Supplementary Materials: Synthesis, Structures and Chemistry of the Metallaboranes of Group 4–9 with M₂B₅ Core Having a Cross Cluster M–M Bond

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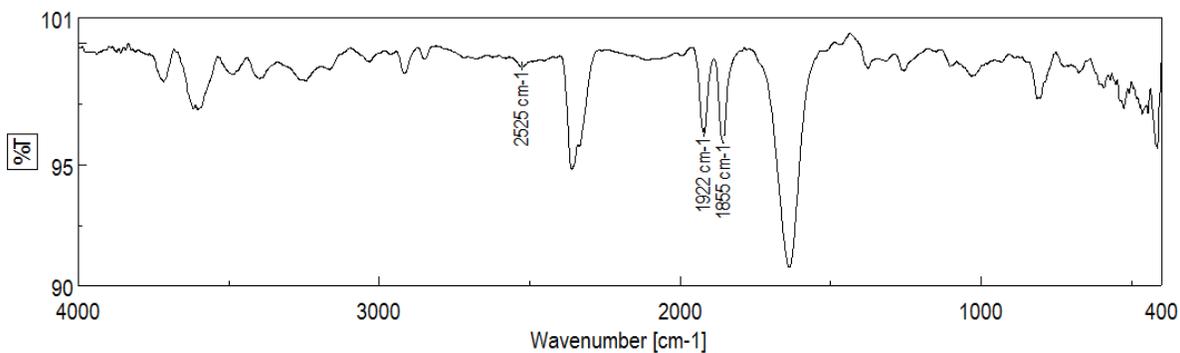
Figure S3. IR spectrum of compound **1**.
