}, H_{-8} 7.79 H_{-6}, H_{-7} 7.50	$J_{2,3}$ 6.2 $J_{5,8}$ 0.3 $J_{6,7}$ 6.2 $J_{5,6}$ 8.8 $J_{5,7}$ 1.3	Structure:  T 33°	754
$C_{15}H_{12}CrO_3$	324	$(h^6-C_{12}H_{12})Cr(CO)_3$	$CDCl_3$	CH_3 2.58 H_{-2}, H_{-3} 7.11 H_{-5}, H_{-8} 6.18 H_{-6}, H_{-7} 5.52	$J_{2,3}$ 5.5 $J_{5,8}$ 0.2 $J_{6,7}$ 5.5 $J_{5,6}$ 7.1 $J_{5,7}$ 1.1	Structure:  T 33°	754

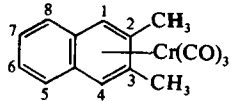
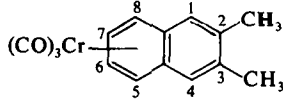
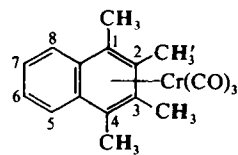
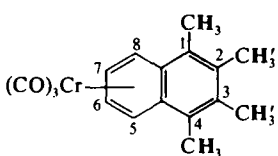
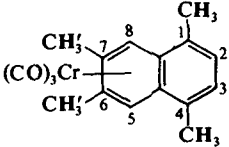
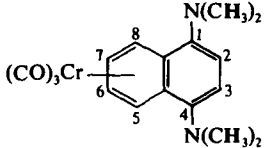
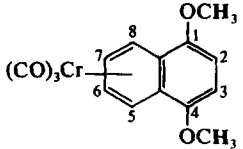
$C_{15}H_{12}CrO_3$	325	$(h^6-C_{12}H_{12})Cr(CO)_3$	$CDCl_3$	H_{-1}, H_{-4} 6.10 H_{-5}, H_{-8} 7.54 H_{-6}, H_{-7} 7.38	$J_{1,4}$ 0.3 $J_{5,8}$ 0.3 $J_{6,7}$ 6.9 $J_{5,6}$ 8.3 $J_{5,7}$ 1.3	Structure: 	754
$C_{15}H_{12}CrO_3$	326	$(h^6-C_{12}H_{12})Cr(CO)_3$	$CDCl_3$	CH_3 2.25 H_{-1}, H_{-4} 7.33 H_{-5}, H_{-8} 6.07 H_{-6}, H_{-7} 5.45	$J_{1,4}$ 0.2 $J_{5,8}$ 0.2 $J_{6,7}$ 5.7 $J_{5,6}$ 6.9 $J_{5,7}$ 1.0	T 33° Structure: 	754
$C_{17}H_{16}CrO_3$	327	$(h^6-C_{14}H_{16})Cr(CO)_3$	CCl_4	CH_3 2.30 H_{-5}, H_{-8} 7.83 H_{-6}, H_{-7} 7.44	$J_{5,8}$ 0.3 $J_{6,7}$ 6.2 $J_{5,6}$ 8.7 $J_{5,7}$ 1.15	T 33° Structure: 	754
$C_{17}H_{16}CrO_3$	328	$(h^6-C_{14}H_{16})Cr(CO)_3$	CCl_4	CH_3 2.65 CH'_3 2.97 H_{-5}, H_{-8} 6.25 H_{-6}, H_{-7} 5.48	$J_{5,8}$ 0.2 $J_{6,7}$ 5.7 $J_{5,6}$ 7.0 $J_{5,7}$ 1.0	T 33° Structure: 	754
				CH_3 2.48 CH'_3 2.33		T 33°	

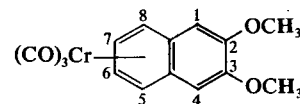
TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{17}H_{16}CrO_3$	329	$(h^6-C_{14}H_{16})Cr(CO)_3$	$CDCl_3$	H_{-2}, H_{-3} 7.06 H_{-5}, H_{-8} 6.12 CH_3 2.55	— — —	Structure: 	754
				CH_3 2.31	—	T 33°	
$C_{17}H_{18}CrN_2O_3$	330	$(h^6-C_{14}H_{18}N_2)Cr(CO)_3$	$CDCl_3$	H_{-2}, H_{-3} 6.78 H_{-5}, H_{-8} 6.48 H_{-6}, H_{-7} 5.51	$J_{2,3}$ 5.9 $J_{5,8}$ 0.2 $J_{6,7}$ 5.9 $J_{5,6}$ 6.9 $J_{5,7}$ 1.0	Structure: 	754
				CH_3 2.80		T 33°	
$C_{15}H_{12}CrO_3$	331	$(h^6-C_{12}H_{12}O_2)Cr(CO)_3$	$CDCl_3$	H_{-2}, H_{-3} 6.50 H_{-5}, H_{-8} 6.41 H_{-6}, H_{-7} 5.47	$J_{2,3}$ 5.8 $J_{5,8}$ 0.2 $J_{6,7}$ 5.8 $J_{5,6}$ 6.8 $J_{5,7}$ 1.0	Structure: 	754
				CH_3 3.92		T 33°	

C₁₅H₁₂CrO₅ 332 (h⁶-C₁₂H₁₂O₂)Cr(CO)₃CDCl₃

H₋₁, H₋₄ 6.67 J_{1,4} 0.2
 H₋₅, H₋₈ 6.01 J_{5,8} 0.2
 H₋₆, H₋₇ 5.40 J_{6,7} 5.6
 J_{5,6} 6.5
 J_{5,7} 1.0

Structure:



754

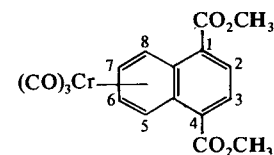
CH₃ 3.92

T 33°

C₁₇H₁₂CrO₇ 333 (h⁶-C₁₄H₁₂O₄)Cr(CO)₃CDCl₃

H₋₂, H₋₃ 8.04 J_{2,3} 6.1
 H₋₅, H₋₈ 7.26 J_{5,8} 0.2
 H₋₆, H₋₇ 5.54 J_{6,7} 6.1
 J_{5,6} 7.4
 J_{5,7} 1.15

Structure:



754

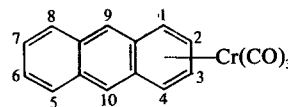
CH₃ 4.0

T 33°

C₁₇H₁₀CrO₃ 334 (h⁶-C₁₄H₁₀)Cr(CO)₃C₆D₆

H₋₁, H₋₄ 5.68 —
 (5.03m)*
 H₋₂, H₋₃ 4.92 —
 (4.57m)*

Structure:



753

H₋₅, H₋₈ 7.30 —
 (6.65m)*

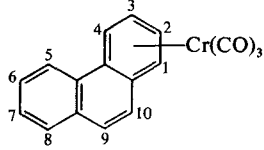
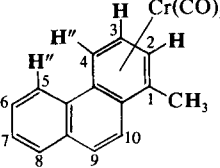
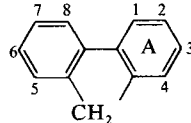
H₋₆, H₋₇ 7.07 —
 (6.65m)*

H₋₉, H₋₁₀ 7.49 —
 (7.15bs)*

T 33°

755

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{17}H_{10}CrO_3$	335	$(h^6-C_{14}H_{10})Cr(CO)_3$	$CDCl_3$	H_{-1}	6.01	—	Structure: 	753 728
				H_{-2}, H_{-3}	5.52	—		
				H_{-4}	6.62	—		
				H_{-5}	8.31	—		
				H_{-6}, H_{-7}	7.68	—		
				H_{-8}				
				H_{-9}	7.62	—		
$C_{18}H_{12}CrO_3$	336	$(h^6-C_{15}H_{12})Cr(CO)_3$	$CDCl_3$	H_{-2}, H_{-3}	5.53	—	Structure: 	728
				H_{-4}	6.58	—		
				H_{-5}	8.3	—		
				$H_{-6}-H_{-10}$	7.67	—		
				CH_3	2.67	—		
$C_{16}H_{10}CrO_3$	337	$(h^6-C_{13}H_{10})Cr(CO)_3$	$(CD_3)_2CO$	H_{-1}	5.97m	—	$C_{13}H_{10} =$ 	746 70
				H_{-2}	5.32m	—		
				H_{-3}	5.32m	—		
				H_{-4}	5.75m	—		
				$H_{-5}-H_{-8}$	7.35m	—		
				H_{-9}	3.87s	—		

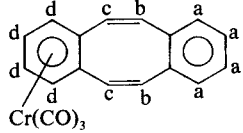
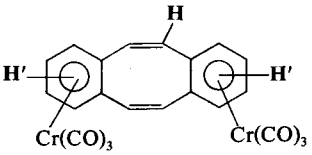
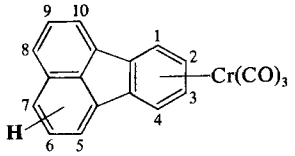
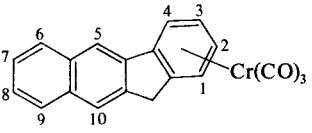
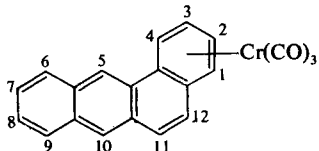
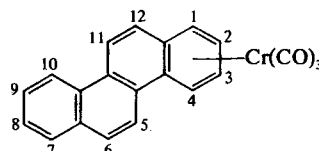
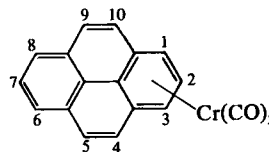
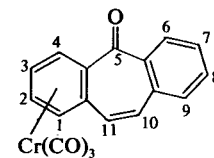
$C_{19}H_{12}CrO_3$	338	$(h^6-C_{16}H_{12})Cr(CO)_3$	—	H_a 7.35 H_b 6.88 H_c 6.71 H_d 5.65	—	Structure: 	962
$C_{22}H_{12}Cr_2O_6$	339	$(h^6, h^6-C_{16}H_{12})[Cr(CO)_3]_2$	—	H 6.77 H' 5.74	—	Structure: 	962
$C_{19}H_{10}CrO_3$	340	$(h^6-C_{16}H_{10})Cr(CO)_3$	$CDCl_3$	H_{-1}, H_{-4} 6.28 H_{-2}, H_{-3} 5.54 H ~7.73	—	Structure:  T 33°	753
$C_{20}H_{12}CrO_3$	341	$(h^6-C_{17}H_{12})Cr(CO)_3$	Diglyme	H_{-1} 6.01 H_{-2}, H_{-3} 5.57 H_{-4} 6.37 H_{-5} 8.17 H_{-6}, H_{-9} 7.93 H_{-10} H_{-7}, H_{-8} 7.52	—	Structure:  T 110°	753

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References	
$C_{21}H_{12}CrO_8$	342	$(h^6-C_{18}H_{12})Cr(CO)_3$	Diglyme	H_{-1}	6.20	—	Structure: 	753
				H_{-2}, H_{-3}	5.75	—		
				H_{-4}	7.07	—		
				H_{-5}	9.07	—		
				H_{-6}, H_{-9}	8.22	—		
				H_{-7}, H_{-8}	7.72	—		
				H_{-11}		—		
				H_{-10}	8.43	—		
				H_{-12}	7.37	—		
						T 110°		
$C_{21}H_{12}CrO_3$	343	$(h^6-C_{18}H_{12})Cr(CO)_3$	$CDCl_3$	H_{-1}	6.20	—	Structure: 	753
				H_{-2}, H_{-3}	5.62	—		
				H_{-4}	6.78	—		
				H_{-5}, H_{-11}	8.60	—		
				H_{-6}	8.07	—		
				H_{-7}, H_{-8}	7.72	—		
				H_{-9}	7.22	—		
				H_{-10}	8.67	—		
				H_{-12}	8.02	—		
						T 33°		
$C_{19}H_{10}CrO_3$	344	$(h^6-C_{16}H_{10})Cr(CO)_3$	$CDCl_3$	H_{-1}, H_{-3}	5.62	—	Structure: 	753
				H_{-2}	6.02	—		
				H_{-4}, H_{-10}	7.50	—		
				H_{-5}, H_{-9}	7.79	—		
				H_{-6}, H_{-7}	7.91	—		
				H_{-8}		—		
						T 33°		

$C_{18}H_{10}CrO_4$	345	$(h^6-C_{15}H_{10}O)Cr(CO)_3$	$CDCl_3$	H_{-1}, H_{-2}	5.35	—
				H_{-3}	5.7dt	—
				H_{-4}	6.28dd	—
				H_{-6}	8.2m	—
				H_{-7}, H_{-8}	7.55m	—
				H_{-9}		
				H_{-10}, H_{-11}	7.09–6.5q	J_{10}
$C_9H_{18}B_3CrN_3O_3$	346	$[h^6-B_3N_3(CH_3)_6]Cr(CO)_3$	$CDCl_3$	$N-CH_3$	2.89	—
				$B-CH_3$	0.71	—
$C_{13}H_9CrNO_3$	347	$(h^6-C_6H_5 \cdot NC_4H_4)Cr(CO)_3$	$(CD_3)_2CO$	H	~5.9, 5.3	—
				H'	7.07t	—
				H''	6.20t	—
$C_{15}H_{13}CrNO_3$	348	$(h^6-C_6H_5 \cdot NC_6H_8)Cr(CO)_3$	$(CD_3)_2CO$	H	5.8m	—
				H'	5.78s	—
				H''	2.31s	—

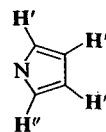
Structure:



738

Hexamethylborazolechromium
tricarbonyl. 100 MHz

756

 $NC_4H_4 =$ 

71

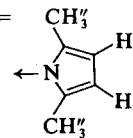
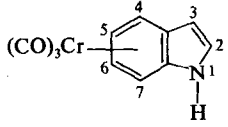
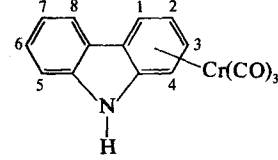
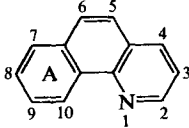
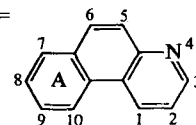
 $NC_6H_8 =$ 

TABLE II—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References							
$C_{11}H_7CrNO_3$	349	$(h^6-C_8H_7N)Cr(CO)_3$	$(CD_3)_2CO$	H_{-1}	10.48m	$J_{1,2}$ 2.6 $J_{1,3}$ 2.0	Structure: 	746						
				H_{-2}	7.48t	$J_{2,3}$ 3.3								
				H_{-3}	6.44m	$J_{3,7}$ 0.9								
				H_{-4}	6.44m	$J_{4,5}$ 6.7 $J_{4,6}$ 0.9 $J_{4,7}$ 0.7								
				H_{-5}	5.27t	$J_{5,6}$ 6.6 $J_{5,7}$ 0.7								
				H_{-6}	5.55t	$J_{6,7}$ 6.9								
				H_{-7}	6.55m	—								
				$C_{15}H_9CrNO_3$	350	$(h^6-C_{12}H_9N)Cr(CO)_3$			$(CD_3)_2CO$	H_{-1}	6.85d	$J_{1,2}$ 6.7	Structure: 	746
										H_{-2}	5.20t	$J_{2,3}$ 6.2		
										H_{-3}	5.70t	$J_{3,4}$ 7.0		
H_{-4}	6.20d	—												
H_{-5}, H_{-6}	~7.30m	—												
H_{-7}		—												
H_{-8}	7.92m	—												
NH	9.80m	—												
$C_{16}H_9CrNO_3$	351	$(h^6-C_{13}H_9N)Cr(CO)_3$	$(CD_3)_2CO$	H_{-10}	7.67m	—	$C_{13}H_9N =$ 	746						
				H_{-9}	5.49m	—								
				H_{-8}	5.49m	—								
				H_{-7}	6.47m	—								
				H_{-6}	7.67m	—								
				H_{-5}	7.67m	—								
				H_{-4}	8.37m	—								
				H_{-3}	7.67m	—								
				H_{-2}	9.06m	—								
						CR complexed with ring A 100 MHz								

$C_{16}H_9CrNO_3$	352	$(h^6-C_{13}H_9N)Cr(CO)_3$	$(CD_3)_2CO$	H_{-10}	7.08m	—
				H_{-9}	5.82m	—
				H_{-8}	5.82m	—
				H_{-7}	6.50m	—
				H_{-6}	7.83m	—
				H_{-5}	7.83m	—
$C_{20}H_{11}CrNO_3$	353	$(h^6-C_{17}H_{11}N)Cr(CO)_3$	$(CD_3)_2CO$	H_{-3}	8.95m	—
				H_{-2}	7.83m	—
				H_{-1}	8.95m	—
				$H_{-1}, H_{-5},$	~7.57m	—
				$H_{-6}, H_{-8},$		
				H_{-9}, H_{-10}		
$C_{47}H_{28}CrN_4O_3Zn$	354	$(h^6-C_{44}H_{28}N_4Zn)Cr(CO)_3$	—	H_{-2}, H_{-3}	5.77m	—
				H_{-4}	6.17	—
				H_{-7}	8.65s	—
				H_{-11}	8.10m	—
				H^*	6.67, 5.79	—
$C_{50}H_{28}Cr_2N_4O_6Zn$	355	$(h^6, h^6-C_{44}H_{28}N_4Zn)[Cr(CO)_3]_2$	—	$H^\dagger$	8.89	—
				$H^\ddagger$	8.19, 7.75	—
				H^*	6.56, 5.80	—
$C_{44}H_{28}N_4Zn$	757	$\alpha, \beta, \gamma, \delta$ -tetraphenyl- porphinzinc	—	$H^\dagger$	8.91	—
				$H^\ddagger$	8.17, 7.74	—
				H^*	6.56, 5.80	—

 $C_{13}H_9N =$ 

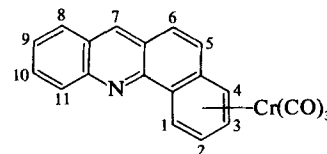
746

Cr complexed with ring A

100 MHz

Structure:

746

 $C_{44}H_{28}N_4Zn = \alpha, \beta, \gamma, \delta$ -tetraphenyl-
porphinzinc

757

*Complexed phenyl ring

†porphin protons

‡Uncomplexed phenyl rings

 $C_{44}H_{28}N_4Zn = \alpha, \beta, \gamma, \delta$ -tetraphenyl-
porphinzinc

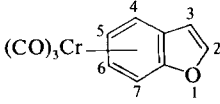
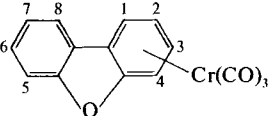
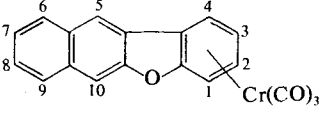
757

*Complexed phenyl rings

†Porphin protons

‡Uncomplexed phenyl rings

TABLE II—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{11}H_6CrO_4$	356	$(h^6-C_8H_6O)Cr(CO)_3$	$(CD_3)_2CO$	H_{-2}	7.70d	$J_{2,3}$ 2.4	Structure: 	746
				H_{-3}	6.87d	$J_{3,7}$ 1.0		
				H_{-4}	6.52q	$J_{4,5}$ 6.2		
				H_{-5}	5.30t	$J_{4,6}$ 1.1		
						$J_{5,6}$ 6.2		
				H_{-6}	5.68t	$J_{5,7}$ 0.8		
						$J_{6,7}$ 7.0		
$C_{15}H_8CrO_4$	357	$(h^6-C_{12}H_8O)Cr(CO)_3$	$(CD_3)_2CO$	H_{-1}	6.97dd	$J_{1,2}$ 6.2	Structure: 	746
				H_{-2}	5.47t	$J_{1,3}$ 1.0		
						$J_{2,3}$ 6.3		
				H_{-3}	5.95t	$J_{2,4}$ 0.6		
				H_{-4}	6.52d	$J_{3,4}$ 6.8		
				H_{-5}, H_{-6}	~ 7.62	—		
				H_{-7}		—		
$C_{19}H_{10}CrO_4$	358	$(h^6-C_{16}H_{10}O)Cr(CO)_3$	$(CD_3)_2CO$	H_{-1}	6.48d	—	Structure: 	746
				H_{-2}	6.03t	—		
				H_{-3}	5.50t	—		
				H_{-4}	7.07d	—		
				H_{-5}	8.63s	—		
				H_{-6}, H_{-9}	8.10m	—		
				H_{-7}, H_{-8}	7.65m	—		
				H_{-10}	8.10m	—		

$C_{26}H_{17}CrO_3P$ 359 ($h^6-C_{23}H_{17}P$)Cr(CO)₃

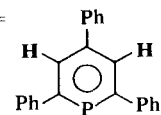
Dioxane

H

6.00d

J_{PH} 4.5

$C_{23}H_{17}P =$



758

$C_{11}H_6CrO_3S$ 360 ($h^6-C_8H_6S$)Cr(CO)₃

(CD₃)₂CO

H₋₂

7.72d

$J_{2,3}$ 5.6

H₋₃

7.27d

$J_{3,7} \sim 0.5$

H₋₄

6.56d

$J_{4,5}$ 6.6

$J_{4,7}$ 0.5

$J_{4,6}$ 1.1

$J_{5,6}$ 6.4

$J_{5,7}$ 1.1

$J_{6,7}$ 6.8

H₋₅

5.54t

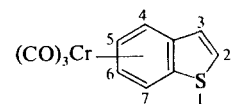
H₋₆

5.72t

H₋₇

6.68d

Structure:



746

$C_{15}H_{14}CrO_3S$ 361 ($h^6-C_{12}H_{14}S$)Cr(CO)₃

—

H₋₂

7.17d

—

H₋₃

6.87d

—

H₋₄

6.55m

—

H₋₆

4.72m

—

H₋₈

3.58q

—

5-CH₃

2.60s

—

7-CH₃

2.20s

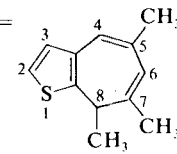
—

8-CH₃

0.37d

—

$C_{12}H_{14}S =$



523

$C_{15}H_8CrO_3S$ 362 ($h^6-C_{12}H_8S$)Cr(CO)₃

(CD₃)₂CO

H₋₁

6.91dd

$J_{1,2}$ 6.3

H₋₂

5.45t

$J_{1,3}$ 1.0

H₋₃

5.90t

$J_{2,3}$ 6.3

H₋₄

6.68d

$J_{2,4}$ 0.9

H₋₅

7.95m

—

H₋₆, H₋₇

7.62m

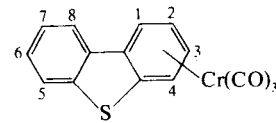
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H₋₈

8.30m

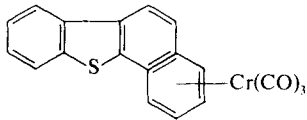
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Structure:



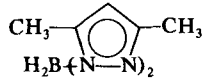
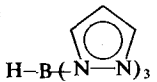
746

TABLE II—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{19}H_{10}CrO_3S$	363	$(h^6-C_{16}H_{10}S)Cr(CO)_3$	—	n.a.		Structure:  Signals at δ 1.75m, 2.32m, 3.12m, 3.38m, 4.10m, in ratio 3:3:1:1:2	746
(7) MIXED LIGANDS							
$C_{14}H_{13}CrNO_3$	364	$(h^5-C_5H_5)Cr[C(OCH_3)C_6H_5]-(NO)(CO)$	$(CD_3)_2CO$	H 5.04s H' 4.61s H'' 7.20m	— — —	—	60
$C_{17}H_{21}CrNO_2$	365	$(h^2-CH_2=CHCN)(h^6-C_6(CH_3)_6)Cr(CO)_2$	$(CD_3)_2CO$	H 0.8–1.0	—	100 MHz compared to free and 6-bonded acrylonitrile (δ 5.0–6.0 and 5.4–6.0 respectively)	75
$C_{27}H_{17}CrNO_2$	366	$(h^6-C_{18}H_{12})Cr(CNC_6H_5)(CO)_2$	—	—	—	$C_{18}H_{12}$ = Triphenylene	76
(8) MISCELLANEOUS DERIVATIVES							
$[C_5H_{11}B_9CrO_3]_2$	367	$[(\pi-(3)-1,2-C_2H_{11}B_9)Cr(CO)_3]^{2-}$	CH_3CN	^{11}B 25.4d* 14.7d* (ratio 1:2)	— —	$C_2H_{11}B_9$ = (3)-1,2-dicarbollide ion Isolated as the tetraethyl ammonium salt *Relative to $BF_3O(Et)_2$	77

$C_4H_8B_3O_4$	368	$Cr(B_3H_8)(CO)_4$	CH_3CN	H	$-7.3b^*$	—	*Bridging hydrogen between boron and chromium	78
				^{11}B	$23.0b^\dagger$			
					$61.3b^\dagger$		†Relative to external $B(OMe)_3$	
$[C_{10}HCr_2O_{10}]^-$	369	$\{[Cr(CO)_5]_2(H)^*\}^-$	THF/ $NaBH_4$	H	-19.17	—	*Hydrogen bridge	915
			THF	H	$-19.47^\dagger$	—	†As the tetraethyl ammonium salt	1027
$[C_{10}HCrO_{10}W]^-$	370	$\{[Cr(CO)_5W(CO)_5](H)^*\}^-$	THF/ $NaBH_4$	H	-15.43	—	*Hydrogen bridge	915
$[C_{10}HCrMoO_{10}]^-$	371	$\{[Cr(CO)_5Mo(CO)_5](H)^*\}^-$	THF/ $NaBH_4$	H	-15.31	—	*Hydrogen bridge	915
$C_8H_3CrNO_5$	372	$Cr(NC-CH=CH_2)(CO)_5$	$(CD_3)_2CO$	H	$6.2-5.5$	—	—	75
$C_8H_7CrNO_6$	373	$Cr[NH=C(CH_3)OCH_3](CO)_5$	C_6D_6	H	$5.38s$	—	—	79
				H'	$1.68s^*$	—	* CH_3 <i>syn</i> to H	
				H''	$2.38s$	—		
			C_6D_6	H	$6.47s$	—	* CH_3 <i>anti</i> to H	79
				H'	$0.70s$	—		
				H''	$2.75s$	—		
$C_{12}H_7CrNO_5$	374	$Cr(NH=CH'.C_6H_5)(CO)_5$	$(CD_3)_2CO$	H	$10.62bd$	$J_{HH'}23$	60 and 100 MHz	80
				H'	$8.62d$	$J_{HH'}23$		
				H''	$7.64m$	—		
$C_{14}H_{12}CrO_6Se$	375	$Cr[Se(C_6H_5)CH'(CH_3'OCH_3'')](CO)_5$	$CDCl_3$	H	$7.63m$	—	—	80
				H'	$5.20q$	—		
				H''	$1.60d$	—		
				H'''	$3.55s$	—		

TABLE III
Molybdenum complexes

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
(1) <i>MONOHAPTO LIGANDS</i>							
$C_{19}H_{27}BMoN_6O_3$	1	$[H_2B(3,5-(CH_3)_2Pz)_2]Mo(CO)_3^-$ $(CH_3)(C_5H_8N_2)$	$CDCl_3$	n.a.	—	Signals at δ 6.12s, 5.85s, 5.58s, 2.62s, 2.43s, 2.40s, 1.95s, 1.87, 1.71 and 0.3b, in ratio 1:1:1:3:3:3:3:2:1:6:1	81
						$H_2B(3,5-(CH_3)_2Pz)_2 = C_5H_8N_2 =$  3,5-dimethylpyrazole	
$C_{14}H_{15}MoN_6O_3$	2	$[HB(Pz)_3]Mo(CO)_3(CH_2CH_3)^-$	—	H 3.62 H' 1.40	—	$H-B(Pz)_3 =$  $H-B-(N-N)_3$	53
$C_{25}H_{21}MoO_5P$	3	$Mo[C(CH_3)OCH_3][P(C_6H_5)_3]-(CO)_4$	C_6D_6	H 2.50s H' 4.10s H'' 7.34m	— — —	—	945
$[C_8H_3MoO_5]^-$	4	$[Mo(CO)_5(C\equiv CCH_3)]^-$	CH_2Cl_2	H 1.74	—	Isolated as the bis (triphenyl phosphine) iminium salt	19
$[C_{17}H_{13}^- MoNO_6]^-$	5	$[Mo(CO)_5(COCH_3)]^-$	CH_2Cl_2	H 2.24 H' 3.28	— —	Isolated as quaternary methyl ammonium salt $[N(CH_3)_4]^+$	33
$[C_{12}H_{15}^- MoNO_6]^-$	6	$[Mo(CO)_5(COC_6H_5)]^-$	CH_2Cl_2	H 7.36 H' 3.04	—	Isolated as quaternary methyl ammonium salt $[N(CH_3)_4]^+$	33

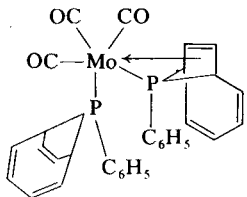
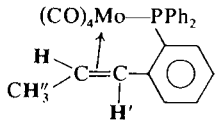
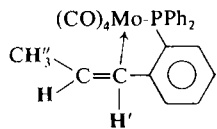
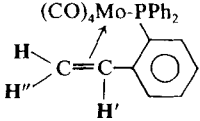
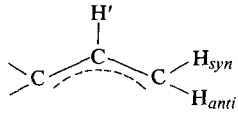
$C_9H_9MoNO_3Si$	7	$Mo[C=NSi(CH_3)_3](CO)_3$	C_6H_6	H	-0.01	—	—	1017
$C_9H_9MoNO_3Sn$	8	$Mo[C=NSn(CH_3)_3](CO)_3$	C_6H_6	H	0.12	$J(^{119}SnH) 60$ $J(^{117}SnH) 57$	—	1017
(2) DIHAPTO LIGANDS								
$[C_{14}H_6Cl-MoO_{11}]^-$	9	$[(h^2-C_4H_2O_3)_3Mo(CO)_2(Cl)]^-$	THF	H	4.22*	$J 5$	$C_4H_2O_3 =$ Maleic anhydride Isolated as lithium salt	1021
$[C_{14}H_6ClMoN_3O_8]^-$	10	$[(h^2-C_4H_2NH'O_2)_3Mo(CO)_2(Cl)]^-$	THF	H H'	4.10* 8.90s	$J 5$	$C_4H_2NHO_2 =$ Maleimide Isolated as lithium salt *Centre of AB quartet	1021
$C_{31}H_{26}MoO_3P_2$	11		$CDCl_3$		3.3-3.05 6.25-5.45 7.3, 7.26, 7.19 7.0-6.7	— — —	Bridgehead protons Olefinic protons Phenyl protons	83
$C_{25}H_{19}MoO_4P$	12		$CDCl_3$	H H' H''	4.38 5.64 1.92	$J_{HH'} 13.4$ $J_{HH''} 5.9$	—	52
$C_{25}H_{19}MoO_4P$	13		$CDCl_3$	H H' H''	4.96 5.92 1.97	$J_{HH'} 10.5$ $J_{HH''} 6.3$	—	52 1016

TABLE III—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{25}H_{17}MoO_4P$	14		$CDCl_3$	H	3.48	$J_{HH'}14.5$	—	50
				H'	5.98	$J_{H'H''}9.5$		
				H''	3.91	$J_{HH''}2.5$		
(3) TRIHAPTO LIGANDS								
$C_9H_{11}BrMoN_2O_2$	15	$(h^3-CH_2CH'CH_2)Mo(CO)_2-(CH_3CN)_2(Br)$	C_6H_5CN	H_{syn}	3.45d	$J_{HH'}6.0$		84
				H_{anti}	1.30d	$J_{HH'}9.0$		
				H'	4.37m	—		
				H''	1.92s	—		
			$CDCl_3$	H_{syn}	3.36d	$J_{HH'}6.3$	External TMS reference	
				H_{anti}	1.18d	$J_{HH'}9.0$		
				H''	2.14s	—		
			C_6H_6	H_{syn}	3.57d	$J_{HH'}6.1$		
				H_{anti}	1.36d	$J_{HH'}9.0$		
				H''	1.18	—		
$C_{15}H_{15}BrMoN_2O_2$	16	$(h^3-CH_2CH'CH''Ph)Mo(CO)_2-(CH_3CN)_2(Br)$	C_6H_5CN	H_{syn}	3.68d	$J_{HH'}6.0$	—	84
				H_{anti}	1.62d	$J_{HH'}9.0$		
				H'	5.1m	—		
				H''	3.06d	$J_{H'H''}9.5$	—	
$C_9H_{11}ClMoN_2O_2$	17	$(h^3-CH_2CH'CH_2)Mo(CO)_2-(CH_3CN)_2(Cl)$	C_6H_5CN	H_{syn}	3.59d	$J_{HH'}6.0$		84
				H_{anti}	1.01d	$J_{HH'}9.0$		
				H'	4.77	—		
				H''	1.92s	—		

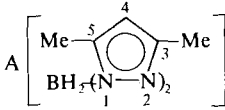
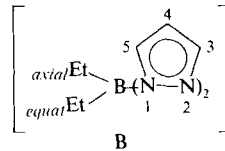
			CDCl ₃	H_{syn} H_{anti} H''	3.33d 1.20d 2.14s	$J_{HH'}$ 6.0 $J_{HH'}$ 9.0 —	External TMS reference	
C ₁₆ H ₁₇ - ClMoN ₂ O ₂	18	(<i>h</i> ³ -CH ₂ C(CH ₃)CH ₂)Mo(CO) ₂ - (C ₅ H ₅ N) ₂ (Cl)	CCl ₄	H_{syn} H_{anti} H'	3.24* 1.33* 2.05	— — —	*Reviewer's assignment	85
C ₉ H ₁₁ IMoN ₂ O ₂	19	(<i>h</i> ³ -CH ₂ CH'CH ₂)Mo(CO) ₂ - (CH ₃ CN) ₂ (I)	C ₆ H ₅ CN	H_{syn} H_{anti} H' H''	3.59d 1.45d 4.56m 1.92s	$J_{HH'}$ 6.0 $J_{HH'}$ 9.4 — —	—	84
C ₁₀ H ₁₁ MoN ₃ O ₂ S	20	(<i>h</i> ³ -CH ₂ CH'CH ₂)Mo(CO) ₂ - (CH ₃ CN) ₂ (SCN)	C ₆ H ₆	H_{syn} H_{anti} H' H''	3.45d 1.45d 4.16m 1.05s	$J_{HH'}$ 6.0 $J_{HH'}$ 9.0 — —	—	84
C ₁₄ H ₁₆ Br ₂ Mo ₂ - N ₂ O ₄	21	[(<i>h</i> ³ -CH ₂ CHCH ₂)Mo(CO) ₂ - (CH ₃ CN)Br] ₂	C ₆ H ₅ NO ₂	H_{syn} H_{anti} H'	3.05d 0.28d 1.83s	$J_{HH'}$ 6.1 $J_{HH'}$ 10.0 —	External TMS reference	84
			CDCl ₃	H_{syn} H_{anti} H'	3.64d 1.55d 2.14s	$J_{HH'}$ 7.0 $J_{HH'}$ 9.7 —	External TMS reference	
			C ₆ H ₆	H_{syn} H_{anti} H'	3.96d 1.53 1.18s	$J_{HH'}$ 6.7 $J_{HH'}$ 9.0 —		
C ₁₄ H ₁₆ Cl ₂ Mo ₂ - N ₂ O ₄	22	[(<i>h</i> ³ -CH ₂ CHCH ₂)Mo(CO) ₂ - (CH ₃ CN)Cl] ₂	C ₆ H ₅ CN	H_{syn} H_{anti} H'	3.60d 1.39d 1.92s	— — —	—	84
			CDCl ₃	H_{syn} H_{anti} H'	3.61 1.58d 2.14s	— — —	External TMS reference	

TABLE III—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{20}H_{30}Mo_2O_{10}$	23	$[(h^3-CH_2CHCH_2)Mo(CO)_2-(n-C_4H_9OH)_2C_2O_4]$	Acetone	H_{syn} 3.61d H_{anti} 1.23d	$J_{HH'}$ 6.7 $J_{HH'}$ 9.0	(CH_3) ₂ CO reference $C_2O_4 =$ 	84
$[C_{10}H_{10}Br_3Mo_2O_4]^-$	24	$\{[(h^3-CH_2CH'CH_2)Mo(CO)_2]_2-(Br)_3\}^-$	Acetone	H_{syn} 3.53 H_{anti} 0.89 H' 3.90m	$J_{HH'}$ 6.7 $J_{HH'}$ 9.2	Acetone as reference	
$[C_{12}H_{14}Br_3Mo_2O_4]^-$	25	$\{[(h^3-CH_2CH'CH''CH''')Mo(CO)_2]_2(Br)_3\}^-$	(CD_3) ₂ CO	H_{syn} ~3.6m H', H'' H_{anti} 0.7d H''' 2.08d	— $J_{HH'}$ 9.2 $J_{H''H'''} 7.5$	Isolated as the quaternary ethyl ammonium salt	86
$[C_{10}H_{10}Cl_3Mo_2O_4]^-$	26	$\{[(h^3-CH_2CH'CH_2)Mo(CO)_2]_2-(Cl)_3\}^-$	Acetone	H_{syn} 3.42d H_{anti} 0.89d H' 3.68m	$J_{HH'}$ 6.9 $J_{HH'}$ 10.0 —		84
$[C_{12}H_{14}Cl_3Mo_2O_4]^-$	27	$\{[(h^3-CH_2C(CH_3)CH_2)Mo(CO)_2]_2(Cl)_3\}^-$	(CD_3) ₂ CO	H_{syn} 2.97s H_{anti} 0.75s H' 2.09s	— — —	Isolated as the quaternary ethyl ammonium salt	86
$[C_{12}H_{14}Cl_3Mo_2O_4]^-$	28	$\{[(h^3-CH_2C(CH_3)CH_2)Mo(CO)_2]_2(Cl)_3\}^-$	(CD_3) ₂ SO	H_{syn} 2.75* H_{anti} 0.8* H' 1.9 H'' 3.2 H''' 1.17	— — — — —	Isolated as the quaternary ethyl ammonium salt [N(CH ₂ CH ₃) ₄] ⁺ *Reviewer's assignment	85

$[\text{C}_{12}\text{H}_{17}\text{Mo}_2\text{O}_7]^-$	29	$\{[(h^3\text{-CH}_2\text{C}(\text{CH}_3)\text{CH}_2)\text{Mo}(\text{CO})_2]_2\text{-CH}_2\text{Cl}_2(\text{OH})_3\}^-$	H_{syn}	2.64*	—	Isolated as the quaternary ethyl ammonium salt	85
			H_{anti}	0.48*	—	$[\text{N}(\text{CH}_2'\text{CH}_3''')_4]^+$	
			H'	1.87	—	*Reviewer's assignment	
			H''	3.27	—		
			H'''	1.38	—		
$[\text{C}_{15}\text{H}_{23}\text{Mo}_2\text{O}_7]^-$	30	$\{[(h^3\text{-CH}_2\text{C}(\text{CH}_3)\text{CH}_2)\text{Mo}(\text{CO})_2]_2\text{-}(\text{CD}_3)_2\text{SO}(\text{OCH}_3)_3\}^-$	H_{syn}	2.61*	—	Isolated as the quaternary ethyl ammonium salt	85
			H_{anti}	0.33*	—	$[\text{N}(\text{CH}_2'''\text{CH}_3^{\text{IV}})_4]^+$	
			H'	1.71	—	*Reviewer's assignment	
			H''	4.82, 3.68	—		
			H'''	3.16	—		
			H^{IV}	1.14	—		
$[\text{C}_{18}\text{H}_{29}\text{Mo}_2\text{O}_7]^-$	31	$\{[(h^3\text{-CH}_2\text{C}(\text{CH}_3)\text{CH}_2)\text{Mo}(\text{CO})_2]_2\text{-}(\text{CD}_3)_2\text{SO}(\text{OEt})\}^-$	H_{syn}	2.6*	—	Isolated as the quaternary ethyl ammonium salt	85
			H_{anti}	0.25*	—	$[\text{N}(\text{CH}_2'\text{CH}_3''')_4]^+$	
			H'	1.80	—	*Reviewer's assignment	
			H''	3.18	—		
			H'''	1.16	—		
$[\text{C}_{30}\text{H}_{29}\text{Mo}_2\text{O}_4\text{S}_3]^-$	32	$\{[(h^3\text{-CH}_2\text{C}(\text{CH}_3)\text{CH}_2)\text{Mo}(\text{CO})_2]_2(\text{SC}_6\text{H}_5)_3\}^-$	H_{syn}	2.99*	—	Isolated as the quaternary ethyl ammonium salt	85
			H_{anti}	0.8*	—	$[\text{N}(\text{CH}_2'''\text{CH}_3^{\text{IV}})_4]^+$	
			H'	2.28	—	*Reviewer's assignment	
			H''	7.7–8.2m, 6.9–7.8m	—		
			H'''	3.48	—		
			H^{IV}	1.36	—		
$\text{C}_{17}\text{H}_{17}\text{BMoN}_8\text{O}_2$	33	$(h^3\text{-CH}_2\text{-CH-CH}_2)\text{Mo}[\text{B}(\text{C}_3\text{H}_3\text{-N}_2)_4](\text{CO})_2$	—	—	—	Complex spectrum, showing the presence of the $[\text{B}(\text{C}_3\text{H}_3\text{N}_2)_4]$ ligand	1022

TABLE III—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{15}H_{20}BBr-MoN_4O_2$	34	$(h^3-CH_2CBrCH_2)Mo(CO)_2-(C_{10}H_{16}BN_4)$	$CDCl_3$	n.a.	—	Signals at δ 5.76s, 3.81s, 2.52s, 2.12, 1.95s, in ratio 1:1:3:3:1. Noninert gas configuration (16 electrons)	81
						$C_{10}H_{16}BN_4 =$ 	
$C_{15}H_{21}BMoN_4O_2$	35	$(h^3-CH_2CH'CH'_2)Mo(CO)_2-(C_{10}H_{16}BN_4)$	$CDCl_3$	H 3.7d* H' 4.3–3.7m H'' 1.59† H₋₃ 8.15d H₋₄ 6.22t H₋₅ 7.43d	J 7.0 — J 9.5 J 2.1, 0.5 J 2.2 J 2.3, 0.5	*More probably H_{syn} and H''_{syn} †More probably H_{anti} and H''_{anti}	81 87
				Et(equat) 0.84b CH₃CH₂ (axial) CH₃CH₂ (axial)-2.4‡	— — —	‡Implies "hydridic" character and suggests that the pseudoaxial methylene hydrogens are intruding into an empty metal orbital	
$C_{15}H_{21}BMoN_4O_2$	36	$(h^3-CH_2CH'CH'_2)Mo(CO)_2-(C_{10}H_{16}BN_4)$	$CDCl_3$	H_{syn} 3.51d* H_{anti} 1.40d* H' 4.04m*	J 7.5 J 10.5 —	^{11}B NMR chemical shift +33.2t ppm relative to external trimethylborate (J 90)	81 87
						$C_{10}H_{16}BN_4 =$ 	

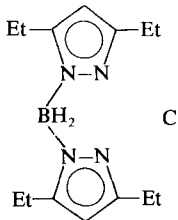
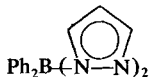
				H_{-4}	5.67s	—	$C_{10}H_{16}BN_4$ as above (A) T60° (limiting high temperature spectrum). Temperature dependent spectrum is consistent with rotation or pseudorotation of the π -allyl group	
				$C_{-3}CH_3$	2.50s	—		
				$C_{-5}CH_3$	2.07s	—		
$C_{19}H_{29}BMoN_4O_2$	37	$(\eta^3\text{-CH}_2\text{CHCH}_3)\text{Mo(CO)}_2\text{-}$ $(C_{14}H_{24}BN_4)$	$CDCl_3$	H	4.27m	—	*Reviewer's assignment Signals at δ 5.90s, 3.51d (J 7), 2.83q (J 7.3), 1.93d (J 2.7), 1.23t (J 7.3) in ratio 2:2:8:2:12 ^{11}B NMR + 33t ppm relative to external trimethylborate (J 76)	81
							$C_{14}H_{24}BN_4 =$	
								
$C_{20}H_{31}BMoN_4O_2$	38	$(\eta^3\text{-CH}_2\text{C(CH}_3\text{)CH}_2)\text{Mo(CO)}_2\text{-}$ $(C_{14}H_{24}BN_4)$	$CDCl_3$	n.a.		—	Signals at δ 5.78s, 3.7–2.8m, 1.69s and 1.4–0.9m in ratio 2:10:3:14. ^{11}B NMR at +32.9t ppm relative to external tri- methylborate (J 80) $C_{14}H_{24}BN_4$ as above (C)	81

TABLE III—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{21}H_{25}BMoN_4O_2$	39	$(h^3-CH_2CPhCH_2)Mo(CO)_2^-$ ($C_{10}H_{16}BN_4$)	$CDCl_3$	n.a.	—	Signals at δ 8.2d (J 2.1), 7.34d (J 2.3), 7.15m, 6.22t (J 2.2), 4.18s, 1.69s, 0.64s, 0.27t (J 7), and -3.8q (J 7) in ratio 2:2:5:2:2:2:5:3:2. ^{11}B NMR + 20.1s relative to external trimethylborate $C_{10}H_{16}BN_4$ as above (B)	81
$C_{21}H_{25}BMoN_4O_2$	40	$(h^3-CH_2CPhCH_2)Mo(CO)_2^-$ ($C_{10}H_{16}BN_4$)	$CDCl_3$	n.a.	—	^{11}B NMR + 33.6t ppm relative to external trimethylborate $C_{10}H_{16}BN_4$ as above (A)	81
$C_{23}H_{21}BMoN_4O_2$	41	$(h^3-CH_2CHCH_2)Mo(CO)_2^-$ ($C_{18}H_{16}BN_4$)	$CDCl_3$	n.a.	—	Signals at δ 8.28s, 7.8–7.1m, 6.9m, 6.53m, 6.30m, 3.0m, 2.31d (J 7), and 1.05d (J 10) in ratio 2:8:2:2:2:1:2:2 $C_{18}H_{16}BN_4 =$  D	81
$C_{24}H_{23}BMoN_4O_2$	42	$(h^3-CH_2C(CH_3)CH_2)Mo(CO)_2^-$ ($C_{18}H_{16}BN_4$)	$CDCl_3$	n.a.	—	Signals at δ 8.18d (J 2), 7.53d (J 2.3), 7.28m, 6.76m, 6.25t (J 2.1), 2.57s, 1.56s, 0.87s in ratio 2:2:5:5:2:2:3:2. ^{11}B NMR + 19.3s ppm relative to external trimethylborate $C_{18}H_{16}BN_4$ as above (D)	81

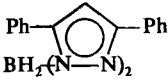
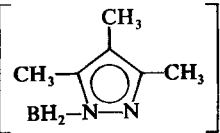
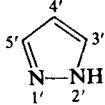
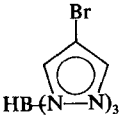
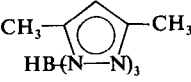
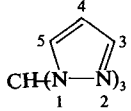
$C_{25}H_{33}BMoN_4O_2$	43	$(h^3-CH_2CPhCH_2)Mo(CO)_2-$ ($C_{14}H_{24}BN_4$)	$CDCl_3$	n.a.	—	—	Signals at δ 7.15m, 5.75m, 4.16d (J 11), 5.03m, 2.23m, and 1.7– 0.7m in ratio 5:2:2:4:4:12 ^{11}B NMR + 33.8 relative to external trimethylborate $C_{14}H_{24}BN_4$ as above (C)	81
$C_{35}H_{29}BMoN_4O_2$	44	$(h^3-CH_2CHCH_2)Mo(CO)_2-$ ($C_{30}H_{24}BN_4$)	$CDCl_3$	n.a.	—	—	Signals at δ 8.1–7.3m, 7.30s, 2.55s, 3.8m, 3.2bd, and 1.08d (J 10) in ratio 10:10:2:1:2:2. ^{11}B NMR + 31.0t ppm relative to external trimethylborate $C_{30}H_{24}BN_4 =$ 	81
$[C_{10}H_{10}Br_3-$ $Mo_2O_4]^-$	45	$\{[(h^3-CH_2CH'CH_2)Mo(CO)_2]_2-$ (Br) $\}_3^-$	$(CD_3)_2CO$	H_{syn} H_{anti} H' H'' H'''	3.46d 0.9d 3.8 comp. 3.61q 1.49t	$J_{HH'}6.5$ $J_{HH'}9.7$ — J 7.6 —	Isolated as quaternary ethyl ammonium salt $[N(CH_2^2CH_3'')_4]^+$	86
$[C_{10}H_{10}Cl_3-$ $Mo_2O_4]^-$	46	$\{[(h^3-CH_2CH'CH_2)Mo(CO)_2]_2-$ (Cl) $\}_3^-$	$(CD_3)_2CO$	H_{syn} H_{anti} H' H'' H'''	3.4d 0.8d 3.7m 3.5q 1.4t	$J_{HH'}65$ $J_{HH'}9.5$ — J 7.4 —	Isolated as quaternary ethyl ammonium salt $[N(CH_2^2CH_3'')_4]^+$	86
$C_{17}H_{25}BMoN_4O_2$	47	$(h^3-CH_2CHCH_2)Mo(CO)_2-$ ($C_{12}H_{20}BN_4$)	$CDCl_3$	n.a.	—	—	Methyl signals at δ 2.5b, 2.06, and 1.87. π -Allyl and other signals at 4.0m, 3.5b and 1.4b $C_{12}H_{20}BN_4 =$ 	81

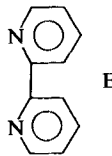
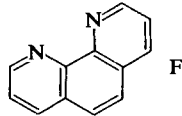
TABLE III—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{18}H_{25}BMoN_6O_2$	48	$(h^3\text{-CH}_2\text{CH}'\text{CH}_2')\text{Mo}(\text{CO})_2\text{-}(\text{C}_{10}\text{H}_{16}\text{BN}_4)(\text{C}_3\text{H}_4\text{N}_2)$	CDCl_3	H	4.2m*	—	$\text{C}_{10}\text{H}_{16}\text{BN}_4$ as above (B)	81
				H'	3.38d†	$J\ 7$	$\text{C}_3\text{H}_4\text{N}_2 =$ 	87
				H''	1.57d‡	$J\ 9.5$		
				H_{-3}	7.79d	$J\ 2$		
				H_{-4}	6.17t	$J\ 2.2$		
				H_{-5}	7.69d	$J\ 2.4$	*More probably H'	
				Et(equat)	0.34	—	†More probably H_{syn} and H''_{syn}	
				Et(axial)	0.9m	—	‡More probably H_{anti} and H''_{anti}	
				$\text{H}_{-3'}$	7.98d	—		
				$\text{H}_{-4'}$	6.17t	$J\ 2.2$		
				$\text{H}_{-5'}$	7.06d	—		
$C_{14}H_{12}BBr_3\text{-}MoN_6O_2$	49	$(h^3\text{-CH}_2\text{CH}'\text{CH}_2)\text{Mo}(\text{CO})_2\text{-}[\text{HB}(4\text{-BrPz})_3]^*$	CDCl_3	NH	8.70bs	—		
				H_{syn}	3.78	—	Pz stands for 1-pyrazolyl	88
				H_{anti}	1.70d	$J\ 9.0$		
				H'	3.78	—	$\text{HB}(4\text{-BrPz})_3 =$ 	
$C_{15}H_{14}BBr_3\text{-}MoN_6O_2$	50	$(h^3\text{-CH}_2\text{C}(\text{CH}_3)\text{CH}_2)\text{Mo}(\text{CO})_2\text{-}[\text{HB}(4\text{-BrPz})_3]^*$	CDCl_3	H_{syn}	3.66	—	*See below	88
				H_{anti}	1.66	—		
				H'	1.78	—		
$C_{20}H_{27}BMoN_6O_2$	51	$(h^3\text{-CH}_2\text{CH}'\text{CH}_2)\text{Mo}(\text{CO})_2\text{-}[\text{HB}(3,5\text{-(CH}_3)_2\text{Pz})_3]^*$	CDCl_3	H_{syn}	3.66d	$J\ 7$	*See below	88
				H_{anti}	1.93d	$J\ 10$	$\text{HB}(3,5\text{-(CH}_3)_2\text{Pz})_3 =$ 	
				H'	4.1	—		
$C_{21}H_{29}BMoN_6O_2$	52	$(h^3\text{-CH}_2\text{C}(\text{CH}_3)\text{CH}_2)\text{Mo}(\text{CO})_2\text{-}[\text{HB}(3,5\text{-(CH}_3)_2\text{Pz})_3]^*$	CDCl_3	H_{syn}	4.49	—		
				H_{anti}	1.50	—		
				H'	1.25	—	*See below	88

$C_{26}H_{31}BMoN_6O_2$	53	$(h^3-CH_2C(C_6H_5)CH_2)Mo(CO)_2-[HB(3,5-(CH_3)_2Pz)_3]^*$	$CDCl_3$	H_{syn} H_{anti} H'	4.05s 1.54s 6.9–6.5m	— — —		88
$[C_{15}H_{15}MoN_6O_2]^+$	54	$[(h^3-CH_2CH'CH_2)Mo(CO)_2-(C_{10}H_{10}N_6)]^+$	—	H_{syn} H_{anti} H'' H_{-3} H_{-4} H_{-5}	3.58m 1.38d 8.42s 8.15b 6.33t 7.98d	— J 8.5 J 2.5 J 2.9	Isolated as the PF_6^- salt $C_{10}H_{10}N_6 =$ 	89
$C_{24}H_{32}Mo_2N_8O_4$	55	$[(h^3-CH_2CH'CH_2)Mo(CO)_2-(NCN(CH_2^III)CH_2^{IV}CH_2^{IV})_2(N(CH_2^VI)C\equiv N)_2]^*$	$CDCl_3$	H_{syn} H_{anti} H' H'' H''' H^{IV} H^V H_{trans}^V H^{VI}	3.14d 1.08d 3.8m 2.95s 3.72d 5.8m 5.45d 5.36d 3.62s	$J_{HH'}$ 6.5 $J_{HH'}$ 9.5 — — $J_{H''H^{IV}}$ 5.5 — J_{cis} 7 J_{trans} 18 —	External TMS *The two cyanamide monoanions are in bridging positions	90
$C_{32}H_{40}Mo_2N_8O_4$	56	$[(h^3-CH_2CH'CH_2)Mo(CO)_2-(NCN(CH_2^{III}CH_2^{IV})_2)_2(N(CH_2^{VI}CH_2^{VII})C\equiv N)_2]^*$	$CDCl_3$	H_{syn} H_{anti} H' H'' H''' H_{cis}^{IV} H_{trans}^{IV} H^V H^{VI} H^{VII}	3.14d 1.08d 3.8m 3.76d 5.95m 5.43d 5.35d 4.40d 6–5.5 ~5.4d	$J_{HH'}$ 6.5 $J_{HH'}$ 9.5 — $J_{H''H^{III}}$ 5.5 — J_{cis} 8 J_{trans} 17 $J_{H^VH^{VI}}$ 6.2 — —	External TMS *The two cyanamide monoanions are in bridging positions	90

*The stereochemical non-rigidity of these complexes, manifested in their temperature dependent spectra, is attributed to rotation of the tridentate tris(1-pyrazolyl) borate ligand rather than of the π -allyl group

TABLE III—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{15}H_{13}IMoN_2O_2$	57	$(h^3-CH_2CH'CH_2)Mo(CO)_2^-$ ($C_{10}H_8N_2$)(I)		H_{syn} 3.31d H_{anti} 1.50d H' 3.5m	$J_{HH'}$ 6 $J_{HH'}$ 9 —	HMDS as reference. 100 MHz $C_{10}H_8N_2 =$  E	91
$C_{17}H_{15}MoN_3O_2S$	58	$(h^3-CH_2C(CH'_3)CH_2)Mo(CO)_2^-$ ($C_{10}H_8N_2$)(NCS)		H_{syn} 3.03s H_{anti} 1.47s H' 1.01	— — —	HMDS as reference (τ 9.95) 100 MHz $C_{10}H_8N_2$ as above (E)	91
$C_{19}H_{15}MoN_3O_2S$	59	$(h^3-CH_2C(CH'_3)CH_2)Mo(CO)_2^-$ ($C_{12}H_8N_2$)(NCS)		H_{syn} 3.20s H_{anti} 1.55s H' 0.72s	— — —	HMDS as reference. 100 MHz $C_{12}H_8N_2 =$  F	91
$[C_{20}H_{18}MoN_3O_2]^+$	60	$[(h^3-CH_2CH'CH_2)Mo(CO)_2^-]$ ($C_{10}H_8N_2$)(C_5H_5N)] $^+$		H_{syn} 3.56d H_{anti} 1.80 H' 3.5m	$J_{HH'}$ 6 $J_{HH'}$ 9 —	HMDS as reference. 100 MHz Isolated as tetrafluoroborate $C_{10}H_8N_2$ as above (E)	91
$[C_{21}H_{20}MoN_3O_2]^+$	61	$[(h^3-CH_2C(CH'_3)CH_2)Mo(CO)_2^-]$ ($C_{10}H_8N_2$)(C_5H_5N)] $^+$		H_{syn} 3.33s H_{anti} 1.77s H' 1.15s	— — —	HMDS as reference. 100 MHz Isolated as the tetrafluoroborate $C_{10}H_8N_2$ as above (E)	91
$[C_{22}H_{18}MoN_3O_2]^+$	62	$[(h^3-CH_2CH'CH_2)Mo(CO)_2^-]$ ($C_{12}H_8N_2$)(C_5H_5N)] $^+$		H_{syn} 3.70d H_{anti} 1.88d H' 3.5m	$J_{HH'}$ 6 $J_{HH'}$ 9 —	HMDS as reference. 100 MHz Isolated as the tetrafluoroborate $C_{12}H_8N_2$ as above (F)	91

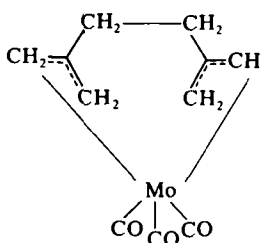
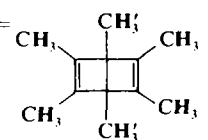
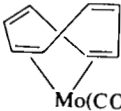
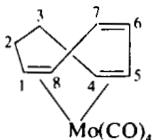
$C_8H_{15}ClMoN_2O_2$	63	$(h^3-CH_2C(CH_3)CH_2)Mo(CO)_2-(C_2H_8N_2)(Cl)$	$(CD_3)_2SO$	H_{syn} H_{anti} H'	3.0 0.78 0.78	— — —	$C_2H_8N_2$ = ethylene diamine	85
$C_{11}H_{12}MoO_3$	64		—	n.a.	—	—	Signals at δ 3.35s, 2.32s, 2.15s in ratio 1:1:1	55
(4) TETRAHAPTO LIGANDS								
$C_8H_6MoO_4$	65	$(h^4-C_4H_6)Mo(CO)_4$	—	H	1.60s	—	C_4H_6 = 	55
$C_8H_4MoO_4$	66	$(h^4-C_4H_4)Mo(CO)_4$	—	H	4.06	—	C_4H_4 = cyclobutadiene	54
$C_{12}H_{12}MoO_4$	67	$(h^4-C_4(CH_3)_4)Mo(CO)_4$	—	H	1.94	—	$C_4(CH_3)_4$ = tetramethyl cyclobutadiene	54
$C_{60}H_{40}Br_2Mo_2O_4$	68	$\{[h^4-C_4(C_6H_5)_4]Mo(CO)_2\}_2(Br)_2^*$	—	H	7.24s	—	*Bridging Br ligands	961
$C_{68}H_{56}Br_2Mo_2O_4$	69	$\{[h^4-C_4(p-C_6H_4CH_3)_4]Mo(CO)_2\}_2(Br)_2^*$	—	H H'	7.16q 2.31s	J 8 —	*Bridging Br ligands	961
$C_{16}H_{12}MoO_{12}$	70	$[h^4-C_4(CO_2CH_3)_4]Mo(CO)_4$	—	H	3.5s	—	Tetrakis (methoxy-carbonyl) cyclobutadiene	92
$C_{16}H_{18}MoO_4$	71	$[h^4-C_6(CH_3)_6]Mo(CO)_4$	$CDCl_3$	H H'	1.90s 1.00s	—	$C_6(CH_3)_6$ = 	56

TABLE III—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{12}H_8MoO_4$	72	$(h^4-C_8H_8)Mo(CO)_4$	—	H 5.54s 4.20s	—	Structure: 	909
$C_{12}H_{10}MoO_4$	73	$(h^4-C_8H_{10})Mo(CO)_4$	—	$\left. \begin{array}{l} H_{-1}, H_{-4} \\ H_{-5}, H_{-8} \end{array} \right\} 4.94s$ $H_{-2}, H_{-3} \quad 2.84s$ $H_{-6}, H_{-7} \quad 5.95s$	— — —	Structure: 	909
$C_{12}H_{12}MoO_4$	74	$(h^4-C_8H_{12})Mo(CO)_4$	CCl_4	$=CH \quad 4.59$ $CH_2 \quad 2.43$	— —	$C_8H_{12} = 1,5$ -cyclooctadiene Free olefin δ 5.53 and 2.31.	1020 93
			CCl_4	$=CH \quad 4.69$ $CH_2 \quad 2.53$	— —	Concluded that unlike the case of complexed conjugated dienes the double bonds are functioning independently and are not greatly changed by coordination	
			C_6H_6	$=CH \quad 4.15$ $CH_2 \quad 1.70$	— —		
$C_{14}H_{10}MoO_4$	75	$(h^4-C_{10}H_{10})Mo(CO)_4$	C_6D_6	$H_{-1} \quad \sim 2.8$ $H_{-2}, H_{-10} \sim 4.1$ $H_{-3}, H_{-9} \sim 4.15$ $H_{-4}, H_{-5} \sim 1.9$ $H_{-6} \quad \sim 1.75$ $H_{-7} \quad \sim 5.6$ $H_{-8} \quad \sim 5.15$	$J_{2,3} \quad 9$ $J_{6,7} \quad 8$ $J_{7,8} \quad 11, J_{1,7} \quad 1$ $J_{1,8} \quad 8$	$C_{10}H_{10} =$ Bullvalene	94

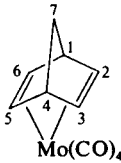
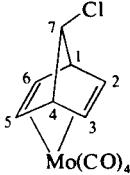
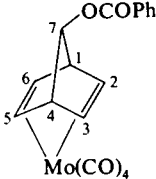
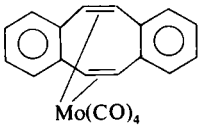
$C_{11}H_8MoO_4$	76		$CDCl_3$	H_1, H_4	3.76	—	—	58
				H_2, H_3	4.94	—		
				H_5, H_6	1.38	—		
				H_7				
$C_{11}H_8MoO_4$	77	$(h^4-C_7H_8)Mo(CO)_4$	CH_2Cl_2	^{13}C	-22.0	—	To high field from CS_2	95
					-25.4	—		
			$CHCl_3$	^{13}C	-22.4	—	C_7H_8 = norbornadiene	
					-26.0	—		
$C_{11}H_7ClMoO_4$	78		$CDCl_3$	H_1, H_4	3.82	—	—	58
				H_2, H_3	4.64	—		
				H_5, H_6	4.79	—		
				H_7	3.65	—		
$C_{18}H_{12}MoO_6$	79		$CDCl_3$	H_1, H_4	4.00	—	—	58
				H_2, H_3	4.70	—		
				H_5, H_6	4.81	—		
				H_7	4.48	—		
$C_{20}H_{12}MoO_4$	80	$(h^4-C_{16}H_{12})Mo(CO)_4$	—	H	5.77	—	Structure:	962
				H'	7.15	—		

TABLE III—cont.

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Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_8H_8MoO_4$	81	$(h^4-C\dot{H}_2=CH'CH''=O)_2Mo(CO)_2$	$CDCl_3$	H_{cis}	3.67	—	All signals shifted upfield to free ligand by 2.72 (H_{cis}), 4.15 (H_{trans}) 2.72 (H'), and 1.27 (H'') ppm	96
				H_{trans}	2.24	—		
				H'	3.67	—		
				H''	8.20	—		
(5) PENTAHAPTO LIGANDS								
(a) Mono-carbonyl derivatives								
$C_{42}H_{35}As_2ClMoO$	82	$(h^5-C_5H_5)(Mo(CO)(AsPh_3)_2(Cl))$	$CDCl_3$	H	5.05	—	—	97
$C_{15}H_{23}I_2MoNO$	83	$(h^5-C_5H_5)Mo(CO)(I)_2\{N=C[C(CH_3)_3]_2\}$	$CDCl_3$	H	5.67s	—	—	98
				H'	1.42, 1.13	—	—	
$C_{17}H_{19}I_2MoNO$	84	$(h^5-C_5H_5)Mo(CO)(I)_2\{N=CC-(CH_3)_3C_6H_5\}$	$CDCl_3$	H	5.44s	—	T +40°	99
				H'	1.56, 1.32	—		
				H''	7.62, 7.38	—		
				H	5.56s	—	T -40°	
				H'	1.55, 1.29	—		
				H''	7.71, 7.39	—		
$C_{18}H_{35}ClMoOP_2$	85	$(h^5-C_5H_5)Mo(CO)(PEt_3)_2(Cl)$	$CDCl_3$	H	5.10	—	—	97
$C_{18}H_{35}IMoOP_2$	86	$(h^5-C_5H_5)Mo(CO)(PEt_3)_2(I)$	$CDCl_3$	H	5.69	—	—	97
$C_{30}H_{59}IMoOP_2$	87	$(h^5-C_5H_5)Mo(CO)[P(n-C_4H_9)_3]_2(I)$	CS_2	H	4.84br	—	—	100
$C_{14}H_{16}MoNO_2P$	88	$(h^5-C_5H_5)Mo(CO)(NO)[P(CH_3)_2-C_6H_5]$	CS_2	H	5.12	$J_{PH} 1.5$	—	101
				H'	1.78d, 1.74d	$J_{PH'} 8.5, 8.2$		
				H''	7.35m			

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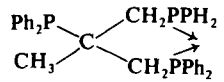
$C_{24}H_{20}MoNO_2P$	89	$(h^5-C_5H_5)Mo[P(C_6H_5)_3](NO)(CO)$	C_6D_6	H	4.86	$J_{PH} 0.8$	—	946
$C_{37}H_{31}ClMoOP_2$	90	$(h^5-C_5H_5)Mo(CO)(Cl)(PCH_2Ph)_2$	CD_2Cl_2	H	4.83, 4.58 and 4.88	—	Two cyclopentadienyl signals at —62° due to <i>cis</i> - and <i>trans</i> - isomers	102
				H'	2.12	—		
$C_{32}H_{29}ClMoOP_2$	91	$(h^5-C_5H_5)Mo(CO)(PPh_2CH_2-CH_2Ph)_2P(Ph)_2$	$CDCl_3$	H	4.63	—	—	97
$C_{32}H_{29}IMoOP_2$	92	$(h^5-C_5H_5)Mo(CO)(PPh_2CH_2-CH_2Ph)_2P(Ph)_2$	$CDCl_3$	H	br.	—	—	97
$C_{46}H_{42}ClMoOP_3$	93	$(h^5-C_5H_5)Mo(CO)(triphos)(Cl)$	$CDCl_3$	H	5.33s	—	triphos = 	103
$C_{32}H_{27}ClMoOP_2$	94	$(h^5-C_5H_5)Mo(CO)(Pf=Pf)(Cl)$	$CDCl_3$	H	4.45s	—	$Pf=Pf = cis-Ph_2PCH=CHPPh_2$	103
$C_{12}H_{21}ClMoOP_2$	95	$(h^5-C_5H_5)Mo(CO)(Pm-Pm)(Cl)$	$CDCl_3$	H	5.02s, 4.97s	—	$Pm-Pm = (CH_3)_2PCH_2CH_2P-(CH_3)_2$. Other signals at 1.83s, 1.74s, 1.67s, 1.56s, 1.40s, 1.15s, and 1.02s	103
$C_{42}H_{35}ClMoOP_2$	96	$(h^5-C_5H_5)Mo(CO)(PPh_3)_2(Cl)$	$CDCl_3$	H	4.91	—	—	97
$C_{42}H_{35}IMoO_3P_2$	97	$(h^5-C_5H_5)Mo(CO)[P(OPh)_3]_2(I)$	$CDCl_3$	H	4.75	—	—	97
$C_{42}H_{36}MoOP_2$	98	$(h^5-C_5H_5)Mo(CO)[P(C_6H_5)_3]_2(H)$	$CDCl_3$	H	5.43	—	—	98
				H'	7.40m	—	—	
$C_{35}H_{14}MoNOP$	99	$(h^5-C_5H_5)Mo(CO)(PPh_3)[N=CC(CH_3)_3C_6H_5]$	$CDCl_3$	H	5.39s	—	—	99
				H'	1.21	—	—	
				H''	7.30	—	—	
$C_{31}H_{27}MoN_2OP$	100	$(h^5-C_5H_5)Mo(CO)[P(C_6H_5)_3]_2[p-N_2C_6H_4CH_3]$	CD_3COCD_3	H	5.42	—	—	104
				H'	7.50	—	—	
$C_{24}H_{20}MoNO_2P$	101	$(h^5-C_5H_5)Mo(CO)(NO)(PPh_3)$	$CDCl_3$	H	5.19d	$J 0.8$	—	59

TABLE III—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{25}H_{20}MoNO_2P$	102	$(\eta^5-C_5H_5)Mo(CO)(NCO)PPh_3$	$CDCl_3$	H 4.79m, 5.24s	—	—	59
$C_{12}H_{23}ClMoO_7P_2$	103	$(\eta^5-C_5H_5)Mo(CO)IP(OCH_3)_3I_2(Cl)$	$CDCl_3$	H H' 5.32 3.86, 3.77, 3.69	— —	—	105
$C_{12}H_{23}IMoO_7P_2$	104	$(\eta^5-C_5H_5)Mo(CO)IP(OCH_3)_3I_2(I)$	$CDCl_3$	H H' 5.25 3.87, 3.78 3.68	—	—	105
$C_{12}H_{24}MoO_7P_2$	105	$(\eta^5-C_5H_5)Mo(CO)IP(OCH_3)_3I_2(H'')$	$CDCl_3$	H H' H'' 5.20 3.68, 3.48 -7.46t	— — $J_{PH''} 64.5$	—	105
$C_{12}H_{23}Cl_3MoO_7P_2Sn$	106	$(\eta^5-C_5H_5)Mo(CO)IP(OCH_3)_3I_2(SnCl_3)$	$CDCl_3$	H H'' 5.35 3.76	— $J_{PH'} 12$	—	105 106
$C_{42}H_{35}ClMoOSb_2$	107	$(\eta^5-C_5H_5)Mo(CO)(SbPh_3)_2(Cl)$	$CDCl_3$	H 5.39	—	—	97
$C_{42}H_{35}IMoOSb_2$	108	$(\eta^5-C_5H_5)Mo(CO)(SbPh_3)_2(I)$	$CDCl_3$	H 5.25	—	—	97
<i>(b) Di-carbonyl derivatives</i>							
$C_{20}H_{18}AsIMoO_2$	109	$(\eta^5-C_5H_5)Mo(CO)_2(AsPh_2CH_3)(I)$	$CDCl_3$	H 5.45	—	—	97
$C_{25}H_{20}AsClMoO_2$	110	$(\eta^5-C_5H_5)Mo(CO)_2(AsPh_3)(Cl)$	$CDCl_3$	H 5.62	—	—	97
$C_{25}H_{20}AsIMoO_2$	111	$(\eta^5-C_5H_5)Mo(CO)_2(AsPh_3)(I)$	$CDCl_3$	H 5.60	—	—	97

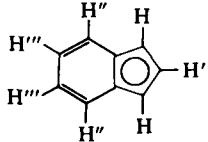
$C_{28}H_{29}AsMoO_2^-$ Sn	112	$(h^5-C_5H_5)Mo(CO)_2(AsPh_3)-$ [Sn(CH ₃) ₃]	CDCl ₃	H	4.87	—	—	107
$C_7H_5Br_3MoO_2$	113	$(h^5-C_5H_5)Mo(CO)_2(Br)_3$	SO ₂	H	6.31	—	100 MHz	108
$C_7H_5Cl_3MoO_2$	114	$(h^5-C_5H_5)Mo(CO)_2(Cl)_3$	Acetone	H	6.11	—	100 MHz	108
$C_7H_5I_3MoO_2$	115	$(h^5-C_5H_5)Mo(CO)_2(I)_3$	Acetone	H	6.49	—	100 MHz	108
$C_{11}H_7IMoO_2$	116	$(h^5-C_9H_7)Mo(CO)_2(I)$	Acetone	H H' H'' H'''	6.32 5.39 7.32 7.64	$J_{HH'}2$ $J_{H''H'''}7, 3$	$C_9H_7 =$ 	109
$C_8H_5ClHgMoO_3$	117	$(h^5-C_5H_5)Mo(HgCl)(CO)_3$	CS ₂	H	5.80s	—	Hexamethyldisiloxane reference	185
$C_{16}H_{23}MoNO_2$	118	$(h^5-C_5H_5)Mo(CO)_2\{N=C[C-(CH_3)_3]_2\}$	Toluene	H H' H H'	5.35s 1.07 5.12s 1.02	— — — —	T 25° T -60°	98 110
			C_7D_{14}	H H' H H'	5.65 1.18 5.68 1.17	— — — —	T 25° T -60°	
$C_{18}H_{19}MoNO_2$	119	$(h^5-C_5H_5)Mo(CO)_2\{N=CC-(CH_3)_3C_6H_5\}$	CDCl ₃	H H' H''	5.83 1.20 7.42	— — —	—	99
$[C_{18}H_{20}^- MoNO_2]^+$	120	$(h^5-C_5H_5)Mo(CO)_2\{NH=C-(CH_3)_3C_6H_5\}^+$	C_6D_6	H H' H''	4.69s 0.73 7.0	— — —	Isolated as the chloride	99
$C_{20}H_{15}MoNO_2$	121	$(h^5-C_5H_5)Mo(CO)_2\{N=C-(C_6H_5)_2\}$	CDCl ₃	H H'	4.95, 4.89 7.52br	— —	—	111

TABLE III—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{13}H_9MoN_3O_4$	122	$(h^5-C_5H_5)Mo(CO)_2(N_2C_6H_4NO_2-p)CS_2$		H	5.76	—	104
$C_{13}H_{10}MoN_2O_2$	123	$(h^5-C_5H_5)Mo(CO)_2(N_2C_6H_5)$	CS_2	H	5.62	—	104
$C_{14}H_{12}MoN_2O_2$	124	$(h^5-C_5H_5)Mo(CO)_2(N_2C_6H_4-CH_3-p)$	CS_2	H	5.66	—	104
$C_{14}H_{12}MoN_2O_3$	125	$(h^5-C_5H_5)Mo(CO)_2(N_2C_6H_4-OCH_3-p)$	CS_2	H	5.63	—	104
$C_7H_5MoNO_3$	126	$(h^5-C_5H_5)Mo(C'O)_2NO$	$CDCl_3$	H	5.57s	—	59
			CD_3COCD_3	H	5.76s	—	60
			CS_2	H	5.53	$^{13}C + 99.2d (J_{CH}175)$ and $^{13}C' - 345$ in CH_2Cl_2 as solvent relative to CS_2	95
$C_{14}H_{12}MoO_4S$	127	$(h^5-C_5H_5)Mo(CO)_2[OS(O)CH_2Ph]$	SO_2	H	3.51, 3.69	$J_{12.5}$	Temperature -37° 112
$C_{10}H_{15}MoO_2P$	128	$(h^5-C_5H_5)Mo(CO)_2[P(CH_3)_3](H'')$	Toluene	H	4.60	$J_{PH} < 0.3$	<i>cis</i> -isomer 113
				H'	0.83	$J_{PH'} 9.4$	T -38° 1023
				H''	-6.59	$J_{PH''} 66.6$	
				H	4.47	$J_{PH} 1.0$	<i>trans</i> -isomer
				H'	0.85	$J_{PH'} 9.0$	100 MHz
				H''	-5.89	$J_{PH''} 23.0$	T -38°
$[C_{19}H_{35}MoO_2-P_2]^+$	129	$[(h^5-C_5H_5)Mo(CO)_2(PEt_3)_2]^+$	$CDCl_3$	H	5.51t	$J_{1.0}$	Isolated as the iodide 100

C ₁₃ H ₂₀ IMoO ₂ P 130	(h ⁵ -C ₅ H ₅)Mo(CO) ₂ (PEt ₃)(I)	CS ₂	H	5.26s	—	<i>cis</i> -isomer <i>trans</i> -isomer	100
			H	5.09d	J _{PH} 2		
C ₁₉ H ₃₂ ClMoO ₂ P 131	(h ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(n-C ₄ H ₉) ₃]- (Cl)	CDCl ₃	H	5.36	—	<i>cis</i> -isomer T 38°	114
C ₁₉ H ₃₂ IMoO ₂ P 132	(h ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(n-C ₄ H ₉) ₃]- (I)	CDCl ₃	H	5.37	—	<i>cis</i> -isomer T 38°	114
			H	5.21	—	<i>trans</i> -isomer	
		CS ₂	H	5.22	—		100
C ₁₉ H ₃₂ IMoO ₂ P 133	(h ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(n-C ₄ H ₉) ₃]- (I)	THF	H	5.42	—	—	115
[C ₁₉ H ₃₂ MoO ₂ P]- 134	{(h ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(n-C ₄ H ₉) ₃]}-	THF	H	4.83	—	—	115
C ₁₉ H ₃₃ MoO ₂ P 135	(h ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(n-C ₄ H ₉) ₃]- (H')	THF	H	5.21	—	—	115
			H'	-6.46	J _{PH} 50.6		
		CDCl ₃	H	5.31	—	<i>cis</i> -isomer T 50°	114
			H'	-6.60	J _{PH} 64.9		
			H	5.15	J _{PH} 1.0	<i>trans</i> -isomer	
			H'	-6.53	J _{PH} 22.4		
C ₂₅ H ₃₈ IMoO ₂ P 136	(h ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(C ₆ H ₁₁) ₃](I)	CDCl ₃	H	5.48	—	—	97
C ₁₅ H ₁₆ BrMoO ₂ P 137	(h ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(CH ₃) ₂ Ph]- (Br)	CDCl ₃	H	5.30s	—	<i>cis</i> -isomer	116
			H'	1.96d, 1.94d	J 9.8		
		CDCl ₃	H	5.31	J _{PH} 0.5	<i>cis</i> -isomer 31° 100 MHz	117
			H'	1.97, 1.94	J _{PH} 9.0, 8.7		
			H	4.98	J _{PH} 2.3	<i>trans</i> -isomer	
			H'	1.94	J _{PH} 8.9		

TABLE III—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{15}H_{16}ClMoO_2P$	138	$(\eta^5-C_5H_5)Mo(CO)_2[P(CH_3)_2Ph](Cl)$	$CDCl_3$	H	5.32s	—	<i>cis</i> -isomer	116
				H'	1.85d, 1.83d	$J_{PH} 9.8$		
			$CDCl_3$	H	5.33	$J_{PH} 0.5$	<i>cis</i> -isomer	117
				H'	1.85, 1.81	$J_{PH} 9.7, 9.4$		
				H	4.99	$J_{PH} 2.4$	<i>trans</i> -isomer	
				H'	—	—		
$C_{15}H_{16}IMoO_2P$	139	$(\eta^5-C_5H_5)Mo(CO)_2[P(CH_3)_2Ph](I)$	$CDCl_3$	H	5.27s	—	<i>cis</i> -isomer	116
				H'	2.09d, 2.05	$J_{PH} 9.8$		
				H	5.02d	$J_{PH} 2.0$	<i>trans</i> -isomer	116
				H'	1.94d	$J_{PH} 9.7$		
			$CDCl_3$	H	5.29	$J_{PH} 0.5$	<i>cis</i> -isomer	117
				H'	2.10, 2.06	$J_{PH} 8.9, 8.7$	100 MHz	
				H	5.03	$J_{PH} 2.3$	<i>trans</i> -isomer	
				H'	1.93	$J_{PH} 9.1$	T 31°	
			$CDCl_3$	H	4.73	—	<i>cis</i> -isomer T 38°	114
				H	4.62	$J_{PH} 2.3$	<i>trans</i> -isomer	
$C_{15}H_{17}MoO_2P$	140	$(\eta^5-C_5H_5)Mo(CO)_2[P(CH_3)_2Ph](H')$	$CDCl_3$	H	5.22	—	<i>cis</i> -isomer T 50°	114
				H'	-6.15	$J_{PH} 65.6$		
				H	4.98	$J_{PH} 1.0$	<i>trans</i> -isomer	
				H'	-6.06	$J_{PH} 23.3$		
			$CHCl_2F$	H	5.22	$J_{PH} < 0.3$	<i>cis</i> -isomer	117
				H'	-6.15	$J_{PH} 65.6$		
H''	1.77	$J_{PH} 9.0$						

			H	4.98	$J_{PH} 1.0$	} <i>trans</i> -isomer	
			H'	-6.06	$J_{PH'} 23.3$		
			H''	1.82	$J_{PH''} 8.8$		
$C_{22}H_{24}AlMoO_2P$	141	$(h^5-C_5H_5)Mo(CO)_2[P(CH_3)Ph_2] \cdot [Al(CH_3)_2]$	C_6D_6	H	5.16	—	118
				H'	2.0	$J_{PH'} 8.0$	
				H''	-0.31br	—	
$C_{41}H_{38}ClMoO_2P_3$	142	$[(h^5-C_5H_5)Mo(CO)_2\{PPh_2-(CH_2)_2PPh\}(Cl)]$	$CDCl_3$	H	4.79s	—	5
$[C_{33}H_{29}MoO_2P_2]^+$	143	$[(h^5-C_5H_5)Mo(CO)_2(PPh_2CH_2-CH_2Ph_2P)]^+$	$CDCl_3$	H	4.74s	—	100
						Isolated as the iodide	
$[C_{25}H_{20}MoO_2P]^-$	144	$[(h^5-C_5H_5)Mo(CO)_2(PPh_3)]^-$	THF	H	4.76	—	115
$C_{25}H_{20}^-BrMoO_2P$	145	$(h^5-C_5H_5)Mo(CO)_2(PPh_3)(Br)$	$CDCl_3$	H	5.36	—	114
				H	5.05	—	<i>cis</i> -isomer <i>trans</i> -isomer T 38°
$C_{25}H_{20}^-ClMoO_2P$	146	$(h^5-C_5H_5)Mo(CO)_2(PPh_3)(Cl)$	$CDCl_3$	H	5.39	—	<i>cis</i> -isomer T 38°
			$CDCl_3$	H	5.49s	—	100 MHz
			$CDCl_3$	H	5.56	—	97
$C_{25}H_{20}IMoO_2P$	147	$(h^5-C_5H_5)Mo(CO)_2(PPh_3)(I)$	$CDCl_3$	H	4.96s	—	100 MHz
			$CDCl_3$	H	5.42, 5.16	—	97
			$CDCl_3$	H	5.43	—	<i>cis</i> -isomer
			$CDCl_3$	H	5.13	—	<i>trans</i> -isomer T 38°
			THF	H	5.36, 5.06	$J_{PH} 2.0$	115
			CS_2	H	5.01s	—	<i>cis</i> -isomer*
				H	4.84d	$J_{PH} 2.0$	<i>trans</i> -isomer*
						*Reviewer's assignment	100

TABLE III—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References		
$C_{25}H_{21}MoO_2P$	148	$(\eta^5-C_5H_5)Mo(\eta^5-C_5H_5)[P(C_6H_5)_3](CO)_2$	—	H	5.20	$J_{PH} < 0.3$	cis-isomer	958	
				H'	-5.33				$J_{PH'} 64$
				CDCl ₃	H	5.00	$J_{PH} 1.0$	trans-isomer	119
					H'	-6.14			
			THF		H	5.06s	—	—	115
					H'	-5.56d	$J_{PH'} 48.0$		
			THF	H	5.11	—	—	115	
				H'	-5.49	$J_{PH'} 51.6$			51.6
$C_{26}H_{20}MoNO_3P$	149	$(\eta^5-C_5H_5)Mo(CO)_2(NCO)(PPh_3)$	CDCl ₃	H	5.35s	—	—	59	
$C_{28}H_{29}GeMoO_2P$	150	$(\eta^5-C_5H_5)Mo(CO)_2(PPh_3)[Ge(CH_3)_3]$	CDCl ₃	H	4.82	—	—	120	
				H'	0.58	—	—		
$C_{28}H_{29}MoO_2PSn$	151	$(\eta^5-C_5H_5)Mo(CO)_2(PPh_3)[Sn(CH_3)_3]$	CDCl ₃	H	4.79	$J_{PH} 1.0$	—	107	
$C_{43}H_{35}MoO_2PSn$	152	$(\eta^5-C_5H_5)Mo(CO)_2(PPh_3)(SnPh_3)$	THF	H	4.87	$J_{PH} 1.0$	—	115	
$C_{26}H_{23}MoO_4PS$	153	$(\eta^5-C_5H_5)Mo[P(C_6H_5)_3](SO_2CH_3)(CO)_2$	CDCl ₃	H	5.35s	—	—	960	
				H'	7.58m	—	—		
				H''	3.22s	—	—		—
$[C_{10}H_{14}MoO_3P]^-$	154	$\{(\eta^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]\}^-$	THF	H	4.94	—	—	115	
$C_{10}H_{14}BrMoO_3P$	155	$(\eta^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3](Br)$	CDCl ₃	H	5.50s, 5.38d	$J 1-2$	—	121	
				H'	3.74d	$J_{PH'} 12$	—		

$C_{10}H_{14}ClMoO_5P$ 156	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3](Cl)$	$CDCl_3$	H	5.55	—	<i>cis</i> -isomer	114
			H	5.40	$J_{PH} 2.2$	<i>trans</i> -isomer T 38°	
			H	5.51	—	<i>cis</i> -isomer	114
			H	5.35	$J_{PH} 2.3$	<i>trans</i> -isomer	
$C_{10}H_{14}IMoO_5P$ 157	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3](I)$	$CDCl_3$	H	4.97s	—	100 MHz	119
		$CDCl_3$	H	5.53s, 5.39d	$J 2.0$	—	121
			H'	3.76d	$J_{PH'} 12$		
		$CDCl_3$	H	5.53	—	<i>cis</i> -isomer	114
			H	5.38	$J_{PH} 2.1$	<i>trans</i> -isomer T 38°	
		$CDCl_3$	H	5.47s, 5.38d	$J 2.0$		121
			H'	3.72d	$J_{PH'} 12$		
		THF	H	5.37	$J_{PH} 2.0$	—	115
		CS_2	H	5.28s	—	<i>cis</i> -isomer*	100
			H	5.19d	$J_{PH} 1.8$	<i>trans</i> -isomer*	
$C_{10}H_{15}MoO_5P$ 158	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]-(H')$	$CDCl_3$	H	5.38	—	<i>cis</i> -isomer	114
			H'	−6.98	$J_{PH'} 68.7$		
			H	5.29	$J_{PH} 1$	<i>trans</i> -isomer	
			H'	−6.19	$J_{PH'} 26.8$	T 50°	
		$CDCl_3$	H	5.34s	—	100 MHz	119
			H'	−6.74d	$J_{PH'} 61.8$		
		$CDCl_3$	H	5.23s, 5.05d	$J 1-2$	—	121
			H'	3.62d,	$J_{PH'} 12$		
				3.55d			
			H''	−6.7	$J_{PH''} 61.3$		
		THF	H	5.30	—	—	115
			H'	−6.71	$J_{PH'} 62.3$		
$C_{10}H_{14}HgBr-MoO_5P$ 159	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]-(HgBr)$	$CDCl_3$	H	5.45d	$J 1-2$	—	121
			H'	3.80d	$J_{PH'} 12$		

TABLE III—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{10}H_{14}HgCl-MoO_5P$	160	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]-(HgCl)$	$CDCl_3$	H	5.40d	J_{1-2}	—	121
				H'	3.75d	$J_{PH'} 12$		
$C_{10}H_{14}HgI-MoO_5P$	161	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]-(HgI)$	$CDCl_3$	H	5.42d	J_{1-2}	—	121
				H'	3.78d	$J_{PH'} 12$		
$C_{13}H_{23}MoO_8P_2$	162	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]_2$	$CDCl_3$	H	5.10	J_2	—	121
				H'	3.72d	$J_{PH'} 12$		
$C_{12}H_{20}MoO_8P_2$	163	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3] \cdot [P(O)(OCH_3)_2]$	$CDCl_3$	H	5.32q		T 38°	122
				H', H''	3.65d	J_{11-3}		
					3.63d	J_{12-0}		
$C_{10}H_{14}Br_3-MoO_5PSn$	164	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]-(SnBr_3)$	$CDCl_3$	H	5.48	$J_{PH} 1.0$	<i>trans</i> -isomer	106
				H'	3.78	$J_{PH'} 12$		
$C_{10}H_{14}Cl_3-MoO_5PSn$	165	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]-(SnCl_3)$	$CDCl_3$	H	5.50	$J_{PH} 1.0$	<i>trans</i> -isomer	106
				H'	3.79	$J_{PH'} 12$		
$C_{10}H_{14}I_3-MoO_5PSn$	166	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]-(SnI_3)$	$CDCl_3$	H	5.49	$J_{PH} 1.0$	<i>trans</i> -isomer	106
				H'	3.80	$J_{PH'} 12$		
$C_{28}H_{29}MoO_5-PSn$	167	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]-(SnPh_3)$	THF	H	5.17	$J_{PH} 0.8$	—	115
$[C_{13}H_{23}MoO_8-P_2]^+$	168	$\{(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]_2\}^+$	$CDCl_3$	H	5.03t	$J_{PH} 0.8$	Isolated as tetraphenylborate	23
				H'	3.52mt		Temperature 38°	
$C_{11}H_{20}IMoO_5P$	169	$(h^5-C_5H_5)Mo(CO)_2[P(OEt)_3](I)$	CS_2	H	5.28s	—	<i>cis</i> -isomer*	100
				H	5.18d	$J_{PH} 1.8$	<i>trans</i> -isomer*	
							*Reviewer's assignment	

$[C_{10}H_{15}MoO_8-P_2]^+$	170	$\{(h^5-C_5H_5)Mo(CO)_2[P(OCH_2-CH_3)_3]_2\}^+$	$CDCl_3$	H H'	5.05t 1.27t	$J_{PH} 0.7$ $J_{HH'} 7.5$	Isolated as tetraphenylborate T 38°	122
$C_{17}H_{30}MoO_8P_2$	171	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_2-CH_3)_3][P(O)(OCH_2CH_3)_2]$	$CDCl_3$	H H', H''	5.32q 1.33t 1.26t	$J 0.8, 0.5$ $J 7.0$ $J 7.0$	T 38°	122
$C_{22}H_{30}MoO_8P_2$	172	$(h^5-C_5H_5)Mo(CO)_2[P(OC_3H_7)_3][P(O)(OC_3H_7)_2]$	$CDCl_3$	H	5.49t	$J_{PH} < 1$	T 38°	123
$C_{28}H_{30}MoO_6P_2$	173	$(h^5-C_5H_5)Mo(CO)_2[P(OC_3H_7)_2-Ph][P(O)(OC_3H_7)Ph]$	$CDCl_3$	H	5.11t	$J_{PH} < 1$	T 38°	123
$C_{34}H_{30}MoO_4P_2$	174	$(h^5-C_5H_5)Mo(CO)_2[P(OC_3H_7)_2-Ph_2][P(O)Ph_2]$	$CDCl_3$	H	5.05t	$J_{PH} < 1$	T 38°	123
$[C_{25}H_{35}MoO_8-P_2]^+$	175	$\{(h^5-C_5H_5)Mo(CO)_2[P(OC_3H_7)_3]_2\}^+$	CD_3COCD_3	H	5.62t	$J_{PH} 0.7$	T 38° Isolated as tetraphenylborate	123
$[C_{31}H_{35}MoO_6-P_2]^+$	176	$\{(h^5-C_5H_5)Mo(CO)_2[P(OC_3H_7)_2Ph]_2\}^+$	CD_3COCD_3	H	5.36t	$J_{PH} 0.7$	T 38° Isolated as tetraphenylborate	123
$[C_{37}H_{35}MoO_4-P_2]^+$	177	$\{(h^5-C_5H_5)Mo(CO)_2[P(OC_3H_7)_2Ph]_2\}^+$	CD_3COCD_3	H	5.43t	$J_{PH} 0.7$	T 38° Isolated as tetraphenylborate	123
$C_{22}H_{40}MoO_8P_2$	178	$(h^5-C_5H_5)Mo(CO)_2[P(OCH(CH_3)_2)_3][P(O)(OCH(CH_3)_2)_2]$	$CDCl_3$	H H', H''	5.28q 1.32d 1.27q	$J 0.9, 0.4$ $J 6.2$ $J 6.2, 2.1$	T 38°	122
$[C_{25}H_{47}MoO_8-P_2]^+$	179	$\{(h^5-C_5H_5)Mo(CO)_2[P(OCH(CH_3)_2)_3]_2\}^+$	$CDCl_3$	H H'	5.12t 1.30d	$J_{PH} 0.7$ $J_{HH'} 6.5$	Isolated as tetraphenylborate T 38°	122
$[C_{31}H_{50}MoO_8-P_2]^+$	180	$\{(h^5-C_5H_5)Mo(CO)_2[P(On-C_4H_9)_3]_2\}^+$	$CDCl_3$	H	5.07t	$J_{PH} 0.8$	Isolated as tetraphenylborate	122
$C_{12}H_{15}MoO_5P$	181	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_2)_3-CCH_3](H')$	$CDCl_3$	H H'	5.25 -6.60d	— $J_{PH'} 58.0$	100 MHz	119

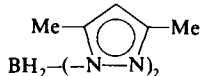
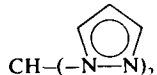
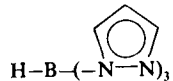
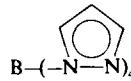
TABLE III—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{15}H_{23}MoO_5PSn$	182	$(\eta^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3-CCH_3][Sn(CH_3)_3]$	$CDCl_3$	H	5.05	$J_{PH} 0.8$	—	107
$C_{15}H_{16}BrMoO_4P$	183	$(\eta^5-C_5H_5)Mo(CO)_2[P(OCH_3)_2-Ph]Br$	$CDCl_3$	H	5.02	$J_{PH} 2.4$	} <i>trans</i> -isomer T 31° 100 MHz	117
				H'	3.74	$J_{PH'} 12.6$		
				H	5.32	$J_{PH} < 0.2$		
				H'	3.66, 3.58	$J_{PH'} 13.7, 11.8$		
$C_{15}H_{16}ClMoO_4P$	184	$(\eta^5-C_5H_5)Mo(CO)_2[P(OCH_3)_2-Ph](Cl)$	$CDCl_3$	H	5.09	$J_{PH} 2.3$	} <i>trans</i> -isomer 31° 100 MHz	117
				H'	3.73	$J_{PH'} 12.6$		
				H	5.33	$J_{PH} < 0.2$		
				H'	3.68, 3.60	$J_{PH'} 13.5, 11.5$		
$C_{15}H_{16}IMoO_4P$	185	$(\eta^5-C_5H_5)Mo(CO)_2[P(OCH_3)_2-Ph](I)$	$CDCl_3$	H	5.02	$J_{PH} 2.3$	} <i>trans</i> -isomer 31° 10 MHz	117
				H'	3.76	$J_{PH'} 12.1$		
				H	5.30	$J_{PH} < 0.2$		
				H'	3.62, 3.55	$J_{PH'} 13.0, 11.7$		
$C_{15}H_{17}MoO_4P$	186	$(\eta^5-C_5H_5)Mo(CO)_2[P(OCH_3)_2-Ph](H'')$	$CHCl_2F$	H	5.04	$J_{PH} 0.9$	} <i>trans</i> -isomer T -65° 100 MHz	117
				H'	3.59	$J_{PH'} 12.7$		
				H''	-6.10	$J_{PH''} 23.4$		
				H	5.22	$J_{PH} < 0.2$		
				H'	3.54, 3.42	$J_{PH'} 13.6, 11.7$		
				H''	-6.49	$J_{PH''} 63.2$		
$[C_{25}H_{20}MoO_5-P]^-$	187	$\{(\eta^5-C_5H_5)Mo(CO)_2[P(OPh)_3]\}^-$	THF	H	4.24	—	—	115
$C_{25}H_{20}ClMoO_5P$	188	$(\eta^5-C_5H_5)Mo(CO)_2[P(OPh)_3](Cl)$	$CDCl_3$	H	5.08s	—	—	121

			CDCl ₃	H	4.96	—	<i>cis</i> -isomer 38°	114
			CDCl ₃	H	4.96s	—	100 MHz	119
C ₂₅ H ₂₀ IMoO ₅ P	189	(<i>h</i> ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(OPh) ₃](I)	CDCl ₃	H	4.91s	—	100 MHz	119
			CDCl ₃	H	5.02s	—	—	121
			CDCl ₃	H	5.03	—	<i>cis</i> -isomer	114
			Acetone	H	5.06s	—	100 MHz	124
			THF	H	5.05	—	—	115
			CS ₂	H	4.96s	—	—	100
C ₂₅ H ₂₁ MoO ₅ P	190	(<i>h</i> ⁵ -C ₅ H ₅)Mo(CO) ₂ P(OPh) ₃ (H')	CDCl ₃	H	4.84s	—	100 MHz	119
				H'	-6.61d	<i>J</i> _{PH'} 70.8	—	
			CDCl ₃	H	4.87s	—	—	121
				H'	-6.68d	<i>J</i> _{PH'} 72	—	
			CDCl ₃	H	4.84	—	<i>cis</i> -isomer T 50°	114
				H'	-6.72	<i>J</i> _{PH'} 73.0	—	
				H	4.54	<i>J</i> _{PH} 1.0	<i>trans</i> -isomer	
				H'	-6.30	<i>J</i> _{PH'} 29.0	—	
			THF	H	4.86	—	—	115
				H'	-6.62	<i>J</i> _{PH} 71.3	—	
			CDCl ₃	H	4.80s	—	100 MHz	124
				H'	-6.63d	<i>J</i> _{PH'} 72	—	
C ₂₇ H ₂₀ F ₃ ⁻ MoO ₇ P	191	(<i>h</i> ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(OPh) ₃]- (OCOCF ₃)	CDCl ₃	H	5.09s	—	100 MHz	124
C ₂₅ H ₂₀ Cl ₃ ⁻ MoO ₅ PSn	192	(<i>h</i> ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(OPh) ₃]- (SnCl ₃)	CDCl ₃	H	5.14	<i>J</i> _{PH} 1.0	<i>trans</i> -isomer	106
C ₂₈ H ₂₉ MoO ₅ PSn	193	(<i>h</i> ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(OC ₆ H ₅) ₃]- [Sn(CH ₃) ₃]	CDCl ₃	H	4.59s	—	100 MHz	107
				H'	7.41, 7.37	—	—	124
				H''	0.24	<i>J</i> (Sn-H) 47	—	

TABLE III—*cont.*

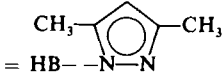
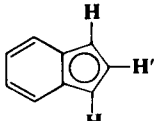
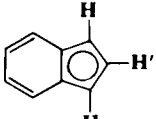
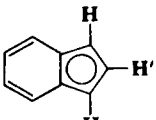
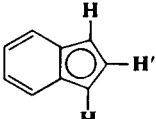
Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{43}H_{35}MoO_3PSn$	194	$(h^5-C_5H_5)Mo(CO)_2[P(OPh)_3]-(SnPh_3)$	THF	H 4.64	J_{PH} 0.8	—	115
$[C_{25}H_{20}MoO_2-Sb]^-$	195	$[(h^5-C_5H_5)Mo(CO)_2(SbPh_3)]^-$	THF	H 4.86	—	—	115
$C_{25}H_{20}IMoO_2Sb$	196	$(h^5-C_5H_5)Mo(CO)_2(SbPh_3)(I)$	$CDCl_3$	H 5.59	—	—	97
			$CDCl_3$	H 5.44	—	<i>cis</i> -isomer T 38°	114
				H 5.24	—	<i>trans</i> -isomer	
			THF	H 5.57	—	—	115
			$CDCl_3$	H 5.45s	—	<i>cis</i> -isomer	100
				H 5.23s	—	<i>trans</i> -isomer	
$C_{25}H_{21}MoO_2Sb$	197	$(h^5-C_5H_5)Mo(CO)_2(SbPh_3)(H')$	THF	H 5.30	—	—	115
				H' -6.07	—	—	
$C_{28}H_{29}MoO_2-SbSn$	198	$(h^5-C_5H_5)Mo(CO)_2(SbPh_3)-[Sn(CH_3)_3]$	$CDCl_3$	H 4.98	—	—	107
$C_{43}H_{35}MoO_2-SbSn$	199	$(h^5-C_5H_5)Mo(CO)_2(SbPh_3)-(SnPh_3)$	THF	H 5.10	—	—	115
$C_{14}H_{12}MoO_4S$	200	$(h^5-C_5H_5)Mo(CO)_2[S(O)_2CH_2Ph]$	SO_2	H 4.22s	—	T -37°	112
$C_7H_5F_2MoO_2-PS_2$	201	$(h^5-C_5H_5)Mo(CO)_2(S_2PF_2)$	$CDCl_3$	H 5.50	—	—	125
$C_{26}H_{20}Mo_2O_4Te_2$	202	$[(h^5-C_5H_5)Mo(CO)_2(TeC_6H_5)]_2$	CS_2	H 5.12s	—	—	126

$C_{19}H_{23}BMoN_4O_2^-$	203	$(h^5-C_7H_7)^*Mo(CO)_2(C_{10}H_{16}BN)_4$	$CDCl_3$	H	5.34s	—	Remaining signals at δ 5.70s, 5.64s, 2.47s, 2.42s, 2.13s, 2.10s, in ratio 1:1:3:3:3:3	81
							$C_{10}H_{16}BN_4 =$ 	
$[C_{19}H_{17}MoN_6O_2]^+$	204	$\{(h^5-C_7H_7)Mo(CO)_2(C_{10}H_{10}N_6)\}^+$		H	5.23	—	$C_{10}H_{10}N_6 =$ 	89
							Isolated as the hexafluorophosphate	
$C_{18}H_{17}BMoN_6O_2^-$	205	$(h^5-C_7H_7^*)Mo(CO)_2[HB(Pz)_3]$	$CDCl_3$	H*	5.34s	—	$HB(Pz)_3 =$ 	
							$C_7H_7 =$ 	
$C_{19}H_{17}BMoN_8O_2^-$	206	$(h^5-C_3H_3)Mo(CO)_2[B(Pz)_4]$	$CDCl_3$	H	5.28	—	$B(Pz)_4 =$ 	53
$C_{21}H_{19}BMoN_8O_2^-$	207	$(h^5-C_7H_7^\dagger)Mo(CO)_2[B(Pz)_4]$	$CDCl_3$	H†	5.24s	—		
			CS_2	H†	5.03	—		

*Fluxional pentohapto- C_7H_7 ligand assuming the bis (1-pyrazolyl)borate ligand to be bidentate. Alternative possibilities are a heptahapto- C_7H_7 ligand and a monodentate ($C_{10}H_{16}BN_4$) ligand, or a fluxional trihapto- C_7H_7 ligand and bidentate ($C_{10}H_{16}BN_4$) ligand if a 16-electron compound

†Hydrogens equivalent due to fluxional behaviour of the C_7H_7 ligand. Alternative formulations containing tridentate $RB(Pz)_3$ and $h^3-C_7H_7$ ligands or a monodentate $RB(Pz)_3$ and planar $h^7-C_7H_7$ ligands are considered less likely

TABLE III—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{24}H_{29}BMoN_6O_2$	208	$(h^5-C_7H_7^*)Mo(CO)_2[HB(3,5-(CH_3)_2Pz)_3]I$	$CDCl_3$	H^* 5.26	—	$HB(3,5-(CH_3)_2Pz)_3$  $= HB-N-N$	53
$C_{29}H_{22}BrMoO_2P$	209	$(h^5-C_9H_7)Mo(CO)_2(PPh_3)(Br)$	CD_3COCD_3	H 6.16br, 5.41br H' 5.19t	—	$C_9H_7 =$ 	127
$C_{29}H_{22}ClMoO_2P$	210	$(h^5-C_9H_7)Mo(CO)_2(PPh_3)(Cl)$	CD_3COCD_3	H 6.26br, 5.38br H' 5.30	—		127
$C_{23}H_{34}BrMoO_2P$	211	$(h^5-C_9H_7)Mo(CO)_2[P(n-C_4H_9)_3](Br)$	CD_3COCD_3	H 6.19br, 5.54br H' 5.35t	— —	$C_9H_7 =$ 	127
$C_{14}H_{16}BrMoO_3P$	212	$(h^5-C_9H_7)Mo(CO)_2[P(OCH_3)_3](Br)$	CD_3COCD_3	H 5.94br, 5.74br H' 5.18t	—		127

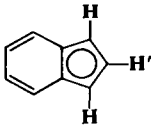
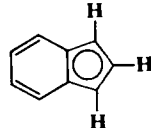
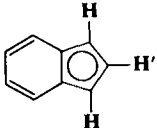
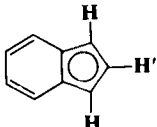
$C_{14}H_{16}ClMoO_5P$ 213	$(\eta^5-C_9H_7)Mo(CO)_2[P(OCH_3)_3]-(Cl)$	CD_3COCD_3	H H'	6.04br, 5.78br 5.26t	—		127
$C_{14}H_{16}IMoO_5P$ 214	$(\eta^5-C_9H_7)Mo(CO)_2[P(OCH_3)_3](I)$	$o-C_6H_4Cl_2$	H H'	~5.6	$J_{HH'}2.9$		117
$C_{29}H_{22}IMoO_2P$ 215	$(\eta^5-C_9H_7)Mo(CO)_2(PPh_3)(I)$	$o-C_6H_4Cl_2$	H H'	4.9 5.93 4.88	$J_{HH'}3.0$	T 31° <i>cis</i> -isomer T 31° <i>cis</i> -isomer	117
$C_{19}H_{18}IMoO_2P$ 216	$(\eta^5-C_9H_7)Mo(CO)_2[P(CH_3)_2Ph](I)$	$o-C_6H_4Cl_2$	H H'	5.77, 5.14 4.84	$J_{HH'}3.0$	T 31° <i>cis</i> -isomer	117
$C_{29}H_{22}IMoO_2Sb$ 217	$(\eta^5-C_9H_7)Mo(CO)_2(SbPh_3)(I)$	$o-C_6H_4Cl_2$	H H'	5.93, 5.46 4.88	$J_{HH'}3.0$	T 31° <i>cis</i> -isomer	117
$C_{29}H_{26}ClMoO_2P$ 218	$(\eta^5-C_9H_{11})Mo(CO)_2(PPh_3)(Cl)$	$CDCl_3$	H	4.28, 4.73, 5.27	—	The cyclopentadienyl protons of the π -tetrahydroindenyl ligand	134
$C_{14}H_{20}ClMoO_5P$ 219	$(\eta^5-C_9H_{11})Mo(CO)_2[P(OCH_3)_3]-(Cl)$	$CDCl_3$	H	4.71, 4.81, 5.27	—	The cyclopentadienyl protons of the π -tetrahydroindenyl ligand	134
$C_{29}H_{26}ClMoO_5P$ 220	$(\eta^5-C_9H_{11})Mo(CO)_2[P(OPh)_3](Cl)$	$CDCl_3$	H	4.16, 4.41, 4.50	—	The cyclopentadienyl protons of the π -tetrahydroindenyl ligand	134
(c) <i>Tri-carbonyl derivatives</i>							
$[C_8H_5MoO_3]^-$ 221	$[(\eta^5-C_5H_5)Mo(CO)_3]^-$	Acetone	H H' H''	5.00s 3.47q 1.47tt	— $J_{NH'}2$ $J_{H'H''}8$	Isolated as the quaternary ethyl ammonium salt $[N(CH_2CH'_3)_4]$	129
		THF	H	5.01	—	—	115

TABLE III—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{26}H_{19}MoO_3P$	222	$(h^5-C_5H_4PPh_3)Mo(CO)_3$	$CHCl_3$	H	5.49, 5.23	$J\ 2.5$	—	66
$C_{20}H_5AsF_{10}MoO_3$	223	$(h^5-C_5H_5)Mo(CO)_3(As(C_6F_5)_2)$	$CDCl_3$	H	5.56	—	^{19}F NMR chemical shifts 124.1, 153.1, 161.6 ppm relative to CCl_3F	130
$C_8H_5BrMoO_3$	224	$(h^5-C_5H_5)Mo(CO)_3Br$	$CDCl_3$	H	5.62s	—	—	131
$C_8H_5ClMoO_3$	225	$(h^5-C_5H_5)Mo(C'O)_3(Cl)$	$CDCl_3$	H	5.72s	—	—	131
			$CDCl_3$	H	5.29	—	—	132
			$CHCl_3$	H	5.63	—	$^{13}C + 97.9d$ ($J_{CH}175$) relative to CS_2 in benzene $^{13}C' - 32.6$ relative to CS_2 in CH_2Cl_2 as solvent	95
$C_8H_5IMoO_3$	226	$(h^5-C_5H_5)Mo(CO)_3(I)$	CS_2	H	5.33	—	—	100
			THF	H	5.74	—	—	115
$C_{12}H_7BrMoO_3$	227	$(h^5-C_9H_7)Mo(CO)_3(Br)$	CD_3COCD_3	H	6.28d	—	$C_9H_7 =$ 	127
				H'	5.82t			
$C_{12}H_7ClMoO_3$	228	$(h^5-C_9H_7)Mo(CO)_3(Cl)$	CD_3COCD_3	H	6.19d	—		127
				H'	5.82t	—		

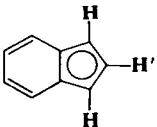
$C_{12}H_7IMoO_3$	229	$(h^5-C_9H_7)Mo(CO)_3(I)$	CD_3COCD_3	H H'	6.32d 5.79t	—		127
$C_{12}H_{11}ClMoO_3$	230	$(h^5-C_9H_{11})Mo(CO)_3(Cl)$	$CDCl_3$	H	4.14, 4.47	—	The cyclopentadienyl protons of the π -tetrahydroindenyl ligand	134
$C_8H_6MoO_3$	231	$(h^5-C_5H_5)Mo(CO)_3(H')$	$CDCl_3$	H'	—5.52	—	—	67
			Hexane	H	5.30	—	—	66
				H'	—5.52	—	—	
			THF	H	5.54	—	—	115
				H'	—5.59	—	—	
$C_8H_6MoO_3$	232	$(h^5-C_5H_5)Mo(CO)_3(H)$	Toluene	H	4.6	—	—	132
$[C_{26}H_{20}MoO_3^-P]^+$	233	$[(h^5-C_5H_4PPh_3)Mo(CO)_3(H')^+]$	CF_3CO_2H	H H'	5.91, 5.69 —5.34	$J 2.5$	—	66
$C_{11}H_{14}GeMoO_3$	234	$(h^5-C_5H_5)Mo(CO)_3[Ge(CH_3)_3]$	$CDCl_3$	H H'	5.24 0.62	—	—	63 64
			C_6H_6	H H'	4.58 0.61	—	—	120
$C_{14}H_{20}GeMoO_3$	235	$(h^5-C_5H_5)Mo(CO)_3[Ge(CH_2-CH'_2)_3]$	C_6H_6	H H', H''	4.65 1.18m	—	—	120
				H	5.33	—	40 MHz	135
$C_{26}H_{20}GeMoO_3$	236	$(h^5-C_5H_5)Mo(CO)_3[Ge(C_6H_5)_3]$	$CDCl_3$	H H'	5.21 7.36*	—	*Midpoint of broad overlapping multiplet	65
$C_8H_5BrHgMoO_3$	237	$(h^5-C_5H_5)Mo(CO)_3(HgBr)$	$CDCl_3$	H	5.49	—	—	136
			SO_2	H	5.62	—	—	
$C_8H_5ClHgMoO_3$	238	$(h^5-C_5H_5)Mo(CO)_3(HgCl)$	$CDCl_3$	H	5.51	—	—	136
			SO_2	H	5.64	—	—	

TABLE III—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_8H_5HgIMoO_3$	239	$(h^5-C_5H_5)Mo(CO)_3(HgI)$	$CDCl_3$	H 5.34	—	—	136
			SO_2	H 5.61	—		
$[C_8H_8MoNO_3]^+$	240	$[(h^5-C_5H_5)Mo(CO)_3(NH_2)]^+$	$C_6H_5NO_2$	H 5.7 H' 1.18	—	Isolated as the tetraphenylborate	137
$[C_8H_8MoN_2O_3]^+$	241	$[(h^5-C_5H_5)Mo(CO)_3(N_2H_4)]^+$	$C_6H_5NO_2$	H 5.91 H' 3.38, 3.23	—	Isolated as the tetraphenylborate	137
$C_9H_5MoNO_3S$	242	$(h^5-C_5H_5)Mo(CO)_3(NCS)$	$CDCl_3$	H 5.67s	—	—	131
$C_{10}H_5F_3MoO_3$	243	$(h^5-C_5H_5)Mo(CO)_3(OCOCF_3)$	Acetone	H 5.88s	—	100 MHz	138
$C_{11}H_8MoO_3S$	244	$(h^5-C_5H_5)Mo[OS(O)CH=C=CH_2](CO)_3$	$CDCl_3$	H 6.38 H' 5.04, 5.5	$J_{HH'}$ 2 $J_{H'H'}$ 15	—	944
$C_{12}H_{10}MoO_3S$	245	$(h^5-C_5H_5)Mo[OS(O)C(CH_3)=C=CH_2](CO)_3$	$CDCl_3$	H 2.04 H' 4.95 5.4	$J_{HH'}$ 18 $J_{H'H'}$ 14	—	944
$C_{17}H_{12}MoO_3S$	246	$(h^5-C_5H_5)Mo[OS(O)C(C_6H_5)=C=CH_2](CO)_3$	$CDCl_3$	H 5.2, 5.7	J_{HH} 15	—	944
$C_{20}H_5F_{10}MoO_3P$	247	$(h^5-C_5H_5)Mo(CO)_3[P(C_6F_5)_2]$	$CDCl_3$	H 5.62	J_{PH} 2.2	^{19}F NMR chemical shift 126.4, 153.3, 162.1 ppm relative to CCl_3F	130
$C_{11}H_{14}MoO_3Pb$	248	$(h^5-C_5H_5)Mo(CO)_3[Pb(CH_3)_3]$	$CHCl_3$	H 5.28 H' 1.17	— $J(^{207}Pb-H)$ 44.5	—	65
$C_{26}H_{20}MoO_3Pb$	249	$(h^5-C_5H_5)Mo(CO)_3[Pb(C_6H_5)_3]$	$CDCl_3$	H 5.26 H' 7.38	—	—	65

$C_9H_5MoNO_3S$	250	$(h^5-C_5H_5)Mo(CO)_3(SCN)$	$CDCl_3$	H	5.67s	—	—	131
$C_8H_8MoO_3Si$	251	$(h^5-C_5H_5)Mo(CO)_3(SiH_3)$	$(C_2H_5)_2O$	H	5.35s	—	—	68
				H'	3.85s			
$C_{11}H_{14}MoO_3Si$	252	$(h^5-C_5H_5)Mo(CO)_3[Si(CH_3)_3]$	$CDCl_3$	H	5.30	—	—	63
				H'	0.07	—	—	
			—	H	5.20	—	—	139
				H'	0.06	—	—	
$C_8H_5Br_3O_3^-$ MoSn	253	$(h^5-C_5H_5)Mo(SnBr_3)(CO)_3$	—	H	5.72	—	—	948
$C_8H_5Cl_3O_3^-$ MoSn	254	$(h^5-C_5H_5)Mo(SnCl_3)(CO)_3$	—	H	5.83	—	—	943
$C_{14}H_{10}Cl_2O_3^-$ MoSn	255	$(h^5-C_5H_5)Mo[Sn(Cl)_2C_6H_5](CO)_3$	—	H	5.5	—	—	948
$C_8H_5I_3O_3$ MoSn	256	$(h^5-C_5H_5)Mo(SnI_3)(CO)_3$	—	H	5.67	—	—	948
$C_{11}H_{14}MoO_3Sn$	257	$(h^5-C_5H_5)Mo(CO)_3[Sn(CH_3)_3]$	$CHCl_3$	H	5.41	—	—	65
				H'	0.48	$J(^{117}Sn-H) 47.0$	—	140
						$J(^{119}Sn-H) 49.0$	—	132
			$CDCl_3$	H	5.24	—	—	63
				H'	0.43	$J(^{117}Sn-H) 46.3$	—	64
						$J(^{119}Sn-H) 48.3$	—	
			C_6H_6	H	4.52	—	—	141
				H'	0.50	$J(^{117}Sn-H) 46.5$	—	
						$J(^{119}Sn-H) 48.7$	—	
$C_{10}H_{11}ClMoO_3^-$ Sn	258	$(h^5-C_5H_5)Mo(CO)_3[Sn(CH_3)_2Cl]$	CCl_4	H	5.37	—	—	65
				H'	0.98	$J(^{117}Sn-H) 45.6$	—	132
						$J(^{119}Sn-H) 47.7$	—	

TABLE III—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)		Remarks	References
$C_8H_5Cl_3MoO_3 \cdot Sn$	259	$(h^5-C_5H_5)Mo(CO)_3(SnCl_3)$	$CDCl_3$	H	5.66	—	—	142
$C_{26}H_{20}MoO_3Sn$	260	$(h^5-C_5H_5)Mo(CO)_3[Sn(C_6H_5)_3]$	$CDCl_3$	H	5.26	—	—	132
			Acetone	H	5.55	—	—	65
			THF	H	7.43m	—	—	115
$C_9H_8MoO_5S$	261	$(h^5-C_5H_5)Mo(SO_2CH_3)(CO)_3$	$CDCl_3$	H	5.49s	—	—	960
				H'	3.29s	—	—	960
$C_{10}H_{10}MoO_5S$	262	$(h^5-C_5H_5)Mo(SO_2CH_2CH_3)(CO)_3$	$CDCl_3$	H	5.75s	—	—	960
				H'	3.12q	$J_{H'H''} 7.5$	—	960
				H''	1.25t	—	—	960
$C_{15}H_{12}MoO_5S$	263	$(h^5-C_5H_5)Mo(SO_2CH_2C_6H_5)(CO)_3$	$CDCl_3$	H	5.62s	—	—	960
				H'	4.25s	—	—	960
				H''	7.35m	—	—	960
$C_8H_5F_2MoO_3 \cdot PS_2$	264	$(h^5-C_5H_5)Mo(CO)_3[SP(S)F_2]$	$CDCl_3$	H	5.71	—	^{19}F NMR chemical shift 12.4 ppm relative to CCl_3F in CH_2Cl_2 ($J_{PF} 1204$)	125
$C_{14}H_{10}MoO_3Te$	265	$(h^5-C_5H_5)Mo(CO)_3(TeC_6H_5)$	CS_2	H	5.28s	—	—	126
(d) Derivatives containing two or more transition metal atoms								
$C_{38}H_{30}Mo_2 \cdot N_2O_2$	266	$\{(h^5-C_5H_5)Mo(CO)[N=C-(C_6H_5)_2]\}_2$	$CDCl_3$	H	4.79s	—	—	111
				H'	7.22b	—	—	111

$C_{22}H_{37}HgMo_2O_{12}P_3$	267	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3Hg- \{ (h^5-C_5H_5)Mo(CO)[P(OCH_3)_3]_2 \}]$	$CDCl_3$	$\begin{matrix} H \\ H' \end{matrix}$	$\begin{matrix} 5.06 \\ 3.64, 3.44 \end{matrix}$	—	—	105
$C_{24}H_{30}Mo_2O_4$	268	$\{ [h^5-C_5(CH_3)_5]Mo(CO)_2 \}_2$	$CHCl_3$	$\begin{matrix} H \end{matrix}$	1.89s	—	Hexamethyldisiloxane used as reference	187
$C_{22}H_{18}Mo_2O_4$	269	$[(h^5-C_9H_9)Mo(CO)_2]_2$	C_6BrF_5	$\begin{matrix} H \\ H' \end{matrix}$	$\begin{matrix} 4.78 \\ 5.0 \end{matrix}$	—	$C_9H_9 \approx$	204
				$\begin{matrix} H'' \\ H''' \end{matrix}$	$\begin{matrix} 5.95 \\ 2.43, 1.8-1.7 \end{matrix}$	—	$T 55^\circ$	
$C_{20}H_{28}HgMo_2O_{10}P_2$	270	$\{ (h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]_2 (Hg) \}$	$CDCl_3$	$\begin{matrix} H \\ H' \end{matrix}$	$\begin{matrix} 5.40d \\ 3.75d \end{matrix}$	$\begin{matrix} J 1.0 \\ J_{PH'} 12 \end{matrix}$	—	121
$C_{26}H_{40}Mo_2O_{10}P_2$	271	$\{ (h^5-C_5H_5)Mo(CO)_2[P(OCH_2CH_3)_3]_2 \}$	$CDCl_3$	$\begin{matrix} H \\ H' \end{matrix}$	$\begin{matrix} 5.03d \\ 1.34t \end{matrix}$	$\begin{matrix} J 1.5 \\ J 7.5 \end{matrix}$	38°	122
$C_{32}H_{40}Mo_2O_{10}P_2$	272	$\{ (h^5-C_5H_5)Mo(CO)_2[P(OC_3H_7)_3]_2 \}$	$CDCl_3$	$\begin{matrix} H \end{matrix}$	4.90d	$J_{PH} 1.7$	$T 38^\circ$	123
$C_{32}H_{52}Mo_2O_{10}P_2$	273	$\{ (h^5-C_5H_5)Mo(CO)_2[P(OCH_2CH_3)_3]_2 \}$	$CDCl_3$	$\begin{matrix} H \\ H' \end{matrix}$	$\begin{matrix} 5.07d \\ 1.32d \end{matrix}$	$\begin{matrix} J 1.6 \\ J 6.5 \end{matrix}$	$T 38^\circ$	122
$C_{38}H_{64}Mo_2O_{10}P_2$	274	$\{ (h^5-C_5H_5)Mo(CO)_2[P(O-n-C_4H_9)_3]_2 \}$	$CDCl_3$	$\begin{matrix} H \end{matrix}$	5.03	—	$T 38^\circ$	122
			$CDCl_3$	$\begin{matrix} H \end{matrix}$	5.17	$J_{PH} 1.2$	—	205
$C_{44}H_{40}Mo_2O_6P_2$	275	$\{ (h^5-C_5H_5)Mo(CO)_2[P(OC_6H_5)_3]_2 \}$	$CDCl_3$	$\begin{matrix} H \end{matrix}$	4.72s(br)	—	$T 38^\circ$	123

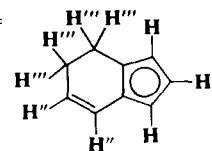


TABLE III—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{33}H_{25}Mo_2O_5P$	276	$[(h^5-C_5H_5)Mo(CO)_3]\{[(h^5-C_5H_5)Mo(CO)_2(PPh_3)]\}$	$CDCl_3$	H 5.22s H' 4.90d	— $J_{PH} 1.9$	—	205
$C_{16}H_{10}Mo_2O_6$	277	$[(h^5-C_5H_5)Mo(CO)_3]_2$	$CHCl_3$	H 5.38s H 5.48	— —	Hexamethyldisiloxane used as reference. 100 MHz	206 916
$C_{28}H_{18}Mo_2O_6$	278	$\{[(h^5-C_5H_4(C_6H_5))Mo(CO)_3]\}_2$		H 5.20 H' 7.19	— —	100 MHz	206
$C_{16}H_{10}Cl_2Mo_2O_6Sn$	279	$[(h^5-C_5H_5)Mo(CO)_3]_2(SnCl_2)$	$CDCl_3$	H 5.59	—	—	142
$C_{16}H_{10}HgMo_2O_6$	280	$[(h^5-C_5H_5)Mo(CO)_3]_2(Hg)$	$CDCl_3$	H 5.41	—	—	142
$C_{16}H_{10}HgMo_2O_6$	281	$[(h^5-C_5H_5)Mo(CO)_3]_2(Hg)$	$CDCl_3$ SO_2	H 5.28 H 5.40	— —	—	136
$C_{18}H_{16}Mo_2O_6Sn$	282	$[(h^5-C_5H_5)Mo(CO)_3]_2[Sn(CH_3)_2]$	$CDCl_3$	H 5.35 H' 0.85	— $J(^{117}Sn-H') 35.8$ $J(^{119}Sn-H') 37.4$	—	65
$C_{24}H_{15}Mo_3O_9Ti$	283	$[(h^5-C_5H_5)Mo(CO)_3]_3Ti$	Acetone	H 5.48	—	—	207
$C_{22}H_{26}Mo_2O_6Si_2$	284	$[(h^5-Me_3SiC_5H_4)Mo(CO)_3]_2$	CS_2	H 5.18t, 5.08t	—	100 Mhz	208
$C_{26}H_{20}AuMoO_6P$	285	$(h^5-C_5H_5)Mo(CO)_3(AuPPh_3)$	$CDCl_3$	H 5.30	—	—	62
$C_{26}H_{20}AuMoO_6P$	286	$(h^5-C_5H_5)Mo(CO)_3[AuP(OPh)_3]$	$CDCl_3$	H 4.91	—	—	62

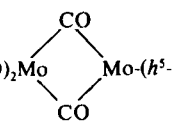
$C_{25}H_{26}As_3^-$ $CuMoO_3$	287	$(h^5-C_5H_5)Mo(CO)_3^-$ $\left[Cu(AsCH_3) \left(As \begin{array}{c} CH_3 \\ \\ \text{C}_6\text{H}_4 \\ \\ CH_3 \end{array} \right)_2 \right]$	$CDCl_3$	H	5.16	—	—	62
$C_{26}H_{38}AuMo-$ O_3P	288	$(h^5-C_5H_5)Mo(CO)_3[AuP(C_6H_{11})_3]$	$CDCl_3$	H	5.23	—	—	62
$C_{39}H_{32}Mo_2^-$ O_3P_2	289	$[(h^5-C_5H_5)Mo(CO)_2][(h^5-C_5H_5)-$ $Mo(CO)] [C_6H_5)_2PCH''=$ $CH''P(C_6H_5)_2]$		H, H'	4.60s	—	—	957
				H''	7.7-7.2	—	—	
$C_{12}H_5CoHg-$ MoO_7	290	$(h^5-C_5H_5)Mo(CO)_3HgCo(CO)_4$	$CDCl_3$	H	5.44	—	—	136
$C_{15}H_{11}Mn-$ MoO_8Sn	291	$[(h^5-C_5H_5)Mo(CO)_3][Sn(CH_3)_2]-$ $[Mn(CO)_5]$	CCl_4	H	5.35	—	100 MHz	140
				H'	0.80	$J(^{119}Sn-H') 36.9$		
$C_{18}H_{15}MoO_3Ti$	292	$(h^5-C_5H_5)_2TiMo(CO)_3(h^5-C_5H_5)$	—	H	5.67	—	—	209
				H'	6.44	—	—	
$C_{33}H_{25}Mo_2^-$ O_5P	293	$(h^5-C_5H_5)(CO)_2Mo$  $Mo-(h^5-$ $C_5H_5)(CO)[P(C_6H_5)_3]$	$CDCl_3$	H	5.11s	—	—	161
				H'	4.72d	$J_{PH'} 1.5$		
				H''	7.44	—		
$C_{16}H_{10}Cl_2-$ Mo_2O_6Sn	294	$[(h^5-C_5H_5)Mo(CO)_3]_2(SnCl_2)$	—	H	5.65	—	—	943 948

TABLE III—*cont.*

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Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{16}H_{10}Br_2Mo_2O_6Sn$	295	$[(h^5-C_5H_5)Mo(CO)_3]_2(SnBr_2)$	—	H 5.67	—	—	948
$C_{16}H_{10}I_2Mo_2O_6Sn$	296	$[(h^5-C_5H_5)Mo(CO)_3]_2(SnI_2)$	—	H 5.67	—	—	948
$C_{20}H_{20}Mo_2O_6Sn$	297	$[(h^5-C_5H_5)Mo(CO)_3]_2[Sn(C_2H_5)_2]$	—	H 5.52	—	—	948
$C_{26}H_{20}Mo_2O_6Sn$	298	$[(h^5-C_5H_5)Mo(CO)_3]_2[Sn(C_5H_5)_2]$	—	H 5.59	—	—	948
$C_{18}H_{10}Mo_2N_2O_6S_2Sn$	299	$[(h^5-C_5H_5)Mo(CO)_3]_2[Sn(SCN)_2]$	—	H 5.78	—	—	948
$C_{16}H_{10}Mo_2N_2O_{10}Sn$	300	$[(h^5-C_5H_5)Mo(CO)_3]_2[Sn(NO_2)_2]$	—	H 5.61	—	—	948
$C_{22}H_{26}Mo_2O_6Si_2$	301	$\{[h^5-C_5H_5Si(CH_3)_3]Mo(CO)_3\}_2$	—	H 5.20t H' 4.90t 0.16	— — —	—	1033
$C_{28}H_{22}Mo_2O_6$	302	$(h^5-C_{20}H_{16})[Mo(CH_3)(CO)_3]_2$	—	n.a.	—	Complex spectrum	1024
$C_{57}H_{46}Mo_2O_4P_2Sn$	303	$[(h^5-C_5H_5)Mo(CO)_2PPh_3]_2\cdot Sn(CH_3)_2$	C_2Cl_4 - CH_2Cl_2	H 5.05	$J_{PH} 0.8$	—	107
$C_{15}H_{12}Mo_2O_5$	304	$[(h^5-C_5H_5)_2Mo(H_2)]Mo(CO)_5$	—	H $\sim 4.9t$ H' 18.5	— —	—	212

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(6) HEXAHAPTO LIGANDS

C ₁₃ H ₁₄ MoO ₃	305	[<i>h</i> ⁶ -C ₆ H ₅ C(CH ₃) ₃]Mo(CO) ₃	CDCl ₃	¹ H ¹ H'	5.58m 1.28s	— —	—	143
C ₂₇ H ₂₂ As ₂ MoO ₂	306	[<i>h</i> ⁶ -C ₆ H ₅ As(C ₆ H ₅)CH ₂ As-(C ₆ H ₅) ₂]Mo(CO) ₂	CDCl ₃	¹ H ¹ H' ¹ H''	~5 ~4 ~7	—	100 MHz	144
C ₁₂ H ₁₄ MoO ₃ Sn	307	[<i>h</i> ⁶ -C ₆ H ₅ Sn(CH ₃) ₃]Mo(CO) ₃	CDCl ₃	¹ H ¹ H'	5.57m 0.38s	— —	<i>J</i> (¹¹⁷ Sn-H) 53.1	143
			CCl ₄	¹ H ¹ H'	5.46 0.33	— —	<i>J</i> (¹¹⁹ Sn-H) 55.7, 57.0	145 146
C ₁₁ H ₁₀ MoO ₃	308	(<i>h</i> ⁶ -1,3-(CH ₃) ₂ C ₆ H ₄)Mo(CO) ₃	CH ₂ Cl ₂	C ₋₁ C ₋₂ C ₋₃ C ₋₄ C ₋₅ C ₋₆ C-CH ₃ CO	115.6 96.4 115.6 92.7 98.2 92.7 21.5 223.1	— — — — — — — —	32	
C ₁₁ H ₁₀ MoO ₃	309	[<i>h</i> ⁶ -1,4-(CH ₃) ₂ C ₆ H ₄]Mo(CO) ₃	CDCl ₃	¹ H ¹ H'	5.63 2.16	—	T 33°	147 1009
C ₁₂ H ₁₂ MoO ₃	310	(<i>h</i> ⁶ -1,3,5-(CH ₃) ₃ C ₆ H ₃)Mo(CO) ₃	CH ₂ Cl ₂	C ₁ , C ₃ , C ₅ C-CH ₃ C ₂ , C ₄ , C ₆ CO	117.1 21.2 94.7 223.7	— — — — —	148 1009	

TABLE III—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{13}H_{14}MoO_3$	311	$(h^6-1,2,4,5-(CH_3)_4C_6H_2)Mo(CO)_3$	CH_2Cl_2	C_{-1}, C_{-2} 118.8 C_{-4}, C_{-5} $C-CH_3$ 19.1 C_{-3}, C_{-6} 101.1 CO 224.4	— — — —		148
$C_{24}H_{21}MoO_3P$	312	$[h^6-C_6H_4-2-CH_2'-1-P(2-CH_3C_6H_4)_2]Mo(CO)_3$	$CDCl_3$	H 5.9–5.0 H' 2.8, 2.35, 2.2, 2.18 H'' 7.3–6.8	— — —	—	149
$C_{13}H_{16}MoO_3Si$	313	$[h^6-C_6H_4-1-CH_2'-4-Si(CH_3)_3]Mo(CO)_3$	$CDCl_3$	H_2, H_6 5.40 H_3, H_5 5.77 H' 2.25 H'' 0.23	— — — —	T 33°	147
$C_{12}H_{13}MoNO_3$	314	$[h^6-C_6H_4-1-CH_2'-4-N(CH_3)_2]Mo(CO)_3$	$CDCl_3$	H_2, H_6 5.90 H_3, H_5 5.19 H' 2.11 H'' 2.78	— — — —	T 33°	147
$C_{14}H_{19}MoNO_3Si$	315	$[h^6-C_6H_4-1-N(CH_3)_2-4-Si(CH_3)_3]Mo(CO)_3$	$CDCl_3$	H_2, H_6 5.16 H_3, H_5 5.89 H' 2.84 H'' 0.23	— — — —	T 33°	147
$[C_{10}H_7MoO_3]^+$	316	$[(h^6-C_7H_7)Mo(CO)_3]^+$	H_2SO_4	H 5.7	—	C_7H_7 = tropylium cation	910

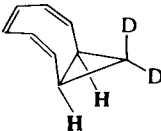
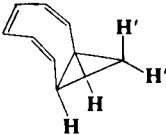
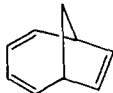
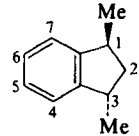
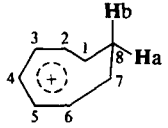
$C_{10}H_8MoO_3$	317	$(h^6-C_7H_8)Mo(CO)_3$	CH_2Cl_2	CH_2 CH CO	28.0 61.3, 98.1, 103.7 220.6	— — — —		148
$C_{10}H_8MoO_3$	318	$(1,2,3,4,5,6-h^6-C_7H_8)Mo(CO)_3$	CCl_4	H_{-7exo} H_{-7endo}	2.45d 3.02	— —	—	955
$C_{13}H_{14}MoO_3$	319	$\{1,2,3,4,5,6-h^6-3,7,7-(CH_3)_3-C_7H_3\}Mo(CO)_3$	CCl_4	$7-CH_{3exo}$ $7-CH_{3endo}$	0.30 1.40	— —	—	955
$C_{14}H_{16}MoO_3$	320	$\{1,2,3,4,5,6-h^6-2,3,7,7-(CH_3)_4-C_7H_4\}Mo(CO)_3$	$CDCl_3$	$7-CH_{3exo}$ $7-CH_{3endo}$	0.23 1.37	— —	—	955
$C_{11}H_8MoO_3$	321	$(1,2,3,4,5,6-h^6-C_8H_8)Mo(CO)_3$	$CDCl_3$	H_1, H_6 H_2, H_5 H_3, H_4 H_7, H_8	4.48 5.14 6.23 4.96	— — — —	T -40° Cyclooctatetraene protons give a sharp signal at 80°	911 912 150 1020
$C_{15}H_{16}MoO_3$	322	$(h^6-C_8H_4(CH_3)_4)Mo(CO)_3$		n.a.	—	—	$C_8H_4(CH_3)_4 = 1,3,5,7$ -tetra- methylcyclooctatetraene Temperature dependence of NMR spectra analysed	151 913
$C_{12}H_8D_2MoO_3$	323	$(h^6-C_9H_8D_2)Mo(CO)_3$	C_6D_6	H	0.6s	—	$C_9H_8D_2 =$ 	152
$C_{12}H_{10}MoO_3$	324	$(h^6-C_9H_{10})Mo(CO)_3$	C_6D_6	H H'	0.6 0.4, 0.2	J 4.5	$C_9H_{10} =$ 	152
Olefinic signals at 5.2, 4.8, 4.5								

TABLE III—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{12}H_{10}MoO_3$	325	$(h^6-C_9H_{10})Mo(CO)_3$	C_6D_6	n.a.		—	Signals at δ 4.5 sext., 3.4m, 2.8t, 1.0t, 0.2t (J 12.5) in ratio 2:4:2:1:1 $C_9H_{10} =$ 	152
$C_{14}H_{14}MoO_3$	326	$(h^6-C_{11}H_{14})Mo(CO)_3$	—	H_{-4}	5.52d	—	100 MHz $C_{11}H_{14} =$ 	153
(7) HEPTAHAPTO LIGANDS								
$[C_{20}H_{15}Fe-MoO_3]^+$	327	$[h^7-C_7H_6Fc]Mo(CO)_3]^+$		H	5.43s	—	Isolated as the tetrafluoroborate Fc = Ferrocene	154
$[C_{11}H_9MoO_3]^+$	328	$[(h^7-C_8H_9)Mo(CO)_3]^+$	SO_2	H_{-1}	4.42	$J_{H_1, H_2} 8.0$	Isolated as tetrafluoroborate $C_8H_9 =$ 	155
				H_{-2}	6.13	$J_{H_2, H_3} 7.5$		910
				H_{-3}	6.62	$J_{H_3, H_4} 10$		955
				H_{-4}	5.94	$J_{H_4, H_5} 10$		
				H_{-5}	6.62	$J_{H_5, H_6} 7.5$		

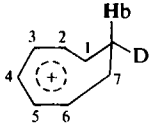
				H_{-6}	6.13	J_{H_6, H_7}	8.0		The homotropylium structure (I) is preferred over the corresponding planar cyclooctatrienyl structure largely on the basis of the large chemical shift difference between the inside and outside C-8 protons	
				H_{-7}	4.42	$J_{H_7, H_{8a}}$	8.5			
				H_{-8a}	3.47	$J_{H_7, H_{8a}}$	8.5			
				H_{-8b}	-0.15	$J_{H_{8a}, H_{8b}}$	12.0			
						$J_{H_{8b}, H_{8b}}$	9.0			
						$J_{H_7, H_{8b}}$	9.0			
		H_2SO_4		H_1, H_7	4.37	—			Remaining signals at δ 6.49, 6.05	150
				H_{8a}	3.37	—				
				H_{8b}	-0.15	—				
$[C_{11}H_8DMoO_3]^+ + 329$	$[(h^7-C_8H_8D)Mo(CO)_3]^+$	D_2SO_4		H_1, H_7	4.25	—			$C_8H_8D =$	
				H_3, H_4, H_5	6.43, 6.0	—				150
				H_{8b}	-0.20	—				
(8) MIXED LIGANDS										
(a) Mono-carbonyl derivatives										
$C_{13}H_{26}MoO_7P_2$	330	$(h^5-C_5H_5)Mo(CO)[P(OCH_3)_3]_2$	$CDCl_3$	H	5.08	—			—	105
		(CH_3^a)		H'	3.69, 3.59,	—				
					3.50					
				H''	-0.27t	$J_{PH''}$	10.5			
$C_{14}H_{13}MoNO_3$	331	$(h^5-C_5H_5)Mo(CO)(NO)[C-(OCH_3)_6C_6H_5^a]$	CD_3COCD_3	H	5.44	—			—	60
				H'	4.51	—				
				H''	7.21					
$C_{15}H_{15}MoNO_3$	332	$(h^5-C_5H_5)Mo(CO)(NO)[C(OCH_3)_2CH_3C_6H_5^a]$	CD_3COCD_3	H	5.37s	—			—	60
				H'	4.70q	—				
				H''	7.11m					

TABLE III—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{34}H_{25}ClMoO$	333	$[h^4-C_4(C_6H_5)_4](h^5-C_5H_5)Mo(CO)-$ (Cl)	$CDCl_3$	H	5.45s	—	—	158
				H'	7.32b	—	—	
$C_{38}H_{33}BrMoO$	334	$(h^5-C_5H_5)Mo(h^4-C_4(p-C_6H_4-$ $CH_3)_4)(Br)(CO)$	—	H	5.29s	—	—	961
				H'	7.0s	—	—	
				H''	2.20s	—	—	
$C_{34}H_{26}MoO$	335	$[h^4-C_4(C_6H_5)_4](h^5-C_5H_5)Mo(CO)-$ (H'')	—	H	4.61s	—	—	159
				H'	7.3–7.0 m	—	—	
				H''	–6.83s	—	—	
			C_6H_6	H	4.61s	—	—	159
				H''	–6.83s	—	—	
(b) Di-carbonyl derivatives								
$C_{26}H_{20}F_3MoO_2P$	336	$(h^5-C_5H_5)Mo(CF_3)[P(C_6H_5)_3]-$ (CO) ₂	CH_2Cl_2	F	–11.3d	—	—	956
$C_{20}H_{35}MoO_2P$	337	$(h^5-C_5H_5)Mo(CO)_2[P(n-C_4H_9)_3]-$ (CH ₃)	$CDCl_3$	H	5.15	—	cis-isomer T 38°	114
				H'	0.02	$J_{PH'} 9.3$		
				H	4.83	$J_{PH} 1.3$		
				H'	0.24	$J_{PH'} 2.4$	trans-isomer	160
			CD_3CN	H	4.97d	$J_{PH} 1.5$		
				H'	0.13d	$J_{PH'} 2.5$		
				H''	1.5, 0.9m	—	—	
$C_{16}H_{19}MoO_2P$	338	$(h^5-C_5H_5)Mo(CO)_2[P(CH_3)_2Ph]-$ (CH ₃)	$CDCl_3$	H	4.71	$J_{PH} 1.4$	trans-isomer	117
				H'	0.30	$J_{PH'} 2.8$		
				H''	1.82	$J_{PH''} 8.5$		

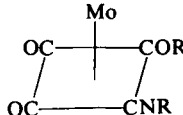
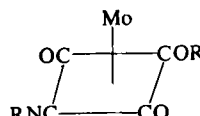
$C_{26}H_{23}MoO_2P$	339	$(\eta^5-C_5H_5)Mo(CO)_2[P(C_6H_5)_3]-(CH_3)_3$	$CDCl_3$	H	5.08	$J_{PH} < 0.3$	} <i>cis</i> -isomer 100 MHz T 31°	161
				H'	-0.18	$J_{PH'} 11.8$		
				H''	1.68, 1.65	$J_{PH''} 8.2, 8.0$		
			CD_3CN	H	4.70s	—	} —	160
				H'	0.39d	$J_{PH'} 2.5$		
				H''	7.39m	—		
			<i>o</i> -C ₆ H ₄ Cl ₂	H	4.45d	$J_{PH} 1.5$	} —	114
				H'	0.39d	$J_{PH'} 3.0$		
				H''	7.3m	—		
$C_{11}H_{17}MoO_5P$	340	$(\eta^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]-(CH_3)_3$	$CDCl_3$	H	5.03	—	} <i>cis</i> -isomer T 38°	122
				H'	-0.08	$J_{PH'} 11.0$		
				H''	4.70	$J_{PH''} 1.4$		
			$CDCl_3$	H	0.58	$J_{PH} 2.3$	} <i>trans</i> -isomer T 38°	121
				H'	5.20s	—		
				H''	0.00d	$J 10.0$		
			$CDCl_3$	H	3.53d	$J 11.5$	} <i>cis</i> -isomer	114
				H'	5.05d	$J 1.5$		
				H''	0.30d	$J 3.2$		
			$CDCl_3$	H	3.62d	$J 12.0$	} <i>trans</i> -isomer T 38°	160
				H'	5.25s, 5.10d	$J 1.2$		
				H''	0.33d	$J_{PH'} 3.0$		

TABLE III—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{16}H_{19}MoO_4P$	341	$(\eta^5-C_5H_5)Mo(CO)_2[P(OCH_3)_2Ph]-(CH_3)$	$CDCl_3$	H	4.84	$J_{PH} 1.6$	$trans$ -isomer	117
				H'	3.62	$J_{PH'} 12.5$		
				H''	0.32	$J_{PH''} 3.0$		
				H	5.05	$J_{PH} < 0.5$	cis -isomer T 38° 100 MHz	
				H'	3.46, 3.42	$J_{PH'} 13.0, 11.8$		
				H''	-0.21	$J_{PH''} 11.6$		
$C_{26}H_{23}MoO_5P$	342	$(\eta^5-C_5H_5)Mo(CO)_2[P(OC_6H_5)_3]-(CH_3)$	$CDCl_3$	H	4.70s	—	cis -isomer 100 MHz	124
				H'	0.29d	$J_{PH'} 11$		
				H	4.51s	—	$trans$ -isomer	
				H'	0.30d	$J_{PH'} 3$		
			$CDCl_3$	H	4.72	—	cis -isomer	114
				H'	0.27	$J_{PH'} 10.3$		
				H	4.53	$J_{PH} 1.2$	$trans$ -isomer T 38°	
				H'	0.29	$J_{PH'} 2.6$		
			CD_3CN	H	4.60d	$J_{PH} 1.5$	—	160
				H'	0.27d	$J_{PH'} 3.0$		
				H''	7.3m	—		
$C_{27}H_{25}MoO_2P$	343	$(\eta^5-C_5H_5)Mo(CO)_2(PPh_3)(CH_2-CH_3)$	$CDCl_3$	H H', H''	4.71d 1.47-1.69m	$J_{PH} 1.44$ —	Hexamethyldisiloxane used as internal standard	162

			CDCl ₃	H	4.67s	—	<i>cis</i> -isomer*	124
				H	4.51d	<i>J</i> 1.2	<i>trans</i> -isomer	
				H', H''	1.2–1.7	—	100 MHz	
							*Reviewer's assignment	
C ₂₇ H ₂₃ MoO ₅ P	344	(<i>h</i> ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(OPh) ₃]- (CH' = CH'')	CDCl ₃	H	4.63s	—	<i>cis</i> -isomer*	124
				H	4.49d	<i>J</i> 1.4	<i>trans</i> -isomer	
				H'	6.02m	—	100 MHz	
				H''	4.72, 4.53,	—	*Reviewer's assignment	
					4.37			
					2.15d	<i>J</i> 3.2		
					2.07d	<i>J</i> 3.2		
C ₂₉ H ₂₅ MoO ₅ P	345	(<i>h</i> ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(OPh) ₃]- (CH ₂ C≡CCH ₃)	CDCl ₃	H	5.12s,	<i>J</i> 1.5	—	163
					5.01d			
				H', H''	2.0 comp.			
C ₁₄ H ₁₂ MoO ₂	346	(<i>h</i> ⁵ -C ₅ H ₅)Mo(CO) ₂ (CH ₂ Ph)	SO ₂	H	2.88	—	T -37°	112
C ₃₂ H ₂₇ MoO ₂ P	347	(<i>h</i> ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(C ₆ H ₅ ''') ₃]- (CH ₂ C ₆ H ₅)	CDCl ₃	H	5.27	—	Structure uncertain (see below)	164
				H'	1.25s	—		
				H'', H'''	7.6–7.1	—		
			CDCl ₃	H	4.68*	<i>J</i> _{PH} 1.4	<i>trans</i> -isomer, 38°	114
				H'	2.19*	<i>J</i> _{PH} 2.0	*Not consistent with data reported by Craig and Green (ref. 164)	
C ₂₂ H ₂₃ MoO ₄ P	348	(<i>h</i> ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(OCH ₃) ₂ - Ph](CH ₂ Ph)	CDCl ₃	H	4.69	<i>J</i> _{PH} 1.6	<i>trans</i> -isomer	117
				H'	3.53	<i>J</i> _{PH} 11.9		
				H''	2.78	<i>J</i> _{PH} 2.9		
				H	4.90	<i>J</i> _{PH} < 0.2	<i>cis</i> -isomer	
				H'	—	<i>J</i> _{PH} —		
				H''	—	<i>J</i> _{PH} —		
							T 31°	
							MHz	

