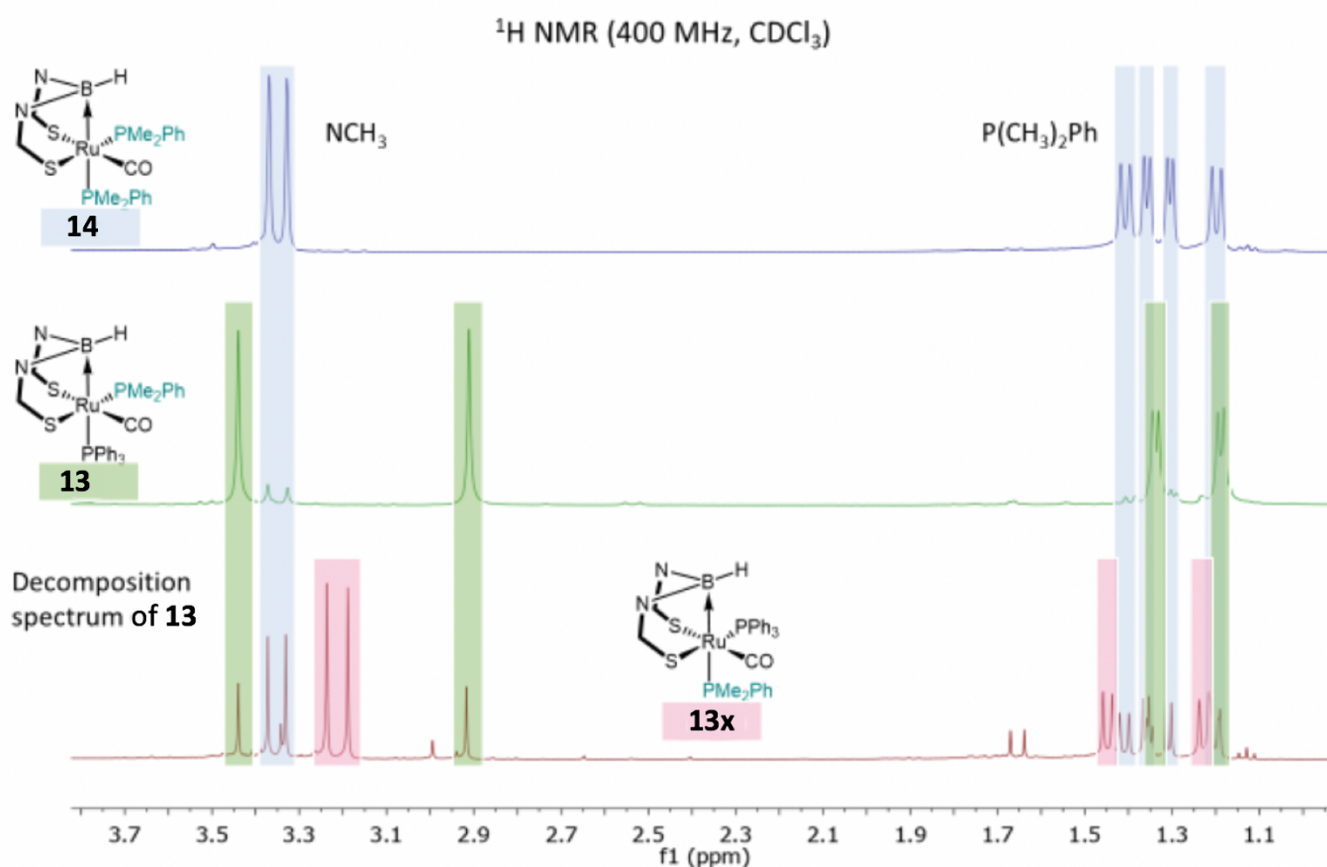


**Methimazolyl Based Diptych Bicyclo-[3.3.0]-Ruthenaboratranes**

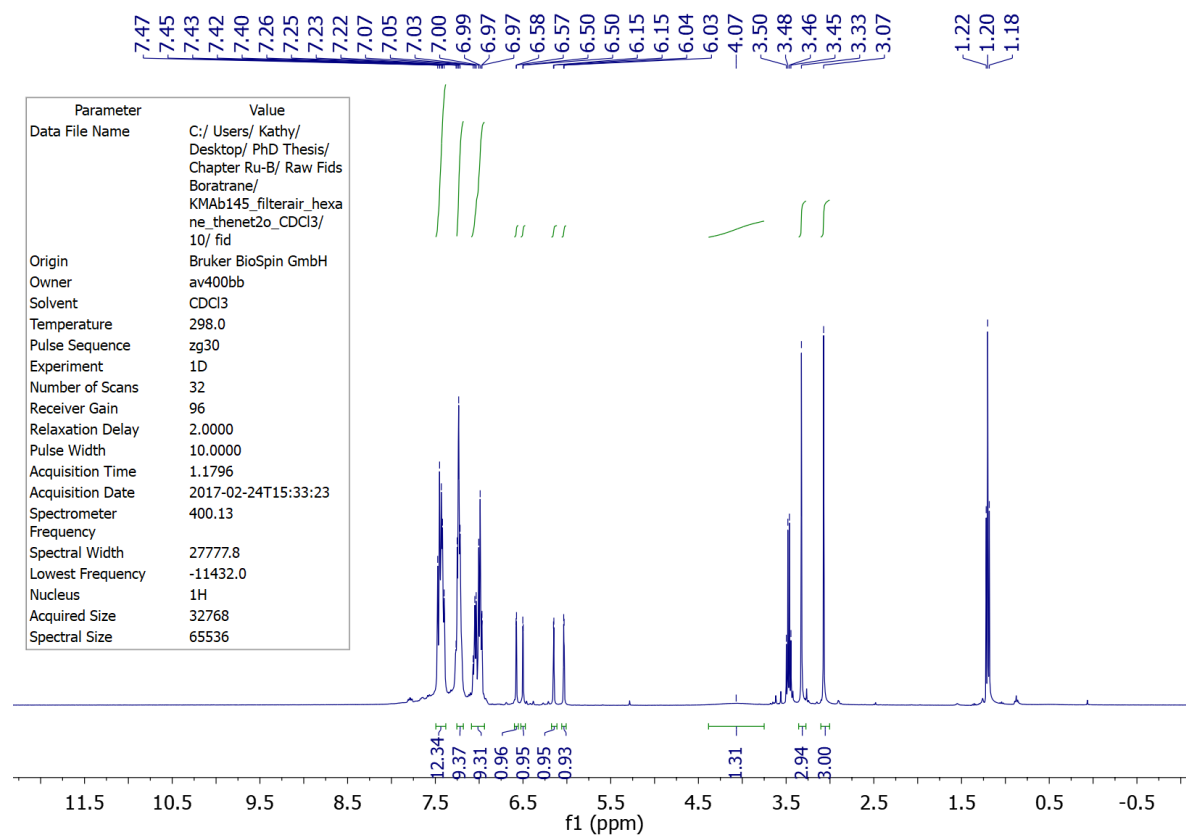
Chenxi Ma<sup>a</sup> and Anthony F. Hill<sup>\*a</sup>

**Figure S1. Comparison of the methyl regions in the <sup>1</sup>H NMR spectra of 13, 14 and the decomposition spectrum of 13 in CDCl<sub>3</sub> to identify isomer 13x**

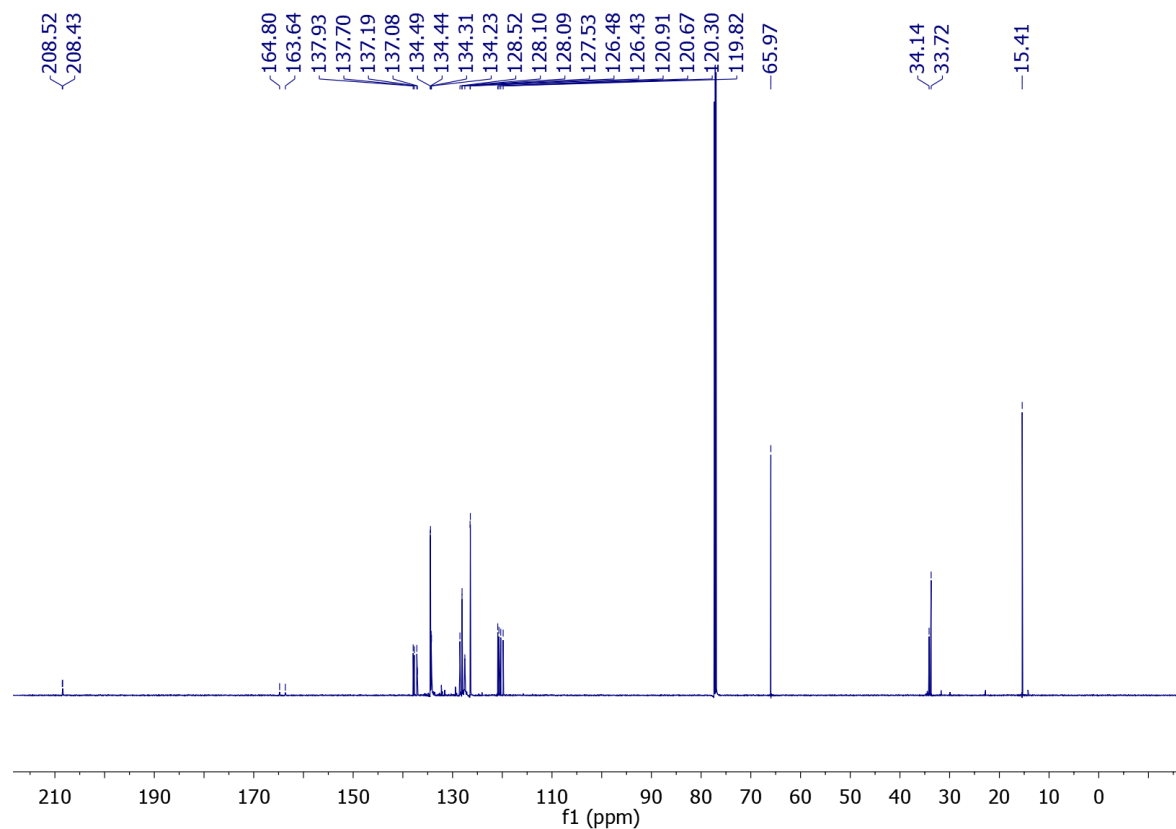


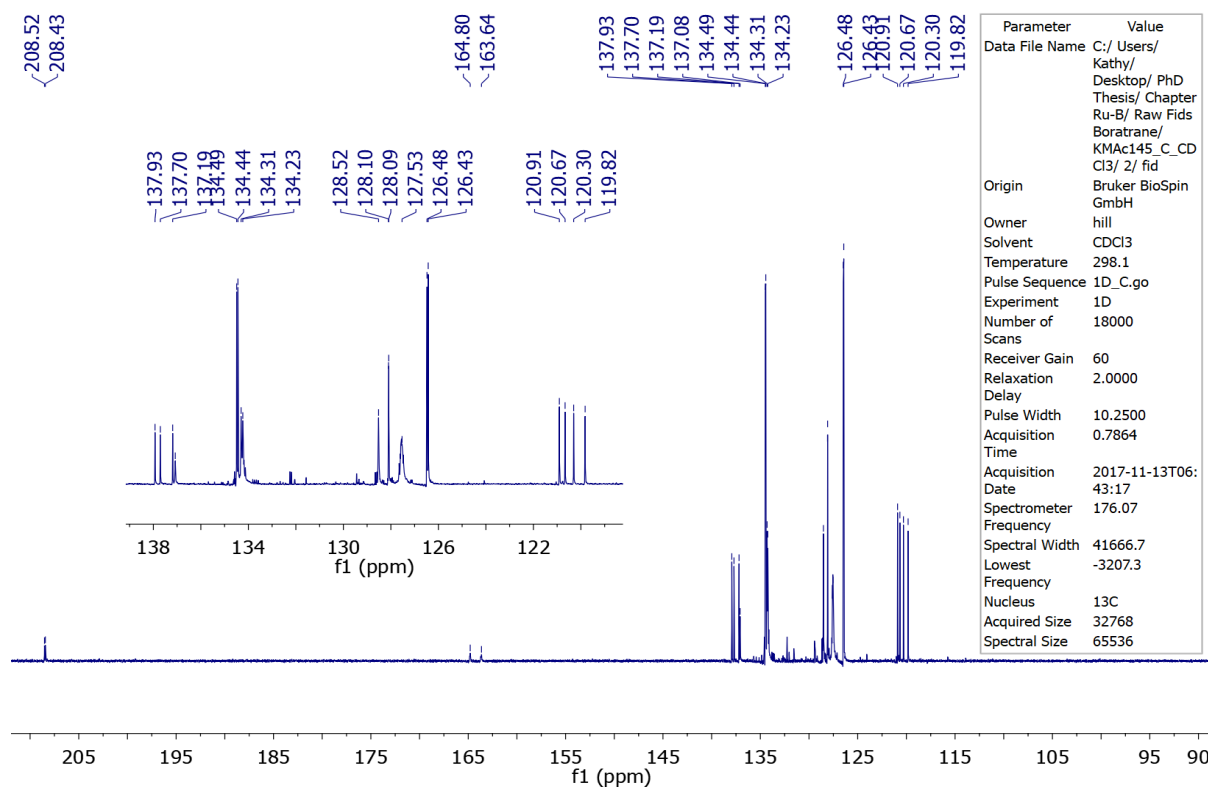
# [Ru{BH(mt)<sub>2</sub>}(CO)(PPh<sub>3</sub>)<sub>2</sub>] (5)

