ELECTRONIC SUPPORTING INFORMATION

Base Metal Complexes featuring a New Pyrazole-Derived PCP-Pincer Ligand

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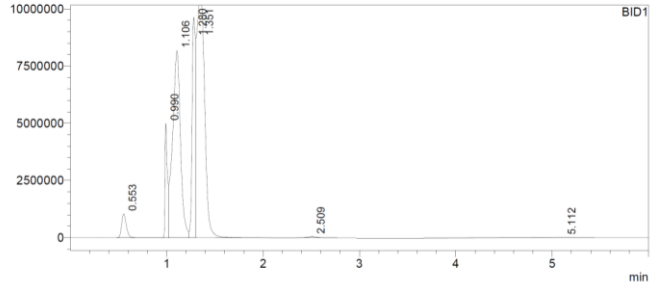
NMR DATA S3-S20

Headspace-GC data

[Mn(κ^3*P,C,P*-PCP-*i*Pr)(CO)$_3$] (6)

The septum of the microwave vial was penetrated with a Hamilton syringe and 200 µL of the headspace was taken up and injected in the GC.

<Chromatogram>



<Peak Table>

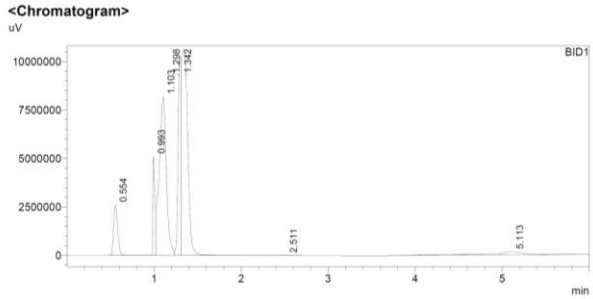
BID1

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	0.553	3509316	1038483	14672.123	ppm		H2
2	0.990	8330159	4994621	0.000			
3	1.106	46847644	8179265	0.000		V	
4	1.280	23280318	9633214	0.000		V	
5	1.351	60977730	10589149	0.000		V	
6	2.509	402168	58071	0.000			
7	5.112	397335	10285	0.000			
Total		143744672	34503087				

[Co(κ^3*P,C,P*-PCP-*i*Pr)(CO)$_2$] (9)

The septum of the microwave vial was penetrated with a Hamilton syringe and 200 µL of the headspace was taken up and injected in the GC.

<Chromatogram>



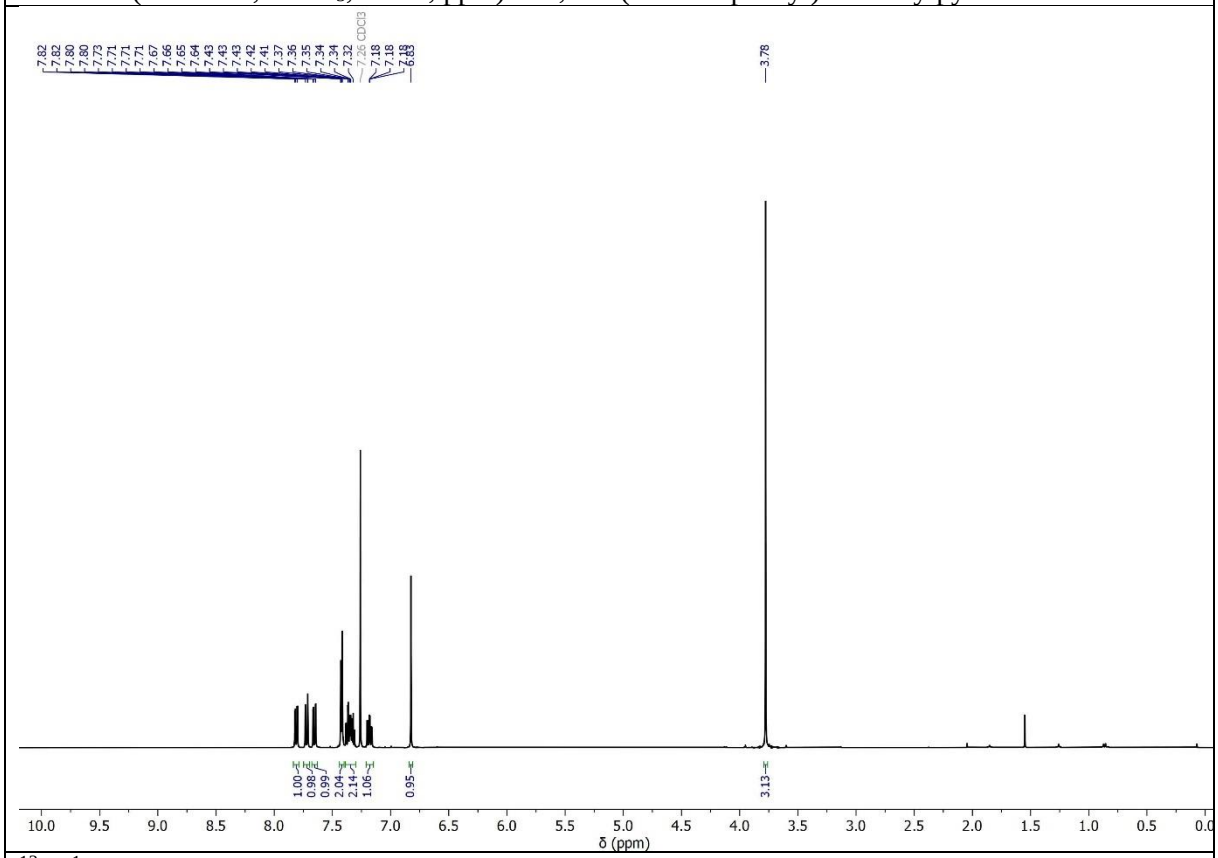
<Peak Table>

BID1

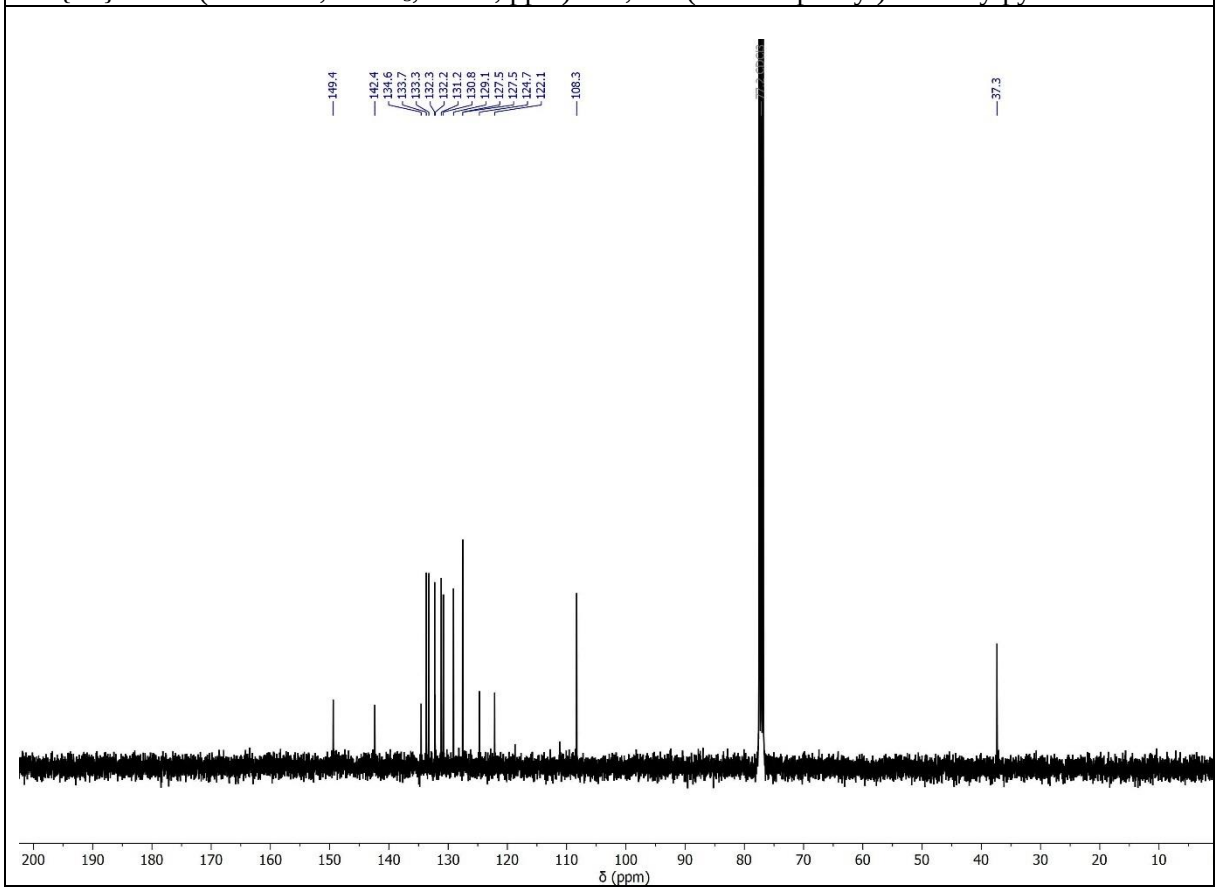
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	0.554	8324048	2606409	34802.067	ppm		H2
2	0.993	8726095	5109459	0.000			
3	1.103	45994345	8194778	0.000		V	
4	1.298	24257430	10252043	0.000		V	
5	1.342	51601570	10632172	0.000		V	
6	2.511	57498	8820	0.000			
7	5.113	4936138	161076	0.000			
Total		143897124	36964759				

NMR data

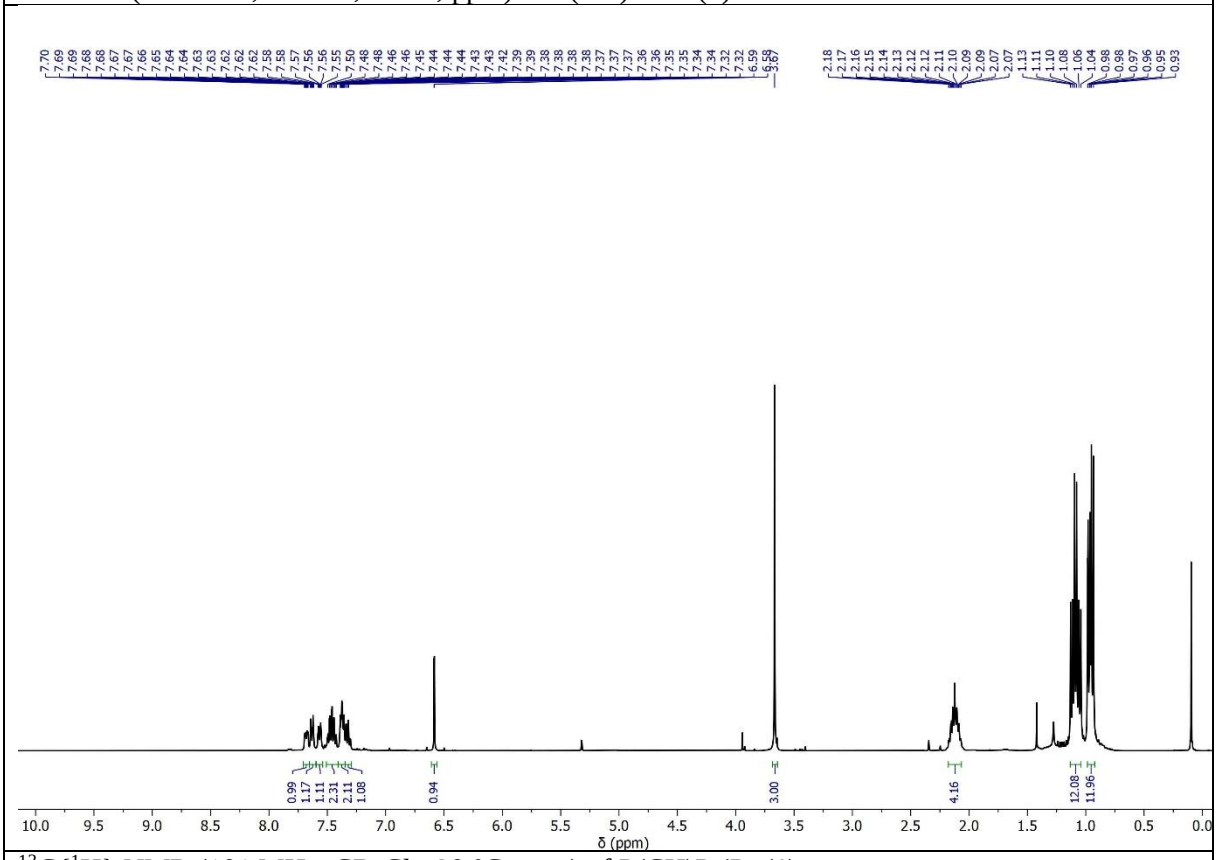
^{1}H NMR (400 MHz, $CDCl_3$, 20 °C, ppm) of 3,5-Di(2-bromophenyl)-1-methylpyrazole



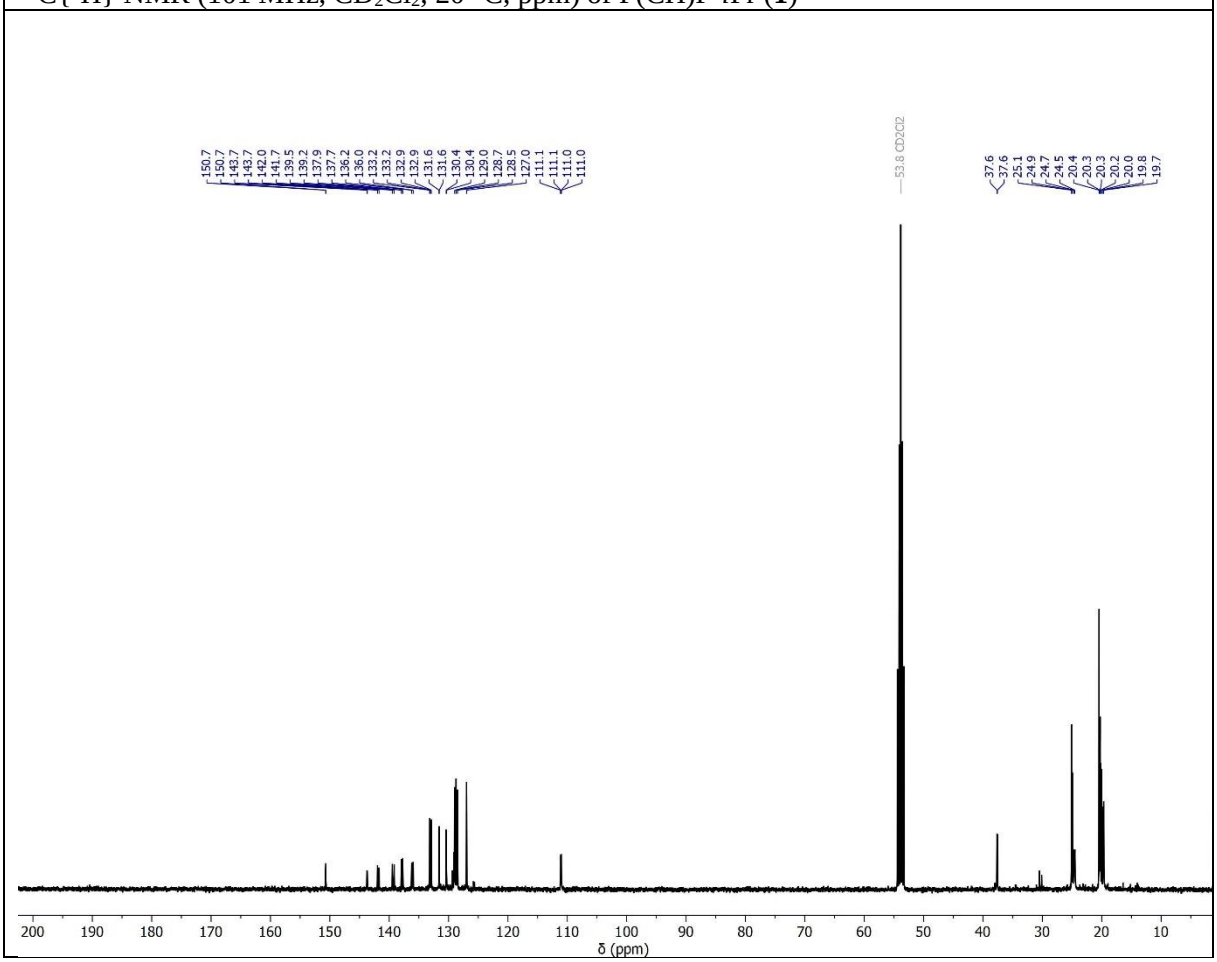
$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$, 20 °C, ppm) of 3,5-Di(2-bromophenyl)-1-methylpyrazole