TABLE III—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References		
$C_{32}H_{27}MoO_5P$	349	$(h^5-C_5H_5)Mo(CO)_2[P(OPh)_3]-(CH_2^iPh)$	$CDCl_3$	H	4.63	—	<i>cis</i> -isomer. Methylene protons nonequivalent due to lack of symmetry of <i>cis</i> -isomer	114		
				H'	2.96	$J_{PH} 10.2$				
					2.60	$J_{PH} 11.0$				
						$J_{gem} 10.3$				
				H	4.45	$J_{PH} 1.3$			<i>trans</i> -isomer T 38°	
				H'	2.76	$J_{PH} 2.7$				
			$CDCl_3$	H	4.61s, 4.43d	$J_{PH} 1.3$	100 MHz	124		
				H'	2.73d	$J_{PH'} 2.7$				
			$CDCl_3$	H	4.45d	$J_{PH} 1.3$	100 MHz	165		
				H	2.76d					
$C_{31}H_{25}MoO_5P$	350	$(h^5-C_5H_5)Mo(CO)_2(PPh_3)(C_6H_5^i)$	$CDCl_3$	H	4.84d	$J_{PH} 1.33$	Hexamethyldisiloxane used as internal standard	162		
				H'	7.29— 7.49m	—				
$C_{14}H_{17}MoNO_3$	351	$(h^5-C_5H_5)Mo(CO)_2(COCH_3^-)[C=NC(CH_3)_3]$	$CDCl_3$	H	5.34	—	<i>cis</i> -isomer, viz.: 	167		
				H'	2.46	—				
				H''	1.50	—				
				$CDCl_3$	H	5.19			—	<i>trans</i> -isomer, viz.: 
					H'	2.57			—	
					H''	1.52			—	

			CS ₂	H	5.15	—	cis-isomer	
				H'	2.27			
				H''	1.47			
				H	5.01	—	trans-isomer	
				H'	2.35			
				H''	1.50			
C ₁₆ H ₁₉ MoNO ₃	352	(<i>h</i> ⁵ -C ₅ H ₅)Mo(CO) ₂ (COCH ₃)- (CNC ₆ H ₁₁)	CS ₂	H	5.28s	—	cis-isomer	166
				H'	2.55s			
				H	5.15s	—	trans-isomer	
				H'	2.63s			
C ₁₅ H ₂₃ MoO ₃ P	353	(<i>h</i> ⁵ -C ₅ H ₅)Mo(CO) ₂ (PEt ₃)- (COCH ₃)	CCl ₄	H	5.08	—	—	168
				H'	2.45	—		
C ₂₁ H ₃₅ MoO ₃ P	354	(<i>h</i> ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(<i>n</i> -C ₄ H ₉) ₃]- (COCH ₃)	CDCl ₃	H	5.00d	<i>J</i> 1.0	100 MHz	169
				H'	2.49	—		
			CD ₃ CN	H	5.12d	<i>J</i> _{PH} 1.0	—	160
				H'	2.47s	—		
				H''	1.5, 0.9m	—		
C ₂₇ H ₂₃ MoO ₃ P	355	(<i>h</i> ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(C ₆ H ₅) ₃]- (COCH ₃)	CDCl ₃	H	5.02d	<i>J</i> 2.0	100 MHz	169
				H'	2.62s	—		161
				H''	7.43m	—		
			CD ₃ CN	H	4.79d	<i>J</i> _{PH} 1.0	—	160
				H'	2.81s	—		
				H''	7.3m	—		
C ₂₉ H ₂₃ MoO ₃ P	356	(<i>h</i> ⁵ -C ₆ H ₅)Mo(CO) ₂ (COCH ₃)- (PPh ₂ C≡CPh)	CDCl ₃	H	5.19d	<i>J</i> 2.0	—	170
				H'	2.59s	—		
C ₁₅ H ₂₆ MoN ₃ - O ₃ P	357	(<i>h</i> ⁵ -C ₅ H ₅)Mo(CO) ₂ {P[N(CH ₃) ₂] ₃ }-	CCl ₄	H	5.10	—	—	168
		(COCH ₃)		H'	2.43	—		

TABLE III—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{12}H_{17}MoO_6P$	358	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]-(COCH_3)$	$CDCl_3$	H	5.14d	J 1.0	100 MHz	169
				H'	2.53	—		
			CCl_4	H	5.22	—	—	168
				H'	2.50	—		
			CD_3CN	H	5.28d	J_{PH} 1.5	—	160
				H'	2.47s			
$C_{15}H_{23}MoO_6P$	359	$(h^5-C_5H_5)Mo(CO)_2[P(OEt)_3]-(COCH_3)$	$CDCl_3$	H	5.09	J 1.0	100 MHz	169
				H'	2.48			
				H''	3.62d	$J_{PH'}$ 10		
$C_{14}H_{17}MoO_6P$	360	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]-CCH_3](COCH_3)$	$CDCl_3$	H	5.21d	J 1.5	100 MHz	169
				H'	2.52	—		
$C_{27}H_{23}MoO_6P$	361	$(h^5-C_5H_5)Mo(CO)_2[P(OC_6H_5)_3]-(COCH_3)$	$CDCl_3$	H	4.74d	J 1.0	100 MHz	169
				H'	2.13	—		
			CD_3CN	H	4.86d	J_{PH} 1.0	—	160
				H'	2.20s	—		
				H''	7.3m			
$C_{22}H_{37}MoO_3P$	362	$(h^5-C_5H_5)Mo(CO)_2[P(n-C_4H_9)_3]-(COCH_2CH_3)$	$CDCl_3$	H	5.02d	J 1.0	100 MHz	169
				H'	2.91q	J 7.2		
$C_{13}H_{19}MoO_6P$	363	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_3)_3]-(COCH_2CH_3)$	$CDCl_3$	H	5.13d	J 1.1	100 MHz	169
				H'	2.94q	J 7.2		
				H''	0.6t	J 7.2		
$C_{28}H_{25}MoO_3P$	364	$(h^5-C_5H_5)Mo(CO)_2(PPh_3)-(COCH_2CH_3)$	$CDCl_3$	H	4.95d	J 1.5	100 MHz	169
				H'	3.02q	J 7.0		
				H''	0.91t	J 7.0		

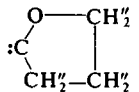
$C_{16}H_{25}MoO_6P$	365	$(h^5-C_5H_5)Mo(CO)_2[P(OC_2H_5)_3]-(COCH_2CH_3)$	$CDCl_3$	H H' H''	5.19d 3.00q 0.94t	J_{1-1} J_{7-4} J_{7-4}	100 MHz	169
$C_{15}H_{19}MoO_6P$	366	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_2)_3-CCH_3](COCH_2CH_3)$	$CDCl_3$	H H' H''	5.15d 2.91q 0.85t	J_{1-0} J_{7-3} J_{7-3}	100 MHz	169
$C_{28}H_{25}MoO_6P$	367	$(h^5-C_5H_5)Mo(CO)_2[P(OPh)_3]-(COCH_2CH_3)$	$CDCl_3$	H H' H''	4.72d 2.50q 0.72t	J_{1-0} J_{7-0} J_{7-0}	100 MHz	169
$C_{29}H_{25}MoO_3P$	368	$(h^5-C_5H_5)Mo(CO)_2[P(C_6H_5^{IV})_3]-(COCH_2CH''=CH_2''')$	$CDCl_3$	H H' H'' H''' H ^{IV}	4.92d 3.69d 5.80 4.86, 4.75 7.36	$J_{PH} 1.0$ $J_{H'H''} 6.9$ $J_{H''H'''} 17.0, 10.8$ $J_{H'''H'''} 2.4$ —	<i>trans</i> -isomer 100 MHz	164
$C_{30}H_{27}MoO_3P$	369	$(h^5-C_5H_5)Mo(CO)_2[P(C_6H_5^V)_3]-(COCH_2CH''=CH'''CH_3^{IV})$	$CDCl_3$	H H' H'' H''' H ^{IV} H ^V	4.95 3.68 5.39 5.19 1.61 7.40	$J_{PH} 1.0$ $J_{H'H''} 5.0$ $J_{H''H'''} 6.0$ $J_{H'''H'''} 6.0$ — —	<i>trans</i> -isomer 100 MHz	164
$C_{17}H_{21}MoO_6P$	370	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_2^{IV})_3-CEt](COCH_2CH''=CH_2''')$	$CDCl_3$	H H' H'' H''' H ^{IV} Et	5.52d 3.84d 5.86 4.90, 4.71 4.51d 1.07	$J_{PH} 1.2$ $J_{H'H''} 7.5$ $J_{H''H'''} 17.0, 10.0$ $J_{H'''H'''} 2.1$ $J_{PH^{IV}} 5.2$ —	<i>trans</i> -isomer 100 MHz	164

TABLE III—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References	
C ₂₀ H ₂₁ MoNO ₃	371	(h ⁵ -C ₅ H ₅)Mo(CO) ₂ (COCH ₂ Ph)-[C=NC(CH ₃) ₃]	CDCl ₃	H	5.25	—	cis-isomer	167	
				H'	4.15, 4.08	—			
				H''	1.48	—			
				H	5.12	—			trans-isomer
				H'	4.24	—			
				H''	1.48	—			
			C ₆ D ₆	H	4.98	—	cis-isomer		
				H'	4.37, 4.30	—			
				H''	0.9	—			
				CS ₂	H	4.90	—		trans-isomer
					H'	4.57	—		
					H''	0.9	—		
CS ₂	H	5.13	—		cis-isomer				
	H'	3.91	—						
	H''	1.38	—						
	CS ₂	H	4.99	—	trans-isomer				
		H'	4.07	—					
		H''	1.46	—					
C ₂₂ H ₂₃ MoNO ₃		372	(h ⁵ -C ₅ H ₅)Mo(CO) ₂ (CNC ₆ H ₁₁)-(COCH ₂ Ph)	CS ₂	H	5.20s	—	cis-isomer	166
					H'	3.94s	—		
					H	5.05s	—	trans-isomer	
	H'				4.04s	—			
C ₂₇ H ₁₉ MoO ₃ P	373	(h ⁵ -C ₅ H ₅)Mo(CO) ₂ [P(n-C ₄ H ₉ '') ₃](COCH ₂ C ₆ H ₅)	CDCl ₃	H	5.05d	J _{PH} 1.1	trans-isomer 100 MHz	164	
				H'	4.19	—			

			H''	7.05	—		
			H'''	2.18–0.78	—		
				comp.			
$C_{35}H_{27}MoO_3P$	374	$(h^5-C_5H_5)Mo(CO)_2(PPh_2C\equiv CPh)-$	$CDCl_3$	H	5.09d	$J_{PH} 2.0$	—
		$(COCH_2Ph)$		H'	4.28s	—	
$C_{33}H_{27}MoO_3P$	375	$(h^5-C_5H_5)Mo(CO)_2[P(C_6H_5''')_3]-$	$CDCl_3$	H	4.98d	$J_{PH} 1.2$	<i>trans</i> -isomer
		$(COCH_2C_6H_5'')$		H'	4.30s	—	100 MHz
				H'', H'''	7.42	—	
$C_{21}H_{23}MoO_6P$	376	$(h^5-C_5H_5)Mo(CO)_2[P(OCH_2'')_3]-$	$CDCl_3$	H	5.25d	$J_{PH} 1.3$	<i>trans</i> -isomer
		$CCH_2^{IV}CH_3^V(COCH_2C_6H_5'')$		H'	4.15s	—	100 MHz
				H''	7.29	—	
				H'''	4.33d	$J_{PH} 5.0$	
				H^{IV}	1.84	—	
				H^V	0.81m	—	
$C_{33}H_{27}MoO_6P$	377	$(h^5-C_5H_5)Mo(CO)_2[P(OC_6H_5''')_3]-$	$CDCl_3$	H	4.92d	$J_{PH} 1.2$	<i>trans</i> -isomer
		$(COCH_2C_6H_5'')$		H'	3.79s	—	100 MHz
				H'', H'''	7.36	—	
$C_{32}H_{25}MoO_3P$	378	$(h^5-C_5H_5)Mo(CO)_2(PPh_3)-$	$CDCl_3$	H	5.09	$J_{PH} 1.33$	Hexamethyldisiloxane used as
		(COC_6H_5)					internal standard
$C_{27}H_{25}MoO_3P$	379	$(h^5-C_5H_5)Mo(CO)_2(PPh_3)-$	$CDCl_3$	H	4.84	$J_{PH} 1.2$	T 38°
		(CH_2OCH_3')		H'	4.74	$J_{PH'} 3.6$	
				H''	3.38	—	
$C_{27}H_{25}MoO_6P$	380	$(h^5-C_5H_5)Mo(CO)_2[P(OC_6H_5)_3]-$	$CDCl_3$	H	4.78	—	} <i>cis</i> -isomer
		(CH_2OCH_3')		H'	obs.	—	
				H''	3.31	—	
				H	4.62	$J_{PH} 1.2$	} <i>trans</i> -isomer
				H'	4.60	$J_{PH'} 3.6$	
				H''	3.56	—	

TABLE III—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$[\text{C}_{29}\text{H}_{26}^-\text{MoO}_3\text{P}]^+$	381	$[(\eta^5\text{-C}_5\text{H}_5)\text{Mo}(\text{CO})_2[\text{P}(\text{C}_6\text{H}_5)_3]\text{-}(\text{C}_4\text{H}_6\text{O})]^+$	CDCl_3	H	5.83s	—	<i>cis</i> -isomer. Isolated as the bromide. 171 A carbene complex where $\text{C}_4\text{H}_6\text{O} = 2\text{-oxacyclopentylidene}$: 	
				H'	7.46m	—		
				H''	4.61 comp.	—		
					sext.	—		
					3.67 comp.	—		
					sext.	—		
			CDCl_3		1.60bm	—		
				H	5.56d	$J_{\text{PH}} 1.1$	<i>trans</i> -isomer isolated as the bromide	
				H'	7.45m	—		
				H''	5.23t	—		
					4.06bt	—		
			CDCl_3		2.16b quin.	—		
				H	5.16	—	<i>cis</i> -isomer isolated as the tetraphenylborate	
				H'	7.16m	—		
				H''	4.10bm	—		
					3.466m	—		
			CDCl_3		2.33 compt.	—	<i>trans</i> -isomer isolated as the tetraphenylborate	
				H	5.10d	$J_{\text{PH}} 1.0$		
				H'	7.20m	—		
				H''	4.35bt	—		
$[\text{C}_{29}\text{H}_{46}\text{MoO}_3^-\text{P}]^+$	382	$\{(\eta^5\text{-C}_5\text{H}_5)\text{Mo}(\text{CO})_2[\text{P}(\text{C}_6\text{H}_{11})_3]\text{-}[\text{C}(\text{OCH}_2\text{CH}_3)\text{CH}_3]\}^+$	CD_3COCD_3	H	5.87d	$J_{\text{PH}} 0.75$	Isolated as the tetrafluoroborate	172
				H'	4.80	—		
				H''	3.25	—		

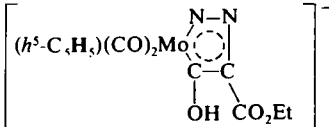
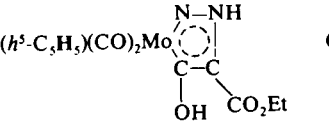
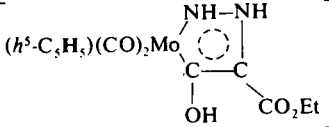
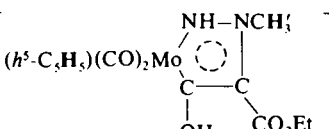
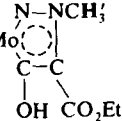
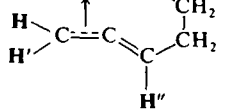
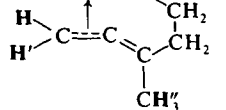
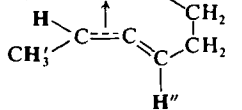
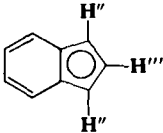
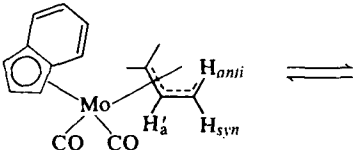
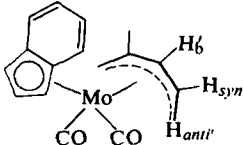
$C_{27}H_{25}MoO_5PS$	383	$(h^5-C_5H_5)Mo(CO)_2[P(OC_6H_5)_3]^-$ (CH_2SCH_3)	C_6H_6	H 4.95 — H' 3.02 J 8.6 H'' 3.91 J 11.5 H'' 2.49 J 0.5	$\left. \begin{array}{l} \\ \\ \end{array} \right\}$ <i>cis</i> -isomer $\left. \begin{array}{l} \\ \\ \end{array} \right\}$ <i>trans</i> -isomer T 38°	114
$[C_{12}H_{11}MoN_2O_5]^-$	384	$(h^5-C_5H_5)(CO)_2Mo$ 		H 5.16s —	Isolated as the quaternary <i>n</i> -butyl ammonium salt 100 MHz	173
$C_{12}H_{12}MoN_2O_5$	385	$(h^5-C_5H_5)(CO)_2Mo$ 	$CDCl_3$	H 5.66s — NH, OH 12.31, 12.57 —	100 MHz	173
$[C_{12}H_{13}MoN_2O_5]^+$	386	$(h^5-C_5H_5)(CO)_2Mo$ 		H 5.59s — NH, OH 11.10, 12.79	Isolated as the PF_6^- salt 100 MHz	173
$[C_{13}H_{15}MoN_2O_5]^+$	387	$(h^5-C_5H_5)(CO)_2Mo$ 		H 5.65s — H' 4.59s — NH, OH 11.91, 12.18 —	Isolated as the PF_6^- salt 100 MHz	173

TABLE III—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{13}H_{14}MoN_2O_5$	388	$(h^5-C_5H_5)(CO)_2Mo$ 		H 5.63s H 4.68s OH 10.03s	— — —	100 MHz	173
$C_{13}H_{12}MoO_3$	389	$(h^5-C_5H_5)(CO)_2Mo-CO$ 	$CDCl_3$	H 3.03 H' 1.29 H'' 3.61	— — —	T -10°	174
$C_{14}H_{14}MoO_3$	390	$(h^5-C_5H_5)(CO)_2Mo-CO$ 	$CDCl_3$	H 3.06 H' 1.40 H'' 1.46	— — —	—	174
$C_{14}H_{14}MoO_3$	391	$(h^5-C_5H_5)(CO)_2Mo-CO$ 	$CDCl_3$	H 3.84 H' 1.19 H'' 3.81	— — —	—	174

$C_{11}H_{15}BMoN_2O_2$	392	$(h^5-C_5H_5)(CO)_2Mo$		$CDCl_3$	H H' H''	5.6s 11.3s 3.4s	— — —	—	175
$C_{19}H_{14}MoN_2O_2$	393	$(h^5-C_5H_5)(CO)_2Mo$		CS_2	H	5.15s	—	—	176
$C_{14}H_{11}MoNO_3$	394	$(h^5-C_5H_5)(CO)_2Mo-CO$		Acetone	H H'	5.38s 4.00s	— —	—	177
$C_{10}H_{10}MoO_2$	395	$(h^3-CH_2CH'CH_2)(h^5-C_5H_5)Mo-(CO)_2$	C_6H_6	H_{syn} H_{syn'} H_{anti} H_{anti'} H'	2.77 2.70 1.64 1.02 3.61	— — — — —	—		178
			$(CD_3)_2CO$	H	5.26s	—	—	T 38°	123

TABLE III—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{14}H_{12}MoO_2$	396	$(h^3-CH_2CH'CH_2)(h^5-C_9H_7)Mo-(CO)_2$	CS_2	H	2.24d,	J 7, 11	$C_9H_7 =$ 	109
				H'	0.85d	—		
				H''	3.30	$J_{H''H'''}2$		
				H'''	5.87	—		
				H'''	5.56	—		
			C_6H_6	H_{syn}	3.60	—	T 5° 100 MHz  $\rightleftharpoons$ 	178
				$H_{syn'}$	2.39	—		
				H_{anti}	-0.68	—		
				$H_{anti'}$	1.15	—		
				H'a	3.37	—		
				H'b	0.15	—		

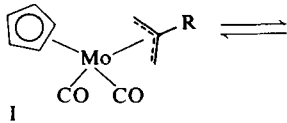
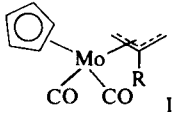
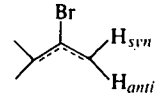
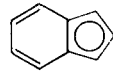
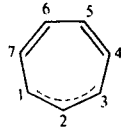
$C_{11}H_{12}MoO_2$	397	$(h^3-CH_2C(CH_3)CH_2)(h^5-C_5H_5)-Mo(CO)_2$	C_6H_6	H_{syn} H_{anti} H'	2.91 1.79 1.96	— — —	T 5° 100 MHz  I	178 179
							 II	
							Conformation I predominates when R = H, Conformation II pre- dominates when R = CH ₃	
$C_{13}H_{14}MoO_2$	398	$(h^3-CH_2C(CH_3)CH_2)(h^5-C_9H_7)-Mo(CO)_2$	C_6H_6	H_{syn} H_{anti} H'	3.68 -0.58 1.63	— — —	T 5° 100 MHz	178
$C_{10}H_9BrMoO_2$	399	$(h^3-CH_2CBrCH_2)(h^5-C_5H_5)Mo(CO)_2$	C_6H_6	H_{syn} H_{anti}	3.25 2.04	— —	 T 5° 100 MHz	178
$C_{14}H_{11}BrMoO_2$	400	$(h^3-CH_2CBrCH_2)(h^5-C_9H_7)Mo(CO)_2$	C_6H_6	H_{syn} H_{anti}	3.89 -0.35	— —	T 5° 100 MHz $C_9H_9 =$ 	178

TABLE III—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{10}H_9ClMoO_2$	401	$(h^3-CH_2CClCH_2)(h^5-C_5H_5)Mo-(CO)_2$	C_6H_6	H_{syn} 3.30 H_{anti} 2.02	—	T 5° 100 MHz	178
$C_{14}H_{11}ClMoO_2$	402	$(h^3-CH_2CClCH_2)(h^5-C_9H_7)Mo-(CO)_2$	C_6H_6	H_{syn} 4.02 H_{anti} -0.39	— —	T 5° 100 MHz	178
$C_{28}H_{20}MoO_2$	403	$[h^3-C_3(C_6H_5)_3](h^5-C_5H_5)Mo(CO)_2$	CS_2	H 4.84 H' 7.2	— —	$C_3=\Delta$	180
$C_{14}H_{12}MoO_2$	404	$(1,2,3-h^3-C_7H_7)(h^5-C_5H_5)Mo-(CO)_2$	$CCl_2F_2/$ Toluene- d_8 (2:1)	H 4.07s H_{-1}, H_{-3} 3.76t H_{-2} 1.13t H_{-4}, H_{-7} 6.20m H_{-5}, H_{-6} 5.19d	— $J_{H_{-1}, H_{-3}}$ 6.6 $J_{H_{-2}, H_{-1}}$ 7.0 $J_{H_{-4}, H_{-5}}$ 4.9 —	T -107° 100 MHz $C_7H_7 =$	181
							
			CCl_3F/CS_2 (1:2)	H 5.10s H_{-1}, H_{-3} 4.27t* H_{-2} 2.10* H_{-4}, H_{-7} 6.0t H_{-5}, H_{-6} 5.00d	— $J_{6,7}$ $J_{6,7}$ — —	T -110° *The terminal allylic protons (viz. H_{-1}, H_{-3}) normally give signals to higher field than the central allylic proton in π -allyl and butadiene complexes. The reverse order in this complex is attributed to the magnetic anisotropy of the uncomplexed diene moiety, although the possibility of the complex having a σ -bonded C_7H_7 ring with additional co-ordination from one of the other double bonds cannot be ruled out	182
			$CHFCl_2$	H_{-1} 2.32 H_{-2} 4.59 H_{-3} 6.50 H_{-4} 5.40			

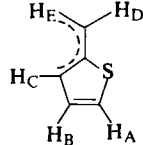
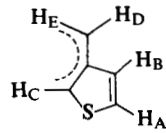
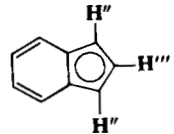
C ₁₄ H ₁₂ MoO ₂	405	(h ³ -CH ₂ ² C ₆ H ₅ ²)(h ⁵ -C ₅ H ₅)Mo(CO) ₂	C ₆ BrF ₃	H	5.31s	—	T -30°	914
				H'	2.82d,	J 3		
				H''	1.81d	—		
					7.09, 7.03,	—	T -30° 100 MHz	178
					6.88, 6.31,	—		
					5.20	—		
			C ₆ BrF ₃	H _{syn}	2.80	—	α-Proton of the 1,2,α-trihapto-benzyl group δ 6.30	183
				H _{anti}	1.80	—		
C ₁₅ H ₁₄ MoO ₂	406	(1,2,7-h ³ -4-CH ₂ C ₆ H ₄ CH ₃)-(h ⁵ -C ₅ H ₅)Mo(CO) ₂	CDCl ₃	n.m.		—	—	183
C ₂₀ H ₂₄ MoO ₂	407	[1,2,7-h ³ -3,5-CH ₂ C ₆ H ₃ (<i>iso</i> -C ₃ H ₇) ₂](h ⁵ -C ₅ H ₅)Mo(CO) ₂	Toluene-d ₈	n.m.		—	—	183
C ₁₈ H ₁₄ MoO ₂	408	(h ³ -CH ₂ C ₆ H ₅)(h ⁵ -C ₉ H ₇)Mo(CO) ₂	C ₆ H ₆	H _{syn}	4.14	—	T 5° 100 MHz	178
				H _{anti}	-0.21	—		
							α-Proton of the 1,2,α-trihapto-benzyl group δ 2.13	184
C ₁₂ H ₁₀ MoO ₂ S	409	(h ³ -2-CH ₂ C ₄ H ₃ S)(h ⁵ -C ₅ H ₅)Mo(CO) ₂	C ₆ D ₅ CD ₃	H	4.64s	—	2-CH ₂ C ₄ H ₃ S =	
				H _A	6.67d	J 6.0		
				H _B	6.35dd	J 6.2		
				H _C	4.51d	J 2		
				H _D	3.51d	J 4		
				H _E	1.92d	J 4		

TABLE III—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{12}H_{10}MoO_2S$	410	$(h^5\text{-}3\text{-CH}_2\text{C}_4\text{H}_3\text{S})(h^5\text{-C}_5\text{H}_5)\text{Mo}(\text{CO})_2$	$C_6D_5CD_3$	H	4.56s	—	3-CH ₂ C ₄ H ₃ S = 	184
				H _A	6.50dd	$J\ 6.2$		
				H _B	6.03d	$J\ 6$		
				H _C	4.7	—		
				H _D	3.18d	$J\ 4$		
				H _E	1.53	—		
$C_{33}H_{25}MoNO_2$	411	$(h^5\text{-C}_5\text{H}_5)\text{Mo}[h^3\text{-(C}_6\text{H}_5)_2\text{C}\equiv\text{N}\equiv\text{C-(C}_6\text{H}_5)_2](\text{CO})_2$	$CDCl_3$	H	4.76s	—	—	959
				H'	7.3m	—		
$C_{33}H_{25}MoNO_2$	412	$[h^3\text{-(C}_6\text{H}_5)_2\text{CNC(C}_6\text{H}_5)_2](h^5\text{-C}_5\text{H}_5)\text{Mo(CO)}_2$	$CDCl_3$	H	4.76s	—	—	111
				H'	7.30br	—		
$C_9H_{10}MoO_2S$	413	$[h^5\text{-C}_5\text{H}_5)\text{Mo(CO)}_2(\pi\text{-CH}_2=\text{S}\cdot\text{CH}_3)$	CS_2	H	5.15	—	Hexamethyldisiloxane used as reference	185
				H'	2.67, 1.89	$J\ 6$		
				H''	1.88	—		
$C_{13}H_{12}MoO_2S$	414	$(h^5\text{-C}_9\text{H}_7)\text{Mo(CO)}_2(\pi\text{-CH}_2=\text{S}\cdot\text{CH}_3)$	CS_2	H	1.83(?)	$J\ 6$	$C_9H_7 =$ 	109
				H'	1.64s	—		
				H''	5.62	—		
				H'''	5.96	—		
$C_{15}H_7F_5MoO_2$	415	$(h^7\text{-C}_7\text{H}_7)\text{Mo(CO)}_2(\text{C}_6\text{F}_5)$		H	5.75s	—	—	156 157

(c) Tri-carbonyl derivatives

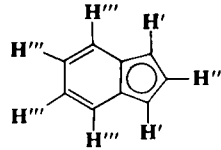
C ₉ H ₃ F ₃ MoO ₃	416	(h ⁵ -C ₅ H ₅)Mo(CO) ₃ (CF ₃)	CS ₂	H	5.59	—	—	132
			CHCl ₃	H	5.55	—	—	95
			C ₆ H ₆	¹³ C	100.9d*	J _{CH} 175	*Relative to CS ₂	956
			CH ₂ Cl ₂	F	-11.9d	—	—	—
C ₉ H ₇ DMoO ₃	417	(h ⁵ -C ₅ H ₅)Mo(CO) ₃ (CH ₂ D)	CH ₃ CN		—	J _{HH} ± 8.9*	*Calculated from J _{H-D}	186
			C ₆ H ₆		—	J _{HH} ± 8.8*	Values taken as evidence for a strong π-donor effect from the filled metal d-orbitals to the methyl group.	949
			CS ₂		—	J _{HH} ± 9.1*		—
C ₉ H ₈ MoO ₃	418	(h ⁵ -C ₅ H ₅)Mo(CO) ₃ (CH ₃)	Toluene	H	4.7	—	—	132
			CDCl ₃	H	5.32	—	—	65
				H'	0.40	—	—	—
			CCl ₄	H	5.28	—	—	168
				H'	0.34	—	—	—
C ₁₄ H ₁₈ MoO ₃	419	[h ⁵ -C ₅ (CH ₃) ₅]Mo(CO) ₃ (CH ₃)	CS ₂	H	1.87s	—	Hexamethyldisiloxane used as reference	187
				H'	-0.03	—	—	—
C ₁₃ H ₁₀ MoO ₃	420	(h ⁵ -C ₉ H ₇)Mo(CO) ₃ (CH ₃)	CS ₂	H	-0.43s	—	C ₉ H ₇ =	109
				H'	5.69	J _{H'H} 3		—
				H''	5.35	—		—
				H'''	7.19	—		—
C ₁₀ H ₁₀ MoO ₃	421	(h ⁵ -C ₅ H ₅)Mo(CO) ₃ (C ₂ H ₅)	CDCl ₃	H	5.25	—	—	132
			CS ₂	H	5.20	—	¹³ C + 101.1d (J _{CH} 175) relative to CS ₂ ion benzene	95

TABLE III—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)		Remarks	References
$C_{11}H_{12}MoO_3$	422	$(h^5-C_5H_5)Mo(CO)_3(iso-C_3H_7)$	Toluene	H	4.8	—	—	132
$C_{11}H_{11}BrMoO_3$	423	$(h^5-C_5H_5)Mo(CO)_3(CH_2CH_2''-CH_2'''Br)$	CS ₂	H H', H'' H'''	5.13s 2.0, 1.5 3.17t	— — J 7	—	189
$C_{12}H_{13}BrMoO_3$	424	$(h^5-C_5H_5)Mo(CO)_3(CH_2CH_2'-CH_2CH_2''Br)$	CS ₂	H H' H''	5.32s 1.89br, 1.66br 3.39t	— — J 6	—	189
$C_{12}H_{10}MoO_3$	425	$(h^5-C_5H_5)Mo(CO)_3(CH_2C\equiv CCH_3)$	CDCl ₃	H H', H''	5.52s 1.88 comp.	— —	—	163
			CS ₂	H', H''	1.79	$J_{H'H''}0$	—	944
$C_{17}H_{12}MoO_3$	426	$(h^5-C_5H_5)Mo(CH_2C\equiv CC_6H_5)(CO)_3$	CS ₂	H	2.0	—	—	944
$C_{14}H_{14}MoO_3$	427	$(h^5-C_5H_5)Mo(CO)_3[C\equiv C(CH_2)_3CH_3]$	CDCl ₃	H	5.49s	—	—	190
$C_{16}H_{10}MoO_3$	428	$(h^5-C_5H_5)Mo(CO)_3(C\equiv CC_6H_5)$	CDCl ₃	H H'	5.57s 7.4-6.2m	— —	—	190
$C_{15}H_{12}MoO_3$	429	$(h^5-C_5H_5)Mo(CO)_3(CH_2C_6H_5)$	CDCl ₃	H H'	5.17s 2.88s	— —	—	166

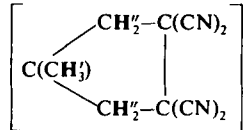
			CS ₂	H	5.14s	—	—	914
				H'	2.88s	—		
				H''	7.13s	—		
C ₁₆ H ₁₄ MoO ₃	430	(h'-4-CH ₂ C ₆ H ₄ '''CH ₃ ')(h ⁵ -C ₅ H ₅)- Mo(CO) ₃		H	5.17s	—	—	183
				H'	2.92s	—		
				H''	2.27s	—		
				H'''	7.04	—		
C ₁₆ H ₁₄ MoO ₃	431	(1,2,7-h ³ -4-CH ₂ C ₆ H ₄ '''CH ₃)- (h ⁵ -C ₅ H ₅)Mo(CO) ₃	CDCl ₃	H	~5.3	—	T -30° *Estimated from published spectra	183
				H'	~2.95, 1.9*	—		
				H''	~2.25	—		
				2-H''', 6-H'''	~5.3, 4.5*	—		
				3-H''', 5-H'''	~6.9*	—		
				H	~5.2	—	T +60°	
				H'	~2.45*	—		
				H''	~2.2	—		
				2-H''', 6-H'''	~5.9*	—		
				3-H''', 5-H'''	~6.8*	—		
C ₂₁ H ₂₄ MoO ₃	432	{h'-3,5-CH ₂ C ₆ H ₃ ^{IV} [CH''(CH ₃ ''') ₂]} CDCl ₃ (h ⁵ -C ₅ H ₅)Mo(CO) ₃		H	5.15s	—	—	183
				H'	2.93s	—		
				H''	2.81 hept.	—		
				H'''	1.21d	—		
				H ^{IV}	6.90d, 6.72m	—		

TABLE III—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{21}H_{24}MoO_3$	433	{1,2,7- h^3 -3,5- $CH_2C_6H_3^{IV}[CH''-(CH_3''')_2]_2$ }(h^5 - C_5H_5) $Mo(CO)_3$	Toluene- d_8	H	~4.9	—	T -24° *Estimated from published spectra	183
				H'	~3.2, 1.6*	—		
				H''	~2.7*	—		
				H'''	~1.2	—		
				2- H^{IV} , 6- H^{IV}	~6.4, 4.5*	—		
				4- H^{IV}	~6.9*	—		
				H	~4.9	—		
				H'	~2.3*	—		
				H''	~2.7*	—		
				H'''	~1.2	—		
				2- H^{IV} , 6- H^{IV}	~5.4*	—		
				4- H^{IV}	~6.7*	—		
$C_{15}H_{11}FMoO_3$	434	(h^5 - C_5H_5) $Mo(CO)_3(CH_2C_6H_4$ -F- <i>m</i>)	CH_2Cl_2	—	—	^{19}F NMR chemical shift + 0.93 ppm relative to FC_6H_5	191	
$C_{15}H_{11}ClMoO_3$	435	(h^5 - C_5H_5) $Mo(CO)_3(CH_2C_6H_4$ -Cl- <i>p</i>)	$CDCl_3$	H	5.19s	—	—	166
				H'	2.84s	—	—	
				H''	7.11s	—	—	
$C_{16}H_{14}MoO_4$	436	(h^5 - C_5H_5) $Mo(CO)_3(CH_2C_6H_4$ -OCH ₃ - <i>p</i>)	$CDCl_3$	H	5.15s	—	—	166
				H'	2.94s	—	—	
$C_{14}H_{11}MoNO_3$	437	(h^5 - C_5H_5) $Mo(CO)_3\left(CH_2-\text{C}_6\text{H}_4\text{N}\right)$	$CDCl_3$	H	5.14	—	—	192
				H'	2.61	—	—	

$C_{14}H_{11}MoNO_3$	438	$(h^5-C_5H_5)Mo(CO)_3\left(CH_2-\text{C}_6H_4-N\right)$	$CDCl_3$	H H'	5.30 2.76	—	—	192
$C_{13}H_{10}MoO_3S$	439	$(h^5-2-CH_2C_4H_3S)(h^5-C_5H_5)Mo(CO)_3$	$CDCl_3$	H H' H''	5.23s 3.12s 6.90, 6.83, 6.77	— — —	—	184
$C_{13}H_{10}MoO_3S$	440	$(h^5-3-CH_2C_4H_3S)(h^5-C_5H_5)Mo(CO)_3$	$CDCl_3$	H H' H''	5.10s 2.88s 7.1-7.0, 6.78b	— — —	—	184
$C_{11}H_{10}MoO_5$	441	$(h^5-C_5H_5)Mo(CO)_3[CH_2C(O)OCH_3]$	CS_2	H H' H''	5.35s 1.70s 3.48s	— — —	—	129
$C_{12}H_{12}MoO_5$	442	$(h^5-C_5H_5)Mo(CO)_3[CH_2C(O)OCH_2CH_3]$	CS_2	H H' H'' H'''	5.37s 1.69s 3.93q 1.18t	— — $J_{H''H'''}7$ —	—	129
$C_{12}H_3F_7MoO_4$	443	$(h^5-C_5H_5)Mo(CO)_3(CO\eta-C_3F_7)$	$CHCl_3$	H	5.55	—	$^{13}C + 97.9d$ (J 175) relative to CS_2 in benzene	95
$C_{16}H_{12}MoO_4$	444	$(h^5-C_5H_5)Mo(CO)_3(CH_2COC_6H_5)$	$CDCl_3$	H H' H''	5.35s 2.63s 7.82m, 7.43m	— — —	—	473
$C_{15}H_3F_5MoO_4$	445	$(h^5-C_5H_5)Mo(CO)_3(COC_6F_5)$	$CDCl_3$	H	5.50s	—	—	193

TABLE III—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)		Remarks	References
$C_{18}H_{12}MoN_4O_3$	446	$(h^5-C_5H_5)Mo(CO)_3$ 		H 5.86 H' 1.84 H'' 3.20, 3.68	— — —	—		194
$C_9H_7BrMoO_3$	447	$(h^5-C_5H_5)Mo(CO)_3(CH_2Br)$	CS_2	H 5.15s H' 3.72s	— —	—		195
$C_9H_7ClMoO_3$	448	$(h^5-C_5H_5)Mo(CO)_3(CH_2Cl)$	CS_2	H 5.42s H' 4.08	— —	—		195
			$CDCl_3$	H 5.47 H' 4.18	— —	—		166
$C_{10}H_7MoNO_3$	449	$(h^5-C_5H_5)Mo(CO)_3(CH_2CN)$	$CDCl_3$	H 5.50 H' 1.42 H 5.46 H' 1.40	— — — —	—		166 163
$C_{10}H_8MoO_5$	450	$(h^5-C_5H_5)Mo(CO)_3(CH_2CO_2H)$	$CDCl_3$	H 5.14s H' 1.75s	— —	—		196
$C_{10}H_9MoNO_4$	451	$(h^5-C_5H_5)Mo(CO)_3(CH_2CONH_2)$	Acetone	H 5.38s H' 1.78s H'' 5.89bs	— — —	—		196
$C_{22}H_{23}MoNO_3$	452	$(h^5-C_5H_5)Mo(CO)_3[C(CH_2Ph)=NC_6H_{11}]$	$(CD_3)_2SO$	H 5.54s H' 5.30s 5.72s	— — —	— Syn-form Anti-form		166

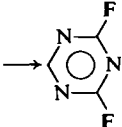
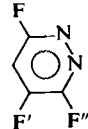
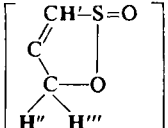
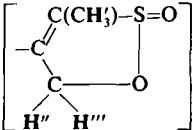
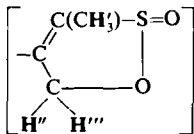
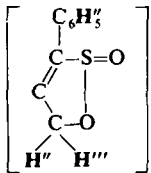
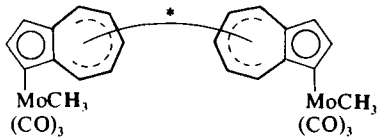
$C_{22}H_{22}Cl-MoNO_3$	453	$(h^5-C_5H_5)Mo(CO)_3[C(CH_2^2C_6H_4Cl-p)=NC_6H_{11}]$	$(CD_3)_2SO$	H H'	5.57s 5.31s 5.74s	— — —	Syn-form Anti-form	166
$C_{23}H_{25}MoNO_3$	454	$(h^5-C_5H_5)Mo(CO)_3[C(CH_2^2C_6H_4OCH_3-p)=NC_6H_{11}]$	$(CD_3)_2SO$	H H'	5.51s 5.39s 5.69s	— — —	Syn-form Anti-form	166
$C_{11}H_5F_2MoN_3O_3$	455	$(h^5-C_5H_5)Mo(CO)_3(h^1-C_3N_3F_2)$	$CHCl_3$	F	42.0	—	$C_3N_3F_2 =$ 	197
$C_{12}H_5F_3MoN_2O_3$	456	$(h^1-C_4N_2F_3)(h^5-C_5H_5)Mo(CO)_3$	$CHCl_3$	F F' F''	n.m. n.m. 107.4	— — J 31.0, 31.0	$C_4N_2F_2 =$ 	197
$C_{10}H_7MoNO_4$	457	$(h^5-C_5H_5)Mo(CO)_3(CH_2NCO)$	CS_2	H H'	5.43s 3.69s	— —	—	198
$C_{10}H_{10}MoO_4$	458	$(h^5-C_5H_5)Mo(CO)_3(CH_2OCH_3)$	CS_2	H H' H''	5.29s 4.59s 3.25s	— — —	—	195
$C_{10}H_{10}MoO_3S$	459	$(h^5-C_5H_5)Mo(CO)_3(h^1-CH_2SCH_3)$	CS_2	H H' H''	5.38 2.38 2.18	— — —	Hexamethyldisiloxane used as reference $^{13}C + 99.6d$ (J_{CH} 175) relative to CS_2 in CH_2Cl_2 as solvent	185
$C_{11}H_8MoO_3S$	460	$(h^5-C_5H_5)Mo(CO)_3$ 	$CDCl_3$	H H' H'' H'''	5.58s 6.42t 5.10 5.48	— $J_{H'H''}$ 2.5 $J_{H''H'''}$ 15 $J_{H'H''}$ 2.5	—	163

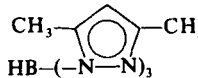
TABLE III—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{12}H_{10}MoO_5S$	461	$(h^5-C_5H_5)-Mo(CO)_3$ 	$CDCl_3$	H 5.58s H' 2.05t H'' 5.06 H''' 5.43	— $J_{H'H''} 2.0$ $J_{H''H'''} 14.5$ $J_{H'H'''} 2.0$	—	163
$C_{12}H_{10}MoO_5S$	462	$(h^5-C_5H_5)-Mo(CO)_3$ 		H' 2.40 H'' 5.19 H''' 5.55	$J_{H'H''} 2.0$ $J_{H''H'''} 14.0$ $J_{H'H'''} 2.0$	—	156
$C_{17}H_{12}MoO_5S$	463	$(h^5-C_5H_5)Mo(CO)_3$ 	$CDCl_3$	H 5.29s H' 7.48s H'' 5.24 H''' 5.72	— — — —	—	163
(d) Derivatives containing two or more transition metal atoms							
$C_{44}H_{40}Mo_2O_6P_2$	464	$[(h^5-C_5H_5)Mo(CO)_2(COCH_3)]_2$ (Pf—Pf)	$CDCl_3$	H 4.92t H' 2.66s	$J 0.5$ —	100 MHz (Pf—Pf)=(Ph ₂ PCH ₂ CH ₂ PPh ₂)	210
$C_{44}H_{36}Mo_2O_6P_2$	465	$[(h^5-C_5H_5)Mo(CO)_2(COCH_3)]_2$ (Pf≡Pf)	$CDCl_3$	H 5.01d H' 2.51s	$J 1.5$ —	100 MHz (Pf≡Pf)=(Ph ₂ PC≡CPPh ₂)	210

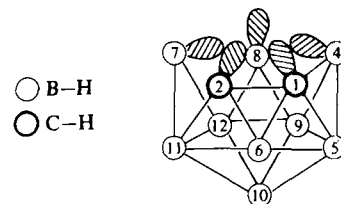
$C_{44}H_{40}Mo_2O_6 \cdot P_2$	466	$[(h^5-C_5H_5)Mo(CO)_2(COCH_3)]_2 \cdot [P(C_6H_5)_2CH_2CH_2(C_6H_5)_2P]$	$CDCl_3$	H	4.88s	—	—	161
				H'	2.69m			
				H''	7.38m			
$C_{46}H_{40}Mo_2O_6 \cdot P_2$	467	$[(h^5-C_5H_5)Mo(CO)_2(COCH_3)]_2 \cdot [P(C_6H_5)_2CH_2C \equiv CCH_2(C_6H_5)_2P]$	$CDCl_3$	H	5.08s	—	100 MHz	211
				H'	7.58, 7.50	—		
				H''	3.37d	J 6		
$C_{61}H_{57}Mo_3O_9 \cdot P_3$	468	$[(h^5-C_5H_5)Mo(CO)_2(COCH_3)]_3 \cdot \{[PPh_2(CH_2)_2]_2PPh\}$	$CDCl_3$	H	~ 4.8	—	100 MHz	5
$C_{56}H_{48}Mo_2O_6 \cdot P_2$	469	$[(h^5-C_5H_5)Mo(CO)_2(COCH_2C_6H_5)]_2(Pf-Pf)$	$CDCl_3$	H	4.89t	J 0.5	100 MHz	210
				H'	4.41s			
				H''	7.3–7.1 comp.			
$C_{20}H_{14}Mo_2O_8S$	470	$(h^5-C_5H_5)Mo(CO)_3(C \begin{array}{l} \text{---} CH_2Mo(CO)_3(h^5-C_5H_5) \\ \text{---} S=O \\ \text{---} O \\ \text{---} C \end{array} \begin{array}{l} H'' \\ H''' \end{array})$		H	5.56, 5.52	—	—	163
				H'	~ 2.0	—		
				H'', H'''	~ 5.3	—		
$C_{28}H_{22}Mo_2O_6$	471		$CHCl_3$	H	0.14		Signals at 6.28dd (J 2, 3), 5.99, 5.13d (J 3), 4.38t (J 3), 3.27b, ($J \sim 10$), 1.41b n.a.	109

*Dimerization believed to be due to the formation of a carbon-carbon bond between unspecified positions of the two seven-membered rings rather than to metal-metal bonds

TABLE III—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References	
(9) MISCELLANEOUS MOLYBDENUM COMPLEXES								
$[\text{C}_{10}\text{HMo}_2\text{O}_{10}]^-$	472	$[\text{Mo}_2(\text{CO})_{10}(\text{H})]^-$	CH_3OH	H	-12.5	—	Isolated as sodium salt <i>cis</i> -isomer $J_{\text{H}13\text{C}} 4.3$. <i>trans</i> -isomer $J_{\text{H}13\text{C}} 4.3$ or ≤ 3.0	199
			THF	H	-12.15	—	Hydrogen bridging between the two metal atoms	915
$[\text{C}_{10}\text{HMoO}_{10}\text{W}]^-$	473	$[\text{MoWH}(\text{CO})_{10}]^-$	THF	H	-12.37	—	Hydrogen bridging between the two metal atoms	915
$\text{C}_{12}\text{H}_{11}\text{BMoN}_6\text{O}_3^-$	474	$[\text{HB}(\text{Pz})_3]\text{Mo}(\text{CO})_3(\text{H})$	CH_2Cl_2	H	-3.3	—	$\text{HB}(\text{Pz})_3 =$  $\text{HB}-(\text{N}-\text{N})_3$	53
$\text{C}_{18}\text{H}_{23}\text{BMoN}_6\text{O}_3^-$	475	$[\text{HB}(3,5\text{-(CH}_3)_2\text{Pz})_3]\text{Mo}(\text{CO})_3(\text{H})$	CH_2Cl_2	H	-3.5	—	$\text{HB}(3,5\text{-(CH}_3)_2\text{Pz}) =$  $\text{HB}-(\text{N}-\text{N})_3$	53
$[\text{C}_5\text{H}_{10}\text{B}_{10}\text{MoO}_5]^{2-}$	476	$[\text{B}_{10}\text{H}_{10}\text{COMoCO}(\text{CO}_3)]^{2-}$	CH_3CN	—			A metalloborane isolated as the tetrabutyl ammonium salt. ^{11}B NMR chemical shifts 24.70 (J 123), 28.95 (J 148), 31.28sh, 36.40sh, relative to trimethylborate at 32 MHz	200

$[\text{C}_5\text{H}_{10}\text{B}_{11}\text{MoO}_5]^-$	477	$[(\text{B}_{10}\text{H}_{10}\text{COH})\text{Mo}(\text{CO})_4]^-$	CH_3CN	—	—	—	A metalloborane isolated as the tetramethylammonium salt. ^{11}B NMR chemical shifts 16.4 (<i>J</i> 108), 23.71 (<i>J</i> 124), 27.67 (<i>J</i> 128), 31.38sh, 33/35sh, relative to trimethylborate at 32 MHz	200
$\text{C}_{18}\text{H}_{24}\text{MoN}_2\text{O}_4$	478	$\text{Mo}(\text{CO})_4[\text{N}(\text{C}_6\text{H}_{11})=\text{CH}.\text{CH}=(\text{C}_6\text{H}_{11})\text{N}]$	CDCl_3	H	8.25	—	—	201
$\text{C}_{30}\text{H}_{22}\text{MoO}_4\text{P}_2$	479	$\text{Mo}(\text{CO})_4 \left(\begin{array}{c} \text{Ph}_2\text{P} \\ \text{H} \end{array} \text{C}=\text{C} \begin{array}{c} \text{PPh}_2 \\ \text{H} \end{array} \right) (\text{CH}_3)_2\text{CO}$		H	8.52	$J_{\text{PH}} 47, 8$	60 and 100 MHz	202
$[\text{C}_6\text{H}_{14}\text{B}_9\text{MoO}_3]^-$	480	$[(\pi\text{-(3)-1,2-B}_9\text{C}_2\text{H}_{11})\text{Mo}(\text{CO})_3\text{-(CH}_3)]^-$		H	-0.49	—	A dicarbollyl derivative isolated as the tetramethyl ammonium salt. $[(3)\text{-1,2-B}_9\text{C}_2\text{H}_{11}]^{2-}$ ion:	203



sp^3 orbitals directed at vacant 3-vertex formed by removal of β -atom 3

TABLE III—cont.

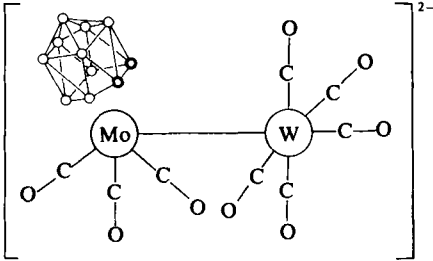
Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$[\text{C}_{10}\text{H}_{11}\text{MoO}_8\text{-W}]^{2-}$	481	$[(\pi\text{-}(3)\text{-}1,2\text{-B}_9\text{C}_2\text{H}_{11})\text{Mo}(\text{CO})_3\text{-W}(\text{CO})_5]^{2-}$		CH -2.5 to -2.8	—	Isolated as the tetramethyl ammonium salt Proposed structure:	203
							
$\text{C}_{14}\text{H}_{12}\text{MoO}_6\text{Se}$	482	$(\text{CO})_5\text{Mo}[\text{Se}(\text{C}_6\text{H}_5)\text{CH}'(\text{CH}_3')\text{-}(\text{OCH}_3'')]$	CDCl_3	H 7.65m H' 5.15q H'' 1.58d H''' 3.53s	— — — —		80

TABLE IV
Tungsten complexes

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
(1) MONOHAPTO LIGANDS							
$C_{25}H_{21}AsO_5W$	1	$W[C(CH_3)OCH_3][As(C_6H_5)_3](CO)_4$	C_6D_6	H	2.48s	—	945
				H'	3.99s	—	
				H''	7.34m	—	
$C_{25}H_{21}O_5PW$	2	$W[C(CH_3)OCH_3][P(C_6H_5)_3](CO)_4$	C_6D_6	H	2.42s	—	945
				H'	4.00s	—	
				H''	7.34m	—	
			$CHCl_3$	H	2.50	—	17
$[C_{24}H_{18}O_5PW]^-$	3	$\{W(COCH_3)[P(C_6H_5)_3](CO)_4\}^-$	CH_2Cl_2	H	2.10s	—	945
				H'	7.34m	—	
				H''	3.47q	—	
				H'''	1.10t	—	
$[C_{29}H_{20}O_5SbW]^-$	4	$\{W(COC_6H_5)[Sb(C_6H_5)_3](CO)_4\}^-$	CH_2Cl_2	H	7.34m	—	945
				H'	3.35	—	
				H''	0.97	—	
$C_{25}H_{22}NO_4PW$	5	$W[C(CH_3)NH''CH_3][P(C_6H_5)_3](CO)_4$	C_6H_6	H	2.11	—	947
				H'	2.70	$J_{H'H''} 5.0$	

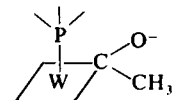


TABLE IV—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{25}H_{22}NO_4PW$	6	$W[C(CH_3)NH''CH_3][P(C_6H_5)_3]-(CO)_4$	$CHCl_3$	H	2.17	—	CH_3 groups <i>cis</i> to each other	947
				H'	2.40	$J_{H'H''} 5.3$		
			C_6H_6	H	2.00	—		
				H'	1.60	—		
$[C_8H_3O_5W]^-$	7	$[W(C\equiv CCH_3)(CO)_5]^-$	CH_2Cl_2	H	1.59	—	Isolated as the bis(triphenylphosphine) iminium salt	19
$C_8H_6O_6W$	8	$W[C(CH_3)=OCH_3](CO)_5$	$CHCl_3$	H	2.80	—	—	17
				H'	4.45	—		
			C_6H_6	H	2.31	—		33
				H'	3.83	—		
$C_9H_8O_6W$	9	$W[C(CH_3)=OCH_2CH_3''](CO)_5$	$CDCl_3$	H	2.93t	$J_{HH'} 0.45$	60 and 100 MHz	39
				H'	4.98			
				H''	1.61t			
$C_{12}H_{14}O_6W$	10	$W[C(CH_2CH_2CH_2CH_3''')=OCH_2''CH_3^{IV}](CO)_5$	$CDCl_3$	H	3.30t	—	60 and 100 MHz	39
				H'	$\sim 1.40m$	—		
				H''	0.93t	—		
				H'''	5.11q	—		
				H ^{IV}	1.65t	—		
$C_{13}H_8O_6W$	11	$W[C(C_6H_5)=OCH_3](CO)_5$	C_6H_6	H	7.04	—	—	33
				H'	3.96	—		
$C_{14}H_{10}O_6W$	12	$W[C(C_6H_5)=OCH_2CH_3''](CO)_5$	$CDCl_3$	H	7.28m	—	60 and 100 MHz	39
				H'	4.90q	—		
				H''	1.62t	—		

$[\text{C}_7\text{H}_5\text{O}_6\text{W}]^-$	13	$[\text{W}(\text{COCH}_3)(\text{CO})_5]^-$	CH_2Cl_2	H H'	2.37 3.30	—	Isolated as the $(\text{CH}_3)_4\text{N}^+$ salt	33
$[\text{C}_{12}\text{H}_5\text{O}_6\text{W}]^-$	14	$[\text{W}(\text{COC}_6\text{H}_5)(\text{CO})_5]^-$	CH_2Cl_2	H H'	7.38 3.06	—	Isolated as the $(\text{CH}_3)_4\text{N}^+$ salt	33
$\text{C}_8\text{H}_7\text{NO}_5\text{W}$	15	$\text{W}[\text{C}(\text{CH}_3)\text{NH}''\text{CH}_3'](\text{CO})_5$	CHCl_3	H H'	2.92 3.55	$J_{\text{HH}''} 0.95$ $J_{\text{HH}'} 0.95$ $J_{\text{H}'\text{H}''} 4.9$	CH_3 groups <i>trans</i> to each other	947
			C_6H_6	H H'	2.24 2.68	— —		
$\text{C}_8\text{H}_7\text{NO}_5\text{W}$	16	$\text{W}[\text{C}(\text{CH}_3)\text{NH}''\text{CH}_3'](\text{CO})_5$	CHCl_3	H H'	2.75 3.16	$J_{\text{HH}''} 0.9$ $J_{\text{HH}'} 0.45$ $J_{\text{H}'\text{H}''} 5.1$	CH_3 groups <i>cis</i> to each other	947
$\text{C}_6\text{HNO}_5\text{W}$	17	$\text{W}(\text{C}=\text{NH})(\text{CO})_5$	$(\text{CH}_3)_2\text{CO}$	H	5.58	—	—	1017
$\text{C}_9\text{H}_9\text{NO}_5\text{SnW}$	18	$\text{W}(\text{C}=\text{NSn}(\text{CH}_3)_3)(\text{CO})_5$	C_6H_6	H	0.10	$J(^{119}\text{Sn}-\text{H}) 60$ $J(^{117}\text{Sn}-\text{H}) 56$	—	1017

(2) DIHAPTO LIGANDS

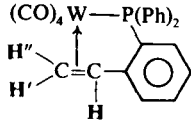
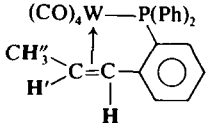
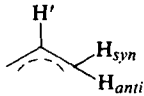
$\text{C}_{24}\text{H}_{17}\text{O}_4\text{PW}$	19		CDCl_3	H H' H''	5.64 3.75 3.23	$J_{\text{HH}''} 9.0$ $J_{\text{H}'\text{H}''} 3.0$ $J_{\text{HH}'} 14.0$	—	50
$\text{C}_{25}\text{H}_{19}\text{O}_4\text{PW}$	20		CDCl_3	H H' H''	5.58 4.67 2.18	$J_{\text{HH}''} 10.0$ $J_{\text{H}'\text{H}''} 6.2$	— —	52

TABLE IV—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
(3) TRIHAPTO LIGANDS							
$C_{18}H_{25}BN_6O_2W$	21	$(h^3\text{-CH}_2\text{CHCH}_2)W(C_3H_4N_2)\text{-}(C_{10}H_{16}BN_4)(CO)_2$	$CDCl_3$	n.a.		$C_3H_4N_2 = \text{pyrazole}$  $C_{10}H_{16}BN_4 = Et_2B\text{-}(N\text{-}N\text{<})_2$ Signals at δ 7.9d (J 2.0), 7.72d (J 2.3, 0.5), 7.14m, 6.20t (J 2.2), 3.2m and s, 1.8d (J 8.0), ~0.9m and 0.38s, in ratio 3:2:1:3:3:2:5:5	81
$C_7H_5BrO_4W$	22	$(h^3\text{-CH}_2\text{CH}'\text{CH}_2)W(CO)_4Br$	C_6F_6	H_{syn} 3.84d H_{anti} 3.13d H' 5.44m	J 7 J 11 —	Major isomer Benzene reference 	213
				H_{syn} 3.11 H_{anti} 2.17 H' 4.98m	J 8 J 9 —	Minor isomer 	
$C_7H_5IO_4W$	23	$(h^3\text{-CH}_2\text{CH}'\text{CH}_2)W(CO)_4I$	C_6F_6	H_{syn} 4.15d H_{anti} 3.24d H' ~5.29m	J 7 J 11 —	Major isomer Benzene reference	213

H_{syn}	3.32d	$J 5$
H_{anti}	2.32d	$J 9$
H'	$\sim 5.29m$	—

Minor isomer

(4) TETRAHAPTO LIGANDS

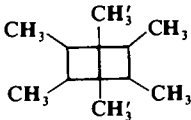
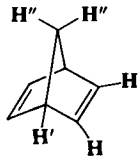
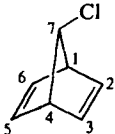
$C_{14}H_{16}O_2W$	24	$(h^4-C_6H_8)_2W(CO)_2$	CS_2	CH	4.67dd 2.83bs	$J 6, 3$ —	$C_6H_8 = 1,4\text{-cyclohexadiene}$	214
				CH_2	2.09dd 1.76dd	$J 11, 3, 1$ $J 11, 3, 1$	$T 37^\circ$	
$C_8H_4O_4W$	25	$(h^4-C_4H_4)W(CO)_4$	—	H	4.02	—	$C_4H_4 = \text{cyclobutadiene}$	54
$C_{12}H_{12}O_4W$	26	$[h^4-C_4(CH_3)_4]W(CO)_4$	—	H	2.14	—	$C_4(CH_3)_4 = \text{tetramethyl-cyclobutadiene}$	54
$C_{16}H_{18}O_4W$	27	$[h^4-C_6(CH_3)_6]W(CO)_4$	$CDCl_3$	H H'	2.00s 0.95s	— —	$C_6(CH_3)_6 =$ 	56
$C_{12}H_{12}O_4W$	28	$(1,2,5,6-h^4-C_8H_{12})W(CO)_4$	CS_2	H_{-1}, H_{-2} H_{-5}, H_{-6}	4.45bs	—	$C_8H_{12} = 1,5\text{-cyclooctadiene}$	214
				H_{-3}, H_{-4} H_{-7}, H_{-8}	2.62bs	—	$T 37^\circ$	
			C_6H_6	H	1.83, 3.86	—	—	93
$C_{11}H_8O_4W$	29	$(h^4-C_7H_8)W(CO)_4$	CS_2	H H' H''	4.63t 3.96bs 1.08s	— — —	$C_7H_8 =$ 	214

TABLE IV—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{11}H_7ClO_4W$	30	$(h^4-C_7H_7Cl)W(CO)_4$	$CDCl_3$	H_{-1}, H_{-4} 3.91 H_{-2}, H_{-3} 4.36 H_{-5}, H_{-6} 4.50 H_{-7} 3.44	— — — —	$C_7H_7Cl =$ 	58
(5) PENTAHAPTO LIGANDS							
$C_{15}H_{23}I_2NOW$	31	$(h^5-C_5H_5)W(I)_2[N=C(C(CH_3)_3)_2](CO)$	$CDCl_3$	H 5.77s H' 1.40, 1.18	— —	—	98
$C_{17}H_{19}I_2NOW$	32	$(h^5-C_5H_5)W(I)_2[N=C(C_6H_5)_3](CO)$	$CDCl_3$	H 5.58, 5.50, 5.52, 5.43, 4.54 H' 7.56, 7.43, 7.49, 7.45 H'' 1.34, 1.33, 1.37, 1.31, 1.39	— — — — — — —	at T $-40^\circ, -20^\circ, 0^\circ, +20^\circ, 40^\circ$ resp. at T $-40^\circ, -20^\circ, 0^\circ, +20^\circ$ — at T $-40^\circ, -20^\circ, 0^\circ, +20^\circ, +40^\circ$	99
$C_{24}H_{20}NO_2PW$	33	$(h^5-C_5H_5)W(NO)(PPh_3)(CO)$	C_6D_6	H 4.79d	$J_{PH} 0.6$	—	59 946
$C_{42}H_{35}ClOP_2W$	34	$(h^5-C_5H_5)W(Cl)(PPh_3)_2(CO)$	$CDCl_3$	H 5.02	—	—	108
$C_7H_5Br_3O_2W$	35	$(h^5-C_5H_5)W(Br)_3(CO)_2$	$(CH_3)_2CO$	H 6.40	—	100 MHz	108
$C_7H_5Cl_3O_2W$	36	$(h^5-C_5H_5)W(Cl)_3(CO)_2$	$(CH_3)_2CO$	H 6.34	—	100 MHz	108
$C_7H_5I_3O_2W$	37	$(h^5-C_5H_5)W(I)_3(CO)_2$	$(CH_3)_2CO$	H 6.40	—	100 MHz	108

C ₁₆ H ₂₃ NO ₂ W	38	(h ⁵ -C ₅ H ₅)W{N=C[C(CH ₃) ₃] ₂ }- (CO) ₂	Toluene	H	5.45	—	T 25°	98
				H'	1.12	—		
				H	4.98	—		
				H'	0.97	—		
C ₁₈ H ₁₉ NO ₂ W	39	(h ⁵ -C ₅ H ₅)W{N=C(C ₆ H ₅)- C(CH ₃) ₃ }(CO) ₂	C ₆ D ₁₁ CD ₃	H	5.65	—	T 25°	99
				H'	1.08	—		
				H	5.60	—		
				H'	7.41	—		
C ₂₀ H ₁₅ NO ₂ W	40	(h ⁵ -C ₅ H ₅)W{N=C(C ₆ H ₅) ₂ }(CO) ₂	CDCl ₃	H	5.98s	—	—	111
				H'	7.37b	—		
				H	5.60	—		
				H'	7.41	—		
C ₃₃ H ₂₅ NO ₂ W	41	(h ⁵ -C ₅ H ₅)W{N[C(C ₆ H ₅) ₂] ₂ }(CO) ₂	CHCl ₃	H	4.77s	—	—	111
				H'	7.25b	—		
				H	5.81	—		
				H'	7.27	—		
C ₁₃ H ₁₀ N ₂ O ₂ W	42	(h ⁵ -C ₅ H ₅)W(N ₂ C ₆ H ₅)(CO) ₂	CDCl ₃	H	5.81	—	—	215
				H'	7.27	—		
				H	5.66s	—		
				H	5.91s	—		
C ₇ H ₅ NO ₃ W	43	(h ⁵ -C ₅ H ₅)W(NO)(CO) ₂	CDCl ₃ (CD ₃) ₂ CO	H	5.66s	—	—	59 60
				H	5.91s	—		
				H	4.83	—		
				H'	1.15	—		
C ₁₀ H ₁₅ O ₂ PW	44	(h ⁵ -C ₅ H ₅)W{P(CH ₃) ₃ }(H")- (CO) ₂	C ₆ H ₆	H	4.83	—	—	216
				H'	1.15	—		
				H"	-7.33	J _{WH} 45		
				H	4.38	J _{PH} 0.5	<i>cis</i> -isomer at -28° 100 MHz	113 1025
			—	H'	0.78	J _{PH'} 9.3		
				H"	-8.32	J _{PH''} 68.3		
				H	4.23	J _{WH} 48	<i>trans</i> -isomer at -28° 100 MHz	113 1025
				H'	0.79	J _{PH'} 9.5		
				H"	-7.51	J _{PH''} 24.0		
				H	4.23	J _{WH} 48		

TABLE IV—cont.

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Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{13}H_{21}O_2PW$	45	$(h^5-C_5H_5)W[P(CH_2CH''_3)_3]-(H'')(CO)_2$	C_6H_6	H	4.74	—	—	216
				H'	1.2	—		
				H''	0.6	—		
				H'''	-7.77	$J_{WH'''} 45$		
			—	H	4.69	$J_{PH} < 0.3$	<i>cis</i> -isomer at -28° 100 MHz	113
				H'''	-8.31	$J_{PH'''} 64.3$		
						$J_{WH'''} 47.5$		
				H	4.55	$J_{PH} 0.8$		
				H'''	-7.76	$J_{PH'''} 22.4$ $J_{WH'''} 47.5$	<i>trans</i> -isomer at -28° 100 MHz	113
$C_{13}H_{20}ClO_2PW$	46	$(h^5-C_5H_5)W(Cl)[P(C_2H_5)_3]-(CO)_2$	$C_6H_5NO_2$	H	5.66	—	—	137
				H'	1.91, 1.05	—		
$[C_{10}H_9O_2-P_2W]^+$	47	$\{(h^5-C_5H_5)W[P(CH_2CH''_3)_3]_2-(CO)_2\}^+$	$C_6H_5NO_2$	H	5.63	—	Isolated as PF_6^- salt	137
				H'	2.03	—		
				H''	1.1	—		
$C_{19}H_{33}O_2PW$	48	$(h^5-C_5H_5)W[P(n-Bu)_3](H')(CO)_2$	$CDCl_3$	H	5.50s	—	100 MHz	119
				H'	-7.90	—		
$C_{25}H_{20}ClO_2PW$	49	$(h^5-C_5H_5)W(Cl)[P(C_6H_5)_3](CO)_2$	$(CH_3)_2CO$	H	5.7	—	—	137
				H'	7.5, 7.4	—		
$C_{25}H_{21}O_2PW$	50	$(h^5-C_5H_5)W[P(C_6H_5)_3](H'')(CO)_2$	$CDCl_3$	H	5.25s	—	100 MHz	119
				H''	-8.00	$J_{PH''} 54.0$		
			C_6H_6	H	4.70	—		
				H'	7.0	—		
				H''	-7.48	$J_{WH''} 45$		

				H	4.33	$J_{PH} < 0.3$	} <i>cis</i> -isomer at -27°	113
				H''	-6.97	$J_{PH''} 66.1$		
				H	4.23	$J_{PH} 0.8$	} <i>trans</i> -isomer at -27°	113
				H''	-7.19	$J_{PH''} 21.4$		
C ₁₀ H ₁₄ BrO ₅ PW	51	(h ⁵ -C ₅ H ₅)W(Br)[P(OCH ₃) ₃](CO) ₂	CDCl ₃	H	5.62s	—	100 MHz	121
					5.47d	$J 2.0$		
				H'	3.73d	$J 12.0$		
					3.70d			
C ₁₀ H ₁₄ ClO ₅ PW	52	(h ⁵ -C ₅ H ₅)W(Cl)[P(OCH ₃) ₃](CO) ₂	CDCl ₃	H	5.67s	—	100 MHz	121
					5.48d	$J 2.0$		
				H'	3.75d	$J 12.0$		
C ₁₀ H ₁₄ IO ₅ PW	53	(h ⁵ -C ₅ H ₅)W(I)[P(OCH ₃) ₃](CO) ₂	CDCl ₃	H	5.60s	—	100 MHz	121
					5.45d	$J 1-2$		
				H'	3.70d	$J 12$		
C ₁₀ H ₁₅ O ₅ PW	53a	(h ⁵ -C ₅ H ₅)W[P(OCH ₃) ₃](H'')(CO) ₂	CDCl ₃	H	5.40s	—	60 and 100 MHz	121
					5.15d	$J 1-2$		
				H'	3.53d	$J_{PH'} 12$		
					3.62d			
				H''	-7.85 sext.	$J_{PH''} 66$ $J_{WH''} 46$		
			C ₆ H ₆	H	4.95	—		216
				H'	3.29	—		1025
				H''	-7.70	$J_{WH''} 45$		
C ₁₃ H ₁₇ O ₅ PW	54	(h ⁵ -C ₅ H ₅)W[P(OCH ₂) ₃ CEt](H')(CO) ₂	CDCl ₃	H	5.24s	—	100 MHz	119
				H'	-8.28	$J_{PH'} 58.0$		
C ₂₅ H ₂₁ O ₅ PW	55	(h ⁵ -C ₅ H ₅)W[P(OC ₆ H ₅) ₃](H')(CO) ₂	CDCl ₃	H	4.81s	—	100 MHz	119
				H'	-8.14	$J_{PH'} 75.4$		
C ₂₆ H ₂₀ AuO ₃ PW	56	(h ⁵ -C ₅ H ₅)W(AuPPh ₃)(CO) ₃	CDCl ₃	H	5.38	—	—	62

TABLE IV—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_8H_5BrO_3W$	57	$(h^5-C_5H_5)W(Br)(CO)_3$	$CDCl_3$	H	5.74s	—	—	131
$C_8H_5ClO_3W$	58	$(h^5-C_5H_5)W(Cl)(CO)_3$	$CDCl_3$	H	5.74s	—	—	131
$C_8H_5IO_3W$	59	$(h^5-C_5H_5)W(I)(CO)_3$	$CDCl_3$	H	5.70s	—	—	131
$C_{25}H_{26}As_3^-$ CuO_3W	60	$(h^5-C_5H_5)W\{Cu(AsCH_3)[AsC_6H_3-2,6(CH_3)_2]_2\}(CO)_3$	$CDCl_3$	H	5.20	—	—	62
$C_{11}H_{14}GeO_3W$	61	$(h^5-C_5H_5)W[Ge(CH_3)_3](CO)_3$	$CDCl_3$	H	5.33	—	—	64
				H'	0.62	—	—	63
			C_6H_6	H	5.3	—	—	120
				H'	0.63	—	—	120
$C_{14}H_{20}GeO_3W$	62	$(h^5-C_5H_5)W(GeCH_2CH_3)_3(CO)_3$	—	H	5.37	—	40 MHz	135
				H'	1.14	—	—	120
			C_6H_6	H	4.63	—	—	120
				H'	1.16	—	—	120
$C_{26}H_{20}GeO_3W$	63	$(h^5-C_5H_5)W[Ge(C_6H_5)_3](CO)_3$	$CDCl_3$	H	5.36	—	—	65
				H'	7.45	—	—	65
$C_8H_6O_3W$	64	$(h^5-C_5H_5)W(H')(CO)_3$	C_6H_6	H	4.59	—	—	216
				H'	-7.16	$J_{WH'}^{37}$	—	216
			Hexane	H	5.35	—	—	66
				H'	-7.33	—	—	66
			$CDCl_3$	H'	-7.30	$J(^{183}W-H') 37.5$	—	67
							220 MHz	219

			CDCl ₃	H'	-7.3	$J(^{183}\text{W}-\text{H}')$ 36.7 $J(^{13}\text{CO}-\text{cis H}')$ 18.5 $J(^{13}\text{CO}-\text{trans H}')$ 5.5	T -70°	220
							The structure deduced is that with the hydrogen atom and the carbon atoms of the carbonyl groups lying at the corners of a square. The molecule is fluxional and undergoes rapid intramolecular interchange of hydride and carbonyl positions. The barrier to interconversion for most hydrides is sufficiently low (10-13 kcal) for averaged spectra to be observed in NMR experiments performed at room temperature and may have led to erroneous interpretations of quantities of <i>cis</i> - and <i>trans</i> -isomers of hydrides in the literature. The barriers are higher for methyl complexes (17-20 kcal for molybdenum derivatives) and halides (>22 kcal)	
C ₁₂ H ₅ Co- HgO ₇ W	65	(<i>h</i> ⁵ -C ₅ H ₅)W(CO) ₃ HgCo(CO) ₄	CDCl ₃	H	5.65	—	40 and 60 MHz	136
C ₁₂ H ₁₃ Br- MgO ₄ W	66	(<i>h</i> ⁵ -C ₅ H ₅)W(CO) ₃ MgBr. THF	C ₆ H ₆	H	4.56s	—	THF gives signals at δ 4.00t and 1.42	120
[C ₈ H ₈ NO ₃ W] ⁻	67	[(<i>h</i> ⁵ -C ₅ H ₅)W(NH ₃)(CO) ₃] ⁻	C ₆ H ₅ NO ₂	H H'	5.76 1.56	—	Isolated as the tetraphenylborate	137
[C ₈ H ₉ N ₂ - O ₃ W] ⁻	68	[(<i>h</i> ⁵ -C ₅ H ₅)W(N ₂ H ₄)(CO) ₃] ⁻	C ₆ H ₅ NO ₂	H H'	5.9 3.48 3.28	— — —	Isolated as the tetraphenylborate	137

TABLE IV—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{26}H_{20}O_3PbW$	69	$(h^5-C_5H_5)W[Pb(C_6H_5)_3](CO)_3$	$CDCl_3$	H	5.43	—	—	65
				H'	7.5m	—		
$C_9H_5NO_3SW$	70	$(h^5-C_5H_5)W(SCN)(CO)_3$	$CDCl_3$	H	5.79s	—	—	131
$C_8H_8O_3SiW$	71	$(h^5-C_5H_5)W(SiH_3)(CO)_3$	Et_2O	H	5.50s	—	—	68
				H'	3.82s	—		
$C_{11}H_{14}O_3SiW$	72	$(h^5-C_5H_5)W[Si(CH_3)_3](CO)_3$	$CDCl_3$	H	5.44	—	—	139
				H'	0.14	—		
				H	5.38	—		63
				H'	0.09	—		
$C_{11}H_{11}F_3O_3-SnW$	73	$(h^5-C_5H_5)W[Sn(CH_3)_2CF_3](CO)_3$	$CHCl_3$	H	0.4	$J(^{117}Sn-H)$ 48 $J(^{119}Sn-H)$ 50	60 and 100 MHz	221
				F	47.5	$J(^{117}Sn-F)$ 210 $J(^{119}Sn-F)$ 220	CFC_3 reference	221
$C_{11}H_{14}O_3SnW$	74	$(h^5-C_5H_5)W[Sn(CH_3)_3](CO)_3$	$CHCl_3$	H	5.47	—	60 and 100 MHz	65
				H'	0.60m	$J(^{117}Sn-H')$ 46.4 $J(^{13}C-H')$ 129		146
			$CDCl_3$	H	5.33	—	—	64
				H'	0.45	—		63
$C_{26}H_{20}O_3SnW$	75	$(h^5-C_5H_5)W[Sn(C_6H_5)_3](CO)_3$	$CDCl_3$	H	5.39	—	—	65
				H'	7.42m	—		
$C_{14}H_{10}Cl_2-O_3SnW$	76	$(h^5-C_5H_5)W[Sn(Cl)_2C_6H_5](CO)_3$	—	H	5.52	—	—	948

$C_8H_5Br_3O_3-SnW$	77	$(h^5-C_5H_5)W(SnBr_3)(CO)_3$	—	H	5.81	—	—	948
$C_8H_5Cl_3O_3SnW$	78	$(h^5-C_5H_5)W(SnCl_3)(CO)_3$	—	H	5.98	—	—	943 142
$C_8H_5I_3O_3SnW$	79	$(h^5-C_5H_5)W(SnI_3)(CO)_3$	—	H	5.76	—	—	948
$C_{15}H_{11}MnO_8-SnW$	80	$(h^5-C_5H_5)W(CO)_3[Sn(CH_3)_2Mn-(CO)_5]$	CCl_4	H H'	5.41 0.82	— $J(SnH') 37.3$	100 MHz	140
$C_{13}H_{16}O_3W$	81	$[h^5-C_5(CH_3)_5]W(H')(CO)_3$	CS_2	H H'	2.20s -6.85s	— —	T 37°	214
$C_{26}H_{19}O_3PW$	82	$[h^5-C_5H_4P(C_6H_5)_3]W(CO)_3$	$CHCl_3$	H H'	5.49 5.22 ~7.85	— $J 2.5$ —	—	66
$C_{26}H_{19}BF_3-O_3PW$	83	$[h^5-C_5H_4P(C_6H_5)_3]W(CO)_3(BF_3)$	CH_2Cl_2/Et_2OBF_3	n.m.	—	—	—	66
$[C_{26}H_{20}O_3PW]^+$	84	$\{[h^5-C_5H_4P(C_6H_5)_3]W(H'')(CO)_3\}^+$	CF_3CO_2H	H H' H''	6.00 5.73 ~7.85 -7.15	$J 2.5$ — $J_{WH''} 36$	—	66
(6) HEXAHAPTO LIGANDS								
$C_9H_6O_3W$	85	$(h^6-C_6H_6)W(CO)_3$	CS_2	H	5.23	—	T 37°	214
$C_{10}H_8O_3W$	86	$(h^6-C_6H_5CH_3)W(CO)_3$	CS_2	H H'	5.2 comp. 2.38s	— —	T 37°	214
$C_{11}H_{10}O_3W$	87	$[h^6-1,4-C_6H_4(CH_3)_2]W(CO)_3$	CS_2	H H'	5.23s 2.31s	— —	T 37°	214
			$CDCl_3$	H H'	5.56 5.45 2.31	— — —	T 33°	147 1009

TABLE IV—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{12}H_{12}O_3W$	88	$[h^6-1,3,5-C_6H_3(CH_3)_3]W(CO)_3$	CS_2	H	4.90s	—	T 37°	214
				H'	2.41s	—		
			CH_2Cl_2	^{13}CH	90.9	—	Relative to TMS at 22.62 MHz. Corresponding chemical shifts of free ligand are: 127.6, 138.6, 21.4 and 181.5 resp.	148 1009
				$^{13}CCH_3$	111.1	—		
				$^{13}CH_3$	20.9	—		
				^{13}CO	212.6	6		
$C_{13}H_{14}O_3W$	89	$[h^6-1,2,4,5-C_6H_2(CH_3)_4]W(CO)_3$	CH_2Cl_2	^{13}CH	97.3	—	Relative to TMS at 22.62 MHz. Corresponding chemical shifts of free ligand are: 131.6, 134.4, 19.2 and 181.5 resp.	148
				$^{13}CCH_3$	107.9	—		
				$^{13}CH_3$	18.9	—		
				^{13}CO	213.7	—		
$C_{12}H_{13}NO_3W$	90	$\{h^6-C_6H_4-1(CH_3)-4[N(CH_3)_2]-W(CO)_3\}$	$CDCl_3$	H ₋₂	5.68	$J^* 7.1$	$J^* = J + J'$ $J^\dagger = J_A + J_B$ T 33°	147
				H ₋₃	5.16	$J^\dagger 3.8$		
				H'	2.23	—		
				H''	2.81	—		
$C_{13}H_{16}O_3SiW$	91	$[h^6-C_6H_4-1(CH_3)-4(Si(CH_3)_3)]-W(CO)_3$	$CDCl_3$	H ₋₂	5.24	$J^* 6.45$	T 33° $J^*, J^\dagger$ (see above)	147
				H ₋₃	5.55	$J^\dagger 2.5$		
				H'	2.42	—		
				H''	0.23	—		
$C_{14}H_{19}NO_3SiW$	92	$[h^6-C_6H_4-1(N(CH_3)_2)-4(Si(CH_3)_3)]W(CO)_3$	$CDCl_3$	H ₋₂	5.10	$J^* 7.2$	T 33° $J^*, J^\dagger$ (see above)	147
				H ₋₃	5.66	$J^\dagger 4.0$		
				H'	2.88	—		
				H''	0.23	—		

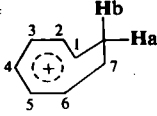
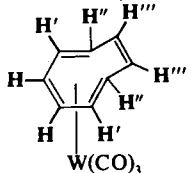
[C ₁₁ H ₉ O ₃ W] ⁺	93	[(<i>h</i> ⁶ -C ₈ H ₉)W(CO) ₃] ⁺	SO ₂	H ₋₁ , H ₋₇	4.29	$J_{1,2} = J_{6,7} 8.9$	C ₈ H ₉ = 	155
				H ₋₂ , H ₋₆	5.98	$J_{2,3} = J_{5,6} 7.5$		
C ₁₀ H ₈ O ₃ W	94	(h ⁶ -C ₇ H ₈)W(CO) ₃	CS ₂	H ₋₃ , H ₋₅	6.57	$J_{3,4} = J_{4,5} 10$	C ₇ H ₈ = cycloheptatriene Olefinic signals at δ 6.13dd (<i>J</i> 5, 2), 4.88 comp., 3.6 comp., and CH ₂ at ~3.6. T 32° 22.62 MHz. Corresponding chemical shifts for the free ligand are: 121.3, 127.3, 131.3, 28.7 and 181.5	214
				H ₋₄	5.80	—		
				Ha	3.79	$J_{1a} = J_{7,a} 8.5$		
				Hb	0.28	$J_{1b} J_{7,b} 9.0$		
						$J_{a,b} 11.5$		
C ₁₁ H ₈ O ₃ W	95	(h ⁶ -C ₈ H ₈)W(CO) ₃	CH ₂ Cl ₂	n.a.	—	—	T 5°. Structure: 	222
				¹³ CH	52.3	—		
					94.2	—		
					101.7	—		
				¹³ CH ₂	28.7	—		
C ₁₁ H ₈ O ₃ W	95	(h ⁶ -C ₈ H ₈)W(CO) ₃	—	¹³ CO	211.6	—	T 37°	214
				H	5.32s	—		
				H'	4.37d	<i>J</i> 10		
				H''	5.52d	<i>J</i> 10		
				H'''	6.24bs	—		
(7) HEPTAHAPTO LIGANDS	96	(h ⁷ -C ₇ H ₇)W(I)(CO) ₂	C ₆ H ₅ Br	H	5.3bs	—	*Reviewers assignment	214
				H'	4.53bd	<i>J</i> 11		
				H''	5.5bd	<i>J</i> 11		
				H'''	6.16bs	—		
C ₉ H ₇ IO ₂ W	96	(h ⁷ -C ₇ H ₇)W(I)(CO) ₂	CHCl ₃	H	5.37s	—	T 37°	214

TABLE IV—*cont.*

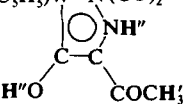
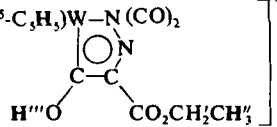
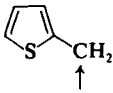
Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
(8) MIXED LIGANDS							
(a) Monohapto/pentahapto derivatives							
$C_{14}H_{13}NO_3W$	97	$(h^5-C_5H_5)W[C(C_6H_5)=OCH_3]-(NO)(CO)$	$(CD_3)_2CO$	H	5.54s	—	60
				H'	7.23m	—	
				H''	4.36s	—	
$C_{26}H_{23}O_2PW$	98	$(h^5-C_5H_5)W(CH_3)[P(C_6H_5)_3]-(CO)_2$	$CDCl_3$	H	4.73d	$J_{PH} 1.5$	161
				H'	0.58d	$J_{PH} 2.5$	
				H''	7.41m	—	
$C_{11}H_{17}O_3PW$	99	$(h^5-C_5H_5)W(CH_3)[P(OCH_3)_3]-(CO)_2$	$CDCl_3$	H	5.30s	60 and 100 MHz	121
					5.14d		
				H'	0.41d		
				H''	3.60d		
					3.53d		
$C_{11}H_{10}N_2O_4W$	100	$(h^5-C_5H_5)W-N(CO)_2$ 	—	H	5.43s	100 MHz	173
				H'	1.61s		
				H''	13.63s		
					13.21s		
$[C_{12}H_{11}N_2O_5W]^-$	101	$(h^5-C_5H_5)W-N(CO)_2$ 	—	H	5.18s	Isolated as the tetra- <i>n</i> -butyl ammonium salt	173
				H'	4.19q		
				H''	1.33t		
				H'''	10.33s		

TABLE IV—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{32}H_{20}F_3O_3PW$	108	$(h^5-C_5H_5)W(COC_6F_5)P(C_6H_5)_3-(CO)_2$	$CDCl_3$	H	5.13d	$J_{PH} 4.5$	—	193
				H'	7.40m	—		
$C_9H_7DO_3W$	109	$(h^5-C_5H_5)W(CH_2D)(CO)_3$	C_6H_6	n.m.		$J_{HH} \pm 10.0$	—	186
			CH_3CN	n.m.		$J_{HH} \pm 10.0$		949
			CS_2	n.m.		$J_{HH} \pm 10.2$		
$C_9H_8O_3W$	110	$(h^5-C_5H_5)W(CH'_3)(CO)_3$	$C_6H_5CH_3$	H	4.71	—	60 and 100 MHz	65
				H'	0.56	—		
				^{13}CH	+92.4	—		32
				$^{13}CH_3$	-28.9	—		
				^{13}CO	+239.2	—	<i>cis</i> -isomer	
					+217.8	—	<i>trans</i> -isomer	
$C_{11}H_{11}BrO_3W$	111	$(h^5-C_5H_5)W(CH_2CH_2CH_2Br)-(CO)_3$	CS_2	H	5.37s	—	—	189
				H'	3.25t	$J 7$		
$C_{12}H_{13}BrO_3W$	112	$(h^5-C_5H_5)W(CH_2CH_2CH_2CH_2Br)(CO)_3$	CS_2	H	5.35s	—	—	189
				H'	1.84b	—		
					1.57b	—		
				H''	3.35t	$J 6$		
$C_9H_7BrO_3W$	113	$(h^5-C_5H_5)W(CH_2Br)(CO)_3$	CS_2	H	5.54	—	—	195
				H	3.86			
$C_9H_7ClO_3W$	114	$(h^5-C_5H_5)W(CH_2Cl)(CO)_3$	CS_2	H	5.53s	—	—	195
				H'	4.15s	—		
$C_{12}H_{10}O_3W$	115	$(h^5-C_5H_5)W(CH_2C \equiv CCH_3)(CO)_3$	CS_2	H	1.9-1.7dt	—	—	944

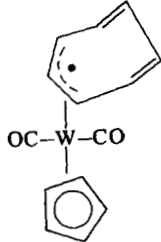
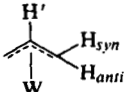
$C_{17}H_{12}O_3W$	116	$(h^5-C_5H_5)W(CH_2C\equiv CC_6H_5)-(CO)_3$	CS_2	H	2.18	—	—	944
$C_{10}H_8O_3W$	117	$(h^5-C_5H_5)W(CO)_3(CH_2CO_2H)$	$CDCl_3$	H H'	5.20s 1.92s	— —	—	196
$C_{10}H_9NO_4W$	118	$(h^5-C_5H_5)W(CO)_3(CH_2CONH_2)$	$CDCl_3$	H H' H''	5.25s 1.94s 4.87bs	— — —	—	196
$C_{10}H_{10}O_4W$	119	$(h^5-C_5H_5)W(CH_2OCH_3)(CO)_3$	CS_2	H H' H''	5.39s 4.54s 3.21s	— — —	—	195
$C_{17}H_{12}O_4W$	120	$(h^5-C_5H_5)W(CH'=CH''COC_6H_5''')(CO)_3$	$CDCl_3$	H H' H'' H'''	5.63 9.53 7.53 7.88 7.41	— $J_{H'H''} 16$ — — —	Hexamethyldisiloxane reference	223
$C_{17}H_{11}BrO_4W$	121	$(h^5-C_5H_5)W(CH'=CH''COC_6H_5'''-p-Br)(CO)_3$	$CDCl_3$	H H' H'' H''' H'''_{ortho} H'''_{meta}	5.75 9.58 7.47 7.85 7.67	— $J_{H'H''} 16.2$ — — —	Hexamethyldisiloxane reference	223
$C_{16}H_{14}O_3W$	122	$(h'-4-CH_2C_6H_4CH_3''')(h_5-C_5H_5)W(CO)_3$	$CDCl_3$	H H' H'' H'''	5.60s 2.99s 7.07m 2.27s	— — — —	—	183
$C_{14}H_{11}NO_3W$	123	$(h^5-C_5H_5)W(\alpha-CH_2-C_5H_4N)-(CO)_3$	CS_2	H H' H'' H'' H'' H'' _{ti}	5.49s 2.91s 7.39t 6.89t 8.29d	— — $J 8$ $J 8$ $J 4$	—	177

TABLE IV—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{14}H_{11}NO_3W$	124	$(h^5-C_5H_5)W(\gamma-CH_2'-C_5H_4N)(CO)_3$	CS_2	H	5.33s	—	—	192
				H'	2.76s	—		
				H''	6.99	—		
					8.29	—		
$C_{13}H_{10}O_3SW$	125	$(h'-2-CH_2C_4H_3S)(h^5-C_5H_5)W(CO)_3$	$CDCl_3$	H	5.29s	—	2- $CH_2C_4H_3S =$ 	184
				H'	3.18s	—		
				H''	6.93, 6.86,	—		
					6.80, 6.77, 6.71	—		
$C_{13}H_{10}O_3SW$	126	$(h'-3-CH_2C_4H_3S)(h^5-C_5H_5)W(CO)_3$	$CDCl_3$	H	5.20s	—	3- $CH_2C_4H_3S =$ 	184
				H'	2.95s	—		
				H''	~7.1, 6.95d,	—		
					6.75	—		
$C_{14}H_{10}O_3W$	127	$(h^5-C_5H_5)W(h'-C_6H_5)(CO)_3$	—	H	5.38	—	—	206
				H'	6.84	—		
					7.18	—		
					6.47	—		
$C_{14}H_5F_3O_3W$	128	$(h^5-C_5H_5)W(h'-C_6F_5)(CO)_3$	THF	F _{ortho}	96.7	—	56.4 and 94.1 MHz	224
				F _{meta}	163.5	—		
				F _{para}	159.0	J 19.5		
$C_{16}H_5F_3N_2O_3W$	129	$(h^5-C_5H_5)W[h'-3,4-C_6F_3(CN)_2](CO)_3$	THF	F ₋₂	62.0	J _{2,5} 12.3	56.4 and 94.1 MHz	224
				F ₋₅	134.7	J _{5,6} 26.0		
				F ₋₆	78.4	J _{2,6} 4.35		

C ₁₃ H ₅ F ₄ NO ₃ W	130	(<i>h</i> ⁵ -C ₅ H ₅)W(4- <i>h'</i> -C ₅ F ₄ N)(CO) ₃	THF	F ₋₂ F ₋₃	98.1 104.4	—	56.4 and 94.1 MHz	224
C ₁₂ H ₅ F ₇ O ₄ W	131	(<i>h</i> ⁵ -C ₅ H ₅)W(COC ₃ F ₇)(CO) ₃	CHCl ₃ C ₆ H ₆	H ¹³ C	5.65 98.7d	— <i>J</i> _{CH} 175	— High field from CS ₂ 25.14 MHz	95
C ₁₅ H ₅ F ₅ O ₄ W	132	(<i>h</i> ⁵ -C ₅ H ₅)W(COC ₆ F ₅)(CO) ₃	CDCl ₃ THF	H F _{<i>ortho</i>} F _{<i>meta</i>} F _{<i>para</i>}	5.64s 141.8 164.0 157.4	— — — —	— 56.4 and 94.1 MHz	193 224
[C ₆ H ₁₄ B ₉ -O ₃ W] ⁻	133	[(<i>π</i> -(3)-1,2-B ₉ C ₂ H ₁₁)W(CH ₃)-(CO) ₃] ⁻	—	H	-0.54	—	Isolated as the tetramethyl-ammonium salt	203
<i>(b) Dihapto/pentahapto derivatives</i>								
C ₉ H ₁₀ O ₂ SW	134	(<i>h</i> ⁵ -C ₅ H ₅)W(CH ₂ =S·CH ₃ ')-(CO) ₂	CS ₂	H H' H''	5.29 2.64 2.05 2.04	<i>J</i> 6.0	Hexamethyldisiloxane reference	185
<i>(c) Trihapto/pentahapto derivatives</i>								
C ₃₇ H ₃₃ NO ₂ W	135	(<i>h</i> ⁵ -C ₅ H ₅)W[<i>h</i> ^{3*} -C(<i>p</i> -C ₆ H ₄ -CH ₃) ₂ N=C(<i>p</i> -C ₆ H ₄ CH ₃) ₂](CO) ₂		H H' H H' H H' H H'	4.55 2.52, 2.29, 2.20, 2.15 4.57 2.54, 2.30, 2.22, 2.09 4.60 2.51, 2.20 4.68 2.29	 } T -20° } T 0° } T 10° } T 70°		1026
*σ-π bonding								

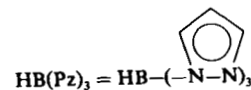
TABLE IV—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References	
$C_{14}H_{12}O_2W$	136	$(h^5-C_5H_5)W(h^3-C_7H_7)(CO)_2$	CS_2	H H'	5.21s 4.71s	— —	T 37° 	214
(d) Tetrahapto/pentahapto derivatives								
$C_{12}H_{14}OW$	137	$(h^5-C_5H_5)W(h^4-C_6H_8)(H'')(CO)$	C_6H_6	H H'	4.43d 4.8m*	— —	TMS external reference	226
					3.71m*	—	$C_6H_8 = 1,4\text{-cyclohexadiene}$	159
					3.08m*	—		
					2.68m*	—	*integral ratios:	
					2.48m*	—	1:2:1:1:1:2	
					2.37m*	—		
				H''	-7.87d	—		
(9) COMPLEXES WITH TWO TUNGSTEN ATOMS								
(a) Trihapto derivatives								
$[C_{10}H_{10}Cl_3-O_4W_2]^-$	138	$\{[(h^3-CH_2CH'H_2)W(CO)_2]_2-(Cl)_3\}^-$	$(CD_3)_2CO$	H _{syn} H _{anti} H' H'' H'''	3.22d 1.16d $\sim 3.1m$ 3.56q 1.44t	$J_{HH'} \sim 7$ $J_{HH''} \sim 8.6$ — — —	Bridging Cl ligands Isolated as the $(CH_3'''CH_2'')_4N^+$ salt 	86

$[\text{C}_{12}\text{H}_{14}\text{Cl}_3\text{-O}_4\text{W}_2]^-$	139	$\{[(h^3\text{-CH}_2\text{C}(\text{CH}_3)\text{CH}_2)\text{W}(\text{CO})_2]_2\text{-}(\text{CD}_3)_2\text{CO}(\text{Cl})_3\}^-$	$(\text{CD}_3)_2\text{CO}$	H_{syn} H_{anti} H' H'' H'''	2.92s 1.18s 2.33s 3.58q 1.42q	— — — — —	Bridging Cl ligands Isolated as the $(\text{CH}_3''' \text{CH}_2'')_4\text{N}^+$ salt	86
$\text{C}_9\text{H}_5\text{Cl}_3\text{O}_6\text{W}_2$	140	$(h^3\text{-CH}_2\text{CH}'\text{CH}_2)\text{W}_2(\text{CO})_6(\text{Cl})_3$	C_6F_6	H_{syn} H_{anti} H'	3.47d 1.50d 3.1m	J 7 J 9 —	—	213
<i>(b) Pentahapto derivatives</i>								
$\text{C}_{15}\text{H}_{12}\text{W}_2\text{O}_5$	141	$(h^5\text{-C}_5\text{H}_5)_2\text{W}(\text{H}')_2[\text{W}(\text{CO})_3]$	—	H H'	4.90 —12 to —18	— —	—	212
$\text{C}_{20}\text{H}_{22}\text{Al}_2\text{O}_6\text{-W}_2$	142	$\{(h^5\text{-C}_5\text{H}_5)\text{W}[\text{Al}(\text{CH}_3)_2](\text{CO})_3\}_2$	$\text{C}_6\text{H}_5\text{CH}_3$	H H'	5.12 —0.17	— —	Bridging $(\text{CH}_3)_2\text{Al}$ ligands	218
$\text{C}_{24}\text{H}_{30}\text{Al}_2\text{-O}_6\text{W}_2$	143	$\{(h^5\text{-C}_5\text{H}_5)\text{W}[\text{Al}(\text{CH}_2\text{CH}'')_2](\text{CO})_3\}_2$	$\text{C}_6\text{H}_5\text{CD}_3$	H H' H''	5.1 1.19t 0.14q	— — —	Bridging CO and Al Et ₂ ligands, viz: $\begin{array}{c} \text{W}-\text{CO}-\text{Al} \\ \\ \text{Al}-\text{CO}-\text{W} \end{array}$	218
$\text{C}_{16}\text{H}_{10}\text{HgO}_6\text{W}_2$	144	$[(h^5\text{-C}_5\text{H}_5)\text{W}(\text{CO})_3]_2\text{Hg}$	CDCl_3	H	5.54	—	40 and 60 MHz	136
$\text{C}_{38}\text{H}_{30}\text{N}_2\text{O}_2\text{W}_2$	145	$\{(h^5\text{-C}_5\text{H}_5)\text{W}[\text{N}=\text{C}(\text{C}_6\text{H}_5)_2](\text{CO})_2\}_2$	CHCl_3	H H'	5.36s 7.37b	— —	<i>trans</i> -isomer	111
$\text{C}_{16}\text{H}_{10}\text{Cl}_2\text{O}_6\text{-SnW}_2$	146	$[(h^5\text{-C}_5\text{H}_5)\text{W}(\text{CO})_3]_2(\text{SnCl}_2)$	—	H	5.83	—	—	948 943
$\text{C}_{16}\text{H}_{10}\text{Br}_2\text{O}_6\text{-SnW}_2$	147	$[(h^5\text{-C}_5\text{H}_5)\text{W}(\text{CO})_3]_2(\text{SnBr}_2)$	—	H	5.78	—	—	948
$\text{C}_{16}\text{H}_{10}\text{I}_2\text{O}_6\text{-SnW}_2$	148	$[(h^5\text{-C}_5\text{H}_5)\text{W}(\text{CO})_3]_2(\text{SnI}_2)$	—	H	5.75	—	—	948

TABLE IV—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{20}H_{20}O_6SnW_2$	149	$[(\eta^5-C_5H_5)W(CO)_3]_2[Sn(C_2H_5)_2]$	—	H 5.70	—	—	948
$C_{26}H_{20}O_6SnW_2$	150	$[(\eta^5-C_5H_5)W(CO)_3]_2[Sn(C_5H_5)_2]$	—	H 5.73	—	—	948
$C_{16}H_{10}N_2O_{10}SnW_2$	151	$[(\eta^5-C_5H_5)W(CO)_3]_2[Sn(NO_2)_2]$	—	H 5.70	—	—	948
$C_{20}H_{20}O_6S_2SnW_2$	152	$[(\eta^5-C_5H_5)W(CO)_3]_2[Sn(SC_2H_5)_2]$	—	H 5.58	—	—	948
$C_{18}H_{10}N_2O_6S_2SnW_2$	153	$[(\eta^5-C_5H_5)W(CO)_3]_2[Sn(SCN)_2]$	—	H 5.80	—	—	948
$C_{28}H_{18}O_6W_2$	154	$[(\eta^5-C_5H_4 \cdot C_6H_5)W(CO)_3]_2$	—	H 5.22s H' 7.19s	—	—	206
$C_{22}H_{26}O_6Si_2W_2$	155	$\{[(\eta^5-C_5H_4 \cdot Si(CH_3)_3)W(CO)_3]_2\}$	CS_2	H 5.30t 5.12t H' 0.18	— — —	100 MHz	208
(10) MISCELLANEOUS DERIVATIVES							
$C_{12}H_{11}BN_6O_3W$	156	$W[HB(Pz)_3](H)(CO)_3$	CH_2Cl_2	H -2.5	—	TMS external	53



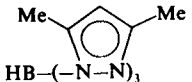
$C_{18}H_{23}BN_6O_3W$	157	$W[HB(3,5-Me_2Pz)_3](H)(CO)_3$	CH_2Cl_2	H	-2.4	—	$HB(3,5-Me_2Pz)_3 =$  $HB-(N-N)_3$	53
$C_{10}H_{16}N_2O_4W$	158	$W[N(CH_3)_2CH_2CH_2N(CH_3)_2](CO)_4$	$CHCl_3$	H H'	3.05s 2.87s	— —	T 37°	214
$C_{24}H_{18}NO_4PW$	159	$W[N\equiv CCH_3](PPh_3)(CO)_4$	C_6D_6	H	0.40	$J_{PH} 1.5$	—	79
$C_{30}H_{22}O_4P_2W$	160	$W[P(C_6H_5)_2CH'=CH'P(C_6H_5)_2](CO)_4$ <i>cis</i>	$(CH_3)_2CO$	H H'	7.9 7.75 8.58	— $J_{PH} 41, 15$	60 and 100 MHz	202
$C_8H_3NO_5W$	161	$W(CH_2=CHCN)^*(CO)_5$	$(CD_3)_2CO$	H	5.0-6.0	—	TMS external reference *σ-bond	75
$C_{14}H_{12}O_6SeW$	162	$W[Se(C_6H_5)CH'(CH_3'OCH_3''')](CO)_5$	$CDCl_3$	H H' H'' H'''	7.40m 5.12q 1.57d 3.52s	— — — —	—	80
$[C_{10}HO_{10}W_2]^-$	163	$[W_2(H)(CO)_{10}]^-$	THF	H H H	-12.52 -12.60 -12.58	— — $J_{13CH} 4.3, 3.5$ $J(^{183}W-H) 42.1$	Borohydride salt Tetramethylammonium salt Sodium Salt	915 199

TABLE V
Manganese complexes

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)		Remarks	References
(1) <i>MONOHAPTO LIGANDS</i>								
(a) <i>Monocarbonyl derivatives</i>								
$C_{14}H_{39}MnO_{13}P_4$	1	$Mn(CH_3)[P(OCH_3)_3]_4(CO)$	—	$\begin{matrix} H \\ H' \end{matrix}$	$\begin{matrix} -0.60 \text{ quint.} \\ 3.55bs \end{matrix}$	$\begin{matrix} — \\ — \end{matrix}$	—	970
(b) <i>Dicarbonyl derivatives</i>								
$C_{12}H_{30}MnO_{11}P_3$	2	$Mn(CH_3)[P(OCH_3)_3]_3(CO)_2$	—	$\begin{matrix} H \\ H' \end{matrix}$	$\begin{matrix} -0.54 \text{ quint.} \\ 3.67t \end{matrix}$	$\begin{matrix} — \\ — \end{matrix}$	—	970
$C_{27}H_{38}MnO_{12}P_3$	3	$Mn(COC_6H_5)[P(OCH_3)_3CCH_2-CH_3]_3(CO)_2$	CH_2Cl_2	$\begin{matrix} H \\ H' \end{matrix}$	$\begin{matrix} 7.22 \\ 4.16b \end{matrix}$	$\begin{matrix} — \\ — \end{matrix}$	<i>trans</i> -isomer	815
(c) <i>Tricarbonyl derivatives</i>								
$C_{16}H_{33}MnO_3P_2$	4	$Mn(CH_3)[P(CH_2CH_3)_2]_2(CO)_3$	C_6H_6	$\begin{matrix} H \\ H' \\ H'' \end{matrix}$	$\begin{matrix} -0.50t \\ 1.53 \text{ comp.} \\ 1.02 \text{ comp.} \end{matrix}$	$\begin{matrix} J\ 7 \\ — \\ — \end{matrix}$	—	816
			THF	$\begin{matrix} H \end{matrix}$	$-0.80t$	$J\ 7$		
$C_{20}H_{25}MnO_3P_2$	5	$Mn(CH_3)[P(CH_3)_2C_6H_5]_2(CO)_3$	C_6H_6	$\begin{matrix} H \\ H' \end{matrix}$	$\begin{matrix} -0.72t \\ 1.37d \end{matrix}$	$\begin{matrix} J\ 7.8 \\ J\ 7.4 \end{matrix}$	—	816
			THF	$\begin{matrix} H \\ H'' \end{matrix}$	$\begin{matrix} -0.92t \\ 7.35 \end{matrix}$	$\begin{matrix} J\ 7.8 \\ — \end{matrix}$		

$C_{30}H_{29}MnO_3P_2$	6	$Mn(CH_3)[P(C_6H_5)_2CH_3](CO)_3$	CH_2Cl_2	H	-0.65t	$J 7.8$	—	816
				H'	1.69d	$J 7.3$		
				H''	7.43	—		
			CS_2	H	-1.04t	$J 7.8$		
				H'	1.62d	$J 7.2$		
				H''	7.43	—		
			C_6H_6	H	-0.47t	$J 7.4$		
				H'	1.82d	$J 6.8$		
			THF	H	-0.93t	$J 7.4$		
				H''	7.40	—		
			CH_2Cl_2	H	-0.63t	$J 7.5$		
				H'	1.92d	$J 7.0$		
				H''	7.47	—		
			CS_2	H	-1.04t	$J 7.4$		
				H'	1.87d	$J 7.4$		
				H''	7.31	—		
$C_{38}H_{36}MnO_3P_3$	7	$Mn(CH_3)[(P(C_6H_5)_2CH_2CH_2)_2PC_6H_5](CO)_3$	C_6H_6	H	0.38s	—	100 MHz	5
				H'	~ 7.3	—		
				H''	~ 2	—		
$C_{29}H_{25}MnO_3P_2$	8	$Mn(CH_3)[P(C_6H_5)_2CH_2P-(C_6H_5)_2](CO)_3$	—	H	0.007	—	—	968
				H'	3.27	—		
$C_{30}H_{27}MnO_3P_2$	9	$Mn(CH_3)[P(C_6H_5)_2CH_2CH_2P-(C_6H_5)_2](CO)_3$	—	H	-0.85	—	—	968
				H'	2.23	—		
$C_{30}H_{25}MnO_4P_2$	10	$Mn(COCH_3)[P(C_6H_5)_2CH_2P-(C_6H_5)_2](CO)_3$	—	H	2.73s	—	—	968
				H'	4.60	—		
$C_{31}H_{27}MnO_4P_2$	11	$Mn(COCH_3)[P(C_6H_5)_2CH_2CH_2P-(C_6H_5)_2](CO)_3$	C_6H_6	H	2.34s	—	—	968

TABLE V—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{10}H_{21}MnO_9P_2$	12	$Mn(CH_3)[P(OCH_3)_3]_2(CO)_3$	C_6H_6	H	-0.05t	J 7.5	—	816
				H'	3.45	J 10.8		
			THF	H	-0.50t	J 7.6		
			CS_2	H	-0.60t	J 7.6		
				H'	3.58	J 10.9		
$C_{40}H_{33}MnO_9P_2$	13	$Mn(CH_3)[P(OC_6H_5)_3]_2(CO)_3$	C_6H_6	H	0.48t	J 8.0	—	816
			THF	H	-0.13t	J 8.0		
				H'	7.20	—		
			CS_2	H	-0.60t	J 8.0		
				H'	7.04	—		
$C_{36}H_{30}FMnO_3P_2$	14	$Mn(h^1-m-CH_2C_6H_4F)[P(C_6H_5)_2-CH_2CH_2P(C_6H_5)_2](CO)_3$	CH_2Cl_2	F	+1.74	—	Relative to C_6H_5F	191
$C_{25}H_{20}MnO_4P$	15	$Mn[CH(CH_2COCH_3)_o-C_6H_4-PPh_2](CO)_3$	—	δ_A	2.46	J_{PH} 6.8	CHCH ₂ from an ABX system	817
				δ_B	2.84	$J_{H'H'}$ 20.1		
				δ_X	3.85	—		
$C_{27}H_{22}MnO_7P$	16	$[h^1-C(CO_2CH_3)=CHCO_2CH_3]-Mn[P(C_6H_5)_3](CO)_3$ * <i>trans</i>	CCl_4	H	6.19d	J 4	* The CO of the CO_2Me group vicinal to the $Mn(CO)_3$ group is coordinated to the metal	818
				H'	3.59s, 3.42s	—		
				H''	7.46m	—		
$C_{35}H_{31}MnO_7P_2$	17	$Mn(h^1-C_6H_5)[P(OPh)_2CH_3]_2(CO)_3$	—	H	1.73t	J 2	—	819
				H	1.73t	J 4		820
$C_{21}H_{27}MnO_9P_2$	18	$(h^1-C_6H_5)Mn[P(OCH_3)_3CCH_2-CH_3]_2(CO)_3$	CH_2Cl	H	7.55, 6.85 (ratio 2:3)		<i>trans</i> -isomer	815
				H'	4.16t	J_{PH} 4.7* J_{PP} 110 $\pm$ 40†	* Separation of two outside absorptions of the triplet † Calculated	

$C_{33}H_{54}F_3MnO_3P_2$	19	$Mn(h^1-C_6F_5)[P(n-Bu)_3]_2(CO)_3$	$(CH_3)_2CO$	F_{ortho}	97.5	—	$(C_6F_5: \delta 163)$	821
				F_{meta}	163.0	—		
				F_{para}	162.6	—		
$C_{35}H_{24}F_5MnO_3P_2$	20	$Mn(h^1-C_6F_5)(PPh_2CH_2CH_2PPh_2)(CO)_3$	$(CH_3)_2CO$	F_{ortho}	95.6	$J_{ortho} 19.5$		821
				F_{meta}	164.0	$J_{meta} \leq 0.7$		
				F_{para}	162.3	$J_{PF} 1.1$		
$C_{21}H_{34}FMnO_9P_2$	21	$Mn(h^1-m-C_6H_4F)[P(OEt)_3]_2(CO)_3$	CH_2Cl_2	F	+4.89	—	Relative to C_6H_5F	191
$C_{21}H_{34}FMnO_9P_2$	22	$Mn(h^1-p-C_6H_4F)[P(OEt)_3]_2(CO)_3$	CH_2Cl_2	F	+11.75	—	Relative to C_6H_5F	191
$C_{21}H_{10}F_5MnO_9P_2$	23	$Mn(h^1-C_6F_5)[P(OEt)_3]_2(CO)_3$	$(CH_3)_2CO$	F_{ortho}	-97.5	$J_{ortho} 19.3$		821
				F_{meta}	-164.6	$J_{meta} \leq 0.7$		
				F_{para}	-162.9	$J_{PF} 2.5$		
$C_{13}H_{10}F_5MnO_3S_2$	24	$Mn(h^1-C_6F_5)[S(CH_3)CH_2CH_2SCH_3](CO)_3$	$(CH_3)_2CO$	F_{-2}, F_{-6}	105.3	$J_{2,3} 30.5$ $J_{2,5} 10.5$ $J_{2,6} 7.1$ $J_{2,4} \leq 0.7$ $J_{3,4} 19.4$ $J_{3,5} 4.5$		821
				F_{-3}, F_{-5}	164.1			
				F_{-4}	161.3	—		
$C_{33}H_{24}MnN_2O_3P$	25	$Mn(h^1-o-C_6H_4 \cdot N=NC_6H_5)(PPh_3)(CO)_3$	CS_2	H	7.83dd 7.70dt 7.15-6.64m	— — —	100 MHz	176
$C_{17}H_{33}MnO_4P_2$	26	$Mn(COCH_3)[P(CH_2CH^H)_3]_2(CO)_3$	C_6H_6	H H' H''	2.52 1.55 comp. 0.95 comp.	— — —	—	816
			THF	H	2.32	—		

TABLE V—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References	
$C_{21}H_{25}MnO_4P_2$	27	$Mn(COCH_3)[P(CH_3)_2C_6H_5]_2(CO)_3$	C_6H_6	H	2.69	—	CH ₃ CO <i>cis</i> to both P ligands	816	
				H'	1.25	—			
			CH_2Cl_2	H'	1.42	—			
				THF	H''	7.46			—
			C_6H_6	H	2.10	—	CH ₃ CO <i>trans</i> to one P ligand		
				H'	1.47d	<i>J</i> 7.9			
			CH_2Cl_2	H'	1.73d	<i>J</i> 7.9			
				H''	7.40	—			
			THF	H''	7.44	—			
			$C_{31}H_{29}MnO_4P_2$	28	$Mn(COCH_3)[P(C_6H_5)_2CH_3]_2(CO)_3$	C_6H_6	H		2.05
H'	1.92d	<i>J</i> 7.9							
CH_2Cl_2	H	1.77				—			
	H'	2.04d				<i>J</i> 7.8			
	H''	7.42				—			
CS_2	H	1.52				—	<i>J</i> 8.0		
	H'	1.95d							
H''	7.35	—							
THF	H''	7.42				—			
$C_{29}H_{25}MnO_4P_2$	29	$Mn(COCH_3)[P(C_6H_5)_2H']_2(CO)_3$				C_6H_6	H	2.52	—
			H'	6.14d	<i>J</i> 380				
			CS_2	H	2.32	—			
				H'	5.85d	<i>J</i> 380			

C ₁₁ H ₂₁ MnO ₁₀ P ₂	30	Mn(COCH ₃)[P(OCH ₃) ₃] ₂ (CO) ₃	C ₆ H ₆	H	2.82	—	CH ₃ CO <i>trans</i> to one P ligand and <i>cis</i> to the other	816					
				H'	3.47	<i>J</i> 11							
			CS ₂	H	2.30	—							
				H'	3.63	<i>J</i> 10.9							
			THF	H	2.35	—							
			C ₆ H ₆	H	2.78	—			CH ₃ CO <i>cis</i> to both P ligands				
			CS ₂	H	2.35	—							
C ₁₅ H ₂₁ MnO ₁₀ P ₂	31	Mn(COCH ₃)[P(OCH ₂) ₃ CCH ₃ '] ₂ (CO) ₃	CH ₂ Cl ₂	H	2.48	—	CH ₃ CO <i>cis</i> to both P ligands	816 822					
				H'	4.27	<i>J</i> 4.7							
			H''	7.84	—								
			C ₁₇ H ₂₅ MnO ₁₀ P ₂	32	Mn(COCH ₃)[P(OCH ₂) ₃ CCH ₃ '] ₂ (CO) ₃	CDCl ₃			H	2.43s	—	CH ₃ CO <i>cis</i> to both P ligands	823
									H'	4.17bd	<i>J</i> _{PH'} 1.0		
						H''			1.20q	<i>J</i> 7	60 and 100 MHz		
						H'''			0.81t	<i>J</i> 7			
C ₄₁ H ₃₃ MnO ₁₀ P ₂	33	Mn(COCH ₃)[P(OC ₆ H ₅) ₃] ₂ (CO) ₃	C ₆ H ₆	H	3.02	—	CH ₃ CO <i>trans</i> to one P ligand	816					
				CS ₂	H	2.35			—				
			H'	7.05	—								
			THF	H	2.55	—							
				H'	7.17	—							
C ₁₃ H ₂₅ MnO ₁₀ P ₂	34	Mn[P(OCH ₃) ₃] ₂ [COCH(CH ₃) ₂](CO) ₃	CCl ₄	H	0.82d	<i>J</i> 7	—	824					
				H'	1.28d	<i>J</i> 7							
C ₂₂ H ₂₇ MnO ₁₀ P ₂	35	(h ¹ -COC ₆ H ₅)Mn[P(OCH ₂) ₃ -CCH ₂ CH ₃] ₂ (CO) ₃	CH ₂ Cl ₂	H	7.12	—	<i>trans</i> -isomer • Separation of two outside absorptions of the triplet † Calculated	815					
				H'	4.72t	<i>J</i> _{PH'} 4.6* <i>J</i> _{PP} 70 ± 20†							
			H	7.32	—	<i>cis</i> -isomer							
				H'	4.25t				<i>J</i> _{PH'} 5.0* <i>J</i> _{PP} 5 ± 2†				

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)		Remarks	References
$C_{36}H_{28}FMnO_4P_2$	36	$Mn(m-COC_6H_4F)(PPh_2CH_2CH_2-PPh_2)(CO)_3$	CH_2Cl_2	F	+1.26	—	Relative to C_6H_5F	191
$C_{36}H_{28}FMnO_4P_2$	37	$Mn(p-COC_6H_4F)(PPh_2CH_2CH_2-PPh_2)(CO)_3$	CH_2Cl_2	F	-0.36	—	Relative to C_6H_5F	191
<i>(d) Tetracarbonyl derivatives</i>								
$C_{23}H_{18}AsMnO_4$	38	$Mn(CH_3)[As(C_6H_5)_3](CO)_4$	C_6H_6	H	-0.03	—	<i>cis</i> -isomer	825
			THF	H	-0.33	—		
				H'	7.48	—		
			CS_2	H	-0.45	—		
				H'	7.37	—		
$C_{11}H_{18}MnO_4P$	39	$Mn(CH_3)[P(CH_2CH_3)_3](CO)_4$	C_6H_6	H	-0.25	J 7.6	<i>cis</i> -isomer	825
				H'	1.4 comp.	—		
			THF	H	-0.47	J 7.6		
$C_{13}H_{14}MnO_4P$	40	$Mn(CH_3)[P(CH_3)_2C_6H_5](CO)_4$	C_6H_6	H	-0.31	J 8.9	<i>cis</i> -isomer	825
				H'	1.16	J 8.4		
			THF	H	-0.53	J 8.7		
				H''	7.45	—		

C ₁₇ H ₁₄ MnO ₄ P	41	Mn(CH ₃)[P(C ₆ H ₅) ₂ H'](CO) ₄	C ₆ H ₆	H	-0.05	J 12.0	cis-isomer	825					
				H'	5.85	J 364							
			THF	H	-0.32	—							
				H'	5.88	J 364							
C ₁₈ H ₁₆ MnO ₄ P	42	Mn(CH ₃)[P(C ₆ H ₅) ₂ CH ₃](CO) ₄	C ₆ H ₆	H	-0.25	J 8.6	cis-isomer	825					
				H'	1.46	J 7.9							
			CS ₂	H	-0.56	J 8.6							
				H'	1.86	J 7.9							
C ₂₃ H ₁₈ MnO ₄ P	43	Mn(CH ₃)[P(C ₆ H ₅) ₃](CO) ₄	C ₆ H ₆	H	-0.14	J 7.6	cis-isomer	825					
				H'	7.33	—							
			THF	H	-0.50	J 7.6							
				H'	7.47	—							
C ₁₁ H ₂₁ MnN ₃ O ₄ P	44	Mn(CH ₃)[P{N(CH ₃) ₂] ₃ }(CO) ₄	CHCl ₃	H	-0.23	J 7.7	—	971					
				H'	2.70d	J 9.5							
			C ₈ H ₁₂ MnO ₇ P	45	Mn(CH ₃)[P(OCH ₃) ₃](CO) ₄	C ₆ H ₆			H	-0.03	J 8.4	cis-isomer	825
									H'	3.18	J 11.2		
CS ₂	H	-0.38	J 8.4										
	H'	3.66	J 11.2										
THF	H	-0.33	J 8.4										

TABLE V—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	Refer- ences
$C_{10}H_{12}MnO_7P$	46	$Mn(CH_3)[P(OCH_2)_3CCH''_3](CO)_4$	$CDCl_3$	H	-0.34	—	<i>cis</i> -isomer	823
				H'	4.23	$J_{PH'} 4.5$		
				H''	0.81	—		
			C_6H_6	H	0.15	$J 8.6$	—	825
				H'	3.30	$J 4.5$		
			CS_2	H	-0.38	$J 8.6$		
				H'	4.25	$J 4.5$		
				H''	7.17	—		
			THF	H	-0.38	$J 8.1$		
				H'	4.25	$J 4.5$		
				H''	7.65	—		
$C_{11}H_{14}MnO_7P$	47	$Mn(CH_3)[P(OCH_2)_3CCH''_2-CH_3'''](CO)_4$	$CDCl_3$	H	-0.33	—	—	823
				H'	4.26	$J_{PH'} 4.4$		
				H''	1.20	$J 7.0$		
				H'''	0.80	$J 7.0$		
$C_{23}H_{18}MnO_7P$	48	$Mn(CH_3)[P(OC_6H_5)_3](CO)_4$	C_6H_6	H	0.22	$J 8.8$	<i>cis</i> -isomer	825
			CS_2	H	-0.17	$J 8.8$		
				H'	7.12	—		
			THF	H	-0.10	$J 8.8$		
				H'	7.25	—		
$C_{23}H_{18}MnO_4Sb$	49	$Mn(CH_3)[Sb(C_6H_5)_3](CO)_4$	C_6H_6	H	-0.08	—	<i>cis</i> -isomer	825
			CS_2	H	-0.36	—		
				H'	7.37	—		

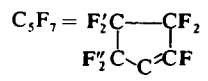
			THF	H	-0.33	—		
				H'	7.48	—		
C ₂₅ H ₁₈ MnO ₄ P	50	Mn(CH ₂ C≡CH')[P(C ₆ H ₅ ') ₃](CO) ₄	CDCl ₃	H	0.86	J _{HH} 3.0	—	827
					0.78	J _{PH} 7.5		
				H'	2.02t	—		
				H''	7.38	—		
C ₂₇ H ₁₅ F ₇ MnO ₄ P	51	Mn(h ¹ -C ₅ F ₇)(PPh ₃)(CO) ₄	(CH ₃) ₂ CO	F	41.8m*	—	<i>cis</i> -isomer 	463
				F'	53.2m*	—		
				F''	20.0m	—		
				F	41.6m*	—	<i>trans</i> -isomer T 35° * Relative to CF ₃ CO ₂ H	
				F'	53.4m*	—		
				F''	22.0m*	—		
C ₂₄ H ₁₅ BrMnO ₄ P	52	[Mn=C=CP(C ₆ H ₅) ₃](Br)(CO) ₄	—	H	7.30	—	—	828
C ₂₇ H ₂₂ MnO ₆ P	53	Mn[C(CH ₂ CO ₂ CH ₃)=CH ₂ ']·[P(C ₆ H ₅ ') ₃](CO) ₄	CDCl ₃	H	4.72s	—	—	827
				H'	2.02s	—		
				H''	5.84s,	—		
					4.85s	—		
				H'''	7.40m	—		
C ₂₈ H ₂₄ MnO ₆ P	54	Mn[C(CH ₂ CO ₂ CH ₂ CH ₃)=CH ₂ '']·[P(C ₆ H ₅ ^{IV}) ₃](CO) ₄	CDCl ₃	H	4.74s	—	—	827
				H'	2.31q	J 6		
				H''	1.12t	J 6		
				H'''	5.87s,	—		
					4.87s	—		
				H ^{IV}	7.41m	—		

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{27}H_{21}ClMnO_6P$	55	$Mn[C(CH_2CO_2CH_2Cl)=CH'_2]\cdot [P(C_6H_5''')_3](CO)_4$	$CDCl_3$	H, H''	4.90,	—	—	827
					4.83	—		
				H'	4.05s	—		
				H''	5.87s	—		
$C_8H_2F_3MnO_5$	56	$Mn[CH=C(CF_3)CH'=O](CO)_4$	—	H''''	7.43m	—	60 and 100 MHz	458
				H	7.43q	J 1.5		
				H'	9.37s	—		
				F	64.3d	J 1.5		
$C_9H_4F_3MnO_5$	57	$Mn[CH=C(CF_3)C(CH_3)=O]\cdot (CO)_4$	—	H	7.32q	J 1.8	60 and 100 MHz	458
				H'	2.56s	—		
				F	64.6d	J 1.8		
$C_9H_5MnO_6$	58	$Mn[C(CH=O)=CH'C-(CH_3'')=O](CO)_4$	CCl_4	H	10.43s	—	—	829
				H'	7.37s	—		
				H''	2.49s	—		
$C_9H_7MnO_6$	59	$Mn[C(CH_2OH')=CH''C-(CH_3''')=O](CO)_4$	$CDCl_3$	H	5.19s	—	—	827
				H'	3.19	—		
				H''	7.35s	—		
				H''''	2.43s	—		
$C_{11}H_{11}MnO_6$	60	$Mn[C(C(CH_3)_2OH')=CH''C-(CH_3''')=O](CO)_4$	$CDCl_3$	H	1.64s	—	—	827
				H'	2.13s	—		
				H''	7.13s	—		
				H''''	2.13s	—		
$C_{10}H_9MnO_7$	61	$Mn[C(CH_2OH)=C(CH_2OH)-C(CH_3)=O](CO)_4$	$CDCl_3$	n.a.		—	Signals at δ 4.3 and 2.39	827

$C_{14}H_9MnO_5$	62	$Mn[C(C_6H_5)=CH'C(CH'_3)=O]-(CO)_4$	$(CH_3)_2CO$	H H' H''	7.38s 6.98s 2.28s	— — —	—	829
$C_{10}H_7MnO_7$	63	$Mn[C(CO_2CH_3)=CH'C-(CH'_3)=O](CO)_4$	CCl_4	H H' H''	3.82s 7.17s 2.42s	— — —	—	829
$C_{12}H_9MnO_9$	64	$Mn[C(CO_2CH_3)=C(CO_2CH_3)-C(CH'_3)=O](CO)_4$	CCl_4	H H''	3.88s, 3.76s 2.68s	— — —	—	829
$C_{14}H_7MnO_6$	65	$Mn[C(CH=O)=CH'C-(C_6H'_5)=O](CO)_4$	CCl_4	H H' H''	10.63s 8.43s 7.94m	— — —	—	829
$C_{14}H_9MnO_6$	66	$Mn[C(CH_2OH')=CH''C-(C_6H'_5)=O](CO)_4$	$CDCl_3$	H H' H'' H'''	5.27s 2.40 7.27 8.04-7.53m	— — — —	—	827
$C_{16}H_{13}MnO_6$	67	$Mn[C[C(C(CH_3)_2OH')=CH''C-(C_6H'_5)=O](CO)_4$	$CDCl_3$	H H' H'' H'''	1.70s 2.10 7.27s 7.91-7.54m	— — — —	—	827
$C_{19}H_{11}MnO_5$	68	$Mn[C(C_6H_5)=CH'C-(C_6H_5)=O](CO)_4$	CCl_4	H H'	8.0-7.9bs, 7.44s 7.69s	— — —	—	829
$C_{15}H_8MnO_7$	69	$Mn[C(CO_2CH_3)=CH'C-(C_6H'_5)=O](CO)_4$	CCl_4	H H' H''	3.88s obs. 7.60- 7.40bs, 8.10- 7.80bs	— — — — —	—	829

TABLE V—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{26}H_{20}MnO_6P$	70	$(h^1\text{-CH=CHCO}_2\text{CH}_3)\text{Mn-}$ $[\text{P}(\text{C}_6\text{H}_5)_3](\text{CO})_4$ <i>trans</i>	CCl_4	H	8.50q, 6.16q	$J_{\text{PH}} 8$ $J_{\text{PH}} 2$ $J_{\text{HH}} 18$	—	818
				H'	3.57s	—		
				H''	7.36m	—		
$C_{28}H_{22}MnO_8P$	71	$[h^1\text{-C}(\text{CO}_2\text{CH}_3)=\text{CHCO}_2\text{CH}_3]\text{-}$ $\text{Mn}[\text{P}(\text{C}_6\text{H}_5)_3](\text{CO})_4$ <i>cis</i>	CDCl_3	H	5.32d	$J 1.5$	—	818
				H'	3.69s, 3.16s	— —		
				H''	7.38m	—		
$C_{10}H_7MnO_8$	72	$[h^1\text{-C}(\text{CO}_2\text{CH}_3)=\text{CHCO}_2\text{CH}_3]\text{-}$ $\text{Mn}(\text{CO})_4^*$ <i>trans</i>	CCl_4	H	6.55s	—	* The CO of the CO_2Me group vicinal to the $\text{Mn}(\text{CO})_4$ group is coordinated to the metal	818
				H'	3.89s, 3.81s	—		
$C_{15}H_7MnO_9$	73	$\text{Mn}[\text{C}(\text{CO}_2\text{H})=\text{C}(\text{CO}_2\text{H})\text{-}]$ $\text{C}(\text{C}_6\text{H}_5)=\text{O}](\text{CO})_4$	$(\text{CH}_3)_2\text{CO}$	H	10.42s	—	—	829
				H'	7.57s	—		
$C_{17}H_{11}MnO_9$	74	$\text{Mn}[\text{C}(\text{CO}_2\text{CH}_3)=\text{C}(\text{CO}_2\text{CH}_3)\text{-}]$ $\text{C}(\text{C}_6\text{H}_5)=\text{O}](\text{CO})_4$	CCl_4	H	3.90s, 3.67s	— —	—	829
				H'	7.51s	—		
$C_{29}H_{21}AsFMnO_4$	75	$\text{Mn}(h^1\text{-}m\text{-CH}_2\text{C}_6\text{H}_4\text{F})(\text{AsPh}_3)\text{-}$ $(\text{CO})_4$	CH_2Cl_2	F	+1.53	—	Relative to $\text{C}_6\text{H}_5\text{F}$	191
$C_{29}H_{21}FMnO_4P$	76	$\text{Mn}(h^1\text{-}m\text{-CH}_2\text{C}_6\text{H}_4\text{F})(\text{PPh}_3)(\text{CO})_4$	CH_2Cl_2	F	+1.65	—	Relative to $\text{C}_6\text{H}_5\text{F}$	191
$C_{24}H_{18}MnO_4P$	77	$\text{Mn}(h^1\text{-}o\text{-CH}_2\text{CH}_2\text{C}_6\text{H}_4\text{PPh}_2)\text{-}$ $(\text{CO})_4$	CDCl_3	H	2.95, 1.35	— —	—	227

C ₂₄ H ₁₈ MnO ₄ P	78	Mn(<i>h</i> ¹ - <i>o</i> -CH(CH ₃)C ₆ H ₄ PPh ₂)-(CO) ₄	CDCl ₃	H H'	3.40q 1.77d	J _{PH} 2.5 J _{HH'} 7.3	—	227
C ₂₆ H ₂₀ MnO ₅ P	79	Mn{ <i>h</i> ¹ - <i>o</i> -C[(CH ₃)COCH ₃]-C ₆ H ₄ P(C ₆ H ₅) ₂ }(CO) ₄	CDCl ₃	H H'	2.08s, 1.90s ~7.4m	— — —	—	830
C ₁₆ H ₁₆ MnO ₇ P	80	(<i>h</i> ¹ -C ₆ H ₅)Mn[P(OCH ₃) ₃ CCH ₂ -CH ₃](CO) ₄	CH ₂ Cl ₂	H H'	7.58, 6.98 4.13	— — J _{PH'} 4.5*, 4.7†	<i>cis-trans</i> mixture * Separation between 3rd and 4th lines (and † separation between 1st and 3rd lines) of quartet	815
C ₂₈ H ₁₉ AsFMnO ₄	81	Mn(<i>h</i> ¹ - <i>m</i> -C ₆ H ₄ F)(AsPh ₃)(CO) ₄	CH ₂ Cl ₂	F	+2.02	—	Relative to C ₆ H ₅ F	191
C ₂₈ H ₁₉ AsFMnO ₄	82	Mn(<i>h</i> ¹ - <i>p</i> -C ₆ H ₄ F)(AsPh ₃)(CO) ₄	CH ₂ Cl ₂	F	+9.08	—	Relative to C ₆ H ₅ F	191
C ₂₂ H ₃₁ FMnO ₄ P	83	Mn(<i>h</i> ¹ - <i>m</i> -C ₆ H ₄ F)[P(<i>n</i> -Bu) ₃](CO) ₄	CH ₂ Cl ₂	F	+2.63	—	Relative to C ₆ H ₅ F	191
C ₂₂ H ₃₁ FMnO ₄ P	84	Mn(<i>h</i> ¹ - <i>p</i> -C ₆ H ₄ F)[P(<i>n</i> -Bu) ₃](CO) ₄	CH ₂ Cl ₂	F	+9.97	—	Relative to C ₆ H ₅ F	191
C ₂₈ H ₁₉ FMnO ₄ P	85	Mn(<i>h</i> ¹ - <i>m</i> -C ₆ H ₄ F)(PPh ₃)(CO) ₄	CH ₂ Cl ₂	F	+2.08	—	Relative to C ₆ H ₅ F	191
C ₂₈ H ₁₉ FMnO ₄ P	86	Mn(<i>h</i> ¹ - <i>p</i> -C ₆ H ₄ F)(PPh ₃)(CO) ₄	CH ₂ Cl ₂	F	+9.26	—	Relative to C ₆ H ₅ F	191
C ₁₃ H ₁₃ FMnO ₇ P	87	Mn(<i>h</i> ¹ - <i>m</i> -C ₆ H ₄ F)[P(OCH ₃) ₃](CO) ₄	CH ₂ Cl ₂	F	+2.49	—	Relative to C ₆ H ₅ F	191
C ₁₃ H ₁₃ FMnO ₇ P	88	Mn(<i>h</i> ¹ - <i>p</i> -C ₆ H ₄ F)[P(OCH ₃) ₃](CO) ₄	CH ₂ Cl ₂	F	+9.48	—	Relative to C ₆ H ₅ F	191
C ₁₆ H ₁₉ FMnO ₇ P	89	Mn(<i>h</i> ¹ - <i>m</i> -C ₆ H ₄ F)[P(OEt) ₃](CO) ₄	CH ₂ Cl ₂	F	+2.86	—	Relative to C ₆ H ₅ F	191
C ₁₆ H ₁₉ FMnO ₇ P	90	Mn(<i>h</i> ¹ - <i>p</i> -C ₆ H ₄ F)[P(OEt) ₃](CO) ₄	CH ₂ Cl ₂	F	+9.78	—	Relative to C ₆ H ₅ F	191
C ₂₈ H ₁₉ FMnO ₇ P	91	Mn(<i>h</i> ¹ - <i>m</i> -C ₆ H ₄ F)[P(OPh) ₃](CO) ₄	CH ₂ Cl ₂	F	+2.32	—	Relative to C ₆ H ₅ F	191
C ₂₈ H ₁₉ FMnO ₇ P	92	Mn(<i>h</i> ¹ - <i>p</i> -C ₆ H ₄ F)[P(OPh) ₃](CO) ₄	CH ₂ Cl ₂	F	+9.20	—	Relative to C ₆ H ₅ F	191

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References	
$C_{28}H_{15}AsF_5MnO_4$	93	$Mn(1-h^1-C_6F_5)(AsPh_3)(CO)_4$	$(CH_3)_2CO$	F_{-2}, F_{-6}	99.0	$J_{2,4} \leq 0.7$, $J_{2,5} 9.6$, $J_{2,6} 8.5$	Free ligand (C_6F_6) δ 163	821
				F_{-3}, F_{-5}	162.4	$J_{3,4} 19.4, J_{3,5} 3.4$		
				F_{-4}	160.2	$J_{2,3} 29.4$		
$C_{15}H_5F_3MnNO_4$	94	$Mn(1-h^1-C_6F_5)(NC_5H_5)(CO)_4$	$(CH_3)_2CO$	F_{-2}, F_{-6}	106.5	$J_{2,4} \leq 0.7$, $J_{2,5} 10.2, J_{2,6} 7.6$	$(C_6F_6 \delta 163)$	821
				F_{-3}, F_{-5}	162.9	$J_{2,3} 29.6$, $J_{3,4} 19.2, J_{3,5} 3.7$		
				F_{-4}	160.2			
$C_{24}H_{18}AsMnO_5$	95	$Mn(COCH_3)[As(C_6H_5)_3](CO)_4$	C_6H_6	H	2.50	—	<i>cis</i> -isomer	825
			THF	H	2.40	—		
				H'	7.45	—		
			CS_2	H	2.36	—	<i>trans</i> -isomer	
				H'	7.33	—		
			C_6H_6	H	2.62	—		
			THF	H	2.59	—		
				H'	7.45	—		
			CS_2	H	2.50	—		
				H'	7.33	—		
			—	H	2.47	—	<i>cis</i> -isomer	820
				H	2.67	—	<i>trans</i> -isomer	
$[C_6H_5IMnO_5]^-$	96	$[Mn(COCH_3)(I)(CO)_4]^-$	$(CD_3)_2CO$	H	2.79s, 2.19s	—	Mixture of <i>cis</i> and <i>trans</i> -isomers	831
						—		

			DMS- <i>d</i> ₆	H	2.57s, 2.13s	—	Isolated as Lithium salt	
			THF	H	2.87	—	—	1015
C ₁₂ H ₁₆ MnNO ₅	97	Mn(COCH ₃)(NH ₂ C ₆ H ₁₁)(CO) ₄	C ₆ H ₆	H	2.70	—	<i>cis</i> -isomer	825
			THF	H	2.62	—		
C ₁₃ H ₁₈ MnNO ₅	98	Mn(COCH ₃)[NH(CH ₃)C ₆ H ₁₁](CO) ₄	C ₆ H ₆	H	2.67	—	<i>cis</i> -isomer	825
			THF	H	2.63	—		
C ₁₂ H ₁₀ MnNO ₅	99	Mn(COCH ₃)(NH ₂ C ₆ H ₅)(CO) ₄	C ₆ H ₆	H	2.70	—	<i>cis</i> -isomer	825
			THF	H	2.55	—		
C ₁₁ H ₈ MnNO ₅	100	Mn(COCH ₃)(NC ₅ H ₅)(CO) ₄	C ₆ H ₆	H	2.73	—	<i>cis</i> -isomer	825
			THF	H	2.65	—		
C ₁₂ H ₁₈ MnO ₅ P	101	Mn(COCH ₃)[P(CH ₂ CH ₃) ₃](CO) ₄	C ₆ H ₆	H	2.63	—	<i>cis</i> -isomer	825
				H'	1.48 comp.	—		
				H''	0.70 comp.	—		
			THF	H	2.50	—		
C ₁₄ H ₁₄ MnO ₅ P	102	Mn(COCH ₃)[P(CH ₃) ₂ C ₆ H ₅](CO) ₄	C ₆ H ₆	H	2.47	—	<i>cis</i> -isomer	825
				H'	1.38	<i>J</i> 9.0		
			THF	H	2.40	—		
				H''	7.45	—		
C ₁₈ H ₁₄ MnO ₅ P	103	Mn(COCH ₃)[P(C ₆ H ₅) ₂ H'']](CO) ₄	C ₆ H ₆	H	2.55	—	<i>cis</i> -isomer	825
				H''	6.35	<i>J</i> 385		
			CS ₂	H	2.45	—		
				H'	7.42	—		
				H''	6.33	<i>J</i> 385		

TABLE V—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	Refer- ences	
$C_{19}H_{16}MnO_5P$	104	$Mn(COCH_3)[P(C_6H_5)_2CH_3](CO)_4$	C_6H_6	H	2.40	—	<i>cis</i> -isomer	825	
				H''	1.78	<i>J</i> 8.4			
			THF	H	2.28	—			
				H'	7.47	—			
				H''	2.13	<i>J</i> 8.8			
			CS_2	H	2.25	—			
				H'	7.35	—			
				H''	2.02	<i>J</i> 8.6			
$C_{24}H_{18}MnO_5P$	105	$Mn(COCH_3)[P(C_6H_5)_3](CO)_4$	C_6H_6	H	2.42	—	<i>cis</i> -isomer	825	
				THF	H	2.28			—
				H'	7.43	—		832	
				CS_2	H	2.22			—
			H'		7.33	—			
			$(CD_3)_3CO$	H	2.32	—			
			C_6H_6	H	2.68	—		<i>trans</i> -isomer	
				THF	H	2.57	—		
				H'	7.43	—			
				CS_2	H	2.49	—		
					H'	7.33	—		
				$(CD_3)_2CO$	H	2.63	—		
				$CDCl_3$	H	2.70s, 2.37s	—		
			THF	^{55}Mn	1970	—	Relative to aqueous $KMnO_4$: 14.858 MHz	833	

$C_9H_{12}MnO_8P$	106	$Mn(COCH_3)[P(OCH_3)_3](CO)_4$	C_6H_6	H	2.57	—	}	<i>cis</i> -isomer	825
				H'	3.24	$J_{11.2}$			
			THF	H	2.45	—			
				H	2.45	—			
			CS_2	H'	3.70	$J_{11.2}$	}	<i>trans</i> -isomer	
				C_6H_6	H	2.62			
			C_6H_6	H'	3.10	$J_{11.8}$			
				CS_2	H	2.47			
		H'	3.60	$J_{11.8}$					
	$C_{11}H_{12}MnO_8P$	$Mn(COCH_3)[P(OCH_2)_3CCH'_3](CO)_4$	$CDCl_3$	H	2.42s	—	<i>cis</i> -isomer 100 MHz	823	
H'				4.15	$J_{5.7}$	927			
H''				0.82	—				
C_6H_6			H	2.70	—		825		
			H'	3.57	$J_{4.6}$				
			H''	−0.08	—				
THF			H	2.43	—				
			H'	4.25	$J_{4.6}$				
			H''	0.90	—				
$C_{12}H_{14}MnO_8P$			108	$Mn(COCH_3)[P(OCH_2)_3CCH'_2CH''_3](CO)_4$	$CDCl_3$	H	2.53s	—	<i>cis</i> -isomer 60 and 100 MHz
	H'	4.30				$J_{PH} 4.4$			
	H''	1.20				$J_{PH} 6.9$			
	H'''	−0.81				$J_{H''H'''} 7.0$			
$C_{24}H_{18}MnO_8P$	109	$Mn(COCH_3)[P(OC_6H_5)_3](CO)_4$	C_6H_6	H	2.58	—	<i>cis</i> -isomer	825	
				H	2.47	—			
			THF	H'	7.23	—			
				H	2.37	—			
			CS_2	H'	7.10	—			
				H	2.37	—			

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{24}H_{18}MnO_5Sb$	110	$Mn(COCH_3)_4[Sb(C_6H_5)_3](CO)_4$	C_6H_6	H	2.47	—	cis-isomer	825
				H	2.50	—		
				H'	7.45	—		
			CS_2	H	2.45	—		
				H'	7.35	—		
			—	H	2.53	—	cis-isomer	820
$C_{11}H_6MnNO_5$	111	$Mn(\alpha-COCH_2C_5H_4N)(CO)_4$	$(CD_3)_2CO$	H	4.0s	—	—	177
				H' _{α}	8.99d	J 7		
				H' _{β}	7.63	—		
				H' _{γ}	8.05dt	J 7.2		
$C_9H_{10}MnNO_5$	112	$Mn[COCH_2CH_2N(CH_3)_2](CO)_4$	—	H	2.62 comp.	—	—	177
				H'	2.86s	—		
$C_{17}H_{16}MnO_8P$	113	$(h^1-COC_6H_5)Mn[P(OCH_2)_3-CCH_2CH_3](CO)_4$	CH_2Cl_2	H	7.36	—	cis-isomer	815
				H'	4.31d	$J_{PH'}$ 5.0		
				H	7.38	—	trans-isomer	
				H'	4.22d	$J_{PH'}$ 4.5		
$C_8H_7MnO_5S$	114	$Mn(COCH_2CH_2SCH_3)(CO)_4$	CS_2	H	~2.4	—	Reference hexamethyldisiloxane	185
				H'	2.59	—		
$C_{27}H_{15}F_4^-$ $MnNO_4P$	115	$Mn(\gamma-h^1-C_5F_4N)[P(C_6H_5)_3](CO)_4$	$CHCl_3$	F _{α}	100.4	—		197
				F _{β}	112.2	—		

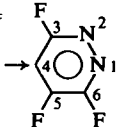
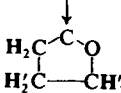
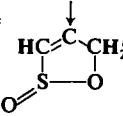
$C_{26}H_{15}F_3^-$ MnN_2O_4P	116	$Mn(4-h^1-C_4F_3N_2)(PPh_3)(CO)_4$	$CHCl_3$	F_{-3} 52.5 F_{-5} 95.4 F_{-6} 109.0	$J_{3,6}$ 28.2 $J_{3,5}$ 16.9 $J_{5,6}$ 28.2	$C_4F_3N_2 =$ 	197
$C_{13}H_6Mn_2O_{10}$	117	$Mn(h^1-C_4H_6O)[Mn(CO)_5](CO)_4$	—	H 3.67t H' 1.95q H'' 4.85t	J 7.5 J 7.5 J 7.5	$C_4H_6O =$ 	834
$C_{25}H_{18}MnO_6PS$	118	$Mn(h^1-C_3H_3O_2S)[P(C_6H_5)_3](CO)_4$	$CDCl_3$	H 5.87s H' 5.03, 4.75	— J 15	$C_3H_3O_2S =$  100 MHz	827
$C_{22}H_{27}F_3MnO_4P$	119	$Mn(1-h^1-C_6F_5)[P(n-Bu)_3](CO)_4$	$(CH_3)_2CO$	F_{-2}, F_{-6} 100.7 F_{-3}, F_{-5} 162.6 F_{-4} 161.5	$J_{2,4} \leq 0.7$ $J_{3,4}$ 19.4 J_{PF-4} 0.8	$(C_6F_5 \delta$ 163)	821
$C_{28}H_{15}F_5MnO_4P$	120	$Mn(1-h^1-C_6F_5)(PPh_3)(CO)_4$	$(CH_3)_2CO$	F_{-2}, F_{-6} 99.3 F_{-3}, F_{-5} 162.6 F_{-4} 161.5	$J_{2,4} \leq 0.7$, $J_{2,5}$ 9.4, $J_{2,6}$ 8.7 $J_{2,3}$ 29.3, $J_{3,4}$ 19.3, $J_{3,5}$ 3.6 J_{PF-3} 0.9, J_{PF-4} 1.8		821