## <sup>1</sup>H NMR Spectrum of Complex 5

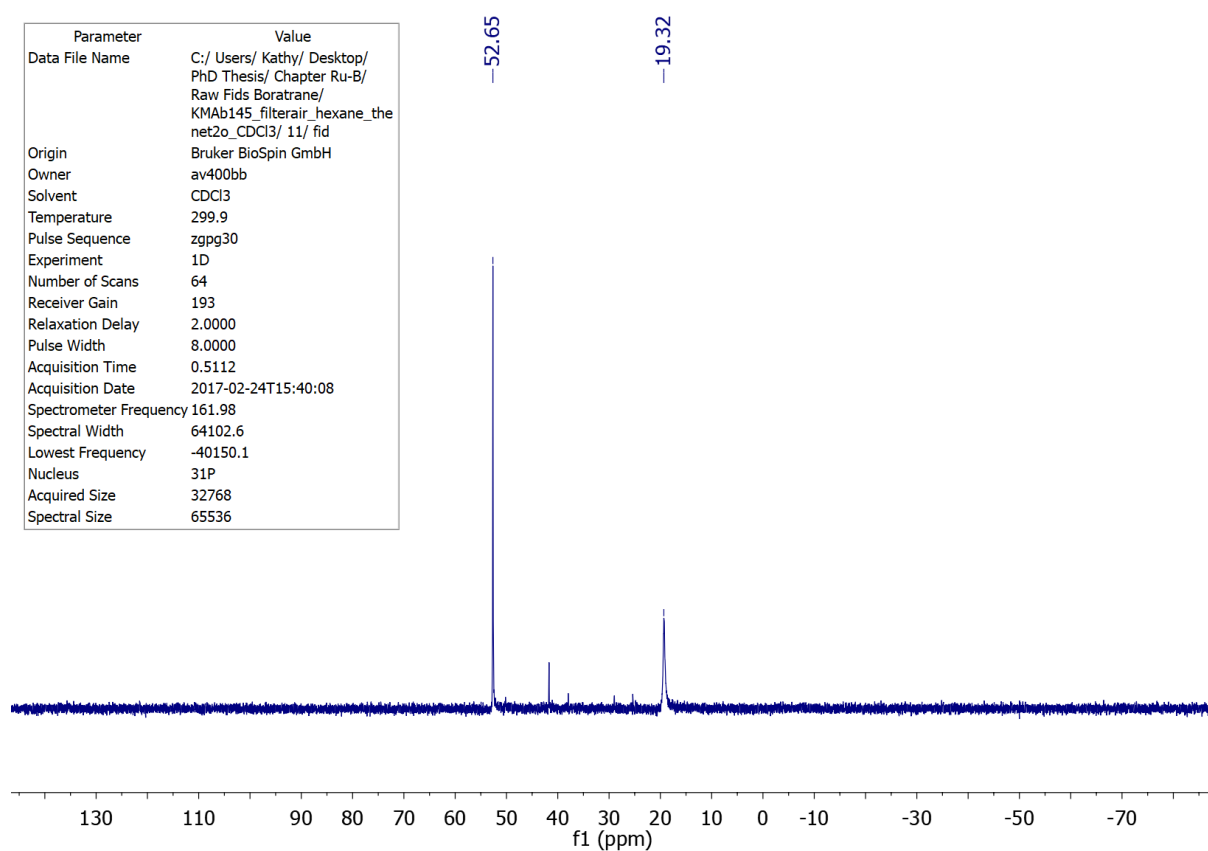


## <sup>13</sup>C{<sup>1</sup>H} NMR Spectrum of Complex 5



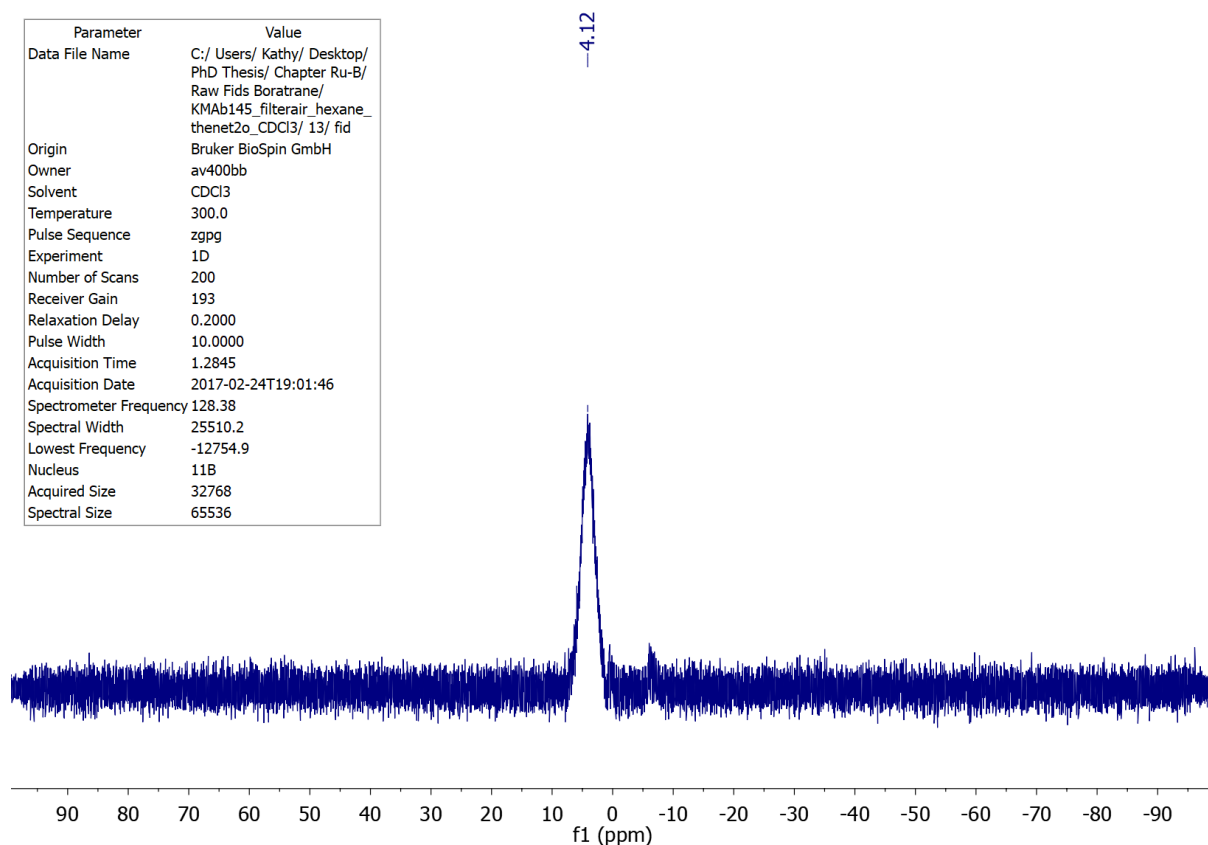


### <sup>31</sup>P{<sup>1</sup>H} NMR Spectrum of Complex 5



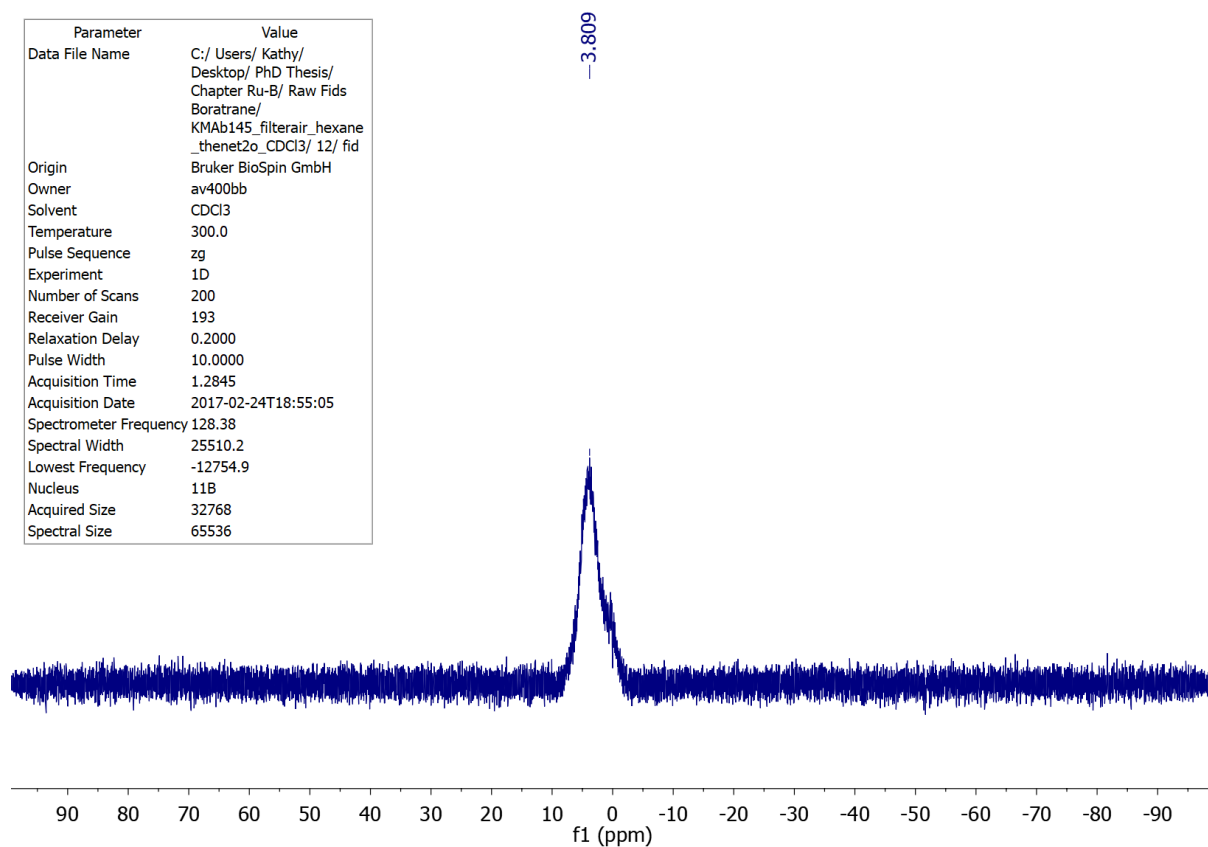
### $^{11}\text{B}\{^1\text{H}\}$ NMR Spectrum of Complex 5

Parameter	Value
Data File Name	C:/ Users/ Kathy/ Desktop/ PhD Thesis/ Chapter Ru-B/ Raw Fids Boratrane/ KMAB145_filterair_hexane_ thenet2o_CDCl3/ 13/ fid
Origin	Bruker BioSpin GmbH
Owner	av400bb
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zgpg
Experiment	1D
Number of Scans	200
Receiver Gain	193
Relaxation Delay	0.2000
Pulse Width	10.0000
Acquisition Time	1.2845
Acquisition Date	2017-02-24T19:01:46
Spectrometer Frequency	128.38
Spectral Width	25510.2
Lowest Frequency	-12754.9
Nucleus	11B
Acquired Size	32768
Spectral Size	65536



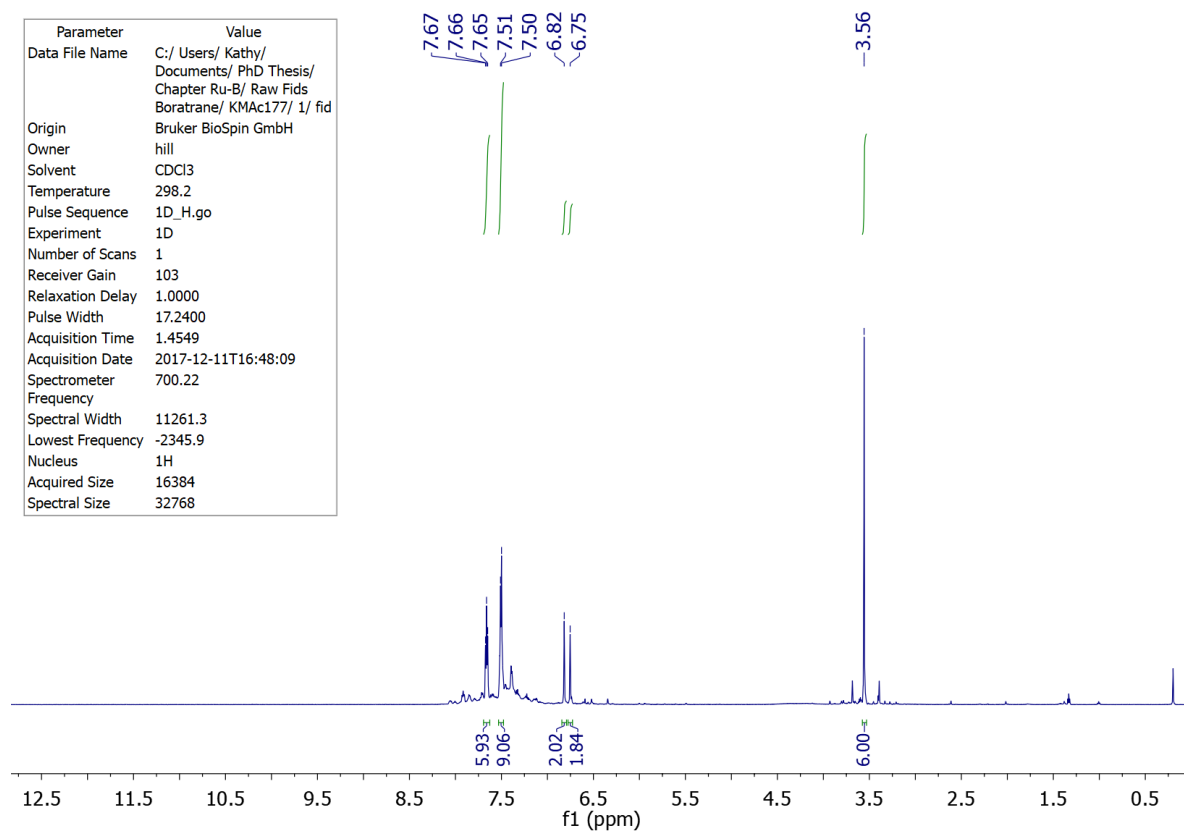
### $^{11}\text{B}$ NMR Spectrum of Complex 5

Parameter	Value
Data File Name	C:/ Users/ Kathy/ Desktop/ PhD Thesis/ Chapter Ru-B/ Raw Fids Boratrane/ KMAB145_filterair_hexane_ thenet2o_CDCl3/ 12/ fid
Origin	Bruker BioSpin GmbH
Owner	av400bb
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zg
Experiment	1D
Number of Scans	200
Receiver Gain	193
Relaxation Delay	0.2000
Pulse Width	10.0000
Acquisition Time	1.2845
Acquisition Date	2017-02-24T18:55:05
Spectrometer Frequency	128.38
Spectral Width	25510.2
Lowest Frequency	-12754.9
Nucleus	11B
Acquired Size	32768
Spectral Size	65536

