Electronic Supporting Information for

The „chemical tug-of-war" in carborane clusters: distinct tuning on different sides of the cluster

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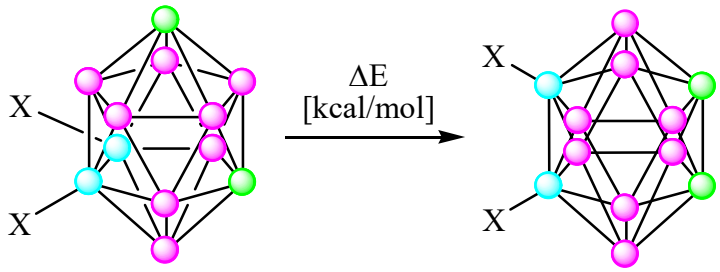
Table of Contents

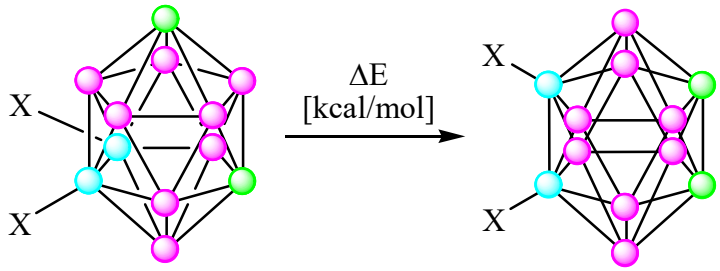
Computational results and details

Table S1. Test of different method, using def2-TZVP basis set.



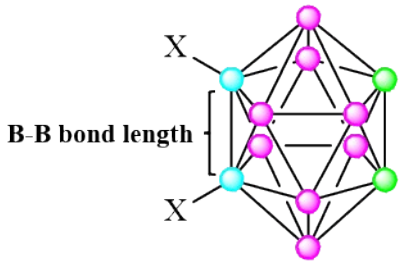
X	B3LYP	ωB97X-D	M06-2X	BP86	PBEh1BE	PW6B95	B3LYP-D3	B3PW91	B3PW91-D3	LNO-CCSD(T)
SH	15.4	15.8	16.1	14.3	15.0	15.4	15.2	15.2	14.9	15.2
S^-	18.6	19.0	19.2	17.1	18.1	18.6	18.4	18.2	18.0	12.7
NH_2	15.3	15.4	15.7	14.3	14.8	15.3	15.1	15.0	14.8	15.0

Table S2. Test of different method, using aug-cc-pVTZ basis set.



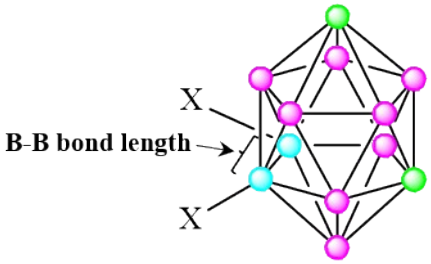
X	B3LYP	ωB97X-D	M06-2X	BP86	PBEh1BE	PW6B95	B3LYP-D3	B3PW91	B3PW91-D3	LNO-CCST(T)
SH	15.4	15.8	15.9	14.3	14.9	15.3	15.2	15.1	15.0	15.2
S^-	18.5	19.0	19.2	16,5	18.0	18.5	18.4	18.2	18.0	18.7
NH_2	15.3	15.3	15.7	14.2	14.8	15.2	15.1	15.0	14.9	15.0

Table S3. Test of different method for the B-B bond length in *o*-carborane, using def2-TZVP basis set.



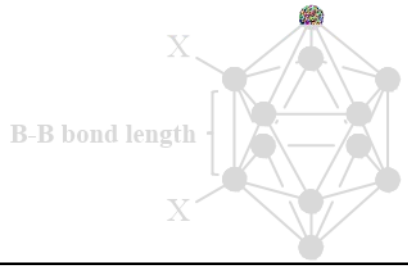
X	B3LYP	ωB97X-D	M06-2X	BP86	PBEh1BE	PW6B95	B3LYP-D3	B3PW91	B3PW91-D3
SH	1.786	1.780	1.785	1.794	1.793	1.785	1.801	1.796	1.797
S^-	1.950	1.926	1.915	1.960	1.931	1.924	1.949	1.936	1.939
NH_2	1.822	1.812	1.806	1.830	1.812	1.807	1.820	1.818	1.818

Table S4. Test of different method for the B-B bond length in *m*-carborane, using def2-TZVP basis set



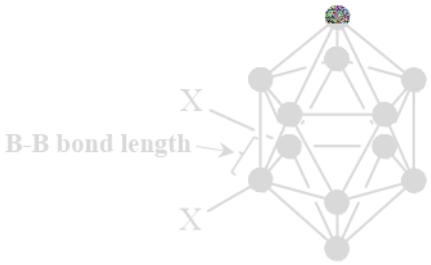
X	B3LYP	ωB97X-D	M06-2X	BP86	PBEh1BE	PW6B95	B3LYP-D3	B3PW91	B3PW91-D3
SH	1.797	1.789	1.791	1.803	1.805	1.799	1.816	1.808	1.808
S^-	1.982	1.956	1.938	1.992	1.957	1.951	1.980	1.966	1.966
NH_2	1.844	1.828	1.822	1.851	1.833	1.827	1.842	1.836	1.837

Table S5. Test of different method for the B-B bond length in *o*-carborane, using aug-cc-pVTZ basis set



X	B3LYP	ωB97X-D	M06-2X	BP86	PBEh1BE	PW6B95	B3LYP-D3	B3PW91	B3PW91-D3
SH	1.799	1.790	1.778	1.806	1.792	1.784	1.800	1.796	1.796
S^-	1.942	1.917	1.909	1.943	1.926	1.918	1.941	1.931	1.930
NH_2	1.823	1.810	1.806	1.831	1.816	1.808	1.820	1.819	1.816

Table S6. Test of different method for the B-B bond length in *m*-carborane, using aug-cc-pVTZ basis set



X	B3LYP	ωB97X-D	M06-2X	BP86	PBEh1BE	PW6B95	B3LYP-D3	B3PW91	B3PW91-D3
SH	1.814	1.798	1.790	1.820	1.804	1.792	1.815	1.808	1.809
S^-	1.975	1.945	1.931	1.984	1.953	1.947	1.974	1.958	1.960
NH_2	1.845	1.828	1.824	1.852	1.835	1.828	1.843	1.838	1.835

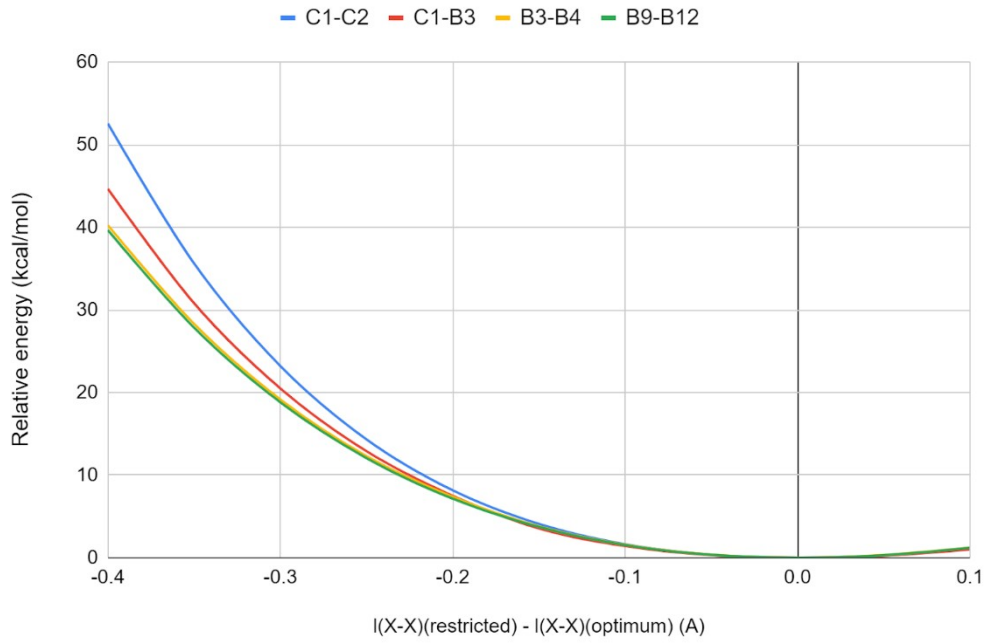
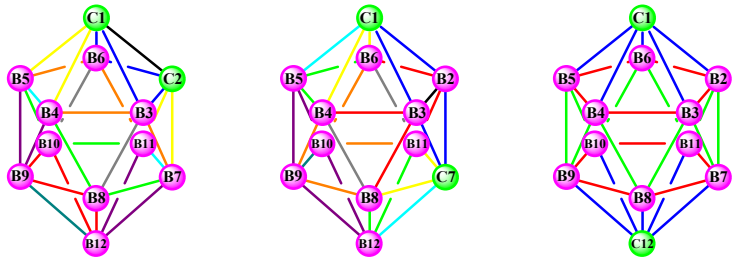


Figure S1. The difference in the energy compared to the optimized structure depending on the amount of shrinking in different bonds of *o*-carboranes. The trend is the opposite compared to the bond elongation, possibly due to the increasing distortion compared to the regular icosahedral geometry and the higher electronic repulsion in the more electronegative carbon atoms.



***o*-carborane** ***m*-carborane** ***p*-carborane**

Figure S2. The chemically different bonds in in the three different isomers of *closo*-dicarbadodecaboranes.

Table S7. The Bader analysis of the restricted systems at the B3LYP/aug-cc-pVTZ level of theory

C1-C2	electron density	type	B9-B12	electron density	type	C1-B4	electron density	type	B4-B5	electron density	type
opt	0.1866	BCP	opt	0.1197	BCP	opt	0.1239	BCP	opt	0.1165	BCP
0.1	0.1534	BCP	0.1	0.1031	BCP	0.1	0.1063	BCP	0.1	0.09914	RCP
0.2	0.1277	BCP	0.2	0.08947	BCP	0.2	0.09196	RCP	0.2	0.08642	RCP
0.3	0.108	BCP	0.3	0.07835	RCP	0.3	0.08024	RCP	0.3	0.07671	RCP
0.4	0.09295	RCP	0.4	0.06936	RCP	0.4	0.0704	RCP	0.4	0.06728	RCP
0.5	0.08155	RCP	0.5	0.06213	RCP	0.5	0.06172	RCP	0.5	0.06037	RCP

Table S8. The difference in the energy (in kcal/mol) compared to the optimized structure depending on the amount of elongation in different bonds of the restricted systems in *ortho*-carborane.

Elongation / Bond	-0.15	-0.10	-0.05	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.40	0.50
C1-C2	4.1	1.6	0.4	0.0	0.3	1.0	2.1	3.4	4.8	6.4	9.5	12.6
C1-B3	3.5	1.4	0.3	0.0	0.2	1.0	2.3	3.7	5.4	7.3	11.6	16.3
C1-B4	3.8	1.5	0.4	0.0	0.3	1.1	2.3	3.9	5.6	7.5	11.7	16.2
B3-B4	3.8	1.6	0.4	0.0	0.3	1.2	2.6	4.4	6.5	8.9	14.2	20.3
B3-B8	3.9	1.6	0.4	0.0	0.3	1.2	2.5	4.3	6.3	8.6	13.6	19.1
B4-B5	3.8	1.6	0.4	0.0	0.3	1.2	2.6	4.4	6.5	8.9	14.3	20.5
B4-B8	3.8	1.6	0.3	0.0	0.3	1.2	2.5	4.1	6.2	8.4	13.4	19.1
B4-B9	3.7	1.6	0.3	0.0	0.3	1.1	2.5	4.1	6.1	8.2	13.3	18.8
B8-B9	3.6	1.5	0.3	0.0	0.3	1.1	2.4	4.0	6.0	8.2	13.2	18.7
B9-B12	3.7	1.5	0.3	0.0	0.3	1.2	2.5	4.3	6.3	8.6	13.7	19.3

Table S9. The difference in the energy (in kcal/mol) compared to the optimized structure depending on the amount of elongation in different bonds of the restricted systems in *meta*-carborane.

Elongation / Bond	-0.15	-0.10	-0.05	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.40	0.50
C1-B2	4.1	1.7	0.4	0.0	0.3	1.1	2.4	4.0	5.9	7.9	12.4	17.0
C1-B4	3.7	1.6	0.3	0.0	0.3	1.2	2.3	3.8	5.6	7.4	11.7	16.3
C1-B5	3.7	1.5	0.3	0.0	0.3	1.0	2.3	3.8	5.5	7.3	11.4	15.9
B2-B3	3.8	1.5	0.3	0.0	0.3	1.2	2.6	4.5	6.8	9.3	15.2	22.0
B2-B6	4.0	1.7	0.4	0.0	0.4	1.3	2.8	4.7	6.9	9.3	15.0	21.4
B4-B5	3.8	1.6	0.4	0.0	0.4	1.3	2.7	4.5	6.6	9.0	14.4	20.6
B4-B8	3.9	1.5	0.4	0.0	0.3	1.3	2.7	4.5	6.5	8.8	14.0	19.8
B4-B9	3.8	1.5	0.4	0.0	0.4	1.2	2.5	4.2	6.2	8.5	13.6	19.2
B5-B9	3.8	1.7	0.4	0.0	0.3	1.2	2.5	4.3	6.3	8.6	13.7	19.4
B9-B10	3.6	1.4	0.4	0.0	0.3	1.1	2.5	4.2	6.2	8.4	13.5	19.2

Table S10. The difference in the energy (in kcal/mol) compared to the optimized structure depending on the amount of elongation in different bonds of the restricted systems in *para*-carborane.

