

Supporting Information for:  
“Assessing the Donor Ability of Boratabenzene and  
9-Borataphenanthrene Anions through Metal  
Complexes with Carbonyl Ligands”

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Figure S-1:  $^1\text{H}$  NMR spectrum of **1Cr** in  $\text{CD}_3\text{CN}$  (\*residual diethyl ether)

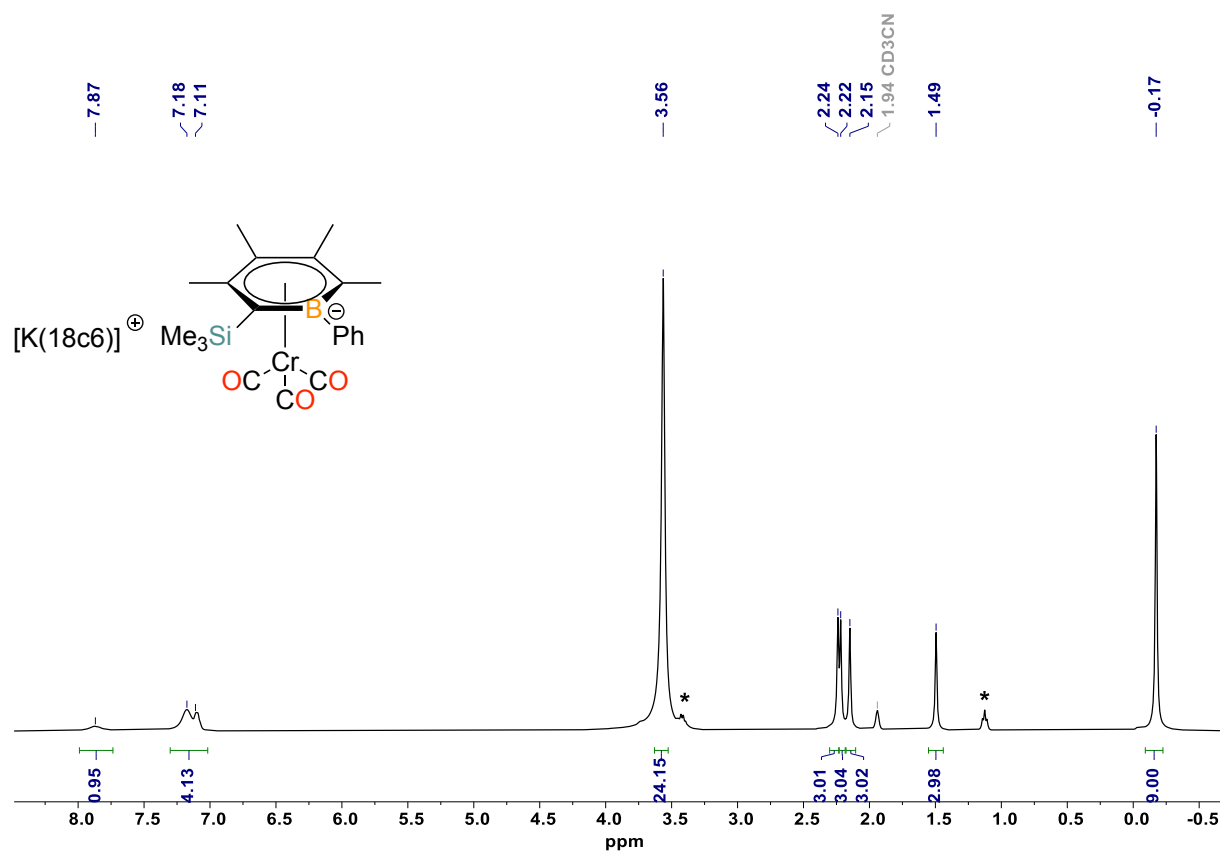


Figure S-2: Expansion of  $^1\text{H}$  NMR spectrum of **1Cr** in  $\text{CD}_3\text{CN}$  (\*residual diethyl ether).

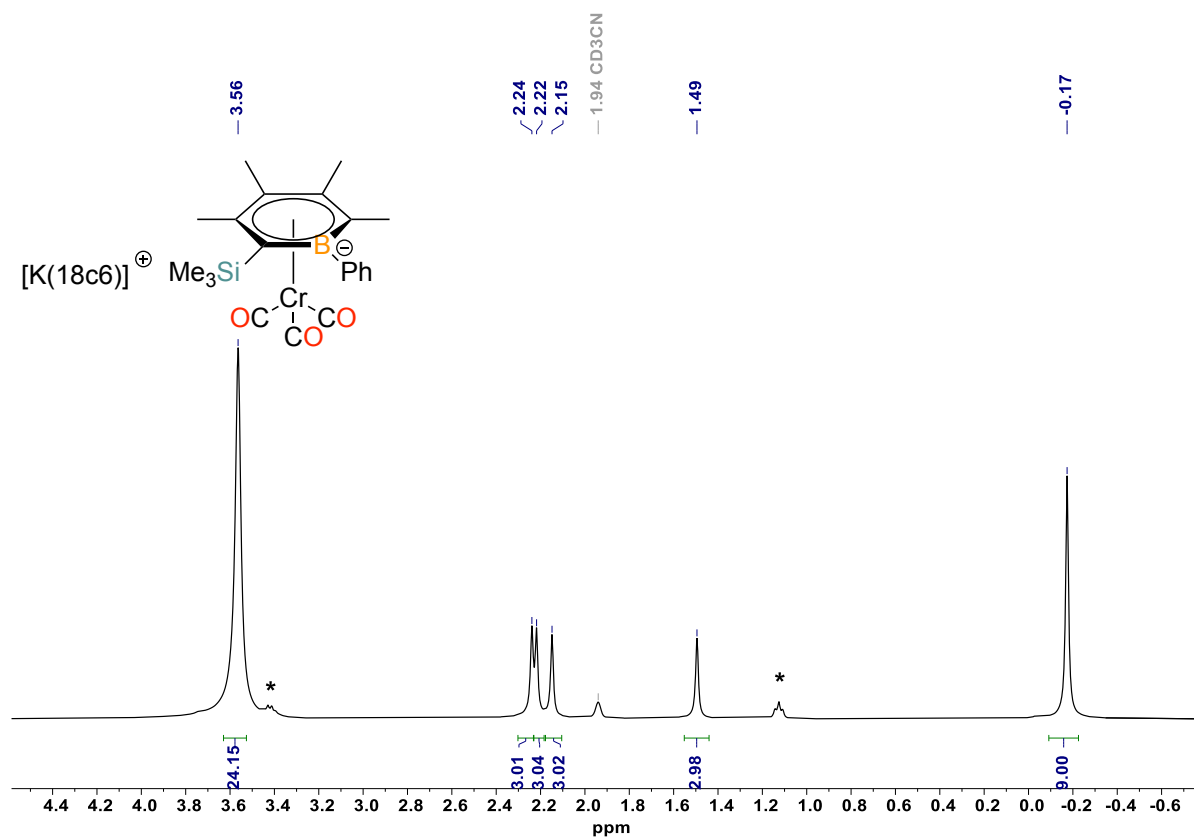


Figure S-3:  $^1\text{H}$  Variable Temperature-NMR spectra of **1Cr** in  $\text{C}_6\text{D}_6$  (\*residual diethyl ether).

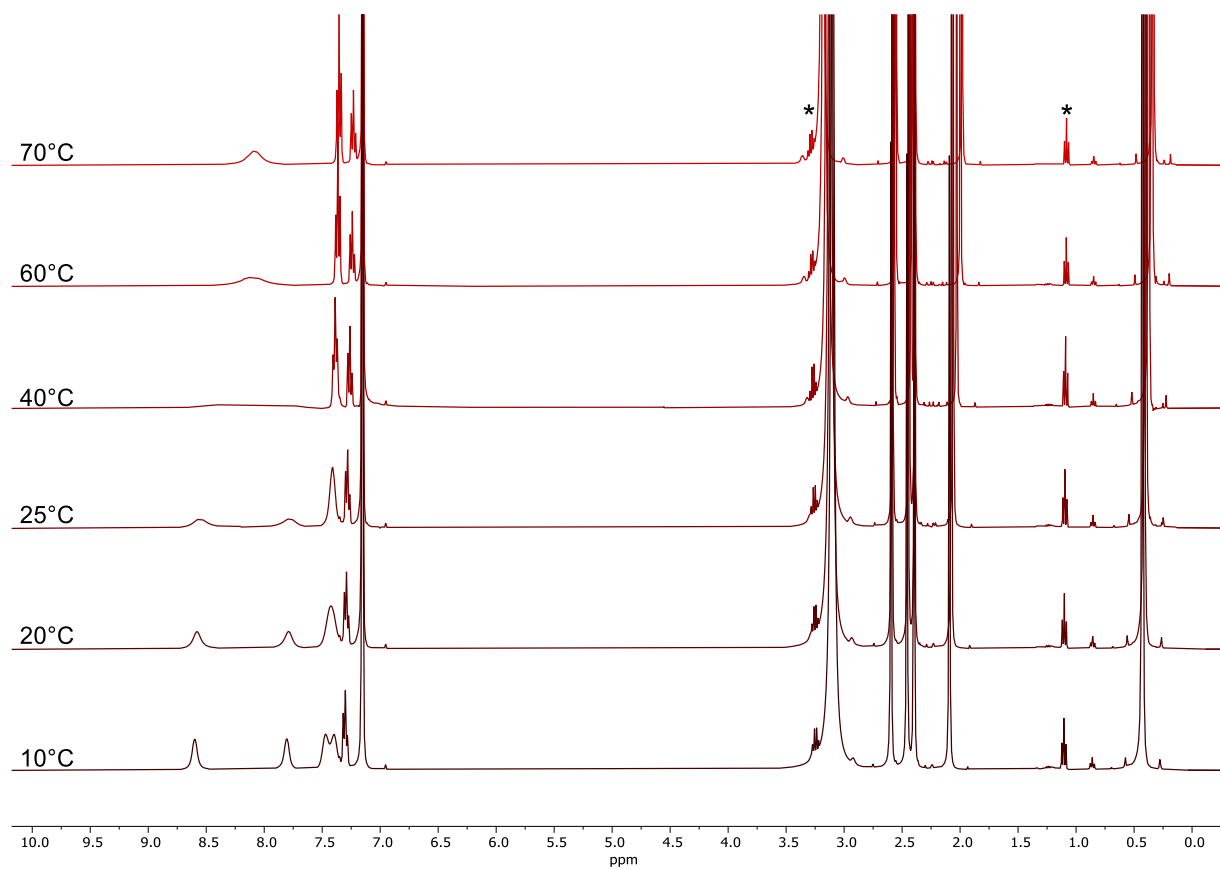


Figure S-4:  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1Cr** in  $\text{CD}_3\text{CN}$  ( $^*\text{CD}_3\text{CN}$ ).

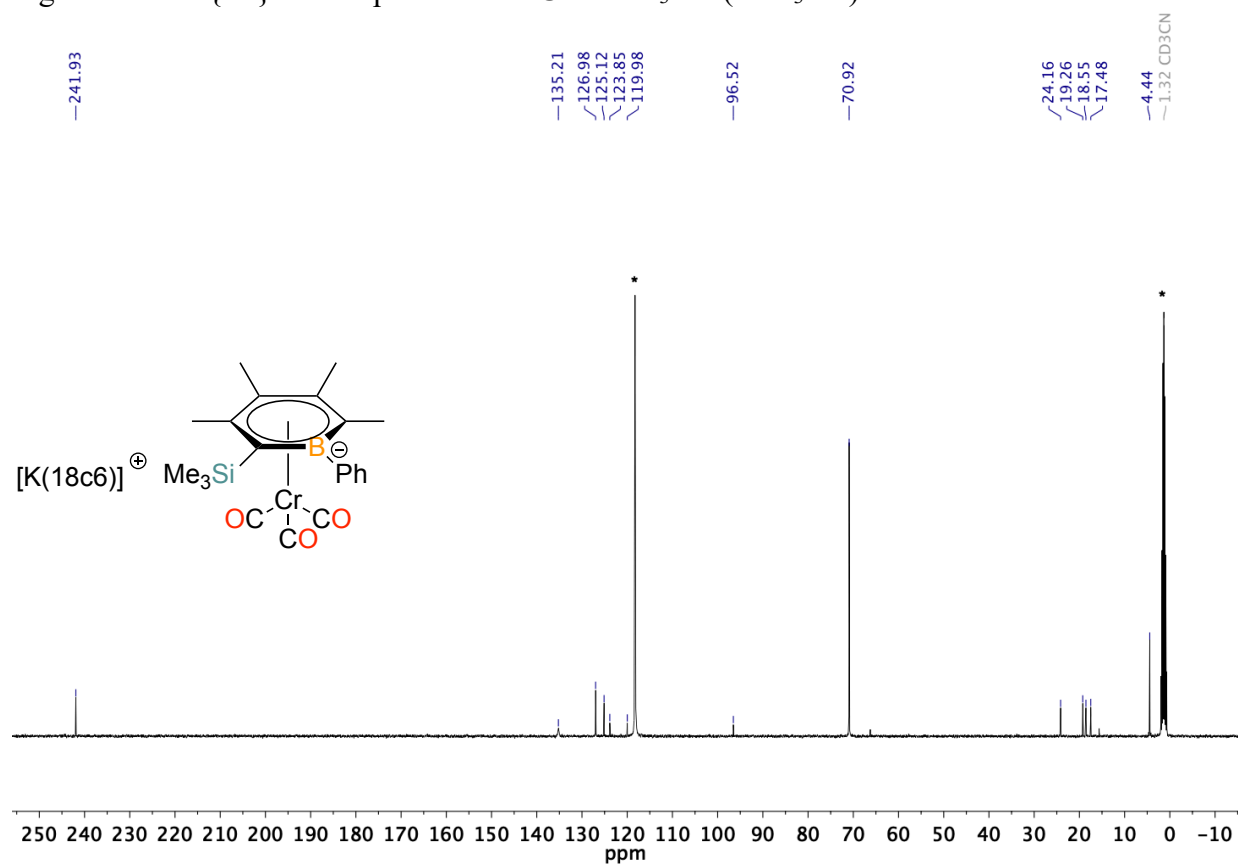


Figure S-5: Expansion of  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1Cr** in  $\text{CD}_3\text{CN}$  ( $^*\text{CD}_3\text{CN}$ ).

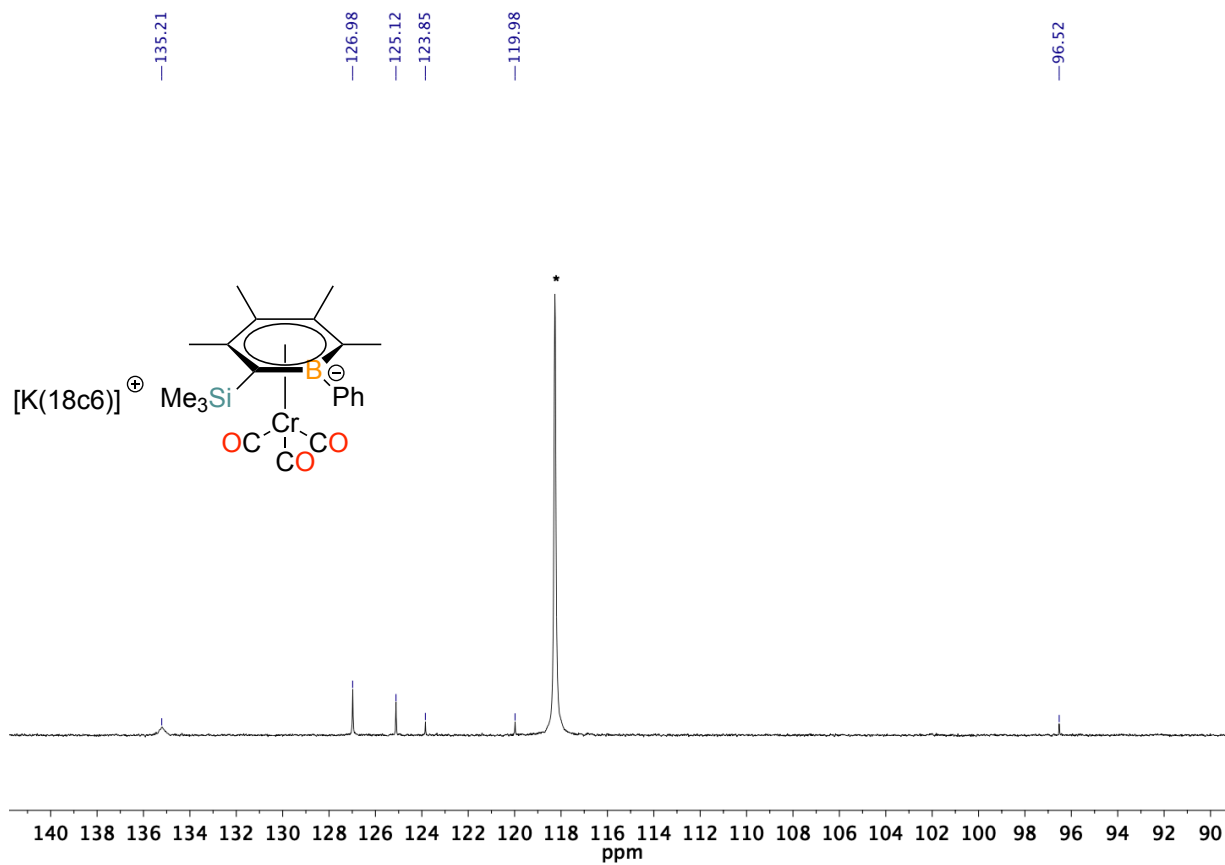


Figure S-6: Expansion of  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1Cr** in  $\text{CD}_3\text{CN}$  (\*diethyl ether).

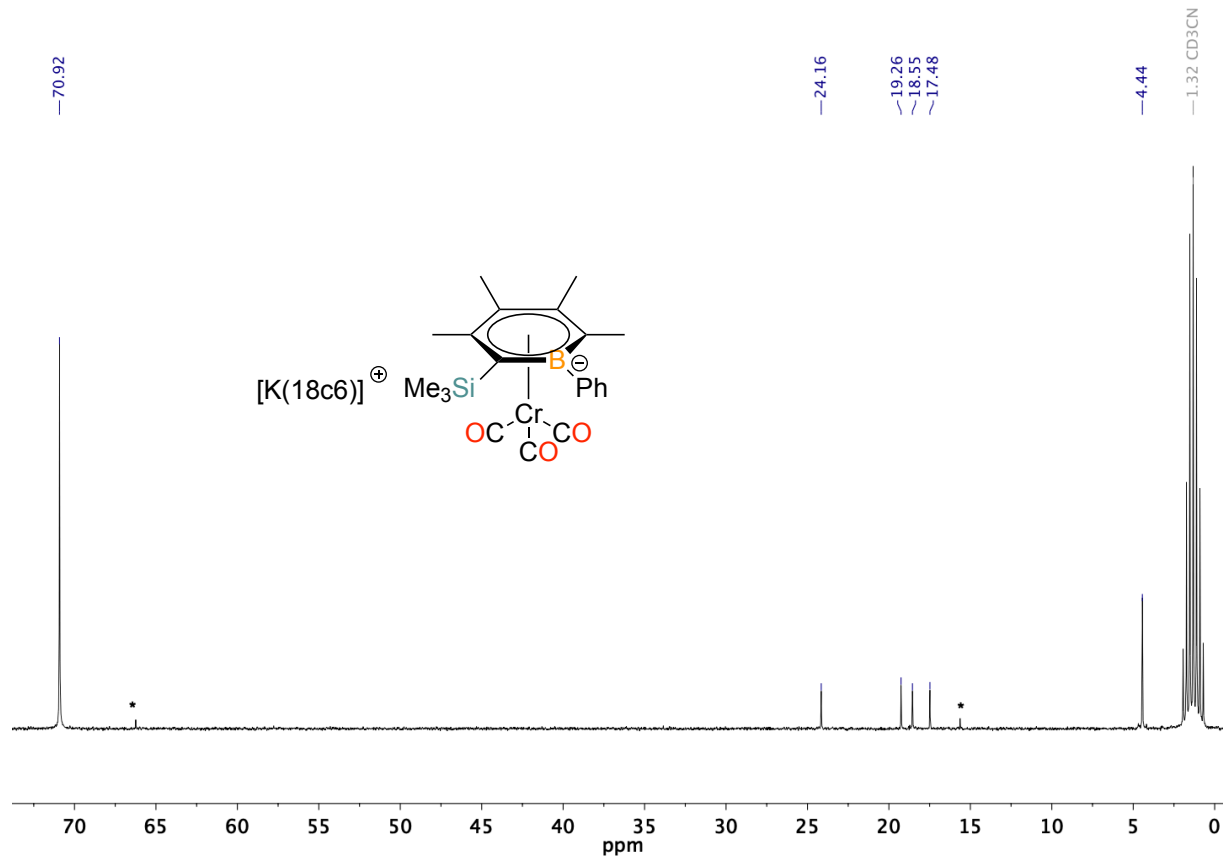




Figure S-7:  $^{11}\text{B}$  NMR spectrum of **1Cr** in  $\text{CD}_3\text{CN}$ .

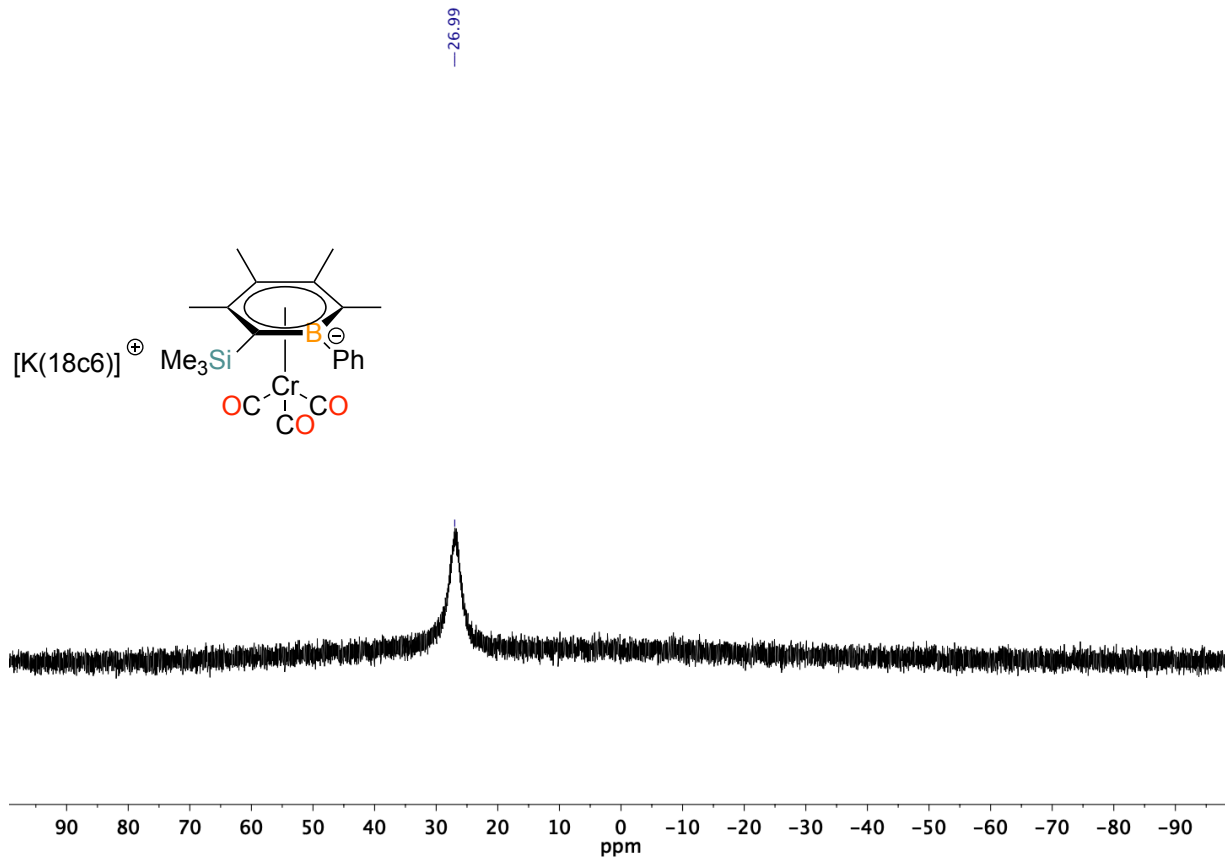


Figure S-8: FT-IR spectrum of **1Cr**.

