Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

A Combined Experimental and Theoretical Study of Bimetallic Bis- and Tris-homocubane Analogues

*Benson Joseph,[a] Rini Prakash,[a] Kriti Pathak,[a] Thierry Roisnel,[b] Samia Kahlal,[b] Jean-François Halet,[*b] and Sundargopal Ghosh[*a]*

[a]*Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036, India. E-mail: sghosh@iitm.ac.in.*

[b]*Univ Rennes, CNRS, Institut des Sciences Chimiques de Rennes, UMR 6226, F-35000 Rennes, France. E-mail: halet@univ-rennes1.fr.*

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I Supplementary Data

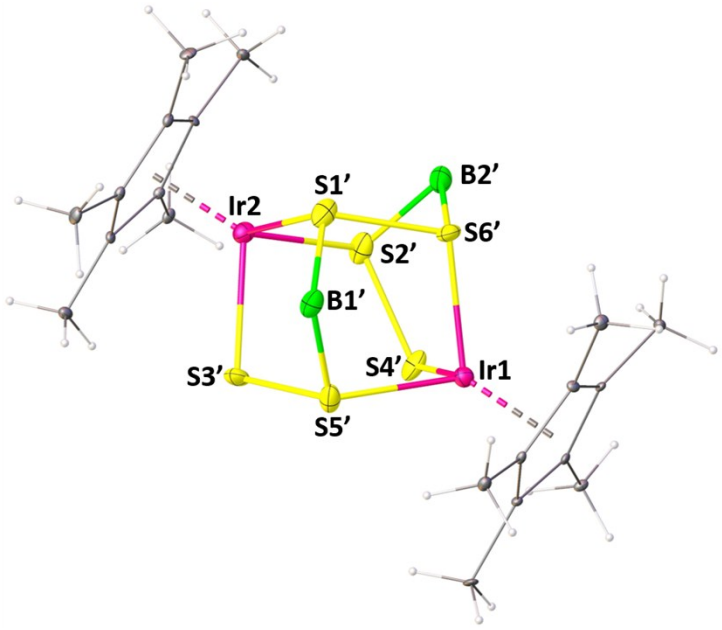


Figure S1. Molecular structure of compound **3**. Selected bond distances (Å) and angle (°): B1'-S5' 1.89(6), B2'-S6' 1.85(6), S1'-Ir2 2.354(9), S2'-Ir2 2.324(10), S1'-S6' 2.130(18), S2'-S4' 2.066(19); S5'-B1'-S1' 101(3).

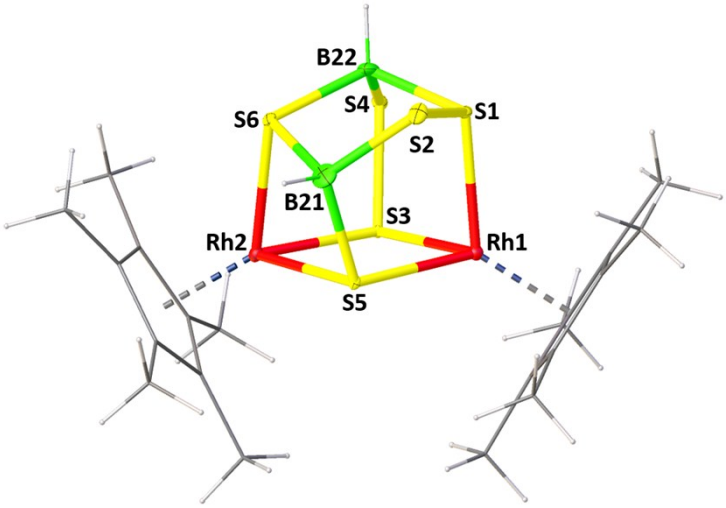


Figure S2. Molecular structure of compound **5**. Selected bond distances (Å) and angles (°): B22-S4 2.0965(18), B22-S1 1.938(7), S1-Rh1 2.3440(13), S6-Rh2 2.3688(14), S1-S2 2.080(2); B22-S1-S2 100.0(3), B21-S2-S1 92.6(2), B21-S6-Rh2 87.0(2).

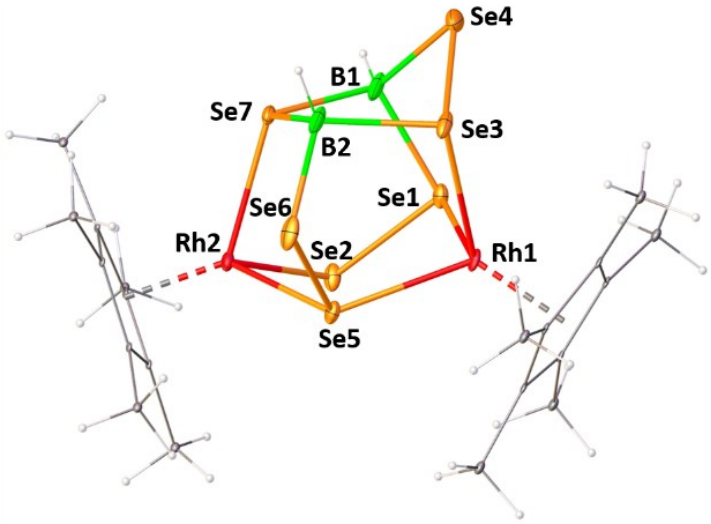


Figure S3. Molecular structure of compound **7**. Selected bond distances (Å) and angles (°): Rh1 -Se1 2.451(2), Rh2-Se7 2.472(2), Se1-B1 2.06(2), Se7 -B2 2.02(2), Se1-Se2 2.330(2), Se5-Se6 2.361(2); Se1-Rh1-Se5 92.46(7), Se5-Rh2-Se2 87.50(7).

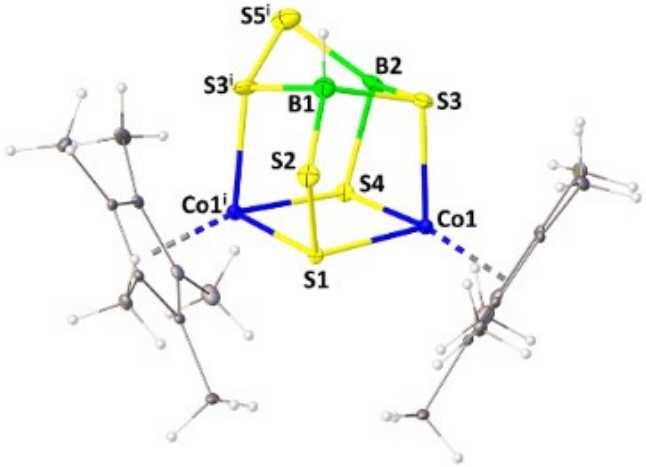


Figure S4. Molecular structure of compound **8**. Selected bond distances (Å) and angles (°): B1-S2 1.883(6), B2-S5 1.861(9), S3-S5 1.906(2), S1-Co1 2.2340(7), B2-S5 1.861(9); S2-B1-S3 108.52(19), B1-S2-S1 94.84(17), B1-S3-B2 94.1(3), B1-S3-Co1 105.06(16).

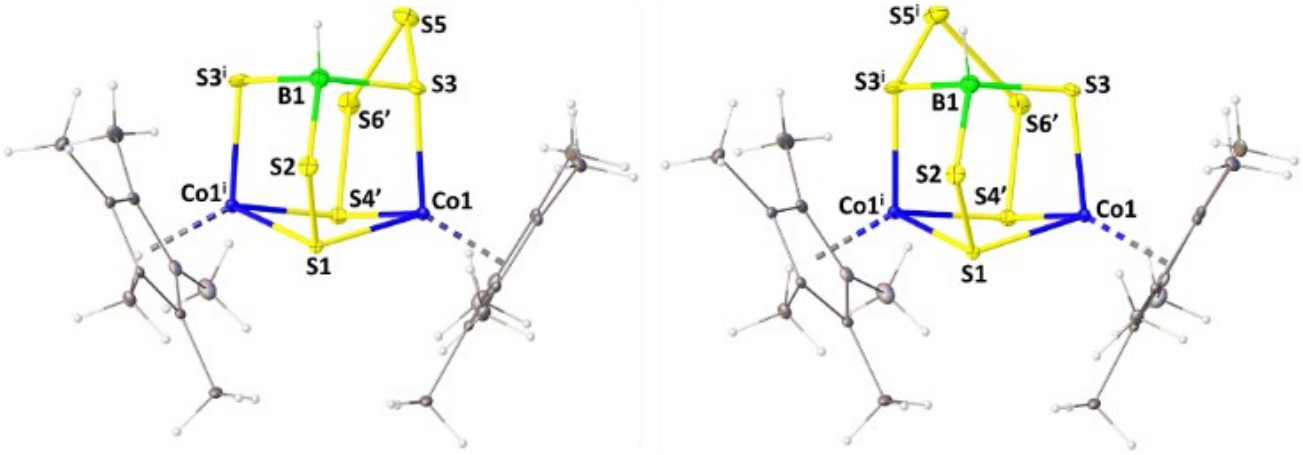
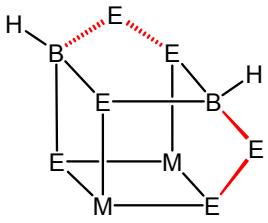


Figure S5. Molecular structures of compound **10**. Selected bond distances (Å) and angles (°): S3-Co1 2.2453(9), B1-S3 1.942(3), S6'-S5 2.503(8), S4' S6' 2.117(12), S4' Co1 2.269(6); S2-S1-Co1 105.79(4), Co1-S1-Co1 95.80(4), S6'-S4'-Co1 103.8(4), S3-Co1-S4' 101.3(3).

Crystal Data for 5: Formula, $C_{20}H_{32}B_2Rh_2S_6$; M_r = 692.25; crystal system, monoclinic; space group, $P2_1/n$; unit cell, a = 11.6036(15) Å, b = 16.221(2) Å, c = 14.2437(19) Å, α = 90°, β = 99.797(5)°, γ = 90°; V = 2641.9(6) Å^3; Z = 4; ρ_{calc} = 1.740 g/cm^3; μ = 1.731 mm^{-1}; *F(000)* = 1392.0; R_1 = 0.0428; wR_2 = 0.0982; 6034 independent reflections [2θ ≤ 54.97°] and 281 parameters.

Crystal data for 7 : Formula, $C_{23}H_{39}B_2Rh_2Se_7$; M_r = 1095.70; crystal system, monoclinic; space group $P2_1/n$; unit cell, a = 10.2132(14) Å, b = 19.541(2) Å, c = 15.563(2) Å, α = 90°, β = 96.078(6)° γ = 90°; V = 3088.7(7) Å^3; Z = 4; ρ_{calcd} = 2.356 g/cm^3; μ = 9.331 mm^{-1}; *F(000)* = 2060; R_1 = 0.1506; wR_2 = 0.3257; 5695 independent reflections [2θ ≤ 54.984°] and 204 parameters.



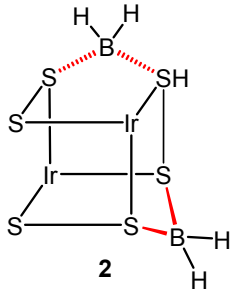
1-2, 5-6, 8 and 10

Bishomocubanes

PSEPT
5*n+15*n+k =
5*8+15*2+2 = 72

CVE
2Cp*M{2*(5+9)=28}+6E(6*6=36)+2BH{2*(3+1)=8}=72
M = Ir, Rh, Co; E = S, Se

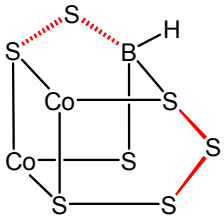
Bishomocubanes with a missing bond



2

PSEPT
5*n+15*n+k =
5*8+15*2+2 = 72
When a bond breaks, 2 electrons should be added, 72+2=74

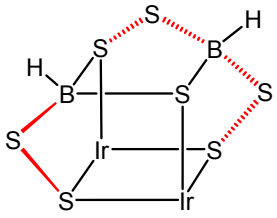
CVE
2Cp*Ir{2*(5+9)=28}+6S(6*6=36)+2BH_2{2*(3+2)=10}=74



9

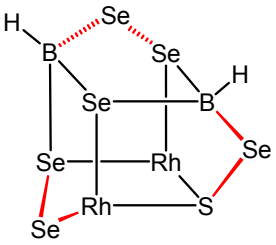
CVE
2Cp*Co{2*(5+9)=28}+7S(7*6=42)+BH{(3+1)=4}=74

Trishomocubanes



3

PSEPT
5*n+15*n+k =
5*9+15*2+3 = 78



7

CVE
2Cp*Ir{2*(5+9)=28}+7S(7*6=42)+2BH{2*(3+1)=8}=78

CVE
2Cp*Rh{2*(5+9)=28}+7Se(7*6=42)+2BH{2*(3+1)=8}=78

n-k vertex 3-connected polyhedron with k vertices inserted into edges

Scheme S1. Cluster Valence Electron (CVE) counts of compounds **1**-**10**. PSEPT stands for Polyhedral Skeletal Electron Pair Theory

II Spectroscopic details

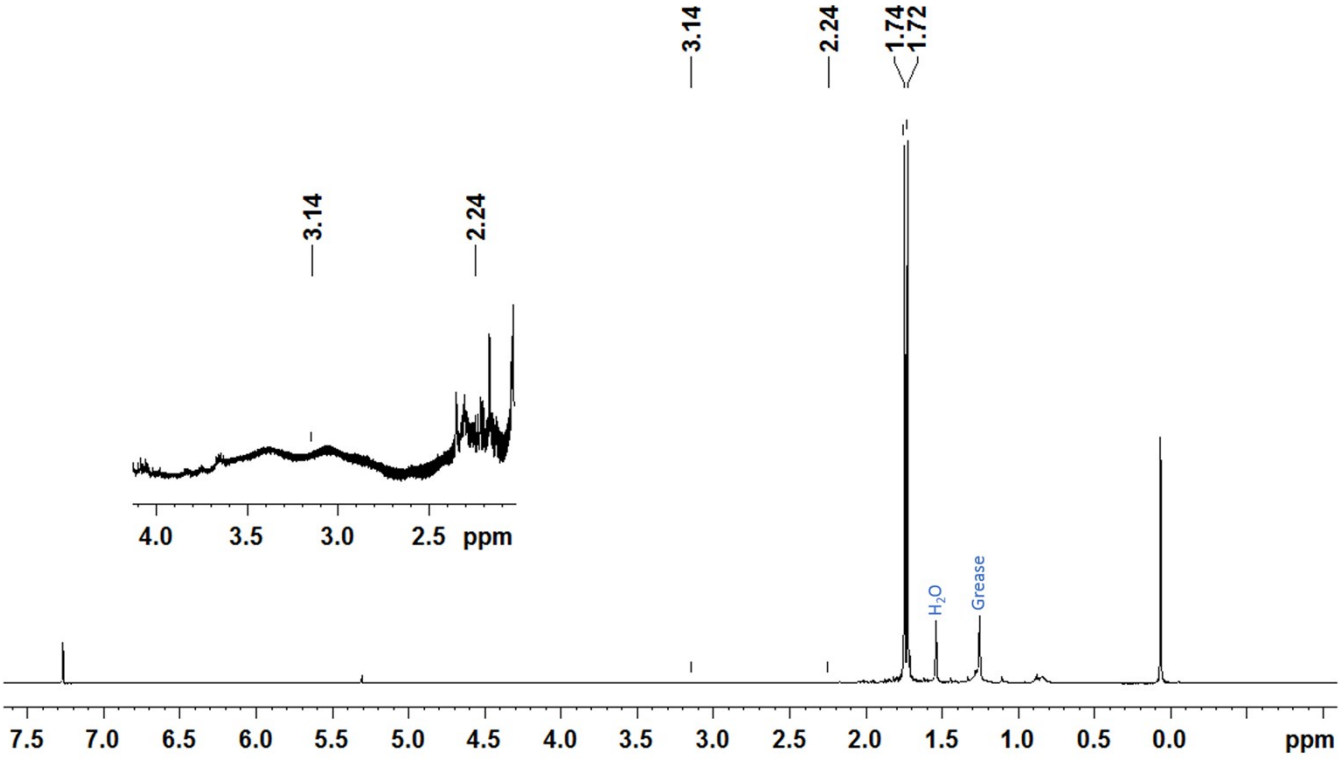


Figure S6. ^{1}H NMR spectrum of compound **1**.

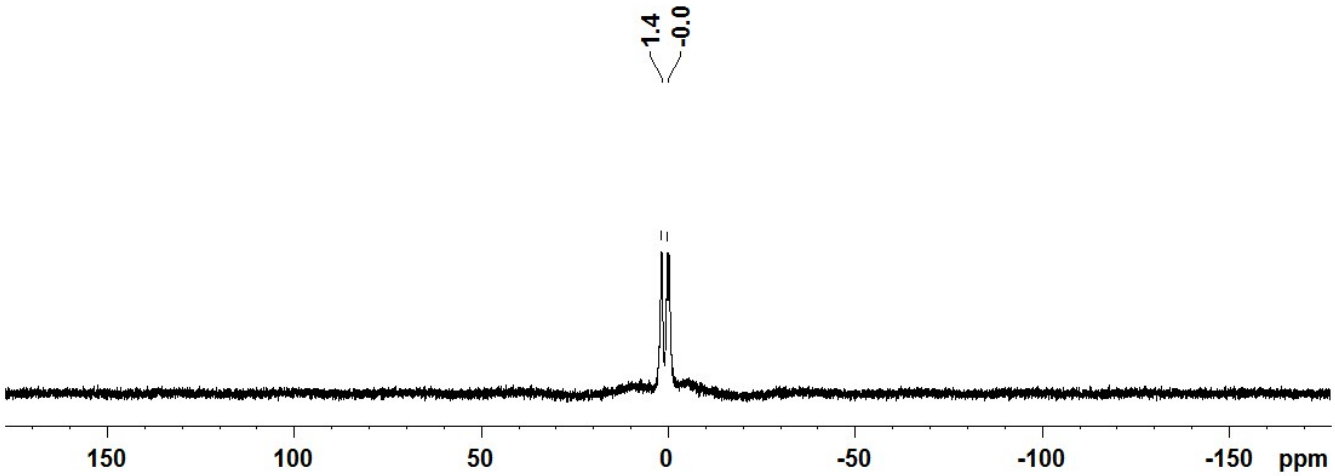


Figure S7. ^{11}B{^{1}H} NMR spectrum of compound **1**[1].

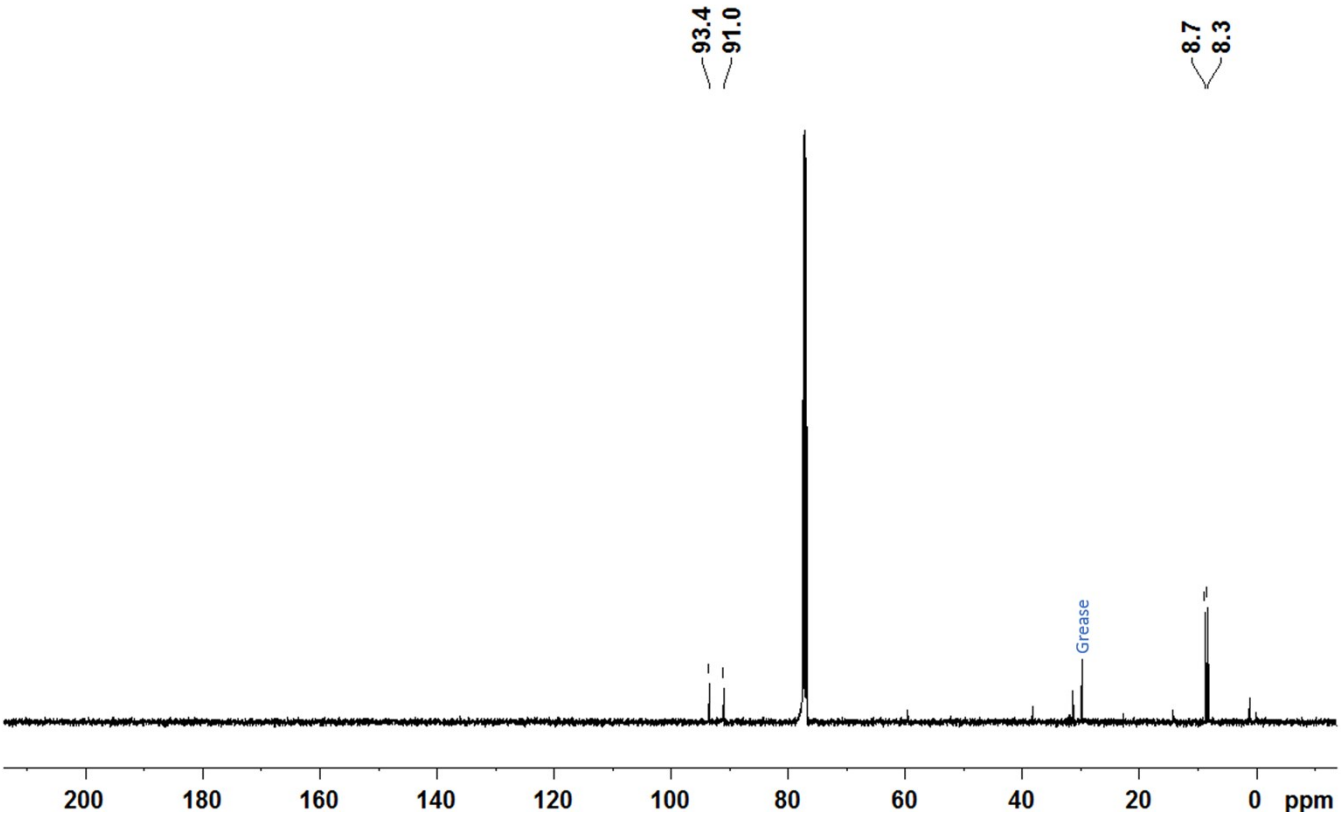


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of compound **1**.