Elongation / Bond	-0.15	-0.10	-0.05	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.40	0.50
C1-B2	3.7	1.6	0.2	0.0	0.3	1.1	2.3	3.8	5.6	7.5	11.8	16.5
B2-B3	3.7	1.5	0.3	0.0	0.3	1.2	2.6	4.4	6.5	8.9	14.4	20.6
B2-B7	3.9	1.6	0.3	0.0	0.2	1.1	2.7	4.3	6.3	8.6	13.9	19.5

Table S11. The length of the different bonds in case of substitution on boron atom 3 (in Å) in *o*-carborane at the B3LYP/aug-cc-pVTZ level of theory

Substituent / Bond	H	NH_2	PH_2	CH_3	SiH_3	OH	SH	Cl	O^-	S^-
1-2	1.62	1.60	1.61	1.62	1.62	1.63	1.62	1.62	1.56	1.55
1-3	1.72	1.78	1.74	1.74	1.73	1.74	1.73	1.73	2.49	2.20
1-4	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.63	1.66
1-5	1.69	1.68	1.69	1.69	1.69	1.70	1.69	1.69	1.70	1.68
1-6	1.72	1.72	1.72	1.72	1.72	1.71	1.72	1.72	1.71	1.72
2-3	1.72	1.78	1.73	1.74	1.73	1.74	1.73	1.73	2.49	2.20
2-6	1.72	1.72	1.72	1.72	1.72	1.71	1.72	1.72	1.71	1.72
2-7	1.69	1.69	1.69	1.69	1.69	1.68	1.69	1.69	1.63	1.66
2-11	1.69	1.68	1.69	1.69	1.69	1.70	1.69	1.69	1.70	1.68
3-4	1.77	1.78	1.78	1.79	1.78	1.80	1.78	1.78	2.04	1.89
3-7	1.77	1.78	1.78	1.79	1.78	1.80	1.78	1.78	2.04	1.89
3-8	1.76	1.77	1.77	1.77	1.77	1.76	1.76	1.76	1.68	1.72
4-5	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.80	1.80
4-8	1.78	1.78	1.78	1.77	1.77	1.78	1.78	1.78	1.83	1.80
4-9	1.77	1.78	1.78	1.77	1.78	1.77	1.77	1.77	1.77	1.79
5-6	1.77	1.77	1.77	1.77	1.77	1.78	1.78	1.78	1.76	1.76
5-9	1.77	1.78	1.77	1.77	1.77	1.77	1.78	1.78	1.76	1.76
5-10	1.78	1.78	1.78	1.78	1.78	1.77	1.78	1.78	1.77	1.77
6-10	1.76	1.75	1.76	1.76	1.76	1.76	1.76	1.76	1.77	1.76
6-11	1.77	1.77	1.77	1.77	1.77	1.78	1.78	1.78	1.76	1.76
7-8	1.78	1.78	1.77	1.77	1.77	1.78	1.78	1.78	1.83	1.80
7-11	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.80	1.80
7-12	1.77	1.78	1.78	1.77	1.78	1.77	1.77	1.77	1.77	1.79
8-9	1.79	1.78	1.79	1.79	1.79	1.79	1.79	1.79	1.78	1.78
8-12	1.79	1.78	1.79	1.79	1.79	1.79	1.79	1.79	1.78	1.78
9-10	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.79
9-12	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.82	1.79
10-11	1.78	1.78	1.78	1.78	1.78	1.77	1.78	1.78	1.77	1.77
10-12	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.79
11-12	1.77	1.78	1.78	1.77	1.77	1.77	1.78	1.78	1.76	1.76

Table S12. The length of the different bonds in case of substitution on boron atom 4 (in Å) in *o*-carborane at the B3LYP/aug-cc-pVTZ level of theory

Substituent / Bond	H	NH_2	PH_2	CH_3	SiH_3	OH	SH	Cl	O^-	S^-
1-2	1.62	1.61	1.62	1.62	1.62	1.61	1.62	1.62	1.62	1.63
1-3	1.72	1.70	1.71	1.71	1.71	1.72	1.71	1.72	1.64	1.67
1-4	1.69	1.76	1.71	1.71	1.70	1.74	1.72	1.70	2.36	1.85
1-5	1.69	1.69	1.69	1.69	1.69	1.68	1.69	1.69	1.66	1.68
1-6	1.72	1.71	1.72	1.72	1.72	1.72	1.71	1.72	1.72	1.72
2-3	1.72	1.72	1.72	1.71	1.72	1.71	1.72	1.71	1.75	1.73
2-6	1.72	1.71	1.72	1.72	1.71	1.72	1.71	1.72	1.71	1.71
2-7	1.69	1.69	1.69	1.69	1.69	1.70	1.69	1.69	1.67	1.68
2-11	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69
3-4	1.77	1.80	1.78	1.79	1.78	1.80	1.78	1.79	2.15	1.85
3-7	1.77	1.78	1.78	1.77	1.78	1.78	1.77	1.77	1.79	1.79
3-8	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76
4-5	1.78	1.80	1.78	1.79	1.79	1.81	1.78	1.79	2.11	1.86
4-8	1.78	1.79	1.78	1.79	1.79	1.79	1.78	1.78	1.81	1.83
4-9	1.77	1.79	1.78	1.79	1.78	1.78	1.78	1.78	1.76	1.82
5-6	1.77	1.78	1.78	1.77	1.78	1.77	1.78	1.77	1.78	1.78
5-9	1.77	1.77	1.78	1.77	1.77	1.78	1.78	1.78	1.78	1.77
5-10	1.78	1.78	1.78	1.78	1.78	1.77	1.78	1.77	1.78	1.78
6-10	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.73	1.75
6-11	1.77	1.77	1.77	1.77	1.78	1.77	1.77	1.77	1.77	1.77
7-8	1.78	1.77	1.78	1.78	1.78	1.77	1.78	1.78	1.77	1.78
7-11	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78
7-12	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77
8-9	1.79	1.79	1.78	1.79	1.78	1.79	1.79	1.79	1.85	1.79
8-12	1.79	1.79	1.79	1.79	1.79	1.78	1.79	1.79	1.78	1.78
9-10	1.79	1.78	1.79	1.79	1.79	1.79	1.78	1.79	1.79	1.79
9-12	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78
10-11	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.77	1.78
10-12	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.81	1.79
11-12	1.77	1.77	1.77	1.78	1.77	1.78	1.77	1.78	1.78	1.78

Table S13. The length of the different bonds in case of substitution on boron atom 8 (in Å) in *o*-carborane at the B3LYP/aug-cc-pVTZ level of theory

Substituent / Bond	H	NH_2	PH_2	CH_3	SiH_3	OH	SH	Cl	O^-	S^-
1-2	1.62	1.63	1.62	1.62	1.62	1.63	1.63	1.62	1.63	1.63
1-3	1.72	1.71	1.72	1.72	1.72	1.72	1.72	1.71	1.73	1.73
1-4	1.69	1.68	1.69	1.69	1.69	1.68	1.69	1.69	1.69	1.69
1-5	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.68	1.68
1-6	1.72	1.72	1.71	1.72	1.72	1.72	1.72	1.72	1.71	1.71
2-3	1.72	1.72	1.72	1.72	1.72	1.72	1.72	1.71	1.73	1.73
2-6	1.72	1.71	1.72	1.72	1.72	1.72	1.71	1.72	1.71	1.71
2-7	1.69	1.68	1.69	1.69	1.69	1.68	1.69	1.69	1.69	1.69
2-11	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.68	1.68
3-4	1.77	1.78	1.77	1.77	1.77	1.78	1.78	1.78	1.76	1.76
3-7	1.77	1.77	1.78	1.77	1.77	1.78	1.78	1.78	1.76	1.76
3-8	1.76	1.78	1.76	1.77	1.76	1.78	1.76	1.77	1.89	1.89
4-5	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78
4-8	1.78	1.80	1.79	1.79	1.78	1.81	1.79	1.78	1.91	1.91
4-9	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.78	1.78	1.78
5-6	1.77	1.77	1.77	1.77	1.78	1.77	1.77	1.78	1.78	1.78
5-9	1.77	1.77	1.78	1.77	1.77	1.77	1.77	1.77	1.77	1.77
5-10	1.78	1.77	1.78	1.78	1.78	1.78	1.78	1.78	1.77	1.77
6-10	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.77	1.77
6-11	1.77	1.78	1.77	1.77	1.78	1.77	1.77	1.78	1.78	1.78
7-8	1.78	1.81	1.78	1.79	1.78	1.81	1.79	1.78	1.91	1.91
7-11	1.78	1.77	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78
7-12	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.78	1.78	1.78
8-9	1.79	1.82	1.79	1.80	1.80	1.80	1.79	1.79	1.90	1.90
8-12	1.79	1.80	1.80	1.80	1.80	1.80	1.79	1.79	1.90	1.90
9-10	1.79	1.78	1.79	1.79	1.79	1.78	1.79	1.79	1.79	1.79
9-12	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78
10-11	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.77	1.77
10-12	1.79	1.79	1.79	1.79	1.79	1.78	1.79	1.79	1.79	1.79
11-12	1.77	1.78	1.78	1.77	1.78	1.77	1.78	1.77	1.77	1.77

Table S14. The length of the different bonds in case of substitution on boron atom 9 (in Å) in *o*-carborane at the B3LYP/aug-cc-pVTZ level of theory

Substituent / Bond	H	NH_2	PH_2	CH_3	SiH_3	OH	SH	Cl	O^-	S^-
1-2	1.62	1.63	1.62	1.62	1.62	1.63	1.63	1.62	1.63	1.63
1-3	1.72	1.72	1.72	1.72	1.72	1.72	1.72	1.72	1.71	1.71
1-4	1.69	1.68	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.70
1-5	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.70
1-6	1.72	1.72	1.72	1.72	1.72	1.72	1.72	1.72	1.71	1.71
2-3	1.72	1.71	1.72	1.72	1.72	1.71	1.71	1.72	1.72	1.72
2-6	1.72	1.71	1.71	1.72	1.72	1.71	1.71	1.72	1.72	1.72
2-7	1.69	1.70	1.69	1.69	1.69	1.69	1.69	1.69	1.70	1.70
2-11	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.70	1.70
3-4	1.77	1.78	1.78	1.78	1.78	1.78	1.78	1.77	1.78	1.78
3-7	1.77	1.77	1.77	1.77	1.78	1.77	1.77	1.77	1.76	1.76
3-8	1.76	1.76	1.76	1.76	1.76	1.75	1.76	1.76	1.75	1.75
4-5	1.78	1.79	1.78	1.78	1.78	1.79	1.79	1.79	1.76	1.77
4-8	1.78	1.77	1.78	1.77	1.77	1.78	1.77	1.78	1.78	1.77
4-9	1.77	1.80	1.78	1.79	1.78	1.80	1.78	1.78	1.90	1.84
5-6	1.77	1.78	1.77	1.78	1.78	1.78	1.78	1.77	1.78	1.78
5-9	1.77	1.79	1.78	1.79	1.78	1.80	1.78	1.78	1.90	1.84
5-10	1.78	1.77	1.77	1.77	1.78	1.78	1.77	1.78	1.78	1.77
6-10	1.76	1.75	1.76	1.76	1.76	1.75	1.76	1.76	1.75	1.75
6-11	1.77	1.77	1.77	1.77	1.78	1.77	1.77	1.77	1.76	1.76
7-8	1.78	1.77	1.78	1.78	1.78	1.77	1.77	1.77	1.77	1.77
7-11	1.78	1.79	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78
7-12	1.77	1.78	1.78	1.77	1.77	1.77	1.78	1.77	1.77	1.78
8-9	1.79	1.82	1.80	1.80	1.79	1.82	1.80	1.79	1.91	1.86
8-12	1.79	1.79	1.78	1.78	1.79	1.79	1.79	1.79	1.79	1.78
9-10	1.79	1.83	1.80	1.80	1.79	1.82	1.80	1.79	1.91	1.86
9-12	1.78	1.79	1.79	1.79	1.79	1.79	1.78	1.78	1.89	1.85
10-11	1.78	1.77	1.78	1.78	1.78	1.77	1.77	1.77	1.77	1.77
10-12	1.79	1.78	1.79	1.78	1.79	1.79	1.79	1.79	1.79	1.78
11-12	1.77	1.78	1.77	1.77	1.77	1.77	1.78	1.77	1.77	1.78

Table S15. The length of the different bonds in case of substitution on boron atom 2 (in Å) in *m*-carborane at the B3LYP/aug-cc-pVTZ level of theory