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{28}H_{15}F_3MnO_7P$	121	$Mn(1-h^1-C_6F_5)[P(OPh)_3](CO)_4$	$(CH_3)_2CO$	F_{-2}, F_{-6} 100.1 F_{-3}, F_{-5} 162.5 F_{-4} 160.0	$J_{2,4} \leq 0.7$, $J_{1,5} 9.5, J_{2,6} 8.4$ $J_{2,3} 29.3$, $J_{3,4} 19.5, J_{3,5} 3.4$ $J_{PF} 1.4$, $J_{PF} 2.4$		821
$C_{28}H_{15}F_3MnO_4Sb$	122	$Mn(1-h^1-C_6F_5)(SbPh_3)(CO)_4$	C_6H_6	F_{-2}, F_{-6} 98.1 F_{-3}, F_{-5} 162.3 F_{-4} 160.0	$J_{2,4} \leq 0.7$ — —		821
			$(CH_3)_2CO$	F_{-2}, F_{-6} 97.4 F_{-3}, F_{-5} 162.1 F_{-4} 160.0	$J_{2,4} \leq 0.7$, $J_{2,5} 9.5, J_{2,6} 8.5$ $J_{2,3} 29.5$, $J_{3,4} 19.3, J_{3,5} 3.2$		821
$C_{17}H_{10}MnNO_4$	123	$Mn(1-h^1-C_6H_4CH=NC_6H_5)(CO)_4$	—	H 8.5–8.0	—	—	835
$C_{16}H_9MnN_2O_4$	124	$Mn(1-h^1-C_6H_4N=NC_6H_5)(CO)_4$	CS_2	H 7.20dd, 7.98dd, 8.1dd H' ~ 7.4	— — — —	100 MHz	176
(e) Pentacarbonyl derivatives							
$C_6H_2DMnO_5$	125	$Mn(CH_2D)(CO)_5$	C_6H_6	—	$J_{HH} \pm 9.7$	—	949
			CS_2	—	$J_{HH} \pm 9.8$		

$C_6H_5MnO_5$	126	$Mn(CH_3)(CO)_5$	THF	^{55}Mn	2265	—	Reference aq. $KMnO_4$ 14·858 MHz	833
			CCl_4	H	-0·1s	—	—	927
								836
			C_6H_6	H	-0·23	—	—	825
			THF	H	-0·16 (-0·10)*	—		*1015
			CS_2	H	-0·11	—		
			CH_2Cl_2	H	-0·12	—	—	816
$C_6H_5FMnO_5$	127	$Mn(CH_2F)(CO)_5$	THF	^{55}Mn	2130	—	Reference aq. $KMnO_4$	833
			CCl_4	H	5·62d	J_{HF} 47·5	—	
$C_6HF_7MnO_5$	128	$Mn(CHF_2)(CO)_5$	THF	^{55}Mn	1970	—	Reference aq. $KMnO_4$	833
			CCl_4	H	7·23t	J_{HF} 48·5	—	837
$C_6F_3MnO_5$	129	$Mn(CF_3)(CO)_5$	THF	^{55}Mn ^{19}F				833 838
$C_7HCl_2F_2MnO_5$	130	$Mn(CCl_2CHF_2)(CO)_5$	C_6F_6	H	6·09	J_{HF} 61·0		653
				F	105·2	—		
$C_7HCl_2F_2MnO_5$	131	$Mn(CF_2CHCl_2)(CO)_5$	C_6F_6	H	6·26	J_{HF} 11·0		653
				F	47·2	—		
$C_7HF_4MnO_5$	132	$Mn(CF_2CHF_2)(CO)_5$	—	H	5·32	J_{FH} 5·3	Reference hexamethyldisiloxane	839
				F	59·8	$J_{FH'} < 1$		
				F'	121·5	$J_{F'H}$ 58		
$C_8HF_6MnO_5$	133	$Mn[CH(CF_3)_2](CO)_5$	—	H	3·0m	—	100 MHz	455
				F	53·3d	J_{HF} 12	94·1 MHz	454
$C_8F_7MnO_5$	134	$Mn[CF(CF_3)_2](CO)_5$	liquid	F	+163·3	—	—	954
				F'	+67·6	—		

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_8ClF_4MnO_5$	135	$Mn(CF_2CCl=CF_2)(CO)_5$	—	F	44.9	$J_{FF'}$ 6.5*		460
				F'	89.0*, 84.2†	$J_{FF'}$ 32.1† $J_{F'F''}$ 35.8	* F' <i>cis</i> to Cl † F' <i>trans</i> to Cl	
$C_{10}H_3F_6MnO_5$	136	$Mn[CF_2CF'=C(F'')CF_2'''CH_3]-(CO)_5$ <i>trans</i>	—	F	59.5m	$J_{FF'}$ 20.0, $J_{FF''}$ 33.5, $J_{FF'''} 3.2$		840
				F'	152.5m	$J_{F'F''}$ 132.2, $J_{F'H} 2.6$		
				F''	166.4m	$J_{F''F'''} 13.5$, $J_{F''H} 2.6$		
				F'''	93.3m	$J_{F'''H} 18.8$		
$C_9HF_6MnO_5$	137	$Mn[CH(CF_3)CF'=CF_2''](CO)_5$	$CDCl_3$	H	2.78dd	J_{HF} 11.9, $J_{HF'} 41.3$		234
				F	57.0	$J_{FF'}$ 5.6		235
				F'	161.0	$J_{F'F''}$ 29.8*, $J_{F'F'''} 111.8$		
				F''	107.1*, 119.3†	$J_{F''F'''} 81.0$, $J_{HF''} 1.0^*$ $J_{HF'''} 3.2^\dagger$	* F'' <i>cis</i> to F' † F'' <i>trans</i> to F'	
$C_8H_3MnO_5$	138	$Mn(CH_2C\equiv CH')(CO)_5$	$CDCl_3$	H	1.36d	J 3	—	163
				H'	2.21t	—	—	841
$C_9H_5MnO_5$	139	$Mn(CH_2C\equiv CCH_3)(CO)_5$	$CDCl_3$	H	1.36q	J 3	—	163
				H'	1.82t	—	—	
$C_9H_5MnO_5$	140	$Mn(CH_2C\equiv CCH_3)(CO)_5$	CS_2	H	1.3	—	—	944
				H'	1.73	$J_{HH'}$ 2.8		

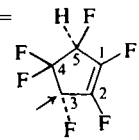
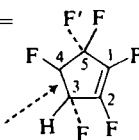
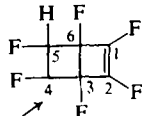
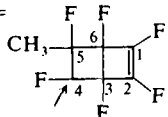
$C_{14}H_7MnO_5$	141	$Mn(CH_2C\equiv CC_6H_5)(CO)_5$	CS_2	H	1.58	—	—	944
$C_8H_3MnO_6$	142	$(h^1-CH=CHCH'O)Mn(CO)_5$ <i>cis</i>	$CDCl_3$	H	8.35bs,	—	T -20° 100 MHz	818
				H'	6.90-7.28b	—		
					9.55-	—		
					9.80bs	—		
$C_9H_5MnO_7$	143	$(h^1-CH=CHCO_2CH_3)Mn(CO)_5$ <i>cis</i>	CCl_4	H	7.79d,	J 12	—	818
				H'	7.04d	—		
					3.70s	—		
$C_9H_3MnO_9$	144	$[h^1-C(CO_2H)=CHCO_2H]Mn-$ $(CO)_5$ <i>trans</i>	$(CH_3)_2CO$	H	9.90s	—	External benzene reference	818
$C_{11}H_7MnO_9$	145	$[h^1-C(CO_2CH_3)=CHCO_2-$ $CH_3]Mn(CO)_5$ <i>trans</i>	CCl_4	H	7.07s	—		818
				H'	3.73s	—		
$C_{10}HF_6MnO_5$	146	$Mn(h^1-C_5HF_6)(CO)_5$	—	F_{-1}	158	—	$C_5HF_6 =$	842
				F_{-2}	132	—		
				F_{-3}	132	—		
				F_{-4}	115	J 237	T 34°	
					99	—		
				F_{-5}	196	$J_{FH} 56$		
$C_{10}HF_6MnO_5$	147	$Mn(h^1-C_5HF_6)(CO)_5$	—	F_{-1}	156	—	$C_5HF_6 =$	842
				F_{-2}	142	—		
				F_{-3}	163	$J_{FH} 163$		
				F_{-4}	136	—		
				F_{-5}	121	$J_{5,5'} 253$		
				F'_{-5}	77	—		

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{11}HF_6MnO_5$	148	$Mn(h^1-C_6HF_6)(CO)_5$	$CHCl_3$	H	5.14d	$J_{FH} 50.0$	$C_6H_6F_6 =$ 	240
				F_{-1}	121.7	—		
				F_{-2}	119.1	—		
				F_{-3}	138	—		
				F_{-4}	156.5	—		
				F_{-5}	189.2	$J_{FH} 50.0$		
				F_{-6}	177.1	—		
$C_{12}H_3F_6MnO_5$	149	$Mn(h^1-C_7H_3F_6)(CO)_5$	$CHCl_3$	F_{-1}	45.4	—	$C_7H_3F_6 =$ 	469
				F_{-2}	41.4	—		
				F_{-3}	81.0	—		
				F_{-4}	36.6	—		
				F_{-5}	72.4	—		
				F_{-6}	109.0	—		
$C_7HF_2MnO_5$	150	$Mn(h^1-CF=CHF')(CO)_5$	—	H	5.7dd	$J_{HF} 25.0$ $J_{HF'} 80.0$	<i>cis</i> -isomer	843
			—	F	+50.1dd	—	Relative to trifluoroacetic acid	
			—	F'	+142.2dd	$J_{FF'} \sim 2.4$		844
			—	H	5.57q	—	<i>cis</i> -isomer	
			—	H	7.47q	—	<i>trans</i> -isomer	

			CDCl ₃	H	5.7	J_{HF} 10.2, 80	<i>cis</i> -isomer	845
				H	8.1	J 25, 86	<i>trans</i> -isomer	
			—	H	8.1	J_{HF} 10.2	<i>trans</i> -isomer	843
						J_{HF} 86.5		
C ₈ F ₅ MnO ₅	151	Mn(<i>h</i> ¹ -CF=C(F')CF ₃ '')(CO) ₅	C ₆ H ₁₂	F	131q	$J_{\text{FF}'}$ 2.2	<i>cis</i> -isomer Relative to CCl ₃ F external	415
				F'	65.1q	$J_{\text{F}'\text{F}''}$ 7.6		
				F''	64.1dd	$J_{\text{FF}''}$ 13		
			CDCl ₃	F	95	$J_{\text{FF}'}$ 127	<i>trans</i> -isomer	
				F'	165	$J_{\text{F}'\text{F}''}$ 12		
				F''	67	$J_{\text{FF}''}$ 23		234
			CS ₂	F	95	$J_{\text{FF}'}$ 127		
				F'	165	$J_{\text{F}'\text{F}''}$ 12		
				F''	67	$J_{\text{FF}''}$ 23		
C ₈ ClF ₄ MnO ₅	152	Mn(<i>h</i> ¹ -CF=C(Cl)CF ₃ ')(CO) ₅	—	F	25.5	$J_{\text{FF}'}$ 8.8	—	460
				F'	59,	24.3		
					60.3	—		
C ₈ H ₂ F ₃ MnO ₅	153	Mn(<i>h</i> ¹ -C(CF ₃)=CH ₂)(CO) ₅	—	H	5.61,	J_{FH} 2	—	458
					6.46			
				F	60.1	—		
C ₈ HF ₆ MnO ₅	154	Mn(<i>h</i> ¹ -C(CHF ₂)=C(F')CF ₃ '')(CO) ₅	CDCl ₃	H	6.8	J_{HF} 60.0	CF ₃ <i>cis</i> to CHF ₂	235
						$J_{\text{HF}'}$ ~0.5		
				F	93.5m	$J_{\text{FF}'}$ 9.8		
				F'	81.4m	$J_{\text{F}'\text{F}''}$ 7.8		
				F''	63.1m	$J_{\text{FF}''}$ 4.9		

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_9H_5F_6MnO_5$	155	$Mn[h^1-CF=C(F')CF_2''CHF_2''']-(CO)_5$	$CDCl_3$	H	5.94	$J_{HF'''} 53.5$	<i>trans</i> -isomer	238 235
						$J_{HF''} 4.6$		
						$J_{HF} 1.0$		
				F	97.6	$J_{FF'} 126.5$		
						$J_{FF''} 17.8$		
$C_{10}H_3F_6MnO_5$	156	$Mn[h^1-CF=C(F')CF_2''CF_2'''CH_3]-(CO)_5$	—	F'	160.2m	$J_{F'F''} 14.1$	<i>trans</i> -isomer	840
						$J_{F'F'''} 3.4$		
				F''	118.6m	$J_{F''F'''} 8.5$		
				F'''	137.6m	—		
				H	1.73m	$J_{HF'''} 18.2$		
						$J_{HF''} 2.4$		
						$J_{HF} 2.6$		
				F	93.3	$J_{FF'} 129.0$		
$C_{12}H_9F_6GeMnO_5$	157	$Mn[h^1-CF=C(F')CF_2''CF_2'''Ge-(CH_3)_3](CO)_5$	$CDCl_3$			$J_{FF''} 25.8$	<i>trans</i> -isomer	238
						$J_{FF'''} 5.5$		
				F'	153.5	$J_{F'F''} 12.9$		
						$J_{F'F'''} 5.5$		
				F''	117.5m	—		
				F'''	110.3m	—		
				H	0.42	—		
				F	96.1	$J_{FF'} 124$		
$C_{12}H_9F_6GeMnO_5$	157	$Mn[h^1-CF=C(F')CF_2''CF_2'''Ge-(CH_3)_3](CO)_5$	$CDCl_3$			$J_{FF''} 27$	<i>trans</i> -isomer	238
						$J_{FF'''} 6$		
				F'	154.1	$J_{F'F''} 12$		
				F''	112.0	—		
				F'''	151.9	$J_{F'F'''} 6$		

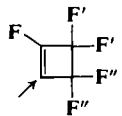
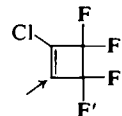
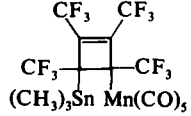
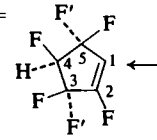
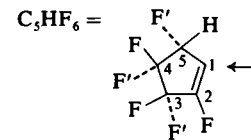
$C_{12}H_9F_6MnO_3Sn$	158	$Mn[h^1-C(CF_3)=C(CF_3)Sn-(CH_3)_3](CO)_5$	C_6H_{12}	F	49.7, 50.9	— —	<i>trans</i> -isomer	415
$C_9F_5MnO_5$	159	$Mn[h^1-CF=CF', CF''=CF''']-(CO)_5$ <i>cis</i>	$CDCl_3$	F F' F'' F''' F'''	73.0 57.1 158.0 108 119.4	$J_{FF'} 34^*$ $J_{F'F''} 16$ $J_{F'F'''} 128^\dagger$ $J_{F''F'''} 27^*$ $J_{F'''}F''' 76^\ddagger$	* <i>cis</i> -coupling † <i>trans</i> -coupling ‡ Geminal coupling F''' <i>cis</i> to F'' F''' <i>trans</i> to F''	238 239
$C_9F_5MnO_5$	160	$Mn(h^1-CF=CF'-CF''=CF''')-(CO)_5$ <i>trans</i>	$CDCl_3$	F F' F'' F''' F'''	87.2 150.3 176.0 99.3 110.6	$J_{FF'} 130$ $J_{FF''} 9$ $J_{FF'''} 16$ $J_{FF'''} 5$ $J_{F'F''} 35$ $J_{F'F'''} 13$ $J_{F'F'''} 3$ $J_{F''F'''} 114$ $J_{F''F'''} 28$ $J_{F'''}F''' 56$ —	F''' <i>trans</i> to F'' F''' <i>cis</i> to F'' F''' <i>trans</i> to F'' F''' <i>cis</i> to F'' F''' <i>trans</i> to F'' F''' <i>cis</i> to F'' F''' <i>cis</i> to F'' F''' <i>trans</i> to F''	238
$C_9F_5MnO_5$	161	$Mn(h^1-C_4F_5)(CO)_5$	CS_2	F F' F''	118.6 123.7 117.7	— — —	$C_4F_5 =$ 	232 236
$C_9ClF_4MnO_5$	162	$Mn(h^1-C_4ClF_4)(CO)_5$	CH_2Cl_2	F F'	110.3 115.2	—	$C_4ClF_4 =$ 	846

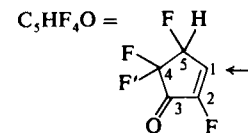
TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{16}H_9F_{12}^- MnO_3Sn$	163	$Mn[h^1-C_4(CF_3)_4Sn(CH_3)_3](CO)_5$	C_6H_{12}	n.a.	—	F NMR δ 51.0q (J 1.9), 53.8 (J 17), 56.9q (J 20), 57.0 (J 17) ppm relative to CCl_3F Structure: 	415 847
$C_{10}F_7MnO_5$	164	$Mn(h^1-C_5F_7)(CO)_5$	Acetone	F	43.4m	—	463
				F'	41.6m	—	
				F''	52.6m	—	
				F'''	21.4m	—	
						Relative to trifluoroacetic acid external T 35°	
$C_{10}HF_6MnO_5$	165	$Mn(h^1-C_5HF_6)(CO)_5$	—	F_{-2}	123	—	842
				F_{-3}	116	$J_{F_3F'_3}$ 258	
				F'_{-3}	111	—	
				F_{-4}	207	J_{F_4H} 50	
						 T 34°	

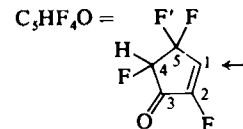
$C_{10}HF_6MnO_5$	166	$Mn(h^1-C_5HF_6)(CO)_5$	—	F_{-5}	97	—	842
				F'_{-5}	86	$J_{F_5F'_5}$ 257	
				F_{-2}	122	—	
$C_{10}HF_4MnO_6$	167	$Mn(h^1-C_5HF_4O)(CO)_5$	—	F_{-3}, F'_{-3}	118	—	842
				F_{-4}	121	$J_{F_4F'_4}$ 243	
				F'_{-4}	129	—	
				F_{-5}	183	J_{F_5H} 50	
				F_{-2}	119	—	
$C_{10}HF_4MnO_6$	168	$Mn(h^1-C_5HF_4O)(CO)_5$	—	F_{-4}	120	$J_{F_4F'_4}$ 280	842
				F'_{-4}	125	—	
				F_{-5}	187	J_{F_5H} 50	
				F_{-2}	117	—	
				F_{-4}	205	J_{F_4H} 50.6	
				F_{-5}	87	$J_{F_5F'_5}$ 259	
				F'_{-5}	101	—	



T 34°
Measured relative to $CFCO_2H$ and
converted to CCl_3F scale by
adding 78 ppm to observed value

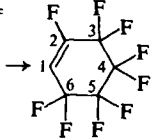
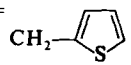


T 34°
Measured relative to $CFCO_2H$ and
converted to CCl_3F scale by
adding 78 ppm to observed values



T 34°
Measured relative to $CFCO_2H$ and
converted to CCl_3F scale by
adding 78 ppm to observed values

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{11}F_9MnO_5$	169	$Mn(h^1-C_6F_9)(CO)_5$	CS_2	F_{-2}	97.7	—	$C_6F_9 =$ 	232
				F_{-3}	124.9	—		236
				F_{-4}	143.5	—		
				F_{-5}	141.6	—		
				F_{-6}	96.4	—		
$C_7H_5MnO_5S$	170	$Mn(CH_2SCH_3)(CO)_5$	CS_2	H	1.88	—	Reference hexamethyldisiloxane	185
				H'	2.18	—		
$C_{12}H_7MnO_5$	171	$Mn(CH_2C_6H_5)(CO)_5$	CCl_4	H	2.36s	—	—	836
				H'	7.07	—		
			$(CD_3)_2CO$	H	2.42	—		
				H'	7.16	—		
			SO_2	H	2.36	—	$T - 37^\circ$	112
$C_{12}H_6FMnO_5$	172	$Mn(h^1-m-CH_2C_6H_4F)(CO)_5$	CH_2Cl_2	F	0.51	—		475
$C_7H_3MnO_7$	173	$Mn(CH_2CO_2H)(CO)_5$	$CHCl_3$	H	1.30s	—	—	196
$C_7H_4MnNO_6$	174	$Mn(CH_2CONH_2)(CO)_5$	$CHCl_3$	H	1.23s	—	—	196
				H'	5.23s	—		
$C_{10}H_5MnO_5S$	175	$(h^1-2-CH_2C_4H_3S)Mn(CO)_5$	$CDCl_3$	H	2.65s	—	$2-CH_2C_4H_3S =$ 	184
				H'	6.86, 6.80,	—		
					6.72	—		
$C_{10}H_5MnO_5S$	176	$(h^1-3-CH_2C_4H_3S)Mn(CO)_5$	$CDCl_3$	H	2.36s	—	—	184
				H'	$\sim 7.1, 6.86d,$ 6.72	—		

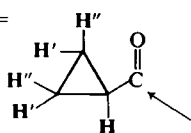
$C_{10}H_8F_4^-$ GeMnO ₅	177	Mn[CF ₂ CF ₂ Ge(CH ₃) ₃](CO) ₅	CDCl ₃	H F	0.43 23.3*, 28.1†	— — —	TMS external • Low field from CF ₃ CO ₂ H † High field from CF ₃ CO ₂ H	848
C ₉ H ₁₁ MnO ₅ Si	178	Mn[CH ₂ Si(CH ₃) ₃](CO) ₅	C ₆ H ₆	H H'	-0.78s 0.12	— —	100 MHz	849
C ₁₁ H ₅ MnO ₅	179	Mn(<i>h</i> ¹ -C ₆ H ₅)(CO) ₅	CH ₂ Cl ₂ (CD ₃) ₂ CO	H H	7.10 7.67- 6.97 comp.	— — —	— —	815 836
C ₁₂ H ₇ MnO ₅	180	Mn(<i>h</i> ¹ - <i>p</i> -C ₆ H ₄ CH ₃)(CO) ₅	CS ₂ or THF	H H'	7.25, 6.85 2.22	<i>J</i> _{ortho} — —	7.2 — —	242
C ₁₁ H ₄ ClMnO ₅	181	Mn(<i>h</i> ¹ - <i>o</i> -C ₆ H ₄ Cl)(CO) ₅	CCl ₄	H	7.53, 7.22, 6.96	— —	—	243
C ₁₁ H ₄ ClMnO ₅	182	Mn(<i>h</i> ¹ - <i>m</i> -C ₆ H ₄ Cl)(CO) ₅	CCl ₄	H	7.40, 6.90	— —	—	243
C ₁₁ H ₄ ClMnO ₅	183	Mn(<i>h</i> ¹ - <i>p</i> -C ₆ H ₄ Cl)(CO) ₅	CS ₂ or THF or CCl ₄	H	7.45, 7.04	<i>J</i> _{ortho} —	8.5 —	242 243
C ₁₁ H ₄ FMnO ₅	184	Mn(<i>h</i> ¹ - <i>m</i> -C ₆ H ₄ F)(CO) ₅	CH ₂ Cl ₂ CHCl ₃ C ₆ H ₁₂	F F F	0.70 0.50 0.14	— — —	High field from C ₆ H ₅ F	191
C ₁₁ H ₄ FMnO ₅	185	Mn(<i>h</i> ¹ -4-C ₆ H ₄ F)(CO) ₅	CH ₂ Cl ₂ CHCl ₃ C ₆ H ₁₂	F F F	7.63 7.31 7.25	— — —	To high field from C ₆ H ₅ F	191

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References	
$C_{11}F_5MnO_5$	186	$Mn(h^1-C_6F_5)(CO)_5$	C_6H_6	F_{-2}, F_6	103.5	$J_{2,4} \leq 0.7$	To high field from CCl_3F using C_6F_6 as internal reference	821
				F_{-3}, F_{-5}	161.3	$J_{3,4} 19.5$		
				F_4	157.5	—		
			$(CH_3)_2CO$	F_{-2}, F_{-6}	102.5	$J_{2,3} 28.1$	T 35°	244
						$J_{2,5} 9.2$		
						$J_{2,6} 8.3$		
			THF	F_{-3}, F_{-5}	162.7	$J_{3,4} 19.1$		
						$J_{3,5} 2.8$		
				F_{-4}	158.7	—		
			THF	F_{-2}, F_{-6}	104.3	—		
				F_{-3}, F_{-5}	161.2	—		
				F_{-4}	157.5	—		
			THF	F_{-2}, F_{-6}	103.1	—	224	
				F_{-3}, F_{-5}	162.2	$J_{3,4} 18.8$		
F_{-4}	158.7	—						
$C_{12}F_4MnNO_5$	187	$Mn(h^1-4-C_6F_4CN)(CO)_5$	$CHCl_3$	F_{-2}, F_{-6}	58.0	—	To high field from CF_3CO_2H (external)	246
				F_{-3}, F_{-5}	23.4	—		245
$C_{13}F_3MnN_2O_5$	188	$Mn[h^1-3,4-C_6F_3(CN)_2](CO)_5$	THF	F_{-2}	69.1	$J_{2,6} 12.6$	T 35°	244
				F_{-5}	135.4	$J_{2,5} 3.95$		925
				F_{-6}	85.7	$J_{5,6} 26.43$		
$C_{12}HF_4MnO_7$	189	$Mn(h^1-4-C_6F_4CO_2H)(CO)_5$	$CHCl_3$	F_{-2}, F_{-6}	62.3	—	To high field from CF_3CO_2H	245
				F_{-3}, F_{-5}	24.6	—		
$C_{14}H_5F_4MnO_7$	190	$Mn(h^1-4-C_6F_4CO_2CH_2CH_3)(CO)_5$	$CHCl_3$	F_{-2}, F_{-6}	63.2	—	To high field from CF_3CO_2H	245
				F_{-3}, F_{-5}	25.1	—		

C ₇ H ₃ MnO ₆	191	Mn(COCH ₃)(CO) ₅	CCl ₄	H	2.58s	—	—	836
			CH ₂ Cl ₂	H	2.57	—	—	825
			C ₆ H ₆	H	2.24	—	—	816
			THF	H	2.57	—	—	
			CS ₂	H	2.55	—	—	
			THF	⁵⁵ Mn	1895	—	Relative to aq. KMnO ₄	833
C ₇ H ₂ ClMnO ₆	192	Mn(COCH ₂ Cl)(CO) ₅	(CD ₃) ₂ CO	H	4.64s	—	—	836
			THF	Mn	1855	—	—	837
								833
C ₇ H ₂ FMnO ₆	193	Mn(COCH ₂ F)(CO) ₅	CCl ₄	H	4.20d	J 50	—	837
								836
			THF	⁵⁵ Mn	2010	—	—	833
C ₇ HF ₂ MnO ₆	194	Mn(COCHF ₂)(CO) ₅	CCl ₄	H	4.85t	J 59	—	837
								836
			CDCl ₃	H	4.85t	J 59	—	
				⁵⁵ Mn	1970	—	—	833
C ₇ F ₃ MnO ₆	195	Mn(COCF ₃)(CO) ₅	THF	⁵⁵ Mn	1850	—	—	833
C ₈ H ₅ MnO ₆	196	Mn(COCH ₂ CH ₃)(CO) ₅	(CD ₃) ₂ CO	H	2.98q	J 7	—	836
				H'	0.91t	J 7	—	
				⁵⁵ Mn	1950	—	—	833
C ₈ H ₄ ClMnO ₆	197	Mn(COCH ₂ CH ₂ Cl)(CO) ₅	CCl ₄	H	~ 3.40	—	A ₂ B ₂ system	836
								837
C ₉ H ₇ MnO ₆	198	Mn(COCH ₂ CH ₂ CH ₃)(CO) ₅	CCl ₄	H	2.85t	J 6.5	—	836
				H'	1.85-0.75	—	—	

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_9H_7MnO_6$	199	$Mn[COCH(CH_3)_2](CO)_5$	CCl_4	H	3.05q	$J_{6.5}$	—	836
				H'	1.02d	$J_{6.5}$		
			$(CD_3)_2CO$	H	3.24q	—		
				H'	1.00	—		
			THF	^{55}Mn	1885	—		833
$C_{10}H_9MnO_6$	200	$Mn[COC(CH_3)_3](CO)_5$	CCl_4	H	1.11s	—	—	836
$C_8F_3MnO_6$	201	$Mn(COCF=CF_2)(CO)_5$	$CDCl_3$	F	141.6	$J_{FF'} 40.6^*$	Relative to $CFCl_3$ • F' <i>cis</i> to F † F' <i>trans</i> to F	234
				F'	84.1*	$J_{FF'} 111.5^\dagger$		
				F'	127.7†	$J_{F'F'} 92.5$		
			—	F	64.9	$J_{FF'} 40.6^*$	Relative to CF_3CO_2H external * F' <i>cis</i> to F † F' <i>trans</i> to F	843
				F'	7.4*	$J_{FF'} 111.5^\dagger$		
				F'	51.0†	$J_{FF'} 92.5$		
$C_9HF_4MnO_6$	202	$Mn[COCF=C(F')CHF_2](CO)_5$	$CDCl_3$	H	6.40	$J_{HF''} 51.8$	F' <i>trans</i> to F	234
						$J_{HF'} 14.6$		235
						$J_{HF} 3.0$		
				F	144.5	$J_{FF'} 129.0$		
						$J_{FF''} 2.0$		
						$J_{F'F''} 18.6$		
$C_9H_5MnO_6$	203	$Mn(COC_3H_5)(CO)_5$	CS_2	H	2.46tt	—	COC ₃ H ₅ = 	929
				H'	0.68m	$J_{HH'} 4.8$		
				H''	1.01m	$J_{HH''} 7.4$		

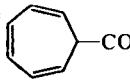
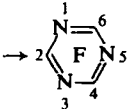
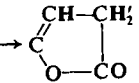
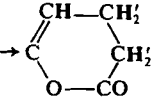
$C_{13}H_7MnO_6$	204	$Mn(COCH_2C_6H_5)(CO)_5$	$(CD_3)_2CO$	H	4.24s	—	—	836
				H'	7.23s	—	—	
			THF	^{55}Mn	2035	—	—	833
$C_8H_3MnO_7$	205	$Mn(COCOCH_3)(CO)_5$	C_6H_6	H	1.63s	—	—	851
$C_{12}H_5MnO_6$	206	$Mn(COC_6H_5)(CO)_5$	CH_2Cl_2	H	7.45	—	—	815
			THF or CS_2	H	7.36	—	—	242
$C_{13}H_7MnO_6$	207	$Mn(p-COC_6H_4CH_3)(CO)_5$	THF or CS_2	H	7.19	—	—	242
				H'	2.24	—	—	
$C_{12}H_4ClMnO_6$	208	$Mn(o-COC_6H_4Cl)(CO)_5$	THF	H	7.25	—	—	243
$C_{12}H_4ClMnO_6$	209	$Mn(m-COC_6H_4Cl)(CO)_5$	CCl_4	H	7.34	—	—	243
$C_{12}H_4ClMnO_6$	210	$Mn(p-COC_6H_4Cl)(CO)_5$	CCl_4 or THF or CS_2	H	7.37	—	—	243
								242
								82
$C_{12}H_4FMnO_6$	211	$Mn(m-COC_6H_4F)(CO)_5$	CH_2Cl_2	F	1.48	—	To low field from C_6H_5F	191
$C_{12}H_4FMnO_6$	212	$Mn(p-COC_6H_4F)(CO)_5$	$(CD_3)_2CO$	H	7.72–7.07	—	—	836
			CH_2Cl_2	F	1.64	—	Low field from C_6H_5F	191
			THF	^{55}Mn	1950	—	—	833
$C_{13}H_7MnO_7$	213	$Mn(p-COC_6H_4OCH_3)(CO)_5$	$(CD_3)_2CO$	H	7.25dd	J 8	—	836
				H'	3.85s	—	—	
$C_{13}H_7MnO_6$	214	$Mn(COC_7H_7)(CO)_5$	C_6D_6	H	2.79*, 4.97, 6.3, 6.18	— — — —	* Integral ratios 1 : 2 : 2 : 2 respectively $COC_7H_7 =$ 	438

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{10}F_4MnNO_5$	215	$Mn(4-h^1-C_5F_4N)(CO)_5$	$CHCl_3$	F_{-2}, F_{-6} 17.5* F_{-3}, F_{-5} 31.5* F_{-2}, F_{-6} 99.5†	— — $J_{2,3}$ 30 $J_{2,5}$ 24.4 $J_{2,6}$ 12.7 $J_{3,5}$ 2.4	* High field from CF_3CO_2H 56.46 MHz † High field from CCl_3F	246 197
$C_9F_3MnN_2O_5$	216	$Mn(4-h^1-C_4F_3N_2)(CO)_5$	$CHCl_3$	F_{-3} 53.1 F_{-5} 96.4 F_{-6} 107.1	$J_{3,5}$ 16.9 $J_{5,6}$ 31.0 $J_{3,6}$ 31.0	$C_4F_3N_2 =$ 	197
$C_8F_2MnN_3O_5$	217	$Mn(2-h^1-C_3F_2N_3)(CO)_5$	$CHCl_3$	F 41.8	—	$C_3F_2N_3 =$ 	197
$C_9H_3MnO_7$	218	$Mn(h^1-C_4H_3O_2)(CO)_5$	C_6H_6	H 5.01t H' 2.57d	— —	$C_4H_3O_2 =$ 	852
$C_{10}H_3MnO_7$	219	$Mn(h^1-C_5H_3O_2)(CO)_5$	C_6H_6	H 4.97t H' 2.03	— —	$C_5H_3O_2 =$ 	852

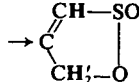
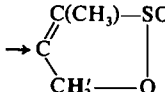
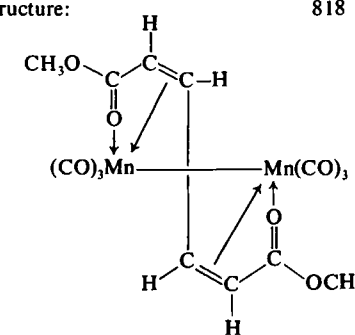
$C_9H_8MnO_5S$	220	$Mn(2-h^1-C_4H_3S)(CO)_5$	$CDCl_3$	H	7.7-6.8m	—	C_4H_3S = thiophene ligand	484
$C_8H_3MnO_7S$	221	$Mn(h^1-C_3H_3O_2S)(CO)_5$	$CDCl_3$	H H'	6.48t 5.11, 5.53	$J_{HH'} 2.5$ $J_{H'H'} 1.5$	$C_3H_3O_2S =$ 	163
$C_9H_8MnO_7S$	222	$Mn(h^1-C_4H_5O_2S)(CO)_5$	$CDCl_3$	H H'	2.20 5.13, 5.52	$J_{HH'} 2$ $J_{H'H} 15$	$C_4H_5O_2S =$ 	163 156
(2) MIXED TRANSITION METAL COMPLEXES WITH MONOHAPTO MANGANESE LIGANDS								
$C_{13}H_8Mn_2O_{10}$	223	$\{Mn[h^1-C(CH_3)_2OCH_2CH_3](CO)_4\}Mn(CO)_5$		H H' H''	3.13 4.70 1.53	— — —	—	834
$C_{15}H_9MnMoO_5$	224	$Mn\{h^1-[(h^5-C_5H_4)Mo(h^5-C_5H_5)(CO))] (CO)_4$	C_6H_6	H H'	4.33t, 4.43t 4.16s	$J 1.7$ —	—	853
$C_{14}H_{10}MnO_4Re$	225	$Mn\{h^1-[(h^5-C_5H_4)Re(H')(h^5-C_5H_5)] (CO)_4$		H H' H''	3.88t, 4.80t —14.7 4.03s	$J 2.0$ — —	—	853
$C_{15}H_9MnO_4W$	226	$Mn\{(h^5-C_5H_4)W(h^5-C_5H_5)(CO)) (CO)_4$		H H'	4.42t, 4.44t 4.17s	$J 1.8$ —	—	853

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
(3) DIHAPTO LIGANDS							
$C_{14}H_{10}Mn_2O_{10}$	227	$[Mn(CO)_3]_2(CH_3O_2C \cdot CH=CH)_2 (CH_3)_2CO$		H	5.10q,	Structure: 	818
				H'	4.18q 3.46s		
$[C_{43}H_{36}MnO_4P_2]^+$	228	$\{(h^2-CH_2=CHCH_3)Mn-[P(C_6H_5)_3]_2(CO)_4\}^+$	SO ₂	H	7.63bd	Isolated as the perchlorate 40 MHz	855
$C_6H_5MnO_4S$	229	$(h^2-CH_2=S-CH_3)Mn(CO)_4$	CS ₂	H	2.35, 1.85	Reference hexamethyldisiloxane	185
				H'	2.06		
(4) TRIHAPTO LIGANDS							
$C_{24}H_{20}MnO_3P$	230	$(h^3-CH_2 \cdots CH' \cdots CH_2)Mn-[P(C_6H_5)_3](CO)_3$	CS ₂	H _{syn}	2.04dq	—	929
				H _{anti}	1.64dq		
				H'	3.72m		
				H''	7.26m		

$C_{25}H_{20}MnO_4P$	231	$\{O, \overset{1}{C}, \overset{2}{C}, \overset{3}{C}, h^3-CH_3COC(CH_3)-$ $C_6H_4-O[P(C_6H_5)_2]Mn(CO)_3$	$CDCl_3$	H H'	2.53s, 2.33s ~ 7.4m	— — —	—	830
$C_{10}H_9MnO_5$	232	$(h^3-CH_3CH' \cdot CH'' \cdot CH''' \cdot$ $COCH_3^{IV})Mn(CO)_4$	$CDCl_3$	H H' H'' H''' H ^{IV}	1.91d 3.35 sext. 5.55q 2.5d 2.19s	$J_{HH'} 6.0$ $J_{H'H''} 10.0$ $J_{H'H'''} 10.0$ — —	H' and H''' <i>anti</i> to H''	856
$C_{15}H_7D_4MnO_5$	233	$(h^3-CD_3CH \cdot CH' \cdot CD^*COC_6H_5)-$ $Mn(CO)_4$	$CDCl_3$	H H' H''	3.56d 5.83d 7.67	$J_{HH'} 12.1$ — —	H and D* <i>anti</i> to H' 100 MHz	857 858
$C_{15}H_{11}MnO_5$	234	$(h^3-CH_3CH' \cdot CH'' \cdot CH''' \cdot$ $COC_6H_5^{IV})Mn(CO)_4$	$CDCl_3$	H H' H'' H''' H ^{IV}	1.93d 3.64 sext. 5.87q 3.23d 7.6m	$J_{HH'} 6.1$ $J_{H'H''} 12.0$ $J_{H'H'''} 9.8$ — —	—	856
$C_{16}H_{13}MnO_5$	235	$(h^3-CH_3CH_2CH'' \cdot CH''' \cdot CH^V \cdot$ $COC_6H_5^V)Mn(CO)_4$	$CDCl_3$	H H' H'' H''' H ^{IV} H ^V	1.18t 2.13qd 3.59td 5.77dd 3.13d 7.85–7.40	$J_{H'H''} 7.0$ $J_{H'H'''} 7.1$ $J_{H''H'''} 10.1$ $J_{H'''}H^{IV} 10.0$ — —	H'' and H ^{IV} <i>anti</i> to H''' 100 MHz	857
$C_9H_7MnO_4S$	236	$(h^3-2-CH_2C_4H_3S)Mn(CO)_4$	$CDCl_3$	H ₋₁ H ₋₂ H ₋₃ H ₋₄ H ₋₅	7.16d n.m. 5.23 3.62d 1.92	J_6 — J_4 J_6 J_6	$2-CH_2C_4H_3S = H_5$ 	184

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_9H_5MnO_4S$	237	$(h^3\text{-}3\text{-CH}_2C_4H_3S)Mn(CO)_4$	$CDCl_3$	H_{-1} H_{-2} H_{-3} H_{-4} H_{-5}	n.m. 7.53dd 5.23s 3.39d 1.66d	— $J_{5,2}$ — J_4 J_4	$3\text{-CH}_2C_4H_3S =$ 	184
(5) PENTAHAPTO LIGANDS								
(a) Monocarbonyl derivatives								
$[C_{24}H_{20}^- AsMnNO_2]^+$	238	$\{(h^5\text{-}C_5H_5)Mn[As(C_6H_5)_3]\text{-(NO)(CO)}\}^+$	$(CD_3)_2CO$	H H'	5.83s 7.58s	— —	Hexafluorophosphate salt	337 859
$[C_{18}H_{32}^- MnNO_2P]^+$	239	$\{(h^5\text{-}C_5H_5)Mn[P(C_4H_9)_3]\text{-(NO)(CO)}\}^+$	$(CD_3)_2CO$	H H'	5.73 0.9–2.0m	$J_{PH} 2.0$ —	Hexafluorophosphate salt	337
$[C_{24}H_{38}^- MnNO_2P]^+$	240	$\{(h^5\text{-}C_5H_5)Mn[P(C_6H_{11})_3]\text{-(NO)(CO)}\}^+$	$(CD_3)_2CO$	H H'	5.88d 1.3–2.2m	$J_{PH} 1.2$ —	Hexafluorophosphate	337
$[C_{27}H_{26}^- MnNO_2P]^+$	241	$\{(h^5\text{-}C_5H_5)Mn[P(CH_2C_6H_5)_3]\text{-(NO)(CO)}\}^+$	$(CD_3)_2CO$	H H' H''	5.34d 3.78d, 3.56d 7.35s	$J_{PH} 1.4$ — — —	Hexafluorophosphate salt	337
$[C_{12}H_{20}^- MnNO_3P]^+$	242	$\{(h^5\text{-}C_5H_5)Mn[P(OCH_2CH_3)_3]\text{-(NO)(CO)}\}^+$	$(CD_3)_2CO$	H H' H''	5.84d 4.44, 4.32, 4.20 1.53, 1.42, 1.31	$J_{PH} 1.6$ — — — —	Hexafluorophosphate salt	337

$[\text{C}_{14}\text{H}_{16}^-\text{MnNO}_2\text{P}]^+$	243	$\{(h^5\text{-C}_5\text{H}_5)\text{Mn}[\text{P}(\text{CH}_3)_2\text{C}_6\text{H}_5^-](\text{NO})(\text{CO})\}^+$	$(\text{CD}_3)_2\text{CO}$	H H' H''	5.69bs, (5.63)* 2.20d 7.62bs	J_{PH} 1.9 $J_{\text{PH}'}$ 11.2 — —	Isolated as PF_6^- salt	860 *101
$[\text{C}_{45}\text{H}_{43}\text{Mn}_2\text{-N}_2\text{O}_3\text{P}_3]^{2+}$	244	$\{(h^5\text{-C}_5\text{H}_5)_2\text{Mn}_2[(\text{PPh}_2\text{CH}_2\text{-CH}_2)_2\text{PPh}](\text{NO})_2(\text{CO})\}^{2+}$	$(\text{CD}_3)_2\text{CO}$	H	5.5b, 4.96b	— —	Isolated as the PF_6^- di-salt 100 MHz	5
$[\text{C}_{32}\text{H}_{29}^-\text{MnNO}_2\text{P}_2]^+$	245	$\{(h^5\text{-C}_5\text{H}_5)\text{Mn}(\text{NO})(\text{CO})\text{-}[\text{P}(\text{C}_6\text{H}_5)_2(\text{CH}_2'')_2(\text{C}_6\text{H}_5)_2\text{P}]\}^+$	$(\text{CD}_3)_2\text{CO}$	H H' H'' H'''	5.62d 7.63 7.32 2.85b	J 2 — — —	Isolated as the hexafluoro-phosphate	859
$[\text{C}_{38}\text{H}_{34}\text{Mn}_2\text{-N}_2\text{O}_4\text{P}_2]^{2+}$	246	$\{[(h^5\text{-C}_5\text{H}_5)\text{Mn}(\text{NO})(\text{CO})]_2\text{-}[\text{P}(\text{C}_6\text{H}_5)_2(\text{CH}_2'')_2(\text{C}_6\text{H}_5)_2\text{P}]\}^{2+}$	$(\text{CD}_3)_2\text{CO}$	H H' H''	5.64s 7.62 2.97	— — —	Isolated as the hexafluoro-phosphate	859
$[\text{C}_{52}\text{H}_{49}\text{Mn}_2\text{-N}_2\text{O}_3\text{P}_2]^{2+}$	247	$\{[(h^5\text{-C}_5\text{H}_5)\text{Mn}(\text{NO})][\{(h^5\text{-C}_5\text{H}_5)\text{-Mn}(\text{NO})(\text{CO})\}[(\text{P}(\text{C}_6\text{H}_5)_2\text{-CH}_2'')_3\text{CCH}_3''']]\}^{2+}$	$(\text{CD}_3)_2\text{CO}$	H H' H'' H'''	5.42d, 5.18, 5.06 7.7b 3.2b 1.01	J 2 — — — — —	Isolated as the hexafluoro-phosphate	859
$\text{C}_{32}\text{H}_{27}\text{MnOP}_2$	248	$(h^5\text{-C}_5\text{H}_5)\text{Mn}[\text{P}(\text{C}_6\text{H}_5)_2\text{CH}''=\text{CH}''\text{P}(\text{C}_6\text{H}_5)_2](\text{CO})$ <i>cis</i>	$(\text{CD}_3)_2\text{CO}/\text{CDCl}_3$	H H' H''	4.10 7.44, 7.32, 7.21 7.91	— — — — —	60 and 100 MHz	202
$[\text{C}_{32}\text{H}_{27}^-\text{MnNO}_2\text{P}_2]^+$	249	$\{(h^5\text{-C}_5\text{H}_5)\text{Mn}(\text{NO})(\text{CO})[\text{P}(\text{C}_6\text{H}_5)_2\text{CH}''=\text{CH}''(\text{C}_6\text{H}_5)_2\text{P}]\}^+$ <i>trans</i>	$(\text{CD}_3)_2\text{CO}$	H H' H''	5.81d 7.80, 7.57, 7.50 n.m.	J 2 — — —	Isolated as the hexafluoro-phosphate	859

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$[\text{C}_{26}\text{H}_{20}^-\text{MnNO}_2\text{P}]^+$	250	$\{(\text{h}^5\text{-C}_5\text{H}_5)\text{Mn}(\text{NO})(\text{CO})\text{-}[\text{P}(\text{C}_6\text{H}_5)_2\text{C}\equiv\text{CC}_6\text{H}_5]\}^+$	$(\text{CD}_3)_2\text{CO}$	H 5.85d H' 7.77, 7.67, 7.56	J 2 —	Isolated as the hexafluorophosphate	859
$[\text{C}_{32}\text{H}_{28}^-\text{MnNO}_2\text{P}_2]^+$	251	$\{(\text{h}^5\text{-C}_5\text{H}_5)\text{Mn}(\text{NO})(\text{CO})\text{-}[\text{P}(\text{C}_6\text{H}_5)_2\text{C}\equiv\text{C}(\text{C}_6\text{H}_5)_2\text{P}]\}^+$	$(\text{CD}_3)_2\text{CO}$	H 5.83d H' 7.78 H'' 7.60	J 2 — —	Isolated as the hexafluorophosphate H' at lower field than H'' since C_6H_5 attached to P ligand	859
$[\text{C}_{38}\text{H}_{30}^-\text{Mn}_2\text{N}_2\text{O}_4\text{P}_2]^{2+}$	252	$\{[(\text{h}^5\text{-C}_5\text{H}_5)\text{Mn}(\text{NO})(\text{CO})]_2\text{-}[\text{P}(\text{C}_6\text{H}_5)_2\text{C}\equiv\text{C}(\text{C}_6\text{H}_5)_2\text{P}]\}^{2+}$	—	H 5.92d H' 7.80	J 2 —	Isolated as the hexafluorophosphate	859
$[\text{C}_{40}\text{H}_{34}\text{Mn}_2\text{N}_2\text{O}_4\text{P}_2]^{2+}$	253	$\{[(\text{h}^5\text{-C}_5\text{H}_5)\text{Mn}(\text{NO})(\text{CO})]_2\text{-}[\text{P}(\text{C}_6\text{H}_5)_2\text{CH}_2\text{C}\equiv\text{CCH}_2\text{-}(\text{C}_6\text{H}_5)_2\text{P}]\}^{2+}$	$(\text{CD}_3)_2\text{CO}$	H 5.74s H' 7.64, 7.57 H'' 3.99d	— — J 3	Isolated as the hexafluorophosphate	859
$[\text{C}_{24}\text{H}_{20}^-\text{MnNO}_2\text{P}]^+$	254	$\{(\text{h}^5\text{-C}_5\text{H}_5)\text{Mn}[\text{P}(\text{C}_6\text{H}_5)_3]\text{-}(\text{NO})(\text{CO})\}^+$	— $(\text{CD}_3)_2\text{CO}$	H 5.56bd H' 7.69s H 5.81d H' 7.78	— — J 2 —	Isolated as the hexafluorophosphate —	860 859 337
$[\text{C}_{24}\text{H}_{20}^-\text{MnNO}_3\text{P}]^+$	255	$(\text{h}^5\text{-C}_5\text{H}_5)\text{Mn}[\text{P}(\text{OC}_6\text{H}_5)_3]\text{-}(\text{NO})(\text{CO})$	Acetone	H 5.65 H' 7.54	J 2 —	Isolated as PF_6^- salt	860 337
$[\text{C}_{24}\text{H}_{20}^-\text{MnO}_2\text{Sb}]^+$	256	$\{(\text{h}^5\text{-C}_5\text{H}_5)\text{Mn}(\text{NO})(\text{CO})\text{-}[\text{Sb}(\text{C}_6\text{H}_5)_3]\}^+$	$(\text{CD}_3)_2\text{CO}$	H 6.02s H' 7.72	— —	Isolated as the hexafluorophosphate	859

(b) Dicarbonyl derivatives

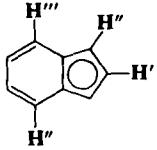
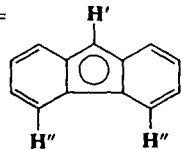
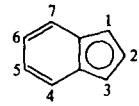
$C_7H_5AsF_3MnO_2$	257	$(h^5-C_5H_5)Mn(AsF_3)(CO)_2$	$(CD_3)_2CO$	H	5.10	—	—	861
$C_7H_5AsMnO_2$	258	$(h^5-C_5H_5)Mn(AsH_3)(CO)_2$	$CDCl_3$	H	4.54s	—	—	862
				H'	3.2s	—		
$[C_8H_5MnNO_2]^-$	259	$[(h^5-C_5H_5)Mn(CN)(CO)_2]^-$	$(CD_3)_2CO$	H	4.22	—	Isolated as $[AsPh_4]^+$ salt	863
				H	4.32s	—	Isolated as sodium salt	
$C_9H_8MnNO_2$	260	$(h^5-C_5H_5)Mn(N\equiv C \cdot CH_3)(CO)_2$	$(CD_3)_2CO$	H	4.41	—	—	864
				H'	2.20	—		865
$C_{11}H_7MnN_2O_2$	261	$(h^5-C_5H_5)Mn(N\equiv CCH'=CH'C\equiv N)(CO)_2$ <i>trans</i>	$(CD_3)_2CO$	H	4.61	—	—	864
				H'	6.52d,	J 16.5		865
					6.36d	J 16.5		
$C_{16}H_{12}MnNO_2$	262	$[h^5-C_5H_5)Mn(N\equiv C \cdot CH'=CH''C_6H_5''')(CO)_2$ <i>trans</i>	$(CD_3)_2CO$	H	4.53	—	—	864
				H'	6.19	$J_{H'H''}$ 16		865
				H''	7.36	—		
				H'''	~ 7.45	—		
$C_{15}H_{12}MnNO_2$	263	$(h^5-C_5H_5)Mn(N\equiv CCH_2C_6H_5)(CO)_2$	$(CD_3)_2CO$	H	4.45	—	—	864
				H'	4.03	—		865
				H''	7.29m	—		
$C_{14}H_5F_3MnNO_2$	264	$(h^5-C_5H_5)Mn(N\equiv CC_6F_3)(CO)_2$	$(CD_3)_2CO$	H	4.64	—	—	865
$C_{14}H_{10}MnNO_2$	265	$(h^5-C_5H_5)Mn(N\equiv C \cdot C_6H_5)(CO)_2$	$(CD_3)_2CO$	H	4.57	—	—	864
				H'	7.57m	—		
$C_{15}H_9F_3MnNO_2$	266	$(h^5-C_5H_5)Mn[N\equiv CC_6H_4-p(CF_3)](CO)_2$	$(CD_3)_2CO$	H	4.63	—	—	864
				H'	7.87	—		865
$C_{15}H_{12}MnNO_2$	267	$(h^5-C_5H_5)Mn[N\equiv CC_6H_4-p(CH_3)](CO)_2$	$(CD_3)_2CO$	H	4.54	—	—	865
				H'	7.48d,	J 7.5		864
					7.32d	J 7.5		
				H''	2.39			

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)		Remarks	References
$C_{15}H_9MnN_2O_2$	268	$(h^5-C_5H_5)Mn[N\equiv CC_6H_4-p(CN)]-(CO)_2$	$(CD_3)_2CO$	H	4.62	—	—		865
				H'	7.87	—	—		864
$C_{17}H_{14}MnNO_4$	269	$(h^5-C_5H_5)Mn[N\equiv CC_6H_4-p(CO_2-CH_2CH_3)](CO)_2$	$(CD_3)_2CO$	H	4.61	—	—		865
				H'	7.75d,	J_8			864
					8.07d	J_8			
				H''	4.36q	J_7			
$C_{14}H_9MnN_2O_4$	270	$(h^5-C_5H_5)Mn[N\equiv CC_6H_4NO_2]-(CO)_2$	$(CD_3)_2CO$	H	4.64	—	—		865
				H'	7.93d,	J_9			864
					8.33d	J_9			
$C_{15}H_{12}MnNO_3$	271	$(h^5-C_5H_5)Mn[N\equiv CC_6H_4-p(OCH_3)](CO)_2$	$(CD_3)_2CO$	H	4.55	—	—		865
				H'	7.03d,	J_8			864
					7.55d	J_8			
				H''	3.85s	—			
$C_7H_5MnN_2O_2$	272	$(h^5-C_5H_5)Mn(N_2)(CO)_2$	$(CD_3)_2CO$	H	4.84s	—	—		866
$C_{12}H_{13}MnN_2O_2$	273	$(h^5-C_5H_5)Mn(C_3H_8N_2)(CO)_2$	Acetone	H	4.55	—	—		710
$[C_7H_5MnNO_3]^+$	274	$[(h^5-C_5H_5)Mn(NO)(CO)_2]^+$	$(CD_3)_2CO$	H	6.14	—	—	T 35°. Isolated the hexafluorophosphate	61 337 859
$C_7H_5F_3MnO_2P$	275	$(h^5-C_5H_5)Mn(PF_3)(CO)_2$	$(CD_3)_2CO$	H	4.98	—	—		861
$C_7H_8MnO_2P$	276	$(h^5-C_5H_5)Mn(PH_3)(CO)_2$	C_6D_6	H	3.70	$J_{PH} 2.8$	—		932
				H'	3.24	$J_{PH'} 327$			

$C_{19}H_{32}MnO_2P$	277	$(h^5-C_5H_5)Mn[P(t-Bu)_3](CO)_2$	THF	^{31}P	-150	$J_{PH} 11$	Relative to phosphoric acid 40.5 MHz	868 972
$C_{20}H_{34}MnO_2P$	278	$(h^5-C_5H_4CH_3)Mn[P(t-Bu)_3](CO)_2$	THF	^{31}P	138	$J_{PH} 11$	Relative to phosphoric acid 40.5 MHz	868 972
$C_{15}H_{16}MnO_2P$	279	$(h^5-C_5H_5)Mn[P(CH_3)_2C_6H_5](CO)_2$	$CDCl_3$	H H' H''	4.32d 1.68d 7.45m	$J_{PH} 2.1$ $J_{PH'} 8.2$ —	—	869
$C_{25}H_{20}MnO_2P$	280	$(h^5-C_5H_5)Mn[P(C_6H_5)_3](CO)_2$	$CDCl_3$	H H'	4.33s 7.38m	— —	—	869
$C_{26}H_{22}MnO_2P$	281	$(h^5-C_5H_4CH_3)Mn[P(C_6H_5)_3](CO)_2$	CCl_4	H H' H''	3.39, 3.54 1.42 6.77 6.88	— — — — —	100 MHz	870
$C_{16}H_{32}Ge_3MnO_2P$	282	$\{(h^5-C_5H_5)Mn\{P[Ge(CH_3)_3]_3\}(CO)_2$	—	^{31}P	+157	$J_{HP} 4.2$	—	868
$C_{17}H_{34}Ge_3MnO_2P$	283	$\{(h^5-C_5H_4CH_3)Mn\{P[Ge(CH_3)_3]_3\}(CO)_2$	—	^{31}P	+154	$J_{HP} 4.4$	—	868
$C_{16}H_{32}MnO_2PSi_3$	284	$\{(h^5-C_5H_5)Mn\{P[Si(CH_3)_3]_3\}(CO)_2$	—	^{31}P	+89.2	$J_{HP} 4.6$	—	868
$C_{16}H_{32}MnO_2PSn_3$	285	$\{(h^5-C_5H_5)Mn\{P[Sn(CH_3)_3]_3\}(CO)_2$	—	^{31}P	+220	$J_{HP} 2.8$	—	868
$C_{17}H_{34}MnO_2PSn_3$	286	$(h^5-C_5H_4CH_3)Mn\{P[Sn(CH_3)_3]_3\}(CO)_2$	—	^{31}P	+216	$J_{HP} 2.7$	—	868
$C_7H_6Cl_3MnO_2Si$	287	$(h^5-C_5H_5)Mn(SiCl_3)(H')(CO)_2$	C_6H_{12}	H H'	5.11 -9.70b	— —	—	402
			CH_3CN	H'	-9.70b	—	—	401

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{26}H_{23}MnO_2Si$	288	$(h^5-C_5H_4CH_3)Mn(SiPh_3)(H')-(CO)_2$	CH_3CN	H	4.30b	—	—	402
				H'	-11.50b	—		
$C_{29}H_{22}AsMnO_2$	289	$(h^5-C_9H_7)Mn[As(C_6H_5)_3](CO)_2$	$CDCl_3$	H	7.11	—	$C_9H_7 =$ 	892
				H', H''	~ 4.6	—		
				H'''	~ 6.8	—		
$C_{29}H_{22}MnO_2P$	290	$(h^5-C_9H_7)Mn[P(C_6H_5)_3](CO)_2$	$CDCl_3$	H	7.14	—	C_9H_7 as above	892
				H', H''	4.50	—		
				H'''	6.87	—		
$C_{33}H_{24}MnO_2P$	291	$(h^5-C_{13}H_9)Mn[P(C_6H_5)_3](CO)_2$	$CDCl_3$	H	7.1	—	$C_{13}H_9 =$ 	892
				H'	4.83d	—		
				H''	~ 7.4	—		
$C_{29}H_{22}MnO_2Sb$	292	$(h^5-C_9H_7)Mn[Sb(C_6H_5)_3](CO)_2$	$CDCl_3$	H	7.30	—	$C_9H_7 =$ 	892
				H_{-1}, H_{-3}	4.99	$J_{1,2}$		
				H_{-2}	4.84	—		
				H_{-4}, H_{-7}	6.72d	—		
				H_{-5}, H_{-6}	7.12d	—		

60 and 100 MHz

$C_{24}H_{19}^-$ AsMnNO ₂	293	$(h^5-C_4H_4N)Mn[As(C_6H_5)_3](CO)_2$	CCl ₄	H_n H_β H'	5.60 4.90 7.37	— — —	—	969
$C_{24}H_{19}MnNO_2P$	294	$(h^5-C_4H_4N)Mn[P(C_6H_5)_3](CO)_2$	CCl ₄	H_n H_β H'	5.51 4.87 7.36	— — —	—	969
$C_{24}H_{19}Mn-$ NO ₂ Sb	295	$(h^5-C_4H_4N)Mn[Sb(C_6H_5)_3](CO)_2$	CCl ₄	H_n H_β H'	5.81 5.01 7.40	— — —	—	969
(c) Tricarbonyl derivatives								
$C_8H_5MnO_3$	296	$(h^5-C_5H_5)Mn(C'O)_3$	CCl ₄	H	4.7	—	—	871
			C ₆ D ₆	H	3.96s	—	—	863
			(CD ₃) ₂ CO	H	5.08	—	T 35°	61
			(CD ₃) ₂ SO	H	4.96	—	100 MHz	872
			—	H	4.75	—	T 32°	7
			C ₆ H ₅ CH ₃	¹³ C ¹³ C'	118d -28	J_{CH} 175	Relative to CS ₂ 8.5 MHz	95 974
$C_8H_4BrMnO_3$	297	$(h^5-C_5H_4Br)Mn(CO)_3$	CDCl ₃	H	4.96t, 4.65	— —	—	873 874
$C_8H_4ClMnO_3$	298	$(h^5-C_5H_4Cl)Mn(CO)_3$	CDCl ₃	H	4.91t, 4.63t	— —	—	873 874
$C_8H_4FMnO_3$	299	$(h^5-C_5H_4F)Mn(CO)_3$	CDCl ₃	H	4.67, 4.43q	— —	—	873
$C_8H_4IMnO_3$	300	$(h^5-C_5H_4I)Mn(CO)_3$	CDCl ₃	H	5.00t, 4.64t	— —	—	873 875 874

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)		Remarks	References
$C_8H_3I_2MnO_3$	301	$(h^5-1,2-C_5H_3I_2)Mn(CO)_3$	$CDCl_3$	H_{-3}, H_{-5}	5.03d	—	—		875
				H_{-4}	4.69	—	—		
$C_8H_3I_2MnO_3$	302	$(h^5-1,3-C_5H_3I_2)Mn(CO)_3$	$CDCl_3$	H_{-2}	5.22t	—	—		875
				H_{-4}, H_{-5}	4.91d	—	—		
$C_9H_7MnO_3$	303	$(h^5-C_5H_4CH_3)Mn(CO)_3$	CCl_4	H	4.57m	—	—		713
				H'	1.97	—	—		876
			$(CD_3)_2SO$	H	4.79s	—	100 MHz		872
$C_9H_6BrMnO_3$	304	$[h^5-1,2-C_5H_3(Br)CH_3]Mn(CO)_3$	CCl_4	H	4.88,	—	—		876
					4.56	—	—		
				H'	2.07	—	—		
$C_9H_6BrMnO_3$	305	$[h^5-1,3-C_5H_3(Br)CH_3]Mn(CO)_3$	CCl_4	H	4.79,	—	—		876
					4.45	—	—		
				H'	1.97	—	—		
$C_9H_6ClMnO_3$	306	$[h^5-1,2-C_5H_3(Cl)CH_3]Mn(CO)_3$	CCl_4	H	4.84,	—	—		876
					4.50	—	—		
				H'	2.08	—	—		
$C_9H_6ClMnO_3$	307	$[h^5-1,3-C_5H_3(Cl)CH_3]Mn(CO)_3$	CCl_4	H	4.78,	—	—		876
					4.41	—	—		
				H'	1.96	—	—		
$C_9H_6IMnO_3$	308	$[h^5-1,2-C_5H_3(I)CH_3]Mn(CO)_3$	CCl_4	H	4.91,	—	—		876
					4.58	—	—		
				H'	2.03	—	—		

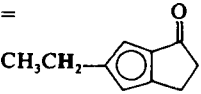
$C_9H_6IMnO_3$	309	$[h^5-1,3-C_5H_3(I)CH_2]Mn(CO)_3$	CCl_4	H	4.82, 4.46	— —	—	876
				H'	1.98	—		
$C_{10}H_9MnO_3$	310	$[h^5-1,2-C_5H_3(CH_2)_2]Mn(CO)_3$	$CDCl_3$	H	4.51	—	—	877
				H'	1.93s	—		
$C_{10}H_9MnO_3$	311	$[h^5-1,3-C_5H_3(CH_2)_2]Mn(CO)_3$	$CDCl_3$	H	4.45	—	—	877
				H'	1.92	—		
$C_{10}H_8ClMnO_3$	312	$[h^5-1,3-C_5H_3(Cl)CH_2CH_2]Mn(CO)_3$	$CDCl_3$	H	4.81d, 4.47t	— —	—	873
				H'	2.27q	—		
				H''	1.11t	—		
$C_{10}H_8IMnO_3$	313	$[h^5-1,3-C_5H_3(I)CH_2CH_2]Mn(CO)_3$	$CDCl_3$	H	4.88d, 4.52t	— —	—	873
				H'	2.28q, 1.12t	— —		
$C_{11}H_{11}MnO_3$	314	$[h^5-1,2-C_5H_3(CH_2CH_3)CH_3]Mn(CO)_3$	—	n.m.		—	H magnetically equivalent	1012
$C_{17}H_{15}MnO_3$	315	$[h^5-1,2-C_5H_3(CH_2CH_3)-CH_2C_6H_5]Mn(CO)_3$	—	n.m.		—	H magnetically equivalent	1012
$C_{12}H_{11}MnO_3$	316	$[h^5-1,2-C_5H_3(CH_2CH_3)-CH=CH_2]Mn(CO)_3$	—	n.m.		—	H magnetically non-equivalent	1012
$C_{12}H_{13}MnO_4$	317	$[h^5-1,2-C_5H_3(CH_2CH_3)CH(OH)-CH_3]Mn(CO)_3$	—	n.m.		—	Two diastereoisomers: H magnetically equivalent in the one isomer, non-equivalent in the other	1012
$C_{11}H_9MnO_4$	318	$[h^5-1,2-C_5H_3(CH_2CH_3)CHO]Mn(CO)_3$	—	n.m.		—	H magnetically non-equivalent	1012

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{12}H_{11}MnO_4$	319	$[h^5-1,2-C_5H_3(CH_2CH_3)COCH_3]-Mn(CO)_3$	—	n.m.	—	H magnetically non-equivalent	1012
$C_{17}H_{13}MnO_4$	320	$[h^5-1,2-C_5H_3(CH_2CH_3)-COC_6H_5]Mn(CO)_3$	—	n.m.	—	H magnetically non-equivalent	1012
$C_{16}H_{13}MnO_3$	321	$[h^5-1,2-C_5H_3(CH_2C_6H_5)CH_3]-Mn(CO)_3$	—	n.m.	—	H magnetically equivalent	1012
$C_{22}H_{15}MnO_4$	322	$[h^5-1,2-C_5H_3(CH_2C_6H_5)-COC_6H_5]Mn(CO)_3$	—	n.m.	—	H magnetically equivalent ($\Delta\nu = 29.4$ Hz)	1012
$C_{19}H_{15}MnO_5$	323	$[h^5-1,2-C_5H_3(p-CH_2C_6H_4-COCH_3(COCH_3)]Mn(CO)_3$	—	n.m.	—	H magnetically equivalent ($\Delta\nu = 36.3$ Hz)	1012
$C_{10}H_9MnO_4$	324	$[h^5-1,2-C_5H_3(CH_2OH)CH_3]-Mn(CO)_3$	—	n.m.	—	H magnetically equivalent	1012
$C_{12}H_{13}MnO_5$	325	$[h^5-1,2-C_5H_3(CH_2OCH_3)_2]-Mn(CO)_3$	—	n.m.	—	H magnetically equivalent ($\Delta\nu = 8.4$ Hz)	1012
$C_{11}H_{11}MnO_3$	326	$[h^5-1,3-C_5H_3(CH_2CH_3)CH_3]-Mn(CO)_3$	—	n.m.	—	H magnetically equivalent	1012
$C_{17}H_{15}MnO_3$	327	$[h^5-1,3-C_5H_3(CH_2CH_3)CH_2-C_6H_5]Mn(CO)_3$	—	n.m.	—	H magnetically equivalent	1012
$C_{12}H_{11}MnO_3$	328	$[h^5-1,3-C_5H_3(CH_2CH_3)CH=CH_2]Mn(CO)_3$	—	n.m.	—	H magnetically equivalent	1012
$C_{12}H_{13}MnO_4$	329	$[h^5-1,3-C_5H_3(CH_2CH_3)CH(OH)CH_3]Mn(CO)_3$	—	n.m.	—	H magnetically equivalent	1012

$C_{10}H_8ClMnO_3$	330	$[h^5-1,3-C_5H_3(CH_2CH_3)Cl]-$ $Mn(CO)_3$	—	n.m.	—	H magnetically equivalent	1012
$C_{11}H_9MnO_4$	331	$[h^5-1,3-C_5H_3(CH_2CH_3)CHO]-$ $Mn(CO)_3$	—	n.m.	—	H magnetically non-equivalent	1012
$C_{12}H_{11}MnO_4$	332	$[h^5-1,3-C_5H_3(CH_2CH_3)COCH_3]-$ $Mn(CO)_3$	—	n.m.	—	H magnetically non-equivalent	1012
$C_{17}H_{13}MnO_4$	333	$[h^5-1,3-C_5H_3(CH_2CH_3)COC_6H_5]-$ $Mn(CO)_3$	—	n.m.	—	H magnetically non-equivalent	1012
$C_{11}H_8ClMnO_4$	334	$[h^5-1,3-C_5H_3(CH_2CH_3)COCl]-$ $Mn(CO)_3$	—	n.m.	—	H magnetically non-equivalent	1012
$C_{12}H_{11}MnO_5$	335	$[h^5-1,3-C_5H_3(CH_2CH_3)CO_2CH_3]-$ $Mn(CO)_3$	—	n.m.	—	H magnetically non-equivalent	1012
$C_{16}H_{13}MnO_3$	336	$[h^5-1,3-C_5H_3(CH_2C_6H_5)CH_3]-$ $Mn(CO)_3$	—	n.m.	—	H magnetically equivalent	1012
$C_{17}H_{13}MnO_4$	337	$[h^5-1,3-C_5H_3(CH_2C_6H_5)COCH_3]-$ $Mn(CO)_3$	—	n.m.	—	H magnetically equivalent	1012
$C_{22}H_{15}MnO_4$	338	$[h^5-1,3-C_5H_3(CH_2C_6H_5)COC_6H_5]-$ $Mn(CO)_3$	—	n.m.	—	H magnetically equivalent	1012
$C_{19}H_{15}MnO_5$	339	$[h^5-1,3-C_5H_3(\mu-CH_2C_6H_4-$ $COCH_3)COCH_3]Mn(CO)_3$	—	n.m.	—	H magnetically equivalent	1012
$C_{10}H_9MnO_4$	340	$[h^5-1,3-C_5H_3(CH_2OH)CH_3]-$ $Mn(CO)_3$	—	n.m.	—	H magnetically equivalent	1012
$C_{12}H_{13}MnO_5$	341	$[h^5-1,3-C_5H_3(CH_2OCH_3)_2]-$ $Mn(CO)_3$	—	n.m.	—	H magnetically equivalent	1012
$C_{14}H_{16}MnO_4$	342	$[h^5-C_5H_3-1,2-(CH_2CH_3)_2-4-$ $(COCH_3)]Mn(CO)_3$	—	n.m.	—	H magnetically non-equivalent	1012

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{14}H_{16}MnO_4$	343	$[h^5-C_5H_3-1,3-(CH_2CH_3)_2-5-(COCH_3)]Mn(CO)_3$	—	n.m.	—	H magnetically non-equivalent	1012
$C_{13}H_{11}MnO_4$	344	$(h^5-C_{10}H_{11}O)Mn(CO)_3$	—	n.m.	—	$C_{10}H_{11}O =$  H magnetically non-equivalent	1012
$C_{13}H_{11}MnO_4$	345	$(h^5-C_{10}H_{11}O)Mn(CO)_3$	—	n.m.	—	$C_{10}H_{11}O =$  H magnetically non-equivalent	1012
$C_{12}H_{13}MnO_3$	346	$[h^5-1,2-C_5H_3(CH_2CH''_2)]-Mn(CO)_3$	$CDCl_3$	H_{-3}, H_{-5} 4.62d H_{-4} 4.43t H' 2.29m H'' 1.13t	— — — —	H' magnetically non-equivalent	877 1012
$C_{12}H_{13}MnO_3$	347	$[h^5-1,3-C_5H_3(CH_2CH''_2)]-Mn(CO)_3$	$CDCl_3$	H 4.51 H' 2.27q H'' 1.12t	— — —	H' magnetically equivalent	877 1012
$C_{11}H_{11}MnO_3$	348	$(h^5-C_5H_4 \cdot CH_2CH_2CH_3)-Mn(CO)_3$	$CDCl_3$	H 4.61	—	—	877

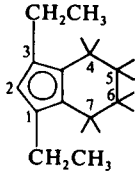
$C_{11}H_{11}MnO_3$	349	$[h^5-C_5H_4 \cdot CH'(CH'_2)_2]Mn(CO)_3$	$CDCl_3$	H H' H''	4.62m 2.58m 1.14d	— — —	—	877
$C_{13}H_{15}MnO_3$	350	$[h^5-1,2-C_5H_3(CH_2CH'_2)CH'''-(CH_3^{IV})_2]Mn(CO)_3$	$CDCl_3$	H H' H'' H''' H ^{IV}	4.55m 2.29q 1.12t 2.54m 1.14d	— — — — —	—	877
$C_{14}H_{17}MnO_3$	351	$[h^5-1,2,4-C_5H_2(CH_2CH'_2)_3]-Mn(CO)_3$	$CDCl_3$	H H' H''	4.55s 2.26m 1.13t	— — —	—	877
$C_{17}H_{23}MnO_3$	352	$(h^5-C_5H_4n-C_9H_{19})Mn(CO)_3$	$CDCl_3$	H	4.61	—	—	877
$C_{16}H_{19}MnO_3$	353	$[h^5-C_9H_5(CH_2CH'_2)_2]Mn(CO)_3$	$CDCl_3$	H ₋₂ H ₋₄ , H ₋₇ H ₋₅ , H ₋₆ H' H''	4.58s 2.4 1.7 2.22q 1.11t	— — — — —	$C_9H_9(CH_2CH_3)_2 =$	877
								
$C_{15}H_{11}MnO_3$	354	$(h^5-C_5H_4 \cdot CH_2Ph)Mn(CO)_3$	$CDCl_3$	H H'	4.60 3.56s	— —	—	877
$C_{11}H_9MnO_3$	355	$[h^5-C_5H_4 \cdot C(CH_3)=CH_2]-Mn(CO)_3$	$CDCl_3$	H ₋₂ , H ₋₅ H ₋₃ , H ₋₄ H'	4.92t 4.68t 1.92	— — —	—	877
$C_{26}H_{19}-AuMnO_3P$	356	$[h^5-C_5H_4AuP(C_6H_5)_3]Mn(CO)_3$	$CDCl_3$	H H'	4.86, 4.57 7.36	— — —	—	979

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{18}H_{12}BrMnO_3$	357	$[h^5-C_5H_4C(C_6H_5)=CH''-C(Br)=CH_2'']Mn(CO)_3$	CCl_4	H	4.65m	—	—	981
				H'	7.2m	—		
				H''	5.1	—		
				H'''	5.35m	—		
$C_{15}H_{15}MnO_6$	358	$[h^5-C_5H_4COCH_2C(CH_3)_2CO_2-CH_3]Mn(CO)_3$	$CDCl_3$	H ₋₂ , H ₋₅	5.38t	—	—	978
				H ₋₃ , H ₋₄	4.81t	—		
				H'	2.87	—		
				H''	1.27s	—		
$C_{16}H_{17}MnO_6$	359	$\{h^5-C_5H_3-1-(CH_3)-2-[COCH_2C-(CH_3)_2CO_2CH_3]\}Mn(CO)_3$	$CDCl_3$	H ₋₃	5.32q	—	—	978
				H ₋₄ , H ₋₅	4.73m	—		
				H'	2.92	—		
				H''	1.29	—		
$C_{10}H_{10}MnNO_3$	360	$[h^5-C_5H_4 \cdot CH(CH_3)NH_2]-Mn(CO)_3$	$(CD_3)_2SO$	H ₋₂ , H ₋₅	4.99d	—	As the hydrochloride salt 100 MHz	872
				H ₋₃ , H ₋₄	5.38s	—		
$C_{11}H_{11}MnO_4$	361	$[h^5-C_5H_4 \cdot C(CH_3)_2OH'']Mn(CO)_3$	$CDCl_3$	H ₋₂ , H ₋₅	4.90t	—	—	877
				H ₋₃ , H ₋₄	4.61t	—		
				H'	1.49s	—		
				H''	1.68s	—		
$C_{17}H_{10}Mn_2O_7$	362	$[h^5, h^5-(C_5H_4)_2CH' \cdot OH'']-[Mn(CO)_3]_2$	—	H	4.8m	—	—	878
				H'	5.12d	—		
				H''	2.16d	—		
$C_{10}H_8MnNO_4$	363	$[h^5-C_5H_4 \cdot C(CH_3)=NOH]-Mn(CO)_3$	$(CD_3)_2SO$	H ₋₂ , H ₋₅	5.30s	—	100 MHz	872
				H ₋₃ , H ₋₄	4.91s	—		

$C_9H_5MnO_4$	364	$(h^5-C_5H_4CH=O)Mn(CO)_3$	$(CD_3)_2SO$	H_{-2}, H_{-5} H_{-3}, H_{-4}	5.78t 5.25t	— —	100 MHz	872
$C_{10}H_7MnO_4$	365	$[h^5-C_5H_3-1(CH'O)-2(CH'_3)]\cdot Mn(CO)_3$	$CDCl_3$	H_{-3} H_{-4} H_{-5} H' H''	4.25 4.81 5.32 9.82s 2.25s	— — — — —	—	877
$C_{10}H_7MnO_4$	366	$[h^5-C_5H_3-1(CH'O)-2(CH'_3)]\cdot Mn(CO)_3$	$CDCl_3$	H_{-2} H_{-4} H_{-5} H' H''	5.31 4.77 5.38 9.65s 2.05s	— — — — —	—	877
$C_{11}H_9MnO_4$	367	$[h^5-C_5H_3-1(CH'O)-2(CH'_2CH'_3'')]Mn(CO)_3$	$CDCl_3$	H_{-3}, H_{-4} H_{-5} H' H'' H'''	4.80d 5.37t 9.51s 2.6m 1.22t	— — — — —	—	877
$C_{11}H_9MnO_4$	368	$[h^5-C_5H_3-1(CH'O)-3(CH'_2CH'_3''')]Mn(CO)_3$	$CDCl_3$	H_{-2}, H_{-5} H_{-4} H' H'' H'''	5.37m 4.83t 9.60s 2.4m 1.19t	— — — — —	—	877
$C_{12}H_9MnO_4$	369	$[h^5-C_5H_4(CH=CHCOCH_3)]\cdot Mn(CO)_3$	—	H_α H_β	5.11 4.82	— —	—	1013
$C_8H_4MnNO_5$	370	$(h^5-C_5H_4NO_2)Mn(CO)_3$	—	H_α H_β	5.80 4.80	— —	—	1013
$C_9H_4MnNO_3$	371	$(h^5-C_5H_4CN)Mn(CO)_3$	—	H_α H_β	5.31 4.83	— —	—	1013

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{10}H_5MnO_5$	372	$[h^5-1,3-C_5H_3(CHO)_2]Mn(CO)_3$	—	H_{-2}	6.05	—	Calculated δ values: 6.15 and 5.62 respectively	1013
				H_{-4}, H_{-5}	5.58	—		
$C_{10}H_3MnN_2O_3$	373	$[h^5-1,3-C_5H_3(CN)_2]Mn(CO)_3$	—	H_{-2}	5.82	—	Calculated δ values: 5.87 and 5.39 respectively	1013
				H_{-4}, H_{-5}	5.37	—		
$C_{12}H_{12}MnNO_4$	374	$[h^5-C_5H_3-1-(NHCOCH_3)-3-(CH_2CH_3)]Mn(CO)_3$	—	H_{-2}	4.35	—	—	1013
				H_{-4}	5.07	—		
				H_{-5}	4.94	—		
$C_{10}H_7MnO_4$	375	$(h^5-C_5H_4 \cdot COCH_3)Mn(CO)_3$	CCl_4	H_{-2}, H_{-5}	5.34	—	—	879
				H_{-3}, H_{-4}	4.79	—		
				H_{-2}, H_{-5}	5.43	—	T 32°	7
				H_{-3}, H_{-4}	4.85	—		
			$(CD_3)_2SO$	H_{-2}, H_{-5}	5.74t	—	100 MHz	872
				H_{-3}, H_{-4}	5.16t	—		
$C_{10}H_4F_3MnO_4$	376	$(h^5-C_5H_4 \cdot COCF_3)Mn(CO)_3$	CCl_4	H_{-2}, H_{-5}	5.71	—	—	879
				H_{-3}, H_{-4}	5.11	—		
$C_{10}H_6BrMnO_4$	377	$(h^5-C_5H_4 \cdot COCH_2Br)Mn(CO)_3$	CCl_4	H_{-2}, H_{-5}	5.44	—	—	880
				H_{-3}, H_{-4}	4.78	—		
$C_{10}H_6IMnO_4$	378	$(h^5-C_5H_4 \cdot COCH_2I)Mn(CO)_3$	CCl_4	H_{-2}, H_{-5}	5.38	—	—	880
				H_{-3}, H_{-4}	4.78	—		
$C_{10}H_6BrMnO_4$	379	$[h^5-1,2-C_5H_3(Br)COCH_3]Mn(CO)_3$	$CDCl_3$	H	5.36,	—	—	873
					5.03b,	—		
					4.79	—		
				H'	2.49s	—		

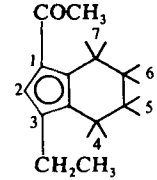
$C_{10}H_6BrMnO_4$	380	$[h^5-1,3-C_5H_3(Br)COCH_3]-$ $Mn(CO)_3$	$CDCl_3$	H	5.60, 5.36, 5.06	— — —	—	873
				H'	2.27s	—		
$C_{10}H_6ClMnO_4$	381	$[h^5-1,2-C_5H_3(Cl)COCH_3]-$ $Mn(CO)_3$	$CDCl_3$	H	5.34, 5.03, 4.76	— — —	—	873
				H'	2.51s	—		
$C_{10}H_6ClMnO_4$	382	$[h^5-1,3-C_5H_3(Cl)COCH_3]-$ $Mn(CO)_3$	$CDCl_3$	H	5.56, 5.36, 5.03	— — —	—	873
				H'	2.29s	—		
$C_{10}H_6FMnO_4$	383	$[h^5-1,3-C_5H_3(F)COCH_3]Mn(CO)_3$	$(CDCl_3)$	H	5.31, 5.18, 4.89	— — —	—	873
				H'	2.26s	—		
$C_{10}H_6IMnO_4$	384	$[h^5-1,3-C_5H_3(I)COCH_3]Mn(CO)_3$	$CDCl_3$	H	5.65, 5.32, 5.08	— — —	—	873
				H'	2.29s	—		
$C_{10}H_5I_2MnO_4$	385	$[h^5-C_4H_2-2,3(I)_2-1(COCH_3)]-$ $Mn(CO)_3$	$CDCl_3$	H	5.47d, 5.25d	— —	—	873
				H'	2.45s	—		
$C_{10}H_5I_2MnO_4$	386	$[h^5-C_4H_2-3,4(I)_2-1(COCH_3)]-$ $Mn(CO)_3$	$CDCl_3$	H	5.96s	—	—	873
				H'	2.29s	—		
$C_{11}H_9MnO_4$	387	$[h^5-1,2-C_5H_3(CH_3)COCH_3]-$ $Mn(CO)_3$	CCl_4	H	2.28	—	—	713
$C_{11}H_9MnO_4$	388	$[h^5-1,3-C_5H_3(CH_3)COCH_3]-$ $Mn(CO)_3$	CCl_4	H	2.02	—	—	713

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{12}H_{11}MnO_4$	389	$[h^5-C_5H_7-2,3(CH_3)_2-1(COCH_3)]-Mn(CO)_3$	$CDCl_3$	H_{-4}	4.63d	—	—	877
				H_{-5}	5.19d	—		
				H'	2.28s,	—		
					1.96s	—		
$C_{12}H_{11}MnO_4$	390	$[h^5-C_5H_7-2,4(CH_3)_2-1(COCH_3)]-Mn(CO)_3$	$CDCl_3$	H_3	4.63d	—	—	877
				H_{-5}	5.10d	—		
				H'	2.33s,	—		
					1.97s	—		
$C_{12}H_{11}MnO_4$	391	$[h^5-C_5H_7-2,5(CH_3)_2-1(COCH_3)]-Mn(CO)_3$	$CDCl_3$	H	4.52s	—	—	877
				H'	2.21s	—		
				H''	2.45s	—		
$C_{12}H_{11}MnO_4$	392	$[h^5-C_5H_7-3,4(CH_3)_2-1(COCH_3)]-Mn(CO)_3$	$CDCl_3$	H	5.26s	—	—	877
				H'	1.99s	—		
				H''	2.28s	—		
$C_{14}H_{13}MnO_6$	393	$[h^5-1,2-C_5H_3(CH_3)COCH_2CH_2-CO_2CH_3]Mn(CO)_3$	CCl_4	H	5.50,	—	—	881
					4.84	—		
				H'	2.29	—		
$C_{14}H_{13}MnO_6$	394	$[h^5-1,3-C_5H_3(CH_3)COCH_2CH_2-CO_2CH_3]Mn(CO)_3$	CCl_4	H	5.50,	—	—	881
					4.84	—		
				H'	2.06	—		

$C_{12}H_{11}MnO_4$	395	$[h^5-1,2-C_5H_3(CH_2CH_3)-COCH_3']Mn(CO)_3$	$CDCl_3$	H	5.30, 4.77, 4.66	— — —	—	873
				H'	2.7m	—		
				H''	1.17t	—		
				H'''	2.31s	—		
$C_{12}H_{11}MnO_4$	396	$[h^5-1,3-C_5H_3(CH_2CH_3)-COCH_3'']Mn(CO)_3$	$CDCl_3$	H	5.35, 5.30, 4.76	— — —	—	873
				H'	2.4m	—		
				H''	1.18t	—		
				H'''	2.28s	—		
$C_{14}H_{15}MnO_4$	397	$[h^5-C_5H_2-2,4(CH_2CH_3)_2-1-(COCH_3'')]Mn(CO)_3$	$CDCl_3$	H ₋₃	4.70d	—	—	877
				H ₋₅	5.15d	—		
				H'	2.3m, 2.7m	— —		
				H''	1.16t	—		
				H'''	2.32s	—		
$C_{14}H_{15}MnO_4$	398	$[h^5-C_5H_2-3,4(CH_2CH_3)_2-1-(COCH_3''')]Mn(CO)_3$	$CDCl_3$	H	5.28s	—	—	877
				H'	2.3m	—		
				H''	1.17t	—		
				H'''	2.27s	—		
$C_{13}H_{13}MnO_4$	399	$\{h^5-C_5H_3-2[CH'(CH_3)]-1-(COCH_3''')\}Mn(CO)_3$	$CDCl_3$	H ₋₃	4.60	—	—	877
				H ₋₄	4.83	—		
				H ₋₅	5.32	—		
				H'	3.32m	—		
				H''	1.17, 1.19	— —		
				H'''	2.33s	—		

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{13}H_{13}MnO_4$	400	$\{h^5-C_5H_3-3[CH'(CH_3)_2]-1-(COCH_3'')\}Mn(CO)_3$	$CDCl_3$	H_{-2}, H_{-5} 5.32 H_{-4} 4.80 H' 2.61m H'' 1.19d H''' 2.29s	— — — — —	—	877
$C_{14}H_{15}MnO_4$	401	$\{h^5-C_5H_3-3[C(CH_3)_3]-1-(COCH_3'')\}Mn(CO)_3$	$CDCl_3$	H_{-2} 5.24 H_{-4} 4.91 H_{-5} 5.42 H' 1.23s H'' 2.30	— — — — —	—	877
$C_{18}H_{23}MnO_4$	402	$\{h^5-C_5H_3-2,4[C(CH_3)_3]_2-1-(COCH_3'')\}Mn(CO)_3$	$CDCl_3$	H_{-3} 5.02d H_{-5} 5.17d H' 1.29s, 1.22s H'' 2.32s	— — — — —	—	877
$C_{16}H_{17}MnO_4$	403	$[h^5-C_9H_9(CH_2CH_3)COCH_3'']Mn(CO)_3$	$CDCl_3$	H_{-2} 5.16s H_{-4} 2.4m H_{-5}, H_{-6} 1.8m H_{-7} 2.8m H' 2.32q H'' 1.17t H''' 2.28s	— — — — — — —	$C_9H_9(CH_2CH_3)COCH_3 =$ 	877
$C_{17}H_{13}MnO_4$	404	$[h^5-1,3-C_5H_3(CH_2Ph)-COCH_3'']Mn(CO)_3$	$CDCl_3$	H 5.35, 5.23, 4.83 H' 3.61s H'' 2.42s	— — — — —	—	877

$C_{19}H_{15}MnO_5$	405	$[h^5-1,2-C_5H_3(p-CH_2C_6H_4-COCH_3)COCH_3'']Mn(CO)_3$	$CDCl_3$	H	5.34t, 4.69d	—	—	877
				H'	4.07q	—		
				H''	2.58s	—		
				H'''	2.33s	—		
$C_{19}H_{15}MnO_5$	406	$[h^5-1,3-C_5H_3(p-CH_2C_6H_4-COCH_3)COCH_3'']Mn(CO)_3$	$CDCl_3$	H	5.38, 5.24, 4.85	—	—	877
				H'	3.69s	—		
				H''	2.59s	—		
				H'''	2.27s	—		
$C_{17}H_{13}MnO_4$	407	$[h^5-1,2-C_5H_3(CH_2CH_3)COPh]Mn(CO)_3$	$CDCl_3$	H	5.14, 4.86, 4.63	—	—	877
				H'	2.8m	—		
				H''	1.16t	—		
$C_{17}H_{13}MnO_4$	408	$[h^5-C_5H_3-3(CH_2CH_3)-1(COPh)]Mn(CO)_3$	$CDCl_3$	H_{-2}, H_{-5}	5.39d	—	—	877
				H_{-4}	4.80t	—		
				H'	2.38m	—		
				H''	1.18t	—		
$C_{22}H_{15}MnO_4$	409	$[h^5-1,2-C_5H_3(CH_2Ph)COPh]Mn(CO)_3$	$CDCl_3$	H	5.17, 4.73, 4.62	—	—	877
				H'	4.11q	—		
$C_{22}H_{15}MnO_4$	410	$[h^5-C_5H_3-3(CH_2Ph)-(COPh)]Mn(CO)_3$	$CDCl_3$	H_{-2}, H_{-5}	5.37d	—	—	877
				H_{-4}	4.85t	—		
				H'	3.63s	—		
$C_{11}H_8ClMnO_4$	411	$[h^5-1,3-C_5H_3(CH_2CH_3)COCl]Mn(CO)_3$	$CDCl_3$	H	5.54, 5.47, 4.88	—	—	873
				H'	2.4m	—		
				H''	1.19t	—		

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_9H_6MnNO_4$	412	$(h^5-C_5H_4 \cdot CONH_2)Mn(CO)_3$	$(CD_3)_2SO$	H_{-2}, H_{-5} 5.64t H_{-3}, H_{-4} 5.01t	— —	100 MHz	872
$C_9H_5MnO_5$	413	$(h^5-C_5H_4 \cdot CO_2H)Mn(CO)_3$	$(CD_3)_2SO$	H_{-2}, H_{-5} 5.58t H_{-3}, H_{-4} 5.11t	— —	100 MHz	872
$C_{11}H_9MnO_5$	414	$[h^5-1,2-C_5H_3(CH_3)CO_2CH_3] \cdot Mn(CO)_3$	CCl_4	H 5.27m, 4.62m	— —	—	713
$C_{11}H_9MnO_5$	415	$[h^5-1,3-C_5H_3(CH_3)CO_2CH_3] \cdot Mn(CO)_3$	CCl_4	H 5.29m, 4.61m H' 2.01	— — —	—	713
$C_{16}H_{17}MnO_6$	416	$\{h^5-C_5H_3-1-(CH_3)-3-[COCH_2C-(CH_3)_2CO_2CH_3]\}Mn(CO)_3$	$CDCl_3$	H_{-2} 5.37q H_{-4} 5.30t H_{-5} 4.73t H' 2.87 H'' 1.28	— — — — —	—	978
$C_{15}H_{15}MnO_6$	417	$\{h^5-C_5H_4COC(CH_3)_2CH_2^*CO_2CH_3\}Mn(CO)_3$	$CDCl_3$	H_{-2}, H_{-5} 5.43t H_{-3}, H_{-4} 4.79t H' 1.38 H'' 2.65	— — — —	—	978
$C_{16}H_{17}MnO_6$	418	$\{h^5-C_5H_3-1-(CH_3)-2-[COC-(CH_3)_2CH_2^*CO_2CH_3]\}Mn(CO)_3$	$CDCl_3$	H_{-3} 5.38q H_{-4}, H_{-5} 4.68m H' 1.34 1.38 H'' 2.73	— — — — —	—	978

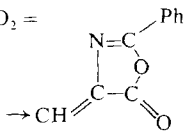
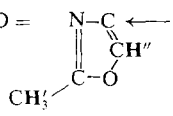
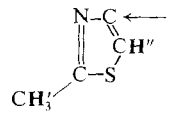
$C_{15}H_{15}MnO_6$	419	$\{h^5-C_5H_5-1-(CH_3)_3-3-[COC-(CH_3)_2CH_2CO_2H]\}Mn(CO)_3$	$CDCl_3$	H_{-2}	5.30m	—	—	978
				H_{-4}	5.30m	—		
				H_{-5}	4.65m	—		
				H'	1.38	—		
				H''	2.63	—		
$C_{12}H_{11}MnO_5$	420	$[h^5-C_5H_5-1-(CH_2CH_2'')-2-(CO_2CH_3')]Mn(CO)_3$	$CDCl_3$	H_{-3}	5.31t	—	Hexamethyldisiloxane reference at 100 MHz	980
				H_{-4}, H_{-5}	4.61d	—		
				H'	2.72m	—		
				H''	1.26s	—		
				H'''	3.74s	—		
$C_{12}H_{11}MnO_5$	421	$[h^5-C_5H_5-1-(CH_2CH_3')-3-(CO_2CH_3'')]Mn(CO)_3$	$CDCl_3$	H_{-2}	5.32	—	Hexamethyldisiloxane reference at 100 MHz	980
				H_{-4}	5.32	—		873
				H_{-5}	4.69	—		
				H'	1.16	—		
				H''	3.79s	—		
$C_{11}H_{11}MnO_3S$	422	$[h^5-1,2-C_5H_3(CH_2CH_3)SCH_3']Mn(CO)_3$	$CDCl_3$	H	4.85, 4.68,	—	—	976
					4.53	—		
				H'	2.33	—		
$C_{11}H_{11}MnO_3S$	423	$[h^5-1,3-C_5H_3(CH_2CH_3)SCH_3']Mn(CO)_3$	$CDCl_3$	H	4.74, 4.58	—	—	976
				H'	2.34	—		
$C_8H_6MnNO_3$	424	$(h^5-C_5H_4NH_2')Mn(CO)_3$	—	H	4.58t,	—	—	882
					4.32t	—		
				H'	3.17b	—		
$C_9H_8MnNO_3$	425	$[h^5-1,2-C_5H_3(CH_3)NH_2']Mn(CO)_3$	CCl_4	H	4.43,	—	—	876
					4.34,	—		
					4.20	—		
				H'	1.93	—		
				H''	2.99	—		

TABLE V—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_9H_8MnNO_3$	426	$[h^5-1,3-C_5H_3(CH_3)NH_2']\text{-Mn(CO)}_3$	CCl_4	H	4.30,	—	—	876
					4.18,	—		
					4.08	—		
				H'	1.93	—		
				H''	2.95	—		
$C_{10}H_{10}MnNO_3$	427	$[h^5-1,3-C_5H_3(CH_2CH''')NH_2'']\text{-Mn(CO)}_3$	$CDCl_3$	H	4.37,	—	—	873
					4.24,	—		
					4.12	—		
				H'	2.26q	—		
				H''	1.09t	—		
				H'''	3.0b	—		
$C_{10}H_{10}MnNO_4$	428	$\{h^5-1,2-C_5H_3[CH(OH)CH_3']\text{-NH}_2''\}\text{Mn(CO)}_3$	$CDCl_3$	H	4.56,	—	—	873
					4.39,	—		
					4.20	—		
				H'	1.44d	—		
				H''	3.7b	—		
$C_{10}H_{10}MnNO_4$	429	$\{h^5-1,3-C_5H_3[CH(OH)CH_3']\text{-NH}_2''\}\text{Mn(CO)}_3$	$CDCl_3$	H	4.59	—	—	873
				H'	4.35	—		
				H''	4.17	—		
$C_{10}H_8MnNO_4$	430	$[h^5-1,2-C_5H_3(COCH_3)NH_2']\text{-Mn(CO)}_3$	$CDCl_3$	H	4.99,	—	—	873
					4.62,	—		
					4.36	—		
				H'	2.31s	—		
				H''	4.88b	—		

$C_{10}H_8MnNO_4$	431	$[h^5-1,3-C_5H_3(COCH_3)NH_2^-]Mn(CO)_3$	$CDCl_3$	H	5.29, 4.82, 4.47	— — —	—	873
				H'	2.27s	—		
				H''	3.46b	—		
$C_{10}H_8MnNO_4$	432	$(h^5-C_5H_4NH'COCH_3^-)Mn(CO)_3$	$CDCl_3$	H	5.11t, 4.60t	— —	—	873
				H'	7.53b	—		
				H''	2.11s	—		
			$(CD_3)_2SO$	H ₋₂ , H ₋₃ H ₋₃ , H ₋₄	5.14s 4.78s	— —	100 MHz	872
$C_{12}H_{10}MnNO_5$	433	$[h^5-1,2-C_5H_3(COCH_3)NH''-COCH_3^-]Mn(CO)_3$	$CDCl_3$	H	5.92, 5.07, 4.73	— — —	—	873
				H'	2.39s	—		
				H''	10.4b	—		
				H'''	2.13s	—		
$C_{12}H_{10}MnNO_5$	434	$[h^5-1,3-C_5H_3(COCH_3)NH''-COCH_3^-]Mn(CO)_3$	$CDCl_3$	H	5.70t, 5.37m	— —	—	873
				H'	2.32s	—		
				H''	8.2b	—		
				H'''	2.13s	—		
$C_{16}H_{12}MnNO_5$	435	$(h^5-C_5H_4 \cdot NH'CO_2CH_2^+Ph^-)Mn(CO)_3$	$CDCl_3$	H	4.93t, 4.55t	— —	—	873
				H'	6.46b	—		
				H''	5.18s	—		
			$(CD_3)_2SO$	H ₋₂ , H ₋₃ H ₋₃ , H ₋₄	5.05s 4.82s	— —	—	872

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{16}H_8Mn_2O_6$	436	$(h^5\text{-}h^5\text{-}C_5H_4 \cdot C_5H_4)[Mn(CO)_3]_2$	$CDCl_3$	H 4.96, 4.74	—	Fulvalene hexacarbonyl dimanganese	883
$C_{18}H_{10}MnNO_5$	437	$(h^5\text{-}C_5H_4 \cdot C_{10}H_6NO_2)Mn(CO)_3$	$(CD_3)_2SO$	H ₋₂ , H ₋₅ 5.96t H ₋₃ , H ₋₄ 5.17t	— —	100 MHz $C_{10}H_6NO_2 =$ 	872
$C_{12}H_8MnO_4$	438	$(h^5\text{-}C_5H_4 \cdot C_4H_4NO)Mn(CO)_3$	CCl_4	H ₋₂ , H ₋₅ 4.73 H ₋₃ , H ₋₄ 5.11 H' 2.47 H'' 7.47	— — —	Reference hexamethyldisiloxane $C_4H_4NO =$ 	871
$C_{12}H_8MnNO_3S$	439	$(h^5\text{-}C_5H_4 \cdot C_4H_4NS)Mn(CO)_3$	CCl_4	H ₋₂ , H ₋₅ 4.73 H ₋₃ , H ₋₄ 5.25 H' 2.67 H'' 6.95	— — —	Reference hexamethyldisiloxane 	871

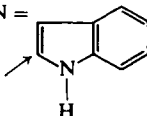
$C_{16}H_{10}MnNO_3$	440	$(h^5-C_5H_4 \cdot C_8H_6N)Mn(CO)_3$	Acetone	H	4.93 5.51	— —		871
$C_{26}H_{23}F_6^-$ $Mn_2O_{11}P$	441	$[h^5, h^5-C_5H_4C(CF_3)-C(CF_3)-O-P(OEt)_3]O$ $C_5H_4[Mn(CO)_3]_2$	—	^{19}F	-11.0	—	Low field from CF_3CO_2H	884
$C_8H_4ClHgMnO_3$	442	$(h^5-C_5H_4 \cdot HgCl)Mn(CO)_3$	$(CD_3)_2SO$	H _{-2, H} ₋₅ H _{-3, H} ₋₄	4.94t 5.02t	— —	—	872
$C_{16}H_9Mn_2O_8P$	443	$[h^5, h^5-C_5H_4P(O)(OH)C_5H_4]Mn(CO)_3]_2$	$(CD_3)_2SO$	H _{-2, H} ₋₅ H _{-3, H} ₋₄	5.52td 5.24t	— —	100 MHz	872
$C_{12}H_{15}MnO_3Si$	444	$[h^5-C_5H_4 \cdot CH_2Si(CH_3)_3]Mn(CO)_3$	—	H H' H''	4.41t, 4.20t 1.55 -0.03	— — —	—	250
$C_{11}H_{13}MnO_3Si$	445	$[h^5-C_5H_4 \cdot Si(CH_3)_3]Mn(CO)_3$	CS_2	H H'	4.67s 0.18	— —	—	208 250
$C_{18}H_{14}Mn_2O_6Si$	446	$[h^5, h^5-C_5H_4 \cdot Si(CH_3)_2C_5H_4]Mn(CO)_3]_2$	—	H H'	4.82s 0.51	— —	—	250
$C_{14}H_{21}MnO_3Si_2$	447	$\{h^5-C_5H_3[Si(CH_3)_3]_2\}Mn(CO)_3$	—	H H'	4.69s 0.18	— —	—	250
$C_{13}H_{19}MnO_3Si_2$	448	$[h^5-C_5H_4 \cdot Si(CH_3)_2Si(CH_3)_3]Mn(CO)_3$	—	H H' H''	4.79t, 4.73t 0.34 0.17	— — —	—	250

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{10}H_{10}MnNO_5S$	449	$[h^5-C_5H_4SO_2N(CH_3)_2]Mn(CO)_3$	$CDCl_3$	H_{-2}, H_{-5} 5.25t H_{-3}, H_{-4} 4.80t H' 2.75s	J 1.0 J 1.0 —	—	885
$C_8H_5MnO_5S$	450	$(h^5-C_5H_4 \cdot SO_2H)Mn(CO)_3$	$(CD_3)_2SO$	H_{-2}, H_{-5} 5.45s H_{-3}, H_{-4} 5.05s	— —	100 MHz	872
$C_{16}H_8Mn_2O_6S_2$	451	$(h^5, h^5-C_5H_4 \cdot SS \cdot C_5H_4) \cdot [Mn(CO)_3]_2$	$(CD_3)_2SO$	H_{-2}, H_{-5} 5.37s H_{-3}, H_{-4} 5.05s	— —	100 MHz	872
$C_7H_4MnNO_3$	452	$(h^5-C_4H_4N)Mn(CO)_3$	CCl_4	H_{-2}, H_{-5} 6.1s H_{-3}, H_{-4} 5.2s	—	$C_4H_4N =$ 	886
$C_9H_8MnNO_3$	453	$[h^5-2,5-C_4H_2N(CH_3)_2]Mn(CO)_3$	CS_2	H_{-3}, H_{-4} 4.9 H' 2.14	—	(see above)	886
$C_9H_8MnNO_3$	454	$[h^5-2,4-C_4H_2N(CH_3)_2]Mn(CO)_3$	CCl_4	H_{-3} 4.87m H_{-5} 5.67m $CH'_3-\alpha$ 2.15s $CH'_3-\beta$ 1.97s	— — — —	$C_4H_4N =$ 	886
$C_{11}H_{12}MnNO_3$	455	$[h^5-2,3,4,5-C_4N(CH_3)_4]Mn(CO)_3$	—	$CH_3-\alpha$ 2.07s $CH_3-\beta$ 1.90s	— —	(See above)	886
$C_{10}H_8MnNO_4$	456	$[h^5-C_4H_2N-2(CH_3)-3(COCH'_3)] \cdot Mn(CO)_3$	CS_2	H_{-4} 5.54d H_{-5} 5.9d H' 2.28s H'' 2.41s	— — — —	(See above)	886

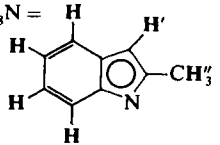
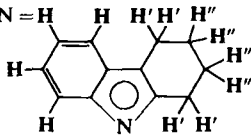
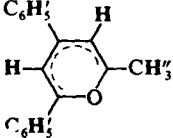
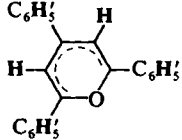
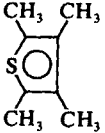
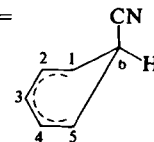
$C_{11}H_{10}MnNO_4$	457	$[h^5-C_4HN-2,4(CH_3)_2-3(COCH_3)]Mn(CO)_3$	CS_2	H_s $CH_3-\alpha$ $CH_3-\beta$ H''	5.72s 2.37s 2.15s 2.37s	— — — —	(See above)	886
$C_{12}H_8MnNO_3$	458	$(h^5-C_9H_8N)Mn(CO)_3$	CS_2	H H' H''	7.3m 5.5s 2.22s	— — —	$C_9H_8N =$ 	886
$C_{15}H_{12}MnNO_3$	459	$(h^5-C_{12}H_{12}N)Mn(CO)_3$	CS_2	H H' H''	$\sim 7.3m$ 2.7m 1.95	— — —	$C_{12}H_{12}N =$ 	886
$C_{14}H_7D_4MnO_4$	460	$\{h^5-CD_3CH=CH'=CD=C(C_6H_5^V)=O\}Mn(CO)_3$	$CDCl_3$	H H' H''	3.58d 5.12d 7.74-7.39	$J_{HH'} 13.2$ — —	100 MHz	857
$C_{14}H_{11}MnO_4$	461	$[CH_3CH=CH'=CH'''=C(C_6H_5^V)=O]Mn(CO)_3$	$CDCl_3$	H H' H'' H''' H^{IV}	1.93d 3.70 sext. 5.28q 5.82d 7.6m	— — — — —	—	856
$C_{15}H_{13}MnO_4$	462	$[CH_3CH_2CH'=CH'''=CH^{IV}=C(C_6H_5^V)=O]Mn(CO)_3$	$CDCl_3$	H H' H'' H''' H^{IV} H^V	1.16t 2.38, 2.07 3.68ddd 5.18dd 5.78d 7.67-7.40	$J^{HH'} 7.0$ $J^{H'H''} 7.0$ $J^{H'H'} 2.0$ $J^{H''H'''} 12.5$ $J^{H'''H^{IV}} 7.1$ — —	100 MHz	857

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{21}H_{15}MnO_4$	463	$(h^5-C_{18}H_{15}O)Mn(CO)_3$	CCl_4	H 5.44s, 4.72s H' 7.85m, 7.35m H'' 1.99s	— — — —	$C_{18}H_{15}O =$ 	829
$C_{26}H_{17}MnO_4$	464	$(h^5-C_{23}H_{17}O)Mn(CO)_3$	$CDCl_3$	H 5.69s H' 8.00m, 7.48s	— — —	$C_{23}H_{17}O =$ 	829
$[C_{11}H_{12}MnO_3S]^+$	465	$\{[h^5-C_4(CH_3)_4S]Mn(CO)_3\}^+$	$(CD_3)_2SO$	H 2.52, 2.43	— —	$C_4(CH_3)_4S =$ 	887
			$(CD_3)_2SO$	H 2.42, 2.36	— —	T 37° Isolated as the perchlorate	888
$C_9H_7MnO_3$	466	$(1,2,3,4,5-h^5-C_6H_7)Mn(CO)_3$	—	H _{-7exo} 1.56 H _{-7endo} 2.25	— —	—	955

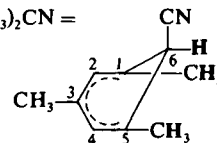
$C_{10}H_9MnO_3$	467	$[1,2,3,4,5-h^5-7-exo-C_6H_6-(CH_3)]Mn(CO)_3$	CCl_4	$H_{-7}endo$ H'	2.58 0.43d	—	—
$C_{10}H_6MnNO_3$	468	$(h^5-C_6H_6CN)Mn(CO)_3$	$CDCl_3$	H_{-1}, H_{-5} H_{-2}, H_{-4} H_{-3} H_{-6}	3.00dd* 5.05dd* 6.00t* 3.60t*	— — — —	—
$C_{13}H_{12}MnNO_3$	469	$[h^5-C_6H_3(CH_3)_3CN]Mn(CO)_3$	$CDCl_3$	H_{-2}, H_{-4} H_{-6} 1,5- CH_3 3- CH_3	4.86s 3.39s 1.73s 2.55s	— — — —	—
$C_{14}H_{14}MnNO_3$	470	$[h^5-C_6H_2(CH_3)_4CN]Mn(CO)_3$	$CDCl_3$	H_{-5} H_{-6} 1- CH_3 2,4- CH_3 3- CH_3	2.86d* 3.43d* 1.76s* 2.07s*, 2.03s* 2.52s*	— — — — — —	—
$C_{10}H_7MnO_3$	471	$(h^5-C_7H_7)Mn(CO)_3$	$(CD_3)_2CO$	H_{-1}, H_{-5} H_{-2}, H_{-4} H_{-3} H_{-6}, H_{-7}	3.53 5.42 7.10 4.70	— — — —	—

$C_6H_6CN =$ 889

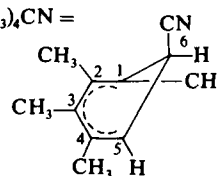


* Reviewer's assignment

$C_6H_3(CH_3)_2CN =$ 889

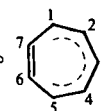


$C_6H_2(CH_3)_4CN =$ 889



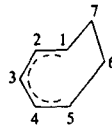
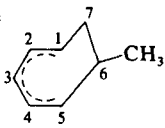
* Reviewer's assignment

$C_7H_7 =$ 438



At T 88° single line at 4.85

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{10}H_9MnO_3$	472	$(h^5-C_7H_9)Mn(CO)_3$	CS_2	H_{-1}, H_{-5}	3.85	$C_7H_9 =$ 	890
				H_{-2}, H_{-4}	5.09q		
				H_{-3}	5.81t		
				H_{-6}, H_{-7}	1.85m, 2.45m		
				H_{-1}, H_{-5}	3.73	$J_{13} = J_{35} - 1.4$ $J_{1,2} = J_{4,5} 9.5$	891
				H_{-2}, H_{-4}	5.01	$J_{2,3} = J_{3,4} 5.8$ $J_{2,4} - 0.4$	
				H_{-3}	5.74	—	
				H_{-6}, H_{-7}	1.75, 2.16	—	
$C_{11}H_{11}MnO_3$	473	$(h^5-C_7H_8CH_3)Mn(CO)_3$	CS_2	H_{-1}	3.55m	$C_7H_8CH_3 =$ 	890
				H_{-2}	5.32q		
				H_{-3}	5.8t		
				H_{-4}	4.78q		
				H_{-5}	3.86d		
				H_{-6}	3.20m		
				$H_{-7} \text{ endo}$	1.98 sext.		
				$H_{-7} \text{ exo}$	0.65 sept.		
				CH_3	0.98		

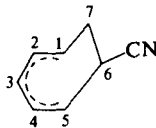
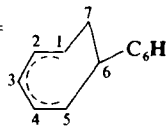
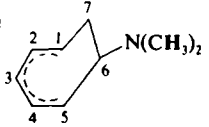
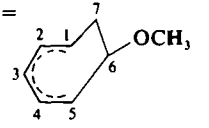
			CS ₂	H_{-1} 3.51 $J_{1,2}$ 8.5; $J_{1,3}$ -2.0; $J_{1,7}$ 4.0, 8.5 H_{-2} 5.24 $J_{2,3}$ 5.6; $J_{2,4}$ -0.2; $J_{2,7}$ -0.8, -0.7 H_{-3} 5.73 $J_{3,4}$ 7.0; $J_{3,5}$ -1.0 H_{-4} 4.71 $J_{4,5}$ 10.0 H_{-5} 3.81 $J_{5,6}$ 4.0; $J_{5,8}$ -2.0 H_{-6} 3.12 $J_{6,7}$ 9.0, 9.0 H_{-7} <i>endo</i> 1.9 $J_{7,7}$ -13.5 H_{-7} <i>exo</i> 0.59 CH_3 0.84 J 6.4	
C ₁₁ H ₈ MnNO ₃	474	(<i>h</i> ⁵ -C ₇ H ₈ CN)Mn(CO) ₃	CDCl ₃	H_{-1}, H_{-5} } 3.40-4.05m — H_{-6} } H_{-2}, H_{-4} 5.32m — H_{-3} 6.08t — H_{-7} <i>endo</i> 2.58m — H_{-7} <i>exo</i> 1.68m —	C ₇ H ₈ CN = 
C ₁₆ H ₁₃ MnO ₃	475	(<i>h</i> ⁵ -C ₇ H ₈ ·C ₆ H ₅)Mn(CO) ₃	CS ₂	H_{-1}, H_{-5} } 4.0m — H_{-6} } H_{-2} 5.44dd — H_{-3} 5.82t — H_{-4} 5.0dd — H_{-7} <i>endo</i> 2.10q — H_{-7} <i>exo</i> 0.90m — H 7.12s —	C ₇ H ₈ ·C ₆ H ₅ = 

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{12}H_{14}MnNO_3$	476	$[h^5-C_7H_8 \cdot N(CH_3)_2]Mn(CO)_3$	$CDCl_3$	H_{-1}, H_{-5} } 3.20–4.20m — H_{-6} } H_{-2}, H_{-4} } 4.95–5.10m — H_{-3} } 5.85t — $H_{-7 \text{ endo}}$ } 1.80m — $H_{-7 \text{ exo}}$ } 0.70m — H } 2.15s —		$C_7H_8N(CH_3)_2$ 	890
$C_{11}H_{11}MnO_4$	477	$(h^5-C_7H_8 \cdot OCH_3)Mn(CO)_3$	CS_2	H_{-1} } 3.20m — H_{-2} } 5.40q — H_{-3} } 5.80t — H_{-4} } 4.95q — H_{-5} } 3.83m — H_{-6} } 4.20 sext. — $H_{-7 \text{ endo}}$ } 2.10 sext. — $H_{-7 \text{ exo}}$ } 0.62 sept. — H } 3.20s —		$C_7H_8 \cdot OCH_3 =$ 	890
			CS_2	H_{-1} } 3.11 H_{-2} } 5.30 H_{-3} } 5.71 H_{-4} } 4.88	$J_{1,2}$ 8.5; $J_{1,3}$ -2.0; $J_{1,7}$ 4.0, 8.5 $J_{2,3}$ 5.6; $J_{2,4}$ -0.2; $J_{2,7}$ -0.8, -0.7 $J_{3,4}$ 7.0; $J_{3,5}$ -1.0 $J_{4,5}$ 10.0		891

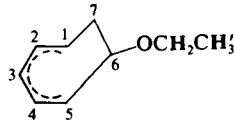
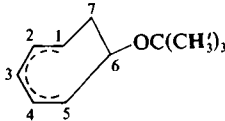
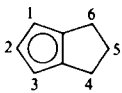
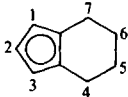
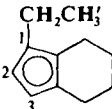
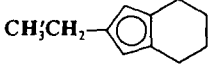
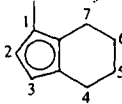
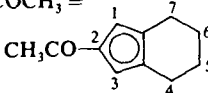
				H_{-5}	3.78	$J_{5,6} 4.0;$ $J_{5,8} -2.0$		
				H_{-6}	4.1	$J_{6,7} 9.0, 9.0$		
				$H_{-7 \text{ endo}}$	2.06	$J_{7,7'} -13.5$		
				$H_{-7 \text{ exo}}$	0.61			
$C_{12}H_{13}MnO_4$	478	$(h^5-C_7H_8 \cdot OCH_2CH_3)Mn(CO)_3$	$CDCl_3$	H_{-1}, H	3.35m	—	$C_7H_8 \cdot OCH_2CH_3 =$	890
				H_{-2}	5.40q	—		
				H_{-3}	5.78t	—		
				H_{-4}	4.95q	—		
				H_{-5}	3.88d	—		
				H_{-6}	4.30 sext.	—		
				$H_{-7 \text{ endo}}$	2.10m	—		
				$H_{-7 \text{ exo}}$	0.65m	—	100 MHz	
				H'	1.10	—		
$C_{14}H_{17}MnO_4$	479	$[h^5-C_7H_8 \cdot OC(CH_3)_3]Mn(CO)_3$	$CDCl_3$	H_{-1}	3.20m	—	$C_7H_8OC(CH_3)_3 =$	890
				H_{-2}	5.50t	—		
				H_{-3}	5.85t	—		
				H_{-4}	5.02tt	—		
				H_{-5}	3.88m	—		
				H_{-6}	4.42m	—		
				$H_{-7 \text{ endo}}$	2.00m	—		
				$H_{-7 \text{ exo}}$	1.00m	—		
				H'	1.30s	—		
					1.25s	—		
$C_{11}H_9MnO_3$	480	$(h^5-C_8H_9)Mn(CO)_3$	$CDCl_3$	H_{-1}, H_{-3}	4.40d	—	$C_8H_9 =$	877
				H_{-2}	4.77t	—		
				H_{-4}, H_{-5}	2.35			
				H_{-6}				

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{12}H_{11}MnO_3$	481	$(h^5-C_9H_{11})Mn(CO)_3$	$CDCl_3$	H_{-1}, H_{-3} 4.43d H_{-2} 4.66t H_{-4}, H_{-7} 2.4m H_{-5}, H_{-6} 1.7m	— — — —	$C_9H_{11} =$ 	877
$C_{14}H_{15}MnO_3$	482	$(h^5-C_9H_{10} \cdot CH_2CH_3)Mn(CO)_3$	$CDCl_3$	H_{-2} 4.59d H_{-3} 4.28d H 2.25q H' 1.10t	— — — —	$C_9H_{10}CH_2CH_3 =$ 	877
$C_{14}H_{15}MnO_3$	483	$(h^5-C_9H_{10}CH_2CH_3)Mn(CO)_3$	$CDCl_3$	H_{-1}, H_{-2} 4.35s H 2.26q H' 1.11t	— — —	$C_9H_{10}CH_2CH_3 =$ 	877
$C_{14}H_{13}MnO_4$	484	$(h^5-C_9H_{10}COCH_3)Mn(CO)_3$	$CDCl_3$	H_{-2} 5.23d H_{-3} 4.59d H_{-4} 2.4m H_{-5}, H_{-6} 1.7m H_{-7} 2.8m H 2.27s	— — — — — —	$C_9H_{10}COCH_3 =$ 	877
$C_{14}H_{13}MnO_4$	485	$(h^5-C_9H_{10}COCH_3)Mn(CO)_3$	$CDCl_3$	H_{-1}, H_{-3} 5.16s H_{-4}, H_{-7} 2.5m H_{-5}, H_{-6} 1.8m H 2.27s	— — — —	$C_9H_{10}COCH_3 =$ 	877

$C_{15}H_{15}MnO_4$	486	$(h^5-C_{12}H_{15}O)Mn(CO)_3$	—	H	4.79	—
				H'	4.42	—
				H''	2.20	—
				H'''	1.12,	—
					1.20	—
$C_{15}H_{15}MnO_4$	487	$(h^5-C_{12}H_{15}O)Mn(CO)_3$	—	H	4.95	—
				H'	4.50	—
				H''	1.99	—
				H'''	1.19,	—
					1.09	—
$C_{15}H_{15}MnO_4$	488	$(h^5-C_{12}H_{15}O)Mn(CO)_3$	—	H	5.03	—
				H'	4.92	—
				H''	1.95	—
				H'''	1.21,	—
					1.10	—
$C_{15}H_{15}MnO_4$	489	$(h^5-C_{12}H_{15}O)Mn(CO)_3$	—	H	4.65	—
				H'	4.53	—
				H''	2.24	—
				H'''	1.15,	—
					0.98	—
$C_{15}H_{15}MnO_4$	490	$(h^5-C_{12}H_{15}O)Mn(CO)_3$	—	H	5.09	—
				H'	4.59	—
				H''	1.99	—
				H'''	1.14,	—
					0.99	—

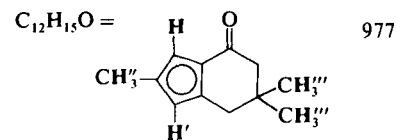
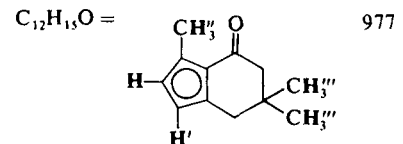
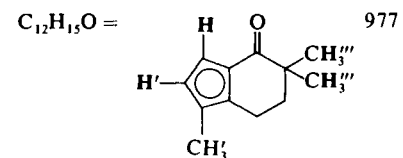
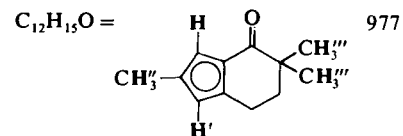
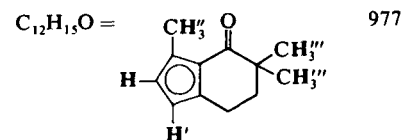
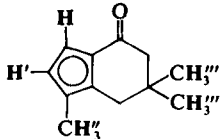
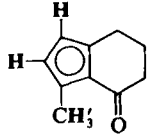
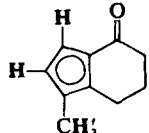
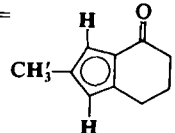


TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{15}H_{15}MnO_4$	491	$(h^5-C_{12}H_{15}O)Mn(CO)_3$	—	H	5.23	—	$C_{12}H_{15}O =$ 	977
				H'	4.69	—		
				H''	1.98	—		
				H'''	1.18, 0.98	—		
$C_{13}H_{11}MnO_4$	492	$[h^5-C_9H_8(CH_3)O]Mn(CO)_3$	CCl_4	H	4.86, 4.53	—	$C_9H_8(CH_3)O =$ 	881
				H'	2.28	—		
$C_{13}H_{11}MnO_4$	493	$[h^5-C_9H_8(CH_3)O]Mn(CO)_3$	CCl_4	H	5.07, 4.99	—	$C_9H_8(CH_3)O =$ 	881
				H'	2.06	—		
$C_{13}H_{11}MnO_4$	494	$[h^5-C_9H_8(CH_3)O]Mn(CO)_3$	CCl_4	H	5.08, 4.57	—	$C_9H_8(CH_3)O =$ 	881
				H'	2.07	—		

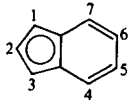
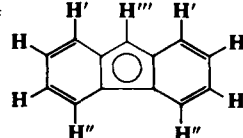
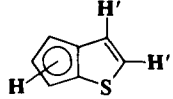
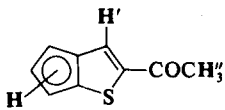
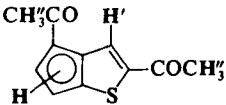
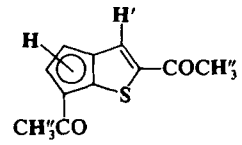
$C_{12}H_7MnO_3$	495	$(h^5-C_9H_7)Mn(CO)_3$	$CDCl_3$	H_{-1}, H_{-3}	5.04	—	60 and 100 MHz	892
				H_{-2}	4.82	—	$C_9H_7 =$	
				H_{-4}, H_{-7}	6.96	—		
				H_{-5}, H_{-6}	7.19	—		
$C_{16}H_9MnO_3$	496	$(h^5-C_{13}H_9)Mn(CO)_3$	$CDCl_3$	H	~ 7.2	—	60 and 100 MHz	892
				H'	~ 7.4	—	$C_{13}H_9 =$	
				H''	~ 8.0	—		
				H'''	5.56s	—		
$C_7H_4MnNO_3$	497	$(h^5-C_4H_4N)Mn(CO)_3$	CCl_4	H_a	6.07	—	100 MHz	969
				H_b	5.21	—		
$C_{10}H_5MnO_3S$	498	$(h^5-C_7H_5S)Mn(CO)_3$	$CDCl_3$	H	5.16, 5.02, 4.83	—	$C_7H_5S =$	976
				H'	7.25d, 6.89d	J 5.5 J 5.5		
$C_{12}H_7MnO_4S$	499	$(h^5-C_9H_7OS)Mn(CO)_3$	$CDCl_3$	H	5.16, 5.12, 4.94	—	$C_9H_7OS =$	976
				H'	7.58	—		
				H''	2.53	—		
$C_{14}H_9MnO_3S$	500	$(h^5-C_{11}H_9O_2S)Mn(CO)_3$	$CDCl_3$	H	5.52d, 5.35d	J 3 J 3	$C_{11}H_9O_2S =$	976
				H'	8.09	—		
				H''	2.61, 2.43	—		

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{14}H_9MnO_5S$	501	$(h^5-C_{11}H_9O_2S)Mn(CO)_3$	$CDCl_3$	H	5.48d, 5.31d	J 3 J 3	$C_{11}H_9O_2S$	976
				H'	7.64	—		
				H''	2.58, 2.57	— —		
(6) <i>HEXAHAPTO LIGANDS</i>								
$C_{12}H_{12}MnNO_2$	502	$[h^6-1,3,5-C_6H_3(CH_3)_3]-Mn(CN)(CO)_2$	$(CD_3)_2CO$	H	5.6bs (5.4)*	—	—	893 889
				H'	2.3bs	—		
$[C_{12}H_{12}MnO_3]^+$	503	$\{[h^6-1,3,5-C_6H_3(CH_3)_3]Mn(CO)_3\}^+ (CD_3)_2CO$		H	6.4s	—	Isolated as PF_6^- salt	893
				H'	2.5s	—		
(7) <i>MIXED LIGANDS</i>								
(a) <i>Monohapto/dihapto ligands</i>								
$C_{25}H_{20}MnO_4P$	504	$[h^2-o-CH_2=CHC_6H_4P-(C_6H_5)_2]Mn(COCH_3)(CO)_3$	$CDCl_3$	H	3.85m, 3.23m, 2.78m	— — —	—	830
				H'	7.3m	—		
				H''	1.39s	—		
(b) <i>Monohapto/pentahapto ligands</i>								
$C_8H_8MnNO_3$	505	$(h^5-C_5H_5)Mn(COCH_3)(NO)(CO)$	CS_2	H	5.04s	—	—	129
				H'	2.57s	—		

$C_8H_8MnNO_4$	506	$(h^5-C_5H_5)Mn(CO_2CH_3)NO(CO)$	CS_2	H	5.10s	—	—	480
				H'	3.46s	—		129
				CS_2	H	5.24s		—
				H'	3.6s	—		
$C_8H_5DMnNO_2$	507	$(h^5-C_5H_5)Mn(CND)(CO)_2$	C_6H_6	H	4.08s	—	—	863
$C_8H_6MnNO_2$	508	$(h^5-C_5H_5)Mn(CNH)(CO)_2$	C_6D_6	H	4.17s	—	—	863
				H'	4.82b	—		
$[C_{13}H_{16}MnN_2O_2]^+$	509	$[(h^5-C_5H_5)Mn(CNC_6H_{11})(NO)(CO)]^+$	$(CD_3)_2CO$	H	5.88s	—	Hexafluorophosphate salt	337
				H'	4.28m,	—		
					2.13–1.52m	—		
$C_{10}H_{11}MnO_3$	510	$(h^5-C_5H_5)Mn[C(CH_3)_3OCH_3](CO)_2$	C_6H_6	H	4.37	—	—	33
				H'	2.33	—		
				H''	3.88	—		
$C_{15}H_{13}MnO_3$	511	$(h^5-C_5H_5)Mn[C(C_6H_5)_3OCH_3](CO)_2$	C_6H_6	H	4.20	—	—	33
				H'	6.89	—		
				H''	3.91	—		
$[C_{14}H_{10}MnO_3]^-$	512	$[(h^5-C_5H_5)Mn(COC_6H_5)(CO)_2]^-$	CH_2Cl_2	H	4.32	—	Isolated as the $[N(CH_3)_4]^+$ salt	33
				H'	7.12	—		
				H''	3.32	—		
<i>(c) Monohapto/hexahapto ligands</i>								
$[C_{14}H_{17}MnNO_2]^+$	513	$\{[h^6-1,3,5-C_6H_3(CH_3)_3]Mn-(CNCH_2CH_3)(CO)_2\}^+$	$(CD_3)_2CO$	H	6.0s	—	Isolated as the PF_6^- salt	893
				H'	2.4s	—		
				H''	4.0q	$J = 7$		
				H'''	1.4t	$J = 7$		
$[C_{31}H_{27}MnNO_2]^+$	514	$[h^6-1,3,5-C_6H_3(CH_3)_3]Mn-[CNC(C_6H_5)_3](CO)_2$	$(CD_3)_2CO$	H	6.3s	—	Isolated as the PF_6^- salt	893
				H'	2.4s	—		
				H'''	7.4m	—		

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
<i>(d) Dihapto/pentahapto ligands</i>							
$C_{10}H_{11}MnO_2$	515	$(h^5-C_5H_5)(h^2-CH_2=CH'CH''_3)-Mn(CO)_2$	$CDCl_3$	H	4.45s	—	894
				H'	1.8–3.5 comp.		
				H''	1.50bd		
$C_{10}H_8MnNO_2$	516	$(h^5-C_5H_5)(h^2-CH_2=CH'CN)-Mn(CO)_2$	—	H	4.6	—	895 75
				H'	1.8–2.8		
$C_{13}H_{17}MnO_6$	517	$(h^5-C_5H_5)[h^2-C(OCH_3)_2=C(OCH_3)_2]Mn(CO)_2$	C_6D_6	H	4.28s	—	T 10° 279
				H'	3.43s		
$C_{12}H_{11}MnO_2$	518	$(h^5-C_5H_5)(h^2-C_5H_6)Mn(CO)_2$	$(CD_3)_2CO$	H	4.61s	—	C ₅ H ₆ = cyclopentadiene 896
				H'	2.95		
$C_{19}H_{16}Mn_2O_4$	519	$[(h^5-C_5H_5)Mn(CO)_2]_2(h^2-C_5H_6)$	$(CD_3)_2CO$	H	4.61s	—	C ₅ H ₆ = cyclopentadiene 896
				H'	2.90		
$C_{12}H_{13}MnO_2$	520	$(h^5-C_5H_5)Mn(h^2-C_5H_8)(CO)_2$	$(CD_3)_2CO$	H	4.61	—	C ₅ H ₈ = Cyclopent-1-ene 974
				H'_{-1}, H'_{-2}	2.71		
$C_{14}H_{15}MnO_2$	521	$(h^5-C_5H_5)Mn(h^2-C_7H_{10})(CO)_2$	$(CD_3)_2CO$	H	4.60	—	C ₇ H ₁₀ = Norbornene * Olefinic protons 974
				H'	3.51*		
$C_{14}H_{13}MnO_2$	522	$(h^5-C_5H_5)Mn(h^2-C_7H_8)(CO)_2$	$(CD_3)_2CO$	H	4.64	—	C ₇ H ₈ = Norbornadiene * Olefinic protons 974
				H'	4.16*		

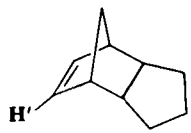
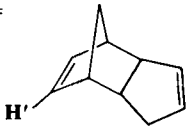
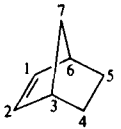
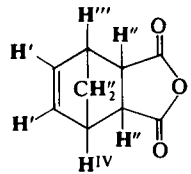
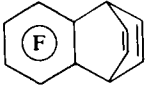
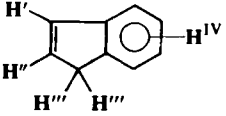
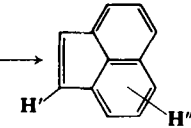
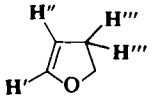
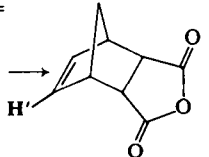
$C_{17}H_{19}MnO_2$	523	$(h^5-C_5H_5)Mn(h^2-C_{10}H_{14})(CO)_2$	$(CD_3)_2CO$	H H'	4.63 3.89*	— —	$C_{10}H_{14} =$	974
								
$C_{17}H_{17}MnO_2$	524	$(h^5-C_5H_5)Mn(h^2-C_{10}H_{12})(CO)_2$	$(CD_3)_2CO$	H H'	4.56 3.6	— —	$C_{10}H_{12} =$	974
								
$C_{14}H_{15}MnO_2$	525	$(h^5-C_5H_5)(h^2-C_7H_{10})Mn(CO)_2$	$CDCl_3$	H H ₋₁ , H ₋₂ H ₋₃ H ₋₄ , H ₋₅ H ₋₆ H ₋₇	4.46 3.39s -0.25d 1.33d 0.28d 2.55s	— — — — — —	$C_7H_{10} =$	894
								
$C_{16}H_{13}MnO_5$	526	$(h^5-C_5H_5)(h^2-C_9H_8O_3)Mn(CO)_2$	$CDCl_3$	H H' H'' H''' H ^{IV}	4.57s 3.20s 3.55bs 0.69d 0.15d	— — — — —	$C_9H_8O_3 =$	894
								
$C_{19}H_{11}F_4MnO_2$	527	$(h^5-C_5H_5)(h^2-C_{12}H_6F_4)Mn(CO)_2$	—	H H'	5.46 3.85, 5.20, 5.82	— — — —	$C_{12}H_6F_4 =$	897
								

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{16}H_{13}MnO_2$	528	$(h^5-C_5H_5)Mn(h^2-C_9H_8)(CO)_2$	$(CD_3)_2CO$	H	4.70	—	$C_9H_8 =$ 	975
				H'	4.59	—		974
				H''	5.15	—		
				H'''	3.51	—		
				H ^{IV}	7.8–6.9	—		
$C_{19}H_{13}MnO_2$	529	$(h^5-C_5H_5)Mn(h^2-C_{12}H_8)(CO)_2$	$(CD_3)_2CO$	H	4.80	—	$C_{12}H_8 =$ 	975
				H'	5.39	—		
				H''	7.82–7.0	—		
$C_{12}H_{11}MnO_3$	530	$(h^5-C_5H_5)Mn(h^2-C_5H_6O)(CO)_2$	$(CD_3)_2CO$	H	4.86	—	$C_5H_6O =$ Cyclopentenone	975 974
$C_{11}H_{11}MnO_3$	531	$(h^5-C_5H_5)Mn(h^2-C_4H_6O)(CO)_2$	$(CD_3)_2CO$	H	4.60s	—	$C_4H_6O =$ 	975
				H'	7.10	—		974
				H''	4.0–3.4	—		
				H'''	3.1–2.1m	—		
$C_{11}H_7MnO_5$	532	$(h^5-C_5H_5)Mn(h^2-C_4H_2O_3)(CO)_2$	$(CD_3)_2CO$	H	5.22s	—	$C_4H_2O_3 =$ maleic anhydride	975
				H'	4.41s	—		974
$C_{16}H_{13}MnO_5$	533	$(h^5-C_5H_5)Mn(h^2-C_9H_6O_3)(CO)_2$	$(CD_3)_2CO$	H	4.78	—	$C_9H_6O_3 =$ 	975
				H'	3.64	—		974

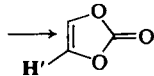
$C_{10}H_7MnO_5$	534	$(h^5-C_5H_5)Mn(h^2-C_3H_2O_3XC O)_2$	$(CD_3)_2CO$	H H'	4.91s 7.22s	— —	$C_3H_2O_3 =$		975 974
(8) COMPLEXES WITH TWO OR MORE MANGANESE ATOMS									
$C_{11}H_5Mn_2NO_9$	535	$Mn_2[C(CH_3)NH_2](CO)_9$	$(CD_3)_2CO$	H H'	2.93s 10.35m	— —	—		973
$C_{12}H_6Mn_2O_{10}$	536	$Mn_2[C(CH_3)OCH_3](CO)_9$	$(CD_3)_2CO$	H H'	3.22s 4.54s	— —	—		973
$C_{13}H_8Mn_2O_{10}$	537	$Mn_2[C(CH_3)OCH_2CH_3](CO)_9$	$(CD_3)_2CO$	H H' H''	3.13s 4.70q 1.53t	— — —	—		973
$C_{17}H_8Mn_2O_{10}$	538	$Mn_2[C(C_6H_5)OCH_3](CO)_9$	$(CD_3)_2CO$	H H	7.38m 4.12s	— —	—		973
$C_{18}H_{10}Mn_2O_{10}$	539	$Mn_2[C(C_6H_5)OCH_2CH_3](CO)_9$	$(CD_3)_2CO$	H H H	7.30m 4.35q 1.39t	— — —	—		973
$C_{16}H_8Mn_2O_6$	540	$(h^5, h^5-C_5H_4-C_5H_4)[Mn(CO)_3]_2$	$(CH_3)_2CO$	H	5.37t, 4.90t	—	Hexamethyldisiloxane as reference		979
$C_{10}H_6Mn_2O_8Se_2$	541	$[Mn(SeCH_3)(CO)_4]_2$	CCl_4	H	1.92	—	—		902
$C_{12}H_{10}Mn_2O_8Se_2$	542	$[Mn(SeCH_2CH_3)(CO)_4]_2$	CCl_4	H H'	2.72q 1.22t	J 7.5 J 7.5	—		902
$C_{14}H_{14}Mn_2O_8Se_2$	543	$[Mn(Se-n-C_3H_7)(CO)_4]_2$	CCl_4	H	2.7t, 1.5m, 1.0t	—	—		902
$[C_{11}H_3Mn_2O_{10}]^-$	544	$\{Mn(COCH_3)(CO)_4[Mn(CO)_5]\}^-$	THF	H	2.81s	—	—		1015
$C_{12}H_3Mn_3O_{12}$	545	$[Mn(H)(CO)_4]_3$	—		Not reported	—	—		900

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
(9) MISCELLANEOUS LIGANDS							
$C_{38}H_{30}^-$ $BrMnO_2P_2$	546	$Mn[P(C_6H_5)_3]_2(Br)(CO)_2$	CCl_4	H 7.29	—	100 MHz	870
$C_{29}H_{25}MnO_3P_2$	547	$Mn[PPh_2(CH_2)_2PPh_2](H)(CO)_3$	—	H -7.8	J_{PH} 45	—	898
$C_{39}H_{31}MnO_3P_2$	548	$Mn(PPh_3)_2(H)(CO)_3$	$CDCl_3$	H -7.4t	J_{PH} 29	100 MHz	899
$C_{29}H_{27}MnO_7P_2$	549	$Mn[P(OPh)_2CH_3]_2(H)(CO)_3$	—	H -8.0t	J_{PH} 45	—	898
				H' 1.9b	—		
$C_{39}H_{31}MnO_9P_2$	550	$Mn[P(OPh)_3]_2(H)(CO)_3$	—	H -8.13t	J_{PH} 50	—	705
				H -8.2t	J_{PH} 50	100 MHz	899
				H -8.0	J_{PH} 50	—	898
$C_{11}H_{12}I_xMnO_3S$	551	$[Mn(C_4(CH_3)_4S)(CO)_3]polyiodide$	$(CD_3)_2CO$	H 2.59,	—	T 37°	888
				2.64,	—		
				2.68	—		
$C_6HF_7MnO_4P$	552	$Mn[P(CF_3)_2F'](H)(CO)_4$	—	*H -6.1	J_{HP} 7	H <i>cis</i> to P ligand * 90 MHz † 84.6 MHz	901
				†F 69.9	J_{HF} 0.7		
				†F' 139.6	J_{FP} 94		
					J_{FF} 988		
$C_6HF_7MnO_4P$	553	$Mn[P(CF_3)_2F'](H)(CO)_4$	—	*H -9.1	J_{HP} 72	H <i>trans</i> to P ligand * 90 MHz † 84.6 MHz	901
				†F 69.1	J_{HF} 31.0, 1.8		
				†F' 134.0	J_{FP} 90		
					J_{FF} 1002		
					J_{FF} 2.2		

C ₇ HF ₉ MnO ₄ P	554	Mn[P(CF ₃) ₃](H)(CO) ₄	—	[*] H †F	-6.7 57.1	J _{HP} <10 J _{FP} 84	H <i>cis</i> to P ligand • 90 MHz † 84.6 MHz	901
C ₇ HF ₉ MnO ₄ P	555	Mn[P(CF ₃) ₃](H)(CO) ₄	—	[*] H †F	-8.5 81	J _{HP} 62 J _{FP} 81	H <i>trans</i> to P ligand • 90 MHz † 84.6 MHz	901
C ₇ H ₄ F ₆ MnO ₄ P	556	Mn[P(CF ₃) ₂ CH ₃](H)(CO) ₄	—	F	63.4	J _{FP} 75	H <i>cis</i> to P ligand 84.6 MHz	901
C ₇ H ₄ F ₆ MnO ₄ P	557	Mn[P(CF ₃) ₂ CH ₃](H)(CO) ₄	—	[*] H [*] H' †F	-8.5 1.83 62.8	J _{HP} 57 J _{HP} 8.0 J _{FP} 72	H <i>trans</i> to P ligand • 90 MHz † 84.6 MHz	901
C ₂₂ H ₁₆ MnO ₄ P	558	Mn(PPh ₃)(H)(CO) ₄	—	H	-6.94d	J _{PH} 34	—	705
			Et ₂ O	H	-6.43	J(³¹ P-H) 34.0 J(¹³ C-H) 5.2 (<i>trans</i>) J(¹³ C-H) 15.7 (<i>cis</i>)	—	199
C ₂₄ H ₁₈ MnO ₄ P	559	Mn[P(Ph) ₂ o-C ₆ H ₄ CH=CH ₂]- (H)(CO) ₄	C ₆ D ₁₂	H	-7.34	J _{PH} 35.2	—	227
C ₂₂ H ₁₆ MnO ₇ P	560	Mn[P(OPh) ₃](H)(CO) ₄	—	H	-7.95d	J _{PH} 55	—	705
C ₅ HMnO ₅	561	Mn(H)(CO) ₅	—	H	-7.5	—	—	705
			Et ₂ O	H	-7.73	J(¹³ C-H) 14 (<i>trans</i>) J(¹³ C-H) 7 (<i>cis</i>)	—	199
			Liquid	⁵⁵ Mn H	2578* 38.7†	—	* Relative to saturated aqueous LiMnO ₄ † Absolute	903

TABLE V—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_4HF_3MnO_4P$	562	$Mn(CO)_4(PF_3)(H)$	Liquid	^{55}Mn 2673 H 39.9†	—	The upfield shifts with increasing substitution of PF_3 for CO is consistent with the assumption that PF_3 is a better σ donor and increases the σ -electron density on the metal	903
$C_3HF_6MnO_3P_2$	563	$Mn(CO)_3(PF_3)_2(H)$	Liquid	^{55}Mn 2742*s H 41.8†	—		903
$C_2HF_9MnO_2P_3$	564	$Mn(CO)_2(PF_3)_3(H)$	Liquid	^{55}Mn 2813	—		903
$CHF_{12}MnOP_4$	565	$Mn(CO)(PF_3)_4(H)$	Liquid	^{55}Mn 2888	—		903
$C_{12}H_7MnO_7S$	566	$Mn(O \cdot SOCH_2C_6H_5)(CO)_5$	SO_2	H 3.95, 3.73	J 12.5	$T -37^\circ$	112
$C_{21}H_{17}MnO_5Sn$	567	$Mn[Sn(Ph)_2CH_2CH_2CH=CH_2] \cdot (CO)_5$	CCl_4	H 5.74 H' 4.87, 4.81	— — —	—	904
$C_8H_3O_7SMn$	568	$Mn[S(O)OCH=C=CH_2](CO)_5$	$CDCl_3$	H 6.48t H' 5.72–4.97	J 2.5 J 2.5	—	841
$C_{12}H_7MnO_7S$	569	$Mn[S(O)OCH_2C_6H_5](CO)_5$	SO_2	H 4.30	—	$T -37^\circ$	112

$C_7H_8B_3MnO_3$	570	$(C_3H_5B_3CH'_3)Mn(CO)_3$	—	H H' H''	3.20 5.10 1.06	—	Structure:	905
							• = BH	
$[C_5H_8B_6MnO_3]^-$	571	$[(C_2H_8B_6)Mn(CO)_3]^-$	$(CD_3)_2CO$	H	-5.70bs	—	Isolated as the tetramethyl ammonium salt Structure:	906
							R = R' = H • = BH	
$[C_7H_{12}B_6MnO_3]^-$	572	$\{[C_2H_6B_6(CH_3)_2]Mn(CO)_3\}^-$	$(CD_3)_2CO$	H	-2.46bs	—	Isolated as the tetramethyl ammonium salt. Structure as above (R = R' = CH ₃)	906
$[C_{11}H_{12}B_6MnO_3]^-$	573	$\{[C_2H_7B_6(C_6H_5)]Mn(CO)_3\}^-$	$(CD_3)_2CO$	CH H'	-4.86bs 7.40bd	—	Isolated as the tetramethyl ammonium salt. Structure as above. (R = H, R' = C ₆ H ₅)	906

TABLE V—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$[\text{C}_5\text{H}_8\text{B}_6\text{MnO}_3]^-$	574	$[\text{Mn}(\text{B}_6\text{C}_2\text{H}_8)(\text{CO})_3]^-$	$(\text{CD}_3)_2\text{CO}$	H 5.7 H' 3.73s $^{11}\text{B}^*$ -20.49, +6.57, +11.57, +18.75	— —	Isolated as the $[\text{N}(\text{CH}_3)_4]^+$ salt * Relative to $\text{BF}_3 \cdot \text{O}(\text{C}_2\text{H}_5)_2$ at 32 MHz	907
$[\text{C}_5\text{H}_{11}\text{B}_9\text{MnO}_3]^-$	575	$\{\text{Mn}[\pi\text{-(3)-1,2-B}_9\text{C}_2\text{H}_{11}](\text{CO})_3\}^-$	—	H -2.48bs	—	Isolated as the $[\text{N}(\text{CH}_3)_4]^+$ salt	203
$[\text{C}_5\text{H}_{13}\text{B}_9\text{MnO}_3]^-$	576	$\{\text{Mn}[\text{B}_9\text{C}_2\text{H}_9(\text{CH}=\text{CH}_2)_2](\text{CO})_3\}^-$	$(\text{CD}_3)_2\text{CO}$	H 6.40dd H' 4.96dd, 4.64dd ^{11}B	J_{cis} 10.5 J_{trans} 17.0 J_{gem} 1.5	Isolated as the Cs^+ salt 60 and 250 MHz	908
$\text{C}_8\text{H}_{11}\text{B}_8\text{MnO}_5$	577	$\text{Mn}[1\text{-(10-CH}_3\text{-1,10-(}\sigma\text{-B}_8\text{C}_2\text{H}_8\text{))-(CO)}_5]$	—	H 2.77s ^{11}B +10.7d	— J 158	* Relative to BF_3OEt_2 32.1 MHz	482
$\text{C}_8\text{H}_{13}\text{B}_{10}\text{MnO}_5$	578	$\text{Mn}[1\text{-(2-CH}_3\text{-1,2-(}\sigma\text{-B}_{10}\text{C}_2\text{H}_{10}\text{))-(CO)}_5]$	—	H 2.08 ^{11}B +2.1, +6.6, +11.3, +12.4	— J 143 J 141 J 169 J 160	— * Relative to BF_3OEt_2 32.1 MHz	482