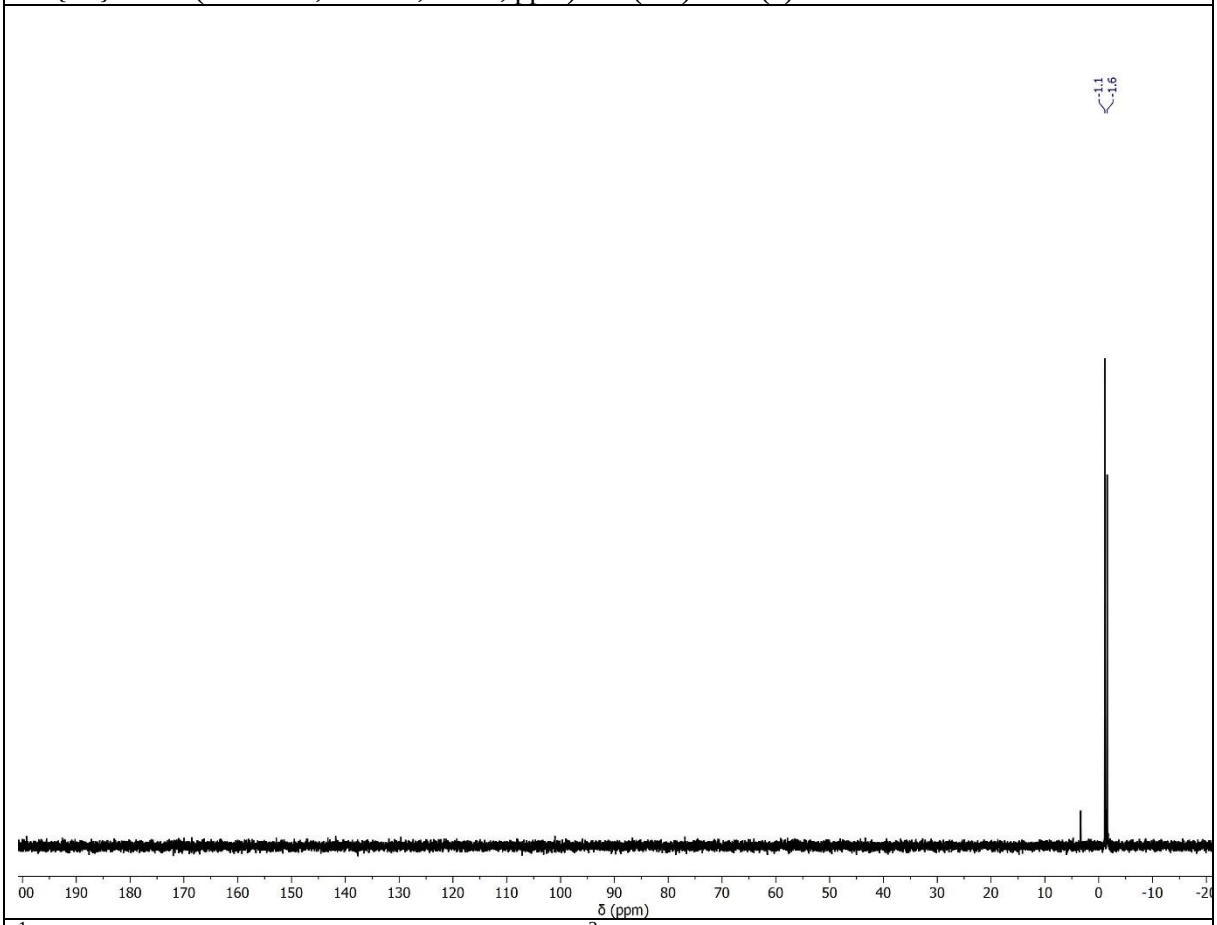
^{1}H NMR (400 MHz, CD_2Cl_2, 20 °C, ppm) of P(CH)P-*i*Pr (**1**)



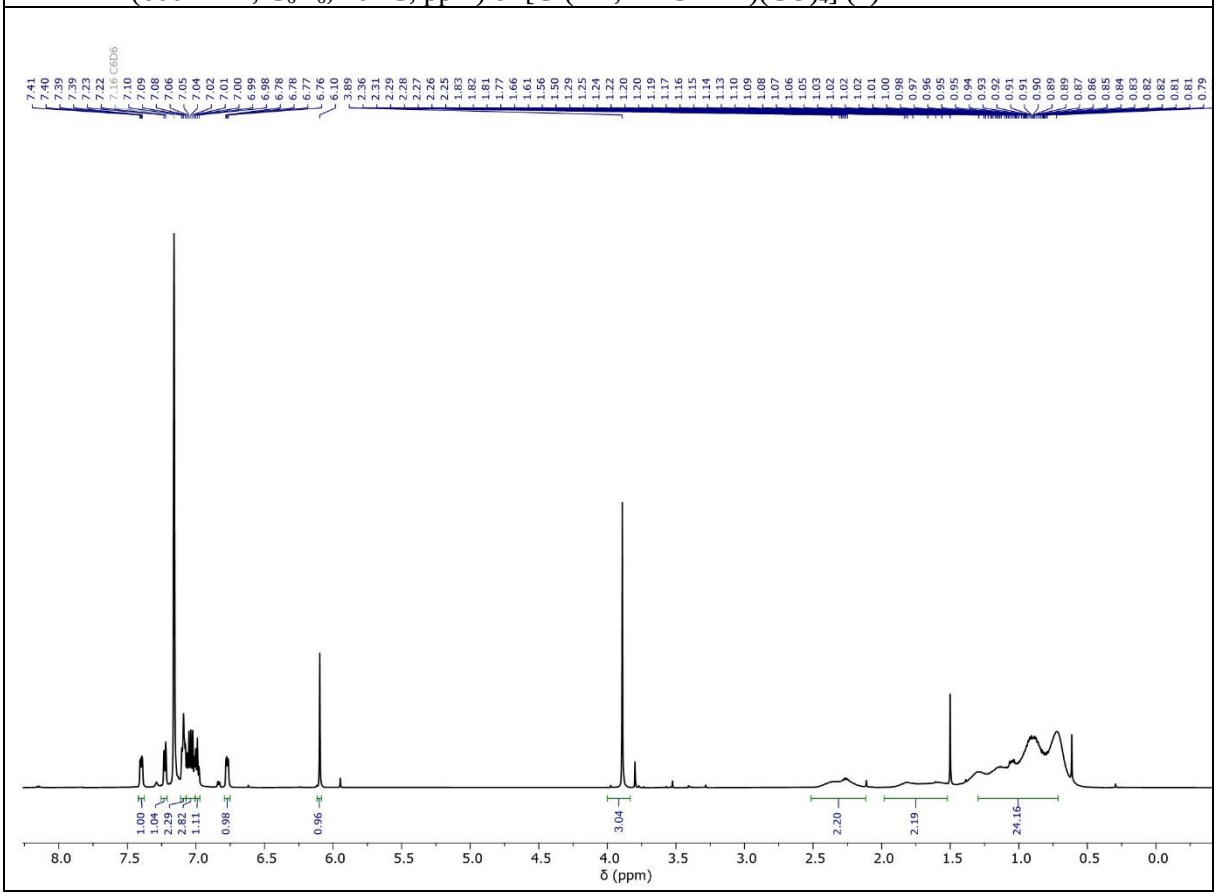
^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2, 20 °C, ppm) of P(CH)P-*i*Pr (**1**)



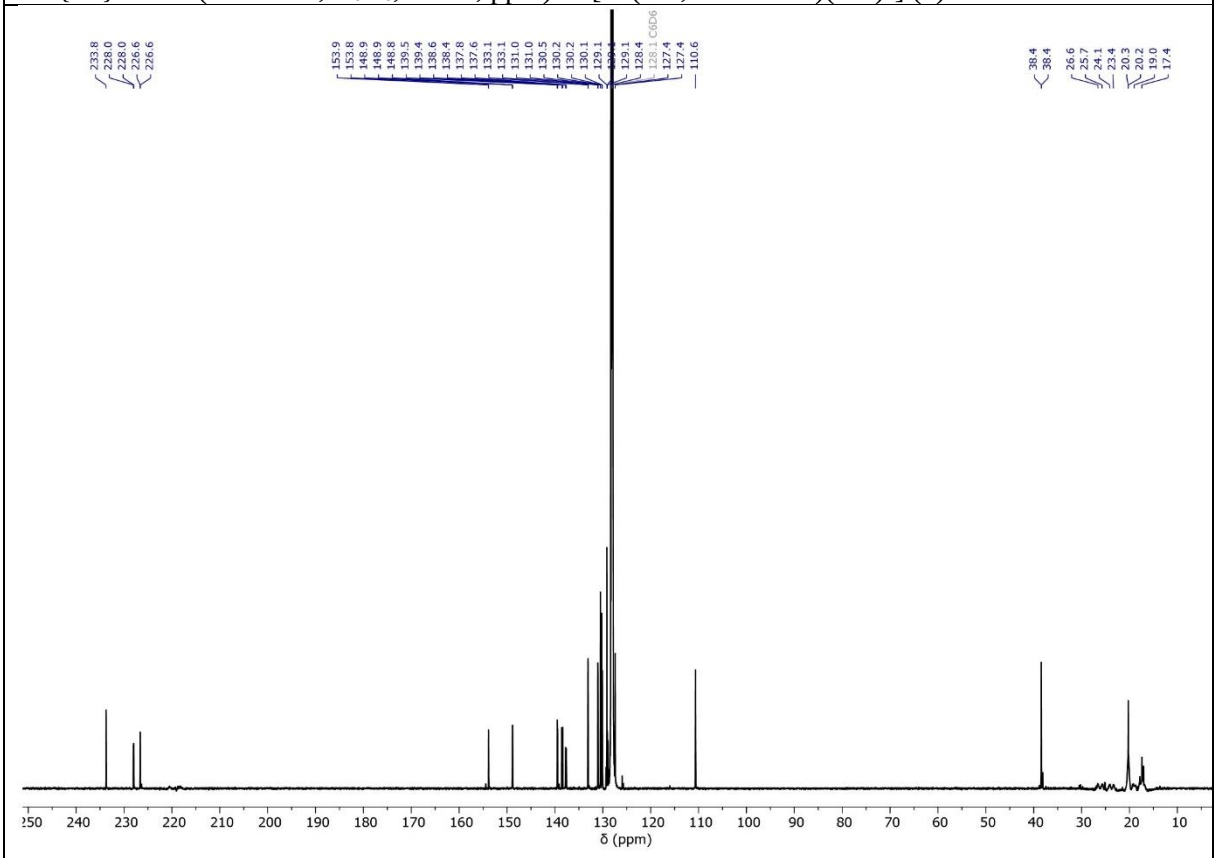
$^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2, 20 °C, ppm) of P(CH)P-*i*Pr (**1**)



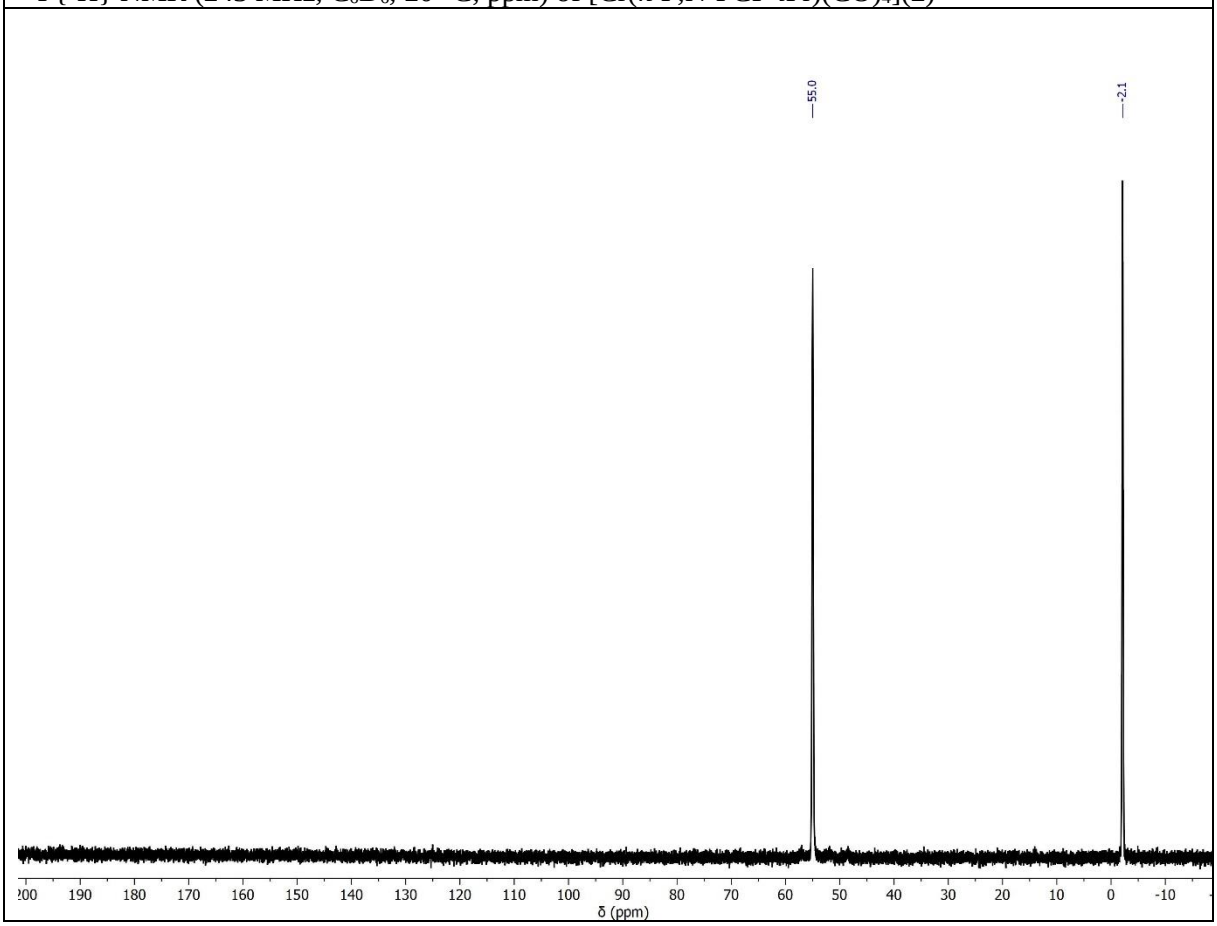
^{1}H NMR (600 MHz, C_6D_6, 20 °C, ppm) of [Cr(κ^{2}P,N-PCP-*i*Pr)(CO)$_4$] (**2**)