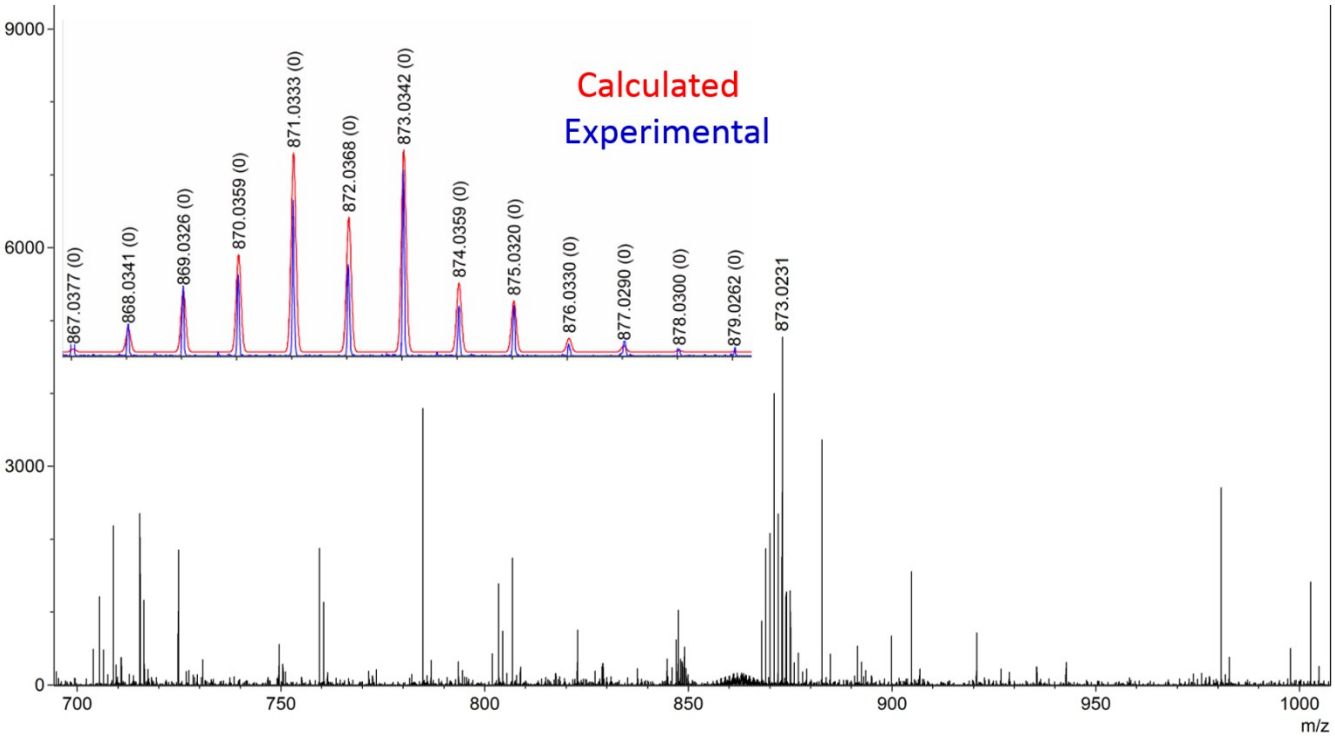


Figure S9. MS (ESI^{+}) spectrum of compound **1**.

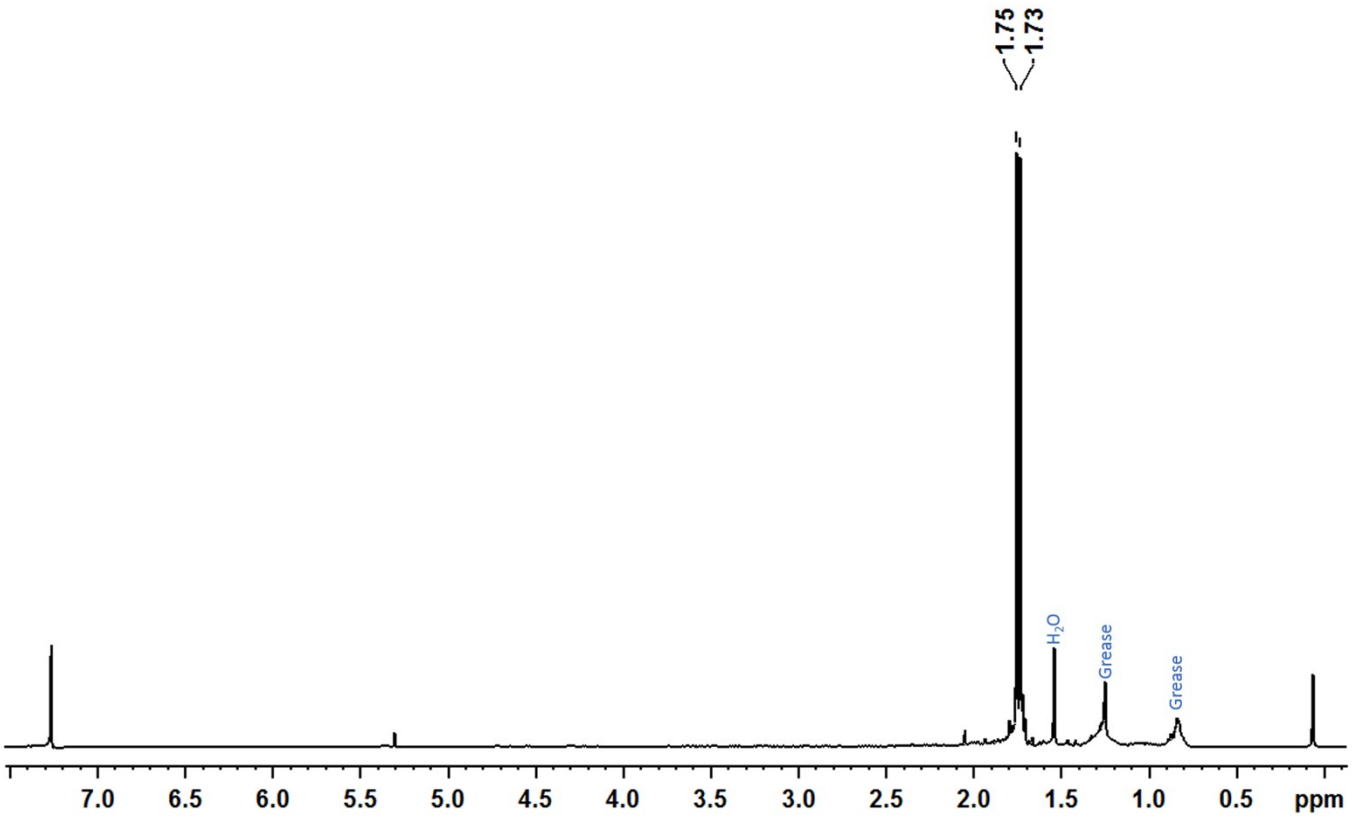


Figure S10. ^{1}H NMR spectrum of compound **2**.

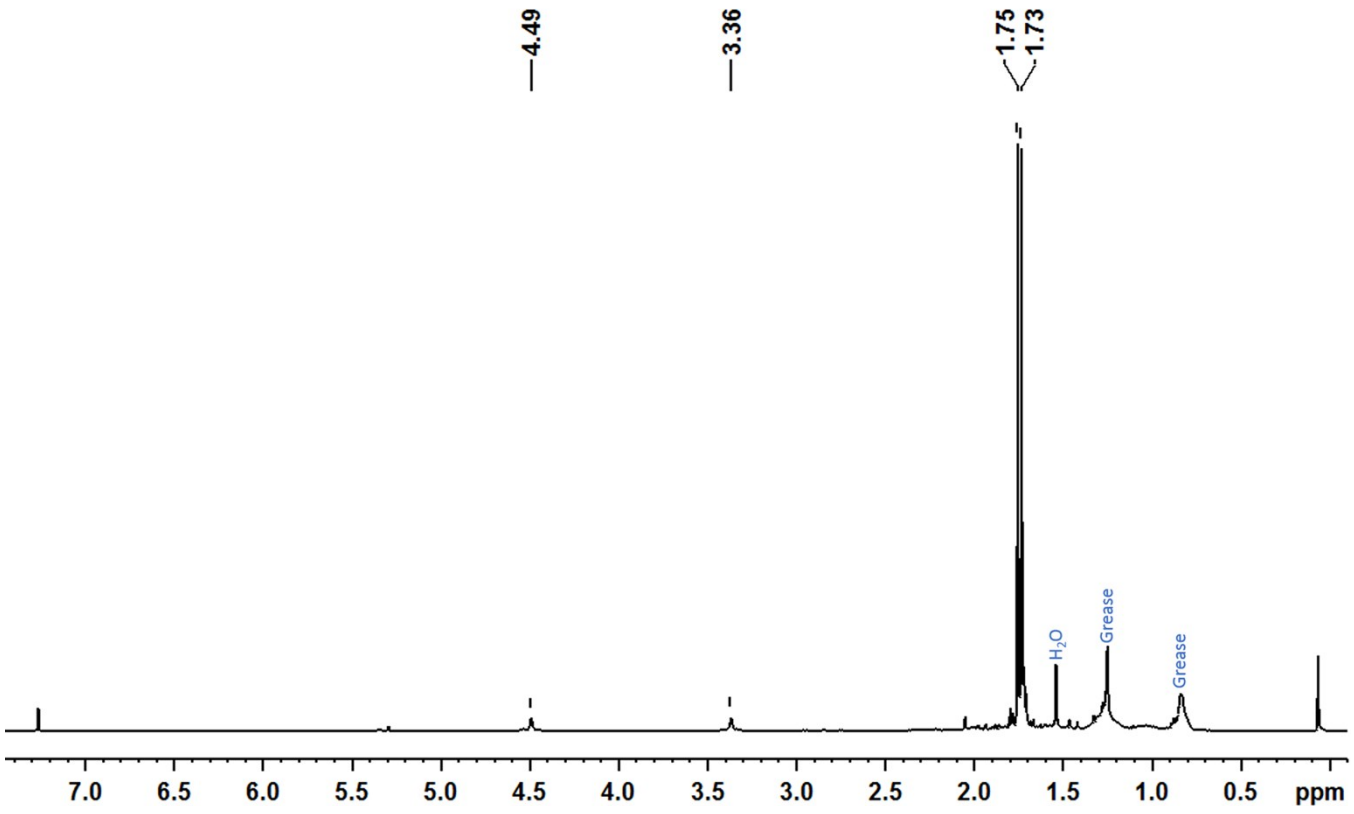


Figure S11. $^{1}H\{^{11}B\}$ NMR spectrum of compound **2**.

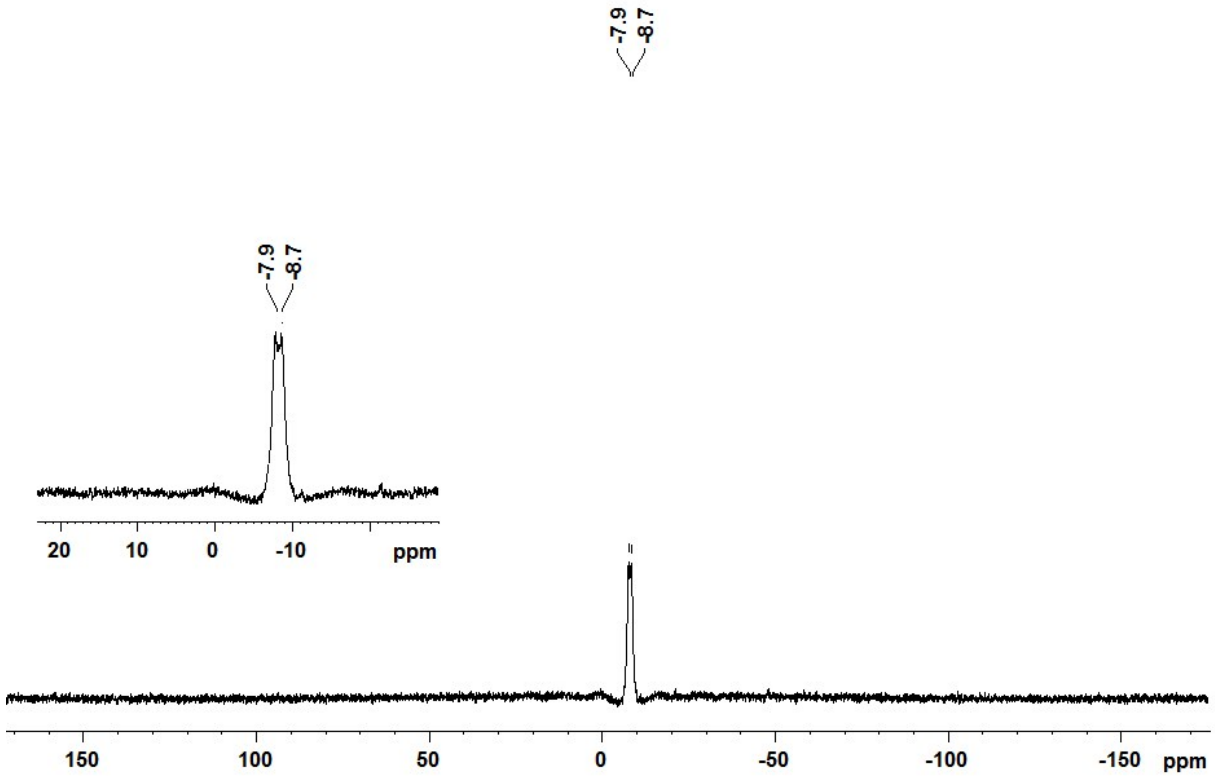


Figure S12. $^{11}B\{^{1}H\}$ NMR spectrum of compound **2**[1].

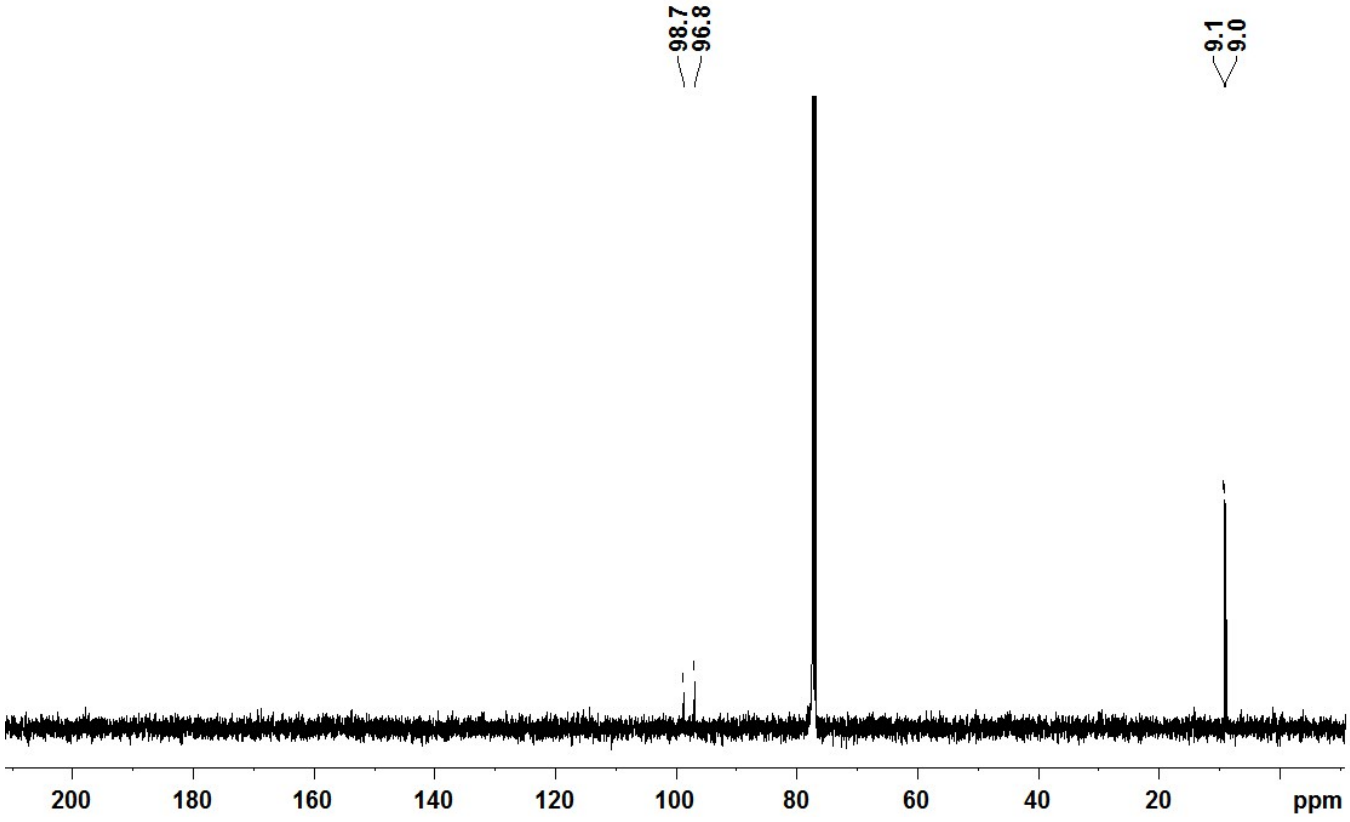


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of compound **2**.

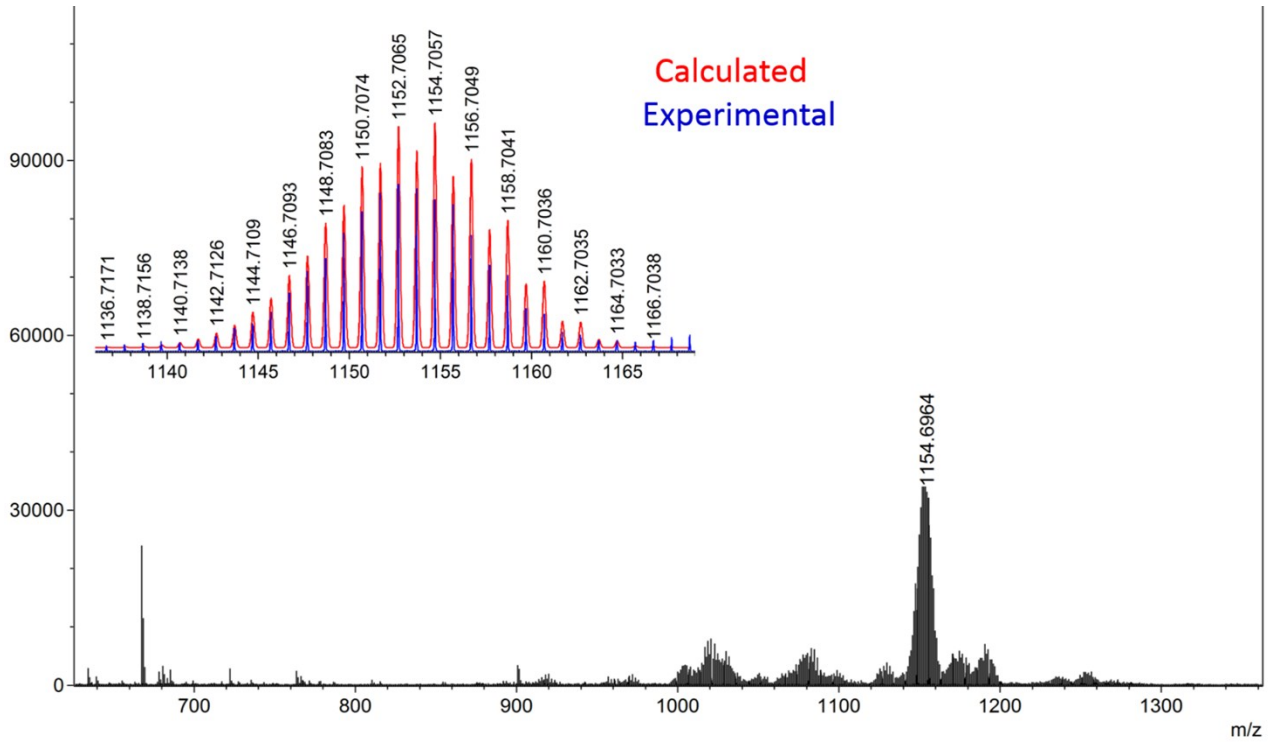


Figure S14. MS (ESI$^+$) spectrum of compound **2**.