Substituent / Bond	H	NH_2	PH_2	CH_3	SiH_3	OH	SH	Cl	O^-	S^-
1-2	1.69	1.74	1.70	1.71	1.70	1.72	1.71	1.70	2.58	1.80
1-3	1.69	1.68	1.69	1.68	1.69	1.68	1.69	1.69	1.63	1.67
1-4	1.71	1.70	1.71	1.71	1.71	1.71	1.70	1.71	1.70	1.71
1-5	1.71	1.70	1.71	1.71	1.71	1.71	1.71	1.71	1.66	1.70
1-6	1.71	1.70	1.70	1.71	1.70	1.71	1.70	1.72	1.66	1.70
2-3	1.78	1.80	1.79	1.80	1.79	1.81	1.79	1.80	2.81	1.87
2-6	1.76	1.78	1.77	1.78	1.77	1.77	1.77	1.77	1.78	1.81
2-7	1.69	1.73	1.71	1.71	1.70	1.72	1.71	1.70	2.58	1.80
2-11	1.76	1.78	1.77	1.78	1.77	1.77	1.77	1.77	1.78	1.81
3-4	1.76	1.77	1.77	1.76	1.77	1.76	1.76	1.76	1.79	1.77
3-7	1.69	1.68	1.69	1.68	1.69	1.68	1.69	1.69	1.63	1.67
3-8	1.76	1.76	1.77	1.76	1.77	1.76	1.76	1.76	1.79	1.77
4-5	1.78	1.77	1.78	1.78	1.78	1.78	1.78	1.78	1.76	1.77
4-8	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.74	1.76
4-9	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.79	1.77
5-6	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.81	1.78
5-9	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.76	1.77
5-10	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.80	1.77
6-10	1.78	1.77	1.78	1.77	1.78	1.77	1.77	1.77	1.78	1.78
6-11	1.77	1.77	1.77	1.76	1.77	1.76	1.77	1.77	1.82	1.75
7-8	1.71	1.70	1.71	1.71	1.71	1.71	1.70	1.71	1.70	1.71
7-11	1.71	1.70	1.70	1.71	1.70	1.71	1.70	1.72	1.66	1.70
7-12	1.71	1.70	1.71	1.71	1.71	1.71	1.71	1.71	1.66	1.70
8-9	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.79	1.77
8-12	1.78	1.77	1.78	1.78	1.78	1.78	1.78	1.78	1.76	1.77
9-10	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.79
9-12	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.76	1.77
10-11	1.78	1.77	1.78	1.78	1.78	1.77	1.77	1.77	1.78	1.78
10-12	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.80	1.77
11-12	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.81	1.78

Table S16. The length of the different bonds in case of substitution on boron atom 4 (in Å) in *m*-carborane at the B3LYP/aug-cc-pVTZ level of theory

Substituent / Bond	H	NH_2	PH_2	CH_3	SiH_3	OH	SH	Cl	O^-	S^-
1-2	1.69	1.68	1.69	1.69	1.69	1.68	1.68	1.69	1.67	1.68
1-3	1.69	1.68	1.69	1.69	1.69	1.69	1.69	1.69	1.65	1.67
1-4	1.71	1.78	1.73	1.73	1.72	1.76	1.74	1.72	2.23	1.87
1-5	1.71	1.70	1.70	1.70	1.70	1.70	1.70	1.71	1.67	1.69
1-6	1.71	1.70	1.71	1.71	1.71	1.71	1.70	1.71	1.69	1.70
2-3	1.78	1.79	1.79	1.78	1.79	1.79	1.79	1.78	1.81	1.80
2-6	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.75	1.75
2-7	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.68	1.68
2-11	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76
3-4	1.76	1.78	1.77	1.78	1.77	1.78	1.77	1.77	2.03	1.84
3-7	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.68	1.70	1.70
3-8	1.76	1.77	1.77	1.76	1.76	1.76	1.77	1.77	1.75	1.75
4-5	1.78	1.79	1.78	1.79	1.79	1.80	1.78	1.78	2.01	1.86
4-8	1.77	1.78	1.77	1.78	1.77	1.78	1.77	1.77	1.80	1.81
4-9	1.78	1.79	1.79	1.79	1.79	1.79	1.78	1.78	1.78	1.83
5-6	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.80	1.79
5-9	1.77	1.77	1.77	1.77	1.77	1.77	1.78	1.77	1.78	1.76
5-10	1.77	1.78	1.77	1.77	1.77	1.77	1.77	1.77	1.78	1.78
6-10	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.76	1.77
6-11	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.76
7-8	1.71	1.70	1.71	1.71	1.71	1.70	1.71	1.71	1.71	1.72
7-11	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.70	1.71
7-12	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.70
8-9	1.78	1.77	1.77	1.77	1.77	1.78	1.77	1.78	1.83	1.78
8-12	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78
9-10	1.79	1.78	1.79	1.79	1.79	1.79	1.79	1.79	1.78	1.79
9-12	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.76	1.77
10-11	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78
10-12	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.78	1.77
11-12	1.78	1.77	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78

Table S17. The length of the different bonds in case of substitution on boron atom 5 (in Å) in *m*-carborane at the B3LYP/aug-cc-pVTZ level of theory

Substituent / Bond	H	NH_2	PH_2	CH_3	SiH_3	OH	SH	Cl	O^-	S^-
1-2	1.69	1.68	1.69	1.69	1.69	1.68	1.68	1.69	1.67	1.68
1-3	1.69	1.68	1.69	1.69	1.69	1.69	1.69	1.69	1.67	1.68
1-4	1.71	1.70	1.71	1.70	1.71	1.70	1.70	1.71	1.67	1.69
1-5	1.71	1.78	1.73	1.73	1.72	1.75	1.74	1.72	2.28	1.87
1-6	1.71	1.70	1.71	1.71	1.71	1.71	1.71	1.71	1.67	1.69
2-3	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.79	1.78	1.78
2-6	1.76	1.77	1.77	1.76	1.77	1.76	1.77	1.76	1.78	1.77
2-7	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.70	1.69
2-11	1.76	1.77	1.76	1.76	1.76	1.77	1.77	1.76	1.74	1.75
3-4	1.76	1.77	1.77	1.76	1.77	1.76	1.77	1.76	1.78	1.77
3-7	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.70	1.69
3-8	1.76	1.77	1.76	1.76	1.76	1.76	1.76	1.76	1.74	1.75
4-5	1.78	1.80	1.78	1.79	1.78	1.80	1.78	1.79	2.06	1.86
4-8	1.77	1.77	1.77	1.76	1.77	1.76	1.77	1.76	1.77	1.77
4-9	1.78	1.78	1.78	1.77	1.78	1.78	1.78	1.78	1.78	1.77
5-6	1.78	1.80	1.78	1.79	1.78	1.79	1.78	1.79	2.06	1.86
5-9	1.77	1.79	1.78	1.79	1.78	1.78	1.78	1.78	1.79	1.82
5-10	1.77	1.79	1.78	1.79	1.78	1.79	1.78	1.78	1.79	1.82
6-10	1.78	1.78	1.78	1.77	1.78	1.77	1.78	1.78	1.78	1.77
6-11	1.77	1.77	1.77	1.76	1.77	1.77	1.77	1.76	1.77	1.77
7-8	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71
7-11	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71
7-12	1.71	1.70	1.71	1.71	1.71	1.71	1.70	1.71	1.71	1.72
8-9	1.78	1.77	1.77	1.78	1.78	1.77	1.77	1.78	1.77	1.78
8-12	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.79	1.77
9-10	1.79	1.78	1.78	1.79	1.78	1.79	1.79	1.79	1.84	1.79
9-12	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.76	1.77
10-11	1.78	1.77	1.77	1.78	1.78	1.77	1.77	1.78	1.77	1.78
10-12	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.76	1.77
11-12	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.79	1.77

Table S18. The length of the different bonds in case of substitution on boron atom 9 (in Å) in *m*-carborane at the B3LYP/aug-cc-pVTZ level of theory

Substituent / Bond	H	NH_2	PH_2	CH_3	SiH_3	OH	SH	Cl	O^-	S^-
1-2	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69
1-3	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.68	1.68
1-4	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71
1-5	1.71	1.70	1.70	1.71	1.71	1.70	1.70	1.71	1.72	1.72
1-6	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71
2-3	1.78	1.79	1.79	1.78	1.79	1.79	1.79	1.78	1.78	1.78
2-6	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.77	1.76
2-7	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69
2-11	1.76	1.77	1.76	1.76	1.76	1.76	1.77	1.76	1.77	1.76
3-4	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.77
3-7	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.68	1.68
3-8	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.77
4-5	1.78	1.77	1.78	1.77	1.78	1.77	1.78	1.78	1.76	1.76
4-8	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77
4-9	1.78	1.80	1.78	1.79	1.78	1.80	1.78	1.78	1.90	1.84
5-6	1.78	1.77	1.78	1.78	1.78	1.78	1.78	1.78	1.79	1.79
5-9	1.77	1.80	1.78	1.79	1.78	1.79	1.79	1.78	1.88	1.83
5-10	1.77	1.77	1.77	1.77	1.77	1.78	1.77	1.77	1.77	1.77
6-10	1.78	1.78	1.78	1.77	1.78	1.77	1.78	1.77	1.76	1.77
6-11	1.77	1.77	1.77	1.76	1.77	1.76	1.77	1.77	1.75	1.75
7-8	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71
7-11	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71
7-12	1.71	1.70	1.71	1.71	1.71	1.70	1.71	1.71	1.72	1.72
8-9	1.78	1.80	1.78	1.79	1.78	1.79	1.79	1.78	1.90	1.84
8-12	1.78	1.77	1.77	1.77	1.78	1.78	1.77	1.78	1.76	1.76
9-10	1.79	1.80	1.79	1.80	1.79	1.80	1.79	1.79	1.92	1.86
9-12	1.77	1.80	1.78	1.79	1.78	1.80	1.78	1.78	1.88	1.83
10-11	1.78	1.78	1.78	1.77	1.78	1.77	1.78	1.77	1.76	1.77
10-12	1.77	1.78	1.77	1.77	1.77	1.77	1.78	1.77	1.77	1.77
11-12	1.78	1.77	1.78	1.78	1.78	1.78	1.78	1.78	1.79	1.79

Table S19. The length of the different bonds in case of substitution on boron atom 2 (in Å) in *p*-carborane at the B3LYP/aug-cc-pVTZ level of theory

Substituent / Bond	H	NH_2	PH_2	CH_3	SiH_3	OH	SH	Cl	O^-	S^-
1-2	1.70	1.76	1.72	1.72	1.72	1.71	1.70	1.71	2.20	1.84
1-3	1.70	1.69	1.70	1.70	1.70	1.71	1.71	1.71	1.66	1.68
1-4	1.70	1.69	1.70	1.70	1.70	1.71	1.71	1.71	1.69	1.70
1-5	1.70	1.69	1.70	1.70	1.70	1.71	1.71	1.71	1.69	1.70
1-6	1.70	1.69	1.70	1.70	1.70	1.71	1.71	1.71	1.66	1.68
2-3	1.78	1.80	1.79	1.80	1.79	1.81	1.80	1.79	2.03	1.86
2-6	1.78	1.80	1.79	1.80	1.79	1.81	1.80	1.79	2.03	1.86
2-7	1.76	1.78	1.77	1.78	1.77	1.78	1.77	1.77	1.79	1.81
2-11	1.76	1.78	1.77	1.78	1.77	1.78	1.77	1.77	1.79	1.81
3-4	1.78	1.78	1.78	1.78	1.78	1.77	1.77	1.78	1.79	1.78
3-7	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76
3-8	1.76	1.76	1.76	1.76	1.76	1.75	1.76	1.76	1.76	1.76
4-5	1.78	1.78	1.78	1.78	1.78	1.79	1.78	1.78	1.78	1.78
4-8	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.74	1.75
4-9	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.77	1.76
5-6	1.78	1.78	1.78	1.78	1.78	1.77	1.77	1.78	1.79	1.78
5-9	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.77	1.76
5-10	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.74	1.75
6-10	1.76	1.76	1.76	1.76	1.76	1.75	1.76	1.76	1.76	1.76
6-11	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76
7-8	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.79
7-11	1.78	1.77	1.78	1.78	1.78	1.79	1.79	1.79	1.82	1.78
7-12	1.70	1.70	1.70	1.70	1.70	1.70	1.70	1.70	1.70	1.71
8-9	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78
8-12	1.70	1.70	1.70	1.70	1.70	1.71	1.70	1.70	1.71	1.70
9-10	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78
9-12	1.70	1.70	1.70	1.70	1.70	1.71	1.71	1.71	1.70	1.71
10-11	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.79
10-12	1.70	1.70	1.70	1.70	1.70	1.71	1.70	1.70	1.71	1.70
11-12	1.70	1.70	1.70	1.70	1.70	1.70	1.70	1.70	1.70	1.71

Table S20. The length of the different bonds in case of substitution on carbon atom 1 (in Å) in *o*-carborane at the B3LYP/aug-cc-pVTZ level of theory