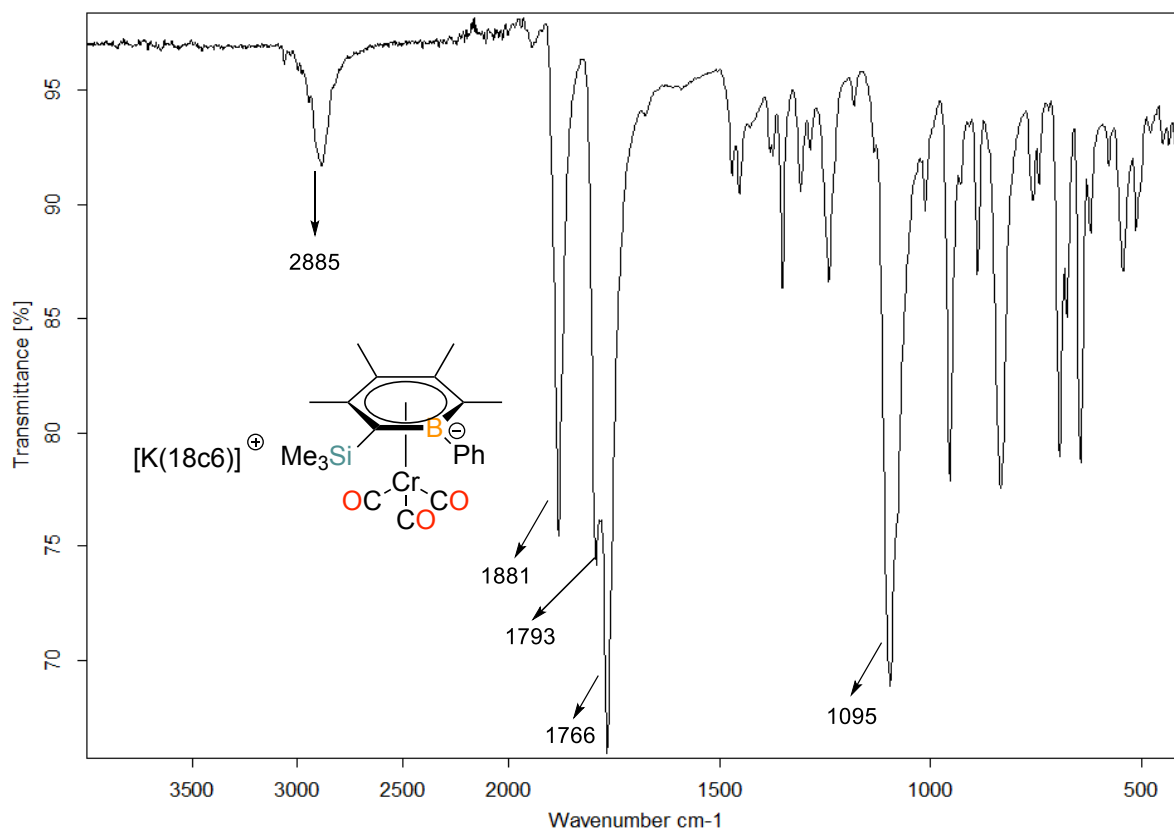


Figure S-9:  $^1\text{H}$  NMR spectrum of **1Mo** in  $\text{CD}_3\text{CN}$  (\*diethyl ether)

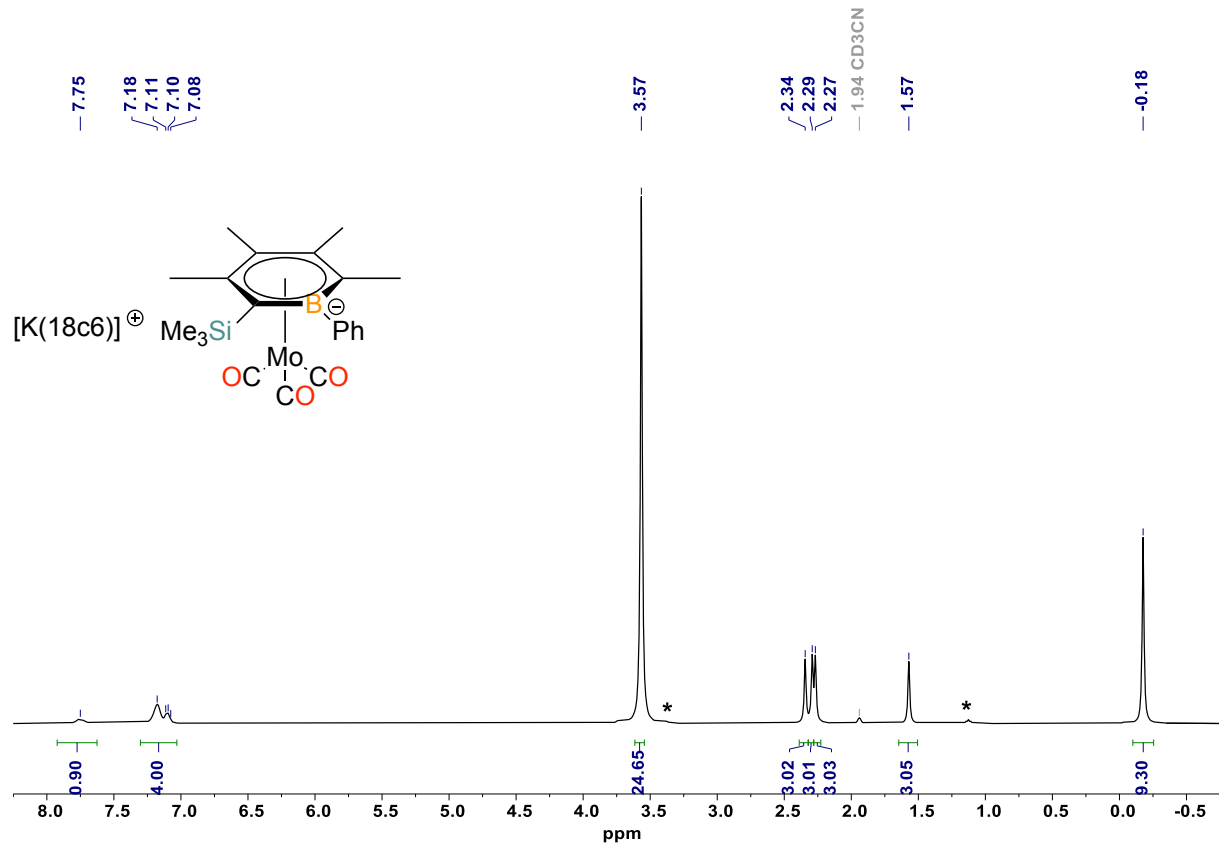


Figure S-10:  $^1\text{H}$  VT-NMR spectra of **1Mo** in  $\text{C}_6\text{D}_6$  (\*diethyl ether and hexanes)

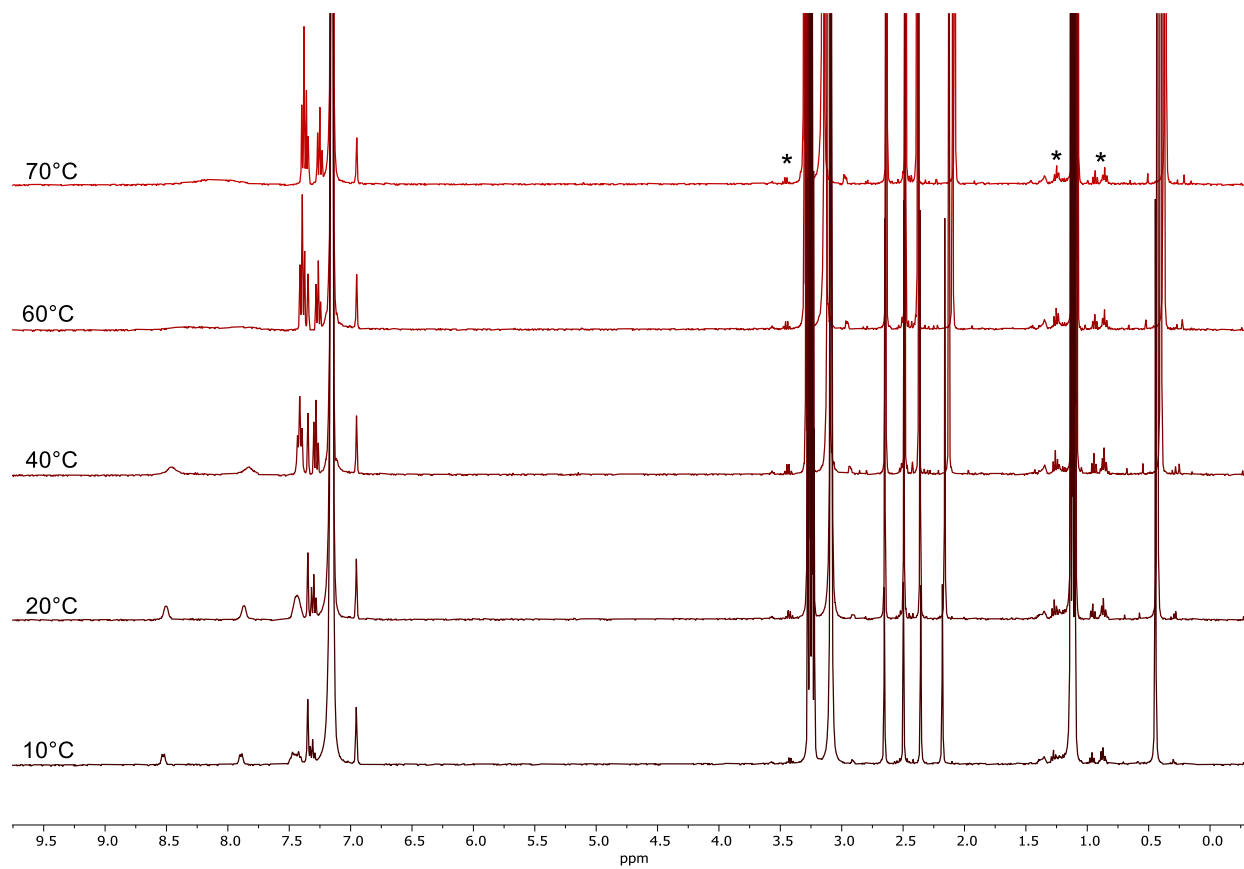


Figure S-11: Expansion of  $^1\text{H}$  NMR spectrum of **1Mo** in  $\text{CD}_3\text{CN}$  (\*diethyl ether).

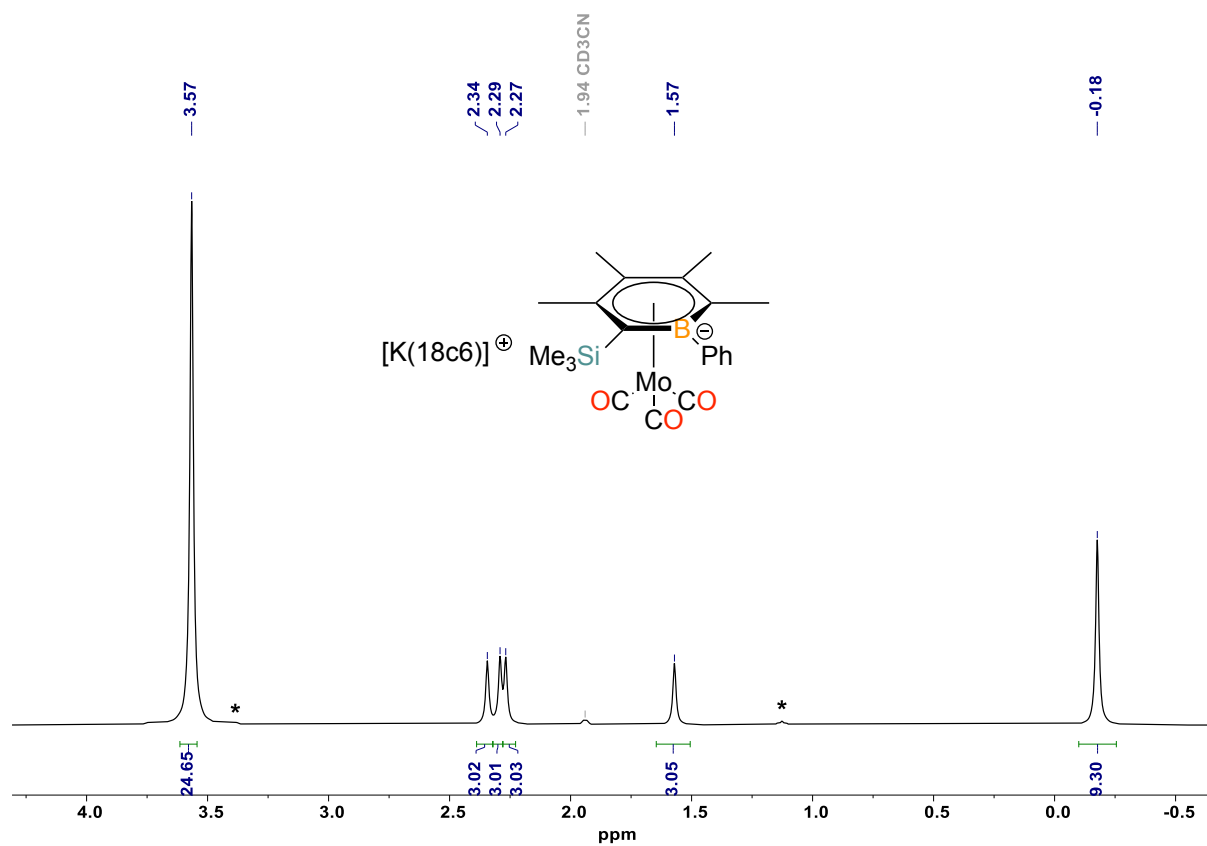


Figure S-12:  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1Mo** in  $\text{CD}_3\text{CN}$  ( $^*\text{CD}_3\text{CN}$ ).

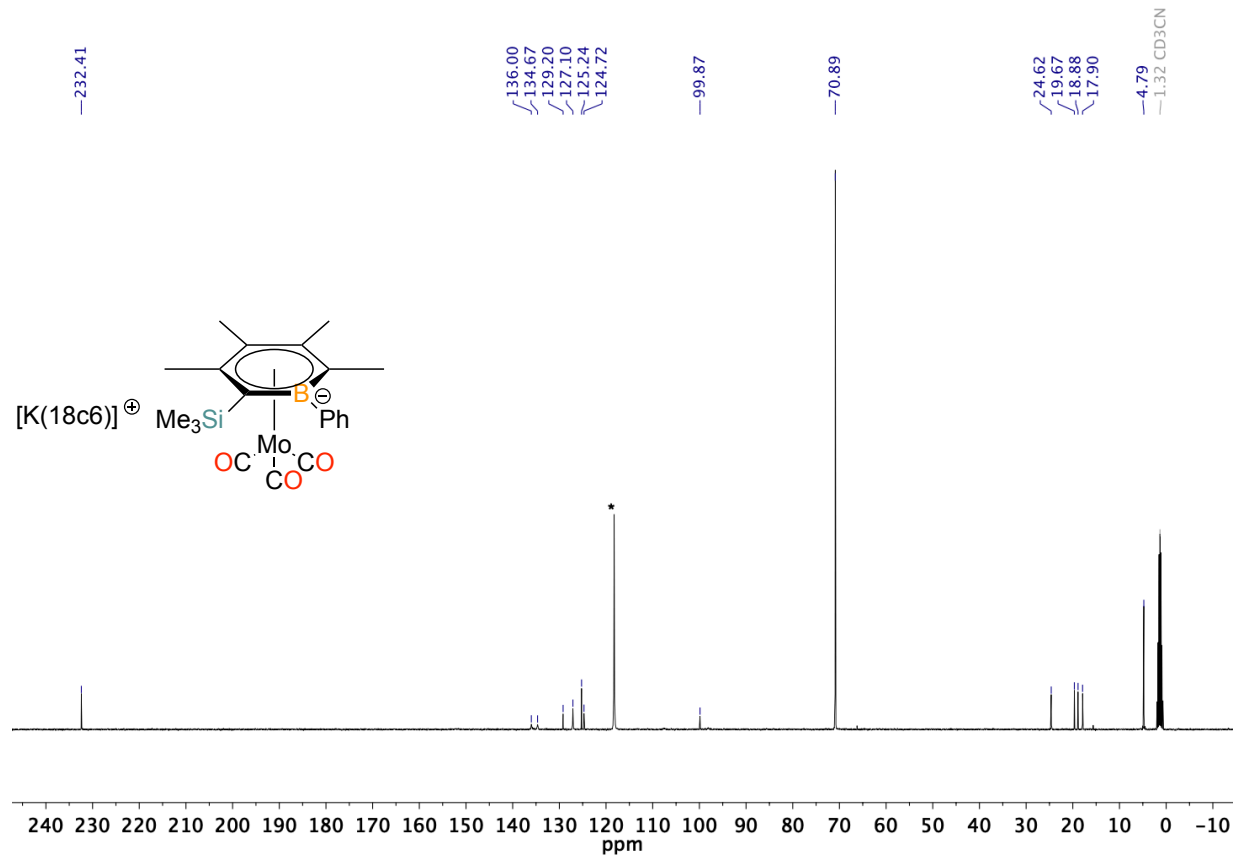


Figure S-13: Expansion of  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1Mo** in  $\text{CD}_3\text{CN}$  ( $^*\text{CD}_3\text{CN}$ ).

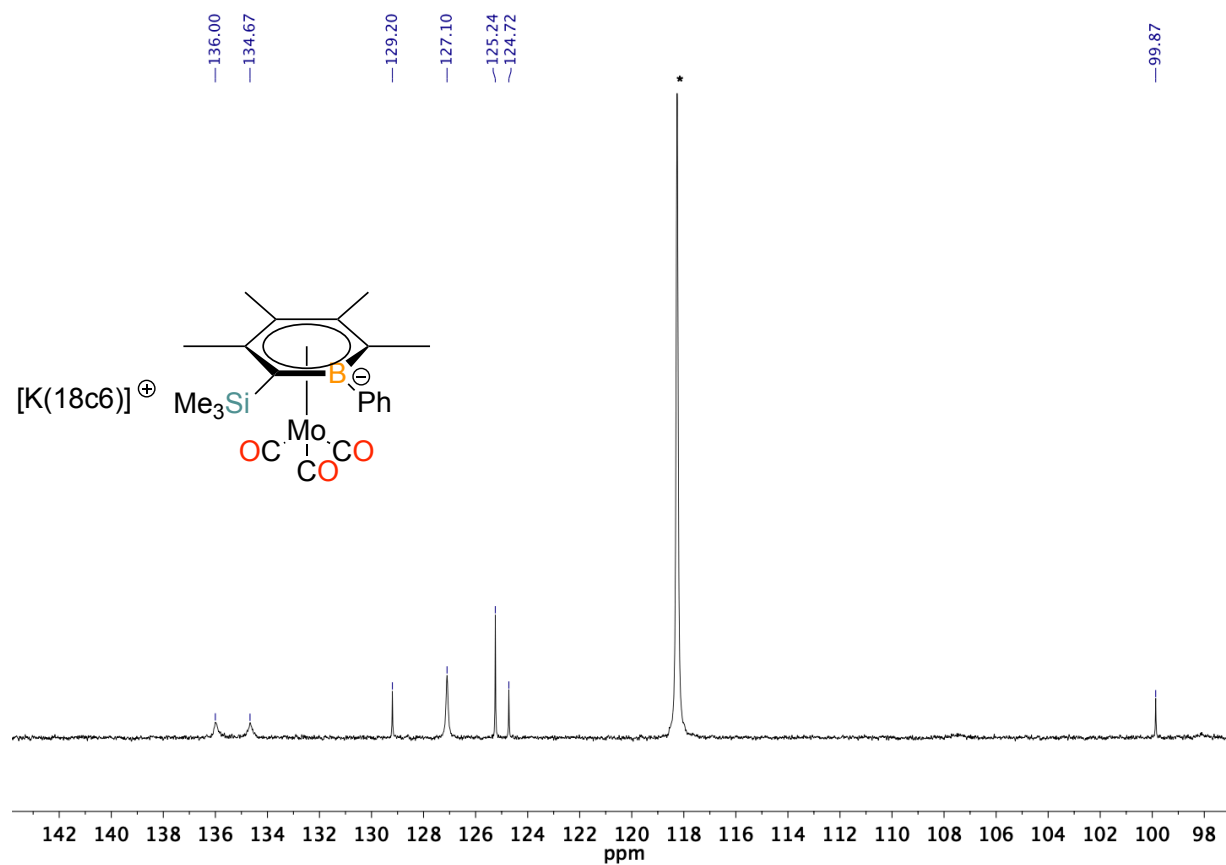


Figure S-14: Expansion of  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1Mo** in  $\text{CD}_3\text{CN}$

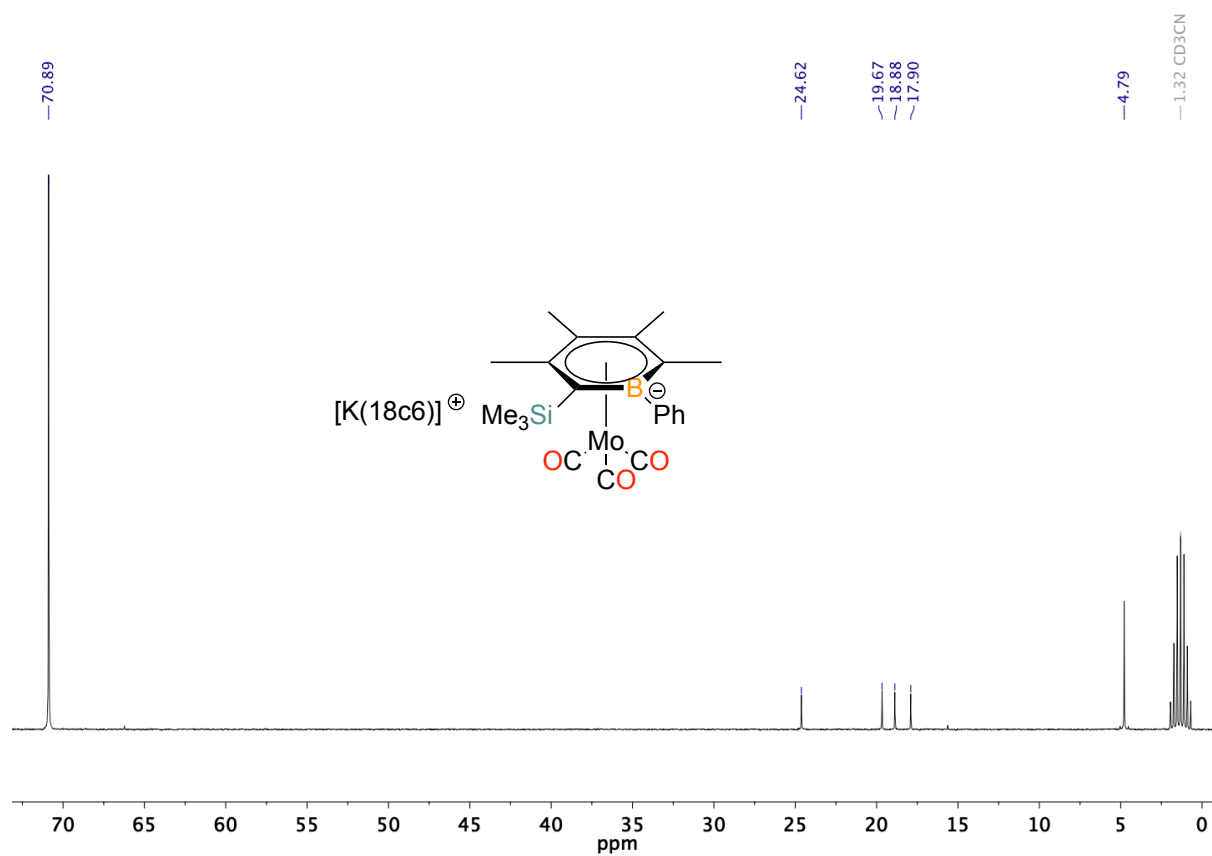




Figure S-15:  $^{11}\text{B}$  NMR spectrum of **1Mo** in  $\text{CD}_3\text{CN}$ .

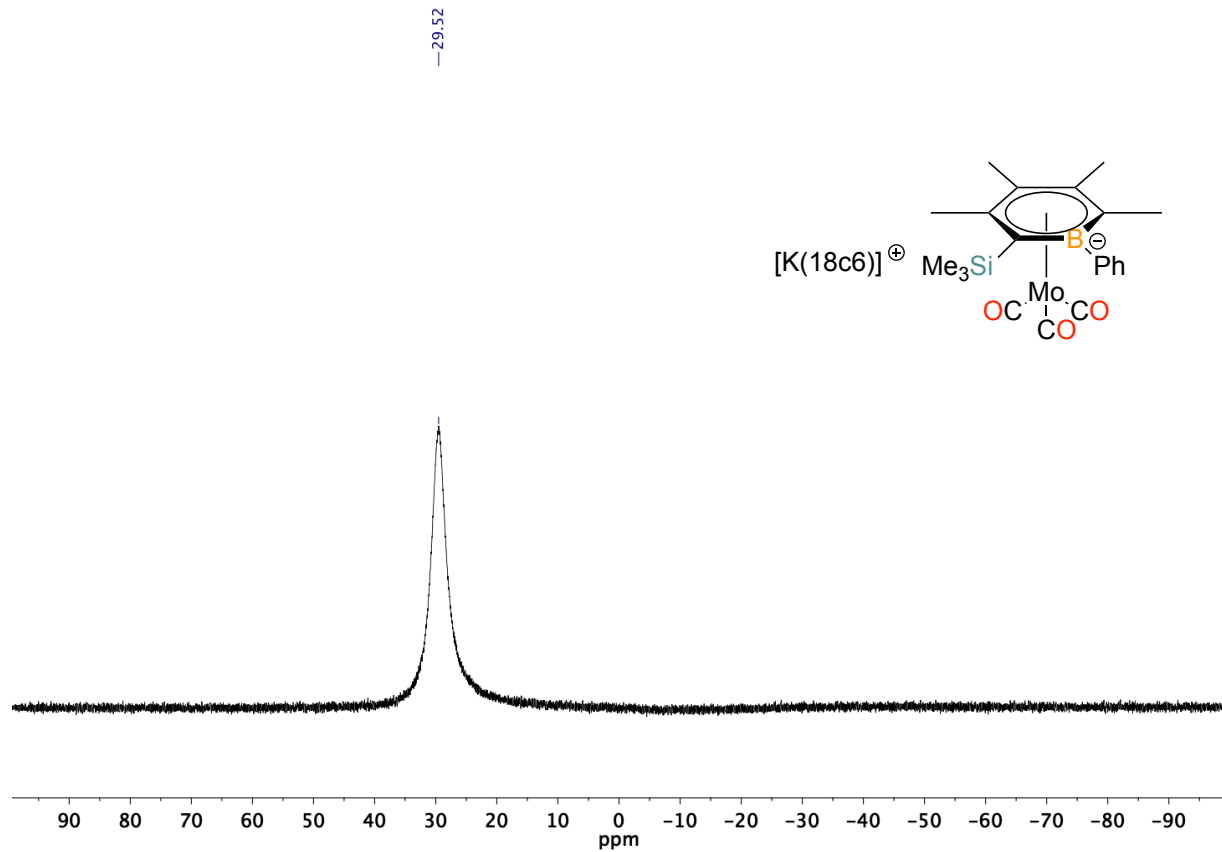


Figure S-16: FT-IR spectrum of **1Mo**.

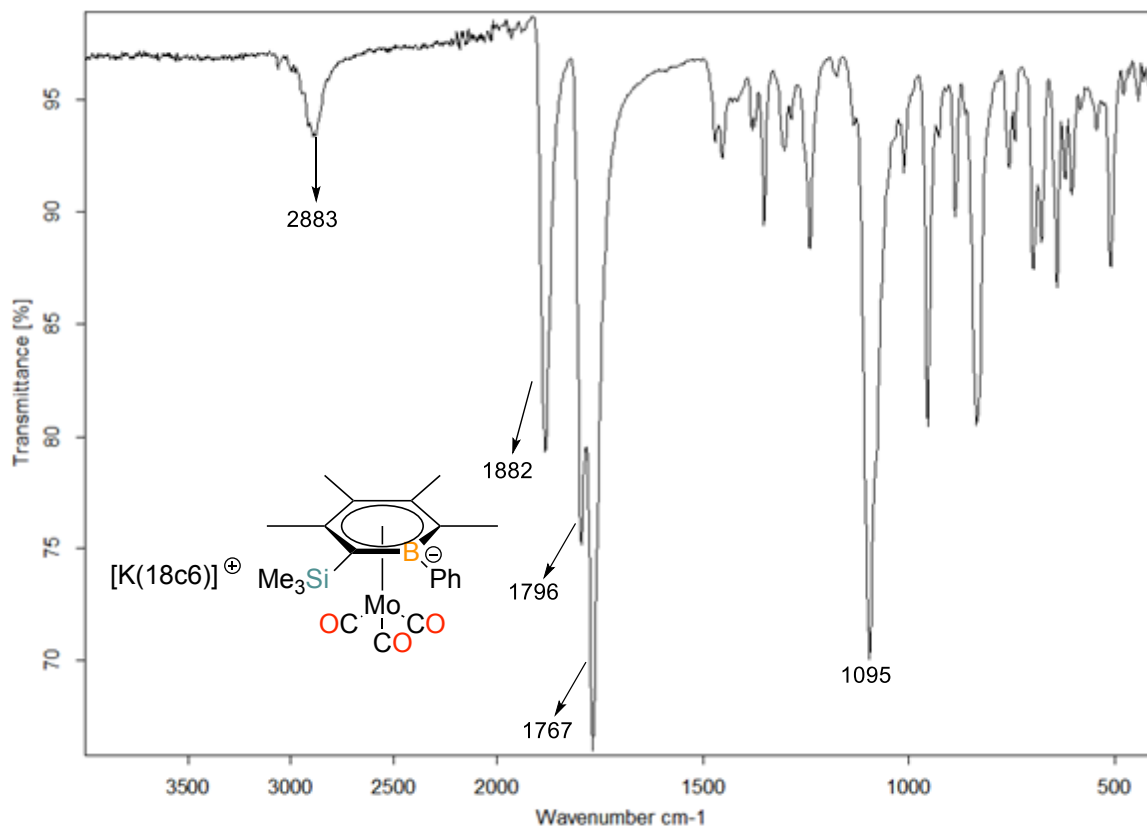


Figure S-17:  $^1\text{H}$  NMR spectrum of **1W** in  $\text{CD}_3\text{CN}$  (\*diethyl ether)

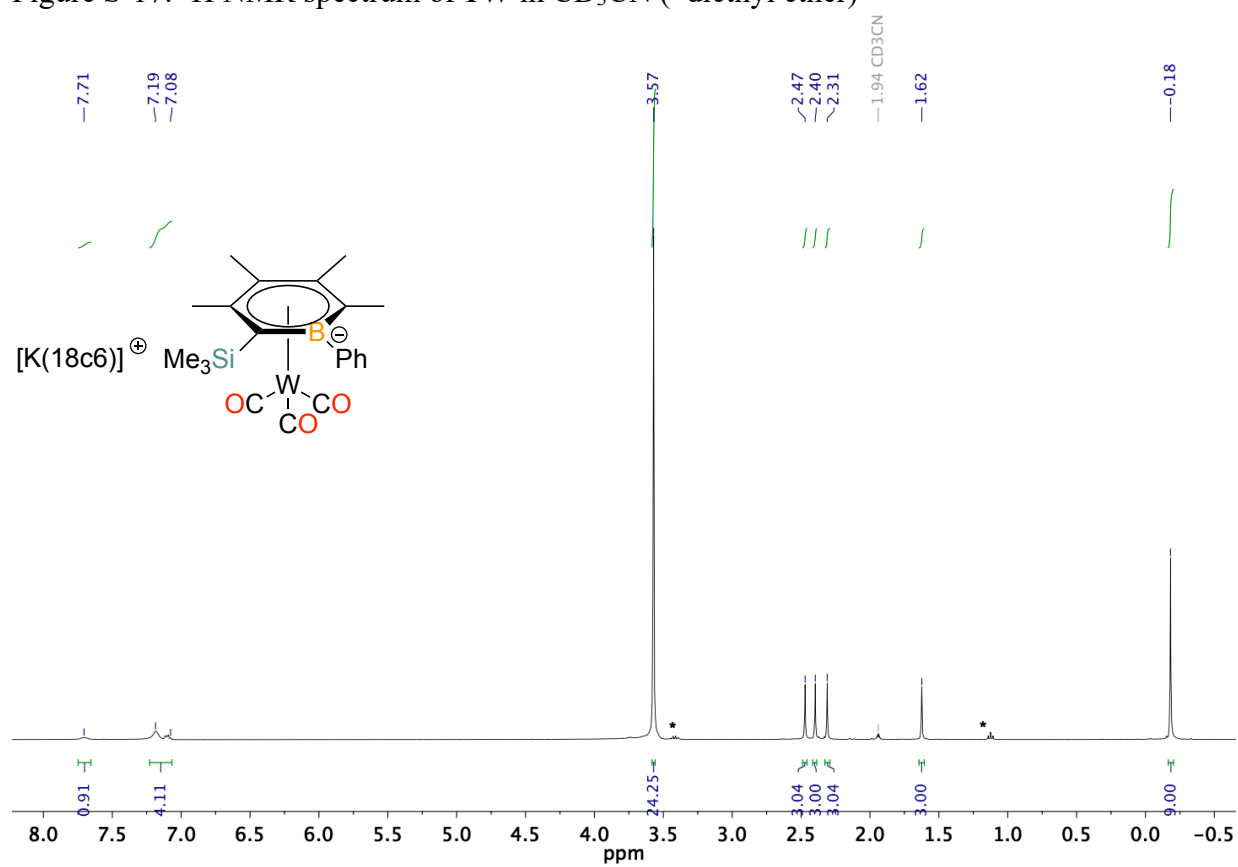


Figure S-18:  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1W** in  $\text{CD}_3\text{CN}$  ( $^*\text{CD}_3\text{CN}$ ).

