SUPPORTING INFORMATION

Cooperative B-H and Si-H Bond Activations by κ²-N,S-chelated Ruthenium Borate Complexes

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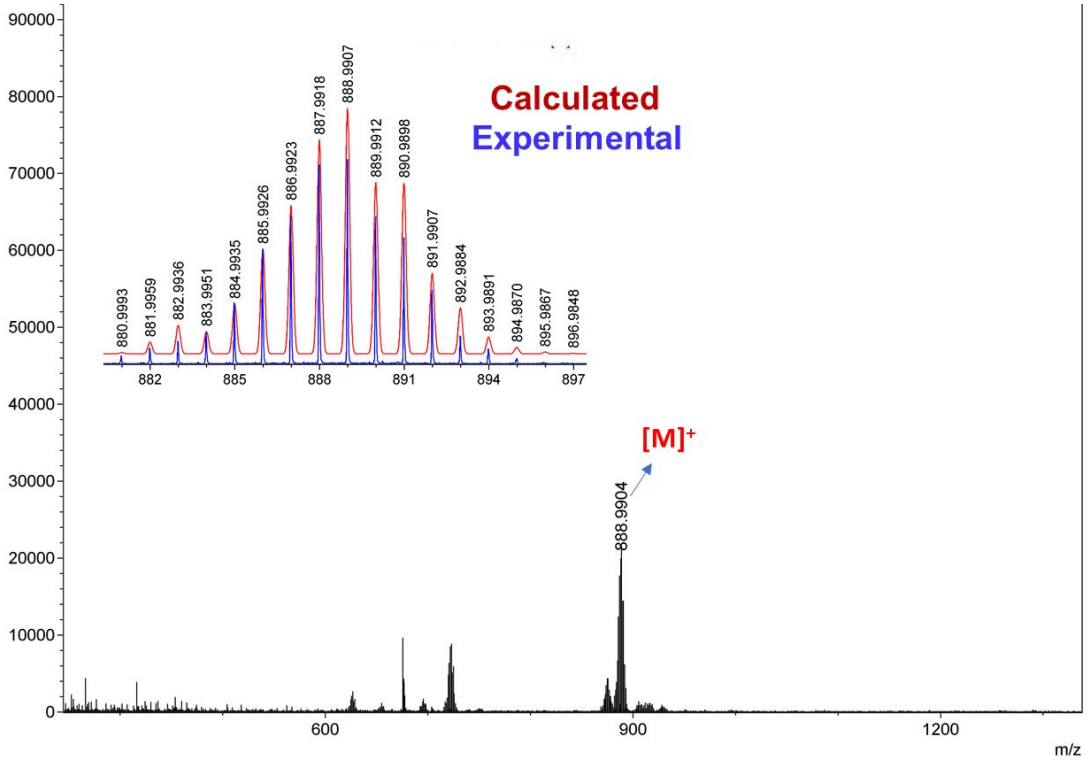

Figure S1. Calculated (red) and experimental (blue) mass spectral isotopic distribution for the fragment of **2**.

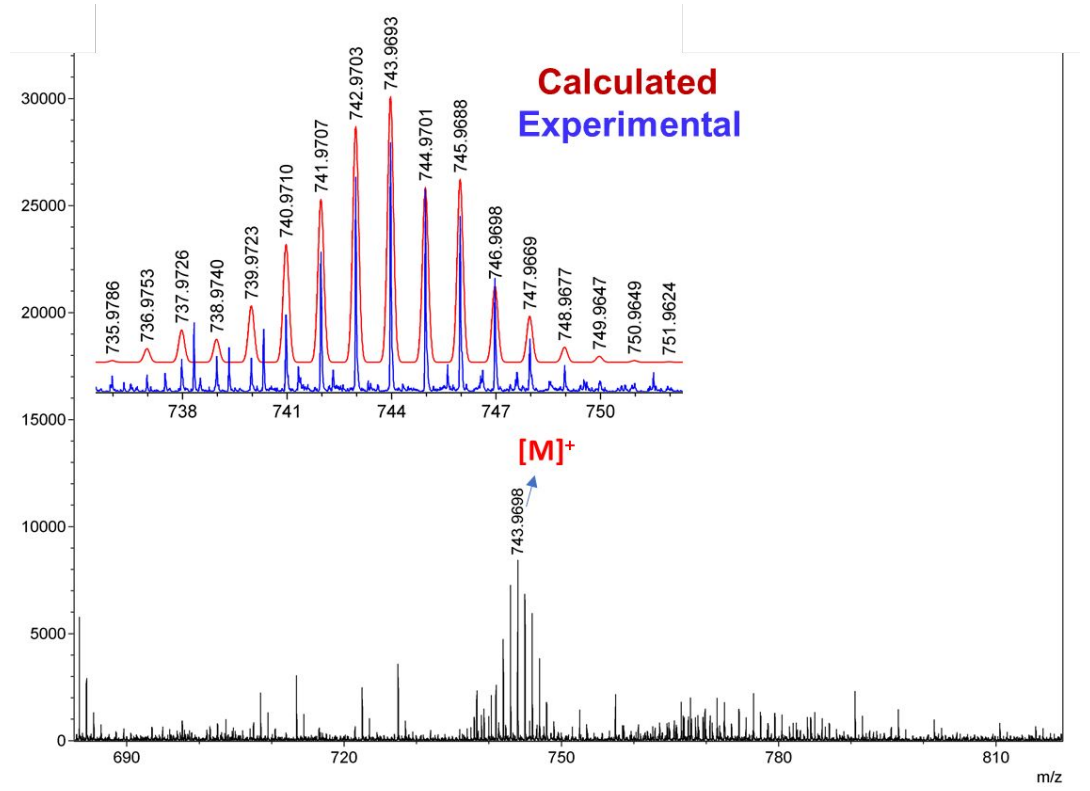

Figure S2. Calculated (red) and experimental (blue) mass spectral isotopic distribution for the fragment of **3**.

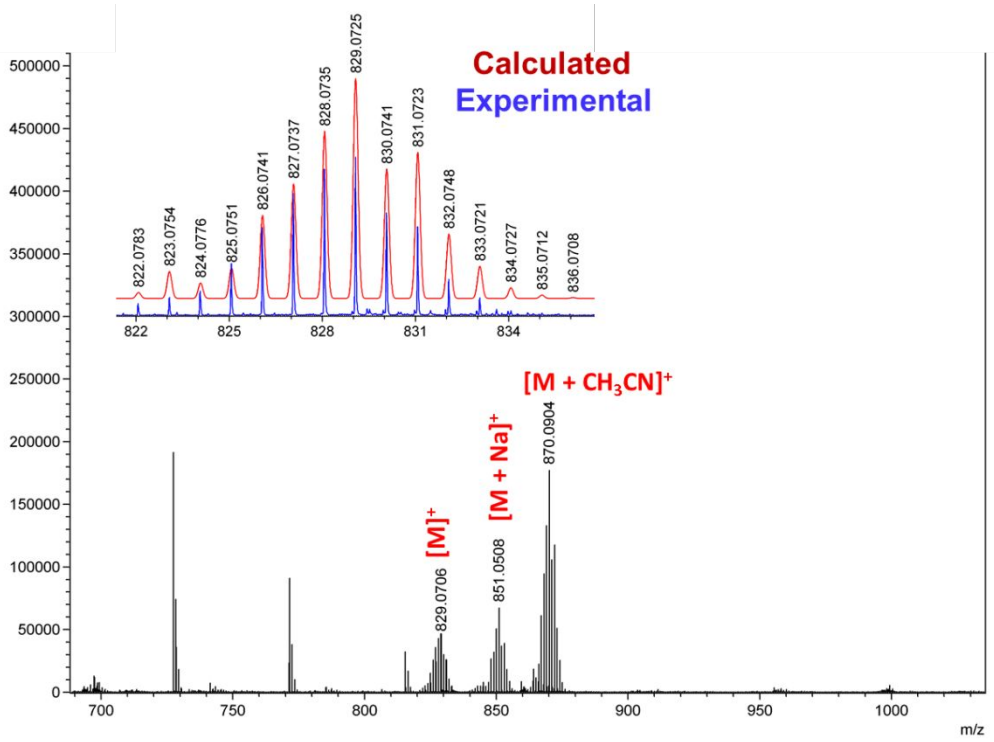

Figure S3. Calculated (red) and experimental (blue) mass spectral isotopic distribution for the fragment of **4**.

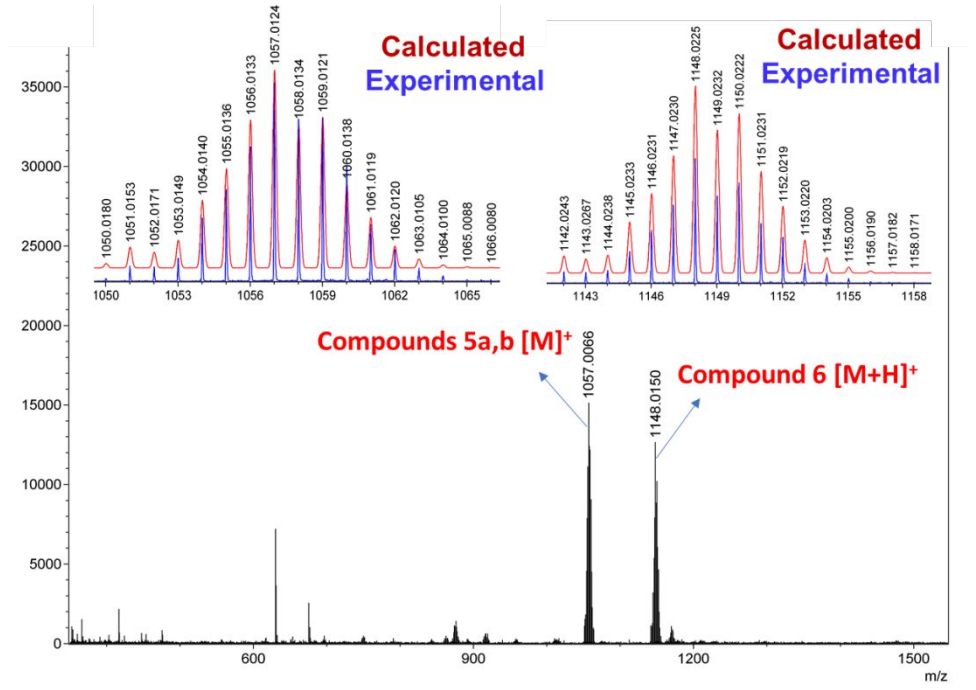

Figure S4. Calculated (red) and experimental (blue) combined mass spectral isotopic distribution for the fragments of **5a, 5b** and **6**.

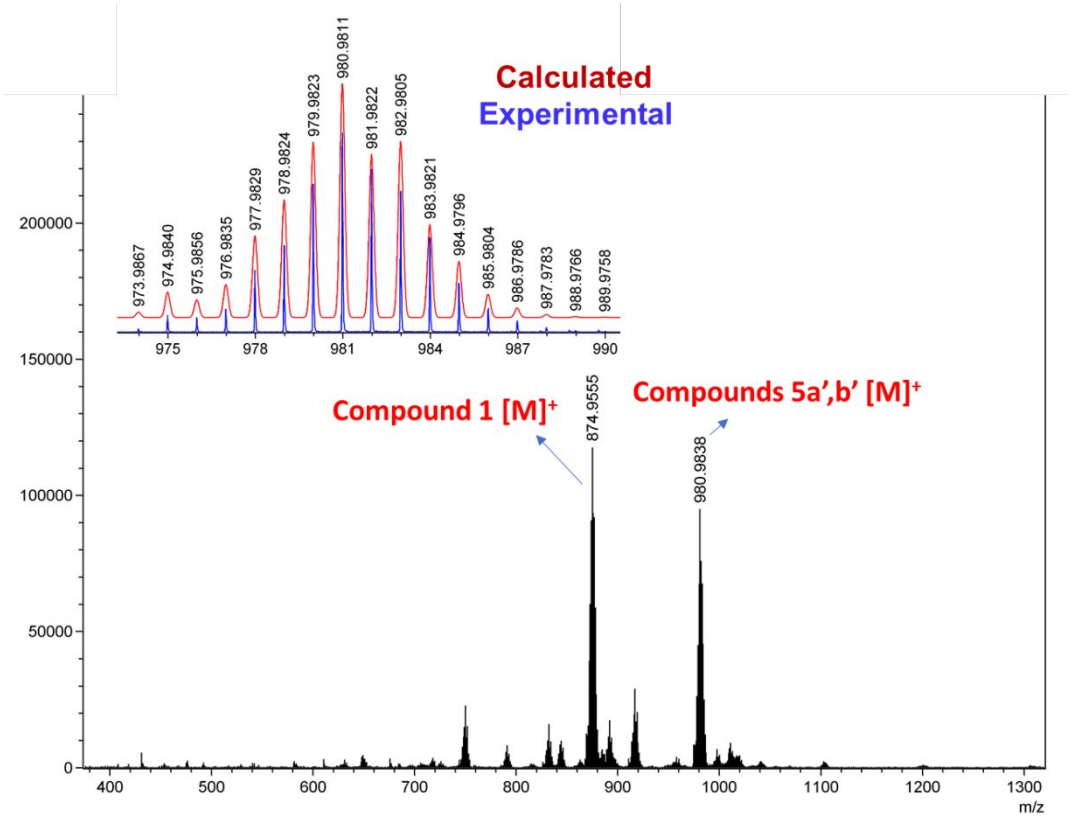

Figure S5. Calculated (red) and experimental (blue) combined mass spectral isotopic distribution for the fragments of **5a'** and **5b'.**

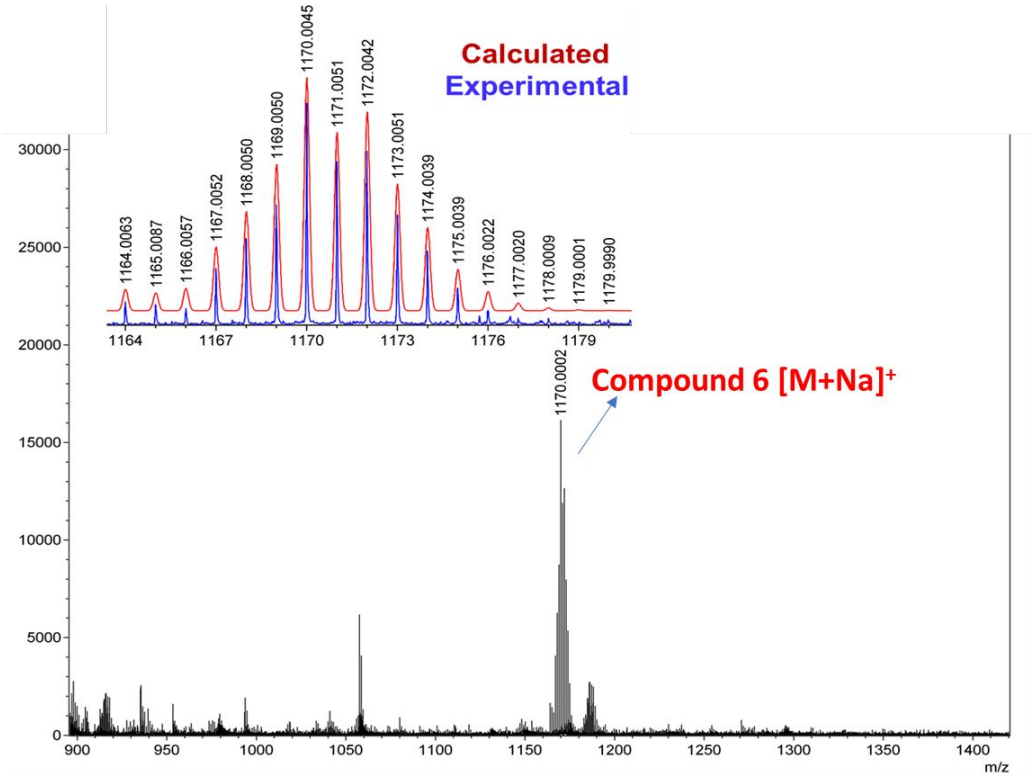

Figure S6. Calculated (red) and experimental (blue) mass spectral isotopic distribution for the fragment of **6**.

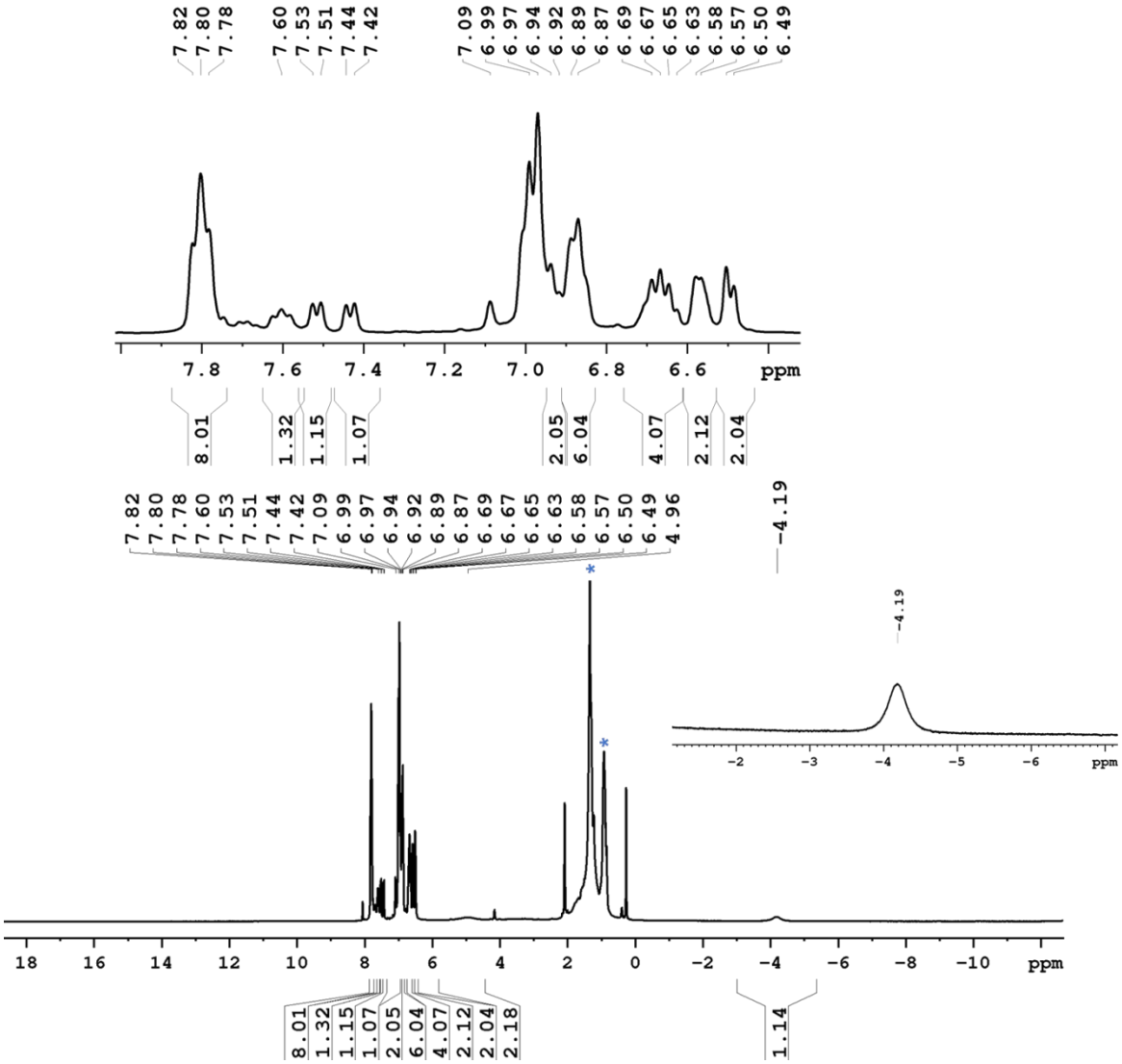

Figure S7. ^{1}H NMR spectrum of **2** in toluene-d_8 (400 MHz) (*= solvent and grease impurities).