Substituent / Bond	H	NH_2	PH_2	CH_3	SiH_3	OH	SH	Cl	O^-	S^-
1-2	1.62	1.68	1.65	1.64	1.65	1.66	1.66	1.64	2.29	1.75
1-3	1.72	1.72	1.72	1.73	1.72	1.73	1.73	1.73	1.99	1.76
1-4	1.69	1.71	1.71	1.70	1.71	1.69	1.70	1.70	1.64	1.72
1-5	1.69	1.71	1.71	1.70	1.71	1.70	1.71	1.70	1.64	1.72
1-6	1.72	1.72	1.72	1.73	1.72	1.72	1.72	1.73	1.99	1.76
2-3	1.72	1.70	1.71	1.71	1.71	1.70	1.71	1.72	1.65	1.69
2-6	1.72	1.70	1.71	1.71	1.71	1.72	1.71	1.72	1.65	1.69
2-7	1.69	1.68	1.69	1.69	1.69	1.69	1.69	1.69	1.67	1.69
2-11	1.69	1.68	1.69	1.69	1.69	1.69	1.69	1.69	1.67	1.69
3-4	1.77	1.78	1.78	1.77	1.77	1.78	1.78	1.78	1.80	1.77
3-7	1.77	1.78	1.78	1.77	1.78	1.77	1.78	1.77	1.79	1.78
3-8	1.76	1.76	1.76	1.76	1.76	1.75	1.76	1.76	1.77	1.77
4-5	1.78	1.77	1.77	1.77	1.77	1.78	1.78	1.79	1.88	1.78
4-8	1.78	1.77	1.77	1.78	1.77	1.78	1.78	1.78	1.78	1.78
4-9	1.77	1.77	1.77	1.77	1.77	1.77	1.78	1.77	1.79	1.78
5-6	1.77	1.78	1.78	1.77	1.77	1.77	1.78	1.78	1.80	1.77
5-9	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.79	1.78
5-10	1.78	1.77	1.77	1.78	1.77	1.77	1.77	1.78	1.78	1.78
6-10	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.77	1.77
6-11	1.77	1.78	1.78	1.77	1.78	1.78	1.78	1.77	1.79	1.78
7-8	1.78	1.78	1.78	1.77	1.77	1.78	1.78	1.78	1.76	1.77
7-11	1.78	1.77	1.78	1.78	1.78	1.78	1.78	1.78	1.77	1.77
7-12	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.78	1.77
8-9	1.79	1.78	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.78
8-12	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.78	1.79
9-10	1.79	1.78	1.79	1.79	1.79	1.78	1.79	1.79	1.79	1.78
9-12	1.78	1.77	1.78	1.78	1.78	1.78	1.78	1.78	1.77	1.78
10-11	1.78	1.78	1.78	1.77	1.77	1.78	1.78	1.78	1.76	1.77
10-12	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.78	1.79
11-12	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.78	1.77

Table S21. The length of the different bonds in case of substitution on carbon atom 1 (in Å) in *m*-carborane at the B3LYP/aug-cc-pVTZ level of theory

Substituent / Bond	H	NH_2	PH_2	CH_3	SiH_3	OH	SH	Cl	O^-	S^-
1-2	1.69	1.71	1.70	1.70	1.70	1.70	1.70	1.70	1.77	1.72
1-3	1.69	1.71	1.71	1.70	1.70	1.70	1.70	1.70	1.77	1.72
1-4	1.71	1.71	1.72	1.72	1.72	1.73	1.73	1.72	1.80	1.75
1-5	1.71	1.74	1.72	1.72	1.73	1.70	1.71	1.71	1.78	1.75
1-6	1.71	1.71	1.73	1.72	1.72	1.73	1.73	1.72	1.79	1.75
2-3	1.78	1.77	1.78	1.78	1.78	1.79	1.79	1.79	1.77	1.77
2-6	1.76	1.77	1.76	1.76	1.76	1.76	1.76	1.77	1.76	1.75
2-7	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.69	1.70
2-11	1.76	1.76	1.76	1.76	1.76	1.77	1.76	1.76	1.77	1.77
3-4	1.76	1.77	1.76	1.76	1.76	1.76	1.76	1.77	1.76	1.75
3-7	1.69	1.69	1.68	1.69	1.69	1.69	1.69	1.69	1.69	1.70
3-8	1.76	1.76	1.76	1.76	1.76	1.77	1.77	1.76	1.77	1.77
4-5	1.78	1.77	1.78	1.77	1.77	1.78	1.78	1.78	1.77	1.77
4-8	1.77	1.77	1.77	1.76	1.77	1.76	1.76	1.77	1.76	1.77
4-9	1.78	1.78	1.78	1.77	1.78	1.77	1.77	1.77	1.77	1.78
5-6	1.78	1.77	1.77	1.77	1.77	1.78	1.78	1.78	1.77	1.77
5-9	1.77	1.76	1.77	1.77	1.77	1.77	1.78	1.77	1.78	1.78
5-10	1.77	1.76	1.77	1.77	1.77	1.77	1.78	1.77	1.78	1.78
6-10	1.78	1.78	1.78	1.77	1.78	1.77	1.77	1.77	1.77	1.78
6-11	1.77	1.76	1.76	1.76	1.77	1.76	1.76	1.77	1.76	1.77
7-8	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.70	1.70
7-11	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.70	1.70
7-12	1.71	1.70	1.71	1.71	1.71	1.71	1.71	1.71	1.71	1.70
8-9	1.78	1.78	1.78	1.77	1.77	1.77	1.77	1.77	1.76	1.77
8-12	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78
9-10	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.79	1.78	1.78
9-12	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77
10-11	1.78	1.78	1.77	1.77	1.77	1.77	1.77	1.77	1.76	1.77
10-12	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77	1.77
11-12	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78

Table S22. The length of the different bonds in case of substitution on carbon atom 1 (in Å) in *p*-carborane at the B3LYP/aug-cc-pVTZ level of theory

Substituent / Bond	H	NH_2	PH_2	CH_3	SiH_3	OH	SH	Cl	O^-	S^-
1-2	1.70	1.71	1.72	1.71	1.72	1.70	1.73	1.71	1.79	1.74
1-3	1.70	1.72	1.71	1.72	1.72	1.72	1.71	1.71	1.79	1.74
1-4	1.70	1.73	1.72	1.71	1.72	1.72	1.73	1.71	1.79	1.74
1-5	1.70	1.70	1.71	1.72	1.71	1.71	1.71	1.71	1.79	1.74
1-6	1.70	1.73	1.72	1.72	1.72	1.73	1.71	1.71	1.79	1.74
2-3	1.78	1.79	1.78	1.78	1.78	1.78	1.78	1.79	1.78	1.77
2-6	1.78	1.77	1.78	1.78	1.78	1.78	1.78	1.79	1.78	1.77
2-7	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76
2-11	1.76	1.77	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76
3-4	1.78	1.77	1.78	1.77	1.78	1.78	1.78	1.79	1.78	1.77
3-7	1.76	1.76	1.76	1.76	1.76	1.76	1.77	1.76	1.76	1.76
3-8	1.76	1.77	1.76	1.76	1.76	1.76	1.77	1.76	1.76	1.76
4-5	1.78	1.78	1.78	1.78	1.78	1.79	1.78	1.79	1.78	1.77
4-8	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76
4-9	1.76	1.75	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76
5-6	1.78	1.78	1.78	1.77	1.78	1.78	1.79	1.79	1.78	1.77
5-9	1.76	1.77	1.77	1.76	1.76	1.76	1.76	1.76	1.76	1.76
5-10	1.76	1.77	1.76	1.76	1.76	1.77	1.76	1.76	1.76	1.77
6-10	1.76	1.75	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.77
6-11	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76	1.76
7-8	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.77	1.77
7-11	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.77	1.77
7-12	1.70	1.71	1.70	1.70	1.70	1.70	1.70	1.70	1.71	1.70
8-9	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.77	1.77
8-12	1.70	1.70	1.70	1.70	1.70	1.70	1.70	1.70	1.71	1.70
9-10	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.77	1.77
9-12	1.70	1.70	1.70	1.70	1.70	1.71	1.70	1.70	1.71	1.70
10-11	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.77	1.77
10-12	1.70	1.71	1.70	1.70	1.70	1.70	1.71	1.70	1.71	1.70
11-12	1.70	1.70	1.70	1.70	1.70	1.70	1.70	1.70	1.71	1.70

Table S23. The length of the different bonds (in Å) in case of substitution with two substituents on the carbon atoms in *o*-carborane

Substituent / Bond	H	1,2-NH_2	1,2-OH	1,2-SH	1-O,2-OH	1-S,2-SH	1,2-O^-	1,2-S^-
1-2	1.62	1.90	1.78	1.83	1.91	2.15	2.13	2.19
1-3	1.72	1.71	1.72	1.72	1.82	1.82	1.79	1.79
1-4	1.69	1.68	1.68	1.68	1.70	1.65	1.70	1.70
1-5	1.69	1.68	1.69	1.69	1.70	1.65	1.70	1.70
1-6	1.72	1.71	1.72	1.72	1.82	1.82	1.79	1.79
2-3	1.72	1.71	1.71	1.72	1.70	1.68	1.79	1.79
2-6	1.72	1.71	1.72	1.72	1.70	1.69	1.79	1.79
2-7	1.69	1.68	1.69	1.68	1.68	1.66	1.70	1.70
2-11	1.69	1.68	1.69	1.69	1.68	1.66	1.70	1.70
3-4	1.78	1.79	1.79	1.79	1.76	1.79	1.78	1.78
3-7	1.78	1.79	1.79	1.79	1.77	1.82	1.78	1.78
3-8	1.76	1.77	1.77	1.77	1.75	1.79	1.77	1.77
4-5	1.78	1.77	1.78	1.78	1.81	1.80	1.79	1.79
4-8	1.78	1.77	1.77	1.77	1.78	1.77	1.77	1.77
4-9	1.77	1.77	1.77	1.77	1.78	1.78	1.78	1.78
5-6	1.78	1.79	1.78	1.79	1.76	1.79	1.78	1.78
5-9	1.77	1.77	1.77	1.77	1.78	1.78	1.78	1.78
5-10	1.78	1.77	1.77	1.77	1.78	1.77	1.77	1.77
6-10	1.76	1.77	1.76	1.78	1.75	1.79	1.77	1.77
6-11	1.78	1.79	1.78	1.79	1.77	1.82	1.78	1.78
7-8	1.78	1.77	1.77	1.77	1.78	1.76	1.77	1.77
7-11	1.78	1.77	1.78	1.78	1.78	1.77	1.79	1.79
7-12	1.77	1.77	1.77	1.77	1.77	1.77	1.78	1.78
8-9	1.79	1.79	1.79	1.79	1.78	1.78	1.78	1.78
8-12	1.79	1.79	1.79	1.79	1.78	1.79	1.78	1.78
9-10	1.79	1.79	1.79	1.79	1.78	1.78	1.78	1.78
9-12	1.78	1.76	1.77	1.77	1.79	1.76	1.77	1.77
10-11	1.78	1.77	1.77	1.77	1.78	1.76	1.77	1.77
10-12	1.79	1.79	1.79	1.79	1.78	1.79	1.78	1.78
11-12	1.77	1.77	1.77	1.77	1.77	1.78	1.78	1.78

Table S24. The length of the different bonds (in Å) in case of substitution with two substituents on the B9-B12 atoms in *o*-carborane

Substituent / Bond	H	9,12-NH_2	9,12-OH	9,12-SH	9-O,12-OH	9-S,12-SH	9,12-O^-	9,12-S^-
1-2	1.62	1.62	1.63	1.62	1.63	1.64	1.61	1.63
1-3	1.72	1.73	1.72	1.72	1.71	1.71	1.72	1.71
1-4	1.69	1.69	1.69	1.69	1.70	1.70	1.71	1.70
1-5	1.69	1.68	1.69	1.69	1.70	1.70	1.71	1.70
1-6	1.72	1.72	1.71	1.72	1.71	1.71	1.72	1.71
2-3	1.72	1.71	1.72	1.71	1.72	1.72	1.72	1.71
2-6	1.72	1.71	1.72	1.71	1.72	1.72	1.72	1.71
2-7	1.69	1.69	1.69	1.70	1.70	1.69	1.71	1.70
2-11	1.69	1.70	1.69	1.69	1.70	1.69	1.71	1.70
3-4	1.78	1.78	1.77	1.78	1.78	1.78	1.77	1.77
3-7	1.78	1.76	1.78	1.77	1.77	1.77	1.77	1.77
3-8	1.76	1.75	1.74	1.76	1.74	1.75	1.75	1.76
4-5	1.78	1.78	1.78	1.79	1.77	1.77	1.75	1.77
4-8	1.78	1.78	1.77	1.77	1.77	1.77	1.78	1.77
4-9	1.77	1.78	1.79	1.78	1.90	1.83	1.90	1.82
5-6	1.78	1.78	1.77	1.78	1.78	1.78	1.77	1.77
5-9	1.77	1.79	1.80	1.78	1.90	1.83	1.90	1.82
5-10	1.78	1.77	1.77	1.78	1.77	1.77	1.78	1.77
6-10	1.76	1.75	1.75	1.76	1.74	1.75	1.75	1.76
6-11	1.78	1.76	1.78	1.77	1.77	1.77	1.77	1.77
7-8	1.78	1.77	1.77	1.77	1.77	1.77	1.78	1.77
7-11	1.78	1.77	1.78	1.78	1.79	1.79	1.75	1.77
7-12	1.77	1.81	1.79	1.79	1.79	1.78	1.90	1.82
8-9	1.79	1.83	1.80	1.80	1.90	1.86	1.91	1.85
8-12	1.79	1.79	1.81	1.79	1.81	1.80	1.91	1.85
9-10	1.79	1.81	1.80	1.81	1.90	1.86	1.91	1.85
9-12	1.78	1.82	1.81	1.80	1.86	1.85	1.98	1.94
10-11	1.78	1.77	1.77	1.77	1.77	1.77	1.78	1.77
10-12	1.79	1.80	1.82	1.79	1.81	1.80	1.91	1.85
11-12	1.77	1.80	1.79	1.79	1.79	1.78	1.90	1.82

Table S25. The length of the different bonds (in Å) in case of substitution with two substituents on the B9-B10 atoms in *m*-carborane