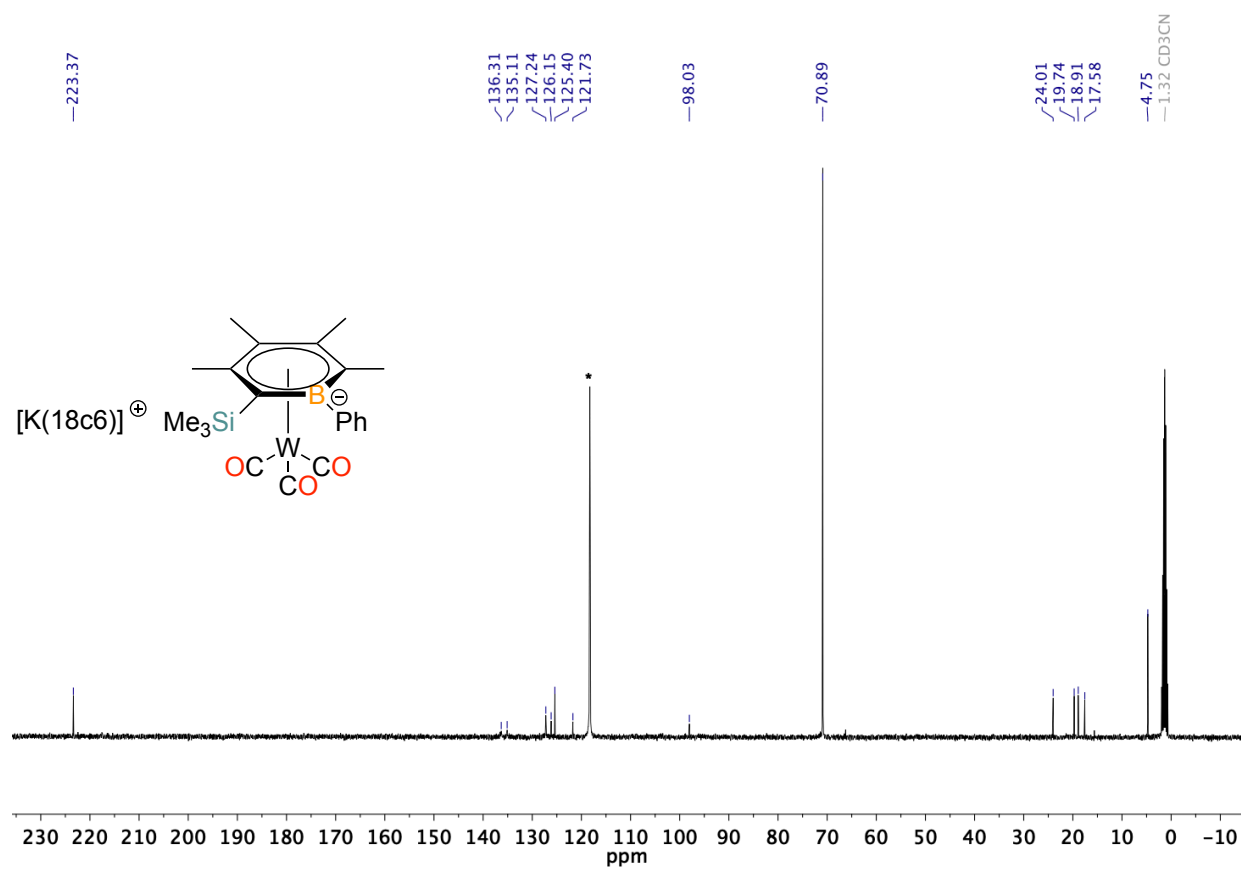


Figure S-19: Expansion of  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1W** in  $\text{CD}_3\text{CN}$  ( $^*\text{CD}_3\text{CN}$ ).

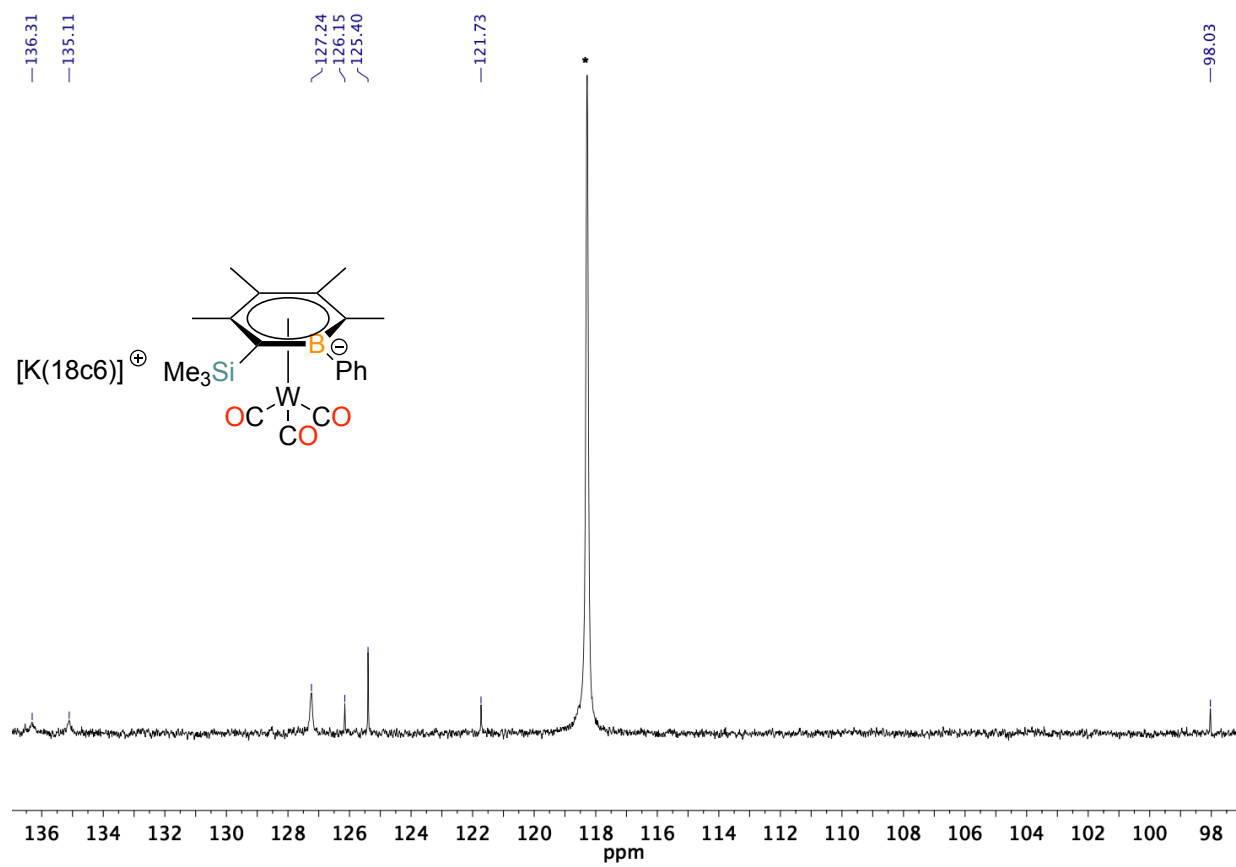


Figure S-20: Expansion of  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1W** in  $\text{CD}_3\text{CN}$  (\*diethyl ether).

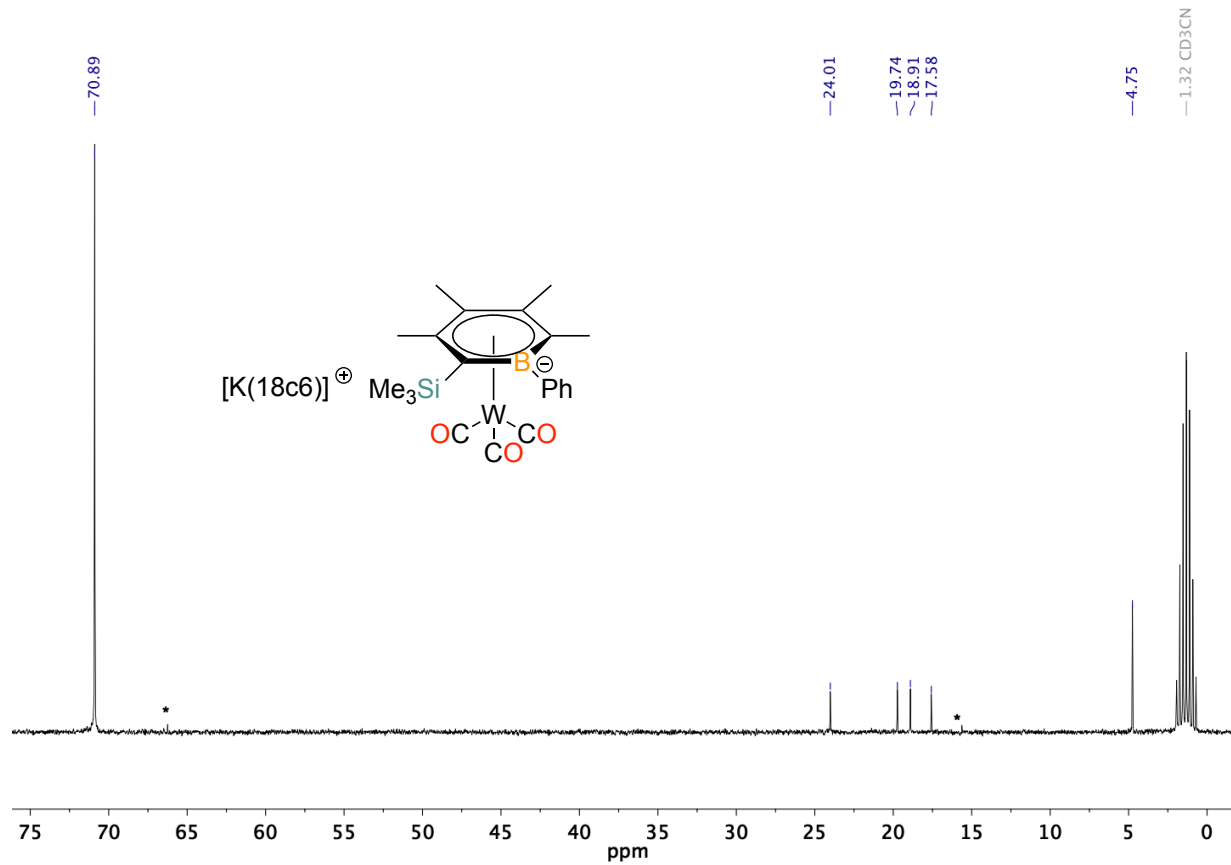


Figure S-21:  $^{11}\text{B}$  NMR spectrum of **1W** in  $\text{CD}_3\text{CN}$ .

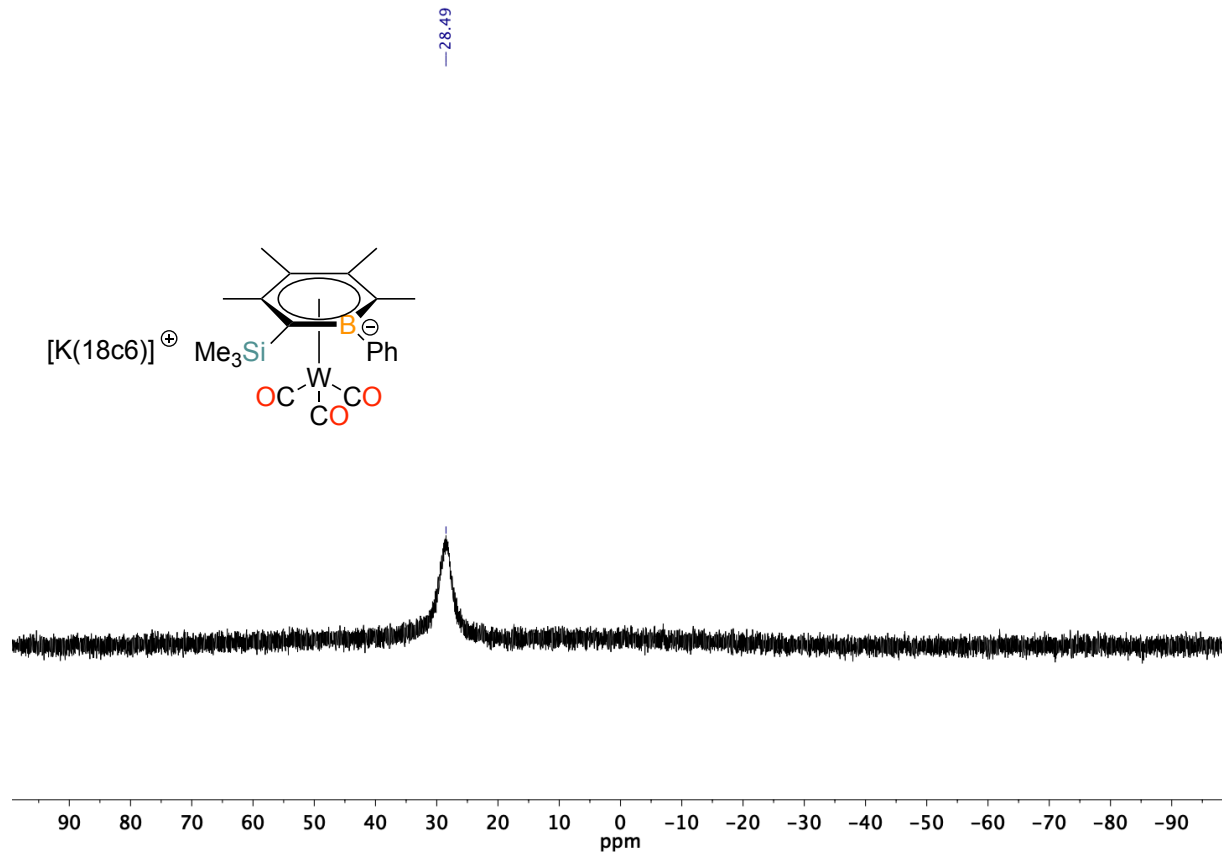


Figure S-22: FT-IR spectrum of **1W**.

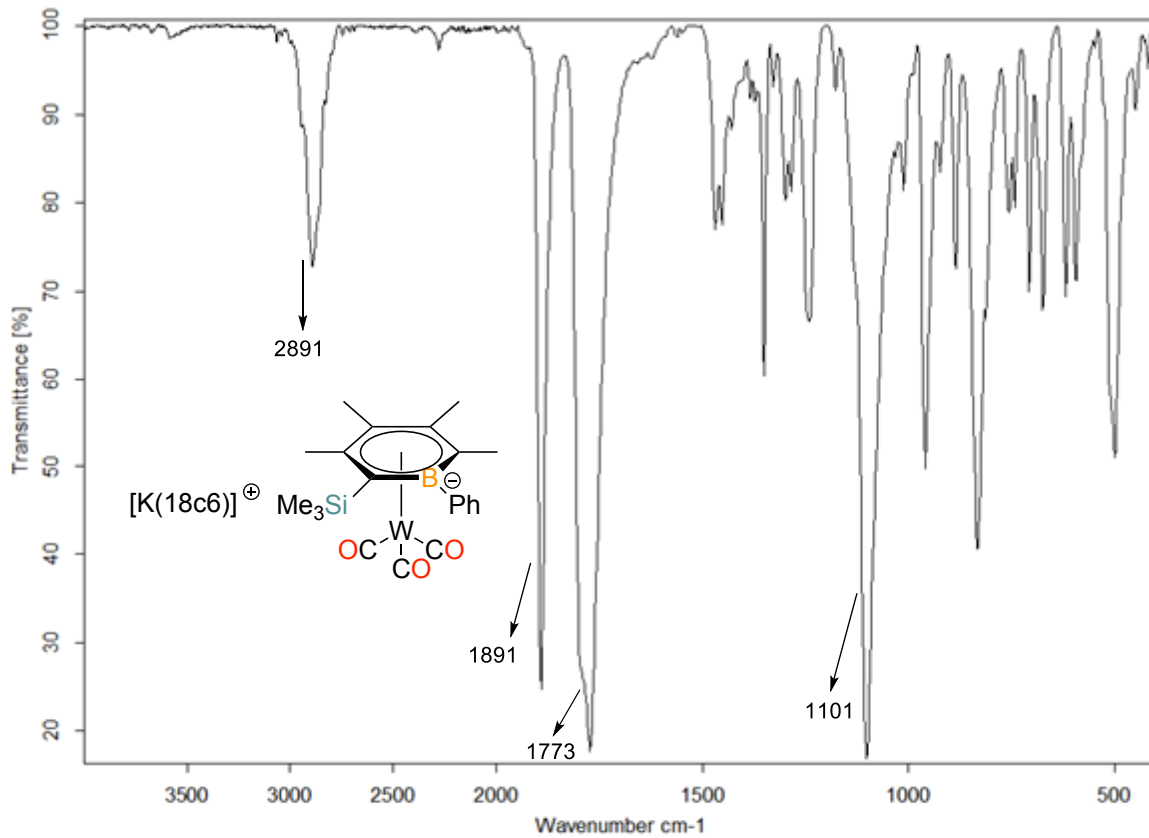




Figure S-23:  $^1\text{H}$  NMR spectrum of **2Mo** in THF- $d_8$  (\*THF- $d_8$ ).

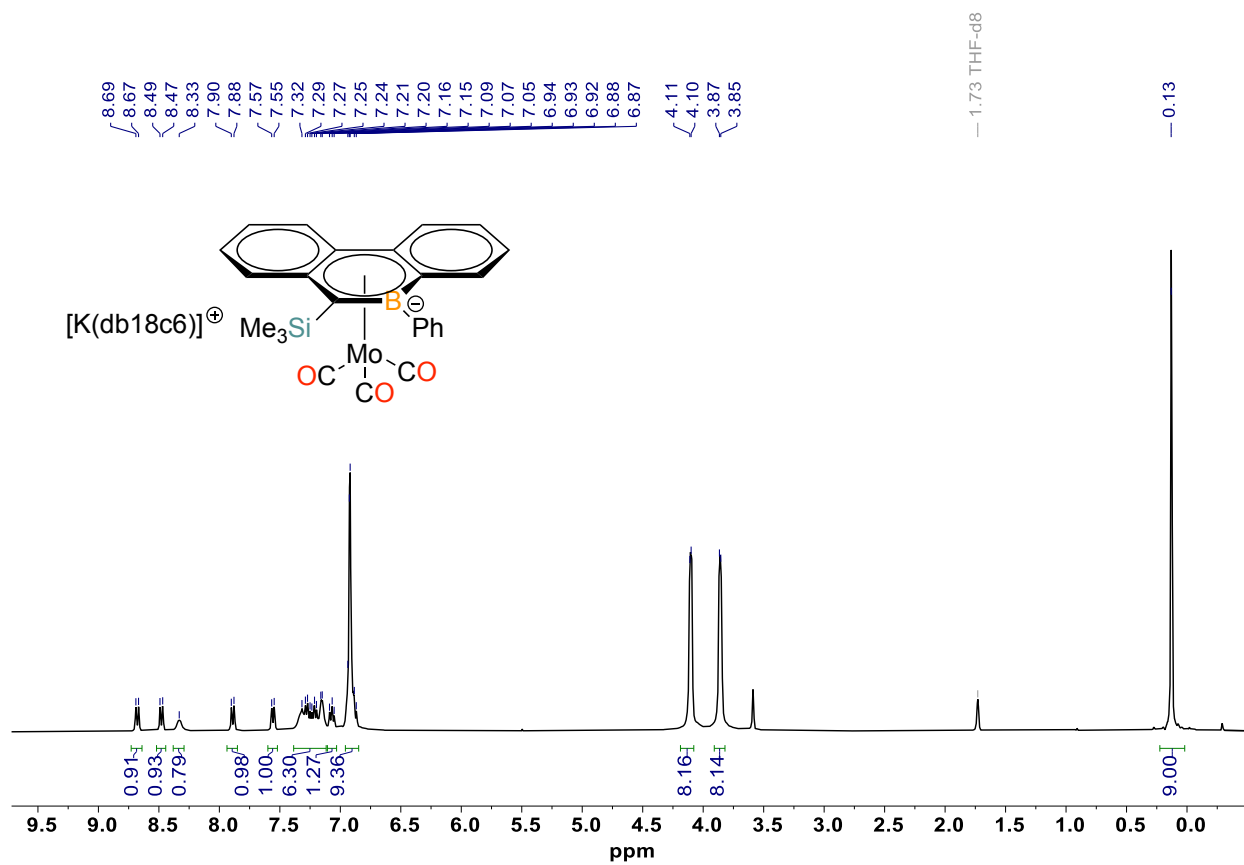


Figure S-24: Expansion of  $^1\text{H}$  NMR spectrum of **2Mo** in  $\text{THF-d}_8$

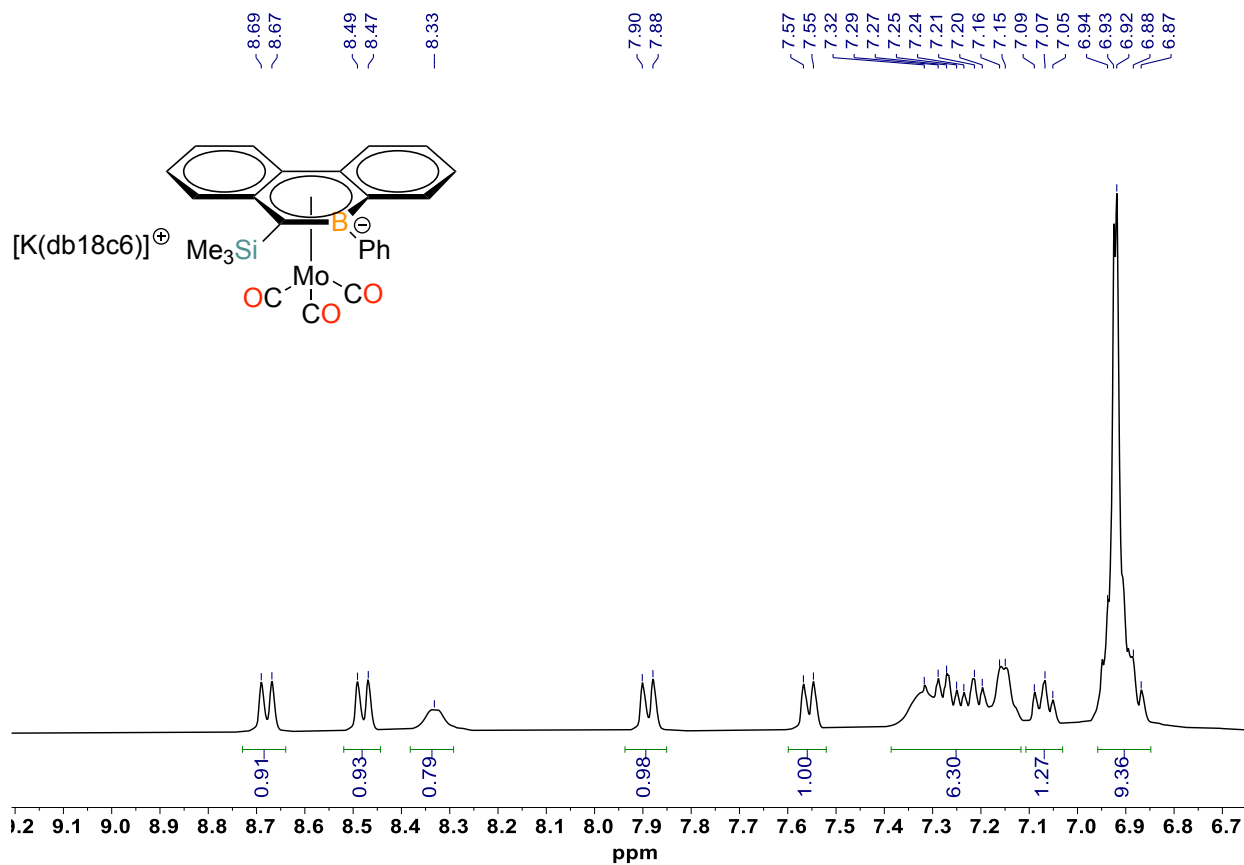


Figure S-25: Expansion of  $^1\text{H}$  NMR spectrum of **2Mo** in THF- $d_8$  (\*THF- $d_8$ ).

