Supplementary Materials: Synthesis of Trithia-borinane Complexes Stabilized in Diruthenium Core: [(Cp*Ru)$_2$(η^1-S)(η^1-CS){(CH$_2$)$_2$S$_3$ BR}] (R = H or SMe)

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I .1 Spectroscopic Details

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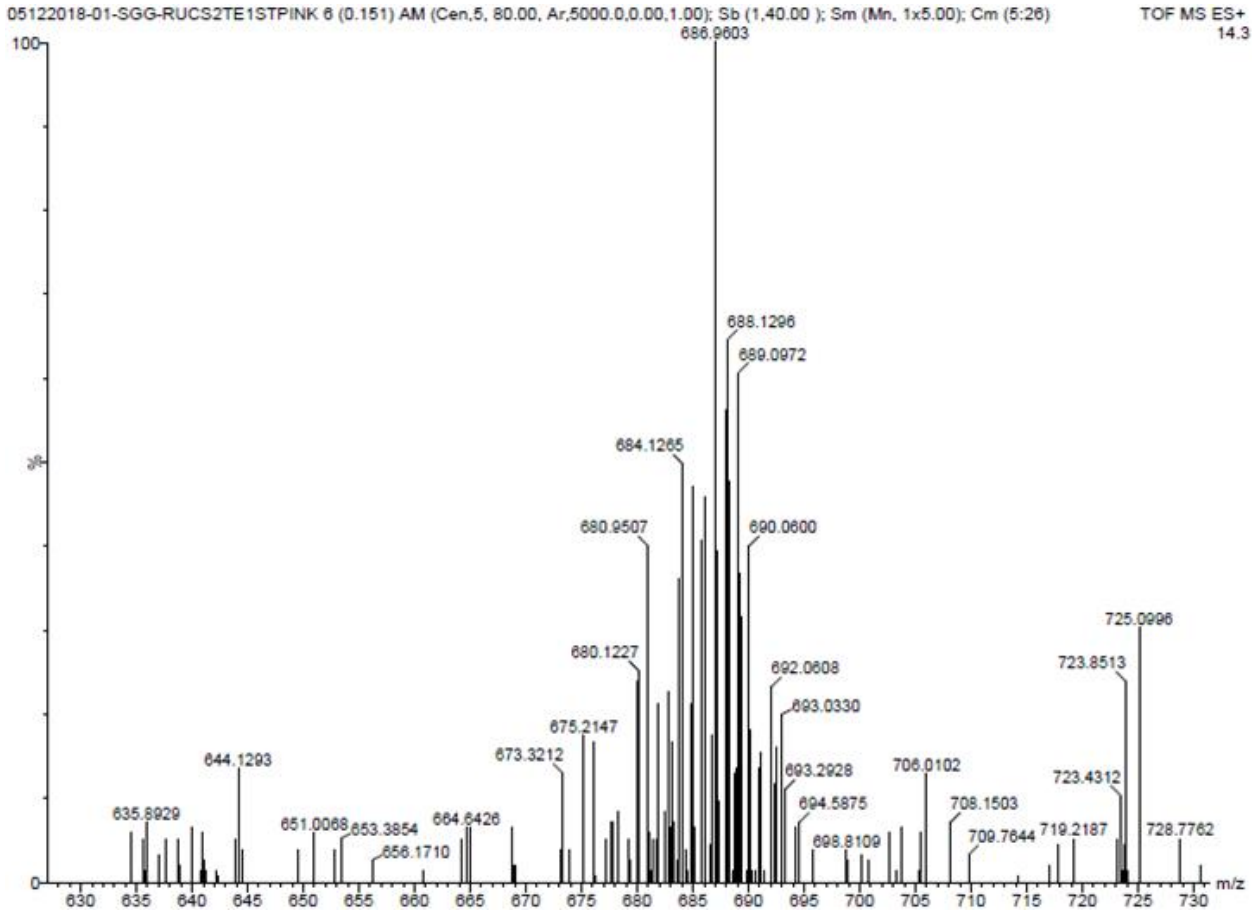
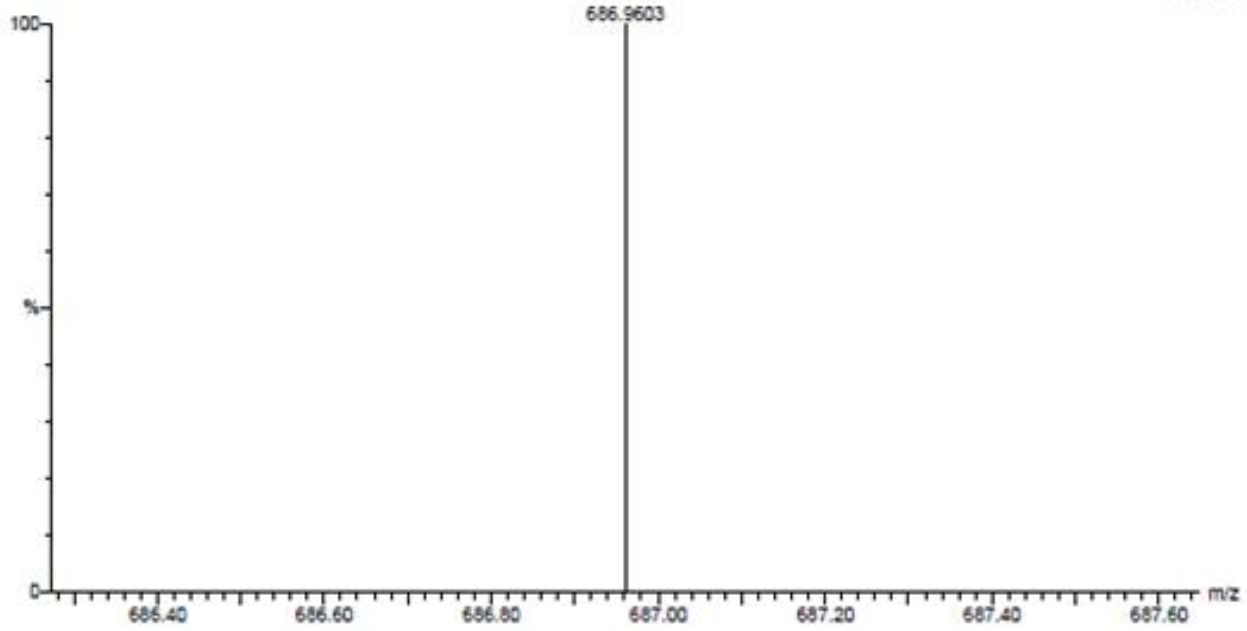


Figure S1. ESI(MS) spectrum of compound **2**.

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
35 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-23 H: 0-36 B: 0-1 S: 0-5 Ru: 0-2
SGG-RUCS2TE1STPINK
05122018-01-SGG-RUCS2TE1STPINK 6 (0.151) AM (Cen,5, 80.00, Ar,5000.0,0.00,1.00); Sb (1,40.00); Sm (Mn, 1x5.00); Cm (5:26) TOF MS ES+
1.43e+001



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
686.9603	686.9601	0.2	0.3	6.5	n/a	C23 H36 B S5 Ru2

Figure S2. HR-MS spectrum of compound **2**.