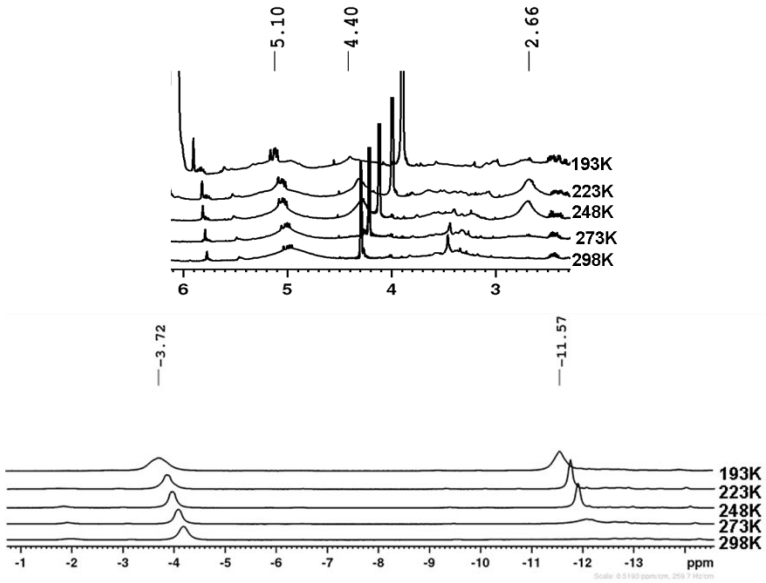

Figure S8. Variable temperature ^{1}H NMR spectrum **2** in toluene-d_8 (500MHz).

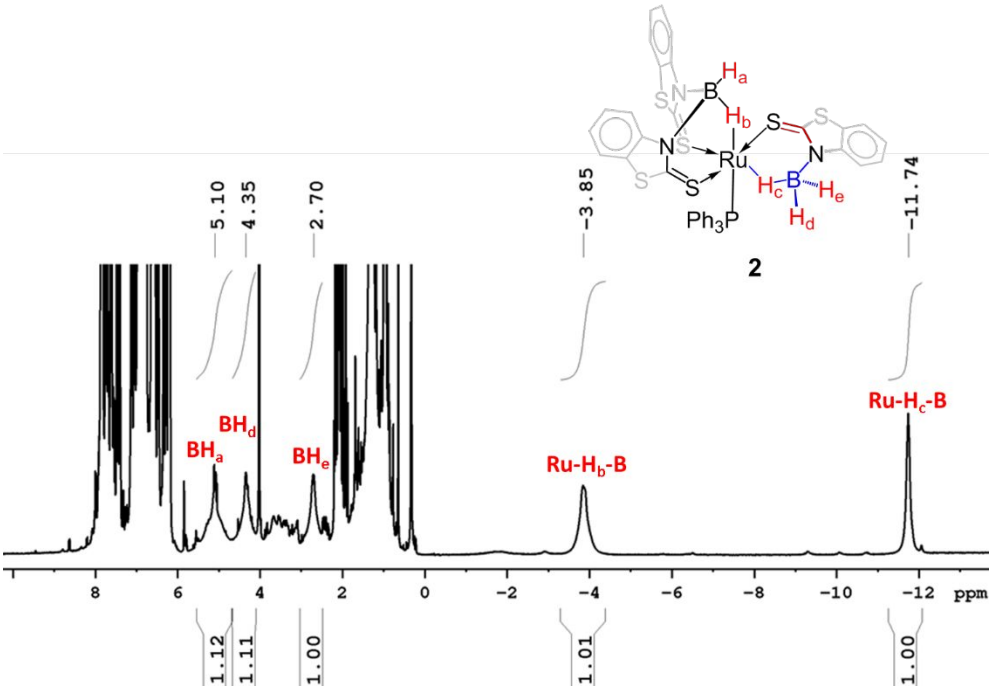

Figure S9. Assignment of BH and Ru-H-B protons in ^{1}H NMR spectrum of **2** at –50°C in toluene-d_8 (500 MHz).

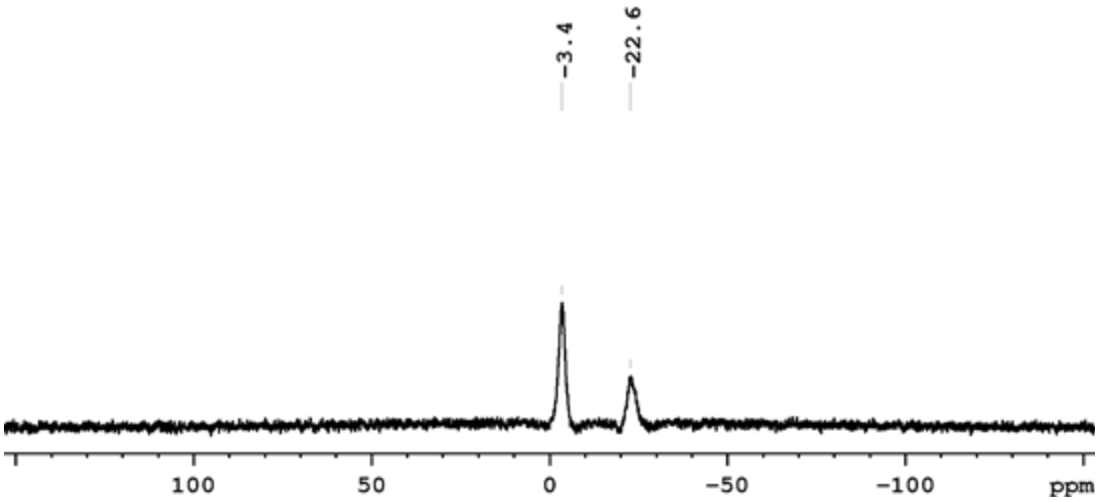

Figure S10. $^{11}B\{^{1}H\}$ NMR spectrum of **2** in $CDCl_3$ (160 MHz).

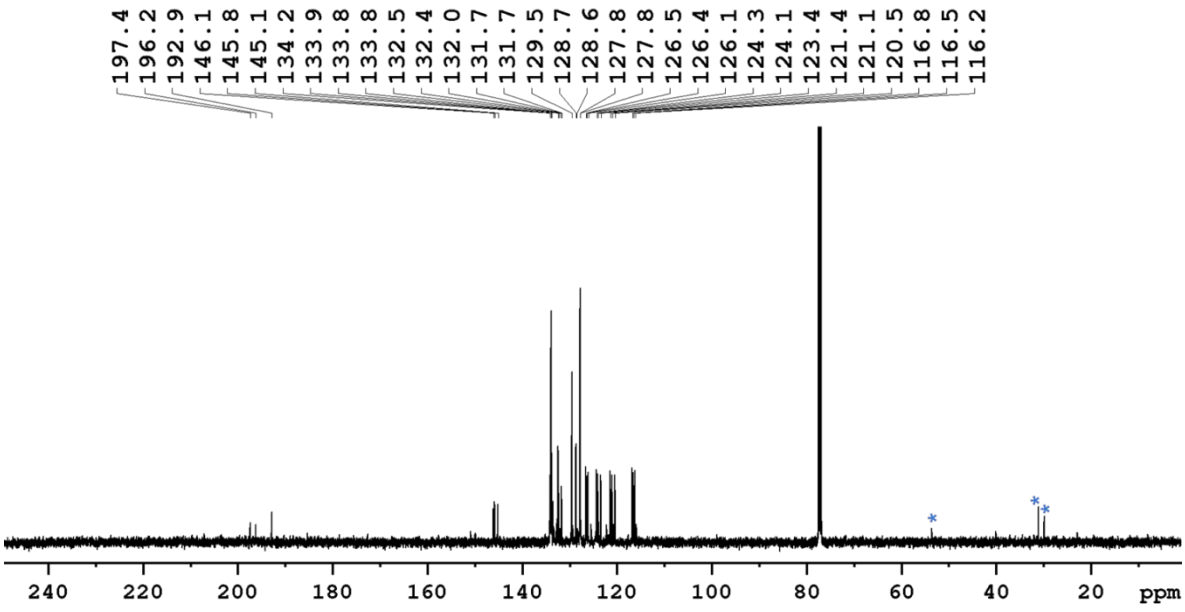

Figure S11. $^{13}C\{^{1}H\}$ NMR spectrum of **2** in $CDCl_3$ (126 MHz) (*= solvent and grease impurities).

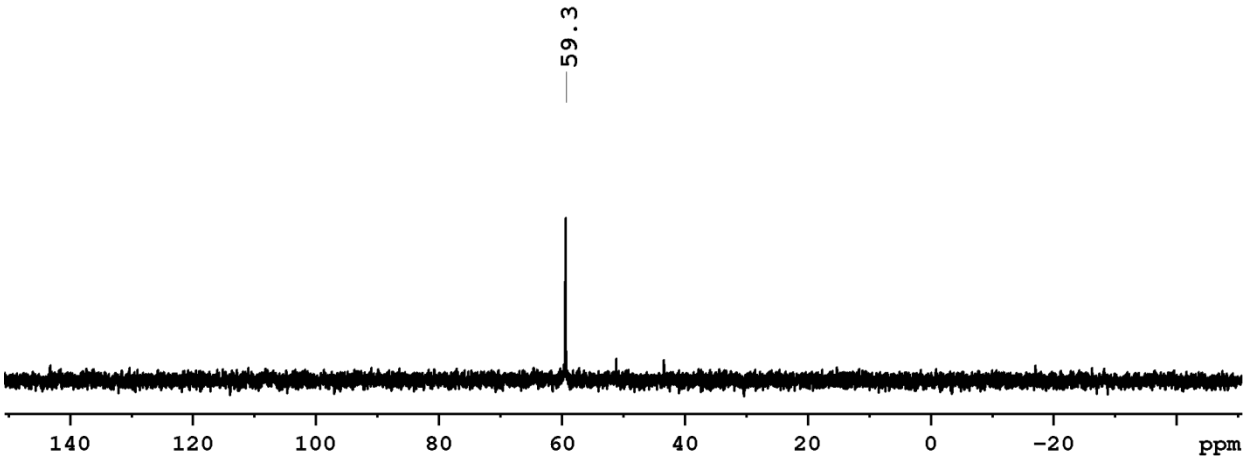

Figure S12. $^{31}P\{^{1}H\}$ NMR spectrum of **2** in $CDCl_3$ (202 MHz).

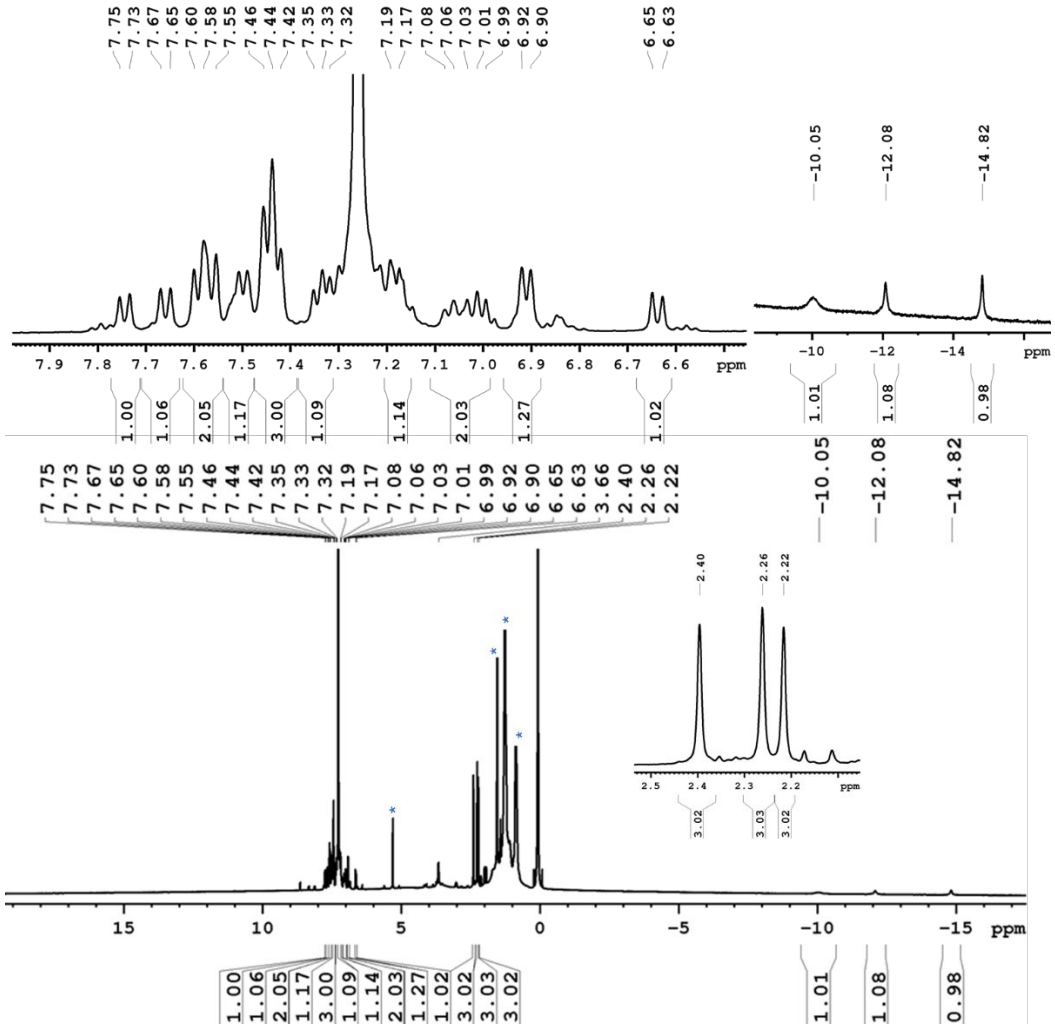

Figure S13. ^{1}H NMR spectrum of **3** in $CDCl_3$ (400 MHz) (*= solvent and grease impurities).

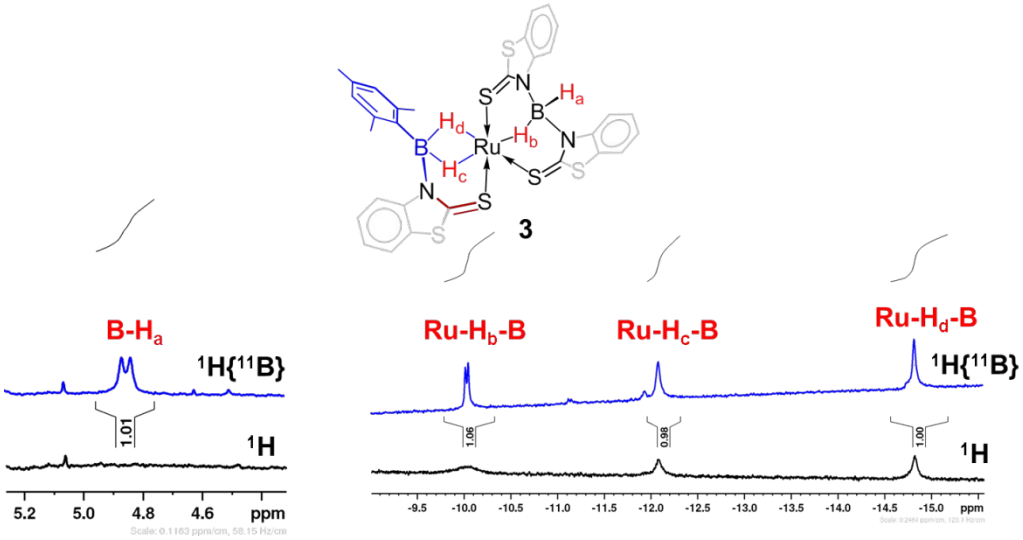

Figure S14. Combined ^{1}H NMR and $^{1}H\{^{11}B\}$ NMR spectra of **3** in $CDCl_3$ (500 MHz).

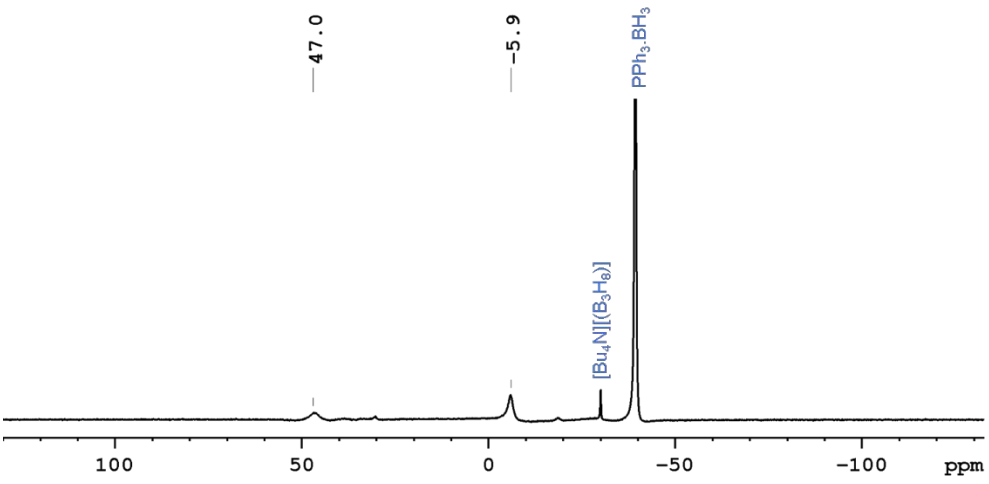

Figure S15. $^{11}B\{^{1}H\}$ NMR spectrum of **3** in benzene-d_6 (160 MHz).