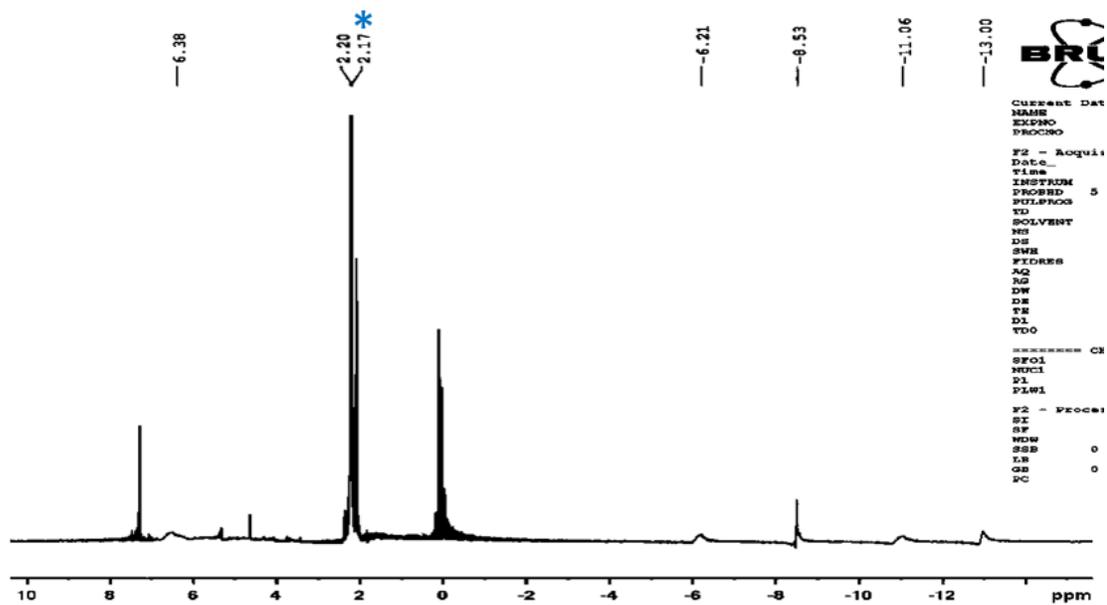
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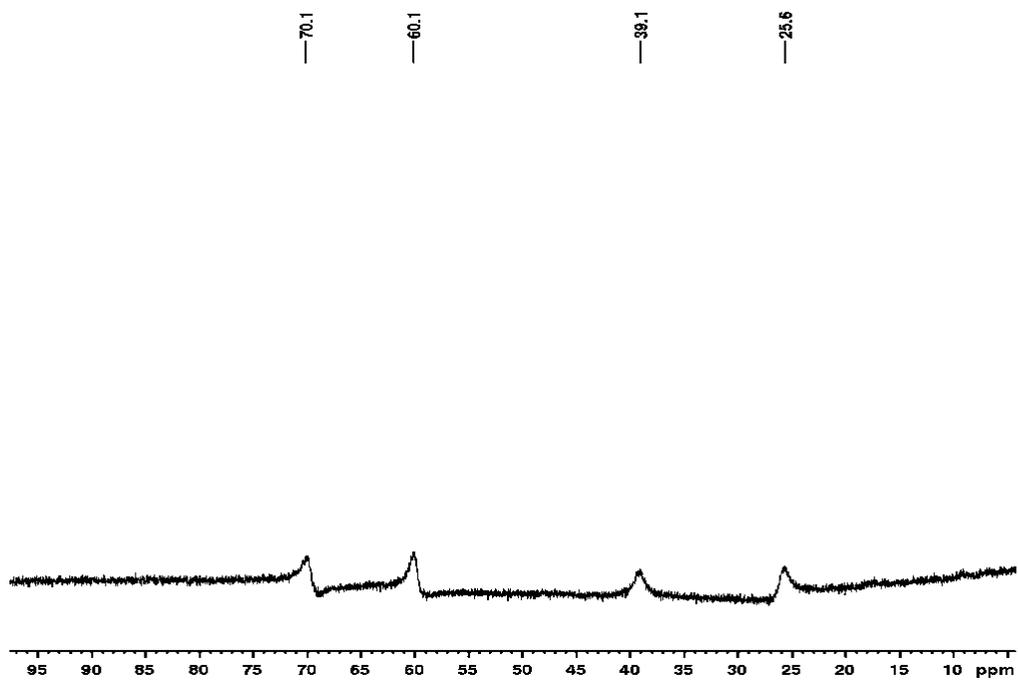
Figure S5. $^{11}B\{^1H\}$ NMR spectrum of compound **2** in CDCl$_3$.
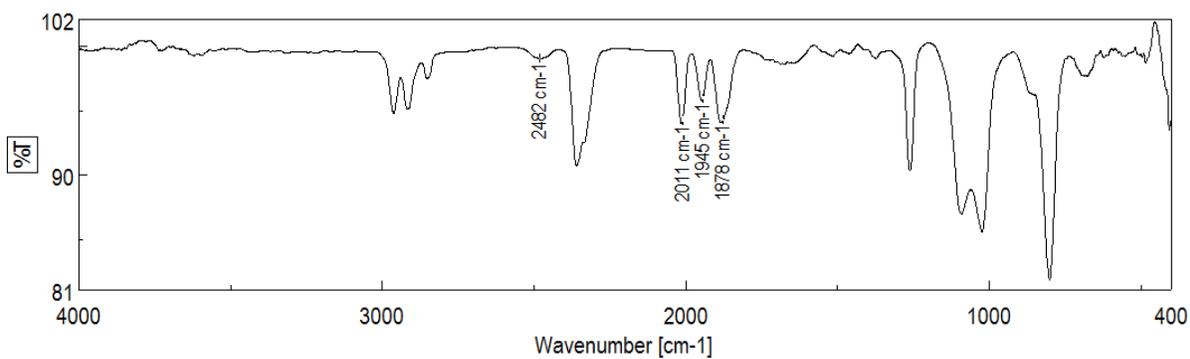
Figure S6. IR spectrum of compound **2.**