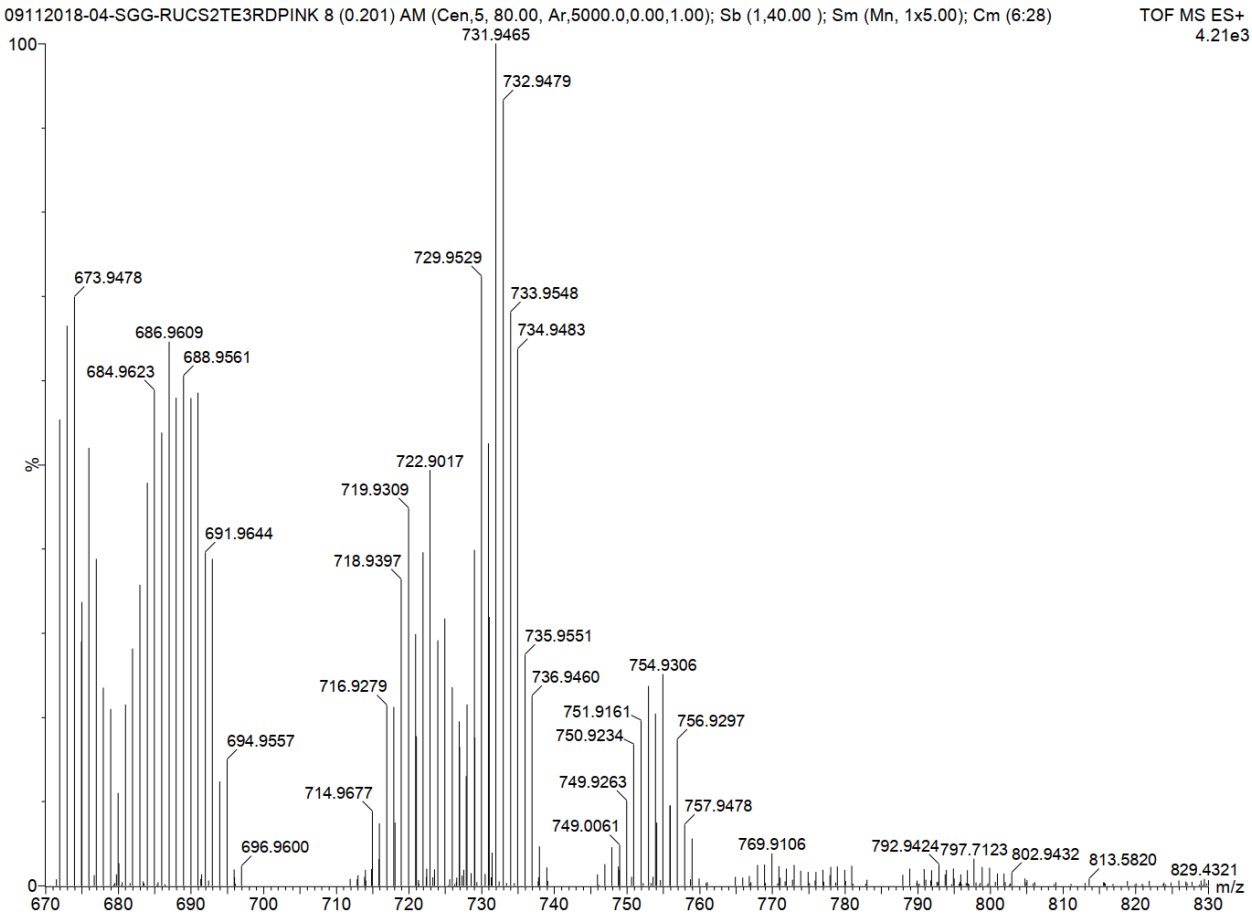
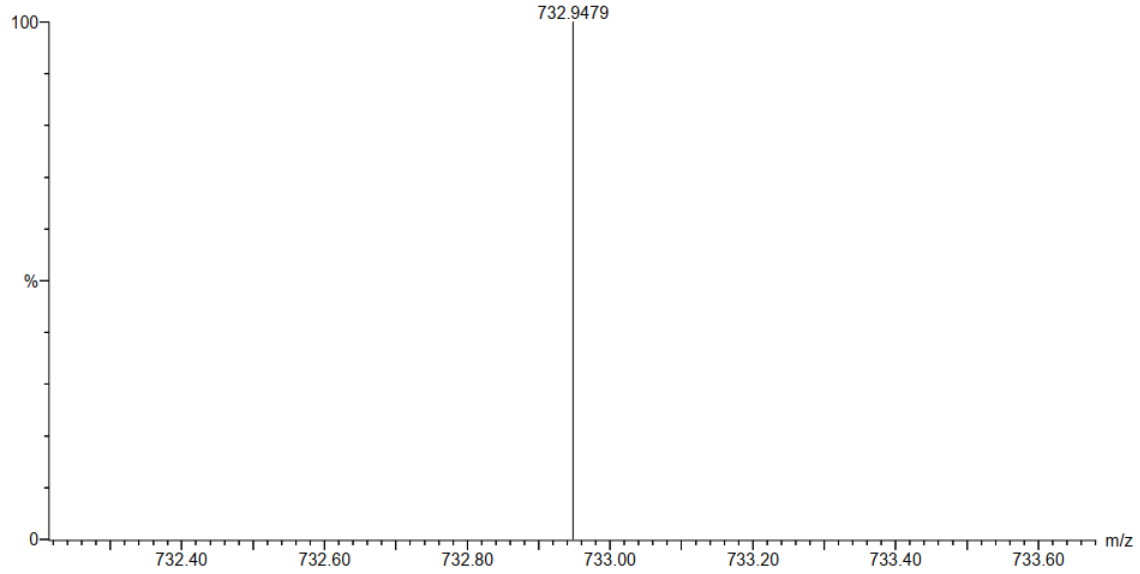


Figure S3. ESI(MS) spectrum of compound **3**.

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
41 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-24 H: 0-38 B: 0-1 S: 0-6 Ru: 0-2
SGG-RUCS2TE3RDPINK
09112018-04-SGG-RUCS2TE3RDPINK 8 (0.201) AM (Cen,5, 80.00, Ar,5000.0,0.00,1.00); Sb (1,40.00); Sm (Mn, 1x5.00); Cm (6:28) TOF MS ES+
3.92e+003



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
732.9479	732.9478	0.1	0.1	6.5	n/a	C24 H38 B S6 Ru2

Figure S4. HR-MS spectrum of compound **3**.

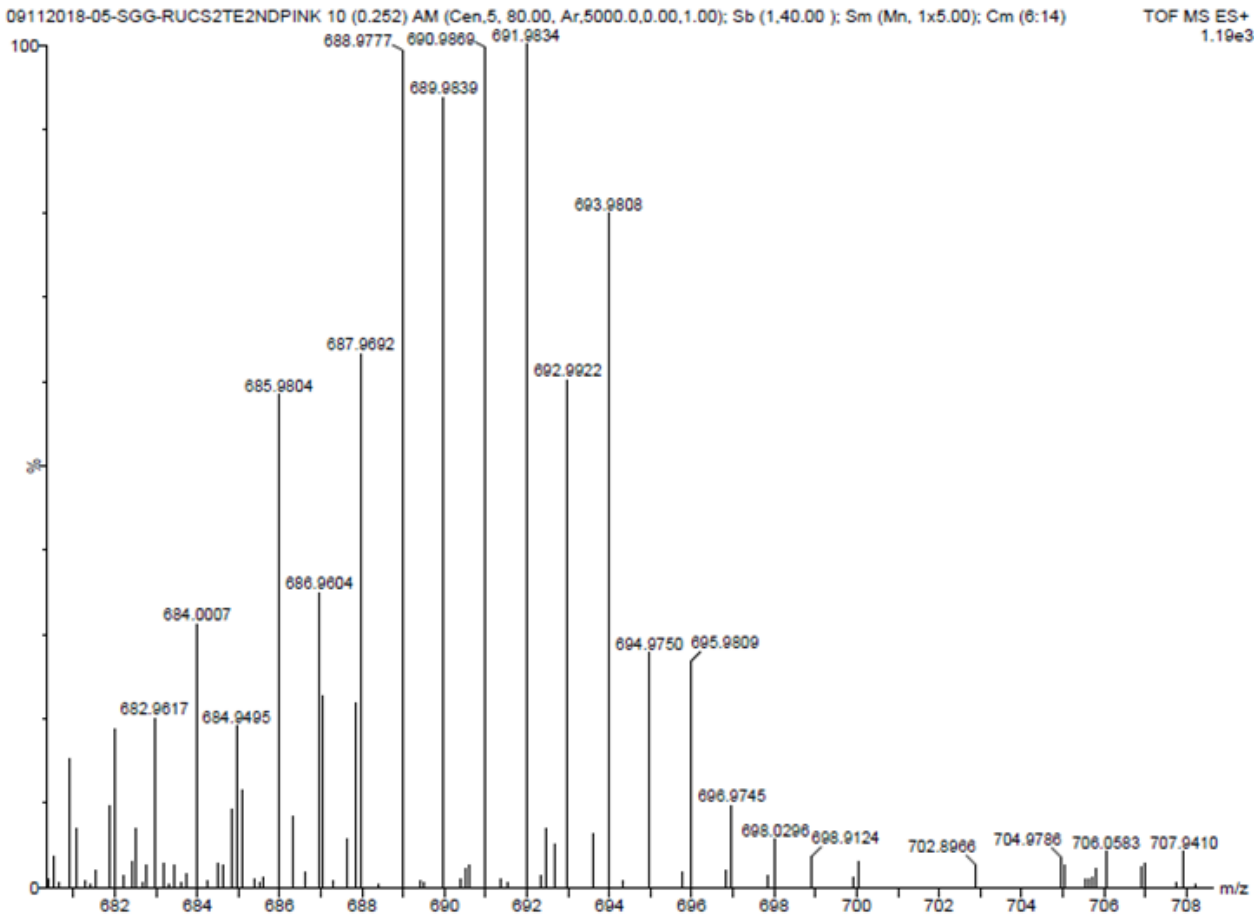
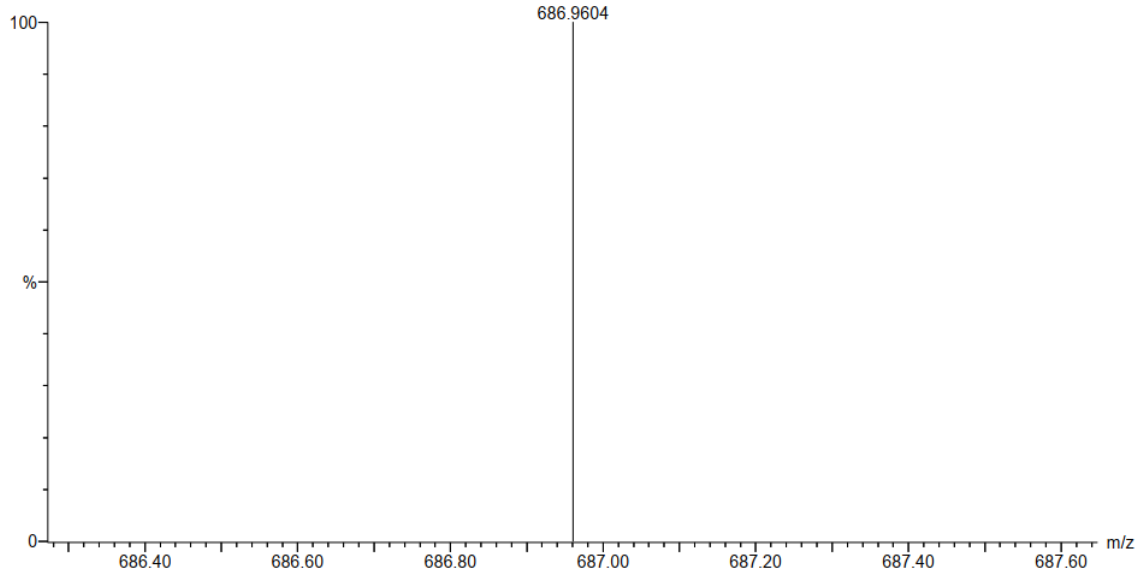


Figure S5. ESI(MS) spectrum of compound **4**.

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
35 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-23 H: 0-36 B: 0-1 S: 0-5 Ru: 0-2

SGG-RUCS2TE2NDPINK 4.15e+002
09112018-05-SGG-RUCS2TE2NDPINK 10 (0.252) AM (Cen,5, 80.00, Ar,5000.0,0.00,1.00); Sb (1,40.00); Sm (Mn, 1x5.00); Cm (6:14)



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
686.9604	686.9601	0.3	0.4	6.5	n/a	C23 H36 B S5 Ru2

Figure S6. HR-MS spectrum of compound **4**.