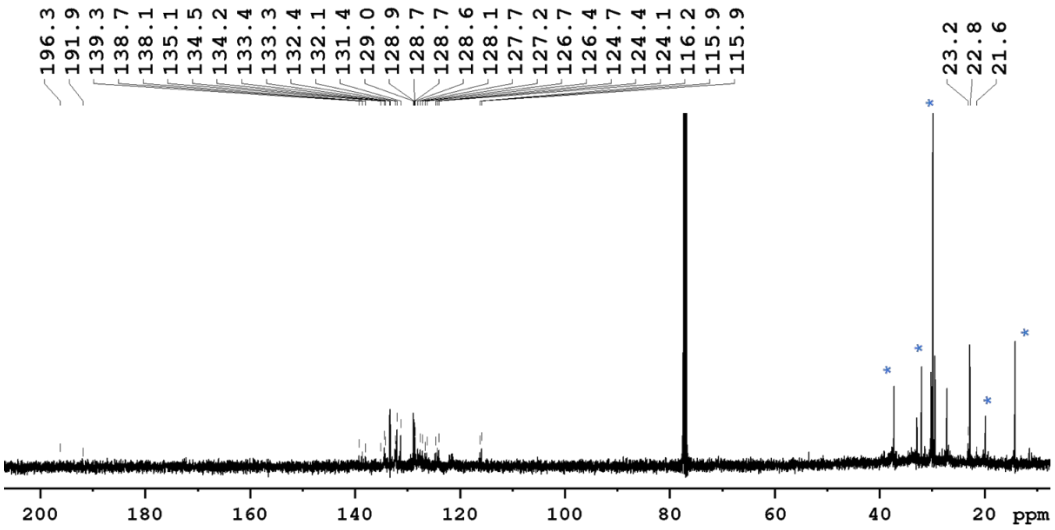

Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of **3** in $CDCl_3$ (202 MHz) (*= solvent and grease impurities).

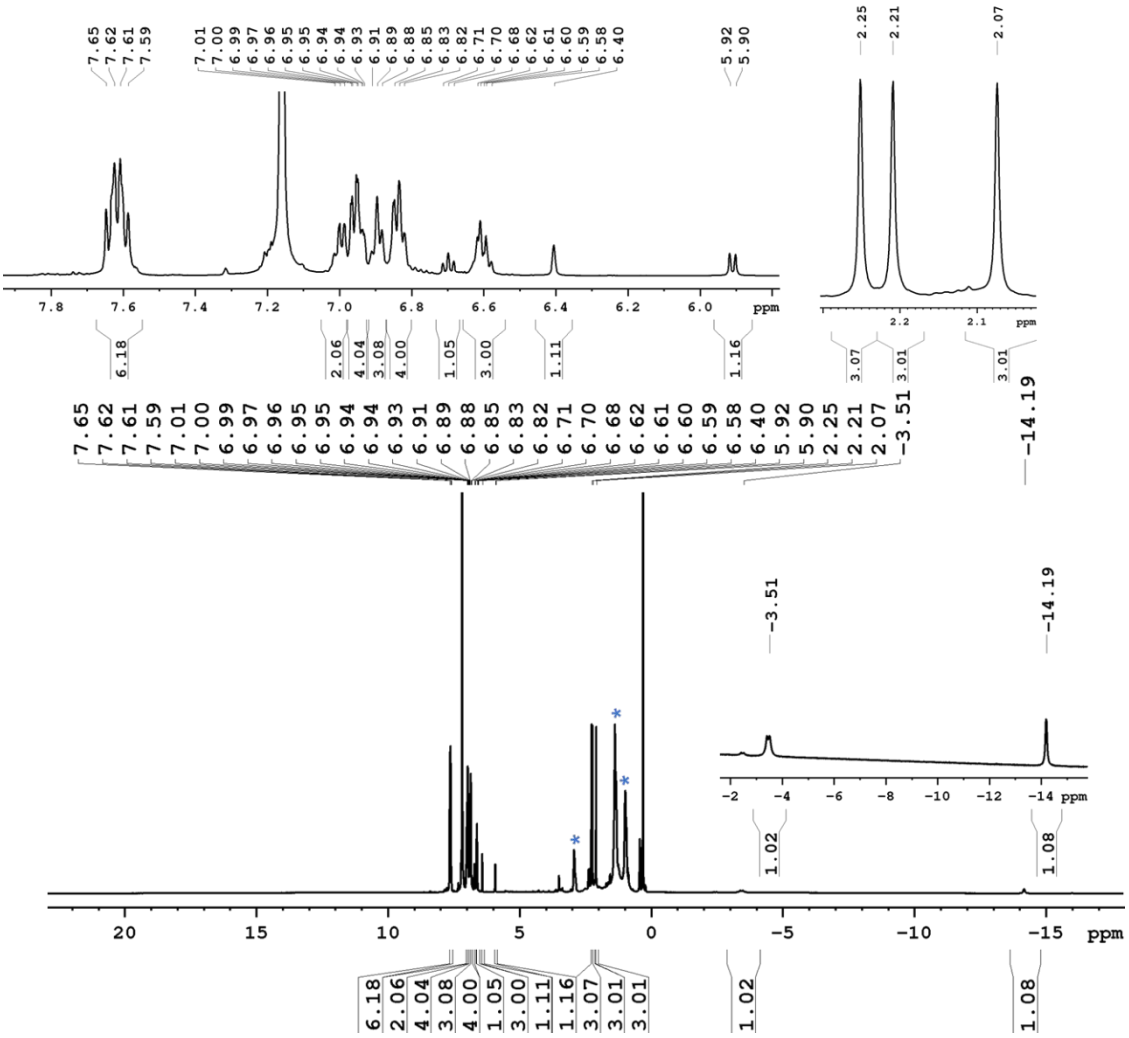

Figure S17. ^{1}H NMR spectrum of **4** in benzene-d_6 (500 MHz) (*= solvent and grease impurities).

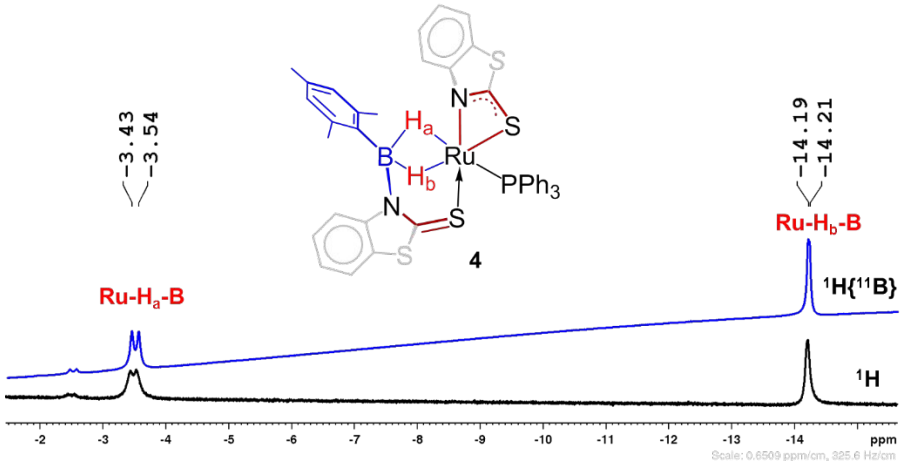

Figure S18. Combined ^{1}H NMR and $^{1}H\{^{11}B\}$ NMR spectra of **4** in benzene-d_6 (500 MHz).

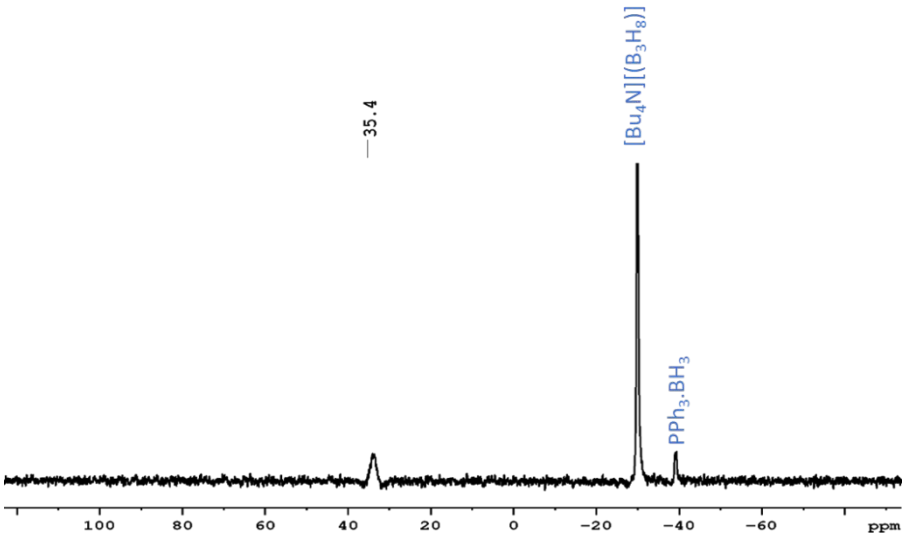

Figure S19. $^{11}B\{^{1}H\}$ NMR spectrum of **4** in benzene-d_6 (160MHz).

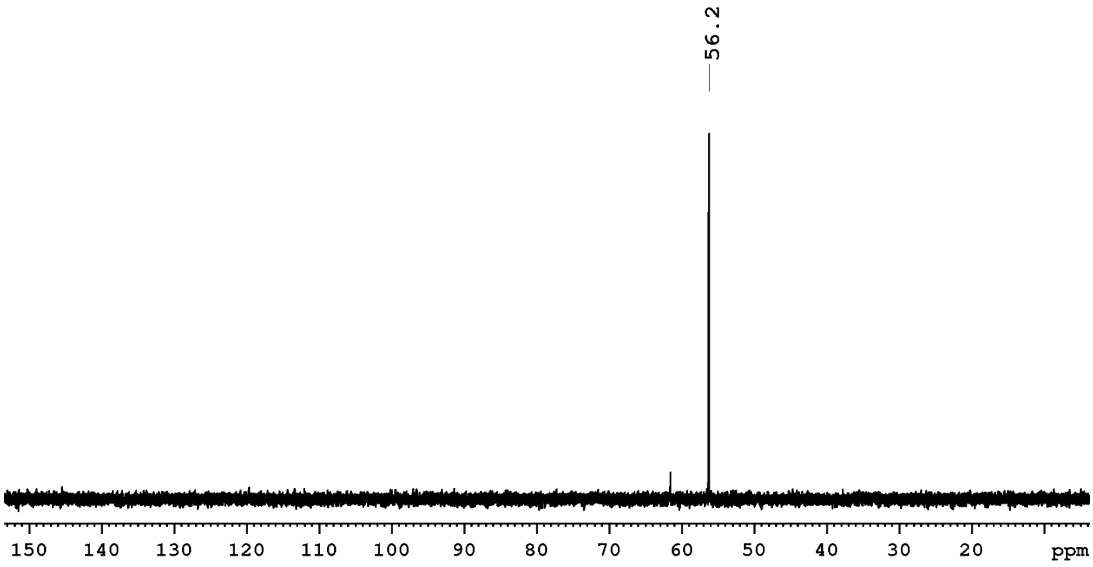

Figure S20. $^{31}P\{^{1}H\}$ NMR spectrum of **4** in benzene-d_6 (202 MHz).

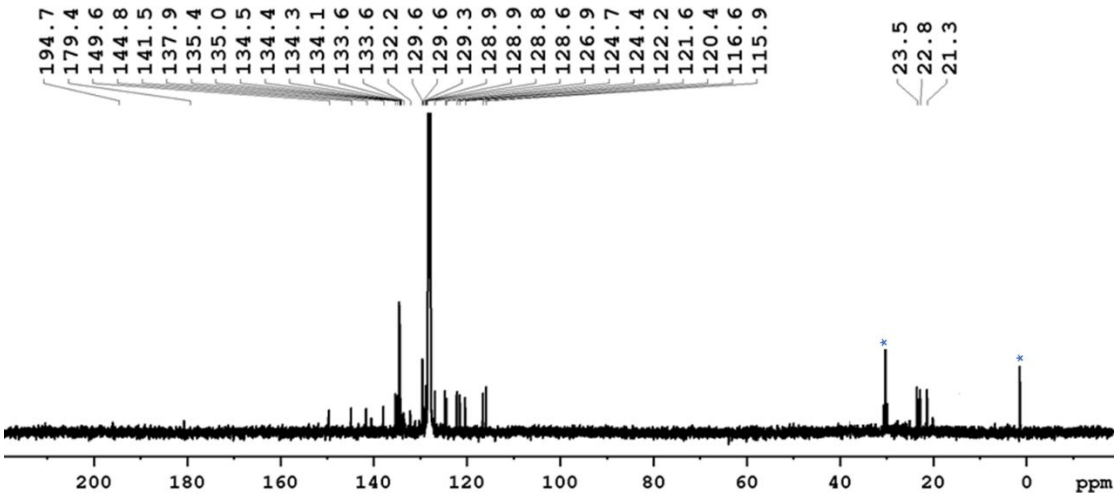

Figure S21. $^{13}C\{^{1}H\}$ spectrum of **4** in benzene-d_6 (202 MHz) (*= solvent and grease impurities).

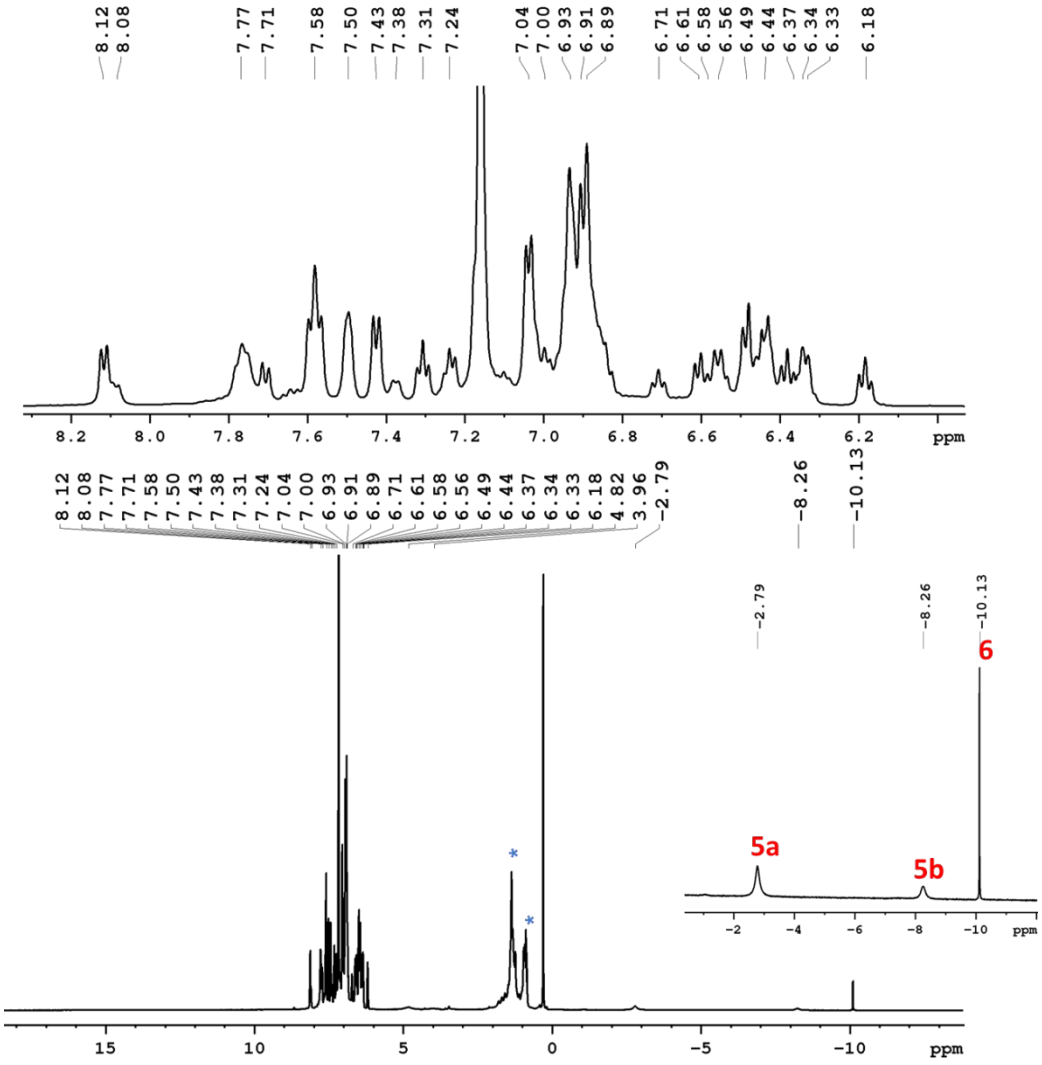

Figure S22. Combined ^{1}H NMR spectrum of **5a, 5b** and **6** in benzene-d_6 (400 MHz) (*= solvent and grease impurities).