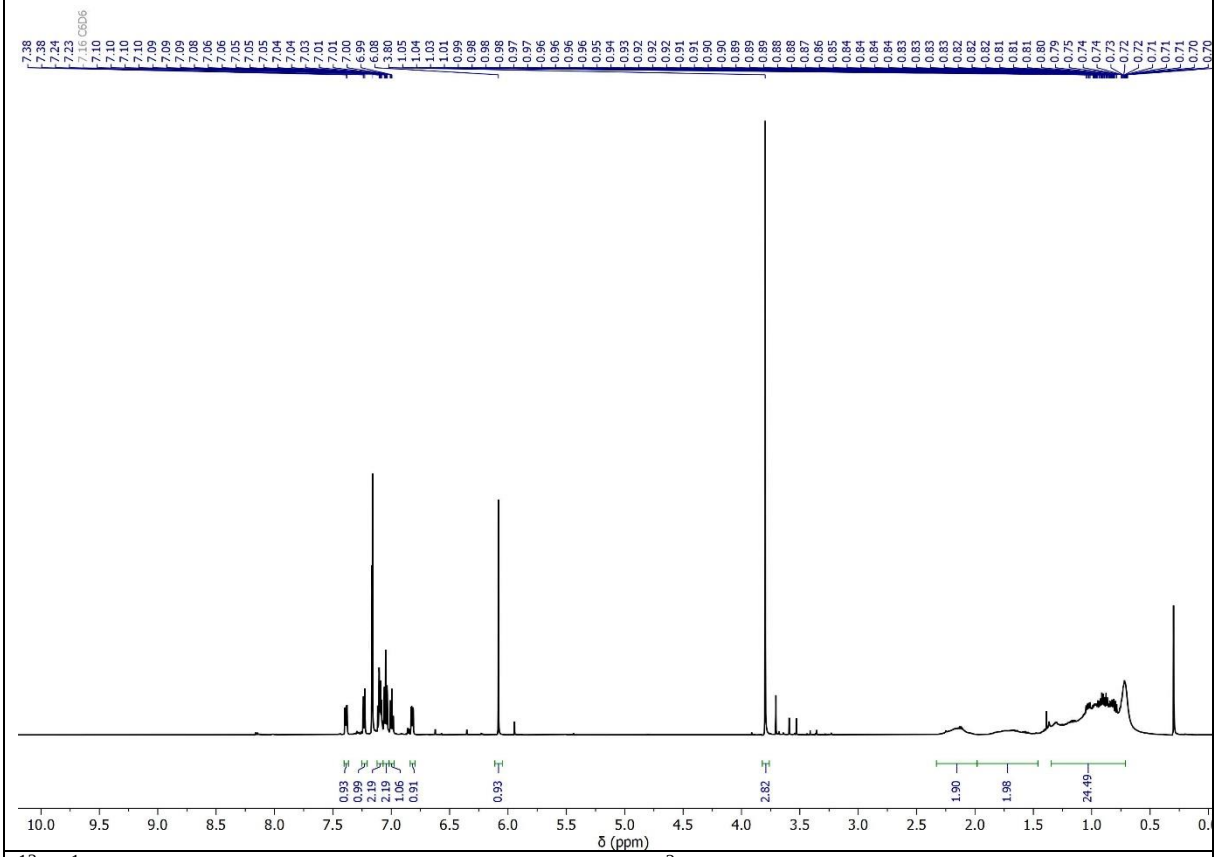
$^{13}C\{^{1}H\}$ NMR (151 MHz, C_6D_6, 20 °C, ppm) of [Cr(κ^{2}P,N-PCP-*i*Pr)(CO)$_4$] (**2**)



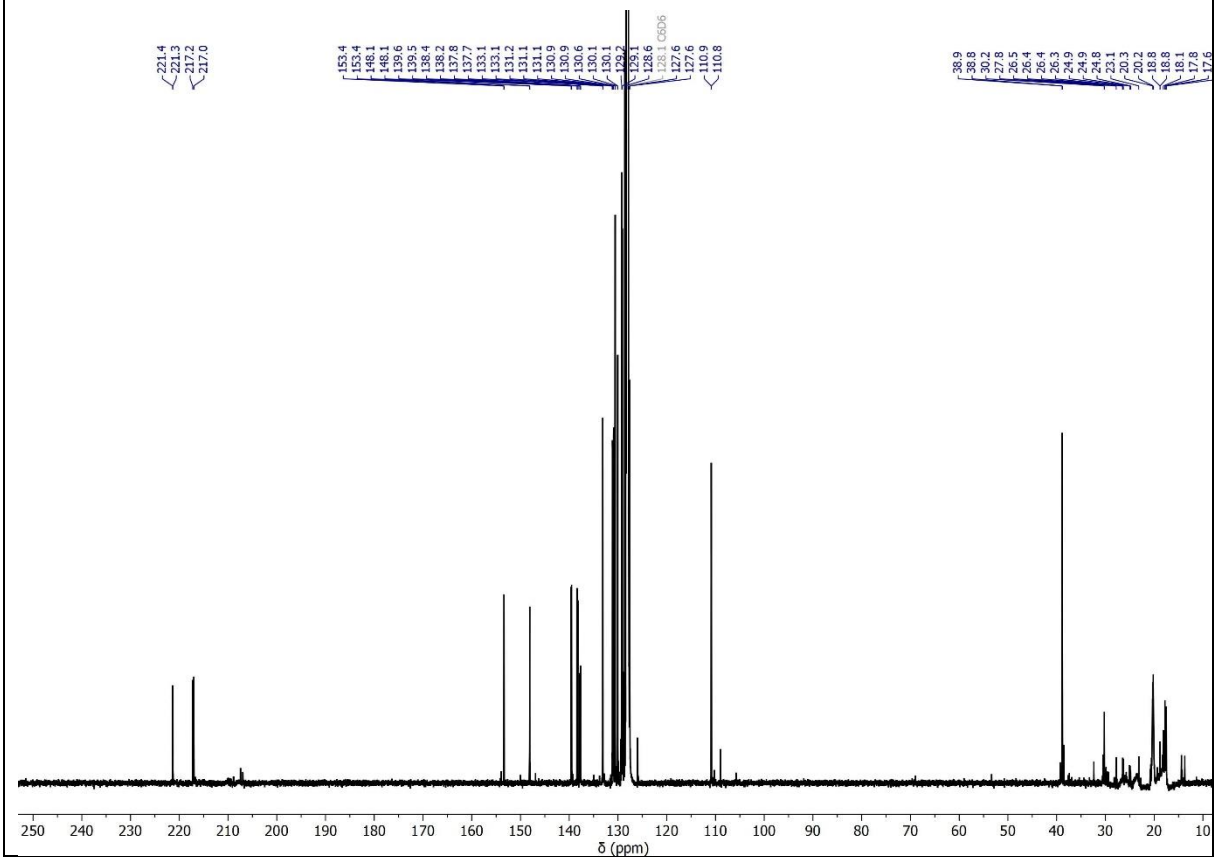
$^{31}P\{^{1}H\}$ NMR (243 MHz, C_6D_6, 20 °C, ppm) of [Cr(κ^{2}P,N-PCP-*i*Pr)(CO)$_4$](**2**)



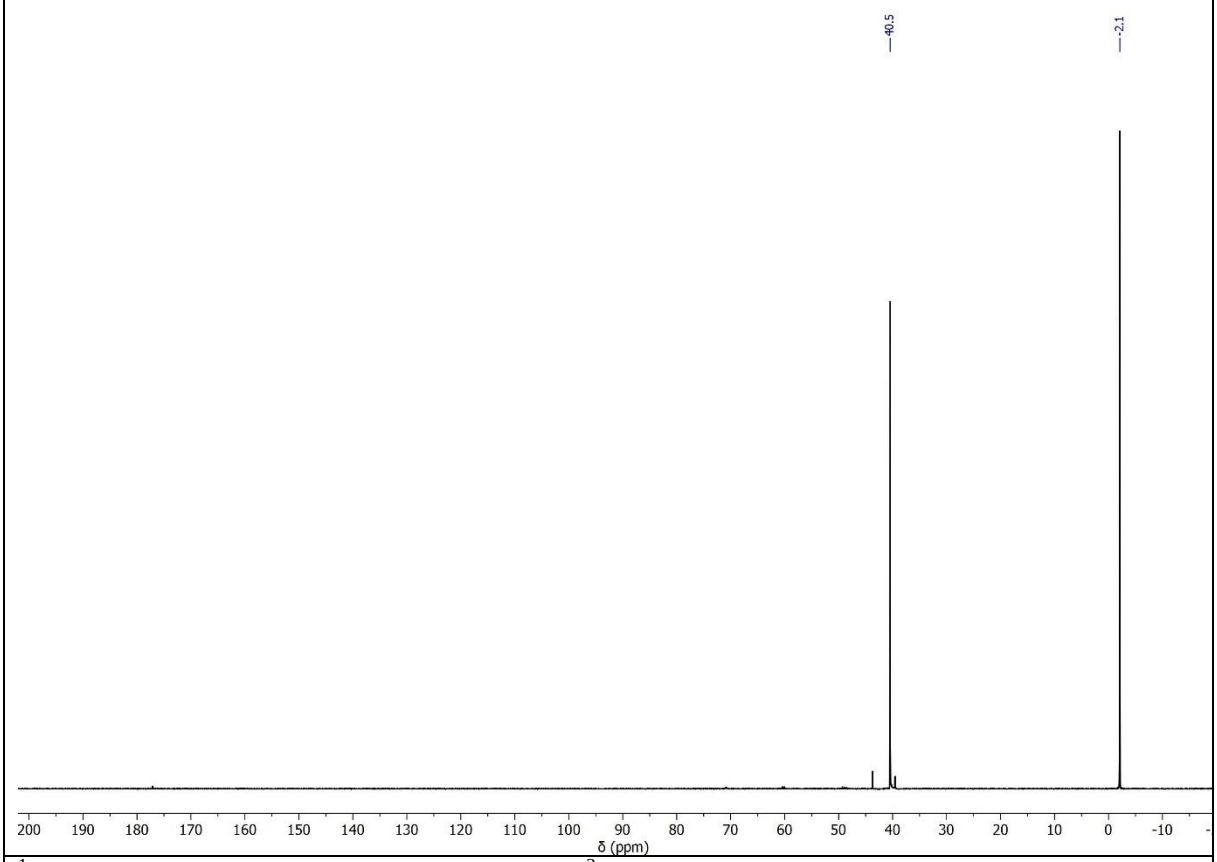
^{1}H NMR (600 MHz, C_6D_6, 20 °C, ppm) of [Mo(κ^{2}P,N-PCP-*i*Pr)(CO)$_4$](**3**)



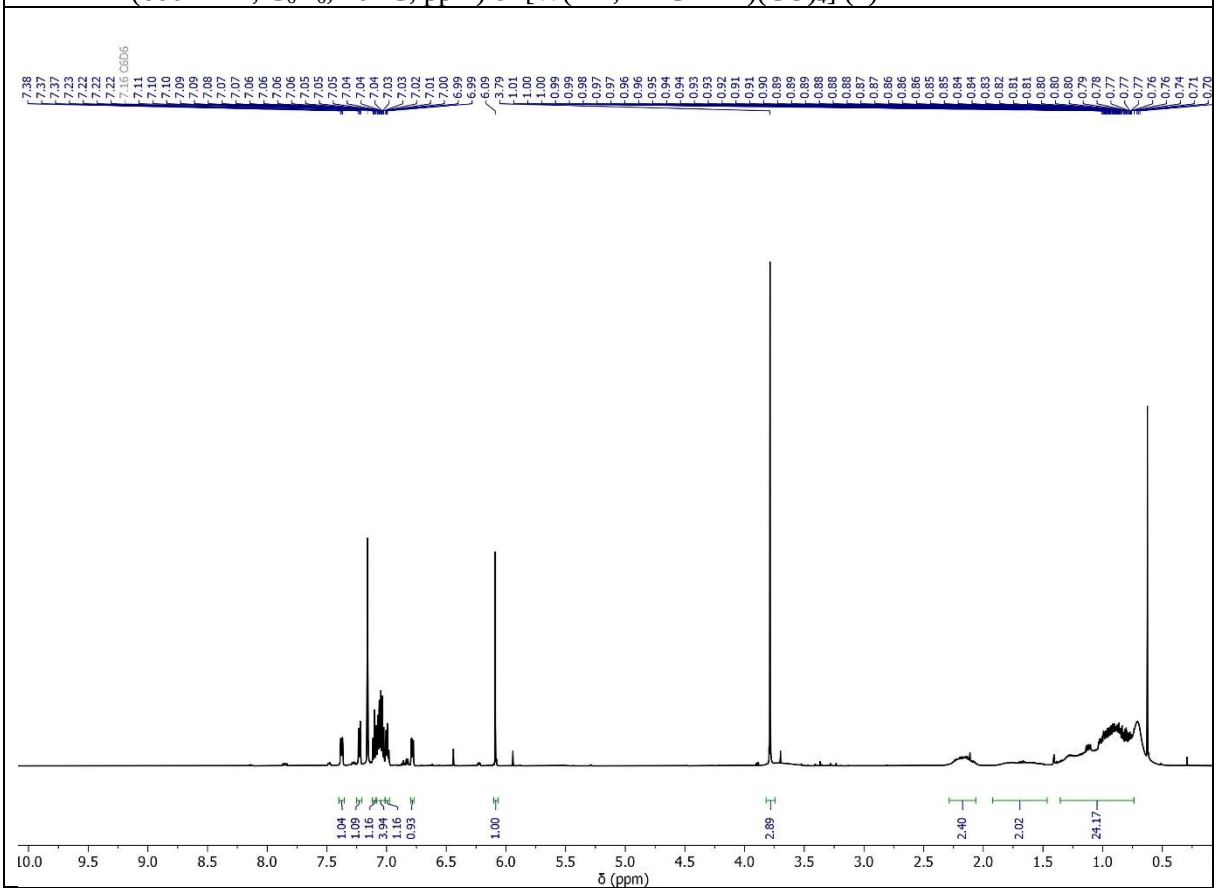
^{13}C{^{1}H} NMR (151 MHz, C_6D_6, 20 °C, ppm) of [Mo(κ^{2}P,N-PCP-*i*Pr)(CO)$_4$] (**3**)