Substituent / Bond	H	9,10-NH_2	9,10-OH	9,10-SH	9-O,10-OH	9-S,10-SH	9,10-O^-	9,10-S^-
1-2	1.69	1.69	1.69	1.69	1.69	1.69	1.68	1.68
1-3	1.69	1.68	1.69	1.69	1.68	1.68	1.68	1.68
1-4	1.71	1.70	1.72	1.70	1.71	1.71	1.71	1.71
1-5	1.71	1.71	1.69	1.71	1.69	1.71	1.74	1.74
1-6	1.71	1.71	1.70	1.72	1.72	1.71	1.71	1.71
2-3	1.78	1.78	1.78	1.78	1.79	1.79	1.78	1.78
2-6	1.76	1.76	1.76	1.76	1.76	1.76	1.77	1.77
2-7	1.69	1.70	1.69	1.69	1.69	1.69	1.68	1.68
2-11	1.76	1.76	1.76	1.76	1.76	1.76	1.77	1.77
3-4	1.76	1.77	1.76	1.76	1.76	1.77	1.77	1.77
3-7	1.69	1.69	1.69	1.69	1.68	1.68	1.68	1.68
3-8	1.76	1.76	1.76	1.77	1.76	1.77	1.77	1.77
4-5	1.78	1.78	1.78	1.78	1.76	1.76	1.78	1.78
4-8	1.77	1.76	1.77	1.77	1.77	1.77	1.76	1.76
4-9	1.78	1.80	1.79	1.79	1.89	1.83	1.81	1.81
5-6	1.78	1.77	1.78	1.78	1.78	1.78	1.78	1.78
5-9	1.77	1.79	1.80	1.77	1.87	1.83	1.83	1.83
5-10	1.77	1.79	1.79	1.79	1.80	1.78	1.83	1.83
6-10	1.78	1.80	1.79	1.78	1.78	1.77	1.81	1.81
6-11	1.77	1.76	1.76	1.77	1.76	1.76	1.76	1.76
7-8	1.71	1.69	1.71	1.70	1.71	1.71	1.71	1.71
7-11	1.71	1.72	1.70	1.71	1.72	1.71	1.71	1.71
7-12	1.71	1.70	1.70	1.71	1.69	1.71	1.74	1.74
8-9	1.78	1.81	1.79	1.79	1.89	1.83	1.81	1.81
8-12	1.78	1.78	1.78	1.78	1.76	1.76	1.78	1.78
9-10	1.79	1.84	1.82	1.81	1.88	1.87	1.98	1.98
9-12	1.77	1.78	1.80	1.78	1.87	1.83	1.83	1.83
10-11	1.78	1.78	1.80	1.78	1.78	1.77	1.81	1.81
10-12	1.77	1.81	1.79	1.78	1.80	1.78	1.83	1.83
11-12	1.78	1.78	1.78	1.78	1.78	1.78	1.78	1.78

Table S26. The length of the different bonds (in Å) in case of substitution with bulky adamantyl (Ad) and *tert*-butyl (*t*Bu) substituents in *o*-carborane systems at the B3LYP/6-31G* level of theory

Substituent / Bond	H	1,2-Ad	9,12-Ad	1,2-*t*Bu	9,12-*t*Bu
1-2	1.62	2.15	1.62	2.01	1.64
1-3	1.72	1.74	1.72	1.73	1.74
1-4	1.70	1.66	1.70	1.68	1.70
1-5	1.70	1.65	1.69	1.67	1.71
1-6	1.72	1.76	1.72	1.75	1.74
2-3	1.72	1.76	1.72	1.75	1.74
2-6	1.72	1.74	1.72	1.73	1.74
2-7	1.70	1.65	1.69	1.67	1.71
2-11	1.70	1.66	1.70	1.68	1.70
3-4	1.78	1.79	1.77	1.78	1.78
3-7	1.78	1.80	1.77	1.79	1.78
3-8	1.76	1.82	1.77	1.80	1.78
4-5	1.78	1.79	1.78	1.78	1.79
4-8	1.78	1.75	1.78	1.76	1.78
4-9	1.78	1.78	1.80	1.78	1.81
5-6	1.78	1.80	1.77	1.79	1.78
5-9	1.78	1.80	1.80	1.79	1.81
5-10	1.78	1.76	1.77	1.76	1.79
6-10	1.76	1.82	1.77	1.80	1.78
6-11	1.78	1.79	1.77	1.78	1.78
7-8	1.78	1.76	1.77	1.76	1.79
7-11	1.78	1.79	1.78	1.78	1.79
7-12	1.78	1.80	1.80	1.79	1.81
8-9	1.79	1.78	1.82	1.79	1.83
8-12	1.79	1.78	1.81	1.78	1.83
9-10	1.79	1.78	1.81	1.78	1.83
9-12	1.78	1.75	1.87	1.76	1.88
10-11	1.78	1.75	1.78	1.76	1.78
10-12	1.79	1.78	1.82	1.79	1.83
11-12	1.78	1.78	1.80	1.78	1.81

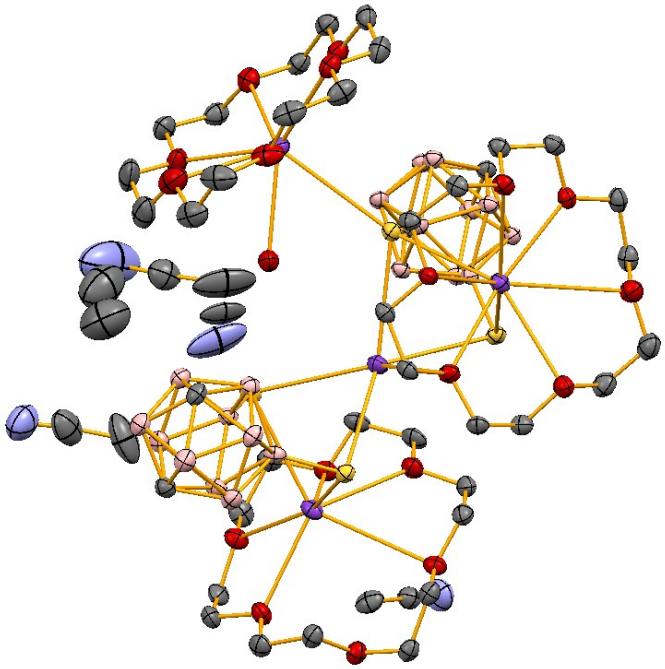


Figure S3. Solid state structure of **5'**. H atoms are omitted for clarity.

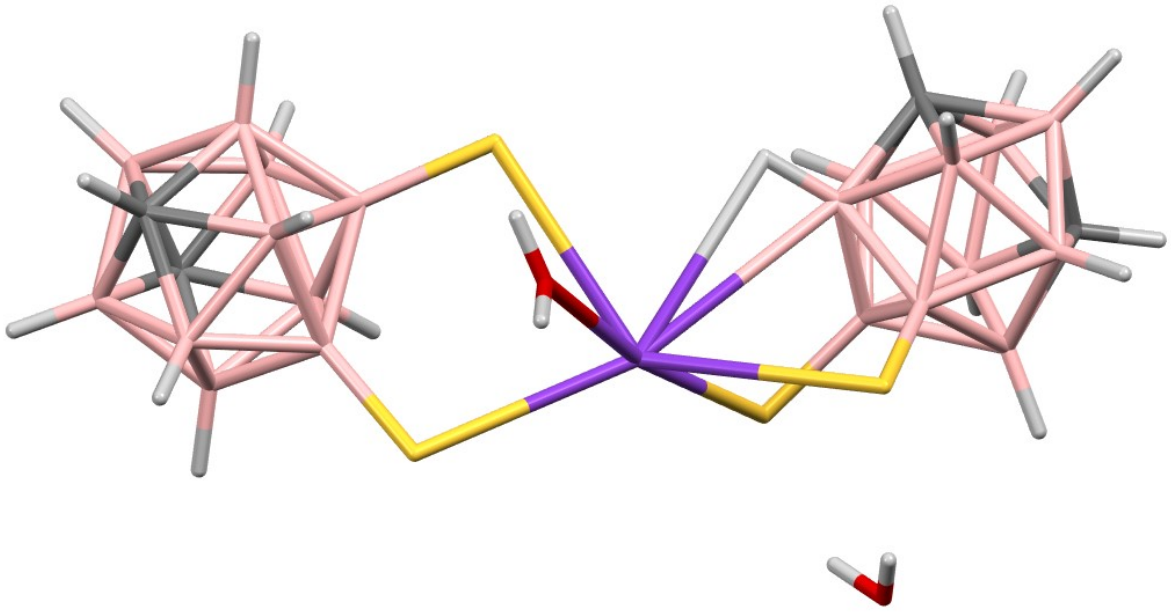


Figure S4. Capped Sticks view of **6**. Solvents and 2.2.2-cryptands were omitted for clarity

Synthetic protocols and characterization

S_2Cl_2 is a toxic material! Please check the safety data sheet prior usage!

All manipulations (unless otherwise stated) were performed under a dry nitrogen atmosphere with exclusion of air and moisture using standard Schlenk techniques. All solvents were dried using standard procedures (toluene, THF, Et_2O over sodium/benzophenone; acetonitrile over CaH_2, CH_2Cl_2 over P_2O_5) and freshly distilled prior to use. Carboranes were purchased from Zhengzhou Yuanli Biological Technology Co. Ltd, and used as received. The ^{1}H, ^{13}C, and ^{11}B NMR spectra were recorded on Bruker AMX 300, DRX 500 spectrometers, and Jeol JNM-ECZL500, using the deuterated solvents ($CDCl_3$, DMSO-*d6*, CD_3OD, CD_2Cl_2, CD_3CN) as internal lock. ^{11}B-NMR and $^{11}B\{^{1}H\}$-NMR chemical shifts were referenced to the external $BF_3{\cdot}OEt_2$. The spectrum simulation was performed with the built-in DNMR module of the Bruker TopSpin program. MestReNova (v.6.0.2-5475) program was used for the baseline correction in the ^{11}B-NMR and $^{11}B\{^{1}H\}$-NMR spectra. Elemental analyses were performed with an Elementar vario MICRO cube analyzer and with a HEKAtech Euro EA CHNS elemental analyzer. IR measurements were performed on a Perkin Elmer Spectrum Two FT-IR spectrometer using the attenuated total reflection (ATR) technique on powdered samples. UV measurements were performed on UNICAM UV4-100 UV/Vis spectrophotometer.

Synthesis of 9,12-$(SH)_2$-1,2-*closo*-$C_2B_{10}H_{10}$ (1) and 9,10-$(SH)_2$-1,7-*closo*-$C_2B_{10}H_{10}$ (2)

To a solution of 1.0 g (7 mmol) of *o*-carborane in 10 mL of CH_2Cl_2 was added to a suspension of 3.7 g (28 mmol) of $AlCl_3$ and 5 mL of CH_2Cl_2 at –50 °C. After that 1.89 g (14 mmol) of S_2Cl_2 (S_2Cl_2 is a toxic material, please check the safety data sheet prior usage) in 5 mL of CH_2Cl_2 was added dropwise to the obtained suspension at –50 °C. After addition it was allowed to warm up slowly (30 min) and then it was heated up and allowed to boil for 12 h. After cooling, the mixture was poured into water. The precipitate obtained was filtered, washed with water. The product was suspended in a solution of 50 mg of NaOH in 50 mL methanol and allowed to stir. 200 mg of $NaBH_4$ was added in small portions to the reaction mixture, and after 2 h of stirring further 200 mg of $NaBH_4$ was added. After 24 hours of stirring, diluted HCl was added to the reaction mixture, until the pH reached 1-2. The raw product was extracted by 3 times using 10-10 mL of ethyl-acetate. After evaporation of the solvent, the raw product was subjected to flash column separation on silica using a mixture of hexane and ethyl-acetate (4:1) as eluent which afforded as white crystals. (1.2 g, 82 % yield)

^{1}H NMR (500.13 MHz, $CDCl_3$): δ 0.59 (s, 2H, SH), 1.69–3.05 (m, 8H, carb-B*H*) 3.52 (s, 2H, carb-C*H*) ^{11}B NMR (160.46 MHz, $CDCl_3$): δ –16.5 (d, 2B, $^1J_{BH}$=178 Hz, carb-*B*H), –14.0 (d, 2B, $^1J_{BH}$=168 Hz, carb-*B*H), –6.6 (d, 2B, $^1J_{BH}$=154 Hz, carb-*B*H), 5.3 (s, 2B, carb-*B*H) ^{11}B{^{1}H} NMR (160.46 MHz, $CDCl_3$): δ –16.5 (s, 2B, carb-*B*H), –14.0 (s, 2B, carb-*B*H), –6.6 (s, 2B, carb-*B*H), 5.3 (s, 2B, carb-*B*H) ^{13}C{^{1}H} NMR (125.77 MHz, $CDCl_3$): δ 47.5 (s, carb-*C*H) Elemental analysis [%]: calculated: C 11.53, H 5.80, S 30.78 found: C 11.83, H 5.64, S 31.84

Applying the same procedure, but starting from *m*-carborane, the corresponding 9,10-$(SH)_2$-1,7-*closo*-$C_2B_{10}H_{10}$ carborane derivative can be obtained with similar yield (1.1 g, 76 % yield).