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
296 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: 0-4   O: 0-4   K: 0-1   Mo: 0-1   W: 0-2

SGG-W2MO
20082018-11-SGG-W2MO 20 (0.503) AM (Cen,5, 80.00, Ar,5000.0,0.00,1.00); Sb (1,40.00); Sm (Mn, 1x5.00); Cm (14:28)   TOF MS ES+
                                                                                                                             5.04e+003
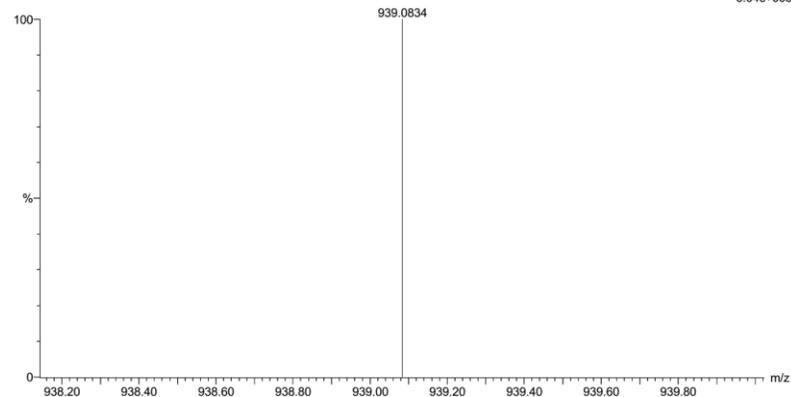
Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
939.0834	939.0853	-1.9	-2.0	10.5	n/a	C24 H38 B4 O4 K Mo W2

Figure S7. HR-MS spectrum of compound **2**.
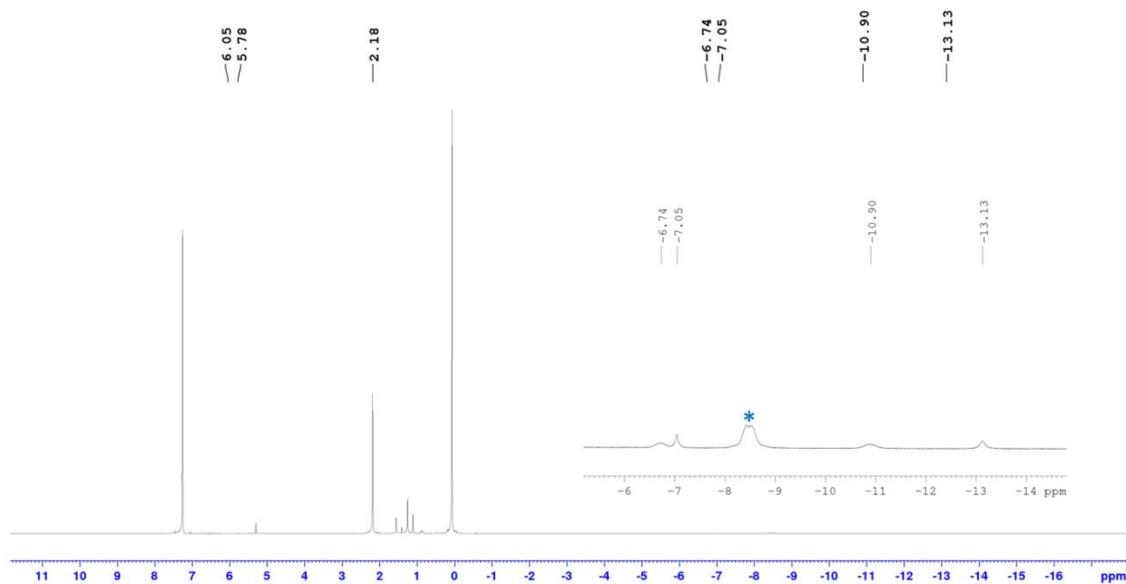
Figure S8. ^{1}H NMR spectrum of compound **3** in CDCl$_3$. (* Peak corresponding to inseparable known {(Cp*W)$_2$B$_5$H$_9$})
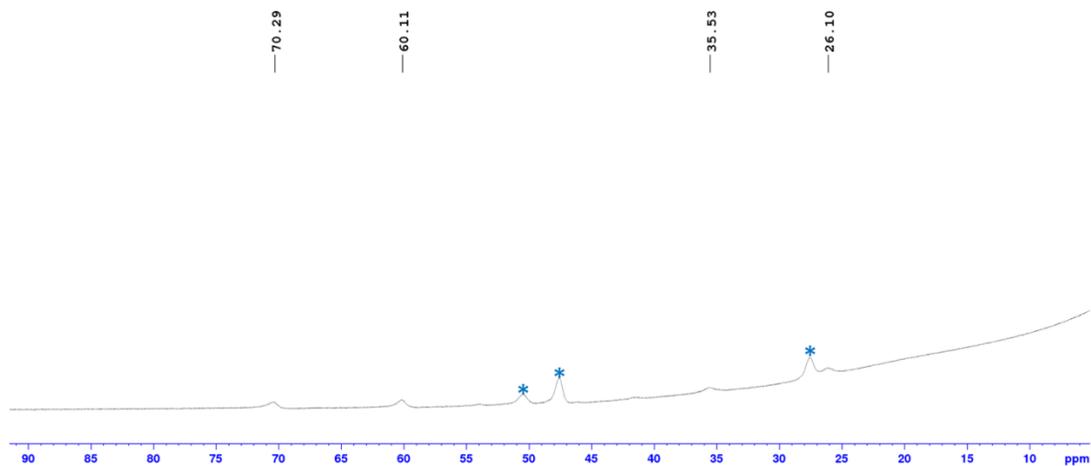
Figure S9. ^{11}B{^{1}H} NMR spectrum of compound **3** in CDCl$_3$. (* Peaks corresponding to inseparable known {(Cp*W)$_2$B$_5$H$_9$})
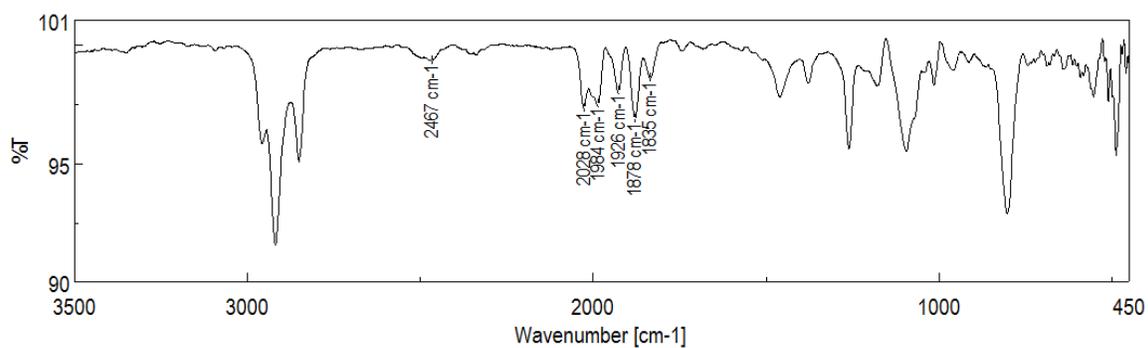
Figure S10. IR spectrum of compound **3**.