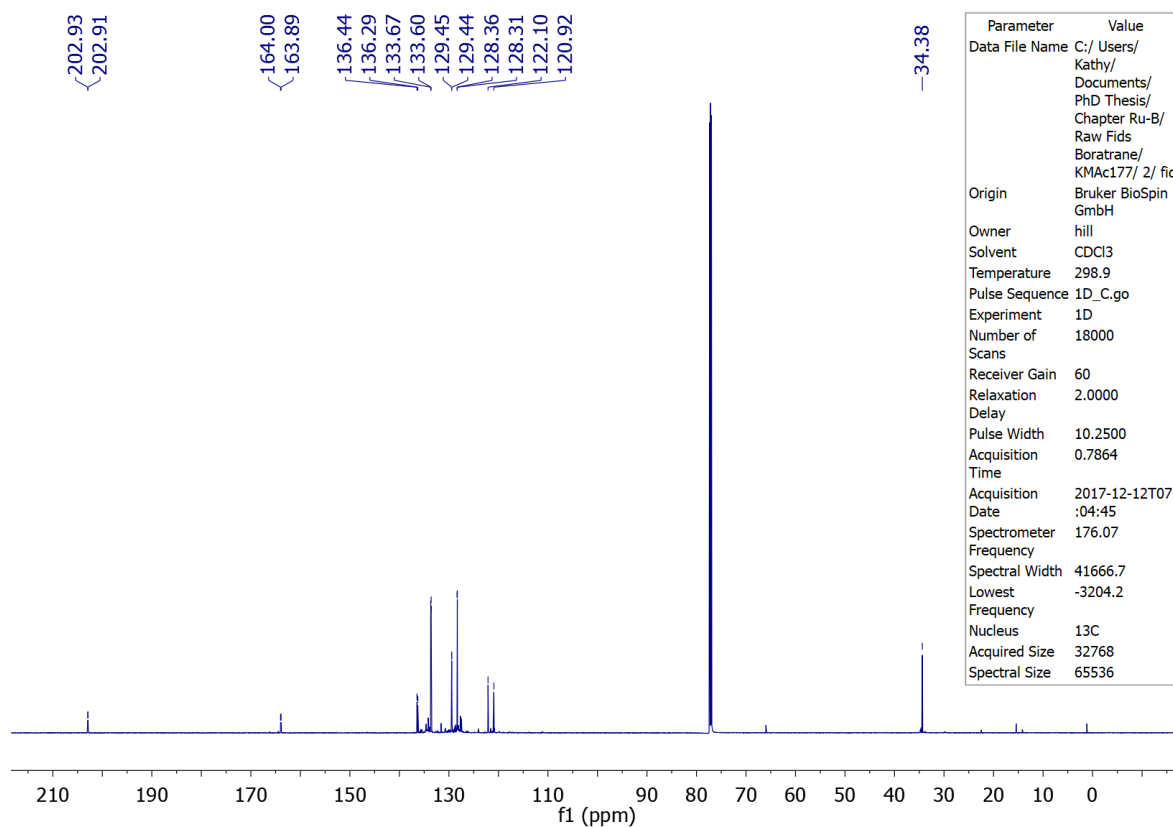


# [Ru{BH(mt)<sub>2</sub>}(CO)<sub>2</sub>(PPh<sub>3</sub>)] (12)

## <sup>1</sup>H NMR Spectrum of Complex 12

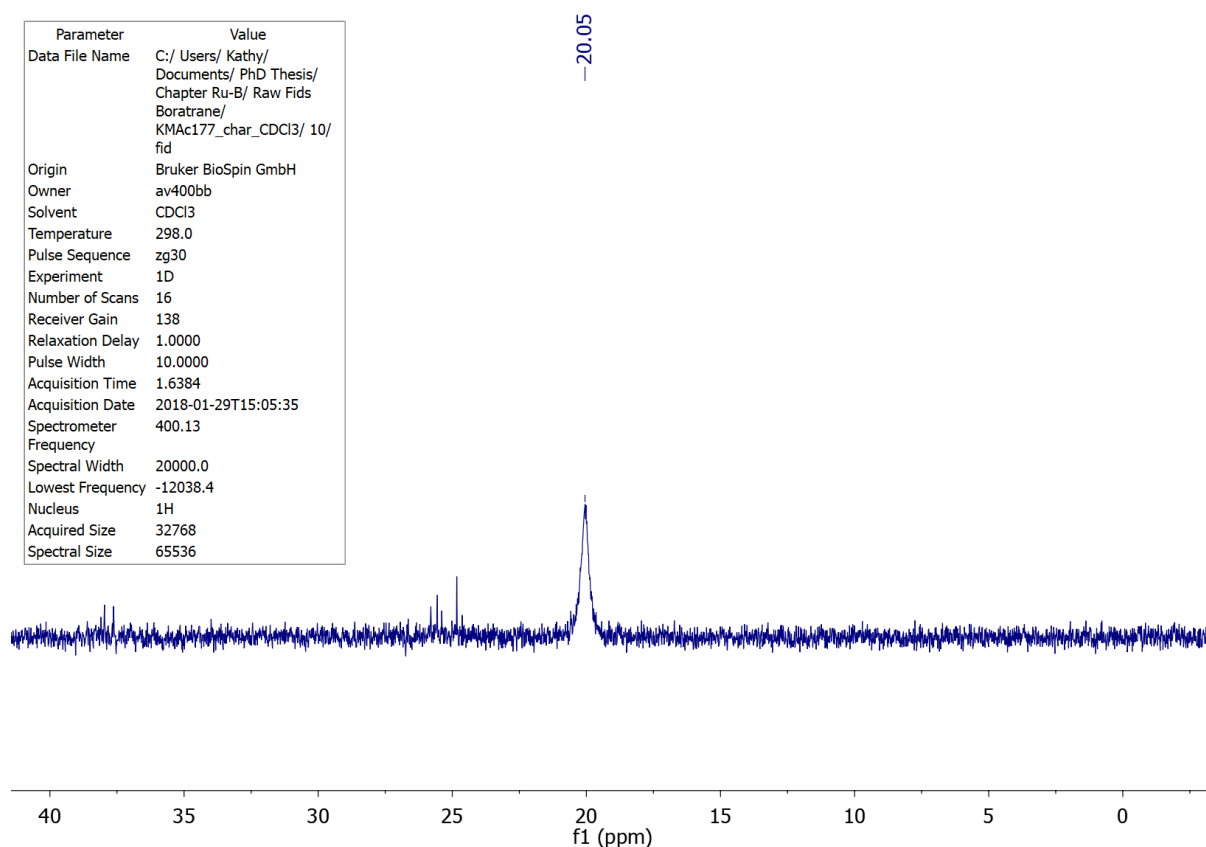


## <sup>13</sup>C{<sup>1</sup>H} NMR Spectrum of Complex 12



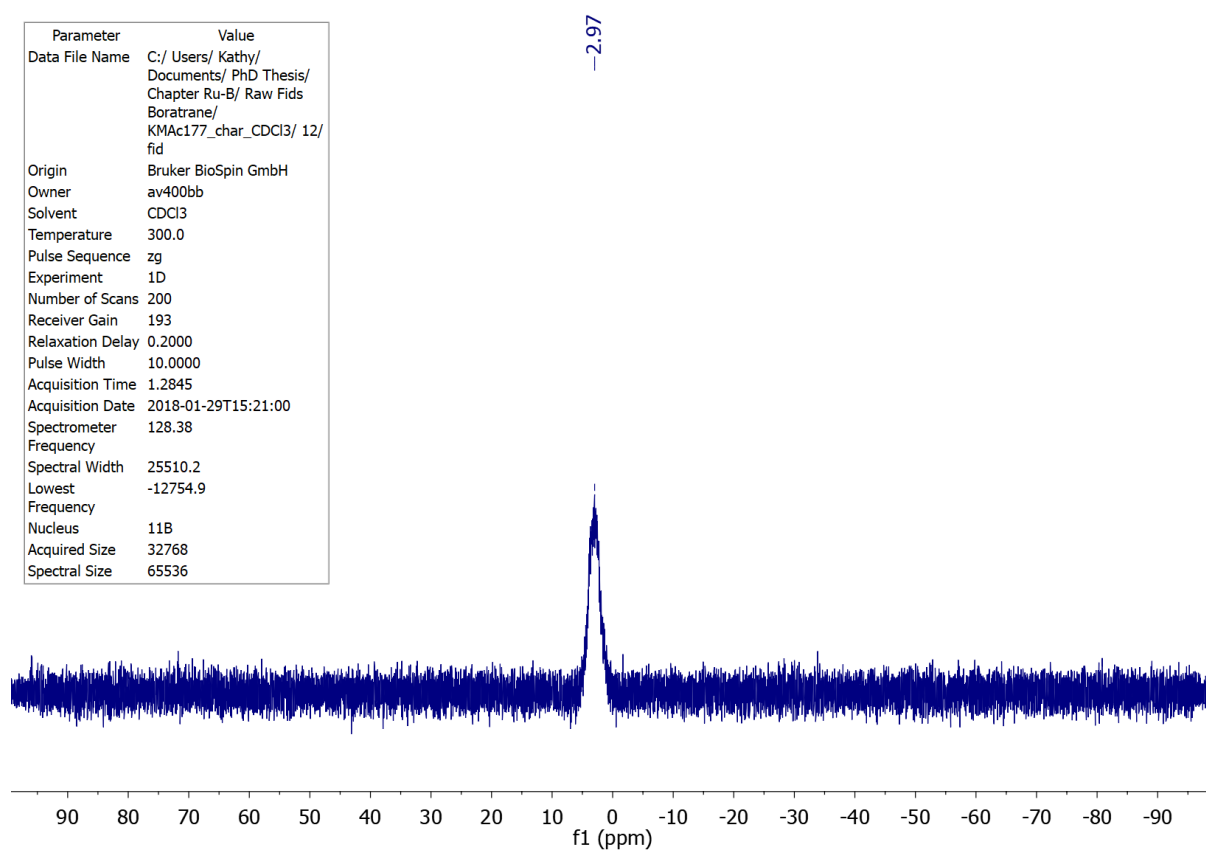
### $^{31}\text{P}\{^1\text{H}\}$ NMR Spectrum of Complex 12

Parameter	Value
Data File Name	C:/Users/Kathy/Documents/PhD Thesis/Chapter Ru-B/ Raw Fids Boratrane/KMAc177_char_CDCl3/ 10/ fid
Origin	Bruker BioSpin GmbH
Owner	av400bb
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	138
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	1.6384
Acquisition Date	2018-01-29T15:05:35
Spectrometer	400.13
Frequency	
Spectral Width	20000.0
Lowest Frequency	-12038.4
Nucleus	$^1\text{H}$
Acquired Size	32768
Spectral Size	65536



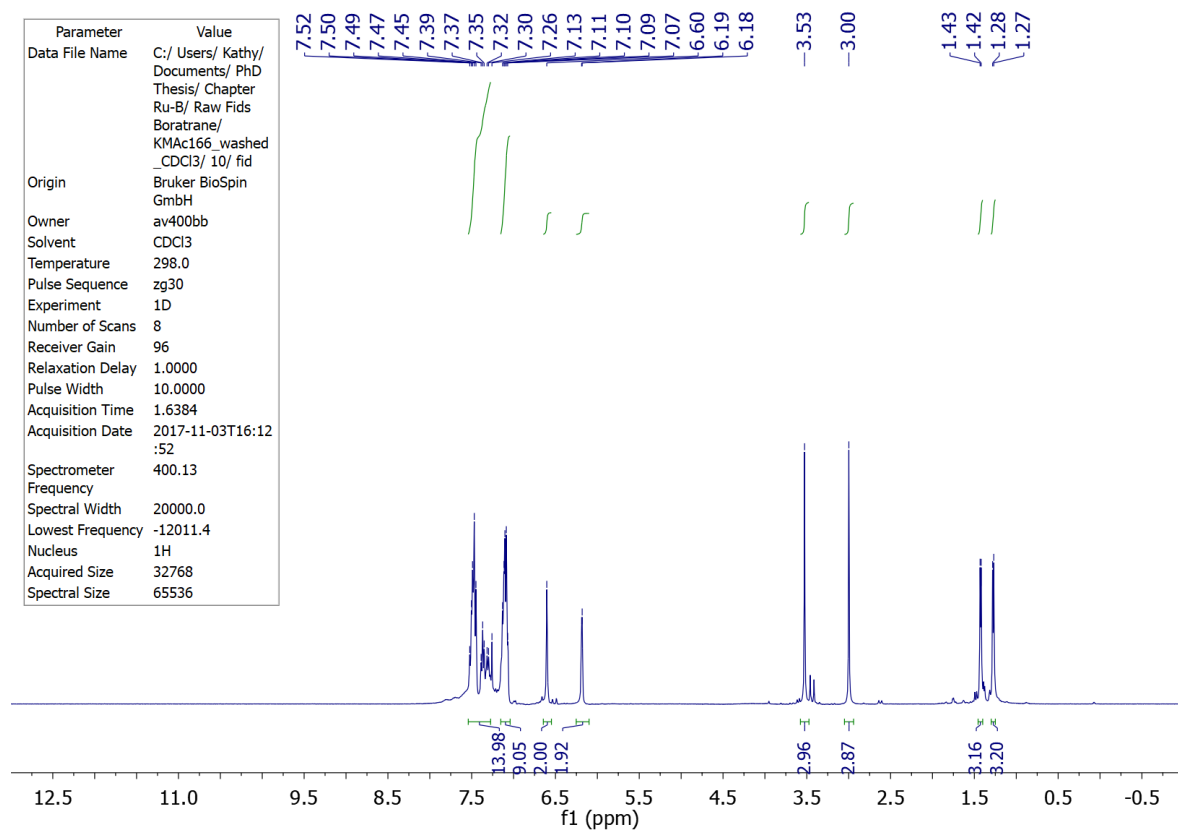
### $^{11}\text{B}$ NMR Spectrum of Complex 12