^{1}H NMR (500.13 MHz, $CDCl_3$): δ 0.57 (s, 2H, S*H*), 1.80–3.33 (m, 8H, carb-B*H*) 2.97 (s, 2H, carb-C*H*) ^{11}B NMR (160.33 MHz, $CDCl_3$): δ –21.0 (d, 2B, $^1J_{BH}$=181 Hz, carb-*B*H), –13.2 (d, 2B, $^1J_{BH}$=170 Hz, carb-*B*H), –5.1 (d, 2B, $^1J_{BH}$=165 Hz, carb-*B*H), –1.8 (s, 2B, carb-*B*H) ^{11}B{^{1}H} NMR (160.33 MHz, $CDCl_3$): δ –21.0 (s, 2B, carb-*B*H), –13.2 (s, 2B, carb-*B*H), –5.1 (s, 2B, carb-*B*H), –1.8 (s, 2B, carb-*B*H) ^{13}C{^{1}H} NMR (125.77 MHz, $CDCl_3$): δ 52.7 (s, carb-*C*H) Elemental analysis [%]: calculated: C 11.53, H 5.80, S 30.78 found: C 11.81, H 5.64, S 29.96

Synthesis of 9,10-$(NH_2)_2$-1,7-*closo*-$C_2B_{10}H_{10}$ (3)

For the hydrolysis of *N,N'*-(1,7-dicarba-*closo*-dodecaboran-9,10-diyl)bis(trifluoroacetamide) we followed the general process of hydrolysis *N*-(1,7-dicarba-*closo*-dodecaboran-9-yl)trifluoroacetamide.[41]

520 mg (1.4 mmol) *N,N'*-(1,7-dicarba-*closo*-dodecaboran-9,10-diyl)bis(trifluoroacetamide) was dissolved in the mixture of 6 mL methanol, 6 mL IPA and 7 mL THF and the solution of 2.68 g (67 mmol) NaOH in 30 mL distilled water was added. The mixture was stirred at room temperature. After 5 days of stirring, 20 mL distilled water was added to the reaction mixture and the solution was extracted by 3 times using 15-15 mL of dichloromethane. After evaporation of the solvent the product was obtained as brownish powder. (210 mg, 86 % yield)

^{1}H NMR (500.13 MHz, $CDCl_3$): δ 0.87 (s, 4H, NH_2), 1.48–2.89 (m, 8H, carb-B*H*) 2.51 (s, 2H, carb-C*H*) ^{11}B NMR (160.46 MHz, $CDCl_3$): δ –27.6 (d, 2B, $^1J_{BH}$=180 Hz, carb-*B*H), –17.1 (d, 2B, $^1J_{BH}$=164 Hz, carb-*B*H), –9.1 (d, 2B, $^1J_{BH}$=158 Hz, carb-*B*H), 2.9 (s, 2B, carb-*B*H) ^{11}B{^{1}H} NMR (160.46 MHz, $CDCl_3$): δ –27.6 (s, 2B, carb-*B*H), –17.1 (s, 2B, carb-*B*H), –9.1 (s, 2B, carb-*B*H), 2.9 (s, 2B, carb-*B*H) ^{13}C{^{1}H} NMR (125.77 MHz, $CDCl_3$): δ 44.9 (s, carb-*C*H)
Elemental analysis [%]: calculated: C 13.78, H 8.10, N 16.08 found: C 15.75, H 8.33, N 14.65

Synthesis and characterization of 4

To a solution of 50 mg (0.29 mmol) **3** in 1.5 mL EtOH was added dropwise to a solution of 20 mg (0.149 mmol) $CuCl_2$ in 1.5 mL of EtOH. The mixture was stirred at room temperature. A pale blue precipitate is observed during the reaction. After 3 hours of stirring, the precipitate obtained was filtered and washed with EtOH, yielding an analytical pure product. (60 mg, 84 % yield). Recrystallization from water at room temperature produced blue crystals suitable for SC-XRD. The low solubility of **4** (several solvents were tried such as water, DMSO, DMF, DCM) does not allow NMR characterization, however IR (**Figure S42**), UV (**Figure S43**) and elemental analysis data are in agreement with the chemical composition obtained by SC-XRD:

The absorption bands around 1568, cm^{-1} are assigned to the asymmetric and symmetric υ(H–N–H) and υ(H–O–H) bending. The asymmetric and symmetric stretching modes of the amino group are observed in the range of 3300–3050 cm^{-1}. The stretching of BH vertices appear around 2610 cm^{-1}, meanwhile the carborane CH is around 3009 cm^{-1} These results are consistent with the DFT-computed IR spectra.
Elemental analysis [%]: calculated: C 9.29, H 5.85, N 10.84, Cl 13.71, found: C 9.35, H 6.37, N 10.73, Cl 13.61

Synthesis of 5

To a solution of 54 mg (0.48 mmol) KO*t*Bu and 133 mg (0.50 mmol) 18-crown-6 in 7 mL of THF was added dropwise to a solution of 50 mg (0.24 mmol) of 9,10-$(S^-)_2$-1,7-*closo*-$C_2B_{10}H_{10}$ in 5 mL of THF. A white precipitate is observed during the reaction. The suspension was stirred overnight at room temperature. After evaporation of the solvent, the white precipitate was washed with a few mL of Et_2O, yielding an analytical pure product. (103 mg, 58% yield – calculated for dried powder, which contains 1.5 eq THF molecule based on the ^{1}H NMR spectra) Recrystallization from acetonitrile solution or acetonitrile-THF mixture at –30 °C afforded as white crystals.

^{1}H NMR (499.71 MHz, DMSO-*d6*): δ 1.76 (m, THF), 2.66 (bs, 4H, carb-C*H*), 3.55 (s, 72H, OCH_2), 3.60 (m, THF) ^{1}H NMR (499.77 MHz, CD_3CN): δ 3.54 (s, 72H, OCH_2) 3.69 (bs, 4H, carb-C*H*) ^{11}B NMR (160.33 MHz, CD_3CN): δ –21.9 (d, 2B, $^1J_{BH}$=182 Hz, carb-*B*H), –16.6 (d, 2B, $^1J_{BH}$=165 Hz, carb-*B*H), –4.0 (d, 2B, $^1J_{BH}$=170 Hz, carb-*B*H), 4.1 (s, 2B, carb-*B*H) ^{11}B{^{1}H} NMR (160.33 MHz, CD_3CN): δ –21.9 (s, 2B, carb-*B*H), –16.6 (s, 2B, carb-*B*H), –4.0 (s, 2B, carb-*B*H), 4.1 (s, 2B, carb-*B*H) ^{13}C{^{1}H} NMR (125.65 MHz, CD_3CN): δ 71.00 (s, 18-crown-6), 71.02 (s, 18-crown-6)

Elemental analysis [%]: calculated (without solvent molecules): calculated: C 35.27, H 6.81, S 9.42 found: C, 34.05, H 6.82, S, 6.66

Synthesis of 6

To a solution of 113 mg (1.0 mmol) KO*t*Bu and 380 mg (1.0 mmol) 2.2.2-Cryptand in 15 mL of THF was added dropwise to a solution of 50 mg (0.24 mmol) of 9,10-$(S^-)_2$-1,7-closo-$C_2B_{10}H_{10}$ in 5 mL of THF. A white precipitate is observed during the reaction. The suspension was stirred overnight at room temperature. After evaporation of the solvent, the white precipitate was washed with a few mL of Et_2O, yielding an analytical pure product. (135 mg, 64% yield – calculated for dried powder, which contains 0.75 eq THF molecule based on the ^{1}H NMR spectra) Recrystallization from acetonitrile solution at –30 °C afforded as white crystals.

^{1}H NMR (500.13 MHz, CD_2Cl_2): δ 1.81 (m, THF), 2.54 (t, 36H, $^3J_{HH}$= 4.6 Hz, NCH_2), 3.34 (bs, 4H, carb-C*H*), 3.53 (t, 36H, $^3J_{HH}$= 4.6 Hz, OCH_2CH_2N), 3.59 (s, 36H, OCH_2CH_2O), 3.68 (m, THF) ^{1}H NMR (500.13 MHz, CD_3OD): δ 1.87 (m, THF), 2.58 (t, 36H, $^3J_{HH}$= 4.5 Hz, NCH_2), 3.16 (bs, 4H, carb-C*H*), 3.57 (t, 36H, $^3J_{HH}$= 4.6 Hz, OCH_2CH_2N), 3.62 (s, 36H, OCH_2CH_2O), 3.73 (m, THF) ^{11}B NMR (160.46 MHz, CD_2Cl_2): δ –21.0 (d, 2B, $^1J_{BH}$=184 Hz, carb-*B*H), –15.5 (d, 2B, $^1J_{BH}$=178 Hz, carb-*B*H), –2.7 (d, 2B, $^1J_{BH}$=174 Hz, carb-*B*H), 5.3 (s,

2B, carb-*B*H) $^{11}B\{^{1}H\}$ NMR (160.46 MHz, CD_2Cl_2): δ –21.0 (s, 2B, carb-*B*H), –15.5 (s, 2B, carb-*B*H), –2.7 (s, 2B, carb-*B*H), 5.3 (s, 2B, carb-*B*H) ^{11}B NMR (160.46 MHz, CD_3OD): δ –23.9 (d, 2B, $^{1}J_{BH}$ =179 Hz, carb-*B*H), –14.3 (d, 2B, $^{1}J_{BH}$=180 Hz, carb-*B*H), –4.9 (d, 2B, $^{1}J_{BH}$=172 Hz, carb-*B*H), 1.5 (s, 2B, carb-*B*H) $^{11}B\{^{1}H\}$ NMR (160.46 MHz, CD_3OD): δ –23.9 (s, 2B, carb-*B*H), –14.3 (s, 2B, carb-*B*H), –4.9 (s, 2B, carb-*B*H), 1.5 (s, 2B, carb-BH) $^{13}C\{^{1}H\}$ NMR (125.65 MHz, CD_2Cl_2): δ 53.8 (s, overlap with the signal of CD_2Cl_2, 2.2.2-cryptand) 67.5 (s, 2.2.2-cryptand), 70.5 (s, 2.2.2-cryptand), the carb-CH signal probably overlap with the signal of CD_2Cl_2 therefore the ^{13}C NMR was measured in CD_3OD solvent. $^{13}C\{^{1}H\}$ NMR (125.77 MHz, CD_3OD): δ 52.0 (s, carb-*C*H), 55.1 (s, 2.2.2-cryptand) 68.8, (s, 2.2.2-cryptand) 71.6 (s, 2.2.2-cryptand)

Elemental analysis [%]: calculated (without solvent molecules): C 41.01, H, 7.60, N 4.95, S 7.55 found: C 39.06, H 7.37, N 4.27, S 3.87 Note: As the crystal structure of **6** contains substantial amount of solvent molecules, CHN measurements produced non-reproducible results.