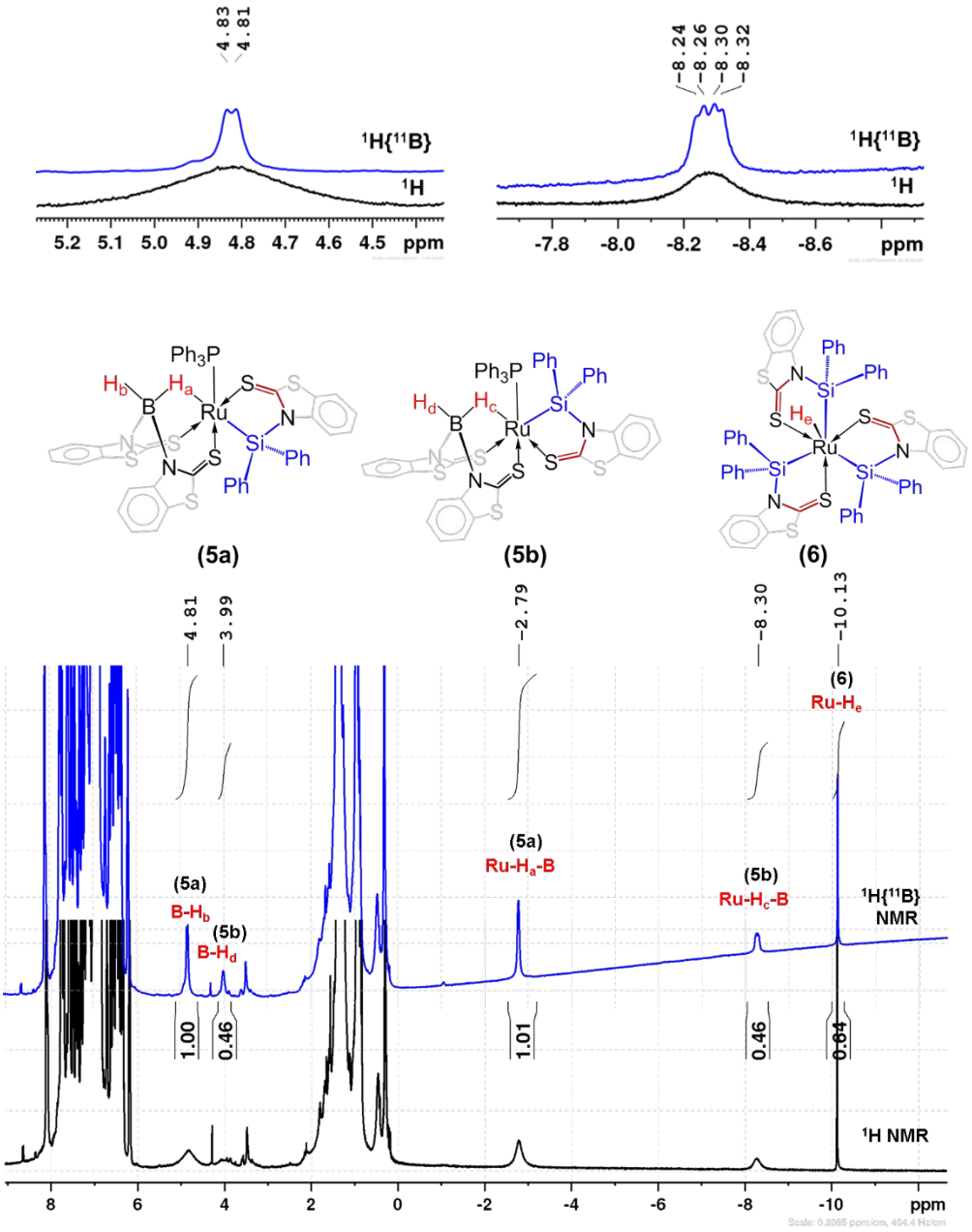

Figure S23. Combined ^{1}H and ^{1}H{^{11}B} NMR spectra of **5a, 5b** and **6** in benzene-d_6 (500 MHz).

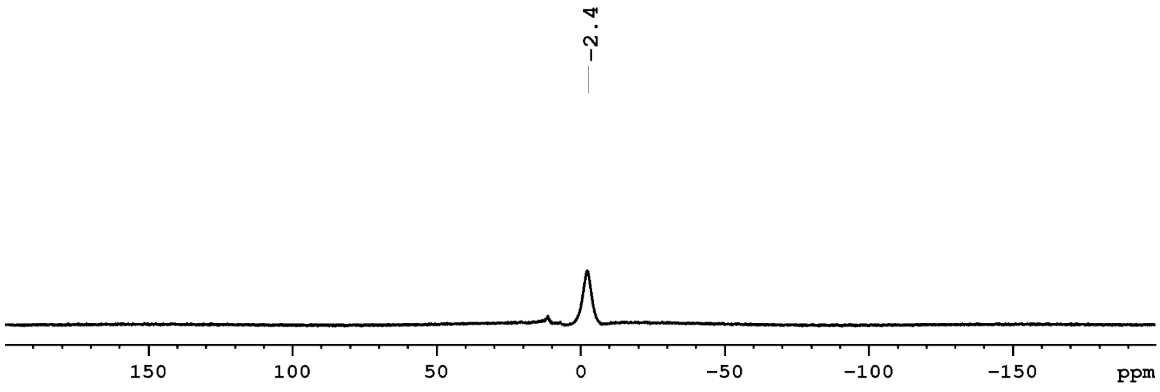

Figure S24. Combined ^{11}B{^{1}H} NMR spectrum of **5a, 5b** and **6** in benzene-d_6 (160 MHz).

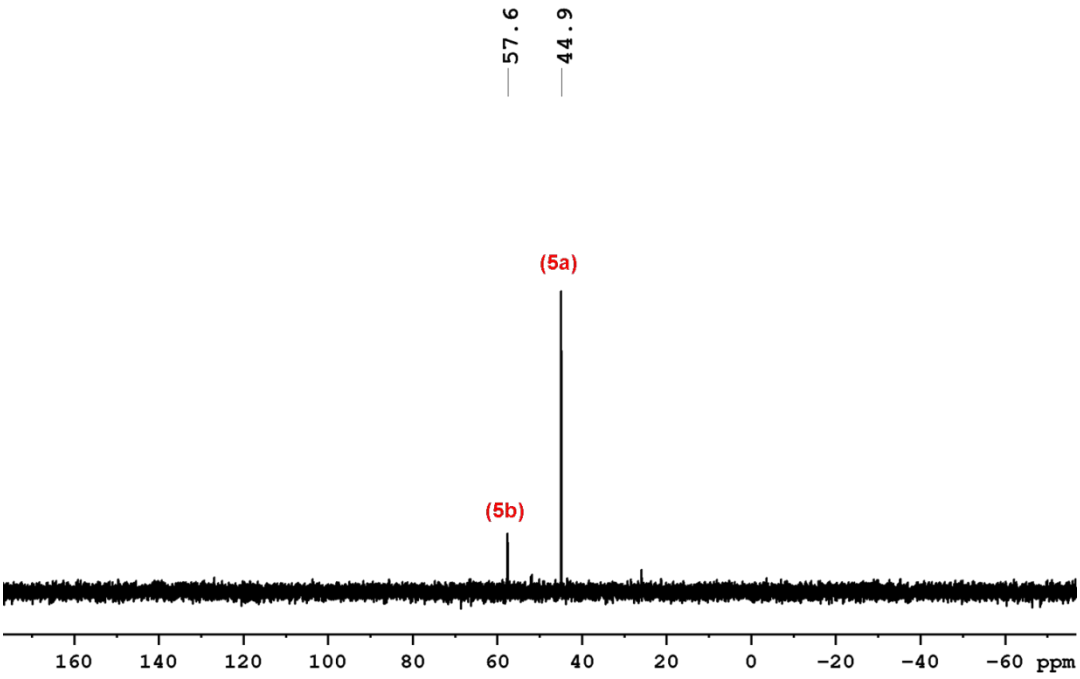

Figure S25. Combined $^{31}P\{^{1}H\}$ NMR spectrum of **5a, 5b** and **6** in benzene-d_6 (202 MHz).

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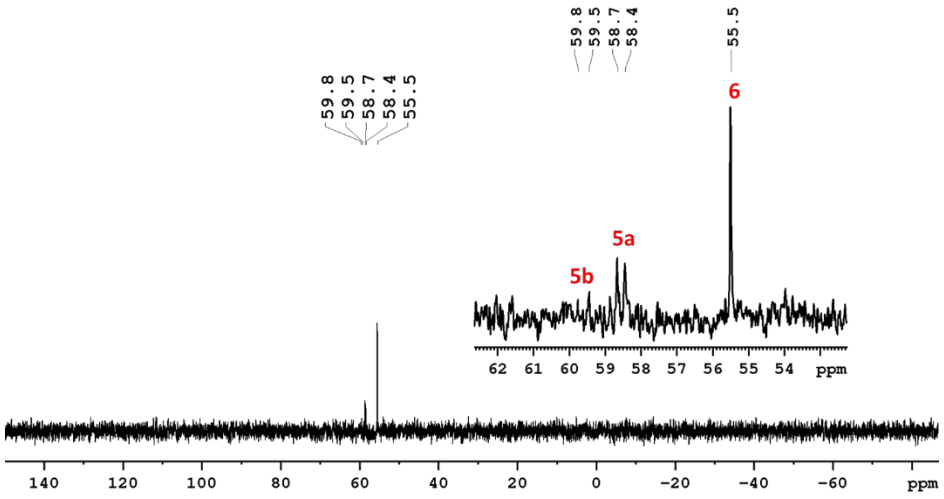


Figure S26. Combined $^{29}Si\{^{1}H\}$ NMR spectrum of **5a, 5b** and **6** in benzene-d_6 (99 MHz).

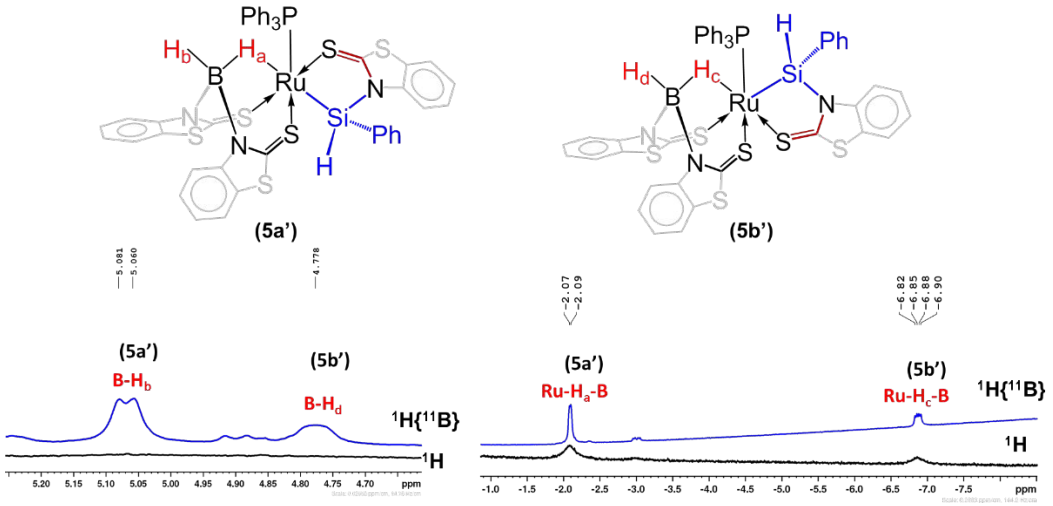


Figure S27. Combined ^{1}H NMR and ^{1}H{^{11}B} NMR spectra of **5a′** and **5b′** in benzene-d_6 (500 MHz).

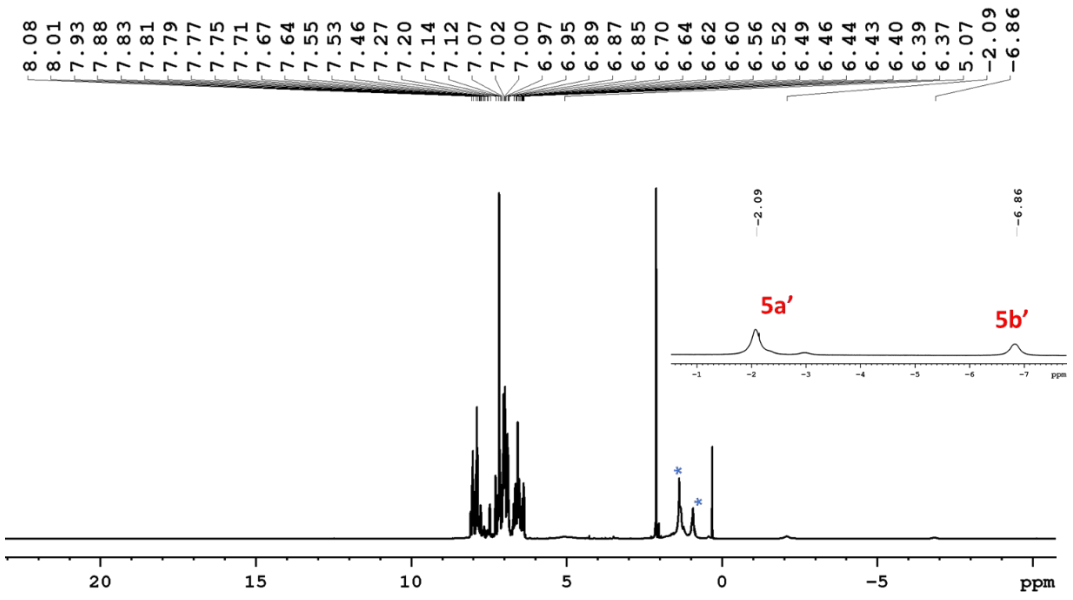


Figure S28. Combined ^{1}H NMR spectrum of **5a′** and **5b′** in benzene-d_6 (400 MHz) (*= solvent and grease impurities).

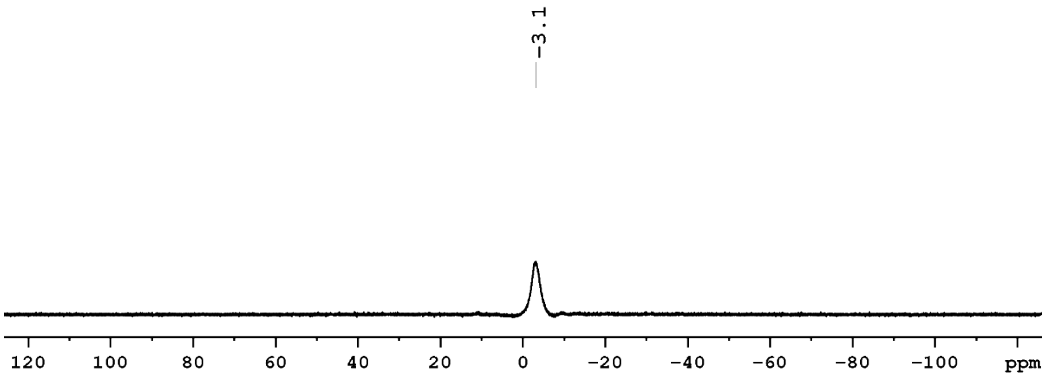


Figure S29. Combined $^{11}B\{^{1}H\}$ NMR spectrum of **5a′** and **5b′** in benzene-d_6 (160MHz).

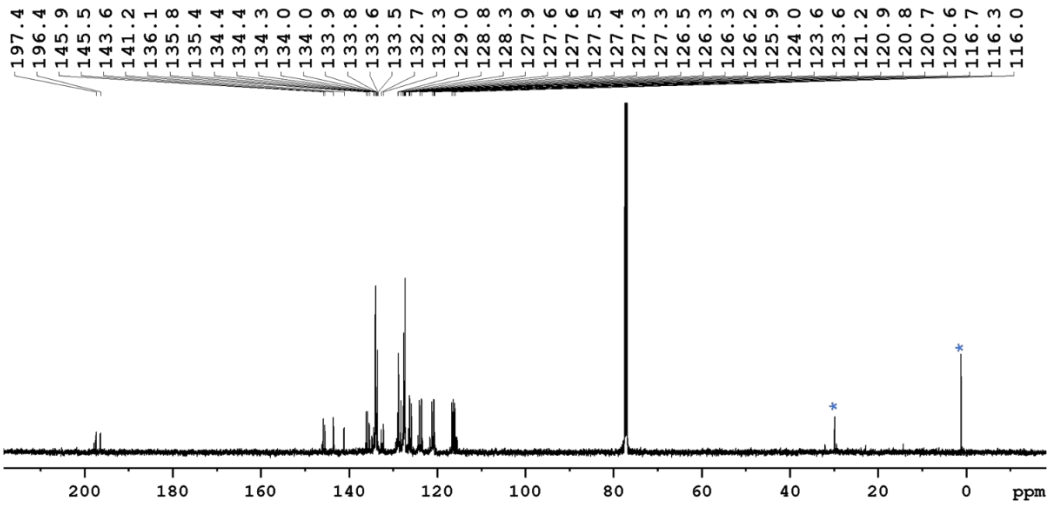


Figure S30. Combined $^{13}C\{^{1}H\}$ NMR spectrum of **5a′** and **5b′** in $CDCl_3$ (126 MHz) (*= solvent and grease impurities).

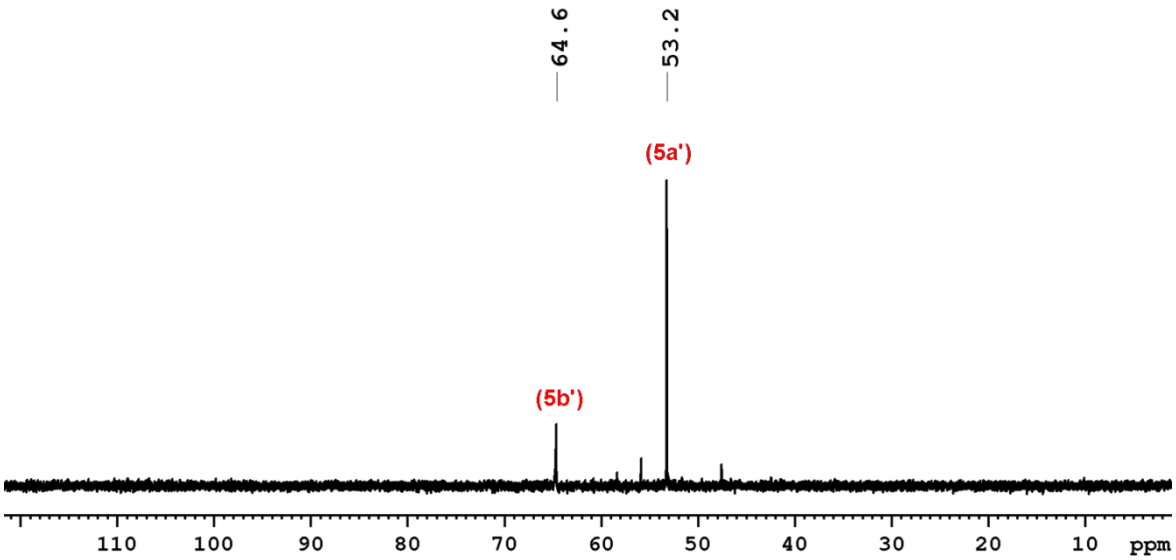


Figure S31. Combined $^{31}P\{^{1}H\}$ NMR spectrum of **5a′** and **5b′** in benzene-d_6 (202 MHz).