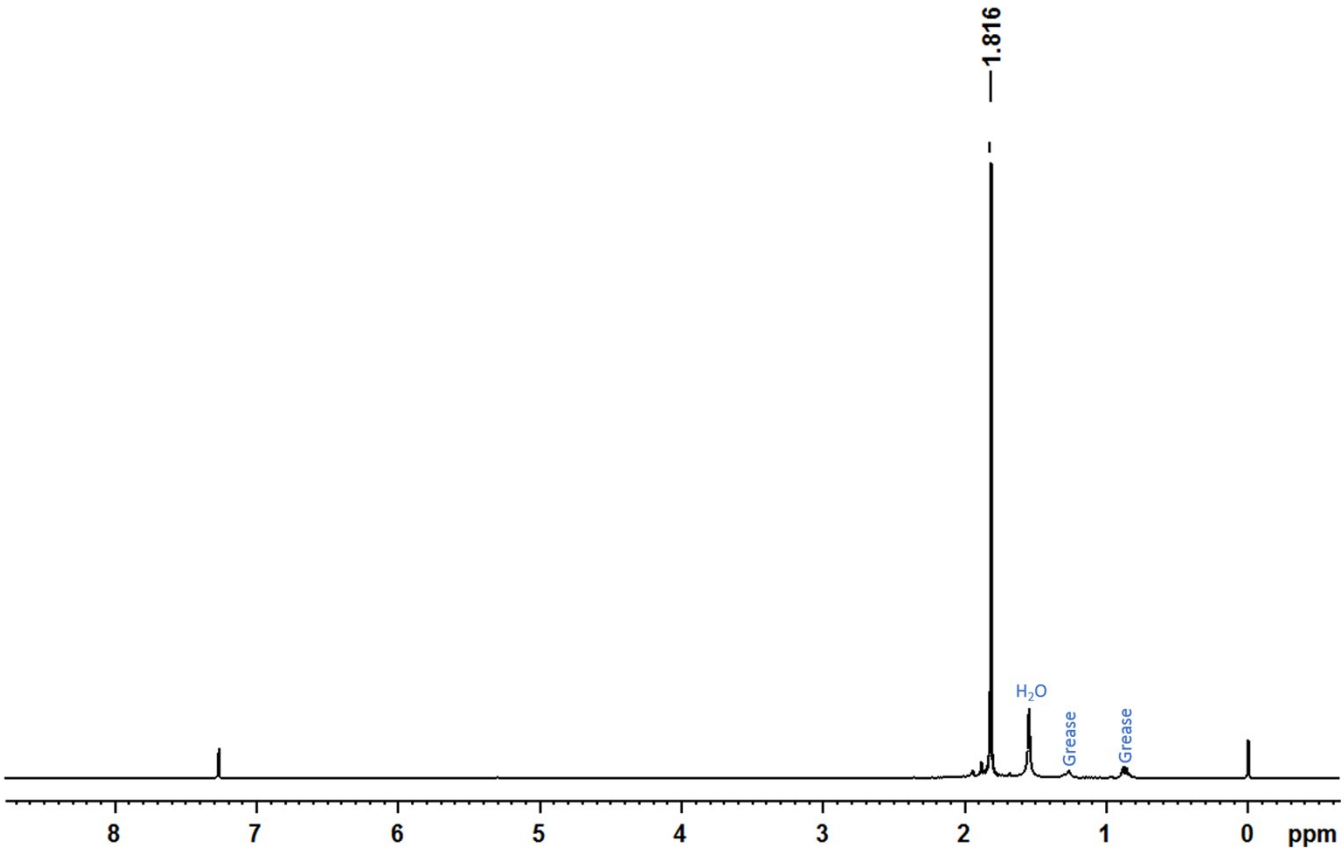


Figure S15. ^{1}H NMR spectrum of compound **3**.

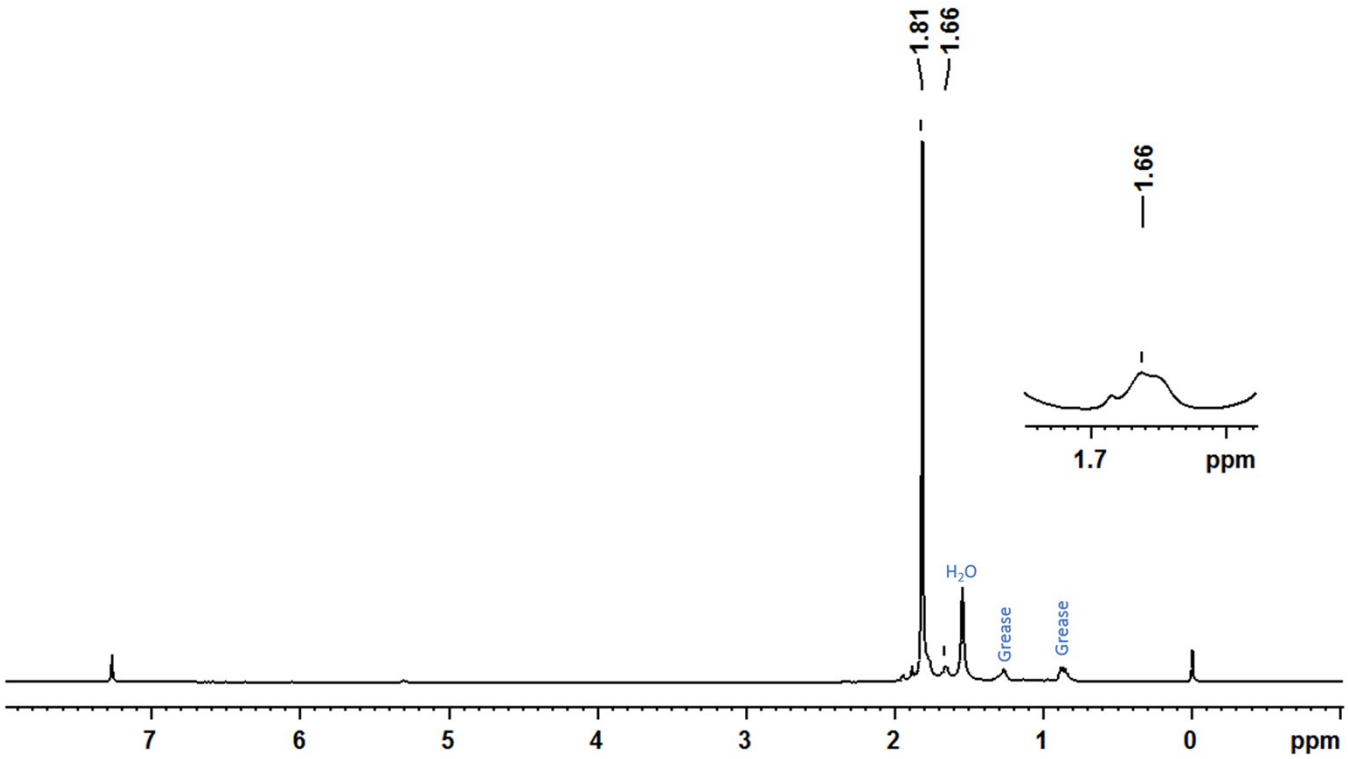


Figure S16. $^{1}H\{^{11}B\}$ NMR spectrum of compound **3**.

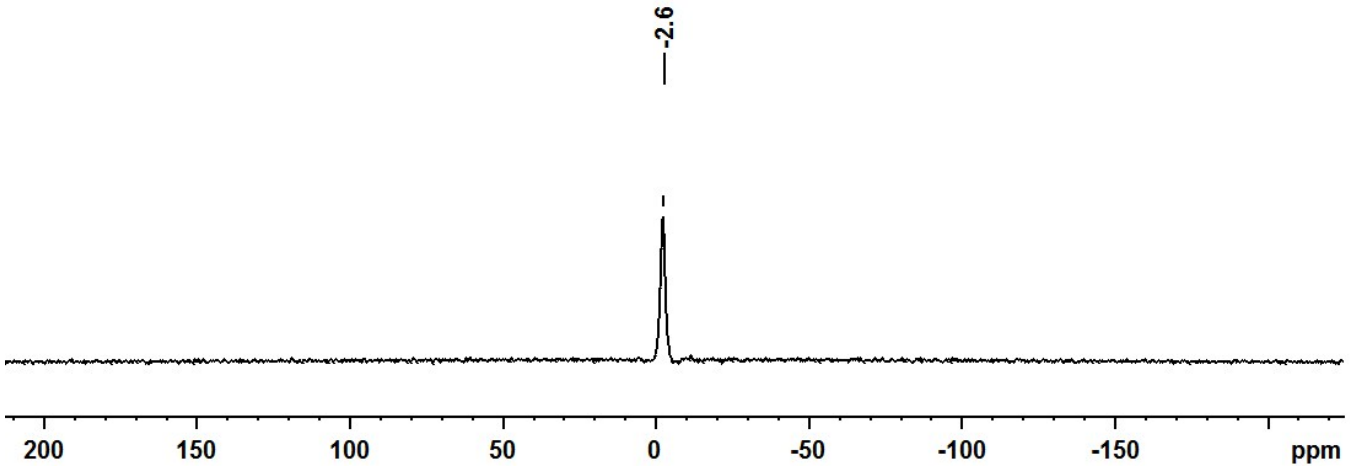


Figure S17. $^{11}B\{^{1}H\}$ NMR spectrum of compound **3**[1].

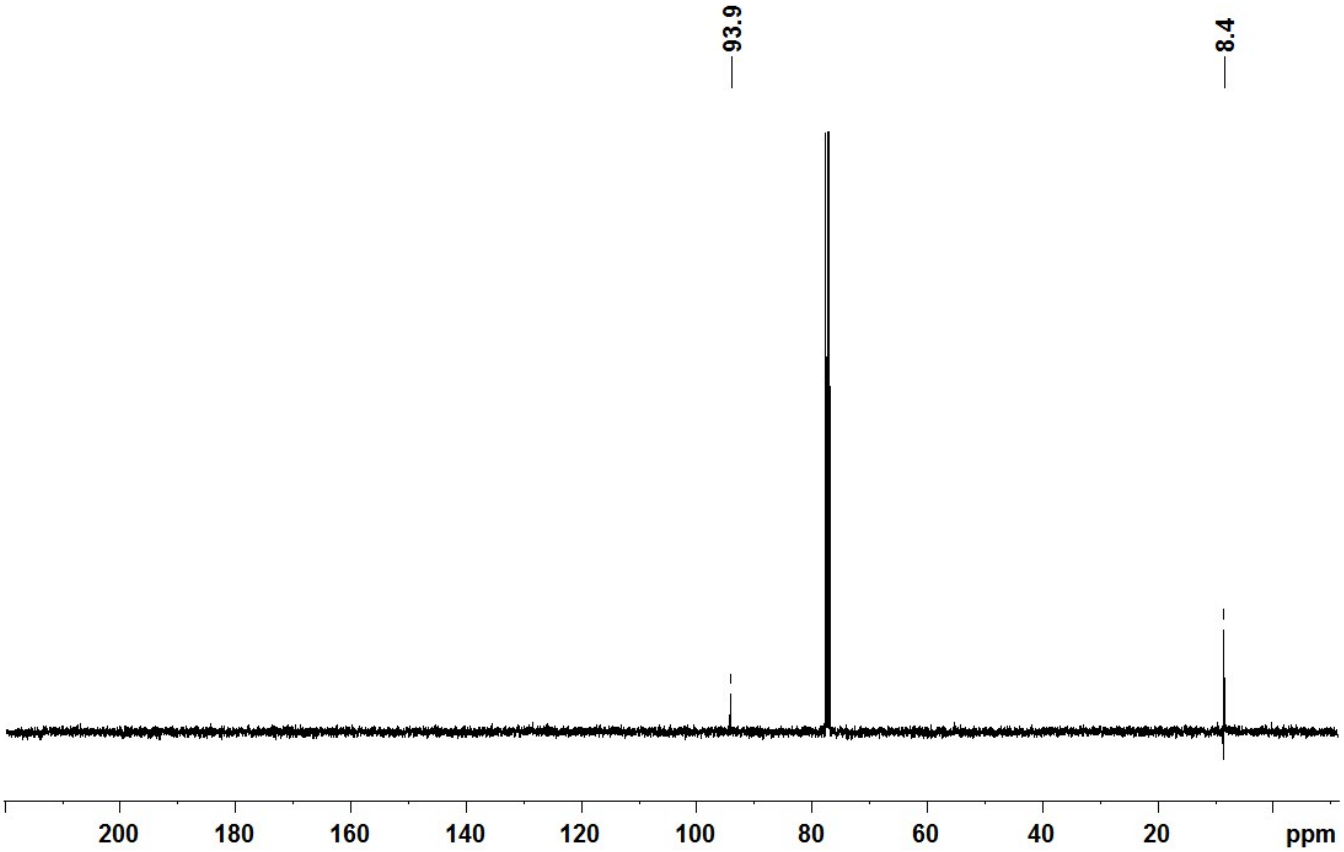


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of compound **3**.

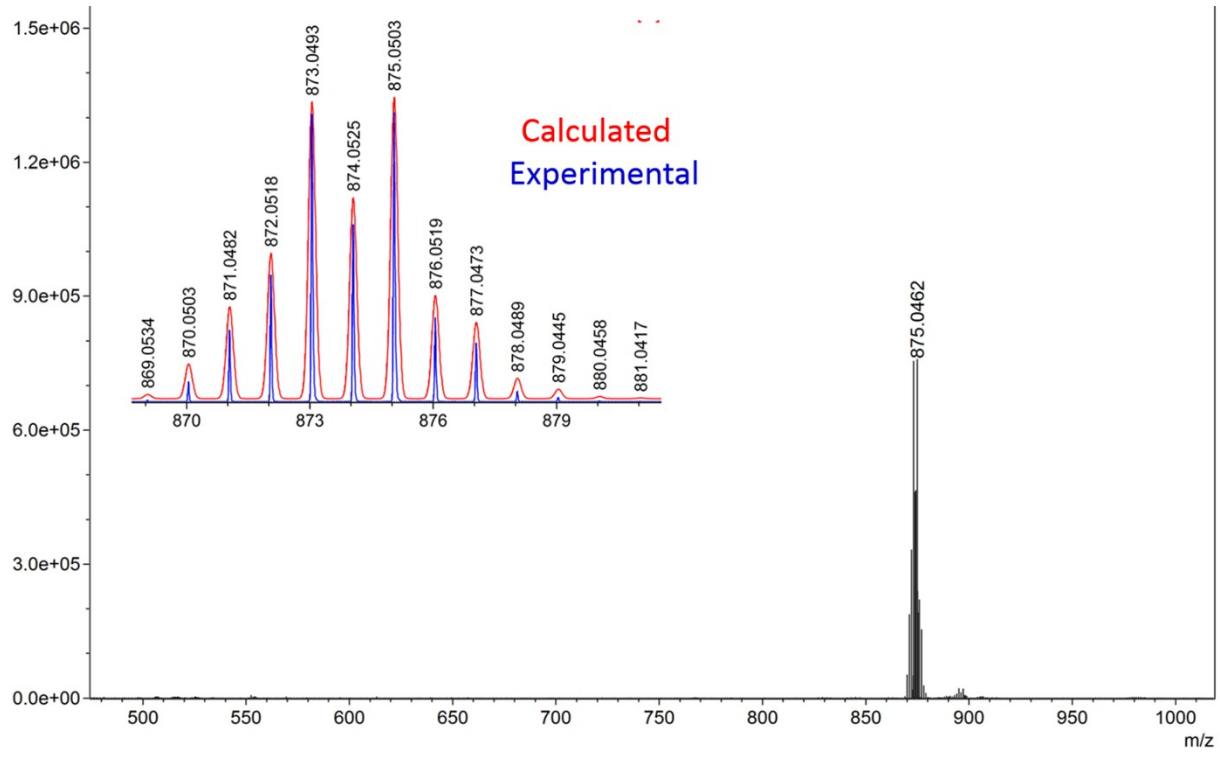


Figure S19. MS (ESI^{+}) spectrum of compound **3**.

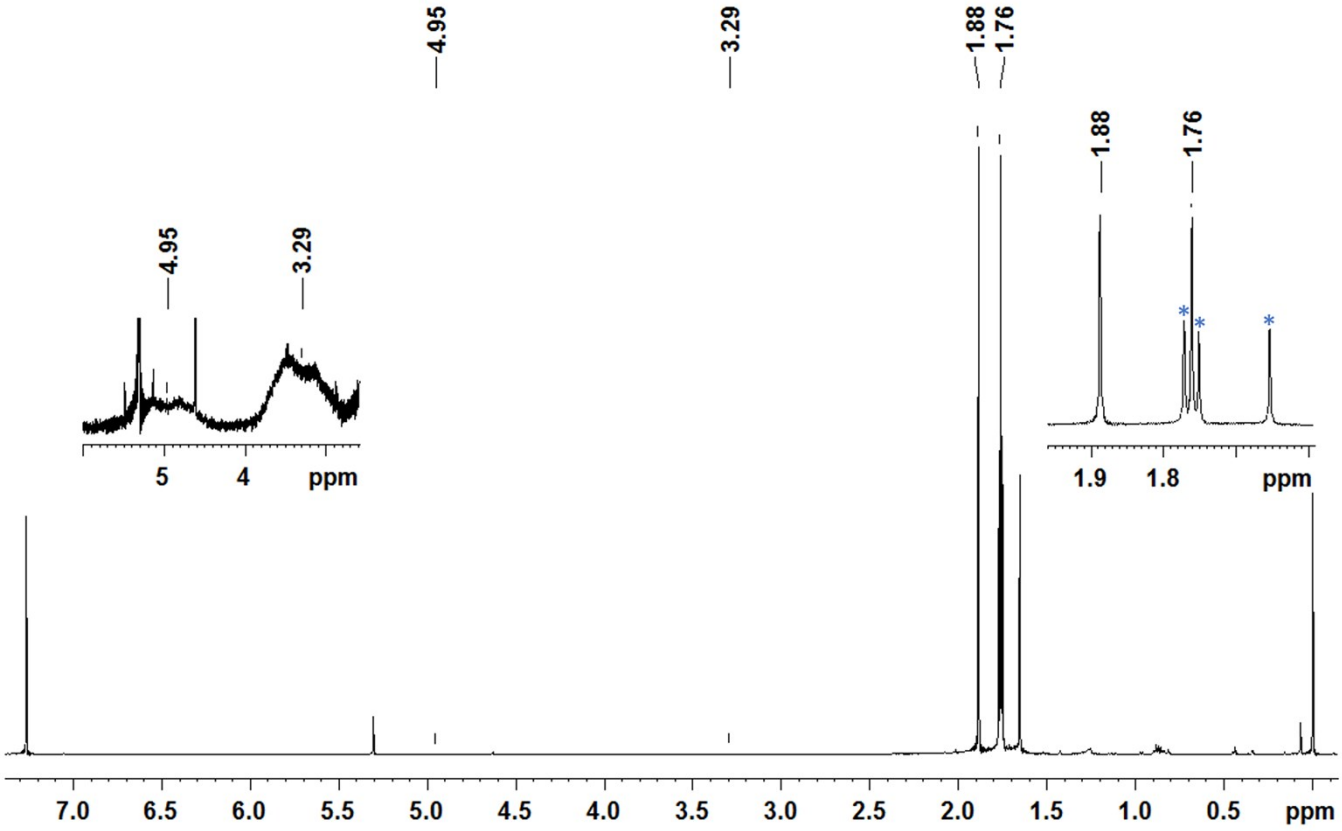


Figure S20. ^{1}H NMR spectrum of compound **4** (*uncharacterized minor compound).