TABLE VI
Rhenium complexes

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
(1) MONOHAPTO LIGANDS							
$C_{24}H_{18}O_4PRe$	1	$Re[\alpha\text{-}h^1\text{-}1,2\text{-}CH_3CH'C_6H_4P\text{-}(C_6H_5)_2](CO)_4$	$CDCl_3$	H 1.98d H' 3.35qd	$J_{HH'}$ 7.3 $J_{HH'}$ 7.3 $J_{PH'}$ 4.0	—	227
$C_{24}H_{18}O_4PRe$	2	$Re[\beta\text{-}h^1\text{-}1,2\text{-}CH_2CH'_2\text{-}C_6H_4P\text{-}(C_6H_5)_2](CO)_4$	$CDCl_3$	H 1.30m H' 3.24m	J_{PH} 2.2 J_{PH} small	—	227
$C_8H_5O_5Re$	3	$Re[\beta\text{-}h^1\text{-}CH=CH'COCH'_3](CO)_4$	$CDCl_3$	H 10.86 H' 7.69 H'' 2.50	$J_{HH'}$ 10.5 — —	Reference hexamethyldisiloxane Carbonyl oxygen lone pair of electrons co-ordinated with the Re atom to give a chelated complex	223
			CH_2Cl_2	H 10.63 H' 7.55 H'' 2.46	J 10.2 — —		
$C_{13}H_7O_5Re$	4	$Re[\beta\text{-}h^1\text{-}CH=CH'CO C_6H_5''](CO)_4$	$CDCl_3$	H 10.90 H' 8.26 H'' ₂ , H'' ₆ 8.05 H'' ₃ , H'' ₄ , H'' ₅ 7.51	$J_{HH'}$ 10.2 — — —		
						Reference hexamethyldisiloxane Chelated complex (see above)	223

TABLE VI—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{16}H_9N_2O_4Re$	5	$Re(1-h^1-2-C_6H_4 \cdot N=NC_6H_5)(CO)_4$	CS_2	H_{-3}	7.13t	—	100 MHz	176
				H_{-4}	$\sim 7.55m$	—		
				H_{-5}	7.92dd	—		
				H_{-6}	8.15dd	—		
				H'	$\sim 7.38m$	—		
$C_7H_9N_2O_5Re$	6	$Re(CONHCH_3)(NH_2^{\prime\prime\prime}CH_3^{\prime\prime\prime})(CO)_4$	$CDCl_3$	H	5.54b	$J_{HH'} 5.1$	60 and 100 MHz	228
				H'	2.83	—		
				H''	4.19b	$J_{H''H'''} 6.4$		
				H'''	2.85	—		
$C_9H_{13}N_2O_5Re$	7	$Re[CONHCH'(CH_3)_2](NH_2^{\prime\prime\prime}-CH_3^{IV})(CO)_4$	$CDCl_3$	H	5.58	$J_{HH'} 8$	60 and 100 MHz	228
				H'	~ 4.10	—		
				H''	1.13	$J_{H'H''} 6.5$		
				H'''	$\sim 3.90b$	$J_{H'''H^{IV}} 6.4$		
				H^{IV}	2.81	—		
$C_{11}H_{17}N_2O_5Re$	8	$Re[CONHCH'(CH_3)_2](NH_2^{\prime\prime\prime}-CH^{IV}(CH_3)_2)(CO)_4$	$CDCl_3$	H	5.35b	—	60 and 100 MHz	228
				H'	4.26	$J_{H'H''} 6.5$		
				H''	1.14	—		
				H'''	4.20b	—		
				H^{IV}	2.95	$J_{H^{IV}H^V} 6.5$		
				H^V	1.26	—		
$C_6H_3O_5Re$	9	$Re(CH_3)(CO)_5$	$CDCl_3$	H	-0.23	—	—	229
$C_7HCl_2F_2O_5Re$	10	$Re(CF_2CHCl_2)(CO)_5$	$CS_2/$ $(CH_3)_2CO$	H	5.80t	J 11.0	*Relative to C_6F_6 (increasing to low field)	230
				F	118.5d*	—		

$C_7HClF_3O_5Re$	11	$Re(CF_2CHClF')(CO)_5$	$CS_2/$ $(CH_3)_2CO$	H F F'	5.59dq 116q*, 101q 26.5	— J_{HF} 5.3, 11.8 $J_{HF'}$ 52.5	*Relative to C_6F_6 (increasing to low field)	230
$C_7HF_4O_5Re$	12	$Re(CF_2CHF_2)(CO)_5$	$CS_2/$ $(CH_3)_2CO$	H F F'	5.13tt 98.4* 42.5d	— J_{HF} 5.7 $J_{HF'}$ 59.0 $J_{FF'} < 1$	*Relative to C_6F_6 (increasing to low field)	230
$C_8H_3F_4O_5Re$	13	$Re(CF_2CF_2CH_3)(CO)_5$	$CS_2/$ $(CH_3)_2CO$	H F F'	1.54t 118.8m* 73.0qt	— J_{HF} 2.5 $J_{HF'}$ 20.0 $J_{FF'}$ 4.5	*Relative to C_6F_6 (increasing to low field)	230
$C_{10}H_3F_8O_5Re$	14	$Re[CF_2CF_2(CF_2)_2CH_3](CO)_5$	$CS_2/$ $(CH_3)_2CO$	F F'	92.2 82.8	— —	*Relative to C_6F_6 (increasing to low field)	230
$C_8H_5O_5Re$	15	$Re(h^1-CH_2-CH'=CH_2)(CO)_5$	$CDCl_3$	H H' H''	1.81d 6.24m 4.59dd, 4.28dd	J 8 — J 2,16 J 2,10	60 and 100 MHz	231
$C_7H_4NO_6Re$	16	$Re(CH_2CONH_2)(CO)_5$	$CDCl_3$	H H'	1.75s 5.27s	— —	—	196
$C_7F_3O_5Re$	17	$Re(h^1-CF=CF_2)(CO)_5$	CS_2	F F' _{cis} F' _{trans}	154.3 96.1 131.7	J_{trans} 120.0 J_{cis} 36.6 J_{gem} 98.0		232
$C_8H_2F_3O_5Re$	18	$Re(h^1-CH=CH'CF_3)(CO)_5$	—	H H' F F	7.46d 6.78q 58.8d 62.2, 65.2	J 14 $J_{H'F}$ 8.5 — — —		233

TABLE VI—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_8F_3O_3Re$	19	$Re(h^1-CF=CF'CF''_2)(CO)_3$ <i>trans</i>	CS_2 or $CDCl_3$	F	93.8	$J_{FF'}$ 14.1		232
				F'	160.5	$J_{F'F''}$ 13		234
				F''	58.0	$J_{FF''}$ 24		
$C_9HF_6O_3Re$	20	$Re(h^1-CF=CF'CF''_2CHE'''_2)(CO)_3$ <i>trans</i>	$CDCl_3$	H	5.95	J_{HF} 1.4 $J_{HF''}$ 4.6 $J_{HF'''} 53.4$		235 234
				F	102.6	$J_{FF'}$ 129.5 $J_{FF''}$ 16.5 $J_{FF'''} 5.3$		
				F'	159.0	$J_{F'F''}$ 14.1 $J_{F'F'''} 3.3$		
				F''	118.7	$J_{F''F'''} 8.3$		
				F'''	138.2	—		
$C_9HF_6O_3Re$	21	$Re(h^1-C(CF_3)=CHCF'_3)(CO)_3$ <i>trans</i>	$CS_2/$ $(CH_3)_2CO$	H	−99	J_{HF} 2.5 $J_{HF'}$ 9.1 $J_{FF'}$ 2.5	*To low field from C_6F_6	230
				F	110.0 quint.*	—		
				F'	112.5dq	—		
$C_9F_3O_3Re$	22	$Re(1-h^1-C_4F_5)(CO)_3$	CS_2	F _{−2}	118.1	—	C_8F_5 = pentafluorocyclobut-1-ene	232
				F _{−3}	122.0	—		236
				F _{−4}	118.6	—		
$C_{10}ClF_6O_3Re$	23	$Re(1-h^1-C_5ClF_6)(CO)_3$	THF	F _{−3}	111.7tt	$J_{3,4}$ 6.70	C_5ClF_6 = 2-chloro-3,3,4,4,5,5-hexafluorocyclopent-1-ene	237
				F _{−4}	129.1 quint.	$J_{4,5}$ 6.70		
				F _{−5}	97.0tt	$J_{3,5}$ 3.74		

C ₁₁ F ₉ O ₃ Re	24	Re(1- <i>h</i> ¹ -C ₆ F ₉)(CO) ₅	CS ₂	F ₋₂	97.0	—	C ₆ F ₉ = nonafluoro- cyclohex-1-ene	232
				F ₋₃	124.8	—		236
				F ₋₄	143.5	—		
				F ₋₅	141.3	—		
C ₉ F ₅ O ₃ Re	25	Re(1- <i>h</i> ¹ -CF=CF'-CF''=CF ₂ ''')- (CO) ₅ <i>cis</i>	CDCl ₃	F	92.5	—		238
				F'	64.3	—		
				F''	166.8	—		
				F _{cis} '''	107.5	—		
				F _{trans} '''	121.5	—		
C ₉ F ₅ O ₃ Re	26	Re(1- <i>h</i> ¹ -CF=CF'-CF''=CF ₂ ''')- (CO) ₅ <i>trans</i>	ether	F	92.4	J _{FF'} 137 J _{FF''} 9 J _{FF_{cis}'''} 6 J _{FF_{trans}'''} 17		238
				F'	150.4	J _{F'F''} 36 J _{F'F_{cis}'''} 4 J _{F'F_{trans}'''} 12		239
				F''	177.8	J _{cis} 28 J _{trans} 117		
				F _{cis} '''	101.4	J _{gem} 60		
				F _{trans} '''	112.2	—		
				F ₋₁	162.0	—		
				F ₋₃	100.4	—		
				F ₋₄	179.9	—		
				F ₋₅ , F ₋₆	122.7	—		
				F	62.0t	J _{FF'} 4.0		
C ₉ F ₅ O ₃ Re	28	Re[1- <i>h</i> ¹ -C(CF ₃)=C=CF ₂](CO) ₅	—	F'	112.2q	—		241
C ₁₂ H ₇ O ₃ Re	29	Re(1- <i>h</i> ¹ -4-C ₆ H ₄ CH ₃)(CO) ₅	CS ₂	H	7.44	J 7.2	—	242
			or THF	H'	6.76 2.25			

C₆F₅ = pentafluoro-
bicyclo[2.2.0]hexa-2,5-
diene)

TABLE VI—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{11}H_4ClO_5Re$	30	$Re(1-h^1-2-C_6H_4Cl)(CO)_5$	CCl_4	H 7.65, 7.16, 6.85	—	—	243
$C_{11}H_4ClO_5Re$	31	$Re(1-h^1-3-C_6H_4Cl)(CO)_5$	CCl_4	H 7.59, 6.94	—	—	243
$C_{11}H_4ClO_5Re$	32	$Re(1-h^1-4-C_6H_4Cl)(CO)_5$	CCl_4	H 7.59, 6.94	—	—	243
			CS_2 or THF	H 7.61, 6.94	—	—	242
$C_{11}F_5O_5Re$	33	$Re(1-h^1-C_6F_5)(CO)_5$	THF	F_{-2}, F_{-6} 101.35	$J_{2,3} = J_{5,6}$ 28.55 $J_{2,4} = J_{4,6}$ 0 $J_{2,6}$ 2.68	T 35° 56.4 MHz	244
				F_{-3}, F_{-5} 163.3	$J_{2,5} = J_{3,6}$ 10.5 $J_{3,5}$ 7.75		
				F_{-4} 159.9	$J_{3,4} = J_{4,5}$ 19.35 —		
$C_{13}HF_4O_5Re$	34	$Re(1-h^1-4-C_6F_4C\equiv CH)(CO)_5$	THF	F_{-2}, F_{-6} 101.95	$J_{2,3}$ 33.4 $J_{2,6}$ 6.4	T 35° 56.4 MHz	244
				F_{-3}, F_{-5} 138.3	$J_{2,5} = J_{3,6}$ 17.6 $J_{3,5}$ 4.2		
$C_{12}F_4NO_5Re$	35	$Re(1-h^1-4-C_6F_4CN)(CO)_5$	$CHCl_3$ or CH_2Cl_2	F_{-2}, F_{-6} 57.7	—	To high field from CF_3CO_2H at 56.4 MHz	245
				F_{-3}, F_{-5} 21.1	—		246

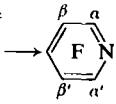
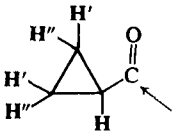
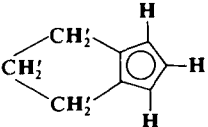
$C_{13}F_3N_2O_5Re$	36	$Re[1-h^1-3,4-C_6F_3(CN)_2(CO)_5]$	THF	F_{-2} 66.2 F_{-5} 134.6 F_{-6} 83.2	$J_{2,5}$ 4.35 $J_{5,6}$ 26.75 $J_{2,6}$ 12.65	T 35°	925 244
$C_{12}H_3F_4O_5ReS$	37	$Re[1-h^1-4-C_6F_4(SCH_3)(CO)_5]$	$CHCl_3$	F_{-2}, F_{-6} 136.5 F_{-3}, F_{-5} 102.1	$J_{2,3} = J_{5,6}$ 29.6 $J_{2,5} = J_{3,6}$ 14.6 $J_{2,6}$ 4.7 $J_{3,5}$ 38		247
$C_{16}F_8NO_5Re$	38	$Re[1-h^1-4-C_6F_4(C_5F_4N)(CO)_5]$	$CHCl_3$	F_{-2}, F_{-6} 101.0 F_{-3}, F_{-5} 139.6 $F_{-\beta},$ 139.6 $F_{-\alpha}$ 90.2	$J_{2,3} = J_{5,6}$ 23.3 $J_{2,5} = J_{3,6}$ 10.9 $J_{2,6}$ 8.0 $J_{3,5}$ 0.5 $J_{\beta\beta'}$ 5.0 $J_{\alpha\beta}$ 18.6 $J_{\alpha\alpha'}$ 13.0 $J_{\alpha\beta'}$ 27.3	$C_5F_4N =$ 	248
$C_9H_5O_6Re$	39	$Re(h^1-CH=CH'.COCH_3')(CO)_5$ <i>cis</i>	CH_2Cl_2	H 8.21 H' 7.62 H'' 2.19	$J_{HH'}$ 13.0 — —	Reference hexamethyldisiloxane	223
$C_9H_5O_6Re$	40	$Re(h^1-CH=CH'.COCH_3')(CO)_5$ <i>trans</i>	$CDCl_3$	H 8.65 H' 6.92 H'' 2.19	$J_{HH'}$ 18.7 — —	Reference hexamethyldisiloxane	223
$C_9H_5O_6Re$	41	$(h^1-COC_3H_5)Re(CO)_5$	CS_2	H 2.37tt H' 0.87m H'' 0.53m	— $J_{HH'}$ 7.6 $J_{HH''}$ 4.6	$COC_3H_5 =$ 	929

TABLE VI—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{14}H_7O_6Re$	42	$Re(h^1-CH=CH' \cdot COC_6H_5)(CO)_5$ <i>cis</i>	CH_2Cl_2	H	8.58	$J_{HH'}$ 13.0	Reference hexamethyldisiloxane 223
				H'	8.34	—	
				H''	7.97,	—	
					7.51	—	
$C_{14}H_7O_6Re$	43	$Re(h^1-CH=CH' COC_6H_5)(CO)_5$ <i>trans</i>	$CDCl_3$	H	8.98	$J_{HH'}$ 18.1	Reference hexamethyldisiloxane 223
				H'	7.67	—	
				H''	7.87,	—	
					7.42	—	
$C_{12}H_5O_6Re$	44	$Re(COC_6H_5)(CO)_5$	CS_2 or THF	H	7.39	—	242
$C_{13}H_7O_6Re$	45	$Re(p-COC_6H_4CH_3)(CO)_5$	CS_2 or THF	H	7.11	—	242
				H'	2.25	—	
$C_{12}H_4ClO_6Re$	46	$Re(o-COC_6H_4Cl)(CO)_5$	CCl_4	H	7.19	—	243
$C_{12}H_4ClO_6Re$	47	$Re(m-COC_6H_4Cl)(CO)_5$	CCl_4	H	7.36	—	243
$C_{12}H_4ClO_6Re$	48	$Re(p-COC_6H_4Cl)(CO)_5$	CCl_4 or CS_2 or THF	H	7.40	—	243
							242 82
$C_7H_3O_7Re$	49	$Re(CO_2CH_3)(CO)_5$	C_6H_6	H	3.62s	—	249
$C_8H_3O_7Re$	50	$Re(CO_2CH_2CH_3)(CO)_5$	C_6H_6	H	4.29q	—	249
				H'	1.27t	—	
$C_{10}F_4NO_5Re$	51	$Re(4-h^1-C_5F_4N)(CO)_5$	$CHCl_3$ or CH_2Cl_2	F_{-2}, F_{-6}	18.0	$J_{2,3} = J_{5,6}$ 30.3	Upfield from CF_3CO_2H 245
						$J_{2,5}$ 25.6	197
				F_{-3}, F_{-5}	30.0	$J_{2,6}$ 3.8	246
						$J_{3,5}$ 13.4	

$C_{16}H_5F_3NO_3Re$	52	$Re[2-h^1-4-C_3F_3N(C_6H_5)](CO)_3$	$CHCl_3$	F_{-3}	88.4	$J_{3,5} < 1.0$		248
				F_{-5}	103.4	$J_{5,6}$	30.8	
				F_{-6}	94.5	$J_{3,6}$	32.1	
$C_{15}H_7N_2O_3Re$	53	$Re[2-h^1-4-C_5H_3N(4-C_3F_4N)](CO)_3$	$CHCl_3$	F_{-3}	97.2	$J_{3,5}$	8.6	248
				F_{-5}	144.1	$J_{5,6}$	21	
				F_{-6}	87.1	$J_{3,6}$	32	
				F'_{-2}, F'_{-6}	89.6	$J_{2,6}$	20.4	
						$J_{2,5}$	27.5	
						$J_{2,6}$	13.1	
				F'_{-3}, F'_{-5}	139.2	$J_{3,5}$	2.3	
$C_9F_3N_2O_3Re$	54	$Re(4-h^1-C_4F_3N_2)(CO)_3$	$CHCl_3$	F_{-3}	53.7	$J_{3,6}$	32.0	197
				F_{-5}	93.8	$J_{3,5}$	16.9	$C_4F_3N_2 =$ trifluoro pyridazinyl
				F_{-6}	106.6	$J_{5,6}$	32.0	
$C_8F_2N_3O_3Re$	55	$Re(2-h^1-C_3F_2N_3)(CO)_3$	$CHCl_3$	F	41.8	—		197
							$C_3F_2N_2 =$ difluoro- <i>s</i> -triazinyl	
(2) DIHAPTO LIGANDS								
$[C_7H_4O_3Re]^+$	56	$[(h^2-CH_2=CH_2)Re(CO)_3]^+$	$(CD_3)_2CO$	H	5.08s	—	Hexafluorophosphate 100 MHz	249
(3) PENTAHAPTO LIGANDS								
$C_7H_5Br_2O_2Re$	57	$(h^5-C_5H_5)Re(Br)_2(CO)_2$	$(CH_3)_2CO$	H	5.96s	—	Hexamethyldisiloxane reference	930
$[C_7H_5NO_3Re]^+$	58	$[(h^5-C_5H_5)Re(NO)(CO)_2]^+$	$(CD_3)_2CO$	H	6.58	—	Hexafluorophosphate T 35	61
$C_8H_5O_3Re$	59	$(h^5-C_5H_5)Re(CO)_3$	—	H	5.37	—	T 32	7
			$(CD_3)_2CO$	H	5.62	—	T 35	61
$C_{13}H_{15}O_3Re$	60	$[h^5-C_5(CH_3)_5]Re(CO)_3$	CS_2	H	2.15s	—	Reference hexamethyldisiloxane	187

TABLE VI—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{12}H_{15}O_3ReSi$	61	$[h^5-C_5H_4 \cdot CH_2Si(CH_3)_3]Re(CO)_3$	—	H	4.94t,	—	—	250
					4.80t	—		
				H'	1.72	—		
				H''	0.02	—		
$[C_8H_5O_3Re]^+$	62	$[(h^5-C_5H_5)Re(Cl)(CO)_3]^+$	$(CH_3)_2CO$	H	6.39	—	Hexachloroantimonate	251
$C_{10}H_7O_4Re$	63	$(h^5-C_5H_4 \cdot COCH_3)Re(CO)_3$	—	H	5.99,	—	T 32	7
				H'	5.43 2.32	—		
$C_{11}H_{13}O_3ReSi$	64	$[h^5-C_5H_4 \cdot Si(CH_3)_3]Re(CO)_3$	CS_2	H	5.22s	—	—	208
				H'	0.15	—	—	250
$C_{14}H_{21}O_3ReSi_2$	65	$h^5-1,3-C_5H_3[Si(CH_3)_3]_2Re(CO)_3$	—	H	5.24s	—	—	250
				H'	0.19	—	—	250
$C_{13}H_{19}O_3ReSi_2$	66	$\{h^5-C_5H_4[Si(CH_3)_2 \cdot Si(CH_3)_3]\}Re(CO)_3$	—	H	5.39t,	—	—	250
					5.26t	—		
				H'	0.28	—		
				H''	0.17	—		
$C_{11}H_9O_3Re$	67	$(h^5-C_8H_9)Re(CO)_3$	C_6D_6	H	4.47–4.43	—	$C_8H_9 =$ 	253
				H'	2.3–2.0	—		

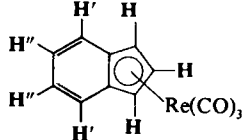
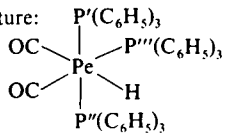
$C_{12}H_7O_3Re$	68	$(h^5-C_6H_7)Re(CO)_3$	—	H H' H''	5.7 7.10 7.43	— — —	Structure: 	109
(4) MIXED LIGANDS								
$C_8H_8NO_4Re$	69	$(h^5-C_5H_5)Re(CO_2CH_3)(NO)(CO)$	CCl_4	H H'	6.0s 3.77s	— —	—	254
$C_9H_9O_3Re$	70	$(h^5-C_5H_5)Re[C(CH_3) \cdots OH'']-(CO)_2$	C_6H_6	H H' H''	4.83 1.94 4.49	— — —	—	255
$C_{10}H_{11}O_3Re$	71	$(h^5-C_5H_5)Re[C(CH_3) \cdots OCH'']-(CO)_2$	C_6H_6	H H H''	4.91 2.06 4.16	— — —	—	255
$C_{13}H_{17}O_3Re$	72	$(h^5-C_5H_5)Re[C(n-C_4H_9) \cdots OCH'']-(CO)_2$	C_6H_6	H H' H''	5.05 1.39 4.17	— — —	—	255
$C_{15}H_{13}O_3Re$	73	$(h^5-C_5H_5)Re[C(C_6H_5) \cdots OCH'']-(CO)_2$	C_6H_6	H H' H''	4.92 7.23 4.19	— — —	—	255
$[C_{14}H_{10}O_3Re]^-$	74	$[(h^5-C_5H_5)Re(COC_6H_5)-(CO)_2]^-$	D_2O	H H'	4.72 3.12	— —	Tetramethylammonium Salt (δ 7.17)	255
$C_{56}H_{46}O_2P_3Re$	75	$Re(H)[P(C_6H_5)_3]_3(CO)_2$	$CDCl_3$	H H''	-3.1t 6.8m	$J_{HP'} = J_{HP''} = 30$ $J_{HP'''} = 18$	Structure: 	256

TABLE VI—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
C ₁₅ H ₃₁ O ₃ P ₂ Re	76	Re(H)[P(C ₂ H ₅) ₃] ₂ (CO) ₃	C ₆ H ₆	H	-6.53t	J _{HP} 20.0	—	257
C ₃₉ H ₃₁ O ₃ P ₂ Re	77	Re(H)[P(C ₆ H ₅) ₃] ₂ (CO) ₃	CDCl ₃	H	-5.35t	J _{HP} 17.5	100 MHz	258
				H'	6.9m	—		256
			C ₆ H ₆	H	-4.48t	J _{HP} 18.0	100 MHz	257
C ₂₈ H ₂₃ O ₃ P ₂ Re	78	Re(H)[P(C ₆ H ₅) ₂ CH ₂ P-(C ₆ H ₅) ₂](CO) ₃	C ₆ H ₆	H	-3.23t	J _{HP} 26.0	100 MHz	257
C ₂₉ H ₂₅ O ₃ P ₂ Re	79	Re(H)[P(C ₆ H ₅) ₂ CH ₂ CH ₂ P-(C ₆ H ₅) ₂](CO) ₃	C ₆ H ₆	H	-5.20t	J _{HP} 26.0	100 MHz	257
C ₄₄ H ₄₀ O ₃ P ₃ Re	80	Re(H){[P(C ₆ H ₅) ₂ CH ₂] ₃ -CCH ₃ }(CO) ₃	C ₆ H ₆	H	-4.82t	J _{HP} 23.5	100 MHz	257
[C ₅ H ₁₁ B ₉ O ₃ Re] ⁻	81	[Re(π -(3)-1,2-B ₉ C ₂ H ₁₁)(CO) ₃] ⁻	—	H	-2.90b	—	Tetramethylammonium salt A carborane derivative	203
C ₁₀ H ₁₆ O ₄ PRe	82	Re(H)P(C ₂ H ₅) ₃ (CO) ₄	C ₆ H ₆	H	-5.66d	J _{HP} 24.5	100 MHz	257
C ₂₂ H ₁₆ O ₄ PRe	83	Re(H)[P(C ₆ H ₅) ₃](CO) ₄	C ₆ H ₆	H	-4.33d	J _{HP} 22.0	100 MHz	257
C ₂₂ H ₁₆ O ₄ PRe	84	Re(H)P(OC ₆ H ₅) ₃ (CO) ₄	C ₆ H ₆	H	-5.68d	J _{HP} 32.5	100 MHz	257
C ₇ F ₃ O ₇ Re	85	Re(OCOCF ₃)(CO) ₅	CH ₂ Cl ₂	F	74.2s	—	94.1 MHz	138
(5) POLYRHENIUM COMPLEXES								
C ₁₅ H ₁₀ O ₄ Re ₂	86	[(h^2 -C ₅ H ₅)Re(CO) ₂] ₂ (CO)*	—	H	5.35s	—	*Bridging CO ligand	259
[C ₆ H ₅ O ₆ Re ₂] ⁻	87	[Re ₂ (H) ₃ (CO) ₆] ⁻	CD ₃ CN	H	-17.49	—	Tetraethylammonium salt	260

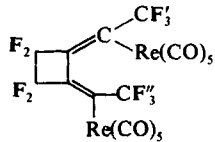
$C_{16}H_8O_6Re_2$	88	$(h^5 : h^5-C_5H_4 \cdot C_5H_4)[Re(CO)_3]_2$	$(CH_3)_2CO$	H	5.54t 6.03t	—	Hexamethyldisiloxane reference	931
$C_{18}H_{16}O_6Re_2Si$	89	$(h^5 : h^5-C_5H_5 \cdot Si(CH_3)_2C_5H_5)-[Re(CO)_3]_2$	—	H H'	5.27s 0.38	—	—	250
$C_{10}H_8O_8Re_2Si$	90	$[Re(H)(CO)_4]_2[Si(CH_3)_2]$	CCl_4	H H'	-10.56b 1.13t*	— J 1.5	Complex contains hydrogen bridged silicon-rhenium bonds *Collapses to a singlet on irradiation at -10.56	261
$C_{20}H_{12}O_8Re_2Si$	91	$[Re(H)(CO)_4]_2[Si(C_6H_5)_2]$	CCl_4	H	-9.56	—	—	261
$C_{18}HF_{11}O_{10}Re_2$	92	$[2,6-h^1 : h^1-C(CF_3)=CH-CF'_2-C(CF''_3)=C(CF'''_3)][Re(CO)_5]_2$	—	H F F' F'' F'''	7.05 62.84 67.72 61.34 43.39 50.29	$J_{HF'}$ 2.9, 7.3 J_{HF} 2.0 $J_{FF'}$ 3.7, 1.7 $J_{FF'}$ 176.0 $J_{F'F''}$ 4.0 $J_{F''F'''} 1.8$	100 MHz and 94.1 MHz	241
$C_{18}F_{10}O_{10}Re_2$	93	$(h^1 : h^1-C_8F_{10})[Re(CO)_5]_2$	—	F F' F''	51.6q 64.0 comp. 44.2 comp.	J 2 — —	Structure: 	239
$[C_{12}H_2O_{12}Re_3]^-$	94	$[Re_3(H)_2(CO)_{12}]^-$	—	H	-17.2	—	Tetraphenylarsonium salt (δ 7.95s)	262
$[C_{12}H_6O_{12}Re_4]^{2-}$	95	$[Re_4(H)_6(CO)_{12}]^{2-}$	$(CH_3)_2CO$	H	-17.4s	—	Complex contains hydrogen bridged rhenium-rhenium bonds Isolated as the tetraphenylarsonium salt	263

TABLE VII

Iron complexes

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
(1) <i>MONOHAPTO LIGANDS</i>								
(a) <i>Dicarbonyl derivatives</i>								
C ₁₉ H ₂₂ F ₃ ⁻ FeIO ₂ P ₂	1	Fe(CF ₃)(I)[P(CH ₃) ₂ Ph] ₂ (CO) ₂	CDCl ₃	H	2.30d, 2.04d	J _{PH} 6.0	100 MHz	264
				F	3.19t	J _{PF} 13.0	94.1 MHz P ligands <i>cis</i> , CO ligands <i>cis</i> , CF ₃ <i>trans</i> to one CO or I ligand	
C ₇ H ₁₁ F ₃ FeO ₂ Sn	2	Fe(CH ₂ CH ₃)[Sn(CH ₃) ₂ CF ₃](CO) ₂	CHCl ₃	H	0.4	J(¹¹⁷ Sn-H) 47 J(¹¹⁹ Sn-H) 49	60 and 100 MHz	221
			CCl ₃ F	F	48.5	J(¹¹⁷ Sn-F) 200 J(¹¹⁹ Sn-F) 209	94.1 MHz	
C ₁₁ H ₁₆ F ₇ FeIO ₂ P ₂	3	Fe(CF ₂ CF ₂ CF ₃)[P(CH ₃) ₂ CH ₂ -CH ₂ P(CH ₃) ₂](I)(CO) ₂	(CH ₃) ₂ CO	F	n.o.	—	94.1 MHz	954
				F'	+115.0	—		
				F''	+78.9	J 12.2		
C ₃₁ H ₂₄ F ₇ FeIO ₂ P ₂	4	Fe(CF ₂ CF ₂ CF ₃)[P(C ₆ H ₅) ₂ CH ₂ -CH ₂ P(C ₆ H ₅) ₂](I)(CO) ₂	(CH ₃) ₂ CO	F	n.o.	—	94.1 MHz	954
				F'	+114.5	—		
				F''	+79.3	J 12.6		
C ₃₁ H ₂₂ F ₇ FeIO ₂ P ₂	5	Fe(CF ₂ CF ₂ CF ₃)[P(C ₆ H ₅) ₂ CH=CHP(C ₆ H ₅) ₂](I)(CO) ₂ <i>cis</i>	(CH ₃) ₂ CO	F	n.o.	—	94.1 MHz	954
				F'	+114.2	—		
				F''	+78.7	J 12.6		
C ₃₁ H ₂₄ F ₇ FeIO ₂ P ₂	6	Fe[CF(CF ₃) ₂][P(C ₆ H ₅) ₂ CH ₂ -CH ₂ P(C ₆ H ₅) ₂](I)(CO) ₂	CH ₂ Cl ₂	F	n.o.	—	94.1 MHz	954
				F'	+64.2	J 8.0		

$C_{31}H_{22}F_7FeIO_2P_2$	7	$Fe[CF(CF_3)_2][P(C_6H_5)_2CH=CHP(C_6H_5)_2](I)(CO)_2$ <i>cis</i>	CH_2Cl_2	F F'	n.o. +64.4	— J 8.0	94.1 MHz	954
$C_{22}H_{17}FeN_2O_3P$	8	$Fe(CH_2CN)[P(C_6H_5)_3](NO)(CO)_2$	CS_2	H H'	2.3s 7.5 comp.	— —	40 MHz	265
$C_{22}H_{18}FeNO_4P$	9	$Fe(COCH_3)[P(C_6H_5)_3](NO)(CO)_2$	CS_2	H H'	2.72s 7.4 comp.	— —	40 MHz	265
$C_{28}H_{22}FeNO_4P$	10	$Fe(COCH_2C_6H_5)[P(C_6H_5)_3](NO)(CO)_2$	CS_2	H H', H''	3.78s 7.3 comp.	— —	40 MHz	265
$C_{25}H_2FeNO_6P$	11	$Fe(COCH_2CO_2CH_2CH_3)[P(C_6H_5)_3](NO)(CO)_2$	CS_2	H H' H'' H'''	2.6s 3.85q 1.12t 7.4 comp.	— — — —	40 MHz	265
<i>(b) Tricarbonyl derivatives</i>								
$C_{11}H_8FeO_4$	12	$Fe[C(C_6H_5)_3 \equiv OCH_3](CO)_3$	$(CD_3)_2CO$	H H'	7.46s 4.85s	— —	— —	266
$C_{23}H_{18}BrFeO_3P$	13	$Fe[o-CH(CH_3)C_6H_4P(Ph)_2](Br)(CO)_3$	$CDCl_3$	H H'	4.17b 2.07d	— $J \sim 5$	—	267
$C_{23}H_{18}ClFeO_3P$	14	$Fe[o-CH(CH_3)C_6H_4P(Ph)_2](Cl)(CO)_3$	$CDCl_3$	H H'	4.24b, 4.54 1.79d, 1.98d	— — $J \sim 4$ $J \sim 4$	Two isomers present	267
<i>(c) Tetracarbonyl derivatives</i>								
$C_7F_7FeIO_4$	15	$Fe[CF(CF_3)_2](I)(CO)_4$	$CHCl_3$	F F'	+77.6 sept. -8.4d	J 11 J 11	T 35°. Positive values to high field from CF_3CO_2H	268

TABLE VII—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_7F_5FeIO_4$	16	$Fe(CF_2CF_2CF_2''(I)(CO)_4$	—	F	61.7	—		269
				F'	114.6	—		
				F''	78.4	—		
			CH_2Cl_2	F	+54.9	—	94.1 MHz	954
				F'	+114.4	—		
				F''	+78.6	$J_{11.4}$		
				C	-6	—	To high field from CS_2 at 8.5 MHz	95
$C_{11}F_{15}FeIO_4$	17	$Fe(CF_2CF_2CF_2''CF_2'''CF_2^{IV}CF_2^VCF_2^{VI}(CO)_4$	CH_2Cl_2	F	53.9	$J_{FF''} 17$	94.1 MHz	954
				F'	110.6	—		
				F''	121.1	—		
				F'''	122.2	—		
				F ^{IV}	123.0	$J_{F^{IV}F^{VI}} 11$		
				F ^V	126.6	—		
				F ^{VI}	81.5	—		
$[C_6H_5FeO_3]^-$	18	$[Fe(COCH_3)(CO)_4]^-$	CH_2Cl_2	H	2.67	—	Isolated as the quaternary methyl ammonium salt	270
$[C_{11}H_5FeO_3]^-$	19	$[Fe(COC_6H_5)(CO)_4]^-$	$(CD_3)_2CO$	H	7.63	—	Isolated as the quaternary methyl ammonium salt	270
				H'	3.37	—	$[N(CH_3)_4]^+$	
$[C_9H_9FeO_3]^-$	20	$[Fe(CONC_4H_9)(CO)_4]^-$	—		n.m.	—	—	919
(2) DIHAPTO LIGANDS								
(a) Dicarboxyl derivatives								
$C_{10}H_{18}F_4FeO_5P_2$	21	$(h^2-CF_2=CF_2)Fe[P(OCH_2)_3]_2(CO)_2$	$CDCl_3$	H	3.66d	$J_{PH} 11.5$	<i>trans</i> -CO ligands, <i>cis</i> -P ligands	272

			CHCl ₃	F	112m*	J 30	* 94.1 MHz	
C ₁₆ H ₃₀ F ₄ FeO ₈ P ₂	22	(h ² -CF ₂ =CF ₂)Fe[P(OCH ₂ -CH ₃) ₃] ₂ (CO) ₂	CDCl ₃	H	4.02q	J _{PH} 7.0	100 MHz <i>trans</i> -CO ligands,	272
				H'	1.32t	J _{PH} 7.0	<i>cis</i> -P ligands	
			CHCl ₃	F	113m*	J 30	* 94.1 MHz	
C ₁₁ H ₁₈ F ₆ FeO ₈ P ₂	23	(h ² -CF ₂ =CF'CF'' ₃)Fe-[P(OCH ₃) ₃] ₂ (CO) ₂	CDCl ₃	H	3.41d	J _{PH} 11.5	100 MHz <i>trans</i> -CO ligands,	272
			CHCl ₃	F	97.2m*	—	<i>cis</i> -P ligands	
				F'	109.2m*	—	* 94.1 MHz	
				F''	67.0 sept.*	—		
C ₄₂ H ₃₄ FeO ₂ P ₂	24	(h ² -o-CH ₂ =CH'.C ₆ H ₄ PPh ₂)Fe-(o-PPh ₂ C ₆ H ₄ CH''=CH ₂ ''')(CO) ₂	C ₆ D ₆	H	2.3m	—	—	51
				H'	2.98m	—		
				H''	n.m.	J _{H''H'''} 17.10		
				H'''	5.50d,	J _{H'''H'''} 0		
					5.10d			
C ₁₈ H ₃₀ F ₈ FeO ₈ P ₂	25	(1,4-h ² -CF ₂ CF ₂ CF ₂ CF ₂)Fe-[P(OCH ₂ CH ₃) ₃] ₂ (CO) ₂ *	CHCl ₃	F	3.8†	—	* <i>cis</i> -dicarbonyl- <i>trans</i> -bis(triethylphosphite) octafluoroferracyclopentane	271
				F'	60.4†	—	†To high field of CF ₃ CO ₂ H (external)	
C ₁₈ H ₃₂ F ₆ FeO ₈ P ₂	26	(1,4-h ² -CHF ₂ CF ₂ CF ₂ CHF)Fe-[P(OCH ₂ CH ₃) ₃] ₂ (CO) ₂ *	CDCl ₃	H	5.30d	J _{HF} 43.0	100 MHz	272
				H'	4.05m	J _{H'H''} 7.0	* <i>cis</i> -dicarbonyl- <i>trans</i> -bis(triethylphosphite) hexafluoroferracyclopentane	
				H''	1.32t	—	†94.1 MHz	
			CHCl ₃	F	69.5m†	—		
				F'	213.0m†	—		
(b) Tricarbonyl derivatives								
C ₇ H ₉ BBBrFeNO ₃	27	[h ² -CH ₂ =CHB(Br)N(CH ₃) ₂]-Fe(CO) ₃	C ₆ H ₆	B	-27.2	—	Reference BF ₃ ·OEt ₂ (external)	273

TABLE VII—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{23}H_{17}FeO_3P$	28	$(h^2-o-CH_2=CH' \cdot C_6H_4PPh_2)-Fe(CO)_3$	C_6D_6	H_{trans}	1.94td	$J_{HH'} 9.8$ $J_{HH} 2.3$ $J_{PH} 9.35$	—	51
				H_{cis}	2.3 sept.	$J_{HH'} 8.5$ $J_{PH} 5.55$		
				H'	4.0m	$J_{PH'} 4.55$		
$C_{25}H_{15}AsF_8FeO_3$	29	$(h^2-CF_2CF_2CF_2CF_2)-Fe(AsPh_3)(CO)_3$	$CHCl_3$	F	-13.1^* , -7.4^*	—	*Low field of CF_3CO_2H †High field of CF_3CO_2H (external)	271
				F'	$+52.9^\dagger$	—		
$C_{25}H_{15}F_8FeO_3P$	30	$(h^2-CF_2CF_2CF_2CF_2)-Fe(PPh_3)(CO)_3$	$CHCl_3$	F	$-4.4d^*$, $+2.8d^\dagger$	$J_{PF} 17$ $J_{PF} 9$	*Low field of CF_3CO_2H †High field of CF_3CO_2H (external)	271
				F'	$+60.8^\dagger$	—		
$C_{13}H_{15}F_8FeO_6P$	31	$(1,4-h^2-CF_2CF_2CF_2CF_2)-Fe[P(OEt)_3](CO)_3$	$CHCl_3$	F	$-1.4d^*$, $+1.8d^\dagger$	$J_{PF} 30.5$ $J_{PF} 18$	*Low field from CF_3CO_2H †High field from CF_3CO_2H (external)	271
				F'	$+60.4^\dagger$	—		
$C_{25}H_{15}F_8FeO_6P$	32	$(1,4-h^2-CF_2CF_2CF_2CF_2)-Fe[P(OPh)_3](CO)_3$	$CHCl_3$	F	$-2.8d^*$, $+0.6m^\dagger$	$J_{PF} 29$	*Low field from CF_3CO_2H †High field from CF_3CO_2H (external)	271
				F'	$+60.0^\dagger$	—		
$C_{25}H_{15}F_8FeO_3Sb$	33	$(1,4-h^2-CF_2CF_2CF_2CF_2)-Fe(SbPh_3)(CO)_3$	$CHCl_3$	F	-8.0^* , -7.3^*	—	*Low field from CF_3CO_2H †High field from CF_3CO_2H (external)	271
				F'	$+59.3^\dagger$	—		
(c) Tetracarbonyl derivatives								
$C_6H_4FeO_4$	34	$(h^2-CH_2=CH_2)Fe(CO)_4$	—	H	2.48s	—	—	274

$C_6BrF_3FeO_4$	35	$(h^2-CFBr=CF_2)Fe(CO)_4$	Petroleum ether	F F'_{cis} F'_{trans}	35.2 10.4 19.4	— $J_{FF'}$ 67 J_{FF} 3 $J_{F'F'}$ 126	To high field of CF_3CO_2H T 35°	268
$C_6ClF_3FeO_4$	36	$(h^2-CFCl=CF_2)Fe(CO)_4$	$CHCl_3$	F F'_{cis} F'_{trans}	38 16 21	— J_{FF} 62 $J_{FF'}$ 2.4 $J_{F'F'}$ 130	To high field from CF_3CO_2H T 35°	268
$C_6Cl_2F_2FeO_4$	37	$(h^2-CCl_2=CF_2)Fe(CO)_4$	CH_2Cl_2	F	6.0s	—	To high field from CF_3CO_2H T 35°	268
$C_6F_4FeO_4$	38	$(h^2-CF_2=CF_2)Fe(CO)_4$	CH_2Cl_2	F	32.0*	—	*To high field from CF_3CO_2H (external). Coupling constants (not reported for this compound) suggest an approach to sp^3 hybridization of the olefinic carbon atoms, but the authors conclude that there is probably no real difference between (I) and (II) since π -electron donation by the olefin is accompanied by back donation from filled d_{xy} orbitals of the iron to π^* -antibonding orbitals of the olefin, a process which is expected to be more efficient for fluoro-olefins than for hydrocarbons:	275 268

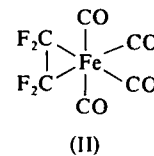
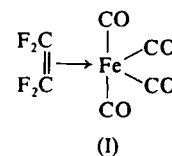
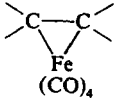


TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_7HF_3FeO_4$	39	$(h^2-CF_2=CHCF_3)Fe(CO)_4$	Liquid	F 10*	J_{FF} 113	*To high field of CF_3CO_2H	268
				F -5.9† -22.8†	$J_{FF'}$ 6, 11	†To low field of CF_3CO_2H T 35°	
$C_7F_6FeO_4$	40	$(h^2-CF_2=CF'CF'_3)Fe(CO)_4$	Liquid	F 18*	J_{FF} 141	*To high field of CF_3CO_2H	268
				15*	$J_{FF'}$ 62.3, 9.7		
				F' 105*	$J_{F'F''}$ 11.5	†To low field of CF_3CO_2H	
				F'' -10†	$J_{FF''}$ 11.6, 2.6	T 35°	
$C_6H_2F_2FeO_4$	41	$(h^2-CH_2=CF_2)Fe(CO)_4$	—	Not reported		The NMR data is interpreted in terms of a cyclic ring structure, viz:  (CO) ₄	276
$C_6HF_3FeO_4$	42	$(h^2-CF_2=CHF)Fe(CO)_4$	—				
$C_{10}F_{12}FeO_4$	43	$[h^2C(CF_3)_2=C(CF_3)_2]Fe(CO)_4$	—				
						The ¹ H NMR signals are shifted well to high field of the vinylic region and the geminal F-F coupling is high (110–138 MHz) and the <i>trans</i> -F-F coupling low	
$C_7H_4FeO_5$	44	$(h^2-CH_2=CH'CH''O)Fe(CO)_4$	$(CD_3)_2CO$	H _{cis} 3.03	—	Corresponding chemical shifts for the free ligands are: δ 6.20, 6.25, 6.25, 9.58 respectively	96
				H _{trans} 2.99	—		
				H' 3.95	—		
				H'' 9.45	—		

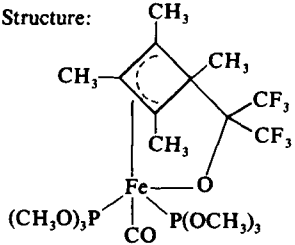
$C_8H_5ClFeO_5$	45	$(h^2-CHCl=CH'COCH_3)Fe(CO)_4$	CCl_4	H	5.07	$J_{HH'}$ 8.6	100 MHz	277
				H'	3.69	—	Reference hexamethyldisiloxane	278 1000
$C_{13}H_7ClFeO_5$	46	$(h^2-CHCl=CH'COPh)Fe(CO)_4$	CCl_4	H	5.35	$J_{HH'}$ 8.0	100 MHz	277
				H'	4.43	—	Reference hexamethyldisiloxane	278 1000
$C_{14}H_9ClFeO_5$	47	$(h^2-CHCl=CH'COC_6H_4CH_3-p)-Fe(CO)_4$	CCl_4	H	5.31	$J_{HH'}$ 8.5	100 MHz	277
				H'	4.42	—	Reference hexamethyldisiloxane	278
$C_{13}H_6BrClFeO_5$	48	$(h^2-CHCl=CH'COC_6H_4Br-p)-Fe(CO)_4$	CCl_4	H	5.32	$J_{HH'}$ 8.0	100 MHz	277
				H'	4.35	—	Reference hexamethyldisiloxane	278
$C_{14}H_9ClFeO_4$	49	$(h^2-CHCl=CH'COC_6H_4OCH_3-p)Fe(CO)_4$	CCl_4	H	5.31	$J_{HH'}$ 8.0	100 MHz	277
$C_{15}H_{10}FeO_7$	50	$(h^2-C_6H_5COCH=CH'CO_2CH_3)-Fe(CO)_4$ <i>cis</i>	CCl_4	H	3.58	J 9.3	Hexamethyldisiloxane as reference	997
				H'	4.14	—	at 100 MHz	
$C_{15}H_{10}FeO_7$	51	$(h^2-C_6H_5COCH=CH'CO_2CH_3)-Fe(CO)_4$ <i>trans</i>	CCl_4	H	3.88	J 9.7	Hexamethyldisiloxane as reference	997
				H'	4.59	—	at 100 MHz	
$C_{10}H_{12}FeO_8$	52	$[h^2-C(OCH_3)_2=C(OCH_3)_2]-Fe(CO)_4$	$(CD_3)_2CO$	H	3.55s	—	T 0°	279
$C_{14}H_{10}FeO_7S$	53	$[h^2-CH(COCH_3)=CH'SO_2Ph]-Fe(CO)_4$ <i>trans</i>	$CDCl_3$	H	3.64	$J_{HH'}$ 8.6	100 MHz	280
				H'	4.35	—	Reference hexamethyldisiloxane	
$C_{19}H_{12}FeO_7S$	54	$[h^2-CH(COPh)=CH'SO_2Ph]-Fe(CO)_4$ <i>cis</i>	$CDCl_3$	H	4.04	$J_{HH'}$ 9.0	<i>cis</i> -isomer	280
				H'	4.24	—	100 MHz	
				H	4.42	$J_{HH'}$ 10	Reference hexamethyldisiloxane	
				H'	4.66	—	<i>trans</i> -isomer	

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{20}H_{14}FeO_7S$	55	$[h^2\text{-CH(COPh)=CH'SO}_2\text{C}_6\text{H}_4\text{-CH}_3\text{-}p]\text{Fe(CO)}_4$		H	4.03	<i>cis</i> -isomer	280
				H'	4.21		
				H	4.40	<i>trans</i> -isomer	
				H'	4.65		
$C_8F_8FeO_4$	56	$(1,4\text{-}h^2\text{-CF}_2\text{CF}_2\text{CF}_2\text{CF}_2\text{-Fe(CO)}_4$	CHCl_3	F	-5.8*	*To low field of $\text{CF}_3\text{CO}_2\text{H}$ †To high field of $\text{CF}_3\text{CO}_2\text{H}$ (external)	271
				F'	+59.2†		
$C_8F_6FeO_4$	57	$(h^2\text{-C}_4\text{F}_6)\text{Fe(CO)}_4$	Liquid	F	98.8	$/J_{AB}/206$ T 35° To high field of $\text{CF}_3\text{CO}_2\text{H}$	268
				F'	34.4q		
$C_{10}F_6FeO_4$	58	$(h^2\text{-C}_6\text{F}_6)\text{Fe(CO)}_4$	CHCl_3	F	158.4*	Structure =	240
				F'	168.6*		
				F''	122.8*		
$C_9F_8FeO_4$	59	$(h^2\text{-C}_5\text{F}_8)\text{Fe(CO)}_4$	CHCl_3	F	96.8*	$C_5F_8 =$	268
				F'	27.3*		

				F''	39.3*	/J _{AB} /251	*To high field of CF ₃ CO ₂ H T 35°	
C ₁₀ F ₁₀ FeO ₄	60	(h ² -C ₆ F ₁₀)Fe(CO) ₄	CHCl ₃	F F' F''	85.0* 24.0* 53.2*	— /J _{AB} /260 /J _{AB} /266	C ₆ F ₀ =	268
							*To high field of CF ₃ CO ₂ H T 35°	
C ₁₂ H ₁₂ FeO ₄	61	(h ² -C ₈ H ₁₂)Fe(CO) ₄	—		n.a.	—	¹ H NMR chemical shifts: δ 5.47m, 3.2, and 2.1 in ratio 2:2:8	281
C ₁₁ H ₁₂ FeO ₄	62	[h ² -C(CH ₃) ₂ =C=C(CH ₃) ₂]- Fe(CO) ₄	CS ₂	H H	1.84s 2.03 1.98 1.77	— — — —	T +30° T -60°	282
C ₈ F ₆ FeO ₄	63	(1,4-h ² -CF ₂ CF'=CF'CF ₂)- Fe(CO) ₄	—	F F'	-4.0 comp.* +71.9 comp.*	— —	*Relative to C ₆ H ₅ CF ₃	283
C ₁₅ H ₈ F ₄ FeO ₄	64	(2,5-h ² -CF ₂ CF ₂ CHPhCHCHO)- Fe(CO) ₄	—		n.m.	—	—	284
(3) TRIHAPTO LIGANDS								
(a) Monocarbonyl derivatives								
C ₂₆ H ₂₈ FeNO ₃ P	65	[h ³ -CH ₂ CHCHCH ₂ C(OH)- (CH ₃) ₂]Fe(PPh ₃)(NO)(CO)	CS ₂	H	1.27s	—	40 MHz Other signals at δ 7.4 comp., 4.0-3.0 comp., 3.0-2.0 comp, and 1.82bs in ratio 15:2:3:2	265

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{27}H_{28}FeNO_3P$	66	$[h^3-CH_2C(CH_3)C(CH_3)CH_2-COCH_3]Fe(PPh_3)(NO)(CO)$	CS_2	n.a.	—	40 MHz Signals at δ 7.5 comp., 3.7–3.2 comp., 2.95d, 2.16s, 1.48d, 0.83s in ratio 15:3:1:3:3:3	265
$C_{18}H_{30}F_6FeO_8P_2$	67	$[1,2,3-h^3-1,2,3,4-C_4(CH_3)_4-4-C(CF_3)_2O]Fe[P(OCH_3)_3]_2(CO)$	—	H 1.84s, 1.79s, 1.73s, 1.12s		Structure: 	284
$C_{24}H_{22}FeNo_2P$	68	$(h^3-C_5H_7)Fe[P(C_6H_5)_3](NO)(CO)$	CS_2	H' F H H'	3.35d 71.4s 4.95* 4.3–3.0*†, 2.0* 7.5	$J_{PH'}$ 10.0 40 MHz	265

$C_5H_7 =$ 

*Integral ratios 2:1:4 respectively
†This result is unusual in that the central hydrogen of a π -allyl complex normally gives a proton resonance signal to lower field than the protons on the two outer carbons

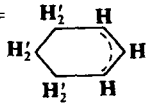
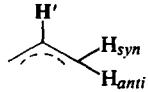
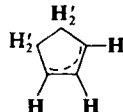
$C_{25}H_{24}FeNO_2P$	69	$(\eta^3-C_6H_9)Fe[P(C_6H_5)_3]-(NO)(CO)$	CS_2	H	4.88*, 3.65*		40 MHz $C_6H_9 =$ 	265
				H'	1.55			
				H''	7.43			
*Integral ratio 1 : 2 respectively								
(b) Dicarbonyl derivatives								
$C_5H_5FeNO_3$	70	$(\eta^3-CH_2CH'CH_2)Fe(NO)(CO)_2$	CCl_4	H_{syn}	3.98d	$J_{HH'} 6.2$		285
				H_{anti}	3.14d	$J_{HH'} 11.4$		
				H'	4.44m	—		
$C_{11}H_{20}FeIO_3P$	71	$(\eta^3-CH_2CH'CH_2)Fe[P(OCH_2CH_3)_3](I)(CO)_2$	—	H	3.92	$J 7$	Signals for π -allyl ligand: Isomer I: δ 3.60d ($J 4$), 3.82 ($J 2.5$), 4.21 sept ($J 7$). Isomer II: δ 3.47d ($J 4$) 3.75d ($J 3$), 4.43 sept ($J 7$).	987
				H'	1.28	$J 7$		
$C_6H_7FeNO_3$	72	$(\eta^3-CH_2CH'CH''CH_3'')Fe-(NO)(CO)_2$	CCl_4	H_{syn}	3.66d	$J_{HH'} 6$	—	285
				H_{anti}	2.78d	$J_{HH'} 10.4$		
				H'	4.04 comp.			
				H''_{anti}				
				H'''	2.05d	$J_{H''H'''} 6$		
$C_9H_{13}FeNO_4$	73	$[\eta^3-CH_2CHCHCH_2C(CH_3)_2OH]Fe(NO)(CO)_2$	CS_2	H	1.31s	—	40 MHz Other signals at δ 4.0 comp., 3.0–1.1 comp., in ratio 3 : 4	265
$C_7H_7FeNO_3$	74	$(\eta^3-CH_2CH'CH''CO_2CH_3'')Fe(NO)(CO)_2$	CCl_4	H_{syn}	3.96d	$J_{HH'} 7.1$	—	285
				H_{anti}	3.12d	$J_{HH'} 11.3$		
				H'	5.17m	—		
				H''_{anti}	3.73d	$J_{H'H''} 10.6$		
				H'''	3.71s	—		

TABLE VII—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_8H_{10}FeO_2$	75	$(h^3-CH_2CH'CH_2)_2Fe(CO)_2$		H_{syn}	2.50	$J_{HH'}$ 6.5	100 MHz T 20°	286
				H_{anti}	1.39	$J_{HH'}$ 12.3		
				H'	4.09	—		
				H_{syn}	3.08	$J_{HH'}$ 6.5	Isomer I T -67°	287
				H_{anti}	1.85	$J_{HH'}$ 12.3		
				H'	4.11	—		
				H_{syn}	1.99	— (Isomer II)	Reference hexamethyldisiloxane The presence of two isomers is attributed to internal rotation of the π -allyl groups, the energy barrier to rotation being estimated to be 4.6 ± 0.8 kcal/mole, viz.	
				H_{anti}	0.96	— T -67°		
				H'	4.11	—		
$C_7H_7FeNO_3$	76	$(h^3-C_5H_7)Fe(NO)(CO)_2$	CS_2	H	5.35 comp.	40 MHz	265	
					4.24t			
				H'	2.1 comp.			



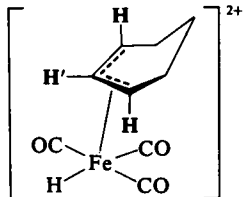
C ₆ H ₅ FeNO ₃	77	(<i>h</i> ³ -C ₆ H ₅)Fe(NO)(CO) ₂	CS ₂	n.a.	—	40 MHz Signals at δ 5.15, 2.1 and 1.0 in ratio 3:4:2	265	
(c) Tricarbonyl derivatives								
C ₆ H ₅ FeClO ₃	78	(<i>h</i> ³ -CH ₂ CH'CH ₂)Fe(Cl)(CO) ₃	CDCl ₃	H _{syn} H _{anti} H'	4.48 3.21 5.11	J _{HH'} 7.7 J _{HH'} 14.7 —	Isomer I* 100 MHz Reference hexamethyldisiloxane	287
				H _{syn} H _{anti} H'	4.22 2.63 5.80	— — —	Isomer II* *Rotational isomers differing in the orientation of the allyl group with respect to the halide ligand	287
C ₆ H ₅ BrFeO ₃	79	(<i>h</i> ³ -CH ₂ CH'CH ₂)Fe(Br)(CO) ₃	CS ₂	H _{syn} H _{anti} H'	4.28 3.41 4.85	J _{HH'} 7.7 J _{HH'} 13.4 —	Isomer I* 100 MHz Reference hexamethyldisiloxane	287
				H _{syn} H _{anti} H'	3.94 2.58 5.7	— — —	Isomer II* *See above	
C ₆ H ₅ FeIO ₃	80	(<i>h</i> ³ -CH ₂ CH'CH ₂)Fe(I)(CO) ₃	CS ₂	H _{syn} H _{anti} H'	4.03 3.67 4.67	J _{HH'} 8.7 J _{HH'} 13 —	Isomer I* 100 MHz Reference hexamethyldisiloxane	287 987
			CCl ₄	H _{syn} H _{anti} H'	4.13 3.77 4.55	J _{HH'} 7.5 J _{HH'} 13 —		
			CS ₂	H _{syn} H _{anti} H'	3.57 2.21 5.83	— — —		Isomer II* *Rotational isomers differing in the orientation of the allyl group with respect to the halide ligand
			CCl ₄	H _{syn} H _{anti} H'	3.75 2.24 5.90	— — —		

TABLE VII—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_6H_5FeNO_6$	81	$(h^3-CH_2CH'CH_2)Fe(NO_3)(CO)_3$	$CDCl_3$	H_{syn} H_{anti} H'	4.70 2.63 5.31	$J_{HH'} 7.5$ $J_{HH'} 15$ —	100 MHz Reference hexamethyldisiloxane	287
$C_6H_5F_3FeO_5$	82	$(h^3-CH_2CH'CH_2)Fe(OCOCF_3)(CO)_3$	$CDCl_3$	H_{syn} H_{anti} H' F	4.68 2.68 5.37tt 75.3*	$J_{HH'} 8$ $J_{HH'} 14$ —	100 and 94.1 MHz	138
$C_9H_5F_3FeO_5$	83	$(h^3-CH_2CH'CH_2)Fe(OCOCF_2CF_3)(CO)_3$	$CDCl_3$	H_{syn} H_{anti} H' F F'	4.69 2.66d 5.40tt 120.0q 83.4t	$J_{HH'} 8$ $J_{HH'} 14$ — $J_{FF} 1.5$ —	100 and 94.1 MHz	138
$C_6H_4Cl_2FeO_3$	84	$(h^3-CH_2C(Cl)(CH_2)Fe(Cl)(CO)_3)$	—	H	4.82b 3.62b	— —	—	288
$[C_7H_7FeO_3]^+$	85	$\{[h^3-CH_2C(CH_3)CH_2]Fe(CO)_3\}^+$	—		n.a.	—	Signals at δ 5.0s, 2.7s, 2.0s, in ratio 2:2:3	920
$C_7H_7ClFeO_3$	86	$[h^3-CH_2C(CH_3)CH_2]Fe(Cl)(CO)_3$	—		n.a.	—	Signals at δ 4.32s, 3.27s, 1.99s	920
$C_{14}H_{13}ClFeO_3$	87	$[h^3-CH(Ph)CH'C(CH_3)_2]Fe(Cl)(CO)_3$	—	H_{anti} H'	4.68d 5.65d	$J 12$ $J 12$	—	289

			H''_{syn}	2.20s	—			
			H''_{anti}	1.57s	—			
$[C_8H_{10}FeO_3]^{2+}$	88	$[(h^3-CH_3CH'CH''CH'''CH_3^{IV})-Fe(H^V)(CO)_3]^{2+}$	HSO ₃ F	H	1.80	$J_{HH'}$ 6.2	Diprotonated <i>trans</i> -piperylene-iron tricarbonyl	290
				H'_{anti}	2.50	$J_{H'H''}$ 11.4		
				H''	6.50	—		
				H'''	6.96	$J_{H''H''''}$ 6.5		
				H^{IV}	1.05	$J_{H^{IV}H^{IV}}$ 6		
						$J_{H^{IV}H^V}$ 11		
					-0.85	$J_{H^{IV}H^V}$ 22.5		
				H^V	-14.67	—		
$[C_9H_{12}FeO_3]^{2+}$	89	$[(h^3-CH_3CH'CH''CH'''CH_2^{IV}-CH_3^V)Fe(H^{VI})(CO)_3]^{2+}$	HSO ₃ F	H	1.84	$J_{HH'}$ 6.2	Diprotonated <i>trans, trans</i> -hexa-2,4-dieneiron tricarbonyl	290
				H'_{anti}	2.50	$J_{H'H''}$ 10.5		
				H''	6.37	—		
				H'''	6.59	$J_{H''H''''}$ 5.5		
				H^{IV}	-0.30	$J_{H^{IV}H^{VI}}$ 22		
				H^V	1.26	$J_{H^{IV}H^V}$ 6.2		
				H^{VI}	-14.64	—		
$[C_9H_9FeO_4]^+$	90	$\{[h^3-CH_2CHCHCH_2COCH_3]-Fe(CO)_3\}^+$	CD ₃ CN	Not reported		$J_{HH'}$ 2.6 $J_{H'H'}$ -23	Isolated as the (AlCl ₄) ⁻ salt. The iron atom formally possesses only 16 electrons but may obtain a closed-shell configuration by intramolecular σ -donation of a lone pair of electrons from the acyl oxygen atom. This restricts rotation about the C ₃ -C ₄ bond and increases the geminal coupling constant and causes these protons (H') to be unequally coupled to the C3 proton (H)	291

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$[\text{C}_9\text{H}_{10}\text{FeO}_3]^{2+}$	91	$(h^3\text{-C}_6\text{H}_9)\text{Fe}(\text{H})(\text{CO})_3$	HSO_3F	H	6.92	—	Diprotonated cyclohexa-1,3-dieneiron tricarbonyl	290
				H'	5.21			
					6.36			
								
$\text{C}_7\text{H}_5\text{FeO}_4$	92	$(h^3\text{-CH}_2\text{---}\overset{(-)}{\text{CH}}'\text{---}\text{CH}''\text{CH}'''\text{=O})\text{-Fe}(\text{CO})_3$	$(\text{CD}_3)_2\text{SO}$	H_{syn}	1.89m	—	The π -bonded allyl anion acts as a four-electron donor. The isomeric hydroxybutadiene anion structure is ruled out by the NMR data	1002
				H_{anti}	1.30m	—		
				H'	5.14m	—		
				H_{syn}''	4.33m	—		
				H'''	6.99	—		
(d) Tetracarbonyl derivatives								
$[\text{C}_{11}\text{H}_{13}\text{FeO}_4]^+$	93	$[h^3\text{-C}(\text{CH}_3)_2\text{---}\overset{+}{\text{C}}\text{H}'\text{---}\text{C}(\text{CH}_3)_2]\text{-Fe}(\text{CO})_4$	$(\text{CD}_3)_2\text{CO}$	H	2.40	—	Tetrafluoroborate	292
					2.30	—		
				H'	5.67	—		
$[\text{C}_{13}\text{H}_{15}\text{FeO}_5]^+$	94	$[h^3\text{-C}(\text{CH}_3)_2\text{---}\overset{+}{\text{C}}(\text{COCH}_3)\text{---}\text{C}(\text{CH}_3)_2]\text{Fe}(\text{CO})_4$	—		—	—	AlCl_4^- salt	292
$[\text{C}_{18}\text{H}_{17}\text{FeO}_5]^+$	95	$[h^3\text{-C}(\text{CH}_3)_2\text{---}\overset{+}{\text{C}}(\text{COC}_6\text{H}_5)\text{---}\text{C}(\text{CH}_3)_2]\text{Fe}(\text{CO})_4$	—		—	—	AlCl_4^- salt	292

(4) TETRAHAPTO LIGANDS

(a) Monocarbonyl derivatives

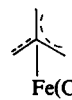
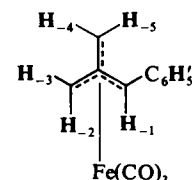
C ₃ H ₆ F ₆ FeOP ₂	96	(<i>h</i> ⁴ -C ₄ H ₆)Fe(PF ₃) ₂ (CO)	—	Not reported	J _{PF} 1300	C ₄ H ₆ = butadiene At low temperatures the PF ₃ groups are non-equivalent. At room temperature the spectra show a time-averaged equivalence indicating fluxional nature comparable to the Bailar twist	293	
C ₉ H ₁₂ FeO	97	(<i>h</i> ⁴ -C ₄ H ₆) ₂ Fe(CO)	C ₆ D ₆	H	4.27, 1.0, −0.35	— — —	C ₄ H ₆ = butadiene 100 MHz Integral ratios = 2 : 2 : 2	294 295
C ₁₁ H ₁₆ FeO	98	[<i>h</i> ⁴ -C ₄ H ₅ (CH ₃)] ₂ Fe(CO)	C ₆ D ₆	H	3.9m, 1.07m, −0.4m	— — —	C ₄ H ₅ (CH ₃) = isoprene Integral ratios = 1 : 2 : 2	295
				H'	1.68s			
C ₁₃ H ₁₆ FeO	99	(<i>h</i> ⁴ -C ₆ H ₈) ₂ Fe(CO)	C ₆ D ₆	H	4.34, 2.54, 1.95, 1.05		C ₆ H ₈ = cyclohexadiene Integral ratios = 2 : 2 : 2 : 2	295
(b) Dicarbonyl derivatives								
C ₂₄ H ₂₁ FeO ₂ P	100	(<i>h</i> ⁴ -C ₄ H ₆)Fe[P(C ₆ H ₅) ₃](CO) ₂	—	H	4.85, 1.75, −0.25		C ₄ H ₆ = butadiene	298
				H'	7.3 comp.			

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{26}H_{23}FeO_3P$	101	$(h^4-C_6H_8O)Fe[P(C_6H_5)_3](CO)_2$	CS_2	H	n.a.	—	C_6H_8O = Hexa-3,5-diene-2-one Signals at 6.0–5.0 comp., 5.0–4.0 comp., 1.91s, 1.5–0.2 comp., in ratio 1:1:4:2 40 MHz	265
				H'	7.4 comp.	—		
$C_{27}H_{25}FeO_3P$	102	$(h^4-C_7H_{10}O)Fe[P(C_6H_5)_3](CO)_2$	CS_2	H	n.a.	—	$C_7H_{10}O$ = 3-methylhexa- 3,5-diene-2-one Signals at δ 5.45d, 1.92d, 1.44d, 0.9(–)0.6 comp., in ratio 1:3:4:2 40 MHz	265
				H'	7.35 comp.	—		
$C_{27}H_{25}FeO_3P$	103	$(h^4-C_7H_{10}O)Fe[P(C_6H_5)_3](CO)_2$	CS_2	H	n.a.	—	$C_7H_{10}O$ = hepta-3,5-diene-2-one Signals at 5.6–4.6 comp., 1.31s, 1.02d, 0.3(–)0.1 comp., in ratio 2:3:3:2. 40 MHz	265
				H'	7.45 comp.	—		
$C_{28}H_{27}FeO_3P$	104	$(h^4-C_8H_{12}O)Fe[P(C_6H_5)_3](CO)_2$	CS_2	H	n.a.	—	$C_8H_{12}O$ = 4,5-dimethylhexa- 3,5-diene-2-one Signals at δ 2.3d, 1.85d, 1.38s, 0.0(–)0.8 comp., in ratio 3:3:4:2 40 MHz	265
				H'	7.4 comp.	—		
$C_{31}H_{25}FeO_2P$	105	$[1,2,3,4-h^4-5-C_5H_5^*(C_6H_5)]-$ $Fe[P(C_6H_5)_3](CO)_2$	$CDCl_3$	H_{-1}, H_{-4}	2.62m	—	*5-Phenylcyclopentadiene	193
				H_{-2}, H_{-3}	5.15m	—		

				H_{-5}	3.85m	—			
				H'	7.03m	—			
					7.34m	—			
$C_{31}H_{26}F_5FeO_2P$	106	$[1,2,3,4-h^4-5-C_5H_5^*(C_6F_5)]-$ $Fe[P(C_6H_5)_3](CO)_2$	$CDCl_3$	H_{-1}, H_{-4}	2.60m	—		*5-Pentafluorophenyl-	193
				H_{-2}, H_{-3}	4.97m	—		cyclopentadiene	296
				H_{-5}	4.15m	—		(<i>exo</i> -isomer)	
				H'	7.30m	—			
$C_{19}H_{11}F_{12}FeO_3P$	107	$[1,2,3,4-h^4-1,2,3,4-C_3(CF_3)_4^*O]-$ $Fe[P(CH_3)_2C_6H_5](CO)_2$	$CDCl_3$	H	2.04d	$J_{PH} 11.0$		100 MHz	297
				H'	7.59m	—		*Tetrakis(trifluoromethyl)	
			$CHCl_2$	F	52.7m	—		cyclopentadiene-5-one	
					54.0m	—		94.1 MHz	
$C_{17}H_{15}F_{12}FeO_6P$	108	$[1,2,3,4-h^4-1,2,3,4-C_3(CF_3)_4^*O]-$ $Fe[P(OCH_2CH_3)_3](CO)_2$	$CDCl_3$	H	4.16q	$J_{PH} 7.0$ $J_{HH'} 7.0$		100 MHz	297
				H'	1.38t	—		*See above	
				F	52.6m	—		94.1 MHz	
					54.9m	—			
$C_{26}H_{23}FeO_2P$	109	$(h^4-C_6H_8)Fe[P(C_6H_5)_3](CO)_2$	—	H	n.a.	—		C_6H_8 = cyclohexadiene	298
				H'	7.5 comp.	—		Signals at δ 4.85, 2.50, 1.6,	
								in ratio 2:2:4.	
$C_{28}H_{25}FeO_3P$	110	$[1,2,3,4-h^4-1-C_6H_7^*(COCH_3)]-$ $Fe[P(C_6H_5)_3](CO)_2$	CS_2	H, H'	n.a.	—		*1-acetylcyclohexa-1,3-diene	265
				H''	7.4 comp.	—		Signals at δ 5.8bd, 4.53 comp.,	
								2.1s, 1.5 comp., in ratio	
								1:1:4:4.	
								40 MHz	
$C_{27}H_{25}FeO_2P$	111	$(h^4-C_7H_{10})Fe[P(C_6H_5)_3](CO)_2$	—	H	n.a.	—		C_7H_{10} = cyclohepta-1,3-diene	298
				H'	7.4 comp.	—		Signals at 4.55, 2.36, 1.83, 1.25,	
								in ratio 2:2:4:2	

TABLE VII—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{27}H_{23}FeO_2P$	112	$(1,2,3,4-h^4-C_7H_8)Fe-[P(C_6H_5)_3](CO)_2$	—	H H'	n.a. 7.35 comp.	— —	C_7H_8 = cyclohepta-1,3,5-triene Signals at δ 4.7 comp., 2.8–1.0, in ratio 2:6.	298
<i>(c) Tricarbonyl derivatives</i>								
$C_7H_6FeO_3$	113	$[h^4-C(CH_2)_3]Fe(CO)_3$	—	H $^{13}C^*$	2.0s −18.8s +87.8s	— — —	Structure:  Fe(CO) ₃	55 920
					+139.8t	J 158	*Relative to CS ₂ (0.0ppm) at 25.1 MHz ^{13}C satellites in 1H NMR spectrum give J_{CH} 162	
$C_{13}H_{10}FeO_3$	114	$(h^4-C_{10}H_{10})Fe(CO)_3$	CCl ₄	H_{-1} H_{-2} H_{-3} H_{-4} H_{-5} H'	4.28d 1.84d 1.84s 2.30d 2.87d 7.11s	$J_{1,4}$ 3.3 $J_{2,5}$ 5.4 — J 3.3 J 5.4 —	Structure:  Fe(CO) ₃	299

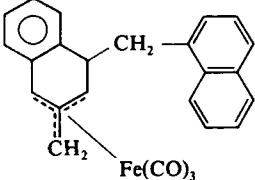
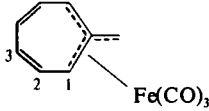
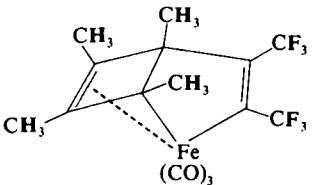
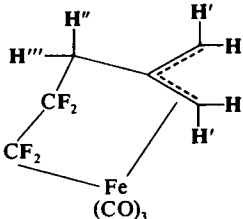
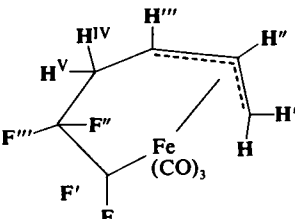
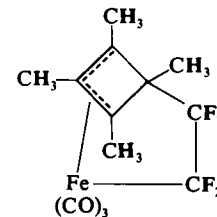
$C_{25}H_{18}FeO_3$	115	$(h^4-C_{22}H_{18})Fe(CO)_3$	CS_2	H^*	7.52m, — 6.92s, — 3.60 comp., — 1.7s, —	Structure	128
							
					1.57s —	*Integral ratio 7:4:5:1:1	
$C_{25}H_{18}FeO_3$	116	$(h^4-C_{22}H_{18})Fe(CO)_3$	—	—	—	Structure: as above but β -naphthyl derivative	128
$C_{11}H_8FeO_3$	117	$(h^4-C_8H_8)Fe(CO)_3$	CS_2	H^*	5.87m, 3.70dd,	Structure:	28
							
					1.40s	*Integral ratio 4:2:2 $J_{1,2}$ 6, $J_{1,3}$ 1)	
						Spectrum unchanged over the temperature range -60 to +140°C	
$C_{15}H_{12}F_6FeO_3$	118	$(h^4-C_{12}H_{12}F_6)Fe(CO)_3$	—	H	2.60s — 2.42s — 1.72q J_{FH} 3.0 1.56s —	Structure:	300
				F	55.2q J_{FF} 18.0 55.4qq J_{FF} 18.0 J_{FF} 3.0		

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_9H_6F_4FeO_3$	119	$(h^4-C_6H_6F_4)Fe(CO)_3$	—	H	2.42	$J_{HH'}$ 2.0	Structure: 	284
				H'	3.38	$J_{HH'}$ 2.0		
				H''	2.60	$J_{H''F}$ 3.0		
				H'''	2.56	$J_{H'''F}$ 3.0		
				F	75m	—		
					106.2m	—		
$C_9H_6F_4FeO_3$	120	$(h^4-C_6H_6F_4)Fe(CO)_3$	—	H	2.68	$J_{HH'}$ 3.0 $J_{HH''}$ 13.0 J_{HF} 5.0	Structure: 	284
				H'	3.46	$J_{H'H''}$ 7.0		
				H''	5.10	$J_{H''H'''} 7.0$		
				H'''	4.68	$J_{H'''H^{IV}} 7.0$		
				H ^{IV}	2.42	$J_{H^{IV}H^V} 14.0$ J_{HF} 14.0		
				H ^V	1.40	$J_{H'''H^V} 7.0$ J_{H^VF} 38.0		
				F	108.5	$J_{FF'}$ 222, $J_{FF''}$ 2.0, $J_{FF'''} 14.0$ $J_{FH^{IV}} 14.0$		
				F'	104.5	$J_{FF'}$ 222		
				F''	87.3	$J_{F''F'''} 236,$ $J_{FF''}$ 2.0, $J_{F'F''} 8.0$		

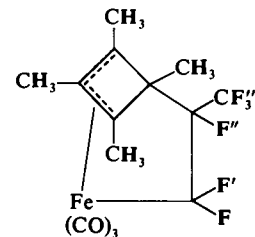
			F'''	76.8	$J_{F''F'''} 236,$ $J_{F'F'''} 1.0,$ $J_{HF'''} 5.6,$ $J_{FF'''} 14$		
$C_{13}H_{12}F_4FeO_3$	121	$(h^4-C_{10}H_{12}F_4)Fe(CO)_3$	—				
			H	2.20s, 1.64s, 1.10s	— — —		
			F	70.8m 120.8m	— —		
$C_{14}H_{12}F_6FeO_3$	122	$(h^4-C_{11}H_{12}F_6)Fe(CO)_3$	—				
			H	2.20s, 1.79s, 1.62s, 1.12s	—		
			F	112.3dm	$J_{FF'} 240$ $J_{FF''} 6.0$		
			F'	107.5dm	$J_{F'F''} 120$ $J_{F'F'''} 3.0$		
			F''	155.0m	$J_{F''F'''} 12.0$		
			F'''	69.3m	$J_{FF'''} 17.0$		

Structure:



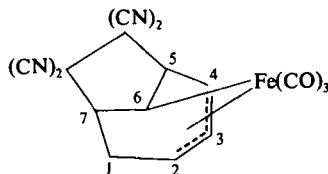
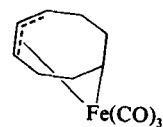
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Structure:



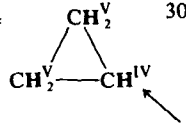
300

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{16}H_8FeN_4O_3$	123	$(2,3,4,6-h^4-C_{13}H_8N_4)Fe(CO)_3$	—	H_{-1}	3.15, 2.38	Structure: 	301
				H_{-2}	4.76		
				H_{-3}, H_{-4}	5.10		
				H_{-5}	4.43		
				H_{-6}	1.68		
				H_{-7}	3.82		
$C_{11}H_{12}FeO_3$	124	$(1,2,3,6-h^4-C_8H_{12})Fe(CO)_3$	—	Not reported		Structure: 	302
$C_7H_6FeO_3$	125	$(h^4-CH_2=CH'-CH'=CH_2)-Fe(CO)_3$	—	H_{syn}	1.90	Relative to CS_2 (0.0 ppm)	1046 201 1035
				H_{anti}	0.22		
				H'	5.37		
				C_{-1}, C_{-4}	157 ± 5		303
				C_{-2}, C_{-3}	112 ± 5		
				CO	-16 ± 5		
				H_{syn}	1.52		
				H_{anti}	0.05		
				H'	4.94		
			C_6D_6			60 and 100 MHz	

$C_7H_3BrFeO_3$	126	$(h^4-CH_2=CH'-CH''=CH'''Br)-Fe(CO)_3$	C_6D_6	H_{syn}	1.19	—	60 and 100 MHz	303
				H_{anti}	-0.44	—		
				H'	4.49	—		
				H''	5.09	—		
				H''_{anti}	1.93	—		
$C_7H_3BrFeO_3$	127	$(h^4-CH_2=CH'-C(Br)=CH_2)-Fe(CO)_3$	C_6D_6	H_{syn}	1.09	—	60 and 100 MHz	303
				H_{anti}	-0.62	—		
				H'	5.29	—		
				H''_{syn}	2.00	—		
				H''_{anti}	0.22	—		
$C_7H_3ClFeO_3$	128	$(h^4-CH_2=CH'-C(Cl)=CH_2)-Fe(CO)_3$	Liquid	H_{syn}	1.58	—	60 and 100 MHz	303
				H_{anti}	-0.21	—		
				H'	5.71	—		
				H''_{syn}	2.23	—		
				H''_{anti}	0.55	—		
$C_7H_4Cl_2FeO_3$	129	$(h^4-ClCH=CH'-CH'=CHCl)-Fe(CO)_3$	—	H	1.99	$^3J_{HH'} 5.9$ $^4J_{HH'} < 0.4$ $J(^{13}C-H) 193.2$	—	991 304
				H'	4.88	$J_{H'H'} 5.9$ $J(^{13}C-H') 176.9$		
$C_9H_8Cl_2FeO_3$	130	$[h^4-CH(Cl)=C'(CH_3)-C'(CH_3)=CH(Cl)]Fe(CO)_3$	C_6H_6	H	1.98s*	$J(^{13}C-H) 191.5$	100 MHz	304
				H'	2.02s†	$J(^{13}C-H) 129.2$	*Half-height width 2.5 Hz †Half-height width 1.5 Hz	
$C_8H_8FeO_3$	131	$(h^4-CH_2=CH-CH=CHCH_3)-Fe(CO)_3$ <i>cis</i>	CCl_4	n.a.	—	—	Signals at δ 5.28d, 2.67t, 1.77d, 1.47dd, 1.03, in ratio 2:1:1:1:3	305
$C_9H_{10}FeO_3$	132	$[h^4-CH_2=CH-CH=C(CH_3)_2]-Fe(CO)_3$	—	n.a.	—	—	Signals at δ 5.27-4.98m, 1.83-1.3m, 1.03s, in ratio 2:5:3	305

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_9H_{10}FeO_3$	133	$(h^4\text{-CH}_3\text{CH=CH-CH=CHCH}_3)\text{Fe(CO)}_3$	—	H 5.0	—	—	306
$C_{10}H_{12}FeO_3$	134	$\{h^4\text{-(CH}_3)_2\text{C=CH-C(CH}_3\text{)=CH}_2\}\text{Fe(CO)}_3$	—	—	—	—	292
$C_9H_{10}FeO_3$	135	$(h^4\text{-CH}_2\text{=CH-CH=CHCH}_2\text{-CH}_3)\text{Fe(CO)}_3$	—	H 5.1m 0.2m	—	—	306
$C_{11}H_{12}FeO_3$	136	$[h^4\text{-CH}_2\text{=C(C}_3\text{H}_5)^*\text{-CH'=CH''CH}_3^{\prime\prime}]\text{Fe(CO)}_3$ <i>trans</i>	$CDCl_3$	H_{syn} 1.92dd H_{anti} 0.92d H' 4.82d H''_{anti} 1.6m H''' 1.25d H^{IV} 1.43 quin. H^V 0.80–0.42m	— — J 8 — J 6 — —	$*C_3H_5 =$  100 MHz	307
$C_{15}H_{14}FeO_4$	137	$[h^4\text{-CH}_2\text{=C}(p\text{-C}_6\text{H}_4\text{OCH}_3^{\prime\prime})\text{-CH'''=CH}^{IV}\text{CH}_3^V]\text{Fe(CO)}_3$ <i>trans</i>	$CDCl_3$	H_{syn} 2.19dd H_{anti} 0.35d H' 7.20 H'' 3.78s H''' 5.55bd H^{IV}_{anti} 1.07dq H^V 1.49d	J_{HH} 2.5 — — — $J_{H''H^{IV}}$ 9 —	—	308
$C_{13}H_{19}FeNO_3$	138	$[h^4\text{-CH}_3\text{CH'=CH''-CH'''=CH}^{IV}\text{(CH}_3^V\text{)NHCH(CH}_3)_2\text{)]Fe(CO)}_3$ <i>trans cis</i>	CD_3OD	H, H^V 1.4 H' 2.52 H'' 5.41 H''' 2.22 H^{IV} 2.7	— — — — —	As the hydrochloride 100 MHz	309 1036

C ₁₆ H ₁₇ FeNO ₃	139	[<i>h</i> ⁴ -CH ₃ CH'=CH''-CH'''= CH ^{IV} CH ^V (CH ₃ ^{VI})NHPh]- Fe(CO) ₃ <i>trans trans</i>	CD ₃ OD	H, H'	~1.4	—	100 MHz	309
				H''	~4.8	—		1036
				H'''	~5.1	—	Oily compound converted into its fluoroborate salt for the NMR determination	
				H ^{IV}	~0.8	—		
				H ^V	~3.30	—		
				H ^{VI}	1.50	—		
C ₁₆ H ₁₇ FeNO ₃	140	[<i>h</i> ⁴ -CH ₃ CH'=CH''-CH'''= CH ^{IV} CH ^V (CH ₃ ^{VI})NHPh]- Fe(CO) ₃ <i>trans cis</i>	CD ₃ OD	H	~1.4	<i>J</i> _{HH'} 6	100 MHz	309
				H'	~2.4	<i>J</i> _{H'H''} 10		
				H''	~5.13	<i>J</i> _{H''H'''} 5		
				H'''	4.80	<i>J</i> _{H'''H^V} 8		
				H ^{IV}	~2.2	<i>J</i> _{H^{IV}H^V} 10		
				H ^V	2.94	<i>J</i> _{H^VH^{VI}} 6		
				H ^{VI}	~1.3	—		
C ₁₇ H ₁₉ FeNO ₃	141	[<i>h</i> ⁴ -CH ₃ CH'=CH''-CH''= CH'CH'''(CH ₃ ^V)NHCH ₂ ^V Ph]- Fe(CO) ₃ <i>trans cis</i>	CD ₃ OD	H	1.43	—	100 MHz As the hydrochloride	309
				H'	~2.3	—		1036
				H''	5.48	—		
				H'''	2.73	—		
				H ^{IV}	1.49	—		
C ₁₈ H ₂₁ FeNO ₃	142	[<i>h</i> ⁴ -CH ₃ CH'=CH''-CH''= CH'''CH'''(CH ₃ ^V)(NHCH- (CH ₃)Ph)Fe(CO) ₃ <i>trans cis</i>	CD ₃ OD	H	1.27	—	(+) Diastereoisomer, as the hydrochloride 100 MHz	309
				H'	~1.7	—		
				H''	~5.5	—		
				H'''	~2.4	—		
				H ^{IV}	1.52	—		
				H	1.28	—	(–) Diastereoisomer, as the hydrochloride	1036
				H'	1.70	—		
				H''	~5.3	—		
				H'''	~2.3	—		
				H ^{IV}	1.38	—		

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{16}H_{16}BrFeNO_3$	143	$[h^4-CH_3CH'=CH''-CH'''=CH^{IV}CH^V(CH_3^{VI})\chi p-NHC_6H_4Br)]Fe(CO)_3$ <i>trans cis</i>	$CDCl_3$	H	1.45	—	100 MHz	309
				H'	2.35	—		
				H''	5.20	—		
				H'''	4.88	—		
				H^{IV}	2.13	—		
				H^V	2.88	—		
				H^{VI}	1.30	—		
$C_{16}H_{16}BrFeNO_3$	144	$[h^4-CH_3CH'=CH''-CH'''=CH^{IV}CH^V(CH_3^{VI})\chi p-NHC_6H_4Br)]Fe(CO)_3$ <i>trans trans</i>	$CDCl_3$	H	1.38	—	100 MHz	309 1036
				H'	1.15	—		
				H''	4.94	—		
				H'''	5.12	—		
				H^{IV}	0.80	—		
				H^V	3.21	—		
				H^{VI}	1.30	—		
$C_{17}H_{19}FeNO_3$	145	$[h^4-CH_3CH'=CH''-CH'''=CH'CH^{IV}(CH_3^V)\chi p-NHC_6H_4CH_3)]Fe(CO)_3$ <i>trans cis</i>	$CDCl_3$	H	1.22	—	100 MHz	309
				H'	~ 2.1	—		
				H''	4.90	—		
				H'''	4.65	—		
				H^{IV}	2.70	—		
				H^V	1.12	—		
$C_{17}H_{19}FeNO_3$	146	$[h^4-CH_3CH'=CH''-CH'''=CH^{IV}CH^V(CH_3^{VI})\chi p-NHC_6H_4CH_3)]Fe(CO)_3$ <i>trans trans</i>	$CDCl_3/C_6D_6$	H	1.22	—	100 MHz	309
				H'	~ 0.9	—		
				H''	4.60	—		
				H'''	4.86	—		

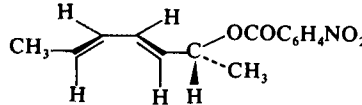
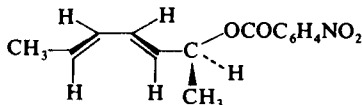
				H^{IV}	0.60	—		
				H^V	3.15	—		
				H^{VI}	1.22	—		
$C_{16}H_{16}^-$ FeN_2O_5	147	$[h^4-CH_3CH'=CH''-CH'''=$ $CH^{IV}CH^V(CH_3^{VI})(m-$ $NHC_6H_4NO_2)]Fe(CO)_3$ <i>trans trans</i>	$CDCl_3$	H	1.40	—	100 MHz	309
				H'	1.20	—		
				H''	4.98	—		
				H'''	5.17	—		
				H^{IV}	0.82	—		
				H^V	3.30	—		
				H^{VI}	1.34	—		
$C_{16}H_{16}^-$ FeN_2O_5	148	$[h^4-CH_3CH'=CH''-CH'''=$ $CH^{IV}CH^V(CH_3^{VI})(p-$ $NHC_6H_4NO_2)]Fe(CO)_3$ <i>trans trans</i>	$CDCl_3$	H	1.40	—	100 MHz	309
				H'	1.00	—		1036
				H''	4.70	—		
				H'''	5.86	—		
				H^{IV}	0.60	—		
				H^V	3.14	—		
				H^{VI}	1.15	—		
$C_7H_6FeO_4$	149	$[h^4-CH_3=CH'-C(OH'')=$ $CH_2''']Fe(CO)_3$	C_6D_6	H_{syn}	1.28dd	—	—	310
				H_{anti}	-0.57dd	—		
				H'	4.94t	—		
				H''	5.88s	—		
				H'''_{syn}	1.88d	—		
				H'''_{anti}	0.11d	—		
$C_9H_8FeO_5$	150	$[h^4-CH_2=CH'-C(OCOCH_3')=$ $CH_2''']Fe(CO)_3$	C_6D_6	H_{syn}	1.15	—	60 and 100 MHz	303
				H_{anti}	-0.57	—		
				H'	5.32	—		
				H''	1.67	—		
				H'''_{syn}	1.98	—		
				H'''_{anti}	0.29	—		

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_9H_8FeO_5$	151	$(h^4\text{-CH}_2=\text{CH}'-\text{CH}''=\text{CH}'''\text{-OCOCH}_3^{\text{IV}})\text{Fe}(\text{CO})_3$ <i>trans</i>	C_6D_6	H_{syn}	1.18	—	60 and 100 MHz	303
				H_{anti}	-0.25	—		
				H'	4.45	—		
				H''	4.90	—		
				H'''_{anti}	3.93	—		
$C_9H_8FeO_5$	152	$(h^4\text{-CH}_2=\text{CH}'-\text{CH}''=\text{CH}'''\text{-OCOCH}_3^{\text{IV}})\text{Fe}(\text{CO})_3$	C_6D_6	H^{IV}	1.57	—	60 and 100 MHz	303
				H	1.80	—		
				H'	4.97	—		
				H''	4.43	—		
				H'''	5.63	—		
$C_{15}H_{12}FeO_5$	153	$[h^4\text{-CH}_2=\text{CH}'-\text{C}(\text{OCOCH}_2^{\text{IV}}\text{-Ph})=\text{CH}_2'']\text{Fe}(\text{CO})_3$	C_6D_6	H_{syn}	1.10	—	60 and 100 MHz	303
				H_{anti}	-0.67	—		
				H'	5.32	—		
				H''	4.96	—		
				H'''_{syn}	2.02	—		
$C_{14}H_{10}FeO_5$	154	$[h^4\text{-CH}_2=\text{CH}'-\text{C}(\text{OCOPh})=\text{CH}_2'']\text{Fe}(\text{CO})_3$	C_6C_6	H'''_{anti}	0.22	—	60 and 100 MHz	303
				H_{syn}	1.23	—		
				H_{anti}	-0.48	—		
				H'	5.54	—		
				H''_{syn}	2.05	—		
$C_{13}H_9FeNO_6S$	155	$[h^4\text{-CH}_2=\text{CH}'-\text{C}(p\text{-OSO}_2\text{C}_6\text{-H}_4^{\text{IV}}\text{NO}_2)=\text{CH}_2'')\text{Fe}(\text{CO})_3$	C_6D_6	H'''_{anti}	0.41	—	60 and 100 MHz	303
				H_{syn}	1.64	—		
				H_{anti}	-0.10	—		

			H'	5.89	—		
			H''	8.59, 8.32	—		
			H''' _{syn}	2.18	—		
			H''' _{anti}	0.67	—		
C ₁₆ H ₁₂ ⁻ FeN ₂ O ₉	156	{h ⁴ -CH ₃ CH'=CH''-CH''= CH'''CH ^{IV} ₂ [1,3,5-OCOC ₆ H ₃ ^V - (NO ₂) ₂]}Fe(CO) ₃ <i>trans trans</i>	CDCl ₃	H, H'	1.49s	—	311
				H''	5.55-5.0m	—	
				H''' _{anti}	1.49q	J _{H''H'''} 7 J _{H'''H^{IV}} 7	
				H ^{IV}	4.51d	—	
				H ^V	9.2s	—	
C ₁₀ H ₁₂ FeO ₄	157	[h ⁴ -CH ₃ CH'=CH''-CH''= CH'''CH ^{IV} (OH ^V)CH ₃ ^{VI}]Fe(CO) ₃ <i>trans trans</i>	CDCl ₃	H	1.39d	J _{HH'} 6	312
				H _{anti}	1.2m	—	
				H''	5.25-4.90m	J _{H''H'''} 7.5 J _{H'''H^{IV}} 7.5	} <i>Endo-isomer</i> (See below)
				H''' _{anti}	1.5-0.9m	—	
				H ^{IV}	3.70m	J _{H^{IV}H^{VI}} 7	
				H ^V	2.05d	J 3.5	
				H ^{VI}	1.30d	J _{H^{IV}H^{VI}} 7	
				H _{anti}	1.46d	J _{HH'} 6	} <i>Exo-isomer</i> (See below)
				H'	1.4m	—	
				H''	5.2m	—	
				H''' _{anti}	0.92t	J _{H''H'''} 8 J _{H'''H^{IV}} 8	
				H ^{IV}	3.57m	—	
				H ^V	1.80s	—	
				H ^{VI}	1.5-1.25m	—	
C ₁₁ H ₁₄ FeO ₄	158	[h ⁴ -CH ₃ CH'=CH''-CH''= CH'''CH ^{IV} (CH ₃ ^V)(OCH ₃ ^{VI})]- Fe(CO) ₃ <i>trans trans</i>	CDCl ₃	H, H'	1.45-1.15m	—	311
				H''	5.25-4.9m	—	
				H'''	0.80t	—	
				H ^{IV}	3.02q	J _{H'''H^{IV}} 8	
				H ^V	1.30d	J _{H^{IV}H^V} 8	
				H ^{VI}	3.31s	—	

TABLE VII—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{12}H_{14}FeO_5$	159	$[h^4\text{-CH}_3\text{CH}'=\text{CH}''-\text{CH}'''=\text{CH}^{\text{IV}}(\text{CH}_3^{\text{V}})(\text{OCOCH}_3^{\text{VI}})]\text{-Fe}(\text{CO})_3$	CDCl_3	H, H' $\text{H}'', \text{H}^{\text{IV}}$ H''' H^{V} H^{VI}	1.40 5.39m, 4.72m, 4.02m 0.88t 1.40 2.00s	— — — $J_{\text{H}''\text{H}'''} 8.5$ $J_{\text{H}'''\text{H}^{\text{IV}}} 8.5$ —	<i>Exo</i> -isomer (See below)	311
$C_{17}H_{14}FeN_2O_9$	160	$\{h^4\text{-CH}_3\text{CH}'=\text{CH}''-\text{CH}'''=\text{CH}^{\text{IV}}(\text{CH}_3^{\text{V}})[1,3,5\text{-OCOC}_6\text{H}_3(\text{NO}_2)_3]\}\text{Fe}(\text{CO})_3$	CDCl_3	H, H' $\text{H}'', \text{H}^{\text{IV}}$ H''' H^{V} H^{VI}	1.7–1.3m 5.4–5.0m 1.10t 1.7–1.3m 9.70s	— — $J_{\text{H}''\text{H}'''} 8$ $J_{\text{H}'''\text{H}^{\text{IV}}} 8$ — —	<i>Endo</i> -isomer, viz.: 	311
			CDCl_3	H, H' $\text{H}'', \text{H}^{\text{IV}}$ H''' H^{V} H^{VI}	1.6–1.35 5.17b 1.02 1.6–1.35 9.50s	— — $J_{\text{H}''\text{H}'''} 8.5$ $J_{\text{H}'''\text{H}^{\text{IV}}} 8.5$ — —		<i>Exo</i> -isomer, viz.: 
$C_{15}H_{14}FeO_4$	161	$[h^4\text{-C}_6\text{H}_5\text{CH}'=\text{CH}''-\text{CH}'''=\text{CH}^{\text{IV}}\text{CH}^{\text{V}}(\text{CH}_3^{\text{VI}})(\text{OH}^{\text{VII}})]\text{-Fe}(\text{CO})_3$	CDCl_3	H H' H'' H''' H^{IV}	7.22s 2.05d 5.78q 5.32q 1.4t	— $J_{\text{H}\text{H}'} 9$ $J_{\text{H}''\text{H}'''} 6$ $J_{\text{H}'''\text{H}^{\text{IV}}} 7$ $J_{\text{H}^{\text{IV}}\text{H}^{\text{V}}} 8$	<i>Endo</i> -isomer (See above)	312

			H^V	3.8m	$J_{H^V H^{VI}}$ 6.5		
			H^{VI}	1.38d	—		
			H^{VII}	1.62s	—		
		CDCl ₃	H	—	—	Exo-isomer (See above)	312
			H'	2.17d	$J_{H' H''}$ 9		
			H''	5.78q	$J_{H'' H'''}$ 5		
			H'''	5.39q	$J_{H''' H^{IV}}$ 8		
			H ^{IV}	1.27t	$J_{H^{IV} H^V}$ 8		
			H ^V	3.68m	$J_{H^V H^{VI}}$ 7.5		
			H ^{VI}	1.40d	—		
			H ^{VII}	1.85s	—		
C ₂₂ H ₁₆ FeN ₂ O ₉	162	{ <i>h</i> ⁴ -C ₆ H ₅ CH'=CH"-CH'''= CH ^{IV} CH ^V (CH ₃ ^{VI}) 1,3,5- OCOC ₆ H ₃ ^{VII} (NO ₂) ₂ }]Fe(CO) ₃				Endo-isomer (See above)	311
		CDCl ₃	H	7.25s	—	}	
			H'	2.22d	$J_{H' H''}$ 9		
			H''	5.84q	$J_{H'' H'''}$ 5		
			H'''	5.55-5.0m	$J_{H''' H^{IV}}$ 9		
			H ^{IV}	1.47t	$J_{H^{IV} H^V}$ 9		
			H ^V	5.55-5.0m	$J_{H^V H^{VI}}$ 6		
			H ^{VI}	1.63d	—		
			H ^{VII}	9.5s	—		
		CDCl ₃	H	7.31s	—	}	
			H'	2.32d	$J_{H' H''}$ 8.5		
			H'', H'''	6.0-4.8m	—		
			H ^V		—		
			H ^{IV}	1.35t	$J_{H''' H^{IV}} \sim 8.5$ $J_{H^{IV} H^V} \sim 8.5$		
			H ^{VI}	1.68d	—		
			H ^{VII}	9.60s	—		
						Exo-isomer (See above)	311

TABLE VII—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_8H_6FeO_4$	163	$(h^4-CH_2=CH-CH=CH-CH=O)Fe(CO)_3$	$CDCl_3$	H	9.32d	$J_{4,1}$	—	313 314
$C_{14}H_{10}FeO_4$	164	$(h^4-C_6H_5CH'=CH''-CH'''=CH^{IV}-CH^{IV}=O)Fe(CO)_3$ <i>trans trans</i>	—	H H' H'' H''' H ^{IV}	7.34s 2.6d 6.07m 1.60q 9.44d	— J_{10} — — J_5	—	315 316
$C_{15}H_{12}FeO_4$	165	$(h^4-p-CH_3C_6H_4CH'=CH'''-CH'''=CH^{IV}-CH^V=O)Fe(CO)_3$ <i>trans trans</i>	—	H H' H'' H''' H ^{IV} H ^V	2.32s 7.2m 2.64d 6.0m 1.52q 9.42d	— — J_9 — — J_4	—	316
$C_9H_8FeO_4$	166	$(h^4-CH_2=CH-CH=CH-COCH_3)Fe(CO)_3$ <i>trans</i>	—	H H	1.25d 3.09d	J_8 J_8	<i>trans</i> -isomer <i>cis</i> -isomer	291
$C_{10}H_8D_2FeO_4$	167	$(h^4-CH_3CH'=CD-CH''=CD-COCH_3''')Fe(CO)_3$ <i>trans trans</i>	$CDCl_3/SO_2$ (2:3)	H H' H'' H'''	~ 1.5 1.66 5.70s 2.1s	— — — —	T -20 to -30	317
$C_{10}H_{10}FeO_4$	168	$(h^4-CH_3CH'=CH''-CH'''=CH^{IV}COCH_3^V)Fe(CO)_3$ <i>trans trans</i>	$CDCl_3/SO_2$ (2:3)	H H'	1.50d 1.65m	$J_{HH'6}$ $J_{H'H''8}$	T -20 to -30	317

			H''	5.35q	$J_{H''H'''} 6$			
			H'''	5.75q	$J_{H'''H^{IV}} 8$			
			H^{IV}	1.35d	—			
			H^V	2.10s	—			
		$CDCl_3$	H	1.45	—		311	
			H'	1.5	—		318	
			H''	5.25	—			
			H'''	5.75	—			
			H^{IV}	1.30	—			
			H^V	2.07	—			
$C_{10}H_{10}FeO_4$	169	$[h^4-CH_3CH'=CH''-CH'''=CH'''COCH_3^{IV})Fe(CO)_3]$ <i>trans cis</i>	$CDCl_3$	H	1.52d	$J_{HH'} 6$	—	311
				H'	2.20m	—		
				H''	5.28m	—		
				H'''	3.02d	$J_{H''H'''} 6.5$		
				H^{IV}	2.09ds	—		
$C_{11}H_{12}FeO_4$	170	$[h^4-CH_3CH'=C(CH_3'')-CH'''=CH^{IV}COCH_3^V)Fe(CO)_3]$ <i>trans trans</i>	$CDCl_3/SO_2$ (2:3)	H	~1.55	—	T -20 to -30	317
				H'	~1.55m	—		
				H''	2.20s	—		
				H'''	5.65d	$J_{H'''H^{IV}} 8$		
				H^{IV}	1.32d	—		
				H^V	2.10s	—		
$C_{11}H_{12}FeO_4$	171	$[h^4-CH_3CH'=CH''-C(CH_3''')=CH^{IV}COCH_3^V)Fe(CO)_3]$ <i>trans</i>	$CDCl_3/SO_2$ (2:3)	H	~1.5	—	T -20 to -30	317
				H'	~1.5m	$J_{H'H''} 7$		
				H''	5.15d	—		
				H'''	2.50s	—		
				H^{IV}	0.90s	—		
				H^V	2.11s	—		
$C_{12}H_{14}FeO_4$	172	$[h^4-(CH_3)_2C=C(COCH_3)-C(CH_3)=CH_2]Fe(CO)_3]$	$(CD_3)_2CO$	n.a.	—		Signals at δ 2.51s, 2.08s, 1.48s, 1.16s, 1.70d, 1.55d	292

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{15}H_{12}FeO_4$	173	$[h^4-C_6H_5CH'=CH''-CH'''=CH^{IV}COCH_3^V]Fe(CO)_3$ <i>trans trans</i>	$CDCl_3/SO_2$ (2:3)	H	7.40s	—	T -20° to -30°	317
				H'	2.65d	$J_{H'H''}$ 8–9		
				H''	5.95m	—		
				H'''	6.05m	—		
				H ^{IV}	1.75d	$J_{H'''H^{IV}}$ 8		
				H ^V	2.20s	—		
			CCl_4	H	7.05s	—	—	312
				H'	2.20d	$J_{H'H''}$ 8		
				H'', H'''	5.80q	—		
				H ^{IV}	1.35d	$J_{H'''H^{IV}}$ 7		
				H ^V	1.10s	—		
$C_{17}H_{16}FeO_4$	174	$[h^4-(CH_3)_2C=C(COC_6H_5)-C(CH_3)=CH_2]Fe(CO)_3$	$(CD_3)_2CO$	n.a.	—	—	Signals at δ 8.20m, 7.80m, 2.02s, 1.38s, 1.33s, 1.78dd.	292
$C_8H_8FeO_5$	175	$[h^4-CH_2=CH'-C(CO_2H'')=CH_2''']Fe(CO)_3$	C_6D_6	H _{syn}	1.48	—	60 and 100 MHz	303
				H _{anti}	-0.02	—		
				H'	6.03	—		
				H''	10.22–11.58	—		
				H' _{syn}	2.33	—		
				H' _{anti}	-0.11	—		
$C_9H_8FeO_5$	176	$[h^4-CH_2=CH'-C(CO_2CH_3')=CH_2''']Fe(CO)_3$	C_6D_6	H _{syn}	1.49	—	60 and 100 MHz	303
				H _{anti}	-0.01	—		
				H'	6.03	—		

				H''	3.45	—		
				H''_{syn}	2.32	—		
				H''_{anti}	-0.09	—		
		$CDCl_3$		H_{syn}	1.95m	—	—	319
				H_{anti}	0.40m	—		
				H'	6.2m	—		
				H''	3.85s	—		
				H''_{syn}	2.42m	—		
				H''_{anti}	0.28m	—		
$C_{13}H_{14}FeO_7$	177	$[h^4 \cdot CH(CO_2CH_2CH''')=CH''' - CH'''=CHCO_2CH_2CH'''] \cdot Fe(CO)_3$	$CDCl_3$	H	5.88	—	—	201
				H'	4.13	—		
				H''	1.25	—		
				H'''	6.06	—		
$C_{22}H_{34}FeO_5$	178	$[CH_3(CH_2)_yCH=CH'-CH''=CH'''(CH_2)_xCO_2CH_3]Fe(CO)_3$ ($x + y = 12$)	—	H, H'''	1.84	$J_{HH'''} 0$	Mixture of isomeric conjugated dienoic fatty esters derived from methyl linoleate $[CH_3(CH_2)_4CH=CHCH_2CH=CH(CH_2)_7CO_2Me]$ $x, y = 4, 8; 5, 7; 6, 6; 7, 5; 8, 4; 9, 3; 10, 2.$ The H,H coupling constants are compatible with 1,4-addition of $Fe(CO)_3$ to the diene to form a nonplanar ring complex, viz.	320
				H', H''	5.00	$J_{H'H''} 4.4 \pm 0.2$		321
						$J_{HH'} = J_{H''H'''} + 8.4$		
						$J_{H'H'''} = J_{HH''} - 1.7$		

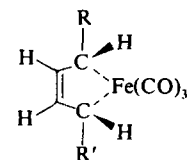


TABLE VII—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References	
$C_7H_6BF_3 \cdot FeO_3S$	179	$(h^4-C_4H_6SO_2BF_3)Fe(CO)_3$	SO_2	H_{-1}	5.15,	$J_{1,2}$ 8.9	Complex formed by reaction of butadieneiron tricarbonyl with SO_2 and BF_3	1048	
					3.02	$J_{1,1}$ 1.9			
				H_{-2}	5.62	$J_{1,2}$ 14.1			
				H_{-3}	6.25	$J_{2,3}$ 7			
						$J_{3,4}$ 8.4, 5.1			
			H_{-4}	3.50, 2.56	—				
$C_{13}H_{16}FeO_3$	180	$[h^4-CH_2=CH-C(=CH_2')CH_2''-CH_2''CH=C(CH_2''')_2]Fe(CO)_3$	C_6H_6	H_{syn}	1.5–2.0	—	—	1006	
				H_{anti}	0.06q	—			
				H'_{anti}	0.25	—			
				H''	2.35d	—			
				H'''	1.5–2.0	—			
$C_{11}H_{10}FeO_3$	181	$[h^4-CH_2=CH'-C(C_4H_5)=CH_2'']Fe(CO)_3$	$(CD_3)_2CO$	H_{syn}	1.90dd	$J_{HH'}$ 7.2	$C_4H_5 = CH_2'''=C-CH^{IV}=CH_2^V$ (Uncomplexed diene system)	303	
				H_{anti}	0.44dd	$J_{HH'}$ 10.3			
						J_{HH} 2.4			
				H'	5.63t	—	60 and 100 MHz		
				H''_{syn}	2.16dd	$J_{H'H''}$ 1.5			
				H''_{anti}	0.49d	$J_{H''H''}$ 2			
				H'''	5.50d	$J_{H'''H'''}$ 1.3			
					5.44d				
				H^{IV}	6.65dd	$J_{H^{IV}H^V}$ 11.0			
				H^V_{syn}	5.28dd	$J_{H^VH^V}$ 2.0			
				H^V_{anti}	5.67dd	$J_{H^{IV}H^V}$ 17.6			

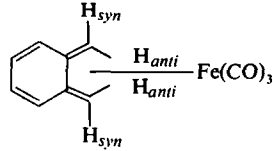
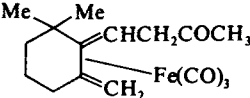
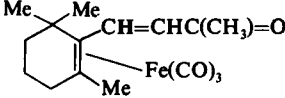
$C_{11}H_8FeO_3$	182	$(h^4-C_6H_8)Fe(CO)_3$	CCl_4	H_{syn} H_{anti}	2.20 -0.05	—		322
$C_{16}H_{14}FeO_3$	183	$(h^4-p-CH_3C_6H_4 \cdot CH=CH-CH'=CH-CH=CH_2) \cdot Fe(CO)_3$ complexed diene	$CDCl_3$	H H' H''_{syn} H''_{anti}	2.28s 1.93t 0.52 (?) 1.77m	— $J 8.7$ $J 8.5$ $J_{H''H''} 2.6$	313	
$C_{16}H_{14}FeO_3$	184	$(h^4-p-CH_3C_6H_4 \cdot CH'=CH-CH=CH-CH=CH_2) \cdot Fe(CO)_3$ complexed diene	$CDCl_3$	H H' H''	2.27s 2.27d 2.05t	— $J 9.5$ $J 9$	313	
$C_{21}H_{16}FeO_3$	185	$(h^4-C_6H_5 \cdot CH'=CH''-CH''=CH'-CH''=CH''C_6H_5) \cdot Fe(CO)_3$ complexed diene	—	H H' H''	7.25d 2.35m 6.9-5.3m	— — —	316	
$C_{22}H_{18}FeO_3$	186	$(h^4-C_6H_5 \cdot CH=CH'-CH'=CH-CH'=CH'-p-C_6H_4CH_3) \cdot Fe(CO)_3$ complexed diene	—	H H' H''	2.34m 6.8-5.1m 2.32s	— — —	316	
$C_{22}H_{18}FeO_3$	187	$(h^4-C_6H_5 \cdot CH=CH-CH'=CH-CH=CH-p-C_6H_4CH_3) \cdot Fe(CO)_3$ complexed diene	—	H H' H''	6.8-5.2 m 2.25m 2.28s	— — —	316	
$C_{23}H_{18}FeO_3$	188	$(h^4-C_6H_5 \cdot CH=CH-CH'=CH''-CH''=CH'-CH=CHC_6H_5) \cdot Fe(CO)_3$ complexed diene	$CDCl_3$	H H' H''	7.27bs 2.27dd 5.30d	— $J 8.7$ $J 7.5$	313	

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{24}H_{20}FeO_3$	189	$(h^4-C_6H_5CH=CH-\underbrace{CH=CH-CH=CH-}_{\text{complexed diene}}CH=CH-p-C_6H_4CH_3)Fe(CO)_3$	$CDCl_3$	H H'	2.28s 2.28s	— —	—	313
$C_{23}H_{18}FeO_3$	190	$(h^4-C_6H_5CH=CH-CH=CH-\underbrace{CH=CH-CH=CH-}_{\text{complexed diene}}C_6H_5)Fe(CO)_3$	$CDCl_3$	H H'	2.25t 2.30d	J 9.3 J 9.3	—	313
$C_{24}H_{20}FeO_3$	191	$(h^4-C_6H_5CH=CH-CH=CH-\underbrace{CH=CH-CH=CH-}_{\text{complexed diene}}CH=CH-CH=CH-p-C_6H_4CH_3)Fe(CO)_3$	$CDCl_3$	H H'	2.31 bs 2.31 bs	— —	—	313
$C_{24}H_{20}FeO_3$	192	$(h^4-C_6H_5CH=CH-CH=CH-\underbrace{CH=CH-CH=CH-}_{\text{complexed diene}}p-C_6H_4CH_3)Fe(CO)_3$	$CDCl_3$	H H'	2.27s 2.27s	— —	—	313
$C_{25}H_{22}FeO_3$	193	$(h^4-p-CH_3C_6H_4-\underbrace{CH=CH-CH=CH-}_{\text{complexed diene}}CH=CH-CH-CH-p-C_6H_4CH_3)Fe(CO)_3$	$CDCl_3$	H H'	2.25 2.25	— —	—	313
$C_{23}H_{30}FeO_4$	194	$\{h^4-[1-C_6H_6(CH_3)_3]CH'=CH'-C(CH_3)_2=CH'-CH'''=CH-C(CH_3)_2=CH-CH_2OH\}Fe(CO)_3$	—	H H' H'' H'''	1.00, 1.66 6.0 1.89 5.30	— — — —	$C_6H_6(CH_3)_3$ = 2,6,6-trimethyl-cyclohexen-1-yl	323

				H^{IV}	2.25	—		
				H^V	3.80d	—		
				H^{VI}	3.50	—		
$C_{23}H_{32}FeO_3$	195	$\{h^4-[1-C_6H_6(CH_3)_3]CH'=CH'-$ $C(CH_3)=CH'-$ $CH'''=CH^{IV}-C(CH_3^V)=$ complexed diene $CH'''CH_2^{VI}OCOCH_3^{VII}\}Fe(CO)_3$	—	H	1.00, 1.64	—	$C_6H_6(CH_3)_3$ —as above	323
				H'	6.0	—		
				H''	1.89	—		
				H'''	5.30	—		
				H^{IV}, H^V	2.30	—		
				H^{VI}	4.20d	—		
				H^{VII}	1.98	—		
$C_{16}H_{12}FeO_4$	196	$(h^4-C_6H_5CH=CH-$ $CH=CH-CH=CH'-$ complexed diene $CH''=O)Fe(CO)_3$	$CDCl_3$	H	2.57t	J 9.0	—	313
				H'	1.57dd	J 4, 8		
				H''	9.30d	J 4		
$C_{16}H_{12}FeO_4$	197	$(h^4-C_6H_5CH=CH-CH=CH'-$ complexed diene $CH=CH-CH''=O)Fe(CO)_3$	$CDCl_3$	H	2.61d	J 9.5	—	313
				H'	2.02t	J 8.5		
				H''	9.52d	J 8.0		
$C_{17}H_{14}FeO_4$	198	$(h^4-CH_3C_6H_4CH''=CH''-$ $CH=CH'''-CH'''=CH^{IV}-$ complexed diene $CH^V=O)Fe(CO)_3$	$CDCl_3$	H	2.30s	—	—	313
				H'	7.17m	—		
				H''	6.47	J 9.0, 15.5		
				H'''	5.63m	—		
				H^{IV}	1.55dd	J 4.5, 8		
				H^V	9.30d	J 4.5		
$C_{17}H_{14}FeO_4$	199	$(h^4-p-CH_3C_6H_4-$ $CH''=CH'''-CH'''=CH^{IV}-$ complexed diene $CH^V=CH^V-CH^{VI}=O)-$ $Fe(CO)_3$	$CDCl_3$	H	2.28s		*AB component of ABXY spectrum	313
				H'	7.12s			
				H''	2.61d	$J_{H''H'''} 9$		
				H'''	5.73	$J_{H'''H'''} 5^*$		
				H^{IV}	2.00t	$J_{H'''H^{IV}} 9$ $J_{H^{IV}H^V} 9$		
				H^V	6.43	$J_{H^VH^V} 15^*$		
				H^{VI}	9.45d	$J_{H^VH^{VI}} 7.5$		

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{23}H_{28}FeO_4$	200	$\{h^4-[1-C_6H_6(CH_3)_3]CH'=$ $CH'-C(CH_3)_2=CH'-$ $CH'''=CH^{IV}-C(CH_3)^V=CH''''-$ $\underbrace{\hspace{10em}}_{\text{complexed diene}}$ $CH=O\}Fe(CO)_3$	—	H 1.00, 1.66 H' 6.0 H'' 1.95 H''' 5.25 H^{IV} 2.7 H^V 2.50	— — — — — —	$C_6H_6(CH_3)_3 = 2,6,6$ - trimethylcyclohexen-1-yl	323 324
$C_{16}H_{20}FeO_4$	201	$(h^4-C_{13}H_{20}O)Fe(CO)_3$	—	n.a.		Structure:  Signals δ 2.5–0.9	325
$C_{16}H_{20}FeO_4$	202	$(h^4-C_{13}H_{20}O)Fe(CO)_3$	—	H 6.24d	—	Structure:  Other signals at δ 2.22–0.88	325
$C_{19}H_{24}FeO_5$	203	$\{h^4-[1-C_6H_6(CH_3)_3]-$ $CH=CH-C(CH_3)=C-$ $\underbrace{\hspace{10em}}_{\text{complexed diene}}$ $HCO_2CH_3\}Fe(CO)_3$	—	H 5.7 H' 3.6	— —	$C_6H_6(CH_3)_3 = 2,6,6$ -trimethyl cyclohexen-1-yl Signals at δ 2.8–0.3	325

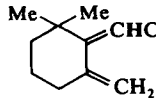
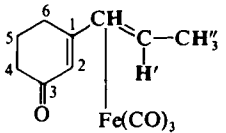
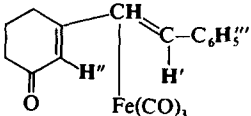
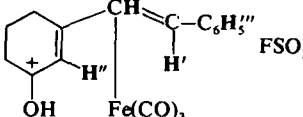
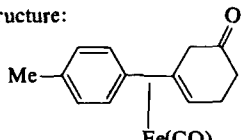
$C_{20}H_{26}FeO_5$	204	$(h^4-C_{17}H_{26}O_2)Fe(CO)_3$		H H' H''	5.25 2.20 4.04q	— — —	$C_{17}H_{26}O_2 =$ 	325 326
$C_{13}H_{12}FeO_7$	205	$(h^4-CH_3O_2C-CH=CH-CH=CH-CH=CHCO_2CH_3)Fe(CO)_3$ complexed diene	C_6D_6	H	3.40, 3.47	— —		326
$C_{15}H_{14}FeO_7$	206	$(h^4-CH_3O_2CCH=CH-CH=CH-CH=CHCO_2CH_3)Fe(CO)_3$ complexed diene	C_6D_6	H	3.46	—		326
$C_{15}H_{14}FeO_7$	207	$(h^4-CH_3O_2C-CH=CH-CH=CH-CH=CHCO_2CH_3)Fe(CO)_3$ complexed diene	C_6D_6	H	3.48, 3.37	— —	—	326
$C_{12}H_{12}FeO_4$	208	$(h^4-C_9H_{12}O)Fe(CO)_3$	$CDCl_3$	H H' H''	4.90d 1.12 dq 1.25 d	J 8 — J 5	Structure: 	307
			$CDCl_3/SO_2$ (2:3)	H ₋₂ H ₋₄ , H ₋₆ H ₋₅ H H' H'' H ₋₂	1.52s 2.75-2.07m 2.0-1.65m 5.45m 1.55 1.55 1.65s	— — — — — — —	T -20° to -30°	317

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{17}H_{14}FeO_4$	209	$(h^4-C_{14}H_{14}O)Fe(CO)_3$	$CDCl_3/SO_2$ (2:3)	H 6.05d H' 2.35d H'' 1.98s H''' 7.35s	$J_{HH'}$ 9 — — —	Structure: 	317
$[C_{17}H_{15}FeO_4]^+$	210	$[(h^4-C_{14}H_{15}O)Fe(CO)_3]^+$	$CDCl_3/SO_2$ (2:3)	H 6.40d H' 3.65d H'' 2.5–2.0 H''' 7.45sd	J 9 — — —	T–20 to –30 Structure: (T–50 to –60) 	317
$C_{12}H_9ClFeO_3$	211	$[h^4-4-ClC_6H_4C(CH_3)=CH_2]-Fe(CO)_3$	—	H_{-2} 2.73 H_{-3}, H_{-5} } 6.93 H_6 } 7.64 H_{syn} 1.79 H_{anti} 0.16	$J_{2,3}$ 5.7 $J_{5,6}$ 8.7 $J_{H'H'}$ 2.6 —	—	327
$C_{16}H_{14}FeO_5$	212	$(h^4-C_{13}H_{14}O_2)Fe(CO)_3$	—	n.m.	—	Structure: 	328

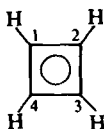
$C_7H_4FeO_3$	213	$(h^4-C_4H_4)Fe(CO)_3$	CCl_4	H	4.00 3.91 3.95s 3.96	— —	$C_4H_4 = \text{cyclobutadiene}$	329
								54 330
			Cyclohexane	^{13}C	$-16.2s^*$ $+131.8d^*$	$J(H-^3H_{-4}) 0$ $J(^{13}C_3-H_3) =$ $J(^{13}C_4-H_4)$ 191.0 $J(^{13}C_2-H_2) =$ $J(^{13}C_4-H_3) =$ $J(^{13}C_1-H_4) =$ $J(^{13}C_3-H_4) 4.2$ $J(^{13}C_1-H_3) =$ $J(^{13}C_2-H_4) 12.8$ *Relative to CS_2 (0.0 ppm)	331 332 333 334 1046	
$C_7H_3ClFeO_3$	214	$(h^4-C_4H_3Cl)Fe(CO)_3$	CCl_4	H_{-2} H_{-3}	3.90s 4.22s	$J_{2,4} 8.6$ $J_{2,3} 0$	1-Chlorocyclobutadiene	335
$C_7H_3FeIO_3$	215	$(h^4-C_4H_3I)Fe(CO)_3$	—	H	4.17, 4.40	— —	1-Iodocyclobutadiene	332
$C_7H_2FeI_2O_3$	216	$(h^4-C_4H_2I_2)Fe(CO)_3$	—	H	4.63	$J 0$	1,2-Di-iodocyclobutadiene	332
$C_7H_2FeI_2O_3$	217	$(h^4-C_4H_2I_2)Fe(CO)_3$	—	H	4.48	—	1,3-Di-iodocyclobutadiene	332
$C_7HFeI_3O_3$	218	$(h^4-C_4HI_3)Fe(CO)_3$	—	H	4.95	—	Tri-iodocyclobutadiene	332

TABLE VII—cont.

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Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_8H_5FeO_3$	219	$(h^4-C_5H_5)Fe(CO)_3$	H_2SO_4	n.a.		—	$C_5H_5 = CH_2$  or  Signals at δ 6.88bs, 5.91bs, 5.09bs, in ratio 1:2:2	336
$C_9H_7FeO_3$	220	$(h^4-C_6H_7)Fe(CO)_3$	H_2SO_4	H H' H₋₂, H₋₄ H₋₃	6.19q 1.78d 5.84d, 5.44d 6.52s	— — — —	$C_6H_7 = CHCH_3$  $CHCH_3$  or	336
$C_9H_8FeO_3$	221	$[h^4-C_4H_2(CH_3)_2]Fe(CO)_3$	CCl_4 Cyclohexane	H H'	3.90 1.76	— —	1,2-Dimethylcyclobutadiene 60 and 100 MHz	339 331 334

$$\begin{aligned}
 J(H_3-H_4) &= 0 \\
 J(^{13}C_3-H_3) &= \\
 J(^{13}C_4-H_4) &= \\
 189.2 \\
 J(^{13}C_2-H_3) &= \\
 J(^{13}C_4-H_3) &= \\
 J(^{13}C_1-H_4) &= \\
 J(^{13}C_3-H_4) &= 4.2 \\
 J(^{13}C_1-H_3) &= \\
 J(^{13}C_2-H_4) &= 12.8
 \end{aligned}$$

$C_9H_6Cl_2FeO_3$	222	$[h^4-C_4H_2(CH_2Cl)_2]Fe(CO)_3$	$CDCl_3$	H H'	4.37s 4.09q	— J 13.1	1,2-Bis-chloromethylcyclobutadiene	338
$C_{10}H_{10}FeO_3$	223	$[h^4-C_4H(CH_3)_3]Fe(CO)_3$	CCl_4	H H'	3.92 1.77, 1.74	J 0.8 — —	Trimethylcyclobutadiene 60 and 100 MHz $J(^{13}C-H)$ 186.7 and 128.3	339
$C_{11}H_{12}FeO_3$	224	$[h^4-C_4H(CH_3)_2CH_2CH_3]Fe(CO)_3$	CCl_4	H H' H'' H'''	3.97s 1.77s, 1.75s 2.07 dq 1.01 dd	— — — J 7.9, 7.2 J 7.9, 7.2	1-Ethyl-2,3-dimethylcyclobutadiene 100 MHz	340
$C_{11}H_{12}FeO_3$	225	$[h^4-C_4(CH_3)_4]Fe(CO)_3$	CCl_4	H	1.68s	J 1.5	Tetramethylcyclobutadiene	339
			CS_2	H	1.73s	$J(^{13}C-H)$ 128.6 —	60 and 100 MHz	341 54
$C_{12}H_{14}FeO_3$	226	$[h^4-C_4(CH_3)_3CH_2CH_3]Fe(CO)_3$	CCl_4	H H' H''	1.76b 2.12q 1.10t	— J 7.4 J 7.4	1-Ethyl-2,3,4-trimethylcyclobutadiene	342
$C_{13}H_{16}FeO_3$	227	$[h^4-C_4(CH_3)_2(CH_2CH_3)_2]Fe(CO)_3$	CCl_4	H H' H''	1.78s 2.1m 1.10dd	— J_{gem} 11 J 7.9, 7.2	1,2-Diethyl-3,4-dimethylcyclobutadiene	342
$C_{13}H_{16}FeO_3$	228	$[h^4-C_4(CH_3)_3CH'(CH_3)_2]Fe(CO)_3$	CCl_4	H H' H''	1.78 1.77 2.42 sept. 1.12d	— — J 6.7 J 6.7	1-Isopropyl-2,3,4-trimethylcyclobutadiene	343
$C_{15}H_{20}FeO_3$	229	$\{h^4-C_4(CH_3)_2[CH'(CH_3)_2]_2\}Fe(CO)_3$	CCl_4	H H' H''	1.82s 2.29m 1.17d, 1.10d	— — J 7.0 J 6.5	1,2-Di-isopropyl-3,4-dimethylcyclobutadiene	343

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{12}H_{14}FeO_3$	230	$\{h^4-C_4H-1,2-(CH_3)_2-3-[CH'-(CH_3)_2]\}Fe(CO)_3$	CCl_4	H	1.79s, 1.78s	Cyclobutadiene derivative	1003
				H'	2.39qq		
				H''	1.02d		
					1.05d		
$C_{27}H_{28}FeO_3$	231	$\{h^4-1,2-C_4[C(CH_3)_3]_2-3,4-(C_6H_5)_2\}Fe(CO)_3$	—	H	0.83	Cyclobutadiene derivative	1004
				H'	6.58–7.0		
$C_{15}H_{20}FeO_3$	232	$[h^4-C_4H_2(C_4H_9)_2]Fe(CO)_3$	—	n.a.	—	1,2-Di- <i>n</i> -butylcyclobutadiene Signals at δ 3.92, 3.88s, 1.98q, 1.35m, 0.88t, in ratio 2:1:4:8:6	331
$C_{13}H_8FeO_3$	233	$(h^4-C_4H_3C_6H_5)Fe(CO)_3$	—	H ₋₂ , H ₋₄	4.467	1-Phenylcyclobutadiene	344
				H ₋₃	4.169		

						$J(^{13}\text{C}_1-\text{H}_3) = 13.3$ $J(^{13}\text{C}_2-\text{H}_3) =$ $J(^{13}\text{C}_4-\text{H}_3) = 4.7$		
			H'	7.02, 7.32				
C ₁₉ H ₁₂ FeO ₃	234	[<i>h</i> ⁴ -C ₄ H ₂ (C ₆ H ₅) ₂]Fe(CO) ₃	Cyclohexane	H 4.50 H' 7.2m	J(H ₃ -H ₄) 0 —	1,2-Diphenylcyclo- butadiene 60 and 100 MHz	334	
					J(¹³ C ₃ -H ₃) 189.5 J(¹³ C ₂ -H ₃) 4.2 J(¹³ C ₁ -H ₃) 12.8			
C ₃₅ H ₂₈ FeO ₃	235	[<i>h</i> ⁴ -C ₄ (<i>p</i> -C ₆ H ₄ CH ₃) ₄]Fe(CO) ₃	CDCl ₃	H 7.1q* H' 2.27	J 7.8 —	Tetra- <i>p</i> -tolylcyclo- butadiene *Centre of AB quartet	345	
C ₉ H ₆ FeO ₄	236	(<i>h</i> ⁴ -C ₄ H ₃ COCH ₃)Fe(CO) ₃	CCl ₄	H ₂ , H ₄ 4.512s H ₃ 4.360s H' 1.960s	— — —	Cyclobutadiene derivative ¹³ C-H coupling constants reported	1005	
C ₁₁ H ₈ FeO ₃	237	[<i>h</i> ⁴ -C ₄ H ₂ (COCH ₃) ₂]Fe(CO) ₃	CDCl ₃	H 4.89s H' 2.25s	— —	1,2-Diacetylcyclobutadiene	338	
C ₁₁ H ₆ Cl ₂ FeO ₃	238	[<i>h</i> ⁴ -C ₄ H ₂ (COCH ₂ Cl) ₂]Fe(CO) ₃	CDCl ₃	H 5.10s H' 4.26s	— —	1,2-Bis-chloroacetylcyclo- butadiene	338	
C ₁₁ H ₆ FeI ₂ O ₃	239	[<i>h</i> ⁴ -C ₄ H ₂ (COCH ₂ I) ₂]Fe(CO) ₃	CDCl ₃	H 5.02s H' 4.02*	— J 10.0	1,2-Bis-iodomethylcyclo- butadiene *Centre of AB quartet (Δν _{AB} = 13.8 Hz)	338	
C ₂₃ H ₁₆ FeO ₃	240	[<i>h</i> ⁴ -C ₄ H ₂ (COCH ₂ C ₆ H ₅) ₂]- Fe(CO) ₃	CDCl ₃	H 4.77s H' 5.17s H'' 7.32s	— — —	1,2-Bis-phenylacetylcyclo- butadiene	338	

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)		Remarks	References
$C_{21}H_{12}FeO_5$	241	$[h^4-C_4H_2(COC_6H_5)_2]Fe(CO)_3$	$CDCl_3$	H H'	5.00s 8.00–7.23m	—	1,2-Dibenzoylcyclobutadiene	338
$C_9H_2FeN_2O_3$	242	$[h^4-C_4H_2(CN)_2]Fe(CO)_3$	$(CD_3)_2CO$	H	5.38s	—	1,2-Dicyanocyclobutadiene	338
$C_9H_2Cl_2FeO_5$	243	$[h^4-C_4H_2(COCl)_2]Fe(CO)_3$	$CDCl_3$	H	5.13s	—	1,2-Dichlorocarbonylcyclobutadiene	338
$C_9H_6FeN_2O_5$	244	$[h^4-C_4H_2(CONH_2)_2]Fe(CO)_3$	$(CD_3)_2SO$	H H'	5.08s 8.12bs, 7.40bs	— — —	1,2-Dicarbamoylcyclobutadiene	338
$C_9H_4FeO_7$	245	$[h^4-C_4H_2(CO_2H)_2]Fe(CO)_3$	$(CD_3)_2CO$	H H'	5.20s 5.85bs	— —	1,2-Dicarboxycyclobutadiene	338
$C_{10}H_6FeO_7$	246	$[h^4-C_4H_2(CO_2CH_3)_2CO_2H'] \cdot Fe(CO)_3$	$CDCl_3$	H H' H''	4.78s, 4.94s 3.86s 10.06bs	— — — —	1-Carboxyl-2-methoxycarbonyl cyclobutadiene	338
$C_{11}H_8FeO_7$	247	$[h^4-C_4H_2(CO_2CH_3)_2]Fe(CO)_3$	$CDCl_3$	H H'	4.77s 3.77s	— —	1,2-Bis-methoxycarbonyl-cyclobutadiene	338
$C_{23}H_{16}FeO_7$	248	$[C(C_6H_5)_3 \equiv CCO_2CH_3]_2Fe(CO)_3$	— —	H H' H H'	7.6, 7.0 3.42 7.9, 7.2 3.27	— — — —	Isomeric tricarbonyl cyclobutadiene iron complexes derived from methyl phenylpropiolate and $Fe_2(CO)_9$	1044
$C_{11}H_6FeO_3$	249	$(h^4-C_8H_6)Fe(CO)_3$	—	H* H†	4.02s 6.95m	— <i>J ortho</i> 8.61, 6.77	Benzocyclobutadiene *Cyclobutadiene protons	330 346

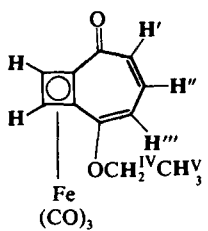
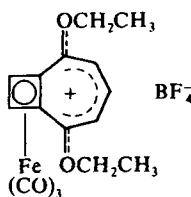
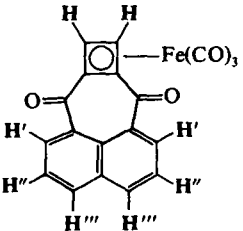
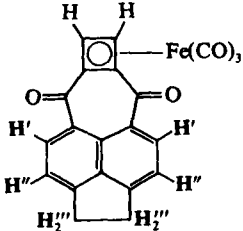
					J_{meta} 0.68 J_{para} 1.57	†Aromatic protons The coupling constants indicate bond fixation in the six-membered ring and reduced π -electron delocalization	
$C_{14}H_{10}FeO_5$	250	$(\eta^4-C_{11}H_{10}O_2)Fe(CO)_3$	—	H 4.95s, 4.82s H' 6.02m H'' 6.75 H''' 5.78	— — $J_{H'H''}$ 13.0 $J_{H''H'''}$ 9.5 $J_{H'H'''}$ 0.4	Structure: 	347
				H^{IV} 4.10q H^V 1.38t	$J_{H^{IV}H^V}$ 7.0	100 MHz	
$C_{16}H_{15}FeO_5$	251	$(\eta^4-C_{13}H_{15}O_2)Fe(CO)_3$	$(CD_3)_2CO$	n.a.		Structure: 	347
						Signals at δ 5.66, 6.88–8.06	

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{19}H_8FeO_5$	252	$(h^4-C_{16}H_8O_2)Fe(CO)_3$	$CDCl_3$	H	5.18s	—	Structure: 	347
				H'	8.89	$J_{H'H''} 7.7$		
				H''	7.64	$J_{H''H'''} 7.6$		
				H'''	8.17	$J_{H'H'''} 1.9$		
$C_{21}H_{10}FeO_5$	253	$(h^4-C_{18}H_{10}O_2)Fe(CO)_3$	$CDCl_3$	H	5.16s	—	Structure: 	347
				H'	8.9	$J_{H'H''} 7.5$		
				H''	7.48	—		
				H'''	3.47	—		
$C_8H_6FeO_3$	254	$(h^4-C_5H_6)Fe(CO)_3$	—	H ₋₁ H ₋₄	2.85m	—	Cyclopenta-1,3-diene No signals below δ 0.0 ppm, indicating absence of protons directly attached to iron	305
				H ₋₂ H ₋₃	5.62t	—		
				H ₋₅	2.69d	J 11.7		
					2.29d	J 11.7		

$C_{10}H_{10}FeO_3$	255	$[h^4-C_5H_4(CH_3)_2]Fe(CO)_3$	C_6D_6	H_{-1}, H_{-4}	2.35t	—	5,5-Dimethylcyclopenta-1,3-diene	348
				H_{-2}, H_{-3}	4.78t	—		
				H'_{exo}	0.50s	—		
				H'_{endo}	1.22s	—		
$C_{13}H_{16}FeO_3$	256	$[h^4-C_5H(CH_3)_3]Fe(CO)_3$	$CDCl_3$	1,4- CH_3	1.51	—	1,2,3,4,5-Pentamethylcyclopenta-1,3-diene	349
				2,3- CH_3	2.13	—	60 and 100 MHz	
				5- CH_3	0.69d	—		
$C_{10}H_{10}FeO_4$	257	$[h^4-C_5H_4(CH_3)CH_2OH''']Fe(CO)_3$	C_6D_6	H_{-1}, H_{-4}	2.25	—	5-Exo-hydroxymethyl-5-endo-methylcyclopentadiene	348
				H_{-2}, H_{-3}	4.72t	—	$ J_{1,2} + J_{1,3} \sim 5$ Hz	
				H'	1.21s	—		
				H''	2.41d	J 5		
				H'''	0.59d	J 5		
				H_{-1}, H_{-4}	2.52t	—	5-Endo-hydroxymethyl-5-exo-methylcyclopentadiene	
				H_{-2}, H_{-3}	4.74t	—	$ J_{1,2} + J_{1,3} \sim 5$ Hz	
				H'	0.68s	—		
				H''	3.62s	—		
				H'''	1.07s	—		
$C_{11}H_{12}FeO_4$	258	$[h^4-C_5H_4(CH_3)CH_2OCH_3''']Fe(CO)_3$	C_6D_6	H_{-1}, H_{-4}	2.39t	—	5-Exo-methoxymethyl-5-endo-methylcyclopentadiene	348
				H_{-2}, H_{-3}	4.75	—		
				H'	1.36s	—		
				H''	2.26s	—		
				H'''	2.86s	—		
				H_{-1}, H_{-4}	2.66t	—	5-Endo-methoxymethyl-5-exo-methylcyclopentadiene	
				H_{-2}, H_{-3}	4.77t	—		
				H'	0.74s	—		
				H''	3.46s	—		
				H'''	3.18s	—		

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References		
$C_{17}H_{16}FeO_6S$	259	$[h^4-5,5-C_6H_4(CH_3)CH_2^p-OSO_2C_6H_4'''CH_3^IV]Fe(CO)_3$	C_6D_6	H_{-1}, H_{-4}	2.07t	—	<i>Endo</i> -methyl derivative $ J_{1,2} + J_{1,3} \sim 5$ Hz	348	
				H_{-2}, H_{-3}	4.58t	—			
				H'	1.14s	—			
				H''	2.96s	—			
				H'''	7.61d,	$J 8.5$			
					6.64d	$J 8.5$			
				H^{IV}	1.72s	—			
				H_{-1}, H_{-4}	2.29t	—			<i>Exo</i> -methyl derivative $ J_{1,2} + J_{1,3} \sim 5$ Hz
				H_{-2}, H_{-3}	4.56t	—			
				H'	0.61s	—			
				H''	4.19s	—			
				H'''	7.81d,	$J 8.5$			
					6.75d	$J 8.5$			
				H^{IV}	1.87s	—			
$C_{12}H_{12}FeO_5$	260	$[h^4-5,5-C_6H_4(CH_3)CO_2-CH_2^qCH_3''']Fe(CO)_3$	C_6D_6	H_{-1}, H_{-4}	2.99t	—	<i>Exo</i> -methylcyclopentadiene derivative $ J_{1,2} + J_{1,3} \sim 5$	348	
				H_{-1}, H_{-3}	4.70t	—			
				H'	0.73s	—			
				H''	4.08q	$J 7$			
				H'''	1.03t	$J 7$			
$C_{14}H_5F_3FeO_3$	261	$[h^4-5-C_6H_5(C_6F_5)]Fe(CO)_3$	C_6D_6	H_{-1}, H_{-4}	2.78m	—	<i>Exo</i> -pentafluorophenyl derivative	193	
				H_{-2}, H_{-3}	4.92m	—			
				H_{-5}	3.75m	—			
$C_{10}H_{16}B_{10}FeO_3$	262	$[h^4-5-exo-C_5H_5(B_{10}C_2H_{11})]-Fe(CO)_3$	C_6H_6	H_{-1}, H_{-4}	2.23	—	$B_{10}C_2H_{11} = o$ -carborane derivative	350	
				H_{-2}, H_{-3}	4.41	—			
				H_{-5}	2.56	—			

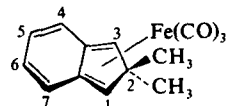
$C_{11}H_{18}B_{10}FeO_3$	263	$[h^4-5-exo-C_5H_5(B_{10}C_3H_{13})]-Fe(CO)_3$	CH_2Cl_2	H_{-1}, H_{-4}	3.19	—	$B_{10}C_3H_{13}$ = 2-methyl- <i>o</i> -carborane derivative 60 and 100 MHz	350 998
				H_{-2}, H_{-3}	—	—		
				H_{-5}	3.19	—		
			$CHCl_3$	H_{-1}, H_{-4}	3.18	—		
				H_{-2}, H_{-3}	5.60	—		
				H_{-5}	3.18	—		
			C_6H_6	H_{-1}, H_{-4}	2.37	—		
				H_{-2}, H_{-3}	4.59	—		
				H_{-5}	2.4	—		
$C_{16}H_{20}B_{10}FeO_3$	264	$[h^4-5-exo-C_5H_5(B_{10}C_8H_{15})]-Fe(CO)_3$	CCl_4	H_{-1}, H_{-4}	2.86	—	$B_{10}C_8H_{15}$ = 2-phenyl- <i>o</i> -carborane derivative	350 998
				H_{-2}, H_{-3}	5.46	—		
				H_{-5}	2.61	—		
			$CHCl_3$	H_{-1}, H_{-4}	2.90	—		
				H_{-2}, H_{-3}	5.52	—		
				H_{-2}	2.62	—		
$C_{10}H_8FeO_3$	265	$(h^4-C_7H_8)Fe(CO)_3$	C_6D_6	n.a.			Spiro[2.4]hepta-4,6-diene iron tricarbonyl Signals at δ 1.47t, 3.18t, 4.05t, 4.39t, in ratio 1:1:1:1	351
$C_{12}H_{12}FeO_3$	266	$(h^4-C_9H_{12})Fe(CO)_3$	—	H_{-6}, H_{-9}	2.95t	—	Spiro[4.4]nona-6,8-diene iron tricarbonyl Other signals at δ 2.0–1.0	352
$C_{14}H_{12}FeO_3$	267	$(h^4-C_{11}H_{12})Fe(CO)_3$	CCl_4	H_{-1}, H_{-3}	3.33s	—	Structure: 	322
				H_{-4}, H_{-7}	7.46m	$J_{4,5}$ 8.62		
				H_{-5}, H_{-6}	7.46m	$J_{5,6}$ 6.64 $J_{4,6}$ 0.98 $J_{4,7}$ 1.07		

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{10}H_2F_6FeO_4$	268	$[h^4-C_5H_2O(CF_3)_2]Fe(CO)_3$	$(CH_3)_2CO$	H_{-3}, H_{-4} 6.57 ^{19}F -4.00s*	— —	2,2-bis-trifluoromethyl cyclopenta-2,4-dien-1-one 100 MHz *Relative to benzotrifluoride at 94.1 MHz	353
$C_{20}H_2F_{10}FeO_4$	269	$[h^4-C_5H_2O(C_6F_5)_2]Fe(CO)_3$	$(CH_3)_2CO$	H_{-3}, H_{-4} 6.62s $^{19}F_{ortho}$ 129.8d $^{19}F_{meta}$ 155.1m $^{19}F_{para}$ 148.8t	— J 18 — J 18	2,2-bis-pentafluorophenyl cyclopenta-2,4-dien-1-one 60 and 100 MHz	354
$C_{24}H_{16}FeO_8$	270	$[C(C_6H_5)_3 \equiv CCO_2CH_3]_2COFe-(CO)_3$	CS_2	H 6.6 H' 3.68s 3.55s	— — —	A tricarbonylcyclopenta- dienoneiron complex derived from methyl phenylpropiolate and $Fe_2(CO)_9$	1044
$C_{20}H_{12}FeO_4$	271	$[h^4-C_5H_2O(C_6H_5)_2]Fe(CO)_3$	—	H_{-2}, H_{-4} ~5.8 H' ~7.1	—	3,4-Diphenylcyclopenta- dienone	355
$C_9H_4D_4FeO_3$	272	$(h^4-C_6H_4D_4)Fe(CO)_3$	CCl_4	H_{-1} 3.26 H_{-3} 5.38 H_{-4} 3.26 H_{-6} 1.58	—	2,5,5,6-Tetradeuterio- cyclohexa-1,3-diene iron tricarbonyl	356
$C_9H_8FeO_3$	273	$(h^4-C_6H_8)Fe(CO)_3$	CCl_4	H_{-1}, H_{-4} 3.18 H_{-2}, H_{-3} 5.30 H_{-5}, H_{-6} 1.68	—	Cyclohexa-1,3-diene iron tricarbonyl	357 358

$C_{10}H_{10}FeO_3$	274	$[h^4-C_6H_7(CH_3)]Fe(CO)_3$	—	H_{-2}, H_{-3}	5.35	—	1-Methylcyclohexa-1,3-diene iron tricarbonyl	358
				H_{-4}	n.a.	—		
				H_{-5}, H_{-6}	2.0–1.7	—		
				H'	1.78	—		
$C_{10}H_{10}FeO_3$	275	$[h^4-C_6H_7(CH_3)]Fe(CO)_3$	$CDCl_3$	H_{-1}	3.20s	—	2-Methylcyclohexa-1,3-diene iron tricarbonyl 100 MHz	359 358
				H_{-3}	5.21d	—		
				H_{-4}	3.04m	—		
				H_{-5}, H_{-6}	1.50b	—		
				H'	2.07s	—		
$C_{10}H_{10}FeO_3$	276	$[h^4-C_6H_7(CH_3)]Fe(CO)_3$	—	H_{-1}, H_{-4}	3.16	—	5-Methylcyclohexa-1,3-diene iron tricarbonyl	358 955
				H_{-2}, H_{-3}	5.50	—		
				H_{-5}	1.4	—		
				H_{-6}	1.9	—		
				H'	0.90d	—		
$C_{11}H_{12}FeO_3$	277	$[h^4-C_6H_6(CH_3)_2]Fe(CO)_3$	—	H_{-1}, H_{-4}	2.95	—	2,5-Dimethylcyclohexa-1,3-diene iron tricarbonyl * C_{-2} methyl signal	358 955
				H_{-3}	5.13d	—		
				H_{-5}, H_{-6}	2.0–1.7	—		
				H'	2.10*	—		
					0.90d	—		
$C_{11}H_{12}FeO_3$	278	$[h^4-C_6H_6(CH_3)_2]Fe(CO)_3$	—	H_{-2}, H_{-3}	4.98	—	1,4-Dimethylcyclohexa-1,3-diene iron tricarbonyl	358
				H_{-5}, H_{-6}	1.75	—		
				H'	1.52	—		
$C_{11}H_{12}FeO_3$	279	$[h^4-C_6H_6(CH_3)_2]Fe(CO)_3$	$CDCl_3$	H_{-2}	5.13s	—	1,3-Dimethylcyclohexa-1,3-diene iron tricarbonyl 100 MHz	359
				H_{-4}	3.08s	—		
				H_{-5}, H_{-6}	1.60m	—		
					1.59s	—		
				H'	2.05s*	—	*3- CH_3	
					1.59s†	—	†1- CH_3	