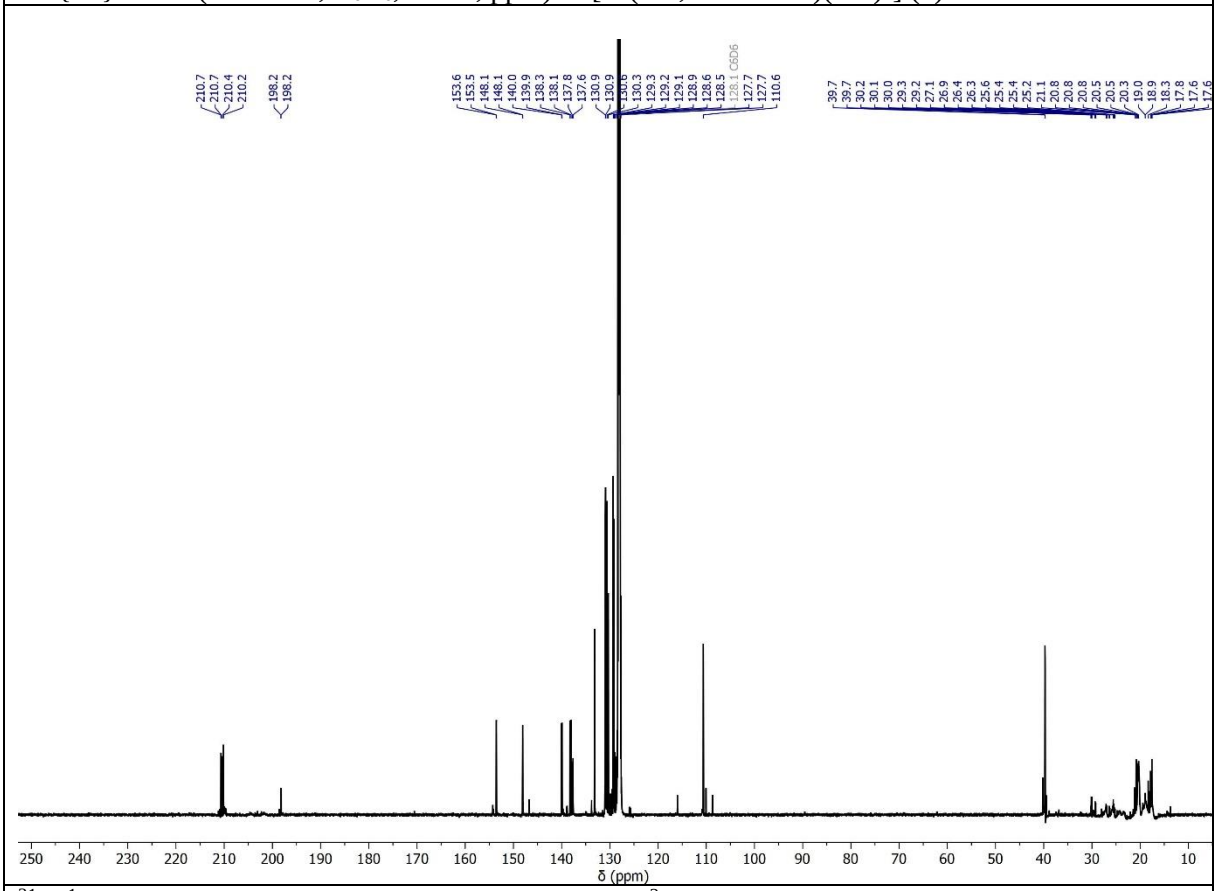
$^{31}P\{^{1}H\}$ NMR (243 MHz, C_6D_6, 20 °C, ppm) of [Mo(κ^{2}P,N-PCP-*i*Pr)(CO)$_4$] (**3**)



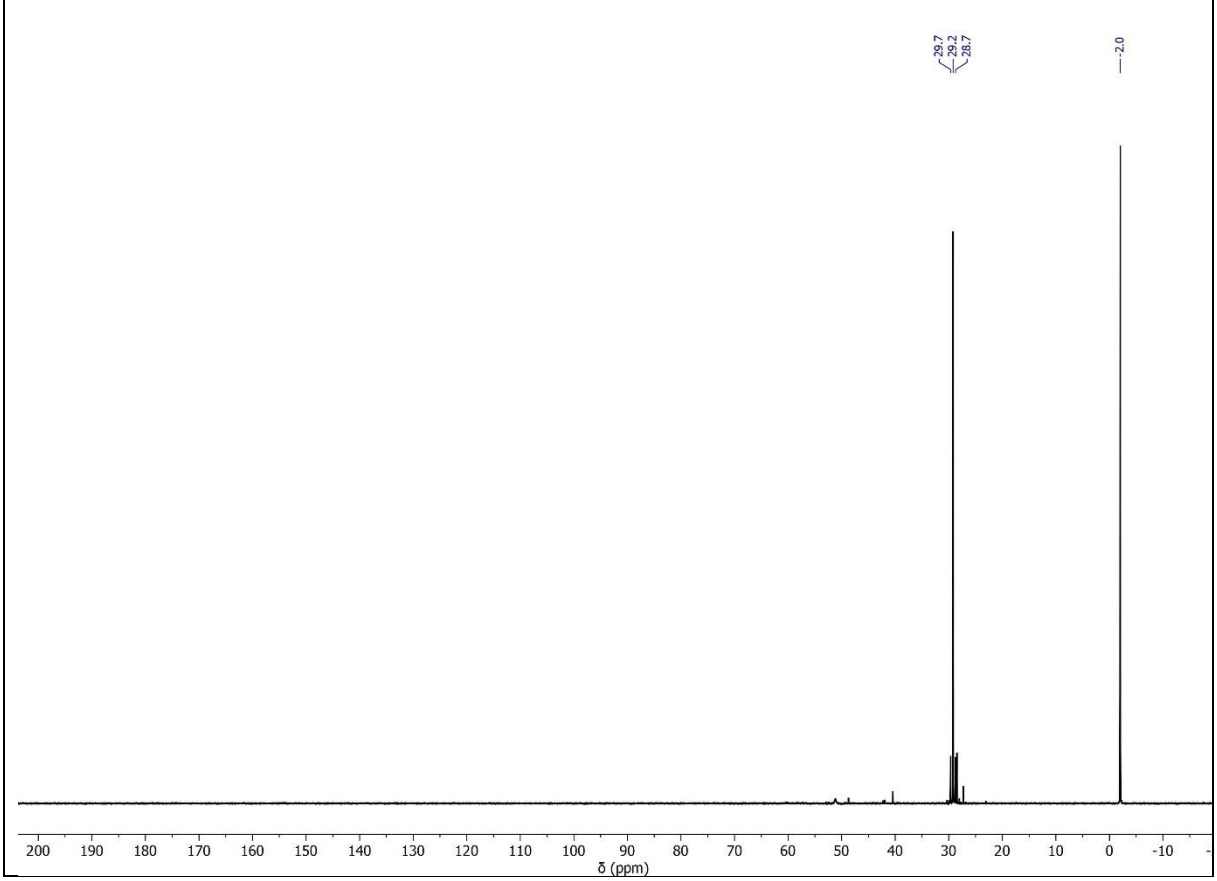
^{1}H NMR (600 MHz, C_6D_6, 20 °C, ppm) of [W(κ^{2}P,N-PCP-*i*Pr)(CO)$_4$] (**4**)



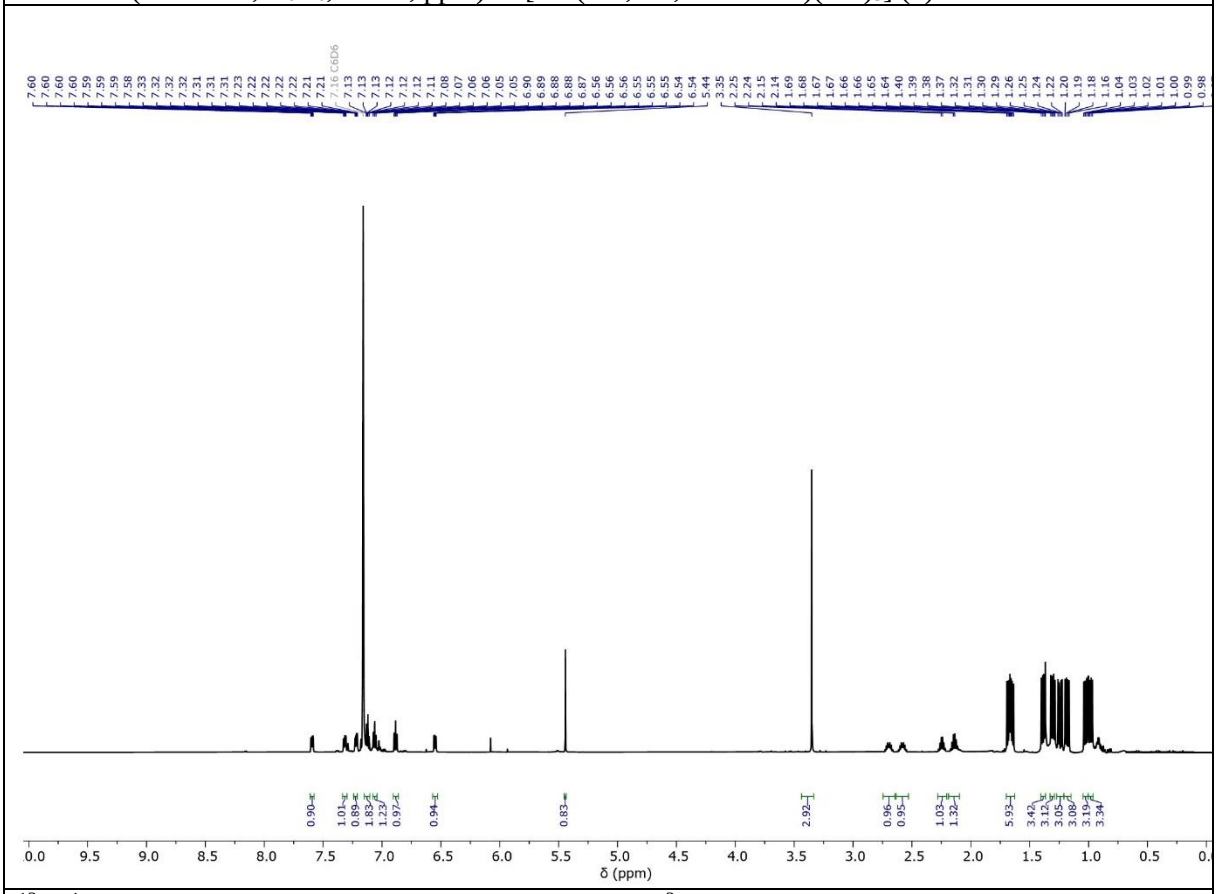
$^{13}C\{^{1}H\}$ NMR (151 MHz, C_6D_6, 20 °C, ppm) of [W(κ^{2}P,N-PCP-*i*Pr)(CO)$_4$] (**4**)



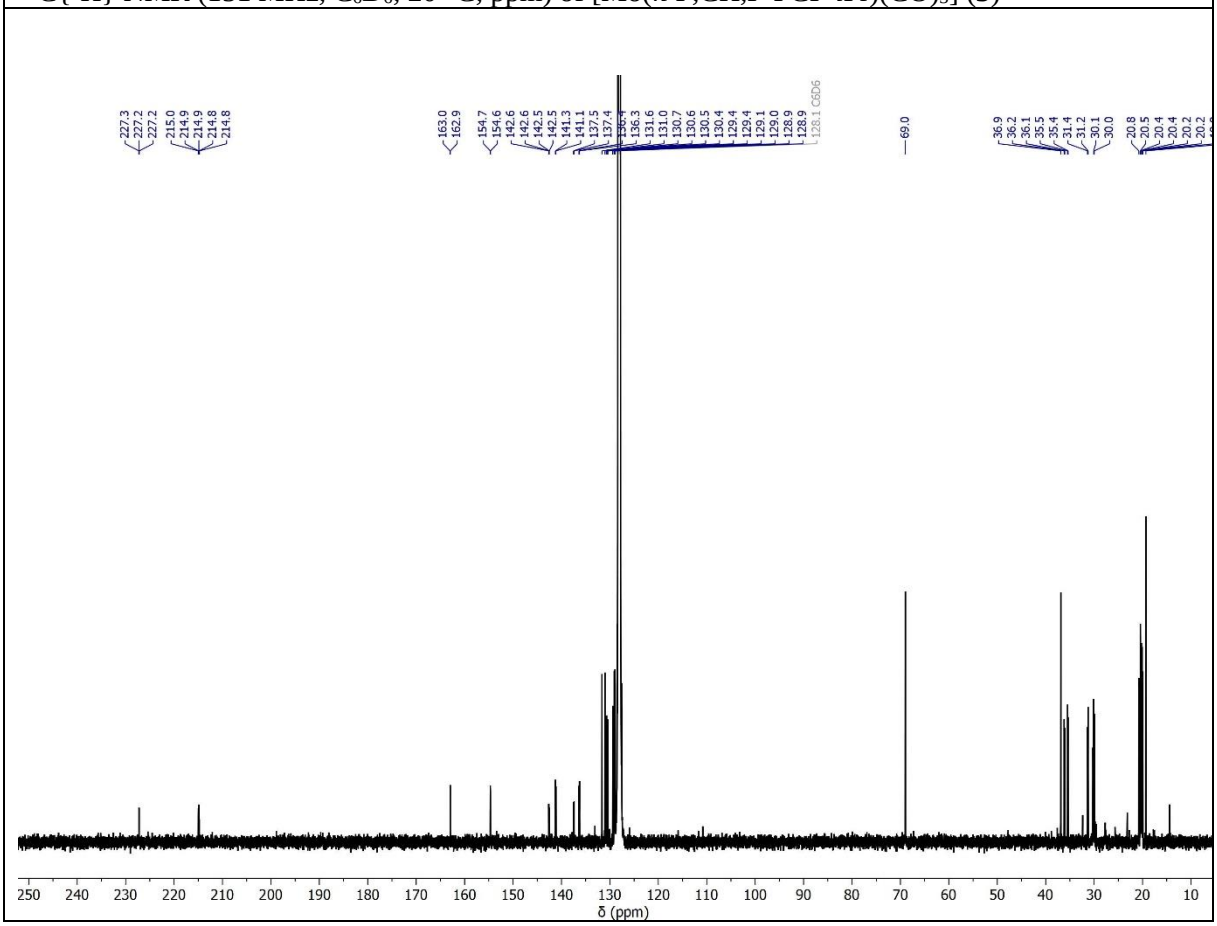
$^{31}P\{^{1}H\}$ NMR (243 MHz, C_6D_6, 20 °C, ppm) of [W(κ^{2}P,N-PCP-*i*Pr)(CO)$_4$] (**4**)



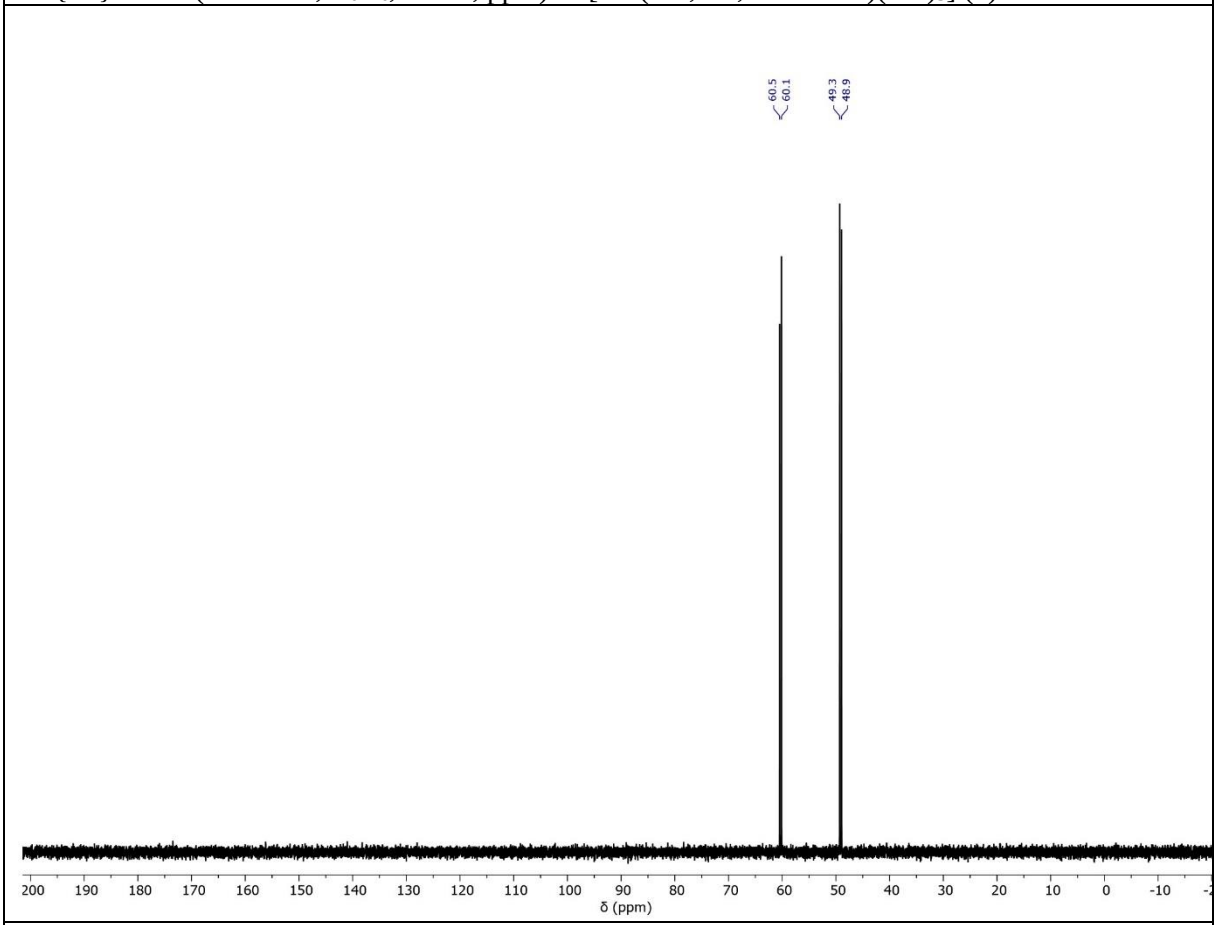
^{1}H NMR (600 MHz, C_6D_6, 20 °C, ppm) of [Mo(κ^3P,CH,P-PCP-*i*Pr)(CO)$_3$] (**5**)