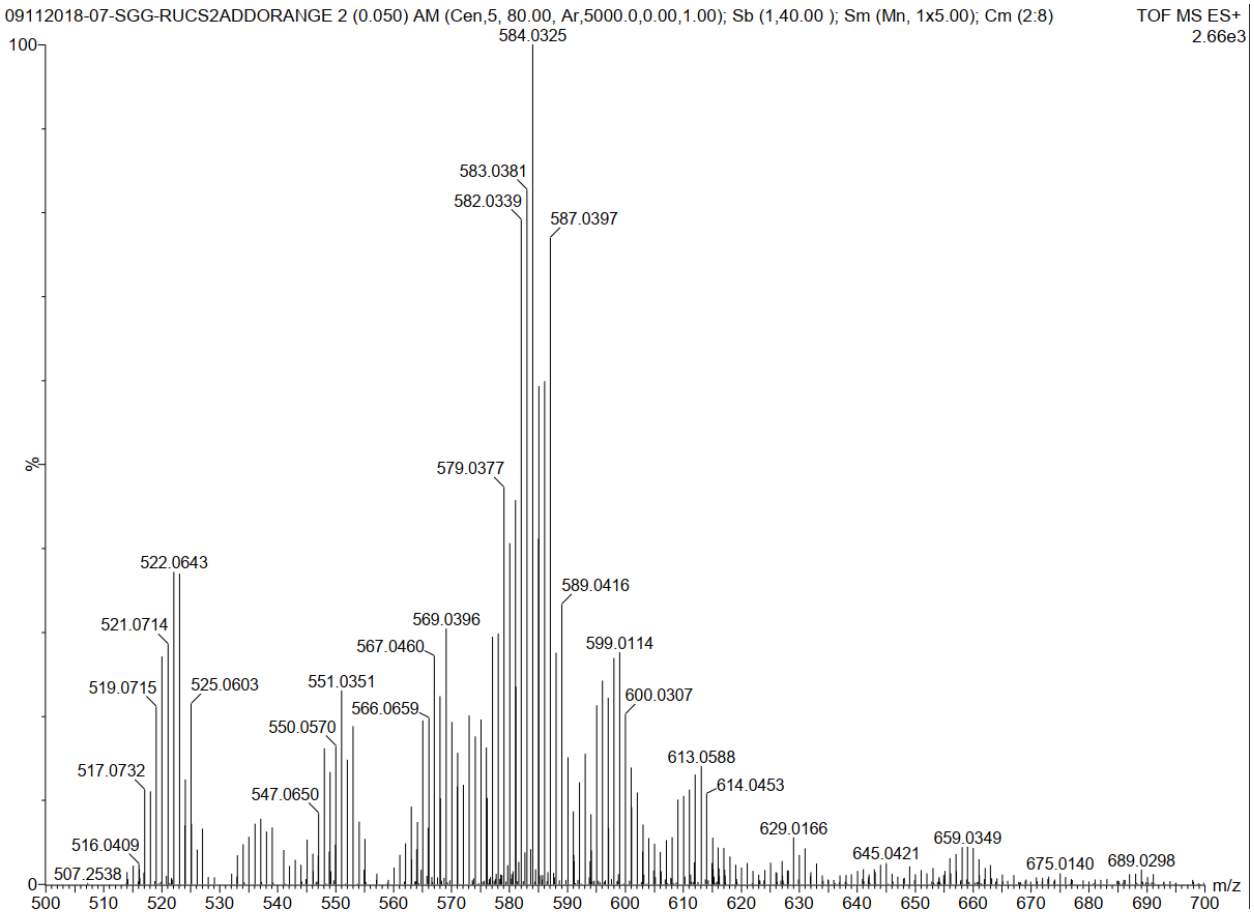


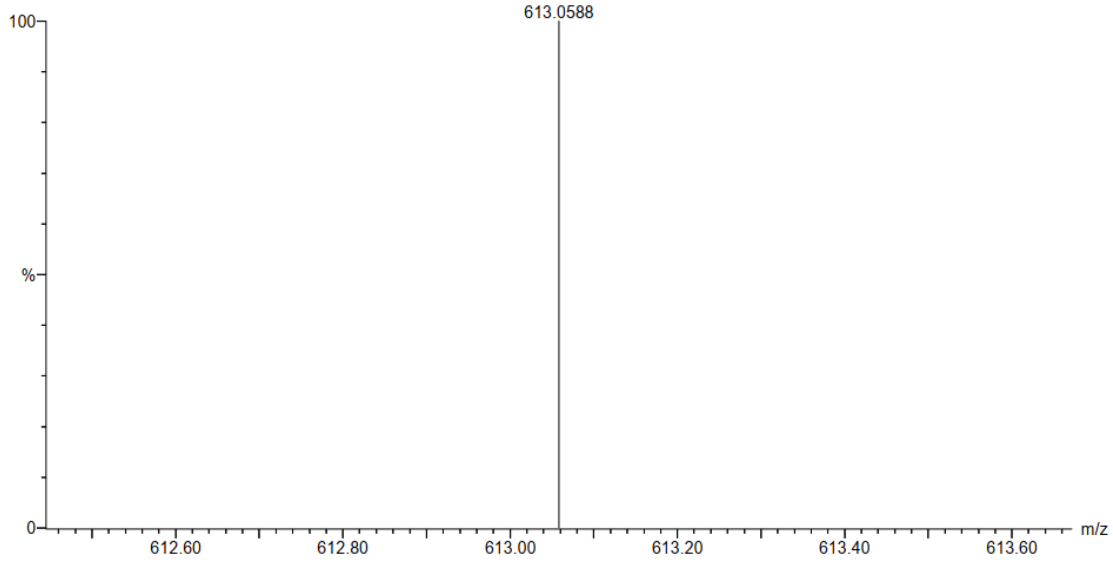
Figure S7. ESI(MS) spectrum of compound **5**.

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
71 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-21 H: 0-37 B: 0-3 Na: 0-1 S: 0-2 Ru: 0-2

SGG-RUCS2ADDORANGE 3.73e+002
09112018-07-SGG-RUCS2ADDORANGE 2 (0.050) AM (Cen,5, 80.00, Ar,5000.0,0.00,1.00); Sb (1,40.00); Sm (Mn, 1x5.00); Cm (2:8)



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
613.0588	613.0601	-1.3	-2.1	4.5	n/a	C21 H37 B3 Na S2 Ru2

Figure S8. HR-MS spectrum of compound **5**.

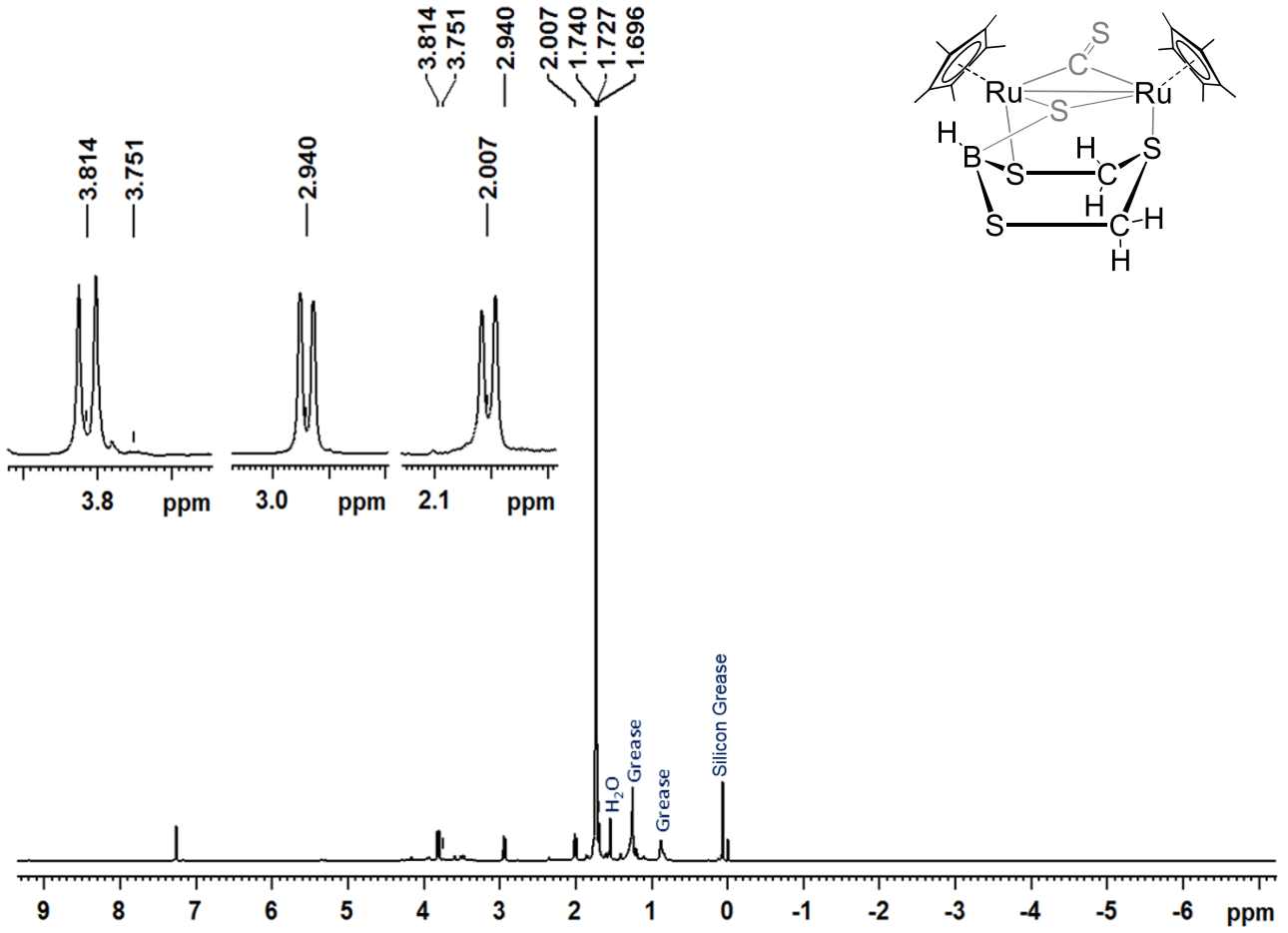


Figure S9. ^{1}H NMR spectrum of compound **2** in $CDCl_3$.