Parameter	Value
Data File Name	C:/Users/Kathy/Documents/PhD Thesis/Chapter Ru-B/ Raw Fids Boratrane/KMAc177_char_CDCl3/ 12/ fid
Origin	Bruker BioSpin GmbH
Owner	av400bb
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zg
Experiment	1D
Number of Scans	200
Receiver Gain	193
Relaxation Delay	0.2000
Pulse Width	10.0000
Acquisition Time	1.2845
Acquisition Date	2018-01-29T15:21:00
Spectrometer	128.38
Frequency	
Spectral Width	25510.2
Lowest Frequency	-12754.9
Frequency	
Nucleus	$^{11}\text{B}$
Acquired Size	32768
Spectral Size	65536

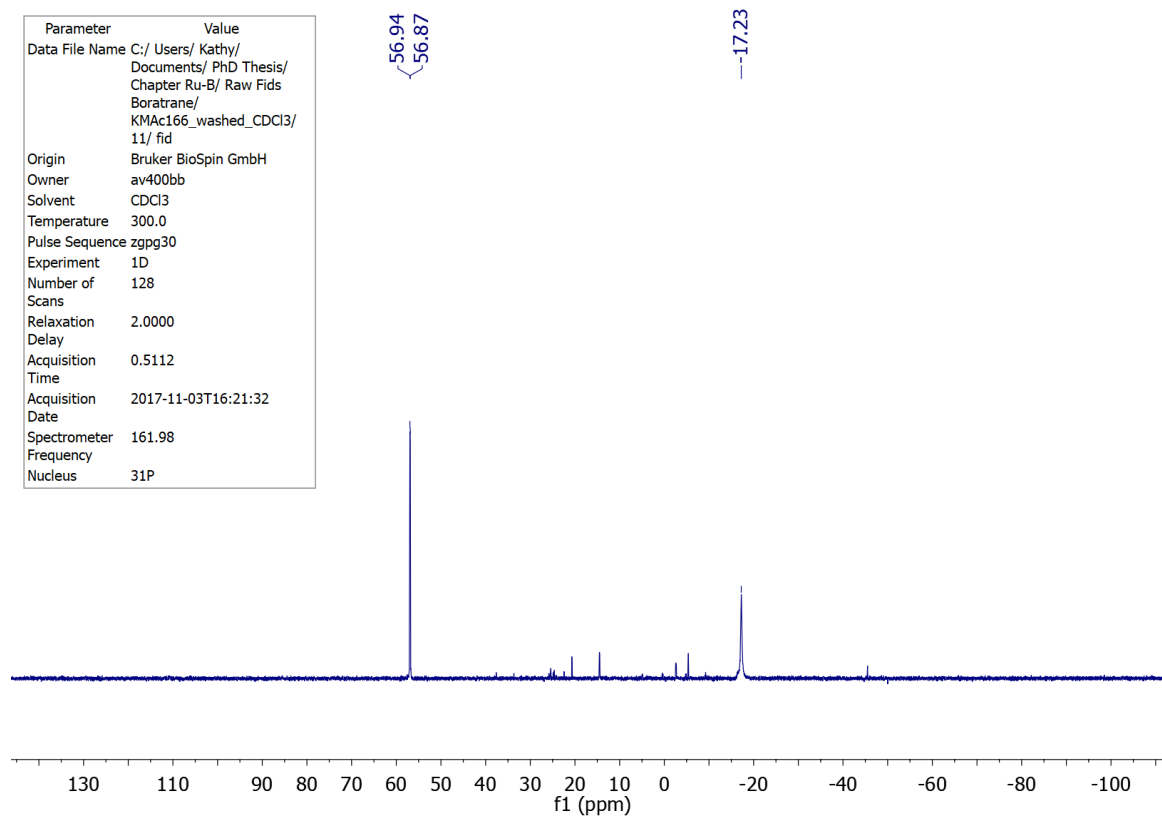


# [Ru{BH(mt)<sub>2</sub>}(CO)(PMe<sub>2</sub>Ph)(PPh<sub>3</sub>)] (13)

## <sup>1</sup>H NMR Spectrum of Complex 13 in CDCl<sub>3</sub>

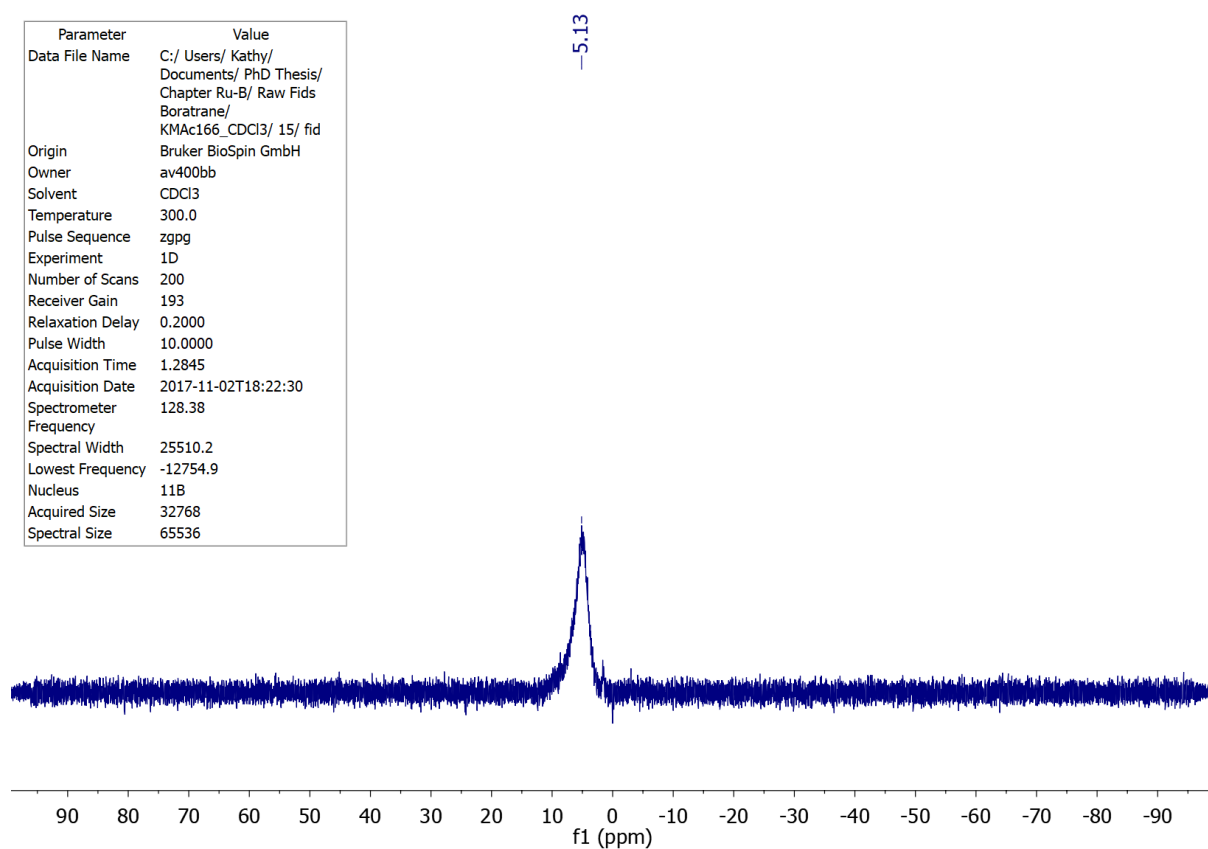


## <sup>31</sup>P{<sup>1</sup>H} NMR Spectrum of Complex 13 in CDCl<sub>3</sub>



# $^{11}\text{B}\{^1\text{H}\}$ NMR Spectrum of Complex 13 in $\text{CDCl}_3$

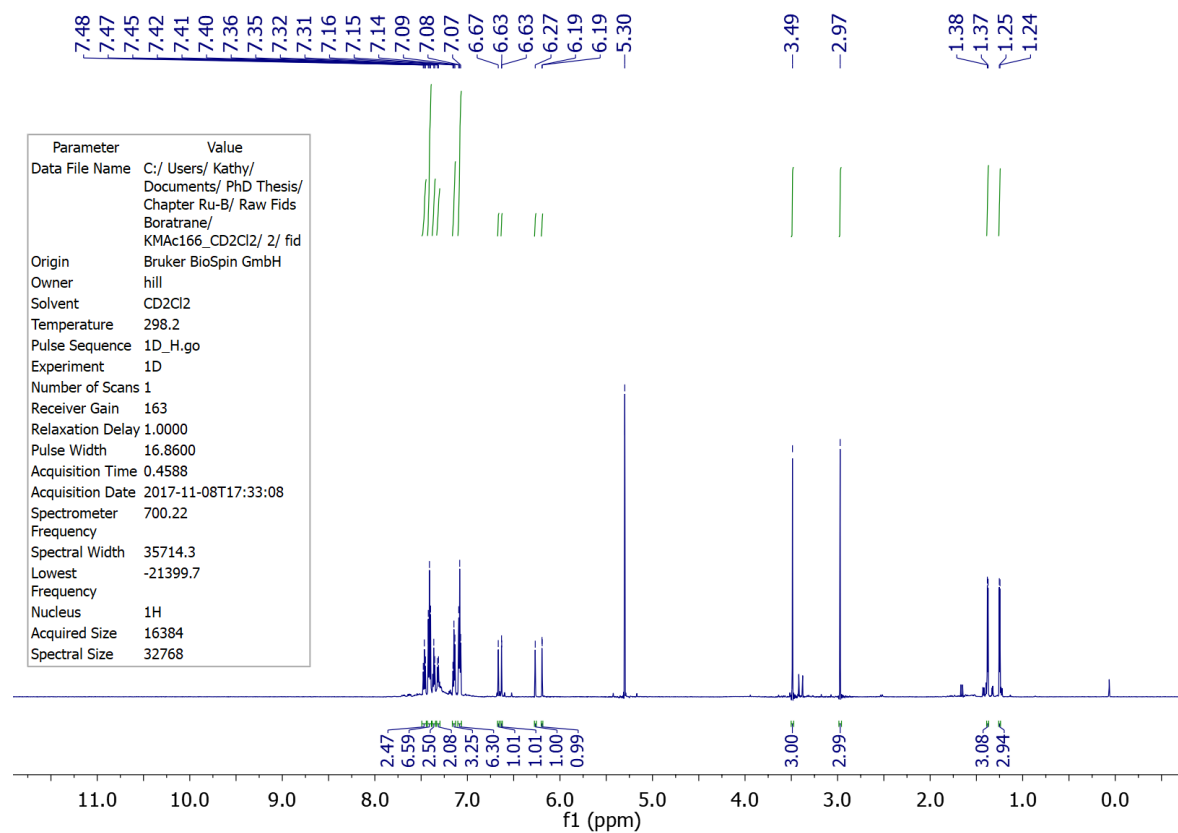
Parameter	Value
Data File Name	C:/Users/Kathy/Documents/PhD Thesis/Chapter Ru-B/ Raw Fids/Boratrane/KMAc166_CDCl3/ 15/ fid
Origin	Bruker BioSpin GmbH
Owner	av400bb
Solvent	$\text{CDCl}_3$
Temperature	300.0
Pulse Sequence	zgpg
Experiment	1D
Number of Scans	200
Receiver Gain	193
Relaxation Delay	0.2000
Pulse Width	10.0000
Acquisition Time	1.2845
Acquisition Date	2017-11-02T18:22:30
Spectrometer	128.38
Frequency	
Spectral Width	25510.2
Lowest Frequency	-12754.9
Nucleus	$^{11}\text{B}$
Acquired Size	32768
Spectral Size	65536