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_9H_8FeO_4$	280	$[h^4-C_6H_7(OH')][Fe(CO)_3]$	—	H_{-1}, H_{-4}	2.82	5-Hydroxycyclohexa-1,3-diene iron tricarbonyl Isomer A (<i>Exo</i> 5-OH)	358 955
				H_{-2}, H_{-3}	5.30		
				H_{-5}	4.16		
				H_{-6}	1.55, 1.25		
				H'	1.55	Isomer B (<i>Endo</i> 5-OH)	
				H_{-1}, H_{-4}	3.20		
				H_{-2}, H_{-3}	5.32		
				H_{-5}	3.81		
				H_{-6}	2.05, 1.70		
				H'	1.67		
$C_{12}H_{12}FeO_6$	281	$[h^4-6,6-C_6H_6(OH)(CH_2CO_2CH_3)][Fe(CO)_3]$	—	Not reported		Ring-expansion studied	360
$C_{10}H_{10}FeO_4$	282	$[h^4-C_6H_7(OCH_3)][Fe(CO)_3]$	—	H_{-2}	5.28d	1-Methoxycyclohexa-1,3-diene iron tricarbonyl	358
				H_{-3}	5.00q		
				H_{-4}	2.7		
				H_{-5}, H_{-6}	1.6		
				H'	3.45		
$C_{10}H_{10}FeO_4$	283	$[h^4-C_6H_7(OCH_3)][Fe(CO)_3]$	—	H_{-1}	3.37	2-Methoxycyclohexa-1,3-diene iron tricarbonyl	358
				H_{-3}	5.02d		
				H_{-4}	2.70		
				H_{-5}, H_{-6}	1.60		
				H'	3.60		
$C_{10}H_{10}FeO_4$	284	$[h^4-C_6H_7(OCH_3)][Fe(CO)_3]$	—	H_{-1}, H_{-4}	2.90	5-Methoxycyclohexa-1,3-diene iron tricarbonyl	358
				H_{-2}, H_{-3}	5.37		

				H_{-5}	3.70	—			
				H_{-6}	1.68	—			
				H'	3.15	—			
		CS_2		H_{-1}, H_{-4}	3.5-2.5m	—	Exo-methoxy group	361	
				H_{-2}, H_{-3}	5.45m	—			
				H_{-5}	3.75m	—			
				H_{-6}	2-1.7m	—			
				H'	3.15s	—			
$C_{11}H_{12}FeO_4$	285	$[h^4-C_6H_6(CH_3)OCH_3]Fe(CO)_3$	—	H_{-2}	5.25	—	1-Methoxy-3-methylcyclohexa-1,3-diene iron tricarbonyl	358	
				H_{-4}	2.9-2.6	—			
				H_{-5}, H_{-6}	1.9-1.2	—			
				H'	2.08	—			
				H''	3.40	—			
$C_{11}H_{12}FeO_4$	286	$[h^4-C_6H_6(CH_3)OCH_3]Fe(CO)_3$	—	H_{-2}, H_{-3}	5.00q	—	1-Methoxy-4-methylcyclohexa-1,3-diene iron tricarbonyl	358	
				H_{-5}, H_{-6}	2.30-1.65	—			
				H'	1.56	—			
				H''	3.44	—			
$C_{11}H_{12}FeO_4$	287	$[h^4-C_6H_6(CH_3)OCH_3]Fe(CO)_3$	—	H_{-2}, H_{-3}	5.3-4.9	—	1-Methoxy-5-methylcyclohexa-1,3-diene iron tricarbonyl	358	
				H_{-4}	2.9-2.6	—		955	
				H_{-5}	n.a.	—			
				H_{-6}	1.9-1.2	—			
				H'	0.95d	—			
				H''	3.40	—			
$C_{11}H_{12}FeO_4$	288	$[h^4-C_6H_6(CH_3)OCH_3]Fe(CO)_3$	—	H_{-2}	5.3-4.9	—	3-Methoxy-1-methylcyclohexa-1,3-diene iron tricarbonyl	358	
				H_{-4}	3.25	—			
				H_{-5}, H_{-6}	1.9-1.2	—			
				H'	1.60	—			
				H''	3.55	—			

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{11}H_{12}FeO_4$	289	$[h^4-C_6H_6(CH_3)OCH_3]Fe(CO)_3$	—	H_{-1}	n.a.	—	5-Methoxy-2-methylcyclohexa-1,3-diene iron tricarbonyl	358
				H_{-3}	5.3	—		
				H_{-4}	2.80	—		
				H_{-5}	n.a.	—		
				H_{-6}	1.5	—		
				H'	2.10	—		
$C_{11}H_{12}FeO_5$	290	$[h^4-C_6H_6(OCH_3)_2]Fe(CO)_3$	—	H_{-2}, H_{-3}	4.9	—	1,4-Dimethoxycyclohexa-1,3-diene iron tricarbonyl	358
				H_{-5}, H_{-6}	2.30–1.70	—		
				H'	3.32	—		
$C_{11}H_{12}FeO_5$	291	$[h^4-C_6H_6(OCH_3)_2]Fe(CO)_3$	—	H_{-1}	3.48	—	2,5-Dimethoxycyclohexa-1,3-diene iron tricarbonyl	358
				H_{-3}	5.17	—		
				H_{-4}	2.68	—		
				H_{-5}	2.10	—		
				H_{-6}	1.7	—		
				H'	3.70*	—		
$C_{10}H_7FeNO_3$	292	$[h^4-C_6H_7(CN)]Fe(CO)_3$	—	H_{-1}, H_{-4}	3.10	—	5-Cyanocyclohexa-1,3-diene iron tricarbonyl	358 361
				H_{-2}, H_{-3}	5.51	—		
				H_{-5}	2.85	—		
				H_{-6}	2.20	—		
					2.02	—		
$C_{11}H_9FeNO_4$	293	$[h^4-C_6H_6(OCH_3)CN]Fe(CO)_3$	—	H_{-1}	3.39	—	5-Cyano-2-methoxycyclohexa-1,3-diene iron tricarbonyl	358
				H_{-3}	5.17	—		

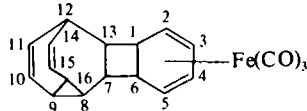
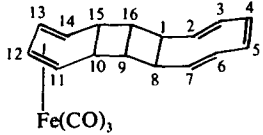
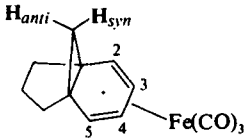
				H₋₄, H₋₅	2.72	—			
				H₋₆	2.10	—			
				H'	3.67	—			
C₁₆H₁₈FeO₇	294	[<i>h</i>⁴-5-C₆H₇CH'(CO₂CH₂^{''}-CH₃^{'''})₂]Fe(CO)₃	—	H₋₁, H₋₄	2.97	—	—	358	
				H₋₂, H₋₃	5.29	—			
				H₋₅	4.09	—			
				H₋₆	2.00	—			
				H'	2.97	—			
				H''	4.09q	—			
				H'''	1.24t	—			
C₁₁H₈FeO₃	295	(<i>h</i>⁴-C₈H₈)Fe(CO)₃	—	H	n.m.	<i>J</i> _{1,2} 6.59 <i>J</i> _{2,3} 4.23 <i>J</i> _{1,3} 1.62 <i>J</i> _{1,4} 0.20	Bicyclo[4.2.0]octa-2,4-diene iron tricarbonyl	346	
C₁₅H₁₆FeO₃	296	[<i>h</i>⁴-C₈H₄(CH₃)₄]Fe(CO)₃	—	H₋₂	2.77	—	1,3,5,7-Tetramethylbicyclo- [4.2.0]octa-2,4,7-triene iron tricarbonyl	362	
				H₋₄	5.22	—			
				H₋₆	2.30	—			
				H₋₈	5.76	—			
				H'	2.03, 1.53	—			
					1.23	—			
C₁₉H₁₆FeO₃	297	(<i>h</i>⁴-C₁₆H₁₆)Fe(CO)₃	CS₂	H₋₁, H₋₆	2.4	—	Structure:	363	
				H₋₂, H₋₅	3.4	—			
				H₋₃, H₋₄	5.4	—			
				H₋₇, H₋₁₃	1.9	—			
				H₋₈, H₋₁₂	1.8	—	T 30		
				H₋₉, H₋₁₁	3.7	—	Temperature-dependent spectra		
				H₋₁₄, H₋₁₆	5.7	—			
				H₋₁₀, H₋₁₅	5.7	—			

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{19}H_{16}FeO_3$	298	$(h^4-C_{16}H_{16})Fe(CO)_3$	$CDCl_3$	H_{-2} to H_{-7} 5.7 $H_{-1}, H_{-8},$ H_{-11}, H_{-14} } 3.3	— —	Structure:  T30	363
$C_{20}H_{24}FeO_4$	299	$[h^4-C_9O(CH_3)_8]Fe(CO)_3$	$CDCl_3$	H_{-12}, H_{-13} 5.3 H_{-10}, H_{-15} 2.6 H_{-9}, H_{-16} 1.95 1-,6- CH_3 0.92s*, 0.85s* 2-,5- CH_3 2.03s†, 1.81s† 3-,4- CH_3 1.67s† 7-,8- CH_3 2.14s‡ 2.11s‡	— — — — — — —	$C_9O(CH_3)_8$ = 1,2,3,4,5,6,7,8-octamethylbicyclo[4.2.0]-nona-2,4,7-trien-9-one *Bridgehead methyls †Methyls of co-ordinated diene ‡Methyls of uncoordinated double bond	341
$C_{13}H_{12}FeO_3$	300	$(h^4-C_{10}H_{12})Fe(CO)_3$	C_6D_6	H_{-2}, H_{-5} 3.38 H_{-3}, H_{-4} 4.90 H_{syn} 0.90 H_{anti} 1.11 n.a.	$J_{2,5} \sim 0$ $J_{2,3} = J_{3,4}$ 6.77 $J_{3,4}$ 4.06 $J_{2,4} = J_{3,5}$ 1.51	Structure:  H_{anti} and H_{syn} labels are present.	1034 742
$C_{30}H_{44}FeO_3$	301	$(h^4-C_{27}H_{44})Fe(CO)_3$	CCl_4		—	$C_{27}H_{44}$ = Cholesta-2,4-diene Olefinic signals at δ 5.62, 5.14	364

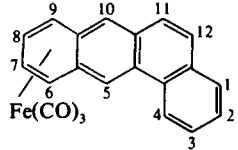
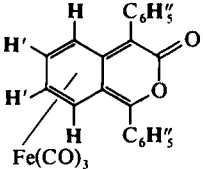
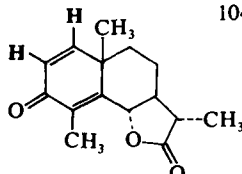
$C_{30}H_{44}FeO_4$	302	$(h^4-C_{27}H_{44}O)Fe(CO)_3$	$CDCl_3$	n.a.	—	$C_{27}H_{44}O$ = Cholesta-5,7-diene-3 β -ol Olefinic signals at δ 5.25, 4.98	364
$C_{31}H_{44}FeO_4$	303	$(h^4-C_{28}H_{44}O)Fe(CO)_3$	$CDCl_3$	n.a.	—	$C_{28}H_{44}O$ = Ergosterol Olefinic signals δ 5.24m	364
$C_{17}H_{10}FeO_3$	304	$(h^4-C_{14}H_{10})Fe(CO)_3$	—	Not reported	$J_{1,2} = J_{3,4}$ 6.29 $J_{2,3}$ 4.21 $J_{1,3} = J_{2,4}$ 1.48 $J_{1,4} \sim 0$	Anthracene iron tricarbonyl Co-ordinated ring	346
					$J_{1,2} = J_{3,4}$ 8.14 $J_{2,3}$ 6.95 $J_{1,3} = J_{2,4}$ 1.26 $J_{1,4}$ 0.63	Unco-ordinated ring	
$C_{21}H_{12}FeO_3$	305	$(h^4-C_{18}H_{12})Fe(CO)_3$	$CDCl_3$	H_{-1}, H_{-2} 7.58 H_{-3} H_{-4} 8.35 H_{-5} 7.83 H_{-6}, H_{-9} 3.78 H_{-7}, H_{-8} 6.40 H_{-10} 7.03 H_{-11}, H_{-12} $\sim$ 7.58	—	Structure: 	365
$C_{24}H_{14}FeO_5$	306	$[h^4-C_9H_4O_2(C_6H_5)_2]Fe(CO)_3$	—	H 3.8m H' 6.0m H'' 7.7-7.2m	—	Structure: 	366

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_9H_6FeO_4$	307	$(h^4-C_6H_6O)Fe(CO)_3$	—	H_{-2}, H_{-5} 3.26m H_{-3}, H_{-4} 5.84m H_{-6} 2.35d	— — —	Cyclohexa-2,4-dien-1-one iron tricarbonyl	358
$C_{10}H_8FeO_4$	308	$[h^4-C_6H_5O(CH_3)]Fe(CO)_3$	—	H_{-2} 3.24s H_{-4} 5.62d H_{-5} 3.12m H_{-6} 2.20 H' 2.20s	— — — — —	3-Methylcyclohexa-2,4-dien-1-one iron tricarbonyl	358
$C_{10}H_8FeO_5$	309	$[h^4-C_6H_5O(OCH_3)]Fe(CO)_3$	—	H_{-2} 2.76d H_{-3} 5.64d H_{-5} 3.46d H_{-6} 2.22	— — — —	4-Methoxycyclohexa-2,4-diene-1-one iron tricarbonyl	358
$C_{11}H_{10}FeO_4$	310	$[2,3,5,6-h^4-4,4-C_6H_4O(CH_3)_2]Fe(CO)_3$	CCl_4	H 4.04, 3.42	—	4,4-Dimethylcyclohexa-2,5-dienone complex	1045
$C_{18}H_{18}FeO_6$	311	$(h^4-C_{15}H_{18}O_3)Fe(CO)_3$	$CDCl_3$	H 3.80, 3.30	—	$C_{15}H_{18}O_3 =$ 	1045
$C_{30}H_{42}FeO_4$	312	$(1,2,4,5-h^5-C_{27}H_{42}O)Fe(CO)_3$	$CDCl_3$	H_{-1}, H_{-2} } 4.06 H_{-4} } 3.18	—	$C_{27}H_{42}O =$ cholesta-1,4-dien-3-one	1045

C ₁₂ H ₁₅ FeNO ₃	313	{ <i>h</i> ⁴ -5-C ₇ H ₉ [N(CH ₃) ₂]}Fe(CO) ₃	—	n.a.	—	Cyclohepta-1,3-diene derivative. Signals at δ 5.4, 2.9, 2.2s, 2.05, 1.35, in ratio 2:3:2:6:2	298	
C ₁₁ H ₁₂ FeO ₄	314	[<i>h</i> ⁴ -5,5-C ₇ H ₈ (CH ₃)OH'']Fe(CO) ₃	—	H ₋₁	3.13	—	Cyclohepta-1,3-diene derivative	367
				H ₋₂ , H ₋₃	5.29	—		
				H ₋₄	2.87	—		
				H ₋₆	1.26	—	T 33.3	
				H ₋₇	2.0	—		
				H'	1.31	—	Europium induced shifts reported	368
				H''	1.67	—		
C ₁₃ H ₁₄ FeO ₆	315	[<i>h</i> ⁴ -C ₇ H ₈ (OH)CH ₂ CO ₂ Me]-Fe(CO) ₃	—	Not reported	—	—	7-Hydroxy-7-methoxy-carbonylmethylcyclohepta-1,3-diene iron tricarbonyl	360
C ₁₂ H ₁₄ FeO ₄	316	[<i>h</i> ⁴ -5-C ₇ H ₉ (OCH ₂ CH ₃)]Fe(CO) ₃	CS ₂	H ₋₁ , H ₋₄ , H ₋₇	3.8–2.6m	—	Cyclohepta-1,3-diene derivative	361
				H ₋₂ , H ₋₃	5.3m	—		
				H ₋₅ , H ₋₆	2.4–1.0m	—		
				H'	3.3q	—		
				H''	1.1t	—		
[C ₁₀ H ₇ FeO ₃] ⁻	317	[(<i>h</i> ⁴ -C ₇ H ₇)Fe(CO) ₃] ⁻	THF	H	4.65	—	Iron tricarbonyl complex of the antiaromatic cycloheptatrienyl anion	369
C ₁₄ H ₁₄ FeO ₅	318	[<i>h</i> ⁴ -C ₈ H ₈ (6-OCH ₃)- (8-COCH ₃)]Fe(CO) ₃	CS ₂	H ₋₁ , H ₋₇	2.55m	—	Bicyclo[5.1.0]octa-2,4-diene derivative	370
				H ₋₂ , H ₋₅ ,	3.1m, 2.7m	—		
				H ₋₃ , H ₋₄	3.2m	—		
				H ₋₆ ,	3.8m	—		
				H ₋₈ ,	2.8s	—		
				H'	3.3s	—		
				H''	Not reported	—		

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References		
$C_{11}H_8Br_2FeO_3$	319	$(h^4-8,8-C_8H_8Br_2)Fe(CO)_3$	CS_2	H_{-1}, H_{-6}	2.6–1.6m	—	Bicyclo[5.1.0]octa-2,4-diene derivative	371	
				H_{-7}					372
				H_{-2}, H_{-5}	3.25m, 2.95b	—			
				H_{-3}, H_{-4}	5.25m	—			
$C_{10}H_8FeO_3$	320	$(1,2,3,4-h^4-C_7H_8)Fe(CO)_3$	C_6D_6	H_{-1}, H_{-4}	2.87	—	C_7H_8 = Cyclohepta-1,3,5-triene	369	
				H_{-2}, H_{-3}, H_{-6}	5.14–4.66	—			
				H_{-5}	5.61	—			
				H_{-7}	2.12	—			
$C_{11}H_8FeO_4$	321	$[h^4-1-C_7H_7(CH'=O)]Fe(CO)_3$	C_6D_6	H_{-2}	6.07d	J 8	Cyclohepta-1,3,5-triene derivative	373	
				H_{-3}, H_{-6}, H_{-7}	2.95–1.62	—			
				H_{-4}, H_{-5}	4.47m	—			
				H'	0.03s	—			
			CS_2	H_{-2}	6.8d	—	T30° 100 MHz	374	
				H_{-3}	3.18t				
				H_{-4}, H_{-5}	4.5m				
				H_{-6}	3.55m				
				H_{-7}	2.43m				
				H'	9.02s				
$C_{12}H_{10}FeO_5$	322	$[h^4-1-C_7H_7(CO_2Me)]Fe(CO)_3$	—	Not reported		Cyclohepta-1,3,5-triene derivative	360		

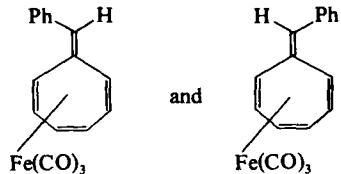
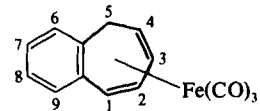
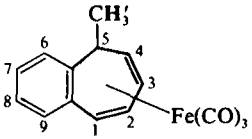
$C_{11}H_8FeO_3$	323	$(2,3,4,5\text{-}h^4\text{-}C_8H_8)Fe(CO)_3$	CS_2	n.a.			$C_8H_8 = 1\text{-Methylenecyclohepta-2,4,6-triene}$ Signals at δ 5.44m, 5.19s, 4.89s, 3.63d (<i>J</i> 7), 2.93t, in ratio 4:1:1:1:1	375
$C_{17}H_{12}FeO_3$	324	$[2,3,4,5\text{-}h^4\text{-}C_8H_7(C_6H_5)]Fe(CO)_3$	—	H	7.2m	—	1-Benzylidenecyclohepta-2,4,6-triene Other signals at δ 6.5d, 5.9–5.2m, 4.0dd*, 2.9t, in ratio 1:4:1:1	376
							*Two signals attributed to presence of two geometrical isomers, viz.:	
								
$C_{14}H_{10}FeO_3$	325	$(h^4\text{-}C_{11}H_{10})Fe(CO)_3$	CCl_4/CH_3CN (1:1)	H_{-1} 3.64 pent. H_{-2}, H_{-3} 5.37 sept. H_{-4} 3.42m H_{-5} 3.10t	— — — —		Structure:	377
								
				H_{-6} to H_{-9}	7.0m	—	100 MHz	

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{15}H_{12}FeO_3$	326	$[h^4-C_{11}H_8(CH_3)]Fe(CO)_3$	CCl_4/CH_3CN	H_{-1} 3.68 pent. H_{-2}, H_{-3} 5.42 pent. H_{-4} 3.27 sept. H_{-5} 3.1m H_{-6} to H_{-9} 7.0m	— — — — —	Structure:  100 MHz	377
$C_{10}H_8FeO_4$	327	$(h^4-C_7H_6O)Fe(CO)_3$	—	H_{-2} 3.05 H_{-3} 5.92 H_{-4} 5.56 H_{-5} 3.33 H_{-6} 2.63 H_{-7} 2.0	— — — — — —	C_7H_6O = Cyclohepta-2,4-dien-1-one T 33.3°	367
$C_{11}H_{10}FeO_3$	328	$[h^4-6-C_7H_7O(OCH_3)]Fe(CO)_3$	—	H_{-2} 3.18 H_{-3}, H_{-4} 5.7 H_{-5} 5.28 H_{-6} 3.91 H_{-7} 2.4, 1.9 H' 3.35	— — — — — —	Europium induced shifts Cyclohepta-2,4-diene-1-one derivative	368 367
$C_{10}H_6FeO_4$	329	$(h^4-C_7H_6O)Fe(CO)_3$	$CDCl_3$	H_{-2} 5.05 H_{-3} 6.58 H_{-4} 2.25	$J_{2,3}$ 11.0 $J_{2,7}$ 2.0 $J_{2,4}$ 1.0 $J_{3,4}$ 8.0 —	C_7H_6O = Cyclohepta-2,4,6-trien-1-one T 33.3° Europium induced shifts	367 368

				H_{-5}, H_{-6}	6.39	—		
				H_{-7}	3.19	—		
$C_{11}H_8FeO_3$	330	$(1,2,3,4-h^4-C_8H_8)Fe(CO)_3$	$CHCl_3$	H_{-1}, H_{-4}	4.55	—	T -155°	378
				H_{-2}, H_{-3}	4.78	—	Singlet at 20° (δ 5.39)	922
				H_{-5}, H_{-8}	6.45	—		1050
				H_{-6}, H_{-7}	6.19	—		
$C_{12}H_3D_7FeO_3$	331	$[h^4-1-C_8HD_6(CH_2D)]Fe(CO)_3$	$CDCl_3$	H	4.56	—	1-Monodeuteriomethyl-2,3,4,5,6,7-hexadeuterio-cyclo-octatetraene iron tricarbonyl	1037
				H'	1.85	—		
				H	4.58	—	1,2,7,8- h^4 -isomer at -145°	
				H	4.32	—	1,2,3,8- h^4 -isomer at -145°	
$C_{12}H_{10}FeO_3$	332	$[h^4-1-C_8H_7(CH_3)]Fe(CO)_3$	—	H	n.a.	—	1-Methylcyclo-octatetraene	921
				H'	1.87s	—	H signals at δ 5.67d, 5.08t, 4.50d at T 30° and at δ 5.95 and 4.38 at T-120.	1050
$C_{16}H_{17}FeNO_4$	333	$[h^4-C_8H_7(CH_2NC_4H_8''O)]Fe(CO)_3$	CS_2	H	5.1m	—	Morpholinomethyl-cyclo-octatetraene	370
				H'	2.8s	—	T 35°	
				H''	3.5t,	J 6		
					2.3t	J 6		
$C_{12}H_{10}FeO_4$	334	$[h^4-C_8H_7CH_2OH'']Fe(CO)_3$	CS_2	H	5.2m	—	Hydroxymethylcyclo-octatetraene iron tricarbonyl	370
				H'	3.85d	J 6	T 29° 100 MHz	
				H''	3.25t	J 6		
$C_{13}H_{12}FeO_4$	335	$[h^4-C_8H_7(CH_2OCH_3'')]Fe(CO)_3$	CS_2	H	5.0m	—	Methoxymethylcyclo-octatetraene iron tricarbonyl	370
				H'	3.7s	—	T 29° 100 MHz	
				H''	3.2s	—		

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{13}H_{12}FeO_4$	336	$\{h^4-C_8H_7[CH'(CH_3)OH''']\}-Fe(CO)_3$	CS_2	H	5.0m	Cyclo-octatetraene derivative T 29° 100 MHz	370
				H'	3.90qd		
				H''	1.30d		
				H'''	1.44d		
$C_{14}H_{14}FeO_4$	337	$\{h^4-C_8H_7[CH'(CH_3)OCH_3''']\}-Fe(CO)_3$	CS_2	H	5.1m	Cyclo-octatetraene derivative T 35	370
				H'	3.55q		
				H''	1.2d		
				H'''	3.1s		
$C_{12}H_8FeO_4$	338	$[h^4-1-C_8H_7(CH'=O)]Fe(CO)_3$	CS_2	H ₋₂ , H ₋₈	6.09	Cyclo-octatetraene derivative T 29 100 MHz	370
				H ₋₃ , H ₋₄	5.34m		
				H ₋₆ , H ₋₇	—		379
				H ₋₅	4.38t		
				H'	9.28s		
$C_{13}H_{10}FeO_4$	339	$[h^4-1-C_8H_7(COCH_3)]Fe(CO)_3$	CS_2	H ₋₃ , H ₋₄	5.16m	Cyclo-octatetraene derivative T 29 100 MHz	370
				H ₋₆ , H ₋₇	—		
				H ₋₅	4.46t		
				H'	2.30s		
$C_{15}H_{12}FeO_5$	340	$[h^4-C_8H_6(COCH_3)_2]Fe(CO)_3$	$CFC l_3$	H	n.a.	Diacylcyclo-octatetraene derivative — mixture of isomers H signals at δ 7.65s, 7.02s, 6.82d (J 3), 6.42d (J 10), 6.06s, 5.94s, 5.04t (J 7), 4.63d (J 7) 4.53d (J 7). T 29 100 MHz	370
				H'	2.40s,		
					2.26s,		
					2.28s		

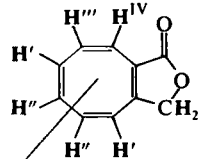
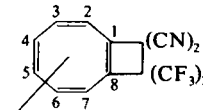
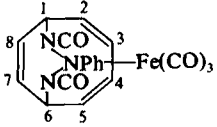
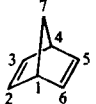
$C_{13}H_{12}FeO_5$	341	$[h^4-2-C_8H_9(CO_2Me)]Fe(CO)_3$	—	Not reported	—	Cyclo-octa-1,3,5-triene derivative	360
$C_{15}H_{12}FeO_7$	342	$[h^4-C_8H_6(CO_2CH_3)_2]Fe(CO)_3$	$CDCl_3$	H_{-2}, H_{-7} 7.28d H_{-3}, H_{-6} 4.09m H_{-4}, H_{-5} 5.09m H' 3.71	J 10 — — —	1,8-Dicarbomethoxy-cyclo-octa-1,3,5,7-tetraene iron tricarbonyl T 35° 60 and 100 MHz	378
$C_{15}H_{10}FeO_3$	343	$(h^4-C_{12}H_{10})Fe(CO)_3$	CCl_4	H^* 4.90bs, 4.60bs, 3.73bs $H^\dagger$ 6.08bs $H^\ddagger$ 7.13s	— — — — —	$C_{12}H_{10}$ = Benzocyclo-octa tetraene *Complexed diene protons $\dagger$ Unco-ordinated double bond protons $\ddagger$ Aromatic protons	380
$C_{13}H_8FeO_3$	344	$(h^4-C_{10}H_8O_2)Fe(CO)_3$	$CDCl_3$	H 4.82, 4.81 H' 4.55 comp. H'' 5.55 H''' 5.95m	— — — J 10.5	Structure: 	378
$C_{17}H_8F_6FeN_2O_3$	345	$(h^4-C_{14}H_8F_6N_2)Fe(CO)_3$	$CDCl_3$	H^{IV} 5.1d H_{-1} 3.34 H_{-2} 5.68 H_{-3} 6.45 H_{-4} 4.42	— $J_{1,2}$ 6.0 $J_{2,3}$ 11.0 $J_{3,4}$ 9.0 $J_{4,5}$ 10.0	$Fe(CO)_3$ 60 and 100 MHz Structure: 	381
				H_{-5} 4.79 H_{-6} 4.60 H_{-7} 4.06 H_{-8} 1.63	$J_{5,6}$ 8.0 $J_{6,7}$ 7.5 $J_{7,8}$ 11.5 $J_{1,8}$ 8.0	$Fe(CO)_3$ 100 MHz $(J_{F,F} 13.0, J_{HF} 4.5)$	

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{19}H_{13}FeN_3O_5$	346	$(h^4-C_{16}H_{13}FeN_3O_2)Fe(CO)_3$	$CDCl_3$	H_{-1}, H_{-6} 5.20 H_{-2}, H_{-5} 3.94 H_{-3}, H_{-4} 5.43 H_{-7}, H_{-8} 6.33	$J_{1,2}$ 9.2 $J_{2,3}$ 8.1 $J_{2,4}$ 1.40 $J_{3,4}$ 4.13 $J_{7,8}$ 8.88 $J_{1,8}$ 7.60 $J_{1,7}$ 0.90	Structure:  100 MHz	381
$C_{11}H_{12}FeO_3$	347	$(h^4-C_8H_{12})Fe(CO)_3$	—	n.a.	—	C_8H_{12} = Cyclo-octa-1,3-diene Signals at δ 4.76q, 3.00m, 1.8m, 1.1m, in ratio 2:2:4:4	281
$C_{11}H_{12}FeO_3$	348	$(h^4-C_8H_{12})Fe(CO)_3$	—	n.a.	—	C_8H_{12} = Cyclo-octa-1,5-diene Signals at δ 3.4m (4H), 2.0m (8H), or at δ 3.7 (4H), 2.4 (8H)	281 922
$C_{10}H_8FeO_3$	349	$(2,3,5,6-h^4-C_7H_8)Fe(CO)_3$	$CDCl_3$	H_{-1}, H_{-4} 3.35m H_{-2}, H_{-3} } 3.15t H_{-5}, H_{-6} } H_{-7} 1.25t	— — —	C_7H_8 = Norbornadiene 	58 382
$[C_{10}H_9FeO_3]^+$	350	$[(2,3,5,6-h^4-C_7H_8)Fe(H')(CO)_3]^+$	FSO_3H/SO_2	H_{-1} 3.32 H_{-2}, H_{-3} 4.75 H_{-4} 4.40 H_{-5}, H_{-6} 4.05 H_{-7} 1.90s H' -7.13	— — — — —	C_7H_8 = Norbornadiene	382

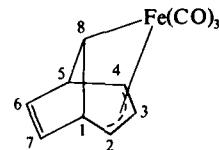
$C_{24}H_{24}FeN_4O_7S_2$	351	$[2,3,5,6-h^4-7,7-C_7H_6(NH'NH''-SO_2-p-C_6H_4'''CH_3^{IV})_2]Fe(CO)_3$	$(CH_3)_2SO$	H	2.92bs	—	Norbornadiene derivative	383
				H'	4.67bs	—		
				H''	7.90bs	—		
				H'''	7.53q	—		
				H ^{IV}	2.40s	—		
$C_{10}H_8FeO_4$	352	$[2,3,5,6-h^4-7-C_7H_7(OH')]-Fe(CO)_3$	$CDCl_3$	H ₋₁ , H ₋₄	3.28 sept.	—	Norbornadiene derivative*	384
				H ₋₂ , H ₋₃	3.02t	—		
				H ₋₅ , H ₋₆	2.92t	—		
				H ₋₇	6.32bd	<i>J</i> 7.5		
				H'	2.0d	<i>J</i> 7.5	*Numbering so that C-7 substituent is syn to C-5C-6 double bond.	
$C_{11}H_{10}FeO_4$	353	$[2,3,5,6-h^4-7,7-C_7H_6(CH_3)OH]-Fe(CO)_3$	$CDCl_3$	n.m.		—	Norbornadiene derivative	383
$C_{12}H_{12}FeO_4$	354	$[2,3,5,6-h^4-7,7-C_7H_6(CH_2'-CH_3')OH''']Fe(CO)_3$	$CDCl_3$	H	3.05m,	—	Norbornadiene derivative	383
					3.00m			
				H'	1.53q	<i>J</i> 7		
				H''	0.84t	<i>J</i> 7		
				H'''	2.15s	—		
$C_{12}H_{10}FeO_4$	355	$[2,3,5,6-h^4-7,7-C_7H_6(CH'=CH_2')OH'']Fe(CO)_3$	$CDCl_3$	H	3.07m	—	Norbornadiene derivative	383
				H'	6.35-5.09	—		
					comp.			
				H''	2.13s	—		
$C_{16}H_{12}FeO_4$	356	$[2,3,5,6-h^4-7,7-C_7H_6(C_6H_5')-OH'']Fe(CO)_3$	$CDCl_3$	H ₋₁ , H ₋₄	3.42m	<i>J</i> 2.5	Norbornadiene derivative	383
				H ₋₂ , H ₋₃	3.08t	<i>J</i> 2.5		
				H ₋₅ , H ₋₆	2.77t	<i>J</i> 2.5		
				H'	7.29m	—		
				H''	2.50s	—		

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{17}H_{12}FeO_5$	357	[2,3,5,6- <i>h</i> ⁴ -7-C ₇ H ₇ -(OCOC ₆ H ₅)Fe(CO) ₃]	CDCl ₃	H ₋₁ , H ₋₄	3.55 oct.	Norbornadiene* derivative	384
				H ₋₂ , H ₋₃	3.09q		
				H ₋₅ , H ₋₆	2.92q		
				H ₋₇	4.50t		
				H'	8.0-7.2 comp.		
$C_{17}H_{10}FeN_2O_9$	358	{2,3,5,6- <i>h</i> ⁴ -7-C ₇ H ₇ [OCOC ₆ H ₅ -3,5(NO ₂) ₂]Fe(CO) ₃ }	CDCl ₃	H ₋₁ , H ₋₄	3.75m	Norbornadiene derivative*	384
				H ₋₂ , H ₋₃	3.23t		
				H ₋₅ , H ₋₆	3.06t		
				H ₋₇	4.7t		
				H' ₂ , H' ₆	9.08d		
$C_{11}H_{10}FeO_6S$	359	[2,3,5,6- <i>h</i> ⁴ -7-C ₇ H ₇ (OSO ₂ -CH ₃)Fe(CO) ₃]	CDCl ₃	H ₋₁ , H ₋₄	3.62m	Norbornadiene derivative*	384
				H ₋₂ , H ₋₃	3.15t		
				H ₋₅ , H ₋₆	2.97m		
				H ₋₇	3.25t		
				H'	—		
$C_{17}H_{14}FeO_6S$	360	[2,3,5,6- <i>h</i> ⁴ -7-C ₇ H ₇ (OSO ₂ - <i>p</i> -C ₆ H ₄ CH ₃)Fe(CO) ₃]	CDCl ₃	H ₋₁ , H ₋₄	3.45m	Norbornadiene derivative*	384
				H ₋₂ , H ₋₃	3.01t		
				H ₋₅ , H ₋₆	2.81t		
				H ₋₇	4.10t		
				H'	7.83m		
				H''	7.73m		
					2.50s		

*Numbering so that C-7 substituent is syn to C-5C-6 double bond

$C_{10}H_6FeO_4$	361	$(2,3,5,6-h^4-C_7H_6O)Fe(CO)_3$	$CDCl_3$	H_{-1}, H_{-4} 3.65q	$J_{2,5}$	Norbornadien-7-one	383
				H_{-2}, H_{-3} } 3.02t	$J_{2,5}$		385
				H_{-5}, H_{-6} }			
$C_{14}H_{12}FeO_3$	362	$[2,3,5,6-h^4-7-C_7H_6(=CH'-CO.OCH_2CH_3''')]Fe(CO)_3$	$CDCl_3$	H_{-1} 3.58m	$J_{2,5}$	7-Carboethoxymethylene norbornadiene*	383
				H_{-2}, H_{-3} } 3.14t	$J_{2,5}$		
				H_{-5}, H_{-6} }			
				H_{-4} 4.64m	$J_{2,5}$		
				H' 4.80s	—		
				H'' 4.12q	J_7		
				H''' 1.27t	J_7		
						*Numbering so that C-7 substituent is syn to the C-5C-6 double bond	
$C_{18}H_{12}FeO_3$	363	$(2,3,5,6-h^4-C_{15}H_{12}O_2)Fe(CO)_3$	$CDCl_3$	H_{-1}, H_{-4} 3.37m	—	$C_{15}H_{12}O_2 = 7$ -Benzoyl methylene-7,8-epoxy-norbornadiene	383
				H_{-2}, H_{-3} 5.44m	$J_{3,5}$		
				H_{-5} 3.00dd	$J_{11,3,5}$		
				H_{-6} 5.15dd	$J_{11,3,5}$	$H^* =$ aromatic protons	
				H_{-8} 5.82	—		
				H^* 7.50m	—		
$C_{15}H_6F_4FeO_3$	364	$(h^4-C_{12}H_6F_4)Fe(CO)_3$	$CDCl_3$	H^* 3.3	—	$C_{12}H_6F_4 =$ Tetrafluorobenz-bicyclo[2.2.2]octatriene	386
				$H^\dagger$ 5.0	—	H^* complexed diene protons	
				F_{ortho} 165.5	—	$H^\dagger$ Bridgehead protons	
				F_{meta} 152.2	—		
$C_{11}H_8FeO_3$	365	$(h^4-C_8H_8)Fe(CO)_3$	$CDCl_3$	H_{-1}, H_{-5} 3.10	$J_{1,2} = J_{4,5} 5.5$	Structure:	387
					$J_{1,8} = J_{5,8} 6.3$		
				H_{-2}, H_{-4} 4.70	$J_{2,3} = J_{3,4} 6.1$		
					$J_{2,8} = J_{4,8} 1.4$		
				H_{-3} 4.30	$J_{1,3} = J_{3,5} 1.2$		
				H_{-6}, H_{-7} 6.30	$J_{1,6} = J_{5,7} 1.1$		
				H_{-8} 0.60	$J_{1,7} = J_{5,6} 1.5$		



T -60 to 120
60, 90 and 220 MHz

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{11}H_{15}FeNO_3$	366	$(h^4\text{-}CH_3CH'=CH''-CH'''=NCH_2^{IV}C_3H_7)Fe(CO)_3$	C_6H_6	H H' H'' H''' H ^{IV}	0.86d 1.95 comp. 3.96q 5.49d 1.75t	— $J_{H'H''}$ 10.0 $J_{H''H'''} 2.9$ — —	100 MHz	388
$C_{18}H_{13}FeNO_3$	367	$(h^4\text{-}C_6H_5CH=CH'-CH''=NC_6H_5''')Fe(CO)_3$	CCl_4	H H' H'' H'''	3.35b 5.65b 7.40 6.70	— — — —	100 MHz	388 389
$C_{15}H_{24}FeN_2O_3$	368	$[h^4\text{-}C_4H_9N=C(CH_3)C(CH_3)=NCH_2C_3H_7]Fe(CO)_3$	—	H H'	1.24s 3.79t	— —	100 MHz	388
$C_{19}H_{16}FeN_2O_3$	369	$[h^4\text{-}C_6H_5N=C(CH_3)C(CH_3)=NC_6H_5]Fe(CO)_3$	C_6H_6	H	1.28s	—	100 MHz	388
$C_{16}H_9FeNO_3$	370	$(1,2,3,4\text{-}h^4\text{-}C_{13}H_9N)Fe(CO)_3$	$(CD_3)_2CO$	H ₋₁₁ , H ₋₄ H ₋₂ , H ₋₃ H ₋₅ to H ₋₉	4.03 6.82 ~ 7.50 —	— — — —	$C_{13}H_9N$ = Acridine	365
$C_{22}H_{23}FeNO_6$	371	$(h^4\text{-}C_{19}H_{23}NO_3)Fe(CO)_3$	—	OCH ₃ NCH ₃ OH =CH	3.84, 3.50 2.34 5.83 6.66*	— — — —	β -Dihydrothebaine iron tricarbonyl. Also signals at δ 4.80d, 5.20d *Aromatic protons	988
$[C_{25}H_{27}FeNO_4]^+$	372	$[(h^4\text{-}C_{22}H_{27}NO_4)Fe(CO)_3]^+$	—	OCH ₃ COCH ₂ - CH ₃	4.40, 3.75 1.25 —	— — —	Propionyl- β -dihydrothebaine iron tricarbonyl hydrofluoroborate. Also signals at δ 5.02, 6.49 (=CH), 7.32 (=CH)	988

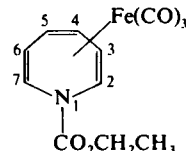
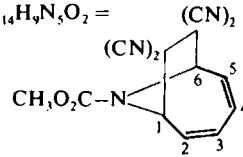
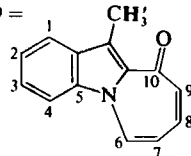
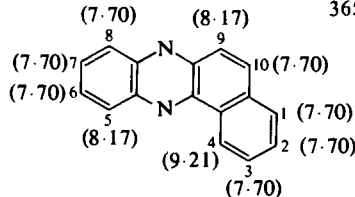
				NHCH_3	4.05	—		
				NHCH_3	9.10	—		
				$=\text{CH}$	7.03*	—		*Aromatic protons
$\text{C}_{22}\text{H}_{20}\text{FeN}_2\text{O}_6$	373	$(h^4\text{-C}_{19}\text{H}_{20}\text{N}_2\text{O}_3)\text{Fe}(\text{CO})_3$	—	OCH_3	3.72, 3.42	—		<i>N</i> -Cyano- β -dihydronorthebaine
				OH	8.55	—		iron tricarbonyl. Also signals
				$=\text{CH}$	6.70*	—		at δ 5.25, 5.54 ($=\text{CH}$)
								*Aromatic protons
$\text{C}_{22}\text{H}_{18}\text{FeN}_2\text{O}_6$	374	$(h^4\text{-C}_{19}\text{H}_{18}\text{N}_2\text{O}_3)\text{Fe}(\text{CO})_3$	—	OCH_3	3.80, 3.60	—		<i>N</i> -Cyanonorthebaine iron
				$=\text{CH}$	6.78d*	—		tricarbonyl. Also signals at
								δ 4.59d, 5.35q
								*Aromatic protons
$\text{C}_{12}\text{H}_{11}\text{FeNO}_5$	375	$(h^4\text{-C}_9\text{H}_{11}\text{NO}_2)\text{Fe}(\text{CO})_3$	CDCl_3	H_{-2}	6.07	—		Structure:
				H_{-3}	4.47	$J_{2,3}$ 6.8		
				$\text{H}_{-4}, \text{H}_{-6}$	5.06	$J_{4,5}$ 7.8		
				H_{-5}	3.54	$J_{5,6}$ 7.8		
				H_{-7}	6.5	$J_{6,7}$ 9		No Fluxional character at T = 0°
$\text{C}_{17}\text{H}_9\text{FeN}_5\text{O}_5$	376	$(2,3,4,5\text{-}h^4\text{-C}_{14}\text{H}_9\text{N}_5\text{O}_2)\text{Fe}(\text{CO})_3$	—	$\text{H}_{-1}, \text{H}_{-6}$	5.75m	$J_{1,2} = J_{5,6}$ 8.8		$\text{C}_{14}\text{H}_9\text{N}_5\text{O}_2 =$
				$\text{H}_{-2}, \text{H}_{-5}$	4.0m	$J_{2,3} = J_{4,5}$ 7.5		
						$J_{2,4} = J_{3,5}$ 1.6		
				$\text{H}_{-3}, \text{H}_{-4}$	5.95m	$J_{3,4}$ 4.5		

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{17}H_{11}FeNO_4$	377	$(6,7,8,9-h^4-C_{14}H_{11}NO)Fe(CO)_3$	$CDCl_3$	H_{-1} to H_{-4} 8.0–7.1m H_{-6}, H_{-8} 5.9–5.4m H_{-7} 6.4–6.1m H_{-9} 3.95–3.65d H' 2.54s	— — — J 8	$C_{14}H_{11}NO =$  100 MHz	391
$C_{15}H_8FeN_2O_3$	378	$(1,2,3,4-h^4-C_{12}H_8N_2)Fe(CO)_3$	$CDCl_3$	H_{-1}, H_{-4} 3.85 H_{-2}, H_{-3} 6.47 H_{-5} to H_{-8} 7.42	— — —	$C_{12}H_8N_2 =$ Phenazine	365
$C_{19}H_{10}FeN_2O_3$	379	$(5,6,7,8-h^4-C_{16}H_{10}N_2)Fe(CO)_3$	$CDCl_3$	H_{-1}, H_{-2}, H_{-3} } 7.60 H_{-9}, H_{-10} } H_{-4} 8.80	— —	$C_{16}H_{10}N_2^* =$  *Values for uncomplexed ligand shown in parentheses	365

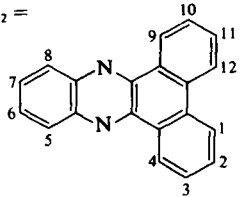
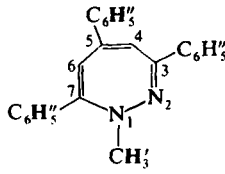
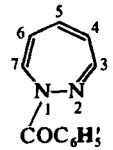
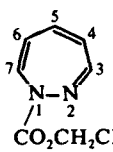
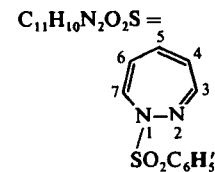
$C_{23}H_{12}FeN_2O_3$	380	$(5,6,7,8-h^4-C_{20}H_{12}N_2)Fe(CO)_3$	$CDCl_3$	H_{-1}, H_{-12} 8.55 H_{-2}, H_{-3} } 7.64 H_{-10}, H_{-11} }	— —	$C_{20}H_{12}N_2 =$		365
				H_{-4}, H_{-9} 9.00 H_{-5}, H_{-8} 3.98 H_{-6}, H_{-7} 6.72	— — —	Values for uncomplexed ligand: δ 8.42 ($H_{-1}, H_{-5}, H_{-8}, H_{-12}$), 7.77 ($H_{-2}, H_{-3}, H_{-6}, H_{-7}, H_{-10}, H_{-11}$), 9.38 (H_{-4}, H_{-9})		
$C_{27}H_{20}FeN_2O_3$	381	$\{4,5,6,7-h^4-C_5H_2N_2(1-CH_3)-[3,5,7-(C_6H'_5)_3]\}Fe(CO)_3$	$CDCl_3$	H_{-4} 4.94d H_{-6} 4.74d H' 2.98s H'' 8.07m 7.75m 7.47–6.88m—	$J_{4,6}$ 2 — — — — —	1-Methyl-3,5,7-triphenyl-1H-1,2-diazepine iron tricarbonyl		390
$C_{10}H_8FeN_2O_4$	382	$[4,5,6,7-h^4-1-C_5H_5N_2(COCH_3)]-Fe(CO)_3$	$CDCl_3$	H_{-3} 6.92 H_{-4} 3.28 H_{-5} 5.11 H_{-6} 4.59 H_{-7} 6.47	$J_{3,4}$ 6 $J_{4,5}$ 7 $J_{4,6}$ 1.6 $J_{5,6}$ 4.3 $J_{6,7}$ 6.7 $J_{5,7}$ 1.7	60 and 100 MHz 1-Acetyl-1H-1,2-diazepine iron tricarbonyl 60 and 100 MHz Calculated chemical shifts and coupling constants reported		390

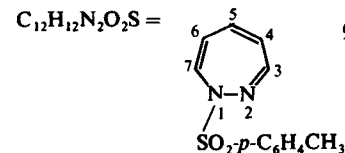
TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{11}H_{10}FeN_2O_4$	383	$[h^4-C_3H_4N_2(1-COCH_3)-(3-CH_3)]Fe(CO)_3$	$CDCl_3$	H_{-4}	3.19dd	$J_{4,5}$ 7.5	1-Acetyl-3-methyl-1 <i>H</i> -1,2-diazepine iron tricarbonyl 60 and 100 MHz	390 *993
					(3.55q)*	$J_{4,6}$ 2		
				H_{-5}	5.09 oct.	$J_{5,6}$ 4.5		
						$J_{5,7}$ 2		
				H_{-6}	4.59 oct.	$J_{6,7}$ 7		
				H_{-7}	6.39dd	—		
$C_{11}H_{10}FeN_2O_4$	384	$[h^4-C_3H_4N_2(1-COCH_3)-(4-CH_3)]Fe(CO)_3$	$CDCl_3$	H_{-3}	6.84s	—	1-Acetyl-4-methyl-1 <i>H</i> -1,2-diazepine iron tricarbonyl 60 and 100 MHz	390
				H_{-5}	4.97bd	$J_{5,6}$ 4.5		
				H_{-6}	4.38dd	$J_{6,7}$ 6.5		
				H_{-7}	6.34dd	$J_{5,7}$ 2		
				H'	2.37s	—		
				H''	1.97s	—		
$C_{15}H_{10}FeN_2O_4$	385	$(h^4-C_{12}H_{10}N_2O)Fe(CO)_3$	$CDCl_3$	H_{-3}	6.79d	J 6	$C_{12}H_{10}N_2O =$ 	993
				H_{-4}	3.2m	J 7, 6, 1.65		
				H_{-5}	5.07m	J 7, 1.8, 0.5		
				H_{-6}	4.64m	J 6.5, 4.4, 1.65		
				H_{-7}	6.5q	J 6.5, 1.8		
				H'	7.4	—		
$C_{11}H_{10}FeN_2O_5$	386	$(h^4-C_8H_{10}N_2O_2)Fe(CO)_3$	—	H_{-3}	7.01	$J_{3,4}$ 6 $J_{3,5}$ 0.5	$C_8H_{10}N_2O_2 =$ 	994 993 392
				H_{-4}	3.32	$J_{4,5}$ 7 $J_{4,6}$ 1.65		

$C_{14}H_{10}FeN_2O_5S$ 387 (h^4 - $C_{11}H_{10}N_2O_2S$) $Fe(CO)_3$	$CDCl_3$	H_{-5}	5.10	$J_{5,6}$ 4.4 $J_{5,7}$ 1.8
		H_{-6}	4.57	$J_{6,7}$ 6.5
		H_{-7}	6.31	—
		H_{-3}	6.94q	J 6, 0.5
		H_{-4}	3.34m	J 7, 6, 1.65
		H_{-5}	4.92m	J 7, 4.4, 1.8, 0.5
		H_{-6}	4.46m	J 6.5, 4.4, 1.65
$C_{15}H_{12}FeN_2O_5S$ 388 (h^4 - $C_{12}H_{12}N_2O_2S$) $Fe(CO)_3$	$CDCl_3$	H_{-7}	6.08q	J 6.5, 1.8
		H'	7.1	—
		H_{-3}	7.08q	J 6, 0.5
		H_{-4}	3.46m	J 7, 6, 1.65
		H_{-5}	5.02m	J 7, 4.4, 1.8, 0.5
$C_8H_4FeO_5$ 389 (h^4 - $C_5H_4O_2$) $Fe(CO)_3$	—	H_{-6}	4.54m	J 6.5, 4.4, 1.65
		H_{-7}	6.24q	J 6.5, 1.8
		n.a.	—	—
$C_{18}H_{10}FeO_5$ 390 (h^4 - $C_{13}H_{10}O_2$) $Fe(CO)_3$	$CDCl_3$	H	3.73s	—
		H^*	7.95–7.2m	—



993



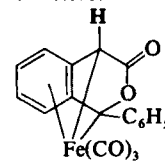
993

α -Pyrone iron tricarbonyl
Signals at δ 6.31, 5.61, 3.01,
in ratio 1:2:1

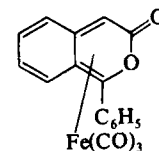
329

Structure:

393



(I)

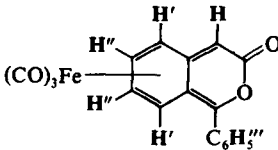
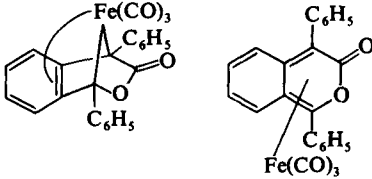


(II)

H^* aromatic protons.

Structure (I) favoured over
(II) for reasons given below
(see diphenyl analogue)

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{18}H_{10}FeO_5$	391	$(h^4-C_{15}H_{10}O_2)Fe(CO)_3$	$CDCl_3$	H	5.77s	—	Structure: 	393
				H'	4.0d	J 6		
					3.5dd	J 6, 1.5		
				H''	6.32–5.97	—		
				H'''	7.74–7.2m	—		
$C_{24}H_{14}FeO_5$	392	$(h^4-C_{21}H_{14}O_2)Fe(CO)_3$	$CDCl_3$	H	8.0–7.2	—	Structure: 	366 394

The NMR spectrum shows only aromatic protons and the σ -bonded structure (I) is therefore favoured over the π -bonded structure (II)

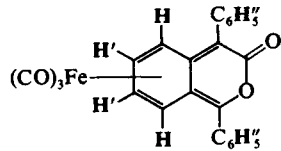
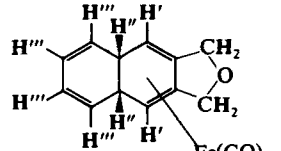
$C_{24}H_{14}FeO_5$	393	$(h^4-C_{21}H_{14}O_2)Fe(CO)_3$	—	H^* H^{**}	3.8 6	— —	Structure:	394
								
$C_{15}H_{12}FeO_4$	394	$(h^4-C_{12}H_{12}O)Fe(CO)_3$	$CDCl_3$	H'' H H'	7.7–7.2 4.61, 4.50* 3.46bs	— $J_{HH} 11$ —	*Reviewer's assignment Structure:	395
								
				H'' H'''	2.85 5.6, 5.3m†	— —	100 MHz *AB quartet †AA'BB' system	
$C_{14}H_{13}BFeO_4$	395	$[h^4-C_6H_5'''-CH_2''OB(CH=CH_2)_2]-Fe(CO)_3$	C_6D_6	H H_{syn}' H_{anti}'	3.20dd 1.63d 0.23d	— $J_{H,H'} 12.0$ $J_{H,H'} 14.5$ $J_{H',H'} < 1$	Benzyloxydivinyl borane iron tricarbonyl	396
				H'' H'''	4.43s 6.8–6.5m	— —	TMS external	
$C_9H_{12}FeO_3Si$	396	$[h^4-(CH_3)_2Si(CH=CH_2)_2]-Fe(CO)_3$	Liquid	H H'	2.4–1.3 0.6, –0.1	— — —	Dimethyldivinylsilane iron tricarbonyl	397

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{12}H_8FeO_4$	397	$(h^4-C_6H_5CH=CH'-CH''=O)-Fe(CO)_3$	$(CD_3)_2CO$	H	6.52	—	Free ligand $[(CD_3)_2CO]$: H 7.63, H' 6.78, H'' 9.75	96
				H'	3.30	—		
				H''	7.78	—		
			CCl_4	H	5.95	—		
				H'	3.13	—		
				H''	7.52	—		
$C_{13}H_{10}FeO_3$	398	$(h^4-p-CH_3'''OC_6H_4CH=CH'-CH''=O)Fe(CO)_3$	$(CD_3)_2CO$	H	6.69	—	Free ligand $[(CD_3)_2CO]$: H 7.61, H' 6.62, H'' 9.67, H''' 3.93	96
				H'	3.34	—		
				H''	7.73	—		
				H'''	3.77	—		
			CCl_4	H	5.97	—	Free ligand: H 7.32, H' 6.61, H'' 9.60	
				H'	3.32	—		
			H''	7.52	—			
	$C_7H_5ClFeO_4$	399	$(h^4-ClCH=CH'=C(CH_3)'''O)-Fe(CO)_3$	—	H	3.61	J 7	—
H'					5.99	—		
$C_{12}H_7ClFeO_4$	400	$(h^4-ClCH=CH'=C(C_6H_5)'''O)-Fe(CO)_3$	—	H	3.78	J 6	—	1000
				H'	6.21	—		
$C_{14}H_{10}FeO_6$	401	$(h^4-C_6H_5COCH=CH'CO_2CH_3)-Fe(CO)_3$ <i>cis</i>	CCl_4	H	5.85	$J_{HH'}$ 6.2	—	997
				H'	3.28	—		
$C_{14}H_{10}FeO_6$	402	$(h^4-C_6H_5COCH=CH'CO_2CH_3)Fe(CO)_3$ <i>trans</i>	CCl_4	H	6.44	J 4.9	Hexamethyldisiloxane as reference at 100 MHz	997
				H'	2.31	—		

(5) PENTAHAPTO LIGANDS

(a) Monocarbonyl derivatives

$C_9H_{14}ClFeO_4P$	403	$(h^5-C_5H_5)Fe[P(OCH_3)_3]-(Cl)(CO)$	$CDCl_3$	H	4.76d	$J_{PH} \sim 1$	T 38°	398
$C_{24}H_{20}ClFeO_4P$	404	$(h^5-C_5H_5)Fe[P(OC_6H_5)_3]-(Cl)(CO)$	$CDCl_3$	H	4.25s	—	T 38°	398
$C_{26}H_{20}BrFeOP$	405	$(h^5-C_5H_5)Fe[P(C_6H_5)_2C \equiv CC_6H_5](Br)(CO)$	$CDCl_3$	H	4.68b	—	60 and 100 MHz	170
				H'	7.6-6.5	—		
				H''	8.2-7.5	—		
$C_{12}H_{20}FeIOP$	406	$(h^5-C_5H_5)Fe[P(C_2H_5)_3](I)(CO)$	$CDCl_3$	H	4.71s	—	T 38°	398
$C_{18}H_{32}FeIOP$	407	$(h^5-C_5H_5)Fe[P(n-C_4H_9)_3](I)(CO)$	$CDCl_3$	H	4.58d	—	T 38°	398
$C_{14}H_{16}FeIOP$	408	$(h^5-C_5H_5)Fe(I)[P(CH_3)_2C_6H_5]-(CO)$	—	H	4.26	$J_{PH} 1.5$	—	990
				H'	2.14,	$J_{PH} 10$		
					1.73	$J_{PH} 9.3$		
				H''	7.34	—		
$C_9H_{14}FeIO_4P$	409	$(h^5-C_5H_5)Fe[P(OCH_3)_3](I)(CO)$	$CDCl_3$	H	4.72d	—	T 38°	398
$C_{12}H_{20}FeIO_4P$	410	$(h^5-C_5H_5)Fe[P(OC_2H_5)_3](I)(CO)$	$CDCl_3$	H	4.70s	—	T 38°	398
$C_{24}H_{20}FeIO_4P$	411	$(h^5-C_5H_5)Fe[P(OC_6H_5)_3](I)(CO)$	$CDCl_3$	H	4.20s	—	T 38°	398 399
$C_7H_8Cl_3FeOSi$	412	$(h^5-C_5H_4CH_3)Fe(SiCl_3)(H)(CO)$	CCl_4	H	5.3t, 5.0t	— —	—	400
				H'	2.2	—		
$C_6H_6Cl_6-FeOSi_2$	413	$(h^5-C_5H_5)Fe(SiCl_3)_2(H')(CO)$	CH_3CN	H	5.43*	—	60 and 100 MHz	400
				H'	-11.64	$J(^{29}Si-H') 20$	*Also a singlet of ~7% intensity at δ 4.62	401
						$J(^{31}Fe-H') 14.5$		402

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$[\text{C}_8\text{H}_5\text{FeN}_2\text{O}]^-$	414	$[(h^5\text{-C}_5\text{H}_5)\text{Fe}(\text{C}'\text{N})_2(\text{C}''\text{O})]^-$	H_2O	^{13}C	+82.6	—	Potassium salt	32
				$^{13}\text{C}'$	+159.0	—		
				$^{13}\text{C}''$	+219.2	—		
$[\text{C}_{26}\text{H}_{23}^- \text{FeNOP}]^+$	415	$\{(h^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CH}_3\text{CN})\text{-}[\text{P}(\text{C}_6\text{H}_5)_3](\text{CO})\}^+$	CDCl_3	H	4.98d	$J_{\text{PH}} 1.5$	Hexafluorophosphate	403
				H'	2.22d	$J_{\text{PH}} 1.5$		
				H''	7.55m			
$[\text{C}_{16}\text{H}_{13}^- \text{FeN}_2\text{O}]^+$	416	$[(h^5\text{-C}_5\text{H}_5)\text{Fe}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{CO})]^+$	CDCl_3	H	5.21s	—	Isolated as the hexafluoro phosphate $\text{C}_{10}\text{H}_8\text{N}_2 = 2,2'\text{-Bipyridine}$	403
$[\text{C}_{32}\text{H}_{29}^- \text{FeOP}_2]^+$	417	$\{(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{P}(\text{C}_6\text{H}_5)_2\text{CH}_2\text{-CH}_2\text{P}(\text{C}_6\text{H}_5)_2](\text{CO})\}^+$	$(\text{CD}_3)_2\text{CO}$	H	5.10	—	Acetone internal reference	404
				H'	7.55	—	Perchlorate	
			—	H	4.83	—		405
				H'	7.58–7.30	—	Tetrafluoroborate	
				H''	3.07–2.58m	—		
$[\text{C}_{42}\text{H}_{35}^- \text{FeOP}_2]^+$	418	$\{(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{P}(\text{C}_6\text{H}_5)_3]_2(\text{CO})\}^+$	$(\text{CD}_3)_2\text{CO}$	H	4.95t	$J_{\text{PH}} 1.5$	Hexafluorophosphate	403
				H'	7.42m	—		
$\text{C}_{21}\text{H}_{30}\text{FeO}_7\text{P}_2$	419	$(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{P}(\text{OC}_3\text{H}_7)_3]\text{-}[\text{P}(\text{O})(\text{OC}_3\text{H}_7)_2](\text{CO})$	CDCl_3	H	5.05t	$J_{\text{PH}} 0.8$	T 30°	398

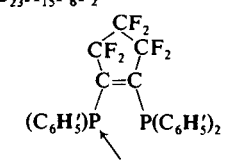
$C_{27}H_{30}FeO_3P_2$	420	$(h^5-C_5H_5)Fe[P(OC_3H_7)_2C_6H_5]-[P(O)(OC_3H_7)C_6H_5](CO)$	$CDCl_3$	H	4.38t	$J_{PH} 1.2$	T 30°	398
$C_{33}H_{30}FeO_3P_2$	421	$(h^5-C_5H_5)Fe[P(OC_3H_7)(C_6H_5)_2]-[P(O)(C_6H_5)_2](CO)$	$CDCl_3$	H	4.47s	—	T 30°	398
$[C_{42}H_{35}FeO_7P_2]^+$	422	$\{(h^5-C_5H_5)Fe[P(OC_6H_5)_3]_2-(CO)\}^+$	—	H H'	4.54s 7.42–7.08m	—	Hexafluorophosphate	405
$C_{27}H_{29}FeOPSi$	423	$(h^5-C_5H_5)Fe[P(C_6H_5)_3]-[Si(CH_3)_3](CO)$	$CDCl_3$	H H' H''	4.17 7.5, 7.3 0.01	— — —	—	406
$C_{27}H_{29}FeO_4PSi$	424	$(h^5-C_5H_5)Fe[P(OC_6H_5)_3]-[Si(CH_3)_3](CO)$	$CDCl_3$	H H' H''	4.16d 7.24 0.41	— — —	—	406
$C_{24}H_{20}Cl_3FeOPSn$	425	$(h^5-C_5H_5)Fe[P(C_6H_5)_3]-[SnCl_3](CO)$	CS_2	H H H'	4.67d 4.79 7.60–7.32	— — —	60 and 100 MHz —	407 408
$C_{32}H_{29}F_6FeOP_2Sn$	426	$(h^5-C_5H_5)Fe(C_{23}H_{15}F_6P_2)-[Sn(CH_3)_3](CO)$	CS_2	H H' H''	4.28d 7.33m –0.08	$J(^{31}P-H) 1.2$ — $J(^{119}Sn-H'') 41.2$	$C_{23}H_{15}F_6P_2 =$ 	407
$C_{22}H_{24}F_3FeOPSn$	427	$(h^5-C_5H_5)Fe[P(C_6H_5)_2CF_3]-[Sn(CH_3)_3](CO)$	CS_2	H H' H'' F	4.57d 7.45m –0.12 58.3d	$J_{PH} 1.2$ — $J(^{119}Sn-H'') 41.2$ $J_{PF} 58$	60 and 100 MHz	407

TABLE VII—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{27}H_{29}FeOPSn$	428	$(h^5-C_5H_5)Fe[P(C_6H_5)_3]-[Sn(CH_3)_3](CO)$	$CDCl_3$	H	4.20d	$J_{PH} 1.2$	—	406
				H'	7.3	—		408
				H''	-0.11	$J(^{119}Sn-H'') 39$		
			CS_2	H	4.23d		60 and 100 MHz	407
				H'	7.40			
				H''	-0.07	$J(^{119}Sn-H'') 40.4$		
$C_{27}H_{29}FeO_4PSn$	429	$(h^5-C_5H_5)Fe[P(OC_6H_5)_3]-[Sn(CH_3)_3](CO)$	$CDCl_3$	H	4.05	—	—	406
				H'	7.22	—		
				H''	0.31	$J(^{119}Sn-H'') 44$		
			CS_2	H	4.57	—	60 and 100 MHz	407
				H'	7.30m	—		
				H''	0.40	$J(^{119}Sn-H'') 44$		
$C_{47}H_{35}F_6-FeOP_2Sn$	430	$(h^5-C_5H_5)Fe(C_{23}H_{15}F_6P_2)-[Sn(C_6H_5)_3](CO)$	CS_2	H	4.50d	$J_{PH} 1.2$	60 and 100 MHz	407
				H'	7.19m	—	$C_{23}H_{15}F_6P_2$ —see above (No. 426)	
$C_{32}H_{31}FeOPSn$	431	$(h^5-C_5H_5)Fe[P(CH_3)_2C_6H_5]-[Sn(C_6H_5)_3](CO)$	CS_2	H	4.33d	$J_{PH} 1.2$	60 and 100 MHz	407
				H'	1.66, 1.40	$J 17.6$		
				H''	7.23m	—		
$C_{37}H_{33}FeOPSn$	432	$(h^5-C_5H_5)Fe[P(C_6H_5)_2CH_3]-[Sn(C_6H_5)_3](CO)$	CS_2	H	4.43d	$J_{PH} 1.2$	60 and 100 MHz	407
				H'	7.33m	—		
				H''	1.57d	—		
$C_{37}H_{30}F_3-FeOPSn$	433	$(h^5-C_5H_5)Fe[P(C_6H_5)_2CF_3]-[Sn(C_6H_5)_3](CO)$	CS_2	H	4.53d	$J_{PH} 1.2$	60 and 100 MHz	407
				H'	7.07m	—		
				F	57.1	—		

$C_{42}H_{35}FeOPSn$	434	$(\eta^5-C_5H_5)Fe[P(C_6H_5)_3]-[Sn(C_6H_5)_3](CO)$	—	H H'	4.38 7.43–6.93	— —	—	408
			CS_2	H H'	4.22d 7.05	$J_{PH} 1.2$ —	60 and 100 MHz	407
$C_8H_8FeOS_3$	435	$(\eta^5-C_5H_5)Fe[CH_3SC(S)-S](CO)$	CS_2	H H'	4.60 2.55	— —	40 MHz T 32.5° Methyltrithiocarbonato-cyclopentadienyl iron carbonyl	409
$C_9H_{10}FeOS_3$	436	$(\eta^5-C_5H_5)Fe[CH_3CH_2^wSC(S)-S](CO)$	CS_2	H H' H''	4.60 1.37t 3.25q	— $J 7.5$ $J 7.5$	40 MHz T 32.5° Ethyltrithiocarbonato-cyclopentadienyl iron carbonyl	409
$C_{13}H_{10}FeOS_3$	437	$(\eta^5-C_5H_5)Fe[C_6H_5^wSC(S)-S](CO)$	CS_2	H H'	4.57 7.43s	— —	40 MHz T 32.5° Phenyltrithiocarbonato-cyclopentadienyl iron carbonyl	409
$[C_6H_5Cl_6^- FeOSi_2]^-$	438	$[(\eta^5-C_5H_5)Fe(SiCl_3)_2(CO)]^-$	CH_3CN	H	4.60	—	Isolated as the tetraphenyl arsonium salt	400
$C_{22}H_{24}AsF_3^- FeOSn$	439	$(\eta^5-C_5H_5)Fe[As(C_6H_5)_2CF_3]-[Sn(CH_3)_3](CO)$	CS_2	H H' H''	4.53s 7.49d —0.03	— — $J(^{119}Sn-H'') 42.2$	60 and 100 MHz	407
			$(CH_3)_2CO$	F	55.6	—		
$C_{27}H_{29}^- AsFeOSn$	440	$(\eta^5-C_5H_5)Fe[As(C_6H_5)_3]-[Sn(CH_3)_3](CO)$	CS_2	H H' H''	4.31s 7.40 0.00	— — $J(^{119}Sn-H'') 40.2$	60 and 100 MHz	407
$C_{42}H_{35}^- AsFeOSn$	441	$(\eta^5-C_5H_5)Fe[As(C_6H_5)_3]-[Sn(C_6H_5)_3](CO)$	CS_2	H H'	4.28s 7.09m	— —	60 and 100 MHz	407
$C_{27}H_{29}^- FeOSbSn$	442	$(\eta^5-C_5H_5)Fe[Sb(C_6H_5)_3]-[Sn(CH_3)_3](CO)$	CS_2	H H' H''	4.42s 7.38m 0.03	— — $J(^{119}Sn-H'') 41.4$	60 and 100 MHz	407

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{42}H_{35}-FeOSbSn$	443	$(h^5-C_5H_5)Fe[Sb(C_6H_5)_3]-[Sn(C_6H_5)_3](CO)$	CS_2	H	4.40s	—	60 and 100 MHz	407
				H'	7.10m	—		
$C_{25}H_{23}-FeO_3PS$	444	$(h^5-C_5H_5)Fe[P(C_6H_5)_3]-(SO_2CH_3)(CO)$	$CDCl_3$	H	4.65d	J 1	—	410
				H'	7.4 comp.	—		
				H''	2.55s	—		
$C_{10}H_{17}-FeO_6PS$	445	$(h^5-C_5H_5)Fe[P(OCH_3)_3]-(SO_2CH_3)(CO)$	$CDCl_3$	H	4.90s	—	—	411
				H'	3.85d	J 11		
				H''	3.0s	—		
$C_{19}H_{35}-FeO_6PS$	446	$(h^5-C_5H_5)Fe[P(OCH_2CH_2CH_2CH_3)_3](SO_2CH_3)(CO)$	$CDCl_3$	H	4.85s	—	—	411
				H'	4.15bq	—		
				H''	1.6–1.0 comp.	—		
				H'''	3.0s	—		
$C_{31}H_{27}-AsFeO_3$	447	$(h^5-C_5H_5)Fe[As(C_6H_5)_3]-(SO_2CH_2C_6H_5)(CO)$	$CDCl_3$	H	4.48s	—	—	410
				H'	7.7 comp.	—		
				H''	4.44, 4.15	J 13.5		
$C_{31}H_{27}-FeO_3PS$	448	$(h^5-C_5H_5)Fe[P(C_6H_5)_3]-(SO_2CH_2C_6H_5)(CO)$	$CDCl_3$	H	4.42d	$J \sim 1$	—	410
				H'	7.5 comp.	—		
				H''	4.26, 3.94	J 13.5		
(b) Dicarboxyl derivatives								
$C_7H_5BrFeO_2$	449	$(h^5-C_5H_5)Fe(Br)(C'O)_2$	$CHCl_3$	C	+85.4	—		32
				C'	+213.2	—		

$C_7H_5ClFeO_2$	450	$(h^5-C_5H_5)Fe(Cl)(C'O)_2$	$CDCl_3$	H	5.02,	—	—	408
					5.06	—	—	132
			CH_3CN	H	5.01	—	—	131
			$CHCl_3$	C	+85.6	—	—	400
				C'	+212.9	—	—	32
$C_7H_5FeIO_2$	451	$(h^5-C_5H_5)Fe(I)(C'O)_2$	CCl_4	H	5.05s	—	—	305
			$CDCl_3$	H	5.01,	—	—	132
					5.04	—	—	131
			$CHCl_3$	C	+84.8	—	—	32
				C'	+213.8	—	—	95
$C_8H_7BrFeO_2$	452	$(h^5-C_5H_4CH_3)Fe(Br)(CO)_2$	$CDCl_3$	H	4.87b	—	—	412
$C_8H_7ClFeO_2$	453	$(h^5-C_5H_4\cdot CH_3)Fe(Cl)(CO)_2$	$CDCl_3$	H	4.91, 4.73	—	—	412
$C_8H_7FeIO_2$	453A	$(h^5-C_5H_4\cdot CH_3)Fe(I)(CO)_2$	$CDCl_3$	H	4.88	—	—	412
$[C_9H_9FeO_3]^+$	454	$[(h^5-C_5H_4\cdot OCH_2CH_3')Fe(CO)_2]^+$	$(CD_3)_2CO$	H	5.4, 5.15	—	Tetrafluoroborate	413
				H'	4.2q	—		
				H''	1.4t	—		
$C_9H_9FeIO_3$	455	$(h^5-C_5H_4OCH_2CH_3')Fe(I)(CO)_2$	$CDCl_3$	H	4.68t,	—	—	413
					4.62t	—		
				H'	3.94q	—		
				H''	1.37t	—		
$C_8H_5FeNO_2$	456	$(h^5-C_5H_5)Fe(C'N)(C''O)_2$	$CHCl_3$	C	+85.9	—		32
				C'	+154.7	—		
				C''	+211.1	—		
$C_9H_5AsF_6FeO_2$	457	$(h^5-C_5H_5)Fe[As(CF_3)_3](CO)_2$	$CFCl_3$	H	4.92	—	100 MHz	414

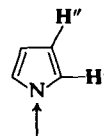
TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{19}H_5AsF_{10}FeO_2$	458	$(h^5-C_5H_5)Fe[As(C_6F_5)_2](CO)_2$	$CDCl_3$	H	4.98	—	—	130
			$CHCl_3$	F_{-2}, F_{-6}	124.2	—		
				F_{-3}, F_{-5}	161.6	—		
				F_{-4}	153.9	—		
$C_{10}H_{14}FeGeO_2$	459	$(h^5-C_5H_5)Fe[Ge(CH_3)_3](CO)_2$	$CHCl_3$	H	4.7	—	—	415
				H'	0.4	—		
$C_{13}H_{20}FeGeO_2$	460	$(h^5-C_5H_5)Fe[Ge(C_2H_5)_3](CO)_2$	—	H	4.70	—	40 MHz	135
				H'	1.08b	—		
$C_8H_8Cl_2^-FeGeO_2$	461	$(h^5-C_5H_5)Fe[Ge(Cl)_2CH_3](CO)_2$	CCl_4	H	5.01s	—	—	416
				H'	1.45s	—		417
$C_9H_{10}Cl_2^-FeGeO_2$	462	$(h^5-C_5H_5)Fe[Ge(Cl)_2CH_2CH_3](CO)_2$	CCl_4	H	5.08	—	—	416
				H'	1.75q	—		
				H''	1.28t	—		
$C_{10}H_{12}Cl_2^-FeGeO_2$	463	$(h^5-C_5H_5)Fe[Ge(Cl)_2C_3H_7](CO)_2$	CCl_4	H	5.04s	—	—	416
				H'	1.75m, 1.08	—		
$C_{10}H_{12}Cl_2^-FeGeO_2$	464	$(h^5-C_5H_5)Fe[Ge(Cl)_2CH'(CH_3)_2](CO)_2$	CS_2	H	4.97s	—	—	416
				H'	1.28 sept.	—		
				H''	1.25d	—		
$C_{14}H_{12}Cl_2^-FeGeO_2$	465	$(h^5-C_5H_5)Fe[Ge(Cl)_2CH_2-C_6H_5](CO)_2$	CS_2	H	4.70	—	—	416
				H'	3.23	—		
				H''	7.19	—		

$C_7H_5Br_3^-$ FeGeO ₂	466	$(h^5-C_5H_5)Fe(GeBr_3)(CO)_2$	—	H	5.30	—	—	999
$C_7H_5Cl_3^-$ FeGeO ₂	467	$(h^5-C_5H_5)Fe(GeCl_3)(CO)_2$	—	H	5.32	—	—	999
$C_7H_5F_3^-$ FeGeO ₂	468	$(h^5-C_5H_5)Fe(GeF_3)(CO)_2$	—	H	5.39	—	—	999
$C_7H_5FeGeI_3O_2$	469	$(h^5-C_5H_5)Fe(GeI_3)(CO)_2$	—	H	5.18	—	—	999
$C_{13}H_{14}FeGeO_8$	470	$(h^5-C_5H_5)Fe[Ge(OCOCH_3)_3]-(CO)_2$	CCl ₄	H H'	5.03 2.02	— —	—	999
$C_{25}H_{20}FeGeO_2$	471	$(h^5-C_5H_5)Fe[Ge(C_6H_4)_3](CO)_2$	CDCl ₃	H	4.74	—	—	418
$C_7H_5^-$ BrFeHgO ₂	472	$(h^5-C_5H_5)Fe(HgBr)(CO)_2$	CDCl ₃	H	5.02	—	—	136
$C_7H_5^-$ ClFeHgO ₂	473	$(h^5-C_5H_5)Fe(HgCl)(CO)_2$	CDCl ₃ CDCl ₃	H H	5.03 4.98	— —	— —	136 142
$C_7H_5FeHgIO_2$	474	$(h^5-C_5H_5)Fe(HgI)(CO)_2$	CDCl ₃	H	5.02	—	—	136
$C_9H_8FeHgO_4$	475	$(h^5-C_5H_5)Fe(HgCO_2CH_3)(CO)_2$	CDCl ₃	H H'	4.95b 2.0b	— —	—	142
$C_8H_5^-$ FeHgNO ₂ S	476	$(h^5-C_5H_5)Fe(HgSCN)(CO)_2$	CDCl ₃	H	5.08	—	—	136
$[C_7H_8FeNO_2]^+$	477	$[(h^5-C_5H_5)Fe(NH_3)(CO)_2]^+$	C ₆ H ₅ NO ₂	H H'	5.2 0.76	— —	Tetraphenylborate	137
$[C_7H_9^-$ FeN ₂ O ₂] ⁺	478	$[(h^5-C_5H_5)Fe(N_2H_4)(CO)_2]^+$	C ₆ H ₅ NO ₂	H H'	5.25 3.7, 3.1	— — —	Tetraphenylborate	137

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$[\text{C}_{13}\text{H}_{12}\text{FeNO}_2]^+$	479	$[(h^5\text{-C}_5\text{H}_5)\text{Fe}(\text{NH}_2\text{C}_6\text{H}_5)(\text{CO})_2]^+$	$(\text{CH}_3)_2\text{CO}$	H 5.7	—	Hexafluorophosphate	419
				H'' 7.3			
			$\text{C}_6\text{H}_5\text{NO}_2$	H 5.6	—		
				H' 2.1	—		
$\text{C}_8\text{H}_5\text{FeNO}_3$	480	$(h^5\text{-C}_5\text{H}_5)\text{Fe}(\text{NCO})(\text{CO})_2$	CD_3CN	H 5.12s	—	—	59
$\text{C}_8\text{H}_5\text{FeNO}_2\text{S}$	481	$(h^5\text{-C}_5\text{H}_5)\text{Fe}(\text{NCS})(\text{CO})_2$	CDCl_3	H 5.14s	—	—	131
$[\text{C}_9\text{H}_8\text{FeNO}_2]^+$	482	$[(h^5\text{-C}_5\text{H}_5)\text{Fe}(\text{NCCH}_3)(\text{CO})_2]^+$	$(\text{CD}_3)_2\text{CO}$	H 5.66s	—	Hexafluorophosphate	403
				H' 2.47s	—		
				H 5.43s	—	—	195
				H' 2.33s	—		
$\text{C}_{20}\text{H}_{12}\text{FeN}_4\text{O}_2$	483	$(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{N}=\text{C}=\text{C}(\text{CN})-\text{C}(\text{CN})_2\text{CH}_2\text{C}_6\text{H}_5](\text{CO})_2$	—	H 5.32	—	—	420
				H' 3.44	—		
				H'' 7.59	—		
$[\text{C}_{14}\text{H}_{10}\text{FeNO}_2]^+$	484	$[(h^5\text{-C}_5\text{H}_5)\text{Fe}(\text{NCC}_6\text{H}_5)(\text{CO})_2]^+$	$(\text{CH}_3)_2\text{CO}$	H 5.8	—	Hexafluorophosphate	419
				H' 7.8	—		
$\text{C}_{11}\text{H}_9\text{FeNO}_2$	485	$(h^5\text{-C}_5\text{H}_5)\text{Fe}(\text{C}_4\text{H}_4\text{N})(\text{CO})_2$	CS_2	H 4.93s	—	$\text{C}_4\text{H}_4\text{N} =$	421
				H' 6.03m	—		
				H'' 5.85d	—		
$\text{C}_{13}\text{H}_{11}\text{FeNO}_3$	486	$(h^5\text{-C}_5\text{H}_5)\text{Fe}(\text{C}_4\text{H}_3\text{N}.\text{COCH}_3)(\text{CO})_2$	CS_2	H 4.75s	—	$\text{C}_4\text{H}_3\text{N} = 2\text{-Acetyl pyrrol-1-yl}$	421
				H' 6.85m,	—		
				6.55m,	—		
				6.05m	—		
				H'' 2.11s	—		



$[\text{C}_{12}\text{H}_{10}^-\text{FeNO}_2\text{P}]^+$	487	$[(h^5\text{-C}_5\text{H}_5)\text{Fe}(\text{C}_5\text{H}_5\text{N})(\text{CO})_2]^+$	$(\text{CD}_3)_2\text{CO}$	H H'	5.64s 7.5m	— —	$\text{C}_5\text{H}_5\text{N} = \text{pyridin-1-yl}$ Hexafluorophosphate	403 419
$\text{C}_{15}\text{H}_{11}\text{FeNO}_2$	488	$(h^5\text{-C}_5\text{H}_5)\text{Fe}(\text{C}_8\text{H}_6\text{N})(\text{CO})_2$	CS_2	H H'	4.94s 6.76m	— —	$\text{C}_8\text{H}_6\text{N} = \text{Indol-1-yl}$	421
$\text{C}_{19}\text{H}_{13}\text{FeNO}_2$	489	$(h^5\text{-C}_5\text{H}_5)\text{Fe}(\text{C}_{12}\text{H}_8\text{N})(\text{CO})_2$	CDCl_3 CS_2	H H' H H'	5.1 8.1, 7.2 5.05s 7.7m, 7.2m	— — — —	$\text{C}_{12}\text{H}_8\text{N} = \text{Carbazol-9-yl}$	421
$\text{C}_9\text{H}_3\text{F}_3\text{FeO}_4$	490	$(h^5\text{-C}_5\text{H}_5)\text{Fe}(\text{OCOCF}_3)(\text{CO})_2$	CDCl_3	H ^{19}F	5.08s 74.2s	— —	100 MHz 94.1 MHz	138 989
$[\text{C}_{10}\text{H}_{11}\text{FeO}_3]^+$	491	$\{[(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{O}=\text{C}(\text{CH}_3)_2](\text{CO})_2]^+\}$	$(\text{CH}_3)_2\text{CO}$	H H'	4.96s 1.70s	— —	Unco-ordinated acetone δ 1.42	422 423
$\text{C}_{11}\text{H}_3\text{F}_7\text{FeO}_4$	492	$(h^5\text{-C}_5\text{H}_5)\text{Fe}(\text{OCOCF}_2\text{CF}_2\text{-CF}_3)(\text{CO})_2$	CDCl_3	H F F' F''	5.02s 116.7q 127.7 81.6t	— J 8 — J 8	100 MHz 94.1 MHz	138
$\text{C}_{14}\text{H}_{12}\text{FeO}_4\text{S}$	493	$(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{OS}(\text{O})\text{CH}_2\text{C}_6\text{H}_5](\text{CO})_2$	SO_2	H	3.43	J 12.6	T -18°	112
$\text{C}_{11}\text{H}_{10}\text{FeO}_4\text{S}$	494	$(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{OS}(\text{O})\text{C}(\text{CH}_3)=\text{C}=\text{CH}_2](\text{CO})_2$	CDCl_3	H H'	2.2 5.35, 4.95	$J_{\text{HH}'} 2.1$ $J_{\text{H}'\text{H}'} 14$	—	944
$\text{C}_{16}\text{H}_{12}\text{FeO}_4\text{S}$	495	$(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{OS}(\text{O})\text{C}(\text{C}_6\text{H}_5)=\text{C}=\text{CH}_2](\text{CO})_2$	CDCl_3	H	5.65, 5.2, 3.59	J 15 J 15	—	944

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$[\text{C}_{13}\text{H}_{20}^-\text{FeO}_2\text{P}]^+$	496	$\{(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{P}(\text{C}_2\text{H}_5)_3](\text{CO})_2\}^+$	CDCl_3	H	5.84d	$J_{\text{PH}} 1.6$	Tetraphenylborate	398
			$(\text{CH}_3)_2\text{CO}$	H	5.48	—	T 38°	424
			$\text{C}_6\text{H}_5\text{NO}_2$	H'	1.98, 1.11	—	Hexafluorophosphate	137
$[\text{C}_{19}\text{H}_{32}^-\text{FeO}_2\text{P}]^+$	497	$\{(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{P}(n\text{-C}_4\text{H}_9)_3](\text{CO})_2\}^+$	CDCl_3	H	4.19d	—	Tetraphenylborate T 38°	398
$\text{C}_{15}\text{H}_{16}\text{FeO}_2\text{P}$	498	$(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{P}(\text{CH}_3)_2\text{C}_6\text{H}_5](\text{CO})_2$	—	H	5.69	$J_{\text{PH}} 1.5$	—	990
				H'	2.32	$J_{\text{PH}'} 11.5$		
				H''	7.60	$J_{\text{PH}''} 3$		
$[\text{C}_{33}\text{H}_{29}^-\text{FeO}_2\text{P}_2]^+$	499	$\{(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{P}(\text{C}_6\text{H}_5)_2\text{CH}_2\text{-CH}_2\text{P}(\text{C}_6\text{H}_5)_2](\text{CO})_2\}^+$	$(\text{CD}_3)_2\text{CO}$	H	5.50	—	Perchlorate	404
				H'	7.50, 7.29	—	Acetone internal reference ($\delta 2.07$)	
$[\text{C}_{25}\text{H}_{20}^-\text{FeO}_2\text{P}]^+$	500	$\{(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{P}(\text{C}_6\text{H}_5)_3](\text{CO})_2\}^+$	$(\text{CD}_3)_2\text{CO}$	H	5.62d	$J_{\text{PH}} 1.5$	Hexafluorophosphate	403
				H'	7.68m	—		
$\text{C}_{19}\text{H}_5\text{F}_{10}^-\text{FeO}_2\text{P}$	501	$(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{P}(\text{C}_6\text{F}_5)_2](\text{CO})_2$	CDCl_3 CHCl_3	H	5.02	—		130
				F₋₂, F₋₆	127.1	—		
				F₋₃, F₋₅	162.0	—		
				F₋₄	154.4	—		
$[\text{C}_{10}\text{H}_{14}^-\text{FeO}_5\text{P}]^+$	502	$\{(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{P}(\text{OCH}_3)_3](\text{CO})_2\}^+$	$(\text{CD}_3)_2\text{CO}$	H	5.64d	$J 1.1$	Tetraphenylborate T 38°	398
$\text{C}_{11}\text{H}_{15}\text{FeO}_5\text{P}$	503	$(h^5\text{-C}_5\text{H}_5)\text{Fe}[\text{P}(\text{O})(\text{OC}_2\text{H}_5)_2](\text{CO})_2$	CDCl_3	H	5.09s	—	T 38°	398

$[C_{16}H_{20}^- FeO_3P]^+$	504	$\{(h^5-C_5H_5)Fe[P(OC_3H_7)_3]-(CO)_2\}^+$	$(CD_3)_2CO$	H	5.19d	J 1.2	*Tetraphenylborate T 38° C ₃ H ₅ = allyl	398
$[C_{19}H_{20}^- FeO_4P]^+$	505	$\{(h^5-C_5H_5)Fe[P(OC_3H_7)_2C_6H_5]-(CO)_2\}^+$	$(CD_3)_2CO$	H	5.12d	J_{PH} 1.3	Tetraphenylborate T 38° *(see above)	398
$[C_{22}H_{20}^- FeO_3P]^+$	506	$\{(h^5-C_5H_5)Fe[P(OC_3H_7)(C_6H_5)_2]-(CO)_2\}^+$	$(CD_3)_2CO$	H	5.38d	J 1.2	Tetraphenylborate T 38° *(see above)	398
$[C_{16}H_{26}^- FeO_3P]^+$	507	$\{(h^5-C_5H_5)Fe[P(O-i-C_3H_7)_3]-(CO)_2\}^+$	$CDCl_3$	H	4.32	J_{PH} 1.4	Tetraphenylborate T 38°	424
$[C_{25}H_{20}^- FeO_3P]^+$	508	$\{(h^5-C_5H_5)Fe[P(OC_6H_5)_3](CO)_2\}^+$	$CDCl_3$	H	4.01s	—	Tetraphenylborate T 38°	398 424 399
$C_{19}H_{15}FeO_3P$	509	$(h^5-C_5H_5)Fe[P(O)(C_6H_5)_2](CO)_2$	$CDCl_3$	H	4.94s	—	T 30°	398
$C_{13}H_{15}FeO_5P$	510	$(h^5-C_5H_5)Fe[P(O)(OC_3H_7)_2]-(CO)_2$	$CDCl_3$	H	5.0s	—	T 38° *(see above)	398
$C_{16}H_{15}FeO_4P$	511	$(h^5-C_5H_5)Fe[P(O)(OC_3H_7)-C_6H_5](CO)_2$	$CDCl_3$	H	4.91s	—	T 30° *(see above)	398
$C_{13}H_{20}FeO_2Pb$	512	$(h^5-C_5H_5)Fe[Pb(C_2H_5)_3](CO)_2$	$CDCl_3$	H	4.77	—	—	132
$C_{25}H_{20}FeO_2Pb$	513	$(h^5-C_5H_5)Fe[Pb(C_6H_5)_3](CO)_2$	$CDCl_3$	H	4.80—4.73	—	—	132
$C_8H_8FeO_2S$	514	$(h^5-C_5H_5)Fe(SCH_3)(CO)_2$	CS_2	H H'	4.87 1.58	— —	T 32.5° 40 MHz	425 188
$C_8H_5F_3FeO_2S$	515	$(h^5-C_5H_5)Fe(SCF_3)(CO)_2$	CH_2Cl_2	F	26.1s	—		1038
$[C_9H_{11}^- FeO_2S]^+$	516	$\{(h^5-C_5H_5)Fe[S(CH_3)_2](CO)_2\}^+$	$(CD_3)_2CO$	H H'	5.77 2.61	— —	Isolated as the iodide	188
$C_9H_{10}FeO_2S$	517	$(h^5-C_5H_5)Fe(SCH_2CH_3)(CO)_2$	CS_2	H H' H''	4.84 2.97q 1.1t	— J 7.2	T 32.5° 40 MHz	425

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
[C ₁₁ H ₁₅ Fe-O ₂ S] ⁺	518	{(<i>h</i> ⁵ -C ₅ H ₅)Fe[S(CH ₂ CH ₃) ₂](CO) ₂ } ⁺	(CD ₃) ₂ CO	H	5.17s	—	Hexafluorophosphate	423
				H'	2.40q	—		
				H''	0.82t	—		
C ₁₃ H ₁₀ FeO ₂ S	519	(<i>h</i> ⁵ -C ₅ H ₅)Fe(SC ₆ H ₅)(CO) ₂	CS ₂	H	4.83	—	100 MHz	414 426 425
				H'	5.17	—		
				H'	7.05	—		
C ₁₄ H ₁₂ FeO ₂ S	520	(<i>h</i> ⁵ -C ₅ H ₅)Fe(<i>p</i> -SC ₆ H ₄ CH ₃)(CO) ₂	CS ₂	H	4.79	—	—	984
				H'	7.02	—		
				H''	2.21	—		
C ₁₃ H ₉ FFeO ₂ S	521	(<i>h</i> ⁵ -C ₅ H ₅)Fe(<i>p</i> -SC ₆ H ₄ F)(CO) ₂	CS ₂	H	4.81	—	—	984
				H'	7.33q	—		
					6.65t	—		
C ₁₃ H ₅ F ₅ FeO ₂ S	522	(<i>h</i> ⁵ -C ₅ H ₅)Fe(SC ₆ F ₅)(CO) ₂	CHCl ₃	H	5.1	—		247
				F ₋₂ , F ₋₆	132.2	$J_{2,4} = J_{4,6} < 1$		
						$J_{2,3} = J_{5,6} 25$		
						$J_{2,6} 1.4$		
				F ₋₃ , F ₋₅	164.5	$J_{3,4} = J_{4,5} 21.2$		
C ₈ H ₅ FeNO ₂ S	523	(<i>h</i> ⁵ -C ₅ H ₅)Fe(SCN)(CO) ₂	CDCl ₃			$J_{2,5} = J_{3,6} 8.2$	—	131
						$J_{3,5} 1.4$		
				F ₋₄	159.3			
C ₉ H ₈ FeO ₂ S ₃	524	(<i>h</i> ⁵ -C ₅ H ₅)Fe[CH ₃ SC(S)-S](CO) ₂	CS ₂	H	5.08	—	T 32.5°	409
				H'	2.60	—		

$C_{10}H_{10}FeO_2S_3$	525	$(h^5-C_5H_5)Fe[CH_3CH_2SC(S)-S]-(CO)_2$	CS_2	H H' H''	5.08 1.25t 3.20q	— J 7.5 J 7.5	T 32.5° 40 MHz	409
$C_{14}H_{10}FeO_2S_3$	526	$(h^5-C_5H_5)Fe[C_6H_5SC(S)-S]-(CO)_2$	CS_2	H H'	5.04 7.39s	— —	T 32.5° 40 MHz	409
$C_{13}H_{10}FeO_2Se$	527	$(h^5-C_5H_5)Fe(SeC_6H_5)(CO)_2$	CS_2	H	5.21	—	—	426
$C_{10}H_{14}FeO_2Si$	528	$(h^5-C_5H_5)Fe[Si(CH_3)_3](CO)_2$	$CHCl_3$	H H'	4.7 0.4	— —	—	415
$C_{10}H_{14}FeO_2Si$	529	$(h^5-C_5H_5)Fe[Si(CH_3)_3](CO)_2$	$CDCl_3$	H H'	4.64s 0.39	— —	—	406
$C_8H_8Cl_2FeO_2Si$	530	$(h^5-C_5H_5)Fe[Si(Cl)_2CH_3](CO)_2$	—	H H'	3.8 0.7	— —	T 33° Presence of two rotational isomers indicated by i.r.	427
$C_7H_5Cl_3FeO_2Si$	531	$(h^5-C_5H_5)Fe(SiCl_3)(CO)_2$	CH_3CN	H	5.13	—	—	400
$C_{25}H_5F_{15}FeO_2Si$	532	$(h^5-C_5H_5)Fe[Si(C_6F_5)_3](CO)_2$	—	H	4.75s	—	—	1039
$C_{10}H_{14}FeO_2Sn$	533	$(h^5-C_5H_5)Fe[Sn(CH_3)_3](CO)_2$	$CDCl_3$	H H'	4.68s 0.32	— J($^{119}Sn-H'$) 47	— —	406 408
			$CHCl_3$	H H'	4.89 0.45	— J($^{119}Sn-H'$) 49	— —	415 140 132 428
$C_9H_{11}ClFeO_2Sn$	534	$(h^5-C_5H_5)Fe[Sn(CH_3)_2Cl](CO)_2$	$CHCl_3$	H H'	4.9 0.8	— J($^{119}Sn-H'$) 40	—	415
$C_{13}H_{20}FeO_2Sn$	535	$(h^5-C_5H_5)Fe[Sn(C_2H_5)_3](CO)_2$	$CDCl_3$	H	4.70	—	—	242

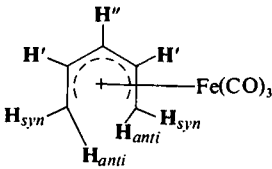
TABLE VII—*cont.*

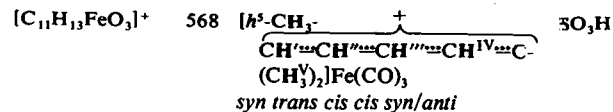
Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{23}H_{20}FeO_2Sn$	536	$(h^5-C_5H_5)Fe[Sn(C_6H_5)_3](CO)_2$	$CDCl_3$	H	4.75	—	—	132
				H	4.90	—	—	408
				H	4.79	—	—	252
				H'	~ 7.4	—	—	
$C_7H_8FeO_2Si$	537	$(h^5-C_5H_5)Fe(SiH_3)(CO)_2$	C_6D_6	n.a.			Two signals at 6.48 and 6.57 in ratio 3:5	982
$C_9H_{12}FeO_2Si$	538	$(h^5-C_5H_5)Fe[Si(CH_3)_2H''](CO)_2$	Liquid	H	4.49s	—	—	983
				H'	0.45d	—	—	
				H''	4.79m	—	—	
$C_9H_{11}ClFeO_2Si$	539	$(h^5-C_5H_5)Fe[Si(CH_3)_2Cl](CO)_2$	$CDCl_3$	H	4.87s	—	—	983
				H'	0.89s	—	—	
$C_{12}H_{20}FeO_2Si_2$	540	$(h^5-C_5H_5)Fe[Si(CH_3)_2Si(CH_3)_3](CO)_2$	—	H	4.73s	—	—	992
				H'	0.37s	—	—	983
				H''	0.12s	—	—	
$C_{14}H_{26}FeO_2Si_3$	541	$(h^5-C_5H_5)Fe[Si(CH_3)_2Si(CH_3)_2Si(CH_3)_3](CO)_2$	$CDCl_3$	H	4.78s	—	—	983
				H'	0.54s	—	—	
				H''	0.23s	—	—	
$C_{16}H_{32}FeO_2Si_4$	542	$(h^5-C_5H_5)Fe[Si(CH_3)_2Si(CH_3)_2Si(CH_3)_2Si(CH_3)_3](CO)_2$	$CDCl_3$	H	4.63s	—	—	983
				H'	0.41s	—	—	
				H''	0.08b	—	—	
$C_{19}H_{15}ClFeO_2-Sn$	543	$(h^5-C_5H_5)Fe[Sn(C_6H_5)_2Cl](CO)_2$	$CDCl_3$	H	4.93	—	—	252
				H'	~ 7.4	—	—	

$C_{13}H_{10}Cl_2\text{-}$ FeO_2Sn	544	$(h^5\text{-}C_5H_5)Fe[Sn(Cl)_2C_6H_5](CO)_2$	$CDCl_3$	H	4.99	—	—	132
				H	5.13	—	—	252
				H'	~7.6	—	—	
$C_{19}H_{16}FeO_5\text{-}$ SSn	545	$(h^5\text{-}C_5H_5)Fe[Sn(OH)(C_6H_5)\text{-}$ $(OS(O)C_6H_5)](CO)_2$	$CDCl_3$	H	4.47s	—	—	429
				H'	7.5m	—	—	
$C_{25}H_{20}FeO_6\text{-}$ S_2Sn	546	$(h^5\text{-}C_5H_5)Fe[Sn(C_6H_5)(OS(O)\text{-}$ $C_6H_5)_2](CO)_2$	$CDCl_3$	H	4.97s	—	—	429
				H'	7.5m	—	—	
$C_7H_5Br_3\text{-}$ FeO_2Sn	547	$(h^5\text{-}C_5H_5)Fe(SnBr_3)(CO)_2$	$CDCl_3$	H	5.17	—	—	142
				H	5.23	—	—	132 106
$C_7H_5Cl_3\text{-}$ FeO_2Sn	548	$(h^5\text{-}C_5H_5)Fe(SnCl_3)(CO)_2$	$CDCl_3$	H	5.18	—	—	142
								132 430
				H	5.26	—	—	252
$C_7H_5FeI_3\text{-}$ O_2Sn	549	$(h^5\text{-}C_5H_5)Fe(SnI_3)(CO)_2$	$CDCl_3$	H	5.51	—	—	408
				H	5.14	—	—	106 132
$C_8H_8FeO_4S$	550	$(h^5\text{-}C_5H_5)Fe(SO_2CH_3)(CO)_2$	$CDCl_3$	H	5.25s	—	—	923
				H'	3.15s	—	—	
$C_9H_{10}FeO_4S$	551	$(h^5\text{-}C_5H_5)Fe(SO_2CH_2CH_3)(CO)_2$	$CDCl_3$	H	5.42s	—	—	923
				H'	3.30q	J 8		
				H''	1.51t	J 8		
$C_{13}H_{18}FeO_4S$	552	$(h^5\text{-}C_5H_5)Fe[SO_2CH_2CH_2\text{-}$ $C(CH_3)_3](CO)_2$	—	Not reported		J_{threo} 4.3 $J_{erythro}$ 13.0	Investigation into the stereochemistry of reactions occurring at iron-carbon σ -bands	431

TABLE VII—*cont.*

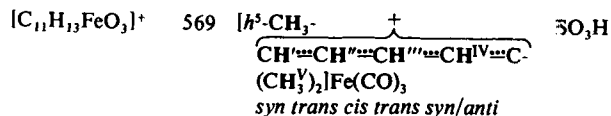
Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)		Remarks	References
$C_{11}H_{10}FeO_4S$	553	$(h^5-C_5H_5)Fe(SO_2CH_2C \equiv CCH_3)(CO)_2$	$CDCl_3$	H H' H''	5.16s 3.68b 1.87t	— — J 2.5	—		163
$C_{12}H_{12}FeO_4S$	554	$(h^5-C_5H_5)Fe(SO_2CH_2CH_2C \equiv CCH_3)(CO)_2$	$CDCl_3$	H H' H'' H'''	5.34s 3.32t 2.92b 1.92t	— J 8 — J 2.5	—		163
$C_{14}H_{12}FeO_4S$	555	$(h^5-C_5H_5)Fe(SO_2CH_2C_6H_5)(CO)_2$	$CDCl_3$	H H' H''	5.10s 4.39s 7.6bs	— — —	—		923 414
			SO_2	H H' H''	5.18s 4.23s 7.54s	— — —	$T - 15^\circ$		
$C_{15}H_{14}FeO_4S$	556	$(h^5-C_5H_5)Fe[SO_2CH'(CH_3)-C_6H_5](CO)_2$	$(CH_3)_2SO$	H H' H'' H'''	4.9s 3.6b 2.30d 7.0b	— — J 6.5 —	—		432
$C_{13}H_{10}FeO_4S$	557	$(h^5-C_5H_5)Fe(SO_2C_6H_5)(CO)_2$	$CDCl_3$	H H'	5.30s 8.0–7.5 comp.	—	60 and 100 MHz		923 414
$C_{14}H_{12}FeO_4S$	558	$(h^5-C_5H_5)Fe(SO_2C_6H_4CH_3)(CO)_2$	$CDCl_3$	H H' H''	5.09s 7.89–7.56m 7.50–7.18m 2.42s	— — — —	—		923

$C_{10}H_3F_3FeO_4S$	559	$(h^5-C_3H_5)Fe(SO_2C_6F_5)(CO)_2$	THF	F_{-2}, F_{-6}	140.5	$J_{2,3}$ 28.05 $J_{2,4}$ 1.7 $J_{2,5} = J_{3,6}$ 9.25 $J_{2,6}$ 0 $J_{3,5}$ 3.0 $J_{3,4}$ 25.2 —	T 35°	244 433
$C_{10}H_{14}FeGeO_4S$	560	$(h^5-C_3H_5)Fe[SO_2Ge(CH_3)_3](CO)_2$	—	F_{-3}, F_{-5}	161.6	—	—	428
$C_{14}H_{12}FeO_4S$	561	$(h^5-C_3H_5)Fe[S(O)OCH_2C_6H_5](CO)_2$	SO ₂	F_{-4}	153.4	—	—	426
$C_{13}H_{10}FeO_2Te$	562	$(h^5-C_3H_5)Fe(TeC_6H_5)(CO)_2$	CS ₂	H	5.23	—	—	426
(c) Tricarbonyl derivatives								
$[C_8H_7FeO_3]^+$	563	$(h^5-CH_2-CH^+-CH^+-CH^+-CH_2)-Fe(CO)_3$ <i>cis cis</i>	SO ₂	H_{syn} H_{anti} H' H''	3.75 2.17 6.26 7.22	$J_{HH'}$ 9.8 $J_{HH'}$ 13 J_{HH} 3.5 $J_{H'H''}$ 6.8 —	Perchlorate Structure:	396
								
$[C_{10}H_{11}FeO_3]^+$	564	$(h^5-CH_3-CH^+-CH^+-CH^+-CH_3)-Fe(CO)_3$ <i>syn trans cis cis trans syn</i>	FSO ₃ H	H H'_{anti} H'' H'''	1.73 2.97 5.67 6.59	— — — —	Internal reference [(CH ₃) ₄ N] ⁺ (δ 3.1) 100 MHz	434



H	1.83	—
H'_{anti}	3.50	—
H''	5.64	—
H'''	6.62	—
H^{IV}	5.47	—
H_{syn}^V	1.83	—
H_{anti}^V	1.34	—

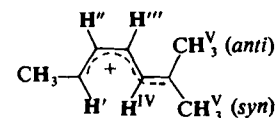
T — 78° 100 MHz
 Internal reference
 $[(CH_3)_4N]^+$
 Fluorosulphate 434



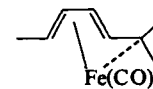
H	1.83	—
H'_{anti}	4.20	—
H''	5.96	—
H'''	6.30	—
H^{IV}	2.40	—

H_{syn}^V	2.06s	—
H_{anti}^V	2.17s	—

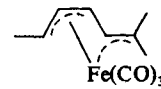
Fluorosulphate 434
 Structure: 317



T — 78° 100 MHz
 Internal reference
 $[(CH_3)_4N]^+$ (δ 3.1)
 This and similar compounds have been classified as pentahapto rather than tetrahapto since the available data has been interpreted in favour of structures of type (I) rather than (II)



(I)



(II)

However this classification should only be regarded as tentative at present

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$[\text{C}_{10}\text{H}_9\text{D}_2\text{FeO}_4]^+$	570	$\begin{array}{c} [h^5\text{-CH}_3-\text{C}^+ \\ \text{CH}'\text{---}\text{CD}\text{---}\text{CH}''\text{---}\text{CD}\text{---}\text{C-} \\ (\text{OH})\text{CH}_3''']\text{Fe}(\text{CO})_3 \\ \text{syn trans cis trans} \end{array}$	$\text{CDCl}_3/\text{SO}_2$ (2:3)	H	1.70d	J 6	Fluorosulphate T -50° to -60° 60 MHz	317
				H'	3.0b	—		
				H''	6.70b	—		
				H'''	2.15	—		
$[\text{C}_{10}\text{H}_{11}\text{FeO}_4]^+$	571	$\begin{array}{c} [h^5\text{-CH}_3-\text{C}^+ \\ \text{CH}'\text{---}\text{CH}''\text{---}\text{CH}'''\text{---}\text{CH}^{\text{IV}}\text{---}\text{C-} \\ (\text{OH})\text{CH}_3^{\text{V}}]\text{Fe}(\text{CO})_3 \\ \text{syn trans cis trans} \end{array}$	H_2SO_4	H	1.70	—	Internal reference CH_2Cl_2	311
				H'	3.00	—		
				H''	5.80	—		
				H'''	6.44	—		
				H ^{IV}	1.45	—		
				H ^V	2.38	—		
			$\text{CDCl}_3/\text{SO}_2$ (2:3)	H	1.75d	J 6	T -50° to -60°	317
				H'	3.05b	—		
				H''	5.80m	—		
				H'''	6.30m	—		
				H ^{IV}	1.45	$J_{\text{H}'''\text{H}^{\text{IV}}}$ 8		
				H ^V	2.15	—		
$[\text{C}_{10}\text{H}_{11}\text{FeO}_4]^+$	572	$\begin{array}{c} [h^5\text{-CH}_3-\text{C}^+ \\ \text{CH}'\text{---}\text{CH}''\text{---}\text{CH}'''\text{---}\text{CH}'\text{---}\text{C-} \\ (\text{OH})\text{CH}_3''']\text{Fe}(\text{CO})_3 \\ \text{syn trans cis cis} \end{array}$	CDCl_3	H	2.15d	—	—	311
				H'	3.4	—		
				H''	5.4m	—		
				H'''	2.1s	—		
$[\text{C}_{11}\text{H}_{13}\text{FeO}_4]^+$	573	$\begin{array}{c} [h^5\text{-CH}_3\text{-CH}'\text{---}\text{C}(\text{CH}_3'')\text{---}\text{CH}'''\text{---} \\ \text{CH}^{\text{IV}}\text{---}\text{C}(\text{OH})\text{CH}_3^{\text{V}}]\text{Fe}(\text{CO})_3 \\ \text{syn trans} \end{array}$	$\text{CDCl}_3/\text{SO}_2$ (2:3)	H	1.70d	J 6	Fluorosulphate T -50° to -60° CH_3' cis to CH_3	317
				H' _{anti}	2.9m	—		
				H''	2.45s	—		
				H'''	6.35d	$J_{\text{H}'''\text{H}^{\text{IV}}}$ 8		
				H ^{IV} _{anti}	1.45d	—		
				H ^V	2.33s	—		

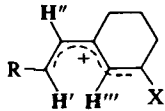
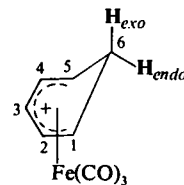
[C ₁₁ H ₁₃ FeO ₄] ⁺	574	$\begin{array}{c} [h^5\text{-CH}_3\text{-} \\ \text{CH}'\text{---CH}''\text{---C(CH}_3''')\text{---CH}^{\text{IV}}\text{---C-} \\ (\text{OH})\text{CH}_3^{\text{V}}\text{]Fe(CO)}_3 \\ \text{syn trans} \end{array}$	CDCl ₃ /SO ₂ (2:3)	H	1.70d	J 6	Fluorosulphate T -50° to -60° CH ₃ ''' cis to C(OH)CH ₃ group	317
				H' <i>anti</i>	2.9m	—		
				H''	5.70d	J _{H'H''} 9		
				H'''	2.61s	—		
				H ^{IV}	0.98s	—		
[C ₁₅ H ₁₃ FeO ₄] ⁺	575	$\begin{array}{c} [h^5\text{-C}_6\text{H}_5\text{-CH}'\text{-CH}''\text{-CH}'''\text{-} \\ \text{CH}'''\text{-C(OH)CH}_3^{\text{IV}}\text{]Fe(CO)}_3 \end{array}$	CDCl ₃ /SO ₂ (2:3)	H	7.50s	—	Fluorosulphate T -50° to -60°	317
				H'	3.80d	J _{H'H''} 9		
				H''	6.6m	—		
				H'''	1.83d	J _{H'H'''} 7		
				H ^{IV}	2.57s	—		
[C ₁₂ H ₁₃ FeO ₄] ⁺	576	$\{[h^5\text{-CH}_3\text{-CH}'\text{=CH}''\text{-C}_6\text{H}_7'''\text{-} \\ (\text{OH})\text{]Fe(CO)}_3\}^+$	CDCl ₃ /SO ₂ (2:3)	H	1.70d	J 5	Fluorosulphate T -50° to -60° Structure:	317
				H''	5.80d	J _{H'H''} 10		
[C ₁₇ H ₁₅ FeO ₃] ⁺	577	$[(h^5\text{-C}_6\text{H}_5\text{-CH}'\text{=CH}''\text{-C}_6\text{H}_8\text{)-} \\ \text{Fe(CO)}_3]^+$	FSO ₃ / CDCl ₃ /SO ₂	H	7.6	—	 (R = CH ₃ ; X = OH)	435
				H'	3.5 or 5.0	—		
				H''	6.8	—		
				H'''	3.0-2.2*	—		
				H ^{IV}	3.5 or 5.0	—		
[C ₈ H ₃ FeO ₃] ⁺	578	[(h ⁵ -C ₅ H ₅)Fe(CO) ₃] ⁺	SO ₂	H	5.84	—	Tetrafluoroborate	305
			(CH ₃) ₂ CO	H	6.13	—	Tetraphenylborate	400
			(CD ₃) ₂ CO	H	6.14	—	Hexafluorophosphate	403

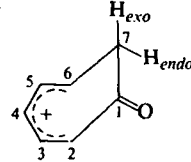
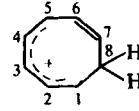
TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$[\text{C}_9\text{H}_7\text{FeO}_3]^+$	579	$[(\eta^5\text{-C}_6\text{H}_7)\text{Fe}(\text{CO})_3]^+$	SO_2	$\text{H}_{-1}, \text{H}_{-5}$ 4.34t	$J_{1,2} = J_{4,5} \sim 6.0$	Tetrafluoroborate Structure:	436 955
				$\text{H}_{-2}, \text{H}_{-4}$ 5.92t	$J_{2,3} = J_{3,4} \sim 5.5$		
				H_{-3} 7.34t	—		
				$\text{H}_{-6\text{exo}}$ 2.02d	—		
				$\text{H}_{-6\text{endo}}$ 3.02dt	$J_{1,6} = J_{5,6} 6.5$ $J_{\text{endo/exo}} 16$		
				$\text{H}_{-1}, \text{H}_{-5}$ 4.27t	—	Tetrafluoroborate	358
				$\text{H}_{-2}, \text{H}_{-4}$ 5.82t	—		
				H_{-3} 7.22t	—		
				H_{-6} 2.57m	—		
$[\text{C}_{10}\text{H}_9\text{FeO}_3]^+$	580	$\{[1,2,3,4,5\text{-}\eta^5\text{-1-C}_6\text{H}_6(\text{CH}_3)]\text{-Fe}(\text{CO})_3\}^+$	$(\text{CD}_3)_2\text{CO}$	H_{-2} 5.87d	$J_{2,3} = J_{3,4} \sim 5.5$	Hexafluorophosphate	436
				H_{-3} 6.68t	—		
				H_{-4} 6.18t	$J_{4,5} \sim 6.0$		
				H_{-5} 4.50t	$J_{5,6\text{endo}} 6.5$		
				$\text{H}_{-6\text{exo}}$ 2.38d	—		
				$\text{H}_{-6\text{endo}}$ 3.16dd	$J_{\text{endo/exo}} 16$		
				H^+ 1.93s	—		
				—	—		
$[\text{C}_{10}\text{H}_9\text{FeO}_3]^+$	581	$\{[1,2,3,4,5\text{-}\eta^5\text{-2-C}_6\text{H}_6(\text{CH}_3)]\text{-Fe}(\text{CO})_3\}^+$	$\text{CF}_3\text{CO}_2\text{H}$	$\text{H}_{-1}, \text{H}_{-5}$ 4.22m	$J_{1,6} = J_{5,6} 7$	Hexafluorophosphate 100 MHz	359
				H_{-3} 7.22d	$J_{3,4} 5.5$		
				H_{-4} 5.87t	$J_{4,5} 6$		



				H_{-6}	3.06dt 2.19d	$J_{6,6}$ 17 —		
				H'	2.29s	—		
$[C_{10}H_9FeO_3]^+$	582	$\{[1,2,3,4,5-h^5-3-C_6H_6(CH_3)]-Fe(CO)_3\}^+$	CF_3CO_2H	H_{-1}, H_{-5} H_{-2}, H_{-4} H_{-6} H'	4.21t 5.89d 2.90m 2.00d 2.88s	$J_{1,2} = J_{4,5}$ 7 — $J_{1,6} = J_{5,6}$ 6 $J_{6,6}$ 19 —	Hexafluorophosphate 100 MHz	359
$[C_{16}H_{21}FeO_3]^+$	583	$\{[h^5-C_6(CH_3)_7]Fe(CO)_3\}^+$	—	n.a.	—		Heptamethylcyclohexadienyl complex Signals at δ 2.66, 2.24, 1.78, 1.48, 0.61, in ratio 1:2:2:1:1. Internal reference $[(CH_3)_4N]^+$	437
$[C_{10}H_9FeO_4]^+$	584	$\{[1,2,3,4,5-h^5-2-C_6H_6(OCH_3)]-Fe(CO)_3\}^+$	—	H_{-1} H_{-3} H_{-4} H_{-5} H_{-6} H'	3.90d 6.99dd 5.89t 4.22t 2.55m 3.79s	— — — — — —	Tetrafluoroborate	358
$[C_{10}H_7FeO_3]^+$	585	$\{(1,2,3,4,5-h^5-C_7H_7)Fe(CO)_3\}^+$	$(CD_3)_2CO$	H_{-1}, H_{-5} H_{-2}, H_{-4} H_{-3}	5.13 6.70 8.48	— — —	Cycloheptatrienyl cation Tetrafluoroborate T — 80° One signal (δ 6.10s) at T 10°	438
$[C_{13}H_{13}FeO_5]^+$	586	$\{[1,2,3,4,5-h^5-1-C_7H_8(CH_2CO_2-Me)]Fe(CO)_3\}^+$	—	Not reported		—		360
$[C_{12}H_{11}FeO_5]^+$	587	$\{[1,2,3,4,5-h^5-1-C_7H_8(CO_2-Me)]Fe(CO)_3\}^+$	—	Not reported		—		360

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$[\text{C}_{10}\text{H}_7\text{FeO}_4]^+$	588	$[(h^5\text{-C}_7\text{H}_7\text{O})\text{Fe}(\text{CO})_3]^+$	—	H_{-2} 4.7	—	$\text{C}_7\text{H}_7\text{O} =$ 	367
				$\text{H}_{-3}, \text{H}_{-5}$ 6.5	—		
				H_{-4} 7.3	—		
				H_{-6} 5.0	—		
				$\text{H}_{-7 \text{ } exo}$ 2.32	$J_{7,7}$ 16.5		
				$\text{H}_{-7 \text{ } endo}$ 3.23	—		
$[\text{C}_{11}\text{H}_9\text{FeO}_3]^+$	589	$[(1,2,3,4,5\text{-}h^5\text{-C}_8\text{H}_9)\text{Fe}(\text{CO})_3]^+$	$\text{FSO}_3\text{H}/\text{SO}_2\text{F}_2$	$\text{H}_{-1}, \text{H}_{-5}$ 4.54m	—	$\text{C}_8\text{H}_9 =$ Cyclo-octatrienyl cation 	439
				$\text{H}_{-2}, \text{H}_{-4}$ 5.88m	—		
				H_{-3} 6.77t	J 7		
				$\text{H}_{-6}, \text{H}_{-7}$ 5.88m	—		
				H_{-8} 2.85m	—		
$[\text{C}_{12}\text{H}_{11}\text{FeO}_3]^+$	590	$\{[1,2,3,4,5\text{-}h^5\text{-3-C}_8\text{H}_8(\text{CH}_3)]\text{-Fe}(\text{CO})_3\}^+$	$\text{FSO}_3\text{H}/\text{SO}_2\text{F}_2$	$\text{H}_{-1}, \text{H}_{-5}$ 4.52m	—	$3\text{-C}_8\text{H}_8(\text{CH}_3) =$ 3-methyl cyclo-octatrienyl cation $T - 80^\circ$ Internal reference CH_2Cl_2 (δ 5.30)	440
				$\text{H}_{-2}, \text{H}_{-4}$ } 5.93m	—		
				$\text{H}_{-6}, \text{H}_{-7}$ }	—		
				H_{-8} 2.95m	—		
				H' 2.72s	—		
$[\text{C}_{12}\text{H}_{11}\text{FeO}_3]^+$	591	$\{[1,2,3,4,5\text{-}h^5\text{-4-C}_8\text{H}_8(\text{CH}_3)]\text{-Fe}(\text{CO})_3\}^+$	$\text{FSO}_3\text{H}/\text{SO}_2\text{F}_2$	$\text{H}_{-1}, \text{H}_{-5}$ 4.52	—	$4\text{-C}_8\text{H}_8(\text{CH}_3) =$ 4-Methyl cyclo-octatrienyl cation $T - 80^\circ$ Internal reference CH_2Cl_2	440
				$\text{H}_{-2}, \text{H}_{-6}$ 5.93	—		
				H_{-7}	—		
				H_{-3} 6.82d	J 7		
				H_{-8} 2.95	—		
				H' 2.65s	—		

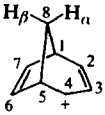
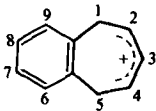
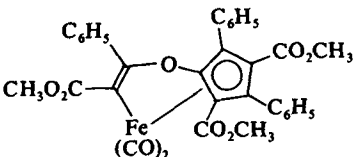
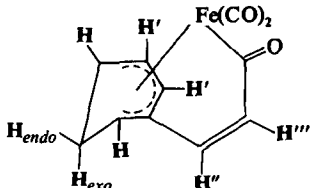
$[C_{11}H_9FeO_3]^+$	592 $[h^5-C_8H_9)Fe(CO)_3]^+$	—	H_{-1}, H_{-5} 3.38m H_{-2}, H_{-4} 4.68t H_{-3} 4.95t	$J_{1,8\alpha}$ 1 $J_{1,8\beta}$ 4 J_6 6	$C_8H_9 =$ 	441
			H_{-6}, H_{-7} 4.24dd $H_{-8\alpha}$ 1.14 $H_{-8\beta}$ 1.70	J_2 $J_{\alpha,\beta}$ 12 —	Isolated as the tetrafluoroborate	
$[C_{11}H_9FeO_3]^+$	593 $[(h^5-C_8H_9)Fe(CO)_3]^+$	H_2SO_4	H_{-1}, H_{-7} 2.52 H_{-2}, H_{-3} 5.38 H_{-5}, H_{-6} 7.74 H_{-4} 1.53, 1.35 H_{-8}	$J_{1,8} = J_{7,8}$ = 4.5, 8 — — $J_{exo/endo}$ 4.8	Bicyclo[5.1.0]octadienyl iron tricarbonyl cation, viz.:	150 439
	594 $\{[2,3,4,5,6-h^5-3-C_8H_8(CH_3)]-Fe(CO)_3\}^+$	FSO_3H/SO_2F_2	H_{-1}, H_{-7} 2.65 $H_{-2},$ 5.05d H_{-4} 7.63d H_{-5}, H_{-6} 5.48 H_{-8} 1.53 H' 2.40	— J_6 5 J_6 — — —	$C_8H_8CH_3 = 3\text{-Methyl}$ bicyclo[5.1.0]octadienyl cation (numbering as above) Internal reference CH_2Cl_2 (δ 5.30) T -62°	440
$[C_{12}H_{11}FeO_3]^+$	595 $\{[2,3,4,5,6-h^5-4-C_8H_8(CH_3)]-Fe(CO)_3\}^+$	FSO_3H/SO_2F_2	H_{-1}, H_{-7} 2.65 H_{-2}, H_{-3} 5.48 H_{-5}, H_{-6} 1.53 H' 3.10	— — — —	$C_8H_8CH_3 = 4\text{-Methyl}$ bicyclo[5.1.0]octadienyl cation (numbering as above) Internal reference CH_2Cl_2 (δ 5.30) T -62°	440
$[C_{13}H_{11}FeO_4]^+$	596 $\{[2,3,4,5,6-h^5-8-C_8H_8(COCH_3)]-Fe(CO)_3\}^+$	SO_2	H_{-1}, H_{-7} 4.07m H_{-2}, H_{-6} 3.60m H_{-3}, H_{-5} 4.65dd H_{-4} 4.95t H_{-8} 2.40s H' 2.05s	— — J_6 J_6 — —	$C_8H_8(COCH_3) = 8\text{-acetyl}$ bicyclo[5.1.0]octadienyl cation (numbering as above) 100 MHz T 29 Isolated as the hexafluorophosphate	370

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$[\text{C}_{14}\text{H}_9\text{FeO}_3]^+$	597	$[(1,2,3,4,5\text{-}h^5\text{-C}_{11}\text{H}_9)\text{Fe}(\text{CO})_3]^+$	$\text{F}_3\text{CO}_2\text{H}$	$\text{H}_{-1}, \text{H}_{-5}$ 5.25 $\text{H}_{-2}, \text{H}_{-4}$ 6.15 H_{-3} 8.2t H_{-6} to H_{-9} 6.94	$J_{1,2} = J_{4,5} = 9$ $J_{2,3} = J_{3,4} = 6.5$ — —	$\text{C}_{11}\text{H}_9 =$  Isolated as the tetrafluoro borate 100 MHz	377
(6) HEXAHAPTO DERIVATIVES							
$\text{C}_{33}\text{H}_{24}\text{FeO}_9$	598	$(h^6\text{-C}_{31}\text{H}_{24}\text{O}_7)\text{Fe}(\text{CO})_2$	CDCl_3	n.a.	—	Structure:  Signals at δ 7.35, 3.70s, 3.52s, 3.48s	1044
$\text{C}_{11}\text{H}_8\text{FeO}_3$	599	$(h^6\text{-C}_9\text{H}_8\text{O})\text{Fe}(\text{CO})_2$	CDCl_3	H 3.71m, 3.48m H' 4.6m, 6.37m H'' 7.33d H''' 5.61d H_{endo} 2.6m H_{exo} 2.05m	— — — — — —	Structure: 	371

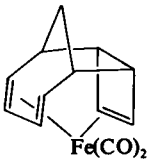
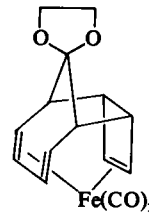
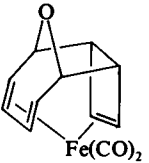
$C_{13}H_{12}FeO_2$	600	$(h^6-C_{11}H_{12})Fe(CO)_2$	—	n.a.	—	Structure:	442
						 Signals at δ 6.45t, 5.7m, 4.55m, 3.45m, 2.6m, 1.40d, 1.05m, in ratio: 2:2:2:2:2:1:1	
$C_{15}H_{14}FeO_4$	601	$(h^6-C_{13}H_{14}O_2)Fe(CO)_2$	—	n.a.	—	Structure:	442
						 Signals at δ 6.35t, 5.75m, 4.25m, 3.55t, 3.3m, 2.3m, in ratio 1:1:1:2:1:1	
$C_{12}H_{10}FeO_3$	602	$(h^6-C_{10}H_{10}O)Fe(CO)_2$	—	n.a.	—	Structure:	442
						 Signals at δ 5.95t, 5.35m, 4.0m, 2.95m, in ratio 1:1:2:1	

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
(7) MIXED HAPTO DERIVATIVES							
(a) Monohapto/tetrahapto							
$C_{10}H_8Cl_3-$ $FeNO_2$	603	$[h^4-exo-1-C_4H_5(CCl_3)]-$ $Fe(CNCH_3)(CO)_2$	$CDCl_3$	n.a.	—	An isocyanide complex Signals at δ 5.40, 3.54, 3.36, 2.89	443
$C_{15}H_8F_3-$ $FeNO_2$	604	$[h^4-exo-1-C_3H_5(C_6F_5)]-$ $Fe(CNCH_3)(CO)_2$	$CDCl_3$	H H'	5.35s, 4.08s, 2.88s 3.38s	— — — —	An isocyanide complex 443
(b) Monohapto/pentahapto							
(i) Monocarbonyl derivatives:							
$C_{25}H_{23}FeOP$	605	$(h^5-C_5H_5)Fe(CH_3)-$ $[P(C_6H_5)_3](CO)$	—	H H' H''	4.25s -0.17d 7.33m	— — —	403
$C_{10}H_{17}FeO_4P$	606	$(h^5-C_5H_5)Fe(CH_3)-$ $[P(OCH_3)_3](CO)$	$CDCl_3$	H H' H''	4.52s -0.13d 3.57d	— J 5 J 11	411
$C_{19}H_{35}FeO_4P$	607	$(h^5-C_5H_5)Fe(CH_3)[P(OCH_2-$ $CH_2'''CH_2'''CH_2''')_3](CO)$	$CDCl_3$	H H' H'' H'''	4.54s -0.17d 3.89d 1.65-0.89 comp.	— J 5 — —	411

$C_{25}H_{23}FeO_4P$	608	$(\eta^5-C_5H_5)Fe(CH_3)-[P(OC_6H_5)_3](CO)$	$CDCl_3$	H H' H''	4.02s 0.10d 7.3m	— J 6 —	—	411
$C_{28}H_{20}ClF_4FeOP$	609	$(\eta^5-C_5H_5)Fe(1-\eta^1-C_4ClF_4)-[P(C_6H_5)_3](CO)$	$CDCl_3$	H H'	4.61s 7.4-7.2m	— —	$C_4ClF_4 = 2\text{-Chloro-3,3,4,4-tetrafluoro-cyclobut-1-ene}$	846
			CH_2Cl_2	F ₋₃ F ₋₄	107.1s 116.2d	— J 15		
$C_{32}H_{25}FeOP$	610	$(\eta^5-C_5H_5)Fe(\eta^1-C\equiv CC_6H_5)-[P(C_6H_5)_3](CO)$	$CDCl_3$	H H'	4.57d 8.0-7.0m	$J_{PH} 1:1$ —	—	190
$C_9H_5F_5FeO_2$	611	$Fe(\eta^5-C_5H_5)(CF_2CF_3)(CO)_2$	CH_2Cl_2	F F'	62.8 82.1	— —		956
$C_{25}H_{20}F_3FeOP$	612	$(\eta^5-C_5H_5)Fe(CF_3)-[P(C_6H_5)_3](CO)$	$CDCl_3$	H F	4.51 -13.7d	— —		956
$C_{34}H_{29}F_5FeOP_2$	613	$(\eta^5-C_5H_5)Fe(CF_2CF_3)[P(C_6H_5)_2-CH_2CH_2P(C_6H_5)_2](CO)$	$(CD_3)_2CO$ CH_2Cl_2	H F F'	4.40s 65.8 81.5	— — —		956
$C_{26}H_{20}F_5FeOP$	614	$(\eta^5-C_5H_5)Fe(CF_2CF_3)-[P(C_6H_5)_3](CO)$	CH_2Cl_2	F F'	65.0 81.7	— —		956
$C_{35}H_{29}F_7FeOP_2$	615	$(\eta^5-C_5H_5)Fe[CF(CF_3)_2][P(C_6H_5)_2CH_2CH_2P(C_6H_5)_2](CO)$	CH_2Cl_2	F	65.0	—		956
$C_{27}H_{20}F_7FeOP$	616	$(\eta^5-C_5H_5)Fe[CF(CF_3)_2]-[P(C_6H_5)_3](CO)$	$CDCl_3$ CH_2Cl_2	H F F'	4.53s 162.9 66.9	— — —		956

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{28}H_{29}FeO_2P$	617	$(h^5-C_5H_5)Fe[CH'(CH_3)OCH_2''-CH_3^{IV}][P(C_6H_5)_3](CO)$	$(CD_3)_2CO$	H	4.26d	J 1.1	—	172
				H'	3.92q	J 7.5		
				H''	1.39d	J 6.2		
				H'''	3.24	—		
				H ^{IV}	0.96	—		
$[C_{26}H_{42}-FeO_2P]^+$	618	$\{(h^5-C_5H_5)Fe[h^1-C(CH_3)^{III}OH]-[P(C_6H_5)_3](CO)\}^+$	SO_2	H	5.12	—	Tetrafluoroborate	172
				H'	3.17s	—		
				H''	1.82, 1.41	—		
$[C_{26}H_{24}-FeO_2P]^+$	619	$\{(h^5-C_5H_5)Fe[h^1-C(CH_3)^{III}OH]-[P(C_6H_5)_3](CO)\}^+$	SO_2	H	4.96	—	Bromide	444
				H'	2.59	—		
				H''	7.56	—		
$[C_{27}H_{44}-FeO_2P]^+$	620	$\{(h^5-C_5H_5)Fe[h^1-(CH_3)^{III}OCH_2']-[P(C_6H_5)_3](CO)\}^+$	$(CD_3)_2CO$	H	5.31d	J 0.9	Tetrafluoroborate	172
				H'	3.29s	—		
				H''	4.45s	—		
				H'''	1.72, 1.45	—		
$[C_{27}H_{26}-FeO_2P]^+$	621	$\{(h^5-C_5H_5)Fe[h^1-C(CH_3)^{III}OCH_2']-[P(C_6H_5)_3](CO)\}^+$	$(CD_3)_2CO$	H	4.97d	J 1.1	Tetrafluoroborate	172
				H'	2.87s	—		
				H''	4.05s	—		
				H'''	7.51s	—		
$[C_{28}H_{46}-FeO_2P]^+$	622	$\{(h^5-C_5H_5)Fe[h^1-C(CH_3)^{III}OCH_2CH_3''']-[P(C_6H_5)_3](CO)\}^+$	$(CD_3)_2CO$	H	5.07d	J 1.0	Tetrafluoroborate	172
				H'	3.15s	—		
				H''	4.53 comp.	—		

				H''' H ^{IV}	1.53t 2.10-1.0 comp.	J 6.9 —		
[C ₂₈ H ₂₈ - FeO ₂ P] ⁺	623	{(h ⁵ -C ₅ H ₅)Fe[h ¹ -C(CH ₃) ^{'''} OCH ₂ CH ₃ ']][P(C ₆ H ₅ ^{IV}) ₃](CO)} ⁺	(CD ₃) ₂ CO	H H' H'' H''' H ^{IV}	5.07d 2.97s 4.30 comp. 1.37t 7.54s	J 1.05 — — J 7.5 —	Tetrafluoroborate	172
C ₂₈ H ₃₁ FeOPSi	624	(h ⁵ -C ₅ H ₅)Fe[CH ₂ Si(CH ₃) ₃]- [P(C ₆ H ₅) ₃](CO)	—	H	-1.2*, -0.2*	J _{PH} 13 J _{HH} 12 J _{PH} 2	*AB part of ABX system (X = P)	445
C ₃₁ H ₂₇ FeOP	625	(h ⁵ -C ₅ H ₅)Fe(CH ₂ C ₆ H ₅)- [P(C ₆ H ₅) ₃](CO)	CDCl ₃	H	1.85q*, 2.54q*	— —	100 MHz *AB part of ABX system (X = P)	165
C ₁₈ H ₁₄ FeN ₂ O	626	(h ⁵ -C ₅ H ₅)Fe(1-h ¹ -2-C ₆ H ₄ N= NC ₆ H ₅ ')(CO)	CS ₂	H H' ₃ H' ₄ H' ₅ H' ₆ H''	4.40s 6.94 7.28m 7.76bm 8.08dd 7.76, 7.28	— — — — — —	100 MHz	176
C ₃₀ H ₂₄ FFeOP	627	(h ⁵ -C ₅ H ₅)Fe(1-h ¹ -4-C ₆ H ₄ F)- [P(C ₆ H ₅) ₃](CO)	—	F	14.6*	—	*To high field relative to C ₆ H ₅ F	446
C ₁₀ H ₆ F ₆ FeN ₂ O	628	(h ⁵ -C ₅ H ₅)Fe[h ¹ -C(CF ₃)= NH'](N≡CCF ₃)(CO)	(CH ₃) ₂ CO CH ₂ Cl ₂	H H' F	5.00s 11.3b 70.5s, 67.5s	— — — —	94.1 MHz	447
C ₈ H ₈ FeINO	629	(h ⁵ -C ₅ H ₅)Fe(CNCH ₃)(I)(CO)	CDCl ₃	H H'	4.75s 3.58s	— —	An isocyanide complex	443

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{28}H_{25}FeO_2P$	630	$(h^5-C_5H_5)Fe(CH=CH'COCH_3)-[P(C_6H_5)_3](CO)$	—	H	9.68	$J_{HH'}$ 16	—	1001
				H'	6.51	—		
$C_{33}H_{27}FeO_2P$	631	$(h^5-C_5H_5)Fe(CH=CHCOC_6H_5)-[P(C_6H_5)_3](CO)$	—	H	10.61	J 16	—	1001
$C_{26}H_{20}F_3FeO_2P$	632	$(h^5-C_5H_5)Fe(COCF_3)-[P(C_6H_5)_3](CO)$	CDCl ₃	H	4.50d	—		956
			CH ₂ Cl ₂	F	79.3s	—		
$C_{20}H_{35}FeO_2P$	633	$(h^5-C_5H_5)Fe(COCH_3)-[P(C_4H_9)_3](CO)$	CDCl ₃	H	4.67s	—	TMS external	448
				H'	2.75s	—		
				H''	1.98–0.79m	—		
$C_{26}H_{41}FeO_2P$	634	$(h^5-C_5H_5)Fe(COCH_3)-[P(C_6H_{11})_3](CO)$	CDCl ₃	H	4.54s	—	—	172
				H'	2.54s	—		
				H''	1.82, 1.28	—		
			CF ₃ CO ₂ H		comp.			
				H	5.05s	—		
				H'	3.07s	—		
$C_{16}H_{19}FeO_2P$	635	$(h^5-C_5H_5)Fe(COCH_3)-[P(CH_3)_2C_6H_5](CO)$		H	4.30d	J 0.7	100 MHz	449 990
				H'	2.48s	—		
				H''	1.78d,	J_{PH} 9.5		
					1.44d	J_{PH} 9.0		
$C_{42}H_{41}FeO_2P_3$	636	$(h^5-C_5H_5)Fe(COCH_3)-[(PPh_2CH_2CH_2)_2PPh](CO)$	CDCl ₃	H	4.17d	J 1	100 MHz	5
				H'	2.41d	J 6		

$C_{26}H_{23}FeO_2P$	637	$(h^5-C_5H_5)Fe(COCH_3)-$ $[P(C_6H_5)_3](CO)$	$CDCl_3$	H H' H''	4.62s 2.52s 7.59m	— — —	TMS external	448
$C_{26}H_{23}FeO_2P$	638	$(h^5-C_5H_5)Fe(COCH_3)-$ $[P(C_6H_5)_3](CO)$	CS_2	H H' H''	4.24 2.17 7.05	— — —	—	444
			CF_3CO_2H	H H' H''	4.96 2.59 7.56	— — —		
$C_{20}H_{35}FeO_3P$	639	$(h^5-C_5H_5)Fe(COCH_3)[P(OCH_2-$ $CH_2'''CH_2'''CH_3'''),_3](CO)$	$CDCl_3$	H H' H'' H'''	4.67s 2.57s 3.97q 1.92-0.83	— — — —	TMS external	448
$C_{26}H_{23}FeO_3P$	640	$(h^5-C_5H_5)Fe(COCH_3)-$ $[P(OC_6H_5)_3](CO)$	$CDCl_3$	H H' H''	4.32s 2.68s 7.45m	— — —	TMS external	448
$C_{21}H_{37}FeO_2P$	641	$(h^5-C_5H_5)Fe(COCH_2CH_3)-$ $[P(n-Bu)_3](CO)$	—	H H' H''	4.38 2.84 0.84t	J_{1-2} $J_{H'H'} 15.8$ $J_{H'H''} 7.5$	—	449
$C_{17}H_{21}FeO_2P$	642	$(h^5-C_5H_5)Fe(COCH_2CH_3)-$ $[P(CH_3'''),_2C_6H_5](CO)$	—	H H' H'' H'''	4.29d 2.78m 0.84t 1.76d, 1.44d	J_{1-4} $J_{H'H'} 16.1$ $J_{H'H''} 7.3$ $J_{PH} 9.5$ $J_{PH} 9.0$		
$C_{22}H_{23}FeO_2P$	643	$(h^5-C_5H_5)Fe(COCH_2CH_3)-$ $[P(C_6H_5)_2CH_3''']](CO)$	—	H H' H'' H'''	4.38 2.38 0.68t 2.02d	J_{1-2} $J_{H'H'} 16.8$ $J_{H'H''} 7.3$ $J_{PH} 9.3$	—	449

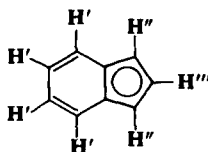
TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{27}H_{25}FeO_2P$	644	$(h^5-C_5H_5)Fe(COCH_2CH_2^o)-[P(C_6H_5''')_3](CO)$	$CDCl_3$	H	4.40s	—	100 MHz	411
				H'	2.70m	—		
				H''	0.60t	J 7		
				H'''	7.3m	—		449
				H	4.32d	J 1.0		
				H'	2.67m	$J_{H'H'}$ 17.0		
$C_{12}H_{19}FeO_3P$	645	$(h^5-C_5H_5)Fe(COCH_2CH_2^o)-[P(OCH_3''')_3](CO)$	—	H	4.56	J 0.9	100 MHz	449
				H'	2.82q	J 7.0		
				H''	0.86q	J 7.0		
				H'''	3.56d	J_{PH} 11.5		
$C_{27}H_{25}FeO_3P$	646	$(h^5-C_5H_5)Fe(COCH_2CH_2^o)-[P(OC_6H_5)_3](CO)$	—	H	5.02d	J 0.6	100 MHz	449
				H'	2.82m	$J_{H'H'}$ 9.5		
				H''	0.88t	$J_{H'H''}$ 7.3		
$C_{18}H_{23}FeO_2P$	647	$(h^5-C_5H_5)Fe[COCH'(CH_2^o)_2]-[P(CH_3''')_2C_6H_5](CO)$	—	H	4.30	J 1.4	100 MHz	449
				H'	3.12 hept.	J 6.5		
				H''	1.0d, 0.8d	J 6.5		
				H'''	1.76d, 1.44d	J_{PH} 9.5 J_{PH} 9.0		
$C_{28}H_{27}FeO_2P$	648	$(h^5-C_5H_5)Fe[COCH'(CH_2^o)_2]-[P(C_6H_5)_3](CO)$	—	H	4.34	J 0.6	100 MHz	449
				H'	2.84 hept.	J 7.0		
				H''	0.88d	J 7.0		
$C_{29}H_{27}FeO_2P$	649	$(h^5-C_5H_5)Fe(COCH_2CH_2^oCH_2''')=CH_2^{IV})[P(C_6H_5)_3](CO)$	$CDCl_3$	H	4.40d	J_{PH} 1.0	—	450
				H'	2.77	$J_{H'H'}$ 16		

				H''	1.90q	$J_{H'H''}$ 7		
				H'''	5.50m	—		
				H ^{IV}	4.90m,	—		
					4.70m			
C ₃₀ H ₂₉ FeO ₂ P	650	(<i>h</i> ⁵ -C ₅ H ₅)Fe(COCH ₂ CH ₂ CH ₂ ''-CH ^{IV} =CH ₂ ^V)/P(C ₆ H ₅) ₃ (CO)	CDCl ₃	H	4.40d	J_{PH} 1.0	—	450
				H'	2.72	$J_{H'H'}$ 17		
				H''	1.25m	$J_{H'H''}$ 7		
				H'''	1.75q	—		
				H ^{IV}	5.60 comp.	—		
				H ^V	4.98m,	—		
					4.75m			
C ₁₁ H ₁₅ FeNO ₂	651	(<i>h</i> ⁵ -C ₅ H ₅)Fe(COCH ₂ CH ₂ N-(CH ₃) ₂)(CO)	CHCl ₃	H	4.46s	—	—	177
				H'	2.84s, 2.41s	—		
C ₁₀ H ₁₂ FeO ₂ S	652	(<i>h</i> ⁵ -C ₅ H ₅)Fe(COCH ₂ CH ₂ -SCH ₃)(CO)	CS ₂	H	4.40	—	Internal reference hexamethyldisiloxane	185
				H'	2.3-2.2	—		
				H''	2.22	—		
C ₃₂ H ₂₇ FeO ₂ P	653	(<i>h</i> ⁵ -C ₅ H ₅)Fe(COCH ₂ C ₆ H ₅ ')-[P(C ₆ H ₅ '') ₃](CO)	—	H	4.14	J_{PH} 1.5	—	990
				H'	4.02,	$J_{H'H'}$ 13.5		
					3.49			
				H''	7.01	—		
				H'''	7.31	—		
C ₂₉ H ₃₁ FeO ₂ -PSi	654	(<i>h</i> ⁵ -C ₅ H ₅)Fe[COCH ₂ Si(CH ₃) ₃]-[P(C ₆ H ₅) ₃](CO)	CDCl ₃	H	4.40s	—	—	983
				H'	2.15s	—		445
				H''	0.01s	—		
(ii) Dicarbonyl derivatives:								
C ₈ H ₇ DFeO ₂	655	(<i>h</i> ⁵ -C ₅ H ₅)Fe(CH ₂ D)(CO) ₂	CH ₃ CN	Not observed		J_{HH} -8.3*	*Calculated values from observations on J_{HD}	186
			C ₆ H ₆			J_{HH} -8.6*		949
			C ₆ H ₁₂			J_{HH} -8.9*		
			CS ₂			J_{HH} -9.0*		

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References	
$C_8H_8FeO_2$	656	$(h^5-C_5H_5)Fe(C'H_3)(C''O)_2$	—	H	4.73s	—	—	403	
				H'	0.17s	—		408	
				Toluene	H	4.30		—	132
				$CHCl_3$	C	+85.3		—	32
					C'	-23.5		—	
					C''	+218.4		—	
$C_{10}H_{12}FeO_3$	657	$(h^5-C_5H_4OCH_2CH_3)Fe-(CH_3''')(CO)_2$	$CDCl_3$		H	4.44t, 4.26t	—	—	413
				H'	3.74q	—			
				H''	1.3t	—			
				H'''	0.1s	—			
$C_{12}H_{10}FeO_2$	658	$(h^5-C_9H_7)Fe(CH_3)(CO)_2$	CS_2	H	-0.49s	—	$C_9H_7 =$	109	
				H'	7.18	—			
				H''	5.23	$J_{H''H'''} 3$			
				H'''	4.79				
$C_9H_{10}FeO_2$	659	$(h^5-C_5H_5)Fe(CH_2CH_3)(CO)_2$	Liquid	H	4.60	—	—	132	
$C_{10}H_{12}FeO_2$	660	$(h^5-C_5H_5)Fe(CH_2CH_2CH_3)(CO)_2$	Liquid	H	4.59	—	—	132	
$C_{10}H_{12}FeO_2$	661	$(h^5-C_5H_5)Fe[CH(CH_3)_2](CO)_2$	Liquid	H	4.58	—	—	132	
$C_{11}H_{14}FeO_2$	662	$(h^5-C_5H_5)Fe[CH_2CH''(CH_3''')_2](CO)_2$	—	H	4.6s	—	—	451	
				H', H''	1.5	—			
				H'''	1.0d	$J 5.2$			



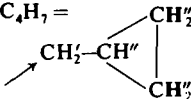
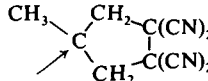
$C_{11}H_{14}FeO_2$	663	$(h^5-C_5H_5)Fe[C(CH_3)_3](CO)_2$	CS_2	H H'	4.65s 1.30s	— —	—	452
$C_8H_5F_3FeO_2$	664	$(h^5-C_5H_5)Fe(CF_3)(CO)_2$	$CHCl_3$ CH_2Cl_2	H F	4.99 -11.6s	— —	—	132 956
$C_9H_6F_4FeO_2$	665	$(h^5-C_5H_5)Fe(CF_2CF_2H)(CO)_2$	—	H F F'	5.18tt 59.0 126.8d	J_{HF} 4.6 $J_{HF'}$ 58.2 — —	—	453
$C_{10}H_5DF_6FeO_2$	666	$(h^5-C_5H_5)Fe[CD(CF_3)_2](CO)_2$	—	H F	4.98 53.6	— —	100 MHz	454
$C_{10}H_6F_6FeO_2$	667	$(h^5-C_5H_5)Fe[CH'(CF_3)_2](CO)_2$	—	H H' F	5.0 2.5m 53.4	— — J_{HF} 12.0	100 MHz	454 455
$C_{11}H_{12}FeO_2$	668	$(h^5-C_5H_5)Fe(C_4H_7)(CO)_2$	C_6D_6	H H' H''	4.35s 1.42d 0.61m, 0.23m	— — — —	$C_4H_7 =$ 	450
$C_{17}H_{12}FeN_4O_2$	669	$(h^5-C_5H_5)Fe(C_{10}H_7N_4)(CO)_2$	—	H H' H''	5.14 1.68 3.38d, 3.02d	— — J 14.5 J 14.5	$C_{10}H_7N_4 =$ 	194
$C_{12}H_{14}FeO_2$	670	$(h^5-C_5H_5)Fe(CH_2^I CH_2^II CH_2^III-CH^IV=CH^V)(CO)_2$	$CDCl_3$	H H' H'' H''' H ^{IV}	4.75 1.55m 2.12m 5.7m 5.05m	— — — — —	—	450