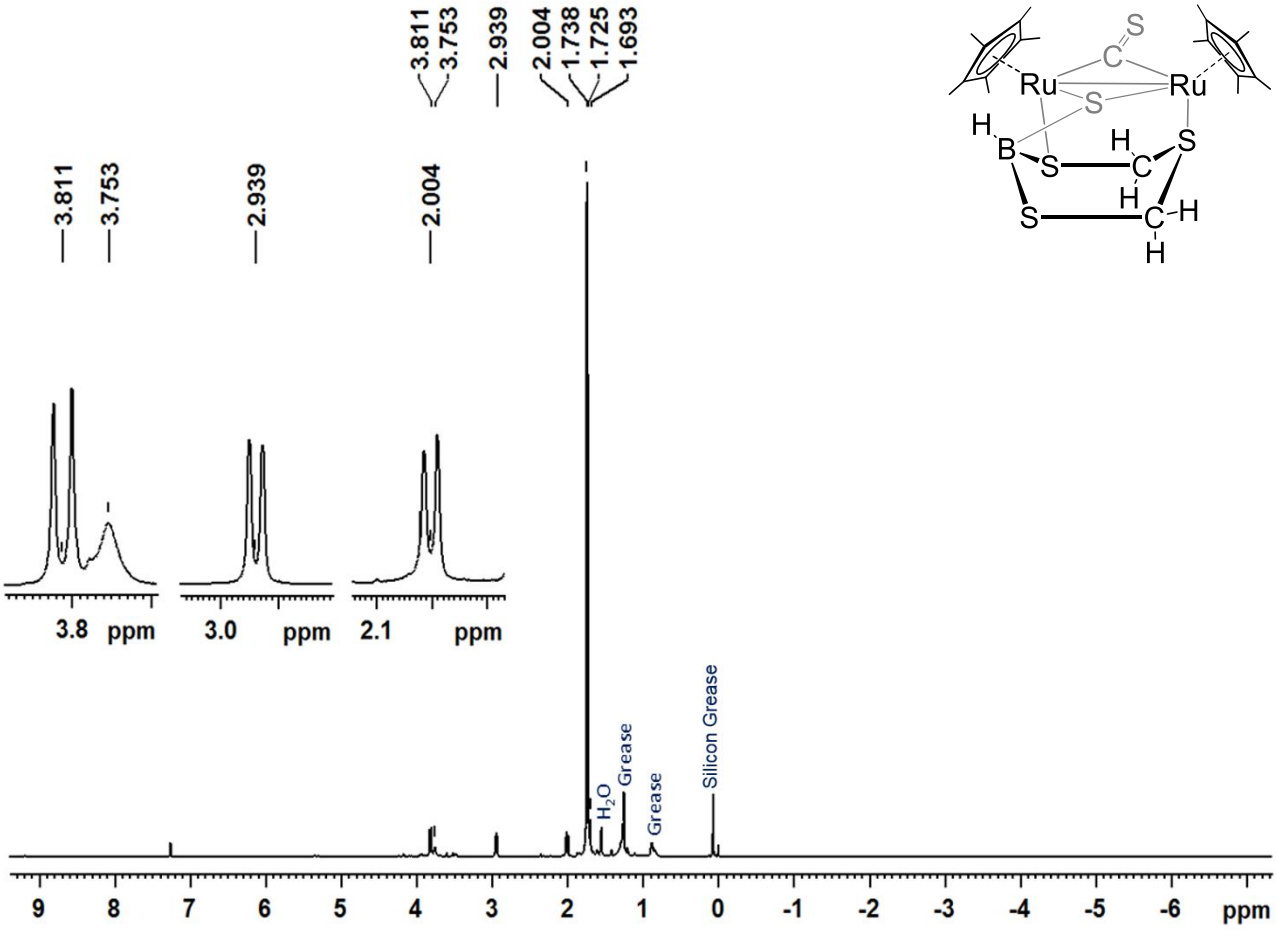


Figure S10. $^{1}H\{^{11}B\}$ NMR spectrum of compound **2** in $CDCl_3$.

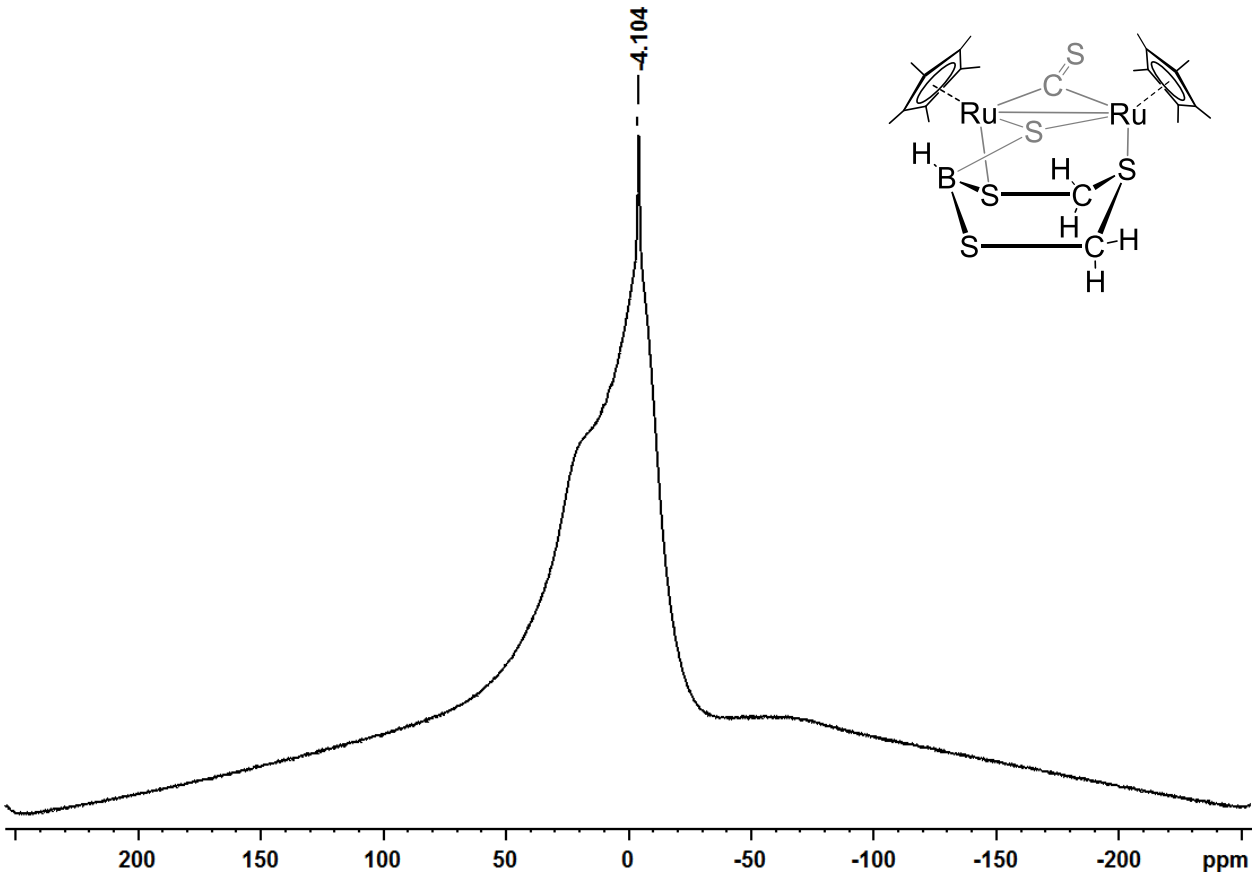


Figure S11. $^{11}B\{^{1}H\}$ NMR spectrum of compound **2** in $CDCl_3$.