NMR spectra of the compounds

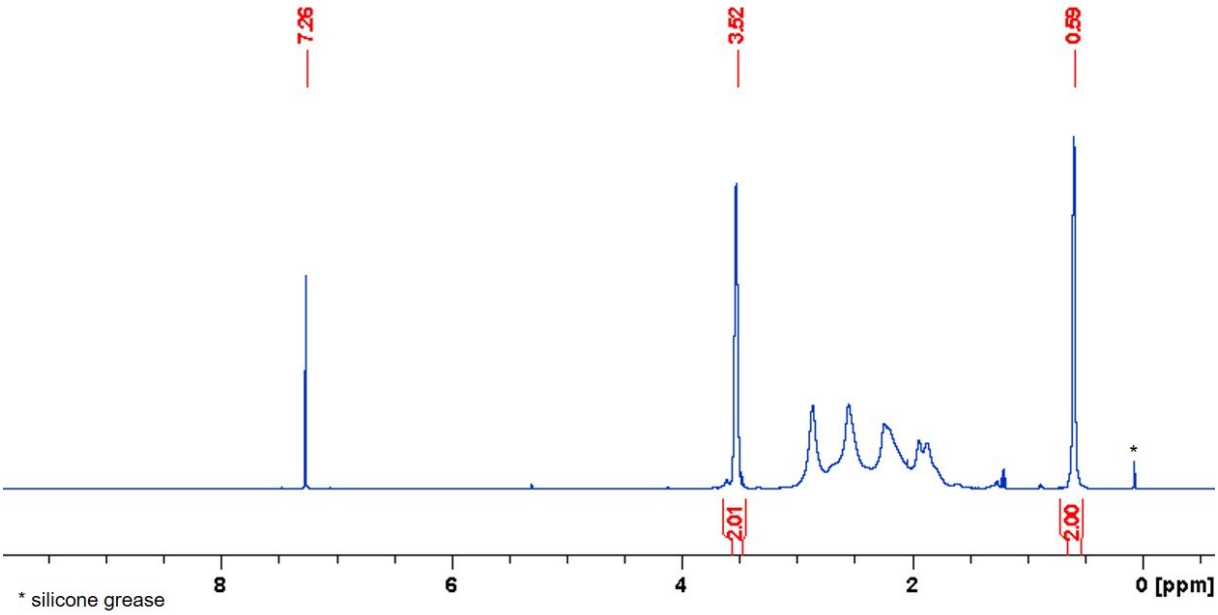


Figure S5. ^{1}H NMR spectra of **1** in $CDCl_3$

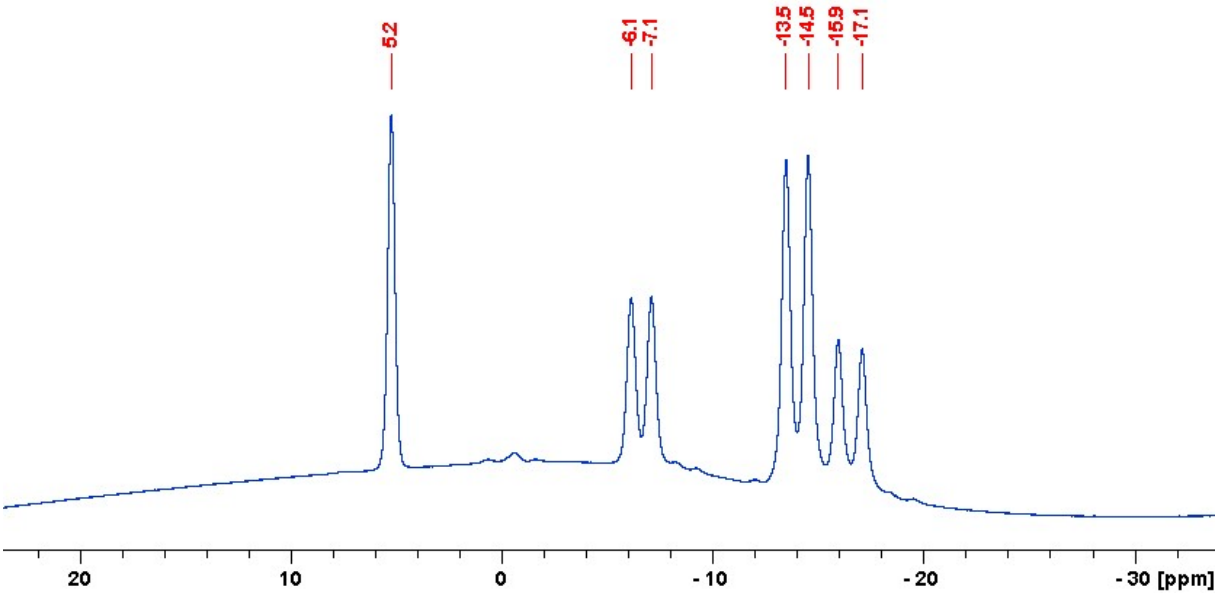


Figure S6. ^{11}B NMR spectra of **1** in $CDCl_3$

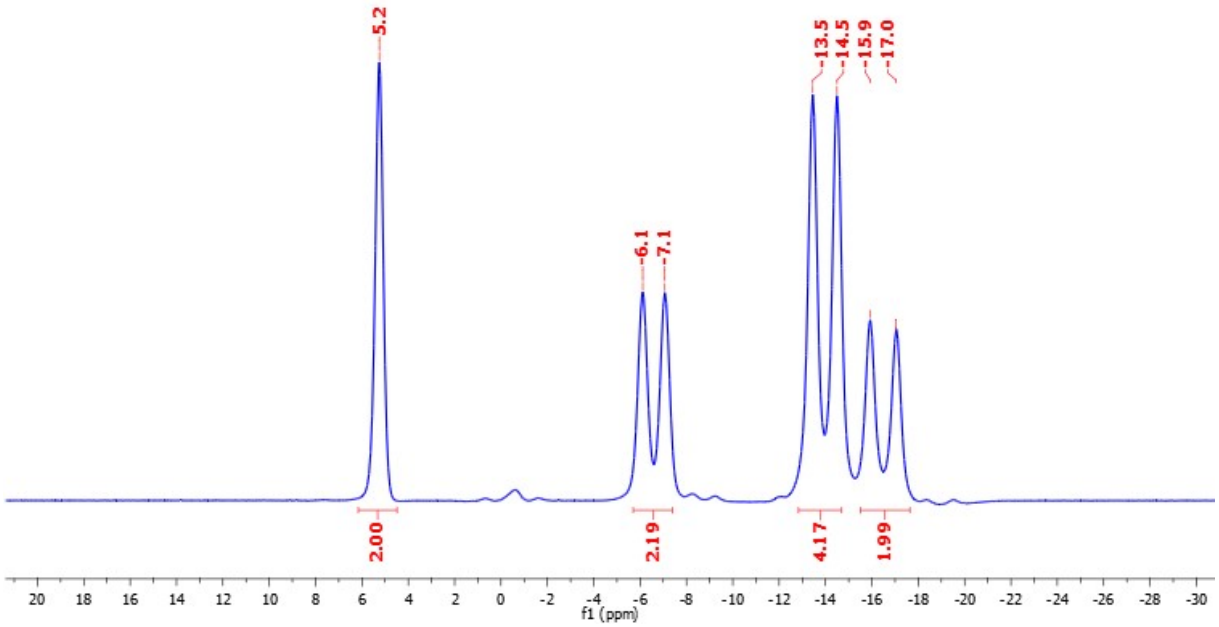


Figure S7. ^{11}B NMR spectra of **1** in $CDCl_3$ (MestReNova program was used for the baseline correction)

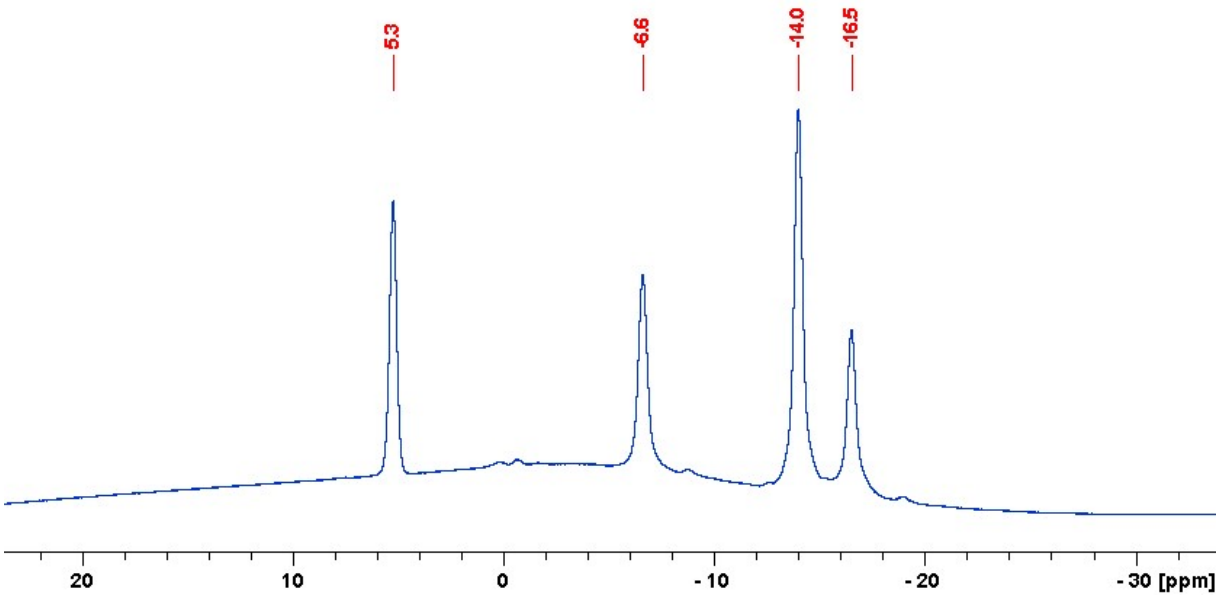


Figure S8. $^{11}B\{^1H\}$ NMR spectra of **1** in $CDCl_3$

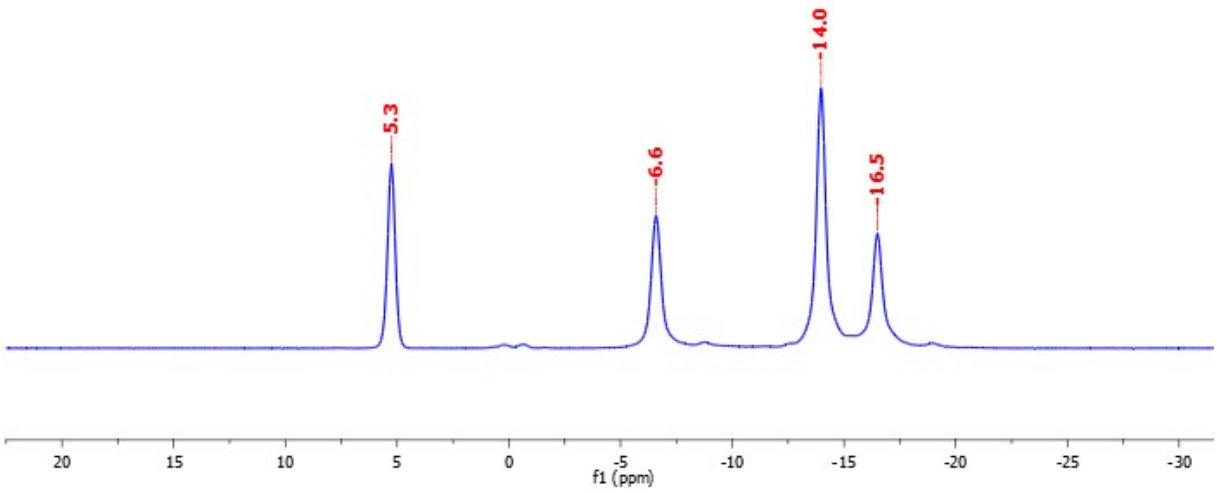


Figure S9. $^{11}B\{^{1}H\}$ NMR spectra of **1** in $CDCl_3$ (MestReNova program was used for the baseline correction)