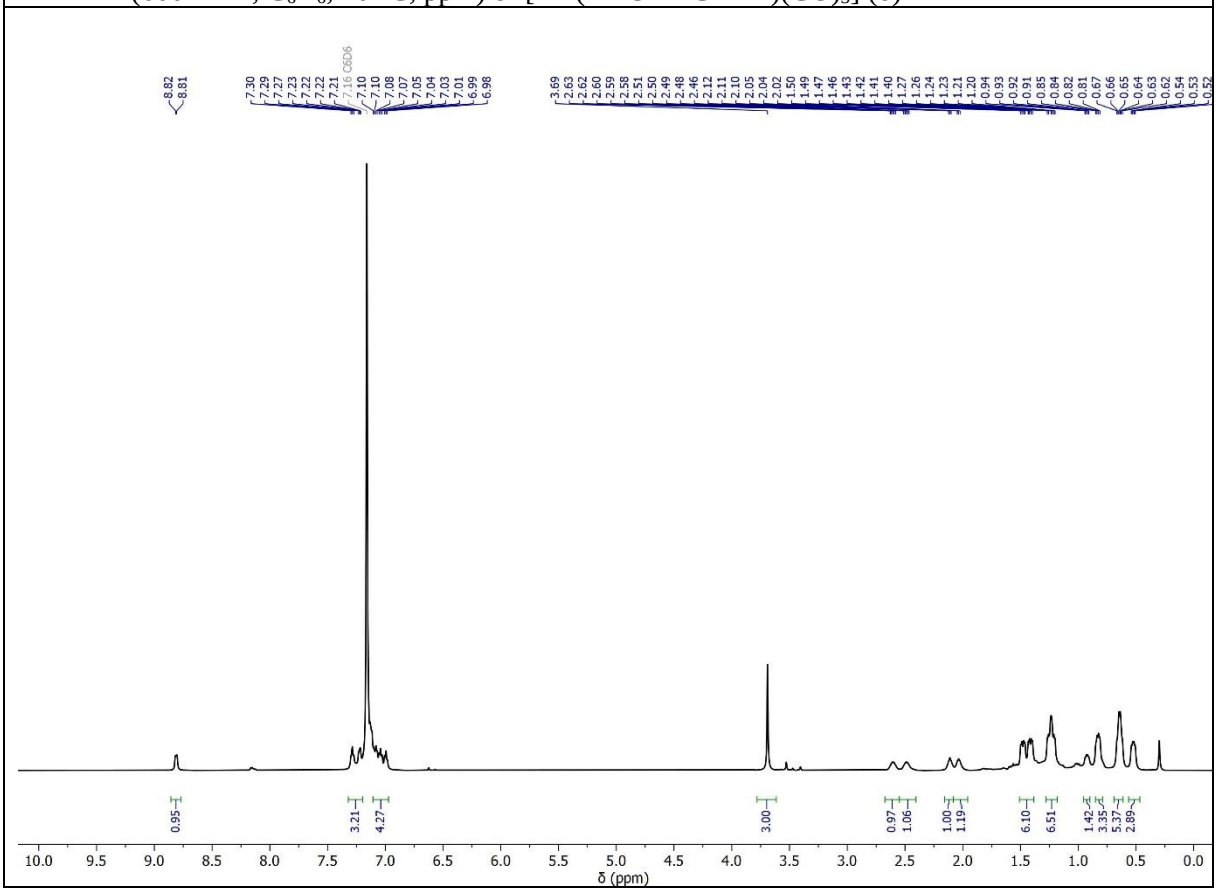
^{13}C{^{1}H} NMR (151 MHz, C_6D_6, 20 °C, ppm) of [Mo(κ^3P,CH,P-PCP-*i*Pr)(CO)$_3$] (**5**)



$^{31}P\{^{1}H\}$ NMR (243 MHz, C_6D_6, 20 °C, ppm) of [Mo(κ^{3}P,CH,P-PCP-*i*Pr)(CO)$_3$] (**5**)



^{1}H NMR (600 MHz, C_6D_6, 20 °C, ppm) of [Mn(κ^3*PCP*-PCP-*i*Pr)(CO)$_3$] (**6**)



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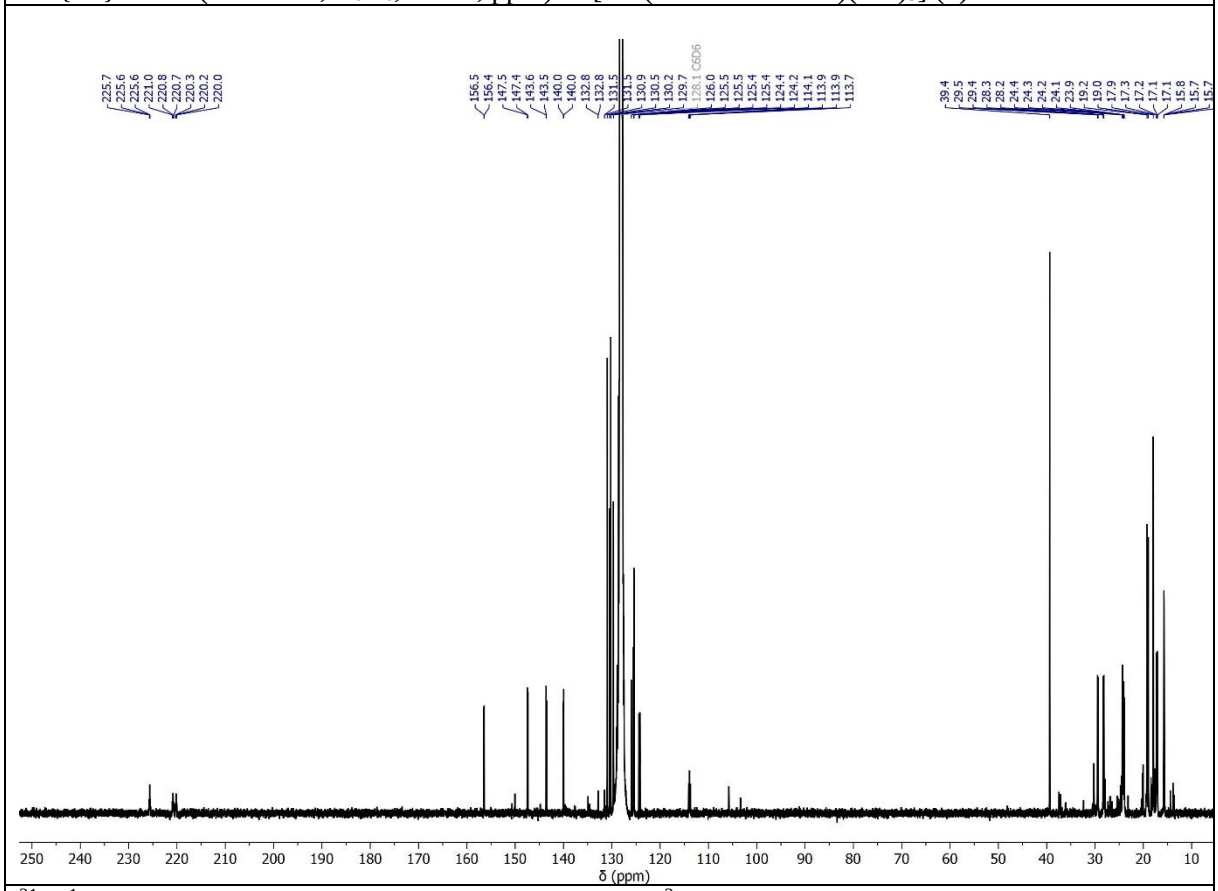

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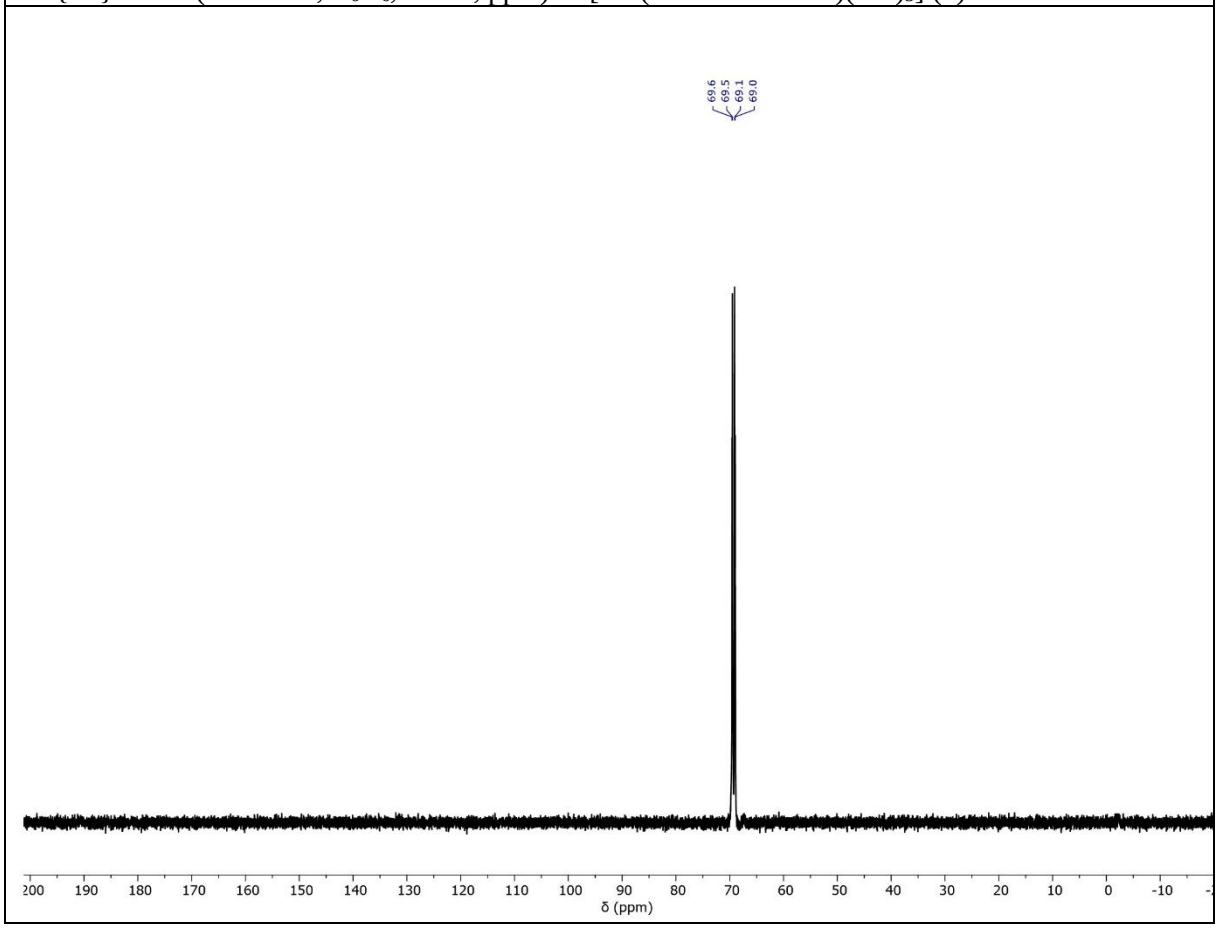
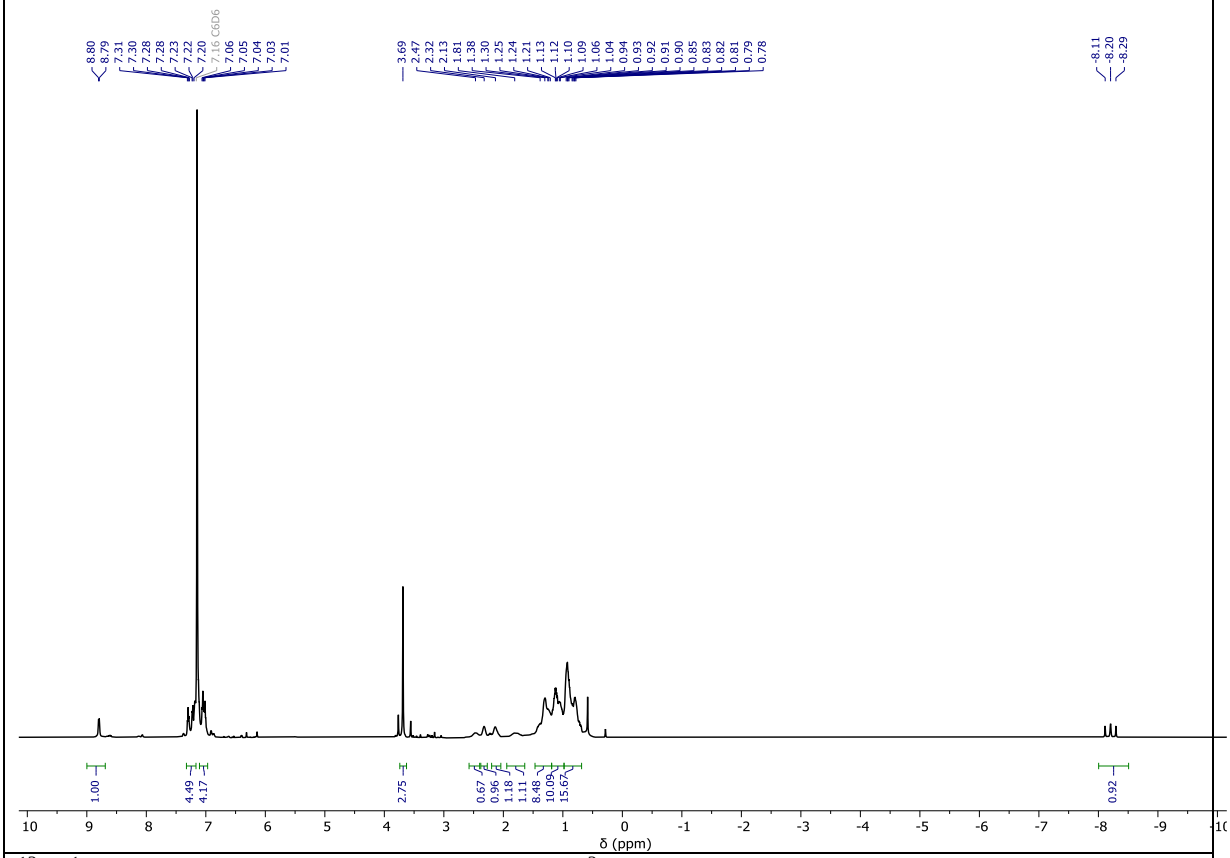
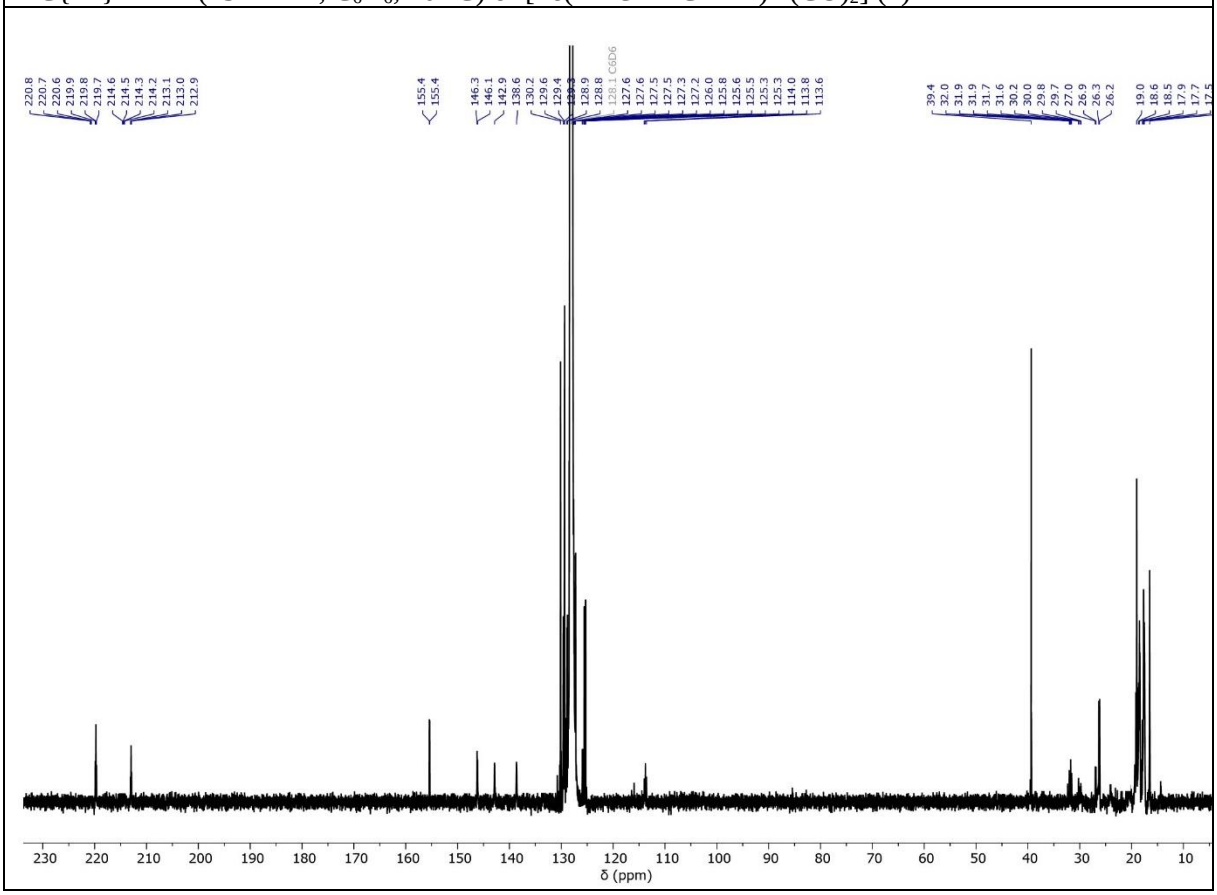