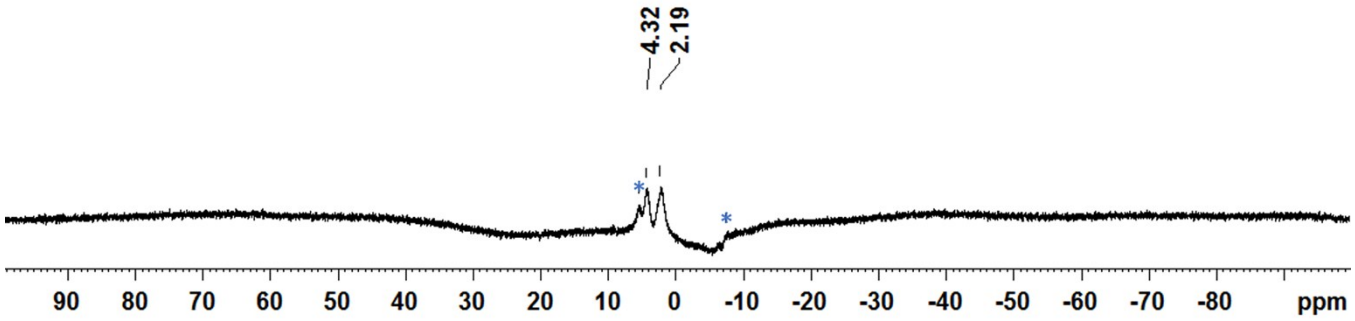


Figure S21. ^{11}B{^{1}H} NMR spectrum of compound **4**[1] (*uncharacterized minor compound).

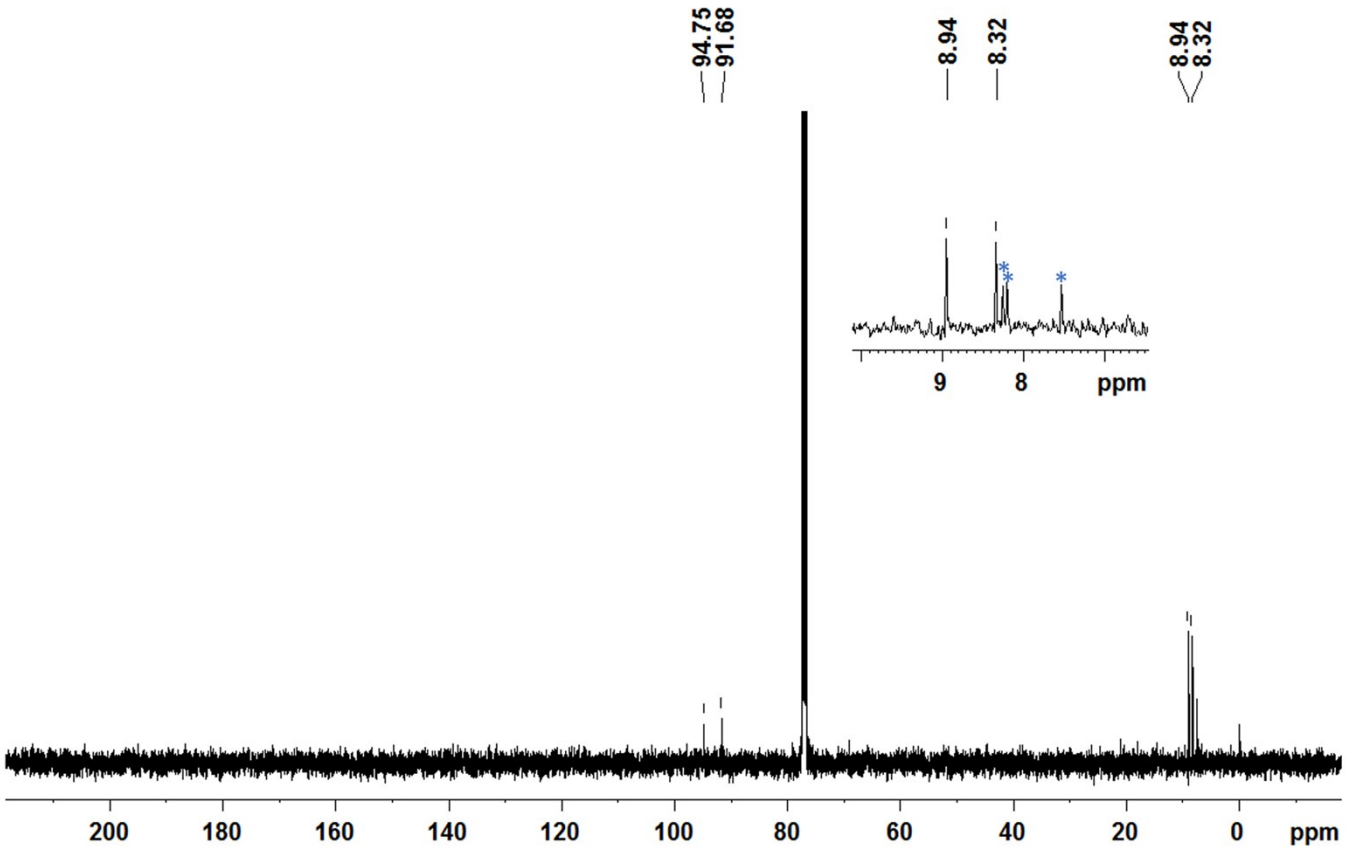


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum of compound **4** (*uncharacterized minor compound).

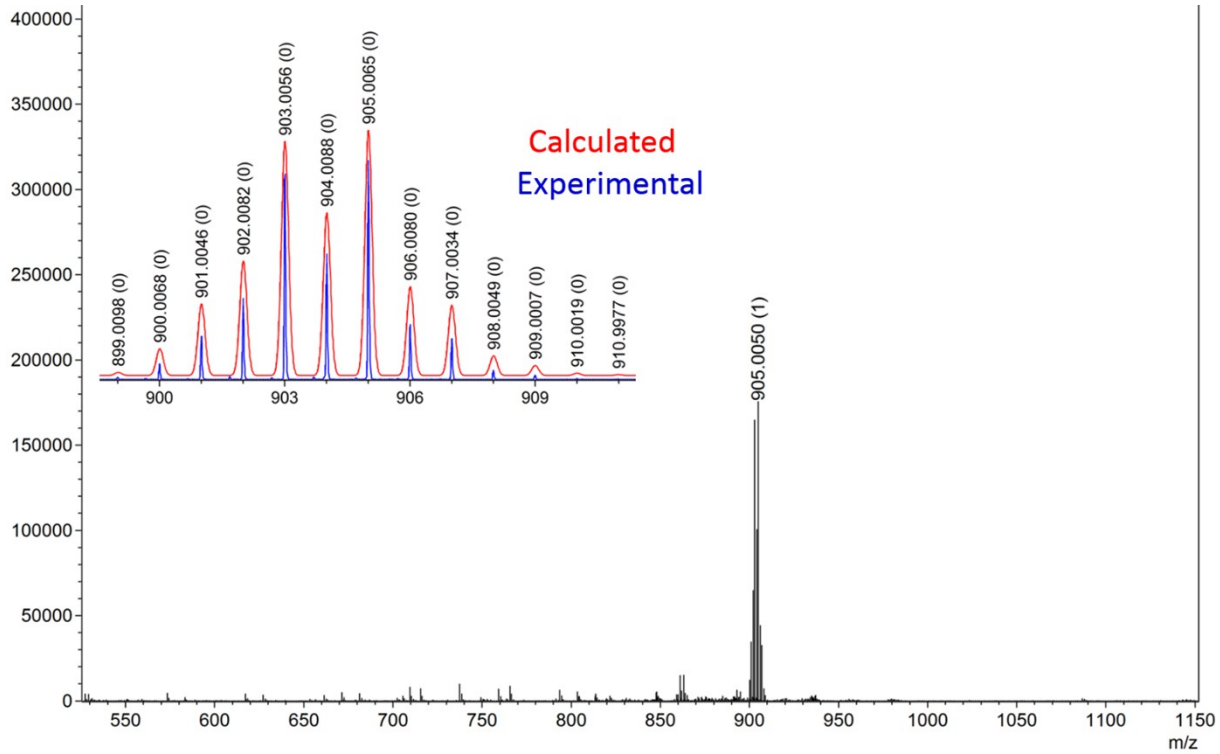


Figure S23. MS (ESI^{+}) spectrum of compound **4**.

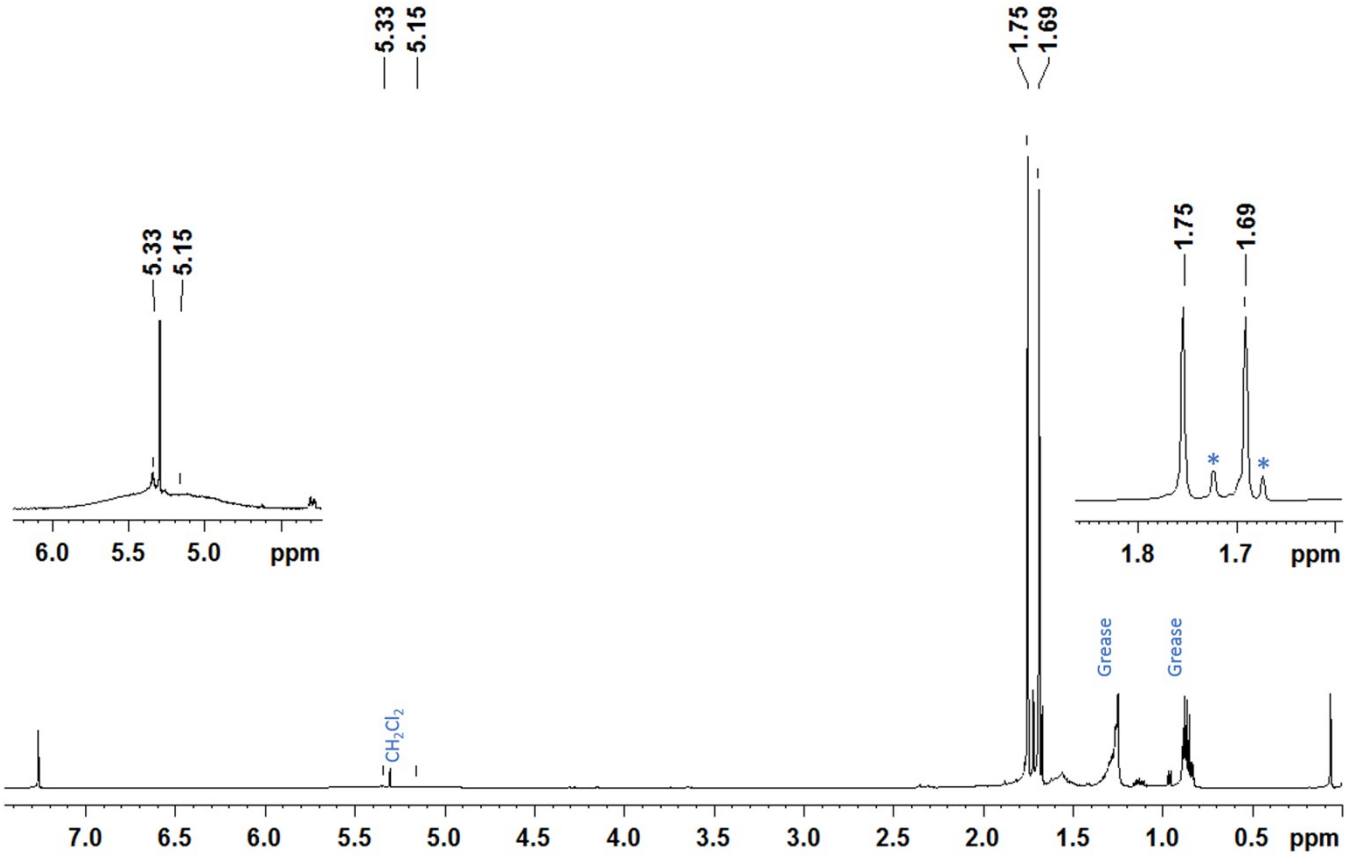


Figure S24. ^{1}H NMR spectrum of compound **7** (*uncharacterized minor compound).

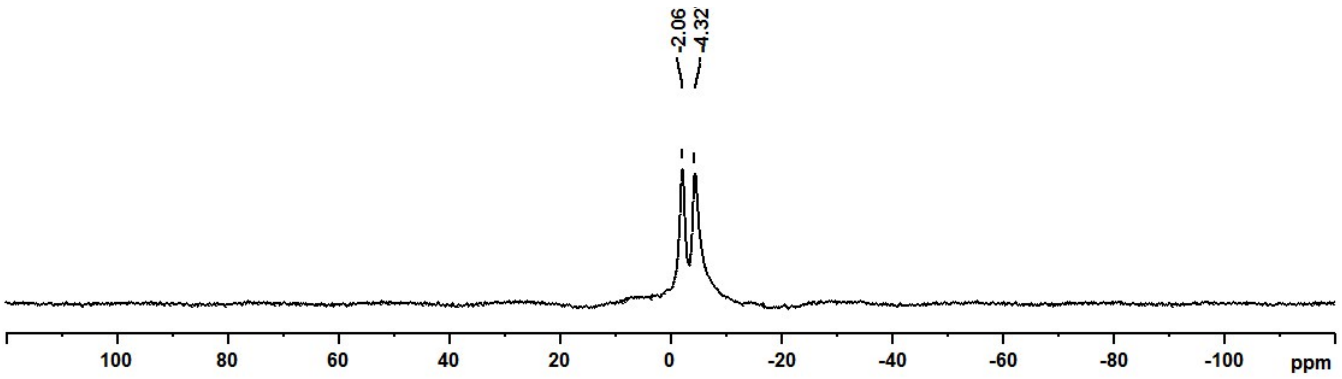


Figure S25. ^{11}B{^{1}H} NMR spectrum of compound **7**[1].

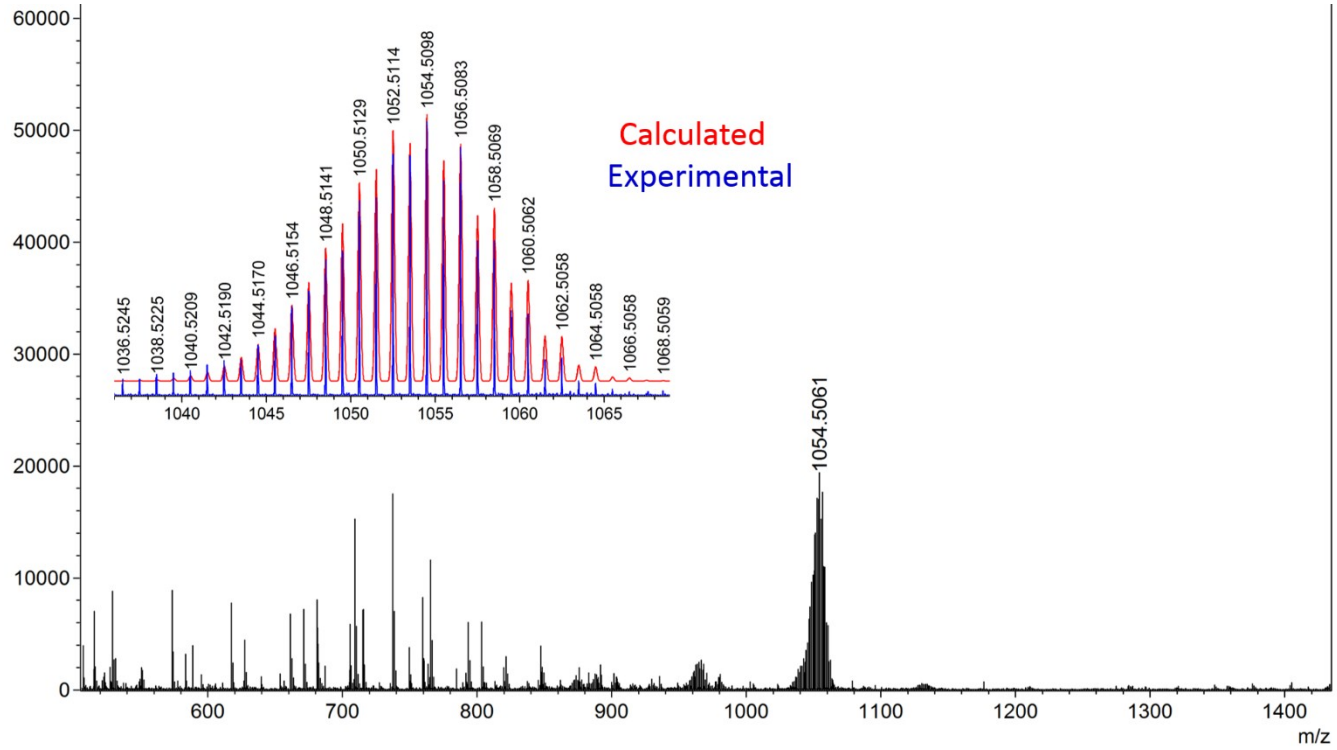


Figure S26. MS(ESI$^+$) spectrum of compound **7**.

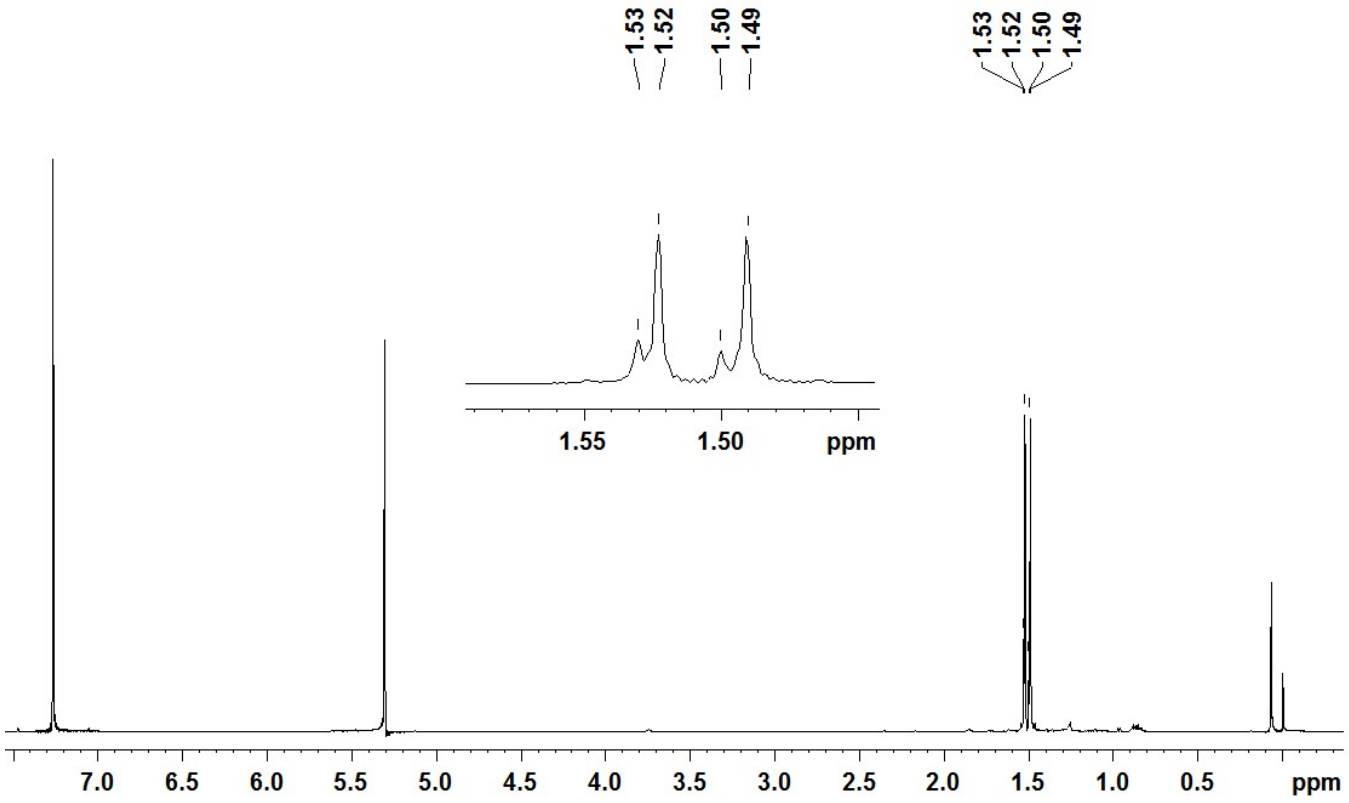


Figure S27. ^{1}H NMR spectrum of compounds **8** and **10**.