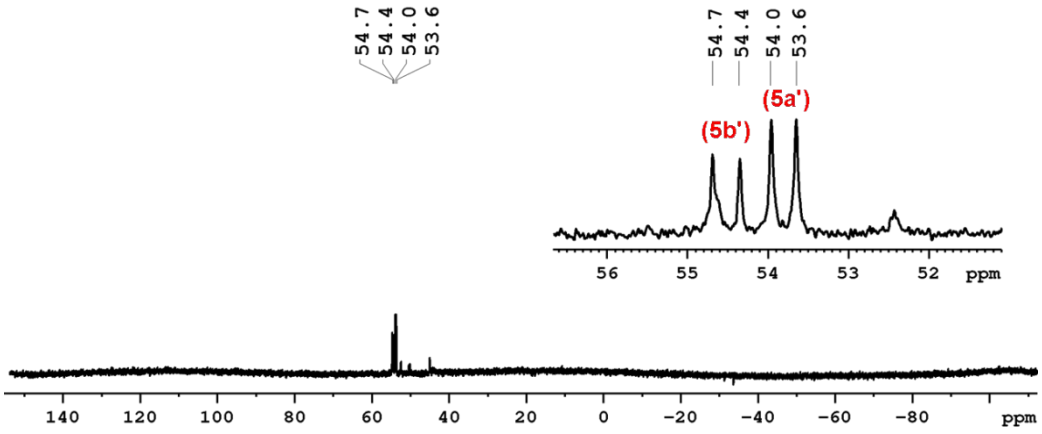


Figure S32. Combined $^{29}Si\{^{1}H\}$ NMR spectrum of **5a′** and **5b′** in benzene-d_6 (99 MHz).

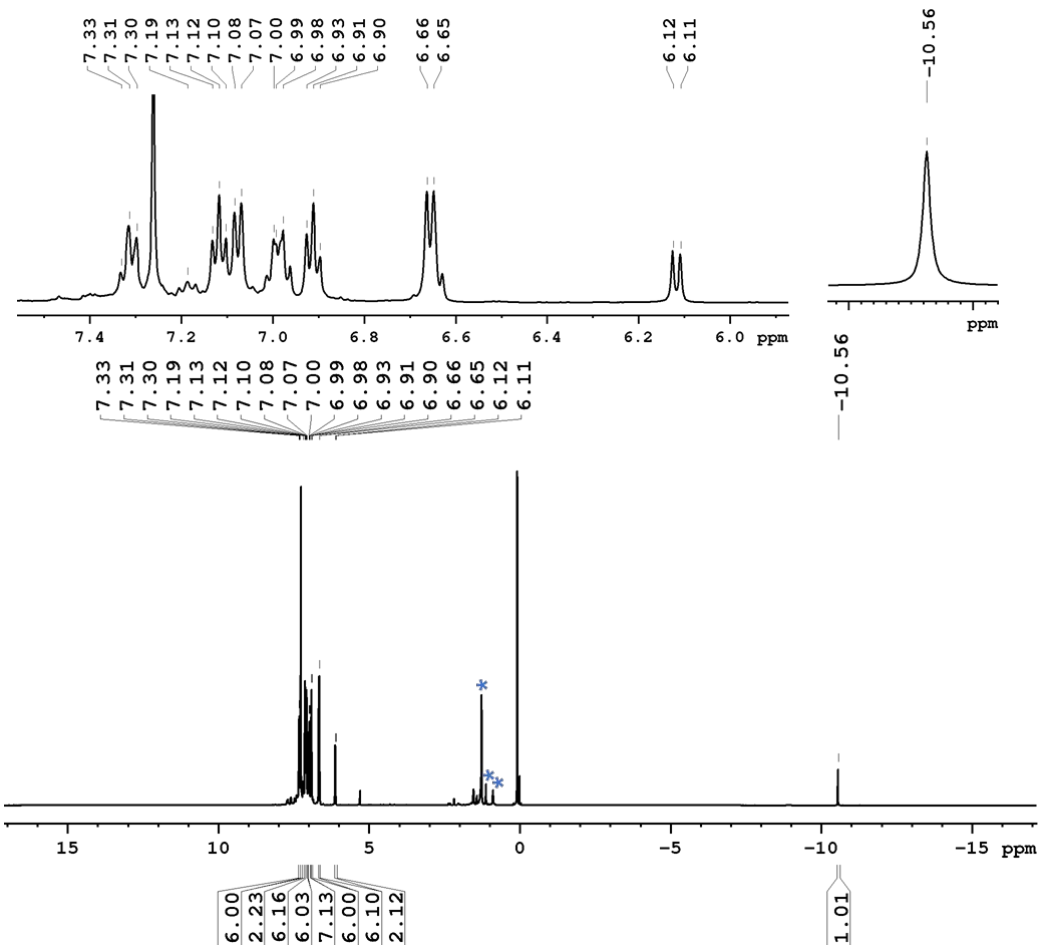


Figure S33. ^{1}H NMR spectrum of **6** in $CDCl_3$ (500 MHz) (*= solvent and grease impurities).

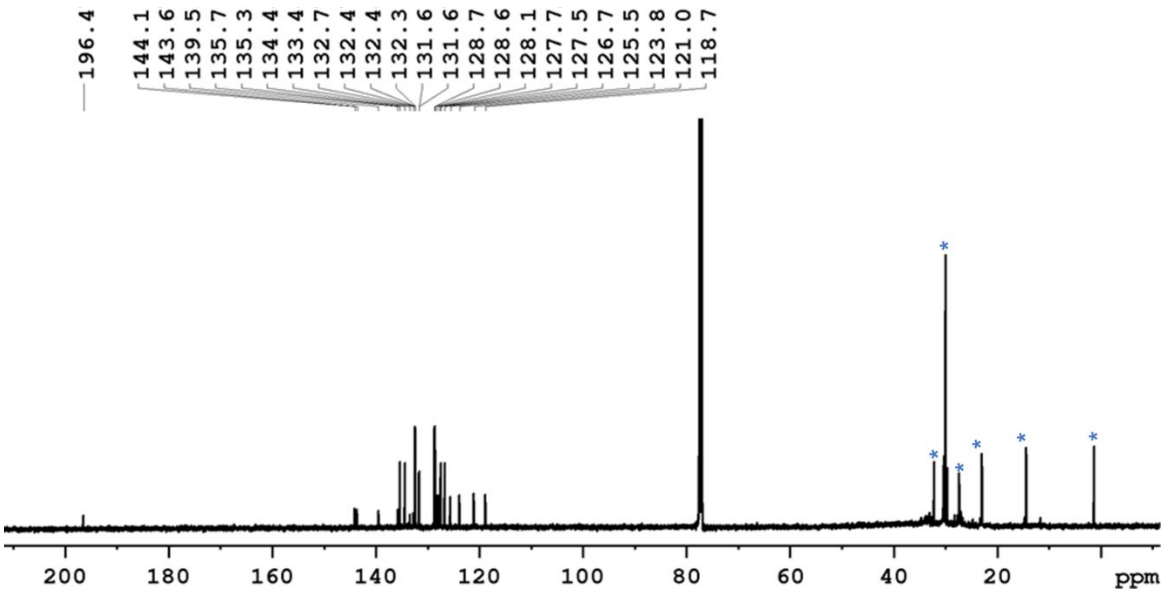


Figure S34. $^{13}C\{^{1}H\}$ NMR spectrum of **6** in $CDCl_3$ (126 MHz) (*= solvent and grease impurities).

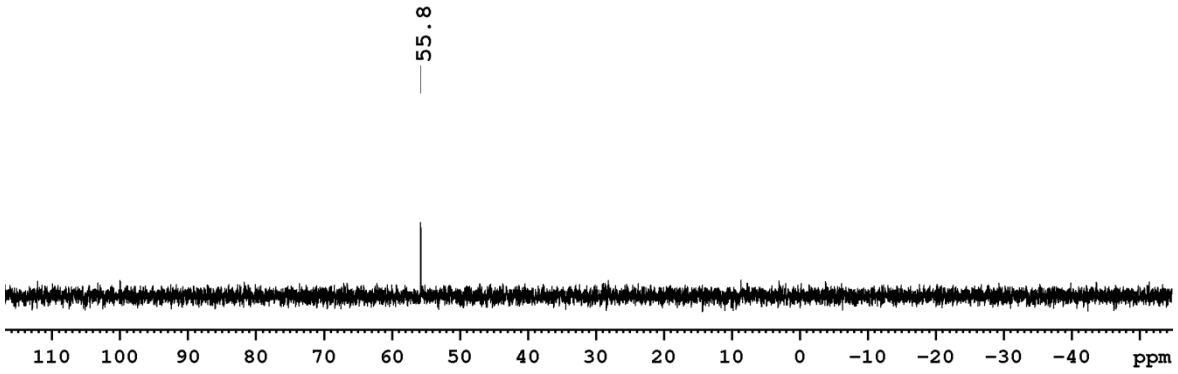


Figure S35. $^{29}Si\{^{1}H\}$ NMR spectrum of **6** in $CDCl_3$ (99 MHz).

II.1 Computational data

Table S1. Selected geometrical parameters and Wiberg bond indices (WBI) of **2-6**.

2				**3**			
	Expt.	Cal.	WBI		Expt.	Cal.	WBI
Ru1-B1	2.646(11)	2.631	0.168	Ru1-B1	2.743	2.683	0.146
Ru1-B2	2.779	2.724	0.124	Ru1-B2	2.122(12)	2.135	0.401
Ru1-P1	2.276(2)	2.410	0.560	Ru1-H2X	1.82(6)	1.744	0.177
Ru1-H1C	1.79(2)	1.724	0.201	Ru1-H3X	1.64(7)	1.743	0.219
Ru1-H2B	1.90(5)	1.763	0.155	Ru1-H4X	1.55(9)	1.689	0.310
B1-H1C	1.16(5)	1.287	0.654	B1-H2X	1.20(6)	1.262	0.702
B1-H1A	1.19(7)	1.200	0.967	B1-H1X	1.17(8)	1.202	0.949
B2-H2B	1.10(5)	1.250	0.718	B2-H3X	1.20(7)	1.364	0.628
B2-H2A	1.11(7)	1.202	0.950	B2-H4X	1.19(9)	1.411	0.529
Ru1-S1	2.373(2)	2.397	0.464	B2-C9	1.591(12)	1.589	0.889
4				**5a**			
	Expt.	Cal.	WBI		Expt.	Cal.	WBI
Ru1-B1	2.156(5)	2.146	0.361	Ru2-Si6	2.303(5)	2.384	0.667
Ru1-H1X	1.80(4)	1.754	0.202	Ru2-B1	2.928	2.830	0.066
Ru1-H2X	1.67(3)	1.713	0.254	Ru2-H1	1.93(14)	1.826	0.088
B1-H1X	1.34(4)	1.344	0.645	Ru2-P1	2.361(5)	2.469	0.428
B1-H2X	1.47(3)	1.393	0.587	Si6-N6	1.980(13)	1.924	0.436
Ru1-P1	2.2994(10)	2.417	0.510	Ru2-S7	2.375(5)	2.375	0.450
Ru1-S1	2.4658(11)	2.346	0.542	Ru2-S9	2.441(5)	2.385	0.443
Ru1-N1	2.127(3)	2.158	0.322	Ru2-S11	2.439(5)	2.405	0.434
B1-C8	1.582(6)	1.592	0.887	B1-H1	1.22(14)	1.248	0.791
5b				**6**			
	Expt.	Cal.	WBI		Expt.	Cal.	WBI
Ru1-Si1	-	2.401	0.572	Ru1-Si1	2.212(5)	2.426	0.499
Ru1-B1	-	2.644	0.160	Ru1-Si2	2.453(5)	2.427	0.510
Ru1-H1	-	1.721	0.179	Ru1-Si3	2.365(5)	2.416	0.530
B1-H1	-	1.273	0.691	Ru1-H1’	1.550	1.586	0.376
Ru1-P1	-	2.445	0.454	Si1-H1’	2.200	2.210	0.194
Si1-N1	-	1.933	0.462	Si2-H1’	2.199	2.257	0.172
Ru1-S1	-	2.385	0.367	Si3-H1’	2.157	2.377	0.131
Ru1-S2	-	2.458	0.280	Si1-N2	1.938(14)	1.919	0.440
Ru1-S3	-	2.417	0.331	S5-Ru1-Si1	162.23(18)	163.10	-
				S3-Ru1-Si2	162.22(16)	162.12	-
				S1-Ru1-Si3	165.12(17)	166.49	-

Table S2. Calculated natural charges (q), natural valence population (Pop) and HOMO – LUMO gaps of **2-6**.

Compound	q_{Ru}	$q_{B/Si}$	q_{B}	q_{P}	**Pop(Ru_{val})**	**Pop(B_{val}/Si_{val})**	**Pop(B_{val})**	**Pop(P_{val})**	ΔE_{H-L} **(eV)**
2	-0.316	-0.081	0.340	1.193	8.290	3.065	2.636	3.790	3.485
3	-0.308	0.337	0.334	-	8.286	2.593	2.640	-	3.390
4	-0.223	0.337	-	1.154	8.202	2.633	-	3.826	3.507
5a	-0.558	1.493	0.329	1.101	8.539	2.492	2.651	3.879	3.363
5b	-0.545	1.406	0.341	1.125	8.524	2.578	2.634	3.856	3.584
6	-0.847	1.521	-	-	8.831	2.463	-	-	3.993

Table S3. Experimentally observed and calculated ^{11}B chemical shifts of **2-5**.

Molecule		**^{11}B NMR**	
		Exp.	Cal.
2	B1	−22.6	−22.0
	B2	−3.5	−3.3
3	B1	−5.9	−5.0
	B2	47.0	35.2
4	B	35.4	31.4
5a	B	−2.4	−3.5
5b	B	−2.4	−5.3
5a'	B	−3.1	−3.4
5b'	B	−3.1	−5.6

Table S4. Topological parameters at selected bond critical points (BCPs) in **2**-**6**.

Molecule	BCP	ρ	H	$\nabla^2\rho$	*ELF*	ε
2	Ru1-P1	0.073	−0.018	0.220	0.205	0.114
	Ru1-H1C	0.051	−0.010	0.363	0.038	1.944
	B1-H1C	0.151	−0.149	−0.071	0.464	0.192
	B1-H1A	0.176	−0.185	−0.213	0.593	0.108
	Ru1-H2B	0.044	−0.008	0.312	0.032	3.260
	B2-H2B	0.172	−0.180	−0.201	0.579	0.175
	B2-H2A	0.184	−0.200	−0.319	0.668	0.104
3	B2-H3X	0.147	−0.157	−0.336	0.725	0.080
	B2-H4X	0.109	−0.100	−0.129	0.526	0.173
	Ru2-H2X	0.045	−0.009	0.330	0.327	1.885
	Ru2-H4X	0.079	−0.018	0.365	0.129	0.244
	B1-H2X	0.168	−0.177	−0.212	0.586	0.184
	B1-H1X	0.184	−0.200	−0.318	0.667	0.104
	B2-C9	0.183	−0.197	−0.368	0.725	0.043
4	Ru1-P1	0.073	−0.019	0.192	0.229	0.684
	Ru1-H2X	0.065	−0.016	0.287	0.105	0.395
	B1-H2X	0.136	−0.139	−0.272	0.678	0.062
	B1-H1X	0.151	−0.160	−0.281	0.653	0.057
	B2-C8	0.182	−0.195	−0.341	0.700	0.044
5a	Ru2-Si6	0.084	−0.041	−0.033	0.683	0.020
	Ru2-P1	0.065	−0.016	0.169	0.212	0.982
	Ru2-S11	0.039	−0.005	0.246	0.036	6.359
	Ru2-H1	0.042	−0.007	0.301	0.030	2.879
	B1-H1	0.168	−0.174	−0.183	0.566	0.154
	B1-H1A	0.182	−0.197	−0.300	0.655	0.090
	Si6-N6	0.068	−0.027	0.378	0.599	0.066
5b	Ru1-Si1	0.082	−0.037	−0.001	0.595	0.072
	Ru1-P1	0.069	−0.018	0.172	0.228	0.914
	Ru1-S1	0.073	−0.016	0.250	0.181	0.256
	Ru1-H1	0.050	−0.010	0.359	0.036	1.772
	B1-H1	0.165	−0.172	−0.214	0.590	0.214
	B1-H1A	0.184	−0.201	−0.325	0.672	0.101
	Si1-N1	0.032	0.001	0.459	0.039	0.182
6	Ru1-Si1	0.059	−0.031	−0.042	0.640	0.584
	Ru1-Si2	0.080	−0.043	−0.097	0.877	0.215
	Ru1-Si3	0.082	−0.044	−0.089	0.840	0.146
	Si1-N2	0.069	−0.029	0.387	0.634	0.021
	S1-Ru1	0.044	−0.097	0.232	0.053	1.593
	S3-Ru1	0.046	−0.010	0.253	0.052	1.821
	S5-Ru1	0.057	−0.010	0.210	0.133	0.806

Electron density, ρ, Total energy density, H, Laplacian of the electron density, $\nabla^2\rho$, Electron localization function, *ELF*,Ellipticity, ε in a.u.

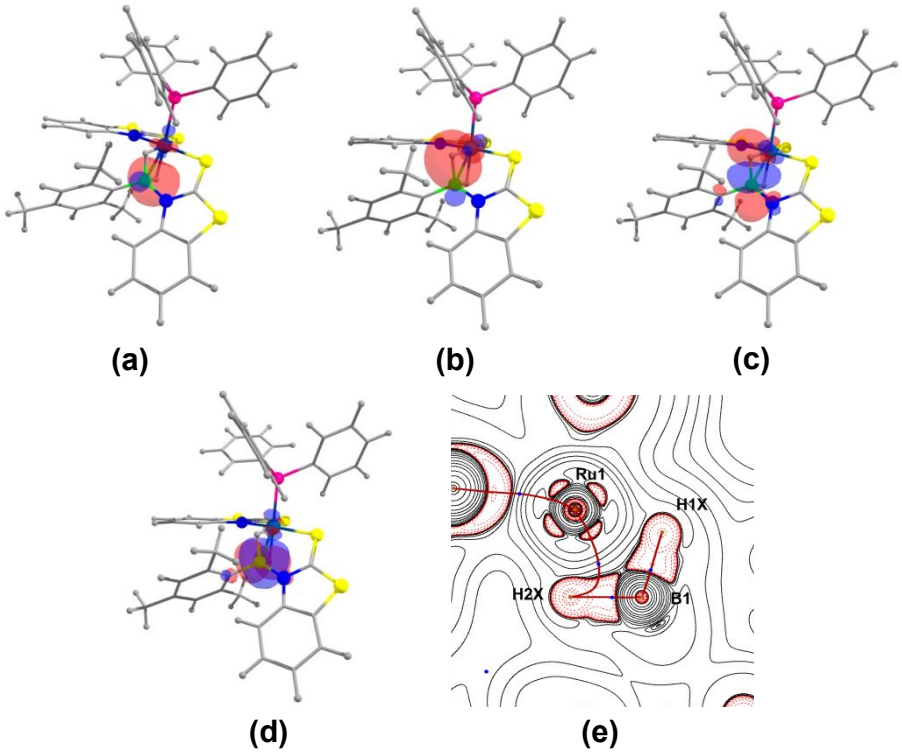


Figure S36. (a-d) NBO donor-acceptor interaction between B-H_2 and Ru in **4**; (e) Contour-line map of the Laplacian of the electron density in the Ru-H_2-B plane of **4.**

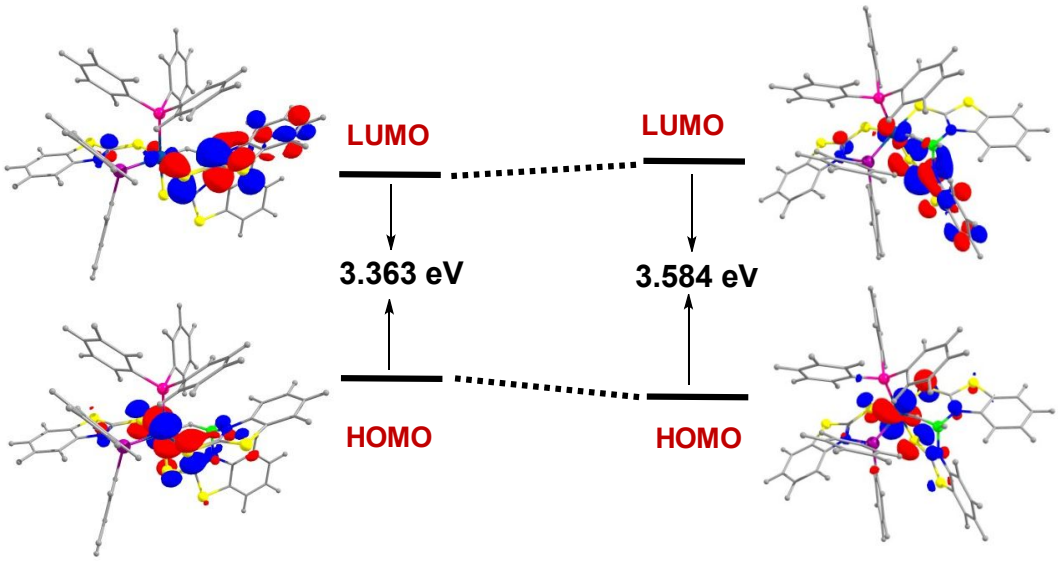


Figure S37. Frontier orbital diagram (MO) of **5a** and **5b** (isovalue ±0.04 [e/bohr^3]$^{1/2}$).