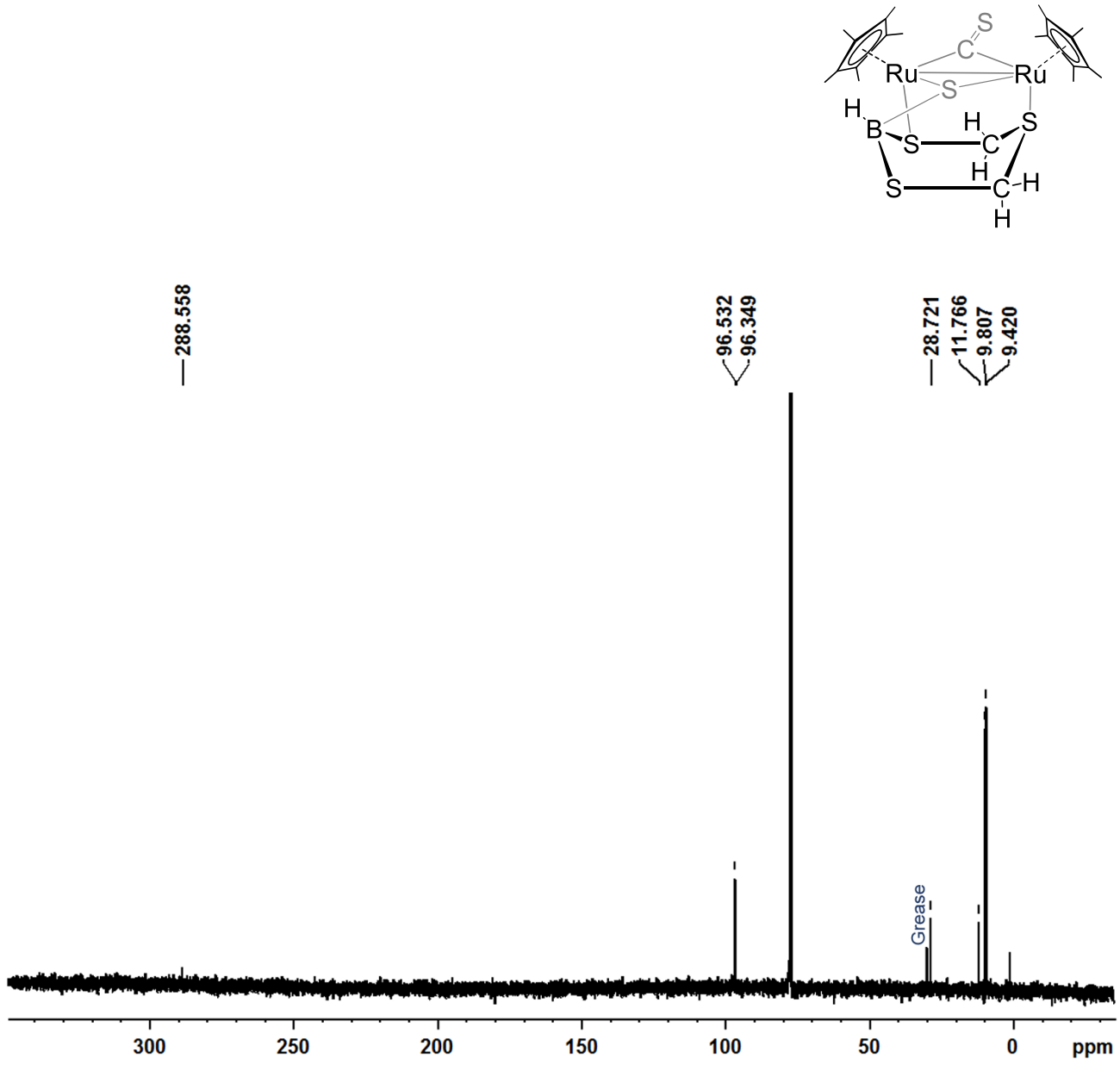


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of compound **2** in $CDCl_3$.

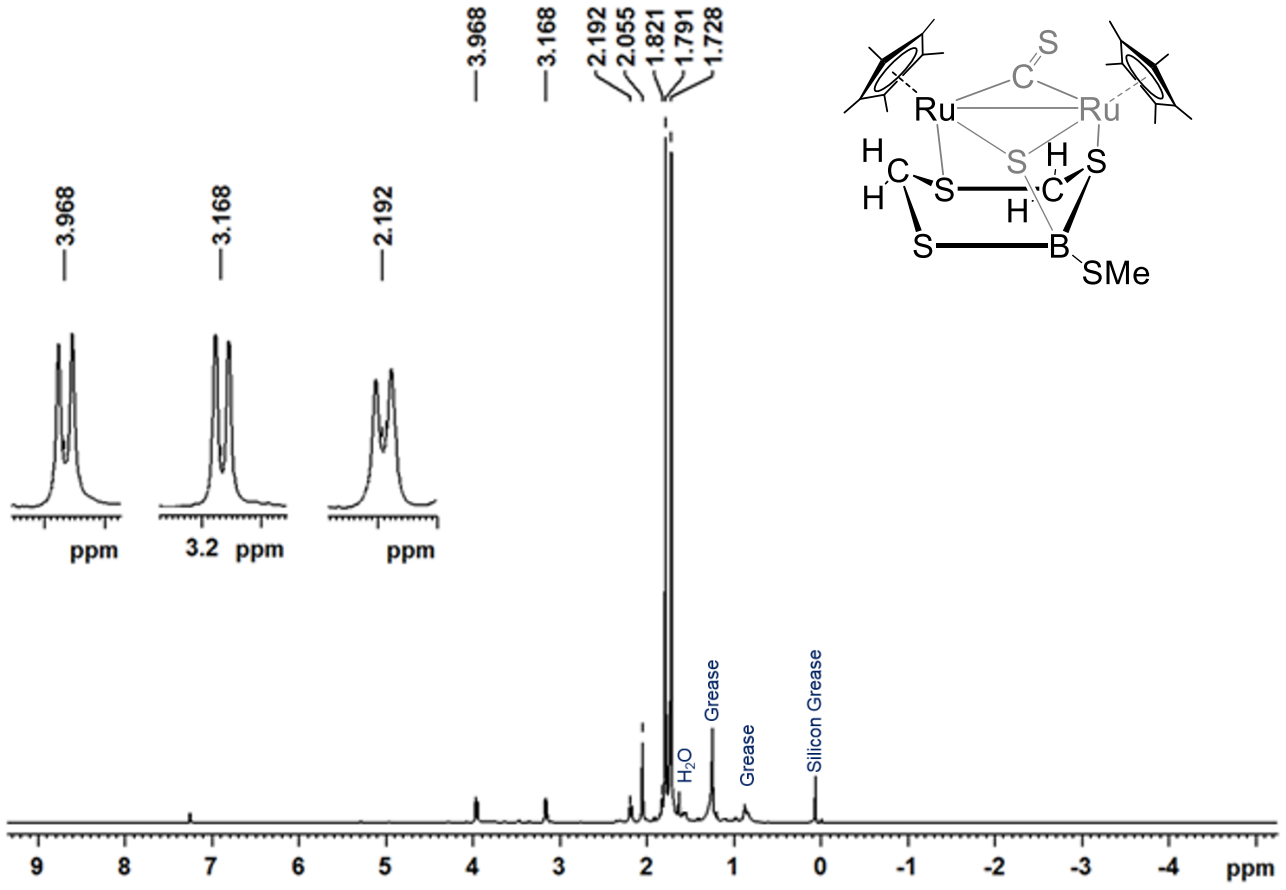


Figure S13. ^{1}H NMR spectrum of compound **3** in $CDCl_3$.

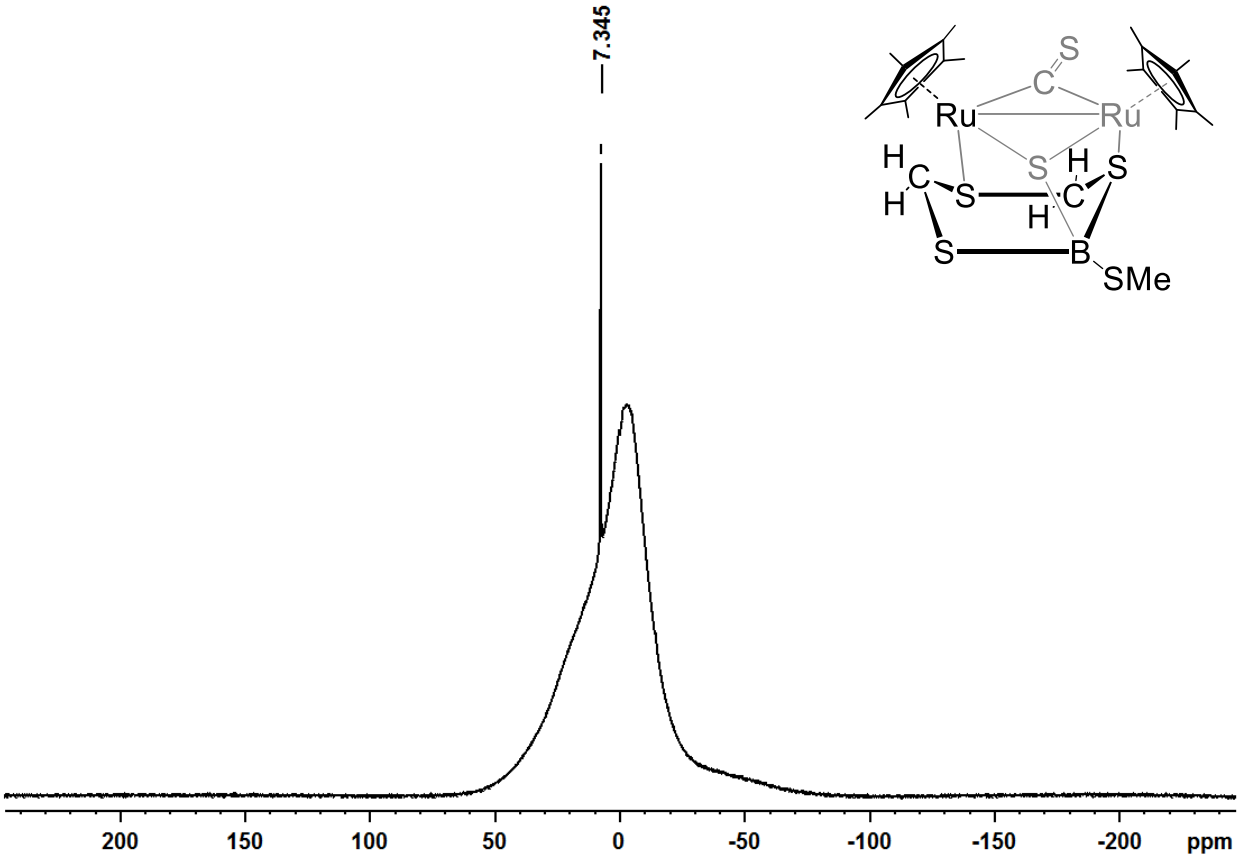


Figure S14. $^{11}B\{^{1}H\}$ NMR spectrum of compound **3** in $CDCl_3$.