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{11}H_{12}FeO_2$	671	$(h^5-C_5H_5)Fe(CH_2CH_2^oCH'''=CH_2^{IV})(CO)_2$	$CDCl_3$	H	4.75	—	—	450
				H'	1.50t	—		
				H''	2.18q	—		
				H'''	5.8m	—		
				H ^{IV}	4.90	—		
			C_6D_6	H	4.6	—	—	451
				H'	1.4 comp.	—		
				H''	2.1 comp.	—		
				H'''	5.9 comp.	—		
				H ^{IV}	4.9 comp.	—		
$C_{12}H_{14}FeO_2$	672	$(h^5-C_5H_5)Fe(CH_2CH_2^oCH'''=CH'''CH_3^{IV})(CO)_2$	$CDCl_3$	H	4.75	—	—	450
				H'	1.40m	—		
				H''	2.10m	—		
				H'''	5.5m	—		
				H ^{IV}	1.65d	—		
$C_{13}H_{16}FeO_2$	673	$(h^5-C_5H_5)Fe[CH_2C(CH_3)_2CH'''=CH_2^{IV}](CO)_2$	C_6D_6	H	4.4s	—	—	451
				H'	1.9s	—		
				H''	1.4s	—		
				H'''	6.1 comp.	—		
				H ^{IV}	5.1 comp.	—		
$C_{10}H_8D_2FeO_2$	674	$(h^5-C_5H_5)Fe(CD_2CH=CH_2)-(CO)_2$	$CDCl_3$	H	5.7m	—	—	456
				H'	4.68m	—		
$C_{10}H_8D_2FeO_2$	675	$(h^5-C_5H_5)Fe(CH_2CH'=CD_2)-(CO)_2$	$CDCl_3$	H	2.08d	—	—	456
				H'	5.7m	—		

$C_{11}H_{12}FeO_2$	676	$(h^5-C_5H_5)Fe[CH_2C(CH_3)=CH_2](CO)_2$	$CDCl_3$	H H' H''	2.06s 1.79s 4.55t	— — —	—	456
$C_{11}H_{11}DFeO_2$	677	$(h^5-C_5H_5)Fe(CHDCH'=CH'CH_3)(CO)_2$ <i>cis</i> and <i>trans</i>	$CDCl_3$	H H' H''	2.12d 5.43m 1.56d	— — —	—	456
$C_{11}H_{12}FeO_2$	678	$(h^5-C_5H_5)Fe(CH_2CH'=CH'CH_3)(CO)_2$	$CDCl_3$	H H' H''	2.12d 5.43m 1.56d	— — —	—	456
$C_{11}H_{11}ClFeO_2$	679	$(h^5-C_5H_5)Fe[CH_2CH'=C(Cl)CH_3](CO)_2$	$CDCl_3$	H H' H''	2.10d 5.7t 2.02s	— — —	—	456
$C_{16}H_{14}FeO_2$	680	$(h^5-C_5H_5)Fe(CH_2CH'=CH'C_6H_5)(CO)_2$	$CDCl_3$	H H' H''	2.30d 6.32 7.29	— J 15 —	—	456
$C_9H_8FeO_2$	681	$(h^5-C_5H_5)Fe(h^1-CH'=CH_2)(CO)_2$	$CDCl_3$	H H' H'' _{cis} H'' _{trans}	4.81 7.14 5.90 5.42	— $J_{H'H''}$ 9.0 $J_{H'H''}$ 17.4 $J_{H''H''}$ 1.4	Internal reference hexamethyldisiloxane	223 201
			CS_2	H H' H'' _{cis} H'' _{trans}	4.42 6.9q 5.83d 5.35d	— $J_{H'H''}$ 9 $J_{H'H''}$ 17	—	457
$C_9H_5F_3FeO_2$	682	$(h^5-C_5H_5)Fe(h^1-CF=CF_2)(CO)_2$	CS_2	F F' _{cis} F' _{trans}	147.3 89.5 139.6	— $J_{FF'}$ 46.8 $J_{FF'}$ 122.4 $J_{F'F'}$ 107.1		232 453

TABLE VII—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{10}H_7F_3FeO_2$	683	$(h^5-C_5H_5)Fe(h^1-C(CF_3)=CH_2)(CO)_2$	CCl_4	H F	6.25*, 5.5† 60.5	— J_{HF} 1.9	100 MHz *Olefinic proton <i>trans</i> to Fe †Olefinic proton <i>cis</i> to Fe	458
$C_{10}H_7F_3FeO_2$	684	$(h^5-C_5H_5)Fe(h^1-CH'=CH''CF_3)(CO)_2$	—	H H' H'' F	4.8 7.91d 6.54q 58.2d	— J 11.5 J_{HF} 8.5 —	—	233 458
$C_{10}H_5F_5FeO_2$	685	$(h^5-C_5H_5)Fe(h^1-CF=CF'CF_3)(CO)_2$ <i>trans</i>	THF	F F' F''	166 86 66	$J_{FF''}$ 13 $J_{FF'}$ 131 $J_{F'F''}$ 66	56.4 and 94.1 MHz	459
$C_{10}H_5ClF_4FeO_2$	686	$(h^5-C_5H_5)Fe(h^1-CF=CClCF_3)(CO)_2$ <i>cis</i> and <i>trans</i>	—	H F F'	5.04 19.4 60.1 58.0	— — $J_{FF'}$ 23.6, 8.7 —	—	460
$C_{11}H_6F_6FeO_2$	687	$(h^5-C_5H_5)Fe(h^1-C(CF_3)=CHCF_3)(CO)_2$ <i>trans</i>	$CHCl_3$	Not reported		J_{HF} 1.5 $J_{HF'}$ 8.5 $J_{FF'}$ 2.0	— —	415
$C_{13}H_{15}F_3FeGeO_2$	688	$(h^5-C_5H_5)Fe(h^1-C(CF_3)=CH'Ge(CH_3)_3)(CO)_2$	$CHCl_3$ C_6H_{12}	H H' H'' F	4.8 7.2q 0.3 59.4d*	— J_{HF} 2 — J_{HF} 2	*External CCl_3F	415

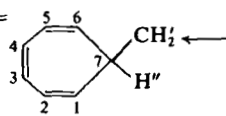
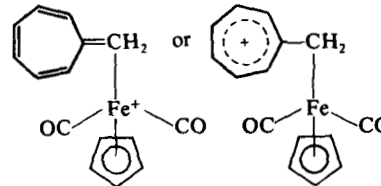
$C_{12}H_{12}FeO_4$	689	$(h^5-C_5H_5)Fe[C(OCOCH_3)=CH''CH_3'''] (CO)_2$	CS_2	H H' H'' H'''	4.89s 1.97s 4.98q 1.41d	— — $J_{6.5}$ $J_{6.5}$	—	461
$C_{13}H_{15}F_3 \cdot FeO_2Si$	690	$(h^5-C_5H_5)Fe[C(CF_3)=CH'Si(CH_3)_3](CO)_2$	$CHCl_3$	H H' H''	4.9 7.0q 0.2	— $J_{HF} 2$ —	—	415
			C_6H_{12}	F	60.1d	$J_{HF} 2$	External CCl_3F	
$C_{14}H_{14}F_6 \cdot FeO_2Sn$	691	$(h^5-C_5H_5)Fe[C(CF_3)=C(CF_3)Sn(CH_3)_3](CO)_2$	C_6H_{12}	F	50.4, 49.4	— —		415
$C_{15}H_{12}FeO_2$	692	$(h^5-C_5H_5)Fe(h^1-CH'=CH''C_6H_5'')(CO)_2$	$CDCl_3$	H H' H'' H'''	4.83 7.66 6.63 7.48–7.08	— $J_{H'H''} 16.0$ — —	Hexamethyldisiloxane as reference	223
$C_{15}H_8F_4FeO_2$	693	$(h^5-C_5H_5)Fe[1-h^1-CH=CH(2,3,5,6-C_6HF_4)](CO)_2$	THF	F_{-2}, F_{-6} F_{-3}, F_{-5}	138.4 138.4	— —	T 35°, 56.4 MHz	244
$C_{11}H_5F_5FeO_2$	694	$(h^5-C_5H_5)Fe[h^1-C(CF_3)=C=CF_2](CO)_2$	—	F F'	60.3t 110.8q	$J_{FF'} 4.0$ —	94.1 MHz	241
$C_{10}H_8FeO_2$	695	$(h^5-C_5H_5)Fe(CH=CH=CH_2)(CO)_2$	CS_2	H H'	4.89 3.92, 3.95	$J_{HH'} 6.5$ — —	—	995
$C_{11}H_{10}FeO_2$	696	$(h^5-C_5H_5)Fe(CH=CH=CH'CH_3')(CO)_2$	CS_2	H H' H''	4.98 4.40 1.47	$J_{HH''} 3.2$ $J_{H'H''} 6.8$ —	—	995

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{11}H_5F_5FeO_2$	697	$(h^5-C_5H_5)Fe(h^1-CF=CF'-CF''=CF_2''')(CO)_2$	$(CH_3)_2O$	F	75.9	$J_{FF'}$ 41 $J_{FF''}$ 7		238
				F'	55.9	$J_{F'F''}$ 14		239
				F''	156.4	$J_{F''F'''_{cis}}$ 25 $J_{F''F'''_{trans}}$ 114		
				F''' _{cis}	108.9	$J_{FF''''}$ 3, $J_{F'F''''}$ 4		
				F''' _{trans}	120.2	$J_{FF''''}$ 3, $J_{F'F''''}$ 13, $J_{F''F''''}$ 79		
$C_{11}H_{10}FeO_3$	698	$(h^5-C_5H_5)Fe(h^1-CH'=CH''COCH_3''')(CO)_2$	CCl_4	H	4.86	—	Hexamethyldisiloxane as reference 100 MHz	462
				H'	8.77	$J_{H'H''}$ 16.4		223
				H''	6.36	—		
				H'''	1.98	—		
$C_{16}H_{12}FeO_3$	699	$(h^5-C_5H_5)Fe(h^1-CH'=CH''COC_6H_5''')(CO)$	$CDCl_3$	H	4.87	—	Hexamethyldisiloxane as reference	223
				H'	9.21	$J_{H'H''}$ 16.3		462
				H''	7.16	—		
				H'''	7.75, 7.32	—		
$C_{17}H_{14}FeO_3$	700	$(h^5-C_5H_5)Fe(h^1-p-CH'=CH''COC_6H_4''')CH_3^{IV}(CO)_2$	—	H	4.89	—	—	462
				H'	9.20	$J_{H'H''}$ 16.3		
				H''	7.15	—		
				H''' _{ortho}	7.67	—		
				H''' _{meta}	7.08	—		
				H ^{IV}	2.32	—		

$C_{11}H_3F_3FeO_2$	701	$(h^5-C_5H_3)Fe(1-h^1-C_4F_3)(CO)_2$	CS_2	F_{-2} 124.1 F_{-3} 123.4 F_{-4} 119.1	— — —	$C_4F_3 = 2,3,3,4,4$ - pentafluorocyclobut-1-ene	232
$C_{11}H_3ClF_4FeO_2$	702	$(h^5-C_5H_3)Fe(1-h^1-C_4ClF_4)(CO)_2$	$CDCl_3$ CH_2Cl_2	H 5.09s F_{-3} 110.9s F_{-4} 115.0s	— — —	$C_4ClF_4 = 2$ -chloro-3,3,4,4- tetrafluorocyclobut-1-ene	846
$C_{12}H_3F_7FeO_2$	703	$(h^5-C_5H_3)Fe(1-h^1-C_5F_7)(CO)_2$	$(CH_3)_2CO$	F_{-2} 47.0m F_{-3} 40.2m F_{-4} 51.8m F_{-5} 22.0m	— — — —	$C_5F_7 = 2,3,3,4,4,5,5$ - Heptafluorocyclopent-1-ene T35 Internal reference CF_3CO_2H	463
$C_{12}H_3ClF_6FeO_2$	704	$(h^5-C_5H_3)Fe(1-h^1-C_5ClF_6)(CO)_2$	THF	F_{-3} 112.6tt F_{-4} 130.0q F_{-5} 99.6s	$J_{3,4}$ 6.82 $J_{4,5}$ 6.82 $J_{3,5}$ 3.65	$C_5ClF_6 = 2$ -Chloro- 3,3,4,4,5,5-hexafluoro- cyclopent-1-ene	237
$C_{12}H_{10}FeO_2$	705	$(h^5-C_5H_3)Fe(5-h^1-C_5H_3)(CO)_2$	$(CH_3)_2CO$	H 5.13 H_{-1}, H_{-4} 6.53bd H_{-2}, H_{-3} 6.18bs H_{-5} 4.09	— $J(^{13}C-H)$ 164* $J(^{13}C-H)$ 162 —	$C_5H_3 =$ Cyclopenta-1,3-diene T -75° 60 and 100 MHz *H satellites are doublets with splitting of ~4.5 Hz	464
			CS_2	H 4.40 H' 5.70	— —	T 30°	924
			CS_2/C_6D_5 - CD_3 (3:1)	n.m.	$J_{1,2} \pm 1.17$ $J_{1,3} \pm 0.01$ $J_{2,3} + 4.66$ $J_{2,4} + 1.15$ $J_{2,5} + 2.02$ $J_{3,4} + 2.02$	100 MHz	465
$C_{14}H_{12}FeO_3$	706	$(h^5-1-C_5H_4COCH_3)Fe(5-h^1-C_5H_3)(CO)_2$	$CDCl_3$	H_{-2}, H_{-5} 5.17t H_{-3}, H_{-4} 4.76t H' 2.35s H'' 5.92s	J_2 J_2 —	$C_5H_3 =$ Cyclopenta-1,3-diene T 30°	466

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{15}H_5F_{11}FeO_2$	707	$(h^5-C_5H_5)Fe(h^1-C_5F_2(CF_3)_3)(CO)_2$	$CHCl_3$ C_6H_{12}	H	4.8	—	$C_5F_2(CF_3)_3 = 1,2$ -Difluoro-3,4,5-tris (trifluoromethyl)-cyclopenta-1,3-diene	415
				F ₋₁	87.5	$J_{1,2}$ 33.5		
				F ₋₂	84.3	$J_{2,3}$ 9.4		
				3-CF ₃ '	63.9m	$J_{3,4}$ 5.7		
				4-CF ₃ '	60.5	$J_{4,5}$ 3.2		
				5-CF ₃ '	62.9	$J_{1,5}$ 7.0		
$C_{13}H_5F_9FeO_2$	708	$(h^5-C_5H_5)Fe(1-h^1-C_6F_9)(CO)_2$	THF and CS_2	F ₋₂	104.5	—	$C_6F_9 = 2,3,3,4,4,5,5,6,6$ -Nonafluorocyclohex-1-ene 94.1 and 56.4 MHz	459 232
				F ₋₃	124.1	—		
				F ₋₄	143.5	—		
				F ₋₅	141.1	—		
				F ₋₆	99.0	—		
$C_{15}H_{14}FeO_2$	709	$(h^5-C_5H_5)Fe(h^1-CH_2C_7H_7)(CO)_2$	CS_2	H'' ₁ , H'' ₆	5.15m	—	$CH_2C_7H_7 =$ 	467
				H'' ₂ , H'' ₅	6.05m	—		
				H'' ₃ , H'' ₄	6.55t	—		
				H'' ₇ , H'	1.80m	—		
				H	4.62s	—		
$[C_{15}H_{13}FeO_2]^+$	710	$[(h^5-C_5H_5)Fe(h^1-CH_2-C_7H_6)(CO)_2]^+$	$(CD_3)_2CO$	H	5.27s	—	Hexafluoroantimonate Structure: 	467
				H'	3.49s	—		
				H''	7.80m	—		

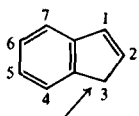
C ₁₄ H ₁₂ FeO ₂	711	(h ⁵ -C ₅ H ₅)Fe(7-h ¹ -C ₇ H ₇)(CO) ₂	C ₆ D ₅ CD ₃	H	4.1s	—	C ₇ H ₇ = Cyclohepta-1,3,5-triene T30	468
				H'	4.8s	—		
				H	4.1s	—	T -50° *Analysed as an AA'XX' system with J _{2,5} = 0	
				H' ₋₂ , H' ₋₅	6.05m	J _{2,3} 11.2*		
						J _{2,4} 1.1*		
				H' ₋₃ , H' ₋₄	5.20m	J _{3,4} 7.5*		
				H' ₋₁ , H' ₋₆	4.32t	J 7		
				H' ₋₇	2.44t	J 7		
C ₁₃ H ₅ F ₃ FeO ₂	712	(h ⁵ -C ₅ H ₅)Fe(2-h ¹ -C ₆ F ₅)(CO) ₂	CHCl ₃	F ₋₁	177.9	—	C ₆ F ₅ = Bicyclo[2.2.0]- hexa-2,5-diene	240
				F ₋₃	107.5	—		
				F ₋₄	187.9	—		
				F ₋₅	129.2	—		
				F ₋₆	123.0	—		
				F ₋₁	97.6	—	Relative to CF ₃ CO ₂ H	469
				F ₋₃	29.8	—		
				F ₋₄	109.0	—		
				F ₋₅	46.0	—		
				F ₋₆	45.2	—		
C ₁₆ H ₁₂ FeO ₂	713	(h ⁵ -C ₅ H ₅)Fe(3-h ¹ -C ₉ H ₇)(CO) ₂	CDCl ₃	H ₋₁ , H ₋₂	6.72d	—	C ₉ H ₇ = 	470 1047
					6.53d	—		
				H ₋₃	3.97	—		
				H ₋₄ to H ₋₇	7.65-6.95	—		
C ₁₀ H ₈ FeO ₂	714	(h ⁵ -C ₅ H ₅)Fe(h ¹ -CH ₂ C≡CH'')(CO) ₂	CS ₂	H	4.76s	—	—	461
				H'	3.97d	J 6.5		
				H''	4.89q	J 6.5		
C ₁₁ H ₁₀ FeO ₂	715	(h ⁵ -C ₅ H ₅)Fe(h ¹ -CH ₂ C≡CCH ₃)(CO) ₂	CDCl ₃	H	4.76s	—	—	163
				H'	2.0-1.6	—		156
					comp.	—		995

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_9H_6FeO_2$	716	$(h^5-C_5H_5)Fe(h^1-C\equiv CH')(CO)_2$	$CDCl_3$	H	4.92s	—	—	471
				H'	1.30s	—		
$C_{10}H_8FeO_2$	717	$(h^5-C_5H_5)Fe(h^1-C\equiv CCH_3)(CO)_2$	CS_2	H	4.93s	—	—	461
				H'	1.79s	—		
$C_{10}H_5F_3FeO_2$	718	$(h^5-C_5H_5)Fe(h^1-C\equiv CCF_3)(CO)_2$	$CDCl_3$	H	5.08s	—	—	472
				F	46.1s	—		
$C_{16}H_{12}FeO_2$	719	$(h^5-C_5H_5)Fe(CH_2C\equiv CC_6H_5)(CO)_2$	$CDCl_3$	H	1.85s	—	—	995
$C_{13}H_{14}FeO_2$	720	$(h^5-C_5H_5)Fe(h^1-C\equiv Cn-C_4H_9)(CO)_2$	$CDCl_3$	H	5.0s	—	—	190
				H'	2.4–0.7	—		
$C_{15}H_{10}FeO_2$	721	$(h^5-C_5H_5)Fe(h^1-C\equiv CC_6H_5)(CO)_2$	$CDCl_3$	H	5.05s	—	—	190
				H'	7.3m	—		
			CS_2	H	4.85s	—	—	472
				H'	7.00m	—		
$C_{15}H_5F_3FeO_2$	722	$(h^5-C_5H_5)Fe(1-h^1-C\equiv CC_6F_5)(CO)_2$	THF	F ₋₂ , F ₋₆	140.8	$J_{2,4}$ 4.4	T 35°	244
				F ₋₃ , F ₋₅	165.6	$J_{3,4}$ 20.45		472
				F ₋₄	162.0	—		
			CS_2	H	5.05s	—		
$C_8H_7BrFeO_2$	723	$(h^5-C_5H_5)Fe(CH_2Br)(CO)_2$	CS_2	H	4.83s	—	—	195
				H'	3.78s	—		
$C_8H_7ClFeO_2$	724	$(h^5-C_5H_5)Fe(CH_2Cl)(CO)_2$	$(CH_3)_2CO$	H	5.09s	—	—	195
				H'	4.24s	—		

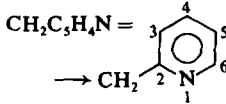
$C_{10}H_{10}FeO_3$	725	$(h^5-C_5H_5)Fe(CH_2COCH_3)(CO)_2$	CCl_4	H	4.90	—	—	132
$C_{15}H_{12}FeO_3$	726	$(h^5-C_5H_5)Fe(CH_2COC_6H_5)(CO)_2$	$CDCl_3$	H	4.76s	—	—	473
				H'	2.31s	—	—	
				H''	7.8, 7.43m	—	—	
$C_{20}H_{12}FeN_4O_2$	727	$(h^5-C_5H_5)Fe[C(CN)_2C(CN)_2-CH_2C_6H_5](CO)_2$	—	H	5.56	—	—	420
				H'	3.85	—	—	
				H''	7.70	—	—	
$C_9H_9FeNO_3$	728	$(h^5-C_5H_5)Fe(CH_2CONH_2)(CO)_2$	$CDCl_3$	H	4.92s	—	—	196
				H'	1.57s	—	—	
				H''	5.45bs	—	—	
$C_9H_8FeO_4$	729	$(h^5-C_5H_5)Fe(CH_2CO_2H)(CO)_2$	$CDCl_3$	H	4.85s	—	—	196
				H'	1.48s	—	—	
				H''	7.65bs	—	—	
$C_{10}H_{10}FeO_4$	730	$(h^5-C_5H_5)Fe(CH_2CO_2CH_3)(CO)_2$	CS_2	H	4.80s	—	—	129
				H'	1.40s	—	—	
				H''	3.46s	—	—	
$C_{12}H_{14}FeO_4$	731	$(h^5-C_5H_5)Fe(CH_2CH_2CO_2-CH_2CH_3)(CO)_2$	CS_2	H	4.76s	—	—	129
				H'	2.24t	} J 8	—	
					1.60t			
				H''	4.00q	J 7	—	
				H'''	1.19t	—	—	
$C_9H_{10}FeO_3$	732	$(h^5-C_5H_5)Fe(CH_2OCH_3)(CO)_2$	CS_2	H	4.70s	—	—	195
				H'	4.73s	—	—	
				H''	3.15s	—	—	
$C_{10}H_{12}FeO_3$	733	$(h^5-C_5H_5)Fe(CH_2CH_2OCH_3)(CO)_2$	CS_2	H	4.76s	—	—	474
				H'	1.69t	—	—	
				H''	3.51t	—	—	
				H'''	3.40s	—	—	

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{10}H_{12}FeO_3$	734	$(h^5-C_5H_5)Fe(CH_2OCH_2CH_3''')-(CO)_2$	Liquid	H	4.69s	—	—	195
				H'	4.83s	—		
				H''	3.37q	—		
				H'''	1.11t	—		
$C_{10}H_6FeO_3$	735	$(h^5-C_5H_5)Fe[C(CF_3)_2OH']-(CO)_2$	$CDCl_3$	H	4.91s	—	100 MHz	475
				H'	2.49b	—		
				F	67.7s	—	56.4 and 94.1 MHz	
$C_{11}H_{12}FeO_3$	736	$(h^5-C_5H_5)Fe(h^1-CH_2OCH_2''-CH'''=CH_2)(CO)_2$	CS_2	H	4.71	—	—	195
				H'	4.76s	—		
				H''	5.05 comp.	—		
				H'''	6.05 comp.	—		
$C_{13}H_{16}FeO_3$	737	$(h^5-C_5H_5)Fe[h^1-CH_2OC(CH_3)_2-CH'''=CH_2^{IV}](CO)_2$	CS_2	H	4.65s	—	—	195
				H'	4.45s	—		
				H''	1.17s	—		
				H'''	5.74q	—		
				H ^{IV}	4.95 comp.	—		
$C_{10}H_{10}FeO_4$	738	$(h^5-C_5H_5)Fe(CH_2OCOCH_3''')-(CO)_2$	CS_2	H	4.81s	—	—	195
				H'	5.08s	—		
				H''	1.86s	—		
$[C_{12}H_{18}FeNO_3]^+$	739	$\{(h^5-C_5H_5)Fe[CH_2OCH_2''CH_2'''-NH(CH_3^{IV})_2](CO)_2\}^+$	SO_2	H	5.10s	—	Hexafluorophosphate	195
				H'	3.95s	—		
				H''	3.35	—		
				H'''	4.05b	—		
				H ^{IV}	3.01s	—		

$C_9H_{10}FeO_2S$	740	$(h^5-C_5H_5)Fe(CH_2SCH_3)(CO)_2$	CS_2	H	4.79	—	Hexamethyldisiloxane as reference	185
				H'	2.32	—		
				H''	2.09	—		
$C_{10}H_{12}FeO_2S$	741	$(h^5-C_5H_5)Fe(CH_2CH_2SCH_3)(CO)_2$	CS_2	H	4.69	—	Hexamethyldisiloxane as reference	185
				H'	2.55t	} J 9		
				H	1.52t			
				H''	2.02s			
$C_{10}H_{12}FeO_2S$	742	$(h^5-C_5H_5)Fe(CH_2SCH_2CH_3)(CO)_2$	CS_2	H	4.76s	—	—	195
				H'	2.27s	—		
				H''	2.39q	—		
				H'''	1.16t	—		
$C_{13}H_{20}FeO_2Si$	743	$(h^5-C_5H_5)Fe[(CH_2)_3Si(CH_3)_3](CO)_2$	$CDCl_3$	H	4.44s	—	—	983
				H'	1.43bs	—		
				H''	-0.08s	—		
$C_{11}H_{16}FeO_2Si$	744	$(h^5-C_5H_5)Fe[CH_2Si(CH_3)_3](CO)_2$	$CDCl_3$	H	4.67s	—	—	983
				H'	-0.36s	—		
				H''	0.00s	—		
$C_{15}H_{14}FeO_2$	745	$(h^5-C_5H_5)Fe(h^1-CH_2CH_2C_6H_5)(CO)_2$	CS_2	H	4.56	—	—	467
$C_{14}H_{12}FeO_2$	746	$(h^5-C_5H_5)Fe(h^1-CH_2C_6H_5)(CO)_2$	$CDCl_3$	H	4.69s	—	—	923
				H'	2.77s	—		
				H''	7.20b	—		
			SO_2	H'	2.69	—	T -18°	112
$C_{15}H_{14}FeO_2$	747	$(h^5-C_5H_5)Fe[h^1-CH'(CH_3)C_6H_5](CO)_2$	$CDCl_3$	H	4.37s	—	—	432
				H'	3.91q	J 7		
				H''	1.58d	J 7		
				H'''	7.02b	—		

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{14}H_{11}FFeO_2$	748	$(h^5-C_5H_5)Fe(h^1-3-CH_2C_6H_4F)(CO)_2$	CH_2Cl_2	F 1.35	—	Relative to C_6H_5F	191
$C_{14}H_7F_3FeO_2$	749	$(h^5-C_5H_5)Fe(h^1-CH_2C_6F_3)(CO)_2$	THF	F ₋₂ , F ₋₆ 144.2 F ₋₃ , F ₋₅ 162.9 F ₋₄ 159.0	$2J_{2,3}$ 21.4 $J_{2,4}$ 0 $J_{2,5}$ 8.1 $J_{3,5}$ 1.8 $J_{3,4}$ 19.9	T35	244 477
$C_{11}H_{20}B_{10}FeO_2$	750	$(h^5-C_5H_5)Fe[h^1-CH_2C_2B_{10}H_{10}(CH_3)](CO)_2$	CCl_4 $CHCl_3$	H 4.92 H', H'' 2.05 H 4.92 H', H'' 2.06	— — — —	—	350
$C_{13}H_{11}FeNO_2$	751	$(h^5-C_5H_5)Fe(h^1-2-CH_2C_5H_4N)(CO)_2$	CS_2	H 4.71s H' 2.55s H'' ₋₃ , H'' ₋₅ 6.90 H'' ₋₄ 7.32t H'' ₋₆ 8.28d	— — — J 8 J 4	$CH_2C_5H_4N =$ 	177
$C_{14}H_{19}FeNO_2$	752	$(h^5-C_5H_5)Fe(h^1-CH_2CH_2C_5H_{10}N)(CO)_2$	CS_2	H 4.62s	—	$CH_2CH_2C_5H_{10}N =$ 2-Piperidinoethyl Other signals at δ 2.27 comp., 1.56s, 1.43bs, in ratio 6:2:6	177

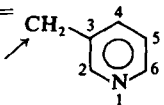
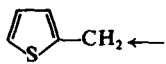
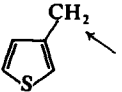
$[C_{13}H_{11}FeNO_2]^+$	753	$[(h^5-C_5H_5)Fe(h^1-3-CH_2C_5H_4N)(CO)_2]^+$	$CDCl_3$	H H' H''	4.62 2.57 9.0-7.0	— — —	Tetrafluoroborate $CH_2C_5H_4N =$	192
								
$C_{12}H_{10}FeO_2S$	754	$(h^5-C_5H_5)Fe(h^1-2-CH_2C_4H_3S)(CO)_2$	$CDCl_3$	H H' H''	~4.6 ~2.9 ~6.8	— — —	$CH_2C_4H_3S =$	184
								
$C_{12}H_{10}FeO_2S$	755	$(h^5-C_5H_5)Fe(h^1-3-CH_2C_4H_3S)(CO)_2$	$CDCl_3$	H H' H''	~4.0 ~2.85 ~6.8	— — —	$CH_2C_4H_3S =$	184
								
$C_{13}H_{10}FeO_2$	756	$(h^5-C_5H_5)Fe(h^1-C_6H_5)(CO)_2$	CCl_4	H	4.79	—	—	408
$C_{15}H_{14}FeO_3$	757	$(h^5-C_5H_5OCH_2CH_3)Fe(h^1-C_6H_5)(CO)_2$	$CDCl_3$	H H' H'' H'''	4.58t, 4.38t 3.40 1.02t 7.5, 6.95	— — — — —	—	413
$C_{13}H_9FFeO_2$	758	$(h^5-C_5H_5)Fe(1-h^1-3-C_6H_4F)(CO)_2$	CH_2Cl_2 —	F F	2.37 1.5	— —	— To high field of C_6H_5F	191 446
$C_{13}H_9FFeO_2$	759	$(h^5-C_5H_5)Fe(1-h^1-4-C_6H_4F)(CO)_2$	CH_2Cl_2	F F	10.92 10.23	— —	— To high field of C_6H_5F	191 446
$C_{13}H_7F_3FeO_2$	760	$(h^5-C_5H_5)Fe(1-h^1-2,3,6-C_6H_2F_3)(CO)_2$	THF	F_{-2} F_{-3} F_{-6}	103.6 144.4 85.6	— — —		925 244

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{13}H_7F_3FeO_2$	761	$(h^5-C_5H_5)Fe(1-h^1-2,3,5-C_6H_2F_3)(CO)_2$	THF	F_{-2}	112.1	$J_{2,3}$ 16.1 $J_{2,5}$ 28.7 J_{H-4F} 6.15 J_{H-6F} 2.4	T 35°	244
				F_{-3}	135.9	$J_{3,5}$ 1.67 J_{H-4F} 10.4 J_{H-6F} 1.75		
				F_{-5}	119.5	J_{H-4F} 8.15 J_{H-6F} 8.15		
$C_{13}H_7F_3FeO_2$	762	$(h^5-C_5H_5)Fe(1-h^1-2,4,5-C_6H_2F_3)(CO)_2$	THF	F_{-2}	84.0	$J_{2,4}$ 15.2 $J_{2,5}$ 3.33 J_{H-3F} 7.2 J_{H-4F} 4.35	T 38°	244
				F_{-4}	143.6	$J_{4,5}$ 20.4 J_{H-3F} 10.65 J_{H-6F} 9.65		
				F_{-5}	146.4	J_{H-3F} 6.55 J_{H-6F} 11.1		
$C_{13}H_6F_4FeO_2$	763	$(h^5-C_5H_5)Fe(1-h^1-2,3,5,6-C_6HF_4)(CO)_2$	$CDCl_3$	F_{-2}, F_{-6}	109.3	$J_{2,3}$ 29.0 $J_{2,5}$ 13.2 $J_{2,6}$ 3.45 J_{H-4F} 7.3	T 35°	244 925
				F_{-3}, F_{-5}	142.0	$J_{3,5}$ 1.2 J_{H-4F} 9.35		
$C_{13}H_5F_5FeO_2$	764	$(h^5-C_5H_5)Fe(1-h^1-C_6F_5)(CO)_2$	THF	F_{-2}, F_{-6}	106.7	$J_{2,3}$ 30.15 $J_{2,4} \sim 1$ $J_{2,6}$ 3.45	T 35°	244 459

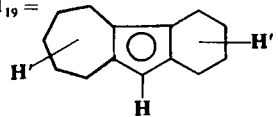
				F_{-3}, F_{-5}	164.3	$J_{2,5}$	8.8		
						$J_{3,5}$	5.7		
				F_{-4}	161.7	$J_{3,4}$	19.6		
$C_{22}H_{19}F_5FeO_2$	765	$(h^5-C_{14}H_{19})Fe(h^1-C_6F_5)(CO)_2$	CS_2	H	4.34s	—		$C_{14}H_{19} =$	
				H'	2.4–1.6	—			985
$C_{13}H_5BrF_4FeO_2$	766	$(h^5-C_5H_5)Fe(1-h^1-C_6BrF_4)(CO)_2$	THF	F_{-2}, F_{-6}	105.2*	$J_{2,3}$	32.3	*Calculated 108.4	478
						$J_{2,5}$	14.8	†Calculated 133.2	
						$J_{2,6}$	6.4		
				F_{-3}, F_{-5}	134.0†	$J_{3,5}$	6.4	(An AA'XX' system)	
$C_{14}H_8F_4FeO_2$	767	$(h^5-C_5H_5)Fe[1-h^1-4-C_6F_4-(CH_3)](CO)_2$	THF	F_{-2}, F_{-6}	109.3	$J_{2,3}$	28.65	(An AA'XX' system)	478
						$J_{2,5}$	11.9		244
						$J_{2,6}$	0		
				F_{-3}, F_{-5}	145.9	$J_{3,5}$	4.1		
$C_{14}H_5F_7FeO_2$	768	$(h^5-C_5H_5)Fe[1-h^1-4-C_6F_4(CF_3)](CO)_2$	THF	F_{-2}, F_{-6}	104.9	$J_{2,3}$	29.0	T 35°	244
						$J_{2,5}$	13.2		
						$J_{2,6}$	7.7		
						$J_{F,F'}$	0		
				F_{-3}, F_{-5}	144.2	$J_{3,5}$	1.8		
						$J_{F,F'}$	21.3		
$C_{16}H_{10}F_4FeO_2$	769	$(h^5-C_5H_5)Fe[1-h^1-4-C_6F_4-(CH_2^1CH''=CH_2''')](CO)_2$	THF	H	4.88s	—		—	478
				H'	3.34d	—			244
				H''	5.74bm	—			
				H'''	5.02d,	—			
					4.88s	—			
				F_{-2}, F_{-6}	108.8	$J_{2,3}$	29.0		
						$J_{2,5}$	13.5		
						$J_{2,6}$	1.6		
				F_{-3}, F_{-5}	146.9	$J_{3,5}$	4.2		

TABLE VII—cont.

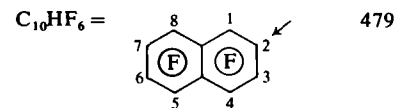
Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{15}H_6F_4FeO_2$	770	$(h^5-C_5H_5)Fe[1-h^1-4-C_6F_4-(CH=CH_2)](CO)_2$	THF	F_{-2}, F_{-6} 108.6	$J_{2,3}$ 27.35 $J_{2,5}$ 12.6 $J_{2,6}$ 3.25 $J_{3,5}$ 3.25		478 244
			—	F_{-3}, F_{-5} 145.6 F_{-2}, F_{-6} 110.4 F_{-3}, F_{-5} 148.0	— — —		233
			THF	H 6.25bs H' ~6.0b H'' 1.90d F_{-2}, F_{-6} 109.4	— — — $J_{2,3}$ 27.35 $J_{2,5}$ 11.8 $J_{2,6}$ 2.35 $J_{3,5}$ 4.3	— (An AA'XX' system)	478
			THF	F_{-2}, F_{-6} 105.1 F_{-3}, F_{-5} 139.4	$J_{2,3}$ 28.5 $J_{2,5}$ 12.8 $J_{2,6}$ 7.3 $J_{3,5}$ 1.55	T 35°	244 925
$C_{14}H_5F_4FeNO_2$	772	$(h^5-C_5H_5)Fe[1-h^1-4-C_6F_4(CN)](CO)_2$	THF	F_{-2}, F_{-6} 105.1 F_{-3}, F_{-5} 139.4	$J_{2,3}$ 28.5 $J_{2,5}$ 12.8 $J_{2,6}$ 7.3 $J_{3,5}$ 1.55	T 35°	244 925
$C_{15}H_5F_3FeN_2O_2$	773	$(h^5-C_5H_5)Fe[1-h^1-3,4-C_6F_3-(CN)_2](CO)_2$	THF	F_{-2} 69.8	$J_{2,5}$ 7.3 $J_{2,6}$ 11.5 $J_{5,6}$ 28.05	56.4 and 94.1 MHz	459 244 925
				F_{-5} 136.0 F_{-6} 86.8	— —		
			THF	F_{-2}, F_{-6} 63.7 F_{-3}, F_{-5} 28.6	— —		
$C_{14}H_6F_4FeO_4$	774	$(h^5-C_5H_5)Fe[1-h^1-4-C_6F_4-(CO_2H)](CO)_2$	CH_2Cl_2 and $CHCl_3$	F_{-2}, F_{-6} 63.7 F_{-3}, F_{-5} 28.6	— —	Relative to CF_3CO_2H	245

$C_{16}H_{10}F_4FeO_4$	775	$(h^5-C_5H_5)Fe[1-h^1-4-C_6F_4(CO_2-CH_2CH_3)](CO)_2$	THF	F_{-2}, F_{-6} 110.0 F_{-3}, F_{-5} 145.3 F_{-2}, F_{-6} 108.2	— — $J_{2,3}$ 29.7 $J_{2,5}$ 13.8 $J_{2,6}$ 5.4 $J_{3,5}$ 2.95	T 35°	925
				F_{-3}, F_{-5} 142.8			244
$C_{19}H_{15}F_3FeO_6$	776	$(h^5-C_5H_5)Fe[1-h^1-3,4-C_6F_3(CO_2-CH_2CH_3)_2](CO)_2$	THF	F_{-2} 83.3 F_{-5} 144.3 F_{-6} 97.3	$J_{2,5}$ 3.15 $J_{5,6}$ 27.65 $J_{2,6}$ 14.5	T 35°	244 925
$C_{14}H_9F_3FeO_3$	777	$(h^5-C_5H_5)Fe[1-h^1-3-C_6HF_3-(OCH_3)](CO)_2$	THF	F_{-2} 79.3 (83.5)* F_{-4} 160.5 (158.8) F_{-5} 142.7 (138.5)	— — —	(1-Monohapto-2,4,5-trifluoro-3-methoxyphenyl)(penta-haptocyclopentadienyl) iron dicarbonyl *Calculated values in parentheses	478
$C_{14}H_8F_4FeO_3$	778	$(h^5-C_5H_5)Fe[1-h^1-3-C_6F_4-(OCH_3)](CO)_2$	THF	F_{-2} 107.4 (111.2)* F_{-4} 165.5 (170.6) F_{-5} 156.3 (166.2) F_{-6} 99.7 (104.8)	— — — —	*Calculated values in parentheses	478
$C_{14}H_8F_4FeO_3$	779	$(h^5-C_5H_5)Fe[1-h^1-4-C_6F_4-(OCH_3)](CO)_2$	THF	F_{-2}, F_{-6} 108.3 (108.6)* F_{-3}, F_{-5} 158.15 (159.8)	$J_{2,3}$ 29.35 $J_{2,5}$ 9.55 $J_{2,6}$ 1.0 $J_{3,5}$ 5.9	*Calculated values in parentheses	478 244
$C_{14}H_8F_4FeO_2S$	780	$(h^5-C_5H_5)Fe[1-h^1-4-C_6F_4-(SCH_3)](CO)_2$	CHCl ₃	H 4.97 H' 2.79 F_{-2}, F_{-6} 109 F_{-3}, F_{-5} 157.7	— — $J_{2,3}$ 30.8 $J_{2,5}$ 12.65 $J_{2,6}$ 3.3 $J_{3,5}$ 4.2		247

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{19}H_{10}F_4^-FeO_2S$	781	$(h^4-C_5H_5)Fe[1-h^1-4-C_6F_4^-(SC_6H_5)](CO)_2$	$CHCl_3$	H	5.05	—	247
				H'	7.03	—	
				F_{-2}, F_{-6}	107.3	$J_{2,3}$ 31.2 $J_{2,5}$ 21.5 $J_{2,6}$ 3.8	
				F_{-3}, F_{-5}	138.4	$J_{3,5}$ 4.7	
$C_{19}H_6F_8FeO_2$	782	$(h^4-C_5H_5)Fe[1-h^1-4-C_6F_4^-(C_6HF_4)](CO)_2$	THF	F_{-2}, F_{-6}	106.6	—	54.6 and 94.1 MHz 479
				F_{-3}, F_{-5}	139.4	—	
				F'_{-2}, F'_{-6}	139.4	—	
				F'_{-3}, F'_{-5}	142.1	—	
$C_{19}H_5F_9FeO_2$	783	$(h^4-C_5H_5)Fe[1-h^1-4-C_6F_4^-(C_6F_5)](CO)_2$	THF	F_{-2}, F_{-6}	106.4	—	54.6 and 94.1 MHz 479
				F_{-3}, F_{-5}	139.2	—	
				F'_{-2}, F'_{-6}	139.2	—	
				F'_{-3}, F'_{-5}	162.9	—	
				F'_{-4}	153.9	—	
$C_{16}H_{12}FeO_2$	784	$(h^4-C_5H_5)Fe(1-h^1-C_9H_7)(CO)_2$	$CDCl_3$	H_{-1}	3.97	—	It was concluded that this complex is not fluxional as has been reported previously 1047
				H_{-2}	6.72	—	
				H_{-3}	6.53	—	
$C_{17}H_5F_7FeO_2$	785	$(h^4-C_5H_5)Fe(2-h^1-C_{10}F_7)(CO)_2$	THF	F_{-1}	83.4	—	$C_{10}F_7$ = Perfluoro- β -naphthyl Other signals at 146.5, 149.4, 152.8, and 160.9 479
				F_{-3}	99.4	—	

$C_{17}H_6F_6FeO_2$	786	$(h^5-C_5H_5)Fe(2-h^1-C_{10}HF_6)-(CO)_2$	THF	F_{-1} 83.2 F_{-3} 101.6	— —
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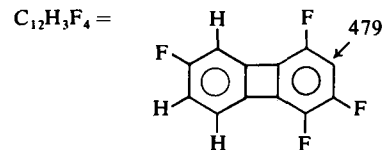


Other signals at 119.7, 123.5,
139.8 and 153.0

(Relative to CCl_3F)

Calculated values reported for
comparison

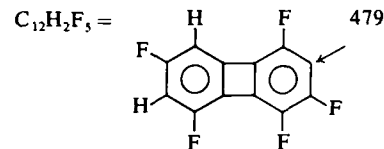
$C_{19}H_8F_4FeO_2$	787	$(h^5-C_5H_5)Fe(2-h^1-C_{12}H_3F_4)-(CO)_2$	THF	n.a.	—
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^{19}F NMR Signals at 88.8 (89)*,
93.1 (93), 95.6 (99), 144.2 (146)
relative to CCl_3F at 56.4 and
94.1 MHz

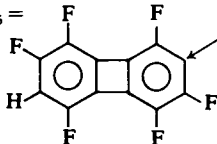
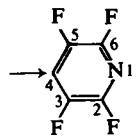
*Calculated values in parentheses

$C_{19}H_7F_5FeO_2$	788	$(h^5-C_5H_5)Fe(2-h^1-C_{12}H_2F_5)(CO)_2$	THF	n.a.	—
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^{19}F NMR Signals at 88.9, 94.3,
124.0, 145.4 relative to
 CCl_3F at 56.4 and 94.1 MHz

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{10}H_6F_6FeO_2$	789	$(h^5-C_5H_5)Fe(2-h^1-C_{12}HF_6)(CO)_2$	THF	n.a.	—	$C_{12}HF_6 =$  ^{19}F NMR signals at 90.1 (89),* 92.9 (93), 123.7 (122), 129.2 (126), 148.2 (146), 154.9 (146) at 56.4 and 94.1 MHz *Calculated values in parentheses	479
$C_{18}H_5F_8FeNO_2$	790	$(h^5-C_5H_5)Fe[1-h^1-4-C_6F_4(4-C_3F_4N)](CO)_2$	$CHCl_3$	F_{-2}, F_{-6} 106.3 F_{-3}, F_{-5} 141.0 F'_{-2}, F'_{-6} 90.6 F'_{-3}, F'_{-5} 139.6	$J_{2,3}$ 28.8 $J_{2,5}$ 12.6 $J_{2,6}$ 6.4 $J_{3,5}$ 2.6 $J_{2,3}$ 21.1 $J_{2,5}$ 29.5 $J_{2,6}$ 13.2 $J_{3,5}$ 2.2	$C_3F_4N =$ 	248
$C_{15}H_8F_5FeNO_2$	791	$(h^5-C_5H_5)Fe[h^1-C(C_6F_5)=NCH_3](CO)_2$	$CDCl_3$	H 5.00s H' 3.58s	— —	—	443
$C_{11}H_{10}FeO_3$	792	$(h^5-C_5H_5)Fe(CH=CH'COCH_3)(CO)_2$	—	H 8.77 H' 6.36	$J_{HH'}$ 16.4 —	—	1001
$C_{16}H_{12}FeO_3$	793	$(h^5-C_5H_5)Fe(CH=CH'COOC_6H_5)(CO)_2$	$CDCl_3$	H 9.21 H' 7.16	$J_{HH'}$ 16.3 —	Hexamethyldisiloxane as reference. 100 MHz	1001

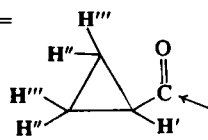
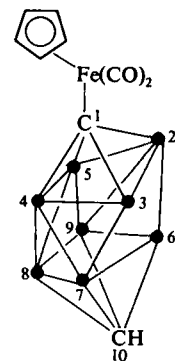
$C_9H_8FeO_3$	794	$(h^5-C_5H_5)Fe(C'OC''H_3)(C'''O)_2$	CS_2	H	4.87s	—	—	129
				H'	2.57s	—		132
				H	4.77	—	40 MHz	444
				H'	2.42	—		
			CF_3CO_2H	H	5.24	—	—	
				H'	3.20	—		
$C_9H_5F_3FeO_3$	795	$(h^5-C_5H_5)Fe(COCF_3)(CO)_2$	C_6H_6	^{13}C	106.3d*	$J(^{13}C-H) 175$	*To high field from CS_2 at 25.1 MHz	95
			$CHCl_3$	^{13}C	86.9	—	^{13}C resonances down field relative to TMS (0.0 ppm)	32
				$^{13}C'$	154.4	—		
				$^{13}C''$	52.0	—		
				$^{13}C'''$	215.7	—		
$C_{10}H_8FeO_3$	796	$(h^5-C_5H_5)(COCH'=CH_2')-Fe(CO)_2$	THF	F	80.1	—	56.4 and 94.1 MHz	459
			$CDCl_3$	H	4.87	—	Hexamethyldisiloxane as reference	223
				H'	6.59	—		
				H_{cis}''	4.89	$J_{cis} 10.0$		
				H_{trans}''	5.33	$J_{trans} 17.0$ $J_{gem} 1.5$		
$C_{16}H_{12}FeO_3$	797	$(h^5-C_5H_5)Fe(COCH'=CH''-C_6H_5''')(CO)_2$	$CDCl_3$	H	4.87	—	Hexamethyldisiloxane as reference	223
				H'	6.96d	$J_{trans} 16.0$		
			$CDCl_3$	H''	6.68d	—	—	432
				H'''	7.68–7.18	—		
				H	4.72s	—		
				H'	4.35q	—		
$C_{11}H_{10}FeO_3$	799	$(h^5-C_5H_5)Fe(h^1-COC_3H_5)(CO)_2$	$CDCl_3$	H''	1.32d	$J 7$	COC ₃ H ₅ =	929
				H'''	7.36s	—		
			CS_2	H	4.72s	—		
				H'	2.38tt	$J_{H'H''} 4.7$		
				H''	0.53m	—		
				H'''	0.86m	$J_{H'H'''} 7.5$		

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_9H_9FeNO_3$	800	$(\eta^5-C_5H_5)Fe(CONH'CH_3'')-(CO)_2$	$CDCl_3$	H 4.94	—	—	418
				H'' 2.88d	—		
			$(CD_3)_2SO$	H' 6.80	—		
$C_9H_8FeO_4$	801	$(\eta^5-C_5H_5)Fe(CO_2CH_3)(CO)_2$	CS_2	H 4.86s	—	—	129
				H' 3.39s	—		
			CS_2	H 4.88	—	—	132
				H' 3.50	—		
$C_9H_8FeO_3$	802	$(\eta^5-C_5H_5)Fe[C(S)OCH_3](CO)_2$	CS_2	H 4.84	—	—	481
				H' 4.03	—		
$C_{12}H_{20}B_{10}FeO_3$	803	$(\eta^5-C_5H_5)Fe[COCH_2C_2B_{10}H_{10}(CH_3)](CO)_2$	$CHCl_3$	H 4.93	—	A 2-methyl-carborane derivative	350
				H' 3.61	—		
				H 1.99	—		
			C_6H_6	H 4.07	—		
				H' 3.29	—		
				H'' 1.42	—		
$C_{10}H_{16}B_{10}FeO_3$	804	$(\eta^5-C_5H_5)Fe(COC_2B_{10}H_{11})(CO)_2$	CCl_4	H 4.96	—	An <i>o</i> -carborane derivative 60 and 100 MHz	350
$C_{10}H_{16}B_{10}FeO_3$	805	$(\eta^5-C_5H_5)Fe(COC_2B_{10}H_{11})(CO)_2$	—	H 4.02	—	An <i>m</i> -carborane derivative	350
$C_9H_{14}B_8FeO_2$	806	$(\eta^5-C_5H_5)Fe(1-\eta^1-1,10-B_8C_2H_9)(CO)_2$	—	H 5.24s	—	*Relative to $BF_3 \cdot O(C_2H_5)_2$ at 32.1 MHz	482

H'_{-10} 6.83bs —
 $^{11}B^*$ 10.8d, J 164
 12.8d J 158

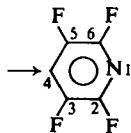
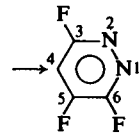
Structure:



● = BH

$C_{10}H_{16}B_8FeO_2$	807	$(h^5-C_5H_5)Fe(1-h^1-10-CH'_3-1,10-B_8C_2H_8)(CO)_2$	—	H	5.06s	—	Structure: see above	482
				H'	2.77s	—	*Relative to $BF_3 \cdot O(C_2H_5)_2$	
				$^{11}B^*$	11.1d	J 159	at 32.1 MHz	
$C_9H_{16}B_{10}FeO_2$	808	$(h^5-C_5H_5)Fe(1-h^1-1,2-B_{10}C_2H_{11})(CO)_2$	C_6H_6	H	3.81	—	A <i>m</i> -carborane derivative	350
$C_{10}H_{18}B_{10}FeO_2$	809	$(h^5-C_5H_5)Fe(1-h^1-2-CH'_3-1,2-B_{10}C_2H_{10})(CO)_2$	—	H	4.93s	—		482
				H'	1.98s	—		
				$^{11}B^*$	3.1d,	J 165	*Relative to $BF_3 \cdot O(C_2H_5)_2$ at	483
					10.1d	J 157	32.1 MHz	
					14.9d	J 154		
$C_{15}H_{20}B_{10}FeO_2$	810	$(h^5-C_5H_5)Fe(1-h^1-2-C_6H'_5-1,2-B_{10}C_2H_{10})(CO)_2$	—	H	4.65s	—	A <i>m</i> -carborane derivative	482
				H'	7.42m	—		
				$^{11}B^*$	3.8d,	J 160	*Relative to $BF_3 \cdot O(C_2H_5)_2$ at	
					10.6d,	J 157	32.1 MHz	
					15.2d	J 155		

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{12}H_5F_4FeNO_2$	811	$(h^5-C_5H_5)Fe(4-h^1-C_5F_4N)(CO)_2$	THF and $CHCl_3$	F_{-2}, F_{-6} 104.0	$J_{2,3}$ 29.6	$C_5F_4N =$ 	459
				F_{-3}, F_{-5} 114.2	$J_{2,6}$ 13.6 $J_{2,5}$ 26.8 $J_{3,5}$ 0.5	56.4 and 94.1 MHz	197
$C_{18}H_{10}F_3FeNO_2$	812	$(h^5-C_5H_5)Fe[2-h^1-4-C_5F_3N-(C_6H_5)](CO)_2$	$CHCl_3$	F_{-3} 104.4	$J_{3,5}$ 2.0	Numbering as above	248
				F_{-5} 154.9	$J_{5,6}$ 28.6		
				F_{-6} 90.2	$J_{3,6}$ 29.8		
$C_{12}H_7F_3FeN_2O_2$	813	$(h^5-C_5H_5)Fe[2-h^1-4-C_5F_3N-(NH_2)](CO)_2$	$CHCl_3$	F_{-3} 188.8	$J_{3,5}$ 7.8	Numbering as above	248
				F_{-5} 172.2	$J_{5,6}$ 28.0		
				F_{-6} 91.7	$J_{3,6}$ 26.7		
$C_{11}H_5F_3FeN_2O_2$	814	$(h^5-C_5H_5)Fe(4-h^1-C_4F_3N_2)(CO)_2$	$CHCl_3$	F_{-3} 55.9	$J_{3,5}$ 19.7	$C_4F_3N_2 =$ 	197
				F_{-5} 98.6	$J_{5,6}$ 32.0		
				F_{-6} 109.2	$J_{3,6}$ 32.0		
$C_{10}H_3F_2FeN_3O_2$	815	$(h^5-C_5H_5)Fe(2-h^1-C_3F_2N_3)(CO)_2$	$CHCl_3$	F_{-4}, F_{-5} 42.9	—	$C_3F_2N_3 =$ 4,6-Difluoro-1,3,5-triazinyl	197

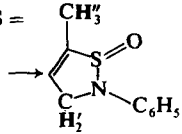
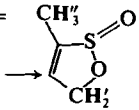
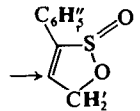
$C_{11}H_2Cl_3FeO_2S$	816	$(h^5-C_5H_5)Fe(2-h^1-C_4Cl_3S)-(CO)_2$	$CDCl_3$	H	5.02	—	$C_4Cl_3S = 3,4,5$ -Tri-chlorothieryl	484
$C_{17}H_{15}FeNO_3S$	817	$(h^5-C_5H_5)Fe(h^1-C_{10}H_{10}NOS)-(CO)_2$	$CDCl_3$	H	5.08	—	$C_{10}H_{10}NOS =$	485
				H'	4.48,	—		
				H''	4.82	—		
					2.36	—		
$C_{11}H_{10}FeO_4S$	818	$(h^5-C_5H_5)Fe(h^1-C_4H_5O_2S)-(CO)_2$	$CDCl_3$	H	5.20s	—	$C_4H_5O_2S =$	163
				H'	5.19,	$J_{H'H'} 14$		156
				H''	5.55	$J_{H'H''} 2$		485
					2.40t			
$C_{16}H_{12}FeO_4S$	819	$(h^5-C_5H_5)Fe(h^1-C_9H_7O_2S)(CO)_2$	$CDCl_2$	H	4.75s	—	$C_9H_7O_2S =$	163
				H'	5.18,	$J_{H'H'} 15$		
				H''	5.55			
					7.42s	—		
(c) <i>Dihapto/tetrahapto</i>								
(i) Dicarbonyl derivatives:								
$C_{12}H_{12}FeO_6$	820	$[h^2-CH(CO_2CH_3)=CH(CO_2-CH_3)]Fe(h^4-C_4H_4)(CO)_2$ <i>cis</i>	—	H	3.37s	—	$C_4H_4 =$ Cyclobutadiene	486
				H'	3.47s	—		
				H''	3.35s	—		
$C_{12}H_{12}FeO_6$	821	$[h^2-CH(CO_2CH_3)=CH(CO_2-CH_3)]Fe(h^4-C_4H_4)(CO)_2$ <i>trans</i>	—	H	4.22s	—	$C_4H_4 =$ Cyclobutadiene	486
				H'	3.4s	—		
				H''	4.46s	—		
$C_{13}H_{12}F_6FeO_3$	822	$[h^2-(CF_3)_2C=O]Fe[h^4-C_4(CH_3)_4](CO)_2$	—	H	1.6, 1.2	—	$C_4(CH_3)_4 =$ Tetramethyl cyclobutadiene	300
				F	80.0m,	—		
					82.8m	—		

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
<i>(d) Dihapto/pentahapto</i>								
<i>(i) Monocarbonyl derivatives:</i>								
$C_{26}H_{24}FeOSn$	823	$(\eta^5-C_5H_5)Fe(\eta^2-CH_2=CH_2)-[Sn(C_6H_5)_3](CO)$	CS_2	H	4.51s	—	—	408
				H'	2.44, 2.30,	—		
					1.80, 1.65	—		
				H''	7.63–7.06	—		
$C_{10}H_{13}BFeN_2O$	824	$(\eta^5-C_5H_5)(Fe \begin{array}{c} CH^1-N-CH_3^3 \\ \quad \$						

$[\text{C}_{11}\text{H}_{11}\text{FeO}_2]^+$	827	$[(h^5\text{-C}_5\text{H}_5)\text{Fe}(h^2\text{-CH}_2=\text{C}=\text{CH}''\text{CH}_3''')(\text{CO})_2]^+$	SO_2	H H' H'' H'''	5.8s 3.07 7.05 2.45 sext.	— $J_{\text{H}'\text{H}''}$ 4 $J_{\text{H}''\text{H}'''}$ 7 $J_{\text{H}'\text{H}'''}$ 3	Perchlorate T -10°	488
$[\text{C}_{16}\text{H}_{13}\text{FeO}_2]^+$	828	$[(h^5\text{-C}_5\text{H}_5)\text{Fe}(h^2\text{-CH}_2=\text{C}=\text{CH}''\text{C}_6\text{H}_5)(\text{CO})_2]^+$	SO_2	H H' H''	5.8s 3.65d 7.3t	— $J_{\text{H}'\text{H}''}$ 4 —	Perchlorate T -10°	488
$[\text{C}_{11}\text{H}_{11}\text{FeO}_2]^+$	829	$[(h^5\text{-C}_5\text{H}_5)\text{Fe}(h^2\text{-CH}_2=\text{CH}'-\text{CH}'=\text{CH}_2)(\text{CO})_2]^+$	—	H H'	5.85s 5.8 comp., 4.0 comp.*	— — — (ratio 4:2)	Hexafluorophosphate *At 100 MHz resolved into two doublets, J 13.7, 7.5	451
(e) Trihapto/pentahapto								
(i) Monocarbonyl derivatives								
$\text{C}_{10}\text{H}_{12}\text{FeO}$	830	$(h^5\text{-C}_5\text{H}_5)\text{Fe}(h^3\text{-CH}_2'''\text{CH}''''\text{CH}'''''\text{CH}_3^{\text{IV}})(\text{CO})$ <i>cis</i> *	CDCl_3	H H' _{syn} H' _{anti} H'' H''', H ^{IV}	4.47 2.62 0.37 4.2 1.65	— $J_{\text{H}'\text{H}''}$ 6.8 $J_{\text{H}'\text{H}'''}$ <0.5 $J_{\text{H}'\text{H}''}$ 11 $J_{\text{H}'\text{H}'}$ 1.8 — —	*H''' <i>anti</i> to H''	450
$\text{C}_{10}\text{H}_{12}\text{FeO}$	831	$(h^5\text{-C}_5\text{H}_5)\text{Fe}(h^3\text{-CH}_2'''\text{CH}''''\text{CH}'''''\text{CH}_3^{\text{IV}})(\text{CO})$ <i>trans</i> *	CDCl_3	H H' _{syn} H' _{anti} H'' H''' H ^{IV}	4.51s 3 1.05 4.2 4.10 0.75	— $J_{\text{H}'\text{H}''}$ 6.8 $J_{\text{H}'\text{H}'''}$ 1.2 $J_{\text{H}'\text{H}''}$ 10.8 $J_{\text{H}'\text{H}'}$ 1.8 — — $J_{\text{H}'''\text{H}^{\text{IV}}}$ 6.3	*H''' <i>syn</i> to H''	450

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{13}H_{12}FeO$	832	$(h^5-C_5H_5)Fe(1,2,7-h^3-C_7H_7)(CO)$	$CDCl_3$	H_{-1}	3.08	—	C_7H_7 = Cyclohepta-1,3,5-trienyl	490
				H_{-2}, H_{-7}	4.75	—		
				H_{-3}, H_{-6}	6.10	—		
				H_{-4}, H_{-5}	5.15	—		
$C_{12}H_{16}FeO$	833	$(h^5-C_5H_5)Fe[1,2,4-h^3-CH_2-C(CH_3)_2-CH=CH_2](CO)$	C_6D_6	H	4.2s	—	—	451
				H'	0.5s	—		
				H_{-1}	2.2 comp.	$J_{cis} 7.5$		
				H_{-2}	2.9 comp.	$J_{trans} 11.3$		
				H_{-4}	2.3d	$J_{gem} 5.3$		
					-0.7d	$J_{gem} 5.3$		
$C_{13}H_{16}FeO_2$	834	$(h^5-C_5H_5)Fe[1,4,5-h^3-COCH_2C(CH_3)_2CH=CH_2](CO)$	C_6D_6	H	4.0s	—		451
				H'	1.0s	—		
				H_{-2}	2.35d	$J_{gem} 14.3$		
					1.8d	$J_{gem} 14.3$		
				H_{-4}	4.2 comp.	—		
				H_{-5}	2.6d	$J_{cis} 9.0$		
					1.9d	$J_{trans} 12.8$		
$C_{12}H_{12}FeO_2$	835	$(h^5-C_5H_5)Fe(1,5,6-h^3-COCH_2CH_2CH=CH_2)(CO)$	$CDCl_3$	H_{-4}	3.31	—	—	174
				H_{-6}	3.22,	—		
					0.82	—		
$C_{13}H_{14}FeO_2$	836	$(h^5-C_5H_5)Fe[1,5,6-h^3-COCH_2CH_2C(CH_3)=CH_2](CO)$	$CDCl_3$	H'	1.21	—	—	174
				H_{-6}	3.38	—		
					0.90	—		

$C_{13}H_{14}FeO_2$	837	$(h^5-C_5H_5)Fe(1,5,6-h^3-$ $COCH_2CH_2CH=C=CHCH_3)-$ $\begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{matrix}$ (CO)	$CDCl_3$	H_{-4} H_{-6} H_{-7}	3.52 4.31 0.85	— — —	—	174	
$C_{10}H_{12}FeO_2$	838	$(h^5-C_5H_5)Fe(1,2,5-h^3-$ $CH_2OCH_2CH=CH_2)(CO)$ $\begin{matrix} 5 & 4 & 3 & 2 & 1 \end{matrix}$	CS_2	H H_{-1} H_{-2} H_{-3} H_{-5}	4.39s 3.15 comp., $J_{cis} 8$ 1.75d $J_{trans} 14$ 4.87 comp. 3.47 comp., 2.95d 6.17d, $J_{gem} 4$ 4.5 $J_{gem} 4$	— — — — —	—	195	
$C_{12}H_{16}FeO_2$	839	$(h^5-C_5H_5)Fe[1,2,5-h^3-$ $CH_2OC(CH_3)_2CH=CH_2](CO)$ $\begin{matrix} 5 & 4 & 3 & 2 & 1 \end{matrix}$	CS_2	H H' H_{-1} H_{-2} H_{-5}	4.36 1.46, 0.91 2.72, $J_{cis} 8$ 1.8–2.0 $J_{trans} 12$ 4.68q 6.22d, } 4.05d } $J_{gem} 5$	— — — — —	—	195	
(f) Tetrahapto/tetrahapto									
$C_{13}H_{14}FeO$	840	$(h^4-CH_2=CH-CH=CH_2)-$ $Fe(h^4-C_8H_8)(CO)$	C_6D_6	n.a.	—	—	$C_8H_8 =$ Cyclo-octatetraene Signals at δ 4.55, 4.3, 1.7, —0.1, in ratio 4 : 1 : 1 : 1	294	
(g) Monohapto/monohapto/pentahapto									
$C_{14}H_8F_3FeNO$	841	$(h^5-C_5H_5)Fe(h^1-C_6F_5)-$ ($CNCH_3$)(CO)	$CDCl_3$	H H'	4.65s 3.35s	— —	An isocyanide complex	443	

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{16}H_{11}F_5^-$ FeN_2O	842	$(\eta^5-C_5H_5)Fe(CNCH_3)(C(C_6F_5)=NCH_3)(CO)$	$CDCl_3$	H	4.70s	—	Isocyanide complexes, existing in two geometrical forms isomeric about the C=N bond	443
				H'	3.28s	—		
				H''	3.55s	—		
				H	4.64s	—		
				H'	3.34s	—		
				H''	3.05s	—		
$[C_{22}H_{19}^-$ $FeN_2O]^+$	843	$[(\eta^5-C_5H_5)Fe(C'NC''H_2C_6'''-H_5)_2(C^{IV}O)]^+$	$CHCl_3$	^{13}C	85.3	—	An isocyanide complex	32
				$^{13}C'$	147.4	—		
				$^{13}C''$	51.4	—		
				$^{13}C'''_{-1}$	132.5	—		
				$^{13}C'''_{-2,6}$	128.0	—		
				$^{13}C'''_{-3,5}$	129.5	—		
				$^{13}C'''_{-4}$	129.0	—		
				$^{13}C^{IV}$	212.1	—		
<i>(h) Monohapto/dihapto/pentahapto</i>								
$C_{31}H_{23}FeN_4OP$	844	$(\eta^5-C_5H_5)Fe(COCH_3)[\eta^2-C(CN)_2=C(CN)_2][P(C_6H_5)_3]$	—	H	5.17d	—	—	194
				H'	2.82s	—		
<i>(8) MISCELLANEOUS COMPLEXES</i>								
$[C_{11}H_{25}^-$ $FeOP_2]^-$	845	$\{Fe[P(Et)_2CH_2CH_2P(Et)_2]-(H)(CO)\}^-$	$(CD_3)_2CO$	H	-10.9	$J_{PH_{cis}}$ 47	Tetraphenylborate 100 MHz	491
$C_{14}H_{30}FeO_4^-$ P_2S	846	$Fe[P(CH_2CH_3)_3]_2(SO_2)(CO)_2$	C_6F_6	H	2.07m	J_{PH} 6.5	100 MHz	264
				H'	1.28m			

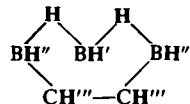
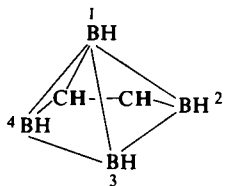
$C_{29}H_{22}^-$ FeO_3P_2	847	$Fe[P(C_6H_5)_2CH=CHP(C_6H_5)_2](CO)_3$	$(CH_3)_2CO$	H	7.54	—	60 and 100 MHz	202
$C_8H_{15}^-$ $BFeN_2O_3$	848	$Fe[N(CH_3)_2B(CH_3)N(CH_3)_2]-(CO)_3$	C_6H_6	^{11}B	-20.0	—	Relative to $BF_3 \cdot OEt_2$ external	273
$C_5H_7B_3FeO_3$	849	$Fe(C_2H_7B_3)(CO)_3$	CCl_4	H H'	+3.7b -7.42q	— J 126	$C_2H_7B_3 =$ 	492
				H'' H'''	-3.70q -5.38s	J 135 —	100 MHz	
				^{11}B	-4.90d	J 135	Relative to $BF_3 \cdot OEt_2$ at 32.2 MHz	
$C_5H_6B_4FeO_3$	850	$Fe(C_2H_6B_4)(CO)_3$	CCl_4	H	-5.58	—	$C_2H_6B_4 =$ 	492
				H_{-1} H_{-2}, H_{-4} H_{-3} $^{11}B_{-1}$ $^{11}B_{-2},$ $^{11}B_{-4}$ $^{11}B_{-3}$	-0.24 6.30 -4.87 +17.7bd -5.16bd -18.9bd	J 160 J 152 J 152 J 160 J 150 J 160	100 MHz Relative to $BF_3 \cdot OEt_2$ at 32.2 MHz	
C_4HFeCl_3Si	851	$Fe(SiCl_3)(H)(CO)_4$	CH_3CN	H	-9.00	—	60 and 100 MHz	402 401

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)		Remarks	References
(9) COMPLEXES CONTAINING TWO OR MORE TRANSITION METALS								
(a) Diiron complexes								
(i) Dicarbonyl derivatives:								
$C_{16}H_{10}As_2F_{12}Fe_2O_2$	852	$\{(h^5-C_5H_5)Fe[As(CF_3)_2](CO)\}_2$	CCl_3F	H	4.57	—	100 MHz	414
$C_{37}H_{32}As_2Fe_2O_2$	853	$[(h^5-C_5H_5)Fe(CO)]_2- [As(C_6H_5)_2CH_2As(C_6H_5)_2]$	$CDCl_3$	H	4.33	—	Bridging carbonyl and bis(diphenylarsino)methane ligands T 38°	493
				H'	7.33b	—		
				H''	1.27b	—		
$C_{18}H_{26}Fe_2I_2O_2P_2$	854	$[(h^5-C_5H_5)Fe(I)(CO)]_2- [P(CH_3)_2CH_2CH_2P(CH_3)_2]$	$CDCl_3$	H	4.66s	—	—	103
$C_{38}H_{32}Fe_2O_2P_2$	855	$[(h^5-C_5H_5)Fe(CO)]_2P(C_6H_5)_2- CH''=CH''P(C_6H_5)_2$	$CDCl_3$	H	4.22	—	Bridging carbonyl and bis(diphenylphosphino)ethylene ligands T 38°	493
				H'	7.47b,	—		
				H''	7.36bd 6.49 sext.	—		
$C_{38}H_{30}Br_2Fe_2O_2P_2$	856	$[(h^5-C_5H_5)Fe(Br)(CO)]_2- [P(C_6H_5)_2C\equiv CP(C_6H_5)_2]$	$CDCl_3$	H	4.52d	J_{PH} 1.9	60 and 100 MHz	494
$C_{38}H_{30}Cl_2Fe_2O_2P_2$	857	$[(h^5-C_5H_5)Fe(Cl)(CO)]_2- [P(C_6H_5)_2C\equiv CP(C_6H_5)_2]$	$CDCl_3$	H	4.53d	J_{PH} 1.9	60 and 100 MHz	494
$C_{38}H_{30}Fe_2I_2O_2P_2$	858	$[(h^5-C_5H_5)Fe(I)(CO)]_2- [P(C_6H_5)_2C\equiv CP(C_6H_5)_2]$	$CDCl_3$	H	4.52d	J_{PH} 1.9	60 and 100 MHz	494

$C_{36}H_{30}Fe_2-O_2P_2$	859	$[(h^5-C_5H_5)Fe(CO)]_2[P(C_6H_5)_2]_2$	CS_2	H	3.99*, 3.87†	—	Bridging $P(C_6H_5)_2$ ligands 100 MHz * <i>cis</i> -isomer † <i>trans</i> -isomer	414
$C_{37}H_{32}Fe_2O_2P_2$	860	$[(h^5-C_5H_5)Fe(CO)]_2-$ $[P(C_6H_5)_2CH_2''P(C_6H_5)_2]$	$CDCl_3$	H H' H''	4.27 7.26b 1.73b	— — —	Bridging carbonyl and bis(diphenyl- phosphino)methane ligands T 38°	495 493
$C_{39}H_{36}Fe_2-O_2P_2$	861	$\{[h^5-C_5H_4(CH_3)]Fe(CO)\}_2-$ $[P(C_6H_5)_2CH_2''P(C_6H_5)_2]$	$CDCl_3$	H H' H'' H'''	4.22, 4.15b, 3.91b 2.42, 2.08 7.34b, 7.22b 1.29b	— — — — — — —	Bridging carbonyl and bis(diphenylphosphino)methane ligands. Mixture of isomers T 38°	493
$C_{46}H_{43}Fe_2-O_2P_3$	862	$[(h^5-C_5H_5)Fe(CO)]_2[P(C_6H_5)_2-$ $CH_2''CH_2''P(C_6H_5)_2CH_2'-$ $CH_2''P(C_6H_5)_2]$	$CDCl_3$	H H' H''	4.13s ~7.3 ~2	— — —	Bridging carbonyl and phosphine ligands 100 MHz	5
$C_{38}H_{34}Fe_2-O_2P_2$	863	$[(h^5-C_5H_5)Fe(CO)]_2[P(C_6H_5)_2-$ $CH_2''CH_2''P(C_6H_5)_2]$	$CDCl_3$	H H' H''	4.08 7.65b, 7.43bd 1.37b 0.88b	— — — — —	Bridging carbonyl and bis(diphenylphosphino) ethane ligands T 38°	493
$C_{40}H_{38}Fe_2-O_2P_2$	864	$\{[h^5-C_5H_4(CH_3)]Fe(CO)\}_2-$ $[P(C_6H_5)_2CH_2''CH_2'''P(C_6H_5)_2]$	$CDCl_3$	H H' H'' H'''	4.15, 3.53 2.06, 1.50 7.67b, 7.43bd 1.29b	— — — — — — —	Bridging carbonyl and bis(diphenylphosphino) ethane ligands T 38°	493

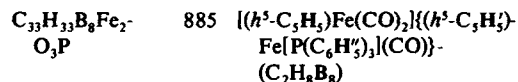
TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{39}H_{36}Fe_2O_2P_2$	865	$[(\eta^5-C_5H_5)Fe(CO)]_2[P(C_6H_5)_2-CH_2^*CH_2^*CH_2^*P(C_6H_5)_2]$	$CDCl_3$	H	4.08	—	Bridging carbonyl and phosphine ligands T 38°	493
				H'	7.67b,	—		
					7.38	—		
				H''	1.38b,	—		
					0.88b	—		
$C_{38}H_{35}Fe_2NO_2P_2$	866	$[(\eta^5-C_5H_5)Fe(CO)]_2[P(C_6H_5)_2-N(CH_2^*CH_2^*)P(C_6H_5)_2]$	$CDCl_3$	H	4.09	—	Bridging carbonyl and phosphine ligands T 38°	493
				H'	7.48b	—		
				H''	2.53m	—		
				H'''	-0.05t	—		
$C_{40}H_{39}Fe_2NO_2P_2$	867	$\{[\eta^5-C_5H_4(CH_3)]Fe(CO)\}_2[P(C_6H_5)_2N(CH_2^*CH_2^*)P(C_6H_5)_2]$	$CDCl_3$	H	4.13,	—	Bridging carbonyl and phosphine ligands T 38°	493
					4.04b,	—		
					3.73b	—		
				H'	1.88,	—		
					1.77,	—		
					1.67	—		
				H''	7.58b,	—		
					7.47b	—		
				H'''	2.49bm	—		
				H ^{IV}	-0.21t	—		
$C_{24}H_{20}Fe_2O_2Se_2$	868	$\{(\eta^5-C_5H_5)Fe[Se(C_6H_5)](CO)\}_2$	CS_2	H	5.54	—	Bridging $Se(C_6H_5)$ ligands Two isomers	426
				H	5.98	—		
$C_{14}H_{16}Fe_2O_2S_2$	869	$\{(\eta^5-C_5H_5)Fe[S(CH_3)](CO)\}_2$	CS_2	H	4.26*	—	Bridging $S(CH_3)$ ligands *Stable isomer	425

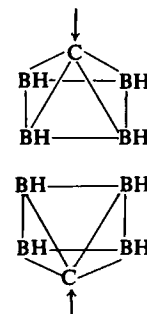
				H'	4.22†	—	†Unstable isomer	
				H'	1.31*,	—	T 32.5° 40 MHz	
					1.58†	—		
		CS ₂	H		4.32	—	—	188
			H'		1.38	—		
C ₁₆ H ₂₀ Fe ₂ - O ₂ S ₂	870	{(h ⁵ -C ₅ H ₅)Fe[S(CH ₂ CH ₃)]-(CO)} ₂	CS ₂	H	4.25*,	—	Bridging S(CH ₂ CH ₃)	425
					4.20†	—	ligands	
				H'	1.69q*,	J 7.2	*Stable isomer	
					1.89q†	J 7.2	†Unstable isomer	
				H''	0.72t*,	—	T 32.5° 40 MHz	
					0.98†	—		
C ₂₀ H ₂₈ Fe ₂ - O ₂ S ₂	871	{(h ⁵ -C ₅ H ₅)Fe[SC(CH ₃) ₃](CO)} ₂	—	H	4.39	—	—	188
				H'	1.03	—		
C ₂₄ H ₂₀ Fe ₂ - O ₂ S ₂	872	{(h ⁵ -C ₅ H ₅)Fe[S(C ₆ H ₅)](CO)} ₂	CS ₂	H	4.49	—	100 MHz	414
				H	4.03	—	Two isomers	425
				H'	7.04	—		426
C ₂₄ H ₂₀ Fe ₂ - O ₂ Te ₂	873	{(h ⁵ -C ₅ H ₅)Fe[Te(C ₆ H ₅)](CO)} ₂	CS ₂	H	5.52	—	Two isomers	426
				H	5.89	—		
(ii) Tricarbonyl derivatives								
C ₂₅ H ₂₀ Fe ₂ - GeO ₃	874	[(h ⁵ -C ₅ H ₅)Fe(CO)] ₂ [Ge(C ₆ H ₅)-(CO)]	CCl ₄	H	4.69	—	cis- and trans- isomers	497
				H	4.53	—	One bridging carbonyl and Ge(C ₆ H ₅) ₂ ligands	
C ₁₉ H ₂₃ Fe ₂ O ₃ P	875	(h ⁵ -C ₅ H ₅) ₂ Fe ₂ [P(CH ₂ CH ₃) ₃]- (CO) ₃	CDCl ₃	H	4.71,	—	T 38°	424
					4.45	—		
C ₂₂ H ₃₁ Fe ₂ O ₃ P	876	(h ⁵ -C ₅ H ₅) ₂ Fe ₂ [P(n-C ₃ H ₇) ₃]- (CO) ₃	CDCl ₃	H	4.57,	—	T 38°	399
					4.29	—		424

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{25}H_{37}Fe_2O_3P$	877	$(h^5-C_5H_5)_2Fe_2[P(n-C_4H_9)_3]-(CO)_3$	$CDCl_3$	H 4.74, 4.47	— —	T 38°	424
$C_{27}H_{25}Fe_2O_3P$	878	$(h^5-C_5H_5)_2Fe_2[P(C_6H_5)_2CH_2-CH_3](CO)_3$	$CDCl_3$	H 4.66, 4.18	$J_{PH} 1.2$	T 38°	424
$C_{16}H_{19}Fe_2O_6P$	879	$(h^5-C_5H_5)_2Fe_2[P(OCH_3)_3]-(CO)_3$	$CDCl_3$	H 4.70, 4.57	— —	T 38°	424 399
$C_{19}H_{25}Fe_2O_6P$	880	$(h^5-C_5H_5)_2Fe_2[P(OCH_2CH_3)_3]-(CO)_3$	$CDCl_3$	H 4.69, 4.54	— —	T 38°	424
$C_{22}H_{31}Fe_2O_6P$	881	$(h^5-C_5H_5)_2Fe_2[P(OCH(CH_3)_2)_3]-(CO)_3$	$CDCl_3$	H 4.72, 4.51	— —	T 38°	424
$C_{25}H_{37}Fe_2O_6P$	882	$(h^5-C_5H_5)_2Fe_2[P(O-n-C_4H_9)_3]-(CO)_3$	$CDCl_3$	H 4.67, 4.52	— —	T 38°	424
$C_{31}H_{25}Fe_2O_6P$	883	$(h^5-C_5H_5)_2Fe_2[P(OC_6H_5)_3]-(CO)_3$	$CDCl_3$	H 4.79, 4.10	— —	T 38°	424 399
$C_{31}H_{25}Cl_2Fe_2O_6PSn$	884	$[(h^5-C_5H_5)Fe(SnCl_2)(CO)_2]-(h^5-C_5H_5)[P(OC_6H_5)_3](CO)_3$	$CDCl_3$	H 4.97, 4.30	— $J_{PH} 1.3$		399



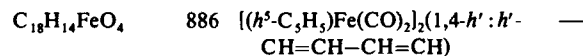
H	4.98s	—
H'	4.45d	$J_{PH} 1.4$
H''	7.8-7.4m	—



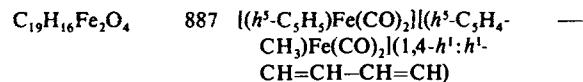
482

 ^{11}B +10.5 J 153Relative to $BF_3 \cdot OEt_2$ at 32.1 MHz

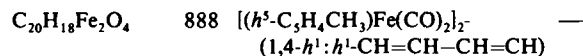
(iii) Tetracarbonyl derivatives:



Not reported



Not reported



Not reported

Fine structure and splitting ($J_{HH}10$) of the ^{13}C satellites were consistent with a fluxional process consisting of 1,3- rather than 1,2-shifts:

499

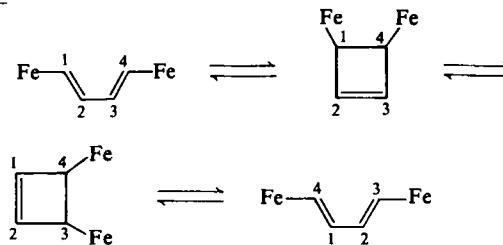


TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{24}H_{36}Fe_2O_4$	889	$\{[h^2-(CH_3)_3CC \equiv CC(CH_3)_3]-Fe(CO)_2\}_2$	CS_2	H 1.35s	—	Bonding interaction proposed between each triple bond with both iron atoms	500
$C_{13}H_{14}Fe_2O_4S_2$	890	$[(h^4-C_7H_8)Fe(CO)]-[Fe(CO)_3][S(CH_3)]_2$	C_6H_6	n.a.	—	C_7H_8 = Norbornadiene Signals at δ 3.20, 2.86b, 1.11s, 0.74s, 0.60s in ratio 4:2:3:2:3	501
			C_6F_6	n.a.	—	Signals at δ 3.70 comp., 3.42 comp., 1.27s, 1.18s, 1.11s in ratio 4:2:2:3:3	
			CS_2	n.a.	—	Signals at δ 3.61t, 3.27d, 1.20s, 1.02s, in ratio 4:2:5:3	
$C_{14}H_{10}Fe_2O_4$	891	$[(h^5-C_5H_5)Fe(CO)_2]_2$	$CDCl_2$	H 4.79	—	Two bridging carbonyl ligands	495
			$CDCl_3$	H 4.855 H 4.862	— —	$\left. \begin{array}{l} trans\text{-isomer} \\ cis\text{-isomer} \end{array} \right\} T -55^\circ$	502 503
$C_{16}H_{14}Fe_2O_4$	892	$\{[h^5-C_5H_4(CH_3)]Fe(CO)_2\}_2$	$CDCl_3$	H 4.55 H' 2.05	— —	Two bridging carbonyl ligands T 38°	493
$C_{24}H_{30}Fe_2O_4$	893	$\{[h^5-C_5(CH_3)_5]Fe(CO)_2\}_2$	CS_2	H 1.62s	—	Hexamethyldisiloxane reference	187
$C_{16}H_{12}Fe_2O_5$	894	$[(h^5-C_5H_5)Fe(CO)_2]-[(h^5-C_5H_4COCH_3)Fe(CO)_2]$	$CDCl_3$	H 4.85s	—	Two bridging carbonyl ligands	466
				H' 5.19t	J 2		
				H' 4.85t	—		
				H'' 2.53s	—		

$C_{18}H_{18}Fe_2O_6$	895	$\{[h^5-C_5H_4(OCH_2CH_3)]Fe(CO)_2\}_2$	$CDCl_3$	H_{-2}, H_{-5}	4.57t	—	Two bridging carbonyl ligands	413
				H_{-3}, H_{-4}	4.25t	—		
				H'	4.05q	—		
				H''	1.37t	—		
$C_{20}H_{26}Fe_2O_4Si_2$	896	$\{[h^5-C_5H_4(Si(CH_3)_3)]Fe(CO)_2\}_2$	C_6H_6	H	4.15t,	—	—	1033
					4.65t	—		
			CS_2	H'	0.33	—		
				H	4.72t,	—	—	208
					4.31t	—		
				H'	0.27	—		
$C_{16}H_{18}B_{10}Fe_2O_4$	897	$(h^5-C_5H_4-C_2B_{10}H_{10}-C_5H_4)-[Fe(CO)_2]_2$	C_6H_6	H	4.58t,	—	Two bridging carbonyl ligands	350
					4.26t	—		
$[C_{14}H_{10}^-BrFe_2O_4]^+$	898	$\{[(h^5-C_5H_5)Fe(CO)_2]_2(Br)\}^+$	—	Not reported		—	Tetrafluoroborate Bridging Br ligand	504
			$(CD_3)_2CO$	H	5.62	—	Tetraphenylborate	412
$[C_{16}H_{14}^-BrFe_2O_4]^+$	899	$\{[h^5-C_5H_4(CH_3)]Fe(CO)_2\}_2-(Br)\}^+$	$(CD_3)_2CO$	H	5.0b	—	Tetraphenylborate	412
$[C_{14}H_{10}^-ClFe_2O_4]^+$	900	$\{[(h^5-C_5H_5)Fe(CO)_2]_2(Br)\}^+$	$(CH_3)_2CO$	Not reported		—	Tetrafluoroborate Bridging Cl ligand	504
			$(CD_3)_2CO$	H	5.29	—	Tetraphenylborate	412
$[C_{16}H_{14}^-ClFe_2O_4]^+$	901	$\{[h^5-C_5H_4(CH_3)]Fe(CO)_2\}_2-(Cl)\}^+$	$(CD_3)_2CO$	H	5.1b	—	Tetraphenylborate	412
$[C_{14}H_{10}^-Fe_2IO_4]^+$	902	$\{[(h^5-C_5H_5)Fe(CO)_2]_2(I)\}^+$	—	Not reported		—	Tetrafluoroborate Bridging iodine ligand	504
			$(CD_3)_2CO$	H	5.22	—	Tetraphenylborate	412
								505
$[C_{16}H_{14}^-Fe_2IO_4]^+$	903	$\{[h^5-C_5H_4(CH_3)]Fe(CO)_2\}_2-(I)\}^+$	$(CD_3)_2CO$	H	5.35	—	Tetraphenylborate Bridging iodine ligand	412

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$[\text{C}_{14}\text{H}_{11}\text{FeO}_4]^+$	904	$\{[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2(\text{H}')\}^+$	—	H	5.24	—	Chloride	1042
				H'	−26.6	—	Bridging H ligand	
			H_2SO_4	H	5.24	—	Hydrogensulphate	1042
				H'	−26.3	—		
				H	5.23	—	Trifluoroacetate	1042
				H'	−26.6	—		
$\text{C}_{14}\text{H}_{10}\text{Br}_2\text{-Fe}_2\text{GeO}_4$	905	$[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2(\text{GeBr}_2)$	THF	H	5.17	—	Hexamethyldisiloxane	506
			CCl_4	H	5.17	—	reference	
$\text{C}_{14}\text{H}_{10}\text{Cl}_2\text{-Fe}_2\text{GeO}_4$	906	$[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2(\text{GeCl}_2)$	THF	H	5.16	—	Hexamethyldisiloxane	506
			CCl_4	H	5.16	—	reference	
$\text{C}_{14}\text{H}_{10}\text{F}_2\text{-Fe}_2\text{GeO}_4$	907	$[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2(\text{GeF}_2)$	THF	H	5.12	—	Hexamethyldisiloxane	506
			CCl_4	H	5.12	—	reference	
$\text{C}_{14}\text{H}_{10}\text{Fe}_2\text{-GeI}_2\text{O}_4$	908	$[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2(\text{GeI}_2)$	THF	H	5.17	—	Hexamethyldisiloxane	506
			CCl_4	H	5.17	—	reference	
$\text{C}_{16}\text{H}_{10}\text{Fe}_2\text{-GeN}_2\text{O}_4\text{S}_2$	909	$[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2[\text{Ge}(\text{NCS})_2]$	THF	H	5.28	—	Hexamethyldisiloxane	506
			CCl_4	H	5.28	—	reference	
$\text{C}_{16}\text{H}_{16}\text{Fe}_2\text{-GeO}_4$	910	$[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2[\text{Ge}(\text{CH}_3)_2]$	CS_2	H	4.77	—	Bridging $\text{Ge}(\text{CH}_3)_2$	507
				H'	0.89	—	ligand	
$\text{C}_{18}\text{H}_{20}\text{Fe}_2\text{-GeO}_4$	911	$[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2[\text{Ge}(\text{C}_2\text{H}_5)_2]$	THF	H	5.02	—	Bridging $\text{Ge}(\text{C}_2\text{H}_5)_2$ ligand	506
			CCl_4	H	4.92	—	Hexamethyldisiloxane reference	

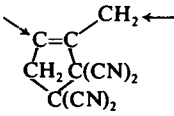
$C_{20}H_{20}Fe_2-$ GeO_4	912	$[(\eta^5-C_5H_5)Fe(CO)_2]_2[Ge(C_3H_5)_2]$	THF CCl_4	H H	5.05 5.05	— —	Hexamethyldisiloxane reference	506
$C_{22}H_{28}Fe_2-$ GeO_4	913	$[(\eta^5-C_5H_5)Fe(CO)_2]_2[Ge(C_4H_9)_2]$	THF CCl_4	H H	5.01 5.01	— —	Hexamethyldisiloxane reference	506
$C_{24}H_{20}Fe_2-$ GeO_4	914	$[(\eta^5-C_5H_5)Fe(CO)_2]_2[Ge(C_3H_5)_2]$	THF	H H'	5.05s 6.36m	— —	Hexamethyldisiloxane reference	506
$C_{26}H_{20}Fe_2-$ GeO_4	915	$[(\eta^5-C_5H_5)Fe(CO)_2]_2[Ge(C_6H_5)_2]$	THF CCl_4	H H	4.71 4.71	— —	Hexamethyldisiloxane reference	506
$C_{16}H_{16}Fe_2-$ GeO_6	916	$[(\eta^5-C_5H_5)Fe(CO)_2]_2-$ $[Ge(OCH_3)_2]$	CCl_4	H H'	5.07 3.62	— —	Hexamethyldisiloxane reference	506
$C_{18}H_{16}Fe_2-$ GeO_8	917	$[(\eta^5-C_5H_5)Fe(CO)_2]_2-$ $[Ge(OCOCH_3)_2]$	THF CCl_4	H H H'	5.06s 4.98s 2.31s	— — —	Hexamethyldisiloxane reference	506
$C_{18}H_{20}Fe_2-$ GeO_4S_2	918	$[(\eta^5-C_5H_5)Fe(CO)_2]_2-$ $[Ge(SC_2H_5)_2]$	CCl_4	H H'	5.08 2.79d 1.33t	— J 7.2 —	Hexamethyldisiloxane reference	506
$C_{14}H_{10}Fe_2-$ HgO_4	919	$[(\eta^5-C_5H_5)Fe(CO)_2]_2(Hg)$	$CDCl_3$ —	H H	4.77 4.79	— —	Bridging Hg atom —	136 508
$[C_{18}H_{14}Fe_2-$ $N_2O_4]^{2+}$	920	$\{[(\eta^5-C_5H_5)Fe(CO)_2]_2-$ $(C_4H_4N_2)\}^{2+}$	CD_3CN	H	5.89	—	Perchlorate Bridging pyrazine ligand Reference CH_3CN (δ 2.00)	404
$[C_{40}H_{34}Fe_2-$ $O_4P_2]^{2+}$	921	$\{[(\eta^5-C_5H_5)Fe(CO)_2]_2-$ $[P(C_6H_5)_2]CH_2CH_2P-$ $(C_6H_5)_2\}^{2+}$	CD_3CN	H H'	5.12 7.44	—	Perchlorate Bridging phosphine ligand Reference CH_3CN (δ 2.00)	404

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{42}H_{34}Fe_2O_4P_2$	922	$[(\eta^5-C_5H_5)Fe(CO)_2]_2-$ $[P(C_6H_5)_2CH_2C\equiv CCH_2-$ $P(C_6H_5)_2]$	$CDCl_3$	H	5.62	—	60 and 100 MHz	211
				H'	7.63,	—		
				H''	7.58 4.03d	— J 6		
$[C_{40}H_{10}Fe_2O_4P_2]^+$	923	$\{[(\eta^5-C_5H_5)Fe(CO)_2]_2-$ $[P(C_6H_5)_2C\equiv CP(C_6H_5)_2]\}^+$	$(CD_3)_2CO$	H	5.79d	$J_{PH} 1.9$	100 MHz Tri-iodide Hexafluorophosphate	494
				H	5.78	$J_{PH} 1.9$		
$C_{14}H_{10}Cl_6FeO_4Si_2$	924	$[(\eta^5-C_5H_5)Fe(CO)_2]^+[(\eta^5-C_5H_5)Fe(SiCl_3)_2(CO)]^-$	CH_3CN	H	5.75,	—	—	400
					4.63	—		
			$(CH_3)_2CO$	H	6.15, 4.60	— —		
$C_{16}H_{14}Cl_6Fe_2O_4Si_2$	925	$\{[(\eta^5-C_5H_4(CH_3))Fe(CO)_3]^+\{[(\eta^5-C_5H_4(CH_3))Fe(SiCl_3)_2(CO)]^-\}$	$(CD_3)_2CO$	H	5.4bs,	—	—	400
					4.0t,	—		
					3.75t	—		
				H'	1.7b,	—		
					1.35s	—		
$C_{14}H_{10}Br_2Fe_2O_4Sn$	926	$[(\eta^5-C_5H_5)Fe(CO)_2]_2(SnBr_2)$	$CDCl_3$	H	5.02	—	—	142
$C_{14}H_{10}Cl_2Fe_2O_4Sn$	927	$[(\eta^5-C_5H_5)Fe(CO)_2]_2(SnCl_2)$	$CDCl_3$	H	5.02	—	—	142
$C_{16}H_{16}Fe_2O_4Sn$	928	$[(\eta^5-C_5H_5)Fe(CO)_2]_2-$ $[Sn(CH_3)_2]$	CS_2	H	4.76s	—	Bridging $Sn(CH_3)_2$ ligand	507
				H'	0.59	$J_{SnH} 36$		

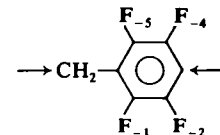
$[\text{C}_{18}\text{H}_{20}\text{Fe}_2\text{O}_4\text{S}_2]^{2+}$	929	$\{[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2\text{-}[\text{S}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{S}(\text{CH}_3)]\}^{2+}$	CD_3CN	H	5.48	—	Bridging thioether ligand Reference CH_3CN (δ 2.00) Perchlorate	404
$\text{C}_{16}\text{H}_{12}\text{Fe}_2\text{O}_4\text{S}_2$	930	$[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2\text{-}(\text{S}\cdot\text{CH}'=\text{CH}'\text{S})$	CDCl_3	H H'	4.45 7.21	— —	Bridging sulphur ligand	509
$\text{C}_{18}\text{H}_{10}\text{Fe}_2\text{N}_2\text{O}_4\text{S}_2$	931	$[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2\text{-}[\text{S}_2\text{C}_2(\text{CN})_2]$	$(\text{CH}_3)_2\text{CO}$	H	5.36s	—	—	510
$\text{C}_{24}\text{H}_{20}\text{Fe}_2\text{O}_4\text{Sn}$	932	$[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2\text{-}[\text{Sn}(\text{C}_5\text{H}_5)_2]$	THF	H	5.00s	—	Bridging $\text{Sn}(\text{C}_5\text{H}_5)$ ligand	511
$\text{C}_{26}\text{H}_{20}\text{Fe}_2\text{O}_8\text{S}_2\text{Sn}$	933	$\{[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2\text{-}[\text{Sn}\{\text{OS}(\text{O})\text{C}_6\text{H}_5\}_2]\}$	—	H H'	4.91s 7.61 comp.	— —	—	512
$\text{C}_{26}\text{H}_{20}\text{Fe}_2\text{O}_8\text{S}_2\text{Sn}$	934	$[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2\text{-}[\text{Sn}(\text{SO}_2\text{C}_6\text{H}_5)_2]$	—	H H'	5.18s 7.73 comp.	— —	—	512
$\text{C}_{17}\text{H}_{16}\text{Fe}_2\text{O}_8\text{S}_2$	935	$[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2\text{-}[\text{SO}_2(\text{CH}_2)_3\text{SO}_2]$	CDCl_3	H H'	5.40s 3.52t, 2.69–2.49m	— <i>J</i> 6 —	—	923
$[\text{C}_8\text{H}_{22}\text{B}_{18}\text{Fe}_2\text{O}_4]^{2-}$	936	$\{[\eta^5\text{-}(3)\text{-}1,2\text{-B}_9\text{C}_2\text{H}_{11}]\text{Fe}(\text{CO})_2\}_2^{2-}$	$(\text{CH}_3)_2\text{CO}$	^{11}B	+20.9d, 9.3d, –0.1d	— — —	Tetramethylammonium Salt	77
$[\text{C}_{18}\text{H}_{20}\text{Fe}_2\text{NO}_4]^+$	937	$\{[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]\{(\eta^5\text{-C}_5\text{H}_5)\text{-Fe}[h\text{-CH}_2\text{CH}_2\text{N}(\text{CH}_3)_2(\text{CO})_2]\}^+\}$	CHCl_3	H	5.05s, 4.96s	— —	Chloride Other signals at δ 4.80, 3.5b, 2.97s, 2.76s, 1.22 comp.	177
$\text{C}_{17}\text{H}_{16}\text{Fe}_2\text{O}_6\text{S}$	938	$[(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2]_2\text{-}(\text{SO}_2\text{CH}_2\text{CH}_2\text{CH}_2'')^*$	CDCl_3	H H' H'' H'''	5.40s 3.72t 2.77–2.33 3.38t	— <i>J</i> 6 — <i>J</i> 6	*Bridging ligand	923

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{24}H_{14}Fe_2-N_4O_4$	939	$[(h^5-C_5H_5)Fe(CO)_2]_2(C_{10}H_4N_4)$	—	H 5.28,	—	$C_{10}H_4N_4$ = bridging ligand 	194
				5.12	—		
				H' 3.50t, 2.60t	J 1.2 —		
$C_{18}H_{14}Fe_2O_4$	940	$[(h^5-C_5H_5)Fe(CO)_2]_2-(CH'=CH'-CH'=CH')^*$	THF	H 4.95s	—	*Bridging butadiene ligand	513
				H' 6.24s†	—		514
							515
							499

†The single absorption of the butadiene protons was attributed to an averaging process caused by rapid valence tautomerism involving a cyclobutene intermediate. Further work has shown that at 60 MHz the single absorption is because of the combination of small chemical shift differences and relatively large coupling constants. The broadening reported at low temperatures is not the result of a slowing down of the proposed valence tautomerism, but is a reflection of increased chemical shift difference as the temperature is lowered. The degeneracy of the butadiene protons observed in THF is removed when C_6D_6 or $CD_3C_6D_5$ is used as solvent, even at 60 MHz, and remains unchanged up to 116°C, showing that the structure is static.

$C_{20}H_{18}Fe_2O_4$	941	$\{[h^5-C_5H_4(CH_3)]Fe(CO)_2\}_2-(CH=CH-CH=CH)^*$		Not reported	—	*Bridging butadiene ligand Analyzed as an A_2B_2 system ($J_{AB} = 10$ Hz)	499
$C_{21}H_{12}F_4Fe_2O_4$	942	$[(h^5-C_5H_5)Fe(CO)_2]_2-(CH_2-C_6F_4)$	$CFCl_3$	F_{-1}, F_{-5} 145.3 F_{-2}, F_{-4} 111.3	— —	$CH_2C_6F_4$ = bridging ligand	477



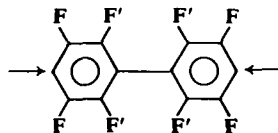
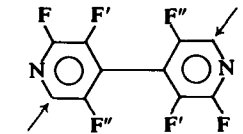
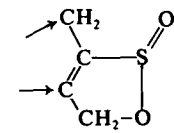
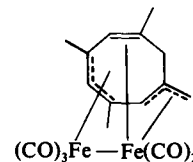
		THF	F_{-1}, F_{-5}	142.9	$J_{1,5}$ 4.4 $J_{1,2}$ 28.1 $J_{1,4}$ 10.9 $J_{2,4}$ 2.1	T 35°	244
			F_{-2}, F_{-4}	108.4			
$C_{26}H_{10}F_8Fe_2O_4$	943	$[(\eta^5-C_5H_5)Fe(CO)_2]_2(C_{12}F_8)$	THF	F F'	107.5 141.9	— —	479
						$C_{12}F_8$ = Bridging ligand	
							
$C_{24}H_{10}F_6Fe_2N_2O_4$	944	$[(\eta^5-C_5H_5)Fe(CO)_2]_2(C_{10}F_6N_2)$	CHCl ₃	F F' F''	89.5 149.6 101.1	$J_{FF'}$ 28.0 $J_{FF'}$ 2.0 $J_{FF''}$ 30.0	248
						$C_{10}F_6N_2$ = bridging ligand	
							
$C_{18}H_{14}Fe_2O_6S$	945	$[(\eta^5-C_5H_5)Fe(CO)_2]_2(C_4H_4O_2S)$	CDCl ₃	H H'	4.97s 4.92s 2.64 2.16	— — J 11 —	163
						$C_4H_4O_2S$ = bridging ligand	
							
$C_{16}H_{18}B_8Fe_2O_4$	946	$[(\eta^5-C_5H_5)Fe(CO)_2]_2(1,10-h^1:h^1-B_8C_2H_8)^*$	—	H ¹¹ B	5.0 +11.6	— J 160	483
						*Bridging ligand Relative to BF ₃ ·OEt ₂	
$C_{28}H_{36}Fe_2O_4$	947	$[h^6-C_6(CH_3)_6]Fe(CO)_2]_2$	C ₆ D ₆	H	1.58s	—	516
						$C_6(CH_3)_6$ = hexamethylbenzene	

TABLE VII—*cont.*

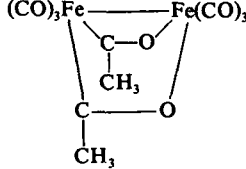
Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
(iv) Pentacarbonyl derivatives:							
$C_{22}H_{15}Fe_2O_5P$	948	$[(h^5-C_5H_5)Fe(CO)][Fe(CO)_3]-[P(C_6H_5)_2]^*(CO)^*$	$CDCl_3$	H	4.87	—	*Bridging ligands 517
$C_{44}H_{34}Fe_2O_5P_2$	949	$(2-h^1:1,2,3-h^3-C_3H_4)Fe_2-[P(C_6H_5)_2]_2(CO)_5$	—	n.a.	—	Signals at δ 3.55, 1.27, and 1.13 in ratio 2:1:1	288
$C_9H_4Fe_2O_5$	950	$(CH_2=C=C=CH_2)Fe_2(CO)_5$	—	n.a.	—	Butatrienediiron pentacarbonyl Signals at δ 4.78 and 4.15	518
$C_{13}H_8Fe_2O_5$	951	$(1,2,3,4,5-h^5:1,5,6,7,8-h^3-C_8H_8)-[Fe(CO)_2]_2(CO)^*$	—	H	4.67s	—	*Bridging carbonyl ligand The complex shows rapid valence tautomerism 519
$C_{17}H_{16}Fe_2O_5$	952	$[1,2,3,4,5-h^5:1,5,6,7,8-h^3-2,4,6,8-C_8H_4(CH_3)_4]-[Fe(CO)_2]_2(CO)^*$	—	—	—	—	*Bridging carbonyl ligand Signals at δ 4.31 and 2.10 362
$C_{17}H_{16}Fe_2O_5$	953	$(h^3:h^5-C_{12}H_{16})[Fe(CO)_3]-[Fe(CO)_2]$	—	n.a.	—	Proposed structure:	362



Signals at δ 2.40, 1.95, 1.85, 1.72, and 1.50

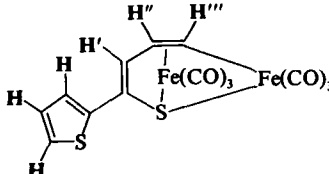
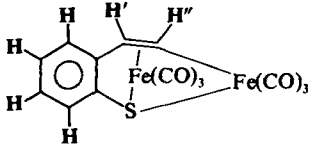
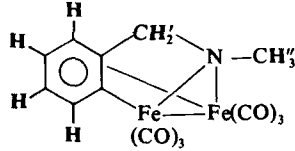
$C_{12}H_8Fe_2O_5$	954	$(h^5-C_5H_5)(1-h^1:1,2-h^2-CH'=CH_2)[Fe(CO)][Fe(CO)_3](CO)^*$	$CDCl_3$	H	5.00	—	*Bridging carbonyl ligand	223
				H'	10.91	—	Hexamethyldisiloxane	
				H'' _{syn}	2.22	$J_{H'H''} 7.3$	reference	
				H''' _{anti}	1.70	$J_{H'H''} 11.8$ $J_{H''H''} 1.4$		
$C_{18}H_{12}Fe_2O_5$	955	$(h^5-C_5H_5)(1-h^1:1,2-h^2-2-CH'=CH''C_6H_5'')[Fe(CO)][Fe(CO)_3](CO)^*$	$CDCl_3$	H	5.08	—	*Bridging carbonyl ligand	223
				H'	11.0	$J_{H'H''} 12.0$	Hexamethyldisiloxane	
				H''	3.28	—	reference	
				H'''	7.08–7.34	—		
$C_{14}H_{10}Fe_2O_6$	956	$(h^5-C_5H_5)(1-h^1:1,2-h^2-2-CH'=CH''COCH_3''')[Fe(CO)][Fe(CO)_3](CO)^*$	$CDCl_3$	H	5.05	—	*Bridging carbonyl ligand	520
				H'	11.34	$J_{H'H''} 10$	Hexamethyldisiloxane	223
				H''	2.20	—	reference	
				H'''	1.93	—	100 MHz	
$C_{19}H_{12}Fe_2O_6$	957	$(h^5-C_5H_5)(1-h^1:1,2-h^2-2-CH'=CH''COC_6H_5'')[Fe(CO)][Fe(CO)_3](CO)^*$	$CDCl_3$	H	5.09	—	*Bridging carbonyl ligand	223
				H'	11.60	$J_{H'H''} 10.0$	Hexamethyldisiloxane	520
				H''	2.96	—	reference	
				H'''	~7.3	—		
$C_{19}H_{12}Fe_2O_6$	958	$(h^5-C_5H_5)(1-h^1:2,3-h^2-3-COCH'=CH''C_6H_5''')[Fe(CO)_2][Fe(CO)_3]$	$CDCl_3$	H	5.07	—	Hexamethyldisiloxane	223
				H'	5.55	$J_{H'H''} 9.3$	reference	
				H''	3.42	—		
				H'''	7.31	—		
(v) Hexacarbonyl derivatives:								
$C_{14}H_{12}As_2F_4Fe_2O_6$	959	$\{1,2-h^2-1,2-[As(CH_3)_2]_2,3,3,4,4-C_4F_4\}[Fe(CO)_3]_2$	$(CD_3)_2CO$	H	2.45s, 1.16s	—	—	521
			$(CH_3)_2CO$	^{19}F	94.74, 96.67, 107.1, 109.1	— — — —		

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{34}H_{20}F_4^-$ $Fe_2O_6P_2$	960	$\{1,2-h^2-1,2-[P(C_6H_5)_2]_2-3,3,4,4-C_4F_4\}[Fe(CO)_3]_2$	$(CH_3)_2CO$	^{19}F 86.95, 88.88, 103.9, 105.9	— — — —		521
$C_{35}H_{20}F_6^-$ $Fe_2P_2O_6$	961	$\{1,2-h^2-1,2-[P(C_6H_5)_2]_2-3,3,4,4,5,5-C_5F_6\}[Fe(CO)_3]_2$	$(CH_3)_2CO$	$^{19}F_{-3}$, F_{-5} $^{19}F_{-5}$ 70.35dm, 99.98dm, 112.4dm, 121.7dt	J 242 J 240 J 236 J 6		521
$C_{10}H_6Fe_2O_8$	962	$(1-h^1-CH_3C=O)_2[Fe(CO)_3]_2$	$CDCl_3$	H 2.82s	—	Proposed structure: 	270
$C_{23}H_{15}Fe_2^-$ O_6P	963	$(h^5-C_5H_5)[Fe(CO)_2][Fe(CO)_4]-[P(C_6H_5)_2]^*$	$CDCl_3$	H 5.04d	J_{PH} 1.2	*Bridging ligand	522 517
$C_{26}H_{24}Fe_2^-$ O_2S_2	964	$[(h^5-C_5H_5)Fe(CO)]_2(p-SC_6H_4CH_3)_2$	$CDCl_3$ CS_2 $CDCl_3$ CS_2	H H' H H' H H' H H' 4.58 2.24 4.40 2.19 4.13 2.30 3.98 2.27	— — — — — — — —	Isomer I Isomer II	984

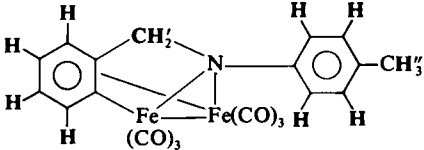
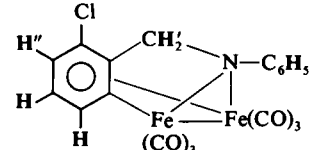
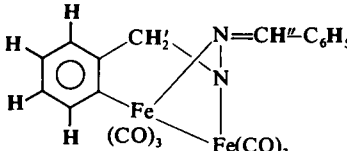
$C_{24}H_{18}F_2^-$ $Fe_2O_2S_2$	965	$[(h^5-C_5H_5)Fe(CO)]_2(p-SC_6H_4F)_2$	$CDCl_3$	H	4.59	—	Isomer I	984
			CS_2	H	4.42	—		
			$CDCl_3$	H	4.17	—	Isomer II	
$C_{26}H_{24}Fe_2^-$ O_4S_2	966	$[(h^5-C_5H_5)Fe(CO)]_2(p-SC_6H_4OCH_3)_2$	CS_2	H	4.38	—	Isomer I	984
				H'	3.69	—		
				H	3.99	—	Isomer II	
				H'	3.74	—		
$C_{18}H_{22}Fe_2^-$ O_4Si_2	967	$[Fe(h^5-C_5H_5)(CO)_2]_2[Si_2(CH_3)_4]$	$CHCl_3$	H	4.79s	—	—	983
				H'	0.45s	—		
$C_{20}H_{26}Fe_2^-$ O_4Si_2	968	$\{[Fe(h^5-C_5H_5)(CO)_2]_2[Si-(CH_3)_2]_2\}(C_2H_4)$	$CDCl_3$	H	4.50s	—	—	983
				H'	0.32s	—		
				H''	0.86s	—		
$C_{20}H_{28}Fe_2^-$ O_4Si_3	969	$[Fe(h^5-C_5H_5)(CO)_2]_2[Si_3(CH_3)_6]$	$CDCl_3$	H	4.78s	—	—	983
				H'	0.52s,	—		
					0.30s	—		
$C_{20}H_{10}Fe_2O_8$	970	$(1-h^1-C_6H_5C=O)_2[Fe(CO)_3]_2$	C_5H_{12}	H	6.65	—	Structure analogous to that above	270 1008
$C_9H_6Fe_2O_6S$	971	$(1-h^1:1,2-h^2-CH=CH_2) \cdot [Fe(CO)_3]_2(CH_3S)^*$	$CDCl_3$	H	8.16	—	*Bridging ligand	201
				H'_{syn}	3.81	—		
				H'_{anti}	2.85	—		

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{10}H_6Fe_2O_6S$	972	(1- <i>h</i> ¹ :1,2- <i>h</i> ² -CH=CH ₂)- [Fe(CO) ₃] ₂ (CH ₂ =CH"S)*	CDCl ₃	H	8.16	—	*Bridging ligand	201
				H' _{syn}	3.82	—		
				H' _{anti}	2.78	—		
				H''	5.70	—		
$C_{14}H_6Fe_2O_6S_2$	973	[C ₄ H ₃ S(C ₄ H ₃ S)][Fe(CO) ₃] ₂	CDCl ₃	H	6.93	—	Structure:	201
				H'	6.34	—		
				H''	5.02	—		
				H'''	8.85	—		
$C_{14}H_6Fe_2O_6S$	974	(C ₈ H ₆ S)[Fe(CO) ₃] ₂	CDCl ₃	H	6.95	—	Structure:	201
				H'	5.40	—		
				H''	8.90	—		
$C_{14}H_9Fe_2NO_6$	975	(C ₈ H ₉ N)[Fe(CO) ₃] ₂	CCl ₄	H	7.55m	—	Structure:	524
				H'	4.04s	—		
				H''	2.84s	—		

T 33.5° 40 MHz

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{20}H_{13}Fe_2NO_6$	979	$(C_{14}H_{13}N)[Fe(CO)_3]_2$	CCl_4	H	7.65m	—	Structure: 	524
				H'	4.40s	—		
				H''	2.32s	—	T 33.5° 40 MHz	
$C_{19}H_{10}ClFe_2NO_6$	980	$(C_{13}H_{10}ClN)[Fe(CO)_3]_2$	$CDCl_3$	H	7.10 m	—	Structure: 	524
				H'	4.46s	—		
				H''	7.90m	—	T 33.5° 40 MHz	
$C_{20}H_{12}Fe_2N_2O_6$	981	$(C_{14}H_{12}N_2)[Fe(CO)_3]_2$	—	H	7.12,	—	Structure: 	388
					7.36s,	—		
					7.58,	—		
					8.07d	—		

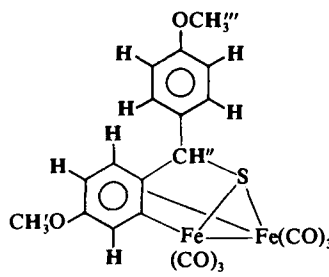
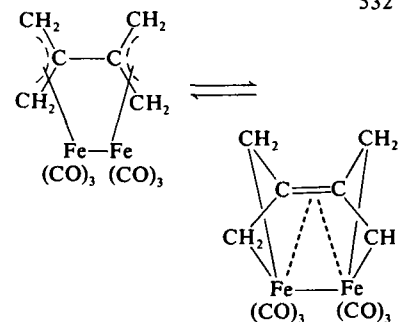
				H'	4.39s	—	100 MHz	
				H''	7.73s	—		
$C_{21}H_{14}Fe_2O_8S$	982	$(C_{15}H_{14}O_2S)[Fe(CO)_3]_2$	$CDCl_3$	H	6.28, 6.67, 7.20, 7.63	— — — —	Structure:	525
				H'	3.70s	—		
				H''	5.43	—		
				H'''	3.83	—		
								
$C_{27}H_{19}Fe_2O_6P$	983	$(1,2,3-h^3:2-h^1-C_3H_4)[Fe(CO)_3]-[Fe(PPh_3)(CO)_3]$	—	H	2.22, 3.48	—	—	288
$C_{13}H_8Fe_2O_6$	984	$(h^5:h^1-C_5H_4CHCH_3)[Fe(CO)_2]-[Fe(CO)_4]$	C_6D_6	n.a.		—	Signals at δ 1.02d, 1.75q, 2.75m, 3.09m, 3.64m in ratio 3:1:1:1:2	351
$C_{13}H_8Fe_2O_7$	985	$(h^5:h^1-1-C_5H_4CH'OCH_3)-[Fe(CO)_2][Fe(CO)_4]$	CS_2	$H_{-2},$ H_{-3}, H_{-4} H_{-5} H' H''	3.69 4.95 4.42 4.96 3.42s	— — — — —	—	526
$C_{21}H_{13}Fe_2NO_6$	986	$[h^2:h^2-CH_3N=C=C(C_6H_5)_2]-[Fe(CO)_3]_2$	C_6D_6	H H'	2.34s 7.70d, 7.20m, 7.0m	— — — —	100 MHz	527

TABLE VII—*cont.*

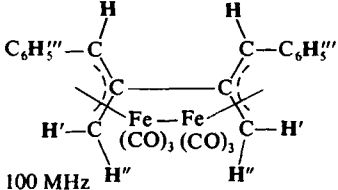
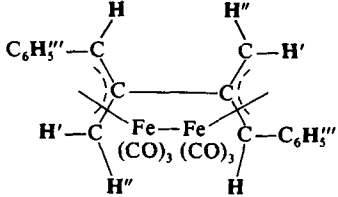
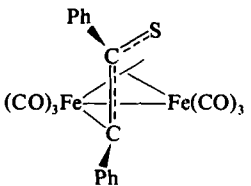
Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{10}H_4Fe_2O_6$	987	(1,2,3,4- h^4 :1,4- h^2 -CH=CH-CH=CH)[Fe(CO) $_3$] $_2$	CDCl $_3$	H_{-1}, H_{-4}	6.78	—	—	201
				H_{-2}, H_{-3}	6.31	—		
$C_{14}H_{12}Fe_2O_6$	988	[1,2,3,4- h^4 :1,4- h^2 -C(CH $_3$)=C(CH $_3$)C(CH $_3$)=C(CH $_3$)]-[Fe(CO) $_3$] $_2$	CDCl $_3$	H	2.26s,	—	—	341
					2.06s	—		
$C_{14}H_8Fe_2O_{10}$	989	(1,2,3,4- h^4 :1,4- h^2 -CH $_3$ O $_2$ CC=CH'-CH'=CCO $_2$ CH $_3$)-[Fe(CO) $_3$] $_2$	CDCl $_3$	H	3.74	—	—	201
			C $_6$ F $_6$	H'	6.54	—	—	528
				H'	3.82s 6.64s	— —		
$C_{16}H_{12}Fe_2O_{10}$	990	(1,2,3,4- h^4 :1,4- h^2 -CH $_3$ CH $_2$ O $_2$ -CC=CH''-CH''=CCO $_2$ CH $_2$ -CH $_3$)[Fe(CO) $_3$] $_2$	CDCl $_3$	H	1.28	—	—	201
				H'	4.20	—		
				H''	6.55	—		
$C_{14}H_6Fe_2O_6$	991	(1,2, α , β - h^4 :2, β - h^2 -1-C $_6$ H $_4$ CH $_{\alpha}$ =CH $_{\beta}$)[Fe(CO) $_3$] $_2$	CDCl $_3$	H_{-3}	7.66d	$J_{3,4} \sim 8.5$	100 MHz	529
				H_{-4}	6.97m	—		
				H_{-5}	7.29m	$J_{5,6} 8.4$		
				H_{-6}	7.80d	—		
				$H_{-\alpha}$	7.10d	$J_{\alpha,\beta} 5.8$		
				$H_{-\beta}$	6.64d	—		
$C_{10}H_4Fe_2O_6$	992	(1,2,3- h^3 :2,3,4- h^3 -CH $_2$ =C=C*=CH $_2$)[Fe(CO) $_3$] $_2$	CS $_2$	H	4.70d, 4.04d	$J 1.8$ —	*The four carbon atoms of the triene are no longer linear	319 530

$C_{14}H_{12}Fe_2O_6$	993	$[1,2,3-h^3:2,3,4-h^3-(CH_3)_2]^-$ $C=C^*=C=C(CH_3)_2[Fe(CO)_3]_2$	CS_2	H	2.14s, 1.96s	—	—	319
$C_{12}H_8Fe_2O_6$	994	$(h^3:h^3-C_6H_8)[Fe(CO)_3]_2$	CCl_4	H	1.66d	—	T 35°	531 532



The separation of the 2 peaks (0.07 ppm) decreases as the temperature is lowered and becomes a sharp singlet at -10° . The 2,2'-bis- π -allylene structure would give two singlets corresponding to the *syn*- and *anti*-protons with a separation of ~ 1 ppm. It is therefore assumed that valence tautomerism occurs rapidly, even at -10° , thus averaging out all the protons. The calculated chemical shift based on this assumption is $\delta 1.65$.

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{24}H_{16}Fe_2O_6$	995	$(h^3:h^3-C_{18}H_{16})[Fe(CO)_3]_2$	$CDCl_3$	H	4.43d		533
				H'	2.25t		
				H''	2.79d		
				H'''	7.22s		
			$CDCl_3$	H	3.60		534
				H	2.71		
				H	3.23		
				H	7.22s		
$C_{20}H_{10}Fe_2O_6S$	996	$h^3:h^3-C_6H_3C=C(C_6H_5)=S-[Fe(CO)_3]_2$	$CDCl_3$	H	2.84s,	Both isomers derived from 1-phenylallene and $Fe_2(CO)_9$ Structure: 	534
					2.90m		
					—		

$C_{13}H_8Fe_2O_6$	997 (1,2,3- h^3 :4,5,5- h^3 - C_7H_8)- [Fe(CO) $_3$] $_2$	—	H_{-1}, H_{-6} 2.7m H_{-2}, H_{-5} 4.2m H_{-3}, H_{-4} 5.1m H_{-7} 3.0m, 2.2m	— — — — —	1,2,3-trihapto-4,5,6-trihaptocyclohepta-1,3,5-trienediiron (Fe—Fe) hexacarbonyl The π -electron system is considered to be divided into two adjacent allyl groups, each of which forms a π -complex with one of the iron atoms. The complex is not fluxional, the spectrum being unchanged down to -100°	535
$C_{14}H_{10}Fe_2O_6$	998 (1,2,6- h^3 :3,4,5- h^3 - C_8H_{10})- [Fe(CO) $_3$] $_2$	$CHCl_2F$	H_{-1}, H_{-6} 2.63 H_{-2}, H_{-5} 3.87 H_{-3}, H_{-4} 4.49 H_{-7}, H_{-8} 1.92, 1.48	— — — — —	<i>cis</i> -1,2,6-trihapto:3,4,5-trihaptocycloocta-1,3,5-triene-diiron hexacarbonyl. In contrast to the above complex this is assigned a skew structure which rapidly oscillates between the two enantiomorphic forms:	536 535 803

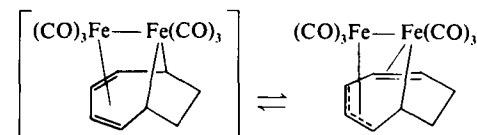
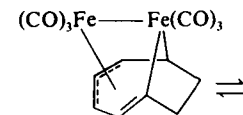
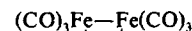


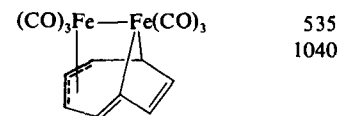
TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{15}H_9Fe_2NO_6$	999	$(C_8H_9)(CN)[Fe(CO)_3]_2$	—	Not reported	—	—	536
$C_{14}H_9Fe_2N_3O_6$	1000	$(C_8H_9)(N_3)[Fe(CO)_3]_2$	—	Not reported	—	Neutral azide complex	536
$[C_{19}H_{14}Fe_2NO_6]^+$	1001	$\{(C_8H_9)(C_3H_5N)[Fe(CO)_3]_2\}^+$	—	Not reported	—	A fluxional molecule giving a non-averaged spectrum at -20° . $[BF_4]^-$ salt	536
$[C_{32}H_{24}Fe_2O_6P]^+$	1002	$\{(C_8H_9)[P(C_6H_5)_3][Fe(CO)_3]_2\}^+$	—	Not reported	—	More rigid than the pyridine adduct and shows a non-averaged spectrum at 37° . $[BF_4]^-$ salt	536
$C_{14}H_8Fe_2O_6$	1003	$(1,2,6-h^3:3,4,5-h^3-C_8H_8) \cdot [Fe(CO)_3]_2$	—	n.a.	—	C_8H_8 = cyclooctatetraene Signals at δ 5.8, 4.6, 4.1, 2.5, of equal intensity Structure originally proposed was the 1,2,3- $h^3:4,5,6-h^3$ -isomer, viz.:	519



in equilibrium with the *cis-h⁴:h⁴* isomer (see 1004)

The structure now regarded as most likely is that of the 1,2,6-*h*³:3,4,5-*h*³-isomer, viz.:



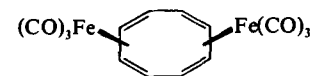
535
1040

by analogy with $C_8H_{10}Fe_2(CO)_6$
(see 998) and $C_8H_8Ru_2(CO)_6$

$C_{14}H_8Fe_2O_6$ 1004 (1,2,3,4-*h*⁴:5,6,7,8-*h*⁴- C_8H_8)-
[Fe(CO)₃]₂

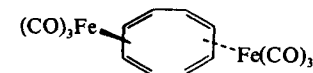
n.a.

cis-isomer, viz.: 519



Signals at δ 5.0, 4.0

trans-isomer, viz.: 519

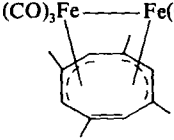
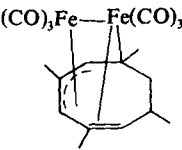


Signals at δ 5.8, 3.3

All three of the above isomers were obtained by the action of $Fe_2(CO)_9$ on cyclooctatetraene
"Wide-line" NMR measurements

537

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{18}H_{16}Fe_2O_6$	1005	$[h^3:h^3-1,3,5,7-C_8H_4(CH_3)_4] \cdot [Fe(CO)_3]_2$	$CDCl_3$	n.a.	—	Structure originally proposed was (I), but by analogy with cyclooctatetraene derivatives it could well be (II), viz.:  (I) or  (II) Signals at δ 5.32, 4.97, 4.16, 3.80 (integrating to one H each) and 2.17, 1.89, 1.68, 1.61 (integrating to three H each)	362

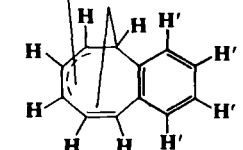
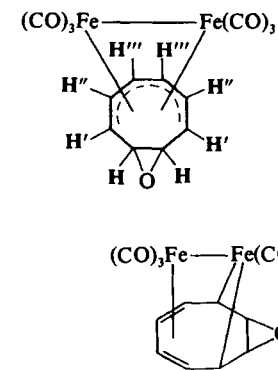
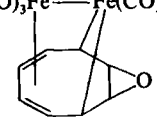
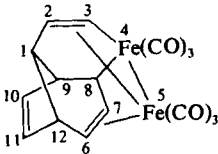
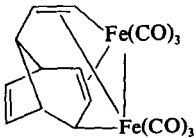
		CS ₂	n.a.	—		<i>trans</i> -isomer of above Signals at δ 5.15, 2.85, 2.24, 1.71, in ratio 1:1:3:3	362
C ₁₈ H ₁₀ Fe ₂ O ₆	1006 (<i>h</i> ³ : <i>h</i> ³ -C ₁₂ H ₁₀)[Fe(CO) ₃] ₂	CCl ₄	H	4.52dd, 4.30dq, 2.91d 6.83	<i>J</i> 2, 4 <i>J</i> 2, 4, 9 <i>J</i> 9	Structure: 	380
C ₁₄ H ₈ Fe ₂ O ₇	1007 (<i>h</i> ⁶ -C ₈ H ₈ O)[Fe(CO) ₃] ₂	CS ₂	H H' H'' H'''	3.13s 4.05d 3.30m 5.51m	— <i>J</i> _{H'H''} 6.5 <i>J</i> _{H''H'''} 9.0 <i>J</i> _{H'''H''''} 11	Structure:  or 	373

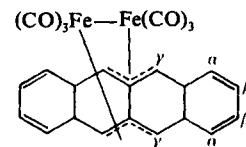
TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{16}H_{10}Fe_2O_6$	1008	$(\eta^6-C_{10}H_{10})[Fe(CO)_3]_2$	—	Not reported	$J_{1,10} = J_{1,11}$ 0 $J_{1,6} = J_{1,8}$ 1.5 $J_{2,3}$ 9.5 $J_{6,8}$ 2.0 $J_{7,9} = J_{7,12}$ 1.3 $J_{9,10}$ 2.5 $J_{10,11}$ 5.9 $J_{11,12}$ 2.5 $J(^{13}C-H_3)$ 155	Structure:  or 	538

$C_{24}H_{12}Fe_2O_6$	1009	$(h^2 : h^3-C_{18}H_{12})[Fe(CO)_3]_2$	$(CD_3)_2CO$	H_α	7.70m	—
				H_β	7.45m	—
				H_γ	5.25s	—

Structure:

365

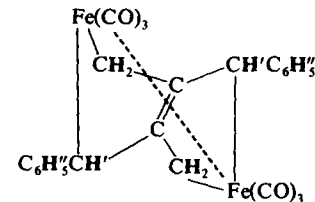


Naphthacenediiron
hexacarbonyl

$C_{24}H_{16}Fe_2O_6$	1010	$(C_{18}H_{16})[Fe(CO)_3]_2$	$CDCl_3$	H	2.92d, 0.80d	J 3.75
				H'	1.77s	—
				H''	7.40m	—

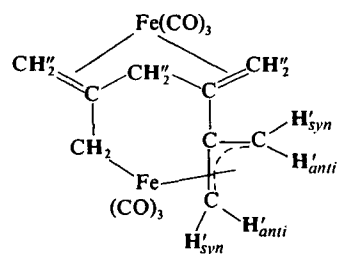
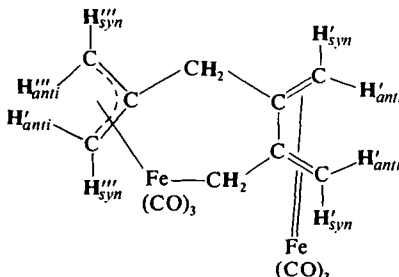
Structure:

533

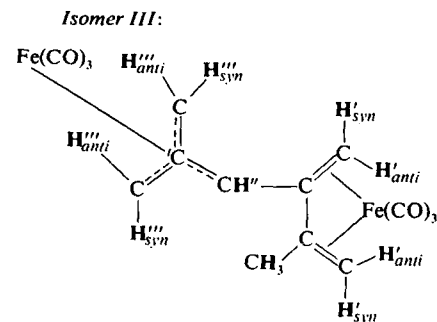


Ancipital co-ordination. The central double bond participates in a bonding interaction with both iron atoms, utilizing both sides [(+) and (-)] of the $p\pi$ -orbital. The inert gas structure for both iron atoms is not realized simultaneously

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{15}H_{12}Fe_2O_6$	1011	$(h^4:h^4-C_9H_{12})[Fe(CO)_3]_2$	$CDCl_3$	H 6.14, 5.85 H'_{syn} 4.15, 4.02 H'_{anti} ~5.8, ~5.6 H'' 5.5–4.8 comp.	<i>J</i> 9.5, 3.0 <i>J</i> 9.5 <i>J</i> 2.5 <i>J</i> 2.5 — —	Isomer I: 	850
			$CDCl_3$	H 6.23d, 5.45d H'_{syn} ~5.6d, ~5.5d H'_{anti} 7.20d, 7.06d H'' 4.37d, 4.27d H'''_{syn} ~4.3s, ~3.95s H'''_{anti} ~5.15, ~4.75	<i>J_{gem}</i> 9.0 <i>J_{gem}</i> 2.5 <i>J_{gem}</i> 2.5 <i>J_{gem}</i> 14.5 — — —	Isomer II: 	

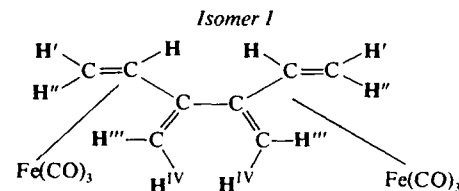
CDCl ₃	H	5.27s	—
	H'_{syn}	5.62d,	$J_{gem} 2.4$
		5.30d	
	H'_{anti}	7.35d,	$J_{gem} 2.4$
		7.26d	
	H''	3.43d	$J_{H''H'''} 2.4$
	H''_{syn}	5.50d,	$J 4.4$
		4.26d	
	H''_{anti}	5.50s,	
		5.02d	



C₁₄H₁₀Fe₂O₆ 1012 (*h*⁴:*h*⁴-C₈H₁₀)[Fe(CO)₃]₂

C ₆ D ₆	H	5.21	—
	H'	1.47	—
	H''	0.05	—
	H'''	-0.13	—
	H^{IV}	2.03	—

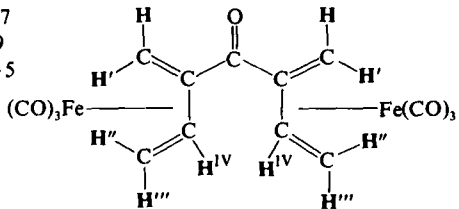
Two diastereoisomers of structure: 303



	H	5.41	—
	H'	1.41	—
	H''	0.07	—
	H'''	-0.25	—
	H^{IV}	1.74	—

Isomer II
60 and 100 MHz
The isomers have identical spectra
in solvents other than benzene

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{15}H_{10}Fe_2O_7$	1013	$(h^4:h^4-C_9H_{10}O)[Fe(CO)_3]_2$	CS_2	H	2.47d	Two diastereoisomers, having identical spectra in solvents other than benzene, of structure:	319
				H'	0.50d		
				H''	0.48dd		
				H'''	1.93d		
				H ^{IV}	6.1m		
					$J_{H''H'''} 2.5$ $J_{H'''H^{IV}} 7$ $J_{H''H^{IV}} 9$ $J_{HH^{IV}} 1.5$		
C_6D_6				H	2.22	Isomer I	303
				H'	-0.05		
				H''	-0.03		
				H'''	1.40		
				H ^{IV}	5.72		
				H	2.31	Isomer II 60 and 100 MHz	
				H'	0.03		
				H''	0.03		
				H'''	1.45		
				H ^{IV}	5.67		

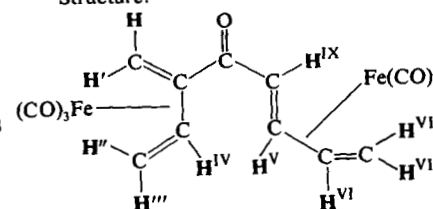
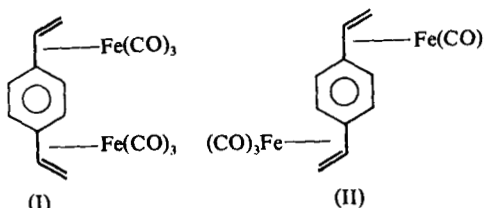
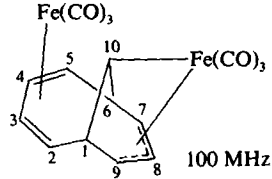
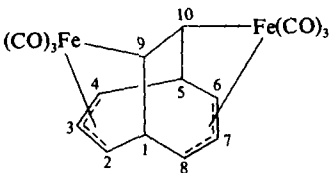
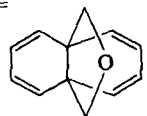
$C_{13}H_{10}Fe_2O_7$	1014	$(h^4:h^4-C_9H_{10}O)[Fe(CO)_3]_2$	$CDCl_3$	H	2.41dd	$J_{HH'} 2.4$ $J_{HH^{IV}} 1.7$	Structure:	303
				H'	0.23dd	$J_{H'H^{IV}} 0.9$		
				H''	0.54dd	$J_{H''H'''} 2.2$ $J_{H''H^{IV}} 9.8$		
				H'''	2.01dd	$J_{H'''H^{IV}} 7.3$		
				H^{IV}	5.98dddd	—	60 and 100 MHz	
				H^V	6.20dddd	$J_{H^VH^{IX}} 7.8$		
				H^VI	5.55dddd	$J_{H^VIH^{IX}} 0.8$ $J_{H^VIH^{VII}} 5.0$ $J_{H^VIH^{VIII}} 7.0$		
				H^{VII}	2.14ddd	$J_{H^{VII}H^{VIII}} 1.1$ $J_{H^{VII}H^{VIII}} 3.0$		
				H^{VIII}	0.94ddd	$J_{H^{VIII}H^{VIII}} 1.1$ $J_{H^{VIII}H^{VIII}} 9.5$		
				H^IX	1.69dd	—		
$C_{16}H_{10}Fe_2O_6$	1015	$[h^4,h^4-1,4-C_6H_4(CH=CH_2)_2]-[Fe(CO)_3]_2$	—	n.m.	—	—	NMR data indicates structure (I) not (II)	1043
								

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{19}H_{12}Fe_2O_7$	1016	(0,1,2,3- h^4 :4,5,6,7- h^4 - O=CH-CH=CH-CH= CH-CH=CH-C ₆ H ₅)- [Fe(CO) ₃] ₂	CDCl ₃	H ₋₁ 7.42s H ₋₂ 5.5-5.9m H ₋₃ 8.70 H ₋₄ 7.75t H ₋₅ , H ₋₆ 5.5-5.9m H ₋₇ 2.59d H' 2.78bs	— — $J_{2,3}$ 11 $J_{3,4} = J_{4,5}$ 8.5 — $J_{6,7}$ 9 —	7-Phenylhepta-2,4,6-trienaldiiron hexacarbonyl	313
$C_{20}H_{14}Fe_2O_7$	1017	(0,1,2,3- h^4 :4,5,6,7- h^4 - O=CH-CH=CH-CH= CH-CH=CH- <i>p</i> -C ₆ H ₄ CH ₃)- [Fe(CO) ₃] ₂	CDCl ₃	H ₋₁ 7.42s H ₋₂ 5.47-5.87 H ₋₃ 1.25dd H ₋₄ 2.42t H ₋₅ , H ₋₆ 5.47-5.87 H ₋₇ 2.20d	— — $J_{2,3}$ 8 $J_{3,4}$ 9 $J_{4,5}$ 9 $J_{6,7}$ 8	7- <i>p</i> -Tolyhepta-2,4,6-trienaldiiron hexacarbonyl	313
$[C_{20}H_{24}Fe_2NO_6]^+$	1018	{[h^4 -CH ₃ CH'=CH"-CH'''= CH ^{IV} -CH ^V (CH ^{VI}) ₂ NH]- [Fe(CO) ₃] ₂ , HCl	CD ₃ OD	H 1.50 H' 2.39 H'' 5.44 H''' 5.17 H ^{IV} 2.07 H ^V 2.70 H ^{VI} 1.38	— — — — — — —	Two diastereoisomers of the hydrochloride Isomer I 100 MHz	309

				H 1.49 H' 2.38 H'' 5.50 H''' 5.22 H^{IV} 2.10 H^V ~2.6 H^{VI} 1.28	— — — — — — —	Isomer II		
C ₁₉ H ₁₆ Fe ₂ O ₇	1019	(<i>h</i> ⁴ : <i>h</i> ⁴ -C ₁₃ H ₁₆ O)[Fe(CO) ₃] ₂	C ₆ D ₆	n.a.			2,3,4,5-Tetramethyl-6,7-dimethylenecyclohepta-2,4-diene-1-one diiron hexacarbonyl. Signals at δ 1.64d, 1.50d, 0.64s (CH ₂ protons in ratio 1:1:2, <i>J</i> 2.4 Hz), 2.08s, 1.03s, 0.78s, 0.55 (CH ₃ protons)	539
C ₁₆ H ₁₀ Fe ₂ O ₆	1020	(1,2,3,4- <i>h</i> ⁴ :7,8,9,10- <i>h</i> ⁴ -C ₁₀ H ₁₀)-[Fe(CO) ₃] ₂	CDCl ₃	H₋₁, H₋₆ 3.8 H₋₂, H₋₅ 3.0 H₋₃, H₋₄ 5.4 H₋₇, H₋₈ } 3.5 H₋₉, H₋₁₀ }	— — — —	Octahaptobicyclo[4.2.2]-deca-2,4,7,9-tetraenediiron hexacarbonyl	540	
C ₁₆ H ₁₀ Fe ₂ O ₆	1021	(<i>h</i> ⁴ : <i>h</i> ⁴ -C ₁₀ H ₁₀)[Fe(CO) ₃] ₂	CS ₂	H₋₁ 3.87 H₋₂ 4.85 H₋₃, H₋₄ 4.6 H₋₅ 2.87 H₋₆ 1.42 H₋₇ 3.32 H₋₈ 3.71	<i>J</i>_{1,8} 7.5 — — <i>J</i>_{5,6} 11.5 <i>J</i>_{6,7} 7.5 <i>J</i>_{7,8} 7.5 —	Structure:	541	
							100 MHz	
				H₋₉, H₋₁₀ 3.05	—			

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{16}H_{10}Fe_2O_6$	1022	$(h^4:h^4-C_{10}H_{10})[Fe(CO)_3]_2$	$CHCl_3$	H_{-1}, H_{-6} 2.81m H_{-2}, H_{-5} 3.62m H_{-3}, H_{-4} 5.20 $H_{-7}, H_{-8}, \sim 4.4$ H_{-9} H_{-10} 0.81	$J_{1,2} 5.1$ $—$ $J_{2,3} = J_{4,5} = 8$ $J_{7,10} = J_{9,10} = 1.4$	Structure: 	542
$C_{16}H_{10}Fe_2O_6$	1023	$(h^4:h^4-C_{10}H_{10})[Fe(CO)_3]_2$	CD_2Cl_2	H_{-1}, H_{-5} 2.96 H_{-2} 4.81 H_{-3} 4.34 H_{-4} 4.71 H_{-6} 4.81 H_{-7} 4.34 H_{-8} 4.71 H_{-9}, H_{-10} 1.92	$J_{1,9} 10.0$ $J_{5,10} 10.0$ $J_{1,2} 7.0$ $J_{2,3} 8.0$ $J_{3,4} 7.0$ $J_{4,5} 8.0$ $J_{5,6} 7.0$ $J_{6,7} 8.0$ $J_{7,8} 7.0$ $J_{1,8} 8.0$ $—$	Structure:  Reference CH_2Cl_2 (δ 5.3) 100 MHz	543
$C_{18}H_{12}Fe_2O_7$	1024	$(h^4:h^4-C_{12}H_{12}O)[Fe(CO)_3]_2$	—	n.m.	—	$C_{12}H_{12}O =$ 	544

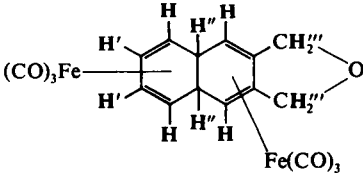
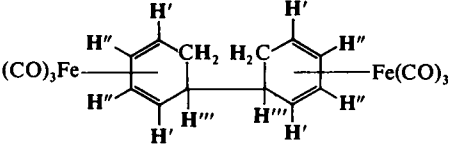
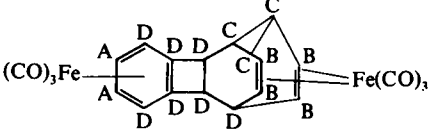
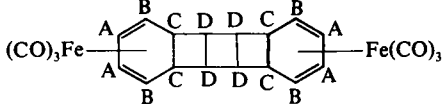
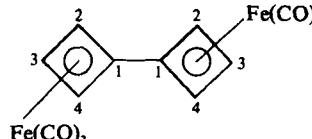
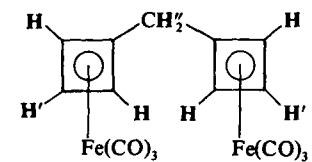
$C_{18}H_{12}Fe_2O_7$	1025	$(h^4:h^4-C_{12}H_{12}O)[Fe(CO)_3]_2$	$CDCl_3$	H H' H''	2.98b 2.84b 5.33–5.15m 2.68b	— — — —	Structure:	395
								
				H'''	4.87–4.55*	J 11	*AB quartet	
$C_{22}H_{14}Fe_2O_6$	1026	$(1,2,3,4-h^4-5,6,7,8-h^4-C_{16}H_{14})[Fe(CO)_3]_2$	—	n.m.		—	$C_{16}H_{14}$ = 9,10-dihydro-2-phenylnaphthalene	1049
$C_{18}H_{14}Fe_2O_6$	1027	$(h^4:h^4-C_{12}H_{14})[Fe(CO)_3]_2$	—	H H' H'' H'''	1.72 2.92 5.18 1.10	— — — —	Structure:	358
								
$C_{22}H_{16}Fe_2O_6$	1028	$(h^4:h^4-C_{16}H_{16})[Fe(CO)_3]_2$	$CDCl_3$	H_A H_B H_C H_D	5.44 3.34 1.67 2.66	— — — —	Structure:	363
								
$C_{22}H_{16}Fe_2O_6$	1029	$(h^4:h^4-C_{16}H_{16})[Fe(CO)_3]_2$	CS_2	H_A H_B H_C H_D	5.2 3.2 2.65 1.9	— — — —	Structure:	363
								

TABLE VII—*cont.*

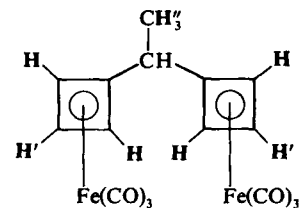
Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{14}H_6Fe_2O_6$	1030	$(h^4:h^4-C_8H_6)[Fe(CO)_3]_2$	CCl_4	H_{-2}, H_{-4} 3.83 H_{-3} 3.79	$J(^{13}C_2-H_2)$ 188.8 $J(^{13}C_3-H_3)$ 187.4	Structure: 	545
$C_{15}H_7Fe_2O_6$	1031	$(h^4:h^4-C_9H_7)[Fe(CO)_3]_2$	SO_2	H 5.33s H' 5.60s H'' 7.26s	$\left. \begin{array}{c} - \\ - \\ - \end{array} \right\}$	Structure: T 40° 	546
				H 5.37d, 5.23d H' 5.62s H'' 7.23s	$\left. \begin{array}{c} - \\ - \\ - \end{array} \right\} J 9$	T -50°	

$C_{16}H_9Fe_2O_6$ 1032 ($h^4:h^4-C_{10}H_9$)[Fe(CO) $_3$] $_2$ —

H	5.24s	—
H'	5.67s	—
H''	1.72s	—

Structure:
T 40°

546



H	5.34d,	J 9
	5.22d	
H'	5.57s	
H''	1.70s	

T 10°

$C_{18}H_{20}B_{10}Fe_2O_6$ 1033 ($h^4:h^4-C_{12}H_{20}B_{10}$)[Fe(CO) $_3$] $_2$ CHCl $_3$

H	5.58	—
H'	3.14	—
H''	3.11	—

Carboranylene-bis-
cyclopentadienediiron
hexacarbonyl
Structure:

350

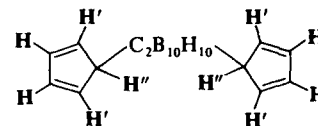
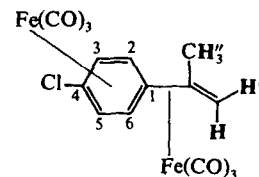
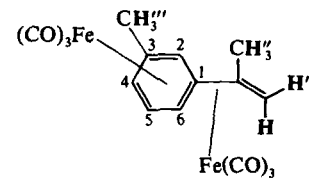
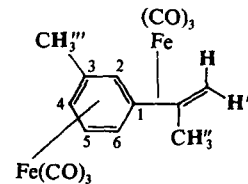


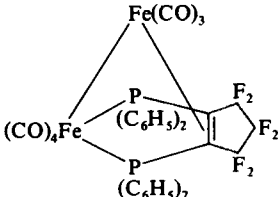
TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{16}H_{12}Fe_2O_6$	1034	$[h^4:h^4-CH_2=C(CH_3)C_6H_4-(CH_3)][Fe(CO)_3]_2$	$CDCl_3$	H	0.32d	$J_{HH'} 2.3$	Two isomers:	547
				H'	1.64d			
				H''	2.07s			
				H'''	1.57s			
				H ₋₂	1.72bs			
				H ₋₄	5.97d	$J_{4,5} 4.5$		
				H ₋₅	6.45dd	$J_{5,6} 6.5$		
				H ₋₆	3.65bd	—		
				H	0.21d	$J_{HH'} 2.4$		
				H'	1.57d			
				H''	2.10s			
				H'''	2.58s			
				H ₋₂	3.70bs			
				H ₋₄	6.05bd	$J_{4,5} 6.0$		
				H ₋₅	3.30dd	$J_{5,6} 5.1$		
				H ₋₆	1.89bd	—		
$C_{15}H_9ClFe_2O_6$	1035	$[h^4:h^4-CH_2=C(CH_3)C_6H_4Cl]-[Fe(CO)_3]_2$	—	H	0.13	$J_{HH'} 2.4$	Structure:	327
				H'	1.56			
				H''	—	—		
				H ₋₂	3.47	$J_{2,3} 6.5$		
				H ₋₃	6.64	$J_{3,5} 2.1$		
				H ₋₅	3.67	$J_{5,6} 5.3$		
				H ₋₆	1.74	$J_{2,6} 1.5$		



$C_{14}H_8Fe_2O_7$	1036	$(h^5-C_5H_5)(1-h^1-2,3-h^2-COCH'=CH_2)[Fe(CO)_2][Fe(CO)_4]$	$CDCl_3$	H H' H'' _{cis} H'' _{trans}	4.90 3.95 2.19 2.57	— — $J_{H'H''}$ 7.0 $J_{H'H''}$ 14.5 $J_{H''H''}$ 1.7	—	223
$C_{20}H_{12}Fe_2O_7$	1037	$(h^5-C_5H_5)(1-h^1-2,3-h^2-COCH'=CH''C_6H_5'')[Fe(CO)_2]-[Fe(CO)_4]$	$CDCl_3$	H H' H'' H'''	5.00 4.74 4.74 7.14-7.70	— — — —	Reference hexa-methyldisiloxane	223
$C_{30}As_2F_{20}Fe_2O_6$	1038	$[Fe(AsC_6F_5)_2(CO)_3]_2$	$CHCl_3$	F ₋₂ , F ₋₆ F ₋₃ , F ₋₅ F ₋₄	122.0 157.4 146.2	— — —		130
$C_{12}H_{18}Ge_3Fe_2O_6$	1039	$Fe_2[Ge(CH_3)_2]_3(CO)_6$	—	H	1.28	—	—	548
$C_{10}H_2F_6Fe_2O_6P_2$	1040	$\{Fe(H)[P(CF_3)_2](CO)_3\}_2$	—	H F H F	-5.82t -105.8* -5.60t -144.4*, -106.6	J_{PH} 44.7 J_{PH} 55.0, 1.0 $ J_{PP} $ 175 J_{PH} 41.8 J_{FF} 8.5	$trans-H$ *Relative to C_6F_6 $cis-H$ *Relative to C_6F_6	549
$C_{30}F_{20}Fe_2O_6P_2$	1041	$\{Fe[P(C_6F_5)_2](CO)_3\}_2$	$CHCl_3$	F ₋₂ , F ₋₆ F ₋₃ , F ₋₅ F ₋₄	123.8 158.8 147.4	— — —		130
$C_{14}H_{18}Fe_2O_6S_2$	1042	$[Fe(CH_3)_3CS(CO)_3]_2$	—	H	1.38, 1.28	—	Two isomers	188

TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References	
(vi) Heptacarbonyl derivatives:								
$C_{36}H_{20}F_6Fe_2O_7P_2$	1043	$\{h^2-C_5F_6[P(C_6H_5)_2]_2\}-[Fe(CO)_3][Fe(CO)_4]$	$(CH_3)_2CO$	F	99.4d, 110.9d, 106.8d, 111.4d, 124.4d, 128.6d	J 264 J 272 J 238	Structure: 	550
$C_{10}H_4Fe_2O_7$	1044	$(2-h^1-1,2,3-h^3-CH_2^{\cdot\cdot}C^{\cdot\cdot}CH_2)-[Fe(CO)_3][Fe(CO)_4]$	—	H	3.77s, 2.40s	— —	T — 67° to +70°	288
(vii) Octacarbonyl derivatives:								
$C_{15}H_6Fe_2O_8$	1045	$Fe_2(CHC_6H_5)(CO)_8$	CCl_4	H H'	6.96s 7.25m	— —	—	986
			$(CD_3)_2CO$	H H'	6.98s 6.65	— —		
$C_{13}F_6Fe_2O_8$	1046	$(h^2:h^2-C_5F_6)[Fe(CO)_4]_2$	—	—	—	—	Hexafluorocyclopentadiene	551
$C_{17}H_{14}Fe_2O_{10}$	1047	$[h^2:h^2-C_5H_4(OCH_2CH_2)_2]-[Fe(CO)_4]_2$	C_6H_6	H H' H''	4.45* 4.5m 1.1t	— — —	1,1-Diethoxycyclopentadiene *Centre of AB quartet	413
$C_{15}H_8Fe_2O_8$	1048	$(h^2:h^2-C_7H_8)[Fe(CO)_4]_2$	C_6D_6	n.a.	—	—	Spiro[2.4]hepta-4,6-dienediiron octacarbonyl. Signals at δ 1.32t, 2.43t, 3.95t, 4.22t, in ratio 1:1:1:1	351

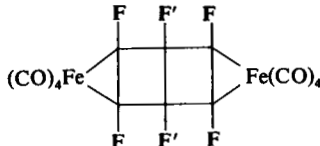
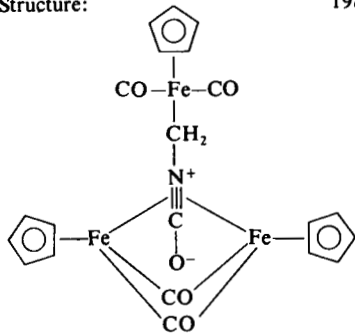
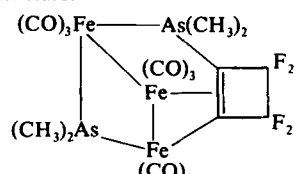
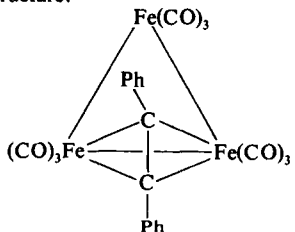
$C_{16}H_{12}Fe_2O_8$	1049	$(h^2: h^2-C_8H_{12})[Fe(CO)_4]_2$	—	n.a.	—	1,5-Cyclooctadiene- diiron octacarbonyl Signals at δ 3.7m, 2.7m, 1.8m (integrating to 4H each)	281
$C_{14}F_6Fe_2O_8$	1050	$(h^2: h^2-C_6F_6)[Fe(CO)_4]_2$	$CHCl_3$	F F'	155.6 135.8	Structure:	240
							
$C_{14}H_{20}Fe_2O_8Si_2$	1051	$[(CH_3)_3SiFe(COH)(CO)_3]_2$	—	H	0.30	—	552
$C_{20}H_{36}Fe_2O_8Si_4$	1052	$\{(CH_3)_3SiFe[COSi(CH_3)_3](CO)_3\}_2$	—	H	0.34, 0.27	—	552
<i>(b) Triiron complexes</i>							
$C_{21}H_{17}Fe_3NO_5$	1053	$(h^5-C_5H_5)_3(CH_2NCO)Fe_3(CO)_4$	CS_2	H	4.85*, 4.48*	Structure:	198
							
				H'	3.07	—	*In ratio 1:2

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{30}H_{24}F_{14}^-$ $Fe_3N_6O_8$	1054	$[(h^1-C_3F_7)Fe(CO)_4]_2^-$ $[Fe(N_2C_{12}H_8)_3]$	—	F 78.4, 114.6, 61.7	— — —	—	269
$C_{17}H_{12}As_2^-$ $F_4Fe_3O_9$	1055	$[h^1:h^2-C_4F_4As(CH_3)_2]^-$ $[As(CH_3)_2][Fe(CO)_3]_3$	$CHCl_3$	n.a.	—	Structure:  Signals at δ 1.05s, 1.56s, 1.70s, 2.15s (integrating to three H each). The ^{19}F NMR spectrum showed eight signals each consisting of 4 lines at 93.6, 98.7, 99.1, 101.2, 101.8, 104.0, 105.2, and 107.6 ppm relative to $CFCl_3$.	550
$C_{23}H_{10}Fe_3O_9$	1056	$(h^2:h^2-C_6H_5C\equiv CC_6H_5)^-$ $[Fe(CO)_3]_3$	CS_2	H 7.3, 6.8, 5.9	—	Structure: 	926

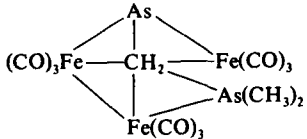
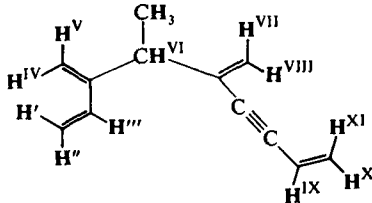
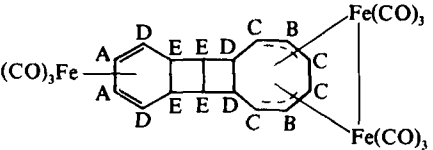
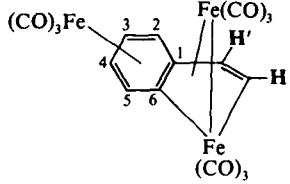
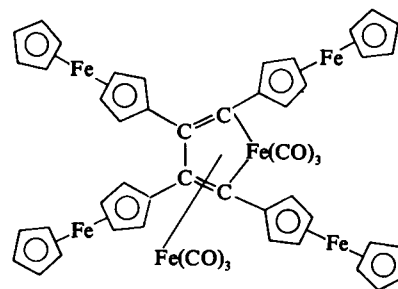
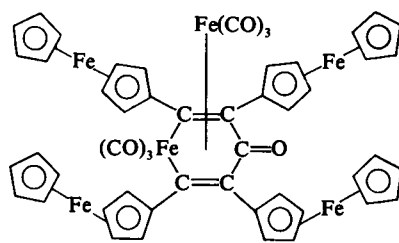
$C_{12}H_8As_2Fe_3O_9$	1057	$(h^2:h^2-AsCH_2)[As(CH_3)_2-Fe(CO)_3]_3$	$(CD_3)_2CO$	n.a.	—	Structure:	550
							
						Signals at δ 3.26s, 2.34s, 1.76 (J 2.1), 2.42, in ratio 3:3:1:1	
$C_{21}H_{14}Fe_3O_9$	1058	$(h^2:h^2:h^3-C_{12}H_{14})[Fe(CO)_3]_3$	C_6D_6	H 1.37d H' 0.28dd H'' 1.68dd H''' 7.27 H^{IV} -0.10d H^V 2.09d H^{VI} 2.15q H^{VII} 4.50q H^{VIII} 3.69d H^{IX} 6.83dd H^X 5.12d H^{XI} 5.59d	$J_{HH^{VI}}$ 6.9 $J_{H'H''}$ 2.5 $J_{H'H'''} 9.3$ $J_{H''H'''} 6.9$ $J_{H'''H^V} 2.0$ $J_{H^VH^VI} 3.2$ $J_{H^{VII}H^{VIII}}$ 3.6 $J_{H^{IX}H^X} 10.0$ $J_{H^{IX}H^{XI}} 16.8$ $J_{H^XH^{XI}} 1.0$ —	Structure:	303
							
						60 and 100 MHz	
$C_{25}H_{16}Fe_3O_9$	1059	$(h^3:h^3:h^4-C_{16}H_{16})[Fe(CO)_3]_3$	$CDCl_3$	H_A 5.15 H_B 3.60 H_C 3.13 H_D 2.71 H_E 1.55	— — — — —	Structure:	363
							

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{17}H_6Fe_3O_9$	1060	$(h^2:h^4:h^4-C_8H_6)[Fe(CO)_3]_3$	$CDCl_3$	H	5.71d	$J_{HH'}$ 5.2	Structure: 	529
				H'	6.73d	—		
				H ₋₂	3.83dd	$J_{2,3}$ 6.1 $J_{2,4}$ 1.5		
				H ₋₃	6.67m	$J_{3,4}$ 4.4		
				H ₋₄	6.43m	$J_{4,5}$ 6.1		
				H ₋₅	3.47dd	$J_{3,5}$ 1.5	100 MHz	
$C_{12}H_8Fe_3O_9S$	1061	$Fe_3(H)[SCH'(CH_3')_2](CO)_9$	$CDCl_3$	H	-22.9	—	μ -Hydrido- μ -isopropylsulphido-triiron nonacarbonyl T 38° 100 MHz	553
				H'	3.0b	—		
				H''	0.91d	J 6.7		
$C_{13}H_{10}Fe_3O_9S$	1062	$Fe_3(H)[SCH_2CH''(CH_3'')_2](CO)_9$	$CDCl_3$	H	-23.1	—	μ -Hydrido- μ - <i>sec</i> -butylsulphido-triiron nonacarbonyl T 38° 100 MHz	553
				H', H''	3.1	—		
				H'''	1.73d,	J 7.3		
					1.26t	J 7.4		
$C_{13}H_{10}Fe_3O_9S$	1063	$Fe_3(H)[SC(CH_3)_3](CO)_9$	$CDCl_3$	H	-22.8	—	μ -Hydrido- μ - <i>tert</i> -butyl sulphidotriiron nonacarbonyl T 38° 100 MHz	553 554
				H'	1.06	—		

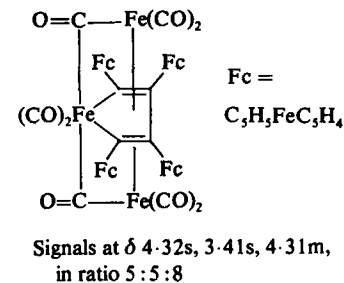
$C_{13}H_7Fe_3NO_{10}$	1064	$Fe_3(H)(CN(CH_3)_2)(CO)_{10}$	—	H H'	-17.8s 4.0s	—	Structure:	555
$C_{18}H_{12}As_2F_4Fe_3O_{10}$	1065	$Fe_3\{[As(CH_3)_2]_2C_4F_4\}(CO)_{10}$	—	Not reported	—	—		556
<i>(c) Tetrairon derivatives</i>								
$C_{24}H_{20}Fe_4O_4$	1066	$(h^5-C_5H_5)_4Fe_4(CO)_4$	$CHCl_3$ CF_3CO_2H	H H	4.84s 5.09	— —	—	557
$C_{52}H_{40}Fe_4O_6P_2$	1067	$(h^5-C_5H_5)_4Fe_4[P(C_6H_5)_2C\equiv CP(C_6H_5)_2](CO)_6$	C_6D_6	H	4.39d, 4.22s	$J_{PH} 1.8$	Structure:	494 498
$C_{52}H_{56}Fe_4O_{12}$	1068	$(h^4:h^4:h^4:h^4-C_{40}H_{56})[Fe(CO)_3]_4$	—	Complex	—	—	β -Carotenetetrairon dodecacarbonyl	558
<i>(d) Pentairon derivatives</i>								
$C_{48}H_{36}Fe_5O_4$	1069	$(h^5-C_5H_5)_4[h^4:h^5:h^5:h^5:h^5:C_5O-(C_5H_4)_4]Fe_5(CO)_3$	$CDCl_3$	H	3.95, 4.46	— —	Tetraferrocenyl cyclopentadienoneiron tricarbonyl	559

TABLE VII—cont.