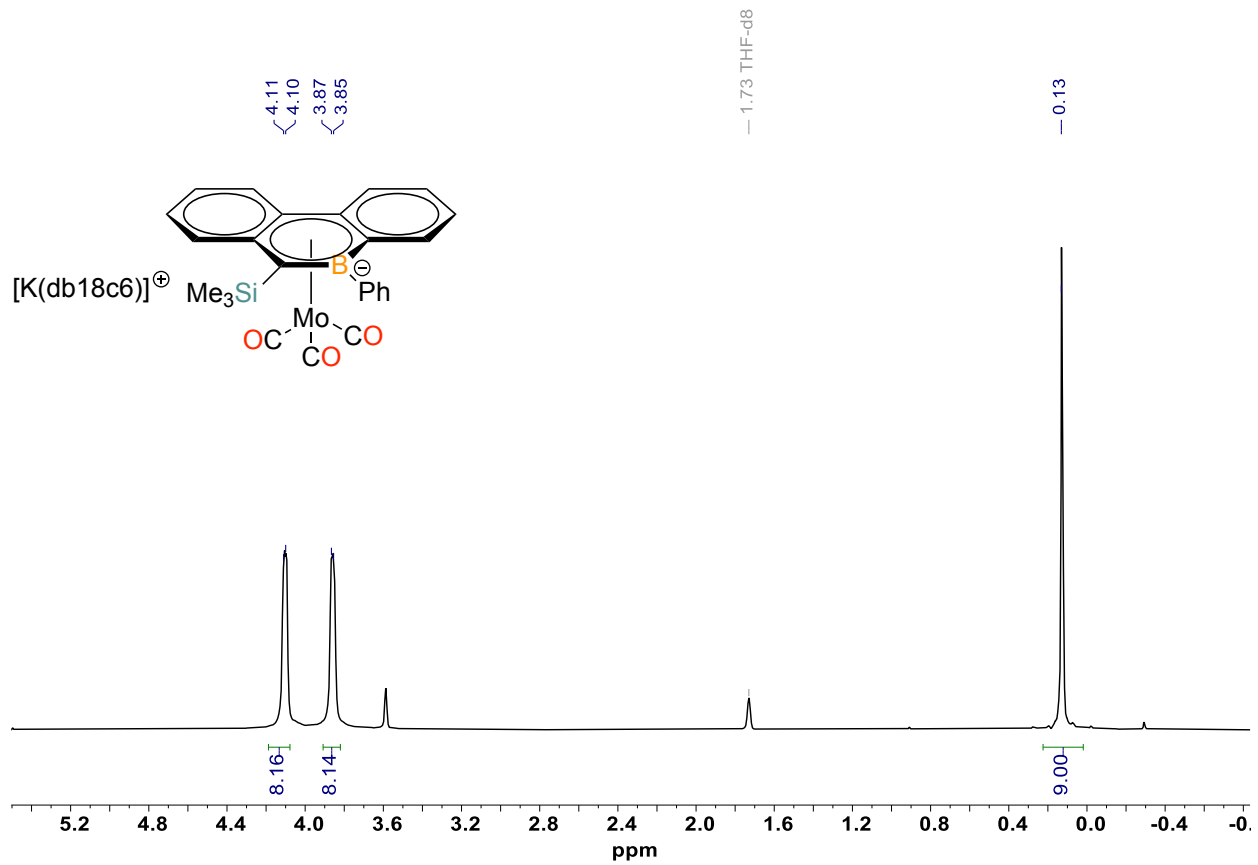


Figure S-26:  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2Mo** in THF- $\text{d}_8$  (\*THF- $\text{d}_8$ ).

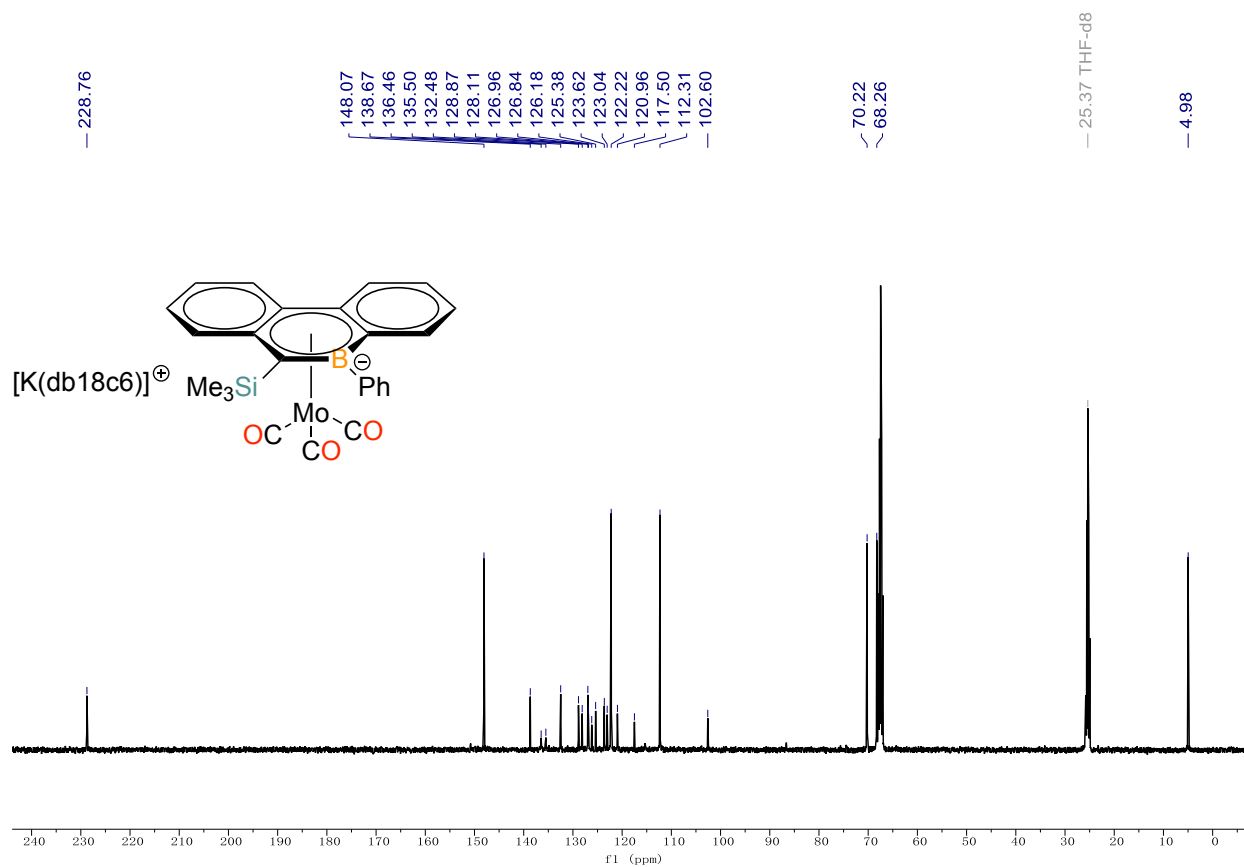


Figure S-27: Expansion of  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2Mo** in THF- $d_8$ .

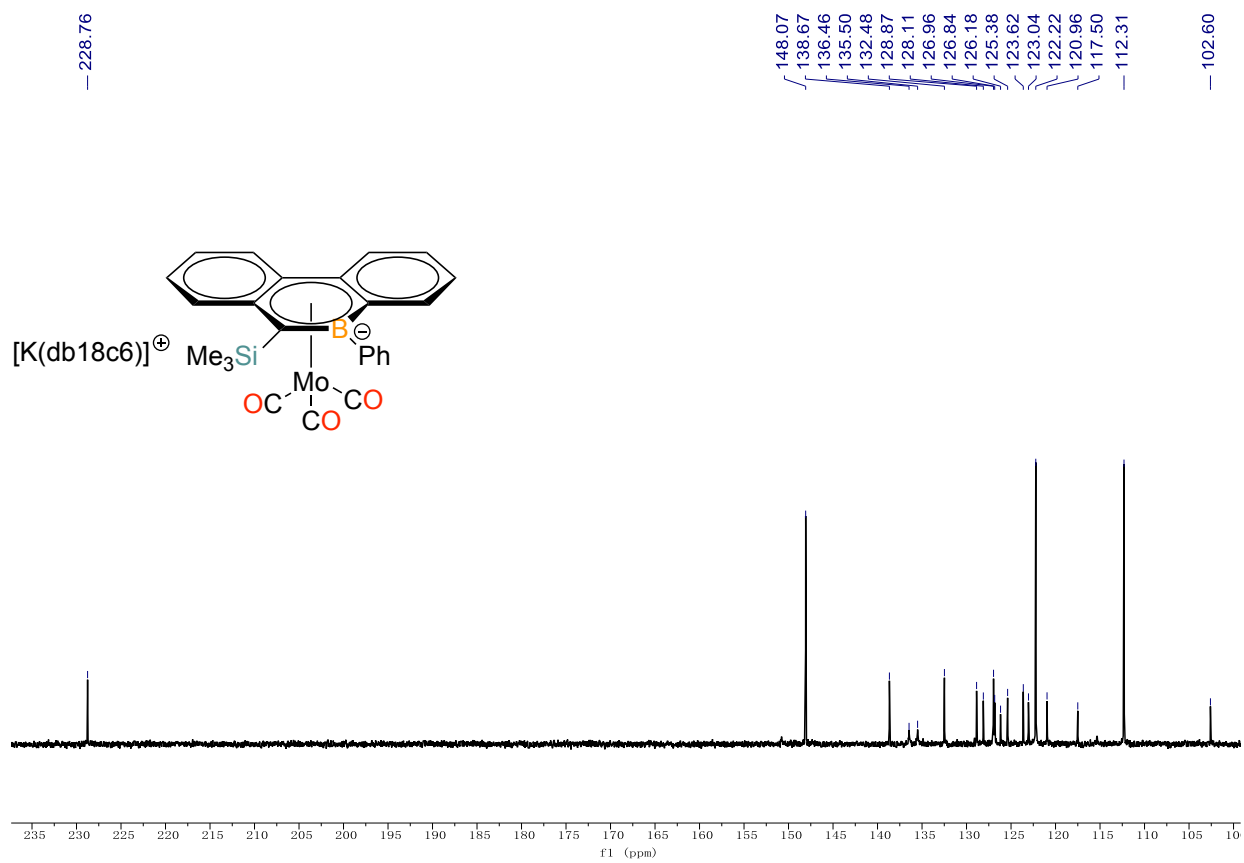


Figure S-28: Expansion of  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2Mo** in THF- $d_8$  (\*THF- $d_8$ ).

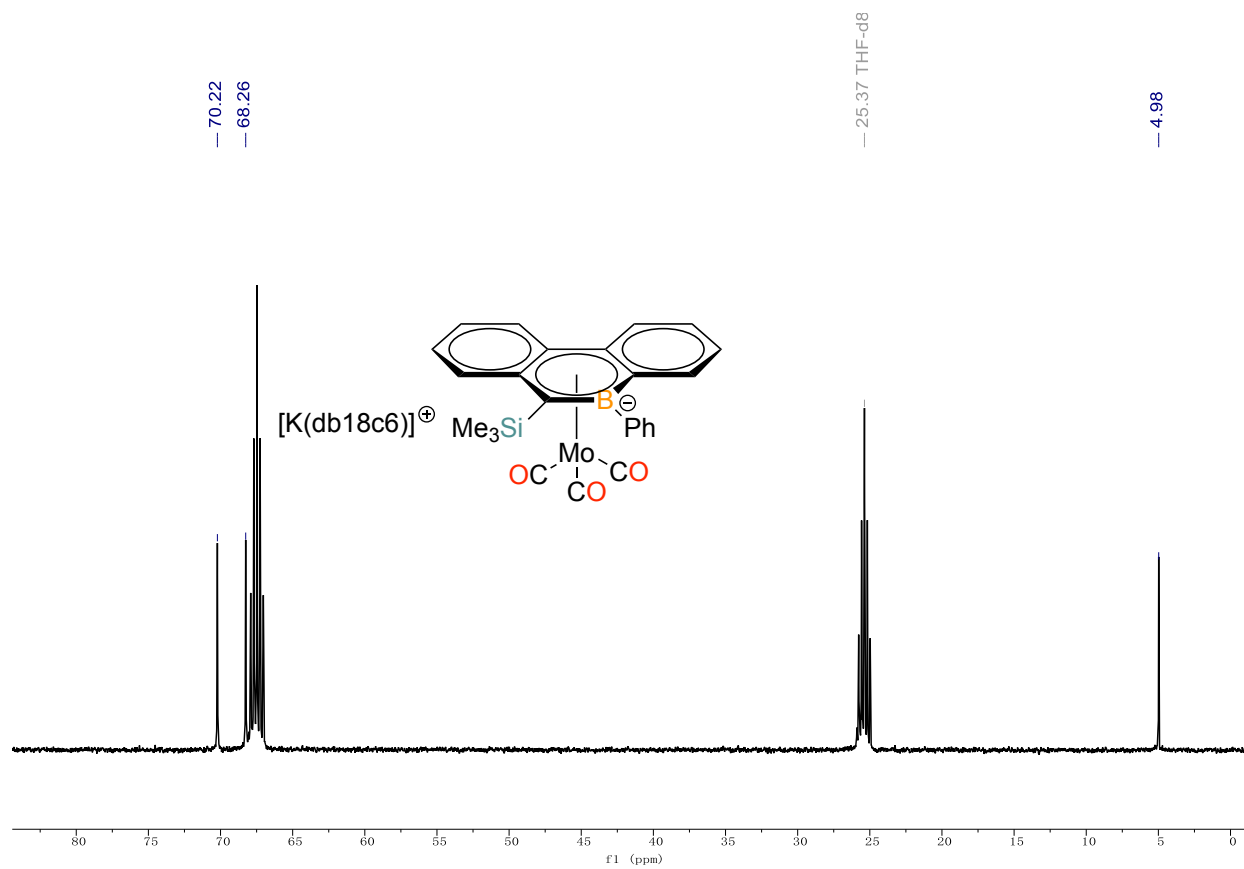


Figure S-29:  $^{11}\text{B}$  NMR spectrum of **2Mo** in THF- $d_8$ .

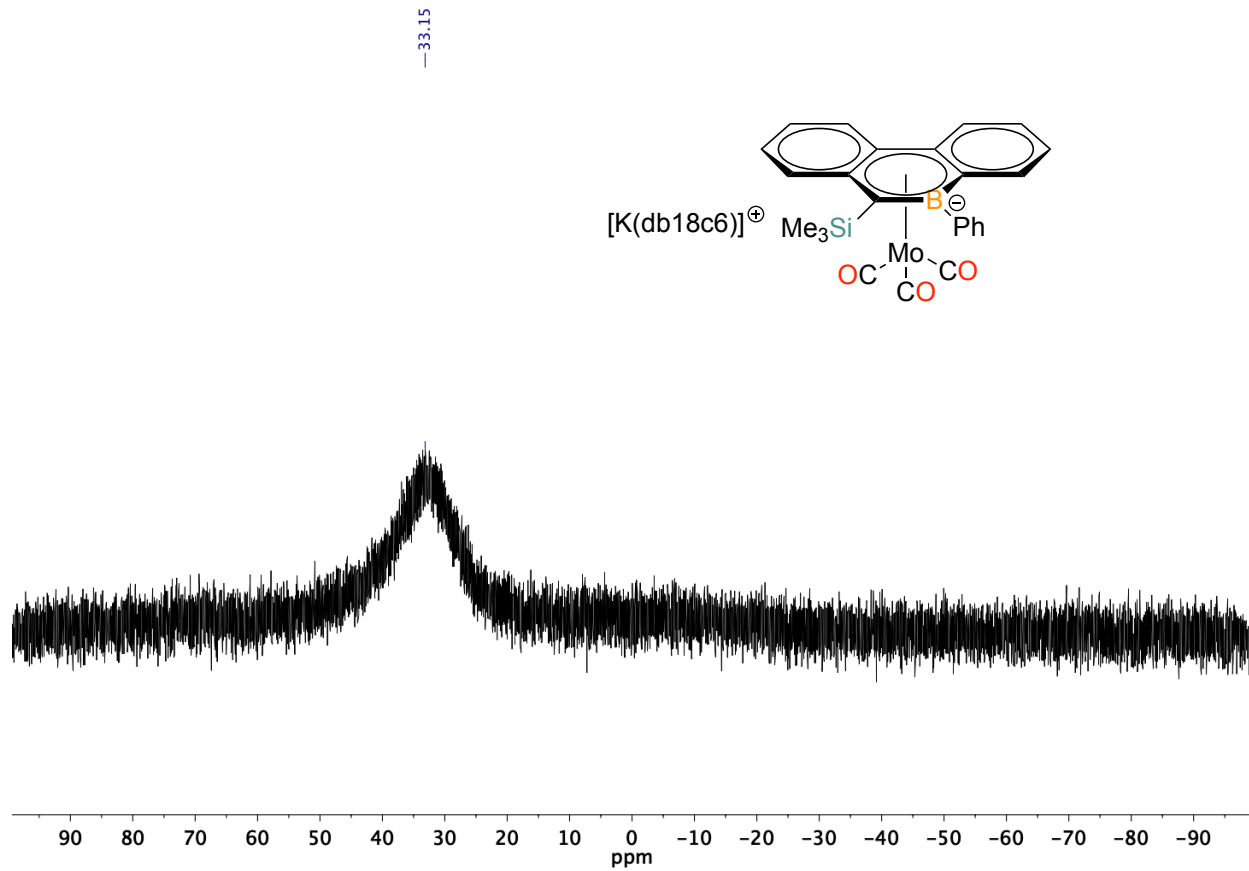


Figure S-30: FT-IR spectrum of **2Mo**.

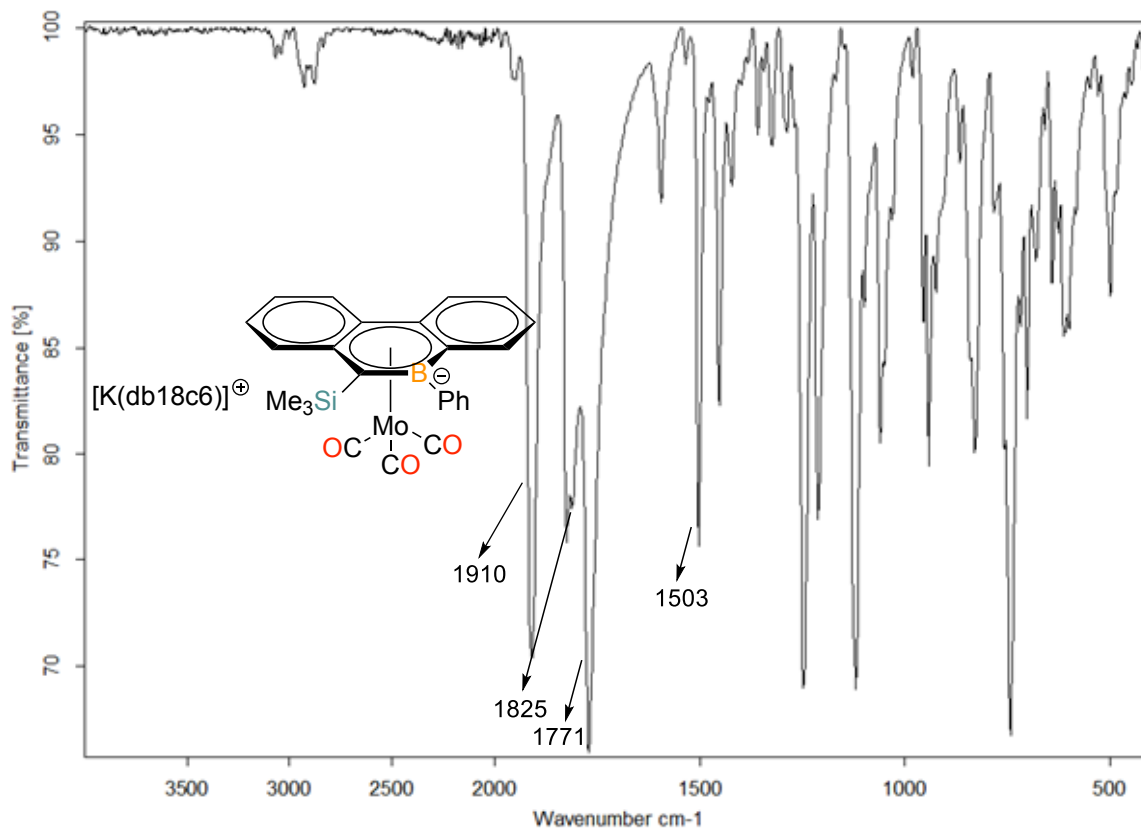




Figure S-31:  $^1\text{H}$  NMR spectrum of **2W** in THF- $d_8$  (\*THF- $d_8$ ).

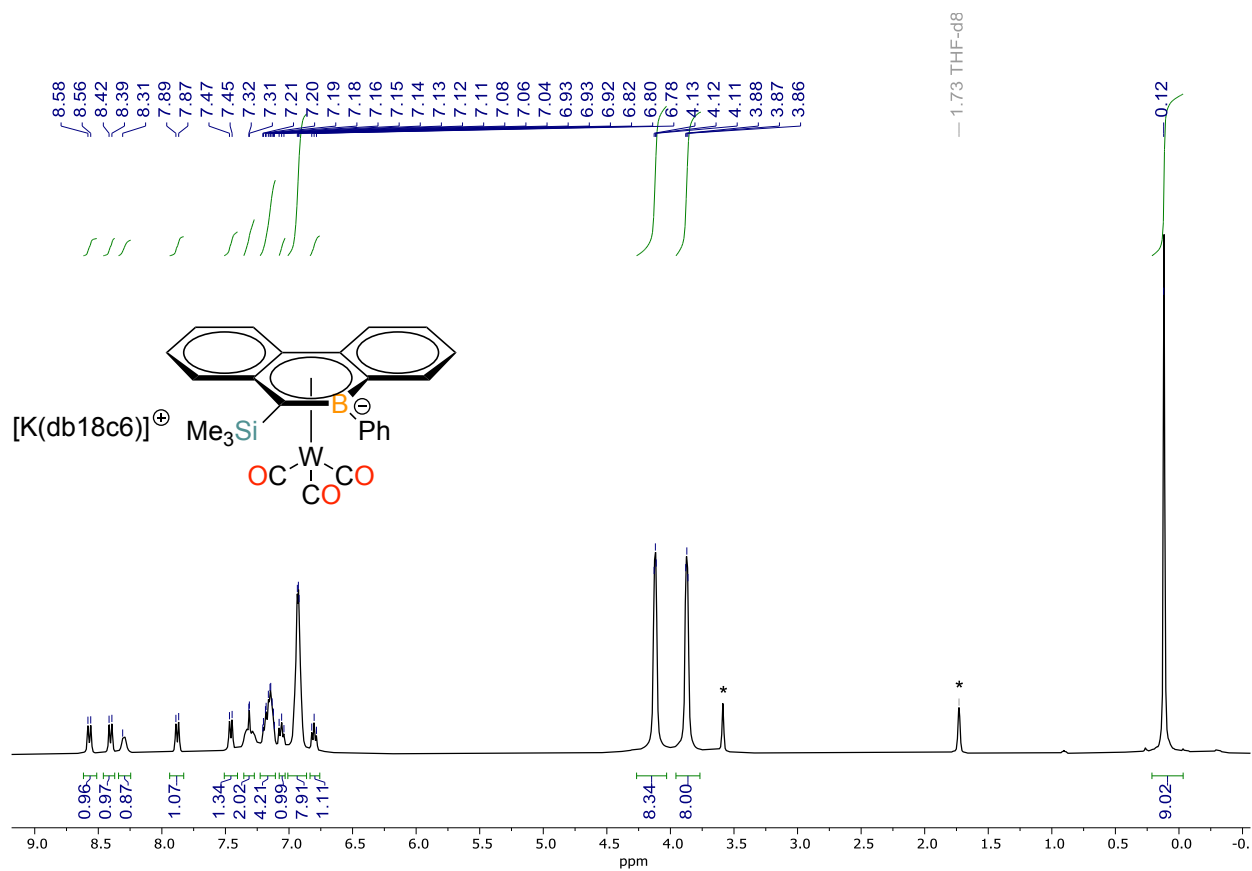


Figure S-32: Expansion of  $^1\text{H}$  NMR spectrum of **2W** in THF- $d_8$  (\* benzene).

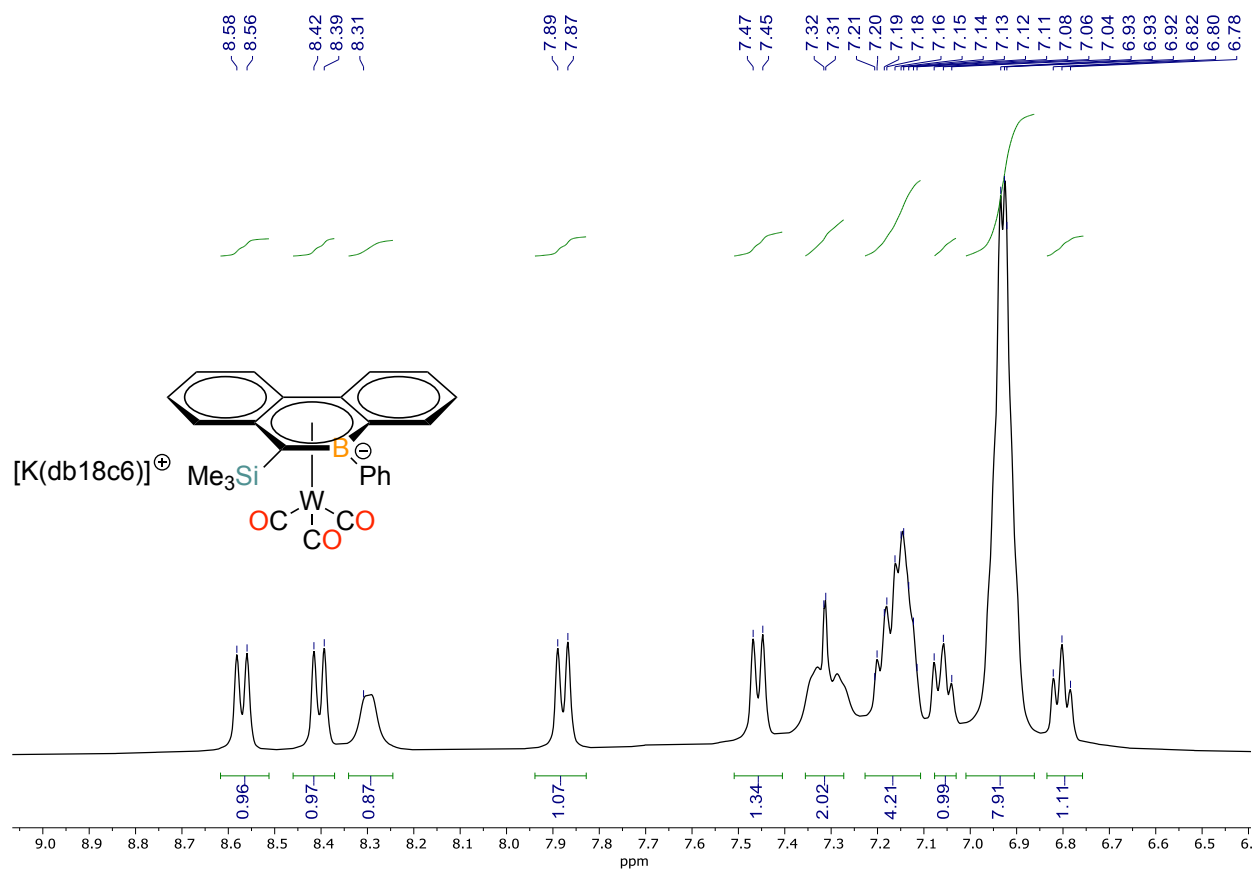


Figure S-33: Expansion of  $^1\text{H}$  NMR spectrum of **2W** in THF- $\text{d}_8$  (\*THF- $\text{d}_8$ ).