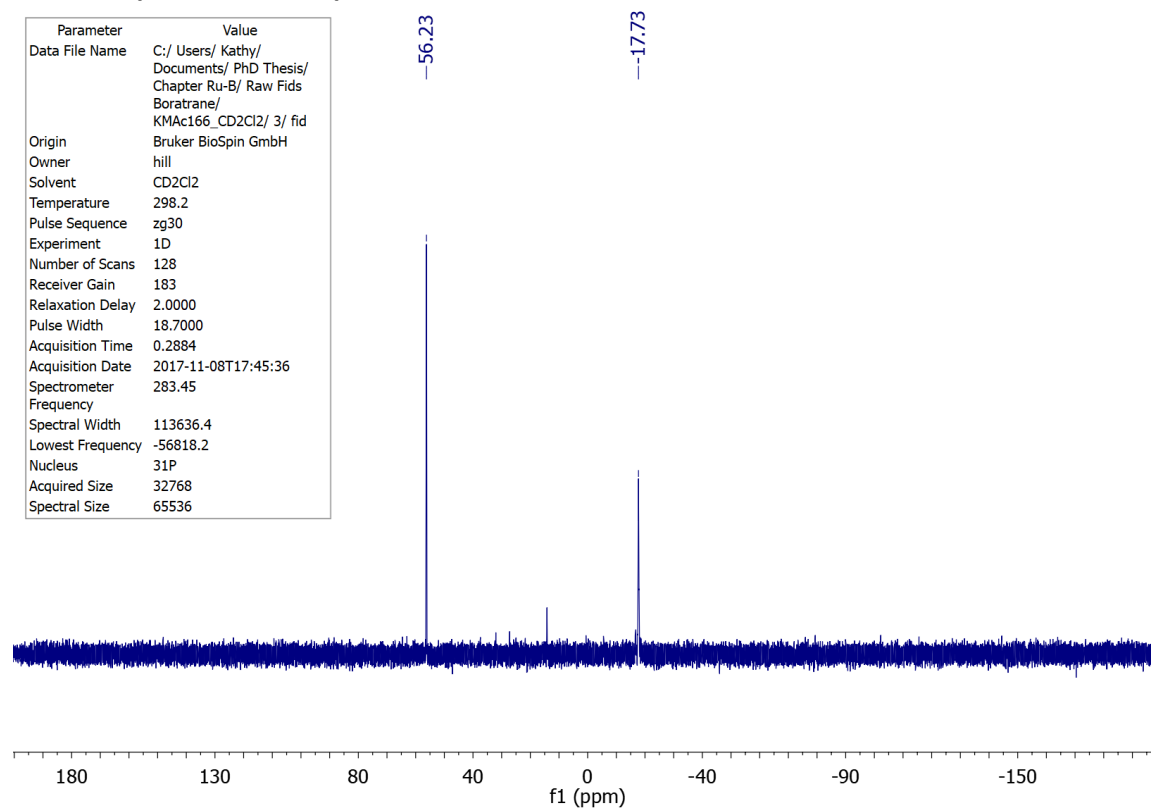


## NMR spectra in CD<sub>2</sub>Cl<sub>2</sub>

### <sup>1</sup>H NMR Spectrum of Complex 13

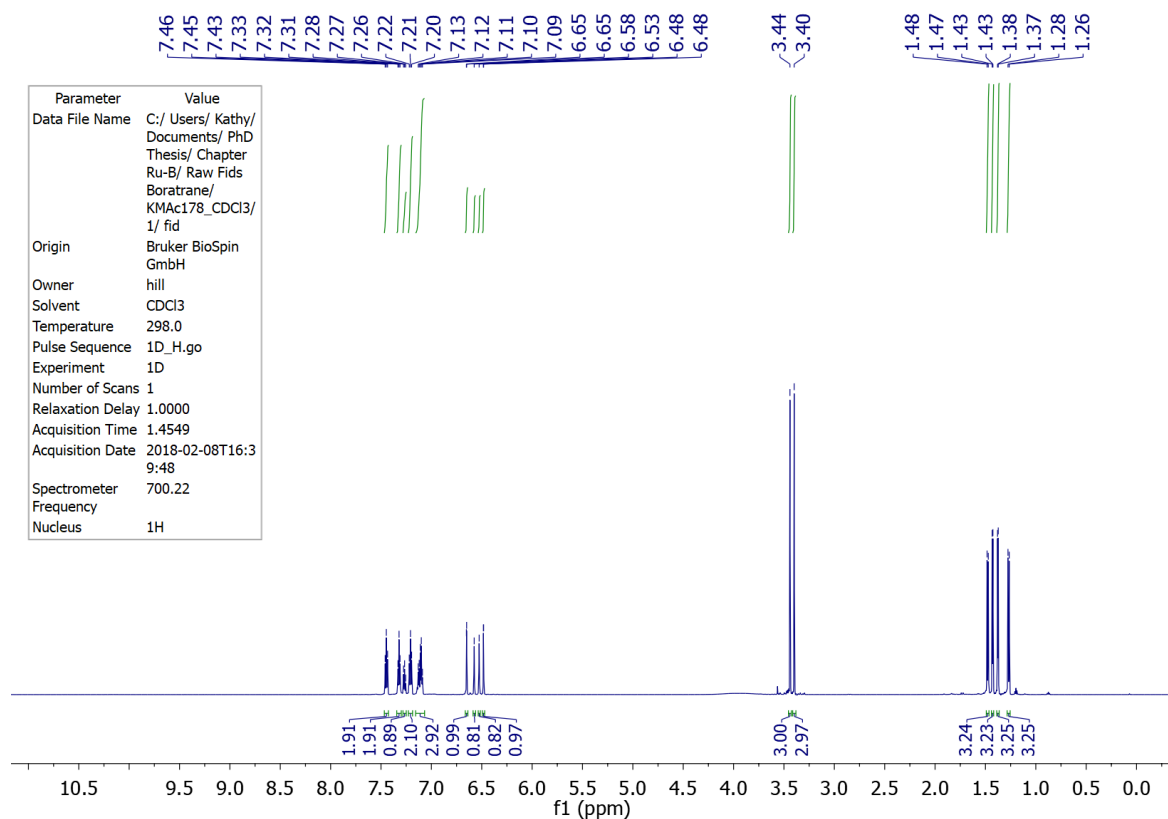


### <sup>31</sup>P NMR Spectrum of Complex 13

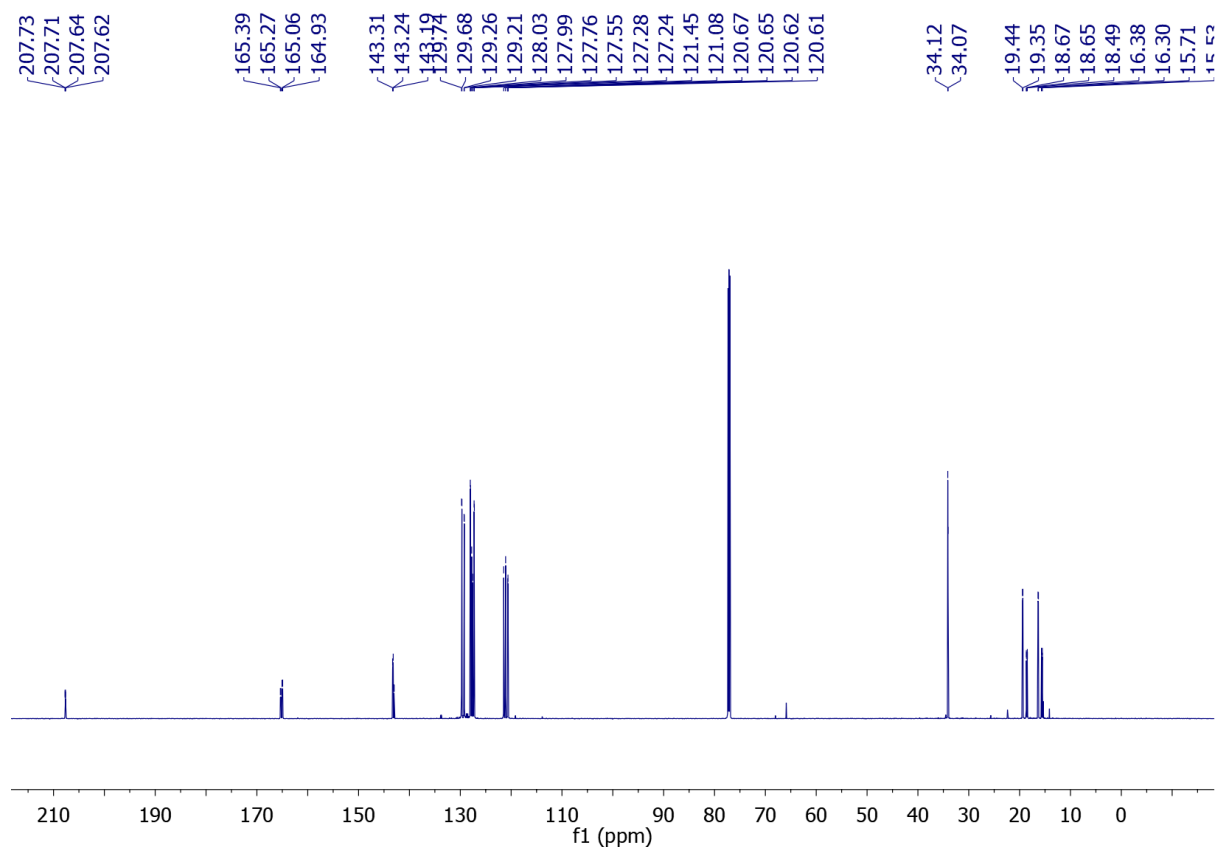


# [Ru{BH(mt)<sub>2</sub>}(CO)(PMe<sub>2</sub>Ph)<sub>2</sub>] (14)

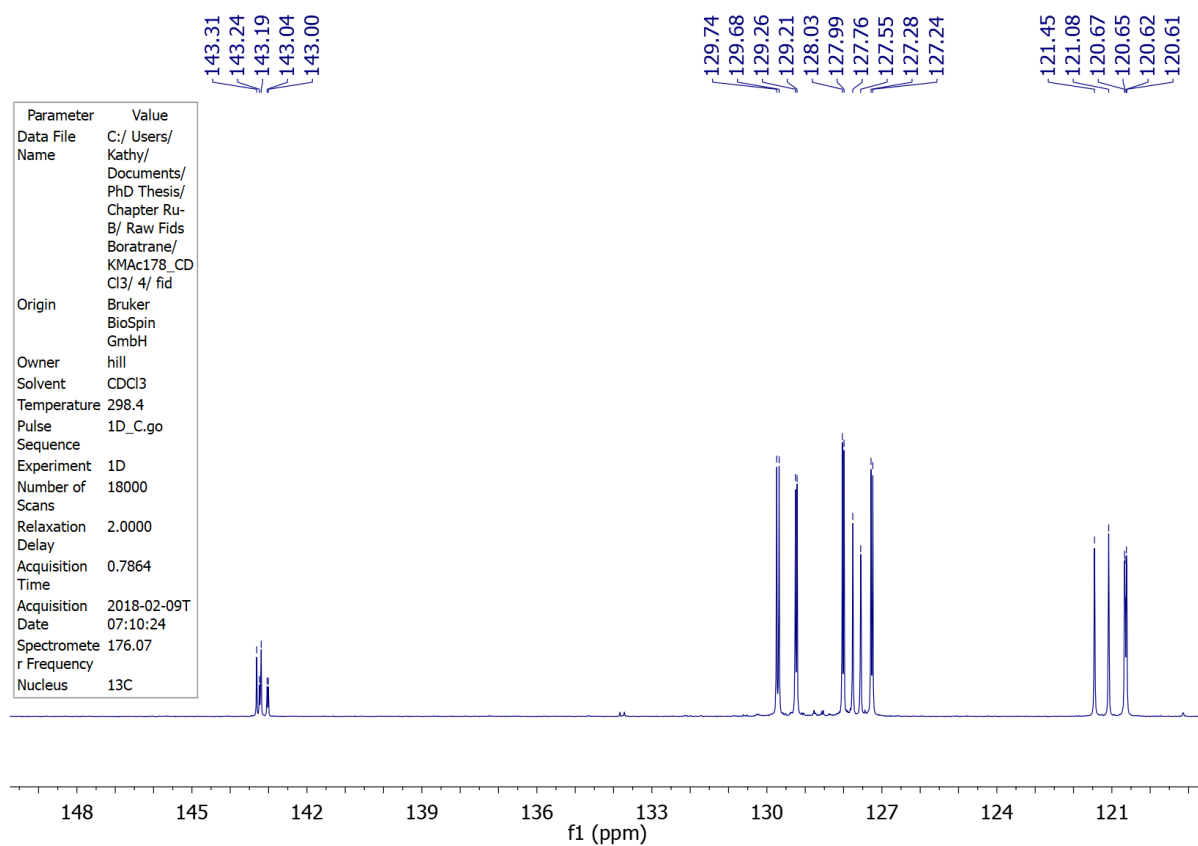
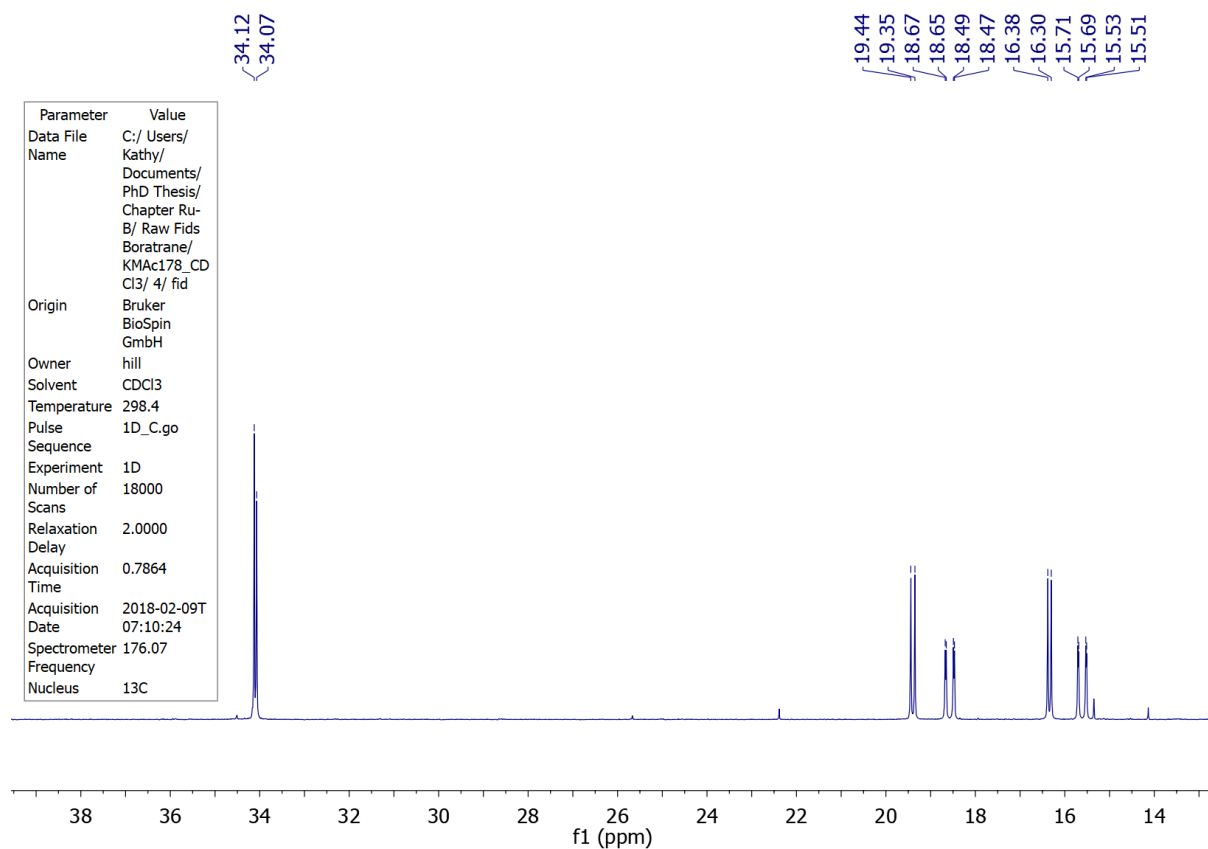
## <sup>1</sup>H NMR Spectrum of Complex 14