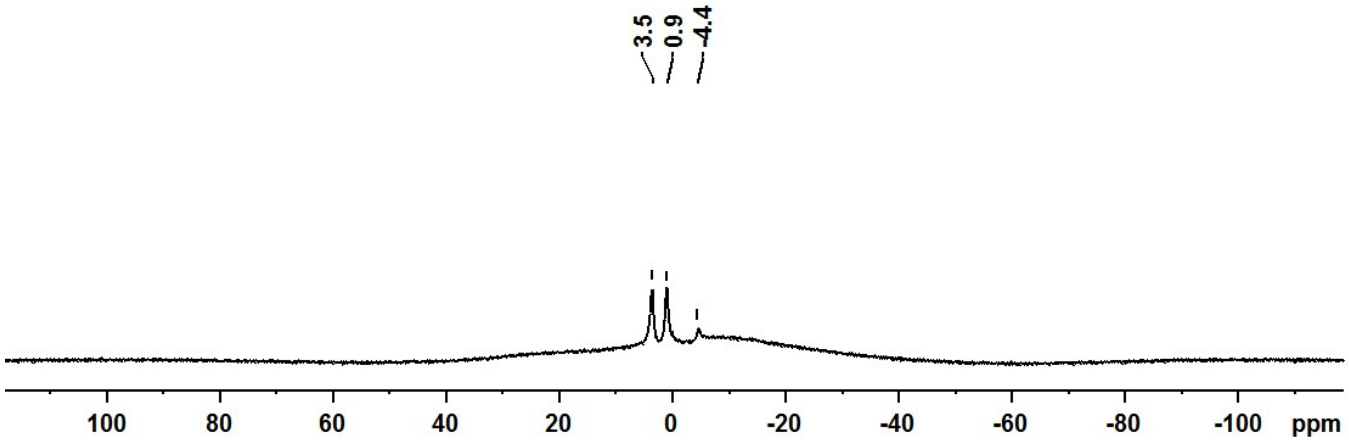


Figure S28. $^{11}B\{^{1}H\}$ NMR spectrum of compounds **8** and **10**[1].

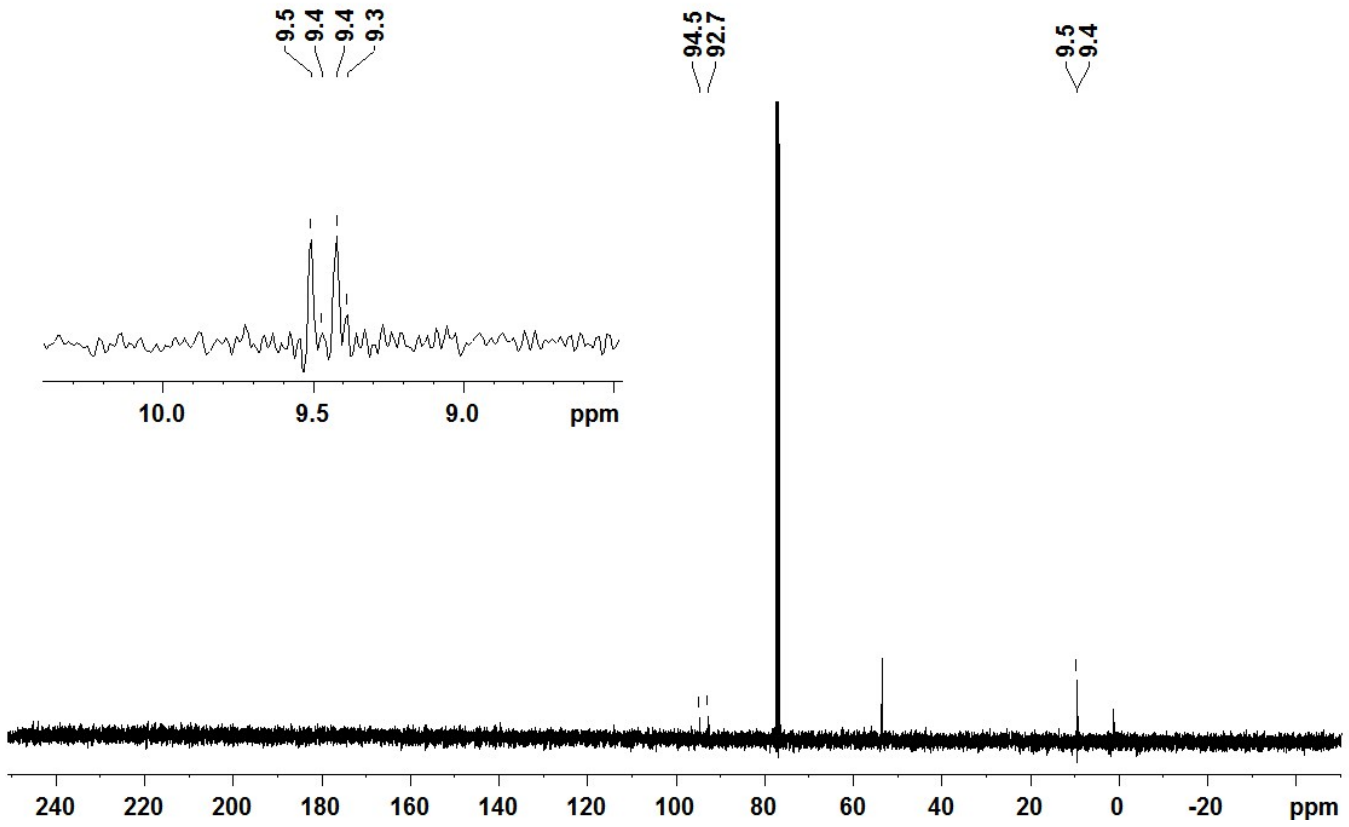


Figure S29. $^{13}C\{^{1}H\}$ NMR spectrum of compounds **8** and **10**.

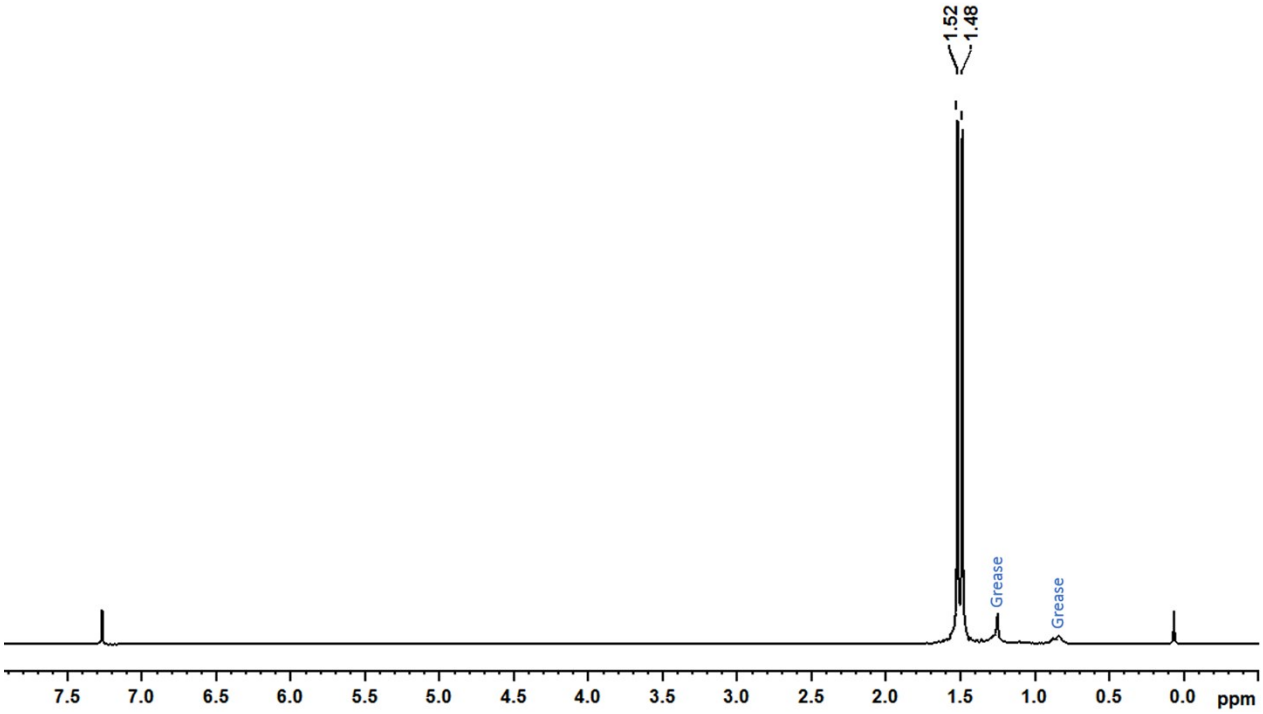


Figure S30. ^{1}H NMR spectrum of compound **8**.

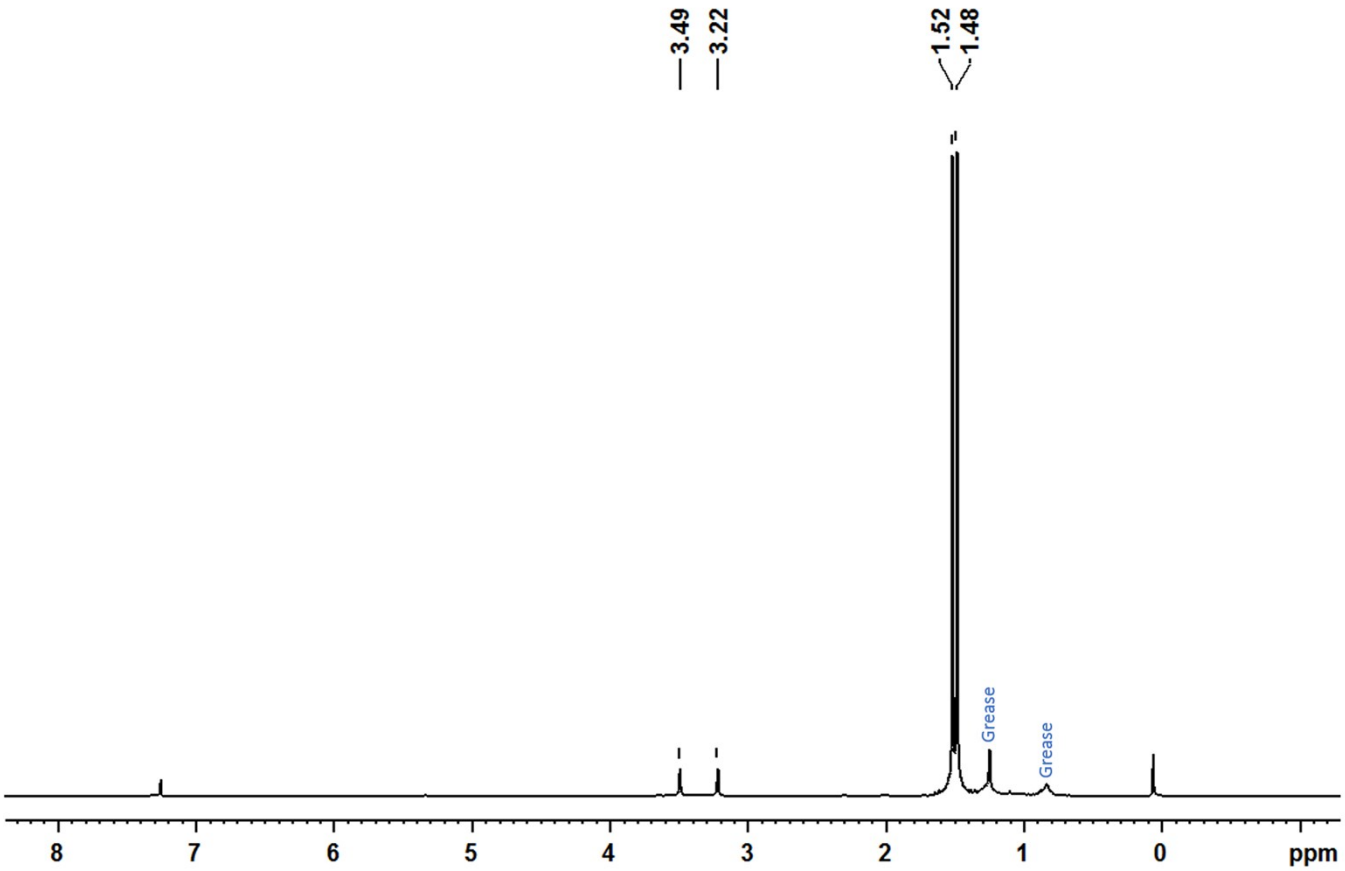


Figure S31. $^{1}H\{^{11}B\}$ NMR spectrum of compound **8**.

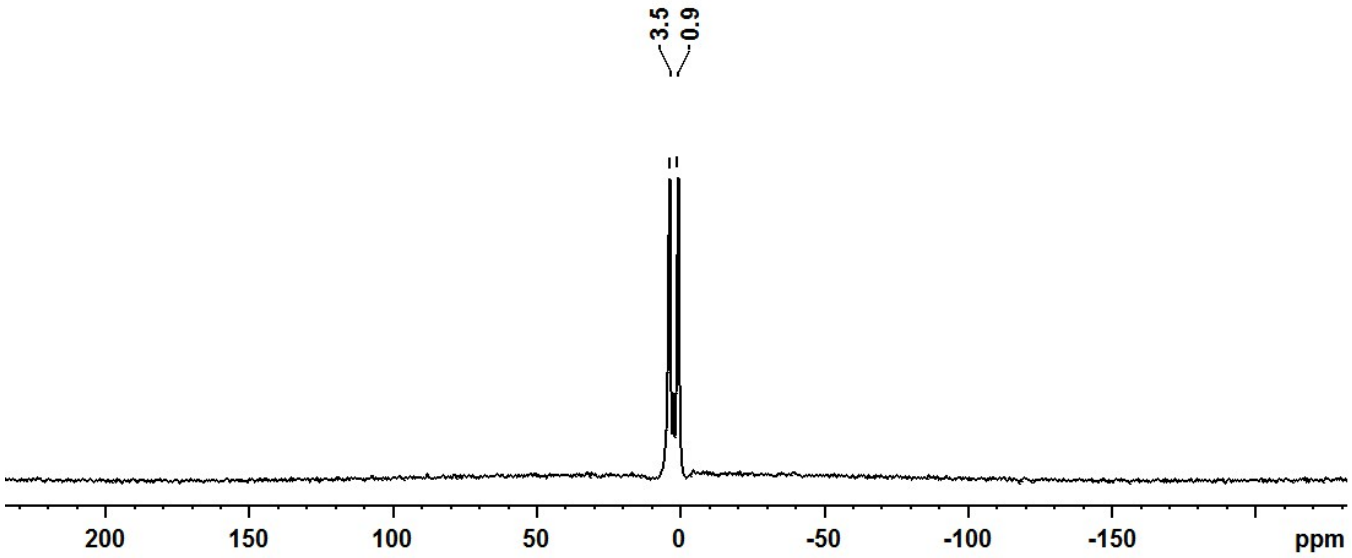


Figure S32. $^{11}B\{^{1}H\}$ NMR spectrum of compound **8**[1].

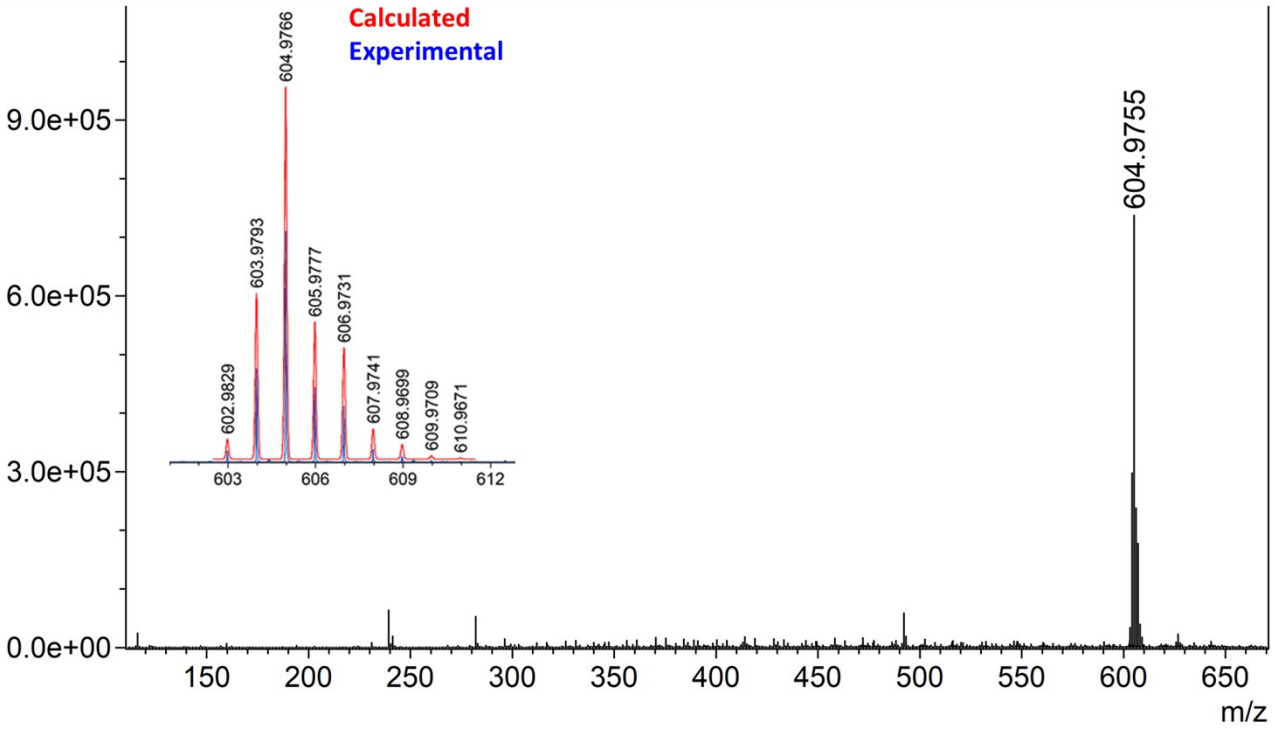


Figure S33. MS (ESI^{+}) spectrum of compound **8**.

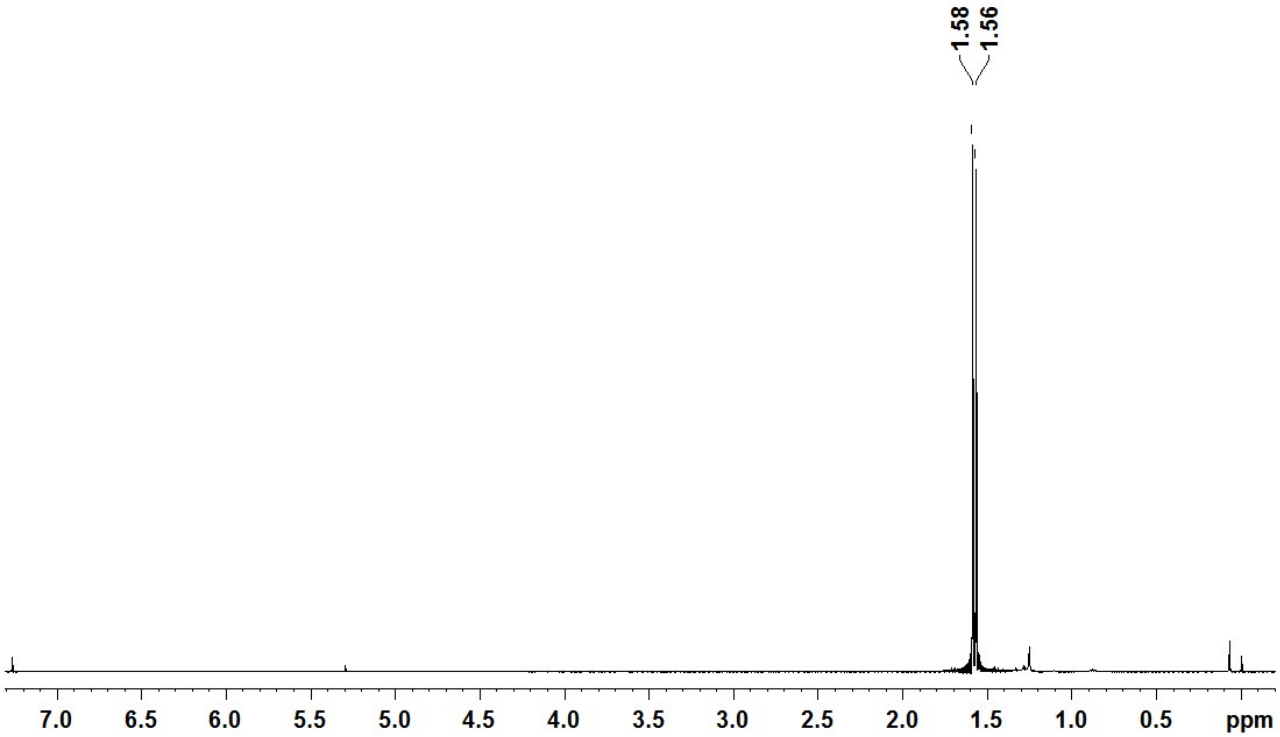


Figure S34. ^{1}H NMR spectrum of compound **9**.