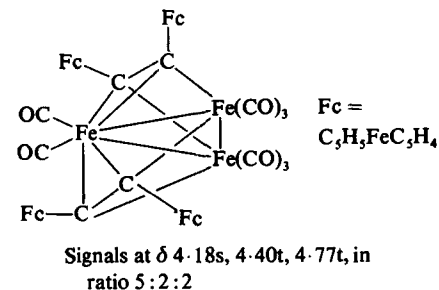
Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{50}H_{36}Fe_6O_6$	1070	$(h^5-C_5H_5)_4[C_4Fe(C_5H_5)]-Fe_3(CO)_6$	$CDCl_3$	H 3.92, 4.25	— —	Structure: 	559
$C_{51}H_{36}Fe_6O_7$	1071	$(h^5-C_5H_5)_4[C_3FeO(C_4H_4)_4]-Fe_3(CO)_6$	$CDCl_3$	H 4.19, 4.35	— —	Structure: 	559

(e) *Heptairon derivatives*

$C_{52}H_{36}Fe_7O_8$ 1072 $[C_4Fe(Fc)_4]Fe_2(CO)_8$ $CDCl_3$ n.a. — Tentative Structure: 559



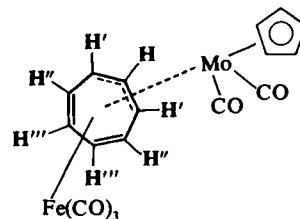
$C_{52}H_{36}Fe_7O_8$ 1073 $[C_2(Fc)_2]_2Fe_3(CO)_8$ $CDCl_3$ n.a. — Tentative structure: 559

(f) *Mixed iron-transition metal complexes*

$C_{11}H_3Co-FeHgO_6$ 1074 $(h^5-C_5H_5)Fe(CO)_2HgCo(CO)_4$ $CDCl_3$ **H** 5.03 — — 136
 $C_{14}H_3CoFe_2O_9$ 1075 $(h^5-C_5H_5)CoFe_2(CO)_9$ — **H** 5.23 — 100 MHz 560

TABLE VII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{13}H_8$ - CrFeO ₇ S	1076	$(h^5-C_5H_5)Fe(CO)_2$ - Cr(SCH ₃)(CO) ₅	C ₆ H ₆	H	4.02	—	—	561
				H'	1.70	—		
$C_{22}H_{10}Fe_2$ - Mn ₂ O ₁₂ S ₂	1077	$\{(h^5-C_5H_5)Fe(CO)_2$ - [S-Mn(CO) ₄] ₂	C ₆ H ₆	H	4.15	—	Bis[tetracarbonylmanganese (cyclopentadienyldicarbonyl iron) sulphide]	141
$C_{15}H_{10}Cl_2$ - FeMoO ₃ Sn	1078	$[(h^5-C_5H_5)Fe(CO)_2](SnCl_2)$ - [$(h^5-C_5H_5)Mo(CO)_3$]	CDCl ₃	H	5.67	—	—	142
					5.41	—		
$C_{17}H_{12}FeMoO_5$	1079	$(h^4:h^3-C_7H_7)[Fe(CO)_3]$ - [$(h^5-C_5H_5)Mo(CO)_2$]	CDCl ₃ / CD ₃ C ₆ D ₃ (4:1)	H	4.82t	—	Structure:	562
				H'	4.37t	—		
				H''	3.77m	—		
				H'''	5.37dd	—		
			CDCl ₃	H	4.98	—	T -71°	
				H'	4.50	—	(at room temperature only two	
				H''	3.83	—	signals at δ 4.57bs (7-membered	
				H'''	5.10	—	ring) and 5.13s (5-membered	
							ring	



$C_{29}H_{23}^-$ FeNiO ₃ P	1080	$(h^5-C_5H_5)Ni(C_6H_5C\equiv CCH_3^-)$ [P(C ₆ H ₅) ₂]Fe(CO) ₃	—	H	4.98	—	Isomer I	996
				H'	7.9–7.0	—		
				H''	3.12d	$J_{PH''}$ 4.8		
				H	5.05	—	Isomer II	
				H'	7.9–7.1	—		
				H''	1.54d	$J_{PH''}$ 13.2		
$C_{34}H_{25}^-$ FeNiO ₃ P	1081	$(h^5-C_5H_5)Ni(C_6H_5C\equiv CC_6H_5^-)$ [P(C ₆ H ₅) ₂]Fe(CO) ₃	CDCl ₃	H	5.07	—	—	996
				H'	8.0–6.8	—		
$C_{30}H_{23}^-$ FeNiO ₃ P	1082	$(h^5-C_5H_5)Ni(C_6H_5C\equiv CCO_2^-CH_3^-)$ [P(C ₆ H ₅) ₂]Fe(CO) ₃	—	H	5.16	—	Isomer I	996
				H'	8.1–7.1	—		
				H''	3.40	—		
				H	5.07	—	Isomer II	
				H'	8–7	—		
				H''	3.86	—		
$C_{26}H_{21}^-$ FeNiO ₇ P	1083	$(h^5-C_5H_5)Ni(CH_3O_2CC\equiv CCO_2^-CH_3^-)$ [P(C ₆ H ₅) ₂]Fe(CO) ₃	—	H	5.18	—	—	996
				H	3.89,	—		
					3.58	—		
				H''	8.1	—		
$C_{21}H_{15}^-$ FeNiO ₄ P	1084	$(h^5-C_5H_5)Ni[P(C_6H_5)_2]Fe(CO)_4$	CDCl ₃	H	5.42	—	Structure:	517
				H'	7.8–7.2	—		1041

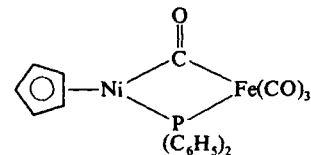
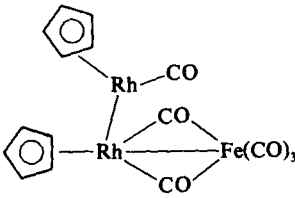


TABLE VII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{22}H_{15}FeNiO_3P$	1085	$(\eta^5-C_5H_5)Fe(CO)_2[P(C_6H_5)_2-Ni(CO)_3]$	C_6D_6	H 5.93d	J_{PH} 1.2	Structure:  $(CO)_2Fe-P(C_6H_5)_2-Ni(CO)_3$	517
$C_{19}H_{24}FeNiO_3$	1086	$[C_8(CH_3)_8]FeNi(CO)_3$	—	H 2.37, 1.87, 1.60	— — —	Structure? [One of the products obtained from tetramethylcyclobutadiene nickel chloride and $Fe(CO)_5$.]	341
$C_{13}H_5FeO_{10}Re$	1087	$\{4-h^1-[Re(CO)_5]-3,4-h^2-[Fe(CO)_4]CH_3C_2COCH'=CH''\}$	—	H 2.21 H' 4.69 H'' 8.85	— $J_{H'H''}$ 13.3	Reference hexamethyldisiloxane	223
$C_{16}H_{10}FeO_6Rh_2$	1088	$(\eta^5-C_5H_5)_2Rh_2Fe(CO)_6$	—	H 5.50	—	Structure:  100 MHz	560

$C_{18}H_{10}Fe_2O_8Rh_2$	1089	$(h-C_5H_5)_2Rh_2Fe_2(CO)_8$	—	H	5.72	—	Structure:	560
$C_{14}H_5Fe_2O_9Rh$	1090	$(h^5-C_5H_5)RhFe_2(CO)_9$	—	H	5.41	—	100 MHz Structure:	560
$C_{16}H_5Fe_3O_{11}Rh$	1091	$(h^5-C_5H_5)RhFe_3(CO)_{11}$	—	H	4.86	—	100 MHz Structure:	560

TABLE VII—*cont.*

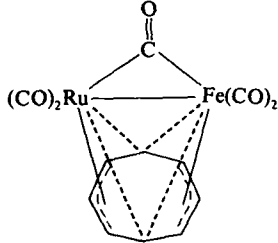
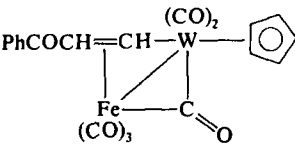
Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{13}H_8FeO_5Ru$	1092	$(C_8H_8)Ru(CO)_2Fe(CO)_3$	—	Not reported	—	Proposed Structure:  Fluxional system giving one sharp signal at ambient temperatures	563
$C_{13}H_2FeO_{13}^-$ Ru_{13}	1093	$Fe(Ru)_3(H)_2(CO)_{13}$	—	H $-18.7s$	—		564
$C_{20}H_{12}FeO_7W$	1094	$(h^5-C_5H_5)(CH'=CH''COC_6H_5'')-[Fe(CO)_4][W(CO)_2]$	$CDCl_3$	H 5.39 H' 8.14 H'' 4.19 H''' 7.98, 7.44	— $J_{H'H''} 10.0$	Structure:  Reference hexamethyl disiloxane	223

TABLE VIII

Ruthenium complexes

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
(1) <i>MONOHAPTO LIGANDS</i>							
(a) <i>Monocarbonyl derivatives</i>							
$C_{22}H_{19}BN_8ORu$	1	$(1-h^1-2-C_6H_4 \cdot N=N \cdot C_6H_5)Ru \cdot [(C_3H_5N_2)_3BH](CO)$	$(CD_3)_2CO$	H_{-3} 6.30 H_{-4} 6.93	— —	Structure	565
				H_{-5} 7.74 H_{-6} 8.29 H' 7.20	— — —	Other signals at δ 6.02t, 7.27d, and 7.77d	
$C_{45}H_{38}^- ClNO_2P_2Ru$	2	$(1-h^1-4-CN \cdot C_6H_4CH_3)Ru(H) \cdot (Cl)[P(C_6H_5)_3]_2(CO)$	$CDCl_3$	H -5.5t	J_{PH} 19	<i>trans</i> -arrangement of phosphine ligands indicated since H gives a triplet due to coupling with two equivalent phosphorus atoms	566
$C_{45}H_{38}^- ClNO_3P_2Ru$	3	$(1-h^1-4-CN \cdot C_6H_4CH_3)Ru(H) \cdot (OCIO_3)[P(C_6H_5)_3]_2(CO)$	$CDCl_3$	H -5.4t	J_{PH} 18		

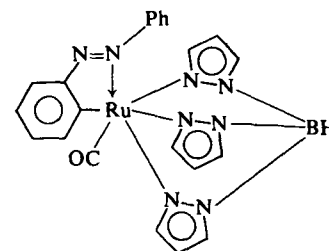


TABLE VIII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
<i>(b) Dicarbonyl derivatives</i>								
$C_{15}H_{22}F_3^-$ IO_8P_2Ru	4	$(CF_3)Ru(I)[P(OCH_2)_3^-CCH_2CH_3]_2(CO)_2$	$CDCl_3$	H	4.30t	$J_{PH} 3.0$	100 MHz	264
				H'	1.3q	—		
				H''	0.8t	—		
				F	0.07s	—		
$C_{20}H_{22}ClF_3^-$ O_2P_2Ru	5	$(1-h^1-CF=CF_2)Ru(Cl)-[P(CH_3)_2C_6H_5]_2(CO)_2$	$CDCl_3$	H	1.86t	$J_{PH} 8.0$	100 MHz	272
				H'	7.44m	—		
			$CHCl_3$	F	161dd	$J_{cis} 37.0$	94.1 MHz	
				F'_{cis}	92.7dt	$J_{gem} 93.0$		
				F'_{trans}	127.6dt	$J_{trans} 108.0$		
$[C_{14}H_9Cl_2^-$ $N_2O_2Ru]^-$	6	$[(1-h^1-2-C_6H_4 \cdot N=N \cdot C_6H_5^-)Ru(Cl)_2(CO)_2]^-$	$(CD_3)_2CO$	H ₋₃	7.08	—	Tetramethylammonium salt (δ 2.92s)	565
				H ₋₄	7.82	—		
				H ₋₅	8.00	—		
				H ₋₆	8.10	—		
				H'	7.37	—		
$C_{17}H_{13}ClN_4^-$ O_2Ru	7	$(1-h^1-2-C_6H_4N=NC_6H_5)Ru(Cl)-(C_3H_4N_2)(CO)_2$	$CDCl_3$	H ₋₃	7.10	—	$C_3H_4N_2$ = imidazol-3-yl	565
				H ₋₄	7.28	—		
				H ₋₅	7.91	—		
				H ₋₆	8.20	—		
				H'	7.26	—		

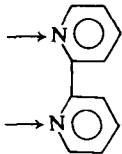
				H''	7.88s, 7.30s, 7.20s	—		
C ₁₉ H ₁₄ ClN ₃ - O ₂ Ru	8	(1- <i>h</i> ¹ -2-C ₆ H ₄ N=NC ₆ H ₅)Ru(Cl)- (C ₅ H ₅ N)(CO) ₂	CDCl ₃	H ₋₃	~ 7.2	—	—	565
				H ₋₄	7.48	—		
				H ₋₅	7.95	—		
				H ₋₆	8.27	—		
				H'	7.18	—		
				H''	8.68	—		
$\left\{ \begin{array}{l} [C_{24}H_{17}N_4- \\ O_2Ru]^+ \\ [C_{14}H_9Cl_2N_2- \\ O_2Ru]^- \end{array} \right\}$	9	$\left\{ \begin{array}{l} [(1-h^1-2-C_6H_4N=NC_6H_5)Ru- \\ (C_{10}H_8N_2)(CO)_2]^+ \\ [(1-h^1-2-C_6H_4N=NC_6H_5)Ru- \\ (Cl)_2(CO)_2]^- \end{array} \right\}$	(CD ₃) ₂ CO	H ₋₃	7.02	—	C ₁₀ H ₈ N ₂ = 	565
				H ₋₄	7.24	—		
				H ₋₅	7.81	—		
				H ₋₆	8.32	—		
				H'	7.54	—		
				H''	9.42, 8.7-8.4	—		
C ₂₃ H ₁₉ BN ₈ O ₂ Ru	10	(1- <i>h</i> ¹ -2-C ₆ H ₄ N=NC ₆ H ₅)Ru- [(C ₅ H ₅ N ₃) ₃ BH](CO) ₂	(CD ₃) ₂ CO	H ₋₃	6.32	—	C ₃ H ₃ N ₂ = pyrazol-1-yl	565
				H ₋₄	6.77	—		
				H ₋₅	6.97	—		
				H ₋₆	8.04	—		
				H'	7.56	—		
				H''	7.92d, 7.32d, 6.24t	—		
C ₁₆ H ₁₂ N ₂ O ₄ Ru	11	(1- <i>h</i> ¹ -2-C ₆ H ₄ N=NC ₆ H ₅)Ru- [O=C(CH ₃) ₂ ···O](CO) ₂	CS ₂	H ₋₃	7.08	—	—	565
				H ₋₄	7.71	—		
				H ₋₅	7.90	—		
				H ₋₆	8.18	—		
				H'	7.37	—		
				H''	1.47s	—		

TABLE VIII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{19}H_{16}N_2O_4Ru$	12	$(1-h^1-2-C_6H_4N=NC_6H_5)Ru-[O=C(CH_3)=CH''=C(CH_3)=O](CO)_2$	CCl_4	H_{-3}	7.18	—	—	565
				H_{-4}	7.64	—		
				H_{-5}	7.84	—		
				H_{-6}	8.12	—		
				H'	7.33	—		
				H''	1.74s,	—		
					1.59s	—		
$C_{32}H_{24}ClN_2O_2PRu$	13	$(1-h^1-2-C_6H_4N=NC_6H_5)Ru(Cl)-[P(C_6H_5)_3](CO)_2$	$CDCl_3$	H_{-3}	7.08	—	—	565
				H_{-4}	7.54	—		
				H_{-5}	8.00	—		
				H_{-6}	8.26	—		
				H'	7.6–7.18	—		
				H''	7.28	—		
$[C_{46}H_{38}NO_2P_2Ru]^+$	14	$\{(h^1-p-CNC_6H_4CH_3)Ru(H)-[P(C_6H_5)_3]_2(CO)_2\}^+$	$CDCl_3$	H	–6.0t*	$J_{PH} 17$	Perchlorate	566
				H	–7.3t†	$J_{PH} 14$		
(c) <i>Tricarbonyl derivatives</i>								
$C_{23}H_{18}BrO_3PRu$	15	$[\alpha-h^1-1,2-CH_3CH'C_6H_4P(C_6H_5)_2]-Ru(Br)(CO)_3$	$CDCl_3$	H	2.03d,	$J 7.5$	—	267
					1.76d	$J 7.5$		
				H'	3.9q			

$C_{23}H_{18}ClO_3PRu$	16	$[\alpha\text{-}h^1\text{-}1,2\text{-}CH_3CH'C_6H_4P(C_6H_5)_2]\text{-}Ru(Cl)(CO)_3$	$CDCl_3$	H H'	1.97d, 1.77d 4.14q	J_7 J_7	—	267
(2) DIHAPTO LIGANDS								
(a) Monocarbonyl derivatives								
$C_{40}H_{35}ClO_2P_2Ru$	17	$(h^2\text{-}O=C\text{-}CH_2CH_3)Ru(Cl)\text{-}[P(C_6H_5)_3]_2(CO)$	—	H H' H''	+4.45q +5.27t -2.14m	$J_7\text{-}5$ —	Relative to CH_2Cl_2 (!) at 100 MHz π -bonded acyl complex	567
(b) Dicarboxyl derivatives								
$C_{20}H_{23}F_3O_2P_2Ru$	18	$(h^2\text{-}CHF=CF_2)Ru[P(CH_3)_2\text{-}C_6H_5]_2(CO)_2$	$CDCl_3$ $CHCl_3$	H H' H'' F F'	4.57dm 1.64t 7.32m 211.0 105.3, 98.5	J_{HF} 66.0 J_{PH} 8.0 — — J_{gem} 170.0	<i>cis</i> -carbonyl ligands; <i>trans</i> - phosphine ligands 100 MHz 94.1 MHz	272
$C_{10}H_{19}F_3O_8P_2Ru$	19	$(h^2\text{-}CHF=CF_2)Ru[P(OCH_3)_3]_2(CO)_2$	$CDCl_3$ $CHCl_3$	H H' F F'	5.57m 3.70d 208.6 104.1	J_{HF} 59.0 $J_{HF'}$ 11.5 J_{PH} 12.0 — J_{gem} 170.0	<i>trans</i> -carbonyl ligands; <i>cis</i> -P ligands 100 MHz 94.1 MHz	272
$C_{20}H_{22}F_4O_2P_2Ru$	20	$(h^2\text{-}CF_2=CF_2)Ru[P(CH_3)_2C_6H_5]_2(CO)_2$	$CDCl_3$	H H' F	1.72t 7.37m 115.2t	J_{PH} 8.0 — —	<i>cis</i> -carbonyl ligands; <i>trans</i> - phosphine ligands 100 MHz 94.1 MHz	272

TABLE VIII—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{10}H_{18}F_4O_8P_2Ru$	21	$(\eta^2-CF_2=CF_2)Ru[P(OCH_3)_3]_2-(CO)_2$	CHCl ₃	F	113.2	$J_{gem} 180 \pm 20$ $J_{trans} -39.6$ $J_{cis} 10.0$ $J_{PF_{trans}} 59.0$ $J_{PF_{cis}} 12.2$	<i>trans</i> -carbonyl ligands; <i>cis</i> -P ligands 94.1 MHz	272
			CDCl ₃	H	3.70d	$J_{PH} 12.5$	Poorly resolved spectrum	568
				F	113.2	$J_{PF} 46.5,$ 26.1 (?)		
$C_{10}H_{18}ClF_3O_8P_2Ru$	22	$(\eta^2-CFCl=CF_2)Ru[P(OCH_3)_3]_2-(CO)_2$	CDCl ₃	H	3.76, 3.72	$J_{PH} 12.0$ $J_{PH} 12.0$	<i>trans</i> -carbonyl ligands; <i>cis</i> -P ligands, 100 MHz 94.1 MHz	272 569
				F	122.0	$J_{PF_{trans}} 46.0$ $J_{PF_{cis}} 7.5$		
				F'	104.8 95.7	$J_{gem} 163.0$ $J_{trans} 44.0$ $J_{cis} 7.5$ $J_{PF'_{trans}} 61.0$ $J_{PF'_{cis}} 14.0$	Comparison of the ¹⁹ F coupling constants with uncoordinated chlorotrifluoroethylene and with the corresponding osmium complex indicates a more substantial change in the geometry of the C ₂ F ₃ Cl ligand coordinated onto Os compared to Ru and suggests that even with extreme bonding situations (i.e. two σ -bonded structures) there are still graduations in bond type dependent on the nature of the metal	

TABLE VIII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{20}H_{22}F_6N_2^-$ O_8P_2Ru	28	$[h^2-C(CN)CF_3=C(CN)CF_3]Ru-$ $[P(OCH_2)_3CCH_2CH_3]_2(CO)_2$	$CDCl_3$	H	4.36d, 4.30d	J_{PH} 4.5	100 MHz	568
				H'	1.3	—		
				H''	0.8	—		
				F	98.7s, 95.0d	J_{PF} 6.0		
$C_{20}H_{22}F_6N_2^-$ O_8P_2Ru	29	$[h^2-C(CN)_2=C(CF_3)_2]Ru-$ $[P(OCH_2)_3CCH_2CH_3]_2(CO)_2$	$CDCl_3$	H	4.38d, 4.30d	J_{PH} 4.5	100 MHz	568
				H'	1.3	—		
				H''	0.8	—	570	
				F	54.4d	J_{PF} 11.5		
$C_{12}H_{18}F_6O_8P_2Ru$	30	$(h^2-C_4F_6)Ru[P(OCH_3)_3]_2(CO)_2$	$CDCl_3$	H	3.64d	J_{PH} 12.0	<i>trans</i> -carbonyl ligands; <i>cis</i> -P ligands. 100 MHz 94.1 MHz. C_4F_6 = hexafluoro-cyclobut-1-ene	272
				F_{-1}, F_{-2}	119.0	—		
				F_{-3}, F_{-4}	124.7, 94.7	J_{gem} 190.0		
$C_{13}H_{18}F_6O_9P_2Ru$	31	$[1,3-h^2-C(CF_3)=C(CF_3)CO]Ru-$ $[P(OCH_3)_3]_2(CO)_2$	$CDCl_3$	H	3.65t	J_{PH} 11.5	1-Rhodiocyclobut-3-ene-2-one derivative 100 MHz ^{19}F signals at 94.1 MHz	297
				F	58.0qt	J_{FF} 9.0		
						J_{PF} 1.0		
					64.2qt	J_{FF} 1.0 J_{PF} 5.0		
$C_{26}H_{22}F_{12}^-$ O_2P_2Ru	32	$[1,4-h^2-C(CF_3)=C(CF_3)-$ $C(CF_3)=C(CF_3)]Ru-$ $[P(CH_3)_2C_6H_5]_2(CO)_2$	$CDCl_3$	H	1.67t	J_{PH} 7.0	1-Rhodio-cyclopent-2,3-diene derivative 100 MHz ^{19}F signals at 94.1 MHz	297
				H'	7.28m	—		
			$CHCl_3$	F	65.6m, 50.2m	— —		

$C_{16}H_{18}F_{12}O_8P_2Ru$	33	$[1,4-h^2-C(CF_3)=C(CF_3)-C(CF_3)=C(CF_3)]Ru-[P(OCH_3)_3]_2(CO)_2$	$CDCl_3$ $CHCl_3$	H F	3.66t 54.6q, 52.3q	$J_{PH} 11.0$ $J_{FF} 3.5$	1-Rhodium-cyclopent-2,3-diene derivative 100 MHz 94.1 MHz	297
$C_{42}H_{34}O_2P_2Ru$	34	$[\alpha,\beta-h^2-1,2-CH_2=CH'-C_6H_4P-(C_6H_5)_2]Ru[1,2-P(C_6H_5)_2C_6H_4-CH''=CH_2](CO)_2$	C_6D_6	H H' H''* H'''	1.9m 2.84m 5.50d, 5.10d	$J_{gem} \sim 0$ $J_{cis} 11.0$ $J_{trans} 17.0$ —	* Overlaid by aromatic proton signals	51
$C_{40}H_{33}O_3P_2Ru$	35	$(h^2-O=C-CH_3)Ru[P(C_6H_5)_3]_2(CO)_2$	—	H H'	+4.83s* -2.08m†	— —	* Upfield from CH_2Cl_2 (!) at 100 MHz † Downfield from CH_2Cl_2 (!) π -bonded acyl complex	567
$C_{21}H_{22}F_6O_3P_2Ru$	36	$[h^2-O=C(CF_3)_2]Ru[P(CH_3)_2-C_6H_5]_2(CO)_2$	$CDCl_3$	H H' F	1.90t 7.60m 75.7s	$J_{PH} 8.0$ — —	94.1 MHz	272
$C_{17}H_{22}F_6O_3P_2Ru$	37	$[h^2-O=C(CF_3)_2]Ru[P(OCH_2)_3-CCH_2CH_3]_2(CO)_2$	$CDCl_3$	H H' H'' F	4.30d 1.3 0.8 68.6d	$J_{PH} 5.0$ — — $J_{PF} 13.0$	100 MHz	568
(c) Tricarbonyl derivatives								
$C_{23}H_{17}O_3PRu$	38	$[\alpha,\beta-h^2-1,2-CH_2=CH'C_6H_4P-(C_6H_5)_2]Ru(CO)_3$	C_6D_6	H _{cis} H _{trans} H'	2.45m 1.62td 3.96 sext.	$J_{cis} 8.5$ $J_{PH} 5.0$ $J_{trans} 9.0$ $J_{gem} 3.0$ $J_{PH} 8.0$ $J_{PH'} 3.5$	—	51

TABLE VIII—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References	
$C_{19}H_{11}F_{12}O_3PRu$	39	$[1,4-h^2-C(CF_3)=C(CF_3)-C(CF_3)=C(CF_3)]Ru[P(CH_3)_2-C_6H_5](CO)_3$	$CDCl_3$	H	1.75d,	J_{PH} 10.0	Mixture of stereoisomers 100 MHz	297	
					1.70d	J_{PH} 13.0			
				H'	7.30m	—			
			$CHCl_3$	F	56.7m, 53.6m	— —	94.1 MHz		
(3) TRIHAPTO LIGANDS									
(a) Dicarbonyl derivatives									
$C_8H_{10}O_2Ru$	40	$(h^3-CH_2\equiv CH'\equiv CH''_2)Ru(CO)_2$	CS_2	H_{syn}	1.88	$J_{HH'}$ 7	100 MHz	571	
					H_{anti}	1.26	$J_{HH''_{syn}}$ 1.5		Two equivalent Π -allyl groups asymmetrically bonded to ruthenium
					H'	4.32	$J_{HH'}$ 11.5		
					H''_{syn}	3.34	J_{HH} small		
					H''_{anti}	2.26	$J_{H'H'}$ 11.5		
			<i>o</i> -C ₆ H ₄ Cl ₂	H_{syn}	1.78	—	}	T 60°	
				H_{anti}	1.18	—			
				H'	4.23	—			
				H''_{syn}	3.28	—			
				H''_{anti}	2.19	—			
				H_{syn}, H''_{syn}	2.53	—	}	T 120°	
				H_{anti}, H''_{anti}	1.73	—			
				H'	4.21	—			
(b) Tricarbonyl derivatives									
$C_6H_5BrO_3Ru$	41	$(h^3-CH_2\equiv CH'\equiv CH_2)Ru(Br)(CO)_3$	—	H_{syn}	4.03	$J_{HH'}$ 7.5 J_{HH} 0	—	572	

			H_{anti}	3.14	$J_{HH'}$ 12.5		
			H'	5.08	—		
$C_6H_5ClO_3Ru$	42	$(h^3-CH_2\equiv CH'\equiv CH_2)Ru(Cl)(CO)_3$	H_{syn}	4.15	$J_{HH'}$ 8.0	—	572
					J_{HH} 0		
			H_{anti}	2.96	$J_{HH'}$ 12.5		
			H'	5.22	—		
$C_6H_5IO_3Ru$	43	$(h^3-CH_2\equiv CH'\equiv CH_2)Ru(I)(CO)_3$	H_{syn}	3.83	$J_{HH'}$ 7.0	—	572
					J_{HH} 0		
			H_{anti}	3.38	$J_{HH'}$ 13.0		
			H'	4.83	—		
$C_7H_7ClO_3Ru$	44	$(h^3-CH_2\equiv C(CH_3)\equiv CH_2)Ru(Cl)(CO)_3$	H_{syn}	3.93	—		572
			H_{anti}	2.86	—		
			H'	2.06	—		

(4) TETRAHAPTO LIGANDS

(a) Monocarbonyl derivatives

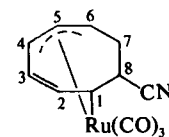
$[C_8H_8Cl_3ORu]^-$	45	$[(2,3,5,6-h^4-C_7H_8)Ru(Cl)_3(CO)]^-$	$CDCl_3$	H_{-1}	4.20bs	$J_{1,2} = J_{1,6}$ 3.0	C_7H_8 = norbornadiene	573
						$J_{1,7} = J_{1,8}$ 1.25	Isolated as the	
				H_{-2}, H_{-6}	5.22t	$J_{2,3} = J_{5,6}$ 4.5	$[P(C_6H_5)_3CH_2^+C_6H_5]^-$ salt	
				H_{-3}, H_{-5}	4.52t	$J_{3,4} = J_{4,5}$ 3.0		
				H_{-4}	3.66bs	$J_{4,7} = J_{4,8}$ 1.50		
				H_{-7}, H_{-8}	1.29t	—		
				H'	7.62,	—		
					7.10	—		
				H''	5.20d	$J_{PH''}$ 14.0		

C₁₂H₉NO₃Ru 49 (1,4,5,6-*h*⁴-8-C₈H₉CN)Ru(CO)₃ —

Not reported

Structure:

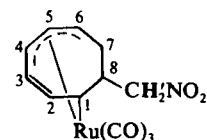
577

C₁₂H₁₁NO₃Ru 50 [1,4,5,6-*h*⁴-8-C₈H₉(CH₂NO₂)]-
Ru(CO)₃ —

H ₋₁	2.52t	<i>J</i> _{1,2} 4.0
		<i>J</i> _{1,9} 4.0
H ₋₂	5.48dd	<i>J</i> _{2,3} 7
H ₋₃	5.66dd	<i>J</i> _{3,4} 4.0
H ₋₄	5.02dd	<i>J</i> _{4,5} 9.0
H ₋₅	4.49t	<i>J</i> _{5,6} 9.0
H ₋₆	5.04m	—
H ₋₇	2.07d	—
H ₋₈	3.14m	—
H'	4.01d	<i>J</i> _{H'H₋₈} 8.0

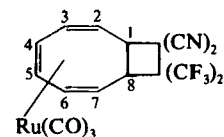
Structure:

577

C₁₇H₈F₆N₂O₃Ru 51 (4,5,6,7-*h*⁴-C₁₄H₈F₆N₂)Ru(CO)₃ CDCl₃

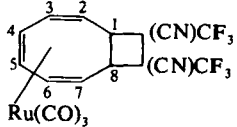
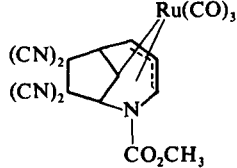
H ₋₁	3.32	<i>J</i> _{1,2} 6.0
H ₋₂	5.55	<i>J</i> _{2,3} 11.0
H ₋₃	6.40	<i>J</i> _{3,4} 9.0
H ₋₄	4.40	<i>J</i> _{4,5} 10.0
H ₋₅	4.92	<i>J</i> _{5,6} 7.5
H ₋₆	4.74	<i>J</i> _{6,7} 12.0
H ₋₇	4.05	<i>J</i> _{7,8} 8.0
H ₋₈	1.73	<i>J</i> _{1,8} 8.0
F	63.2,	<i>J</i> _{F,F} -13.2
	58.8	<i>J</i> _{FH} 4.8

Structure:

381
578

100 MHz

TABLE VIII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{17}H_8F_6N_2O_3Ru$	52	$(4,5,6,7-h^4-C_{14}H_8F_6N_2)Ru(CO)_3$	$CDCl_3$	H_{-1}	3.46	$J_{1,2}$ 6.0	Structure:  100 MHz	381
				H_{-2}	5.71	$J_{2,3}$ 11.0		
				H_{-3}	6.44	$J_{3,4}$ 9.0		
				H_{-4}	4.24	$J_{4,5}$ 10.0		
				H_{-5}	4.88	$J_{5,6}$ 7.0		
				H_{-6}	4.70	$J_{6,7}$ 9.0		
				H_{-7}	4.24	$J_{7,8}$ 10.0		
				H_{-8}	1.71	$J_{1,8}$ 8.0		
				F	67.2,	J_{FF} 0		
					61.3	J_{FH} 1.5		
$C_{17}H_9N_3O_5Ru$	53	$(h^4-C_{14}H_9N_3O_2)Ru(CO)_3$	—	Not reported			Structure: 	391
$C_{10}H_8N_2O_4Ru$	54	$[4,5,6,7-h^4-1-C_5H_5N_2(COCH_3)]-Ru(CO)_3$	$CDCl_3$	H_{-3}	6.92d	$J_{3,4}$ 6 $J_{3,5}$ 0.5	1-Acetyl-1H-1,2-diazepine complex	390

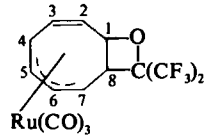
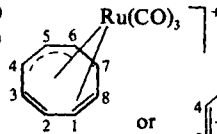
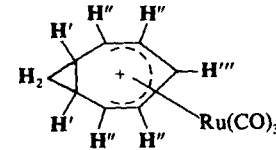
				H ₋₄	3.43 oct.	J _{4,5} 7 J _{4,6} 1.5	60 and 100 MHz				
				H ₋₅	5.36 oct.	J _{5,6} 4.5					
				H ₋₆	4.97m	J _{6,7} 7					
				H ₋₇	6.40dd	J _{5,7} 2					
				H'	2.35s	—					
C ₁₄ H ₈ F ₆ O ₄ Ru	55	(h ⁴ -C ₁₁ H ₈ F ₆ O)Ru(CO) ₃	CDCl ₃	H ₋₁	3.27	J _{1,2} 6.0	C ₁₁ H ₈ F ₆ O =		381		
				H ₋₂	5.64	J _{2,3} 11.0					
				H ₋₃	6.31	J _{3,4} 9.0					
				H ₋₄	4.25	J _{4,5} 10.0	100 MHz				
				H ₋₅	4.62	J _{5,6} 8.0					
				H ₋₆	4.92	J _{6,7} 9.0					
				H ₋₇	4.92	J _{7,8} 9.0					
				H ₋₈	1.85	J _{1,8} 10.0					
				F	71.4, 70.1	J _{FF} -11.2 J _{FH} 2.0, 1.4					
(5) PENTAHAPTO LIGANDS											
C ₂₄ H ₂₀ ClOPRu	56	(h ⁵ -C ₅ H ₅)Ru[P(C ₆ H ₅) ₃](Cl)(CO)	CDCl ₃	H	4.61s	—	100 MHz				
				H'	7.26m	—					
[C ₄₂ H ₃₅ OP ₂ Ru] ⁺	57	{(h ⁵ -C ₅ H ₅)Ru[P(C ₆ H ₅) ₃] ₂ (CO)} ⁺	CDCl ₃	H	4.48s	—	Tetraphenylborate 100 MHz				
				H'	7.24m	—					

TABLE VIII—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$[\text{C}_{11}\text{H}_9\text{O}_3\text{Ru}]^+$	58	$[(\eta^5\text{-C}_8\text{H}_9)\text{Ru}(\text{CO})_3]^+$	$(\text{CD}_3)_2\text{CO}$	H_{-1}	6.48dd	$J_{1,2}$ 2.3 $J_{1,8}$ 8.0	Structure: 	577
				H_{-2}	5.34dd	$J_{2,3}$ 8.0		
				H_{-3}	5.68dd	$J_{3,4}$ 3.9	Isolated as the tetrafluoroborate or hexafluorophosphate 100 MHz	
				$\text{H}_{-4}, \text{H}_{-5}$	5.06 comp.	—		
				H_{-6}	3.70m	—		
$[\text{C}_{11}\text{H}_9\text{O}_3\text{Ru}]^+$	59	$[(\eta^5\text{-C}_8\text{H}_9)\text{Ru}(\text{CO})_3]^+$	CD_3CN	H_{-7}	4.41q	$J_{7,8}$ 8.0	Structure: 	577
				H	2.0	—		
				H'	3.0	—		
				H''	5.3	—		
				H'''	7.7	—		
(6) MIXED LIGANDS								
(a) Pentahapto/monohapto								
(i) Monocarbonyl derivatives:								
$[\text{C}_{26}\text{H}_{42}\text{O}_2\text{PRu}]^+$	60	$\{(\eta^5\text{-C}_5\text{H}_5)\text{Ru}[\eta^1\text{-C}(\text{CH}_3)_2\text{OH}]\text{-P}(\text{C}_6\text{H}_{11})_3\}^+$	SO_2	H	5.49s	—	Tetrafluoroborate	172
				H'	2.93s	—		
				H''	1.8–1.35	—		

[C ₂₇ H ₄₄ O ₂ PRu] ⁺ 61	{(h ⁵ -C ₅ H ₅)Ru[h ¹ -C(CH ₃)=OCH ₂]- (CD ₃) ₂ CO [P(C ₆ H ₁₁) ₃](CO)} ⁺		H	5.70s	—	Tetrafluoroborate	172
			H'	3.15d	J _{PH} 0.4		
			H''	4.37d	J 0.55		
			H'''	1.57, 1.40	—		
[C ₂₈ H ₄₆ O ₂ PRu] ⁺ 62	{(h ⁵ -C ₅ H ₅)Ru[h ¹ -C(CH ₃)-OCH ₂ - (CD ₃) ₂ CO CH ₃ ''']P(C ₆ H ₁₁ ^{IV}) ₃](CO)} ⁺		H	5.63s	—	Tetrafluoroborate	172
			H'	3.12s	—		
			H''	4.60	—		
			H'''	1.56t	J _{H''H'''} 7.2		
			H ^{IV}	2.0-1 comp.	—		
C ₁₈ H ₁₄ N ₂ ORu 63	(h ⁵ -C ₅ H ₅)Ru(1-h ¹ -2-C ₆ H ₄ N= NC ₆ H ₅ ''')(CO)	CS ₂	H	4.85s	—	—	565
			H' ₃	6.94	—		
			H' ₄	7.28	—		
			H' ₅	7.81	—		
			H' ₆	8.08	—		
			H''	7.28	—		
C ₂₆ H ₄₁ O ₂ PRu 64	(h ⁵ -C ₅ H ₅)Ru(COCH ₃)- [P(C ₆ H ₁₁) ₃](CO)	CDCl ₃	H	5.21s	—	—	172
			H'	2.56s	—		
			H''	1.87, 1.32	—		
		CF ₃ CO ₂ H	comp.	—	—		
			H	5.62s	—		
			H'	3.03s	—		
C ₂₆ H ₂₃ O ₂ PRu 65	(h ⁵ -C ₅ H ₅)Ru(COCH ₃)- [P(C ₆ H ₅) ₃](CO)	CDCl ₃	H	4.97s	—	—	172
			H'	2.09s	—		
			H''	7.30 comp.	—		
		CF ₃ CO ₂ H	H	5.35s	—		
			H'	2.53s	—		
			H''	7.55	—		

TABLE VIII—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
(ii) Dicarbonyl derivatives:								
$C_{10}H_{10}O_2Ru$	66	$(\eta^5-C_5H_5)Ru(\eta^1-CH_2CH''=CH_2')-(CO)_2$	$CDCl_3$	H H' H''	5.14s 4.96m, 4.50m, 2.41dd 6.16m	— J 8, 2 —	60 and 100 MHz	231
$C_{10}H_5F_5O_2Ru$	67	$(\eta^5-C_5H_5)Ru(\eta^1-CF=CF'-CF_3'')-(CO)_2$	THF	F F' F''	163.9 85.3 65.6	$J_{FF'}$ 134.5 $J_{F'F''}$ 22.25 $J_{FF''}$ 13.05	94.1 and 56.4 MHz	459
$C_{13}H_5F_9O_2Ru$	68	$(\eta^5-C_5H_5)Ru(1-\eta^1-C_6F_9)(CO)_2$	THF	F ₋₂ F ₋₃ F ₋₄ F ₋₅ F ₋₆	96.3 116.6 134.6 132.3 92.6	— — — — —	C ₆ F ₉ = Perfluorocyclohex-1-ene 94.1 and 56.4 MHz	459
$C_{12}H_{10}O_2Ru$	69	$(\eta^5-C_5H_5)Ru(1-\eta^1-C_5H_5)(CO)_2$	$(CH_3)_2CO$	H H' ₁ H' ₂ , H' ₅ H' ₃ , H' ₄	5.56 4.45 6.61bd 6.17bs	— — — —	T -75° 60 and 100 MHz $\eta^1-C_5H_5$ = cyclopenta-2,4-dien-1-yl	464
			CS ₂ / Toluene- <i>d</i> ₈ (3:1)		n.m.	$J_{1,2} \pm 1.22$ $J_{1,3} \pm 0.10$ $J_{2,3}$ 4.64 $J_{2,4}$ 1.17 $J_{2,5}$ 2.06 $J_{3,4}$ 2.12	T -82° Low temperature studies indicate that rearrangement of the η^1 -C ₅ H ₅ ring occurs predominantly by 1,2-shifts	465

C ₁₃ H ₁₂ O ₂ Ru	70	(η^5 -C ₅ H ₅)Ru[1- <i>h</i> ¹ -1-C ₅ H ₄ (CH ₃)]-(CO) ₂	CS ₂	H	4.91	—	}	T -40°	464		
				H'	2.12	—					
				H'' ₋₂ to H'' ₋₅	n.a.	—					
C ₁₃ H ₁₂ O ₂ Ru	71	(η^5 -C ₅ H ₅)Ru[1- <i>h</i> ¹ -2-C ₅ H ₄ (CH ₃)]-(CO) ₂	CS ₂	H	4.63	—	}	Migration of the metal round the σ -bonded ring takes place by a sequence of 1,2-shifts resulting in ready interconversion of the three isomers at ambient temperature. In the temperature range of 30–60° the signals observed are: δ 4.82s (H), 2.01s (H'), 5.89b and 5.67b (H'')			
				H'	2.06	—					
				H'' ₋₁	3.76d	<i>J</i> 1.2					
				H'' ₋₃ to H'' ₋₅	n.a.	—					
C ₁₃ H ₁₂ O ₂ Ru	72	(η^5 -C ₅ H ₅)Ru[1- <i>h</i> ¹ -3-C ₅ H ₄ (CH ₃)]-(CO) ₂	CS ₂	H	5.01	—	}				
				H'	2.16	—					
				H'' ₋₁	4.16t	<i>J</i> 1.2					
				H'' ₋₂ to H'' ₋₅	n.a.	—					
C ₁₃ H ₅ F ₅ O ₂ Ru	73	(η^5 -C ₅ H ₅)Ru(1- <i>h</i> ¹ -C ₆ F ₅)(CO) ₂	THF	F ₋₂ , F ₋₆	104.25	<i>J</i> _{2,3} 29.6 <i>J</i> _{2,4} 1.4 <i>J</i> _{2,6} 3.7	}	94.1 and 56.4 MHz	459		
				F ₋₃ , F ₋₅	164.3	<i>J</i> _{2,5} = <i>J</i> _{3,6} 9.6 <i>J</i> _{3,5} 6.7					
				F ₋₄	162.5	<i>J</i> _{3,4} 19.7					
C ₁₃ H ₃ F ₃ N ₂ O ₂ Ru	74	(η^5 -C ₅ H ₅)Ru[1- <i>h</i> ¹ -3,4-C ₆ F ₃ (CN) ₂](CO) ₂	THF	F ₋₂	68.9	<i>J</i> _{2,5} 6.45	}	94.1 and 56.4 MHz	459		
				F ₋₅	136.35	<i>J</i> _{5,6} 28.7					
				F ₋₆	85.9	<i>J</i> _{2,6} 11.9					
C ₁₉ H ₁₄ N ₂ O ₂ Ru	75	(η^5 -C ₅ H ₅)Ru(1- <i>h</i> ¹ -2-C ₆ H ₄ N=NC ₆ H ₅)(CO) ₂	(CD ₃) ₂ CO	H	5.28s	—	}	—	565		
				H' ₋₃	6.85	—			581		
				H' ₋₄	7.22	—					
				H' ₋₅	7.60	—					
				H' ₋₆	7.70	—					
				H''	7.31	—					

TABLE VIII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_9H_8O_3Ru$	76	$(\eta^5-C_5H_5)Ru(COCH_3)(CO)_2$	$CDCl_3$	H	5.28s	—	—	172
				H'	2.38s	—		
			CF_3CO_2H	H	5.64s	—		
				H'	3.02s	—		
$C_9H_5F_3O_3Ru$	77	$(\eta^5-C_5H_5)Ru(COCF_3)(CO)_2$	THF	F	81.35	—	94.1 and 56.4 MHz	459
$C_{12}H_5F_4NO_2Ru$	78	$(\eta^5-C_5H_5)Ru(4-\eta^1-C_5F_4N)(CO)_2$	THF	F_{-3}, F_{-5}	111.2	$J_{2,3}$ 28.9 $J_{3,5}$ 2.5	94.1 and 56.4 MHz	459
				F_{-2}, F_{-6}	98.7	$J_{2,5}$ 26.4 $J_{2,6}$ 11.7		
<i>(b) Pentahapto/trihapto</i>								
$C_9H_{10}ORu$	79	$(\eta^5-C_5H_5)Ru(\eta^3-CH_2'''-CH'''''-CH_2)(CO)$	$CDCl_3$	H	4.99s	—	Isomer A 60 and 100 MHz	231
				H'	2.89d,	J 7		
					1.25d	J 11		
				H''	~ 4m	—		
				H	5.14s	—	Isomer B	
				H'	3.03d,	J 7		
					1.77d	J 11		
				H''	~ 4m	—		
<i>(7) MISCELLANEOUS COMPLEXES</i>								
<i>(a) Monocarbonyl derivatives</i>								
$[C_{11}H_{25}OP_2Ru]^+$	80	$\{Ru(H)[P(C_2H_5)_2CH_2CH_2P(C_2H_5)_2](CO)\}^+$	$CDCl_3$	H	-9.4	J_{PH} 20	Tetraphenylborate 100 MHz	491

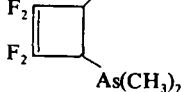
$C_{33}H_{50}^-$ AsClOP ₂ Ru	81	Ru(H)(Cl)[As(CH ₃) ₂ C ₆ H ₅]- [P(C ₃ H ₇) ₂ C ₆ H ₅] ₂ (CO)	C ₆ H ₆	H	-8.46	$J_{PH_{cis}}$ 24.0	<i>trans</i> -P ligands; <i>trans</i> -CO and Cl ligands T 34°	582
$C_{37}H_{58}^-$ AsClOP ₂ Ru	82	Ru(H)(Cl)[As(CH ₃) ₂ C ₆ H ₅]- [P(C ₄ H ₉) ₂ C ₆ H ₅] ₂ (CO)	C ₆ H ₆	H	-8.29	$J_{PH_{cis}}$ 23.0	<i>trans</i> -P ligands; <i>trans</i> -CO and Cl ligands T 34°	582
$C_{35}H_{54}^-$ AsClOP ₂ Ru	83	Ru(H)(Cl)[As(C ₂ H ₅) ₂ C ₆ H ₅]- [P(C ₃ H ₇) ₂ C ₆ H ₅] ₂ (CO)	C ₆ H ₆	H	-8.56	$J_{PH_{cis}}$ 24.0	<i>trans</i> -P ligands; <i>trans</i> -CO and Cl ligands T 34°	582
$C_{49}H_{41}N_3OP_2Ru$	84	Ru(H)(C ₆ H ₅ N ₃ C ₆ H ₅)- [P(C ₆ H ₅) ₃] ₂ (CO)	—	H	-12.33	J_{PH} 26.25	—	583
$C_{31}H_{46}ClOP_3Ru$	85	Ru(H)(Cl)[P(C ₂ H ₅) ₂ C ₆ H ₅] ₃ (CO)	C ₆ H ₆	H	-7.1	$J_{PH_{cis}}$ 24 $J_{PH_{trans}}$ 107	<i>trans</i> -CO and Cl ligands T 34°	582
$C_{31}H_{54}ClOP_3Ru$	86	Ru(H)(Cl)[P(C ₂ H ₅) ₃]- [P(C ₃ H ₇) ₂ C ₆ H ₅] ₂ (CO)	C ₆ H ₆	H	-6.90	$J_{PH_{cis}}$ 26.0 $J_{PH_{trans}}$ 106.0	<i>trans</i> -CO and Cl ligands T 34°	582
$C_{35}H_{54}ClOP_3Ru$	87	Ru(H)(Cl)[P(C ₂ H ₅) ₂ C ₆ H ₅]- [P(C ₃ H ₇) ₂ C ₆ H ₅] ₂ (CO)	C ₆ H ₆	H	-7.14	$J_{PH_{cis}}$ 27.0 $J_{PH_{trans}}$ 110.5	<i>trans</i> -CO and Cl ligands T 34°	582
$C_{37}H_{58}ClOP_3Ru$	88	Ru(H)(Cl)[P(C ₃ H ₇) ₂ C ₆ H ₅] ₃ (CO)	C ₆ H ₆	H	-7.5	$J_{PH_{cis}}$ 25 $J_{PH_{trans}}$ 109	<i>trans</i> -CO and Cl ligands T 34°	582
$C_{40}H_{35}OP_3Ru$	89	Ru(H) ₂ [P(C ₆ H ₅) ₂ CH ₃] ₃ (CO)	—	H	-8.02, -6.80	J_{HH} -6.2 $J_{PH_{cis}}$ -19.5 -27.1 $J_{PH_{trans}}$ +75.4	H <i>cis</i>	584
				H'	1.82, } 1.42 }	$J_{PH'}$ 7.6		

TABLE VIII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References									
C ₂₅ H ₃₄ BrOP ₃ Ru	90	Ru(H)(Br)[P(CH ₃) ₂ C ₆ H ₅] ₃ (CO)	CHCl ₃	H	-7.0	$J_{PH_{cis}}$ 26.5 $J_{PH_{trans}}$ 113	H <i>cis</i> to Br and CO ligands; Br and CO ligands <i>trans</i> to each other	917									
				H'	1.82t, 1.73t, 1.20d	$J_{PH'}$ 3 $J_{PH'}$ 3 $J_{PH'}$ 7											
				H'	1.76t, 1.73t, 1.20d	$J_{PH'}$ 3 $J_{PH'}$ 3 $J_{PH'}$ 7											
			C ₆ H ₆	H'	1.76t, 1.73t, 1.20d	$J_{PH'}$ 3 $J_{PH'}$ 3 $J_{PH'}$ 7											
				C ₂₅ H ₃₄ ClOP ₃ Ru	91	Ru(H)(Cl)[P(CH ₃) ₂ C ₆ H ₅] ₃ (CO)			CHCl ₃	H	-6.6	$J_{PH_{cis}}$ 26.5 $J_{PH_{trans}}$ 105	H <i>cis</i> to Cl and CO ligands; Cl and CO ligands <i>trans</i>	917			
										H'	1.73, 1.10d	— $J_{PH'}$ 7					
H'	1.71t, 1.15d	$J_{PH'}$ 3.5 $J_{PH'}$ 7.5															
C ₆ H ₆	H	-6.82	$J_{PH_{cis}}$ 24.5 $J_{PH_{trans}}$ 114.5				T 34°	582									
	C ₃₃ H ₅₀ ClOP ₃ Ru	93	Ru(H)(Cl)[P(CH ₃) ₂ C ₆ H ₅]- [P(C ₃ H ₇) ₂ C ₆ H ₅] ₂ (CO)						C ₆ H ₆	H	-6.80	$J_{PH_{cis}}$ 25.0 $J_{PH_{trans}}$ 115.0			T 34°	582	
										C ₃₇ H ₅₈ ClOP ₃ Ru	94	Ru(H)(Cl)[P(CH ₃) ₂ C ₆ H ₅]- [P(C ₄ H ₉) ₂ C ₆ H ₅] ₂ (CO)					C ₆ H ₆
C ₄₃ H ₇₀ ClOP ₃ Ru				95	Ru(H)(Cl)[P(C ₄ H ₉) ₂ C ₆ H ₅] ₃ (CO)	C ₆ H ₆	H	-7.10					$J_{PH_{cis}}$ 26.0 $J_{PH_{trans}}$ 110.0	H <i>cis</i> to CO and Cl ligands; CO and Cl ligands <i>trans</i> T 34°			

$C_{33}H_{50}ClO_3P_3Ru$	96	$Ru(H)(Cl)[P(C_3H_7)_2C_6H_5]_2-$ $[P(OCH_3)_2C_6H_5](CO)$	C_6H_6	H	-6.18	$J_{PH_{cis}}$ 23.5 $J_{PH_{trans}}$ 160.5	H <i>cis</i> to CO and Cl ligands; CO and Cl ligands <i>trans</i> T 34°	582
$C_{31}H_{54}ClO_4P_3Ru$	97	$Ru(H)(Cl)[P(C_3H_7)_2C_6H_5]_2-$ $[P(OC_2H_5)_3](CO)$	C_6H_6	H	-6.20	$J_{PH_{cis}}$ 27.5 $J_{PH_{trans}}$ 185.0	H <i>cis</i> to CO and Cl ligands; CO and Cl ligands <i>trans</i> T 34°	582
$C_{55}H_{47}OP_3Ru$	98	$Ru(H)_2[P(C_6H_5)_3]_3(CO)$	$CDCl_3$	H	-8.67* -6.69†	$J_{PH_{cis}}$ 20 $J_{PH_{trans}}$ 74 J_{HH} 6 $J_{PH_{cis}}$ 30, 16	• H <i>cis</i> to CO and H ligands † H <i>cis</i> to H and <i>trans</i> to CO ligand 100 MHz	585
(b) Dicarbonyl derivatives								
$C_{14}H_{32}O_2P_2Ru$	99	$Ru(H)_2[P(C_2H_5)_3]_2(CO)_2$	—	H	-8.48t	J_{PH} 24	—	586
$C_{38}H_{31}ClO_2P_2Ru$	100	$Ru(H)(Cl)[P(C_6H_5)_3]_2(CO)_2$	—	H	-4.53t	J_{PH} 19	—	587
$C_{38}H_{32}O_2P_2Ru$	101	$Ru(H)_2[P(C_6H_5)_3]_2(CO)_2$	—	H	-7.65	—	100 Mhz	588
(c) Tetracarbonyl derivatives								
$C_4H_2O_4Ru$	102	$Ru(H)_2(CO)_4$	—	H	-7.62	—	T -30°	586 588
(d) Pentacarbonyl derivatives								
$[C_5HO_5Ru]^+$	103	$[Ru(H)(CO)_5]^+$	—	H	-8.0	—	—	589
(8) COMPLEXES CONTAINING TWO OR MORE RUTHENIUM ATOMS								
$C_{28}H_{18}Cl_2N_4-$ O_4Ru_2	104	$[(1-h^1-2-C_6H_4N=NC_6H_5)Ru(Cl)-$ $(CO)_2]_2$	$CDCl_3$	H ₋₃ H ₋₄ H ₋₅ H ₋₆ H'	7.10 7.48 7.96 8.20 7.42	— — — — —	—	565

TABLE VIII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{13}H_8O_3Ru_2$	105	$(h^4:h^4-C_8H_8)[Ru(CO)_2]_2(CO)$	CS_2	H 4.8s	—	C_8H_8 = cyclooctatetraene	574
			CS_2	H 4.7s*	—	T -35° * The signal remains as a sharp singlet down to -80° . The structure is assumed to be the same as the analogous iron compound, the NMR equivalence being attributed to fluxional behaviour	590 576
$C_{30}H_{18}N_4O_6Ru_2$	106	$[(1-h^1-2-C_6H_4N=NC_6H_5)-Ru(CO)_3]_2$	—	H 8.3–6.8	—	—	591
$C_{14}H_{12}As_2F_4O_6Ru_2$	107	$\{h^2-C_4F_4[As(CH_3)_2]_2\}[Ru(CO)_3]_2$	$C_6H_5NO_2$	H 2.25s, 1.80s	— —	$C_4F_4[As(CH_3)_2]_2 =$	592
							
			THF	F 110.0 108.2 94.8 92.9	— — — —	94.1 MHz	
$C_{34}H_{20}F_4O_6P_2Ru_2$	108	$\{h^2-C_4F_4[P(C_6H_5)_2]_2\}[Ru(CO)_3]_2$	THF	F* 107.8 105.8	— —	* ^{19}F NMR complex; four major areas upfield from $CFCl_3$	592

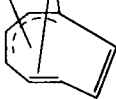
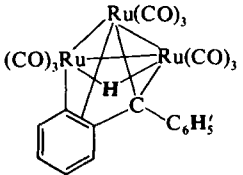
					87.1	—		
					85.2	—		
$C_{35}H_{20}F_6O_6P_2Ru_2$	109	$\{h^2-C_5F_6[P(C_6H_5)_2P_2][Ru(CO)_3]_2$	C_6H_6	F	122.2dm	—	* 3,3,4,4,5,5-hexafluoro-1,2-diphenylphosphinocyclopent-1-ene	592
					114.0dm	—		
					103.3dm	—		
					65.2dm	—		
$C_{14}H_8O_6Ru_2$	110	$(h^3:h^3-C_8H_8)[Ru(CO)_3]_2$	$C_6D_5CD_3/$ CF_2Cl_2 (3:2)	H_{-1}, H_{-6} H_{-2}, H_{-3} H_{-4}, H_{-5} H_{-7}, H_{-8}	2.6 4.3 5.8	— — —	Structure:  A fluxional molecule, the two enantiomeric forms undergoing rapid interconversion at ambient temperature, as in the case of the iron analogue	576 535
			C_6H_{12}	H_{-1}, H_{-6} H_{-2}, H_{-3} H_{-4}, H_{-5} H_{-7}, H_{-8}	2.63 4.3 5.81	— — —	—	590 574
$C_{11}H_6O_7Ru_2$	111	$[h^3:h^1-CH_2-C(CH_2)-CH_2]-[Ru(CO)_3][Ru(CO)_4]$	—	n.a.	—	—	Signals at δ 1.88m, 1.58m, 1.35m, in ratio 1:1:1	55

TABLE VIII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{20}H_{16}Ru_3O_4$	112	$(C_8H_8)_2Ru_3(CO)_4$	$CDCl_3$	H 3.74s*	—	A fluxional metal atom cluster compound * Signal remains as a sharp singlet down to -40°	576 590
$C_{22}H_{10}O_9Ru_3$	113	$(C_{13}H_9)(H)[Ru(CO)_3]_3$	CS_2	H H' -20.2 7.5-7.0	— —	Structure: 	593
$C_{21}H_{16}O_9Ru_3$	114	$(C_{12}H_{15})(H)[Ru(CO)_3]_3$	—	H -20.24d	J 2.7	A cyclododeca-1,5,9-triene derivative. Remaining signals at δ 6.19d, 5.37m, and 3.2-1.5 not assigned	594
$C_{22}H_{16}O_{10}Ru_4$	115	$(C_{12}H_{16})Ru_4(CO)_{10}$	—	n.a.	—	Cyclododeca-1,3-diene derivative. Signals at δ 5.98s, 3.78t (J 10), 2.8m, 1.8m	595

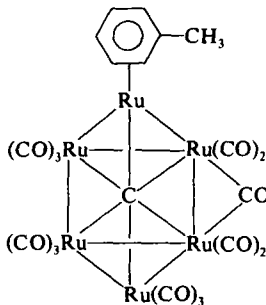
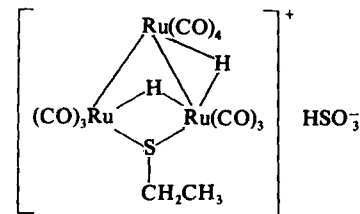
$C_{22}H_8O_{14}Ru_6$	116	$[(\eta^6-C_6H_5CH_3)Ru](C)[Ru(CO)_2]_2-$ $[Ru(CO)_3]_3(CO)$	$CDCl_3$	H H'	5.49 2.15	— —	Proposed structure:	596
 (Carbidotetradecacarbonyl toluenehexaruthenium) 100 MHz								
$C_{23}H_{10}O_{14}Ru_6$	117	$\{[\eta^6-1,3-C_6H_4(CH_3)_2]Ru\}(C)-$ $[Ru(CO)_2]_2[Ru(CO)_3]_3(CO)$	$CDCl_3$	H H'	5.23, 5.30, 5.50 2.22	— — — —	Structure analogous to above	596
$C_{24}H_{12}O_{14}Ru_6$	118	$\{[\eta^6-1,3,5-C_6H_3(CH_3)_3]Ru\}(C)-$ $[Ru(CO)_2]_2[Ru(CO)_3]_3(CO)$	$CDCl_3$	H H'	5.30 2.23	— —	Structure analogous to above	596 1010
$C_{38}H_{32}O_2P_2Ru$	119	$Ru(H)_2[P(C_6H_5)_3]_2(CO)_2$	THF	H	-6.90t	J 23	—	1018
$C_{30}As_2F_{20}O_6Ru_2$	120	$\{Ru[As(C_6F_5)_2](CO)_3\}_2$	$CHCl_3$	F_{-1}, F_{-6} F_{-3}, F_{-5} F_{-4}	121.7 156.2 146.1	— — —	—	130

TABLE VIII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)		Remarks	References
$C_{30}F_{20}O_6P_2Ru_2$	121	$\{Ru[P(C_6F_5)_2](CO)_3\}_2$	$CHCl_3$	F_{-1}, F_{-6} 123.0 F_{-3}, F_{-5} 158.1 F_{-4} 147.1	— — —	—		130
$C_9H_2O_9Ru_3S$	122	$(H)_2(S)[Ru(CO)_3]_3$	$CDCl_3$	H -19.98s	—	—		597
$C_{12}H_6O_{10}Ru_3S$	123	$(H)(SCH_2CH_3)Ru_3(CO)_{10}$	—	H -15.4s H' 2.17q H'' 1.35t	— — —		Bridged hydrido and thiol complex	598 599
$C_{14}H_{10}O_{10}Ru_3S$	124	$(H)[SCH_2(CH_2)_2CH_3]-Ru_3(CO)_{10}$	—	H -15.42s H' 2.16m H'' 1.57m H''' 0.93m	— — — —		Bridged hydrido and thiol complex	598
$[C_{12}H_8O_{10}-Ru_3S]^+$	125	$[(H)_2(SCH_2CH_3)Ru_3(CO)_{10}]^+$	—	H -19.39d, -14.94d H' 2.33q H'' 1.24t	— — — —		Possible structure:	597



$[\text{C}_{12}\text{H}_{12}\text{O}_{12}\text{Ru}_3]^+$	126	$[(\text{H})\text{Ru}_3(\text{CO})_{12}]^+$	H_2SO_4	H	-19.4	—	Reference dimethyl sulphate (δ 6.1) 100 MHz	600
			$(\text{CH}_3)_2\text{CO}$	H	-18.6	—		
$\text{C}_{13}\text{H}_2\text{FeO}_{13}\text{Ru}_3$	127	$(\text{H})_2\text{Ru}_3\text{Fe}(\text{CO})_{13}$	CH_2Cl_2	H	-18.5s	—	—	601
			C_6D_6	H	-18.7s	—		
$\text{C}_{56}\text{H}_{112}\text{O}_8\text{P}_4\text{Ru}_4$	128	$(\text{H})_4\text{Ru}_4[\text{P}(\text{C}_4\text{H}_9)_3]_4(\text{CO})_8$	C_6D_6	H	-16.8m	—	—	602
$\text{C}_{80}\text{H}_{64}\text{O}_8\text{P}_4\text{Ru}_4$	129	$(\text{H})_4\text{Ru}_4[\text{P}(\text{C}_6\text{H}_5)_3]_4(\text{CO})_8$	THF	H	-15.65m	—	—	602
$\text{C}_{20}\text{H}_{40}\text{O}_{20}\text{P}_4\text{Ru}_4$	130	$(\text{H})_4\{\text{Ru}[\text{P}(\text{OCH}_3)_3](\text{CO})_2\}_4$	CDCl_3	H H'	-17.83 quint. 3.74 comp.	$J_{\text{PH}} 7.95$ $J_{\text{PH}'} 12.2$	Symmetrical cyclic structure containing bridging hydrido ligands	603
$\text{C}_{45}\text{H}_{85}\text{O}_9\text{P}_3\text{Ru}_4$	131	$(\text{H})_4\text{Ru}_4[\text{P}(\text{C}_4\text{H}_9)_3]_3(\text{CO})_9$	C_6D_6	H	-16.5m	—	—	602
$\text{C}_{63}\text{H}_{49}\text{O}_9\text{P}_3\text{Ru}_4$	132	$(\text{H})_4\text{Ru}_4[\text{P}(\text{C}_6\text{H}_5)_3]_3(\text{CO})_9$	THF	H	-17.1m, -16.1m	— —	—	602
$\text{C}_{18}\text{H}_{31}\text{O}_{18}\text{P}_3\text{Ru}_4$	133	$(\text{H})_4\{\text{Ru}[\text{P}(\text{OCH}_3)_3](\text{CO})_2\}_3\text{-}$ $[\text{Ru}(\text{CO})_3]$	CDCl_3	H H'	-17.84q 3.77 comp.	$J_{\text{PH}} 7.7$ $J_{\text{PH}'} 12.0$	Cyclic metal cluster	603
$\text{C}_{16}\text{H}_{22}\text{O}_{16}\text{P}_2\text{Ru}_4$	134	$(\text{H})_4\{\text{Ru}[\text{P}(\text{OCH}_3)_3](\text{CO})_2\}_2\text{-}$ $[\text{Ru}(\text{CO})_3]_2$	CDCl_3	H H'	-17.61t 3.69d	$J_{\text{PH}} 6.63$ $J_{\text{PH}'} 12.0$	Cyclic metal cluster	603
$\text{C}_{46}\text{H}_{34}\text{O}_{10}\text{P}_2\text{Ru}_4$	135	$(\text{H})_4\text{Ru}_4[\text{P}(\text{C}_6\text{H}_5)_3]_2(\text{CO})_{10}$	THF	H	-16.9m, -16.1m	— —	—	602
$\text{C}_{23}\text{H}_{31}\text{O}_{11}\text{PRu}_4$	136	$(\text{H})_4\text{Ru}_4[\text{P}(\text{C}_4\text{H}_9)_3](\text{CO})_{11}$	C_6H_6	H	-17.7m	—	—	602

TABLE VIII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{29}H_{19}O_{11}PRu_4$	137	$(H)_4Ru_4[P(C_6H_5)_3](CO)_{11}$	THF	H —17.7m	—	—	602
$C_{14}H_{13}O_{14}PRu_4$	138	$(H)_4\{Ru[P(OCH_3)_3](CO)_2\}-[Ru(CO)_3]_3$	$CDCl_3$	H —17.72d H' 3.69d	J_{PH} 2.65 $J_{PH'}$ 12.2	Cyclic metal cluster	603
$C_{12}H_4O_{12}Ru_4$	139	$(H)_4Ru_4(CO)_{12}$	THF or $CDCl_3$	H —17.6s H —8.6s	—	α -isomer β -isomer	604 605
			CCl_4	H —5.08	—	—	588 606
			C_6H_6	H —17.72	—	α -isomer	588
			Octadeuterio furan	H —17.9s	—	—	602
$C_{13}H_2O_{13}Ru_4$	140	$(H)_2Ru_4(CO)_{13}$	$CDCl_3$	H —18.55s H —9.1	—	α -isomer β -isomer	604 588
			CH_2Cl_2	H —18.6s	—	—	601
			C_6D_6	H —9.1	—	β -isomer	588

TABLE IX

Osmium complexes

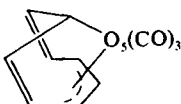
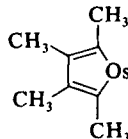
Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
(1) MONOHAPTO LIGANDS								
$C_{12}H_{19}ClF_6O_8OsP_2$	1	$[h^1-C(CF_3)=CHCF_3]Os-P(OCH_3)_3)_2(Cl)(CO)_2$	$CDCl_3$	H	6.82qm	J_{HF} 11.2, J_{HP} 1.0	P ligands <i>trans</i> to each other, (CO) ligands <i>cis</i> to each other	569
				H'	3.76t	$J_{H'P}$ 10.6		
				F	57.7qt,	J_{FF} 14.0		
					54.6q	J_{HP} 2.8, J_{HF} 11.2 J_{FF} 14.0		
$[C_6H_6Br_2O_4Os]^{2-}$	2	$[Os(COCH_3)_2(Br)_2(CO)_2]^{2-}$	$(CD_3)_2CO$	H	2.61s, 2.37s	— —	Isolated as magnesium bromide salt with five THF molecules of solvation	607 939
$C_{22}H_{19}O_3OsP$	3	$Os(CH_3)(H)(PPh_3)(CO)_3$	THF	H	-0.23d, -0.37d	J_{HH} 2.4 J_{PH} 8.5	—	607
$C_{23}H_{21}O_3OsP$	4	$Os(CH_3)_2(PPh_3)(CO)_3$	$(CD_3)_2CO$	H	0.14s, -0.23d	— J_{PH} 8.4	—	607
$C_5H_4O_4Os$	5	$Os(CH_3)(H')(CO)_4$	THF	H	0.00d	$J_{HH'}$ 2.4		607 939
				H'	-7.94q	$J_{HH'}$ 2.4		
$C_5H_3BrO_4Os$	6	$Os(CH_3)(Br)(CO)_4$	CCl_4	H	0.75s	—	—	608
$C_5H_3IO_4Os$	7	$Os(CH_3)(I)(CO)_4$	CCl_4	H	0.86s	—	—	608 939
			$(CD_3)_2CO$	H	0.78s	—	—	607

TABLE IX—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_8H_{12}O_4OsSi$	8	$Os(CH_3)_3[Si(CH_3)_3](CO)_4$	—	H —0.03 H' 0.45s	—	<i>cis</i> -isomer 100 MHz	614
$C_6H_6O_4Os$	9	$Os(CH_3)_2(CO)_4$	C_6D_6	H 0.11s	—	—	608
			THF	H 0.05s	—	—	607
$C_8H_{10}O_4Os$	10	$Os(CH_2CH_3)_2(CO)_4$	CCl_4	H 1.05m H' 1.73m	J 7.5 J 7.5	—	608
$C_{10}H_{10}O_6Os$	11	$Os(COCH_2CH_3)_2(CO)_4$	CCl_4	H 2.71q H' 0.89t	J 7 J 7	—	608
(2) DIHAPTO LIGANDS							
$C_{20}H_{23}F_3O_2OsP_2$	12	$(h^2-CHF=CF_2)Os[P(CH_3)_2-C_6H_5]_2(CO)_2$	$CDCl_3$	H 4.50dm H' 1.85t H'' 7.35m	$J_{HF_{gem}}$ 64.0 J_{PH} 8.0 —	P ligands <i>trans</i> , (CO) ligands <i>cis</i>	569
$C_{10}H_{18}F_4O_8OsP_2$	13	$(h^2-CF_2=CF_2)Os[P(OCH_3)_3]_2(CO)_2$	$CDCl_3$	H 3.70d* F 117.5	J_{HP} 12.3 $J_{PF} + J_{PF}$ 51.5	* 100 MHz P ligands <i>trans</i> , (CO) ligands <i>trans</i>	569
$C_{10}H_{18}ClF_3O_8OsP_2$	14	$[h^2-C(Cl)F=CF_2]Os[P(OCH_3)_3]_2(CO)_2$	$CDCl_3$	H 3.71d*, 3.66d* F 123.0†	J_{PH} 12.0 $J_{FF'}$ 35.0 8.0 J_{PF} 32.0‡ <0.2§	* 100 MHz † 94.1 MHz ‡ <i>trans</i> coupling § <i>cis</i> coupling P ligands <i>cis</i> , (CO) ligands <i>trans</i>	569

				F'	115.0†, 99.8†	$J_{FF'} 178.0$ $J_{PF'} 53.0\pm$ <0.2§		
$C_{10}H_{19}F_3O_8OsP_2$	15	$(h^2\text{-CHF=CF}_2)Os[P(OCH_3)_3]_2\text{-}(CO)_2$	$(CD_3)_2CO$	H H'	5.70dm 3.75d, 3.55d	$J_{HF}^{rem} 66.0$ $J_{HP} 11.0$ 10.0	P ligands <i>cis</i> , (CO) ligands <i>trans</i>	569
			$CDCl_3$	F F	57.0dm 205 comp. 101 comp.	— — —		
$C_{12}H_{18}F_6\text{-}O_8OsP_2$	16	$[h^2\text{-C(CF}_3)_2\equiv C(CF_3)]Os\text{-}[P(OCH_3)_3]_2(CO)_2$	$CDCl_3$ CH_2Cl_2	H F	3.63t 55.1t	$J_{HP} 12.0$ $J_{PF} 2.7$	100 MHz 94.1 MHz P ligands <i>trans</i> , (CO) ligands <i>cis</i>	569
$C_{21}H_{22}F_6\text{-}O_3OsP_2$	17	$[h^2\text{-C(CF}_3)_2=O]Os[P(CH_3)_2\text{-}C_6H_5]_2(CO)_2$	$CDCl_3$ $CHCl_3$	H H' F	1.93m 7.37m 66.2d*	— — $J_{PF_{trans}} 4.0$	P ligands <i>cis</i> , (CO) ligands <i>trans</i> * ^{19}F chemical shift of free ligand 77.2, relative to $CFCI_3$	569
(3) TETRAHAPTO LIGANDS								
$C_{11}H_8O_3Os$	18	$(1,2,3,4\text{-}h^4\text{-}C_8H_8)Os(CO)_3$	CS_2	H₋₁, H₋₄ H₋₂, H₋₃ H₋₅, H₋₈ H₋₆, H₋₇	4.08 5.16 6.11 5.61	$J_{1,2} = J_{3,4} 9.0$ $J_{1,8} = J_{4,5} 9.7$ $J_{1,3} = J_{2,4} 0.5$ $J_{2,3} 5.0$ $J_{3,6} = J_{7,8} 12.1$ $J_{5,7} = J_{6,8} 0.7$ $J_{6,7} 8.0$	C_8H_8 = Cyclo-octatetraene T -100° 100 MHz One singlet at ambient temperature (δ 5.22)	609 610

TABLE IX—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{11}H_8O_3Os$	19	$(1,4,5,6-h^4-C_8H_8)Os(CO)_3$	CCl_4	H_{-1} H_{-4}, H_{-6} H_{-5}	2.55t 5.1m 4.8t	$J_{1,2} = J_{1,8} 4.5$ $J_{4,5} = J_{5,6} 9.5$ —	C_8H_8 = Cyclo-octatetraene Structure: 	611 610
				H_{-2}, H_{-8} H_{-3}, H_{-7}	6.0d 5.1m	$J_{2,3} = J_{7,8} 6.5$ —	100 and 200 MHz On warming this complex isomerizes to the 1,3-diene complex above	
(4) PENTAHAPTO LIGANDS								
$C_{24}H_{20}BrOOSp$	20	$(h^5-C_5H_5)Os[P(C_6H_5)_3](Br)(CO)$	$CDCl_3$	H H'	4.74s 7.20m	— —	100 MHz	579
(5) MIXED LIGANDS								
$C_{14}H_{12}O_6Os_2$	21	$[h^4-C_8H_8Os(CO)_3]Os(CO)_3$	$CDCl_3$	H	2.74s, 2.61s	— —	$C_8H_{12}Os$ = 	610

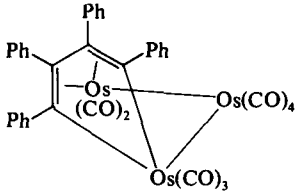
$C_{37}H_{20}O_9Os_3$	22	$[1,4-h^2-\{[H^4-C_4(C_6H_5)_4]Os(CO)_2\}-Os(CO)_3]Os(CO)_4$	—	H	7.05m, 6.80m	— —	Structure:	612
								
(6) MISCELLANEOUS								
(a) Mono-osmium complexes								
$C_{51}H_{45}N_3OOSp_2$	23	$Os[(p-CH_3C_6H_4)_2N_3][P(C_6H_5)_3]_2$ (H)(CO)	—	H	−12.85t	$J_{PH} 18.5$	—	583
$[C_{11}H_{25}OOSp_2]^+$	24	$[Os(PEt_2CH_2CH_2PEt_2)(H)(CO)]^+$	$CDCl_3$	H	−10.4	$J_{PH_{cis}} 21$	Isolated as the tetraphenylborate 100 MHz	491
$C_{26}H_{56}O_2OSp_2$	25	$Os[P(n-Bu)_3]_2(H)_2(CO)_2$	—	H	−9.42t	—	—	586
$C_{38}H_{32}O_2OSp_2$	26	$Os(H)_2[P(C_6H_5)_3]_2(CO)_2$	THF	H	−7.65t	$J 23$	—	1018
$C_{15}H_{29}O_3OSp$	27	$Os[P(n-Bu)_3](H)_2(CO)_3$	—	H	−8.97	$J_{PH} 25$	—	586
$C_{21}H_{17}O_3OSp$	28	$Os[P(C_6H_5)_3](H)_2(CO)_3$	THF	H	−8.00d	$J_{PH} 24$	—	613
$[C_{19}H_{22}IO_3OsP_2]^+$	29	$\{Os[P(CH_3)_2C_6H_5]_2(I)(CO)_3\}^+$	$CDCl_3$	H H'	2.52t 7.40m	$J_{PH} 8.5$ —	Isolated as the iodide	586 569
$[C_4HO_4Os]^-$	30	$[Os(H)(CO)_4]^-$	THF	H	−10.24s, −10.62s*	— —	* Not always observed	607 939
$C_4H_2O_4Os$	31	$Os(H)_2(CO)_4$	Heptane THF	H H	−8.73s −8.84s	— —	—	613 939
$C_7H_{10}GeO_4Os$	32	$Os(H)[Ge(CH_3)_3](CO)_4$	C_6H_6	H H'	−9.11 0.68	— —	100 MHz	1011

TABLE IX—cont.

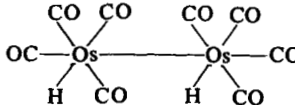
Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_7H_{10}O_4OsSi$	33	$Os[Si(CH_3)_3](H')(CO)_4$	—	H H' 0.56s -9.03s	—	100 MHz	614 940
$C_4HCl_3O_4OsSn$	34	$Os(H)SnCl_3(CO)_4$	CH_2Cl_2	H -8.37s	$J(^{119}Sn-H)$ 136 $J(^{117}Sn-H)$ 129.5	<i>cis</i> -isomer	941
$C_7H_{10}O_4OsSn$	35	$Os[Sn(CH_3)_3](H')(CO)_4$	—	H H' 0.47s -9.62s	—	100 MHz	614
$[C_5HO_5Os]^+$	36	$[Os(H)(CO)_3]^+$	H_2SO_4	H -8.2s	—	Isolated as the hexafluorophosphate. 100 MHz	589
<i>(b) Di-osmium complexes</i>							
$C_8H_2O_8Os_2$	37	$[Os(CO)_4(H)]_2$	C_6H_6	H -10.11s	—	Possible structure:	616
							
$C_{42}H_{32}O_6Os_2$	38	$Os_2(CO)_6(PPh_3)_2(H)_2$	CH_2Cl_2	H -9.46*	—	* Centre of AA'XX' multiplet $ J_{HOsP} + J_{HOsP} = 18.5$ Hz	616
$C_8HCl_3O_8Os_2Sn$	39	$[Os(H)(CO)_4][Os(SnCl_3)(CO)_4]$	—	H -9.55s	—	—	941

TABLE IX—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$[\text{C}_{26}\text{H}_{38}\text{O}_8^- \text{Os}_3\text{P}_2\text{S}]^{2+}$	42	$[\text{Os}_3(\text{PEt}_3)_2(\text{SC}_6\text{H}_5)(\text{H})_3(\text{CO})_8]^{2+}$	H_2SO_4	H -14.97d, -19.44q, -20.73d	J_{PH} 16.0 J_{PH} 18.0, 10.2 J_{PH} 11.2	Structure: 100 MHz using dimethyl sulphate (δ 3.9) as internal reference	617
$[\text{C}_{27}\text{H}_{46}\text{O}_9^- \text{Os}_3\text{P}_3]^{+}$	43	$\{\text{Os}_3(\text{H})[\text{P}(\text{C}_2\text{H}_5)_3]_3(\text{CO})_9\}^{+}$	H_2SO_4	H -19.2b	—	Isolated as the hexafluorophosphate	942
$[\text{C}_{48}\text{H}_{40}\text{O}_9^- \text{Os}_3\text{P}_3]^{+}$	44	$\{\text{Os}_3[\text{PCH}_3(\text{C}_6\text{H}_5)_2]_3(\text{H}')(\text{CO})_9\}^{+}$	CDCl_3	H 2.73d, 2.54d, 2.32d H' -17.58q, -18.33q	J_{PH} 9.4 J_{PH} 9.4 J_{PH} 10.6 J_{PH} 11.3, 8.3 J_{PH} 18.9, 10.6	Isomer A Isolated as the hexafluorophosphate	589

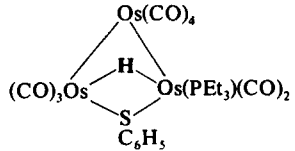
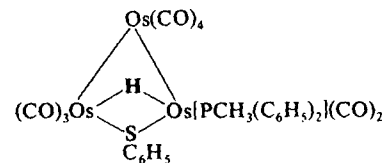
				H	2.72d, 2.51d	J_{PH} 9.5 J_{PH} 9.5	Isomer B 100 MHz
				H'	-18.85t	J_{PH} 9.5	
$C_{21}H_{21}O_9Os_3PS$ 45	$Os_3(PEt_3)(SC_6H_5)(H)(CO)_9$	$CDCl_3$		H	-16.72d	J_{PH} 26.1	Structure: 617
							
$C_{28}H_{19}O_9Os_3PS$ 46	$Os_3[PCH_3(C_6H_5)_2](SC_6H_5)(H')-(CO)_9$	$CDCl_3$		H	2.60d	J_{PH} 9.5	Structure analogous to that above 617 100 MHz
				H'	-16.88d	J_{PH} 28.5	
$[C_{21}H_{22}O_9Os_3PS]^+$ 47	$[Os_3(PEt_3)(SC_6H_5)(H)_2(CO)_9]^+$	H_2SO_4		H	-15.88d, -29.01d	J_{PH} 23.8 J_{PH} 12.4	Dimethylsulphate as internal reference (δ 3.9) 100 MHz 617
$[C_{48}H_{41}O_9Os_3P_3]^{2+}$ 48	$\{Os_3[PCH_3(C_6H_5)_2]_3(H')_2(CO)_9\}^{2+}$	H_2SO_4		H	2.65d, 2.34d, 2.18d	J_{PH} 10.5 J_{PH} 11.0 J_{PH} 11.0	Dimethylsulphate as internal reference (δ 3.9) 100 MHz 589
				H'	-18.97q, -19.38q	J_{PH} 13.0, 6.2 J_{PH} 18.8, 8.9	

TABLE IX—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References	
[C ₂₈ H ₂₀ O ₉ -Os ₃ PS] ⁺	49	{Os ₃ [PCH ₃ (C ₆ H ₅) ₂](SC ₆ H ₅)(H) ₂ (CO) ₉ } ⁺	CH ₃ NO ₂	H*	-15.8d, -18.01d	J _{PH} 26.0 J _{PH} 14.0	Isolated as the hexafluorophosphate Structure:	617	
				H'	2.89d	J 10.5			
				H†	-15.85d,	J _{PH} 26.0			
								</	



$[\text{C}_{36}\text{H}_{28}\text{O}_{10}^- \text{Os}_3\text{P}_2]^{2+}$	52	$\{\text{Os}_3[\text{PCH}_2(\text{C}_6\text{H}_5)_2]_2(\text{H}'')_2(\text{CO})_{10}\}^{2+}$	H_2SO_4	H	2.31d	J_{PH} 10.0	Isomer A	589
				H'	$\sim 7\text{m}$	—		
				H''	-19.30t,	J_{PH} 9.8		
					-19.98t	J_{PH} 7.0	Isomer B Dimethylsulphate as internal reference 100 MHz	
				H	2.73d	J_{PH} 10.5		
				H'	$\sim 7\text{m}$	—		
				H''	-19.14d,	J_{PH} 14.0		
					-19.77q	J_{PH} 18.8, 8.7		
$[\text{C}_{12}\text{H}_7\text{O}_{10}^- \text{Os}_3\text{S}]^+$	53	$[\text{Os}_3(\text{SCH}_2\text{CH}_3)(\text{H}'')_2(\text{CO})_{10}]^+$	H_2SO_4	H	2.46q	—	Dimethylsulphate as internal reference 100 MHz	617
				H'	1.18t	—		
				H''	-17.12s,	—		
					-18.87s	—		
$\text{C}_{12}\text{H}_6\text{O}_{10}\text{Os}_3\text{S}$	54	$[\text{Os}(\text{CO})_3]_2[\text{Os}(\text{CO})_4](\text{SCH}_2\text{CH}_3)(\text{H}'')$	CCl_4	H	2.60	—	Cyclic hydrido and thiol bridged structure proposed	599
				H'	1.50	—		
				H''	-17.5	—		
$\text{C}_{14}\text{H}_{10}\text{O}_{10}\text{Os}_3\text{S}$	55	$[\text{Os}(\text{CO})_3]_2[\text{Os}(\text{CO})_4][\text{SCH}_2(\text{CH}_2)_2\text{CH}_3(\text{H}''')]$	CCl_4	H	2.35m	—	Cyclic hydrido and thiol bridged structure, viz.:	599
				H'	1.50m	—		
				H''	0.95t	—		
				H'''	-17.4s	—		
$\text{C}_{16}\text{H}_6\text{O}_{10}\text{Os}_3\text{S}$	56	$[\text{Os}(\text{CO})_3]_2[\text{Os}(\text{CO})_4](\text{SC}_6\text{H}_5)(\text{H}')$	CCl_4	H	7.27s	—	Cyclic bridged structure as above	599
				H'	-17.0s	—		

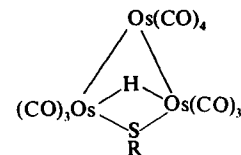
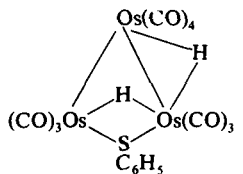
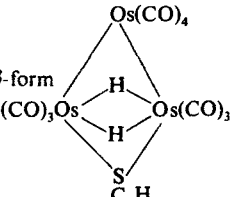


TABLE IX—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
[C ₁₆ H ₇ O ₁₀ Os ₃ S] ⁺	57	{Os ₃ (SC ₆ H ₅)(H') ₂ (CO) ₁₀ } ⁺	H ₂ SO ₄	H*	7.14m	Dimethylsulphate as internal reference (δ 3.9) 100 MHz Structure:	617
				H'*	-16.88s, -19.55s		
						 * α-form	
				H†	7.60m	† β -form	
				H'†	-16.98, -19.43		
							

$[\text{C}_{24}\text{H}_{15}\text{O}_{11}\text{Os}_3\text{P}]^{2+}$	58	$\{\text{Os}_3[\text{PCH}_3(\text{C}_6\text{H}_5)_2](\text{H}')_2(\text{CO})_{11}\}^{2+}$	H_2SO_4	H H' H''	2.79d ~7m -19.58d, -20.00d	J 11.2 — J_{PH} 12.6 J_{PH} 13.5	Dimethylsulphate as internal reference (δ 3.9) 100 MHz	589
$\text{C}_{12}\text{HO}_{12}\text{Os}_3$	59	$\text{Os}_3(\text{H})(\text{CO})_{12}$	H_2SO_4	H	-19.9	—	Dimethylsulphate as internal reference (δ 3.9) 100 MHz	600
$[\text{C}_{12}\text{HO}_{12}\text{Os}_3]^+$	60	$[\text{Os}_3(\text{H})(\text{CO})_{12}]^+$	H_2SO_4	H	-19.1s	—	Dimethylsulphate as internal reference (δ 3.9)	600 942
$\text{C}_{12}\text{H}_2\text{O}_{12}\text{Os}_3$	61	$\text{Os}_3(\text{H})_2(\text{CO})_{12}$	C_6H_6	H	-9.85	—	—	619
$\text{C}_9\text{HO}_9\text{OsRe}$	62	$\text{Os}(\text{H})(\text{CO})_4\text{Re}(\text{CO})_5$	C_6H_6	H	-10.37	—	—	619

TABLE X

Cobalt complexes

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
(1) MONOHAPTO LIGANDS								
(a) Monocarbonyl derivatives								
$C_{27}H_{33}CoF_3^-$ $N_2O_{10}P_3$	1	$Co[1-h^1-3,4-C_6F_3(CN)_2]-$ $[P(OCH_2)_3CCH_2CH_3]_3(CO)$	CH_2Cl_2 $CHCl_3$	H	4.23bs	—	100 MHz	245
				F_{-2}	-9.5	—	Relative to CF_3CO_2H	
				F_{-5}	59.5	—		
				F_{-6}	9.0	—		
(b) Dicarbonyl derivatives								
$C_{22}H_{22}CoF_3^-$ $N_2O_8P_2$	2	$Co[1-h^1-3,4-C_6F_3(CN)_2]-$ $[P(OCH_2)_3CCH_2CH_3]_2(CO)_2$	CH_2Cl_2 $CHCl_3$	H	4.21bs	—		245
				F_{-2}	-7.8	—	Relative to CF_3CO_2H	
				F_{-5}	57.6	—		
				F_{-6}	9.8	—		
$C_{46}H_{30}CoF_3^-$ $N_2O_8P_2$	3	$Co[1-h^1-3,4-C_6F_3(CN)_2]-$ $[P(OC_6H_5)_3]_2(CO)_2$	$CHCl_3$	F_{-2}	-8.85	—	Relative to CF_3CO_2H	245
				F_{-5}	58.3	—		
				F_{-6}	8.28	—		
(c) Tricarbonyl derivatives								
$C_4CoF_6O_3P$	4	$Co(CF_3)(PF_3')(CO)_3$	—	F	-634 Hz	J_{PF} 58	T 25° Relative to CCl_3F , negative values to low field and positive values to high field T -70° <i>cis</i> -isomer	652
						J_{FF} 6		
				F'	886 Hz	J_{PF} 1368		
				F	-659 Hz	J_{PF} 38		
						J_{FF} 3		
		F'	1120Hz	J_{PF} 1373				

$C_{23}H_{16}CoF_4O_3P$	5	$Co(CF_2CHF_2)[P(C_6H_5)_3](CO)_3$	—	F	−590 Hz	J_{PF} 80	} T −70° <i>trans</i> -isomer	653	
				F'	635 Hz	J_{FF} 9			
						J_{PF} 135.1			
				H	5.75tt	J_{HF} 5.5	} —		
						$J_{HF'}$ 57.0			
$C_{26}H_{20}CoF_4O_3P$	6	$Co(h^1-CF_2CF_2CH_2CH'=CH_2) \cdot [P(C_6H_5'')_3](CO)_3$	$CDCl_3$	H'	7.45	—	} 100 MHz	654	
				F	48.2	J_{PF} 30.5			
				F'	121.1	J_{FF} 5.5			
				H	2.75td	$J_{HH'}$ 7.0			
				H'	5.80m	$J_{H'H''_{it}}$ 1.8			
						$J_{H'H''_{trans}}$ 3.5			
				H''	5.20d, 5.05s	—			
$C_{27}H_{22}AsCoF_4O_3$	7	$Co(h^1-CF_2CF_2CH_2C(CH_3)=CH_2)[As(C_6H_5'')_3](CO)_3$	$CDCl_3$	H'''	7.40m	—	} 94.1 MHz	654	
				F	51.1d	J_{PF} 34.0			
				F'	101.2t	J_{HF} 19.0			
				H	2.65	$J_{HF'}$ 19.0			} 100 MHz
				H'	1.9s	—			
				H''	4.90bs, 4.83bs	—			
				H'''	7.45m	—			
$C_{27}H_{22}CoF_4O_3P$	8	$Co(h^1-CF_2CF_2CH_2C(CH_3)=CH_2)[P(C_6H_5''')_3](CO)_3$	$CDCl_3$	F	49.0s	—	} 94.1 MHz	654	
				F'	100.5t	—			
						—			
				H	2.5t	$J_{HF'}$ 19.0	} 100 MHz		
				H'	1.84s	—			
				H''	4.93bs, 4.85bs	—			
				H'''	7.4m	—			
F	50.9d	J_{PF} 29.0	} 94.1 MHz						
F'	100.7t	—							

TABLE X—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{27}H_{26}CoF_6O_3P$	9	$Co(h^1-CF(CF_3)CF_2^2CH_2CH'=CH_2^3)[P(C_6H_5^4)_3](CO)_3$	$CDCl_3$	H	3.2–2.6m	—	100 MHz	654
				H'	5.75m	—		
				H''	5.2bs,	—		
					5.05bs	—		
				H'''	7.4m	—		
				F	145.9m	—		
				F'	65.7m	—		
				F''	98.0dm, 76.0dm	$J_{F''F''} = 270$	94.1 MHz	
$C_{28}H_{22}CoF_6O_3P$	10	$Co(h^1-CF(CF_3)CF_2^2CH_2C(CH_3)=CH_2^3)[P(C_6H_5^4)_3](CO)_3$	$CDCl_3$	H	3.05–2.45m	—	100 MHz	654
				H'	1.85s	—		
				H''	4.92bs,	—		
					4.82bs	—		
				H'''	7.4m	—		
				F	145.0m	—		
				F'	64.4	—		
				F''	98.0dm, 76.5d	$J_{F''F''} = 260$	94.1 MHz	
$C_{28}H_{21}CoFO_3P$	11	$Co(h^1-3-CH_2C_6H_4F)[P(C_6H_5)_3](CO)_3$	CH_2Cl_2	F	+1.25	—	Relative to C_6H_5F	191
$C_{23}H_{16}CoF_2O_4P$	12	$Co(h^1-COCHF_2)[P(C_6H_5)_3](CO)_3$	—	H	5.28t	$J_{PH} 2.2$	—	655
				H'	7.45	—		
$C_{23}H_{17}CoFO_4P$	13	$Co(h^1-COCH_2F)[P(C_6H_5)_3](CO)_3$	THF	H	4.73d	$J_{HF} 49$	—	655
				H'	7.45	$J_{PH} 0.6$		

(d) Tetracarbonyl derivatives

C ₆ HCof ₄ O ₄	14	Co(CF ₂ CHF ₂)(CO) ₄	C ₆ H ₁₂	F	50.3m	—	656
				F'	122.5m	—	
				H	5.30tt	J _{HF} 3.7	
			C ₆ F ₆	F	41.7†	J _{FF'} 4.7	653
				F'	119.3	J _{HF'} 57.1	
						† The difference between this value and that reported above in C ₆ H ₁₂ seems too great to be due to a solvent effect	
C ₆ HCICoF ₃ O ₄	15	Co(CFCICHF ₂)(CO) ₄	C ₆ H ₁₂	H	4.10dd	J _{HF} 3.4	657
				F	69.7	J _{FF'} 20.4, 11.8	
				F'	116.6	J _{HF'} 60.1, 56.9	

(2) DIHAPTO LIGANDS

C ₉ H ₉ CoF ₄ O ₄ Sn	16	(h ² -CF ₂ =CF ₂)Co[Sn(CH ₃) ₃](CO) ₄	CDCl ₃	H	0.33	—	658
				F	41,	—	
					101	—	

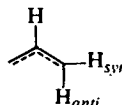
(3) TRIHAPTO LIGANDS

(a) Monocarbonyl derivatives

C ₃₅ H ₃₉ CoOP ₂	17	(1,2,3- <i>h</i> ³ -C ₈ H ₁₃)Co[P(CH ₃)Ph ₂] ₂ (CO)	C ₆ D ₆	H ₋₁ , H ₋₃	3.1m	—	C ₈ H ₁₃ = cyclooctenyl 100 MHz. TMS external	659
				H ₋₂	4.6m	—		
				CH ₂	2.1m, ~1.3	—		
				(ratio 4:6)				
C ₄₅ H ₄₃ CoOP ₂	18	(1,2,3- <i>h</i> ³ -C ₈ H ₁₃)Co(PPh ₃) ₂ (CO)	C ₆ D ₆	H ₋₁ , H ₋₃	3.4m	—	C ₈ H ₁₃ = cyclooctenyl 100 MHz. TMS external	659
				H ₋₂	4.5m	—		
				CH ₂	2.3m, 1.4m	—		
				(ratio 4:6)				

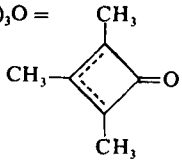
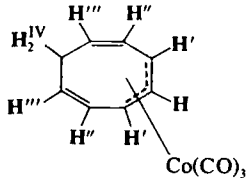
C₈H₁₃ = cyclooctenyl
100 MHz. TMS externalC₈H₁₃ = cyclooctenyl
100 MHz. TMS external

TABLE X—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{45}H_{43}CoO_7P_2$	19	$(1,2,3-h^3-C_8H_{13})Co[P(OPh)_3]_2-(CO)$	C_6D_6	H_{-1}, H_{-3} 4.0m H_{-2} 4.7m CH_2 1.8m 1.3m	— — — —	C_8H_{13} = cyclooctenyl 100 MHz. TMS external	659
(b) Dicarbonyl derivatives							
$C_{18}H_{34}CoO_2P$	20	$(h^3-CH_2 \cdots CH' \cdots CH''CH_3''')Co-[P(n-C_4H_9)_3](CO)_2$	—	H_{syn} 2.17 H_{anti} 1.35 H' 4.42 H''_{anti} 2.60 H''' 1.57 P -41*	$J_{HH'}$ 6.2 J_{PH} 9.5 $J_{HH'}$ 10.4 $J_{H'H''}$ 9.0 $J_{H''H'''} 6.0$ $J_{PH''}$ 2.9 $J_{PH'''} 4.0$ —	 Hexamethyldisiloxane reference * Trimethyl phosphate reference	950 660
$C_{24}H_{22}CoO_2P$	21	$(h^3-CH_2 \cdots CH' \cdots CH''CH_3''')Co-[P(C_6H_5)_3](CO)_2$	—	H_{syn} 2.06 H_{anti} 1.65 H' 4.21 H''_{anti} 2.72 H''' 1.41 P -64*	$J_{HH'}$ 6.0 J_{PH} 9.7 $J_{HH'}$ 10.1 J_{PH} 2.0 $J_{H'H''}$ 9.5 $J_{H''H'''} 6.0$ $J_{PH''} \sim 0$ $J_{PH'''} 4.5$ —	Hexamethyldisiloxane reference * Trimethylphosphate reference	950 660

$C_{31}H_{28}CoO_2P$	22	$(h^3-CH_2 \cdots C(CH_3) \cdots CHCH_2C_6H_5)-$ $Co(PPh_3)(CO)_2$	$CDCl_3$	H	1.66	—	Poorly resolved due to para-	661
				H'	3.18	—	magnetic impurities	
				H''	7.31	—		
$C_{25}H_{22}CoO_4P$	23	$(h^3-CH_2 \cdots CH' \cdots CH. OCOCH_3)-$ $Co[P(C_6H_5'')_3](CO)_2$	$CDCl_3$	H_{syn}	5.76d	$J_{HH'} 7.5$	—	662
				H_{anti}	1.70d	$J_{HH'} 11.2$		
				H'	4.66m	—		
				H''	1.98s	—		
				H'''	7.4m	—		
$C_{25}H_{20}CoF_4O_2P$	24	$(1,2,5-h^3-CH_2=CH'-CH''CF_2-$ $CF_2)Co[P(C_6H_5''')_3](CO)_2$	$CDCl_3$	H	3.35dd	$J_{HH} 6.0$ $J_{HH'} 2.0$	100 MHz	654
				H'	3.25bm	—		
				H, H''	2.0–2.7 comp.	—		
				H'''	7.40m	—		
			C_6H_6	F	108.8m	$J_{PF'} 33.0$	94.1 MHz	
				F'	74.4			
(c) Tricarbonyl derivatives								
$C_7H_7CoO_3$	25	$(h^3-CH_2 \cdots CH' \cdots CH''CH_3'')Co-$ $(CO)_3$	—	Not reported	$J_{HH} < 0.2$ $J_{H'H_{syn}} 6.3$ $J_{H'H_{anti}} 10.5$ $J_{H''H_{syn}} < 0.2$ $J_{H'H''} 10.5$ $J_{H''H'''} 6.5$	$\left. \begin{array}{l} \\ \\ \\ \\ \\ \end{array} \right\} \begin{array}{l} CH_3 \text{ syn to } H' \\ \\ \\ \\ \end{array}$		663
				Not reported	$J_{HH} 0.6$ $J_{H'H_{syn}} 7.1$ $J_{H'H_{anti}} 12.3$ $J_{H''H_{syn}} 1.6$ $J_{H'H''} 6.8$ $J_{H''H'''} 7.0$	$\left. \begin{array}{l} \\ \\ \\ \\ \\ \end{array} \right\} \begin{array}{l} CH_3 \text{ anti to } H' \\ \\ \\ \\ \end{array}$		663

TABLE X—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{10}H_9CoO_4$	26	$[h^3-2,3,4-C_4(CH_3)_3O]Co(CO)_3$	CS_2	H_{-2}, H_{-4} 1.69s H_{-3} 2.06s	— —	$C_4(CH_3)_3O =$ 	664
$C_{10}H_7CoO_3$	27	$(1,2,3-h^3-C_7H_7)Co(CO)_3$	CCl_2F_2	H_{-1}, H_{-3} 4.95t H_{-2} 3.5t $H_{-4}, H_{-7} \sim 6.5b$ $H_{-5}, H_{-6} \sim 5.8b$	— — — —	T -140° One singlet at ambient temperature in CS_2 (δ 5.51), indicating fluxional behaviour	182 369
$C_{11}H_9CoO_3$	28	$(h^3-C_8H_9)Co(CO)_3$	$(CD_3)_2CO$	H 4.70t H', H''' 5.2–5.6 comp. H'' 6.10dd H^{IV} 2.60t	$J_{HH'}$ 8.0 — $J_{H'H''}$ 8.0 $J_{H''H'''} 5.0$ $J_{H'''H^{IV}}$ 8.0	T -50 . 100 MHz Structure: 	665
$C_8H_5CoF_4O_3$	29	$(1,2,5-h^3-CH_2=CH'CH_2'CF_2CF_2')Co(CO)_3$	$CDCl_3$	H 3.3–3.6m H' 4.5 H'' 2.0–2.8m F 108.5m F' 73.2bs	— — — — — } — }	100 MHz 94.1 MHz	654

$C_9H_3CoF_6O_3$	30	$[1,2,5-h^3-CH_2=CH'CH_2''CF_2CF''-(CF_3)]Co(CO)_3$	$CDCl_3$	H	3.5-4.0m	—	100 MHz	654
				H'	4.65	—		
				H''	2.3-3.0m	—		
				F	96.7	$J_{FF} 240$		
					105.3dm			
				F'	161.7bs	$J_{F'F''} 23.0$		
$C_9H_3CoF_4O_3$	31	$[1,2,5-h^3-CH_2=C(CH_3)CH_2''CF_2CF'']Co(CO)_3$	$CDCl_3$	H	3.5bs	—	100 MHz	654
				H'	2.0s	—		
				H''	2.55d,	$J_{H''H'''} 10.0$		
						$J_{H''F} 21.0$		
					2.30d	$J_{H''F} 21.0$		
				F	107.4m	$J_{FF} 45$		
$C_{10}H_7CoF_6O_3$	32	$[1,2,5-h^3-CH_2=C(CH_3)CH_2''CF_2CF''-(CF_3)]Co(CO)_3$	$CDCl_3$	H	3.95bs,	—	100 MHz	654
					3.77bs	—		
				H'	2.0s	—		
				H''	2.5-3.05	—		
					comp.			
				F	106.7dm,	$J_{FF} 230$		
$C_{15}H_7CoF_{12}O_3$	33	$[1,2,7-h^3-CH_2=C(CH_3)CH_2''C(CF_3)=C(CF_3')-C(CF_3'')C(CF_3''')Co(CO)_3]$	$CDCl_3$	H	4.0bs,	—	100 MHz	654
					3.8bs	—		
				H'	2.0s	—		
				H''	2.8m	—		
				F	61.3q	$J_{FF'} 14.0$		
				F', F''	57.5-59.2m	$J_{F'F''} = 14.0$		
$C_{15}H_7CoF_{12}O_3$	33	$[1,2,7-h^3-CH_2=C(CH_3)CH_2''C(CF_3)=C(CF_3')-C(CF_3'')C(CF_3''')Co(CO)_3]$	$CDCl_3$	F'''	52.8q	$J_{F''F'''} 14.0$	100 MHz	654

TABLE X—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
(4) <i>TETRAHAPTO LIGANDS</i>							
$C_{47}H_{35}BrCoOP$	34	$[h^4-C_4(C_6H_5)_4]Co(Br)(PPh_3)(CO)$	$CDCl_3$	H 7.24m	—	$C_4(C_6H_5)_4$ = tetraphenylcyclobutadiene	666
$C_{27}H_{27}CoIOp$	35	$[h^4-C_4(CH_3)_4]Co(I)[P(C_6H_5)_3](CO)$	$CH_2Cl_2/CDCl_3$	H 1.48d H' 7.4m	J_{PH} 3.8 —	Tetramethylcyclobutadiene derivative. 60 and 100 MHz	667
$C_6H_4CoIO_2$	36	$(h^4-C_4H_4)Co(I)(CO)_2$	—	H 4.68s	—	Cyclobutadiene derivative	668
$C_{10}H_{12}CoIO_2$	37	$[h^4-C_4(CH_3)_4]Co(I)(CO)_2$	$CDCl_3$	H 1.81s	—	Hexamethyldisiloxane reference	669
$C_{30}H_{20}BrCoO_2$	38	$[h^4-C_4(C_6H_5)_4]Co(Br)(CO)_2$	$CDCl_3$	H 7.40m	—	—	666
$C_{34}H_{28}BrCoO_2$	39	$[h^4-C_4(p-C_6H_4CH_3)_4]Co(Br)(CO)_2$	$CDCl_3$	H 7.31 H' 2.33	—	—	666
(5) <i>PENTAHAPTO LIGANDS</i>							
(a) <i>Monocarbonyl derivatives</i>							
$C_6H_5CoI_2O$	40	$(h^5-C_5H_5)Co(I)_2(CO)$	$CHCl_3$	H 5.65	—	—	633
$C_6H_6Cl_3CoOSi$	41	$(h^5-C_5H_5)Co(SiCl_3)(H')(CO)$	C_6H_{12}	H 5.13 H' -13.33b	— —	— —	401 402
$C_{24}H_{20}CoOP$	42	$(h^5-C_5H_5)Co[P(C_6H_5)_3](CO)$	C_6H_6	H 4.60d H' 7.0-7.6	— —	—	918 670
$C_7H_8Br_3CoOSn$	43	$(h^5-C_5H_5)Co(Br)[Sn(CH_3)_2Br_2](CO)$	$CDCl_3$	H 5.47s H' 1.70	— J_{SnH} 56	—	671

$C_6H_{11}Br_4-$ $CoOSn_2$	44	$(h^5-C_5H_5)Co[Sn(CH_3)Br_2]_2(CO)$	$CDCl_3$	H H'	5.42s 1.74s	— $J_{SnH'} 50$	—	671
$C_{12}H_{23}CoOSn_2$	45	$(h^5-C_5H_5)Co[Sn(CH_3)_3]_2(CO)$	CS_2	H H'	4.70 0.31	— —	—	637
<i>(b) Dicarbonyl derivatives</i>								
$C_7H_5CoO_2$	46	$(h^5-C_5H_5)Co(CO)_2$	<i>o</i> -chloro- aniline	H	4.63	—	—	672
$C_7H_5Br_4-$ $CoHg_2O_2$	47	$(h^5-C_5H_5)Co(HgBr_2)_2(CO)_2$	<i>o</i> -chloro- aniline	H	4.94	—	—	672
$C_7H_5Cl_4-$ $CoHg_2O_2$	48	$(h^5-C_5H_5)Co(HgCl_2)_2(CO)_2$	<i>o</i> -chloro- aniline	H	4.87	—	—	673 672
$C_7H_5Br_2-$ $CoHgO_2$	49	$(h^5-C_5H_5)Co(HgBr_2)(CO)_2$	<i>o</i> -chloro- aniline	H	4.73	—	—	672
$C_7H_5Cl_2-$ $CoHgO_2$	50	$(h^5-C_5H_5)Co(HgCl_2)(CO)_2$	<i>o</i> -chloro- aniline	H	4.87	—	—	672
$C_7H_5CoHgI_2O_2$	51	$(h^5-C_5H_5)Co(HgI_2)(CO)_2$	<i>o</i> -chloro- aniline	H	4.63	—	—	672
$C_{12}H_{15}CoO_2$	52	$[h^5-C_5(CH_3)_5]Co(CO)_2$	CS_2	H	1.89s	—	Reference hexamethyldisiloxane	187
$C_{11}H_{15}CoO_2Si$	53	$[h^5-C_5H_4CH_2Si(CH_3)_3]Co(CO)_2$	—	H H' H''	4.80t, 4.70t 1.60 0.00	— — — —	—	250
$C_{10}H_{13}CoO_2Si$	54	$[h^5-C_5H_4Si(CH_3)_3]Co(CO)_2$	CS_2	H H'	5.04t, 4.74t 0.13	— — —	—	208

TABLE X—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_9H_9CoO_2$	55	$(1,2,3,4,5-h^5-C_7H_9)Co(CO)_2$	C_6D_6	$\equiv CH$ 4.65 CH_2 1.65, 0.90	— — —	—	1030
(6) MIXED LIGANDS							
$C_{25}H_{23}CoIOP$	56	$(h^5-C_5H_5)Co(COCH_3)(I)-[P(C_6H_5)_3]$	$CDCl_3$	H 4.77s H' 3.37s H'' 7.5m	— — —	—	674
(a) Monocarbonyl derivatives							
$[C_{26}H_{20}CoF_5OP]^+$	57	$\{(h^5-C_5H_5)Co(CF_2CF_3)-[P(C_6H_5)_3](CO)\}^+$	$(CD_3)_2CO$ or CH_3CN	F 60.8 F' 78.0s	J_{FF} 245 J_{PF} 12.3, 32.9	Hexafluorophosphate	675
$C_9H_5BrCoF_7O$	58	$(h^5-C_5H_5)Co(CF_2CF_2CF_3)(Br)(CO)$	C_6H_6	F 62.2bs F' 114.3s F'' 78.9bs	— — —		676
$C_9H_5ClCoF_7O$	59	$(h^5-C_5H_5)Co(CF_2CF_2CF_3)(Cl)(CO)$	C_6H_6	F 65.4bs F' 114.5s F'' 89.3t	— — J 10.4		676
$C_9H_5CoF_7IO$	60	$(h^5-C_5H_5)Co(CF_2CF_2CF_3)(I)(CO)$	THF	F +56 F' +114.1 F'' +79.1	— — —	94.1 MHz	954
$C_9H_5CoF_7IO$	61	$(h^5-C_5H_5)Co[CF(CF_3)_2](I)(CO)$	CH_2Cl_2	H 5.63s F +157.1 F' +64.1	— $J_{FF'}$ 10.8 —		954

$C_{11}H_5CoF_{10}O_3$	62	$(h^5-C_5H_5)Co(CF_2CF_2CF_3^-)(OCOCF_3)(CO)$	$(CH_3)_2CO$	H F F' F''	6.10s 115.6, 116.8 79.8 74.0s	— — — —	100 MHz 94.1 MHz	138
$C_{12}H_5CoF_{12}O_3$	63	$(h^5-C_5H_5)Co(CF_2CF_2CF_3^-)(OCOCF_2CF_3''')(CO)$	$(CH_3)_2CO$	H F F' F'' F'''	6.08s 115.6, 116.8 79.8 118.8 83.6	— — — — —	100 MHz 94.1 MHz	138
$C_{13}H_5CoF_{14}O_3$	64	$(h^5-C_5H_5)Co(CF_2CF_2CF_3^-)(OCOCF_2''CH_2^VCF_3^V)(CO)$	$CDCl_3$	F F' F'' F''' F ^{IV} F ^V	59.5q 116.8, 115.6 79.8t 116.2t 127.4 81.5t	J 11 — — J 11 J 9 — J 9	94.1 MHz	138
$\{C_{27}H_{20}^-CoF_7OP\}^+$	65	$\{(h^5-C_5H_5)Co(CF_2CF_2CF_3^-)[P(C_6H_5)_3](CO)]^+\}$	$(CH_3)_2CO$ or CH_3CN	F F' F''	56.8bq 115d 74.8t	J_{FF} 246 $J_{FF'}$ 11.4 —	Perchlorate	675
$C_{13}H_5CoF_{15}IO$	66	$(h^5-C_5H_5)Co(CF_2CF_2CF_3''CF_2'''-CF_2^{IV}CF_2^VCF_3^{VI})(I)(CO)$	$(CH_3)_2CO$	H F F' F'' F''' F ^{IV} F ^V F ^{VI}	5.90s 54.0 110.7 121.1 122.1 123.1 126.5 81.8	— $J_{FF''}$ 17 — — — $J_{F^IVF^VI}$ 10 — —	94.1 MHz	954

TABLE X—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{36}H_{20}CoF_5O_2$	67	$[h^4-C_4(C_6H_5)_4]Co(h^1-C_6F_5)(CO)_2$	$CDCl_3$	H 7.30 F_{ortho} 108.5m F_{meta} 164.7m F_{para} 163.4	— $J_{o,m} 24.6$ $J_{m,p} 19.2$ —		666
$C_{40}H_{28}CoF_5O_2$	68	$[h^4-C_4(p-C_6H_4CH_3)_4]Co-(h^1-C_6F_5)(CO)_2$	$CDCl_3$	H 7.20 H' 2.24 F 107.1m, 162.0m, 163.2m	J 8 — $J_{o,m} 22.8$ $J_{m,p} 18.7$ —		666
$C_{11}H_5CoF_6O$	69	$(h^5-C_5H_5)Co(h^2-C_5F_6)(CO)$		Not reported	—	Two isomers C_5F_6 = hexafluorocyclopentadiene	551
$C_{17}H_{25}CoO$	70	$(1,2,3-h^3-C_8H_{13})Co(h^4-C_8H_{12})(CO)$	Toluene- d_8	H₋₁, H₋₃ 2.8m H₋₂ 6.0t =CH' 3.7m, 3.2m CH₂, CH₂' 2.5m, 2.0m, 1.6m, 1.3m	— — — — —	T 0°, 100 MHz TMS external C_8H_{13} = cyclooctenyl C_8H_{12} = cycloocta-1,5-diene ratio 2:6:4:6	659
(7) COMPLEXES WITH TWO OR MORE COBALT ATOMS							
(a) Dicobalt derivatives							
$C_{60}H_{40}Co_2F_6O_2S_2$	71	$\{[h^4-C_4(C_6H_5)_4]Co(CO)\}_2(SCF_3)_2^*$	$CDCl_3$ CH_2Cl_2	H 7.5–7.1 F 32.3	— —	100 MHz * Bridging SCF_3 ligands	677

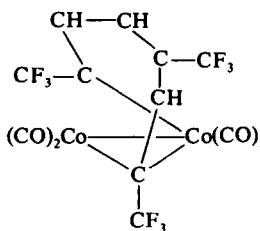
$C_{16}H_{10}Cl_4Co_2 \cdot FeGe_2O_6$	72	$[(\eta^5-C_5H_5)Co]_2[(GeCl_2)_2 \cdot Fe(CO)_4]^*(CO)_2^*$	$CDCl_3$	H	5.52	—	* Bridging ligands	678
$C_{16}H_{22}Co_2O_2Sn$	73	$\{(\eta^5-C_5H_5)Co[Sn(CH_3)_2](CO)\}_2$	CS_2	H H'	4.61 0.75	— —	—	637
$C_{18}H_{22}Co_2O_4$	74	$Co_2(C_2H_2)[CH \equiv CC(CH_3)_2](CO)_4$	—	H	5.7d, 3.8d, 1.5s	— — —	—	953
$C_{22}H_{30}Co_2O_4$	75	$Co_2[HC \equiv CC(CH_3)_3](CO)_4$	—	H	5.7m, 3.8s, 1.5s, 1.1s	— — — —	—	953
$C_{13}H_3Co_2F_9O_4$	76	$Co_2(CF_3C_2H)_3(CO)_4$	CCl_4	H	6.51, 6.32, 4.02	— — —	—	953
				F	58.2, 58.4, 64.4	— — —		
			$CDCl_3$	H	6.39s, 6.28s, 3.99s	— — —	Structure proposed:	679
				F	58.6, 58.9, 64.8	— — —		

TABLE X—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{14}H_5Co_2F_9O_4$	77	$(CF_3C_2CH_3)(CF_3C_2H')_2Co_2(CO)_4$	$CDCl_3$	H	1.65	—	—	680
				H'	6.47,	—		
					6.13	—		
				F	57.25,	—		
					57.32,	—		
$C_{14}H_2Co_2F_{12}O_4$	78	$(CF_3C_2CF_3)(CF_3C_2H)_2Co_2(CO)_4$	$CDCl_3$	H	6.39s,	—	Structure analogous to that above	679
					4.01s	—		
				F	61.4q,	—	Isomer I	
					51.1q	—		
				F'	64.0s,	—		
					57.8s	—	Isomer II	679 953
				H	6.59s	—		
$C_{15}HCo_2F_{15}O_4$	79	$(CF_3C_2CF_3)_2(CF_3C_2H)Co_2(CO)_4$	CCl_4	H	6.51s	—	Structure analogous to that above	679
				F	61.8q,	—		
			$CDCl_3$		59.5q,	—		
					55.4q,	—		
					52.2q	—		
				F'	57.6s	—		
						—		
$C_{16}H_3Co_2F_{13}O_4$	80	$(CF_3C_2CF_3)_2(CF_3C_2CH_3)Co_2(CO)_4$	CCl_4	H	1.28s	—	—	680
				F	59.2m,	—		
					55.1m,	—		
					50.5m	—		

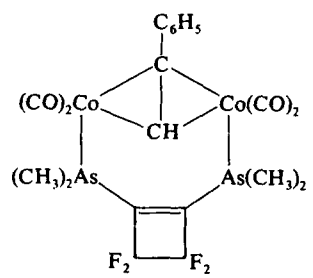
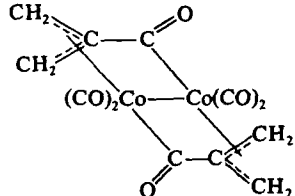
$C_{16}Co_2F_{18}O_4$	81	$(CF_3C_2CF_3)_3Co_2(CO)_4$	$CDCl_3$	F	59.1q 55.3 sept. 52.0q	— — —	Structure analogous to that above	679 681
			CCl_4	F	53.2, 56.5, 60.4	— — —		953
$C_{44}H_{33}Co_2F_3O_4P_2$	82	$(CF_3C_2CH_3)Co_2[P(C_6H_5)_3]_2(CO)_4$	$CDCl_3$	H H' F	2.15s 7.37m 45.8s	— — —	—	680
$C_{48}H_{31}Co_2F_5O_4P_2$	83	$(C_6F_5C_2H)Co_2[P(C_6H_5)_3]_2(CO)_4$	$CDCl_3$	H	7.35m	—	—	681
$C_{54}H_{35}Co_2F_5O_4P_2$	84	$(C_6H_5C_2C_6F_5)Co_2[P(C_6H_5)_3]_2(CO)_4$	$CDCl_3$	H	7.08m	—	—	681
$C_{20}H_{18}As_2Co_2F_4O_4$	85	$(C_6H_5C_2H)Co_2\{[As(CH_3)_2]_2C_4F_4\}(CO)_4$	—	n.a.	—	—	Proposed structure:	682
							 Signals at δ 1.45, 1.56, 5.50, 7.1–7.3, in ratio 6:6:1:5	
$C_{16}H_{20}Co_2O_4$	86	$\{[h^4-CH_2=C(CH_3)-C(CH_3)=CH_2]Co(CO)_2\}_2$	$CHCl_3$	H H'	2.16, 1.63 1.81	— — —	—	357

TABLE X—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{14}F_{12}Co_2O_4$	87	$[(h^4-C_5F_6)Co(CO)_2]_2$	—	not reported	—	C_5F_6 = hexafluorocyclopentadiene	551
$C_{18}H_{16}Cl_2Co_2O_4Sn$	88	$[(h^4-C_7H_8)Co(CO)_2]_2Sn(Cl)_2$	CD_2Cl_2	—	—	Norbornadiene derivative. One signal associated with the olefinic protons (δ 4.18s) which split into two peaks of equal intensity at -95°	683
$C_{30}H_{26}Co_2O_4Sn$	89	$[(h^4-C_7H_8)Co(CO)_2]_2Sn(C_6H_5)_2$	CD_2Cl_2	—	—	Norbornadiene derivative. One olefinic signal (δ 3.84)	683
$C_{12}H_8Co_2O_6$	90	$\{[CH_2 \cdots C(CO) \cdots CH_2]Co(CO)_2\}_2$	$CDCl_3$	H 3.61s, 2.28s	— —	Structure: 	532
$C_{16}H_{14}Co_2O_4Si$	91	$[h^5: h^5-C_5H_4Si(CH_3)_2C_5H_4]Co(CO)_2$	—	H 5.12t, 4.80t H' 0.38	— — —	—	250
$C_{25}H_{17}Co_2O_5P$	92	$(h^2: h^2-CH \equiv CH)\{Co[P(C_6H_5)_3](CO)_2\} [Co(CO)_3]$	CS_2	H 5.03d H' 7.3m	J_{PH} 2.9 —	—	684 685

$C_{21}H_{18}As_2 \cdot Co_2F_4O_5$	93	$(C_6H_5C \equiv CH')Co_2\{[As(CH_3)_2]_2C_4F_4\}(CO)_5$	—	H H' H''	7.1–7.6 3.83 1.32*	— — —	T 30° * At T –50° this signal split into three peaks at δ 1.19, 1.27, and 1.31 in ratio 1:1:2	682
$C_{31}H_{27}Co_2O_5P$	94	$[h^4-C_4(CH_3)_4][Co(CO)_2]\{Co-[P(C_6H_5)_3](CO)_3\}$	$CDCl_3$	H H'	1.92 7.6m	— —	Tetramethylcyclobutadiene derivative	669
$C_{46}H_{30}As_2 \cdot Co_2F_6O_6$	95	$(2-h^1:3-h^1-CF_3C \equiv CCF_3)[CoAs-(C_6H_5)_3(CO)_3]_2$	$CHCl_3$	F	–15.1	—	Relative to benzotrifluoride at 56.4 MHz	686
$C_{36}H_{24}Co_2 \cdot F_6O_6P_2$	96	$(2-h^1:3-h^1-CF_3C \equiv CCF_3)[Co-(CO)_3]_2[PPH_2(CH_2)_2PPH_2]$	$CHCl_3$	F	–13.4t	J_{PF} 9.4	Relative to benzotrifluoride at 56.4 MHz	686
$C_{46}H_{30}Co_2 \cdot F_6O_6P_2$	97	$(2-h^1:3-h^1-CF_3C \equiv CCF_3)\{Co-[P(C_6H_5)_3](CO)_3\}_2$	$CHCl_3$	F F	–15.08 –14.86	— —	T –30° (Relative to benzotrifluoride) T –60° (ide at 94.1 MHz)	686
$C_8H_2Co_2O_6$	98	$(h^2:h^2-CH \equiv CH)[Co(CO)_3]_2$	CS_2	H	–4.0s	$J(^{13}C-H)$ 222.3 $J(^{13}C \equiv C-H)$ 15.3 J_{HH} 1.0	100 MHz Structure with C_{2v} symmetry of co-ordinated acetylene proposed and vibrational frequencies compared to that of electronically excited state. Change in hybridization ($sp \rightarrow sp^2$) confirmed by $J(^{13}C-H)$ which is intermediate between that of acetylene and ethylene	687 685
$C_9H_4Co_2O_6$	99	$(h^2:h^2-CH \equiv CCH_3)[Co(CO)_3]_2$	CCl_4	H H'	5.97 2.75	$J(^{13}C-H)$ 220 ± 2 $J(^{13}C-H')$ 132	100 MHz	687
$C_9HCo_2F_3O_6$	100	$(h^2:h^2-CH \equiv CCF_3)[Co(CO)_3]_2$	CCl_4	H F	6.1 –11.1s	— —	100 MHz Relative to benzotrifluoride at 94.1 MHz	353

TABLE X—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{10}H_3Co_2F_3O_6$	101	$(h^2 : h^2 \cdot CH_3C \equiv CCF_3)[Co(CO)_3]_2$	CCl_4	H	2.70s	—	—	680
				F	52.09s	—		
$C_{10}H_6Co_2O_6$	102	$(h^2 : h^2 \cdot CH_3C \equiv CCH_3)[Co(CO)_3]_2$	CCl_4	H	2.64	—	100 MHz	687
			$CDCl_3$	H	2.65s	—		680
$C_{12}H_{10}Co_2O_7$	103	$[CH \equiv CC(OCH_3)(CH_3)_2]Co_2(CO)_6$	—	H	6.01s	—	—	688
				H'	3.23s	—		
				H''	1.50s	—		
$C_{14}HCo_2F_5O_6$	104	$(h^2 : h^2 \cdot CH \equiv CC_6F_5)[Co(CO)_3]_2$	CCl_4	H	6.45	—	100 MHz	354
				F	137.9d	J_{FF} 23		
					154.7t	J_{FF} 23		
					162.3t	J_{FF} 23		
$C_{20}Co_2F_{10}O_6$	105	$(h^2 : h^2 \cdot C_6F_5C \equiv CC_6F_5)[Co(CO)_3]_2$	CCl_4	F_{ortho}	58.9q	—	Relative to CF_3CO_2H at 56.4 MHz	689
				F_{meta}	82.8m	—		
				F_{para}	74.9t	—		
$C_{22}H_6Co_2F_8O_8$	106	$[h^2 : h^2 \cdot (p-C_6F_4OCH_3)C \equiv C(p-C_6F_4OCH_3)][Co(CO)_3]_2$	CCl_4	H	4.5	—	Relative to CF_3CO_2H	689
				F_{ortho}	61.3m	—		
				F_{meta}	81.1m	—		
$C_{10}H_4Co_2O_7$	107	$(h^2 : h^2 \cdot CH \equiv CCOCH_3)[Co(CO)_3]_2$	CCl_4	H	6.18s	—	—	690
				H'	2.43s	—		
$C_{14}H_{12}Co_2O_7$	108	$[h^2 : h^2 \cdot (CH_3)_3CC \equiv CCOCH_3]Co(CO)_3]_2$	CCl_4	H	1.38s	—	—	690
				H'	2.48s	—		

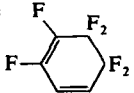
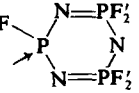
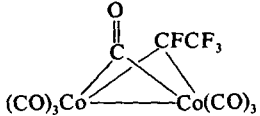
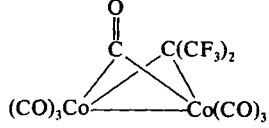
$C_{12}Co_2F_6O_6$	109	$(h^2:h^2-C_6F_6)[Co(CO)_3]_2$	—	n.a.	—	—	$C_6F_6 = $ 	691
$C_{28}H_{18}Co_2Fe_2O_6$	110	$(h^2:h^2-FcC\equiv CFc)[Co(CO)_3]_2$	$CDCl_3$	H	4.24	—	Fc = ferrocenyl Signals at 36.2, 49.7, 59.0, and 89.7 ppm relative to benzonitrile, in ratio 2:2:1:1	559
$C_{14}H_5Co_2F_5N_3P_3$	111	$[h^2:h^2-C_6H_5C\equiv C(F_5N_3P_3)]-[Co(CO)_3]_2$	C_6H_6	F F'	49.8 68.2	$J_{PF} 970$ $J_{PF} 910$	$F_5N_3P_3 = $ 	692
$C_{14}H_{18}Co_2Ge_2O_6$	112	$[h^2:h^2-(CH_3)_3GeC\equiv CGe(CH_3)_3]-[Co(CO)_3]_2$	CCl_4	H	0.47s	—	—	690
$C_{14}H_{18}Co_2GeO_6Si$	113	$[h^2:h^2-(CH_3)_3GeC\equiv CSi(CH_3)_3]-[Co(CO)_3]_2$	CCl_4	H	0.55s, 0.40s	— —	—	690
$C_{11}H_{10}Co_2O_6Sn$	114	$[h^2:h^2-CH\equiv CSn(CH_3)_3]-[Co(CO)_3]_2$	CCl_4	H H'	6.25s 0.42	$J(^{117}Sn-H) 53$ $J(^{119}Sn-H') 56$	—	690
$C_{15}H_{18}Co_2O_6Sn$	115	$[h^2:h^2-(CH_3)_3CC\equiv CSn(CH_3)_3]-[Co(CO)_3]_2$	CCl_4	H H'	1.35s 0.43	$J(^{117}Sn-H') 55$ $J(^{119}Sn-H') 58$	—	690
$C_{14}H_{18}Co_2O_6SiSn$	116	$[h^2:h^2-(CH_3)_3SiC\equiv CSn(CH_3)_3]-[Co(CO)_3]_2$	CCl_4	H H'	0.30s 0.42	$J(^{117}Sn-H') 55$ $J(^{119}Sn-H') 58$	—	690
$C_{14}H_{18}Co_2O_6Sn_2$	117	$[h^2:h^2-(CH_3)_3SnC\equiv CSn(CH_3)_3]-[Co(CO)_3]_2$	CCl_4	H	0.40	$J(^{117}Sn-H) 53$ $J(^{119}Sn-H) 56$	—	690

TABLE X—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)		Remarks	References
$C_{10}Co_2F_6O_6$	118	$(h^1:h^2-CF_2=CF-CF=CF_2)-[Co(CO)_3]_2$	—	F	26.2b, 36.7d	J 75 J 16.5	Relative to benzotrifluoride at 56.4 MHz	283
$C_{10}H_4Co_2O_6$	119	$(h^4-C_4H_4)[Co(CO)_2][Co(CO)_4]$	—	H	4.58s	—	—	668
$C_{14}H_{12}Co_2O_6$	120	$[h^4-C_4(CH_3)_4][Co(CO)_2]-[Co(CO)_4]$	$CDCl_3$	H	1.67s	—	Hexamethyldisiloxane as reference	669
$C_9Co_2F_4O_7$	121	$(CFCF_3)[Co(CO)_3]_2(CO)$	$CFCl_3$	F F'	50.0q 70.8d	J 12 J 12	Structure: 	656 1031
$C_{10}Co_2F_6O_7$	122	$[C(CF_3)_2][Co(CO)_3]_2(CO)$	—	F	49.5s	—	94.1 MHz Structure: 	454 455
$C_{10}Co_2F_4O_8$	123	$(1,2-h^1:h^1-CF_2CF_2)[Co(CO)_4]_2$	—	F	31.8	—	—	658

(b) Tricobalt derivatives

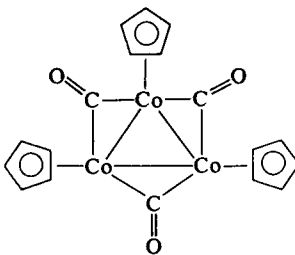
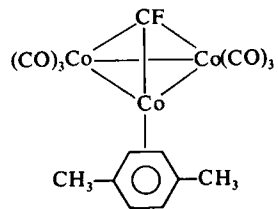
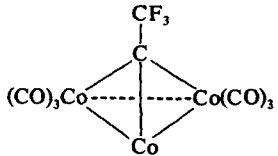
$C_{18}H_{15}Co_3O_3$	124	$[(\eta^5-C_5H_5)Co(CO)]_3$	C_6H_6	H	4.56	—	Structure:	557
								
$C_{15}H_{10}Co_3FO_6$	125	$[\eta^6-p-C_6H_4(CH_3)_2](CF)Co-[Co(CO)_3]_2$	CS_2	H	5.55	—	Structure:	693
								
$C_{16}H_{12}Co_3FO_6$	126	$[\eta^6-1,3,5-C_6H_3(CH_3)_3](CF)Co-[Co(CO)_3]_2$	CS_2	H	5.44	—	Structure analogous to that above	693
$C_{16}H_{13}Co_3O_6$	127	$[\eta^6-1,2-C_6H_4(CH_3)_2](CCH_3)Co-[Co(CO)_3]_2$	—	H	5.93, 5.44	—	Structure analogous to that above	693
				H'	3.64	—		
$C_{16}H_{13}Co_3O_6$	128	$[\eta^6-1,4-C_6H_4(CH_3)_2](CCH_3)Co-[Co(CO)_3]_2$	—	H	5.49	—	Structure analogous to that above	693
				H'	3.65	—		