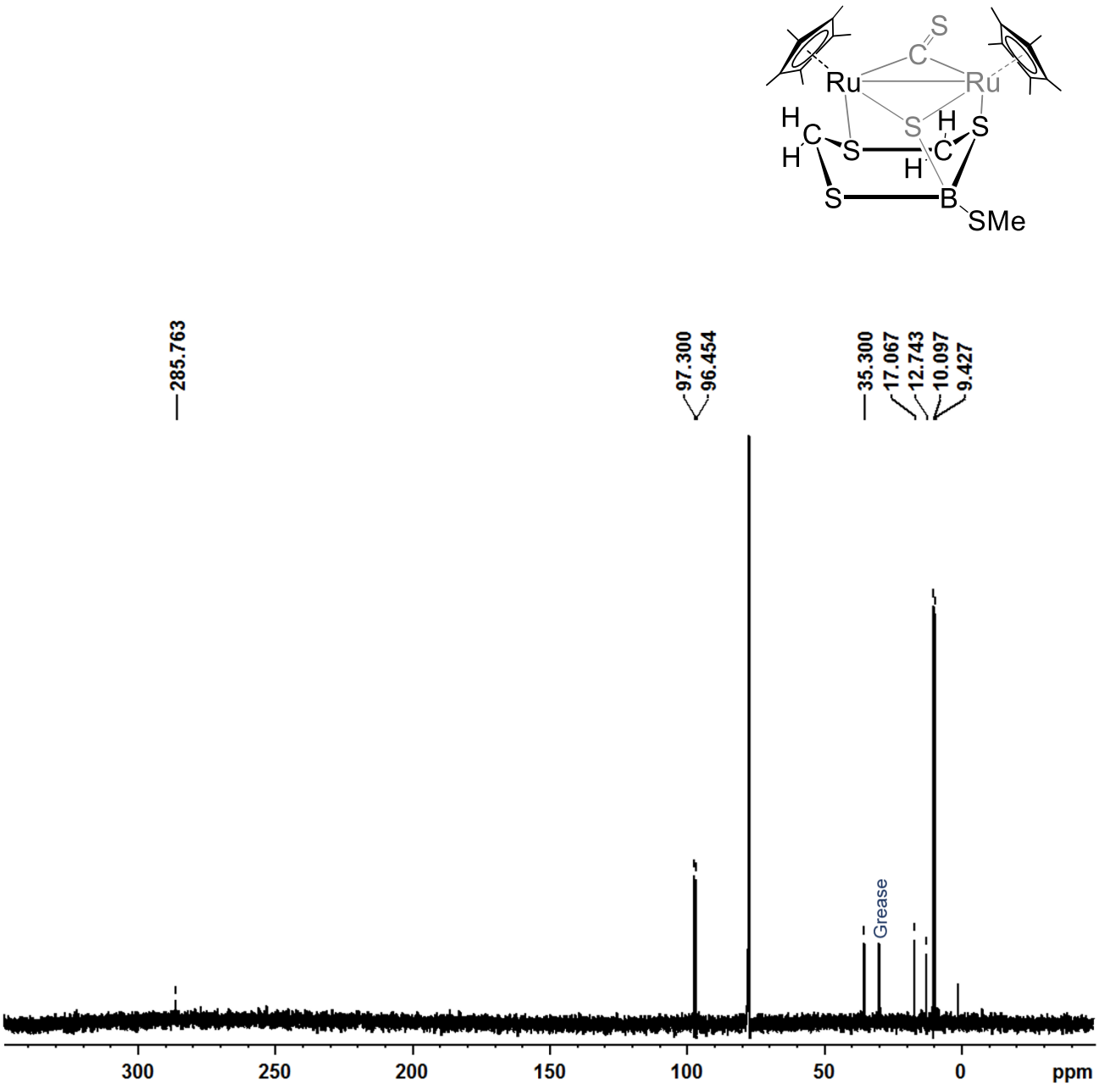


Figure S15. ^{13}C {^{1}H} NMR spectrum of compound **3** in $CDCl_3$.

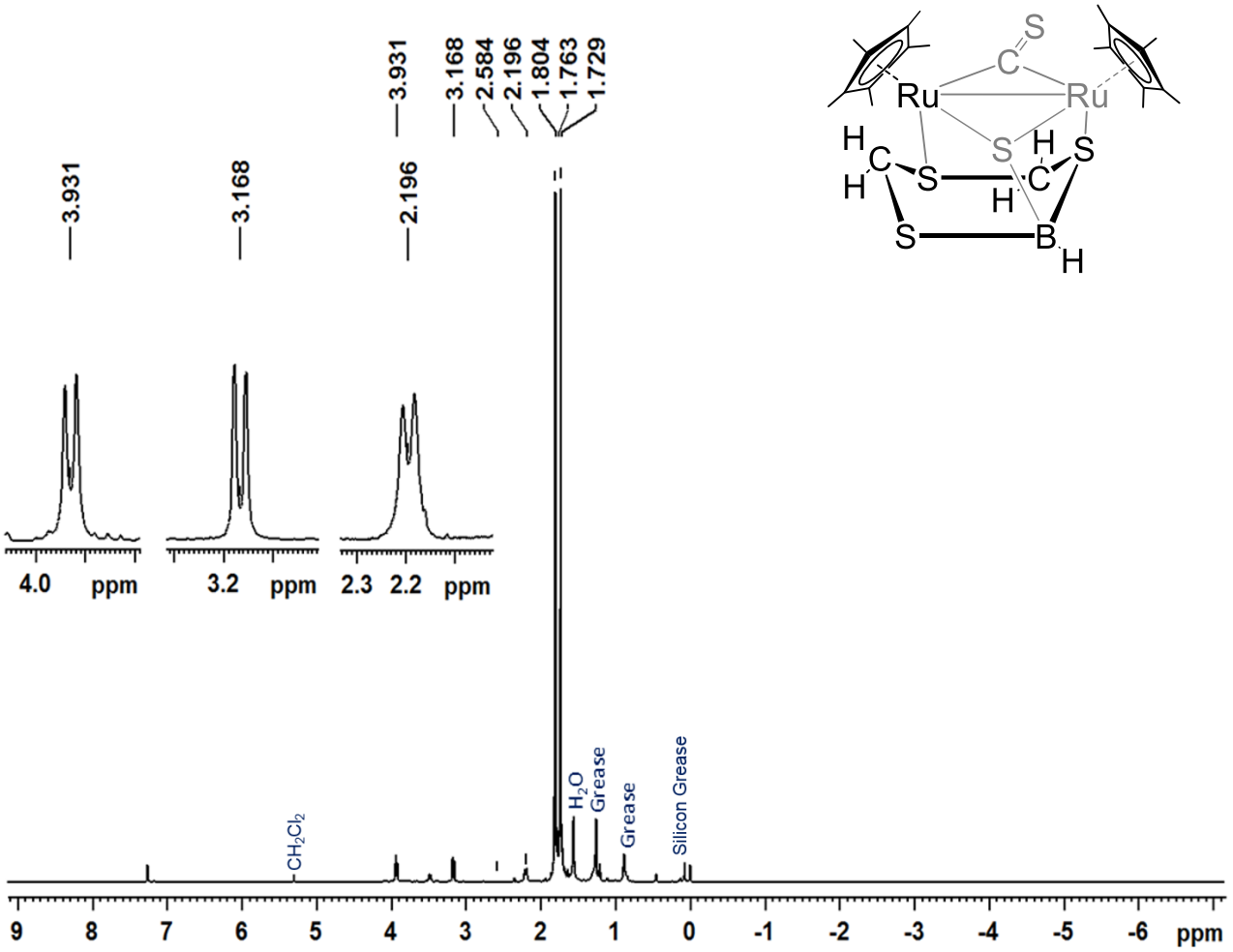


Figure S16. ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

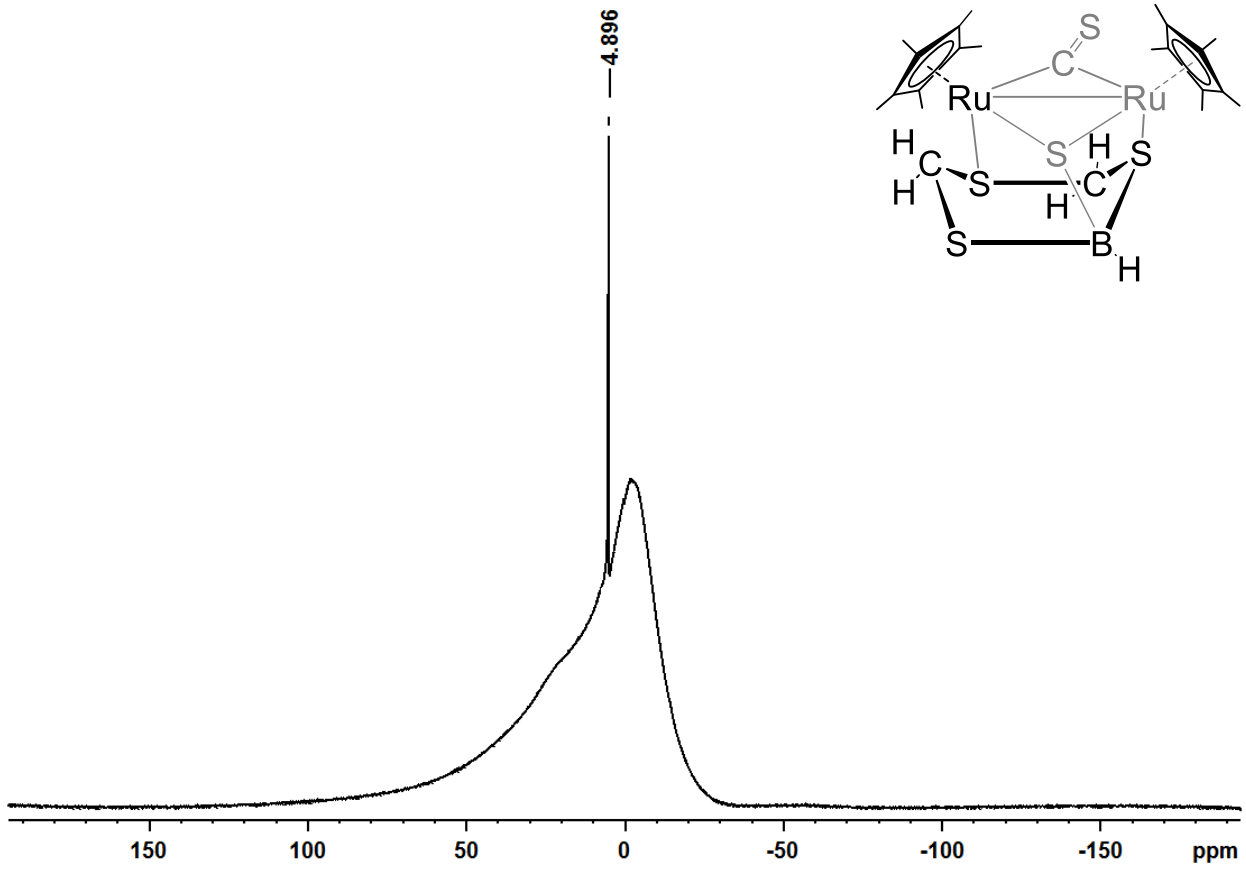


Figure S17. $^{11}B\{^{1}H\}$ NMR spectrum of compound **4** in $CDCl_3$.