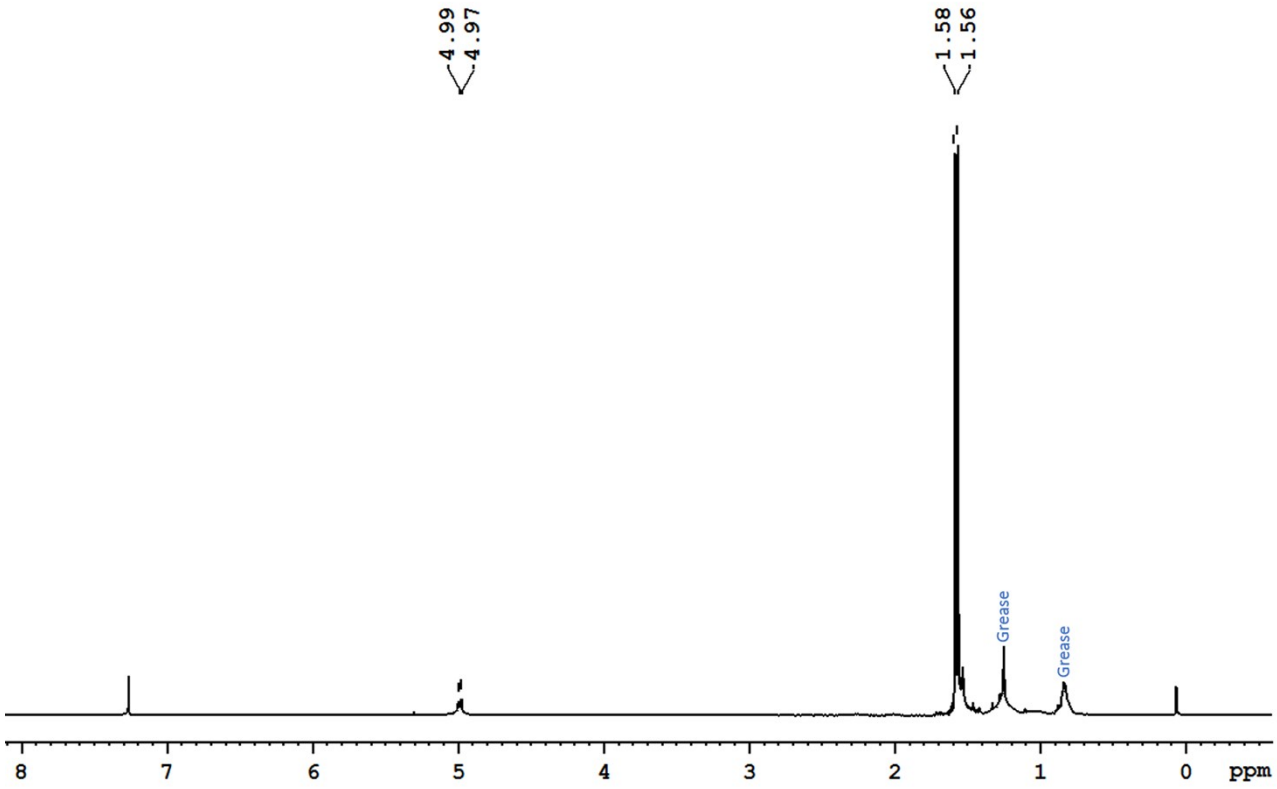


Figure S35. $^{1}H\{^{11}B\}$ NMR spectrum of compound **9**.

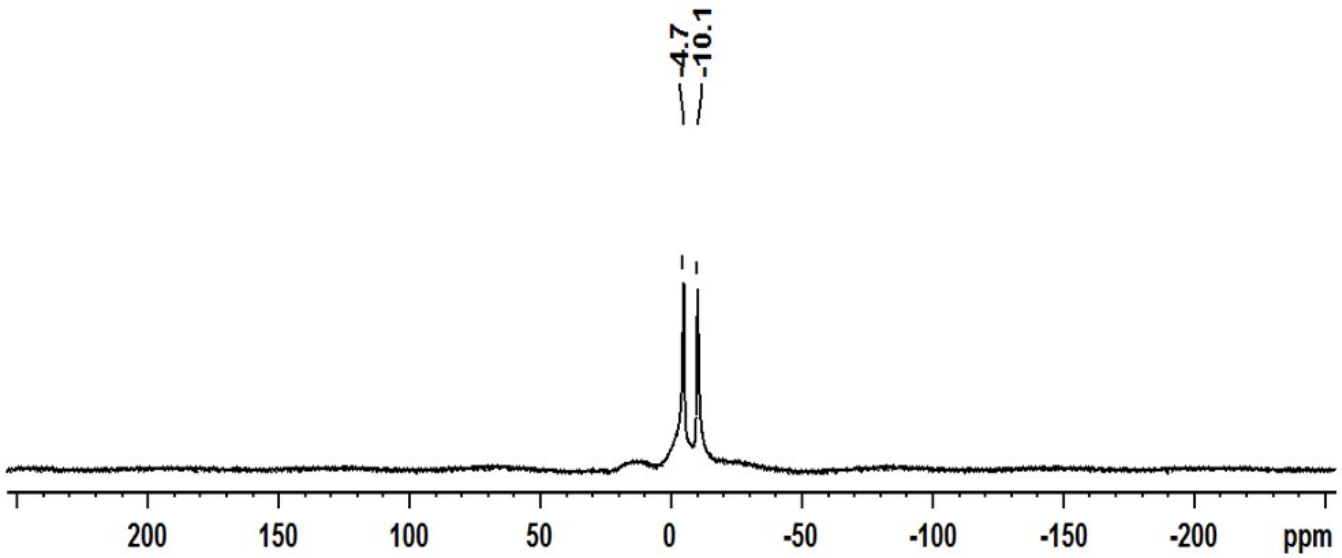


Figure S36. $^{11}B\{^{1}H\}$ NMR spectrum of compound **9**[1].

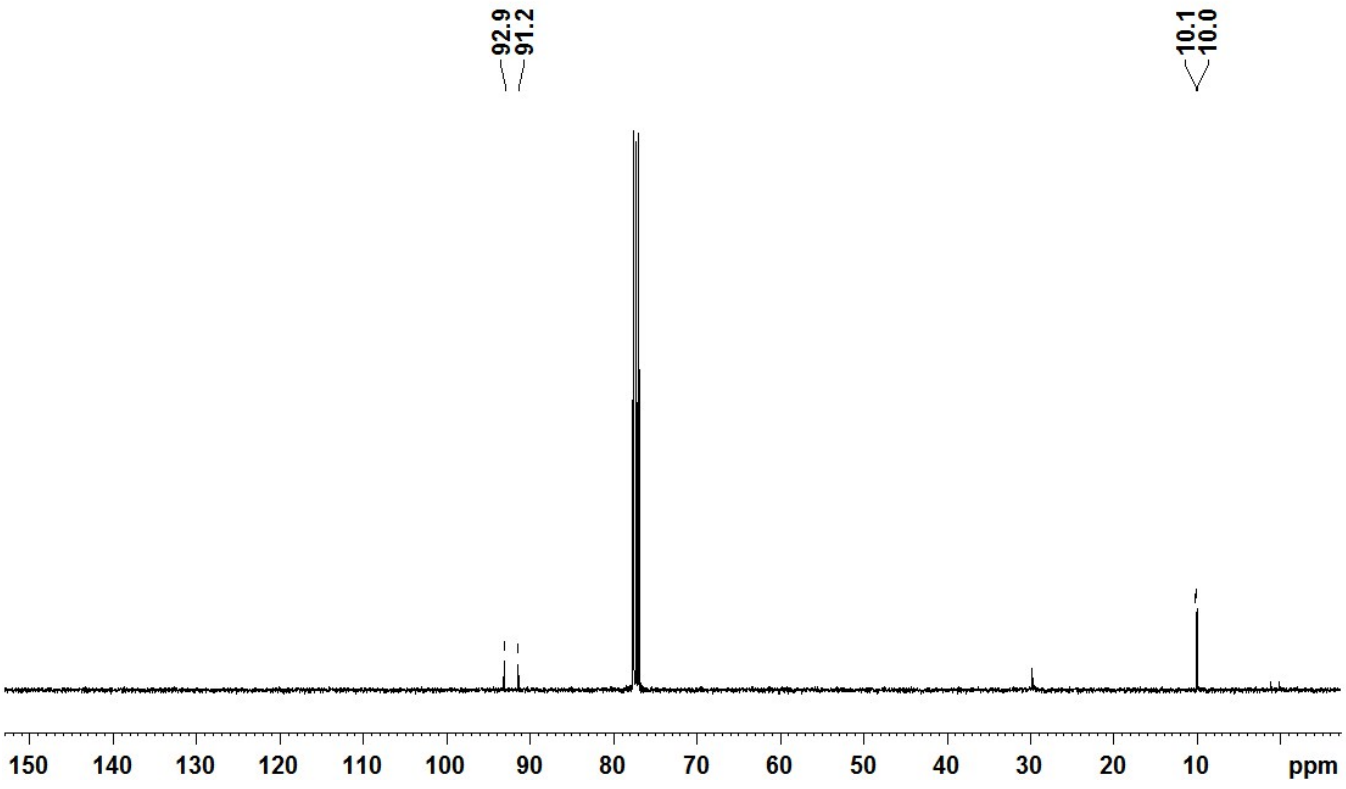


Figure S37. $^{13}C\{^{1}H\}$ NMR spectrum of compound **9**.

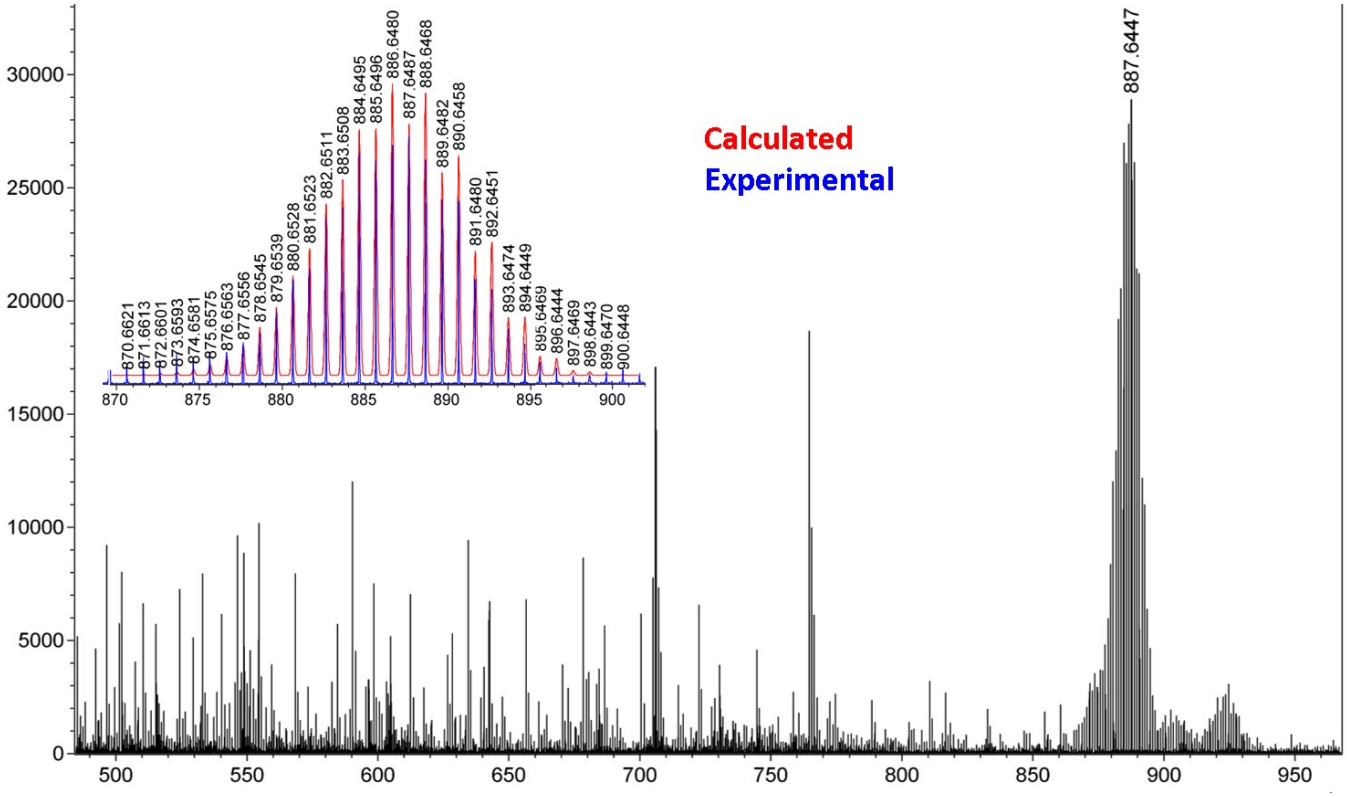


Figure S38. MS (ESI$^+$) spectrum of compound **9**.

III Computational Data

Table S1: Experimental and calculated bond lenghts (average) and their Wiberg bond indices (WBI) (avaerage) of **1**-**4** and **7**-**10**.

		1	**2**	**3**	**4**	**7**	**8**	**9**	**10**
M-E	Exp	2.357	2.464	2.342	2.337	2.457	2.243	--	2.249
	Cal	2.395	2.516	2.395	2.390	2.510	2.277	2.407	2.277
	WBI	0.688	0.717	0.669	0.674	0.707	0.732	0.745	0.736
B-μ_3E	Exp	1.971	2.179	1.990	1.959	2.056	1.987	--	1.942
	Cal	1.967	2.103	1.931	1.962	2.091	1.936	2.089	2.062
	WBI	0.881	0.897	0.908	0.885	0.915	0.903	0.919	0.715
B-μE	Exp	1.855	1.895	2.358	1.899	2.043	1.872	--	1.912
	Cal	1.878	2.019	2.377	1.908	2.033	1.893	2.032	1.866
	WBI	1.037	1.054	0.803	0.992	1.026	1.015	1.029	1.105
E-E	Exp	2.100	2.377	2.077	1.987	2.344	1.990	--	2.150
	Cal	2.104	2.403	2.103	2.090	2.377	2.091	2.831	2.090
	WBI	0.954	0.914	0.954	0.976	0.957	0.993	0.958	1.025

Table S2: Experimentally observed and calculated ^{11}B chemical shifts of **1-4** and **7-10**.

		1	**2**	**3**	**4**	**7**	**8**	**9**	**10**
B1	Exp	1.4	-7.9	-2.6	4.2	-2.0	3.4	-4.8	-4.5
	Cal	6.99	12.89	-8.48	1.00	12.78	4.83	9.43	2.02
B2	Exp	-0.1	-8.7	-2.6	1.6	-4.1	0.9	-10.0	--
	Cal	-1.91	2.82	-8.48	6.14	9.90	3.39	8.23	--

Table S3: Calculated (DFT) energies of the HOMO and LUMO (eV) and HOMO-LUMO gaps ($\Delta E = E_{LUMO} - E_{HOMO}$, eV) for compounds **1-10**.

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
HOMO	-5.41	-5.24	-4.94	-5.20	-5.42	-5.25	-4.97	-5.60	-5.37	-4.72
LUMO	-1.21	-1.44	-1.18	-1.41	-1.74	-1.80	-2.03	-1.99	-2.06	-2.37
E	4.20	3.80	3.76	3.79	3.68	3.40	2.94	3.61	3.31	2.35

Table S4: DFT-calculated MO compositions for compounds **1**-**10**

	M		**μ-E**		**μ_3-E**		**B**	
	HOMO	**LUMO**	**HOMO**	**LUMO**	**HOMO**	**LUMO**	**HOMO**	**LUMO**
1	26.78	38.72	32.66	6.27	19.12	26.20	1.34	2.38
2	5.61	25.66	70.95	24.73	13.41	30.33	2.48	2.36
3	22.65	39.74	48.91	17.93	10.94	10.16	2.15	2.47
4	10.61	39.64	76.54	18.7	7.80	14.18	2.80	0.62
5	16.07	41.59	48.46	3.63	17.07	26.38	5.46	1.14
6	7.50	39.88	67.41	5.98	13.9	28.33	2.15	0.83
7	19.03	39.57	55.49	8.80	12.40	21.47	0.99	0.94
8	10.69	48.88	61.19	3.32	16.27	21.75	2.28	1.60
9	6.52	47.42	69.87	5.07	15.51	23.66	2.70	1.40
10	17.45	35.19	46.15	7.34	25.94	31.24	3.97	1.87

Table S5: Calculated natural charges (q) and natural valence population (pop) of **1-10**.

		1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
M1	q	-0.1302	-0.2841	-0.1730	-0.1181	-0.4221	-0.5426	-0.5431	-0.4210	-0.5142	-0.5142
	pop	9.1022	9.2582	9.1488	9.0887	9.3930	9.5181	9.5221	9.3873	9.4845	9.4046
M2	q	-0.0880	-0.2641	-0.1730	-0.1253	-0.3847	-0.5121	-0.5347	-0.3877	-0.4878	-0.4227
	pop	9.0580	9.2171	9.1488	9.0984	9.3523	9.4839	9.5134	9.3533	9.4558	9.3905
B1	q	-0.3044	-0.4234	-0.4041	-0.3465	-0.3119	-0.4290	-0.4617	-0.3505	-0.4694	-0.3241
	pop	3.2802	3.3953	3.3861	3.3216	3.2871	3.4028	3.4353	3.3269	3.4426	3.2963
B2	q	-0.3463	-0.4660	-0.4041	-0.3485	-0.3526	-0.4714	-0.4578	-0.3082	-0.4261	--
	pop	6.0018	3.4387	3.3861	3.3278	3.3291	3.4437	3.4303	3.2828	3.3994	--
E1	q	-0.0398	-0.0161	-0.1164	-0.0561	-0.0505	-0.0125	-0.0323	-0.0572	-0.0225	-0.0605
	pop	5.9979	5.9922	6.0726	6.0138	6.0053	5.9938	6.0055	6.0113	5.9956	6.0145
E2	q	-0.0430	-0.0049	-0.1164	-0.0381	-0.0460	-0.0111	-0.0013	-0.0528	-0.0173	-0.0308
	pop	6.0018	5.9881	6.0726	5.9964	6.0024	5.9867	5.9768	6.0088	5.9922	5.9756
E3	q	0.1285	0.2303	0.2174	-0.0477	0.2143	0.2921	-0.0795	0.2158	0.2845	-0.0307
	pop	5.8058	5.7205	5.7251	6.0056	5.7300	5.6640	6.0522	5.7319	5.6746	5.9659
E4	q	0.1368	0.2813	0.2290	0.1379	0.1822	0.3179	0.2769	0.1658	0.3374	-0.1448
	pop	5.8210	5.6924	5.7043	5.7914	5.7797	5.6589	5.6822	5.6870	5.6289	6.1145
E5	q	0.2154	0.3102	0.2289	0.1383	0.2597	0.3431	0.2954	0.2600	0.2979	0.2229
	pop	5.7254	5.6485	5.7044	5.7946	5.6854	5.6222	5.6814	5.7977	5.6792	5.7235
E6	q	0.0688	0.2813	0.2175	0.1241	0.1576	0.2958	0.3479	0.1328	0.2591	0.2160
	pop	5.8834	5.7388	5.7251	5.8348	5.8033	5.6739	5.6166	5.8311	5.7094	5.7313
E7	q	--	--	--	0.2215	--	--	0.3783	--	--	0.1648
	pop	--	--	--	5.7137	--	--	5.5822	--	--	5.7831

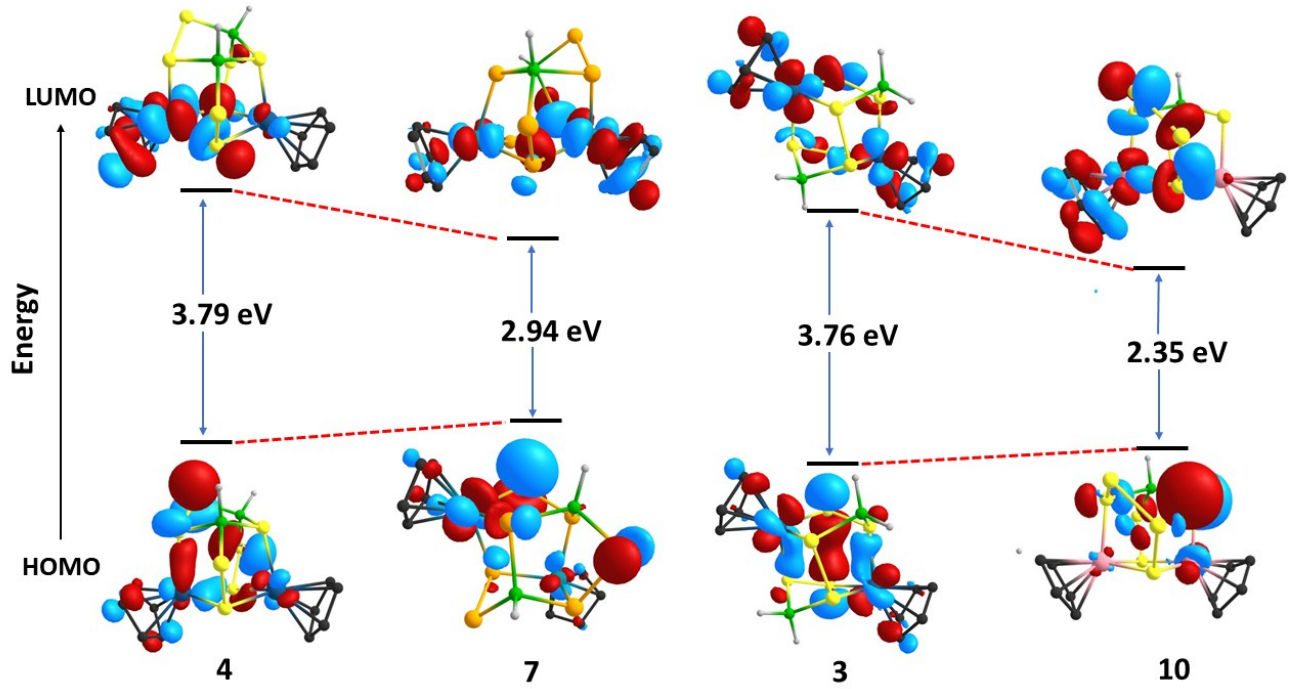


Figure S39. Frontier molecular orbital (MO) diagram of **4** and **7** (trishomocubanes) and **3** and **10** (bishomocubanes with broken edge). Isosurfaces are plotted at an isovalue of 0.04 $(e/bohr^3)^{1/2}$. Methyl groups of Cp* are removed for clarity.