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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
95 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-24   H: 0-39   B: 0-4   O: 0-4   W: 0-3

SGG-W2B4W
04012019-01-SGG-W2B4W 126 (3.170) AM (Cen,5, 80.00, Ar,5000.0,0.00,1.00); Sb (1,40.00); Sm (Mn, 1x5.00); Cm (112:130)   TOF MS ES+
3.25e+002

987.1727

100

%

0
986.20   986.40   986.60   986.80   987.00   987.20   987.40   987.60   987.80

			-1.5		
Minimum:					
Maximum:		5.0	10.0	50.0	

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
987.1727	987.1749	-2.2	-2.2	12.0	n/a	C24 H39 B4 O4 W3

Figure S11. HR-MS spectrum of compound **3**.
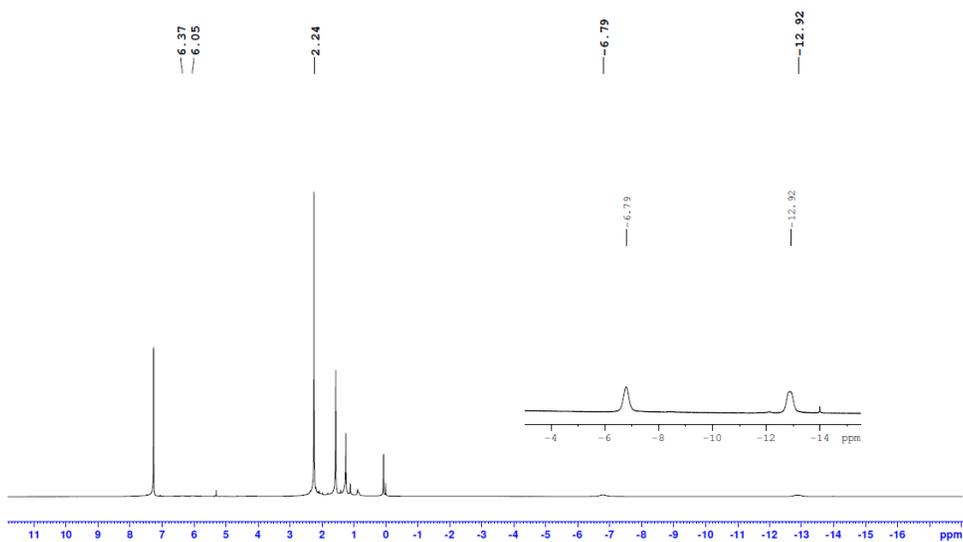
Figure S12. ^{1}H NMR spectrum of compound **4** in CDCl$_3$.