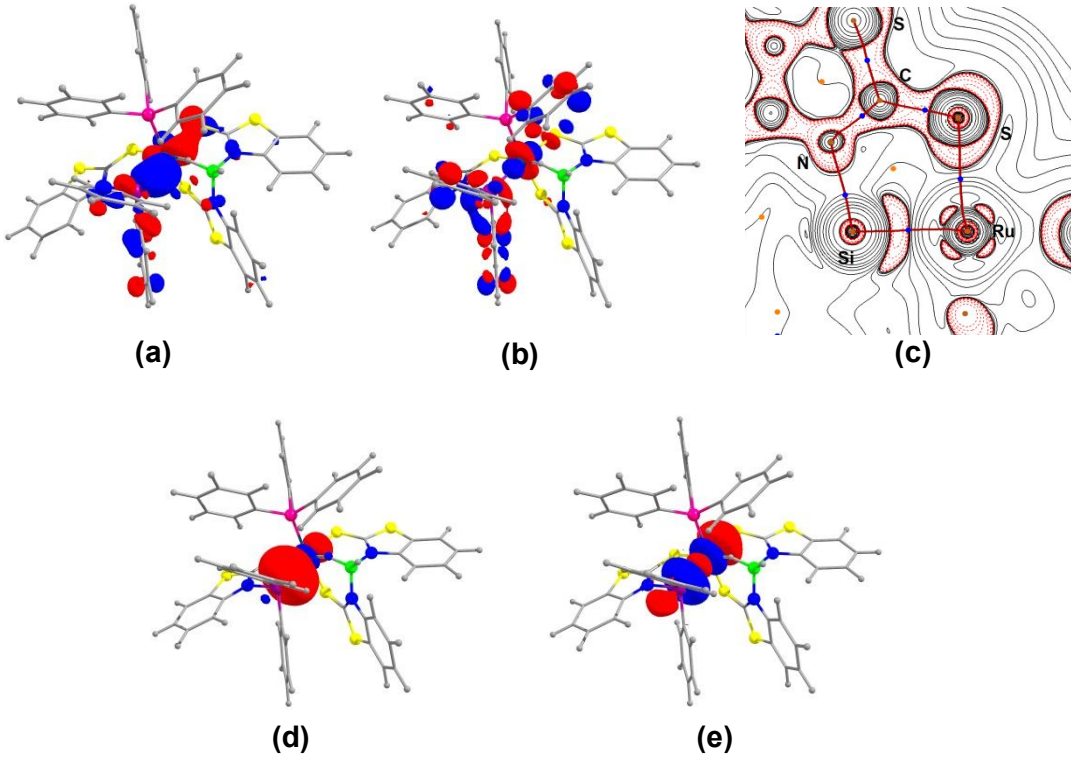


Figure S38. (a) and (b) HOMO-4 and LUMO+4 of **5b** involving Ru-Si bonding and antibonding interactions; (c) Contour-line map of the Laplacian of the electron density in the S-Ru-Si plane of **5b** and (d,e) Bonding and antibonding interactions between Ru-Si in **5b** obtained from NBO analysis.

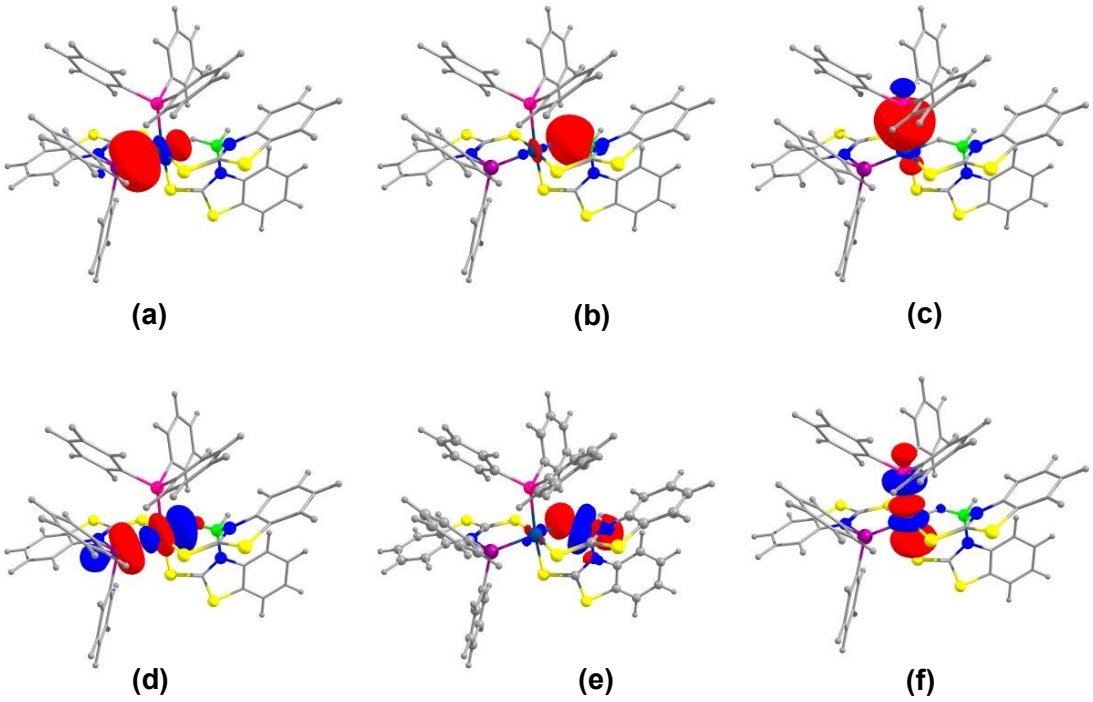


Figure S39. Bonding and antibonding interactions between Ru-Si (a,d), Ru-H-B (b,e) and Ru-P (c,f) in **5a** obtained from NBO analysis.

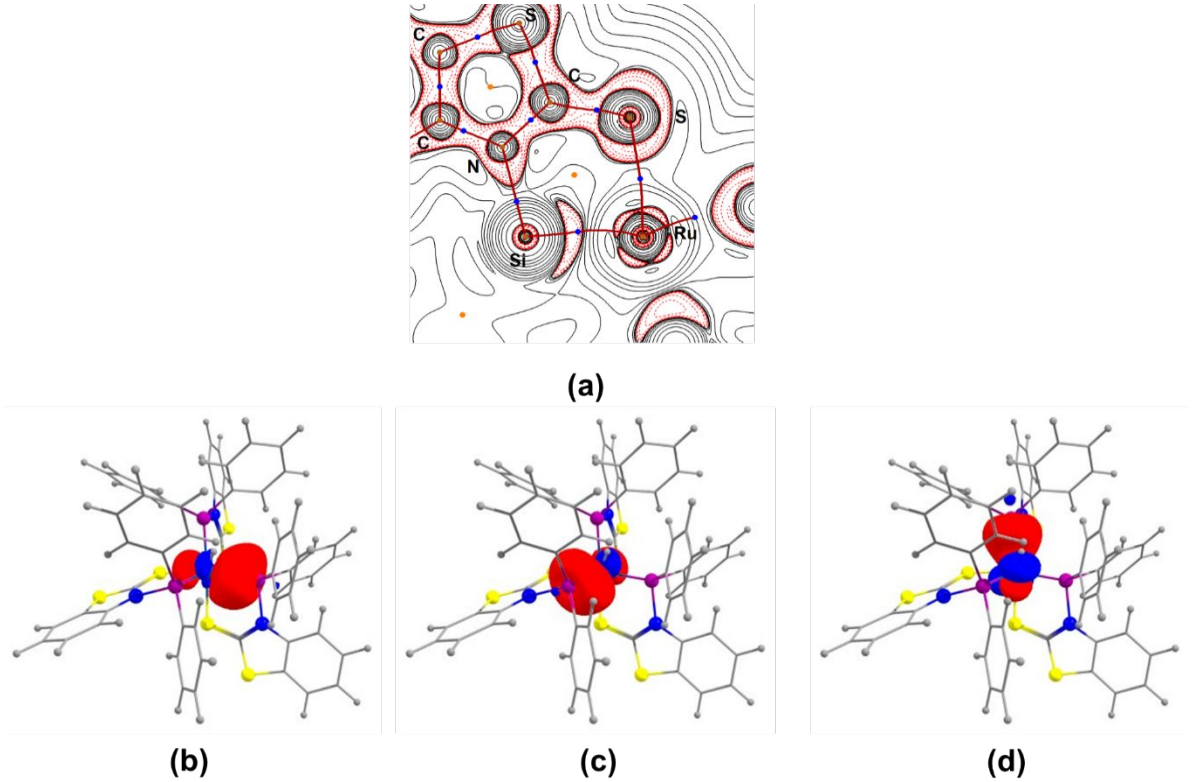
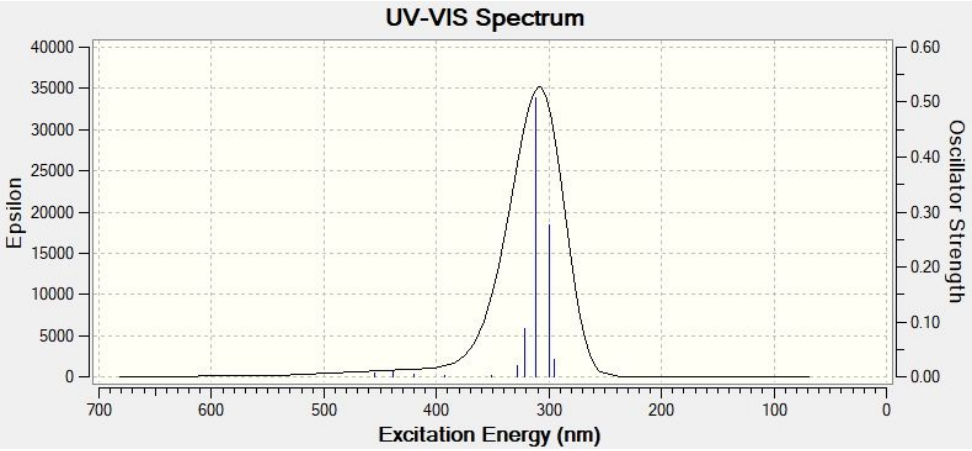


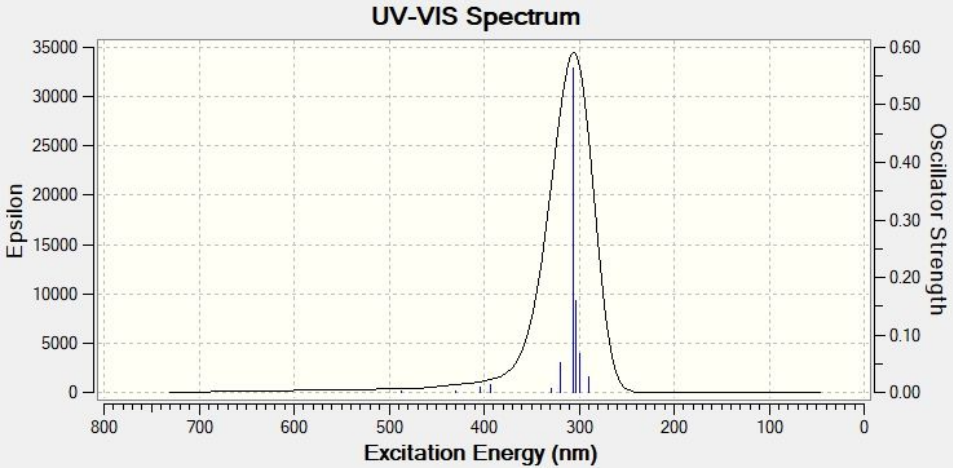
Figure S40. Contour-line map of the Laplacian of the electron density in the S-Ru-Si plane of **6** and (b-d) Bonding interactions of Ru-Si in **6** obtained from NBO analysis.

II.2 TD-DFT results



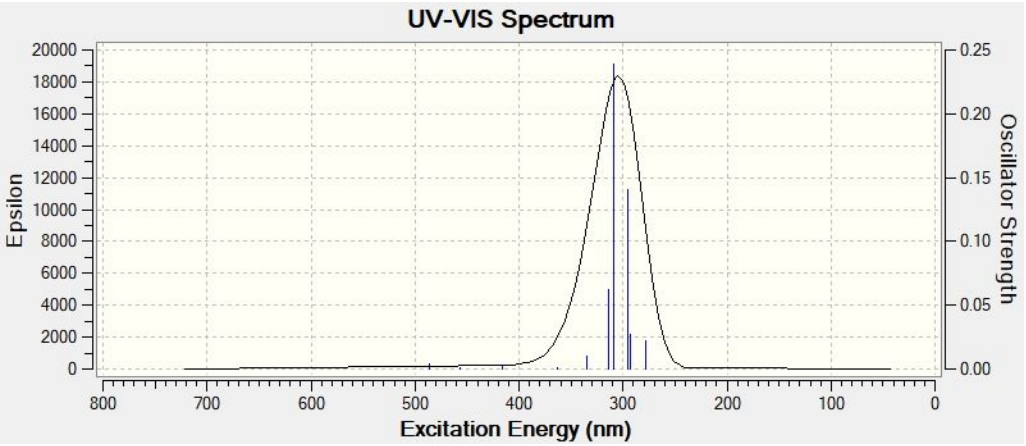
FigureS41. Calculated UV-Vis absorption spectra of **2** at CAM-B3LYP/LANL2DZ/6-31G(d,p) level.

Excited State 1: Singlet-A 2.7246 eV 455.06 nm f=0.0074 <S**2>=0.000
Excited State 2: Singlet-A 2.8251 eV 438.87 nm f=0.0102 <S**2>=0.000
Excited State 3: Singlet-A 2.9520 eV 420.00 nm f=0.0038 <S**2>=0.000
Excited State 4: Singlet-A 3.1537 eV 393.14 nm f=0.0033 <S**2>=0.000
Excited State 5: Singlet-A 3.5303 eV 351.20 nm f=0.0026 <S**2>=0.000
Excited State 6: Singlet-A 3.7846 eV 327.60 nm f=0.0208 <S**2>=0.000
Excited State 7: Singlet-A 3.8570 eV 321.45 nm f=0.0876 <S**2>=0.000
Excited State 8: Singlet-A 3.9762 eV 311.82 nm f=0.5082 <S**2>=0.000
Excited State 9: Singlet-A 4.1444 eV 299.16 nm f=0.2772 <S**2>=0.000
Excited State 10: Singlet-A 4.2003 eV 295.18 nm f=0.0316 <S**2>=0.000



FigureS42. Calculated UV-Vis absorption spectra of **3** at CAM-B3LYP/LANL2DZ/6-31G(d,p) level.

Excited State 1:	Singlet-A	2.5446 eV	487.25 nm	f=0.0025	<S**2>=0.000
Excited State 2:	Singlet-A	2.8804 eV	430.44 nm	f=0.0029	<S**2>=0.000
Excited State 3:	Singlet-A	3.0678 eV	404.14 nm	f=0.0081	<S**2>=0.000
Excited State 4:	Singlet-A	3.1531 eV	393.21 nm	f=0.0141	<S**2>=0.000
Excited State 5:	Singlet-A	3.7654 eV	329.27 nm	f=0.0064	<S**2>=0.000
Excited State 6:	Singlet-A	3.8847 eV	319.16 nm	f=0.0514	<S**2>=0.000
Excited State 7:	Singlet-A	4.0475 eV	306.33 nm	f=0.5633	<S**2>=0.000
Excited State 8:	Singlet-A	4.0810 eV	303.81 nm	f=0.1593	<S**2>=0.000
Excited State 9:	Singlet-A	4.1423 eV	299.32 nm	f=0.0671	<S**2>=0.000
Excited State 10:	Singlet-A	4.2872 eV	289.20 nm	f=0.0277	<S**2>=0.000



FigureS43. Calculated UV-Vis absorption spectra of **4** at CAM-B3LYP/ LANL2DZ/6-31G(d,p) level.