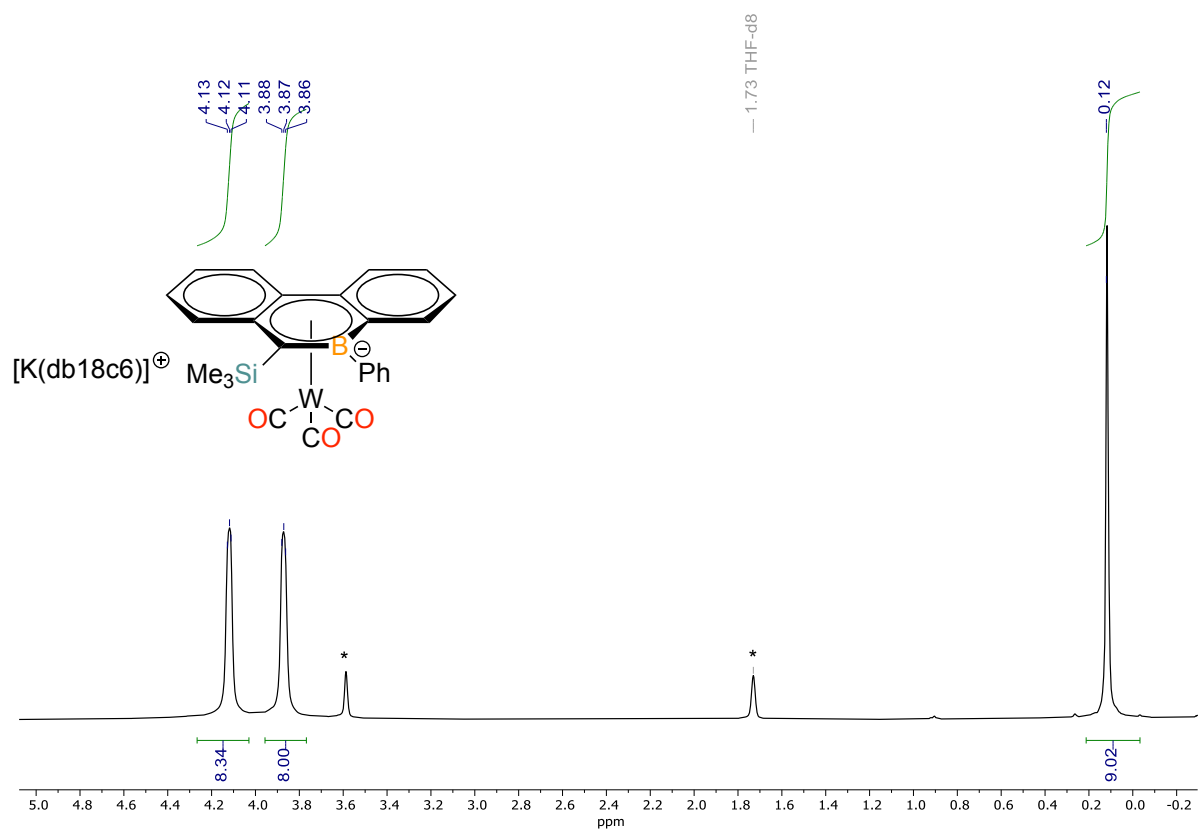


Figure S-34:  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2W** in THF- $\text{d}_8$  (\*THF- $\text{d}_8$ ).

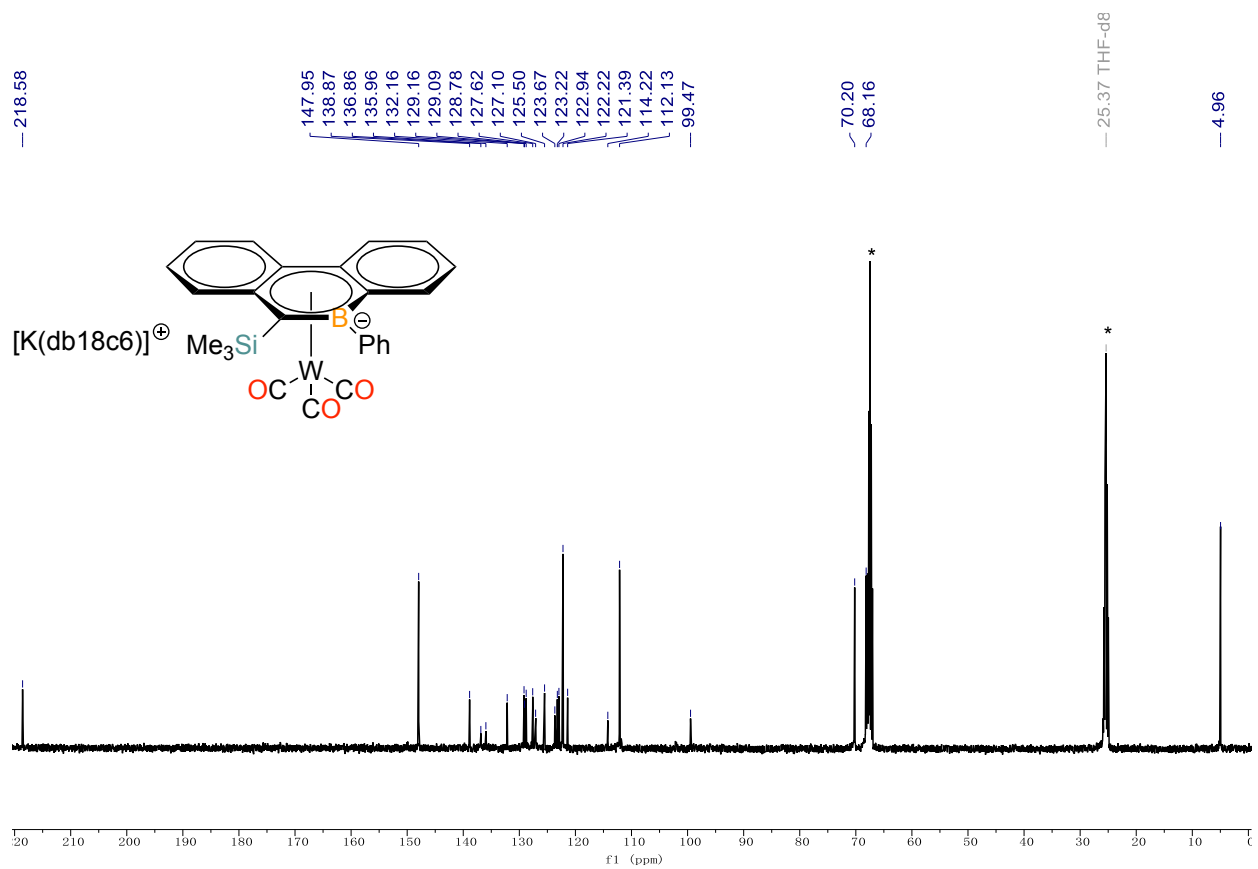


Figure S-35: Expansion of  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2W** in THF- $d_8$ .

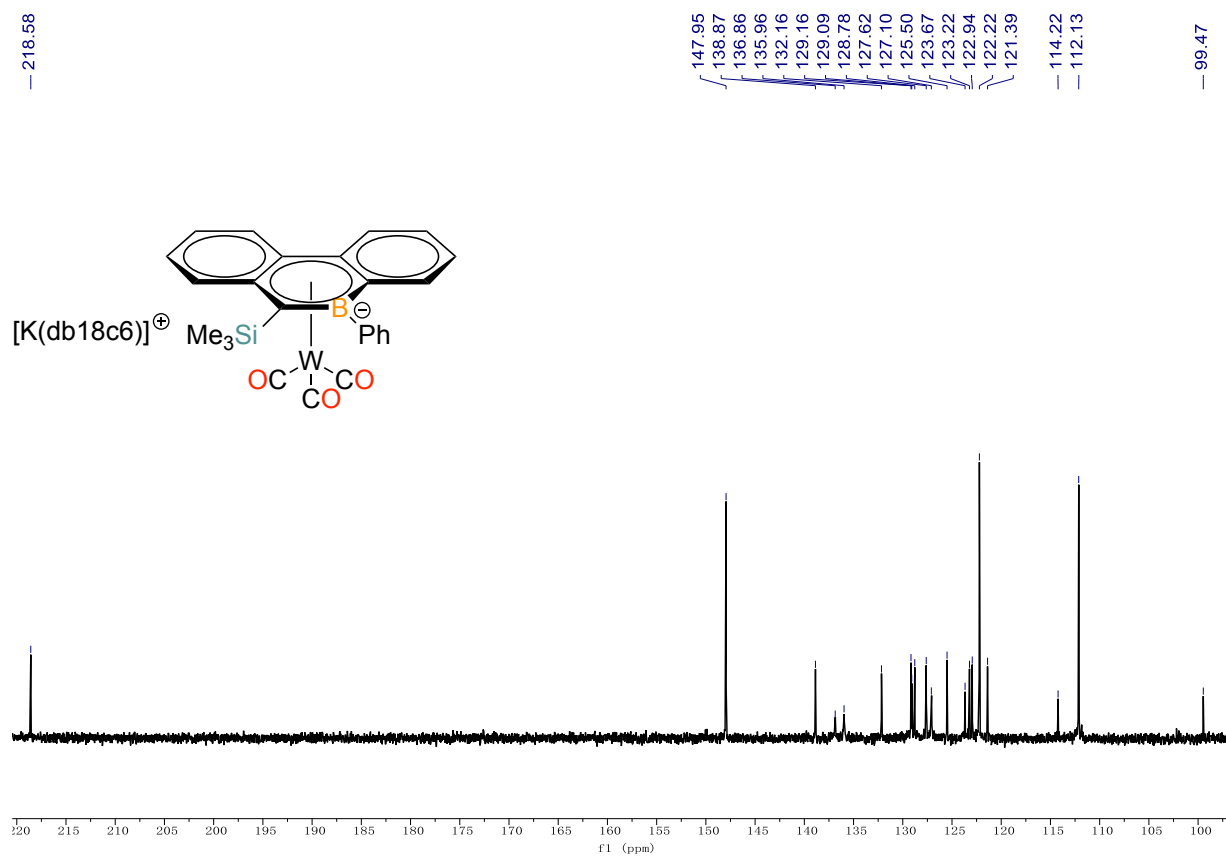


Figure S-36: Expansion of  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2W** in THF- $\text{d}_8$  (\*THF- $\text{d}_8$ ).

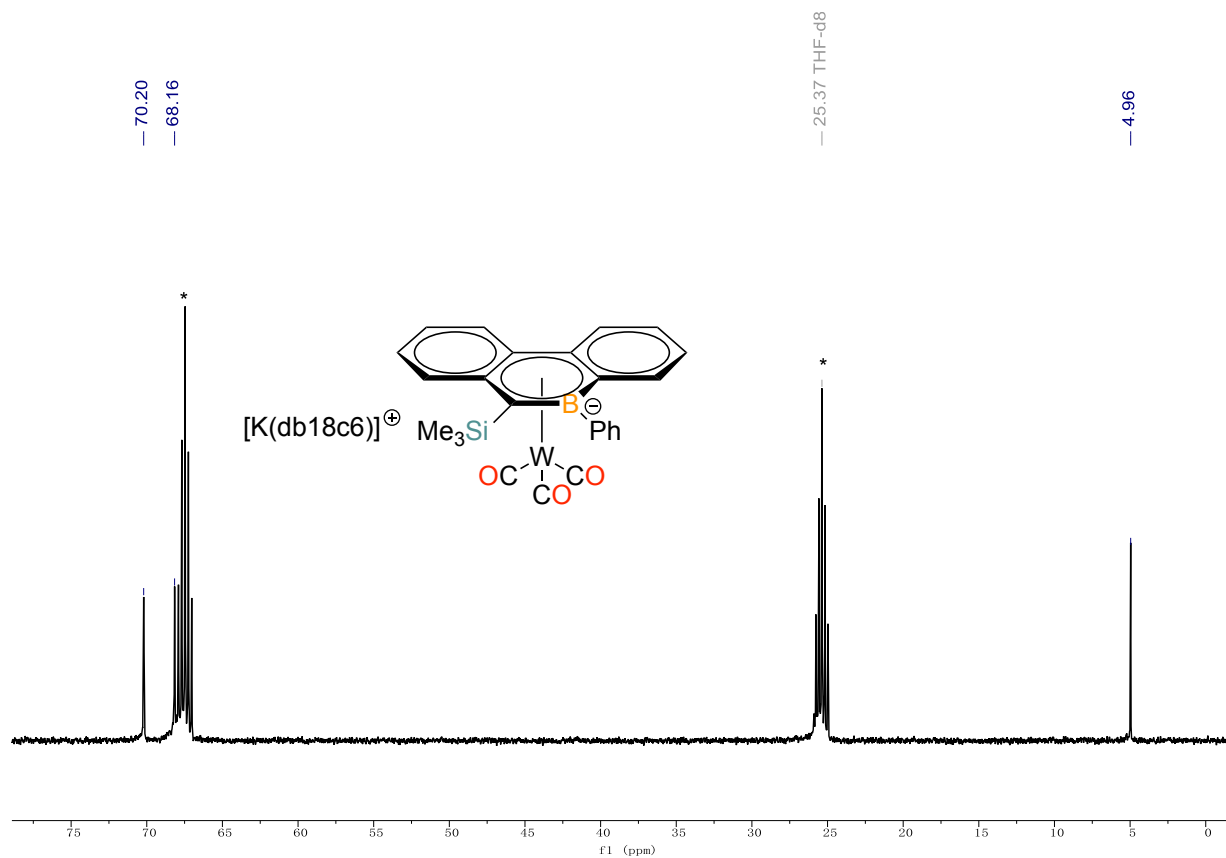


Figure S-37:  $^{11}\text{B}$  NMR spectrum of **2W** in THF- $d_8$ .

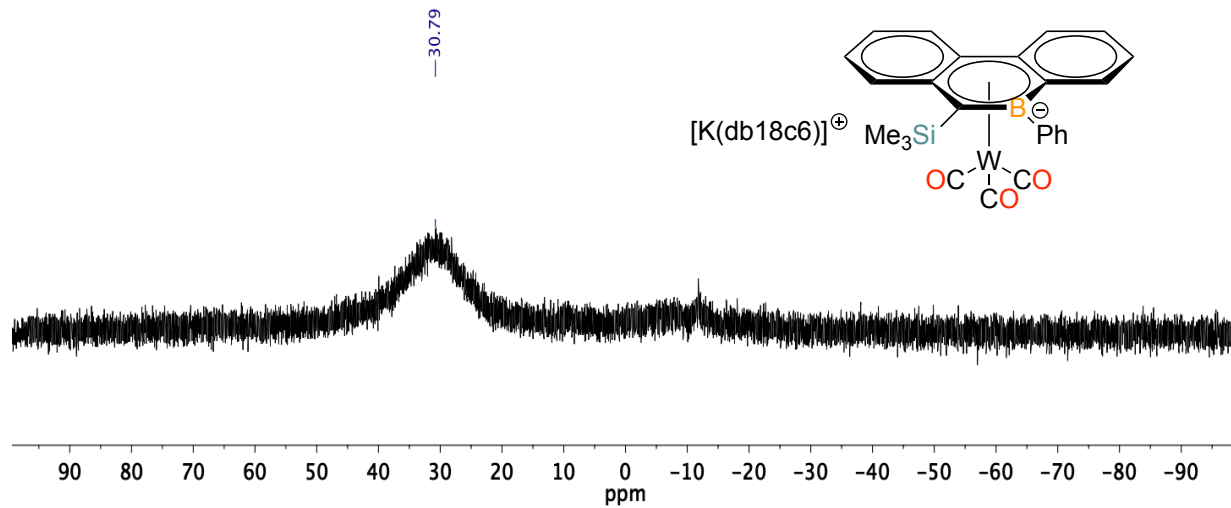


Figure S-38: FT-IR spectrum of **2W**.

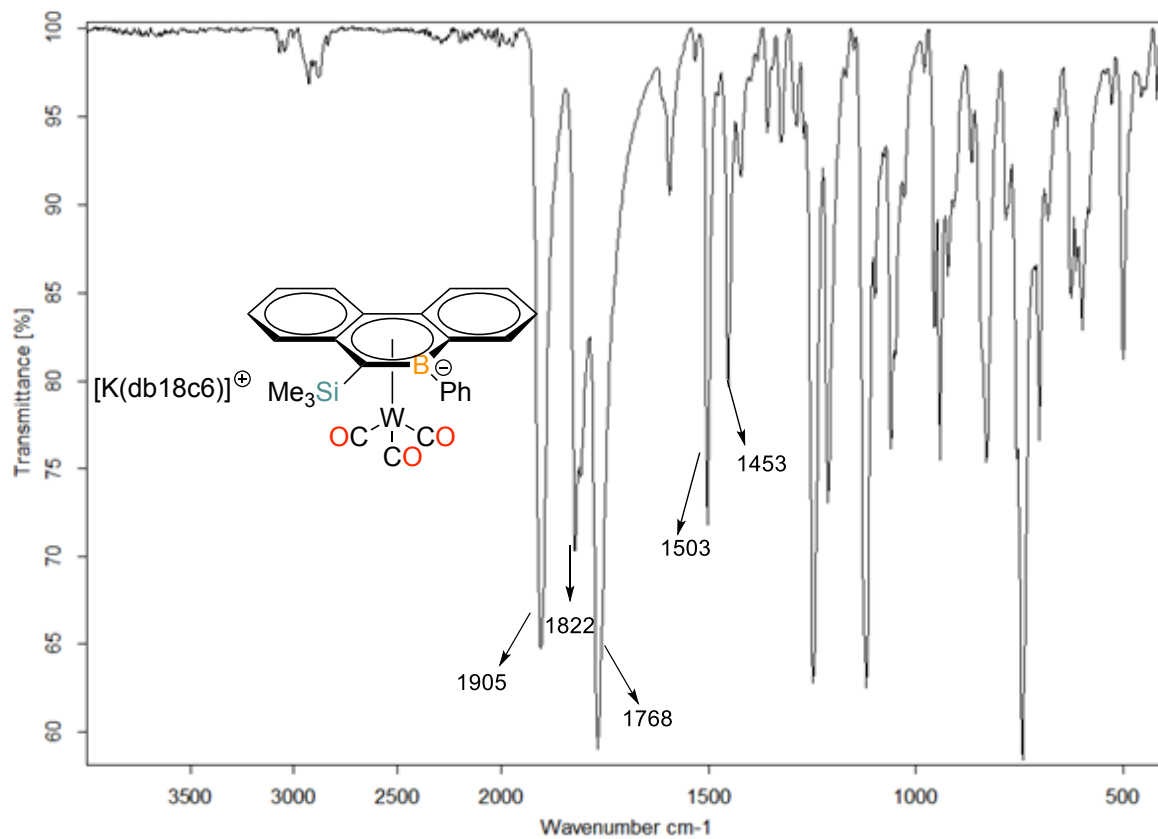




Figure S-39:  $^1\text{H}$  NMR spectrum of **1Rh** in  $\text{C}_6\text{D}_6$ .

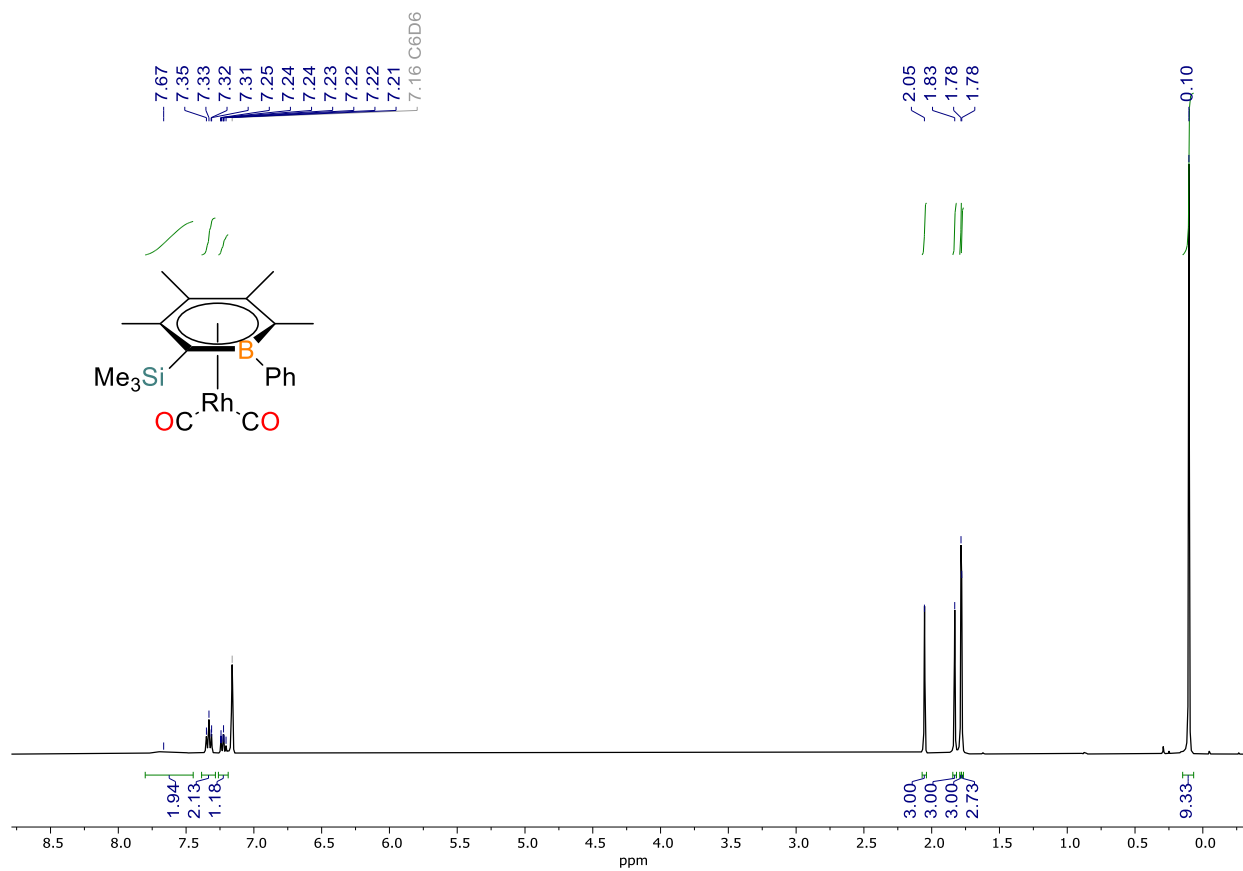


Figure S-40: Expansion of  $^1\text{H}$  NMR spectrum of **1Rh** in  $\text{C}_6\text{D}_6$ .

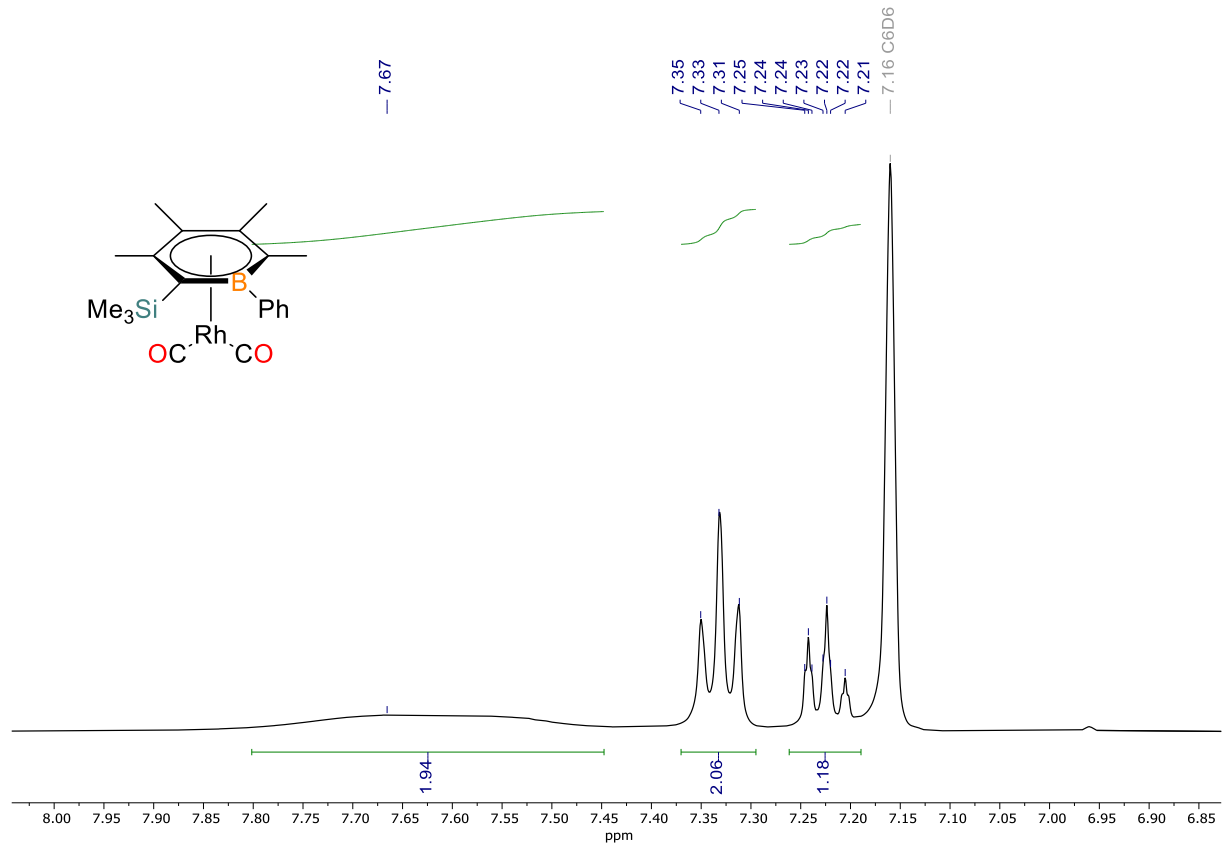


Figure S-41: Expansion of  $^1\text{H}$  NMR spectrum of **1Rh** in  $\text{C}_6\text{D}_6$ .

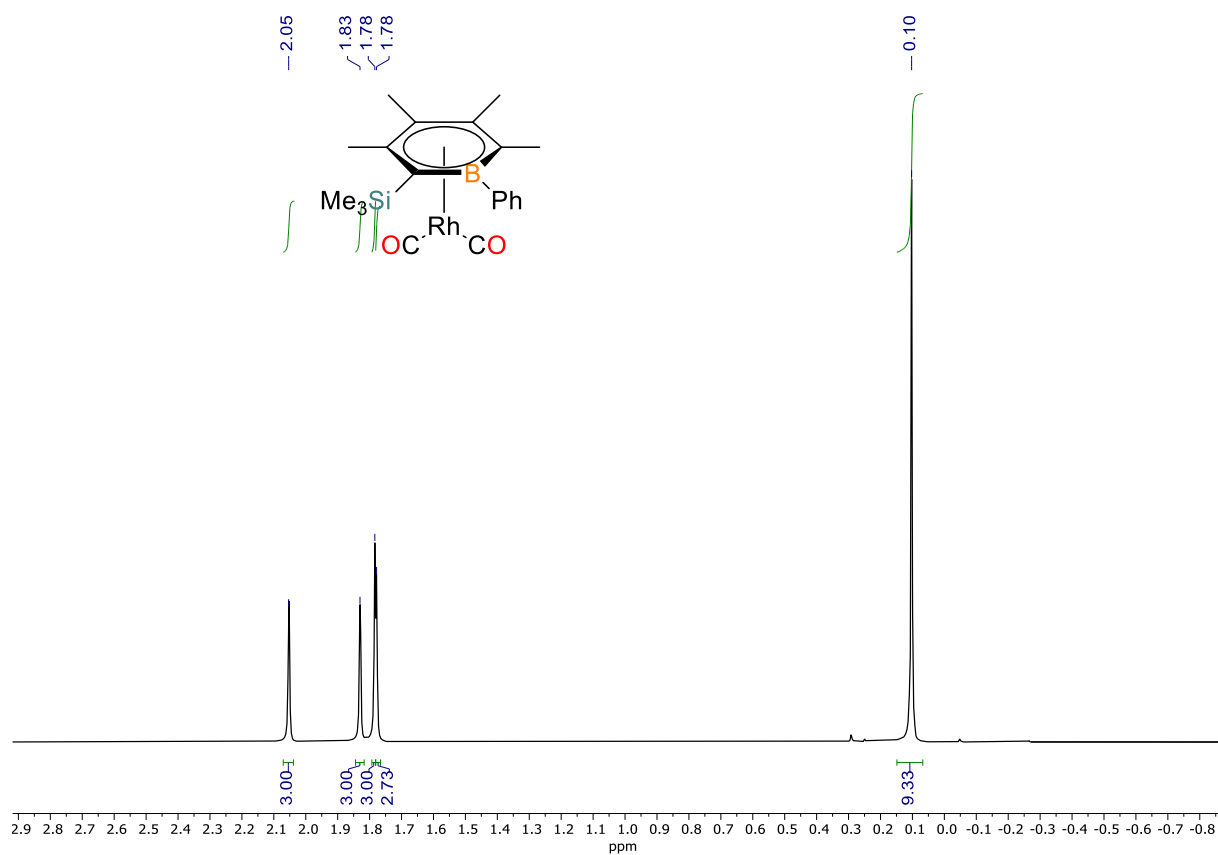


Figure S-42:  $^1\text{H}$  VT-NMR spectra of **1Rh** in  $\text{C}_6\text{D}_6$ .