^{1}H NMR (600 MHz, C_6D_6, 20 °C) of [Fe(κ^{3}*PCP*-PCP-*i*Pr)H(CO)$_2$] (**7**)



^{13}C{^{1}H} NMR (151 MHz, C_6D_6, 20 °C) of [Fe(κ^{3}*PCP*-PCP-*i*Pr)H(CO)$_2$] (**7**)



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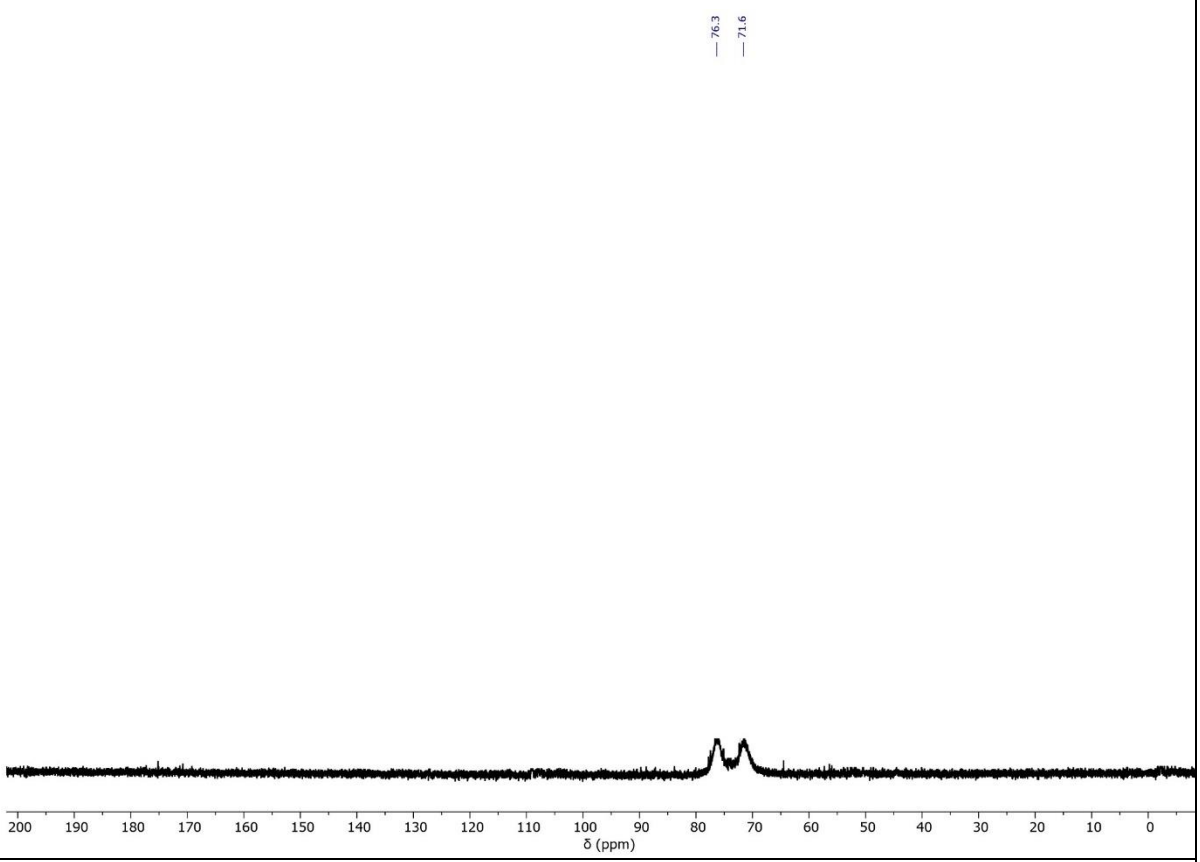
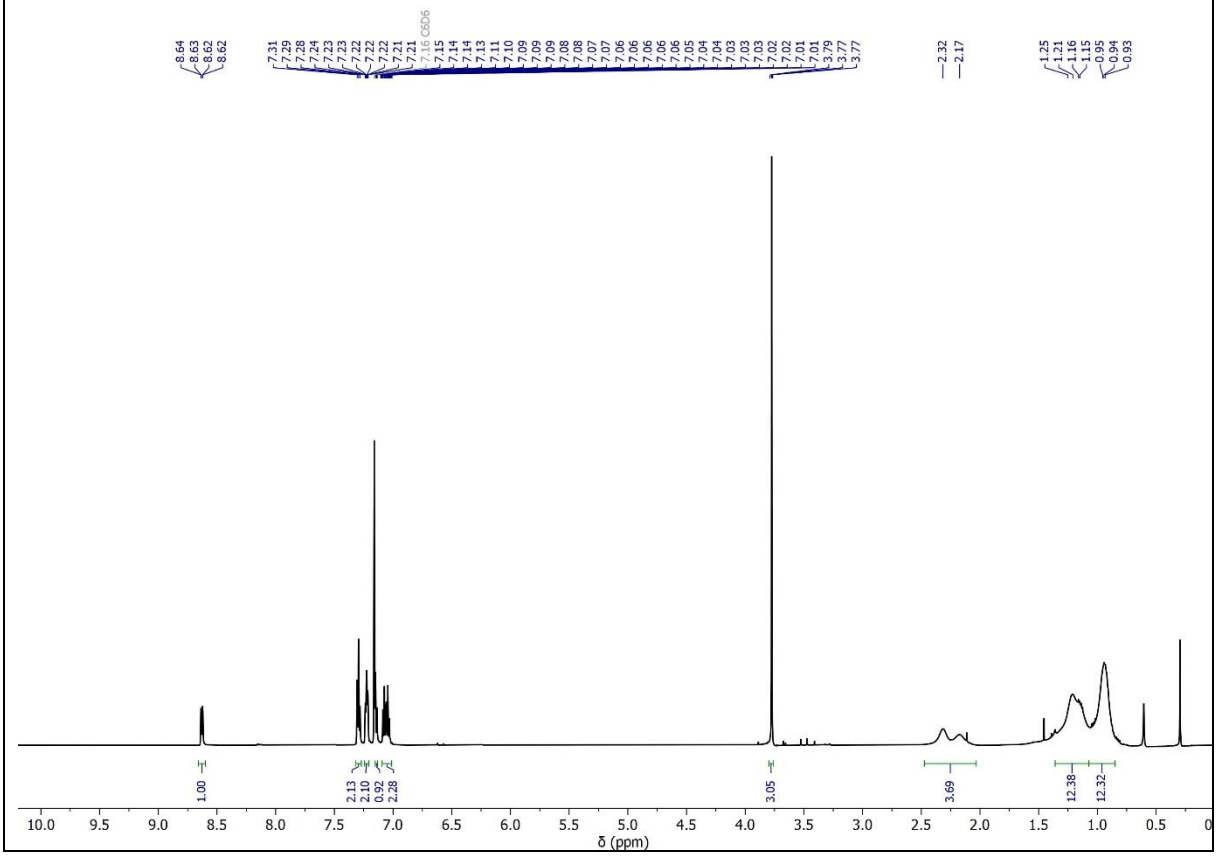
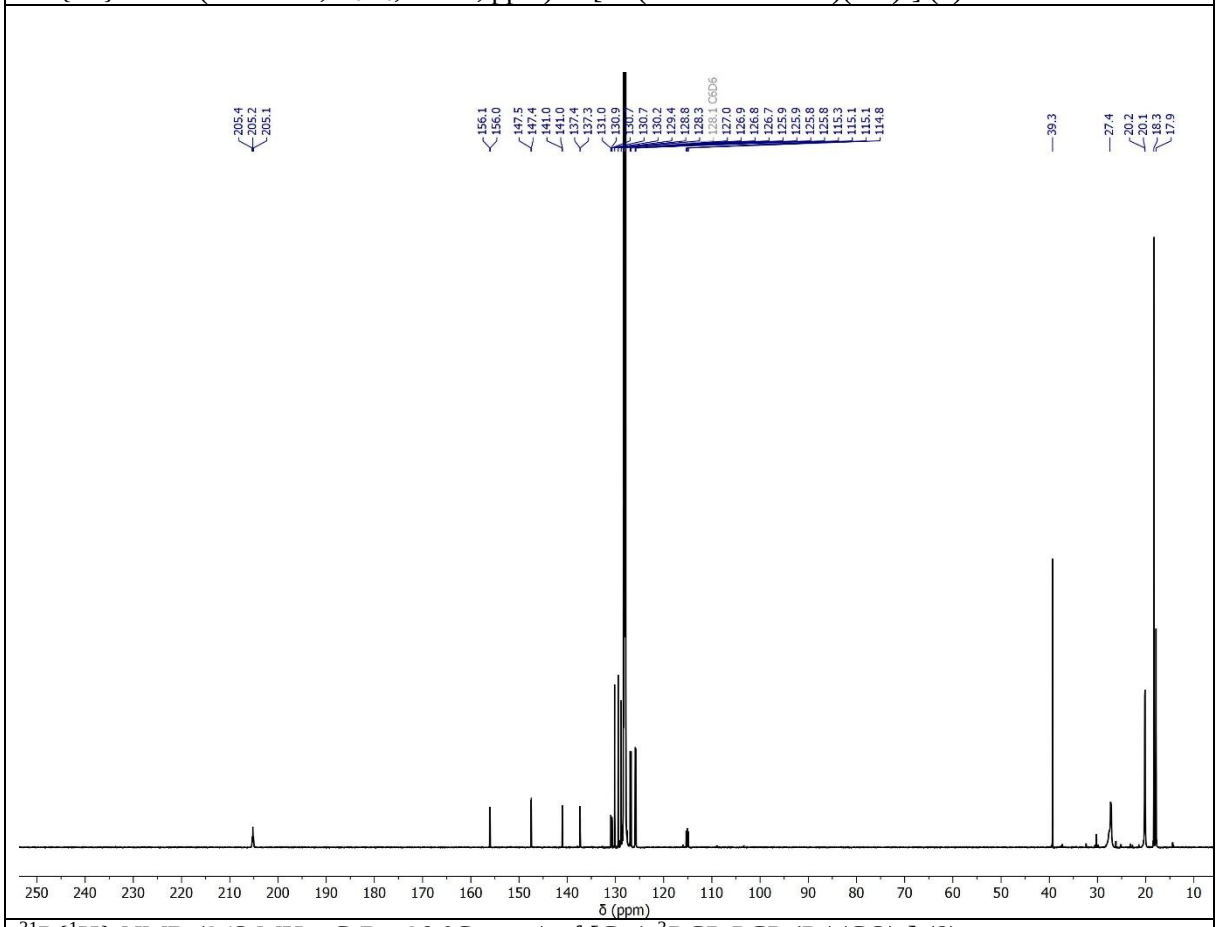


^{1}H NMR (600 MHz, C_6D_6, 20 °C, ppm) of [Co(κ^3*PCP*-PCP-*i*Pr)(CO)$_2$] (**8**)



$^{13}C\{^{1}H\}$ NMR (151 MHz, C_6D_6, 20 °C, ppm) of [Co(κ^3*PCP*-PCP-*i*Pr)$(CO)_2$] (**8**)