79.0
76.2
41.0
35.8

100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 ppm
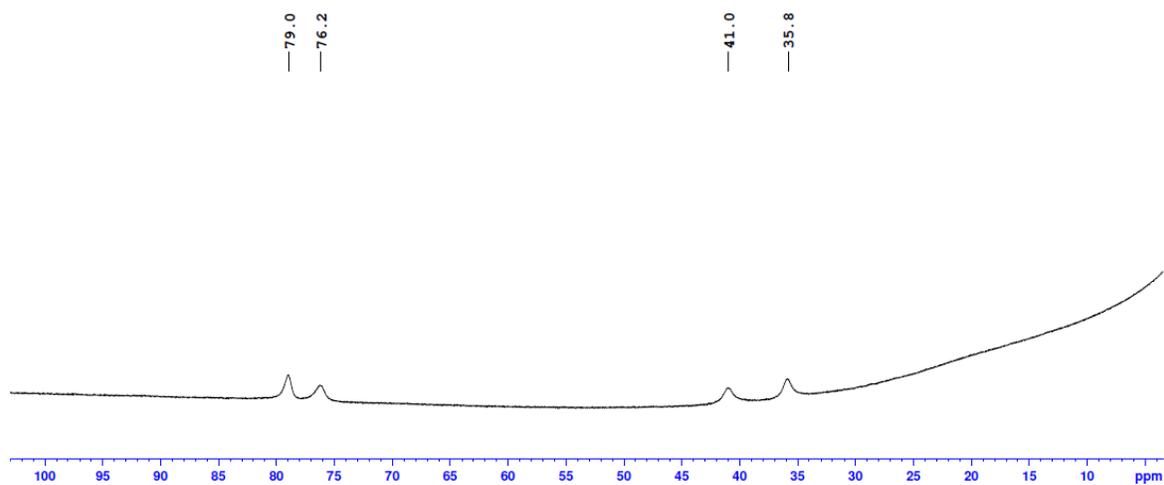
Figure S13. $^{11}B\{^1H\}$ NMR spectrum of compound **4** in CDCl$_3$.

%T

101

90

80

4000   3000   2000   1000   400
Wavenumber [cm-1]

2482 cm-1
1984 cm-1
1918 cm-1
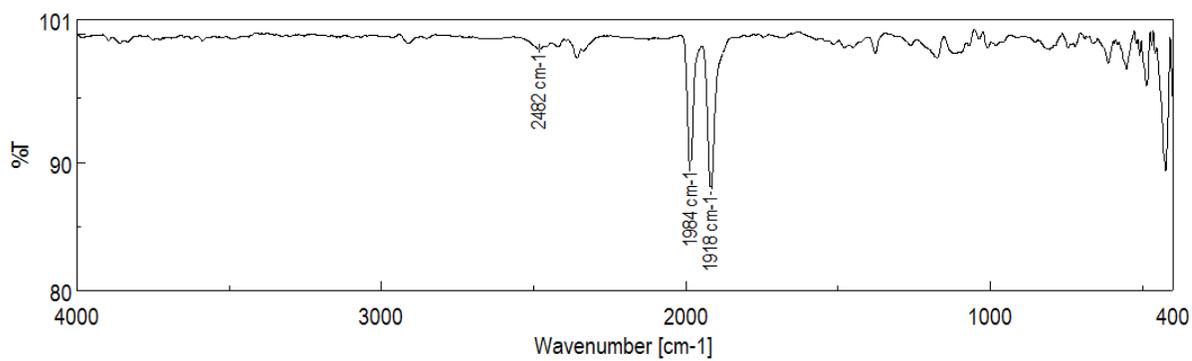
Figure S14. IR spectrum of compound **4**.