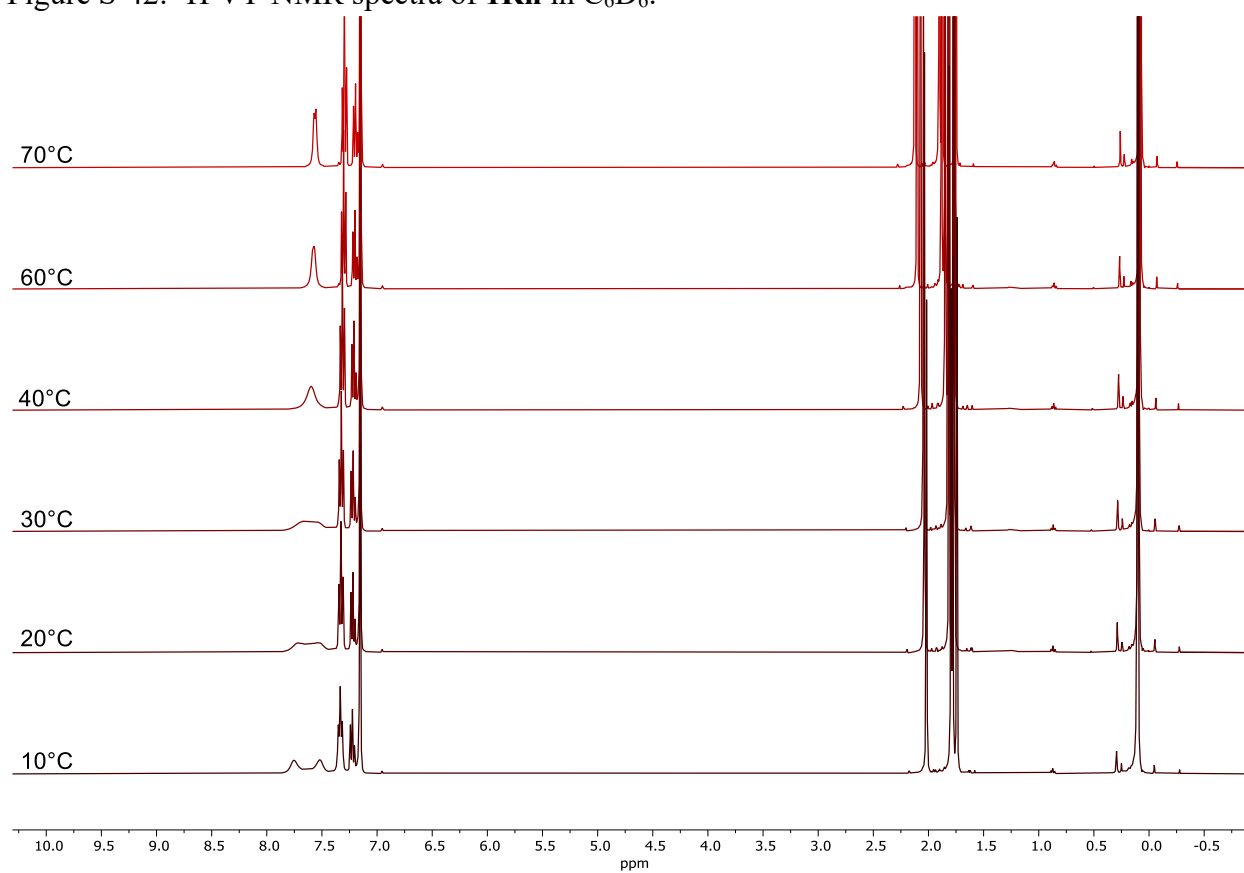


Figure S-43:  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1Rh** in  $\text{C}_6\text{D}_6$ .

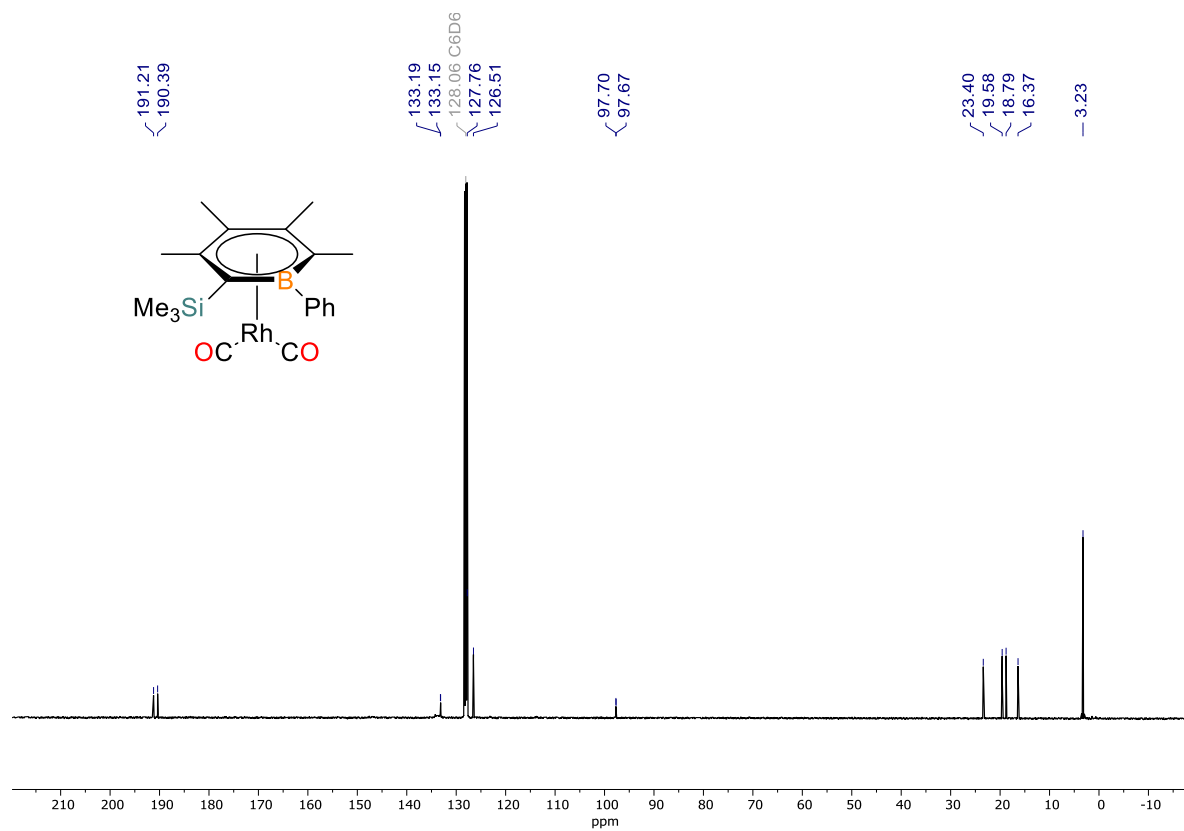


Figure S-44: Expansion of  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1Rh** in  $\text{C}_6\text{D}_6$ .

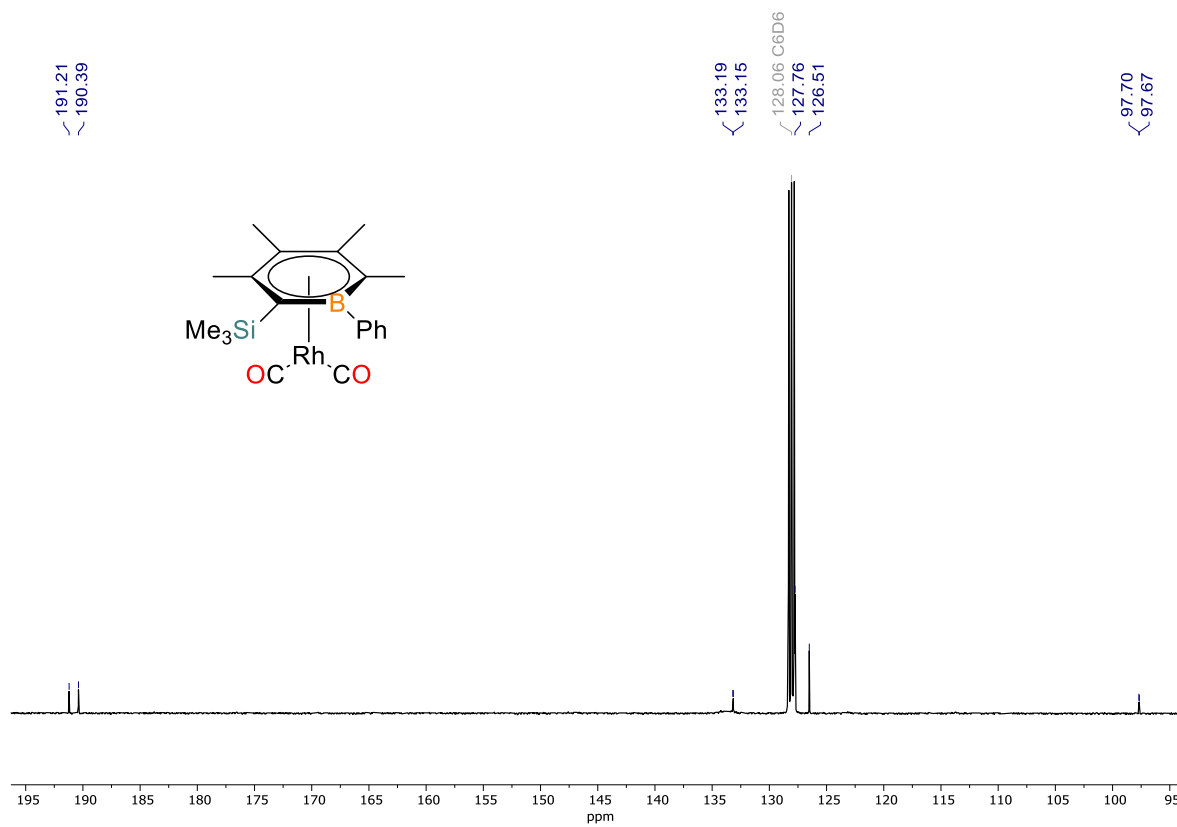


Figure S-45: Expansion of  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1Rh** in  $\text{C}_6\text{D}_6$ .

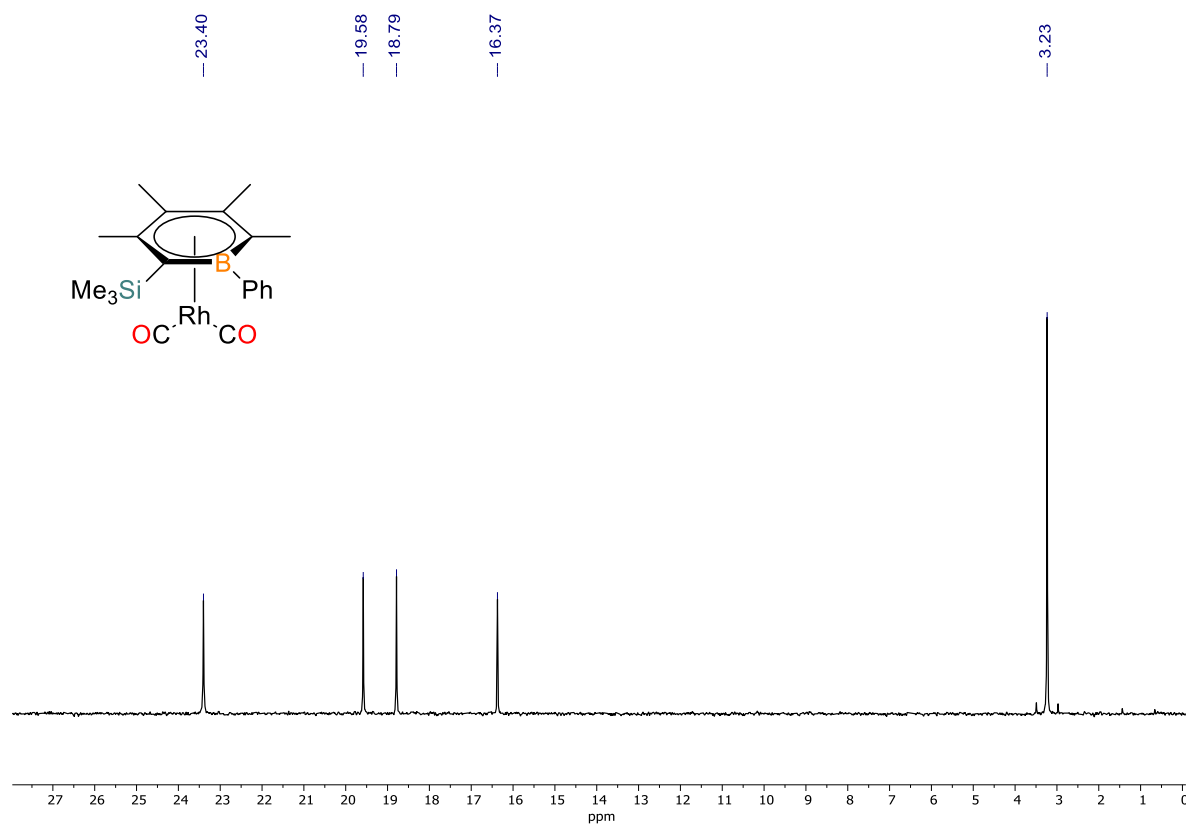


Figure S-46:  $^{11}\text{B}$  NMR spectrum of **1Rh** in  $\text{C}_6\text{D}_6$ .

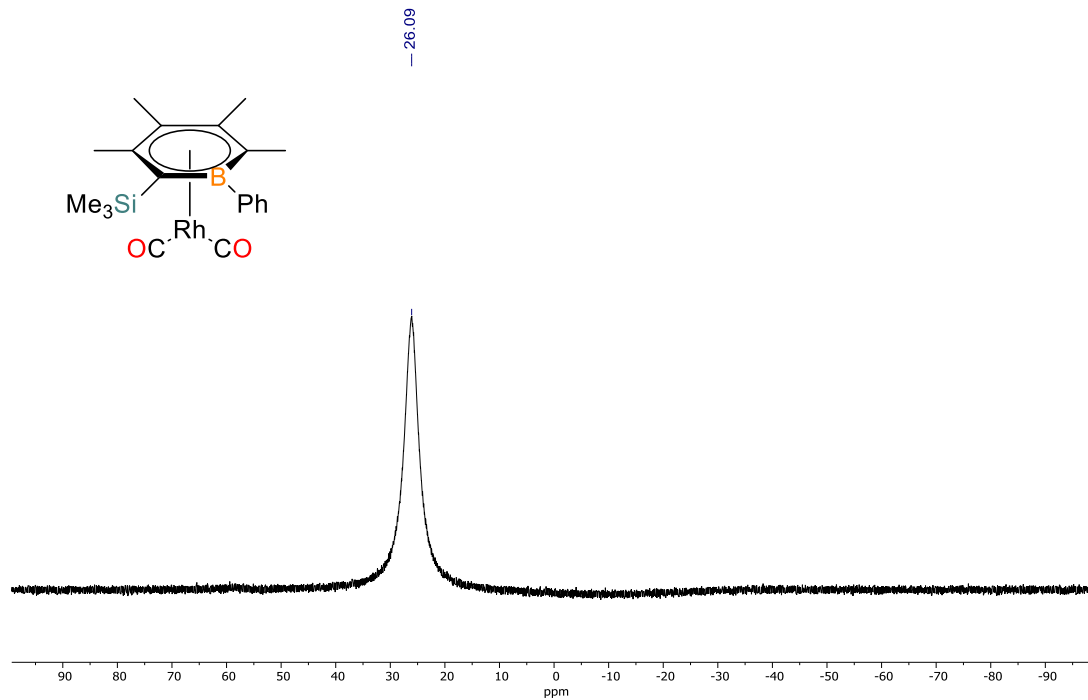




Figure S-47: FT-IR spectrum of **1Rh**.

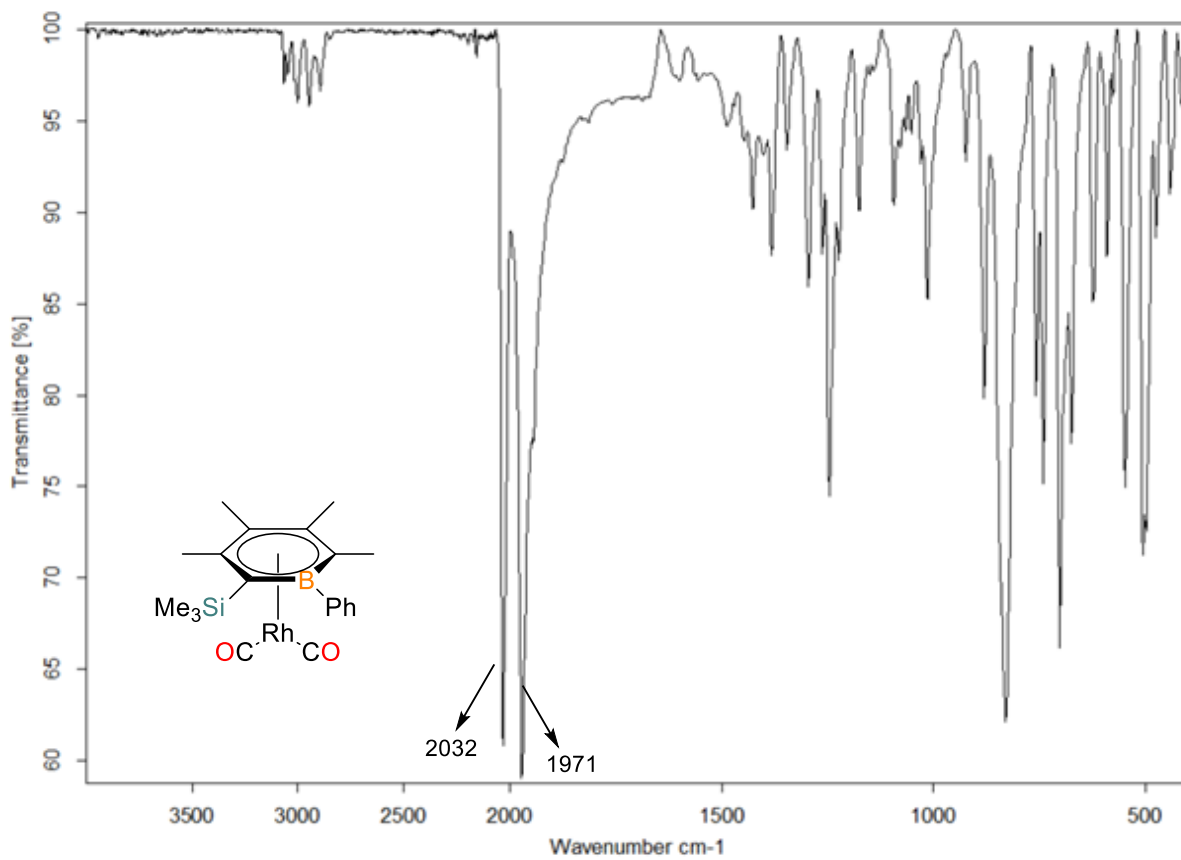


Figure S-48:  $^1\text{H}$  NMR spectrum of **2Rh** in  $\text{C}_6\text{D}_6$ .

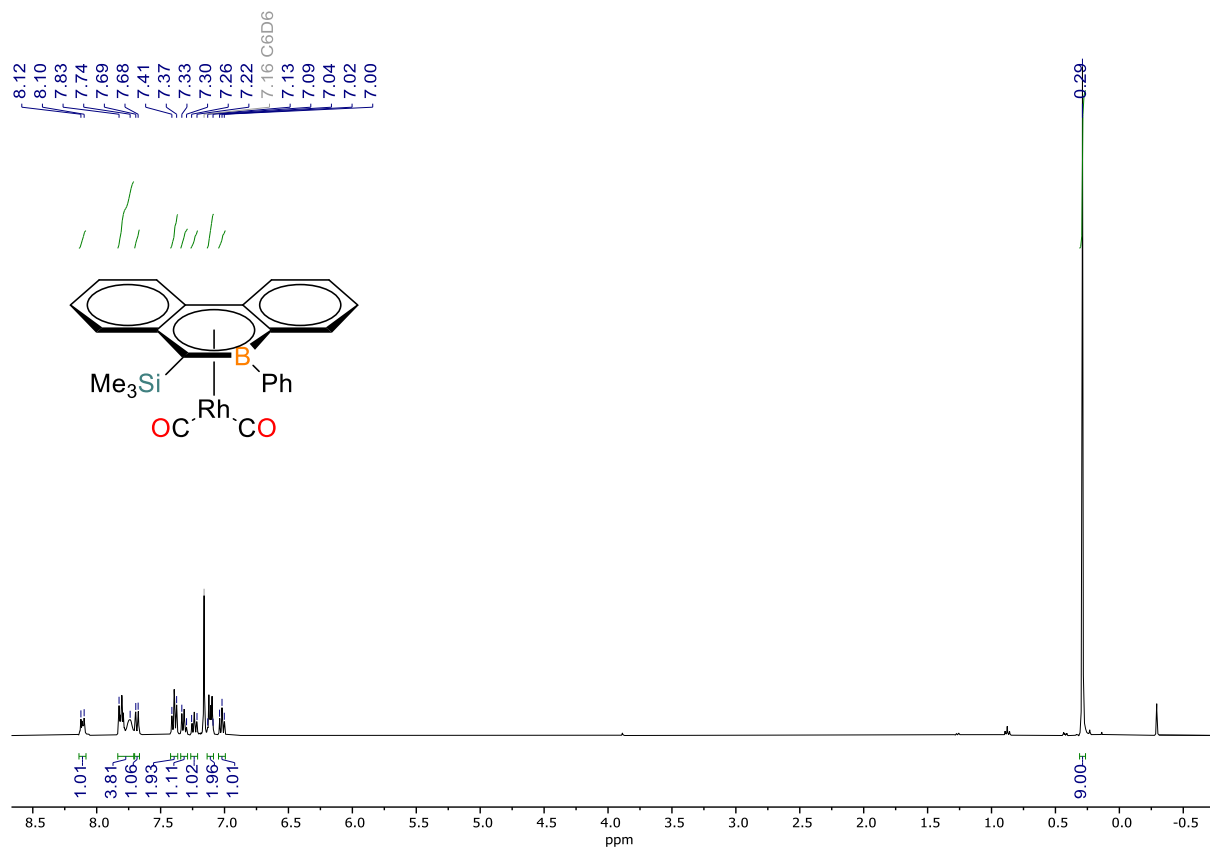


Figure S-49: Expansion of  $^1\text{H}$  NMR spectrum of **2Rh** in  $\text{C}_6\text{D}_6$ .

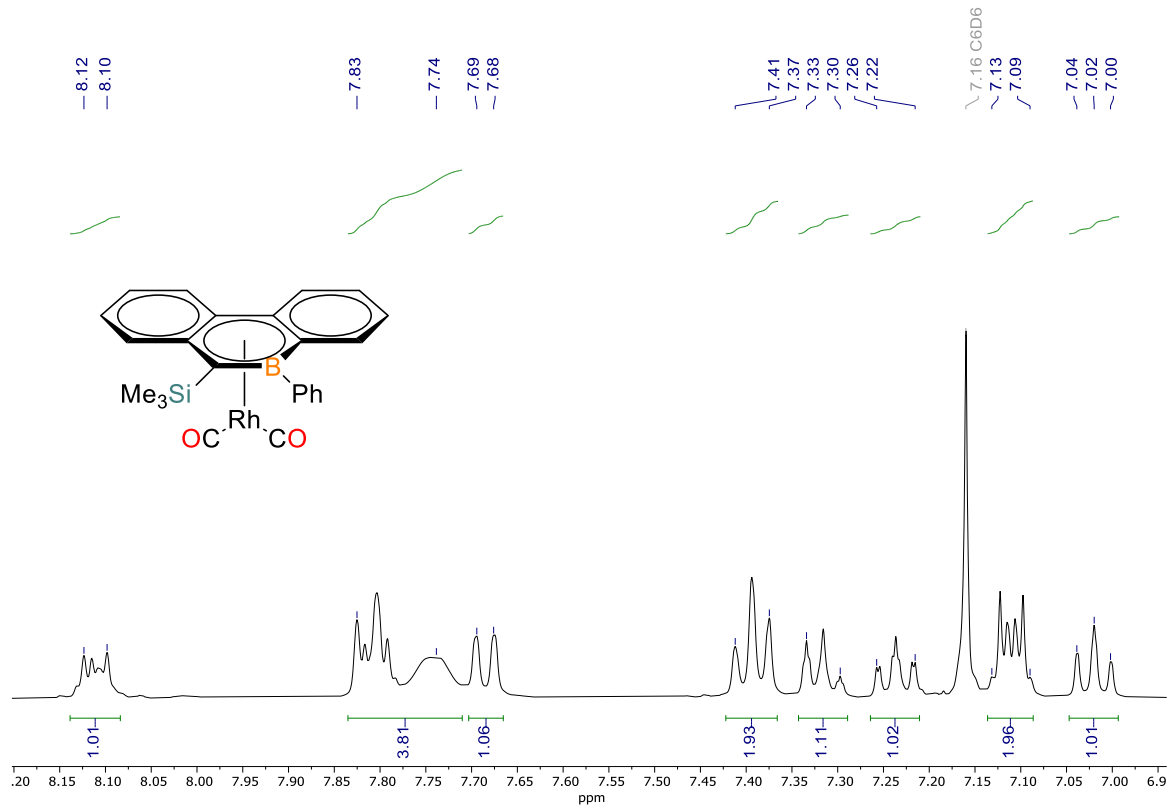


Figure S-50:  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2Rh** in  $\text{C}_6\text{D}_6$ .