Excited State 1:	Singlet-A	2.5509 eV	486.04 nm	f=0.0041	<S**2>=0.000
Excited State 2:	Singlet-A	2.7129 eV	457.02 nm	f=0.0008	<S**2>=0.000
Excited State 3:	Singlet-A	2.9834 eV	415.58 nm	f=0.0021	<S**2>=0.000
Excited State 4:	Singlet-A	3.4191 eV	362.62 nm	f=0.0011	<S**2>=0.000
Excited State 5:	Singlet-A	3.7021 eV	334.90 nm	f=0.0105	<S**2>=0.000
Excited State 6:	Singlet-A	3.9545 eV	313.53 nm	f=0.0619	<S**2>=0.000
Excited State 7:	Singlet-A	4.0098 eV	309.20 nm	f=0.2393	<S**2>=0.000
Excited State 8:	Singlet-A	4.1981 eV	295.33 nm	f=0.1405	<S**2>=0.000
Excited State 9:	Singlet-A	4.2412 eV	292.33 nm	f=0.0274	<S**2>=0.000
Excited State 10:	Singlet-A	4.4485 eV	278.71 nm	f=0.0221	<S**2>=0.000

Table S5. Electronic transition configurations for **2-4** by TD-DFT calculations.

Compounds	Excited state	Major transition configurations
2	1	HOMO-1->LUMO (21%), HOMO-1->LUMO+3 (13%), HOMO->LUMO (11%)
	2	HOMO->LUMO (18%), HOMO->LUMO+7 (10%)
	3	HOMO->LUMO (17%), HOMO->LUMO+3 (31%)
	4	HOMO-3->LUMO (17%), HOMO-3->LUMO+3 (32%)
	5	HOMO-1->LUMO+3 (14%), HOMO-1->LUMO+7 (13%), HOMO-1->LUMO+9 (11%)
	6	HOMO-3->LUMO+7 (11%), HOMO-3->LUMO (9%)
	7	HOMO->LUMO (14%), HOMO->LUMO+1 (24%), HOMO->LUMO+3 (11%)
	8	HOMO-2->LUMO (13%), HOMO-1->LUMO+2 (10%), HOMO->LUMO (11%), HOMO->LUMO+1 (37%)
	9	HOMO-1->LUMO+2 (64%), HOMO-2->LUMO (8%)
	10	HOMO-1->LUMO (24%), HOMO->LUMO (15%)
3	1	HOMO->LUMO (35%), HOMO->LUMO+1 (12%), HOMO->LUMO+3 (25%)
	2	HOMO-2->LUMO (11%), HOMO->LUMO+5 (12%)
	3	HOMO-5->LUMO (12%), HOMO-5->LUMO+3 (11%)
	4	HOMO-7->LUMO (11%), HOMO-2->LUMO (12%)
	5	HOMO-2->LUMO+1 (19%), HOMO-2->LUMO+5 (10%)
	6	HOMO-1->LUMO (17%), HOMO->L+1 (18%), HOMO->LUMO+2 (25%)
	7	HOMO->LUMO+1 (34%), HOMO->LUMO+2 (15%), HOMO->LUMO+3 (14%)
	8	HOMO-1->LUMO (22%), HOMO->LUMO+2 (20%)
	9	HOMO->LUMO (20%), HOMO->LUMO+2 (16%), HOMO->LUMO+3 (13%)
	10	HOMO-1->LUMO (15%), HOMO->LUMO (12%)
4	1	HOMO-1->LUMO (12%), HOMO->LUMO (26%), HOMO->LUMO+1 (22%)
	2	HOMO-5->LUMO (11%), HOMO-5->LUMO+1 (11%), HOMO-1->LUMO (23%), HOMO-1->LUMO+1 (18%)
	3	HOMO-2->LUMO (10%)
	4	HOMO-2->LUMO (13%), HOMO-2->L+1 (10%)
	5	HOMO-7->LUMO+7 (2%), HOMO-5->LUMO+4 (4%), HOMO-5->LUMO+7 (5%)
	6	HOMO-7->LUMO+7 (2%), HOMO-2->LUMO+4 (6%), HOMO-2->LUMO+7 (7%)
	7	HOMO-1->LUMO (25%), HOMO-1->LUMO+1 (13%), HOMO->LUMO (11%)
	8	HOMO->LUMO+2 (59%)
	9	HOMO-5->LUMO+1 (13%), HOMO-1->LUMO (15%), HOMO->LUMO (32%), HOMO->LUMO+2 (16%)
	10	HOMO-5->LUMO (21%), HOMO-1->LUMO+1 (17%), HOMO->LUMO+1 (27%)

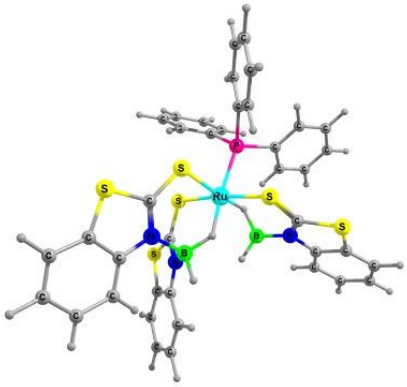


Figure S44. Optimized geometry of **2**.

Cartesian coordinates for the calculated structure of **2** (in Å).

Ru	0.134874000	-0.263191000	-0.240161000	H	3.653370000	-3.944433000	0.893119000
C	1.758560000	2.133547000	-1.747342000	C	4.024990000	-4.839824000	-1.023926000
C	2.742610000	4.419539000	-1.720805000	H	4.575377000	-5.676363000	-0.601961000
C	3.341274000	5.669584000	-1.853240000	C	3.838255000	-4.746674000	-2.402594000
H	3.891670000	5.929971000	-2.751947000	H	4.240910000	-5.512147000	-3.060436000
C	3.211842000	6.576375000	-0.804826000	C	3.132639000	-3.668972000	-2.932171000
H	3.669417000	7.557822000	-0.886275000	H	2.981078000	-3.586904000	-4.004732000
C	2.492884000	6.234124000	0.346294000	C	2.611176000	-2.688049000	-2.088798000
H	2.394866000	6.956456000	1.151465000	H	2.072777000	-1.847221000	-2.510970000
C	1.895108000	4.985478000	0.479995000	C	3.636731000	-0.347443000	0.707889000
H	1.332963000	4.718942000	1.366949000	C	4.826592000	-0.555373000	0.005814000
C	2.028806000	4.064031000	-0.562727000	H	4.900146000	-1.364579000	-0.713223000
C	-2.346184000	-1.917221000	-1.460553000	C	5.923597000	0.278479000	0.223027000
C	-4.409599000	-0.922846000	-1.452530000	H	6.841716000	0.111250000	-0.333558000
C	-5.393534000	0.056977000	-1.300333000	C	5.844352000	1.317329000	1.147318000
H	-5.144151000	1.041050000	-0.927476000	H	6.700544000	1.964786000	1.315711000
C	-6.709069000	-0.250395000	-1.633315000	C	4.658756000	1.527937000	1.850500000
H	-7.472969000	0.512040000	-1.513583000	H	4.584171000	2.341049000	2.566990000
C	-7.061388000	-1.514760000	-2.114190000	C	3.556882000	0.705084000	1.627666000
H	-8.094845000	-1.732926000	-2.365640000	H	2.631442000	0.891362000	2.163365000
C	-6.090551000	-2.498577000	-2.274802000	C	1.966879000	-2.401612000	2.042448000
H	-6.348731000	-3.483003000	-2.652303000	C	2.795430000	-2.192197000	3.146351000
C	-4.774919000	-2.188606000	-1.942442000	H	3.573189000	-1.436275000	3.109914000
C	-2.343452000	0.219369000	1.793878000	C	2.631449000	-2.959646000	4.300603000
C	-3.717804000	1.925395000	1.116623000	H	3.280051000	-2.787114000	5.155234000
C	-4.242486000	2.941807000	0.311381000	C	1.647299000	-3.943329000	4.355697000
H	-3.920789000	3.042672000	-0.718664000	H	1.522071000	-4.540103000	5.255053000
C	-5.159591000	3.831235000	0.863587000	C	0.822195000	-4.159061000	3.251944000
H	-5.565116000	4.623580000	0.241458000	H	0.050472000	-4.922896000	3.286823000
C	-5.554999000	3.730257000	2.201126000	C	0.977690000	-3.391074000	2.101235000
H	-6.272436000	4.434888000	2.610458000	H	0.327285000	-3.559766000	1.246359000
C	-5.016142000	2.742321000	3.020382000	N	1.496094000	2.775248000	-0.606151000
H	-5.296745000	2.670590000	4.066535000	N	-2.796782000	0.938434000	0.747847000
C	-4.092641000	1.857477000	2.470600000	N	-3.039226000	-0.797100000	-1.174196000
C	2.790046000	-2.779259000	-0.705988000	P	2.130531000	-1.433559000	0.437348000
C	3.504737000	-3.861894000	-0.178981000	S	1.252720000	0.573297000	-2.188869000

S	2.722319000	3.092987000	-2.858963000
S	-1.059580000	-0.871552000	1.774200000
S	-3.194299000	0.594262000	3.280235000
S	-0.682443000	-2.185111000	-1.361368000
S	-3.367689000	-3.213597000	-2.053931000
B	0.584519000	2.209399000	0.538646000
B	-2.413710000	0.573606000	-0.719443000
H	1.011959000	2.581489000	1.608669000
H	-0.559813000	2.534046000	0.373025000
H	-2.822284000	1.430555000	-1.456962000
H	-1.188079000	0.656641000	-0.955610000
H	0.856463000	0.965450000	0.730915000

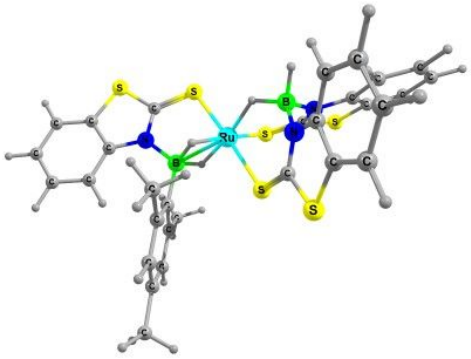


Figure S45. Optimized geometry of **3**.

Cartesian coordinates for the calculated structure of **3** (in Å).

B	2.247845000	-0.574345000	-0.861669000
B	-2.193790000	-0.153888000	0.100172000
C	-5.162719000	-1.957825000	-1.577842000
C	-6.513378000	-1.976559000	-1.914560000
H	-6.934534000	-2.812309000	-2.464439000
C	-7.303666000	-0.898961000	-1.529649000
H	-8.360123000	-0.889852000	-1.780026000
C	-6.739592000	0.168639000	-0.825828000
H	-7.362598000	1.007855000	-0.531420000
C	-5.389648000	0.187736000	-0.488893000
H	-4.969821000	1.022468000	0.054882000
C	-4.583630000	-0.892014000	-0.864795000
C	-2.734568000	-2.235535000	-1.149797000
C	-2.740123000	1.167769000	0.794080000
C	-3.261381000	1.130649000	2.109044000
C	-3.703155000	2.306573000	2.720451000
H	-4.107005000	2.254927000	3.730363000
C	-3.645447000	3.541295000	2.072651000
C	-3.139145000	3.570187000	0.773022000
H	-3.097210000	4.519346000	0.241061000
C	-2.685481000	2.415050000	0.130295000
C	-3.369075000	-0.163722000	2.878391000
H	-3.954661000	-0.027391000	3.791902000
H	-2.382105000	-0.540566000	3.172077000
H	-3.851481000	-0.953139000	2.291453000
C	-4.095237000	4.802257000	2.761708000
H	-3.285882000	5.229423000	3.366827000
H	-4.937165000	4.614148000	3.435336000
H	-4.400513000	5.566772000	2.040874000
C	-2.163105000	2.536086000	-1.280378000
H	-1.089059000	2.322503000	-1.326715000
H	-2.319212000	3.546207000	-1.669578000
H	-2.657481000	1.837486000	-1.964743000
C	1.749608000	1.625599000	0.313361000
C	3.156423000	3.132909000	-1.084434000
C	3.863472000	4.114560000	-1.772993000
H	3.970262000	5.112606000	-1.359749000
C	4.414489000	3.789561000	-3.009315000
H	4.965150000	4.541441000	-3.566155000
C	4.244441000	2.508248000	-3.542950000
H	4.656607000	2.273558000	-4.519835000
C	3.544021000	1.523976000	-2.851383000
H	3.397861000	0.539788000	-3.281449000
C	3.010375000	1.830426000	-1.595045000
C	2.613426000	-2.037634000	1.250635000
C	4.509926000	-1.274823000	0.212487000
C	5.327120000	-0.625002000	-0.715377000
H	4.899277000	-0.036980000	-1.516254000
C	6.708543000	-0.742763000	-0.596050000
H	7.343233000	-0.237015000	-1.317546000
C	7.288503000	-1.494043000	0.430180000
H	8.368960000	-1.569735000	0.505328000
C	6.485585000	-2.149927000	1.358382000
H	6.922364000	-2.741581000	2.156760000
C	5.104100000	-2.032879000	1.236020000
N	-3.205098000	-1.074454000	-0.628703000

N	2.282973000	0.983203000	-0.749562000
N	3.106582000	-1.276288000	0.250872000
Ru	-0.207764000	-0.935991000	0.158589000
S	-1.135389000	-2.743299000	-1.047600000
S	-3.965836000	-3.177735000	-1.950152000
S	0.625993000	0.980439000	1.383198000
S	2.293610000	3.288401000	0.429803000
S	1.000232000	-2.380696000	1.595583000
S	3.871258000	-2.754622000	2.238806000
H	1.099381000	-1.083229000	-0.986507000
H	2.696034000	-0.892011000	-1.931283000
H	-1.205628000	0.126384000	-0.797820000
H	-1.606470000	-0.952359000	1.105236000

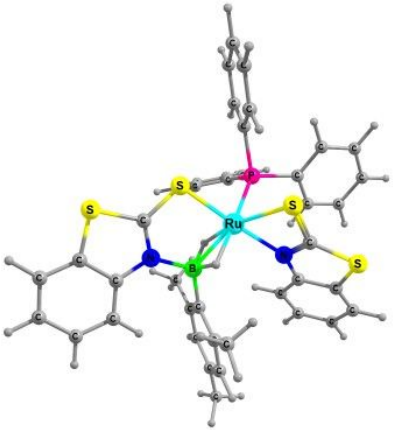


Figure S46. Optimized geometry of **4**.

Cartesian coordinates for the calculated structure of **4** (in Å).

B	-1.929675000	-0.176494000	-0.366046000
C	1.363227000	1.774682000	-2.043449000
C	1.195002000	4.042248000	-1.096308000
C	1.192930000	5.366607000	-0.664464000
H	1.682438000	6.142385000	-1.245383000
C	0.550628000	5.670294000	0.533444000
H	0.537308000	6.697250000	0.886810000
C	-0.078071000	4.666234000	1.281740000
H	-0.578262000	4.923265000	2.210931000
C	-0.080544000	3.344324000	0.852750000
H	-0.582433000	2.565715000	1.415791000
C	0.560295000	3.023977000	-0.348171000
C	-2.755104000	1.083471000	0.151650000
C	-3.216737000	2.081502000	-0.738953000
C	-3.904853000	3.193843000	-0.245820000
H	-4.256085000	3.947461000	-0.948731000
C	-4.154751000	3.366571000	1.116257000
C	-3.706607000	2.374807000	1.989513000
H	-3.903688000	2.476725000	3.055729000
C	-3.018002000	1.247080000	1.533083000
C	-3.008614000	1.972291000	-2.230116000
H	-3.518097000	2.785472000	-2.754799000
H	-3.394025000	1.027432000	-2.629216000
H	-1.946409000	2.017855000	-2.492675000
C	-4.868099000	4.591135000	1.624862000
H	-5.667035000	4.902436000	0.944293000
H	-4.177384000	5.438241000	1.718783000
H	-5.310070000	4.418277000	2.610678000
C	-2.588951000	0.208932000	2.541363000
H	-2.945946000	0.464284000	3.543183000
H	-1.498119000	0.112223000	2.591168000
H	-2.982785000	-0.783467000	2.294092000
C	-4.064222000	-1.813942000	-0.351724000
C	-5.104677000	-0.929537000	-0.046432000
H	-4.904358000	0.121841000	0.104927000
C	-6.401570000	-1.423668000	0.054515000
H	-7.205667000	-0.733587000	0.291980000
C	-6.687375000	-2.776925000	-0.145911000
H	-7.708026000	-3.137526000	-0.061408000
C	-5.665886000	-3.665899000	-0.462686000
H	-5.871353000	-4.718265000	-0.631938000
C	-4.368292000	-3.171921000	-0.564164000
C	-1.969303000	-2.617262000	-0.856388000
C	1.892494000	-1.212281000	2.214674000
C	0.766073000	-1.961647000	2.570253000
H	0.080133000	-2.293959000	1.796221000
C	0.525493000	-2.279804000	3.905203000
H	-0.351217000	-2.864940000	4.169016000
C	1.403106000	-1.845254000	4.898237000
H	1.211571000	-2.087673000	5.939993000
C	2.526611000	-1.099087000	4.549010000
H	3.216031000	-0.758023000	5.316653000

C	2.775551000	-0.787437000	3.211725000
H	3.656228000	-0.210389000	2.947578000
C	3.089832000	-2.435679000	-0.152232000
C	3.742515000	-3.256845000	0.772689000
H	3.719928000	-3.010692000	1.829713000
C	4.417914000	-4.398338000	0.344060000
H	4.917479000	-5.031729000	1.072137000
C	4.451056000	-4.727000000	-1.010221000
H	4.976388000	-5.618357000	-1.342310000
C	3.804715000	-3.910099000	-1.935834000
H	3.822709000	-4.159473000	-2.993079000
C	3.124357000	-2.770373000	-1.509575000
H	2.622968000	-2.134284000	-2.231626000
C	3.554728000	0.413388000	0.404332000
C	4.789110000	0.181002000	-0.206230000
H	4.988763000	-0.773119000	-0.683060000
C	5.768417000	1.174354000	-0.206714000
H	6.724568000	0.983633000	-0.686350000
C	5.523230000	2.402519000	0.402780000
H	6.287296000	3.175083000	0.400130000
C	4.291173000	2.639019000	1.012307000
H	4.086261000	3.596290000	1.482967000
C	3.309504000	1.650938000	1.009832000
N	0.677141000	1.769010000	-0.912942000
N	-2.692694000	-1.526852000	-0.504491000
P	2.190271000	-0.873521000	0.389141000
Ru	0.165176000	-0.325137000	-0.811777000
S	1.552601000	0.258554000	-2.808725000
S	1.936574000	3.363337000	-2.532428000
S	-2.926283000	-4.073081000	-0.972735000
S	-0.315382000	-2.594254000	-1.166714000
H	-0.888140000	-0.367226000	0.539199000
H	-1.373355000	0.045570000	-1.570017000
H	2.349878000	1.847267000	1.478290000

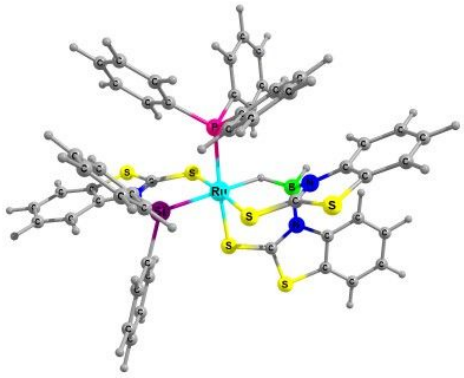


Figure S47. Optimized geometry of **5a**.