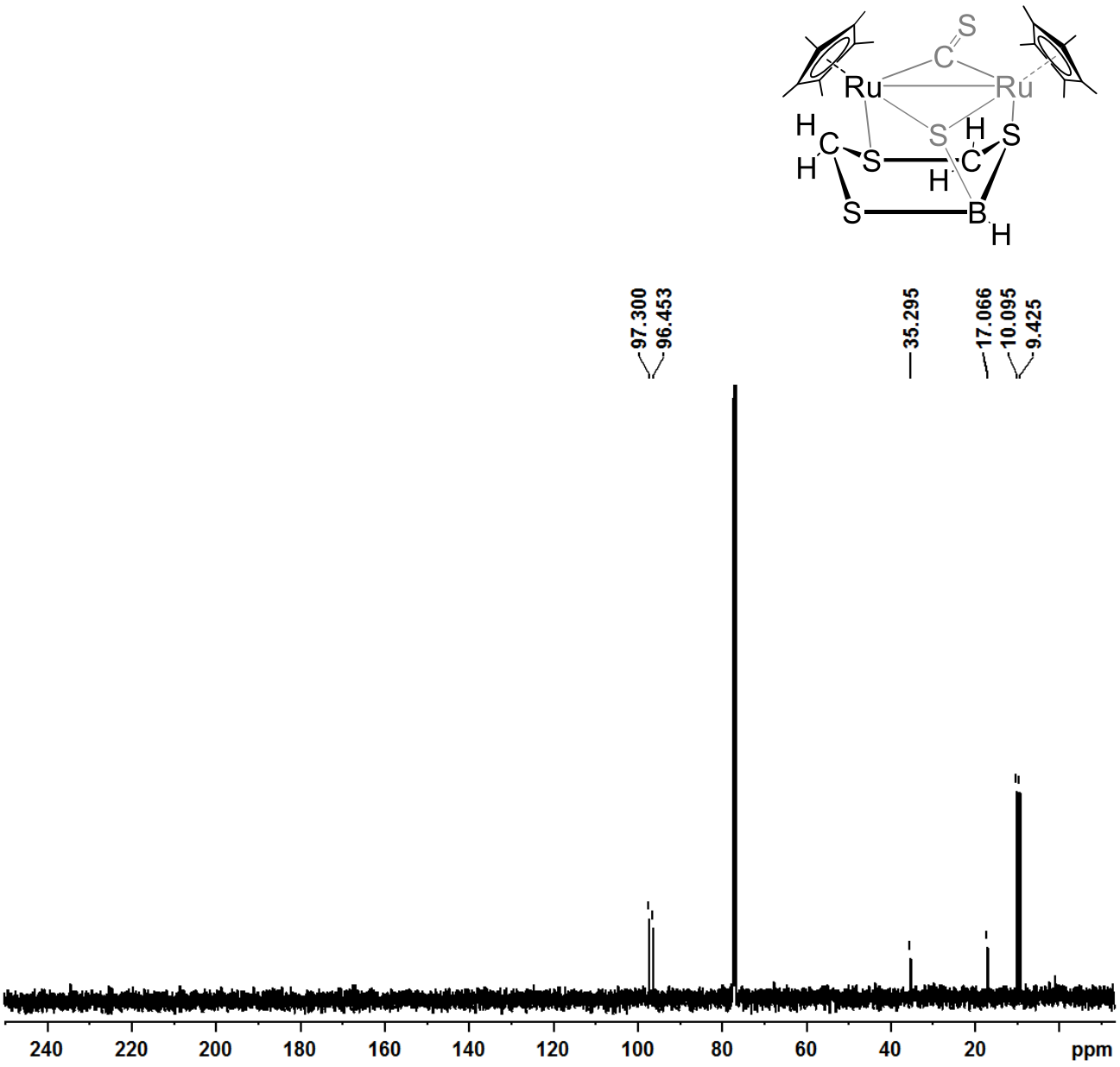


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of compound **4** in $CDCl_3$.

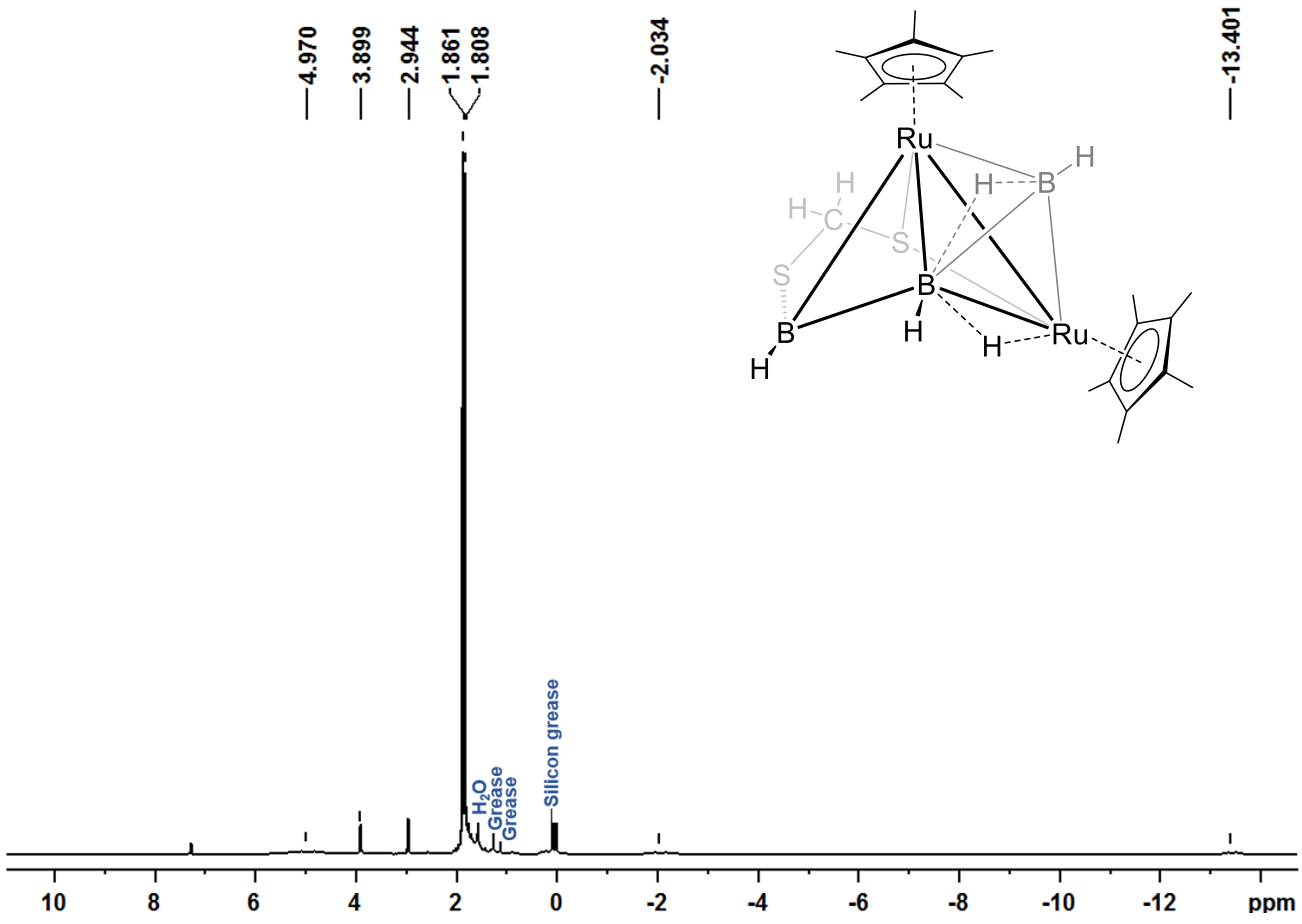


Figure S19. ^{1}H NMR spectrum of compound **5** in $CDCl_3$.