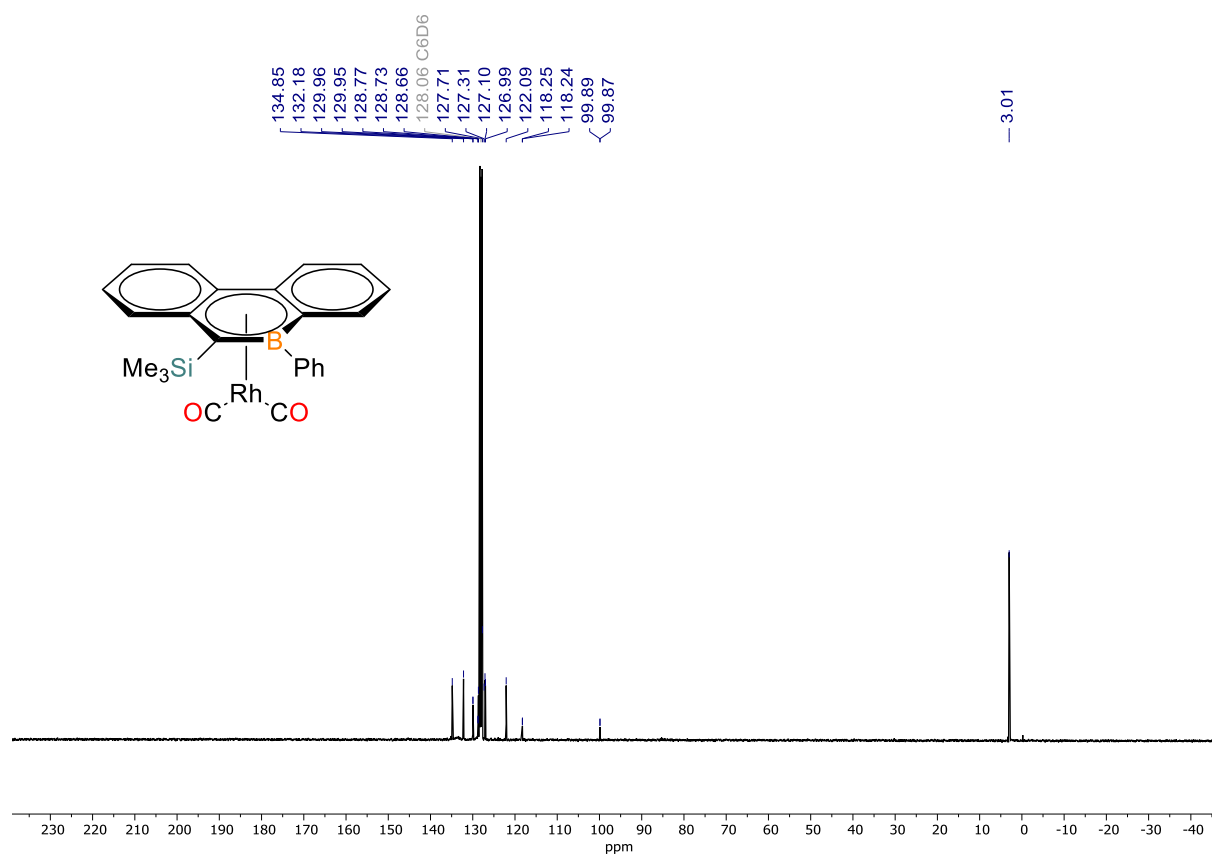


Figure S-51: Expansion of  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2Rh** in  $\text{C}_6\text{D}_6$ .

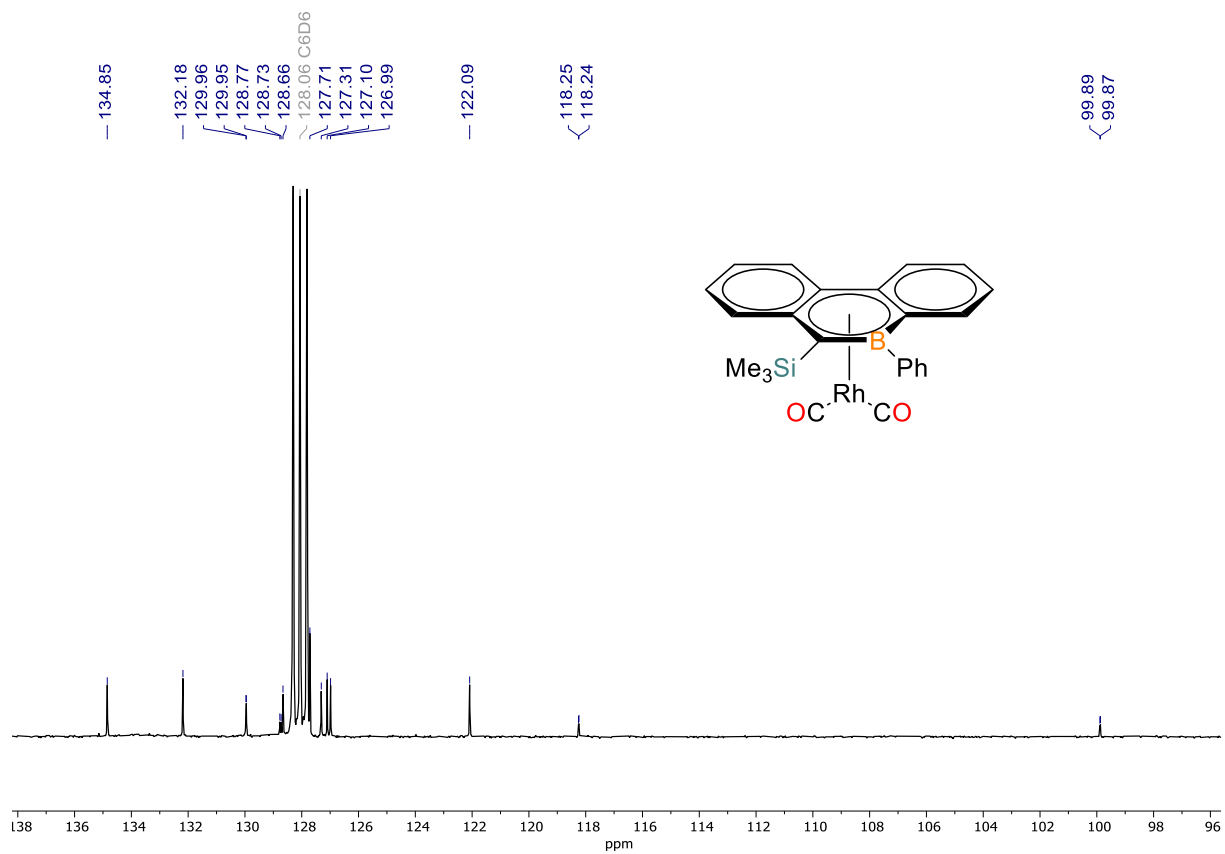


Figure S-52:  $^{11}\text{B}$  NMR spectrum of **2Rh** in  $\text{C}_6\text{D}_6$ .

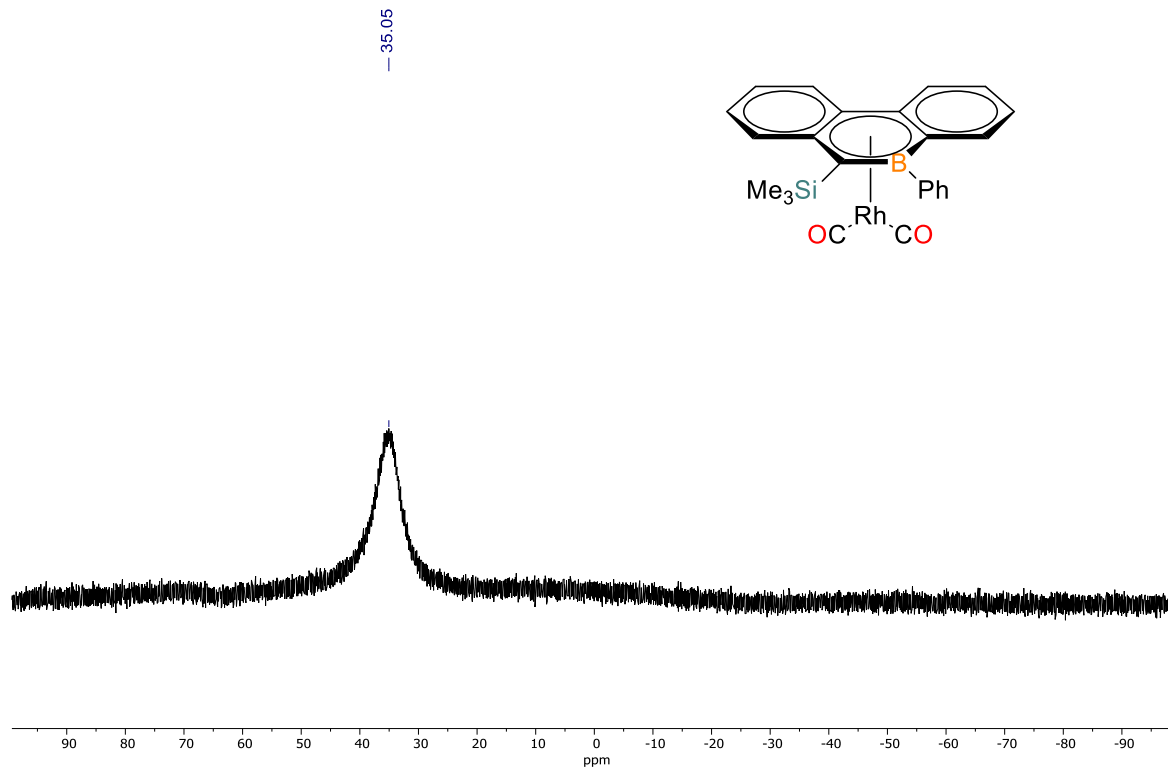
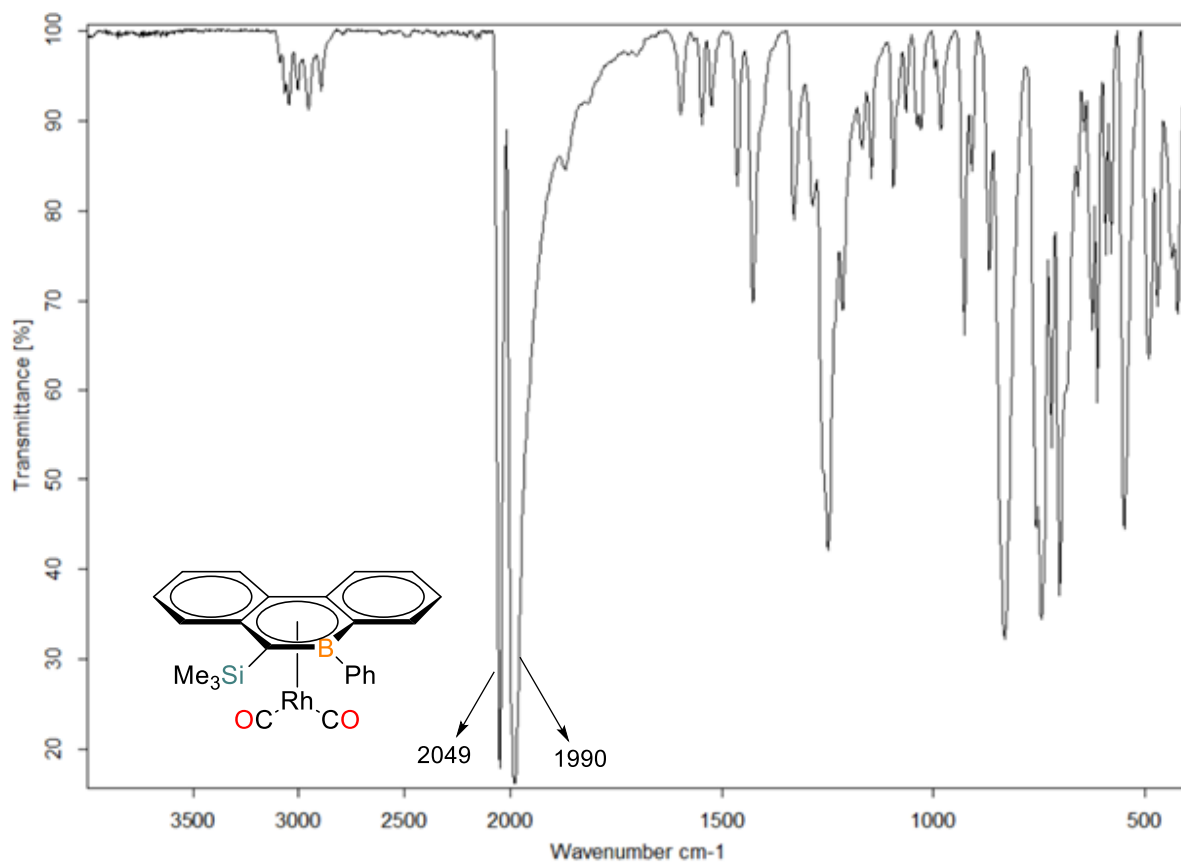


Figure S-53: FT-IR spectrum of **2Rh**.



**Table S2:** X-ray crystallographic details for the metal complexes with **L1** and **L2**.

	<b>1Cr</b>	<b>1Mo</b>	<b>1W</b>	<b>2Mo</b>	<b>2W</b>	<b>1Rh</b>	<b>2Rh</b>
CCDC	2203739	2203740	2203741	2203742	2203743	2203744	2203745
Empirical Formula	C <sub>33</sub> H <sub>50</sub> BCrKO <sub>9</sub> Si, 2(C <sub>6</sub> H <sub>6</sub> )	C <sub>33</sub> H <sub>50</sub> BMoKO <sub>9</sub> Si, 2(C <sub>6</sub> H <sub>6</sub> )	C <sub>33</sub> H <sub>50</sub> BKO <sub>9</sub> SiW	C <sub>46</sub> H <sub>48</sub> BCl <sub>2</sub> KMoO <sub>9</sub> Si	C <sub>46</sub> H <sub>48</sub> BCl <sub>2</sub> KO <sub>9</sub> SiW	C <sub>20</sub> H <sub>26</sub> BO <sub>2</sub> Rh Si	C <sub>24</sub> H <sub>22</sub> BO <sub>2</sub> RhSi
FW (g/mol)	876.95	920.89	852.57	989.68	1077.59	440.22	484.22
Crystal System	Triclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space Group	P -1	P -1	C 2/c	C c	C c	P 2 <sub>1</sub> /c	P 2 <sub>1</sub> /n
a (Å)	11.350(1)	11.2735(3)	33.118(1)	14.3574(3)	14.3661(4)	17.3967(5)	12.3516(9)
b (Å)	11.5688(11)	11.8132(4)	11.7793(3)	32.3930(7)	32.3267(8)	7.7875(2)	13.2338(9)
c (Å)	18.8139(18)	18.8859(6)	20.0868(6)	9.8045(2)	9.8108(2)	15.7760(4)	13.6808(9)
α (deg)	74.292(4)	73.690(1)	90	90	90	90	90
β (deg)	86.768(3)	81.302(1)	108.163(1)	102.3096(8)	102.329(1)	105.7830(9)	95.797(3)
γ (deg)	77.513(3)	78.301(1)	90	90	90	90	90
V (Å <sup>3</sup> )	2321.9(4)	2351.86(13)	7445.6(4)	4455.04(16)	4451.14(2)	2056.70(1)	2224.8(3)
Z	2	2	4	4	4	4	4
D <sub>c</sub> (g cm <sup>-3</sup> )	1.254	1.300	1.521	1.476	1.608	1.422	1.446
Radiation λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Temp (K)	150	150	150	150	150	150	150
R1 [I > 2(σ)I] <sup>a</sup>	0.0442	0.0356	0.0248	0.0190	0.0248	0.0181	0.0591
wR2 (F <sup>2</sup> ) <sup>a</sup>	0.1404	0.0992	0.0847	0.0596	0.0714	0.0460	0.1519
GOF (S) <sup>a</sup>	1.145	1.144	1.222	1.191	1.186	1.093	1.215

<sup>a</sup>  $R1(F[I > 2(I)]) = \sum ||F_o| - |F_c|| / \sum |F_o|$ ;  $wR2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$ ;  $S(\text{all data}) = [w(F_o^2 - F_c^2)^2 / (n - p)]^{1/2}$  ( $n$  = no. of data;  $p$  = no. of parameters varied);  $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$  where  $P = (F_o^2 + 2F_c^2)/3$  and  $a$  and  $b$  are constants suggested by the refinement program.



## **Theoretical calculations**

The theoretical calculations were carried out by using Gaussian 16.<sup>2</sup> Geometry optimizations were performed using the B3LYP<sup>3</sup> functional with a standard 6-31+G(d,p)<sup>4</sup> basis set (LANL2DZ basis set for all metals Cr, Mo, W).<sup>5</sup> Frequency analysis were done to obtain the thermodynamic energy corrections and to ensure that the optimized structures were at a minimum. The Cartesian coordinates of the geometry-optimized structures are given below.

**Complex 1Cr**

K	3.39143900	0.20790200	-0.42495100
B	-3.80457900	-0.57226100	0.41311800
Cr	-1.38152600	-0.91169200	0.60423700
O	-1.25586000	-0.27115900	-2.31466800
O	0.49510400	-3.18793600	0.15296200
O	1.11140900	0.65014300	1.06241800
O	1.97365800	0.09157000	-2.79762500
O	2.55618100	2.65723900	-1.76154100
O	4.18701100	2.76652600	0.59059900
O	5.77359500	0.51380000	1.27667000
O	4.98185400	-2.06153600	0.33739100
O	3.48116500	-2.17863300	-2.09680800
Si	-3.27363700	2.36229100	0.84394400
C	-3.13116300	0.51013400	1.28080500
C	-2.40396000	0.08705000	2.43511600
C	-2.13838500	-1.29661100	2.70766400
C	-2.69187800	-2.33752300	1.88707000
C	-3.46228800	-2.03350900	0.73877000
C	-1.90846300	1.08521000	3.47629300
H	-2.13988500	0.72799600	4.48505100
H	-2.39893600	2.04986000	3.36377700
H	-0.82695800	1.25303500	3.42726800
C	-1.33304700	-1.67561500	3.93889500
H	-0.57112200	-0.93025000	4.17284400
H	-0.81538200	-2.62648700	3.80617500
H	-1.97725300	-1.77629000	4.82578400
C	-2.46146800	-3.77870500	2.31953100
H	-2.79020200	-3.92054800	3.35571600
H	-1.40658000	-4.06747900	2.26998900
H	-3.02036500	-4.47894100	1.70070500
C	-3.99465600	-3.17782100	-0.11212200
H	-4.44315000	-2.80366000	-1.03311800
H	-4.77932800	-3.73651800	0.41822700
H	-3.21638300	-3.89642000	-0.39336300
C	-4.92420100	-0.25879400	-0.68070000
C	-6.19570800	0.14239800	-0.21995400
H	-6.35610400	0.26520700	0.84967000
C	-7.26171500	0.38735100	-1.09219100
H	-8.22638600	0.69645700	-0.69604100
C	-7.08586800	0.23573700	-2.47062300
H	-7.90809300	0.42766400	-3.15537700
C	-5.83856700	-0.16926100	-2.95647400
H	-5.68633800	-0.29181600	-4.02655000
C	-4.78204700	-0.41547200	-2.07392500
H	-3.82281200	-0.71831800	-2.48354000
C	-1.67111000	3.36593100	1.15236600
H	-1.51823000	3.65829400	2.19580400
H	-1.72154900	4.28774900	0.55849100
H	-0.78535600	2.80713400	0.83242700
C	-3.64459100	2.69366200	-0.98683200
H	-2.93851200	2.17964300	-1.64754800
H	-3.54567700	3.77348200	-1.16101500
H	-4.65154900	2.39437400	-1.28421800
C	-4.66274500	3.18576200	1.85614500
H	-4.51223300	3.08218500	2.93711800

H	-5.63295100	2.73825400	1.61309000
H	-4.72298500	4.25764100	1.62785800
C	-1.32996500	-0.52091800	-1.16748900
C	-0.26941900	-2.30600600	0.33039400
C	0.09123600	0.06128300	0.89079200
C	1.52770500	1.28112100	-3.43912100
H	0.57210000	1.09603900	-3.94927100
H	2.27285300	1.61344100	-4.17910300
C	1.30947300	2.35308300	-2.39289300
H	0.90618600	3.25243300	-2.88358200
H	0.58143400	2.00671600	-1.64825400
C	2.44609600	3.68003700	-0.77797700
H	1.72609200	3.38812200	-0.00036900
H	2.09809100	4.61749200	-1.24037200
C	3.80875500	3.91719900	-0.16067500
H	4.55172600	4.11627700	-0.94810900
H	3.75588800	4.79642600	0.50021800
C	5.44624100	2.88789800	1.23330300
H	5.46667600	3.78525200	1.87226400
H	6.25195100	2.97694500	0.48787000
C	5.67276000	1.66887000	2.10425300
H	6.60267800	1.80587700	2.67854700
H	4.83912300	1.55690200	2.81364000
C	6.00968700	-0.68467600	2.00856200
H	5.16502400	-0.89216200	2.68301500
H	6.92176000	-0.58450000	2.61798600
C	6.19613600	-1.83259500	1.03806000
H	7.00571800	-1.59619000	0.33023500
H	6.48526000	-2.73180600	1.60524900
C	5.06385400	-3.14665300	-0.58611000
H	5.31243600	-4.07600500	-0.05035400
H	5.85505100	-2.94770500	-1.32499300
C	3.73250000	-3.32311500	-1.28456100
H	3.78703200	-4.22787700	-1.91123200
H	2.92348100	-3.45902200	-0.55427500
C	2.26361000	-2.28362400	-2.84105200
H	1.41693700	-2.42459000	-2.15872300
H	2.31300100	-3.15026100	-3.51926000
C	2.07126500	-1.02905300	-3.66695400
H	2.91161400	-0.89220300	-4.36602800
H	1.14394700	-1.13891200	-4.24813500

**Complex 1Mo**

K	-3.56966700	0.26259200	0.40049100
B	3.88709300	-0.48634300	-0.32285100
O	1.04354000	-0.21539300	2.56441400
O	-0.58218800	-3.38922500	-0.02186700
O	-1.28621700	0.65182700	-1.09648500
O	-2.14793900	0.36049100	2.76653200
O	-2.78192600	2.82653200	1.54088800
O	-4.41391100	2.71394100	-0.81232300
O	-5.95236500	0.38066300	-1.31746000
O	-5.08813700	-2.09919200	-0.19804600
O	-3.57247400	-2.00292000	2.22554700
Si	3.26864100	2.39563200	-0.97470500
C	3.20348300	0.51256200	-1.28303500

C	2.54618600	-0.01981800	-2.44005000	H	-4.80012400	4.17843800	0.61216100
C	2.35365700	-1.43015600	-2.63694600	H	-4.01670500	4.75121600	-0.88843500
C	2.91376900	-2.39474600	-1.72268700	C	-5.67860200	2.75860500	-1.45439000
C	3.63714600	-1.98607200	-0.57407900	H	-5.72209300	3.60424700	-2.15931100
C	2.07381600	0.88510400	-3.57282700	H	-6.48255400	2.88625800	-0.71270200
H	2.40734900	0.48914400	-4.53787100	C	-5.88168900	1.47256200	-2.22959600
H	2.48915800	1.88589700	-3.48113200	H	-6.81713000	1.54531600	-2.80666300
H	0.98331000	0.97841200	-3.61549800	H	-5.04906300	1.32625600	-2.93390800
C	1.66517600	-1.92020500	-3.90026500	C	-6.16014300	-0.87452100	-1.95753300
H	0.88186400	-1.23621000	-4.23030200	H	-5.31326200	-1.10890900	-2.62024500
H	1.19531200	-2.89336800	-3.75576900	H	-7.07724900	-0.84299200	-2.56680700
H	2.38132000	-2.02454300	-4.73004600	C	-6.31159800	-1.95292500	-0.90467800
C	2.76771700	-3.86804000	-2.07404500	H	-7.12346700	-1.68661200	-0.21016500
H	1.72017100	-4.17665700	-2.14089000	H	-6.58023200	-2.89801400	-1.40317400
H	3.25063400	-4.50936300	-1.33902300	C	-5.13534200	-3.11917100	0.79956000
H	3.23119700	-4.07290900	-3.04708200	H	-5.36032000	-4.09010800	0.33154800
C	4.23190300	-3.04910500	0.34027000	H	-5.92835900	-2.89064800	1.52787300
H	4.66182100	-2.59629900	1.23426500	C	-3.79636800	-3.20962200	1.49986600
H	5.04279500	-3.59620000	-0.16173000	H	-3.82340700	-4.06769700	2.19064400
H	3.49441800	-3.78949800	0.66988300	H	-2.98757200	-3.37881800	0.77622700
C	4.93384400	-0.05595700	0.80065400	C	-2.34434400	-2.01542200	2.95971700
C	6.21713400	0.36182400	0.39149600	H	-1.49827200	-2.16246600	2.27775700
H	6.44210200	0.41764400	-0.67205700	H	-2.35164500	-2.84116900	3.68849900
C	7.21482800	0.70808600	1.30923600	C	-2.19278600	-0.70652400	3.70589900
H	8.19172900	1.02733600	0.95322300	H	-3.03151500	-0.55900100	4.40463300
C	6.95517300	0.64451600	2.68126200	H	-1.25522200	-0.74449800	4.27857300
H	7.72411600	0.91537900	3.40034200	Mo	1.32677000	-0.94529700	-0.47660200
C	5.69411600	0.22460400	3.11666100				
H	5.47747000	0.16930500	4.18111900				
C	4.70652800	-0.12267000	2.18967700	<b>Complex 1W</b>			
H	3.73417000	-0.43727200	2.55785900	O	3.30700200	-1.65374700	2.61545300
C	1.64629200	3.31514200	-1.41141300	C	2.06392100	-1.32965800	3.24515700
H	1.51750900	3.52387100	-2.47792400	H	1.23666800	-1.45884900	2.53706800
H	1.64703100	4.28021200	-0.88821100	H	1.89370200	-1.99636700	4.10520100
H	0.76943800	2.75142500	-1.07547700	C	2.11106700	0.10125500	3.73815900
C	3.55340800	2.86276200	0.84132400	H	2.92930400	0.23473500	4.46350900
H	2.83534200	2.36875900	1.50442900	H	1.15569000	0.32596400	4.23314500
H	3.41130800	3.94746000	0.93738100	O	2.30026700	0.96839400	2.62651700
H	4.55547600	2.61986400	1.19993400	C	2.08511700	2.34306100	2.92098700
C	4.67003000	3.19414400	-1.99002300	H	1.10013700	2.47597700	3.39007000
H	4.56378600	3.01293900	-3.06600700	H	2.86352100	2.71003300	3.60859800
H	5.64337800	2.79583400	-1.68230300	C	2.10796900	3.13146900	1.62858000
H	4.68954600	4.28037000	-1.83408900	H	1.88022000	4.18592700	1.85064200
C	1.14704700	-0.48770200	1.42397100	H	1.34441600	2.74490000	0.94101800
C	0.14459000	-2.47315000	-0.18147300	O	3.40394000	3.02678600	1.03370100
C	-0.27768900	0.06463700	-0.85735600	C	3.51121300	3.74084500	-0.19270900
C	-1.73086800	1.60298400	3.31998800	H	2.77120600	3.36870100	-0.91527700
H	-0.77376800	1.47700900	3.84517700	H	3.33217600	4.81514100	-0.02462000
H	-2.48559100	1.97339000	4.03167200	C	4.91067100	3.56130100	-0.74381700
C	-1.53171600	2.59825600	2.19649700	H	5.04550200	4.22801100	-1.61008300
H	-1.14983400	3.54094000	2.61823800	H	5.65500900	3.82898900	0.02173600
H	-0.79426100	2.21214900	1.48060800	O	5.08430800	2.20462700	-1.14405900
C	-2.68785700	3.76449000	0.47461400	B	-3.60133600	0.59416800	-0.68766500
H	-1.96394900	3.41834500	-0.27685600	K	3.73293800	0.18977100	0.40130100
H	-2.35429900	4.74283100	0.85587300	O	-0.93072400	0.93773200	2.29278800
C	-4.05451000	3.92808200	-0.15791900	O	0.38784200	-2.83431200	0.30977900
				O	1.64620200	0.90292100	-1.29517000