Cp* groups have been omitted from the **Figures 47-56** for clarity.

Figure 40. Optimized geometry of compound **1**.

T. E. = −3429.89405171 a. u.

Ir	1.873145000	0.019148000	-0.050390000
C	3.224229000	1.388272000	-1.209646000
C	3.858575000	0.103217000	-1.062823000
C	4.085012000	-0.108973000	0.352354000
C	3.553746000	1.004839000	1.062783000
C	3.012353000	1.943300000	0.090477000
C	2.895188000	2.042658000	-2.512521000
H	3.774393000	2.563051000	-2.905121000
H	2.095305000	2.773317000	-2.404102000
H	2.578327000	1.313644000	-3.257114000
C	4.376512000	-0.760101000	-2.170255000
H	3.773692000	-0.657989000	-3.071742000
H	4.370593000	-1.812723000	-1.889954000
H	5.406679000	-0.489493000	-2.425801000
C	4.803512000	-1.280443000	0.939705000
H	5.885660000	-1.144485000	0.848156000
H	4.538537000	-2.206586000	0.430513000
H	4.569166000	-1.406648000	1.995236000
C	3.625752000	1.241442000	2.537561000
H	4.494671000	1.859876000	2.784508000
H	3.711027000	0.306960000	3.089379000
H	2.737788000	1.757387000	2.902191000
C	2.493281000	3.310387000	0.407502000
H	3.318074000	4.022300000	0.517725000
H	1.928418000	3.315394000	1.339494000
H	1.839225000	3.682725000	-0.380063000
Ir	-1.784112000	0.127652000	0.014630000
C	-3.217836000	1.175301000	-1.368448000
C	-2.631187000	2.135079000	-0.455499000
C	-3.054942000	1.774054000	0.874892000
C	-3.849076000	0.588572000	0.794880000
C	-3.955770000	0.223686000	-0.606996000
C	-3.115317000	1.231614000	-2.858202000
H	-3.325626000	0.264171000	-3.310595000
H	-2.119081000	1.535442000	-3.178127000
H	-3.833236000	1.954577000	-3.258101000
C	-1.917371000	3.389743000	-0.851009000
H	-1.312954000	3.236454000	-1.744596000
H	-1.256654000	3.739754000	-0.058691000
H	-2.629801000	4.193215000	-1.066861000
C	-2.760741000	2.548301000	2.118729000
H	-2.760921000	1.908212000	2.999498000
H	-3.519453000	3.323192000	2.265855000
H	-1.789118000	3.037348000	2.066839000
C	-4.569859000	-0.080939000	1.921955000
H	-5.597549000	0.289207000	1.996693000
H	-4.078602000	0.103187000	2.876148000
H	-4.616177000	-1.160154000	1.780227000
C	-4.787952000	-0.894756000	-1.147757000
H	-5.818606000	-0.560113000	-1.303165000
H	-4.814386000	-1.740310000	-0.461703000
H	-4.404249000	-1.257403000	-2.099825000
S	0.078196000	0.401973000	1.474324000
S	0.060169000	-1.285181000	2.762008000
S	1.376061000	-2.323164000	0.053688000
S	0.005799000	-0.212615000	-1.561954000
S	-1.755829000	-2.217500000	0.437188000
S	-1.297137000	-3.128486000	-1.395790000
B	0.304445000	-2.157323000	-1.583773000
H	0.919600000	-2.475085000	-2.559741000
B	-0.052813000	-2.546328000	1.379911000
H	-0.063273000	-3.665746000	1.798194000

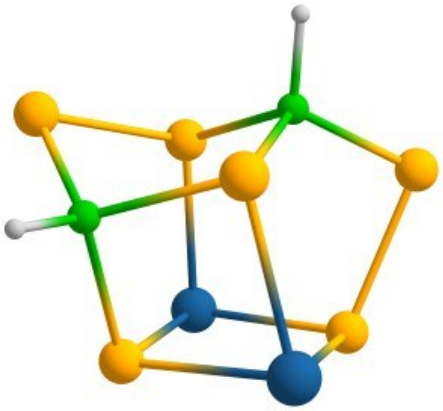


Figure 41. Optimized geometry of compound **2**.
T. E. = −15450.12435840 a. u.

Ir	2.028591000	0.230193000	-0.173025000
C	3.461601000	1.358680000	-1.488178000
C	4.021185000	0.071565000	-1.172795000
C	4.233852000	0.028405000	0.260564000
C	3.769502000	1.254942000	0.816130000
C	3.281439000	2.089022000	-0.270068000
C	3.184284000	1.868243000	-2.865662000
H	4.084268000	2.331265000	-3.282783000
H	2.393077000	2.616319000	-2.866055000
H	2.880600000	1.066153000	-3.536704000
C	4.489060000	-0.955218000	-2.155793000
H	3.892998000	-0.936872000	-3.067239000
H	4.424505000	-1.960940000	-1.742285000
H	5.532819000	-0.777194000	-2.436065000
C	4.902064000	-1.086042000	0.998978000
H	5.989999000	-0.991405000	0.922636000
H	4.622963000	-2.058119000	0.593715000
H	4.638628000	-1.082125000	2.055333000
C	3.865441000	1.674731000	2.247969000
H	4.784712000	2.244558000	2.417514000
H	3.874403000	0.816348000	2.917550000
H	3.026627000	2.307899000	2.536224000
C	2.854265000	3.517510000	-0.142807000
H	3.722235000	4.185347000	-0.157211000
H	2.321024000	3.692861000	0.791231000
H	2.197933000	3.812659000	-0.960761000
Ir	-1.783370000	0.570593000	-0.054309000
C	-3.187080000	1.572543000	-1.500943000
C	-2.522106000	2.574625000	-0.693948000
C	-2.934070000	2.367325000	0.672254000
C	-3.800660000	1.231249000	0.719822000
C	-3.962850000	0.744300000	-0.637929000
C	-3.139289000	1.492493000	-2.992381000
H	-3.383523000	0.492806000	-3.347613000
H	-2.152226000	1.747462000	-3.376399000
H	-3.860551000	2.190839000	-3.428886000
C	-1.745788000	3.741227000	-1.219672000
H	-1.172438000	3.469251000	-2.105360000
H	-1.047361000	4.124281000	-0.476593000
H	-2.416249000	4.561507000	-1.497710000
C	-2.580437000	3.244895000	1.828935000
H	-2.584795000	2.694110000	2.768250000
H	-3.306233000	4.059713000	1.914536000
H	-1.593196000	3.689126000	1.711189000
C	-4.540258000	0.727427000	1.918527000
H	-5.528658000	1.193839000	1.985286000
H	-4.004518000	0.947670000	2.840621000
H	-4.686259000	-0.351196000	1.873974000
C	-4.885578000	-0.353199000	-1.061863000
H	-5.882813000	0.049546000	-1.266613000
H	-4.988334000	-1.111836000	-0.287321000
H	-4.531655000	-0.850548000	-1.963496000
B	0.243304000	-2.082497000	-1.624585000
H	0.846995000	-2.467928000	-2.580957000
B	-0.103607000	-2.261598000	1.565838000
H	-0.176801000	-3.364402000	2.015459000
Se	-1.518995000	-3.046040000	-1.400517000
Se	-1.935605000	-1.839106000	0.617668000
Se	0.134465000	-0.883529000	3.019632000
Se	0.036751000	0.012048000	-1.725639000
Se	0.219580000	0.917447000	1.408249000
Se	1.414213000	-2.198154000	0.117907000

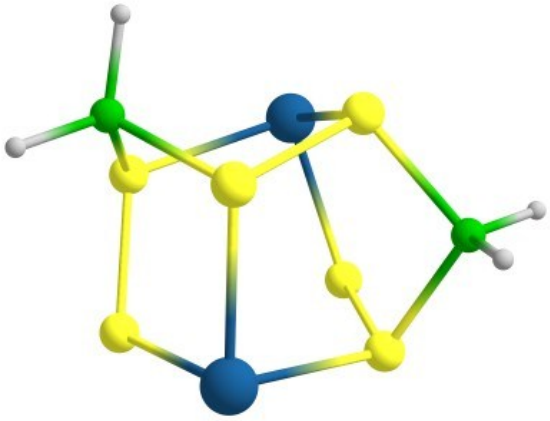


Figure 42. Optimized geometry of compound **3**.

T. E. = −3828.04688178 a. u.

C	4.158000000	-1.059661000	0.486909000
C	4.116898000	0.219395000	1.178318000
C	4.084268000	1.254686000	0.201964000
C	4.082366000	0.634035000	-1.110988000
C	4.173572000	-0.788469000	-0.918398000
C	4.313830000	-1.809727000	-1.999570000
H	3.840240000	-2.750788000	-1.726151000
H	5.374248000	-2.003971000	-2.188519000
H	3.864988000	-1.473138000	-2.932770000
C	4.340006000	-2.397336000	1.131764000
H	5.403838000	-2.618731000	1.268025000
H	3.907285000	-3.192792000	0.527066000
H	3.866796000	-2.436227000	2.112112000
C	4.205373000	0.395933000	2.659923000
H	5.247209000	0.322316000	2.987227000
H	3.636726000	-0.368093000	3.189221000
H	3.822970000	1.366118000	2.972119000
C	4.143936000	2.726242000	0.457676000
H	3.774959000	2.978053000	1.450283000
H	3.550165000	3.283148000	-0.266410000
H	5.177306000	3.079417000	0.382078000
C	4.176724000	1.362039000	-2.414835000
H	3.792139000	0.759933000	-3.236596000
H	5.217614000	1.614541000	-2.642589000
H	3.606518000	2.289929000	-2.393146000
C	-4.084385000	-1.254806000	0.200883000
C	-4.116970000	-0.220337000	1.178141000
C	-4.158045000	1.059307000	0.487780000
C	-4.173590000	0.789315000	-0.917725000
C	-4.082333000	-0.633054000	-1.111536000
C	-4.144062000	-2.726586000	0.455306000
H	-5.177275000	-3.079890000	0.378221000
H	-3.776185000	-2.979141000	1.448129000
H	-3.549347000	-3.282795000	-0.268547000
C	-4.205577000	-0.398023000	2.659604000
H	-3.636072000	0.364948000	3.189513000
H	-3.824181000	-1.368867000	2.970973000
H	-5.247312000	-0.323568000	2.987036000
C	-4.339988000	2.396490000	1.133664000
H	-3.905764000	3.192222000	0.530398000
H	-3.868218000	2.434029000	2.114755000
H	-5.403853000	2.618560000	1.268560000
C	-4.313670000	1.811455000	-1.998074000
H	-5.374066000	2.005578000	-2.187292000
H	-3.864393000	1.475752000	-2.931386000
H	-3.840448000	2.752407000	-1.723674000
C	-4.176776000	-1.359779000	-2.416090000
H	-5.217979000	-1.609577000	-2.645411000
H	-3.608843000	-2.289053000	-2.394390000
H	-3.789641000	-0.757966000	-3.236877000
S	-0.847103000	0.660843000	1.779177000
S	-0.945856000	1.396260000	-1.497856000
S	-0.809379000	-1.860688000	-0.482254000
S	0.809374000	1.860743000	-0.482057000
S	0.945777000	-1.396073000	-1.498102000
S	0.847200000	-0.661238000	1.779085000
Ir	2.239961000	-0.025081000	-0.049734000
Ir	-2.239931000	0.025021000	-0.049637000
B	-0.094371000	-2.269779000	1.260353000
H	-0.997586000	-2.455134000	2.029192000
B	0.094454000	2.269514000	1.260692000
H	0.997733000	2.454712000	2.029487000
H	-0.716421000	3.147285000	1.175025000
H	0.716450000	-3.147569000	1.174462000

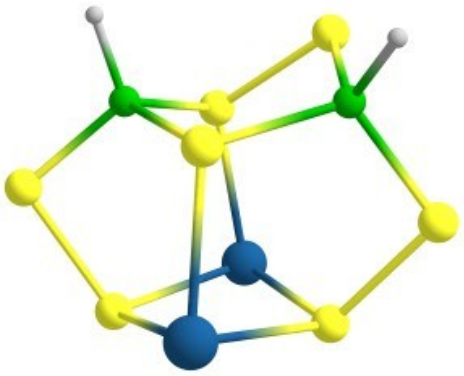


Figure 43. Optimized geometry of compound **4**.

T. E. = −3828.12148953 a. u.

C	-3.996211000	-0.110831000	-0.711489000
C	-3.952492000	0.242806000	0.699430000
C	-3.432416000	-0.878024000	1.413804000
C	-3.113711000	-1.918159000	0.464774000
C	-3.494365000	-1.437405000	-0.845615000
C	-4.577213000	0.741590000	-1.793332000
H	-4.312343000	1.789587000	-1.657502000
H	-5.669453000	0.668056000	-1.790406000
H	-4.223094000	0.437418000	-2.776860000
C	-4.491561000	1.504857000	1.293497000
H	-5.567148000	1.412717000	1.476418000
H	-4.338570000	2.353358000	0.627936000
H	-4.007301000	1.738252000	2.240375000
C	-3.287223000	-0.976379000	2.897884000
H	-2.486259000	-1.659039000	3.177792000
H	-4.215411000	-1.348880000	3.342218000
H	-3.066602000	-0.006846000	3.342249000
C	-2.685731000	-3.313773000	0.796529000
H	-2.065926000	-3.339292000	1.692061000
H	-2.112933000	-3.758703000	-0.016424000
H	-3.554951000	-3.954972000	0.977418000
C	-3.420452000	-2.229032000	-2.111500000
H	-2.567450000	-2.906655000	-2.110472000
H	-4.325597000	-2.832190000	-2.232641000
H	-3.328448000	-1.583283000	-2.983165000
C	3.342760000	-0.813979000	1.510185000
C	3.995298000	-0.045540000	0.501019000
C	3.869639000	-0.752326000	-0.757731000
C	3.149148000	-1.965229000	-0.500782000
C	2.805936000	-2.010371000	0.895129000
C	3.294558000	-0.496557000	2.969917000
H	4.122533000	-0.988072000	3.490633000
H	2.365650000	-0.841065000	3.423052000
H	3.371929000	0.574224000	3.149672000
C	4.765752000	1.217751000	0.713169000
H	4.741729000	1.853941000	-0.170296000
H	4.368545000	1.796352000	1.545488000
H	5.813828000	0.987623000	0.929859000
C	4.510804000	-0.350200000	-2.047601000
H	5.565956000	-0.641541000	-2.063232000
H	4.462349000	0.728322000	-2.196388000
H	4.022463000	-0.820074000	-2.900035000
C	2.869467000	-3.039226000	-1.501731000
H	1.960000000	-3.587188000	-1.260654000
H	2.754712000	-2.632791000	-2.505326000
H	3.696943000	-3.755143000	-1.522559000
C	2.179431000	-3.155788000	1.626229000
H	1.576751000	-3.772864000	0.960881000
H	2.945425000	-3.799354000	2.071158000
H	1.533464000	-2.807187000	2.432036000
Ir	-1.854165000	-0.137314000	-0.007174000
Ir	1.797956000	-0.221868000	-0.021231000
S	-0.043604000	0.013000000	1.508940000
S	-0.062724000	-0.870335000	-1.384033000
S	-1.354108000	2.138425000	-0.629205000
S	-0.290093000	1.889799000	2.387888000
S	-0.128113000	0.448576000	-3.040891000
S	1.718035000	1.924166000	-1.068321000
S	1.384004000	3.508997000	0.214856000
B	0.017352000	2.015109000	-2.019788000
B	-0.375519000	3.025099000	0.844839000
H	0.024388000	2.989965000	-2.710139000
H	-0.929168000	4.034091000	1.180331000

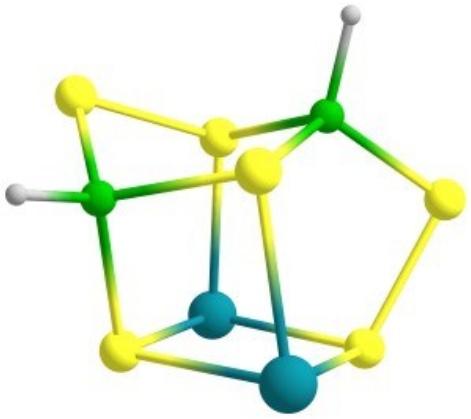


Figure 44. Optimized geometry of compound **5**.

T. E. = −3442.31076930 a. u.

Rh	1.849898000	0.018986000	-0.055722000
C	3.200538000	1.401080000	-1.213532000
C	3.820941000	0.111044000	-1.088448000
C	4.075466000	-0.117625000	0.314700000
C	3.558201000	0.983916000	1.043924000
C	3.006287000	1.933175000	0.092857000
C	2.861311000	2.073062000	-2.504445000
H	3.746511000	2.567779000	-2.916892000
H	2.088850000	2.829257000	-2.374140000
H	2.503440000	1.359541000	-3.245701000
C	4.300296000	-0.750261000	-2.213908000
H	3.676377000	-0.635930000	-3.099469000
H	4.292869000	-1.804634000	-1.940168000
H	5.326171000	-0.487840000	-2.494605000
C	4.798955000	-1.299176000	0.873877000
H	5.879399000	-1.174691000	0.749603000
H	4.509778000	-2.220411000	0.368629000
H	4.597816000	-1.428614000	1.935865000
C	3.645773000	1.201546000	2.520317000
H	4.510056000	1.827415000	2.765623000
H	3.750323000	0.261635000	3.059530000
H	2.756763000	1.702454000	2.903354000
C	2.485868000	3.292152000	0.439379000
H	3.310138000	4.002379000	0.564147000
H	1.922883000	3.277476000	1.372542000
H	1.831563000	3.682227000	-0.339384000
Rh	-1.747105000	0.144800000	0.019505000
C	-3.199840000	1.160563000	-1.369655000
C	-2.591355000	2.139686000	-0.498702000
C	-2.997142000	1.833661000	0.844659000
C	-3.791667000	0.650003000	0.817434000
C	-3.927445000	0.242358000	-0.565832000
C	-3.124893000	1.169480000	-2.861655000
H	-3.359014000	0.192398000	-3.280518000
H	-2.130886000	1.448356000	-3.210507000
H	-3.839192000	1.890726000	-3.271748000
C	-1.856083000	3.362386000	-0.949057000
H	-1.256307000	3.160053000	-1.836145000
H	-1.189344000	3.737442000	-0.173365000
H	-2.555068000	4.167502000	-1.200195000
C	-2.682699000	2.647411000	2.057373000
H	-2.634218000	2.031526000	2.954133000
H	-3.458702000	3.403749000	2.212957000
H	-1.729301000	3.164403000	1.960198000
C	-4.488120000	0.018962000	1.981012000
H	-5.510016000	0.401388000	2.074033000
H	-3.970575000	0.224226000	2.916991000
H	-4.550014000	-1.063158000	1.870594000
C	-4.770474000	-0.890356000	-1.055827000
H	-5.795473000	-0.550605000	-1.236600000
H	-4.814554000	-1.699722000	-0.328369000
H	-4.385744000	-1.305586000	-1.986079000
S	0.091099000	0.429388000	1.497806000
S	0.070499000	-1.256526000	2.762358000
S	1.373581000	-2.314558000	0.047308000
S	0.010999000	-0.190045000	-1.576314000
S	-1.748950000	-2.199097000	0.449044000
S	-1.311958000	-3.090294000	-1.390718000
B	0.301583000	-2.128477000	-1.583286000
H	0.910187000	-2.461150000	-2.559001000
B	-0.044990000	-2.525504000	1.379932000
H	-0.051225000	-3.640337000	1.812655000

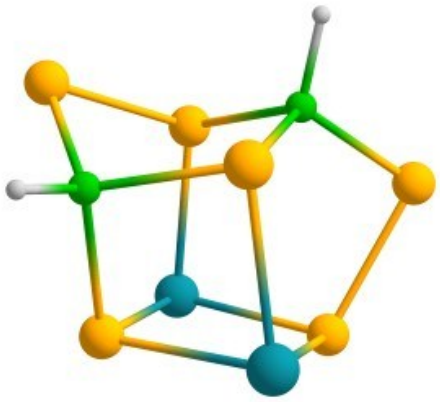


Figure 45. Optimized geometry of compound **6**.