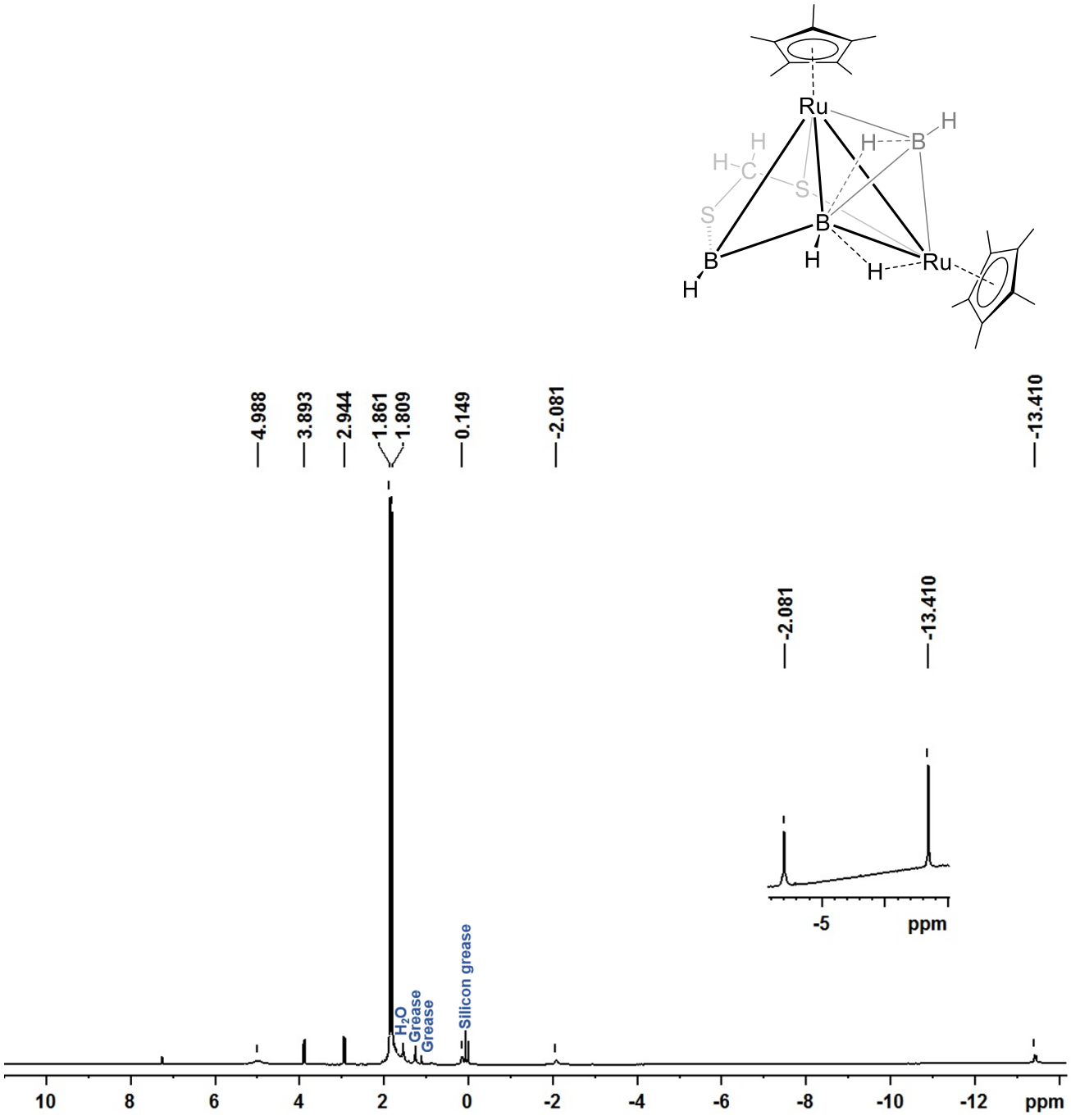


Figure S20. $^{1}H\{^{11}B\}$ NMR spectrum of compound **5** in $CDCl_3$.

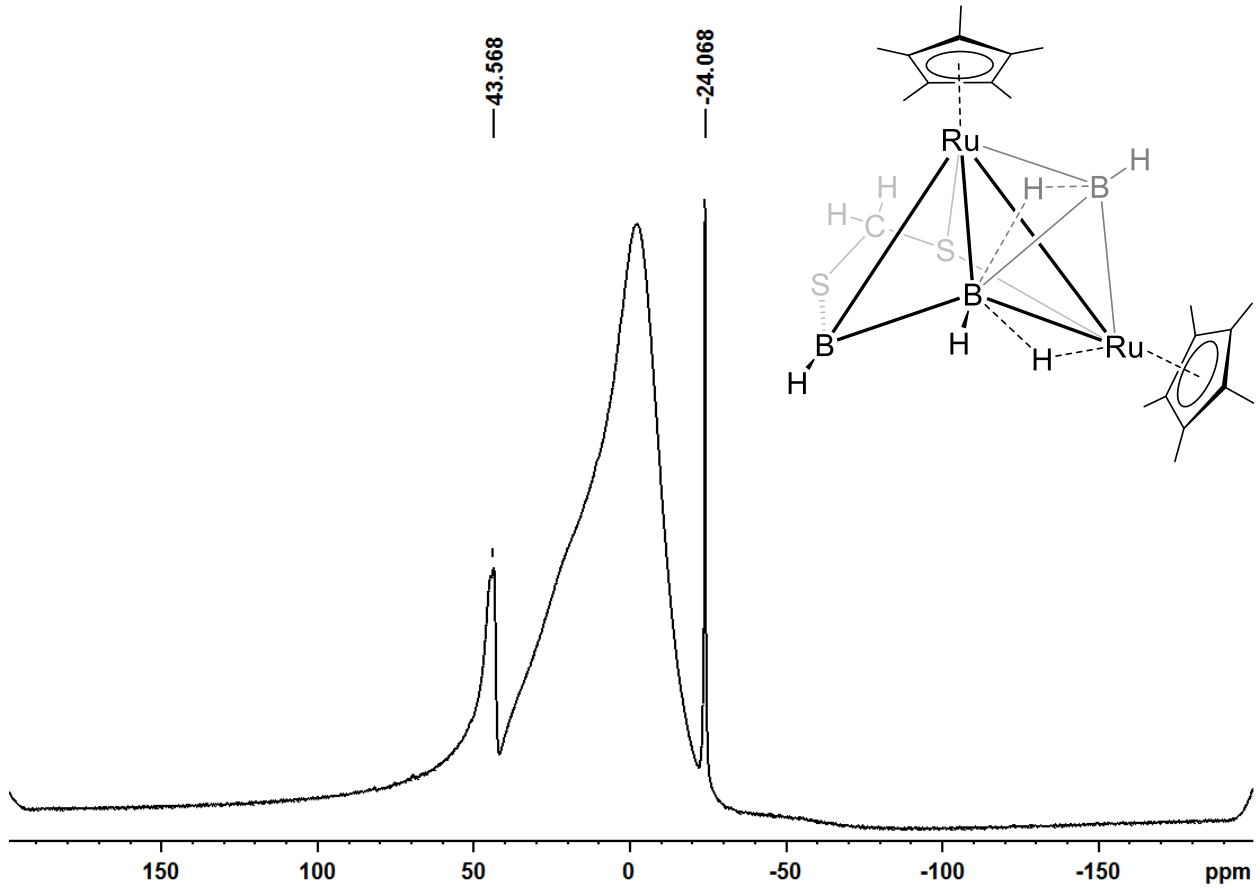


Figure S21. $^{11}B\{^{1}H\}$ spectrum of compound **5** in $CDCl_3$.

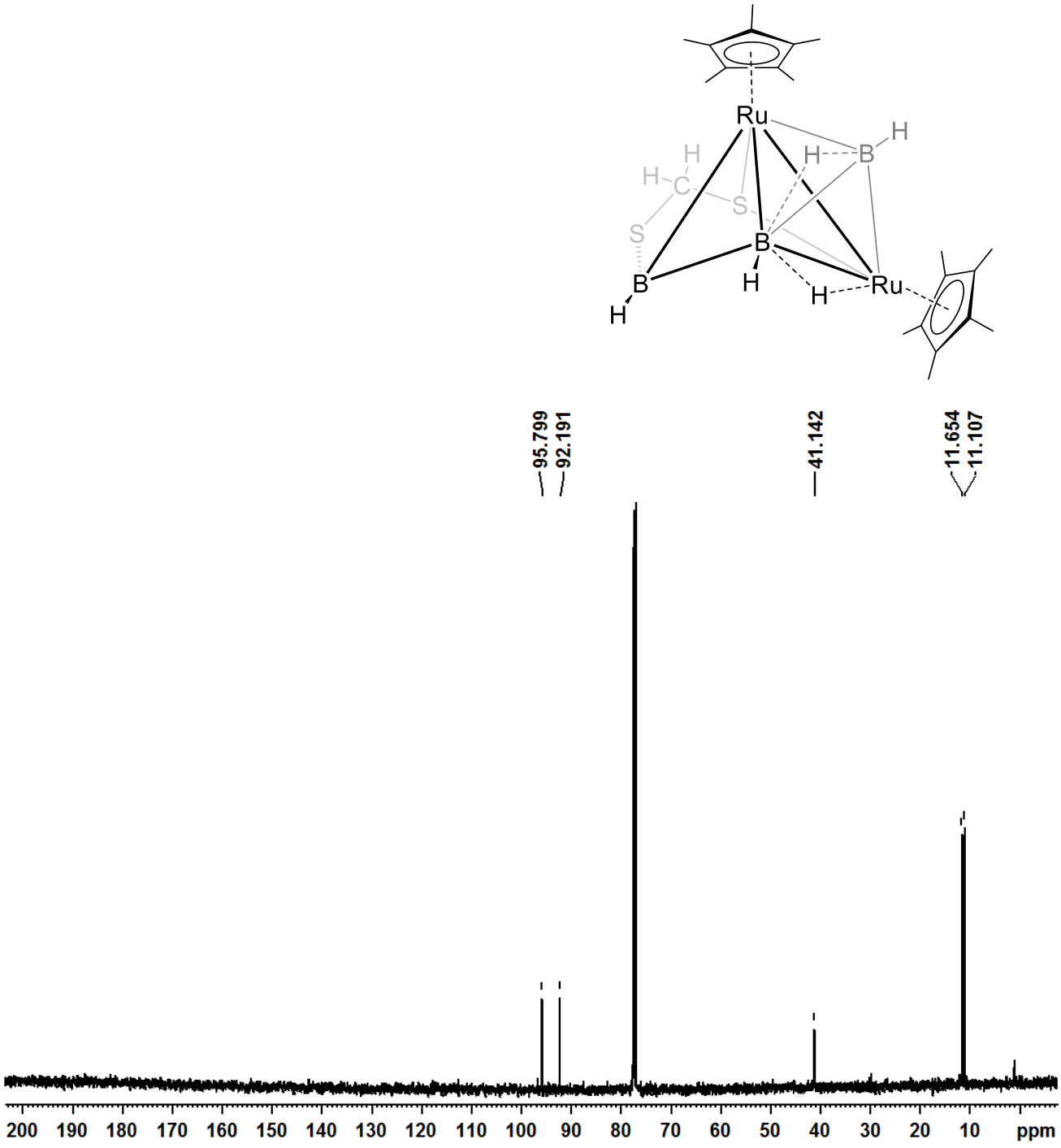


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum of compound **5** in $CDCl_3$.