H	-5.56000200	5.44336800	-0.18015500
C	-5.86231100	3.32595500	-0.49744700
H	-6.94087200	3.41094700	-0.60734900
C	-5.24920300	2.07254200	-0.59196700
H	-5.87048100	1.19829500	-0.77685900
C	-5.84148300	-0.90192700	2.22552700
H	-6.22868900	-0.73406000	3.23851500
H	-6.01217700	-1.95442800	1.97219400
H	-6.44110000	-0.29748800	1.53507800
C	-3.06264500	-1.33647200	3.49816400
H	-2.04231500	-0.94936700	3.59056000
H	-2.98593700	-2.42091000	3.38703300
H	-3.57711200	-1.13552300	4.44730400
C	-3.87520600	1.39489500	2.70162600
H	-4.10098200	1.41369800	3.77613100
H	-4.56896900	2.07069600	2.19749000
H	-2.86400600	1.79296100	2.56700000
C	-0.42330000	-1.52429000	1.17520500
C	-0.37765200	0.80338500	0.15035500
C	0.44499500	-1.13473900	-1.13494400
C	3.69346800	3.49076100	-1.60524800
H	3.33394300	4.04929700	-2.48393900
H	4.73837300	3.77889000	-1.41318200
C	2.82646000	3.84872100	-0.41431800
H	2.84317400	4.94315100	-0.28869800
H	1.78882500	3.53132800	-0.58323400
C	2.64477000	3.56187300	1.94484500
H	1.57693900	3.33488000	1.83475700
H	2.76274100	4.63832800	2.14727500
C	3.22433100	2.77974100	3.10616700
H	4.31604000	2.91926000	3.14901200
H	2.78953600	3.15994300	4.04399300
C	3.44373300	0.57161500	3.97216600
C	2.98251700	-0.85853600	3.75897900
C	3.51189300	-2.71378200	2.33087000
H	2.66201100	-3.21059500	2.81795800
H	4.44644400	-3.06114300	2.79676700
C	3.48296800	-3.07263400	0.85515400
H	3.68443100	-4.15102600	0.75234400
H	2.49095800	-2.86961300	0.43089000
C	4.60026400	-2.62909100	-1.21152000
H	3.62387100	-2.56225200	-1.70943100
H	4.98165100	-3.65716700	-1.33109600
C	5.60316700	-1.66117100	-1.82374400
H	6.52588700	-1.68536300	-1.23462900
H	5.83847100	-1.97946900	-2.85009200
C	4.44900700	0.13599700	-2.96596100
C	4.40081400	1.65248200	-2.94942200
H	4.54421600	0.61975800	3.95811900
H	3.09495700	0.91301700	4.96002300
H	1.88921900	-0.93589800	3.82405600
H	3.42859200	-1.47944600	4.55059600
H	4.96932400	-0.18456300	-3.88169700
H	3.43213800	-0.27948600	-2.97787600
H	3.96122000	2.01313800	-3.89278100
H	5.42351700	2.04956800	-2.86413900

### Complex 2Mo

K	-3.33419200	-0.24351600	0.25819800
B	3.73166800	0.35116600	0.12879100
Mo	1.12121300	0.56415200	-0.25519100
O	-1.46505300	2.30302000	-0.00159800
O	-1.00081500	-1.48313000	-1.24400500
O	0.55212000	-0.53956700	2.61158500
O	-2.86390500	-1.66434900	2.62206400
O	-3.54845800	1.03178200	2.89874700
O	-4.90629000	2.31108000	0.70758300
O	-5.16553100	0.83066400	-1.60665000
O	-4.67427400	-1.91321900	-1.79558000
O	-3.51020000	-3.25569800	0.48310400
Si	3.59124000	-2.23105200	-1.38313300
C	3.27835700	-0.36671500	-1.13251300
C	2.73136400	0.44301600	-2.22062400
C	2.51092700	-0.10688700	-3.53143600
H	2.80115000	-1.13288800	-3.70879100
C	1.99894400	0.61714100	-4.58050900
H	1.88293600	0.14828200	-5.55428300
C	1.62709900	1.96770000	-4.39298900
H	1.20973600	2.54549900	-5.21258900
C	1.81338100	2.54896700	-3.16114500
H	1.54271100	3.59063700	-3.04132700
C	2.38239700	1.84519300	-2.05431000
C	2.67864300	2.55488900	-0.79458700
C	2.36099200	3.93826500	-0.62095600
H	1.85589400	4.48722800	-1.40611200
C	2.69378100	4.61152900	0.53405900
H	2.44982400	5.66666400	0.62844500
C	3.34334500	3.93828100	1.59264500
H	3.60534300	4.47321700	2.50152800
C	3.64189500	2.59973500	1.45745400
H	4.14638200	2.08019200	2.26553500
C	3.34081100	1.86105500	0.27142500
C	4.67846700	-0.26159200	1.25414700
C	4.26231000	-0.63386900	2.54730900
H	3.21161700	-0.56474800	2.81391700
C	5.16551900	-1.11112600	3.50287200
H	4.80525200	-1.39960500	4.48769600
C	6.52540400	-1.21929600	3.19667600
H	7.22880900	-1.58994000	3.93788900
C	6.96965200	-0.84211900	1.92585300
H	8.02475800	-0.91562400	1.67283800
C	6.05675800	-0.37177000	0.97634900
H	6.42456100	-0.08448400	-0.00688200
C	2.13657000	-3.19943500	-2.15754700
H	2.46185000	-4.23840200	-2.30169800
H	1.76759000	-2.83272300	-3.11883600
H	1.28456900	-3.21517100	-1.46933200
C	5.12304400	-2.48927200	-2.48858400
H	5.01901000	-2.02316000	-3.47494500
H	5.31281800	-3.55925700	-2.64175100
H	6.01244500	-2.05785900	-2.01474500
C	3.89564200	-3.18857300	0.22524400
H	3.88435000	-4.25957200	-0.01725400

H	3.10678900	-3.00403900	0.96180600	C	-3.15069300	-1.03107200	0.46220900
H	4.85228800	-2.95832900	0.69855200	C	-2.60807100	-2.19901100	-0.23406600
C	-0.45405400	1.69230700	-0.07852600	C	-2.45640000	-3.46840400	0.42750100
C	-0.13998700	-0.74474700	-0.89901600	H	-2.78846000	-3.54890000	1.45232300
C	0.77651400	-0.12082200	1.53553900	C	-1.95442900	-4.58663200	-0.18955800
C	-2.63826600	-0.97772000	3.85334900	H	-1.89221700	-5.52302000	0.35863800
C	-3.65452400	0.13806200	3.99946400	C	-1.52076400	-4.52000000	-1.53451700
C	-4.37349100	2.18313300	3.03177300	H	-1.11251100	-5.39754700	-2.02732800
H	-4.04338200	2.78626900	3.89243800	C	-1.63003300	-3.33345800	-2.21675100
H	-5.42017200	1.88410400	3.19938100	H	-1.30847900	-3.30476900	-3.25020300
C	-4.27287300	3.01824100	1.77302200	C	-2.18531900	-2.15316800	-1.62633200
H	-4.78123100	3.98154000	1.93959800	C	-2.38926500	-0.93866600	-2.43950100
H	-3.21958400	3.20947500	1.53081400	C	-1.99668300	-0.88293900	-3.81598600
C	-4.77116600	2.95229000	-0.55573700	H	-1.50233000	-1.72802700	-4.27852400
H	-3.71333500	2.98619400	-0.84919400	C	-2.24441700	0.22962000	-4.58629500
H	-5.15052400	3.98618800	-0.50767100	H	-1.94830000	0.23368600	-5.63218000
C	-5.58789800	2.19158500	-1.58250200	C	-2.87520000	1.36509700	-4.02522700
H	-6.65921100	2.23799800	-1.33522500	H	-3.06971000	2.24042300	-4.63898500
H	-5.43438100	2.66374600	-2.56464400	C	-3.24149600	1.34619200	-2.69890000
C	-5.63571200	0.08045200	-2.72338300	H	-3.73174000	2.21165400	-2.26561900
C	-5.87441300	-1.36081200	-2.31226300	C	-3.03613200	0.20417800	-1.85971700
C	-4.76207800	-3.31421600	-1.54541500	C	-4.43644200	1.39918800	0.10902200
H	-4.87081100	-3.85755900	-2.49714800	C	-3.97894700	2.70059700	0.39539100
H	-5.63944700	-3.53234100	-0.91730200	H	-2.91570200	2.91741400	0.35489800
C	-3.50347000	-3.77762100	-0.84267800	C	-4.85840400	3.72712200	0.75440900
H	-3.49360800	-4.87920500	-0.81604100	H	-4.46734000	4.71644200	0.98037300
H	-2.61646000	-3.43001800	-1.38836200	C	-6.23376800	3.48573400	0.82657600
C	-2.30903300	-3.52345300	1.20333300	H	-6.91849000	4.28221700	1.10627500
H	-1.46202100	-3.02660700	0.71321500	C	-6.71757100	2.20777500	0.53219300
H	-2.10655700	-4.60639800	1.22672000	H	-7.78478500	2.00434200	0.57869700
C	-2.46492000	-3.03241100	2.63034900	C	-5.82871100	1.18714900	0.17898700
H	-3.22098500	-3.62759200	3.16495000	H	-6.22763200	0.20046200	-0.04772900
H	-1.49764600	-3.15104100	3.13868200	C	-3.63912500	0.59695600	3.14480200
H	-6.58752300	0.49003000	-3.09134000	H	-2.71087900	1.15216500	2.97112700
H	-4.89739300	0.13173000	-3.53606500	H	-3.74224000	0.44656900	4.22730100
H	-6.21062500	-1.92514100	-3.19769900	H	-4.46951000	1.22068100	2.80929800
H	-6.67001300	-1.40992100	-1.55161400	C	-2.37551700	-2.10551200	3.41390700
H	-3.45748600	0.66993900	4.94437600	H	-2.61230500	-3.17377900	3.47255800
H	-4.67366800	-0.27827100	4.04355700	H	-2.44370600	-1.70983800	4.43523000
H	-2.76827100	-1.66297100	4.70408200	H	-1.33382900	-2.00951200	3.09432900
H	-1.61367900	-0.58569400	3.86814200	C	-5.30204100	-1.92012600	2.52873300
				H	-5.33370700	-2.92087800	2.08139900
				H	-6.08424100	-1.31896600	2.05276100
				H	-5.55605700	-2.02068200	3.59162900
				C	0.66148000	-0.31277300	-1.48941900
				C	-0.56075400	1.50938500	0.09945500
				C	0.18199900	-0.92561200	1.02038500
				C	5.34639500	-2.39370700	-1.22342100
				C	5.00010700	-1.37788600	-2.29572600
				C	5.48733400	0.92908900	-2.84553200
				H	5.74850900	0.49595400	-3.82242200
				H	6.29527200	1.60161400	-2.53877600
				C	4.19974500	1.73082300	-2.97489000
				H	4.30664900	2.44073700	-3.81245700
				H	3.34069200	1.07865600	-3.18054000
				C	2.77546800	3.15565300	-1.68419900
<b>Complex 2W</b>							
K	3.40603500	0.37153400	0.33103300				
B	-3.51474900	0.19183700	-0.36920900				
O	1.68909500	-0.31804700	-2.09048800				
O	-0.31897400	2.62443500	0.40390100				
O	0.93411500	-1.29712400	1.85770600				
O	4.57109400	-2.13972500	-0.05710200				
O	5.43163300	-0.09218600	-1.84913900				
O	4.00463800	2.43773800	-1.75360000				
O	3.02303600	3.07985200	0.70313600				
O	3.21606600	1.46827000	2.96736700				
O	4.33243300	-1.15801300	2.59849400				
Si	-3.59185400	-1.10946500	2.32046700				
W	-0.95520800	-0.32058700	-0.42231300				

H	1.92682800	2.45992500	-1.72965900
H	2.68674100	3.85642200	-2.52980500
C	2.74161600	3.95060100	-0.39024300
H	3.49041400	4.75695200	-0.41129200
H	1.74080800	4.39028000	-0.28617300
C	2.60727300	3.56957800	1.97505700
C	3.41252500	2.87418100	3.05706900
C	3.87392600	0.73461500	3.99386600
H	3.47219200	1.01949200	4.97918300
H	4.95370100	0.95202800	3.98429800
C	3.63999200	-0.74678400	3.77818800
H	4.02641300	-1.29847000	4.65007700
H	2.56618800	-0.94744500	3.67628400
C	4.11980900	-2.52984800	2.26966200
H	3.05852800	-2.70335700	2.04672500
H	4.40973800	-3.17228900	3.11656300
C	4.98446000	-2.89170500	1.07834600
H	6.04121000	-2.67861400	1.30098800
H	4.88103400	-3.97048400	0.88030500
H	3.92059600	-1.38555500	-2.49764600
H	5.53201100	-1.65541400	-3.21906500
H	6.41795100	-2.32090900	-0.98391100
H	5.13957500	-3.40733800	-1.60213800
H	3.07996800	3.24476900	4.04004700
H	4.48259100	3.10951200	2.94238100
H	2.79842100	4.65070700	2.05336900
H	1.53177300	3.39130700	2.10340400

#### Complex 1Rh

B	-0.71100300	-0.55399400	-0.64000300
O	4.13416200	-0.23884100	2.00027100
O	0.03413400	-0.74393900	3.40684400
Rh	1.37226400	-0.33859000	0.71100500
Si	-1.19431200	2.40938700	-0.01960900
C	-0.16909300	0.90430000	-0.68152300
C	1.12652800	1.11584300	-1.21438400
C	2.01319000	-0.00750600	-1.45356300
C	1.54149000	-1.38321600	-1.50636900
C	0.23508900	-1.69457400	-1.10113400
C	1.66688600	2.49792900	-1.54457600
H	0.86103100	3.22558500	-1.61375700
H	2.17416300	2.48643800	-2.51451400
H	2.38366300	2.86582600	-0.80334700
C	3.43727400	0.27623400	-1.90090600
H	3.48300600	0.39677300	-2.99222600
H	4.11568100	-0.53527400	-1.63586000
H	3.83195800	1.18926600	-1.45421600
C	2.49791600	-2.44485200	-2.02051800
H	1.99551400	-3.40166300	-2.15345700
H	3.34036100	-2.60896500	-1.34038300
H	2.91703900	-2.15346800	-2.99004500
C	-0.22924400	-3.14007200	-1.13082300
H	-0.31269300	-3.49990000	-2.16554100
H	-1.21430600	-3.24643400	-0.67640900
H	0.45715900	-3.81442100	-0.60721300
C	-2.22828600	-0.90241100	-0.32148200

C	-2.67998200	-1.57781700	0.82838000
H	-1.97018000	-1.85588100	1.60324200
C	-4.02865800	-1.89539800	1.01455600
H	-4.34246500	-2.40653600	1.92115900
C	-4.97193500	-1.55738100	0.03944400
H	-6.02067000	-1.80384100	0.18114100
C	-4.55034300	-0.90193000	-1.12074900
H	-5.27125700	-0.63795900	-1.89050800
C	-3.19978000	-0.58082300	-1.29140800
H	-2.89546700	-0.06817100	-2.20209500
C	-2.52185500	1.92418500	1.24791800
H	-2.94088600	2.84881800	1.66375800
H	-2.10353400	1.35059600	2.08078000
H	-3.33990800	1.34352100	0.81935500
C	-0.09228000	3.66667200	0.90810400
H	-0.72091600	4.25145900	1.58944200
H	0.42338200	4.37398700	0.25312700
H	0.66386700	3.15789900	1.51596600
C	-2.06029400	3.28529200	-1.47581400
H	-2.78008100	2.61704600	-1.95970000
H	-1.35715600	3.62743700	-2.24260400
H	-2.61128700	4.16199200	-1.11576400
C	3.08993100	-0.27655400	1.50989000
C	0.52529800	-0.59572200	2.37363100

#### Complex 2Rh

B	0.87654000	0.57143900	-0.55578300
O	0.67310900	-0.83807600	3.45118300
O	-3.45286300	0.55546700	2.86648600
Rh	-1.03393600	-0.05613400	1.08311900
Si	1.21495300	-2.46627000	-0.46314100
C	0.21388800	-0.82079000	-0.66060600
C	-1.16206900	-0.88325300	-1.14202400
C	-1.77679200	-2.10381200	-1.57473200
H	-1.15538400	-2.98202900	-1.68156000
C	-3.11169400	-2.19546500	-1.88509600
H	-3.52540900	-3.13906400	-2.22878100
C	-3.94874700	-1.06504700	-1.73615100
H	-5.01201900	-1.14059300	-1.94358600
C	-3.41053900	0.13596800	-1.34433700
H	-4.06860500	0.99182900	-1.26244500
C	-2.01014700	0.29997400	-1.07902300
C	-1.43201000	1.66881900	-0.96523200
C	-2.24159800	2.82373400	-1.08774000
H	-3.31110800	2.74150700	-1.23695800
C	-1.68537200	4.09418200	-1.04796600
H	-2.32922800	4.96230800	-1.15995400
C	-0.30185500	4.26026000	-0.87704100
H	0.13126500	5.25618800	-0.85330600
C	0.50250600	3.13910500	-0.73891100
H	1.57162100	3.26118100	-0.59883600
C	-0.02678200	1.82610100	-0.77401200
C	2.42541800	0.81135000	-0.32139400
C	2.96658700	1.27772900	0.89161900
H	2.31030000	1.44758000	1.74201300
C	4.33504500	1.52425400	1.03818100

H	4.72218600	1.87063600	1.99298800
C	5.20305700	1.32995200	-0.04034500
H	6.26657900	1.52327000	0.06975500
C	4.68855000	0.88929700	-1.26322100
H	5.35129000	0.74198200	-2.11217700
C	3.32034100	0.63247100	-1.39534700
H	2.94286800	0.28713400	-2.35589500
C	2.76829600	-2.30348200	0.61589500
H	2.54652600	-1.91725300	1.61464400
H	3.53687300	-1.66822900	0.17342800
H	3.18868100	-3.30922300	0.74062500
C	1.77035400	-3.05386800	-2.19098600
H	2.44612400	-2.32672700	-2.65318700
H	0.92883600	-3.20479000	-2.87534700
H	2.31042800	-4.00465000	-2.11208800
C	0.17675700	-3.84728800	0.36274800
H	0.83227200	-4.46507900	0.98684000
H	-0.30375000	-4.51482600	-0.35976400
H	-0.60679900	-3.43846000	1.00862300
C	0.04598900	-0.53408600	2.53263900
C	-2.54259200	0.34136200	2.19744000

**[CpCr(CO)<sub>3</sub>]<sup>-</sup>**

C	-1.83314700	-1.15516500	0.38581600
C	1.10558200	1.29769400	-0.75129300
C	-1.83425200	0.70934500	-0.97364600
C	1.10574300	-1.29825100	-0.75025000
C	1.12313300	0.00062500	1.48652000
Cr	0.09078600	-0.00003800	-0.00122500
O	1.73301600	-2.16586800	-1.24844400
H	-1.82209500	2.18422700	0.71904600
C	-1.83424900	-0.71051400	-0.97285000
H	-1.79510100	0.00124800	2.29876600
C	-1.83313600	1.15551400	0.38452500
H	-1.81825800	1.34355300	-1.85037100
H	-1.81824700	-1.34570400	-1.84886300
H	-1.82211700	-2.18350400	0.72148500
C	-1.82295200	0.00064100	1.21668600
O	1.73272800	2.16499100	-1.25020400
O	1.76383300	0.00109800	2.47818400

**[CpMo(CO)<sub>3</sub>]<sup>-</sup>**

C	-2.05829200	-1.15600600	0.38056700
C	1.23966000	1.36954600	-0.78983200
C	-2.05491500	0.71076000	-0.97806100
C	1.23968600	-1.36873800	-0.79118400
C	1.24968600	-0.00071800	1.57387300
O	1.88709200	-2.22489800	-1.28507700
H	-2.06373800	2.18429600	0.71721500
C	-2.05489200	-0.70982000	-0.97874900
H	-2.03918800	-0.00111100	2.29614800
C	-2.05829900	1.15563300	0.38168600
H	-2.05336700	1.34650000	-1.85410700
H	-2.05329700	-1.34468500	-1.85543200
H	-2.06372100	-2.18499100	0.71510700
C	-2.04796200	-0.00058900	1.21351800

O	1.88713900	2.22601500	-1.28309500
O	1.90344200	-0.00118800	2.55792600
Mo	0.09818800	0.00000300	-0.00018700

**[CpW(CO)<sub>3</sub>]<sup>-</sup>**

C	-2.04532300	-1.16708400	0.35615500
C	1.20623600	1.38857400	-0.75852400
C	-2.04038200	0.73405000	-0.96136700
C	1.20661100	-1.35075100	-0.82313800
C	1.21929700	-0.03678700	1.57227700
O	1.84089800	-2.20694800	-1.34193400
H	-2.05339800	2.16894000	0.76944800
C	-2.04023500	-0.68856100	-0.99463800
H	-2.01960200	-0.05390200	2.29797700
C	-2.04559500	1.14886800	0.41033300
H	-2.04076000	1.38893500	-1.82259100
H	-2.04048300	-1.30246000	-1.88553900
H	-2.05288000	-2.20283600	0.66717400
C	-2.02913600	-0.02858900	1.21607100
O	1.84119400	2.26686800	-1.23808200
O	1.86146300	-0.06062000	2.56781700
W	0.07121400	0.00011600	-0.00043100

**[(Mesitylene)Cr(CO)<sub>3</sub>]**

C	1.34585000	0.54016400	-1.31883100
C	-1.51973200	0.51723600	-1.40065700
C	-1.51919700	-1.47209100	0.25297400
C	-1.51908000	0.95447400	1.14876000
O	-2.17794300	0.84944600	-2.30058600
O	-2.17698300	-2.41782100	0.41534900
C	1.35264500	-0.86376300	-1.11487800
C	1.34617700	0.87201900	1.12684400
O	-2.17705900	1.56802200	1.88638400
C	1.34627300	-1.41186500	0.19144200
C	1.35265900	1.39735500	-0.19098000
H	1.33260000	-1.52782800	-1.97264200
C	1.35287700	-0.53331300	1.30535300
H	1.33339500	-0.94423300	2.30929600
H	1.33286500	2.47224900	-0.33708700
Cr	-0.44278400	-0.00012800	0.00000800
C	1.38713100	1.11008300	-2.71482400
H	2.42898800	1.22820600	-3.03745000
H	0.88615000	0.45239000	-3.42980100
H	0.90730400	2.09112700	-2.75980400
C	1.38800900	1.79623100	2.31823600
H	2.43002600	2.01485800	2.58263300
H	0.88885100	2.74506600	2.10541700
H	0.90669400	1.34572300	3.19005600
C	1.38807400	-2.90584100	0.39564100
H	2.43006900	-3.24412800	0.45327700
H	0.88828800	-3.19648300	1.32326200
H	0.90733600	-3.43519800	-0.43102100



<b>[(Mesitylene)Mo(CO)<sub>3</sub>]</b>			
C	1.53179100	-1.17131400	0.81695200
C	-1.63329900	-1.30143200	0.90885900
C	-1.63329900	1.43766900	0.67282800
C	-1.63365000	-0.13628500	-1.58113200
O	-2.28979300	-2.09002900	1.45957900
O	-2.28978700	2.30888200	1.08047700
C	1.54679000	0.12084600	1.40881800
C	1.53142300	-0.12198700	-1.42319000
O	-2.29043600	-0.21878900	-2.53925000
C	1.53168400	1.29335400	0.60567600
C	1.54652700	-1.28060900	-0.60007200
H	1.54798800	0.21350900	2.48975100
C	1.54646200	1.15981600	-0.80929700
H	1.54740400	2.04961400	-1.42999300
H	1.54754600	-2.26306700	-1.06026800
C	1.59325700	-2.40766300	1.67943100
H	2.63969200	-2.67820600	1.86804000
H	1.10799900	-2.24364600	2.64489600
H	1.10780900	-3.25705600	1.19221600
C	1.59256600	-0.25075800	-2.92514400
H	2.63893500	-0.27963600	-3.25389600
H	1.10654500	-1.16849400	-3.26579700
H	1.10773000	0.59628500	-3.41702600
C	1.59309600	2.65847100	1.24514300
H	2.63952300	2.95715700	1.38503600
H	1.10774400	3.41257100	0.62043000
H	1.10778600	2.66117900	2.22441100
Mo	-0.45063500	-0.00003300	0.00006000

<b>[(Mesitylene)W(CO)<sub>3</sub>]</b>			
C	1.57709200	-0.04898700	-1.43083000
C	-1.53465300	-0.05361500	-1.58442700
C	-1.53360100	-1.34631900	0.83917600
C	-1.53381900	1.39907600	0.74672600
O	-2.18645200	-0.08619700	-2.55125300
O	-2.18482000	-2.16765500	1.35101200
C	1.59682600	-1.25139400	-0.66680200
C	1.57730500	1.26382200	0.67194900
O	-2.18504000	2.25303600	1.20205800
C	1.57823900	-1.21363200	0.75749200
C	1.59608500	1.20338200	-0.75138500
H	1.59260600	-2.20869300	-1.17623800
C	1.59698600	0.04922300	1.41679200
H	1.59291400	0.08665000	2.50055500
H	1.59123300	2.12322800	-1.32568600
C	1.63064200	-0.10127900	-2.93718300
H	2.67560100	-0.11336400	-3.27116300
H	1.14196700	-1.00038200	-3.32098000
H	1.14271900	0.76944000	-3.38244200
C	1.63100700	2.59445000	1.37995200
H	2.67600300	2.89013500	1.53546300

H	1.14139900	3.37629200	0.79386500
H	1.14412800	2.54429900	2.35714600
C	1.63309200	-2.49199600	1.55591400
H	2.67835100	-2.77403800	1.73344700
H	1.14424300	-2.37538600	2.52644000
H	1.14616900	-3.31349100	1.02438200
W	-0.35281100	-0.00019700	0.00008700

<b>[CpRh(CO)<sub>2</sub>]</b>			
Rh	0.19615400	-0.00016000	-0.00776600
C	1.50736900	-1.34959200	0.01222500
O	2.30421000	-2.18461800	0.01746400
C	1.50639800	1.35029600	0.01222900
O	2.30229000	2.18621900	0.01748500
C	-1.77461100	-1.14298900	-0.38120800
C	-1.86142000	-0.69816000	0.99742400
C	-1.86131600	0.70318300	0.99333400
C	-1.77540500	1.14028600	-0.38806100
C	-1.82817700	-0.00373200	-1.23276500
H	-1.78385500	-2.17572400	-0.70484400
H	-1.88426200	-1.34035000	1.86714700
H	-1.88461000	1.35038400	1.85933700
H	-1.78516000	2.17114800	-0.71757000
H	-1.81806600	-0.00681900	-2.31325700

<b>[(Mesitylene)Rh(CO)<sub>2</sub>]<sup>+</sup></b>			
O	2.84701200	2.02069600	0.00043200
O	2.64402000	-2.26787500	0.00055200
Rh	0.59622300	-0.02787900	0.00006300
C	-1.44109200	-0.63722100	1.25820000
C	-1.38747100	0.76715000	1.23357000
C	-1.29802500	1.47975000	-0.00043200
C	-1.38718000	0.76678500	-1.23416900
C	-1.44043700	-0.63763600	-1.25840300
C	-1.26289500	2.98636500	-0.00055300
H	-2.29211000	3.36639200	0.00182600
H	-0.76821600	3.38167800	-0.89078900
H	-0.76423400	3.38171800	0.88746200
C	-1.57881000	-1.40958400	-2.54213600
H	-2.64053200	-1.61257400	-2.72950000
H	-1.06577300	-2.37318600	-2.49197000
H	-1.18973800	-0.84805400	-3.39423400
C	2.00951100	1.24359300	0.00022900
C	1.88140600	-1.41605300	0.00028200
C	-1.35132900	-1.31434800	0.00001800
H	-1.39103300	1.32473100	2.16500800
H	-1.39054900	1.32401700	-2.16581500
H	-1.33405800	-2.40085300	0.00024400
C	-1.58040200	-1.40887700	2.54201800
H	-1.19266300	-0.84686700	3.39439400
H	-2.64224400	-1.61237200	2.72819900
H	-1.06680400	-2.37220800	2.49270900

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