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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
2022 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-23   H: 0-38   B: 0-4   O: 0-3   Na: 0-1   Fe: 0-1   W: 0-2

SGG-W2B4FE
04012019-03-SGG-W2B4FE 19 (0.479) AM (Cen,5, 80.00, Ar,5000.0,0.00,1.00); Sb (1,40.00); Sm (Mn, 1x5.00); Cm (8:19)   TOF MS ES+
                                                                                                                           6.92e+003
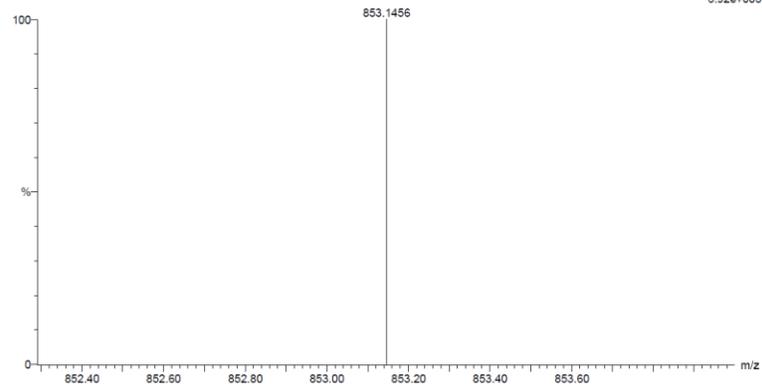
Minimum:				-1.5							
Maximum:		5.0	10.0	50.0							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula					
853.1456	853.1459	-0.3	-0.4	9.5	n/a	C23	H38	B4	O3	Na	Fe	W2

Figure S15. HR-MS spectrum of compound **4**.
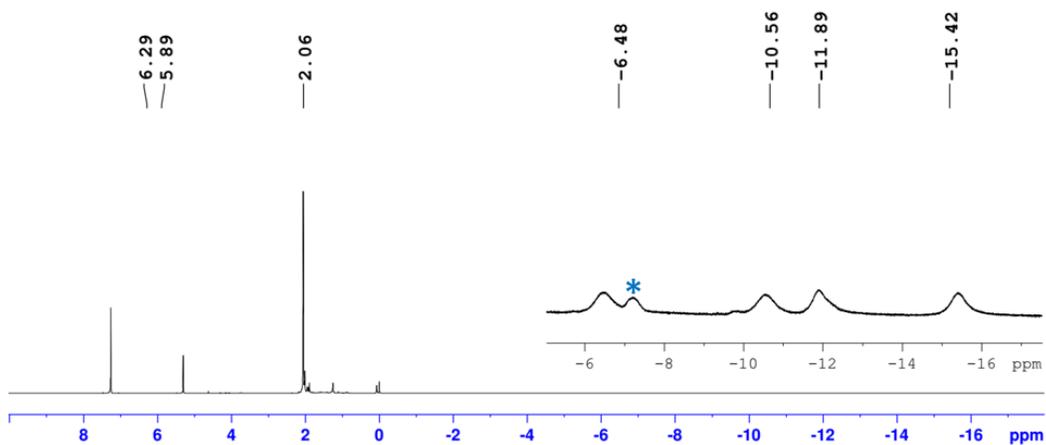
**Figure S16.** ^{1}H NMR spectrum of compound **5** in CDCl$_3$. (* Peak corresponding to inseparable known {(Cp*Mo)$_2$B$_5$H$_9$}.)
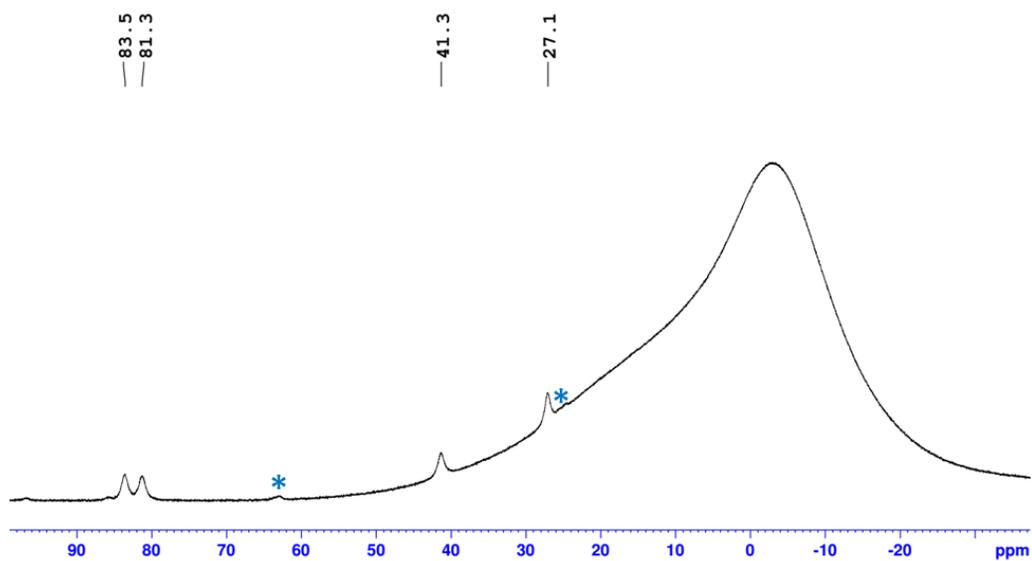
Figure S17. $^{11}B\{^{1}H\}$ spectrum of compound **5** in CDCl$_3$. (* Peaks corresponding to inseparable known {(Cp*Mo)$_2$B$_5$H$_9$}).
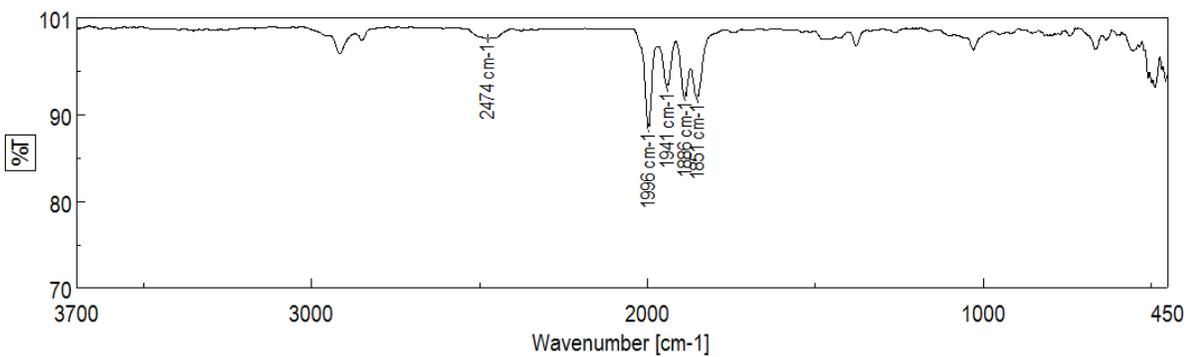