## <sup>13</sup>C{<sup>1</sup>H} NMR Spectrum of Complex 14

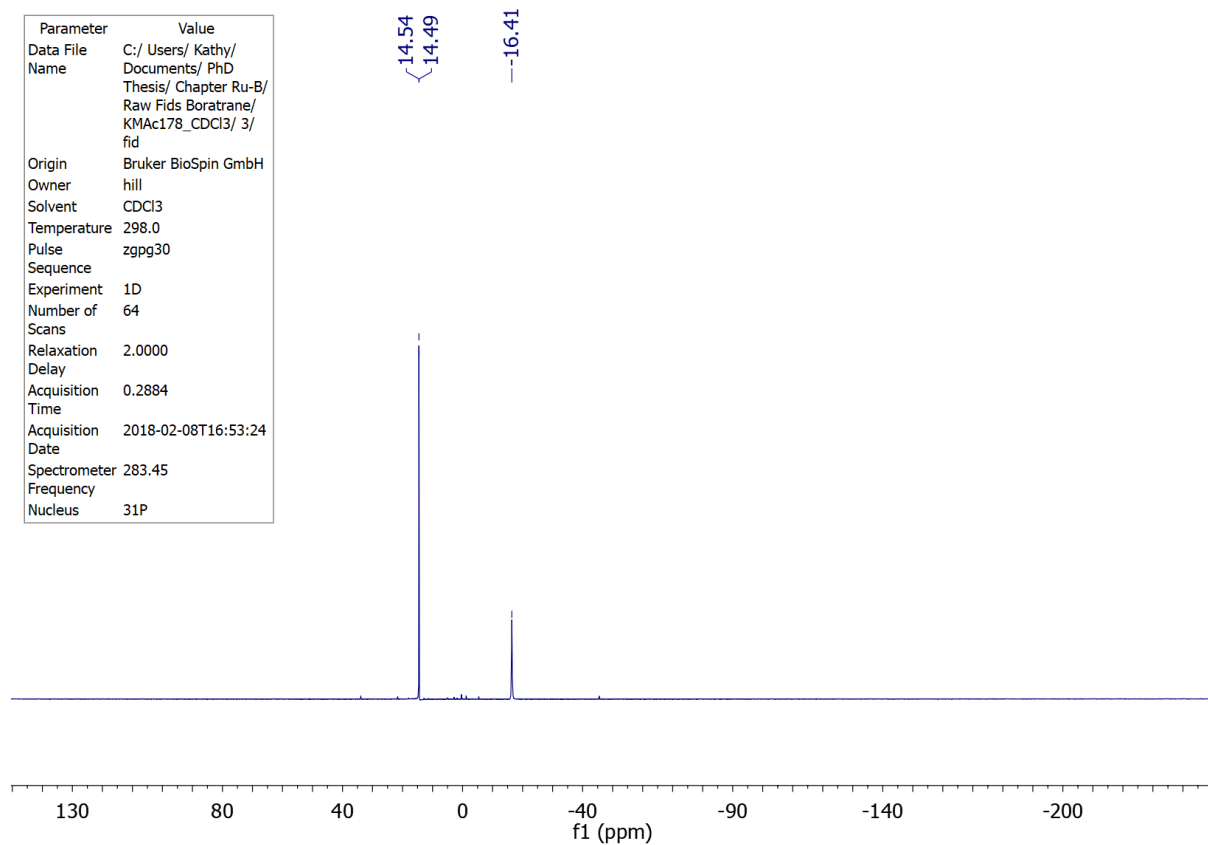


# Expansion of $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of Complex 14



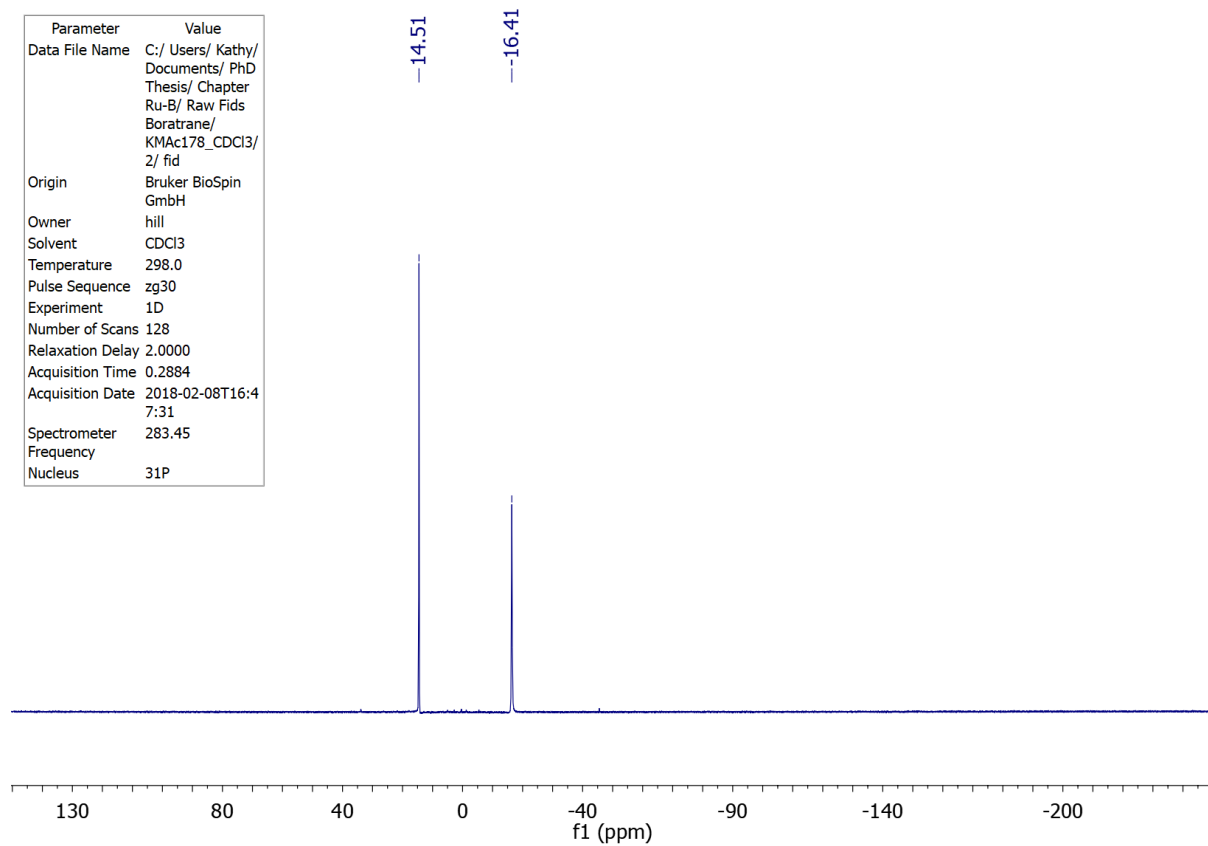
### $^{31}\text{P}\{^1\text{H}\}$ NMR Spectrum of Complex 14

Parameter	Value
Data File Name	C:/Users/Kathy/Documents/PhD Thesis/Chapter Ru-B/Raw Fids Boratrane/KMAc178_CDCl3/3/fid
Origin	Bruker BioSpin GmbH
Owner	hill
Solvent	CDCl3
Temperature	298.0
Pulse	zgpg30
Sequence	
Experiment	1D
Number of Scans	64
Relaxation Delay	2.0000
Acquisition Time	0.2884
Acquisition Date	2018-02-08T16:53:24
Spectrometer	283.45
Frequency	
Nucleus	31P



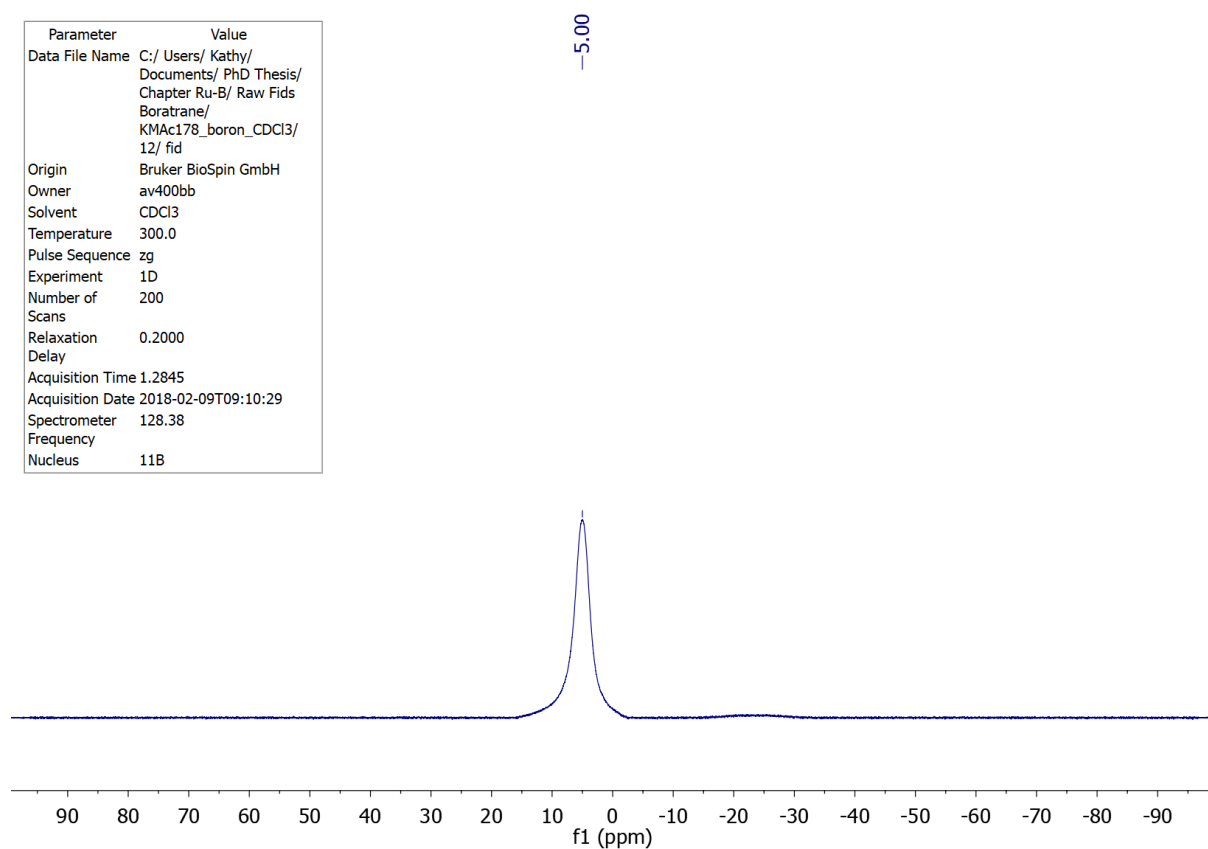
### $^{31}\text{P}$ NMR Spectrum of Complex 14

Parameter	Value
Data File Name	C:/Users/Kathy/Documents/PhD Thesis/Chapter Ru-B/Raw Fids Boratrane/KMAc178_CDCl3/2/fid
Origin	Bruker BioSpin GmbH
Owner	hill
Solvent	CDCl3
Temperature	298.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	128
Relaxation Delay	2.0000
Acquisition Time	0.2884
Acquisition Date	2018-02-08T16:47:31
Spectrometer	283.45
Frequency	
Nucleus	31P



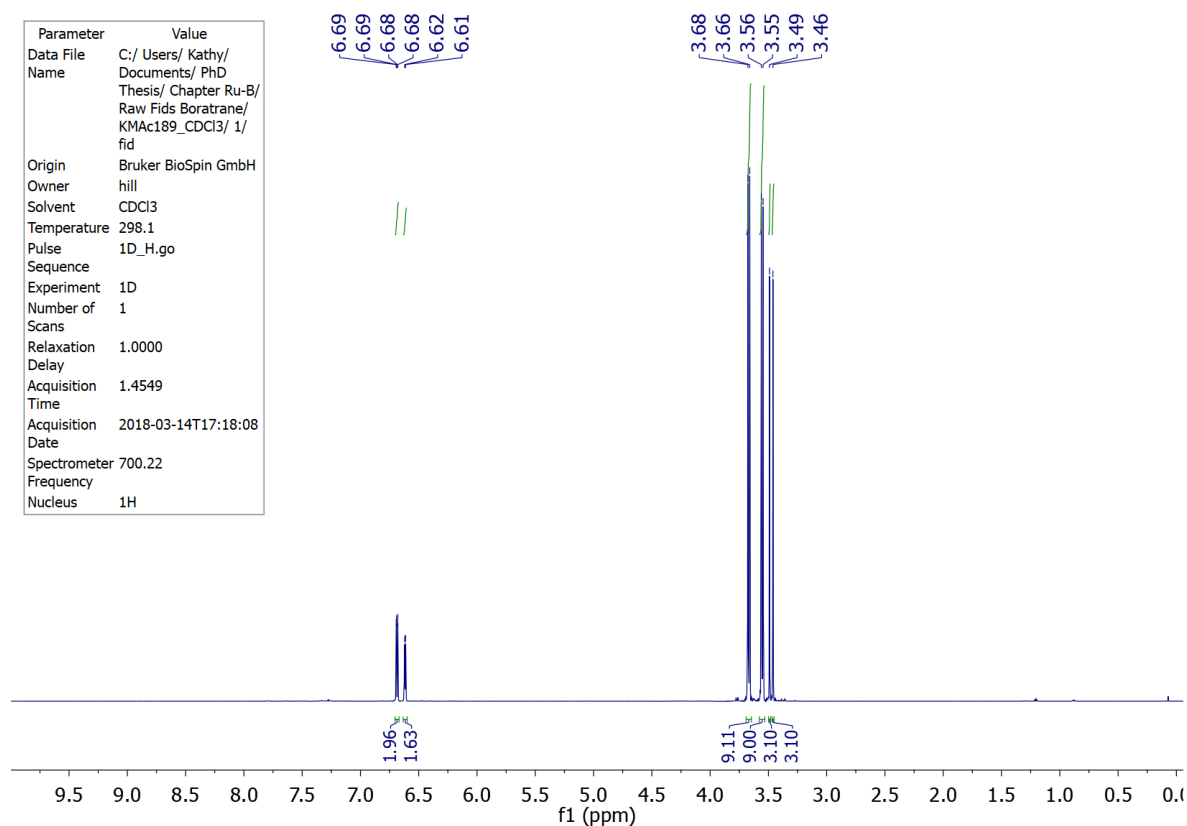
# <sup>11</sup>B NMR Spectrum of Complex 14