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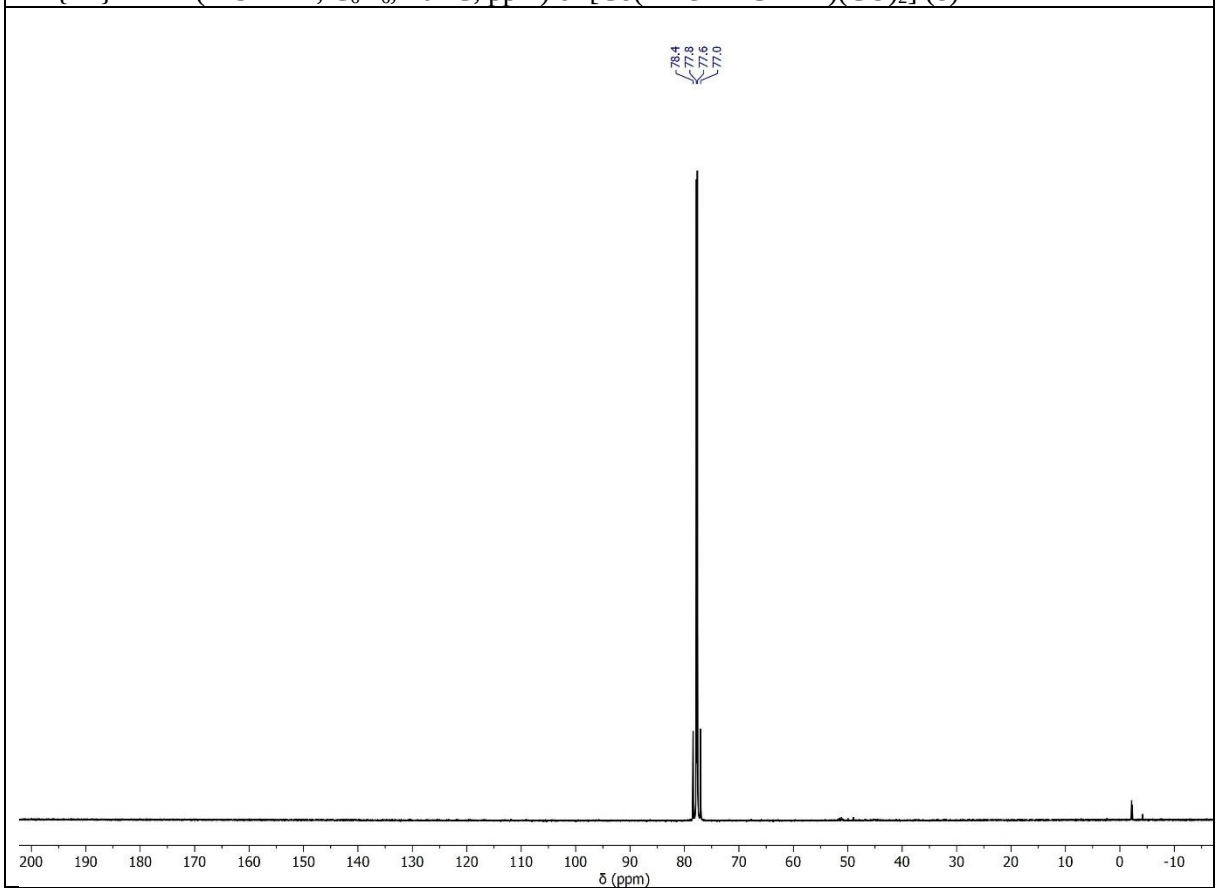
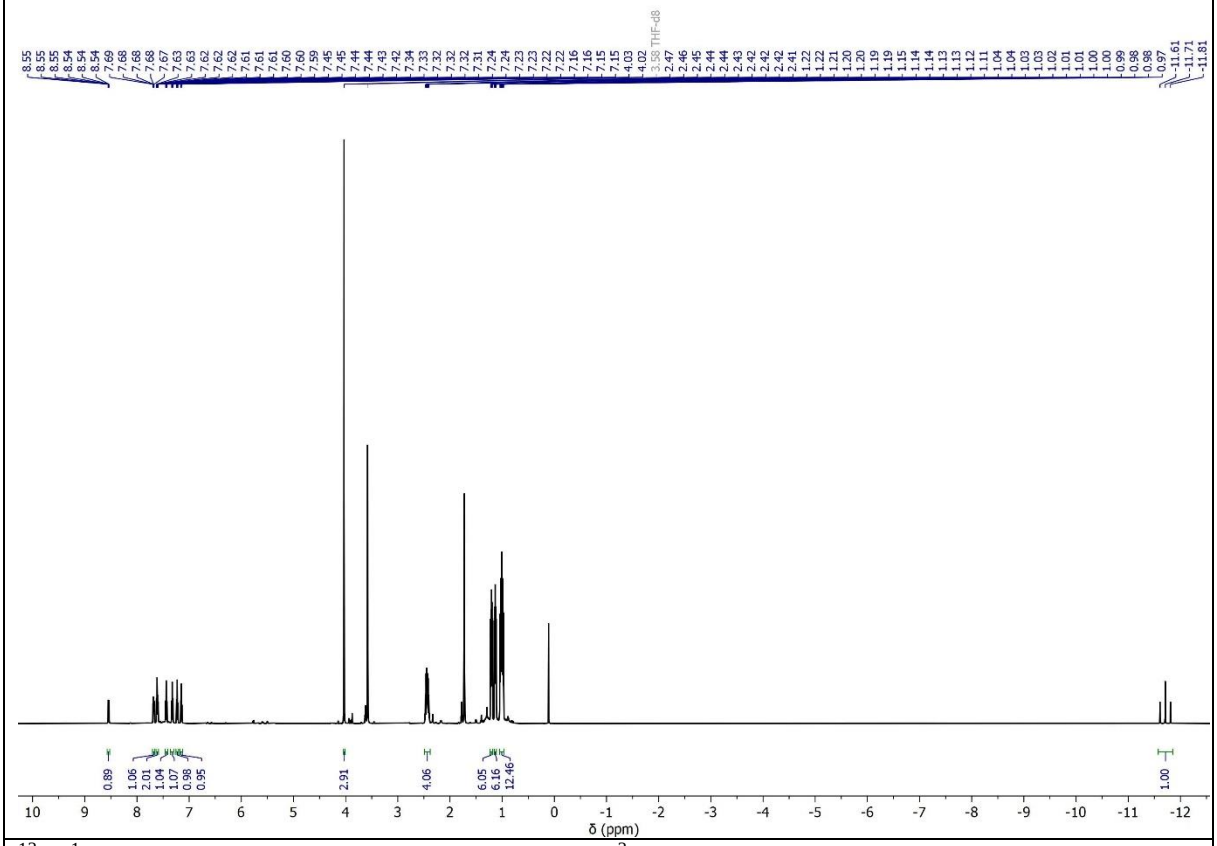


^{1}H NMR (600 MHz, THF-d$_8$, 20 °C) of [Ni(κ^3*PCP*-PCP-*i*Pr)H] (**9**)



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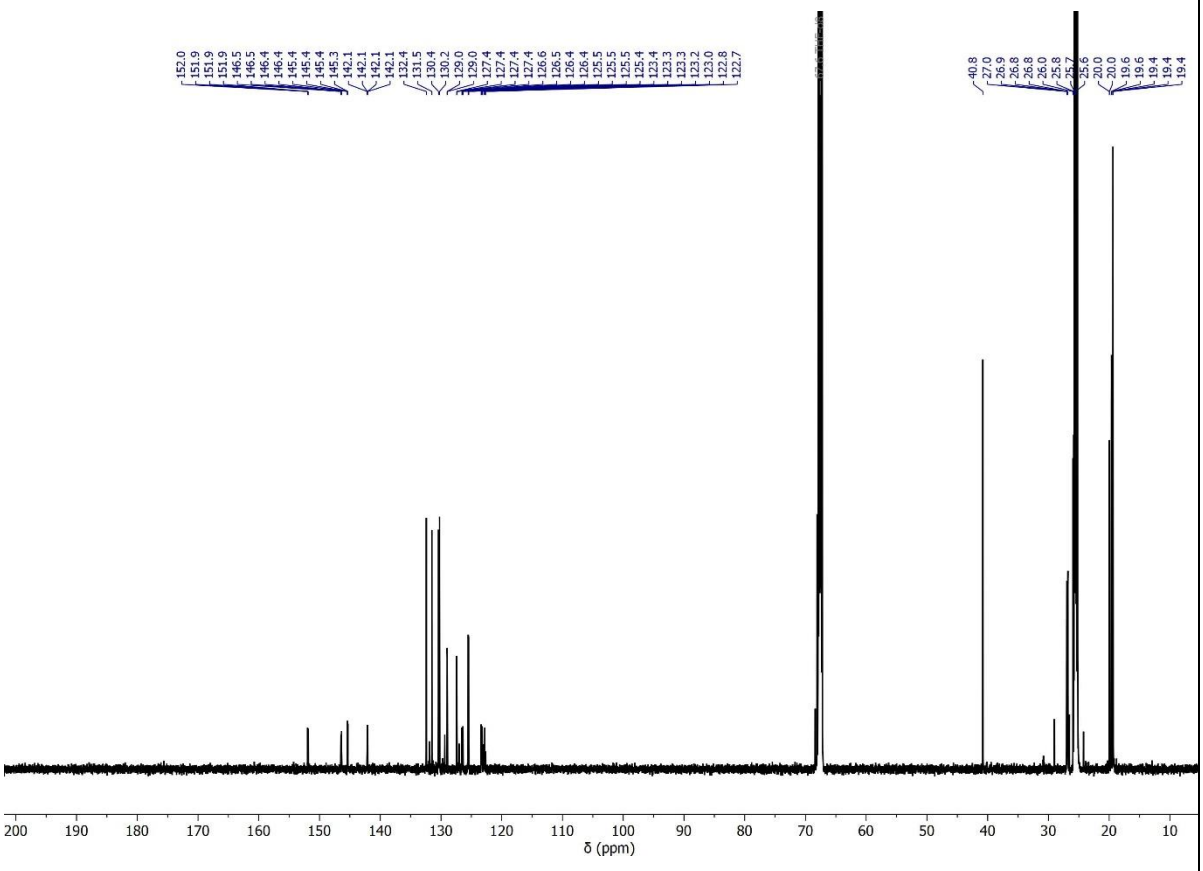

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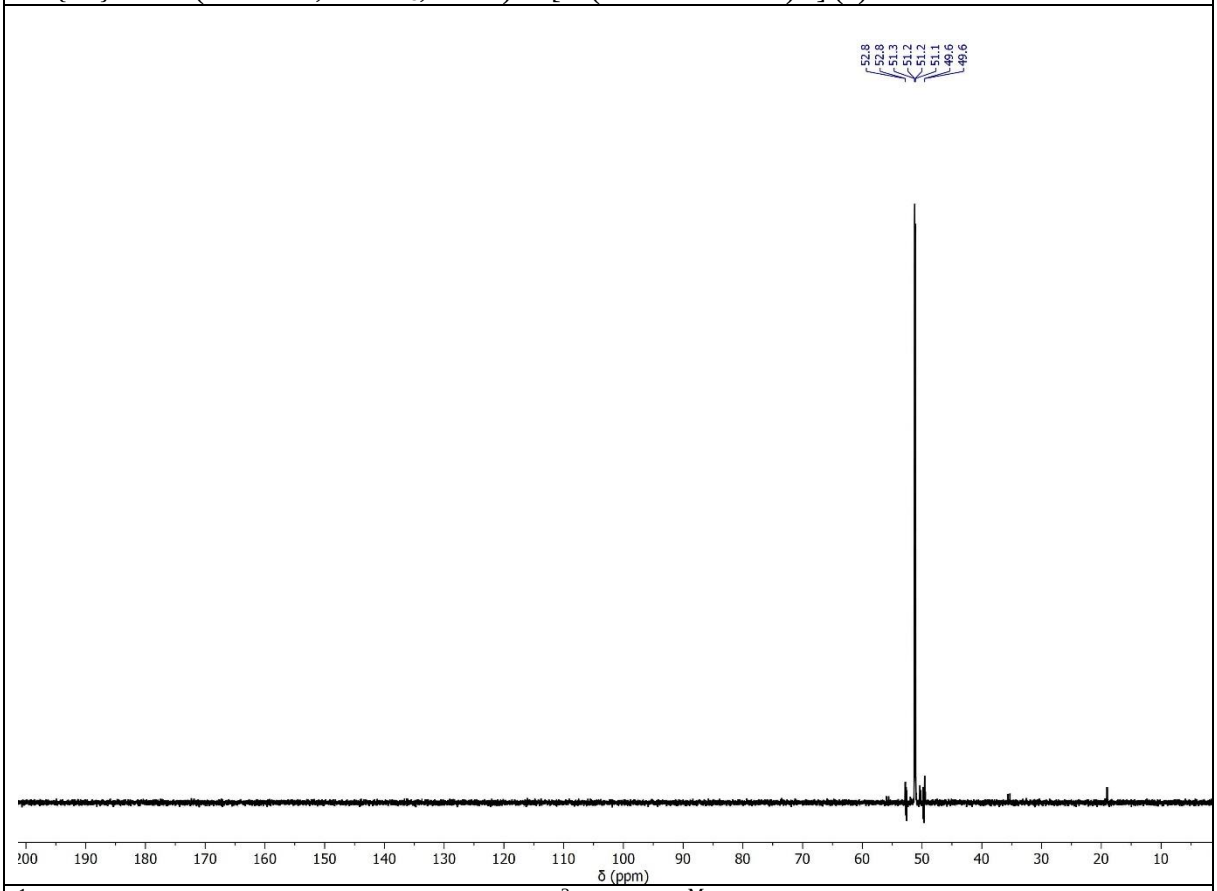
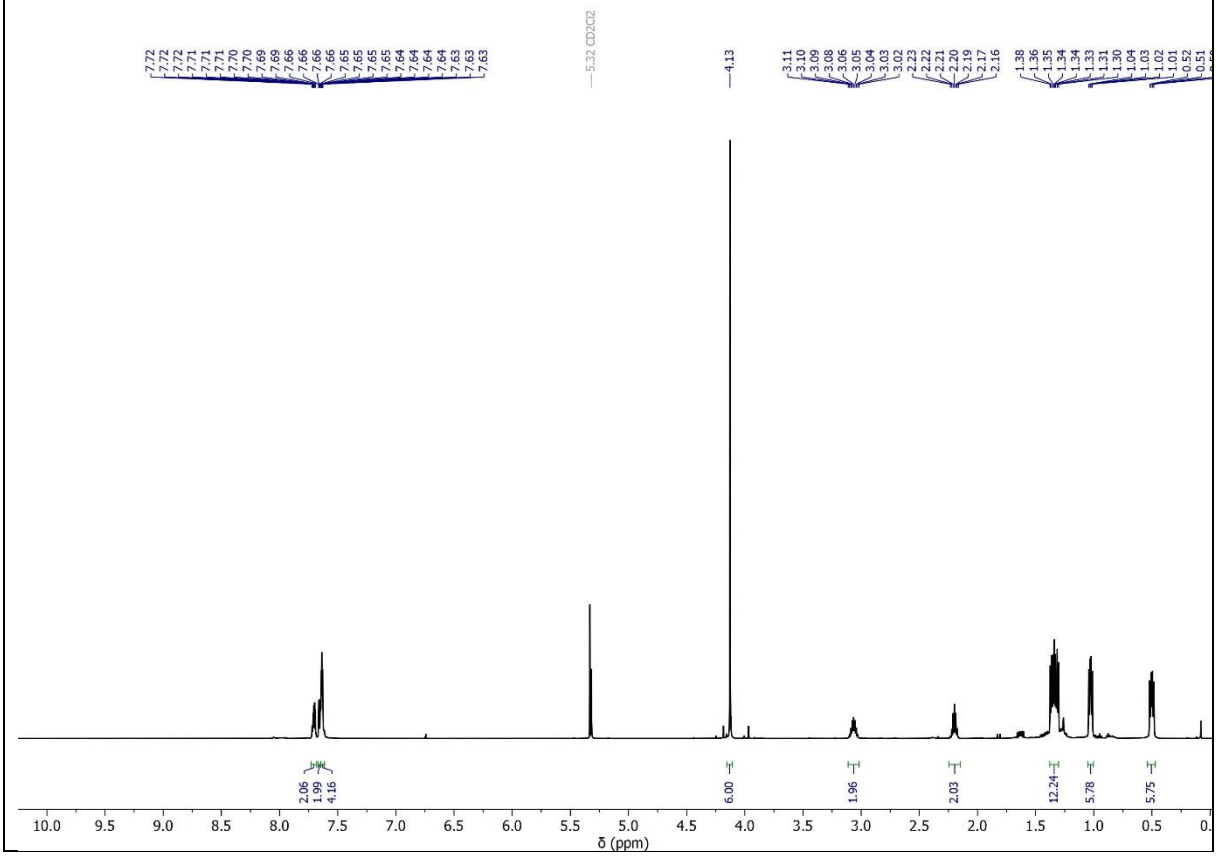