TABLE X—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{17}H_{15}Co_3O_6$	129	$[h^6-1,3,5-C_6H_3(CH_3)_3](CCH'_3)Co-[Co(CO)_3]_2$	CS_2	H	5.45	Structure analogous to that above	694 693
				H'	2.36		
				H''	3.64		
$C_{19}H_{11}Co_3O_6$	130	$(h^6-C_6H_6)(CC_6H_5)Co[Co(CO)_3]_2$	CS_2	H	5.91	Structure analogous to that above	693
				H'	7.46,		
					7.17		
$C_{20}H_{13}Co_3O_6$	131	$(h^6-C_6H_5CH_3)(CC_6H_5)Co-[Co(CO)_3]_2$	CS_2	H	5.62,	Structure analogous to that above	693
					5.86		
				H'	7.41,		
$C_{21}H_{15}Co_3O_6$	132	$[h^6-1,2-C_6H_4(CH_3)_2](CC_6H_5)Co-[Co(CO)_3]_2$	CS_2	H	5.49,	Structure analogous to that above	693
					5.86		
				H'	7.45,		
$C_{21}H_{15}Co_3O_6$	133	$[h^6-1,3-C_6H_4(CH_3)_2](CC_6H_5)Co-[Co(CO)_3]_2$	CS_2	H	5.33,	Structure analogous to that above	693
					5.65		
				H'	7.21,		
$C_{21}H_{15}Co_3O_6$	134	$[h^6-1,4-C_6H_4(CH_3)_2](CC_6H_5)Co-[Co(CO)_3]_2$	—	H	5.49	Structure analogous to that above	693
				H'	7.21,		
					7.41		
$C_{22}H_{17}Co_3O_6$	135	$[h^6-1,3,5-C_6H_3(CH_3)_3](CC_6H_5)Co[Co(CO)_3]_2$	CS_2	H	5.34	Structure analogous to that above	693
				H'	7.20,		
					7.40		

$C_{33}H_{57}^-$ $As_2Co_3O_7$	136	$(CCH_3)Co_3[As(C_4H_9)_3]_2(CO)_7$	—	H H	2.47 2.56	—	—	695 951
$C_{35}H_{29}^-$ $As_2Co_3O_7$	137	$(CCH_3)Co_3(AsMePh_2)_2(CO)_7$	—	H	2.42	—	—	695
$C_{33}H_{57}^-$ $Co_3O_7P_2$	138	$(CCH_3)Co_3[P(C_4H_9)_3]_2(CO)_7$	—	H	2.60s, 2.46t	—	—	695
$C_{45}H_{33}Co_3O_7P_2$	139	$Co_3(CCH_3)[P(C_6H_5)_3]_2(CO)_7$	—	H	2.65	—	—	951
$C_{22}H_{30}AsCo_3O_8$	140	$(CCH_3)Co_3[As(C_4H_9)_3](CO)_8$	—	H H	2.95 3.19	—	—	695 951
$C_{23}H_{16}AsCo_3O_8$	141	$(CCH_3)Co_3(AsMePh_2)(CO)_8$	$CDCl_3$	H	3.06	—	100 MHz	695
$C_{28}H_{18}AsCo_3O_8$	142	$(CCH_3)Co_3[As(C_6H_5)_3](CO)_8$	$CDCl_3$	H	3.10	—	100 MHz	695 951
$C_{22}H_{30}Co_3O_8P$	143	$(CCH_3)Co_3[P(C_4H_9)_3](CO)_8$	$CDCl_3$	H	3.10, 3.08	— —	100 MHz	695 951
$C_{28}H_{36}Co_3O_8P$	144	$(CCH_3)Co_3[P(C_6H_{11})_3](CO)_8$	—	H	2.60	—	—	695
$C_{20}H_{18}Co_3O_8P$	145	$(CCH_3)Co_3(PEt_2Ph)(CO)_8$	—	H	2.95	—	—	695
$C_{28}H_{18}Co_3O_8P$	146	$(CCH_3)Co_3[P(C_6H_5)_3](CO)_8$	$CDCl_3$	H	3.15	—	100 MHz	695 951
$C_{28}H_{18}AsCo_3O_8$	147	$(CC_6H_5)Co_3(AsMePh_2)(CO)_8$	—	H	7.22	—	—	695
$C_{33}H_{20}AsCo_3O_8$	148	$(CC_6H_5)Co_3[As(C_6H_5)_3](CO)_8$	—	H	7.23	—	—	695
$C_{27}H_{32}Co_3O_8P$	149	$(CC_6H_5)Co_3[P(C_4H_9)_3](CO)_8$	—	H	7.15, 7.48	— —	—	695

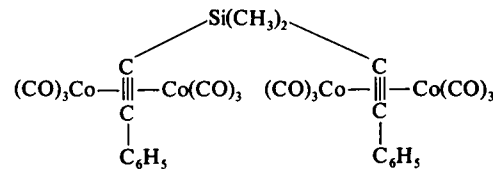
TABLE X—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{33}H_{38}Co_3O_8P$	150	$(CC_6H_5)_3Co_3[P(C_6H_{11})_3](CO)_8$	—	H 7.15, 7.52	—	—	695
$C_{25}H_{20}Co_3O_8P$	151	$(CC_6H_5)_3Co_3(PEt_2Ph)(CO)_8$	—	H 7.22	—	—	695
$C_{33}H_{20}Co_3O_8P$	152	$(CC_6H_5)_3Co_3[P(C_6H_5)_3](CO)_8$	—	H 7.24	—	—	695
$C_{10}BrCo_3O_9$	153	$(CBr)[Co(CO)_3]_3$	—	^{13}C +186.2	—	—	32
$C_{10}Co_3FO_9$	154	$(CF)[Co(CO)_3]_3$	—	F -44.5	—	—	658
$C_{11}Co_3F_3O_9$	155	$(CCF_3)[Co(CO)_3]_3$	—	F 50.3s	—	Structure:	656 658
							
$C_{11}HD_2Co_3O_9$	156	$(CCHD_2)[Co(CO)_3]_3$	$CDCl_3$	H 3.61q	J_{HD} 2.2	—	696
$C_{11}H_2DCo_3O_9$	157	$(CCH_2D)[Co(CO)_3]_3$	$CDCl_3$	H 3.67t	J_{HD} 2.0	—	696
$C_{11}H_3Co_3O_9$	158	$(CCH_3)[Co(CO)_3]_3$	$CFCl_3$	H 3.7s	—	—	656
			$CDCl_3$	H 3.64	—	—	695
			C_6H_6	H 3.10s	$J(^{13}C-H)$ 128	—	696 687 953 951

$C_{12}H_2Co_3F_3O_9$	159	$(CCH_2CF_3)[Co(CO)_3]_3$	—	H	4.3q (4.41q)*	J 9.5	—	458 *953
				F	65.1t (66.1t)*	J 9.5		
$C_{12}H_5Co_3O_9$	160	$(CCH_2CH_3)[Co(CO)_3]_3$	—	H	3.78q	J 7.5	—	688
				H'	1.54t	J 7.5		
$C_{13}H_7Co_3O_9$	161	$(CCH_2CH_2CH_3)[Co(CO)_3]_3$	—	H	1.91m, 3.65t	— J 7.0	—	688
				H'	1.16t	J 7.0		
$C_{14}H_9Co_3O_9$	162	$[CCH_2CH'(CH_3)_2][Co(CO)_3]_3$	—	H	3.67d	J 5.5	—	688
				H'	2.2–1.7m	—		
				H''	1.19d	—		
$C_{13}H_5Co_3O_{11}$	163	$(CCH_2CO_2CH_3)[Co(CO)_3]_3$	—	H	4.6	—	—	658
				H'	3.75	—		
$C_{17}H_7Co_3O_9$	164	$Co_3(CCH_2C_6H_5)(CO)_9$	CCl_4	H	4.02s	—	—	953
				H'	7.11s	—		
$C_{17}H_2Co_3F_5O_9$	165	$(CCH_2C_6F_5)[Co(CO)_3]_3$	CCl_4	H	4.97	—	—	354
			C_6H_6	H	4.41	—		953
				F	143.9m, 155.9t, 161.8m	J_{FF} 18		
$C_{16}H_5Co_3O_9$	166	$(CC_6H_5)[Co(CO)_3]_3$	—	H	7.23	—	—	695
$C_{18}H_7Co_3O_{10}$	167	$[C(p-C_6H_4COCH_3)][Co(CO)_3]_3$	$CDCl_3$	H	7.4d, 7.9d	J 8	—	697
				H'	2.55s	—		
(c) <i>Tetracobalt derivatives</i>								
$C_{14}H_6Co_4O_{10}$	168	$(CH_3C\equiv CCH_3)Co_4(CO)_{10}$	CH_2Cl_2	H	2.70s	—	—	681

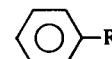
TABLE X—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)		Remarks	References
$C_{14}H_3Co_4F_3O_{10}$	169	$(CH_3C\equiv CCF_3)Co_4(CO)_{10}$	$CDCl_3$	H 2.76	—	—		680
$C_{14}Co_4F_6O_{10}$	170	$(CF_3C\equiv CCF_3)Co_4(CO)_{10}$	$CHCl_3$	F 47.2s, 52.1s	— —	—		681
$C_{18}H_6Co_4O_{10}$	171	$(CH\equiv CC_6H_5)Co_4(CO)_{10}$	CH_2Cl_2	H 7.36m	—	—		681
$C_{24}H_5Co_4F_5O_{10}$	172	$(C_6H_5C\equiv CC_6F_5)Co_4(CO)_{10}$	CCl_4	H 7.35m, 7.71m	— —	—		681
$C_{20}Co_4F_{12}O_{12}$	173	$(CF_3C\equiv CCF_3)_2Co_4(CO)_{12}$	$CHCl_3$	F -10.26 F -9.52	— —	—	T 30° T -60° Relative to benzotrifluoride at 94.1 MHz	686
$C_{30}H_{16}Co_4O_{12}Si$	174	$[(C_6H_5C\equiv C)_2Si(CH_3)_2]-[Co(CO)_3]_4$	—	H 7.2, 7.4 H' 0.9	— — —	—	Structure:	698

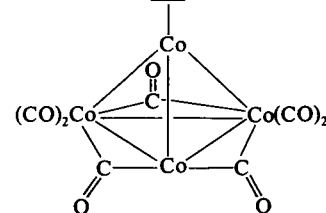


$C_{15}H_6Co_4O_9$	175	$(h^6-C_6H_6)Co_4(CO)_9$	—	—	—	}
$C_{16}H_8Co_4O_9$	176	$(h^6-C_6H_5CH_3)Co_4(CO)_9$	—	—	—	

Structure:



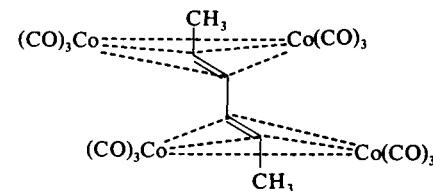
1032

R = H, CH₃

$C_{18}H_6Co_4O_{12}$	177	$Co_4(CH_3C_2C_2CH_3)(CO)_{12}$	CH_2Cl_2	H	2.73s	—
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Structure:

952



$C_{28}H_{10}Co_4O_{12}$	178	$Co_4(C_6H_5C_2C_2C_6H_5)(CO)_{12}$	$CDCl_3$	H	7.45m, 7.60m	—
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952

(d) Pentacobalt derivatives

$C_{18}HCo_5O_{15}$	179	$(C_3H)[Co(CO)_3]_5$	$CDCl_3$	H	6.88	—
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100 MHz

699

The product is derived from chloromethynyltricobalt enneacarbonyl by heating in mesitylene at 130°. The crystal structure is reported

TABLE X—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
<i>(e) Hexacobalt derivatives</i>								
C ₅₈ H ₅₅ Co ₆ O ₁₄ P ₃	180	(CC ₆ H ₅) ₂ Co ₆ (PEt ₂ Ph) ₃ (CO) ₁₄	—	H	6.53	—	—	695
C ₄₉ H ₄₀ Co ₆ O ₁₅ P ₂	181	(CC ₆ H ₅) ₂ Co ₆ (PEt ₂ Ph) ₂ (CO) ₁₅	—	H	6.93	—	—	695
<i>(8) MISCELLANEOUS COBALT COMPLEXES</i>								
CHCoF ₉ OP ₃	182	Co(H)(PF ₃) ₃ (CO)	Ether	H	-11.4	—	—	700
C ₃₇ H ₈₂ CoOP ₃	183	Co(H)[P(C ₄ H ₉) ₃](CO)	C ₆ D ₆	H	-13.9q	J _{PH} 48	—	701 702
C ₄₀ H ₄₀ CoOP ₃	184	Co(H)[P(CH ₃)Ph ₂] ₃ (CO)	THF	H	-13.5q	J _{PH} 50	External TMS	659
C ₅₅ H ₄₆ CoOP ₃	185	Co(H)(PPh ₃) ₃ (CO)	THF	H	-13.0q	J _{PH} 50	External TMS	659
			C ₆ H ₆	H	-12.3q	J _{PH} 48 or 41 (?)	—	703 704
[C ₄ H ₁₁ B ₉ CoO ₂] ⁻	186	{[π -(3)-1,2-B ₉ C ₂ H ₁₁][Co(CO) ₂]} ⁻	CH ₃ CN	B	24.1d* 11.6d* (ratio 1:2)	—	Tetramethylammonium salt * Relative to BF ₃ ·OEt ₂ at 32 MHz	77

$C_{26}H_{55}CoO_2P_2$	187	$Co(H)[P(C_4H_9)_3](CO)_2$	C_6H_{12}	H	-11.15	J_{PH} 49.1	100 MHz	701
			C_6H_6	H	-10.62	J_{PH} 48.6		702
			THF	H	-10.96	J_{PH} 47.6		
			CH_3CO_2Et	H	-10.96	J_{PH} 47.5		
			$CH_3OH/$ $(CH_3)_2CO$	H	-10.94	J_{PH} 46.5		
			CH_3COCH_2- $CHMe_2$	H	-10.77	J_{PH} 46.9		
			Pyridine	H	-10.55	J_{PH} 46.7		
			$(CH_3)_2CO$	H	-10.90	J_{PH} 45.9		
			DMF	H	-10.83	J_{PH} 45.3		
$C_{38}H_{31}CoO_2P_2$	188	$Co(H)[P(C_6H_5)_3](CO)_2$	C_6H_6	H	-10.35t	J_{PH} 41	—	705
								703
$C_{38}H_{31}CoO_8P_2$	189	$Co(H)[P(OC_6H_5)_3](CO)_2$	—	H	-11.9t	J_{PH} 21	—	705
$[C_3H_{20}-$ $B_{18}CoO_3]^-$	190	$[Co(m-B_{18}H_{20})(CO)_3]$	—	Not reported		—	Tetramethylammonium salt	706
$C_{21}H_{16}CoO_3P$	191	$Co(H)[P(C_6H_5)_3](CO)_3$	—	H	-10.7d	J_{PH} 57	—	705
C_4HCoO_4	192	$Co(H)(CO)_4$	Ether	H	-10.0	—	—	700

707
705
708

TABLE XI
Rhodium complexes

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
(1) <i>MONOHAPTO LIGANDS</i>							
(a) <i>Monocarbonyl derivatives</i>							
$C_{38}H_{33}As_2Cl_2ORh$	1	$Rh(CH_3)(AsPh_3)_2(Cl)_2(CO)$	C_6D_6	H 0.22	—	Mixture of both compounds 100 MHz	620
$C_{39}H_{33}As_2Cl_2O_2Rh$	2	$Rh(COCH_3)(AsPh_3)_2(Cl)_2(CO)$	H'	1.53d $J_{PH} 2$			
$C_{18}H_{25}Br_2OP_2Rh$	3	$Rh(CH_3)[P(CH_3)_2Ph]_2(Br)_2(CO)$	C_6H_6	H 0.82	$J_{PH} 5.4$ $J_{RhH} 2.2$ $J 8.0$	T 34°	621
				H' 2.07t, 1.80t			
$C_{18}H_{25}Cl_2OP_2Rh$	4	$Rh(CH_3)[P(CH_3)_2Ph]_2(Cl)_2(CO)$	C_6H_6	H 0.72	$J_{PH} 5.0$ $J_{RhH} 2.1$ $J 8.0$	T 34°	621
				H' 1.97t, 1.74t			
$C_{38}H_{33}Cl_2OP_2Rh$	5	$Rh(CH_3)(Cl)_2[P(C_6H_5)_3]_2(CO)$	$C_6H_5CF_3$	H 0.85	$J_{PH} 5.0$ $J_{RhH} 2.1$	Phosphine ligands <i>trans</i> -orientated and Cl <i>cis</i> Two isomers obtained by the action of acetyl chloride on $RhCl(PPh_3)_3$ Two further signals at δ 2.58 and 3.26 indicates the presence of two isomeric acetyl complexes: $Rh(CH_3)(Cl)_2(PPh_3)_2(CO) \rightleftharpoons Rh(COCH_3)(Cl)_2(PPh_3)_2$	622
				H 1.63m			

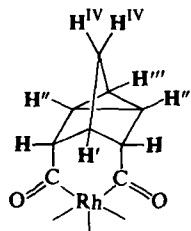
$[\text{C}_3\text{H}_5\text{Cl}_2\text{ORh}]_n$	6	$[\text{Rh}(\text{CH}_2\text{CH}_2)(\text{Cl})_2(\text{CO})]_n$	CDCl_3	H H'	4.0 1.24	J 7 —	Since rhodium(III) is normally hexacoordinate n is probably > 2	623
$\text{C}_{39}\text{H}_{31}\text{F}_4\text{OP}_2\text{Rh}$	7	$\text{Rh}(\text{CF}_2\text{CHF}_2)[\text{P}(\text{C}_6\text{H}_5)_3]_2(\text{CO})$	—	H F F'	5.00tt -74.83b* -34.20d*	J_{HF_a} 9 J_{HF_b} 56 — —	100 MHz T 35° * Relative to C_6F_6 at 94.1 MHz	624
$\text{C}_{39}\text{H}_{32}\text{ClF}_4\text{-OP}_2\text{Rh}$	8	$\text{Rh}(\text{C}_2\text{F}_4\text{H})(\text{PPH}_3)_2(\text{Cl})(\text{H})(\text{CO})$	—	H	-12.6	—	Unstable	625
$\text{C}_{39}\text{H}_{31}\text{F}_4\text{O}_3\text{-P}_2\text{RhS}$	9	$\text{Rh}(\text{CF}_2\text{CHF}_2)[\text{P}(\text{C}_6\text{H}_5)_3]_2(\text{SO}_2)(\text{CO})$	—	H F F'	5.62tt -83.9b* -28.6d*	J_{HF_a} 9 J_{HF_b} 55 — —	100 MHz T 35° * Relative to C_6F_6 at 94.1 MHz	624
$\text{C}_{19}\text{H}_{27}\text{Cl}_2\text{-OP}_2\text{Rh}$	10	$\text{Rh}(\text{CH}_2\text{CH}_2)(\text{Cl})_2[\text{P}(\text{CH}_3)_2\text{-C}_6\text{H}_5]_2(\text{CO})$	CDCl_3	H H' H''	1.9 0.76 2.15t, 2.02t	J 7.5 — J_{PH} 4.5	Phosphorous ligands <i>trans</i> -orientated and Cl <i>cis</i> -orientated T 34°	623
$\text{C}_{21}\text{H}_{29}\text{Cl}_2\text{-OP}_2\text{Rh}$	11	$\text{Rh}[\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2]_2[\text{P}(\text{CH}_3)_2\text{Ph}]_2(\text{Cl})_2(\text{CO})$	C_6H_6	H H' H'' H'''	2.82 1.31 4.37, 4.25 1.97t, 1.90t	J_{PH} 6.2 J_{RHH} 3.3 — J 8.2	T 34°	621
$\text{C}_{40}\text{H}_{32}\text{Cl}_2\text{-F}_3\text{OP}_2\text{Rh}$	12	$\text{Rh}[2\text{-CH}_2\text{C}_6\text{H}_4\text{P}(2\text{-C}_6\text{H}_4\text{CH}_3)_2]_2[\text{P}(p\text{-C}_6\text{H}_4\text{F}_3)(\text{Cl})_2(\text{CO})]$	CDCl_3	H H' H''	2.7-3.9 6.5-8.2 2.13, 2.30	— — —	100 MHz	626
$\text{C}_{43}\text{H}_{41}\text{Cl}_2\text{-OP}_2\text{Rh}$	13	$\text{Rh}[2\text{-CH}_2\text{C}_6\text{H}_4\text{P}(2\text{-C}_6\text{H}_4\text{CH}_3)_2]_2[\text{P}(m\text{-C}_6\text{H}_4\text{CH}_3)(\text{Cl})_2(\text{CO})]$	CDCl_3	H H' H''	2.7-3.9 6.7-7.1 2.05, 2.30, 2.37	— — —	100 MHz	626

TABLE XI—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{43}H_{41}Cl_2 \cdot OP_2Rh$	14	$Rh[2-CH_2C_6H_4P(2-C_6H_4CH_3)_2] \cdot [P(p-C_6H_4CH_3)_3](Cl)_2(CO)$	$CDCl_3$	H H' H''	2.9–3.9 6.6–8.1 2.12, 2.32, 2.38	— — —	100 MHz	626
$C_{39}H_{33}Cl_2 \cdot OP_2Rh$	15	$Rh(CH=CH_2)(Cl)_2[P(C_6H_5)_3]_2(CO)$	$C_6H_5CF_3$	H	5.7–3.4	—	56.5 MHz	622
$C_{40}H_{33}OP_2Rh$	16	$Rh(C\equiv CCH_3)[P(C_6H_5)_3]_2(CO)$	C_6H_6	H	1.47s	—	100 MHz	627
$C_{38}H_{48}OP_3Rh$	17	$Rh(C\equiv CCH_3)[P(C_6H_5)_3]_3(CO)$	C_6H_6	H	1.35s	—	100 MHz	627
$C_{40}H_{33}O_3O_2RhS$	18	$Rh(C\equiv CCH_3)[P(C_6H_5)_3]_2(SO_2)(CO)$	C_6H_6	H	1.47s	—	100 MHz	627
$C_{34}H_{31}Cl_2 \cdot OP_2Rh$	19	$Rh[1,2-C_6H_4(CHCH_3)(PPh_2)] \cdot (Cl)_2[P(CH_3)(C_6H_5)_2](CO)$	$CDCl_3$	H H' H''	3.81t* 1.26d 2.42dd	J 7 J 7 J 11, 2.5	100 MHz * Further split by coupling with ^{31}P and ^{103}Rh	47
$C_{19}H_{25}Br_2 \cdot O_2P_2Rh$	20	$Rh(COCH_3)[P(CH_3)_2Ph]_2(Br)_2(CO)$	$CHCl_3$	H H'	1.69s 2.28t	— J 8.2	T 34°	621
$C_{19}H_{25}Cl_2 \cdot O_2P_2Rh$	21	$Rh(COCH_3)[P(CH_3)_2Ph] \cdot (Cl)_2(CO)$	$CHCl_3$	H H'	1.57s 2.16t, 2.11t	— J 8.0	T 34°	621
$C_{21}H_{29}As_2 \cdot Cl_2ORh$	22	$Rh[COCH(CH_3)_2][As(CH_3)_2Ph]_2 \cdot (Cl)_2(CO)$	$CHCl_3$	H H' H''	3.01m 0.46d 2.08s, 2.00s	— J 6.0 —	T 34°	621

$C_{21}H_{27}As_2-$ Cl_2ORh	23	$Rh(COCH_2CH=CH_2)[As(CH_3)_2-CHCl_3$ $Ph]_2(Cl)_2(CO)$	—	H H'	3.11d 2.04s	— —	T 34°	621
$C_{21}H_{29}As_2-$ Cl_2ORh	24	$Rh[CH_2C(CH_3)=CH_2]-$ $[As(CH_3)_2Ph]_2(Cl)_2(CO)$	C_6H_6	H H' H'' H'''	3.00 1.48 4.42 1.83s, 1.75s	J_{RhH} 3.2 — — —	T 34°	621
(b) Dicarbonyl derivatives								
$C_{22}H_{16}F_4O_2PRh$	25	$Rh(CF_2CHF_2)[P(C_6H_5)_3](CO)_2$	—	H F F'	5.09tt -73.20b* -34.55d*	— — —	100 MHz T 35° • Relative to C_6F_6 at 94.1 MHz	624
$C_{44}H_{30}F_5-$ O_2P_2Rh	26	$Rh(h^1-C_6F_5)[P(C_6H_5)_3]_2(CO)_2$	CH_2Cl_2	F_{ortho} F_{meta} F_{para}	33.8 86.6 86.8	— — —	Relative to CF_3CO_2H at 56.4 and 94.1 MHz	628
$C_{45}H_{30}F_4-$ NO_2P_2Rh	27	$Rh(1-h^1-4-C_6F_4CN)[P(C_6H_5)_3]_2-$ $(CO)_2$	CH_2Cl_2	F_{-2}, F_{-6} F_{-3}, F_{-5}	32.0 60.0	— —	Relative to CF_3CO_2H at 56.4 and 94.1 MHz	628
$C_{46}H_{30}F_3-$ $N_2O_2P_2Rh$	28	$Rh[1-h^1-3,4-C_6F_3(CN)_2]-$ $[P(C_6H_5)_3]_2(CO)_2$	$CHCl_3$	F_{-2} F_{-5} F_{-6}	-3.2 58.0 15.5	— — —	Relative to CF_3CO_2H at 56.4 and 94.1 MHz	628
$C_{47}H_{35}F_4-$ O_4P_2Rh	29	$Rh(1-h^1-4-C_6F_4-CO_2CH_2CH_3)-$ $[P(C_6H_5)_3]_2(CO)_2$	CH_2Cl_2	F	65.2, 34.9	— —	Relative to CF_3CO_2H at 56.4 and 94.1 MHz	628
$C_{41}H_{35}O_3P_2Rh$	30	$Rh(COCH_2CH_3)[P(C_6H_5)_3]_2(CO)_2$	—	H H'	2.93q 0.74t	J 7.5 J 7.5	T 35° 100 MHz	624
$C_{43}H_{30}F_4-$ O_2NP_2Rh	31	$Rh(4-h^1-C_5F_4N)[P(C_6H_5)_3]_2(CO)_2$	$CHCl_3$	F_{-2}, F_{-6} F_{-3}, F_{-5}	22.4 40.0	— —	Relative to CF_3CO_2H at 56.4 and 94.1 MHz	628
$C_{44}H_{30}F_3-$ $N_2O_2P_2Rh$	32	$Rh[4-h^1-2-C_5F_3N(CN)]-$ $[P(C_6H_5)_3]_2(CO)_2$	CH_2Cl_2	F_{-3} F_{-5} F_{-6}	17.5 23.3 11.8	— — —	Relative to CF_3CO_2H at 56.4 and 94.1 MHz	628

TABLE XI—cont.

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{44}H_{30}F_3-N_2O_2P_2Rh$	33	$Rh[5-h^1-2-C_3F_3N(CN)]-[P(C_6H_5)_3]_2(CO)_2$	CH_2Cl_2	F_{-3}	71.1	—	Relative to CF_3CO_2H at 56.4 and 94.1 MHz	628
				F_{-4}	16.2	—		
				F_{-6}	-36.6	—		
(c) Tricarbonyl derivatives								
$C_{23}H_{16}F_4O_3PRh$	34	$Rh(CF_2CHF_2)[P(C_6H_5)_3](CO)_3$	—	H	5.40tt	$J_{HF_n}^5$ $J_{HF_\beta}^{60}$	Relative to C_6F_6 at 94.1 MHz T 35°	624
				F	-113.2b	—		
				F'	-40.90d	—		
(2) DIHAPTO LIGANDS								
$C_{45}H_{38}ClO_2-P_2Rh$	35	$(h^2-C_9H_8O_2)Rh[P(C_6H_5)_3]_2(Cl)$	—	H	0.8-1.5	—		1007
				H'	0.83	—		
				H'', H'''	0.0-0.6	—		
				H ^{IV}	2.15	—		
(a) Monocarbonyl derivatives								
$C_{39}H_{32}ClOP_2Rh$	36	$Rh[h^2-1-CH_2=CH'C_6H_4(PPh_2)]-[P(C_6H_5)_3](Cl)(CO)$	—	H	~3.1	—		47
				H'	~4.2	—		
$C_{21}H_{24}ClN_2-O_3Rh$	37	$Rh[1,4-h^2-COC(CH_3)=C(CH_3)-CO](p-NH_2C_6H_4CH_3)_2-(Cl)(CO)$	$CDCl_3$	H	2.20s	—	T 60° * Centre of AB quartet	629
				H'	4.56s	—		
				H''	7.08*	—		
				H'''	2.28s	—		

$C_{32}H_{36}ClNO_3$ - PRh	38	$Rh[1,4-h^2-COC(CH_3)=C(CH_3)-$ $CO](p-NH_2C_6H_4CH_3'')$ - $[P(C_6H_5)_3](Cl)(CO)$	$CDCl_3$	H H' H'' H'''	2.16s 4.47b 6.97d, 6.39d 2.33s	— — — —	—	629
$C_{41}H_{36}As_2$ - ClO_2Rh	39	$(C_4H_6ORh)(Cl)[As(C_6H_5)_3]_2(CO)$	$CDCl_3$	H H'	1.66, 1.47, 0.76 7.42	— —	A 1-rhodiacyclopentan-2-one derivative 100 MHz	630
(b) Dicarbonyl derivatives								
$C_8H_{10}ClO_2Rh$	40	$Rh(h^2-C_6H_{10})(Cl)(CO)_2$	—		n.a.	—	Signals at δ 2.56, 2.22, and 1.13, in ratio 2:6:2	357
$C_{26}H_{40}Cl_4O_2Rh_4$	41	$[(h^2-CH_3CH_2C\equiv CCH_2CH_3)_2-$ $Rh_2(Cl)_2(CO)]_2$	$CDCl_3$		n.a.	—	Signals at δ 2.3b, 1.57, 1.42, 1.39, 1.20, 1.08 and 0.93	928
(3) TRIHAPTO LIGANDS								
(a) Monocarbonyl derivatives								
$C_{40}H_{35}OP_2Rh$	42	$Rh(h^3-CH_2\cdots CH\cdots CH_2)-$ $[P(C_6H_5)_3]_2(CO)$	C_6H_6	H	4.90m	—	100 MHz T 35° Other signals very broad	631
$C_{41}H_{37}OP_2Rh$	43	$Rh(h^3-CH_2\cdots CH\cdots CH'(CH_3)-$ $[P(C_6H_5)_3]_2(CO)$	C_6H_6	H H' H''	4.88m 3.10b 1.95d	— — J 6.0	T 35° 100 MHz Higher field signals very broad	631
(b) Dicarbonyl derivatives								
$C_5H_5O_2Rh$	44	$Rh(h^3-CH_2\cdots CH\cdots CH_2)(CO)_2$	$CDCl_3$	H_{syn} H_{anti} H'	4.02d 2.40d 5.28m	$J_{HH'}7.2$ $J_{HH'}13.3$ —	—	632

TABLE XI—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
(4) PENTAHAPTO LIGANDS							
(a) Monocarbonyl derivatives							
$C_6H_5I_2ORh$	45	$(h^5-C_5H_5)Rh(I)_2(CO)$	$CHCl_3$	H	5.91	—	633
$C_{18}H_{32}OPRh$	46	$(h^5-C_5H_5)Rh[P(n-C_4H_9)_3](CO)$	C_6H_6	H	5.41t	$J_{HRh} 0.55$ $J_{PH} 0.55$	918
$C_{14}H_{16}OPRh$	47	$(h^5-C_5H_5)Rh[P(CH_3)_2C_6H_5](CO)$	$CDCl_3$	H	5.28	$J_{HRh} 0.6$ $J_{PH} 0.6$	T 40° 60 and 100 MHz 634
				H'	1.81	$J_{H'Rh} 1.6$ $J_{PH'} 9.7$	
				H''	7.43	—	
$[C_{14}H_{16}-BrOPRh]^+$	48	$\{(h^5-C_5H_5)Rh[P(CH_3)_2C_6H_5]-Br(CO)\}^+$	$CDCl_3$	H	6.43	$J_{HRh} 0.4$ $J_{PH} 1.5$	Isolated as the bromide. T 40° 60 and 100 MHz 634
				H'	2.36	$J_{H'Rh} 0^*$ $J_{PH'} 12.6$	
$C_{24}H_{20}OPRh$	49	$(h^5-C_5H_5)Rh[P(C_6H_5)_3](CO)$	$CDCl_3$	H	5.14t	$J_{HRh} 0.6$ $J_{PH} 0.6$	T 30–40° 100 MHz 635
			C_6H_6	H	5.28	$J_{HRh} 0.55$ $J_{PH} 0.55$	
			CCl_4	H'	7.3	—	
$C_9H_{14}O_4PRh$	50	$(h^5-C_5H_5)Rh[P(OCH_3)_3](CO)$	C_6H_6	H	5.44	$J_{HRh} 0.6$ $J_{PH} 1.2$	918
				H'	3.49d	$J_{PH'} 13$	

$C_{11}H_{14}O_4PRh$	51	$(\eta^5-C_5H_5)Rh[P(OCH_3)_3CCH_3]-(CO)$	C_6H_6	H	5.51dd	$J_{HRh} 0.6$ $J_{PH} 1.2$	—	918
				H'	3.70d	$J_{PH'} 5$		
				H''	-0.175	—		
$C_{24}H_{21}ORhSi$	52	$(\eta^5-C_5H_5)Rh[Si(C_6H_5)_3](H'')(CO)$	CCl_4	H	5.27	$J 0.5$	—	636
				H'	7.28	—		
				H''	-11.1b	$J 31.8$		
$C_6H_5Cl_6ORhSi_2$	53	$(\eta^5-C_5H_5)Rh(SiCl_3)_2(CO)$	$CDCl_3$	H	5.79	—	—	636
$C_8H_{11}Cl_4-ORhSi_2$	54	$(\eta^5-C_5H_5)Rh[Si(Cl)_2CH_3]_2(CO)$	$CDCl_3$	H	5.67d	$J_{HRh} 0.8$	—	636
				H'	1.27d	—		
$C_6H_5I_4ORhSn$	55	$(\eta^5-C_5H_5)Rh(SnI_3)(I)(CO)$	$CDCl_3$	H	6.00	—	—	636
$C_{12}H_{23}ORhSn_2$	56	$(\eta^5-C_5H_5)Rh[Sn(CH_3)_3]_2(CO)$	CS_2	H	5.18	—	—	637
				H'	0.32	—		
<i>(b) Dicarbonyl derivatives</i>								
$C_7H_5O_2Rh$	57	$(\eta^5-C_5H_5)Rh(CO)_2$	C_6H_6	H	5.12d	$J_{HRh} 0.7$	—	918
				^{13}C	105.2	$J(^{13}C-H) 1.76$	Relative to CS_2 (0.0 ppm)	580
$C_{12}H_{15}O_2Rh$	58	$[\eta^5-C_5(CH_3)_5]Rh(CO)_2$	$CDCl_3$	H	2.05d	$J_{HRh} 0.4$	—	638
$C_{10}H_{13}O_2RhSi$	59	$[\eta^5-C_5H_4Si(CH_3)_3]Rh(CO)_2$	—	H	5.45t, 5.22t	—	—	250
				H'	0.16	—		
$C_{11}H_7O_2Rh$	60	$(\eta^5-C_9H_7)Rh(CO)_2$	CS_2	H ₋₁ , H ₋₃	5.66	$J_{1,2} 2.9$	Structure:	639
				H ₋₂	6.00	—		
				H ₋₄	7.29	—		
				H ₋₅ , H ₋₆ , H ₋₇	7.00	—	T 30°	

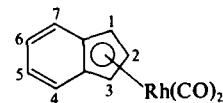


TABLE XI—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
(5) MIXED LIGANDS							
$C_{46}H_{33}N_4-$ OP_2Rh	61	$Rh(C\equiv CCH_3)[C(CN)_2=C(CN)_2]-$ $[P(C_6H_5)_3]_2(CO)$	C_6H_6	H 1.14t	J_{2-4}	100 MHz	627
$C_{47}H_{35}N_4-$ OP_2Rh	62	$Rh(C\equiv CCH_2CH_3)[C(CN)_2=C(CN)_2][P(C_6H_5)_3]_2(CO)$	C_6H_6	H 2.09q H' 0.81t	J_{7-5} J_{7-5}	100 MHz	627
$[C_{15}H_{19}OPRh]^+$	63	$\{(h^5-C_5H_5)Rh(CH_3)[P(CH_3)_2-C_6H_5'''] (CO)]^+$	$CDCl_3$	H 5.15 H' 0.82 H'' 1.65 H''' 6.92	$J_{HRh} 0.4$ $J_{PH} 1.3$ $J_{HRh} 2.2$ $J_{PH'} 5.1$ $J_{H''Rh} 1.1$ $J_{PH''} 11.2$ —	T 40° 60 and 100 MHz Tetraphenylborate	634
$C_{13}H_{16}NORh$	64	$(h^5-C_5H_5)Rh(C\equiv NC_6H_{11})(CO)$	C_6H_6	H 5.48d H' 1.37	$J_{HRh} 0.6$	—	918
$C_{13}H_{18}IO_2Rh$	65	$[h^5-C_5(CH_3)_5]Rh(COCH_3)(I)(CO)$	$CDCl_3$	H 1.95 H' 2.79s	— —	—	638
$[C_{16}H_{16}F_3-$ $O_2PRh]^+$	66	$\{(h^5-C_5H_5)Rh(COCF_3)[P(CH_3)_2-C_6H_5'''] (CO)]^+$	$CDCl_3$	H 5.13 H' 1.73 H'' 6.90	$J_{HRh} 0.4$ $J_{PH} 1.2$ $J_{H'Rh} 1.1$ $J_{PH'} 11.5$ —	T 40° 60 and 100 MHz Tetraphenylborate	634

			CDCl ₃	H	6.34	—	T -20°	
				H'	2.59	$J_{PH'}$ 12.4	Isolated as the Chloride	
				H''	7.56	—		
[C ₁₆ H ₁₉ - O ₂ PRh] ⁺	67	{(h ⁵ -C ₅ H ₅)Rh(COCH ₃)[P(CH ₃) ₂ - C ₆ H ₅ '''](CO)] ⁺	CDCl ₃	H	6.08	J_{HRh} 0.4 J_{PH} 1.0	T 0° 60 and 100 MHz Isolated as the bromide	634
				H'	2.52	—		
				H''	2.39	$J_{H''Rh}$ 1.2 $J_{PH''}$ 11.9		
				H'''	7.52	—		
			CDCl ₃	H	5.32	J_{HRh} 0.4 J_{PH} 1.1	T 40° Isolated as the tetraphenylborate	634
				H'	2.42	—		
				H''	1.87	$J_{H''Rh}$ 1.1 $J_{PH''}$ 11.6		
				H'''	6.93	—		
[C ₁₇ H ₂₁ OPRh] ⁺	68	{(h ⁵ -C ₅ H ₅)Rh(h ³ -CH ₂ -CH=CH ₂)- CH ₂)[P(CH ₃) ₂ C ₆ H ₅ '''](CO)] ⁺	CDCl ₃	H	5.12	J_{HRh} 0.4 J_{PH} 1.1	T 40° 60 and 100 MHz	634
				H'	1.68	$J_{H'Rh}$ 1.2 $J_{PH'}$ 11.4		
				H''	6.89	—		
(6) MISCELLANEOUS COMPLEXES								
C ₃₁ H ₂₆ ClN ₂ - ORh	69	Rh[N(C ₆ H ₅)=CH-CH'=CH'- C ₆ H ₅] ₂ (Cl)(CO)	—	H	8.68	—	—	389
				H'	8.25d	—		
				H''	8.10d	—		
C ₁₉ H ₄₆ OP ₃ Rh	70	Rh(PEt ₃) ₃ (H)(CO)	C ₆ H ₆	H	-11.3	J_{PH} 17 J_{RhH} 4	—	640
C ₃₁ H ₄₆ OP ₃ Rh	71	Rh(PEt ₂ Ph) ₃ (H)(CO)	C ₆ H ₆	H	-10.7	J_{PH} 17 J_{RhH} 4	—	640

TABLE XI—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{37}H_{82}OP_3Rh$	72	$Rh[P(n-Bu)_3]_3(H)(CO)$	C_6H_6	H	-11.2	$J_{PH} 17$	—	640
$C_{40}H_{40}OP_3Rh$	73	$Rh[P(CH_3)Ph_2]_3(H)(CO)$	C_6H_6	H	-9.9	$J_{PH} 13$ J_{RhH^4}	—	640
$C_{30}H_{26}ClF_3 \cdot NOP_2Rh$	74	$Rh[OC(CN)CF_3][P(CH_3)Ph_2]_2 \cdot (Cl)(CO)$	$CDCl_3$	H F	2.01d 78.6d	$J_{PH} 13.0$ $J_{PF} 7.0$	100 MHz	641
$C_{55}H_{37}F_9OP_3Rh$	75	$Rh(H)[P(C_6H_4F)_3]_3(CO)$	CH_2Cl_2	H	-9.82q	$J 14$	T 0° 100 MHz	642
$C_{55}H_{46}OP_3Rh$	76	$Rh(H)[P(C_6H_5)_3]_3(CO)$	CH_2Cl_2	H	-9.69qd	$J_{HRh} \sim 1$ $J_{PH} 14$	T -35° 100 MHz	643 640
			C_6H_6	H H	-9.27b -9.15	— —	T 35° 100 MHz	644
$C_{64}H_{64}OP_3Rh$	77	$Rh(H)[P(p-C_6H_4CH_3)_3]_3(CO)$	$C_6H_5CH_3$	H	-9.02q	$J 13.5$	T 15° 100 MHz	642
$C_{43}H_{42}ClO_7 \cdot P_2Rh$	78	$Rh[P(p-C_6H_4OCH_3)_2]_2(Cl)(CO)$	$CDCl_3$		n.a.	—	Signals at δ 0.80t ($J_{PH} 5$), 2.15s, 2.55t ($J_{PH} 1$), 3.08s, 3.82s (OCH_3) 100 MHz	620
$C_{38}H_{31}O_2P_2Rh$	79	$Rh(H)[P(C_6H_5)_2]_2(CO)_2$	CH_2Cl_2	H	-9.63b	—	T 35° 100 MHz	643
			C_6H_6	H	-9.1b	—		
$C_{17}H_{13} \cdot ClNO_2Rh$	80	$Rh[N(C_6H_5)=CH-CH=CH \cdot C_6H_5](Cl)(CO)_2$	$CDCl_3$	H	8.18t	—	—	389

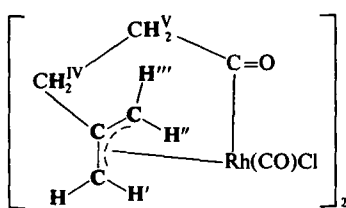
$C_4H_{10}O_2P_2^-$ RhSn	81	$Rh[P(C_6H_5)_3]_2[Sn(CH_3)_3](CO)_2$	$CDCl_3$	H H'	7.19 0.14	— —	—	645
(7) DI- AND TRI-RHODIUM COMPLEXES								
$C_{10}H_{12}Cl_2O_4Rh_2$	82	$\{Rh[1,4-h^2-CO(CH_2)_3](CO)\}_2(Cl)_2$	—		n.a.	—	Signals at δ 3.6, 2.72, 1.65	630
$C_6H_8Cl_2O_2Rh_2$	83	$[Rh(h^2-CH_2=CH_2)(CO)]_2(Cl)_2$	$CDCl_3$ C_6H_6	H H	3.91 3.47	— —	T 34° * Bridging Cl ligands	623
$C_{18}H_{32}Cl_2^-$ O_4Rh_2	84	$\{[Rh(h^2-C(CH_3)_2=CH'-C(CH_3)_2-CH_2''OH^{IV})(CO)]_2(Cl)_2\}$	C_6D_6	H H' H'' H''' H^{IV}	1.64s, 1.62s 3.58s 1.43s, 0.65s 3.44d, 3.54d 6.24b	— — — — — — — —	100 MHz • Bridging Cl ligands	646
$C_{14}H_{16}Cl_2O_4Rh_2$	85	$[Rh(h^4-C_6H_8O)(CO)(Cl)]_2$	$CDCl_3$	H H' H'' H''' H^{IV} H^V	4.13bs 3.15bs 4.46bs 4.90bs 2.93m 2.26m	— — — — — —	Structure: 	647
$C_{16}H_{22}O_2^-$ Rh_7Sn_2	86	$\{(h^5-C_5H_5)Rh[Sn(CH_3)_2](CO)\}_2$	CS_2	H H'	5.13 0.74	— —	—	637

TABLE XI—cont.

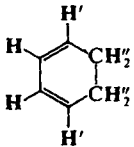
Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)		Remarks	References
$C_{10}H_{10}Cl_2 \cdot O_4Rh_2$	87	$[Rh(CO)_2]_2[CH_2=C(CH_3)-C(CH_3)=CH_2](Cl)_2^*$	$CDCl_3$	$H_{syn}^\dagger$ 2.56m $H_{anti}^\dagger$ 1.13d H' 2.22s	— J 3.5 —	—	* Bridging Cl ligands † <i>Syn</i> or <i>anti</i> to CH_3 groups	648
$C_{10}H_8Cl_2 \cdot O_4Rh_2$	88	$[Rh(CO)_2]_2(C_6H_8XCl)_2^*$	$CDCl_3$	H 5.38dd H' 4.06m	— —	—	$C_6H_8 =$ 	648
				H'' 1.20m	—	—	* Bridging Cl ligands	
$C_{16}H_{10}F_6O_2Rh_2$	89	$[(\eta^5-C_5H_5)Rh(CO)]_2(CF_3C\equiv CCF_3)$	—	H 5.53 F 54.37	— —	—	—	649
$C_{49}H_{35}O_3PRh_2$	90	$Rh_2(C_6H_5C\equiv C \cdot C_6H_5)_2-[P(C_6H_5)_3](CO)_3$	$C_2H_2Cl_4$	H 6.76m H' 7.25m	— —	—	100 MHz	650
$C_{18}H_{15}O_3Rh_3$	91	$[(\eta^5-C_5H_5)Rh(CO)]_3$	—	Not reported	—	—	—	651

TABLE XII

Iridium complexes

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
(1) MONOHAPTO LIGANDS								
(a) Monocarbonyl derivatives								
$C_{18}H_{25}Br_2^-$ $IrOP_2$	1	$Ir(CH_3)(Br)_2[P(CH_3)_2Ph]_2(CO)$	C_6H_6	H H'	0.76t 2.04t, 1.75t	$J_{PH} 5.4$ $J^* 8.0$ $J^* 8.6$	<i>trans</i> -orientation of P ligands, CH ₃ <i>trans</i> to one Br and <i>cis</i> to the other J^* = Separation of outer lines of triplets	759
$C_{18}H_{25}Cl_2^-$ $IrOP_2$	2	$Ir(CH_3)(Cl)_2[P(CH_3)_2Ph]_2(CO)$	C_6H_6	H H'	0.64t 1.94t, 1.66t	$J_{PH} 5.3$ $J^* 8.2$ $J^* 9.0$	<i>trans</i> -orientation of P ligands, CH ₃ <i>trans</i> to one Cl and <i>cis</i> to the other J^* = Separation of outer lines of triplets	759
$C_{18}H_{25}^-$ $BrClIrOP_2$	3	$Ir(CH_3)(Br)(Cl)[P(CH_3)_2Ph]_2(CO)$	C_6H_6	H H'	0.67t 2.00t, 1.73t	$J_{PH} 5.5$ $J^* 8.2$ $J^* 9.0$	<i>trans</i> -orientation of P ligands, CH ₃ <i>trans</i> to Br and <i>cis</i> to Cl J^* = Separation of outer lines of triplets	759
$C_{18}H_{25}^-$ $ClIrOP_2$	4	$Ir(CH_3)(Cl)(I)[P(CH_3)_2Ph]_2(CO)$	C_6H_6	H H'	0.72t 2.09t, 1.84t	$J_{PH} 5.5$ $J^* 7.6$ $J^* 8.6$	<i>trans</i> -orientation of P ligands, CH ₃ <i>trans</i> to I and <i>cis</i> to Cl J^* = Separation of outer lines of triplets	759

TABLE XII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{18}H_{25}I_2^-$ $IrOP_2$	5	$Ir(CH_3)(I)_2[P(CH_3)_2Ph]_2(CO)$	C_6H_6	H H'	0.98t 2.32t, 2.00t $J_{PH} 5.5$ $J^* 7.8$ $J^* 8.6$	<i>trans</i> -orientation of P ligands, CH_3 <i>trans</i> to one I and <i>cis</i> to the other J^* = Separation of outer lines of triplets	759
$C_{28}H_{29}^-$ $BrClIrOP_2$	6	$Ir(CH_3)(Br)(Cl)(PPh_2CH_3)_2(CO)$	$CDCl_3$	H H'	0.35t 2.51t — —	Isomer resulting from <i>trans</i> addition of CH_3Cl to <i>trans</i> - $[Ir(Br)(PPh_2CH_3)_2(CO)]$ Isomer resulting from <i>trans</i> addition of CH_3Br to <i>trans</i> - $[Ir(Cl)(PPh_2CH_3)_2(CO)]$	760
$C_{28}H_{29}Cl_2^-$ $IrOP_2$	7	$Ir(CH_3)(Cl)_2(PPh_2CH_3)_2(CO)$	$CDCl_3$	H H'	0.36t 2.49t — —	Product of <i>trans</i> addition of CH_3Cl to <i>trans</i> - $[Ir(Cl)(PPh_2CH_3)_2(CO)]$	760
$C_{18}H_{22}Cl_5^-$ $IrOP_2$	8	$Ir(CCl_3)(Cl)_2[P(CH_3)_2Ph]_2(CO)$	C_6H_6	H	1.96t, 1.89t $J^* 8.0$ $J^* 9.4$	<i>trans</i> -orientation of P ligands, CCl_3 <i>trans</i> to one Cl and <i>cis</i> to the other J^* = Separation of outer lines of triplets	759
$C_{19}H_{24}As_2^-$ Cl_2IrON	9	$Ir(CH_2CN)(Cl)_2[As(CH_3)_2Ph]_2(CO)$	C_6H_6	H H'	1.72s 2.03s, 1.94s — — —	<i>trans</i> -orientation of As ligands, CH_2CN <i>trans</i> to one Cl and <i>cis</i> to the other	759
$C_{19}H_{24}Cl_2^-$ $IrNOP_2$	10	$Ir(CH_2CN)(Cl)_2[P(CH_3)_2Ph]_2(CO)$	C_6H_6	H H'	1.31t 2.20t, 2.07t $J_{PH} 5.9$ $J^* 8.4$ $J^* 1.2$	<i>trans</i> -orientation of P ligands, CH_2CN <i>trans</i> to one Cl and <i>cis</i> to the other J^* = Separation of outer lines of triplets	759

$C_{19}H_{26}Br_3^-$ $IrOP_2$	11	$Ir(CH_2CH_2Br)(Br)_2[P(CH_3)_2Ph]_2(CO)$	$CDCl_3$	H H'	2.95m, 1.98 2.28t, 2.17t	— — $J^* 7.8$ $J^* 8.6$	$J^* = {}^2J_{PH} + {}^4J_{PH}$ Br ligands <i>cis</i> to each other, phosphine ligands <i>trans</i> since H' gives a triplet (if the phosphine ligands were mutually <i>cis</i> , H' would give a doublet)	761
$C_{20}H_{28}Cl_3^-$ $IrOP_2$	12	$Ir(CH_2CH^*ClCH_2''(Cl)_2-$ $[P(CH_3''')_2Ph]_2(CO)$	$CDCl_3$	H H' H'' H'''	1.5–2.0 3.38m 0.83d 2.17t, 2.10t	— — $J_{H'H''} 6.5$ $J^* 9.6$ $J^* 9.6$	T 34° $J^* = {}^2J_{PH'''} + {}^4J_{PH''}$ (i.e. separation of the outer peaks of the 1:2:1 triplets)	762
$C_{21}H_{30}Cl_3^-$ $IrOP_2$	13	$Ir[CH_2C(CH_3)_2Cl](Cl)_2-$ $[P(CH_3'')_2Ph]_2(CO)$	$CDCl_3$	H H' H''	1.8–2.4 1.14s 2.18t, 2.03t	— — $J^* 8.6$ $J^* 8.6$	T 34° $J^* = {}^2J_{PH''} + {}^4J_{PH''}$	762
$C_{30}H_{26}ClF_6^-$ $IrOP_2$	14	$Ir[C(CF_3)_2](Cl)(PPh_2CH_3)_2(CO)$	—	F	63.7t	$J_{PF} 10.0$	Relative to CCl_3F (0.0 ppm) at 94.1 MHz	454
$C_{20}H_{20}Br_2^-$ IrO_2P_2	15	$Ir(CH_2CH_2OCH_3)(Br)_2-$ $[P(CH_3')_2Ph]_2(CO)$	$CDCl_3$	H H' H''	2.85m, 1.6m 2.96s 2.26t, 2.09t	— — $J^* 8.4$ $J^* 8.4$	$J^* = {}^2J_{PH} + {}^4J_{PH}$	761
$[C_{27}H_{37}Br_2^-$ $IrOP_3]^+$	16	$\{Ir[CH_2CH_2P(CH_3)_2Ph]-$ $(Br)_2[P(CH_3)_2Ph]_2(CO)\}^+$	$CDCl_3$	H H'	1.86d 2.32t, 2.06t	$J_{PH} 14$ $J^* 7.6$ $J^* 1.4$	Isolated as the bromide $J^* = {}^2J_{PH} + {}^4J_{PH}$	761
$C_{40}H_{33}IrOP_2$	17	$Ir(h^1-C\equiv CCH_3)(PPh_3)_2(CO)$	C_6H_6	H	1.48s	—	100 MHz	627

TABLE XII—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{46}H_{33}IrN_4-OP_2$	18	$Ir(h^1-C\equiv CCH_3)(C_6N_4)-(PPh_3)_2(CO)$	$CDCl_3$	H	1.54t	$J\ 2$	100 MHz T 35°	763
$C_{40}H_{33}IrO_3P_2$	19	$Ir(h^1-C\equiv CCH_3)(O_2)(PPh_3)_2(CO)$	C_6H_6	H	1.86t	$J\ 1.5$	100 MHz	627
$C_{43}H_{33}F_6-IrO_2P_2$	20	$Ir(h^1-C\equiv CCH_3)[(CF_3)_2CO]-(PPh_3)_2(CO)$	$CDCl_3$ $CHCl_3$	H F	1.29 +6.95* +9.86*	$J\ 2.5$ $J\ 14$ $J\ 1.5$	*Relative to trifluoromethylbenzene at 35° at 94.2 MHz	627
$C_{40}H_{33}IrO_3-P_2S$	21	$Ir(h^1-C\equiv CCH_3)(PPh_3)_2(SO_2)-(CO)$	C_6H_6	H H	1.53 1.52	$J\ 2$ $J\ 2.5$	T 35°. 100 MHz 100 MHz	763 627
$C_{38}H_{48}IrOP_3$	22	$Ir(h^1-C\equiv CCH_3)(PPh_3)_3(CO)$	C_6H_6	H H	1.40s 1.41	— —	100 MHz T 35°. 100 MHz	627 763
$C_{41}H_{35}IrOP_2$	23	$Ir(h^1-C\equiv CCH_2CH_3)(PPh_3)_2-(CO)$	C_6H_6	H H'	1.98q 0.62t	$J\ 7.5$ $J\ 7.5$	100 MHz	627
$C_{41}H_{35}IrO_3P_2$	24	$Ir(h^1-C\equiv CCH_2CH_3)(O_2)-(PPh_3)_2(CO)$	C_6H_6	H H'	2.28q 0.79t	$J\ 7.5$ $J\ 7.5$	100 MHz	627 763
$C_{41}H_{35}IrO_3P_2S$	25	$Ir(h^1-C\equiv CCH_2CH_3)(PPh_3)_2-(SO_2)(CO)$	C_6H_6	H H'	2.03q 0.47t	$J\ 7.5$ $J\ 7.5$	100 MHz	627
$C_{41}H_{35}IrO_5P_2S$	26	$Ir(h^1-C\equiv CCH_2CH_3)(PPh_3)_2-(SO_4)(CO)$	$CDCl_3$	H H'	2.04q 0.61t	$J\ 7.5$ $J\ 7.5$	100 MHz	627
$C_{43}H_{39}IrOP_2$	27	$Ir[h^1-C\equiv CC(CH_3)_3](PPh_3)_2(CO)$	C_6H_6	H	0.76s	—	100 MHz	627 763
$C_{42}H_{37}IrO_2P_2$	28	$Ir[h^1-C\equiv CC(CH_3)_2OH](PPh_3)_2-(CO)$	C_6H_6	H H'	1.10s 0.92s	— —	100 MHz	627

$C_{42}H_{37}IrO_4P_2S$	29	$Ir[h^1-C\equiv CC(CH_3)_2OH'](PPh_3)_2-(SO_2)(CO)$	C_6H_6	H H'	0.94s 0.74s	— —	100 MHz	627
$C_{53}H_{41}IrOP_2$	30	$Ir(h^1-C\equiv CPh)_2(PPh_3)_2(H)(CO)$	C_6H_6	H	-8.83	J 15.5	—	627
$C_{42}H_{35}ClIrO_3P_2$	31	$Ir(h^1-C\equiv CCO_2CH_2CH_3)-(Cl)(PPh_3)_2(CO)$	—	H H'	3.9q 1.1t	— —	—	764
$C_{20}H_{27}As_2-Cl_2IrO$	32	$Ir[h^1-CH_2CH'=CH_2](Cl)_2-[As(CH_3)_2Ph]_2(CO)$	$CHCl_3$	H H' H'' H'''	2.5d 5.55 quint. 4.3d 2.00s, 1.90s	J 8.0 — — —	<i>Trans</i> orientation of As ligands, $CH_2CH=CH_2$ <i>trans</i> to one Cl and <i>cis</i> to the other T 34°	765
$C_{20}H_{27}-BrClIrOP_2$	33	$Ir[h^1-CH_2CH'=CH_2](Br)-(Cl)[P(CH_3)_2]_2(CO)$	$CHCl_3$	H H' H'' H'''	2.0-2.7 5.4m 4.2m 2.22t, 2.08t	— — — J^* 8.4 J^* 9.0	<i>Trans</i> orientation of P ligands, $CH_2CH=CH_2$ <i>trans</i> to Br and <i>cis</i> to Cl J^* = Separation of outer lines of triplets. T 34°	765
$C_{20}H_{27}Cl_2-IrOP_2$	34	$Ir(h^1-CH_2CH'=CH_2)(Cl)_2-[P(CH_3)_2Ph]_2(CO)$	$CHCl_3$	H H' H'' H'''	2.0-2.7 5.48m 4.25 sext. 2.52t, 2.03t	— — — J^* 8.0 J^* 8.8	T 34° $J^* = {}^2J_{PH'''} + {}^4J_{PH''}$	765
$C_{20}H_{26}As_2-Cl_3IrO$	35	$Ir[h^1-CH_2C(Cl)=CH_2](Cl)_2-[As(CH_3)_2Ph]_2(CO)$	$CHCl_3$	H H' H''	2.70s 4.43s, 4.10s 2.10s, 1.93s	— — —	<i>trans</i> -orientation of As ligands, $CH_2C(Cl)=CH_2$ <i>trans</i> to one Cl and <i>cis</i> to the other T 34°	765
			$CHCl_3$	H H' H''	3.70d, 3.02d 5.39s, 4.86s 1.77s, 1.72s 1.66s	— — — — —	<i>cis</i> -orientation of As and Cl ligands	765

TABLE XII—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{20}H_{26}Cl_3$ - IrOP ₂	36	Ir[h^1 -CH ₂ C(Cl)=CH ₂](Cl) ₂ - [P(CH ₃) ₂ Ph] ₂ (CO)	CHCl ₃	H	2.5-3.7 oct.	—	<i>cis</i> -orientation of P and Cl ligands	765
				H'	5.33d,	J 2.5		
				H''	4.81d	—		
			CHCl ₃		comp.	—	T 34°	765
				H	2.53t	J_{HP} 6.3		
				H'	4.43, 3.91	$J < 1$		
$C_{21}H_{29}As_2$ - Cl ₂ IrO	37	Ir[h^1 -CH ₂ C(CH ₃)=CH ₂](Cl) ₂ - [As(CH ₃) ₂ Ph] ₂ (CO)	CHCl ₃	H	2.71s	—	T 34°	765
				H'	1.30s	—		
				H''	4.17s	—		
				H'''	2.00s,	—		
					1.93s	—		
$C_{21}H_{29}Br_2$ - IrOP ₂	38	Ir[h^1 -CH ₂ C(CH ₃)=CH ₂](Br) ₂ - [P(CH ₃) ₂ Ph] ₂ (CO)	CDCl ₃	H	2.51t	—	T 34° $J^* = {}^2J_{PH'''} + {}^4J_{PH''}$	762
				H'	1.22s	—		
				H''	4.21s, 4.08s	—		
				H'''	2.32t,	J^* 8.0		
					2.19t	J^* 9.0		
$C_{21}H_{29}$ - BrClIrOP ₂	39	Ir[h^1 -CH ₂ C(CH ₃)=CH ₂](Br)- (Cl)[P(CH ₃) ₂ Ph] ₂ (CO)	CHCl ₃	H	2.47t	J_{PH} 6.8	T 34° $J^* = {}^2J_{PH'''} + {}^4J_{PH''}$ P ligands mutually <i>trans</i> , organic ligand <i>trans</i> to Br ligand	765
				H'	1.21s	—		
				H''	4.16s,	—		
					3.94s	—		
				H'''	2.25t	J^* 8.2		
					2.10t	J^* 8.4		

$C_{21}H_{29}Cl_2-$ IrOP ₂	40	Ir[h^1 -CH ₂ C(CH ₃)=CH ₂](Cl) ₂ - [P(CH ₃ ') ₂ Ph] ₂ (CO)	CHCl ₃	H	3-4 sept.*	—	T 34°	765
				H'	2.33s	—	*Non-equivalent methylene H's	
				H''	4.73s	—		
				H'''	Complex†	—	†Probably four overlapping doublets P ligands mutually <i>cis</i> , Cl ligands mutually <i>cis</i> , organic ligand <i>trans</i> to one P ligand	
			CHCl ₃	H	2.44t	J_{PH} 6.4	T 34°	765
				H'	1.23s	—	$J^* = {}^2J_{PH'''} + {}^4J_{PH''}$	
				H''	4.12s,	—	Cl ligands mutually <i>cis</i> , P ligands	
					4.00s	—	<i>trans</i>	
				H'''	2.18t	J^* 8.2	Organic ligand <i>trans</i> to one Cl	
					2.07t	J^* 8.8	ligand	
$C_{21}H_{29}As_2-$ Cl ₂ IrO	41	Ir[h^1 -CH ₂ C(CH ₃)=CH ₂](Cl) ₂ - [As(CH ₃ ') ₂ Ph] ₂ (CO)	CHCl ₃	H	3.41d,	J_{HH} 8.8	*Some poorly resolved fine structure As ligands and Cl ligands mutually <i>cis</i> , organic ligand <i>trans</i> to one As ligand	765
					3.16d			
				H'	—	—		
				H''	4.7s,*	—		
					4.56s	—		
				H'''	1.73s,	—		
					1.68s,	—		
					1.64s,	—		
					1.61s	—		
$C_{21}H_{29}Br_2-$ IrOP ₂	42	Ir[h^1 -CH=C(CH ₃) ₂](Br) ₂ - [P(CH ₃ ') ₂ Ph] ₂ (CO)	CDCl ₃	H	6.48bs	—	T 34°	762
				H'	1.11q,	—		
					1.69q	—		
				H''	2.23t,	—		
					1.94t	—		

TABLE XII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{21}H_{19}Cl_2 \cdot IrOP_2$	43	$Ir[h^1-CH=C(CH_3)_2](Cl)_2 \cdot [P(CH_3)_2Ph]_2(CO)$	$CDCl_3$	H	6.15bs	—	T 34°	762
				H'	1.10q,	—	$J^* = {}^2J_{PH''} + {}^4J_{PH''}$	
					1.67q	—		
				H''	2.09t,	$J^* 8.8$		
					1.84t	$J^* 8.8$		
$C_{21}H_{19}As_2 \cdot Cl_2IrO$	44	$Ir[h^1-CH=C(CH_3)_2](Cl)_2 \cdot [As(CH_3)_2Ph]_2(CO)$	$CDCl_3$	H	6.19bs	—	T 34°	762
				H'	1.22d,	$J_{HH'} 1.0$		
					1.70d	$J_{HH'} 1.2$		
				H''	1.95s,	—		
					1.75s	—		
$C_{40}H_{33}Cl_2 \cdot IrOP_2$	45	$Ir(h^1-CH=C=CH_2)(Cl)_2 \cdot (PPh_3)_2(CO)$	$CDCl_3$	H	5.18m	—	Cl <i>cis</i> , P ligands <i>trans</i> , organic	766
				H'	3.54m	—	ligand <i>trans</i> to one Cl ligand	
$C_{41}H_{35}Cl_2 \cdot IrOP_2$	46	$Ir(h^1-CH=C=CH'CH'_3)(Cl)_2 \cdot (PPh_3)_2(CO)$	$CDCl_3$	H	5.28m	$J_{HH'} 3.0$	Orientation of ligands as above	766
				H'	3.95m	—		
				H''	1.25m	$J_{H'H''} 7$		
$C_{42}H_{37}Cl_2 \cdot IrOP_2$	47	$Ir[h^1-CH=C=C(CH_3)_2](Cl)_2 \cdot (PPh_3)_2(CO)$	$CDCl_3$	H	5.30m	$J_{HH'} 2.7$	Orientation of ligands as above	766
				H'	1.07d	—		
$C_{23}H_{27}Cl_2 \cdot IrOP_2$	48	$Ir(h^1-C_6H_5)(Cl)_2[P(CH_3)_2Ph]_2(CO)$	C_6H_6	H	1.92t,	$J^* 8.8$	<i>trans</i> -orientation of P ligands, C_6H_5 <i>trans</i> to one Cl and <i>cis</i> to the other	759
					1.23t	$J^* 8.8$		
							J^* = separation of outer lines of triplets	
$C_{44}H_{36}Cl_3 \cdot IrOP_2$	49	$Ir(h^1-3-C_6H_4CH_2Cl)(Cl)_2 \cdot (PPh_3)_2(CO)$	—	H	8.10–7.70,	—	Two isomers present	767
					7.70–7.30,	—		

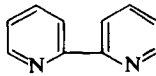
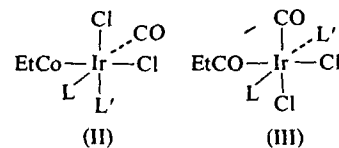
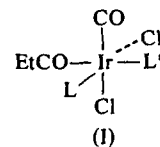
					7.30-6.70	—		
			H'		4.84,	—		
					4.70	—		
$C_{17}H_{21}I_2^-$ IrN_2O_2	50	$Ir(COCH_3)(I)_2(p-NH_2C_6H_4-$ $CH_3)_2(CO)$	$(CD_3)_2SO$	H	3.6	—	—	768
$C_{13}H_{11}I_2^-$ IrN_2O_2	51	$Ir(COCH_3)(I)_2(C_{10}H_8N_2)(CO)$	$(CD_3)_2SO$	H	3.8	—	$C_{10}H_8N_2 =$ 	768
$C_{19}H_{25}Br_2^-$ IrO_2P_2	52	$Ir(COCH_3)(Br)_2[P(CH_3)_2Ph]_2-$ (CO)	C_6H_6	H H'	1.74s 1.96t, 1.88t	— $J^* 8.8$ $J^* 9.8$	<i>trans</i> -orientation of P ligands, COCH ₃ <i>trans</i> to one Br and <i>cis</i> to the other J^* = Separation of outer lines of triplets	759
$C_{19}H_{25}^-$ $BrClIrO_2P_2$	53	$Ir(COCH_3)(Br)(Cl)[P(CH_3)_2-$ $Ph]_2(CO)$	C_6H_6	H H'	1.84s 1.90t, 1.81t	— $J^* 9.0$ $J^* 9.8$	<i>trans</i> -orientation of P ligands, COCH ₃ <i>trans</i> to Cl and <i>cis</i> to Br J^* = Separation of outer lines of triplets	759
			C_6H_6	H H'	1.58s 1.90t, 1.81t	— $J^* 8.2$ $J^* 9.0$	<i>trans</i> -orientation of P ligands, COCH ₃ <i>trans</i> to Br and <i>cis</i> to Cl J^* = Separation of outer lines of triplets	759
$C_{19}H_{25}Cl_2^-$ IrO_2P_2	54	$Ir(COCH_3)(Cl)_2[P(CH_3)_2-$ $Ph]_2(CO)$	C_6H_6	H H'	1.71s 1.85t, 1.75t	— $J^* 8.8$ $J^* 9.2$	<i>trans</i> -orientation of P ligands, COCH ₃ <i>trans</i> to one Cl and <i>cis</i> to the other J^* = Separation of outer lines of triplets	759
			$CDCl_3$	H H' H''	1.65 2.16q* 7.55m	— $J_{PH'} \sim 5$ —	*Quartet formed by overlapping triplets	769

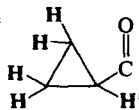
TABLE XII—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{29}H_{29}BrClIrO_2P_2$	55	$Ir(COCH_3)(Br)(Cl)[P(Ph)_2CH_3]_2(CO)$	$CDCl_3$	H	0.70s*	—	*Mixture of isomers in which the $COCH_3$ ligand is <i>trans</i> to the Cl or the Br ligands	760
					0.80s*	—		
				H'	2.58t	—		
$C_{29}H_{29}Cl_2IrO_2P_2$	56	$Ir(COCH_3)(Cl)_2[P(Ph)_2CH_3]_2(CO)$	$CDCl_3$	H	0.70s	—	—	760
				H'	2.58t	—		
$C_{20}H_{27}As_2Cl_2IrO_2$	57	$Ir(COCH_2CH_3)(Cl)_2[As(CH_3)_2Ph]_2(CO)$	$CDCl_3$	H	3.33q	—	*Since each methyl group gives a separate resonance neither As—Ir bond lies in a plane of symmetry through the molecule and the two $AsMe_2Ph$ ligands are in different environments. The structure must therefore be (I) or (II):	770
				H'	0.94t	—		
				*H''	1.74s,	—		
					1.59s,	—		
					1.54s,	—		
					1.45	—		



							Structure (I) is favored since one AsMe ₂ Ph group (the entering ligand L') is readily removed and must therefore lie <i>trans</i> to the labilizing EtCO group. This is the product of kinetic control, and changes slowly into a more thermodynamically stable form (III)	
C ₂₅ H ₂₉ As ₂ - Cl ₂ IrO ₂	58	Ir(COCH ₂ CH ₃)(Cl) ₂ [As(CH ₃) ₂ - Ph][As(Ph) ₂ CH ₃ '] (CO)	CDCl ₃	H H' H'' H'''	3.26q 0.92t 1.63s, 1.39s 1.83s	— — — —	Structure (I) (see above) where L = AsMe ₂ Ph and L' = AsMePh ₂ . Not isolated since it is rapidly converted into the more stable form (III) (see above)	770
C ₃₀ H ₃₁ As ₂ - Cl ₂ IrO ₂	59	Ir(COCH ₂ CH ₃)(Cl) ₂ [As(Ph) ₂ - CH ₃ '] ₂ (CO)	CDCl ₃	H H' H''	3.30q 0.92t 1.52s, 1.91s*	— — — —	Structure (I) (see above) where L = L' = AsPh ₂ Me. Not isolated since rapidly converted into (III) (see above) *Temperature dependent and is therefore the Me signal of the labile ligand L'	770
C ₂₀ H ₂₇ Cl ₂ - IrO ₂ P ₂	60	Ir(COCH ₂ CH ₃)(Cl) ₂ [P(CH ₃) ₂ - Ph] ₂ (CO)	C ₆ H ₆	H H' H''	1.81q 0.13t 2.11t, 2.03t	J 7.2 J 7.2 J* 9.4 J* 9.4	<i>Trans</i> orientation of P ligands, COCH ₂ CH ₃ <i>trans</i> to one Cl and <i>cis</i> to the other J* = Separation of outer lines of triplets	759
C ₄₀ H ₃₅ IrO ₂ P ₂	61	Ir(COCH ₂ CH ₃)(PPh ₃) ₂ (CO)	CH ₂ Cl ₂	H H'	2.30q 0.05t	J 7.25 J 7.25	T 35° 100 MHz	624

TABLE XII—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{21}H_{29}Cl_2-IrO_2P_2$	62	$Ir[COCH(CH_3)_2](Cl)_2[P-(CH_3)_2Ph]_2(CO)$	$CDCl_3$	H H' H''	2.59m 0.34d 2.18t, 2.00t	— $J_{HH'}$ 4.7 $J_{PH''}$ 5.6 —	—	769
$C_{41}H_{35}Cl_2-IrO_2P_2$	63	$(h^1-COC_3H_7)Ir[P(C_6H_5)_3]_2(Cl)_2(CO)$	$CDCl_3$	H H'	0.8m 2.62tt	— —	$COC_3H_7 =$ 	929
$C_{24}H_{27}Cl_2-IrO_2P_2$	64	$Ir(COC_6H_5)(Cl)_2[P(CH_3)_2-C_6H_5]_2(CO)$	$CDCl_3$	H H' H''	7.1m 2.16t, 2.96t 7.5m	— $J_{PH'}$ 4.7 — —	—	769
			C_6H_6	H'	1.95t, 1.66t	J^* 9.0 J^* 9.0	<i>trans</i> -orientation of P ligands, PhCO <i>trans</i> to one Cl and <i>cis</i> to the other J^* = Separation of outer lines of triplets	759
$C_{34}H_{31}Cl_2-IrO_2P_2$	65	$Ir(COC_6H_5)[P(C_6H_5)_2CH_3]_2(Cl)_2(CO)$	—	H	2.46	J_{PH} 9.1	—	1014
$C_{20}H_{27}As_2-Cl_2IrO_3$	66	$Ir(CH_2CO_2CH_3)(Cl)_2[As(CH_3)_2-Ph]_2(CO)$	C_6H_6	H H' H''	2.49s 3.37s 1.93s, 1.97s	— — — —	<i>trans</i> -orientation of As ligands, $CH_2CO_2CH_3$ <i>trans</i> to one Cl and <i>cis</i> to the other	759

$C_{20}H_{27}Cl_2-$ IrO_3P_2	67	$Ir(CH_2CO_2CH_3)(Cl)_2[P(CH_3)_2-$ $Ph]_2(CO)$	C_6H_6	H H' H''	2.25t 3.36s 2.16t, 2.06t	J_{PH} 6.8 — J^* 8.8 J^* 9.4	<i>trans</i> -orientation of P ligand, CH_2CO_2Me <i>trans</i> to one Cl and <i>cis</i> to the other J^* = Separation of outer lines of triplets	759
$C_{40}H_{33}IrO_3-$ P_2S	68	$Ir(CO_2CH_3)(PPh_3)_2(SC)(CO)$	C_6D_6	H	3.0s	—	—	771
$C_{18}H_{23}As_2-$ Cl_2IrO_3	69	$Ir(CO_2H)(Cl)_2[As(CH_3)_2-$ $Ph]_2(CO)$	—	H	2.00, 1.96	—	As ligands <i>trans</i> , carboxy group <i>trans</i> to one Cl T 34°	772
$C_{18}H_{23}Cl_2-$ IrO_3P_2	70	$Ir(CO_2H)(Cl)_2[P(CH_3)_2Ph]_2-$ (CO)	—	H	2.16t, 2.09t	J^* 9.2 J^* 9.0	$J^* = {}^2J_{PH} + {}^4J_{PH}$ P ligands <i>trans</i> , carboxy group <i>trans</i> to one Cl T 34°	772
$C_{19}H_{25}As_2-$ Cl_2IrO_3	71	$Ir(CO_2CH_3)(Cl)_2[As(CH_3)_2-$ $Ph]_2(CO)$	—	H H'	3.29 2.0, 1.92	— — —	As ligands <i>trans</i> , carboxy group <i>trans</i> to one Cl T 34°	772
$C_9H_2Cl_2-$ IrO_3P_2	72	$Ir(CO_2CH_3)(Cl)_2[P(CH_3)_2]_2(CO)$	—	H H'	3.55s 1.75t	— J^* 8.8	$J^* = {}^2J_{PH} + {}^4J_{PH}$ P ligands <i>trans</i> , carboxy group <i>trans</i> to one Cl T 34°	772
$C_{19}H_{25}Cl_2-$ IrO_3P_2	73	$Ir(CO_2CH_3)(Cl)_2[P(CH_3)_2-$ $Ph]_2(CO)$	—	H H'	3.24s 2.14t, 2.01t	— J^* 9.0 J^* 9.0	$J^* = {}^2J_{PH} + {}^4J_{PH}$ Stereochemistry as above T 34°	772
$C_{20}H_{27}As_2-$ Cl_2IrO_3	74	$Ir(CO_2CH_2CH_3)(Cl)_2[As-$ $(CH_3)_2Ph]_2(CO)$	—	H H'	3.81q, 0.97t 2.0	J 7.0 J 7.0 —	Stereochemistry as above T 34°	772

TABLE XII—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{20}H_{27}Cl_2 \cdot IrO_3P_2$	75	$Ir(CO_2CH_2CH_3)(Cl)_2[P(CH_3)_2Ph]_2(CO)$	—	H	3.74q	J 7.2	$J^* = {}^2J_{PH''} + {}^4J_{PH''}$ Stereochemistry as above T 34°	772
				H'	0.98t	J 7.2		
				H''	2.15t,	J^* 9.2		
					2.01t	J^* 9.2		
$C_{24}H_{27}Cl_2 \cdot IrO_3P_2$	76	$Ir(CO_2Ph)(Cl)_2[P(CH_3)_2Ph]_2(CO)$	—	H	2.20t	J^* 9.4	$J^* = {}^2J_{PH} + {}^4J_{PH}$ Stereochemistry as above T 34°	772
					2.19t	J^* 8.8		
<i>(b) Dicarbonyl derivatives</i>								
$C_8H_8Cl_2IrNO_2$	77	$Ir(CH_3)(Cl)_2(C_5H_5N)(CO)_2$	$CDCl_3$	H	1.76*,	—	*Mixture of isomers	769
					1.52*	—		
				H'	8.87	—		
$C_{12}H_{16}AsCl_2 \cdot IrO_2$	78	$Ir(CH_2CH_3)(Cl)_2[As(CH_3)_2Ph](CO)_2$	$CDCl_3$	H	2.79q	—	—	770
				H'	1.92t	—		
				H''	2.00	—		
$C_{17}H_{18}AsCl_2 \cdot IrO_2$	79	$Ir(CH_2CH_3)(Cl)_2[As(Ph)_2CH_3](CO)_2$	$CDCl_3$	H	2.61q	—	—	770
				H'	1.77t	—		
				H''	2.05s	—		
$C_9H_{10}Cl_2 \cdot IrNO_2$	80	$Ir(CH_2CH_3)(Cl)_2(C_5H_5N)(CO)_2$	$CDCl_3$	H, H'	2.15m	—	—	769
				H''	8.56m	—		
			C_6H_6	H	3.14q	$J_{HH'}$ 9		
				H'	1.7t	—		

$C_{40}H_{35}^-$ IrO_2P_2	81	$Ir(CH_2CH_3)(PPh_3)_2(CO)_2$	CH_2Cl_2	H H'	2.89q 0.89t	— —	T 35° 100 MHz	624
$C_8H_{10}Cl_4^-$ Ir_2O_4	82	$[Ir(CH_2CH_3)(Cl)(CO)_2]_2(Cl)_2^*$	$CDCl_3$	H H'	2.8m 1.41t	$J_{HH} \sim 7.5$	*Two bridging Cl ligands	769
$C_{41}H_{33}IrO_2P_2$	83	$Ir(h^1-C \equiv CCH_3)(PPh_3)_2(CO)_2$	C_6H_6	H	1.51s	—	100 MHz	627
$C_{40}H_{33}IrO_3P_2$	84	$Ir(COCH_3)[P(C_6H_5)_3]_2(CO)_2$	$CDCl_3$	H H'	2.20s 7.27m	— —	—	645
$C_{41}H_{35}IrO_3P_2$	85	$Ir(COCH_2CH_3)(PPh_3)_2(CO)_2$	CH_2Cl_2	H H'	2.66q 0.45t	$J 7.5$ —	T 35° 100 MHz	624
			C_6H_6	H H'	2.90q 0.73t	— —		
$C_{46}H_{40}I_2Ir_2^-$ O_8P_2	86	$[Ir(CO_2CH_2CH_3)(I)(PPh_3)(CO)_2]_2$	$CDCl_3$	H H'	3.7q 1.2t	$J 7$ $J 7$	—	768
$C_{40}H_{33}IrO_4P_2$	87	$Ir(CO_2CH_3)[P(C_6H_5)_3]_2(CO)_2$	C_5D_5N	H H'	2.93 7.34	— —	—	773
(c) Tricarbonyl derivatives								
$C_{24}H_{20}IrO_4P$	88	$Ir(COCH_2CH_3)(PPh_3)(CO)_3$	CH_2Cl_2	H H'	2.52q 0.35t	— —	T 35° 100 MHz	624
			C_6H_6	H H'	2.97q 1.03t	$J 7.5$ —		
(2) DIHAPTO LIGANDS								
$C_{29}H_{30}Cl_3^-$ $IrOP_2Sn$	89	$(h^2-CH_2=CH_2)Ir[P(Ph)_2CH_3]_2(SnCl_3)(CO)$	$CDCl_3$	H H'	2.0b, 1.05b 2.44t	— — $J_{PH}, 3.4$	T 34°	774

TABLE XII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{39}H_{34}Cl_3^-$ $IrOP_2Sn$	90	$(h^2-CH_2=CH_2)Ir(PPh_3)_2(SnCl_3)(CO)$	$CDCl_3$	H 1.75b, 0.9b	—	T 34°	774
$C_{29}H_{26}ClF_4^-$ $IrOP_2$	91	$(h^2-CF_2=CF_2)Ir(Cl)[P(C_6H_5)_2CH_3]_2(CO)$	$CDCl_3$	H 7.40m H' 1.95d F 155.5, 166.0	— — — —		775
$C_{39}H_{30}ClF_4^-$ $IrOP_2$	92	$(h^2-CF_2=CF_2)Ir(Cl)(PPh_3)_2(CO)$	$CDCl_3$	F 46 dt, 64 dq	J 154, 41 J 159, 50, 37	To high field of CCl_2FCCL_2F	776
$C_{41}H_{33}IrN_2OP_2$	93	$(h^2-CH(CN)=CH(CN))Ir-(PPh_3)_2(H)(CO)$	CH_2Cl_2	H -11.13	—	—	777
$C_{23}H_{22}^-$ $ClIrN_4OP_2$	94	$Ir[h^2-C(CN)_2=C(CN)_2](Cl)-[P(CH_3)_2Ph]_2(CO)$	$CHCl_3$	H 2.15d, 2.08d	J^* 11.9 J^* 11.6	<i>cis</i> -orientation of P ligands, Cl and CO <i>trans</i> J^* = Separation of lines of doublets	759
$C_{33}H_{26}ClF_6^-$ IrN_2OP_2	95	$[h^2-C(CN)CF_3=C(CN)CF_3]Ir-(Cl)[P(C_6H_5)_2CH_3]_2(CO)$	$CDCl_3$	H 7.34 H' 2.17d, 2.00d F 53.1, 57.9	— J_{PH} 10.8 $J_{PH'}$ 10.8 J_{PF} 12.0 J_{PF} 9.4	100 MHz 94.1 MHz	778
$C_{43}H_{30}ClF_6^-$ IrN_2OP_2	96	$[h^2-C(CN)CF_3=C(CN)CF_3]Ir-(Cl)(PPh_3)_2(CO)$	CH_2Cl_2	F 53.5d, 58.0d	J_{PF} 11.7 J_{PF} 9.3	94.1 MHz	778

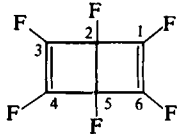
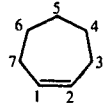
$C_{19}H_{30}ClF_6-$ $IrN_2O_7P_2$	97	$[h^2-C(CN)CF_3=C(CN)CF_3]Ir-$ $(Cl)[P(OEt)_3]_2(CO)$	$CFCl_3$	F	53.8d 58.0d	$J_{PF} 11.7$ $J_{PF} 9.3$		570
$C_{33}H_{26}ClF_6-$ $IrOP_2$	98	$(1,6-h^2-C_6F_6)Ir(Cl)[P(C_6H_5)_2-$ $CH_3]_2(CO)$	$CHCl_3$	H H' F _{-1, F} ₋₆ F _{-2, F} ₋₅ F _{-3, F} ₋₄	7.4 2.06 168.6 181.2 124.4	— $J_{PH'} 7.5$ — — —	$C_6F_6 =$ 	240
$C_{22}H_{36}ClIrO$	99	$(h^2-C_7H_{12})_3Ir(Cl)(CO)$	$CDCl_3$	H _{-1, H} ₋₂ H _{-3, H} ₋₇ H _{-4, H} ₋₅ H ₋₆	4.47bm 2.26bm 1.71bm —	— — — —	$C_7H_{12} =$ 	357
$C_{35}H_{26}ClF_{12}-$ $IrOP_2$	100	$[1,4-h^2-C(CF_3)=C(CF_3)C(CF_3)=$ $C(CF_3)Ir(Cl)[P(C_6H_5)_2-$ $CH_3]_2(CO)]$	$CDCl_3$	H H' F	7.45m 2.25t 48.06q* 51.86q* 56.9m*	— $J_{PH'} 4.0$ $J_{FF} 15.0$ $J_{FF} 15.0$	$*In ratio of 3:3:6 respectively$	779
$C_{39}H_{38}ClIrO_9-$ P_2	101	$[1,4-h^2-C(CO_2CH_3)=C(CO_2-$ $CH_3)C(CO_2CH_3)=C(CO_2-$ $CH_3)Ir(Cl)[P(C_6H_5)_2-$ $CH_3]_2(CO)]$	$CDCl_3$	H H' H''	3.56s, 3.52s, 3.25s 8.0-7.1m 2.25t	— — — — —	—	780
$C_{49}H_{42}ClIrO_9-$ P_2	102	$[1,4-h^2-C(CO_2CH_3)=C(CO_2-$ $CH_3)C(CO_2CH_3)=C(CO_2-$ $CH_3)Ir(Cl)[P(C_6H_5)_3]_2(CO)]$	$CDCl_3$	H H'	3.25s, 3.37s 7.8-7.2m	— — —	—	780
$C_{39}H_{32}Cl_3-$ $IrOP_2Sn$	103	$(h^2-CH\equiv CH)Ir(PPh_3)_2(SnCl_3)-$ (CO)	$CDCl_3$	H	4.60	—	T 34°	774

TABLE XII—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{31}H_{26}ClF_6^-$ $IrOP_2$	104	$[h^2-C(CF_3)\equiv C(CF_3)]Ir(Cl)-$ $[P(C_6H_5)_2CH_2]_2(CO)$	$CDCl_3$	H H' F	7.35m 2.10t 51.7q, 54.4q	— $J_{PH} 4.0$ $J_{FF} 15.0$ $J_{FF} 15.0$		779
$C_{41}H_{30}ClF_6^-$ $IrOP_2$	105	$[h^2-C(CF_3)\equiv C(CF_3)]Ir(Cl)-$ $(PPh_3)_2CO$	CH_2Cl_2	F	-14.2s*, -16.7s*	—	*Two isomers, signals to high field of CCl_2F . CCl_2F	776
$[C_{31}H_{32}^-$ $IrOP_2]^+$	106	$\{[h^2-C(Ph)\equiv C(Ph)]Ir[P(CH_3)_2-$ $Ph]_2(CO)\}^+$	$CDCl_3$	H	1.34d	$J^* 7.7$	Isolated as the tetraphenylborate $J^* = {}^2J_{PH} + {}^4J_{PH}$	761
$C_{30}H_{26}ClF_3^-$ $IrNO_2P_2$	107	$[h^2-O=C(CN)CF_3]Ir(Cl)-$ $[P(C_6H_5)_2CH_2]_2(CO)$	$CDCl_3$	H H' F	7.3m 2.6t 75.5s	— — —	100 MHz 94.1 MHz	641
$C_{40}H_{30}ClF_3^-$ $IrNO_2P_2$	108	$[h^2-O=C(CN)CF_3]Ir(Cl)-$ $(PPh_3)_2(CO)$		F	79.9s	—	94.1 MHz	641
$C_{40}H_{31}F_6^-$ $IrOP_2S$	109	$(h^2-S=C(CF_3)_2)Ir-$ $(PPh_3)_2(H)(CO)$	$CDCl_3$	H	-10.51t	$J_{PH} 16$	100 MHz	781
$C_{38}H_{31}^-$ $IrOP_2S_2$	110	$(h^2-S=C=S)Ir(PPh_3)_2(H)(CO)$	—	H	-11.0	$J_{PH} 21.0$	100 MHz	781
$C_{41}H_{30}ClF_6^-$ $IrOP_2S$	111	$[h^2-S=C=C(CF_3)_2]Ir(Cl)-$ $(PPh_3)_2(CO)^*$	CH_2Cl_2	F	57.5q, 61.3q	$J_{FF} 7.5$ $J_{FF} 7.5$	94.6 MHz *Bonding occurs to the C=S group of the thioketen ligand	775

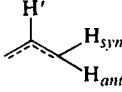
$C_{34}H_{56}Cl_2-Ir_2O_2$	112	$[(\eta^2-C_8H_{14})_2Ir(CO)]_2(Cl)_2^*$	$CDCl_3$	H	4.90t*, 2.23†, 1.61†	— — —	*Two bridging Cl ligands C_8H_{14} = cyclooctene *Olefinic protons †Methylene protons	357
(3) TRIHAPTO LIGANDS								
$[C_{20}H_{27}As_2-ClIrO]^+$	113	$\{(h^3-CH_2CH'CH_2)Ir(Cl)-[As(CH_3)_2Ph]_2(CO)\}^+$	$CHCl_3$	H_{syn} H_{anti} H' H''	4.04 2.82 n.m. 1.77s, 1.72s	$J_{HH'}$ 7.8 $J_{HH'}$ 12.8 — —	T 34°. Isolated at the tetraphenylborate 	765
$[C_{20}H_{27}-ClIrOP_2]^+$	114	$\{(h^3-CH_2CH'CH_2)Ir(Cl)-[P(CH_3)_2Ph]_2(CO)\}^+$	$CHCl_3$	H_{syn} H_{anti} H' H''	4.27 2.99 n.m. 2.05d, 1.99d	$J_{HH'}$ 8.0 $J_{PH'}$ 3.0 $J_{HH'}$ 13.0 $J_{PH'}$ 6.8 J^* 11.2 J^* 11.2	T 34° $J^* = {}^2J_{PH''} + {}^4J_{PH''}$ Isolated as the hexafluorophosphate	765
$C_{40}H_{35}IrOP_2$	115	$(h^3-CH_2CHCH_2)Ir(PPh_3)_2(CO)$	C_6H_6	H	4.40m* 1.82 v.b.*	— —	T 35°. 100 MHz *Broad AX_4 spectrum, temperature and solvent dependent	631
$C_{13}H_{18}AsCl_2-IrO$	116	$(h^3-CH_2C(CH_3)CH''_2)Ir(Cl)_2-[As(CH_3)_2C_6H_5^{IV}](CO)$	$CDCl_3$	H_{syn} H_{syn} H_{anti} H_{anti} H' H''' H^{IV}	4.7s 3.4m 3.87s 3.0d 2.49s 2.08s 7.59m	— J_{HH} 2.6 — J_{HH} 2.6 — — —	—	769

TABLE XII—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$[\text{C}_{21}\text{H}_{29}\text{As}_2\text{-ClIrO}]^+$	117	$\{[h^3\text{-CH}_2\text{C}(\text{CH}_3)\text{CH}_2]\text{Ir}(\text{Cl})\text{-}[\text{As}(\text{CH}_3)_2\text{Ph}]_2(\text{CO})\}$	CHCl_3	H_{syn}	4.30	$J_{\text{HH}} \sim 1$	T 34° Isolated as the hexafluorophosphate	765
				H_{anti}	3.06	$J_{\text{HH}} \sim 1$		
				H'	2.54	—		
				H''	1.92s,	—		
					1.88s	—		
$\text{C}_{23}\text{H}_{22}\text{-AsBr}_2\text{IrO}$	118	$[h^3\text{-CH}_2\text{C}(\text{CH}_3)\text{CH}_2]\text{Ir}(\text{Br})_2\text{-}(\text{AsPh}_3)(\text{CO})$	CDCl_3	H_{syn}	4.7s	—	—	769
				H_{syn}''	3.5b	J 3		
				H_{anti}	4.21s	—		
				H_{anti}''	3.35d	J 3		
				H'	n.m.	—		
$\text{C}_{23}\text{H}_{22}\text{-AsCl}_2\text{IrO}$	119	$[h^3\text{-CH}_2\text{C}(\text{CH}_3)\text{CH}_2]\text{Ir}(\text{Cl})_2\text{-}[\text{As}(\text{C}_6\text{H}_5'')_3](\text{CO})$	CDCl_3	H_{syn}	4.77s	—	—	769
				H_{syn}''	3.4b	$J \sim 3$		
				H_{anti}	4.00s	—		
				H_{anti}''	3.1d	$J \sim 3$		
				H'	2.49s	—		
				H'''	7.68m	—		
$\text{C}_{41}\text{H}_{37}\text{As}_2\text{IrO}$	120	$[h^3\text{-CH}_2\text{C}(\text{CH}_3)\text{CH}_2]\text{Ir}(\text{AsPh}_3)_2\text{-}(\text{CO})$	C_6H_6	H	2.68b, 1.35	—	T 35° 100 MHz	631
				H'	2.30	—		
$\text{C}_{10}\text{H}_{12}\text{Cl}_2\text{-IrNO}$	121	$[h^3\text{-CH}_2\text{C}(\text{CH}_3)\text{CH}_2]\text{Ir}(\text{Cl})_2\text{-}(\text{C}_3\text{H}_5'''\text{N})(\text{CO})$	CDCl_3	H_{syn}	4.2	—	—	769
				H_{syn}''	3.8s	—		
				H_{anti}	4.03s	—		

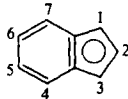
				H''_{anti}	3.7s	—		
				H'	2.74s	—		
				H'''	8.43	—		
$[C_{21}H_{29}^- ClIrOP_2]^+$	122	$\{[h^3-CH_2C(CH_3)CH_2]Ir(Cl)[P-(CH_3)_2Ph]_2(CO)\}^+$	$CHCl_3$	H_{syn}	4.08	$J_{HH} \sim 1$ $J_{PH} < 1$	$J^* = {}^2J_{PH''} + {}^4J_{PH''}$	765
				H_{anti}	3.04	$J_{PH} 6.8, 1$		
				H'	2.46		Isolated as the hexafluorophosphate	
				H''	2.02d, 1.96d	$J^* 10.8$ $J^* 11.3$		
$C_{23}H_{22}Cl_2IrOP$	123	$[h^3-CH_2C(CH_3)CH_2]Ir(Cl)_2-[P(C_6H_5''')_3](CO)$	$CDCl_3$	H_{syn}	4.79d	$J_{PH} 4.5$	—	769
				H''_{syn}, H''_{anti}	2.79s	—		
				H_{anti}	4.2d	$J_{PH} 8.3$		
				H'	2.33d	$J_{PH'} 1.7$		
				H'''	7.77m	—		
$C_{41}H_{37}IrOP_2$	124	$[h^3-CH_2C(CH_3)CH_2]Ir-(PPh_3)_2CO$	C_6H_6	H	1.86	—	T 35°. 100 MHz Temperature dependent	631
$C_{41}H_{37}IrOP_2$	125	$(h^3-CH_2CHCHCH_3)Ir-[P(Ph)_3]_2(CO)$	C_6H_6	H	4.23m	—	T 35°. 100 MHz	631
				H'	2.09b	—	Methyl signal unresolved, other signals broad	
$C_{42}H_{39}IrOP_2$	126	$[h^3-CH_2C(CH_3)CHCH_3']Ir-(PPh_3)_2(CO)$	C_6H_6	H	2.06	—	T 35°. 100 MHz	631
				H'	1.99d	$J 6.0$		
$C_{44}H_{43}IrOP_2$	127	$[h^3-CH_2C(CH_3)CHCH(CH_3)_2]Ir-(PPh_3)_2(CO)$	C_6H_6	H	2.34	—	T 35°. 100 MHz	631
				H'	1.21d	$J 7.0$		

TABLE XII—cont.

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
(4) TETRAHAPTO LIGANDS								
[C ₂₁ H ₂₈ ⁻ IrOP ₂] ⁺	128	{(h ⁴ -CH ₂ CH'CH'CH ₂)Ir-[P(CH ₃) ₂ Ph] ₂ (CO)} ⁺	CDCl ₃	H	2.4m,	—	Isolated as the tetrafluoroborate	761
					0.3m	—		
				H'	5.86m,	—		
					5.25	—		
				H''	2.08d,	J 10.2		
					2.05d,			
					1.75d			
				H	2.45m,	—	Isolated as the perchlorate	
					0.35m	—		
				H'	5.9m,	—		
H''	5.3m	—						
	2.12d,	J 10.3						
	2.07d,	J 10.5						
	1.77d	J 9.8						
[C ₂₂ H ₃₀ ⁻ IrOP ₂] ⁺	129	{[h ⁴ -CH ₂ C(CH ₃)CH''CH ₂]Ir-[P(CH ₃ '') ₂ Ph] ₂ (CO)} ⁺	SO ₂	H	2.6m,	—	T 34°	761
					0.4m	—	Isolated as the tetraphenylborate	
				H'	2.43d	J _{PH'} 3.8		
				H''	4.9m	—		
				H'''	1.96d,	J 10.1	Integral intensities in ratio 1 : 1 : 2 respectively	
					1.86d,	J 10.3		
					1.53d	J 10.1		
[C ₂₃ H ₃₂ ⁻ IrOP ₂] ⁺	130	{[h ⁴ -CH ₂ C(CH ₃)C(CH ₃ ')CH ₂]Ir-[P(CH ₃ ') ₂ Ph] ₂ (CO)} ⁺	CH ₂ Cl ₂	H	2.49m,	—	Isolated as the tetraphenylborate	761
					0.3m	—	T 34°	

				H'	2.27d	$J_{PH} 3.8$		
				H''	1.66q	$J_{PH} 3.0, 4.7$		
				H'''	1.97d,	$J 10.4$		
					1.84d,	$J 10.1$		
					1.46d,	$J 9.6$		
					1.39d	$J 9.6$		
		SO ₂	H		2.51m,	—		
					0.7—0.1m	—		
			H'		2.34d	$J_{PH} 3.8$		
			H''		1.76q	$J_{PH} 3.0, 4.6$		
			H'''		2.13d,	$J 10.0$		
					2.00d,	$J 10.3$		
					1.62d,	$J 9.8$		
					1.56d	$J 9.7$		
(5) PENTAHAPTO LIGANDS								
C ₆ H ₅ I ₂ IrO	131	(<i>h</i> ⁵ -C ₅ H ₅)Ir(I) ₂ (CO)	CDCl ₃	H	6.01s	—	—	782
C ₂₄ H ₂₀ IrOP	132	(<i>h</i> ⁵ -C ₅ H ₅)Ir[P(C ₆ H ₅) ₃](CO)	CCl ₄	H	5.00	$J_{PH} 0.6$	T 40°	783
				H'	7.32	—		
			CDCl ₃	H	4.97	—		782
				H'	8.1—6.9	—		
[C ₂₄ H ₂₁ IrOP] ⁺	133	[(<i>h</i> ⁵ -C ₅ H ₅)Ir[P(C ₆ H ₅) ₃](H)- (CO)] ⁺	(CD ₃) ₂ CO	H	n.m.	—	T 40° 100 MHz	783
				H'	7.56	—	Isolated as the tetraphenylborate	
				H''	-14.42	$J_{PH} 25$		
C ₁₁ H ₁₅ Cl ₂ IrO	134	[<i>h</i> ⁵ -C ₅ (CH ₃) ₅]Ir(Cl) ₂ (CO)	CDCl ₃	H	1.91s	—	—	638
C ₁₁ H ₁₅ I ₂ IrO	135	[<i>h</i> ⁵ -C ₅ (CH ₃) ₅]Ir(I) ₂ (CO)	CH ₂ Cl ₂	H	2.28s	—	—	784
			CDCl ₃	H	2.00s	—	—	638
C ₁₂ H ₁₈ ClIrO ₃ S	136	[<i>h</i> ⁵ -C ₅ (CH ₃) ₅]Ir(Cl)(SO ₂ CH ₃)- (CO)	CDCl ₃	H	1.97s	—	—	638
				H'	3.24s	—		

TABLE XII—*cont.*

Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)		Remarks	References
$C_{17}H_{20}ClIrO_3S$	137	$[h^5-C_5(CH_3)_5]Ir(Cl)-(SO_2C_6H_5)(CO)$	$CDCl_3$	H H'	1.93s 7.67m	— —	—		638
$C_{18}H_{22}ClIrO_3S$	138	$[h^5-C_5(CH_3)_5]Ir(Cl)(p-SO_2-C_6H_4CH_3)(CO)$	$CDCl_3$	H H' H''	1.93s 7.45q 2.40s	— — —	—		638
$C_{17}H_{19}BrClIrO_3S$	139	$[h^5-C_5(CH_3)_5]Ir(Cl)-(p-SO_2C_6H_4Br)(CO)$	$CDCl_3$	H H'	1.95s 7.61d	— —	—		638
$C_{12}H_{15}IrO_2$	140	$[h^5-C_5(CH_3)_5]Ir(CO)_2$	$CDCl_3$	H	219s	—	—		785 638
$C_{11}H_7IrO_2$	141	$(h^5-C_9H_7)Ir(CO)_2$	C_6H_{12}	H_{-1}, H_{-3} H_{-2}	5.56 6.00	$J_{1,2}$ 2.9 —	$C_9H_7 =$ 	639	
				H_{-4}, H_{-7} H_{-5}, H_{-6}	7.17 7.17	— —	T 30°		
(6) MIXED LIGANDS									
(a) Monohapto/monohapto									
$C_{44}H_{42}IrOP_2$	142	$Ir(CH_3)(h-C \equiv CCH_2CH_2CH_2-CH_3)(I)(PPh_3)_2(CO)$	C_6H_6	H H' H''	1.11t 2.66m, 1.52m 0.82t	J 5.5 J 6.0 J 2.0 J 6.5	100 MHz	627	

(b) *Monohapto/dihapto*

C ₄₉ H ₄₃ IrP ₂ O ₉	143	Ir[<i>h</i> ¹ -C(CO ₂ CH ₃)=CHCO ₂ -CH ₃][<i>h</i> ² -C(CO ₂ CH ₃)≡C(CO ₂ CH ₃)](PPh ₃) ₂ (CO)	—	H	3.60, 3.42, — 3.32, 3.23 —	—	777	
C ₄₄ H ₃₃ F ₆ IrOP ₂	144	Ir(<i>h</i> ¹ -C≡CCH ₃)(1,4- <i>h</i> ² -CF ₂ -CF'=CF'CF ₂)(PPh ₃) ₂ (CO)	CDCl ₃ CHCl ₃	H F F'	1.47t +39.7dd, +29.6dd +99.6 comp.	<i>J</i> 2.5 <i>J</i> 144, 42 <i>J</i> 73, 23 —	100 MHz Relative to trifluoromethylbenzene at 35° and 94.2 MHz Two non-equivalent CF ₂ groups	627
C ₄₄ H ₃₃ F ₈ IrOP ₂	145	Ir(<i>h</i> ¹ -C≡CCH ₃)[<i>h</i> ² -C(CF ₃)F=C(CF ₃)F](PPh ₃) ₂ (CO)	C ₆ H ₆ CHCl ₃	H F F'	1.47t +2.73q, +5.22q +104 comp. +124 comp.	<i>J</i> 2.5 <i>J</i> 10 <i>J</i> 10 — —	100 MHz Relative to trifluoromethylbenzene at 35° and 94.2 MHz Two non-equivalent CF ₃ groups	627
C ₄₆ H ₃₃ IrN ₄ -OP ₂	146	Ir(<i>h</i> ¹ -C≡CCH ₃)[<i>h</i> ² -C ₂ (CN) ₄](PPh ₃) ₂ (CO)	CDCl ₃	H	1.68t	<i>J</i> 2.5	100 MHz	627
C ₄₄ H ₃₃ F ₆ -IrOP ₂	147	Ir(<i>h</i> ¹ -C≡CCH ₃)[<i>h</i> ² -C ₂ (CF ₃) ₂](PPh ₃) ₂ (CO)	CDCl ₃	H F	1.74t -10.25 comp., -11.8 comp.	<i>J</i> 1.6 <i>J</i> 6, 3	100 MHz CF ₃ non-equivalent Relative to trifluoromethylbenzene at 35° and 94.2 MHz	627
C ₄₆ H ₃₉ IrO ₅ P ₂	148	Ir(<i>h</i> ¹ -C≡CCH ₃)[<i>h</i> ² -C ₂ (CO ₂ -CH ₃) ₂](PPh ₃) ₂ (CO)	CDCl ₃	H H'	1.52t 2.03	<i>J</i> 2.5 —	100 MHz	627

TABLE XII—cont.

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References	
(c) Monohapto/pentahapto								
$[\text{C}_{25}\text{H}_{23}\text{IrOP}]^+$	149	$\{(\eta^5\text{-C}_5\text{H}_5)\text{Ir}(\text{CH}_3)[\text{P}(\text{C}_6\text{H}_5)_3](\text{CO})\}^+$	CDCl_3	H	6.05	$J_{\text{PH}} 1.2$	Isolated as bromide with 0.5M CH_2Cl_2 solvent of crystallization T 40°	783
				H'	1.15	$J_{\text{PH}} 5.1$		
				H''	7.58	—		
			CDCl_3	H	6.05	$J_{\text{PH}} 1.1$	Isolated as chloride with 0.5M CH_2Cl_2 solvent of crystallization T 40°	
				H'	1.13	$J_{\text{PH}} 5.1$		
				H''	7.57	—		
			CDCl_3	H	6.02	$J_{\text{PH}} 1.2$	Isolated as iodide with 0.5M CH_2Cl_2 solvent of crystallization T 40°	
				H'	1.16	$J_{\text{PH}} 5.0$		
				H''	7.57	—		
$[\text{C}_{26}\text{H}_{23}\text{IrOP}]^+$	150	$\{(\eta^5\text{-C}_5\text{H}_5)\text{Ir}(\text{CH}_2\text{CH}_3)[\text{P}(\text{C}_6\text{H}_5)_3](\text{CO})\}^+$	CDCl_3	H	6.02	$J_{\text{PH}} 1.1$	Isolated as iodide with 0.5M CH_2Cl_2 solvent of crystallization T 40°	783
				H'	1.53, 2.93	—		
				H''	7.60	—		
$(\text{C}_{27}\text{H}_{20}\text{F}_7\text{-IrOP})^+$	151	$\{(\eta^5\text{-C}_5\text{H}_5)\text{Ir}(\text{C}_3\text{F}_7)[\text{P}(\text{C}_6\text{H}_5)_3](\text{CO})\}^+$	CDCl_3	H	6.27	$J_{\text{PH}} 1.0$	Isolated as iodide T 40°	783
				H'	7.63	—		
$[\text{C}_{30}\text{H}_{33}\text{-IrOP}]^+$	152	$\{(\eta^5\text{-C}_5\text{H}_5)\text{Ir}(\text{C}_6\text{H}_{13})[\text{P}(\text{C}_6\text{H}_5)_3](\text{CO})\}^+$	CDCl_3	H	6.00	$J_{\text{PH}} 1.1$	Isolated as iodide with 0.5M CH_2Cl_2 solvent of crystallization T 40°	783
				H'	1.13	—		
				H''	7.60	—		
$[\text{C}_{31}\text{H}_{27}\text{-IrOP}]^+$	153	$\{(\eta^5\text{-C}_5\text{H}_5)\text{Ir}(\text{CH}_2\text{C}_6\text{H}_5)[\text{P}(\text{C}_6\text{H}_5)_3](\text{CO})\}^+$	CDCl_3	H	5.83	$J_{\text{PH}} 1.1$	Isolated as iodide T 40°	783
				H'	3.10, 4.16	—		
				H''	7.64	—		
$\text{C}_{12}\text{H}_{18}\text{IrO}$	154	$\{[\eta^5\text{-C}_5(\text{CH}_3)_3]\text{Ir}(\text{CH}_3)(\text{I})(\text{CO})\}$	CH_2Cl_2	H	2.08	—	—	784
				H'	1.33	—		

$C_{12}H_{13}F_3IrO$	155	$[h^5-C_5(CH_3)_5]Ir(CF_3)(I)(CO)$		H F	2.21 5.0s	— —		784
$C_{13}H_{15}F_3IrO$	156	$[h^5-C_5(CH_3)_5]Ir(CF_2CF_3)(I)(CO)$	CH_2Cl_2	H F F'	2.16 70.5q 82.3t	— J_{FF} 269 $J_{FF'}$ 2.0		784
$C_{14}H_{15}F_7IrO$	157	$[h^5-C_5(CH_3)_5]Ir(CF_2CF_2CF_3)(I)(CO)$	CH_2Cl_2	H F F' F''	2.18 65.6q 115.3q 79.4t	— J_{FF} 280 J 12		784
$C_{17}H_{20}ClIrO$	158	$[h^5-C_5(CH_3)_5]Ir(h^1-C_6H_5)(Cl)(CO)$	$CDCl_3$	H H'	1.73s 7.10m	— —	—	638
$C_{18}H_{22}ClIrO$	159	$[h^5-C_5(CH_3)_5]Ir(h^1-p-C_6H_4CH_3)(Cl)(CO)$	$CDCl_3$	H H' H''	1.77s 7.05q* 2.29s	— — —	*Centre of AB quartet	638
$C_{17}H_{19}BrClIrO$	160	$[h^5-C_5(CH_3)_5]Ir(h^1-p-C_6H_4Br)(Cl)(CO)$	$CDCl_3$	H H'	1.77s 7.20bs	— —	—	638
$[C_{13}H_{18}IrO_2]^+$	161	$\{[h^5-C_5(CH_3)_5]Ir(CH_3)(CO)_2\}^+$	$(CD_3)_2CO$	H H' H''	2.24s 1.16s 7.35, 6.88m	— — —	Isolated as the $B(C_6H_5)_4$ salt	638
$[C_{13}H_{18}IrO_2]^+$	162	$\{[h^5-C_5(CH_3)_5]Ir(CH_3)(CO)_2\}^+$	$CDCl_3$	H H'	2.30s 1.06s	— —	Isolated as the iodide	638
$[C_{14}H_{15}F_4IrO_2]^+$	163	$\{[h^5-C_5(CH_3)_5]Ir(CF_2CF_2I)(CO)_2\}^+$	$(CD_3)_2CO$	H F F'	2.48 65.7 75.2	— — —	Isolated as the hexafluorophosphate	784

(7) MISCELLANEOUS IRIDIUM COMPLEXES

(a) Monocarbonyl derivatives

$C_{17}H_{23}As_2Cl_2IrO$	164	$Ir(Cl)_2[As(CH_3)_2Ph]_2(H)(CO)$	C_6H_6	H H'	-16.1 1.75, 1.73	—	As ligands <i>trans</i> , Cl <i>cis</i>	786
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TABLE XII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$[\text{C}_{25}\text{H}_{34}^- \text{AsClIrOP}_2]^+$	165	$\{\text{Ir}(\text{Cl})[\text{P}(\text{CH}_3)_2\text{Ph}]_2[\text{As}(\text{CH}_3)_2\text{Ph}](\text{H})(\text{CO})\}^+$	—	H	—10.7	J 15.5	$J^* \approx {}^2J_{\text{PH}} + {}^4J_{\text{PH}}$	787
				H'	1.83t, 1.69t	J^* 8.2 J^* 8.2	P ligands <i>trans</i> , Cl and CO ligands <i>trans</i>	
				H''	1.06s	—	Isolated as the tetraphenylborate	
$\text{C}_{37}\text{H}_{31} \text{ClGeIrOP}$	166	$\text{Ir}(\text{Cl})(\text{GePh}_3)(\text{PPh}_3)(\text{H})(\text{CO})$	C_6D_6	H	—8.50	J_{PH} 15.6	0.5M C_6H_{12} Solvent of crystallization	788
$\text{C}_{17}\text{H}_{24}^- \text{ClIrOP}_2$	167	$\text{Ir}(\text{Cl})[\text{P}(\text{CH}_3)_2\text{Ph}]_2(\text{H})_2(\text{CO})$	C_6H_6	H_a	—18.36	J_{PH} 14.1	<i>trans</i> -orientation of P ligands,	759
				H_b	—7.58	J_{PH} 20.2	H_a <i>trans</i> to Cl, H_b <i>cis</i> to Cl	
				H'	1.89t, 1.86t	J_{HH} 8.4 J^* 7.6 J^* 7.6	J^* Separation of outer lines of triplet	
$\text{C}_{25}\text{H}_{34}^- \text{ClIrOP}_3$	168	$\text{Ir}(\text{Cl})[\text{P}(\text{CH}_3)_2\text{Ph}]_3(\text{H})(\text{CO})$	—	H	—9.2	J_{PH} 16, 151	Two P ligands <i>trans</i> , Cl and CO ligands <i>trans</i> Isolated as the tetraphenylborate	787
				H'	1.84t, 1.64t, 1.19q	J_{PH} 8.0 J_{PH} 8.2 J_{PH} 9.7 J_{HH} ~1		
$\text{C}_{21}\text{H}_{32}^- \text{BrIrOP}_2$	169	$\text{Ir}(\text{Br})(\text{PEt}_2\text{Ph})_2(\text{H})_2(\text{CO})$	C_6H_6	H_a	—18.29	J_{PH} 13.5	<i>trans</i> -orientation of P ligands, H_a <i>trans</i> , and H_b <i>cis</i>, to Br	759
				H_b	—8.73	J_{PH} 18.9		
$\text{C}_{21}\text{H}_{31}\text{BrD}^- \text{IrOP}_2$	170	$\text{Ir}(\text{Br})(\text{PEt}_2\text{Ph})_2(\text{D})(\text{H})(\text{CO})$	C_6H_6	H_a	—18.30	J_{PH} 13.5	<i>trans</i> -orientation of P ligands, H_a <i>trans</i> , and H_b <i>cis</i>, to Br	759
				H_b	—8.75	J_{PH} 19.0		

$C_7H_{19}Cl_2-$ $IrOP_2$	171	$Ir(Cl)_2[P(CH_3)_3]_2(H)(CO)$	CH_2Cl_2	H H'	-16.6 1.74	$J_{PH} 12.9$ $J_{PH} 4.2$	P ligands <i>trans</i> , Cl <i>cis</i>	786
$C_{13}H_{39}Cl_2-$ $IrOP_2$	172	$Ir(Cl)_2(PEt_3)_2(H)(CO)$	—	H	-9.2t	$J_{PH} 16.0$	P ligands <i>trans</i> , Cl <i>trans</i>	789
$C_{13}H_{31}Cl_2-$ $IrOP_2$	173	$Ir(Cl)_2[P(CH_3)_2C(CH_3)_3]_2(H)-$ (CO)	—	H H' H''	-15.98t 1.65, 1.53 0.92t	$J_{PH} 10.8$ $J^* 8.7$ $J^* 7.1$ $J^\dagger 14.6$	P ligands <i>trans</i> , Cl <i>cis</i> $J^* = {}^2J_{PH} + {}^4J_{PH}$ $J^\dagger = {}^3J_{PH} + {}^5J_{PH}$	790
$C_{17}H_{39}Cl_2-$ $IrOP_2$	174	$Ir(Cl)_2[P(Et)_2C(CH_3)_3]_2(H)(CO)$	—	H H'	-16.24t 1.19t	$J_{PH} 10.6$ $J^\dagger 12.6$	P ligands <i>trans</i> , Cl <i>cis</i> $J^\dagger = {}^3J_{PH} + {}^5J_{PH}$	790
$C_{21}H_{47}Cl_2-$ $IrOP_2$	175	$Ir(Cl)_2[P(n-C_3H_7)_2C(CH_3)_3]_2-$ (H)(CO)	—	H H'	-15.75 1.1t	$J_{PH} 10.65$ $J^\dagger 13.7$	P ligands <i>trans</i> , Cl <i>cis</i> $J^\dagger = {}^3J_{PH} + {}^5J_{PH}$	790
$C_{23}H_{55}Cl_2-$ $IrOP_2$	176	$Ir(Cl)_2[P(n-C_4H_9)_2C(CH_3)_3]_2-$ (H)(CO)	—	H H'	-16.36 1.27t	$J_{PH} 10.7$ $J^\dagger 14.0$	P ligands <i>trans</i> , Cl <i>cis</i> $J^\dagger = {}^3J_{PH} + {}^5J_{PH}$	790
$C_{19}H_{43}Cl_2-$ $IrOP_2$	177	$Ir(Cl)_2\{P(CH_3)[C(CH_3)_3]_2\}_2-$ (H)(CO)	—	H H' H''	-16.46t 1.8 1.29, 1.25	$J_{PH} 10.9$ $J^* 7.6$ $J^\dagger 13.3$	P ligands <i>trans</i> , Cl <i>cis</i> $J^* = {}^2J_{PH} + {}^4J_{PH}$ $J^\dagger = {}^3J_{PH} + {}^5J_{PH}$	790
$C_{21}H_{47}Cl_2-$ $IrOP_2$	178	$Ir(Cl)_2\{P(Et)[C(CH_3)_3]_2\}_2-$ (H)(CO)	—	H H'	-16.26 1.37t, 1.31	$J_{PH} 11.7$ $J^\dagger 13.2$ $J^\dagger 13.1$	P ligands <i>trans</i> , Cl <i>cis</i> $J^\dagger = {}^3J_{PH} + {}^5J_{PH}$	790
$C_{23}H_{55}Cl_2-$ $IrOP_2$	179	$Ir(Cl)_2\{P(n-C_3H_7)[C(CH_3)_3]_2\}_2-$ (H)(CO)	—	H H'	-16.26 1.39t, 1.32	$J_{PH} 11.9$ $J^\dagger 13.2$ $J^\dagger 13.1$	P ligands <i>trans</i> , Cl <i>cis</i> $J^\dagger = {}^3J_{PH} + {}^5J_{PH}$	790

TABLE XII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{13}H_{31}Br_2^-$ $IrOP_2$	180	$Ir(Br)_2[P(CH_3)_2C(CH_3)_3]_2-$ (H)(CO)	—	H	—15.5t	J_{PH} 10.45	P ligands <i>trans</i> , Br <i>cis</i> $J^* = {}^2J_{PH} + {}^4J_{PH}$ $J^\dagger = {}^3J_{PH} + {}^5J_{PH}$	790
				H'	1.91,	J^* 6.0		
					1.88	J^* 5.8		
				H''	1.22t	$J^\dagger$ 14.0		
$C_{17}H_{39}Br_2^-$ $IrOP_2$	181	$Ir(Br)_2[P(Et)_2C(CH_3)_3]_2(H)(CO)$	—	H	—15.75t	J_{PH} 10.5	P ligands <i>trans</i> , Br <i>cis</i> $J^\dagger = {}^3J_{PH} + {}^5J_{PH}$	790
				H'	1.1t	$J^\dagger$ 13.7		
$C_{21}H_{47}Br_2^-$ $IrOP_2$	182	$Ir(Br)_2[P(n-C_3H_7)_2C(CH_3)_3]_2-$ (H)(CO)	—	H	—15.78t	J_{PH} 10.4	P ligands <i>trans</i> , Br <i>cis</i> $J^\dagger = {}^3J_{PH} + {}^5J_{PH}$	790
				H'	1.27t	$J^\dagger$ 13.7		
$C_{25}H_{55}Br_2^-$ $IrOP_2$	183	$Ir(Br)_2[P(n-C_4H_9)_2C(CH_3)_3]_2-$ (H)(CO)	—	H	—15.78t	J_{PH} 10.45	P ligands <i>trans</i> , Br <i>cis</i> $J^\dagger = {}^3J_{PH} + {}^5J_{PH}$	790
				H'	1.29t	$J^\dagger$ 14.0		
$[C_{25}H_{34}-$ $BrIrOP_3]^+$	184	$\{Ir(Br)[P(CH_3)_2Ph]_3(H)(CO)\}^+$	—	H	—9.74dt	J_{PH} 17, 150*	Two P ligands <i>trans</i> , Br and CO ligands <i>trans</i> $J^* = {}^2J_{PH} + {}^4J_{PH}$ Isolated as the tetraphenylborate *Large P—H coupling is characteristic of a P in <i>trans</i> -position to hydrogen (H) Smaller coupling to other two equivalent P nuclei	787
				H'	1.90t,	J^* 7.8		
					1.67t,	J^* 8.0		
					1.49	J_{PH} 9.4 $J_{HH'} \sim 1$		
$C_{17}H_{23}Br_2^-$ $IrOP_2$	185	$Ir(Br)_2[P(CH_3)_2Ph]_2(H)(CO)$	C_6H_6	H	—15.3	J_{PH} 12.0	P ligands <i>trans</i> , Br <i>cis</i>	786
				H'	2.00,	J_{PH} 5.0		
					1.93	J_{PH} 5.3		

$C_{27}H_{27}^-$ $BrClIrOP_2$	186	$Ir(Br)(Cl)[P(Ph)_2CH_3]_2(H)(CO)$	$CDCl_3$	H	2.60t, 2.57t	— —	P ligands <i>trans</i> Two isomers	760
$C_{17}H_{23}Cl_2^-$ $IrOP_2$	187	$Ir(Cl)_2[P(CH_3)_2Ph]_2(H)(CO)$	C_6H_6	H H'	-15.7 1.88, 1.81	$J_{PH} 12.3$ $J_{PH} 4.5$ $J_{PH} 4.6$	P ligands <i>trans</i> , Cl <i>cis</i>	786
			C_6H_6	H H'	-8.7 1.80	$J_{PH} 17.5$ $J_{PH} 4.2$	P ligands <i>trans</i> , Cl <i>trans</i> The hydride ligand gives a signal to considerably higher field (-13 to -18) when <i>trans</i> orientated with respect to a hydrogen ligand than when it is <i>cis</i> to a halogen (-6 to -10)	
$C_{27}H_{27}Cl_2^-$ $IrOP_2$	188	$Ir(Cl)_2[P(Ph)_2CH_3]_2(H)(CO)$	$CDCl_3$	H	2.48t	—	—	760
$C_{55}H_{46}IrOP_3$	189	$Ir(PPh_3)_3(H)(CO)$	C_6D_6	H	-10.30	$J_{PH} 21.3$	100 MHz	791
$[C_{13}H_{33}^-]$ $IrOP_4^{2+}$	190	$\{Ir[P(CH_3)_2CH_2^+CH_2^+P-(CH_3)_2]_2(H)(CO)\}^{2+}$	—	H H' H'' H'''	-12.0q 2.1, 1.95 2.3m 7.2s 7.93t 6.8	$J_{PH} 16$ — — — — — — $J_{H''H'''} 7.5$	220 MHz <i>trans</i> -isomer Isolated as the $[B(C_6H_5'')_4]_2^{2-}$ salt	792
$C_{55}H_{46}IrO_4P_3$	191	$Ir[P(Ph)_3]_2[P(OPh)_3](H)(CO)$	C_6D_6	H	-11.32	$J_{PH} 13.5, 22.0$	100 MHz	791
$C_{55}H_{46}IrO_{10}P_3$	192	$Ir\{P(OPh)_3\}_3(H)(CO)$	C_6D_6	H H	-11.76 -11q	$J_{PH} 13.0$ $J_{PH} 14$	100 MHz —	791 793
$C_{43}H_{36}^-$ $BrIrOP_2S$	193	$Ir(Br)(PPh_3)_2(SPh)(H)(CO)$	—	H	-15.2t	$J_{PH} 12.0$	P ligands <i>trans</i> , H and Br ligands <i>trans</i>	794
$C_{43}H_{36}^-$ $ClIrOP_2S$	194	$Ir(Cl)(PPh_3)_2(SPh)(H)(CO)$	—	H	-16.1t	$J_{PH} 12.0$	P ligands <i>trans</i> , H and Cl ligands <i>trans</i>	794

TABLE XII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{43}H_{36}IIrOP_2S$	195	$Ir(I)(PPh_3)_2(SPh)(H)(CO)$	—	H $-13.1t$	$J_{PH} 11.9$	P ligands <i>trans</i> , H and I ligands <i>trans</i>	794
$C_{43}H_{31}BrF_5^- IrOP_2S$	196	$Ir(Br)(PPh_3)_2(SC_6F_5)(H)(CO)$	—	H $-14.8t$	$J_{PH} 11.1$	P ligands <i>trans</i> , H and Br ligands <i>trans</i>	794
$C_{43}H_{31}ClF_5^- IrOP_2S$	197	$Ir(Cl)(PPh_3)_2(SC_6F_5)(H)(CO)$	—	H $-15.7t$	$J_{PH} 11.4$	P ligands <i>trans</i> , H and Cl ligands <i>trans</i>	794
$C_{43}H_{31}F_5^- IIrOP_2S$	198	$Ir(I)(PPh_3)_2(SC_6F_5)(H)(CO)$	—	H $-13.1t$	$J_{PH} 10.8$	P ligands <i>trans</i> , H and I ligands <i>trans</i>	794
$C_{49}H_{31}F_{10}^- IrOP_2S_2$	199	$Ir(PPh_3)_2(SC_6F_5)_2(H)(CO)$	CH_2Cl_2	H $-13.2t$	$J_{PH} 11.6$	P ligands <i>trans</i> , H <i>trans</i> to one SC_6F_5 ligand	794
$C_{43}H_{46}ClIrO_4^- P_2Si$	200	$Ir(Cl)(PPh_3)_2[Si(OEt)_3](H)(CO)$	CH_2Cl_2	H -7.0	—	—	795
			$CHCl_3$	H -6.34	—	—	
			C_6H_6	H -6.1	—	—	
$C_{37}H_{31}Cl_4^- IrOP_2Sn$	201	$Ir(Cl)(PPh_3)_2(SnCl_3)(H)(CO)$	CH_2Cl_2	H -9.9	$J_{PH} 10$	56.5 MHz	796
$C_{40}H_{37}Cl_4^- IrO_2P_2Sn$	202	$Ir(Cl)(PPh_3)_2(SnCl_3)(H)(CO). (CH_3)_2CO$	CH_2Cl_2	H $-9.9t$	$J_{PH} 10$	56.5 MHz	796
$C_{40}H_{40}^- BrIrOP_2Sn$	203	$Ir(Br)(PPh_3)_2[Sn(CH_3)_3](H)(CO)$	$CDCl_3$	H —	—	P ligands <i>trans</i> , H and Br ligands <i>cis</i>	797
				H' $-0.03s$	—		
$C_{40}H_{40}^- ClIrOP_2Sn$	204	$Ir(Cl)(PPh_3)_2[Sn(CH_3)_3](H)(CO)$	$CDCl_3$	H' $-0.09s$	—	—	797
			C_6H_6	H -8.8	—		

$C_{43}H_{46}^-$ ClIrOP ₂ Sn	205	Ir(Cl)(PPh ₃) ₂ [Sn(CH ₂ CH ₃) ₃]- (H)(CO)	CDCl ₃ C ₆ H ₆	H' H	6.07 -10.4	— —	—	797
$C_{45}H_{42}^-$ ClIrOP ₂ Sn	206	Ir(Cl)[P(C ₆ H ₅) ₂ CH ₃] ₂ (SnPh ₃)- (H)(CO)	CDCl ₃ C ₆ H ₆	H' H'' H	7.32m 1.8t -5.3	— $J_{PH} 9$ —	P ligands <i>trans</i> , H <i>cis</i> to Cl and <i>trans</i> to Sn ligand	797
$C_{13}H_{32}$ ClIrOP ₂	207	Ir(Cl)[P(CH ₂ CH ₃) ₃] ₂ (H) ₂ (CO)	C ₆ D ₆	H H' H''	-8.27, -19.45 1.68 0.89	$J_{PH} 13.8, 13.2$ $J_{HH} 5.4$ $J_{H'H''} 8.4$ $J_{PH'} 7.5$ —	P ligands <i>trans</i> , H ligands <i>cis</i> , and the chemical shifts of the H ligands indicates that one is <i>cis</i> and the other <i>trans</i> to the Cl ligand	788
$C_{37}H_{32}^-$ ClIrOP ₂	208	Ir(Cl)(PPh ₃) ₂ (H) ₂ CO	CH ₂ Cl ₂	H	-7.3t, -18.4t	$J_{PH} 15$ $J_{PH} 15$	P ligands <i>trans</i> , H ligands <i>cis</i> , one H <i>cis</i> and the other <i>trans</i> to the Cl ligand	796
$C_{13}H_{32}$ IrOP ₂	209	Ir(I)[P(CH ₂ CH ₃) ₃] ₂ (H) ₂ (CO)	C ₆ D ₆	H H' H''	-10.2, -17.5 1.73 0.84	$J_{PH} 18.7$ $J_{PH} 13.9$ $J_{HH} 5.1$ $J_{H'H''} 7.8$ $J_{PH'} 7.2$ —	P ligands <i>trans</i> , H ligands <i>cis</i> to each other, one being <i>cis</i> and the other <i>trans</i> to the I ligand	788
$C_{16}H_{41}^-$ GeIrOP ₂	210	Ir[Ge(CH ₃) ₃][P(CH ₂ CH ₃) ₃] ₂ - (H) ₂ (CO)	C ₆ D ₆	H H'	-11.31, -11.80 0.83	$J_{HH} 4$ $J_{PHtrans} 11.4$ $J_{PHcis} 19.2$ —	P ligands <i>cis</i> , one H ligand <i>cis</i> to both P ligands, and one H <i>trans</i> to one and <i>cis</i> to the other P ligand GeMe ₃ ligand <i>cis</i> to both H's	788
$C_{20}H_{33}^-$ GeIrOP ₂	211	Ir[Ge(CH ₃) ₃][P(CH ₃) ₂ Ph] ₂ - (H) ₂ (CO)	C ₆ D ₆	H H' H''	— 0.93 1.54d	— — $J_{PH''} 8.1$	—	788

TABLE XII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
$C_{40}H_{41}^-$ GeIrOP ₂	212	Ir[Ge(CH ₃) ₃](PPh ₃) ₂ (H) ₂ (CO)	C ₆ D ₆	H	−9.50* −10.50†	$J_{PH_{cis}}$ 19 $J_{PH_{cis}}$ 18 $J_{PH_{trans}}$ 117 J_{HH} 3.5 —	P ligands <i>cis</i> , one H* <i>cis</i> to both P ligands, and one H† <i>trans</i> to one and <i>cis</i> to the other. GeMe ₃ ligand <i>cis</i> to both H's	788 798
				H'	0.80	—		
$C_{33}H_{41}^-$ GeIrOP ₂	213	Ir[Ge(C ₂ H ₅) ₃](PPh ₂ CH ₂ CH ₂ -PPh ₂)(H) ₂ (CO)	—	H	−10.04* −10.82†	$J_{PH_{cis}}$ 11 $J_{PH_{cis}}$ 19 $J_{PH_{trans}}$ 121	One H* <i>cis</i> to both P ligands, and one H† <i>cis</i> to one and <i>trans</i> to the other P ligand	788
				H	1.38	—		
$C_{43}H_{47}^-$ GeIrOP ₂	214	Ir[Ge(CH ₂ CH ₃) ₃](PPh ₃) ₂ (H) ₂ (CO)	C ₆ D ₆	H	−9.77*	$J_{PH_{cis}}$ 22, 16, J_{HH} 4	220 MHz P ligands <i>cis</i>	788 798
					−10.86†	$J_{PH_{cis}}$ 18.5 $J_{PH_{trans}}$ 117	*H <i>cis</i> to both P ligands (8 lines) †H <i>cis</i> to one and <i>trans</i> to the other P ligand (8 lines)	
				H'	1.11	—	GeMe ₃ ligand <i>cis</i> to both H's	
				H''	1.28	—		
$[C_{25}H_{35}^-$ IrOP ₃] ⁺	215	{Ir[P(CH ₃) ₂ Ph] ₃ (H) ₂ (CO)} ⁺	—	H	−9.6 to −12.8		Isolated as the tetraphenylborate Two of the P ligands mutually <i>trans</i>	787
				H'	1.89t 1.18q	— $J_{PH'}$ 9.2 $J_{HH'_{trans}}$ ~ 1	One H <i>cis</i> to all three P ligands and one H <i>cis</i> to two and <i>trans</i> to the other P ligand	
$[C_{40}H_{41}^-$ IrOP ₃] ⁺	216	{Ir[P(C ₆ H ₅) ₂ CH ₃] ₃ (H) ₂ (CO)} ⁺	CDCl ₃	H	−9.03q*, −11.6†	$J_{PH_{cis}}$ 16.7 $J_{PH_{cis}}$ 17.7 $J_{PH_{trans}}$ 119	100 MHz Two P ligands mutually <i>trans</i> *H <i>cis</i> to three P	799

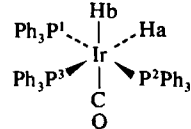
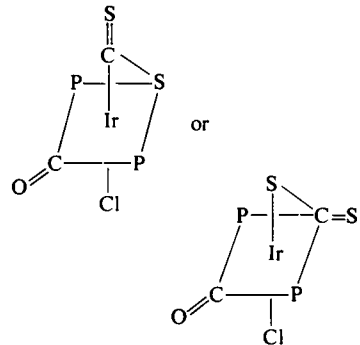
				H'	1·81t, 1·60d	J_{PH} 3·5 J_{PH} 8·0	†H <i>cis</i> to two P and <i>trans</i> to one P Isolated as the tetraphenylborate	
$[C_{55}H_{47}^- IrOP_3]^+$	217	$[Ir(PPh_3)_3(H)_2(CO)]^+$	—	H_b	—9·4qd	J_{HbP_1} 20 J_{HbP_2} 12 J_{HbH_a} 4	100 MHz	781
				H_a	—10·7td, —11·9td	J_{HaP_1} 18 J_{HaP_2} 11·5		
						J_{HaHb} 4	Isolated as the perchlorate	
$C_{37}H_{32}Cl_3^- IrOP_2Sn$	218	$Ir(PPh_3)_2(SnCl_3)(H)_2(CO)$	CH_2Cl_2	H	—9·9t, —12·5t	J_{PH} 10 J_{PH} 10	56·5 MHz	796
$C_{43}H_{32}F_5^- IrOP_2S$	219	$Ir(PPh_3)_2(SC_6F_5)(H)_2(CO)$	CH_2Cl_2	H	—7·9td, —15·0td	J_{PH} 18·0 J_{PH} 15·0 J_{HH} 4·2	—	794
$[C_{38}H_{68}^- IrOP_2S]^+$	220	$\{Ir[P(C_6H_{11})_3]_2(CS)(H)_2(CO)\}^+$	$CDCl_3$	H	—9·95t, —14·05t	J_{PH} 25	Isolated as the perchlorate	771
$C_{45}H_{43}^- IrOP_2Si$	221	$Ir(H)_2[P(C_6H_5)_3]_2[Si(CH_3)_2C_6H_5](CO)$	—	H	—10·0, —11·0	J_{HH} 4 J_{PH} 22, 17 J_{PH} 110·5, 18·5	—	935
$C_{55}H_{47}^- IrOP_2Si$	222	$Ir(H)_2[P(C_6H_5)_3]_2[Si(C_6H_5)_3](CO)$	—	H	—9·5, —10·7	J_{HH} 4·5 J_{PH} 20, 15·5 J_{PH} 110·3, 17·0	—	935

TABLE XII—*cont.*

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Formula	No.	Compound	Solvent		δ (ppm)	Coupling constant (Hz)	Remarks	References
$C_{43}H_{47}^-$ IrO_4P_2Si	223	$Ir(H)_2[P(C_6H_5)_3]_2[Si-(OC_2H_5)_3](CO)$	—	H	—10.2, —11.5	$J_{HH} 4$ $J_{PH} 22, 17$ $J_{PH} 110.5, 18.5$	—	935
$C_{18}H_{22}^-$ $ClIrOP_2S_2$	224	$Ir(Cl)[P(CH_3)_2Ph]_2(CS_2)(CO)$	C_6H_6	H	1.68t	$J^* 8.6$	Structure: 	759
J^* Separation of outer lines of triplet								
<i>(b) Dicarbonyl derivatives</i>								
$C_{38}H_{31}As_2-IrO_2$	225	$Ir(AsPh_3)_2(H)(CO)_2$	CH_2Cl_2 C_6H_6	H H	—12.30s —11.40s	— —	T 35° 100 MHz The hydridodicarbonyliridium (I) complexes of formula	800

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$C_{30}H_{31}IrO_2P_2$	226	$Ir[P(Ph)_2Et]_2(H)(CO)_2$	CH_2Cl_2 $C_6H_5CH_3$ C_5H_5N	H H H	-11.58t -10.99t -11.06t	J 17.5 J 11.0 J 18.5	Ir(H)(CO) ₂ L ₂ (where L = PPh ₃ , P(C ₆ H ₄ F) ₃ , PEtPh ₂ , and AsPh ₃) have a single structure in the solid state but in solution two isomeric pentaco- ordinate species are formed in equilibrium. The equilibria and spectra are temperature and solvent dependent. The appearance of the NMR spectra requires that the ³¹ P-H coupling constants in the two isomers are opposite in sign *T -70°	
$C_{38}H_{31}IrO_2P_2$	227	$Ir(PPh_3)_2(H)(CO)_2$	CS ₂	H	-10.98t* -11.26t*	J 19 J 35		
			—	H	-11.1	—		100 MHz 781
$C_{38}H_{25}F_6-$ IrO_2P_2	228	$Ir[P(C_6H_4F)_3]_2(H)(CO)_2$	$C_6H_5CH_3$	H	-10.58t	J 3.5	T 35°	100 MHz 800
$[C_{26}H_{34}-$ $IrO_2P_3]^{2+}$	229	$\{Ir[P(CH_3)_2Ph]_3(H)(CO)_2\}^{2+}$	CH_2Cl_2	H H'	-8.18q 1.68qt, 1.21d	J_{PH} 16.2 J_{PH}^* 16.8 J_{PH}^* 10.8	T 34° Isolated as the tetraphenylborate J^* values are the separation of outer peaks of triplets (or doublets)	801
$[C_{38}H_{32}As_2-$ $IrO_2]^+$	230	$[Ir(AsPh_3)_2(H)_2(CO)_2]^+$	CDCl ₃	H	-10.5s	—	60 and 100 MHz	799
$[C_{14}H_{32}-$ $IrO_2P_2]^+$	231	$Ir[P(Et)_3]_2(H)_2(CO)_2\}^+$	CDCl ₃	H	-11.4t	J_{PH} 15	60 and 100 MHz Isolated as the tetraphenylborate	799
$[C_{20}H_{44}-$ $IrO_2P_2]^+$	232	$Ir[P(i-C_3H_7)_3]_2(H)_2(CO)_2\}^+$	CDCl ₃	H	-11.8t	J_{PH} 15	60 and 100 MHz Isolated as the tetraphenylborate	799

TABLE XII—*cont.*

Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References
$[\text{C}_{38}\text{H}_{68}^-\text{IrO}_2\text{P}_2]^+$	233	$\{\text{Ir}[\text{P}(\text{C}_6\text{H}_{11})_3]_2(\text{H})_2(\text{CO})_2\}^+$	CDCl_3	H -11.5t	$J_{\text{PH}} 15$	60 and 100 MHz Isolated as the tetraphenylborate	799
$[\text{C}_{22}\text{H}_{32}^-\text{IrO}_2\text{P}_2]^+$	234	$\{\text{Ir}[\text{P}(\text{Et})_2\text{Ph}]_2(\text{H})_2(\text{CO})_2\}^+$	CDCl_3	H -11.0t	$J_{\text{PH}} 15$	60 and 100 MHz Isolated as the tetraphenylborate	799
$[\text{C}_{28}\text{H}_{28}^-\text{IrO}_2\text{P}_2]^+$	235	$\{\text{Ir}[\text{P}(\text{Ph})_2\text{CH}_3]_2(\text{H})_2(\text{CO})_2\}^+$	CDCl_3	H -10.4t H' 2.20	$J_{\text{PH}} 15$ $J_{\text{PH}} 4.0$	60 and 100 MHz Isolated as the tetraphenylborate	799 802
$[\text{C}_{30}\text{H}_{32}^-\text{IrO}_2\text{P}_2]^+$	236	$\{\text{Ir}[\text{P}(\text{Ph})_2\text{Et}]_2(\text{H})_2(\text{CO})_2\}^+$	CDCl_3	H -10.5t	$J_{\text{PH}} 15.0$	60 and 100 MHz Isolated as the tetraphenylborate	799
$[\text{C}_{38}\text{H}_{32}^-\text{IrO}_2\text{P}_2]^+$	237	$\{\text{Ir}[\text{P}(\text{Ph})_3]_2(\text{H})_2(\text{CO})_2\}^+$	CDCl_3	H -9.8t	$J_{\text{PH}} 15$	60 and 100 MHz Isolated as the tetraphenylborate	799
$\text{C}_{11}\text{H}_2\text{Ir}_4\text{O}_{11}$	238	$\text{Ir}_4(\text{H})_2(\text{CO})_{11}$	—	H 4.47	—	—	804
$[\text{C}_{11}\text{H}\text{Ir}_4\text{O}_{11}]^-$	239	$[\text{Ir}_4(\text{H})(\text{CO})_{11}]^-$		H 4.5	—	Trimethylbenzylammonium salt	804
$[\text{C}_{12}\text{H}_2\text{Ir}_4\text{O}_{12}]^{2+}$	240	$[\text{Ir}_4(\text{H})_2(\text{CO})_{12}]^{2+}$	98% H_2SO_4	H -20.0^*	—	100 MHz The neutral complex $\text{Ir}_4(\text{CO})_{12}$ becomes doubly protonated on dissolution in strong acid *Reference Me_2SO_4 in H_2SO_4 (δ CH for Me_2SO_4 taken as 3.9)	600

TABLE XIII
Nickel, palladium, platinum, and copper complexes

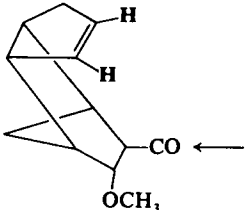
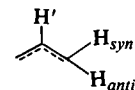
Formula	No.	Compound	Solvent	δ (ppm)		Coupling constant (Hz)	Remarks	References
(1) MONOHAPTO LIGANDS								
$[\text{C}_8\text{H}_{21}\text{As}_2\text{-OPt}]^+$	1	$[\text{Pt}(\text{CH}_3)[\text{As}(\text{CH}_3)_3]_2(\text{CO})]^+$	$(\text{CD}_3)_2\text{CO}$	H	0.65	$J_{\text{PtH}} 62.4$	T 36°	811
				H'	1.75	$J_{\text{PtH}} 24.8$	<i>trans</i> -isomer	
				$^{13}\text{CH}_3$	-6.9	$J_{\text{PtC}} 470$	25.2 MHz	
				$^{13}\text{CH}_3'$	10.0	$J_{\text{PtC}} 42$	Isolated as the hexafluoro-phosphate	
				^{13}CO	178.7	$J_{\text{PtC}} 1000$		
$\text{C}_{31}\text{H}_{30}\text{ClO}_3\text{-PPt}$	2	$\text{Pt}(\text{COC}_{10}\text{H}_{12}\text{OCH}_3)(\text{Cl})\text{-}(\text{PPh}_3)(\text{CO})$	CDCl_3	H	5.5	—	$\text{COC}_{10}\text{H}_{12}\text{OCH}_3 =$	812
								
(2) DIHAPTO LIGANDS								
$\text{C}_{14}\text{H}_8\text{I}_4\text{-Ni}_2\text{O}_2$	3	$[(\eta^2\text{-C}_6\text{H}_4)\text{Ni}(\text{I})_2]_2(\text{CO})_2^*$	CD_3OD	A_2B_2 spectrum centred at ~ 7.67		J 3.5	$\text{C}_6\text{H}_4 = \text{benzyne}$ *Bridging CO ligands	805

TABLE XIII—cont.

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Formula	No.	Compound	Solvent	δ (ppm)	Coupling constant (Hz)	Remarks	References	
(3) TRIHAPTO LIGANDS								
$C_{22}H_{20}INiOP$	4	$(h^3\text{-CH}_2\text{CH}'\text{CH}_2)\text{Ni(I)(PPh}_3\text{)-CO}$	$CDCl_3$	H_{syn}	3.93	$J_{HH'} 7$ $J_{HH'} 13$	T +20° 100 MHz	806 807
				H_{anti}	3.28			
				H'	4.97			
				H_{syn}	3.98	—	T +5°	
				H_{anti}	3.49			
				H'	4.89			
				H_{syn}	4.01	—	T -10°	
				H_{anti}	3.53			
				H'	4.88			
$C_{23}H_{22}INiOP$	5	$(h^3\text{-CH}_2\text{C(CH}_3\text{)CH}_2)\text{Ni(I)-(PPh}_3\text{)(CO)}$	C_6H_5Cl	H_{syn}	3.45	—	T +30° 100 MHz	806
				H_{anti}	2.70			
				H'	1.48			
				H_{syn}	3.45	—	T +10°	
				H_{anti}	2.76			
				H'	1.43			
				H_{syn}	3.45	—	T -10°	
				H_{anti}	2.79			
				H'	1.36			
				H_{syn}	3.46	—	T -20°	
				H_{anti}	2.82			
				H'	1.36			



$C_8H_{10}Cl_2O_2Pd_2$	6	$[(h^3-CH_2CH'CH_2)Pd(Cl)(CO)]_2$	$CDCl_3$	H_{syn} H_{anti} H'	4.82d 3.87 3.54d n.m.	$J_{HH'}$ 7 $J_{HH'}$ 12 $J_{HH'}$ 11 —	T -78°	809
$C_{10}H_{14}Cl_2O_2Pd_2$	7	$[(h^3-CH_2C(CH_3)CH_2)Pd(Cl)(CO)]_2$	$CHCl_3$	H_{syn} H_{anti} H'	3.48b 3.48b 2.17	— — —	T 34°	810
		—	—	H_{syn} H_{anti} H'	4.65d 4.75d 3.35s 3.72s 2.12s	J_{HH} 2.9 J_{HH} 2.9 — — —	T -77°	809
(4) PENTAHAPTO LIGANDS								
$C_{12}H_{20}GeNiO$	8	$(h^5-C_5H_5)Ni[Ge(C_2H_5)_3](CO)$		H H'	5.26 1.07	—	40 MHz	135
C_6H_5CuO	9	$(h^5-C_5H_5)Cu(CO)$	Saturated h.c.	H	~ 5.7	—	T -20°	814
$C_{14}H_5Co_3NiO_9$	10	$(h^5-C_5H_5)Ni[Co_3(CO)_9]$	$(CD_3)_2CO$	H	5.1s	—	—	808
$C_{15}H_{10}FeNi_2O_5$	11	$(h^5-C_5H_5)_2Ni_2(Fe(CO)_3)$	$(CD_3)_2CO$	H	5.4s	—	—	808
$[C_{15}H_{10}Ni_2MnO_5]^-$	12	$\{(h^5-C_5H_5)_2Ni_2[Mn(CO)_3]\}^-$	$(CD_3)_2CO$	H	5.02s	—	Isolated as the tetramethyl ammonium salt	808
(5) MISCELLANEOUS LIGANDS								
$[C_{13}H_{31}AsOPt]^+$	13	$[Pt(AsEt_3)_2(H)(CO)]^+$	$CDCl_3$	H	-5.65	$J_{Pt(H)}$ 768	100 MHz <i>trans</i> -isomer Isolated as the perchlorate	813
$[C_{15}H_{31}OPt_2Pt]^+$	14	$[Pt(PEt_3)_2(H)(CO)]^+$	$CHCl_3$	H	-4.78	—	Isolated as the perchlorate	802

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