Figure S18. IR spectrum of compound **5**.

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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
296 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: 0-4   O: 0-4   Na: 0-1   Cr: 0-1   Mo: 0-2
SGG-MO2B4CR
04012019-02-SGG-MO2B4CR 56 (1.409) AM (Cen,5, 80.00, Ar,5000.0,0.00,1.00); Sb (1,40.00); Sm (Mn, 1x5.00); Cm (46:71)   TOF MS ES+
6.27e+002
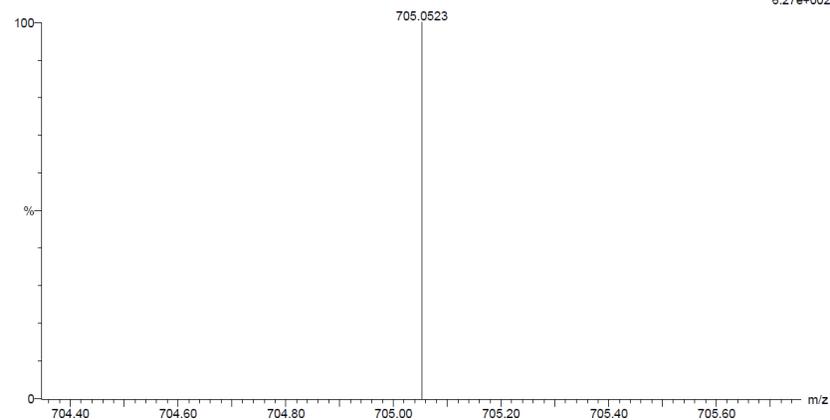
Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
705.0523	705.0553	-3.0	-4.3	7.5	n/a	C24 H38 B4 O4 Na Cr Mo2

Figure S19. HR-MS spectrum of compound **5**.