Parameter	Value
Data File Name	C:/Users/Kathy/Documents/PhD Thesis/Chapter Ru-B/ Raw Fids Boratrane/KMAc178_boron_CDCl3/12/ fid
Origin	Bruker BioSpin GmbH
Owner	av400bb
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zg
Experiment	1D
Number of Scans	200
Relaxation Delay	0.2000
Acquisition Time	1.2845
Acquisition Date	2018-02-09T09:10:29
Spectrometer	128.38
Frequency	
Nucleus	11B

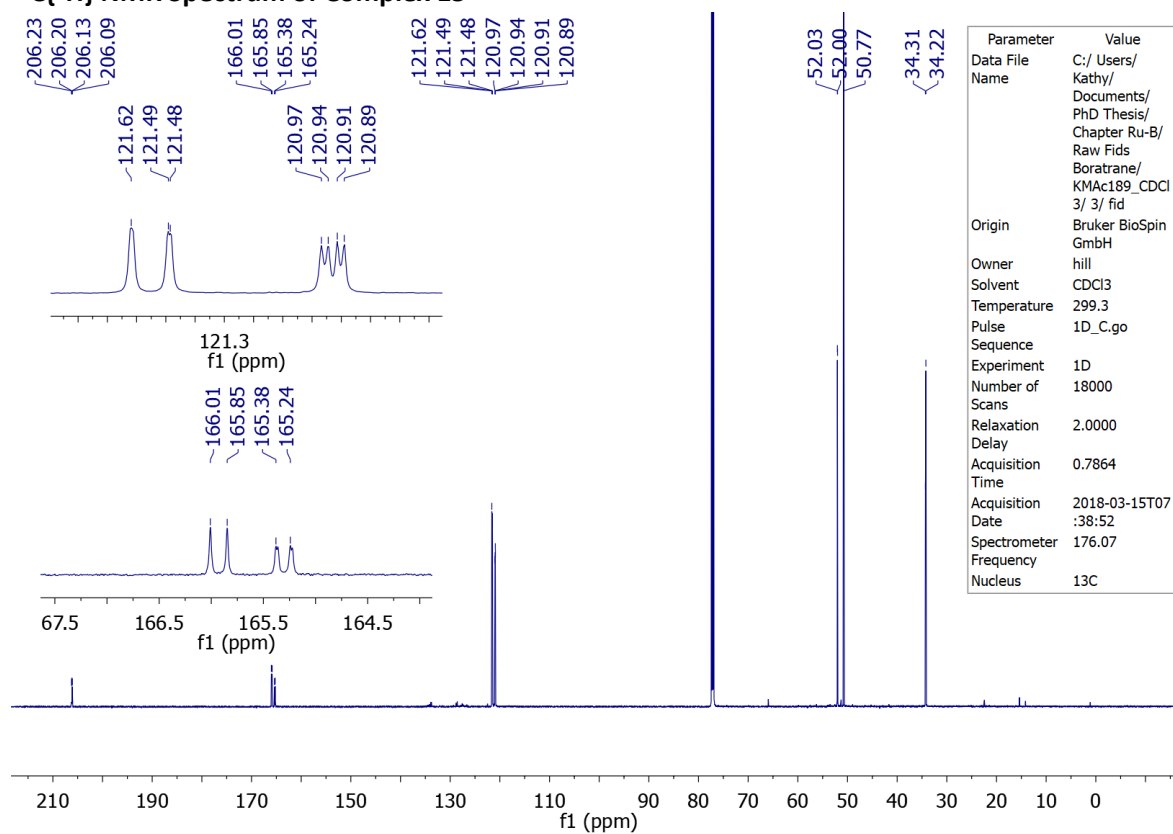


# [Ru{BH(mt)<sub>2</sub>}(CO){P(OMe)<sub>3</sub>}<sub>2</sub>] (15)

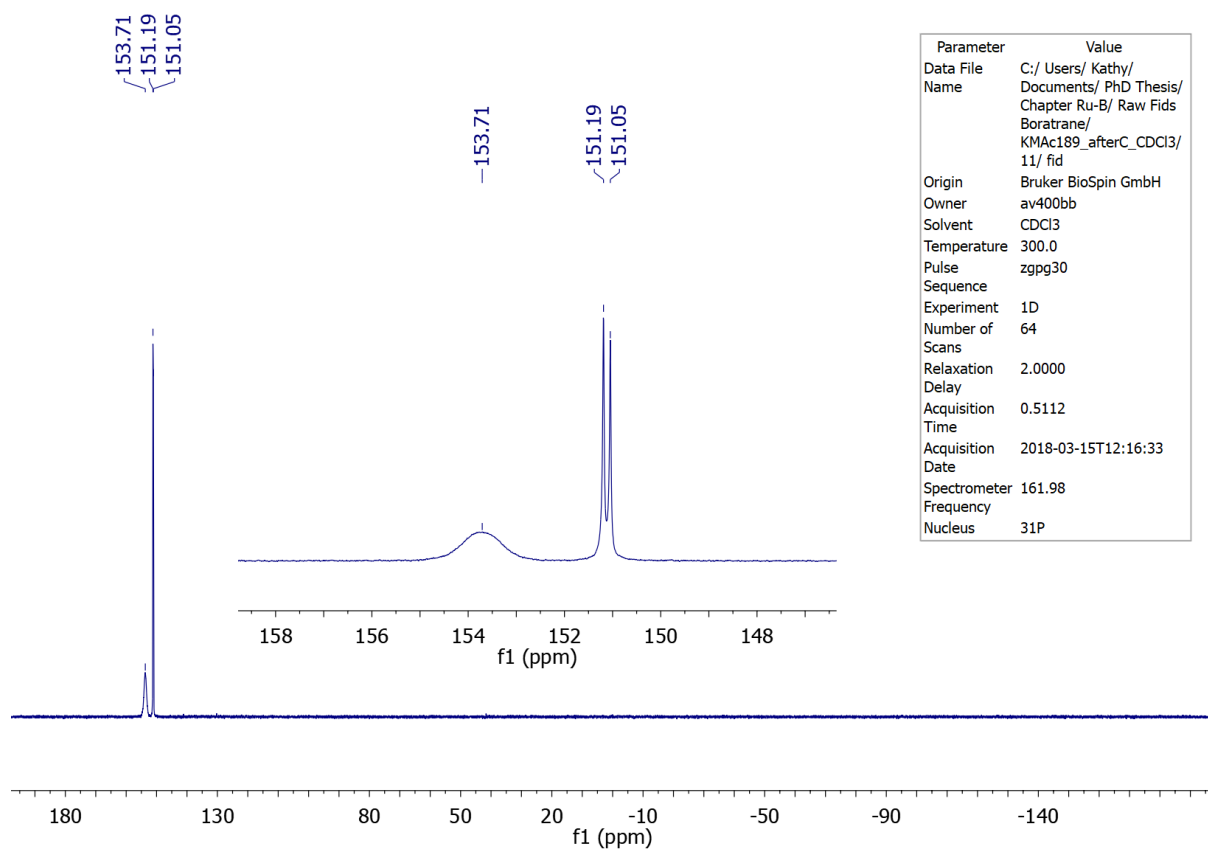
## <sup>1</sup>H NMR Spectrum of Complex 15



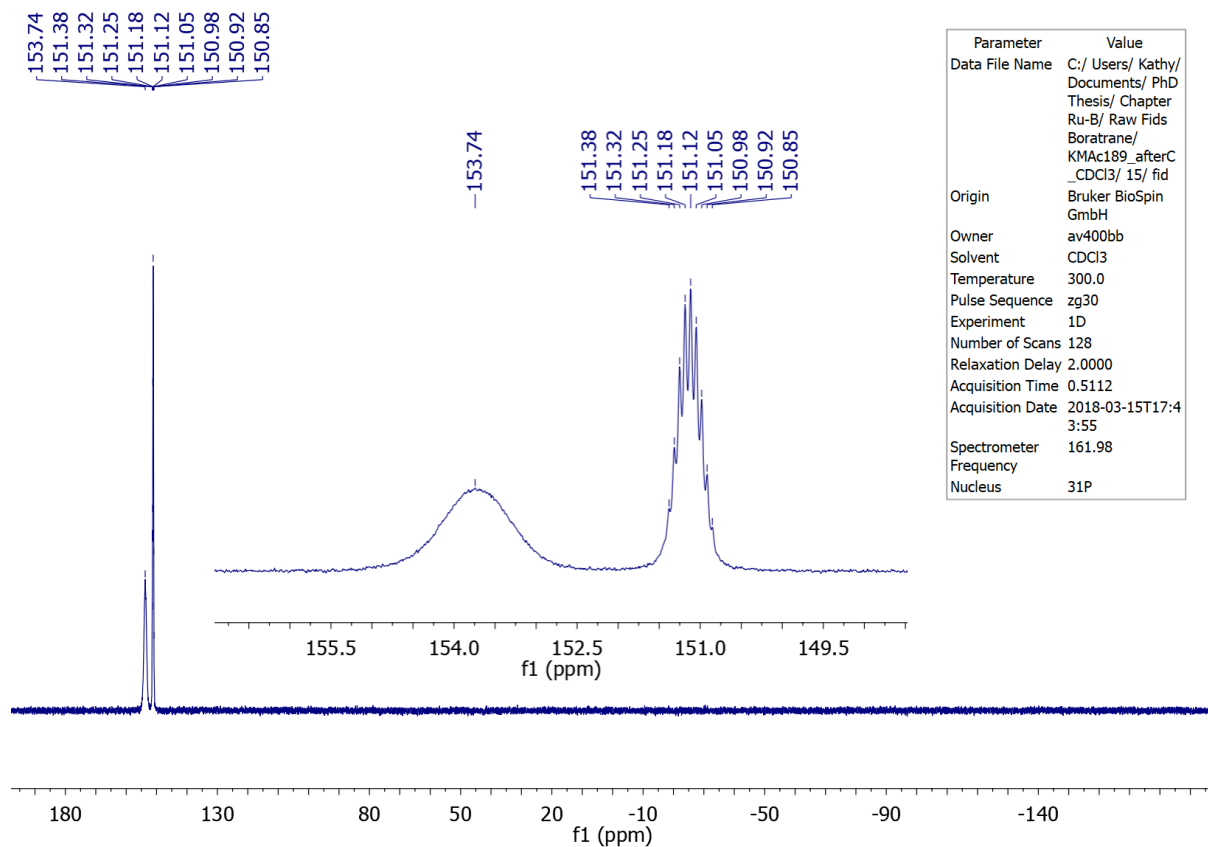
## <sup>13</sup>C{<sup>1</sup>H} NMR Spectrum of Complex 15



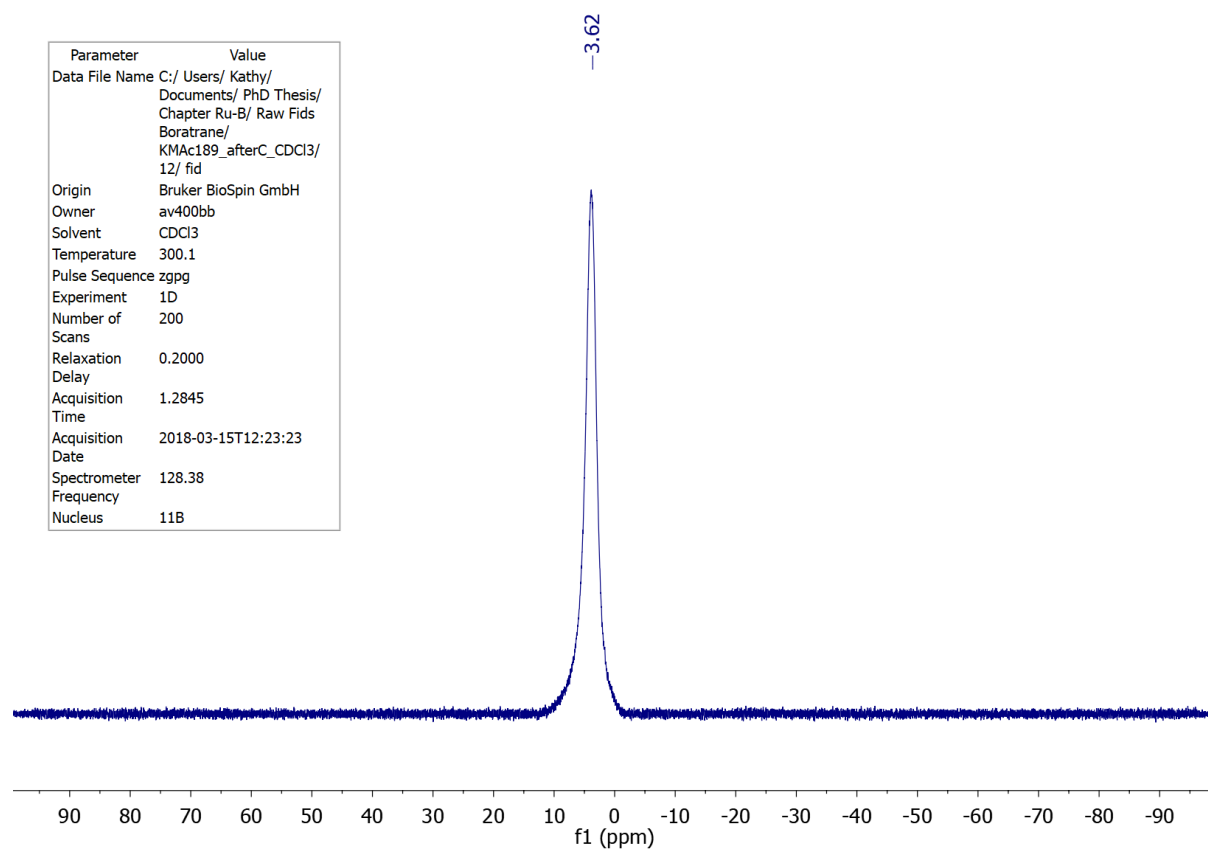
### $^{31}\text{P}\{^1\text{H}\}$ NMR Spectrum of Complex 15