T. E. = −15462.54320020 a. u.

Rh	2.020943000	0.247123000	-0.201113000
C	3.458560000	1.364054000	-1.532474000
C	3.992354000	0.066404000	-1.230677000
C	4.237867000	0.013156000	0.192394000
C	3.802650000	1.238416000	0.761160000
C	3.307602000	2.082459000	-0.310070000
C	3.173308000	1.886394000	-2.903275000
H	4.079922000	2.321308000	-3.336706000
H	2.407908000	2.660805000	-2.889135000
H	2.832007000	1.097248000	-3.571792000
C	4.410652000	-0.968639000	-2.226653000
H	3.786807000	-0.941367000	-3.119208000
H	4.345021000	-1.973049000	-1.810103000
H	5.447557000	-0.807654000	-2.541216000
C	4.902746000	-1.115554000	0.911102000
H	5.990268000	-1.041987000	0.807703000
H	4.596422000	-2.081797000	0.511369000
H	4.668104000	-1.109328000	1.974279000
C	3.928034000	1.649190000	2.192947000
H	4.858161000	2.204885000	2.351317000
H	3.936538000	0.787902000	2.858971000
H	3.104026000	2.293566000	2.498763000
C	2.893110000	3.512426000	-0.162715000
H	3.767072000	4.172635000	-0.170171000
H	2.364441000	3.681197000	0.775278000
H	2.238763000	3.825884000	-0.975524000
Rh	-1.733219000	0.642719000	-0.066318000
C	-3.138414000	1.632845000	-1.521959000
C	-2.450210000	2.638585000	-0.747820000
C	-2.853973000	2.480885000	0.622478000
C	-3.729234000	1.358956000	0.707931000
C	-3.913426000	0.840381000	-0.631241000
C	-3.110509000	1.514717000	-3.010990000
H	-3.366467000	0.508304000	-3.338200000
H	-2.127577000	1.753784000	-3.415480000
H	-3.833036000	2.206142000	-3.457028000
C	-1.646005000	3.768097000	-1.309962000
H	-1.085841000	3.457079000	-2.191258000
H	-0.934054000	4.155035000	-0.581791000
H	-2.296175000	4.597738000	-1.608086000
C	-2.480328000	3.385627000	1.751133000
H	-2.464854000	2.857880000	2.703604000
H	-3.206805000	4.200606000	1.833282000
H	-1.497567000	3.831211000	1.604646000
C	-4.456820000	0.892936000	1.928672000
H	-5.440706000	1.369049000	1.996298000
H	-3.908689000	1.133935000	2.838350000
H	-4.613484000	-0.185102000	1.915160000
C	-4.855017000	-0.254248000	-1.017576000
H	-5.842982000	0.159314000	-1.245467000
H	-4.979079000	-0.979520000	-0.214701000
H	-4.506977000	-0.793534000	-1.897472000
B	0.225810000	-2.035861000	-1.613796000
H	0.816078000	-2.451010000	-2.566365000
B	-0.103346000	-2.181037000	1.578229000
H	-0.181362000	-3.270910000	2.058886000
Se	-1.557720000	-2.966274000	-1.369624000
Se	-1.934311000	-1.751649000	0.642697000
Se	0.158095000	-0.775177000	3.009766000
Se	0.047022000	0.052372000	-1.750716000
Se	0.259193000	1.000463000	1.396357000
Se	1.399751000	-2.163297000	0.119743000

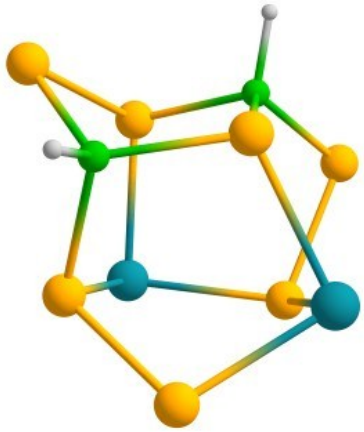


Figure 46. Optimized geometry of compound **7**.

T. E. = −17864.15199980 a. u.

Rh	1.953294000	-0.623247000	0.021335000
Rh	-2.271601000	-0.214403000	-0.169934000
Se	0.920725000	0.277654000	-2.056375000
Se	-1.132929000	-0.846852000	-2.298838000
Se	2.045927000	1.703324000	0.959030000
Se	1.912799000	3.163788000	-0.917181000
Se	-0.292753000	-1.083380000	1.093212000
Se	-0.300116000	0.492377000	2.897027000
Se	-1.179722000	2.086843000	-0.045948000
B	0.242222000	2.189666000	-1.559675000
H	-0.204828000	2.683112000	-2.549366000
B	0.090936000	2.028332000	1.629274000
H	0.074410000	3.076213000	2.200612000
C	3.954382000	-1.212823000	0.922818000
C	3.023053000	-2.257743000	1.166439000
C	2.587313000	-2.774395000	-0.116041000
C	3.278003000	-2.053878000	-1.134650000
C	4.089077000	-1.049349000	-0.505420000
C	4.742821000	-0.473614000	1.954284000
H	5.710539000	-0.963214000	2.104521000
H	4.230340000	-0.448586000	2.914595000
H	4.937103000	0.555536000	1.655569000
C	2.650713000	-2.826259000	2.497103000
H	1.607908000	-3.141907000	2.519147000
H	2.792542000	-2.102779000	3.298252000
H	3.267843000	-3.702228000	2.722638000
C	1.712020000	-3.969241000	-0.320110000
H	1.180802000	-3.918524000	-1.269641000
H	0.968315000	-4.057923000	0.470971000
H	2.309656000	-4.887025000	-0.317585000
C	3.228269000	-2.348591000	-2.597885000
H	3.981641000	-3.102235000	-2.849508000
H	3.432070000	-1.463052000	-3.197283000
H	2.256481000	-2.737963000	-2.899231000
C	5.059469000	-0.142494000	-1.193610000
H	5.212829000	0.779238000	-0.633996000
H	4.713534000	0.133452000	-2.188737000
H	6.034054000	-0.630119000	-1.303202000
C	-3.832184000	-1.021890000	1.265671000
C	-4.109493000	0.349455000	1.006032000
C	-4.379877000	0.489860000	-0.411177000
C	-4.267807000	-0.799386000	-1.005955000
C	-3.883401000	-1.738138000	0.018450000
C	-3.605751000	-1.630988000	2.610010000
H	-2.962230000	-2.508103000	2.551928000
H	-4.560321000	-1.948261000	3.042470000
H	-3.144354000	-0.923679000	3.297349000
C	-4.252516000	1.432131000	2.026630000
H	-4.004664000	2.407767000	1.610793000
H	-3.600893000	1.262293000	2.882365000
H	-5.284867000	1.477721000	2.389657000
C	-4.838187000	1.744112000	-1.082514000
H	-5.908106000	1.900999000	-0.909415000
H	-4.677681000	1.703911000	-2.158678000
H	-4.309161000	2.617061000	-0.701105000
C	-4.593532000	-1.145117000	-2.423155000
H	-4.402886000	-0.312261000	-3.097379000
H	-5.652896000	-1.409414000	-2.505808000
H	-4.014956000	-1.997468000	-2.777622000
C	-3.765820000	-3.219728000	-0.149707000
H	-3.089705000	-3.651314000	0.587495000
H	-3.386960000	-3.481552000	-1.137057000
H	-4.740462000	-3.704631000	-0.028610000

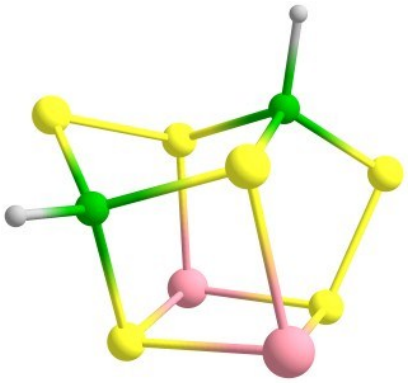


Figure 47. Optimized geometry of compound **8**.

T. E. = −5986.69737691 a. u.

C	-3.480446000	0.736050000	0.898683000
C	-3.739106000	0.171983000	-0.402195000
C	-3.057895000	0.952088000	-1.365789000
C	-2.382304000	2.021671000	-0.675967000
C	-2.689339000	1.905314000	0.712321000
C	-4.061109000	0.259560000	2.192355000
H	-3.425803000	0.522673000	3.037245000
H	-4.183833000	-0.822815000	2.201054000
H	-5.045878000	0.706200000	2.364493000
C	-4.638730000	-0.984859000	-0.692262000
H	-4.727339000	-1.653381000	0.161948000
H	-4.282537000	-1.571833000	-1.538233000
H	-5.642180000	-0.621495000	-0.936401000
C	-3.095524000	0.756106000	-2.846319000
H	-3.263120000	-0.287884000	-3.107298000
H	-2.163310000	1.067459000	-3.315525000
H	-3.906280000	1.346331000	-3.285931000
C	-1.644524000	3.141219000	-1.337888000
H	-2.345140000	3.887485000	-1.726482000
H	-1.048228000	2.782480000	-2.176776000
H	-0.976900000	3.649771000	-0.643872000
C	-2.295364000	2.864972000	1.786900000
H	-3.099968000	3.589957000	1.946737000
H	-1.395641000	3.420411000	1.528233000
H	-2.110952000	2.360165000	2.734082000
B	-0.025604000	-2.398415000	1.432193000
S	0.112732000	0.533838000	1.425437000
S	0.107878000	-1.074015000	2.771782000
S	-1.722578000	-2.056354000	0.515648000
S	0.014985000	-0.133920000	-1.550714000
S	-1.337800000	-2.999446000	-1.304378000
Co	-1.625216000	0.169639000	0.016494000
H	-0.042763000	-3.497060000	1.903576000
B	0.293470000	-2.064230000	-1.536193000
S	1.374257000	-2.223371000	0.088445000
C	3.827304000	-0.124121000	0.411905000
C	3.629903000	-0.057042000	-1.014590000
C	3.025502000	1.199940000	-1.312279000
C	2.773969000	1.874213000	-0.084282000
C	3.295382000	1.053089000	0.983351000
C	4.524873000	-1.228399000	1.136628000
H	4.245851000	-1.259151000	2.188761000
H	4.293168000	-2.201051000	0.704423000
H	5.609236000	-1.087874000	1.082459000
C	4.119390000	-1.063216000	-2.007220000
H	4.041743000	-2.078323000	-1.619240000
H	3.552157000	-1.021573000	-2.936099000
H	5.171101000	-0.881798000	-2.252679000
C	2.736070000	1.722161000	-2.681757000
H	2.455820000	0.924179000	-3.367676000
H	1.925436000	2.448864000	-2.675444000
H	3.624188000	2.216638000	-3.088332000
C	2.229628000	3.257807000	0.078544000
H	3.042532000	3.987965000	0.149453000
H	1.605823000	3.546041000	-0.766550000
H	1.630965000	3.348390000	0.985095000
C	3.326354000	1.430661000	2.429119000
H	4.225117000	2.015940000	2.648703000
H	2.463055000	2.035048000	2.705111000
H	3.333941000	0.553917000	3.074975000
Co	1.736294000	0.024244000	-0.066313000
H	0.885492000	-2.430214000	-2.509756000

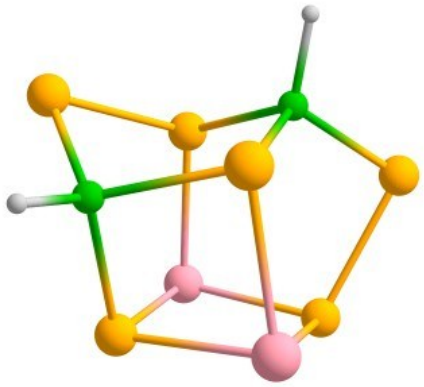


Figure 48. Optimized geometry of compound **9**.
T. E. = –18006.91942400 a. u.

C	-3.427607000	1.460657000	0.711523000
C	-3.705985000	0.826043000	-0.553441000
C	-2.955743000	1.489020000	-1.553999000
C	-2.202102000	2.540271000	-0.922937000
C	-2.541011000	2.543822000	0.465765000
C	-4.078096000	1.135092000	2.018678000
H	-3.438948000	1.396915000	2.861167000
H	-4.308523000	0.073651000	2.100162000
H	-5.017320000	1.686843000	2.129893000
C	-4.705785000	-0.259017000	-0.791061000
H	-4.883316000	-0.851804000	0.104426000
H	-4.386403000	-0.938079000	-1.581125000
H	-5.662731000	0.178752000	-1.093518000
C	-3.015965000	1.209959000	-3.020577000
H	-3.219332000	0.158710000	-3.220690000
H	-2.083186000	1.466378000	-3.520131000
H	-3.815809000	1.799163000	-3.481383000
C	-1.373051000	3.561169000	-1.635309000
H	-2.003179000	4.370712000	-2.018249000
H	-0.846978000	3.125366000	-2.484273000
H	-0.630976000	4.009277000	-0.975649000
C	-2.103977000	3.553900000	1.475937000
H	-2.847820000	4.354916000	1.539083000
H	-1.149947000	4.008482000	1.215026000
H	-2.002134000	3.118758000	2.469180000
B	-0.098901000	-2.005180000	1.662442000
Se	0.312497000	1.123003000	1.268182000
Se	0.212080000	-0.511444000	3.005779000
Se	-1.916917000	-1.558437000	0.731862000
Se	0.051278000	0.059625000	-1.746363000
Se	-1.620806000	-2.882585000	-1.217118000
Co	-1.607584000	0.687996000	-0.099156000
H	-0.200297000	-3.059498000	2.212361000
B	0.190635000	-2.015524000	-1.528510000
Se	1.378341000	-2.089020000	0.194615000
C	4.006788000	-0.031029000	0.226165000
C	3.784302000	-0.143369000	-1.193881000
C	3.274208000	1.105444000	-1.655038000
C	3.107019000	1.961462000	-0.528711000
C	3.587847000	1.255898000	0.634284000
C	4.648337000	-1.066205000	1.091873000
H	4.334253000	-0.973601000	2.130707000
H	4.405398000	-2.075246000	0.762268000
H	5.737620000	-0.958794000	1.061910000
C	4.179045000	-1.305812000	-2.048723000
H	4.062507000	-2.251144000	-1.520055000
H	3.579179000	-1.360611000	-2.956298000
H	5.228575000	-1.222263000	-2.350026000
C	3.016010000	1.468596000	-3.081252000
H	2.706133000	0.606710000	-3.670174000
H	2.238860000	2.225512000	-3.173693000
H	3.928641000	1.870529000	-3.533560000
C	2.684750000	3.396264000	-0.562584000
H	3.554615000	4.054021000	-0.661812000
H	2.024422000	3.600569000	-1.404785000
H	2.162302000	3.683220000	0.349989000
C	3.705732000	1.824454000	2.011735000
H	4.679074000	2.309858000	2.137222000
H	2.937669000	2.571275000	2.208516000
H	3.618971000	1.052941000	2.775805000
Co	1.926722000	0.223411000	-0.241689000
H	0.754903000	-2.494520000	-2.466341000

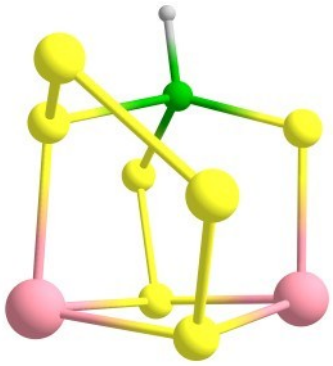


Figure 49. Optimized geometry of compound **10**.

T. E. = −6359.38284708 a. u.

C	3.401586000	1.072965000	-0.774551000
C	3.749623000	0.124364000	0.255191000
C	3.141298000	0.541571000	1.459710000
C	2.439445000	1.777122000	1.201551000
C	2.650798000	2.121247000	-0.163576000
C	3.878142000	1.050781000	-2.191546000
H	3.142092000	1.484653000	-2.867103000
H	4.071351000	0.035193000	-2.532652000
H	4.807204000	1.620899000	-2.294584000
C	4.653853000	-1.052017000	0.092278000
H	4.708263000	-1.379538000	-0.943831000
H	4.325272000	-1.900531000	0.691669000
H	5.666154000	-0.786201000	0.413090000
C	3.261081000	-0.124315000	2.791859000
H	3.507408000	-1.179854000	2.691319000
H	2.334278000	-0.053954000	3.360476000
H	4.051159000	0.349914000	3.383084000
C	1.776374000	2.624063000	2.239806000
H	2.516732000	3.247163000	2.752197000
H	1.279286000	2.016385000	2.994693000
H	1.034421000	3.291199000	1.803300000
C	2.217493000	3.381706000	-0.836077000
H	3.024604000	4.119795000	-0.784492000
H	1.339018000	3.816867000	-0.362926000
H	1.981503000	3.220067000	-1.886479000
B	-0.193018000	-1.709559000	-2.272273000
S	-0.139649000	1.035568000	-1.231188000
S	0.032537000	0.022215000	-3.050507000
S	1.559298000	-1.693913000	-1.186303000
S	-0.037694000	-0.471033000	1.396568000
S	0.196422000	-2.512520000	1.731659000
S	1.612941000	-3.146259000	0.260614000
Co	1.607435000	0.257282000	-0.009356000
H	-0.034856000	-2.573875000	-3.086580000
S	-1.684964000	-1.892485000	-1.210672000
C	-3.880693000	-0.347785000	0.252228000
C	-3.299819000	0.042989000	1.485750000
C	-2.770391000	1.373330000	1.330680000
C	-3.018541000	1.782897000	-0.006619000
C	-3.662699000	0.706506000	-0.696236000
C	-4.660203000	-1.594058000	-0.003781000
H	-4.472873000	-1.983714000	-1.002976000
H	-4.414568000	-2.379548000	0.708842000
H	-5.730611000	-1.380876000	0.085506000
C	-3.324643000	-0.738993000	2.759786000
H	-3.307033000	-1.811961000	2.572370000
H	-2.472104000	-0.498929000	3.394385000
H	-4.232700000	-0.515802000	3.329343000
C	-2.199702000	2.207156000	2.433343000
H	-1.543666000	1.624527000	3.080719000
H	-1.626615000	3.049369000	2.047506000
H	-2.998708000	2.615620000	3.060460000
C	-2.726791000	3.128260000	-0.588333000
H	-3.611687000	3.767402000	-0.505163000
H	-1.908626000	3.628843000	-0.072411000
H	-2.462818000	3.065187000	-1.642776000
C	-4.153915000	0.718825000	-2.107911000
H	-5.211225000	1.001344000	-2.149633000
H	-3.597039000	1.426850000	-2.720292000
H	-4.045260000	-0.264061000	-2.564639000
Co	-1.778149000	0.025329000	-0.011203000

Notes and References

(1) (a) ^{11}B spectra were processed with backward linear prediction algorithm to remove broad ^{11}B background signal from NMR probe and NMR tube; (b) H. Gesmar and J. J. Led, *Chem. Rev*., 1991, **91**, 1413; (c) L. Yang, R. Simionescua, A. Lough and H. Yan, *Dyes and Pigments,* 2011, **91**, 264; (d) R. Weiss and R. N. Grimes, *J. Am. Chem. Soc*., 1978, **100**, 1401.