Cartesian coordinates for the calculated structure of **5a** (in Å).

H	-1.605521000	0.372583000	-1.166040000
H	-3.406981000	0.282308000	-1.828953000
Ru	-0.026768000	0.482110000	-0.253448000
C	-0.588737000	-2.631299000	-2.156652000
C	-1.237668000	-1.799523000	-3.069164000
H	-1.354988000	-0.745442000	-2.850644000
C	-1.732996000	-2.314920000	-4.268877000
H	-2.228511000	-1.650593000	-4.971576000
C	-1.585933000	-3.666559000	-4.565895000
H	-1.970020000	-4.066513000	-5.500526000
C	-0.934437000	-4.504634000	-3.660151000
H	-0.808627000	-5.560481000	-3.884572000
C	-0.434172000	-3.989316000	-2.467761000
H	0.085247000	-4.646432000	-1.776224000
C	1.766157000	-2.897423000	-0.612520000
C	2.100508000	-3.957938000	0.230918000
H	1.427729000	-4.259459000	1.026172000
C	3.301607000	-4.647277000	0.053615000
H	3.545727000	-5.472359000	0.717402000
C	4.178471000	-4.285227000	-0.965092000
H	5.111080000	-4.825797000	-1.102925000
C	3.846126000	-3.229548000	-1.814469000
H	4.515621000	-2.944674000	-2.621549000
C	2.646781000	-2.543576000	-1.641928000
H	2.379402000	-1.743452000	-2.324774000
C	2.752221000	0.921639000	-1.992254000
C	5.213711000	1.317193000	-2.073242000
C	6.566394000	1.568679000	-2.286254000
H	6.961605000	1.669146000	-3.292298000
C	7.394224000	1.697164000	-1.174577000

H	8.452486000	1.895717000	-1.314926000
C	6.869902000	1.584155000	0.117633000
H	7.525280000	1.702285000	0.975255000
C	5.519167000	1.330023000	0.330929000
H	5.117685000	1.257712000	1.334407000
C	4.681701000	1.182062000	-0.778560000
C	2.878521000	-0.523384000	1.902600000
C	3.987482000	-1.322080000	1.589844000
H	4.447900000	-1.250713000	0.609311000
C	4.513456000	-2.226405000	2.512735000
H	5.375216000	-2.829830000	2.240168000
C	3.935404000	-2.362769000	3.772763000
H	4.348748000	-3.063588000	4.493456000
C	2.815054000	-1.599285000	4.097670000
H	2.346391000	-1.703381000	5.073181000
C	2.292730000	-0.696886000	3.170988000
H	1.406784000	-0.126567000	3.443488000
C	2.565291000	2.483713000	1.548813000
C	2.698944000	3.624883000	0.740068000
H	2.555795000	3.546717000	-0.335059000
C	3.014973000	4.868738000	1.281818000
H	3.114767000	5.732035000	0.628879000
C	3.199163000	5.005510000	2.656712000
H	3.442947000	5.975069000	3.083332000
C	3.070985000	3.888213000	3.478608000
H	3.218761000	3.980981000	4.551789000
C	2.762036000	2.643932000	2.928300000
H	2.692987000	1.785421000	3.589976000
C	-0.848877000	-2.968978000	0.745083000
C	-0.422819000	-2.951486000	2.079544000
H	0.451359000	-2.373167000	2.362423000
C	-1.110642000	-3.678536000	3.048720000
H	-0.759765000	-3.665231000	4.076979000
C	-2.246667000	-4.410255000	2.703523000
H	-2.784168000	-4.974274000	3.461084000
C	-2.693668000	-4.405090000	1.384748000
H	-3.585114000	-4.960571000	1.106826000
C	-1.997569000	-3.689979000	0.408838000
H	-2.352298000	-3.702097000	-0.616229000
C	-2.686656000	-0.095240000	1.587480000
C	-4.948456000	-1.124070000	1.752182000
C	-6.156866000	-1.764595000	2.011105000
H	-6.465984000	-1.970692000	3.031112000
C	-6.948016000	-2.150098000	0.932262000
H	-7.892337000	-2.655062000	1.111535000
C	-6.519157000	-1.910416000	-0.376792000
H	-7.128179000	-2.243880000	-1.211930000
C	-5.315447000	-1.260577000	-0.635227000
H	-4.975519000	-1.105548000	-1.652875000
C	-4.529659000	-0.834522000	0.441004000
C	-2.012867000	3.073608000	-0.428186000
C	-4.223244000	4.186465000	-0.742574000
C	-5.368534000	4.960558000	-0.904601000
H	-5.325958000	6.039806000	-0.796097000
C	-6.564025000	4.317493000	-1.211285000
H	-7.470830000	4.900359000	-1.341323000
C	-6.597539000	2.927554000	-1.351695000
H	-7.534207000	2.432879000	-1.591078000
C	-5.451171000	2.155543000	-1.188014000
H	-5.500517000	1.080861000	-1.294764000
C	-4.244840000	2.787416000	-0.877243000
N	-3.297679000	-0.171474000	0.382834000
N	-2.993320000	2.179380000	-0.683369000
N	3.306416000	0.924326000	-0.766699000
B	-2.787846000	0.633106000	-0.859745000
Si	2.117894000	0.793883000	0.741137000
P	0.116151000	-1.968528000	-0.525001000
S	-0.362635000	2.832668000	-0.195777000
S	-2.607030000	4.726295000	-0.370971000
S	-1.095103000	0.363245000	1.876543000
S	-3.723146000	-0.632494000	2.897259000
S	1.111863000	0.737873000	-2.356618000
S	3.939815000	1.153638000	-3.263887000

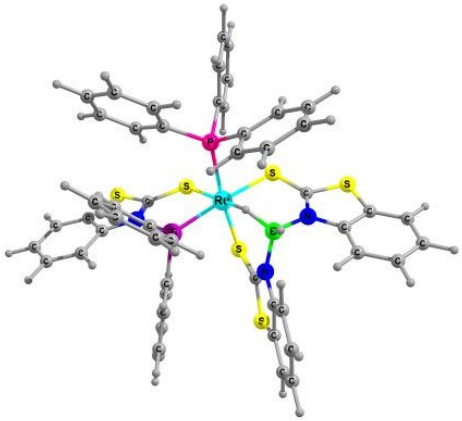


Figure S48. Optimized geometry of **5b**.

Cartesian coordinates for the calculated structure of **5b** (in Å).

Ru	0.065571000	0.439824000	-0.926585000	H	-0.005349000	1.237422000	2.968478000
P	-0.688317000	2.389814000	0.341424000	S	-1.715832000	0.663896000	-2.496937000
C	-2.335152000	2.484482000	1.268598000	S	-4.522629000	-0.347728000	-2.793217000
C	-3.493291000	2.256476000	0.516831000	C	-2.999832000	-0.284146000	-1.923604000
H	-3.408790000	1.982203000	-0.530253000	N	-3.001113000	-1.055342000	-0.824872000
C	-4.752026000	2.405906000	1.093040000	C	-4.182564000	-1.786153000	-0.662023000
H	-5.641367000	2.230900000	0.493720000	C	-4.456984000	-2.730539000	0.331595000
C	-4.869219000	2.786710000	2.430084000	H	-3.710382000	-2.974682000	1.077482000
H	-5.850920000	2.906602000	2.880403000	C	-5.699160000	-3.356030000	0.331940000
C	-3.720076000	3.023201000	3.179696000	H	-5.918084000	-4.091901000	1.099807000
H	-3.799760000	3.328227000	4.219749000	C	-6.663303000	-3.061386000	-0.638291000
C	-2.457657000	2.877429000	2.602309000	H	-7.625911000	-3.563312000	-0.616037000
H	-1.574309000	3.077694000	3.199411000	C	-6.394771000	-2.135782000	-1.642572000
C	-0.898070000	4.029353000	-0.585589000	H	-7.131225000	-1.911140000	-2.407770000
C	-1.092819000	5.205843000	0.149404000	C	-5.150127000	-1.511615000	-1.644981000
H	-1.085439000	5.174599000	1.235246000	S	1.587860000	1.976062000	-2.095321000
C	-1.300061000	6.419614000	-0.499759000	S	4.529011000	2.223511000	-2.189367000
H	-1.443562000	7.324740000	0.084281000	C	3.085532000	1.490238000	-1.511376000
C	-1.331218000	6.470571000	-1.893693000	N	3.366219000	0.608452000	-0.525990000
H	-1.496484000	7.416983000	-2.401518000	C	4.740717000	0.534375000	-0.241672000
C	-1.156085000	5.302329000	-2.629484000	C	5.359560000	-0.230643000	0.749807000
H	-1.185703000	5.328601000	-3.715153000	H	4.776535000	-0.860690000	1.406475000
C	-0.939140000	4.086745000	-1.978398000	C	6.743580000	-0.175832000	0.884185000
H	-0.816920000	3.183286000	-2.563317000	H	7.220104000	-0.774454000	1.654876000
C	0.604862000	2.820625000	1.632606000	C	7.524122000	0.628221000	0.049227000
C	1.552265000	3.823165000	1.403237000	H	8.603006000	0.653029000	0.169143000
H	1.508738000	4.413518000	0.493782000	C	6.921099000	1.402388000	-0.937252000
C	2.559376000	4.065448000	2.337756000	H	7.512454000	2.037882000	-1.589107000
H	3.290483000	4.846089000	2.145738000	C	5.536408000	1.347790000	-1.067740000
C	2.627517000	3.314996000	3.509428000	C	1.983841000	-2.151207000	-1.308031000
H	3.408413000	3.511131000	4.239146000	S	0.987677000	-1.286829000	-2.345813000
C	1.694194000	2.304073000	3.734644000	S	2.582687000	-3.753122000	-1.681194000
H	1.743761000	1.705335000	4.640256000	N	2.351891000	-1.735086000	-0.075419000
C	0.696336000	2.048189000	2.796375000	C	2.975235000	-2.737911000	0.674880000

C	3.316178000	-2.697599000	2.031044000
H	3.090212000	-1.818136000	2.623888000
C	3.933942000	-3.805428000	2.604615000
H	4.197734000	-3.776638000	3.657793000
C	4.210017000	-4.951537000	1.852828000
H	4.693725000	-5.804206000	2.319486000
C	3.848715000	-5.014600000	0.509803000
H	4.035647000	-5.908945000	-0.076242000
C	3.223552000	-3.910208000	-0.062024000
B	2.313438000	-0.217151000	0.301515000
H	2.602416000	-0.111922000	1.465043000
H	1.154692000	0.301542000	0.399181000
Si	-1.331098000	-1.197715000	0.138912000
C	-1.107583000	-3.096964000	-0.127444000
C	-0.794305000	-3.990114000	0.907554000
C	-1.296493000	-3.638412000	-1.411186000
C	-0.670303000	-5.361376000	0.674909000
H	-0.663824000	-3.621124000	1.920849000
C	-1.184723000	-5.006366000	-1.648867000
H	-1.536252000	-2.981367000	-2.243203000
C	-0.868110000	-5.874733000	-0.604058000
H	-0.428193000	-6.027628000	1.499330000
H	-1.344081000	-5.394641000	-2.651684000
H	-0.779606000	-6.942696000	-0.786760000
C	-1.770243000	-1.043044000	1.998791000
C	-0.738341000	-1.300532000	2.920884000
C	-3.022775000	-0.688268000	2.520066000
C	-0.955403000	-1.243556000	4.297490000
H	0.258776000	-1.547017000	2.560017000
C	-3.245036000	-0.623187000	3.896127000
H	-3.841714000	-0.445751000	1.849928000
C	-2.215848000	-0.908202000	4.790596000
H	-0.140401000	-1.460753000	4.983816000
H	-4.226931000	-0.341768000	4.267201000
H	-2.391004000	-0.862277000	5.862288000

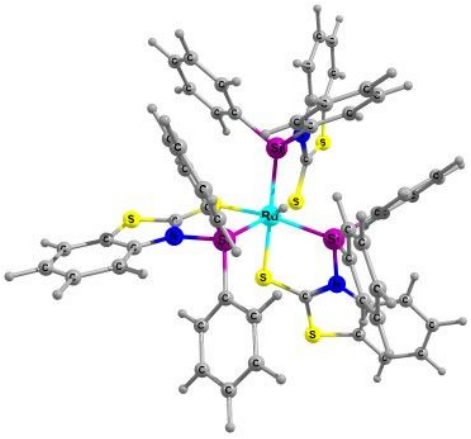


Figure S49. Optimized geometry of **6**.

Cartesian coordinates for the calculated structure of **6** (in Å).

Ru	-0.085444000	-0.058334000	-0.750308000
S	-0.296645000	-2.058460000	-2.218154000
S	1.375474000	-4.459188000	-2.836321000
S	-1.580900000	0.949527000	-2.458062000
S	1.645948000	0.592982000	-2.389755000
S	3.495432000	2.911108000	-2.778714000
N	1.926190000	-2.855428000	-0.883874000
N	1.802657000	2.809486000	-0.829666000
Si	-2.169639000	-0.775643000	0.263867000
Si	1.664357000	-1.370020000	0.302817000
Si	0.319771000	2.125815000	0.201112000
C	1.302870000	-2.246199000	1.970618000
C	1.362351000	-3.635184000	2.157199000
H	1.598464000	-4.288588000	1.323913000
C	1.107150000	-4.212148000	3.401807000
H	1.161693000	-5.292071000	3.514777000
C	0.779923000	-3.410937000	4.494153000
H	0.581679000	-3.859887000	5.464024000
C	0.704511000	-2.028477000	4.329416000
H	0.445367000	-1.388592000	5.168727000
C	0.958963000	-1.458016000	3.082257000
H	0.879310000	-0.378091000	2.981203000
C	3.467614000	-0.734854000	0.461658000
C	4.002085000	-0.408706000	1.717843000
H	3.389746000	-0.510724000	2.608802000
C	5.318624000	0.034226000	1.853178000

H	5.706327000	0.276761000	2.839448000
C	6.134800000	0.155808000	0.730874000
H	7.161756000	0.496846000	0.834020000
C	5.626666000	-0.173024000	-0.525537000
H	6.258049000	-0.094049000	-1.406760000
C	4.310385000	-0.612037000	-0.656501000
H	3.939424000	-0.871889000	-1.642974000
C	2.934448000	-3.830026000	-0.859770000
C	4.002374000	-3.925138000	0.038631000
H	4.127171000	-3.190149000	0.823947000
C	4.900534000	-4.978266000	-0.098877000
H	5.731750000	-5.053548000	0.595685000
C	4.753487000	-5.934464000	-1.109232000
H	5.468922000	-6.746580000	-1.196502000
C	3.691677000	-5.854328000	-2.004916000
H	3.564786000	-6.593338000	-2.789800000
C	2.791894000	-4.800353000	-1.868468000
C	1.026424000	-3.040406000	-1.868221000
C	2.229166000	2.097552000	-1.883868000
C	2.429355000	4.057544000	-0.712806000
C	2.174078000	5.044693000	0.243628000
H	1.414805000	4.893409000	1.000477000
C	2.908378000	6.224532000	0.196928000
H	2.712633000	6.995496000	0.936035000
C	3.886530000	6.436129000	-0.781166000
H	4.446896000	7.366082000	-0.795339000
C	4.143654000	5.464533000	-1.743119000
H	4.895177000	5.621596000	-2.510447000
C	3.406332000	4.284005000	-1.698582000
C	0.963220000	2.265084000	2.002215000
C	2.313383000	2.476773000	2.320436000
H	3.050846000	2.564467000	1.528656000
C	2.742115000	2.568844000	3.645349000
H	3.794855000	2.736336000	3.857808000
C	1.828689000	2.446046000	4.689920000
H	2.161332000	2.523683000	5.721775000
C	0.485412000	2.211744000	4.398909000
H	-0.238695000	2.100137000	5.201790000
C	0.062349000	2.114363000	3.073128000
H	-0.986192000	1.903066000	2.878842000
C	-0.850857000	3.632275000	-0.056639000
C	-1.459996000	4.315908000	1.006744000
H	-1.281822000	3.996748000	2.029083000
C	-2.282424000	5.421610000	0.784793000
H	-2.736580000	5.933611000	1.629779000
C	-2.509360000	5.876343000	-0.512150000
H	-3.146897000	6.739082000	-0.687354000
C	-1.903049000	5.221166000	-1.582922000
H	-2.063037000	5.572424000	-2.599023000
C	-1.087594000	4.114288000	-1.355043000
H	-0.625173000	3.624049000	-2.206518000
C	-3.151565000	0.488935000	-2.059383000
N	-3.519868000	-0.218049000	-0.978127000
S	-4.519419000	0.940617000	-3.059203000
C	-4.904290000	-0.400639000	-0.871842000
C	-5.621337000	0.165619000	-1.940528000
C	-7.009102000	0.080672000	-2.016087000
H	-7.548487000	0.521940000	-2.848310000
C	-7.683465000	-0.581578000	-0.994563000
H	-8.765875000	-0.659863000	-1.030334000
C	-6.977689000	-1.142902000	0.075268000
H	-7.518617000	-1.653830000	0.866025000
C	-5.591380000	-1.061676000	0.149983000
H	-5.052370000	-1.498666000	0.981521000
C	-2.899244000	0.086602000	1.816404000
C	-3.351084000	1.411920000	1.698157000
H	-3.276018000	1.928095000	0.744362000
C	-3.899405000	2.092798000	2.784260000
H	-4.244862000	3.115291000	2.657791000
C	-4.000152000	1.464079000	4.024789000
H	-4.426911000	1.991628000	4.873909000
C	-3.555001000	0.150950000	4.164598000
H	-3.634837000	-0.352131000	5.125108000
C	-3.016352000	-0.529217000	3.071464000
H	-2.699670000	-1.558443000	3.205826000
C	-3.230338000	-3.329278000	-0.612616000
H	-3.605100000	-2.785972000	-1.474995000
C	-3.470995000	-4.699341000	-0.530600000
H	-4.029462000	-5.195757000	-1.320022000
C	-2.995102000	-5.429989000	0.556764000
H	-3.184162000	-6.498242000	0.624338000
C	-2.264370000	-4.781154000	1.549163000
H	-1.870201000	-5.339472000	2.393946000
C	-2.023235000	-3.409980000	1.460943000
H	-1.418001000	-2.944302000	2.233042000
C	-2.516160000	-2.650057000	0.388445000
H	-0.137792000	-0.119438000	0.834233000