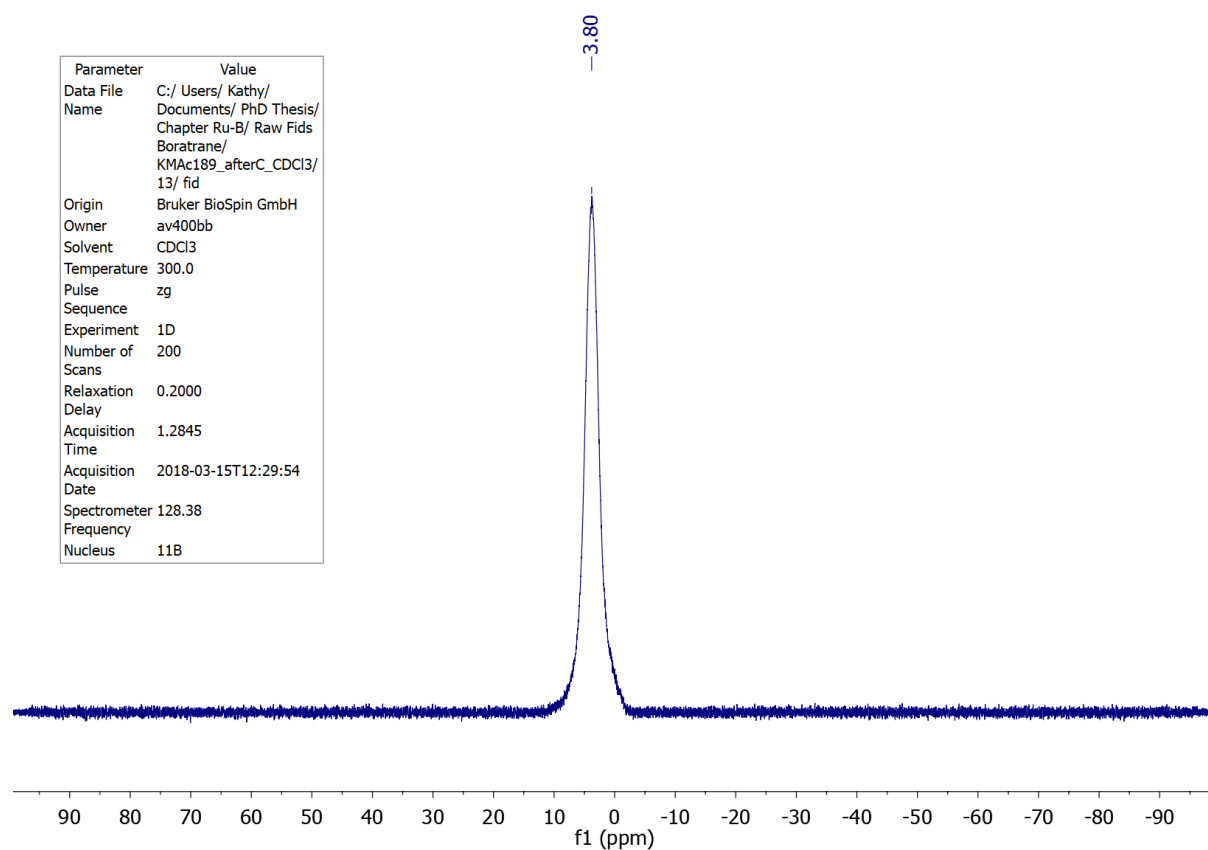
### $^{31}\text{P}$ NMR Spectrum of Complex 15



### $^{11}\text{B}\{^1\text{H}\}$ NMR Spectrum of Complex 15



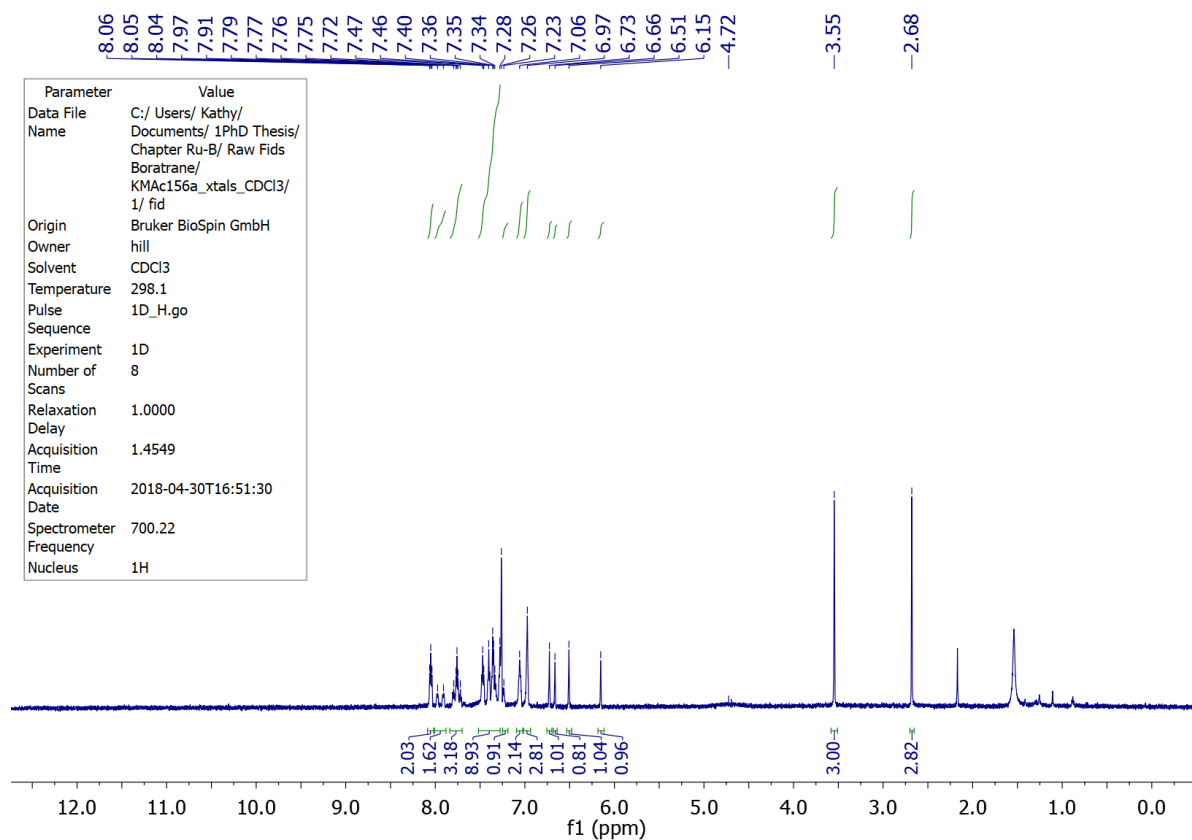
### $^{11}\text{B}$ NMR Spectrum of Complex 15



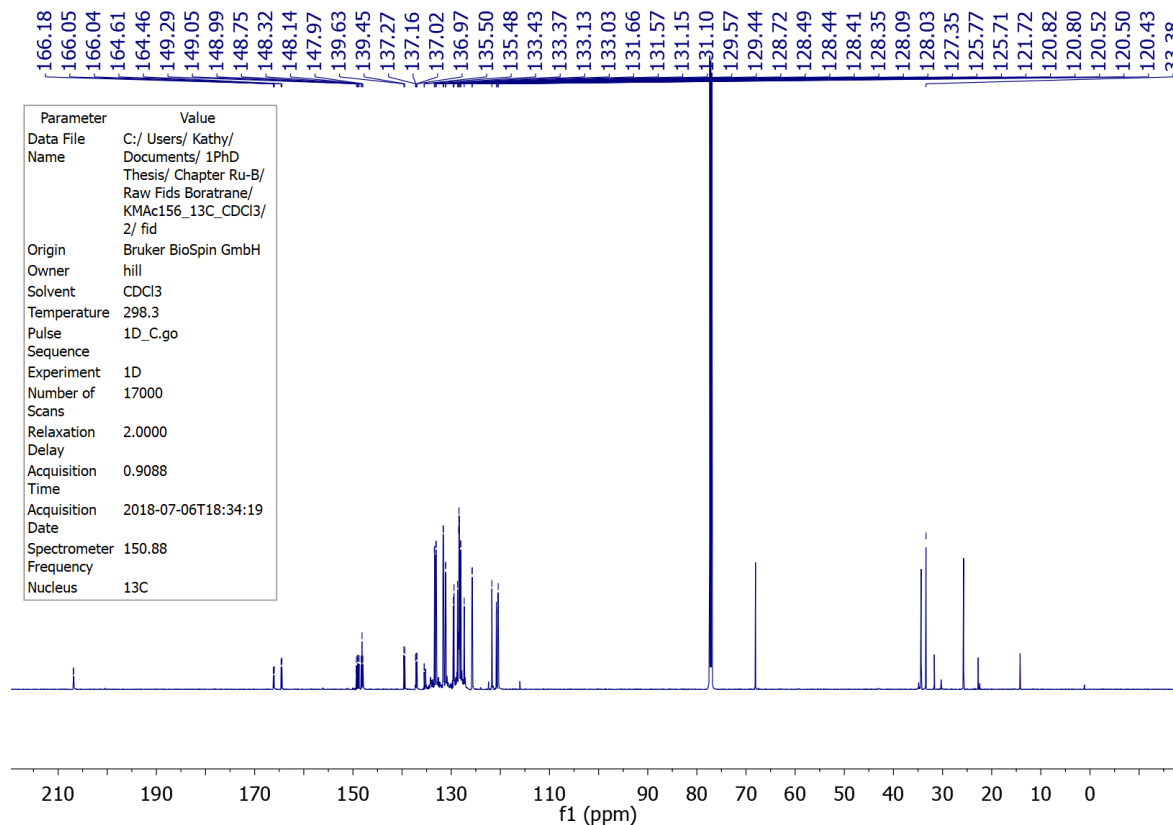


# [Ru{BH(mt)<sub>2</sub>}(CO)(Z-Ph<sub>2</sub>PCH=CHPPH<sub>2</sub>)] (16)

## <sup>1</sup>H NMR Spectrum of Complex 16

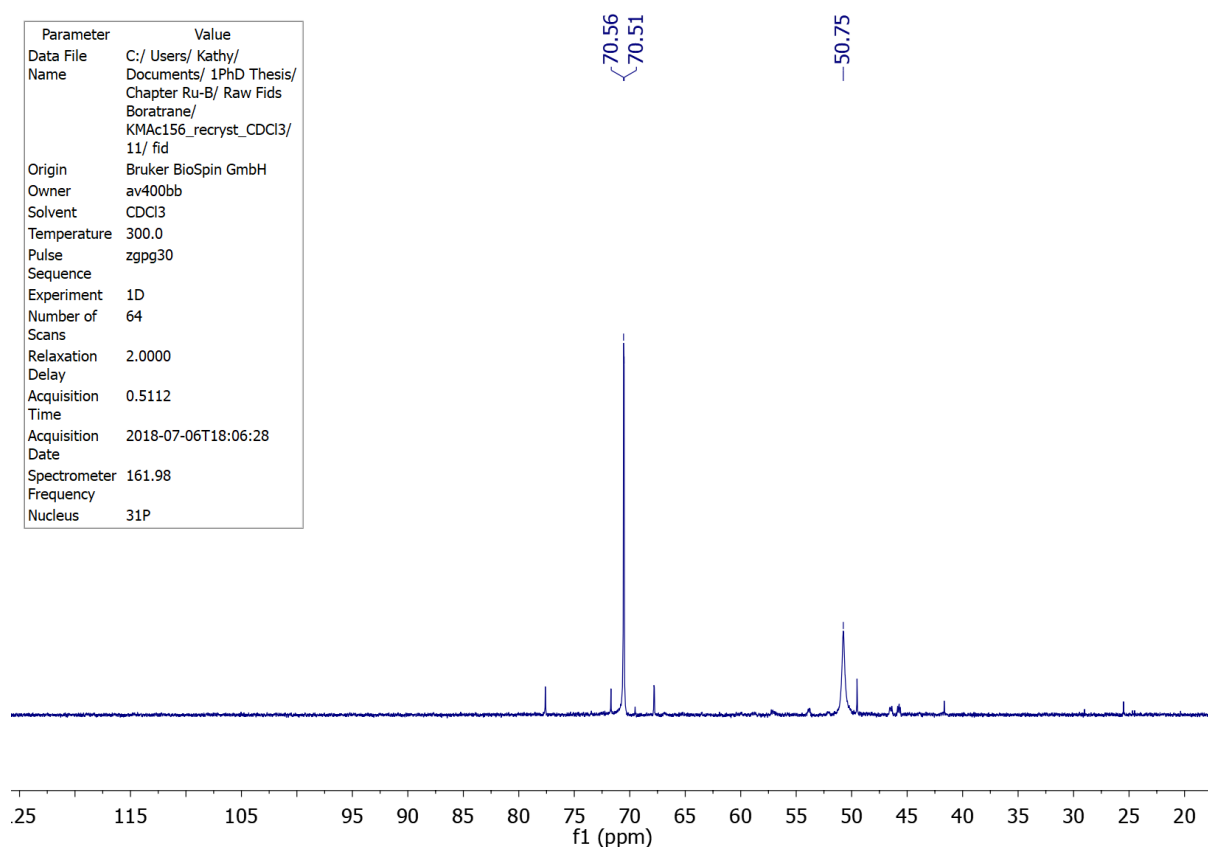


## <sup>13</sup>C{<sup>1</sup>H} NMR Spectrum of Complex 16



### $^{31}\text{P}\{^1\text{H}\}$ NMR Spectrum of Complex 16

Parameter	Value
Data File Name	C:/Users/Kathy/Documents/1PhD Thesis/Chapter Ru-B/ Raw Fids/Boratrane/KMAc156_recryst_CDCl3/11/ fid
Origin	Bruker BioSpin GmbH
Owner	av400bb
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	64
Relaxation Delay	2.0000
Acquisition Time	0.5112
Acquisition Date	2018-07-06T18:06:28
Spectrometer Frequency	161.98
Nucleus	$^{31}\text{P}$



### $^{11}\text{B}\{^1\text{H}\}$ NMR Spectrum of Complex 16

Parameter	Value
Data File Name	C:/Users/Kathy/Documents/1PhD Thesis/Chapter Ru-B/ Raw Fids/Boratrane/KMAc156_recryst_CDCl3/12/ fid
Origin	Bruker BioSpin GmbH
Owner	av400bb
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zgpg
Experiment	1D
Number of Scans	200
Relaxation Delay	0.2000
Acquisition Time	1.2845
Acquisition Date	2018-07-06T18:13:22
Spectrometer Frequency	128.38
Nucleus	$^{11}\text{B}$