^{1}H NMR (600 MHz, CD_2Cl_2, 20 °C) of [Mn(κ^3*PCP*-PCP^{Me}-*i*Pr)(CO)$_3$]BF_4 (**10**)



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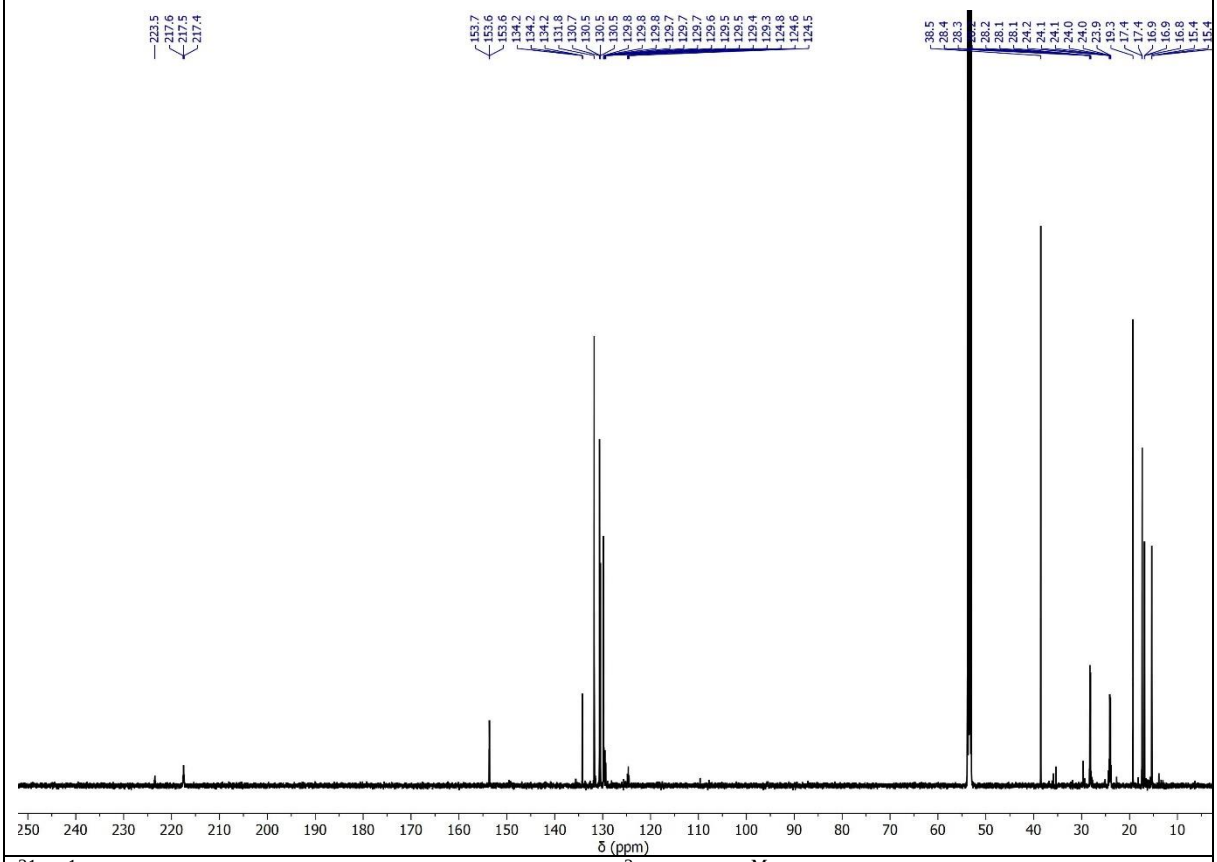
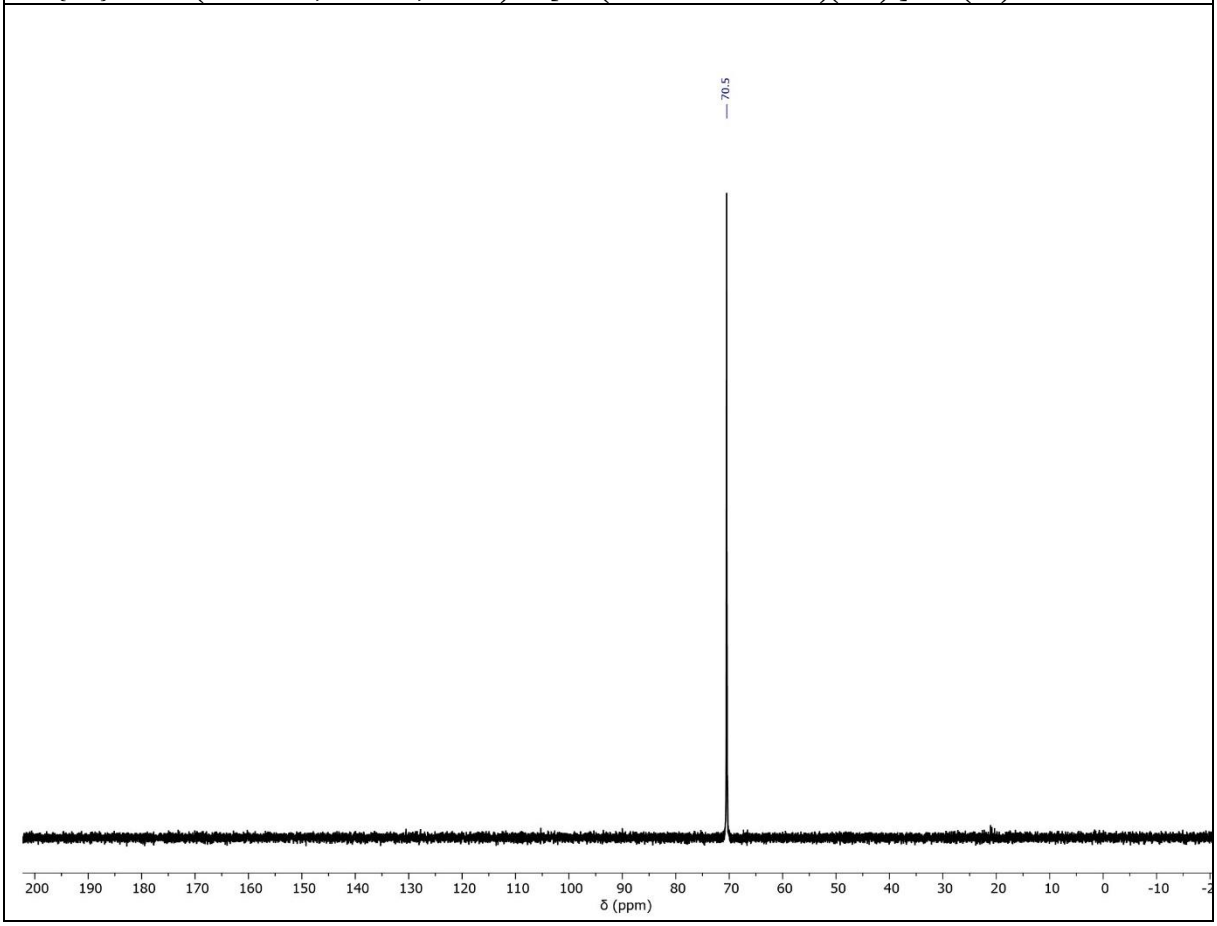
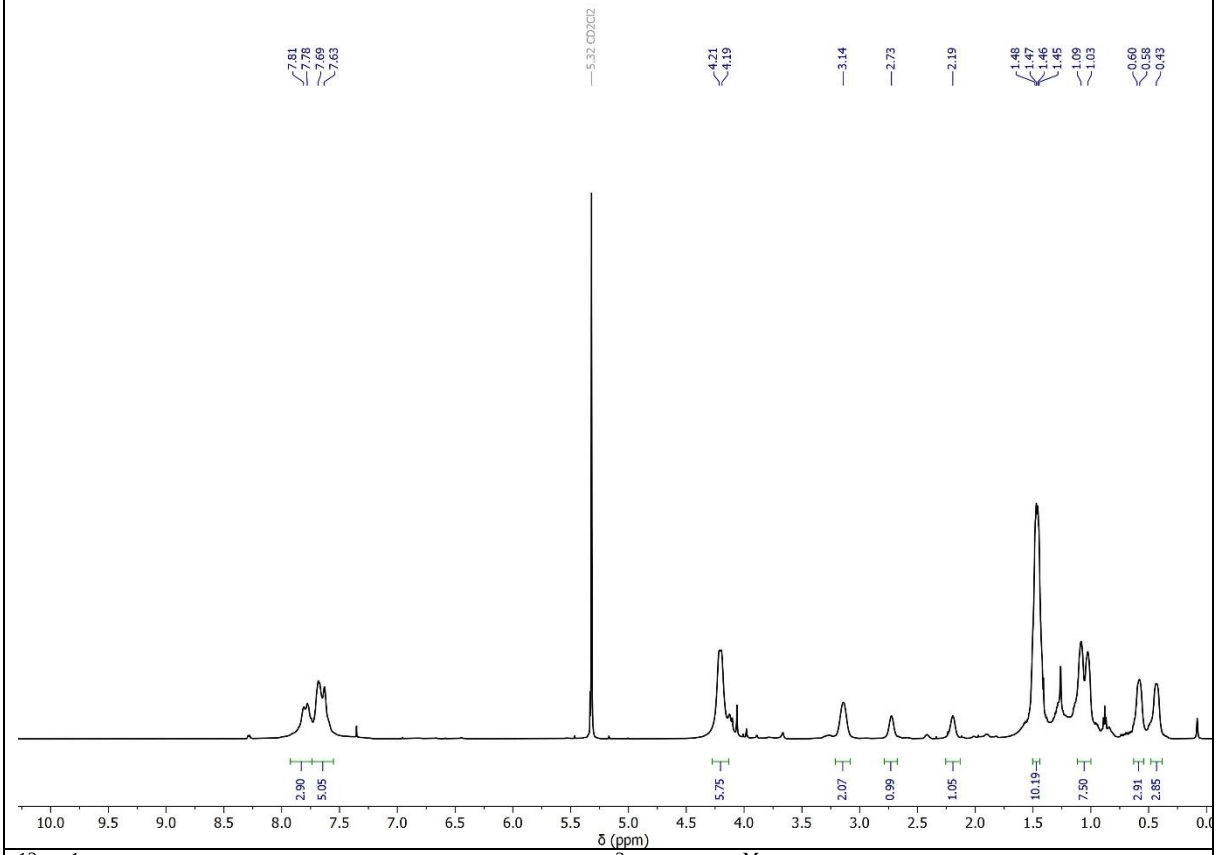


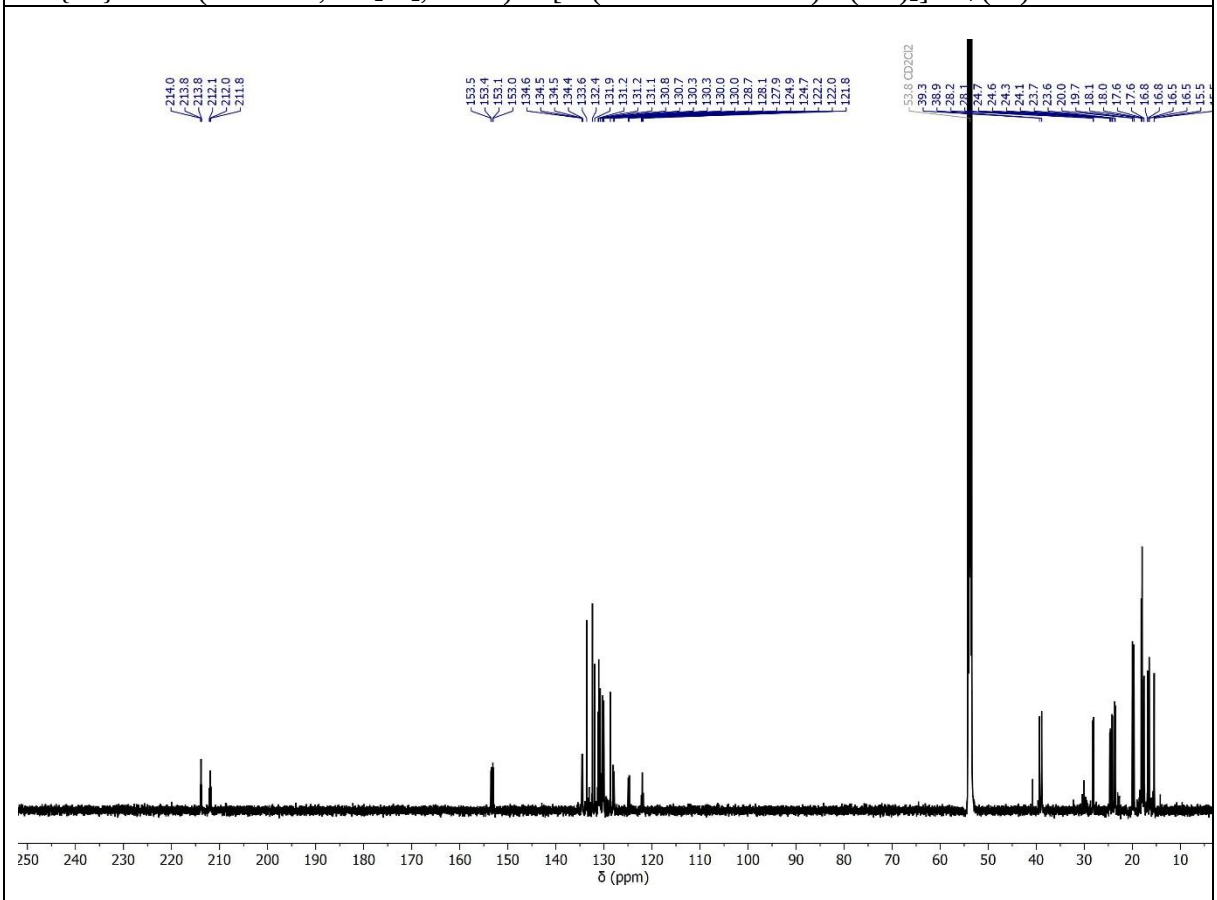
$^{31}P\{^{1}H\}$ NMR (243 MHz, CD_2Cl_2, 20 °C) of [Mn(κ^3*PCP*-PCP^{Me}-*i*Pr)(CO)$_3$]BF_4 (**10**)



^{1}H NMR (600 MHz, CD_2Cl_2, 20 °C) of [Fe(κ^{3}*PCP*-PCP^{Me}-*i*Pr)Cl(CO)$_2$]BF_4 (**11**)



^{13}C{^{1}H} NMR (151 MHz, CD_2Cl_2, 20 °C) of [Fe(κ^{3}*PCP*-PCP^{Me}-*i*Pr)Cl(CO)$_2$]BF_4 (**13**)



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