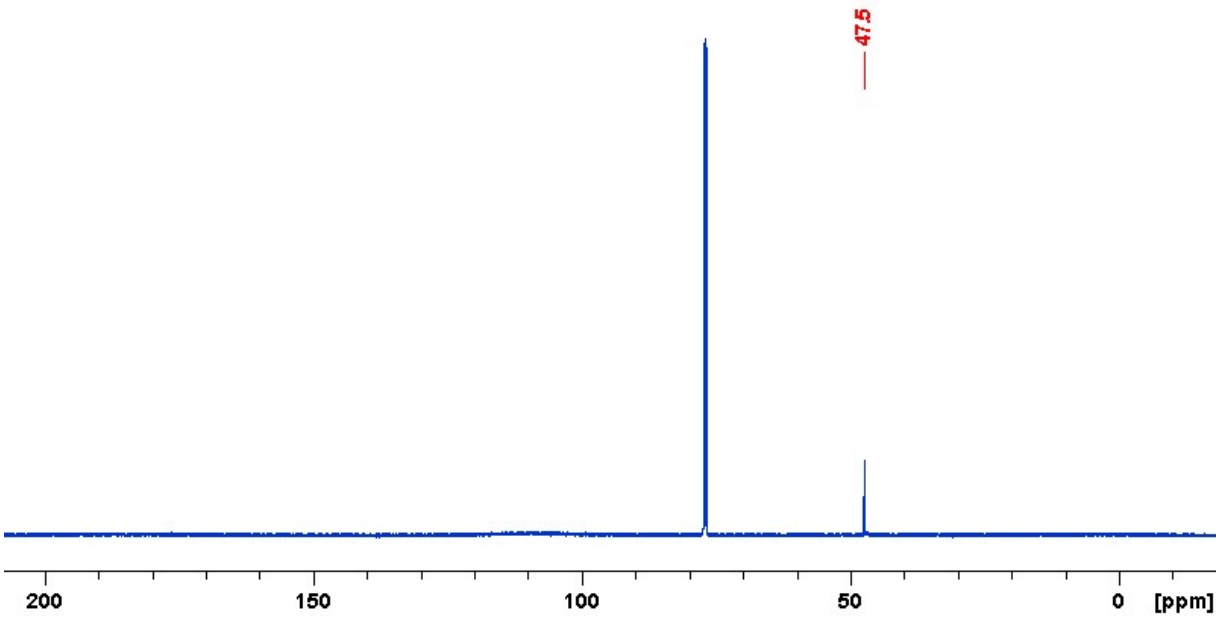


Figure S10. $^{13}C\{^{1}H\}$ NMR spectra of **1** in $CDCl_3$

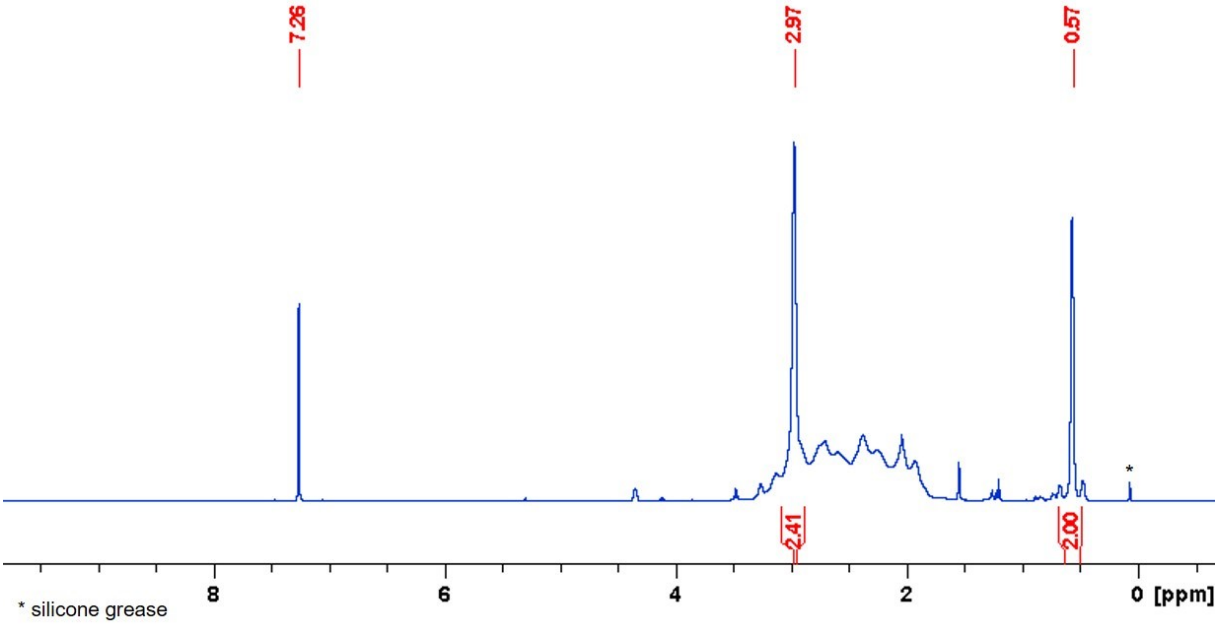


Figure S11. ^{1}H NMR spectra of **2** in $CDCl_3$

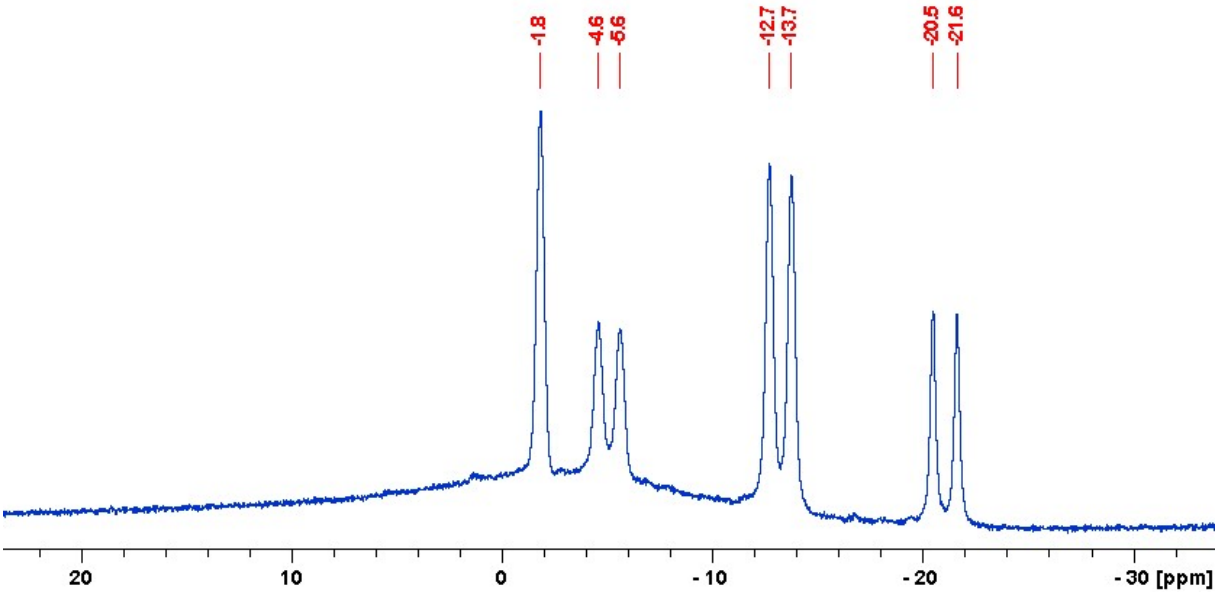


Figure S12. ^{11}B NMR spectra of **2** in $CDCl_3$

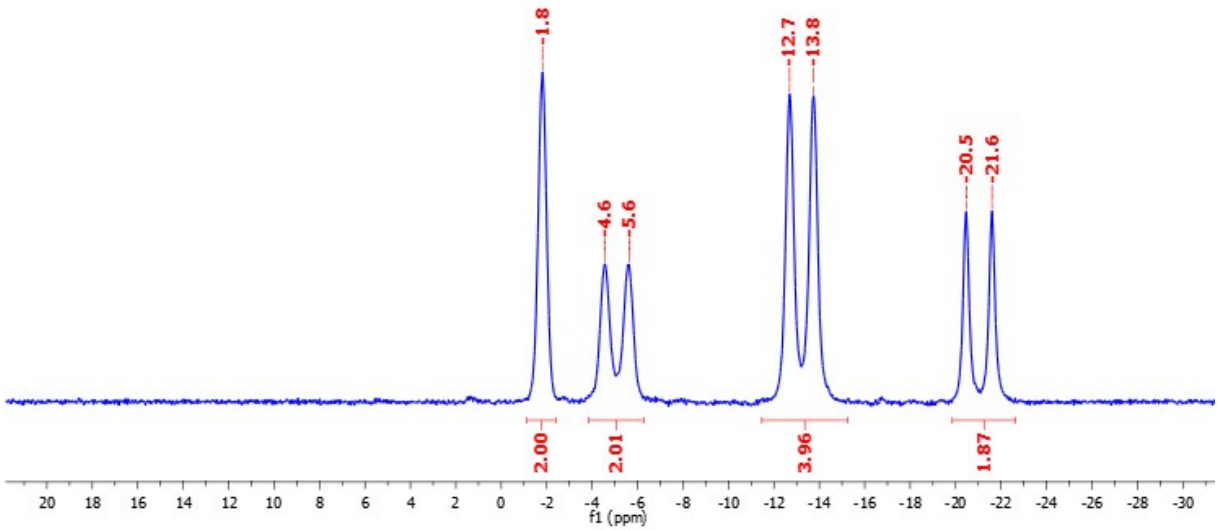


Figure S13. ^{11}B NMR spectra of **2** in $CDCl_3$ (MestReNova program was used for the baseline correction)

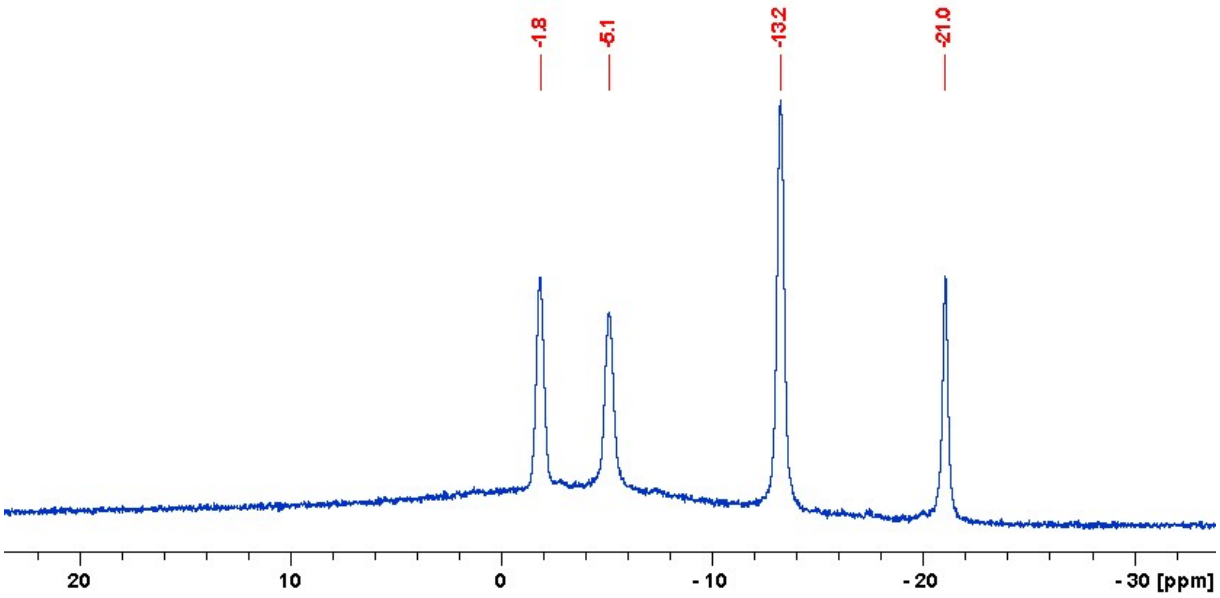


Figure S14. $^{11}B\{^1H\}$ NMR spectra of **2** in $CDCl_3$

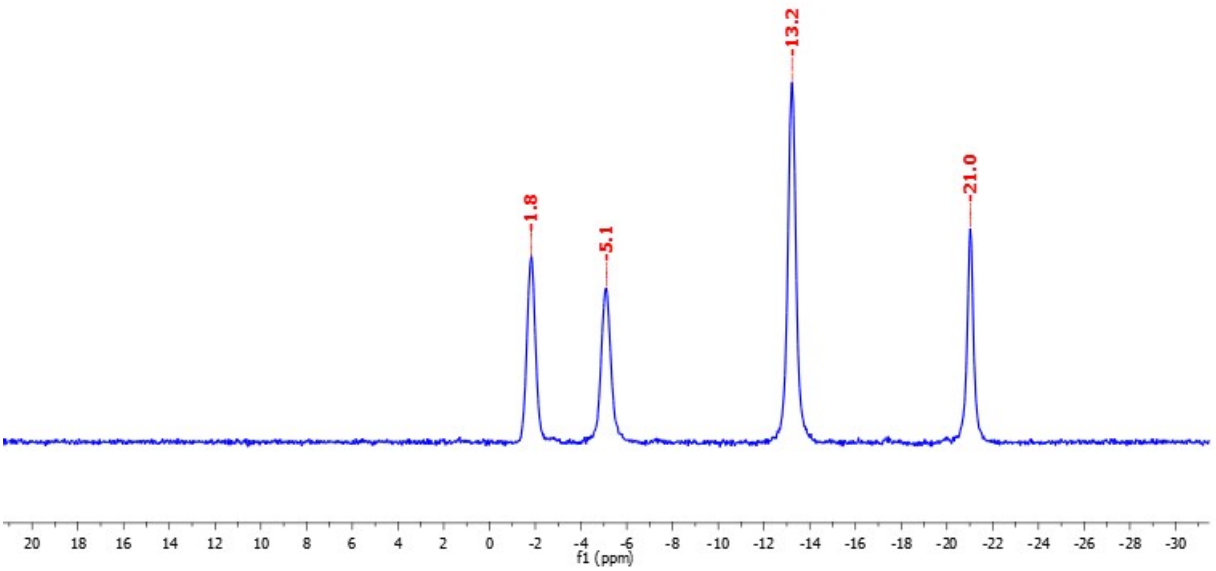


Figure S15. $^{11}B\{^{1}H\}$ NMR spectra of **2** in $CDCl_3$ (MestReNova program was used for the baseline correction)

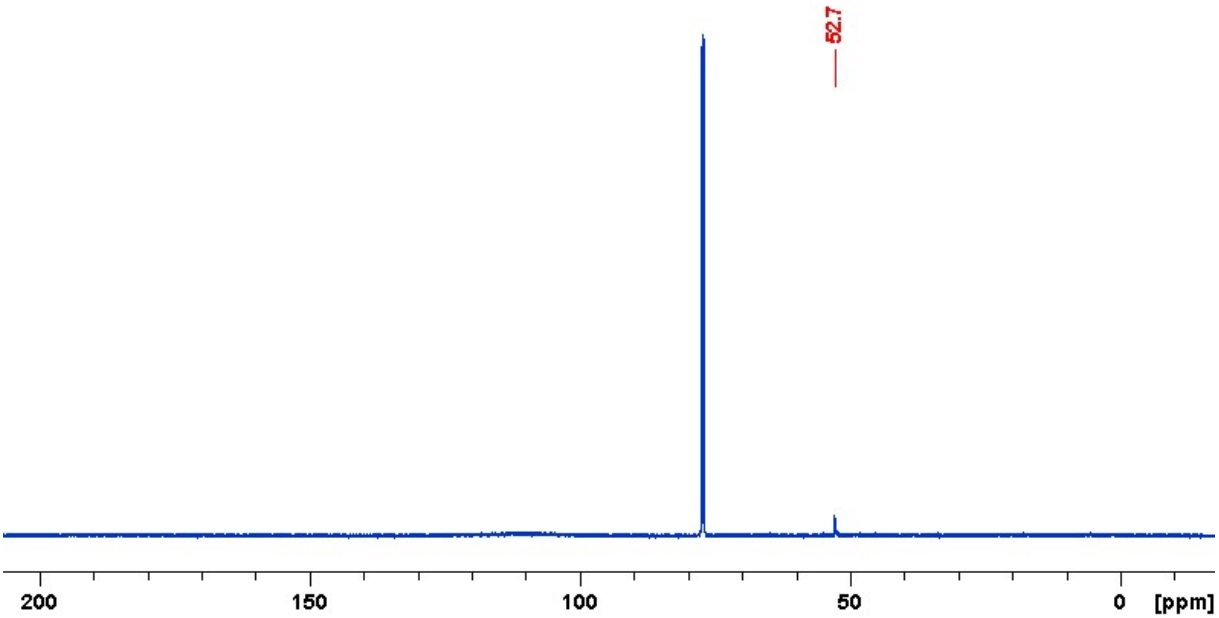


Figure S16. $^{13}C\{^{1}H\}$ NMR spectra of **2** in $CDCl_3$

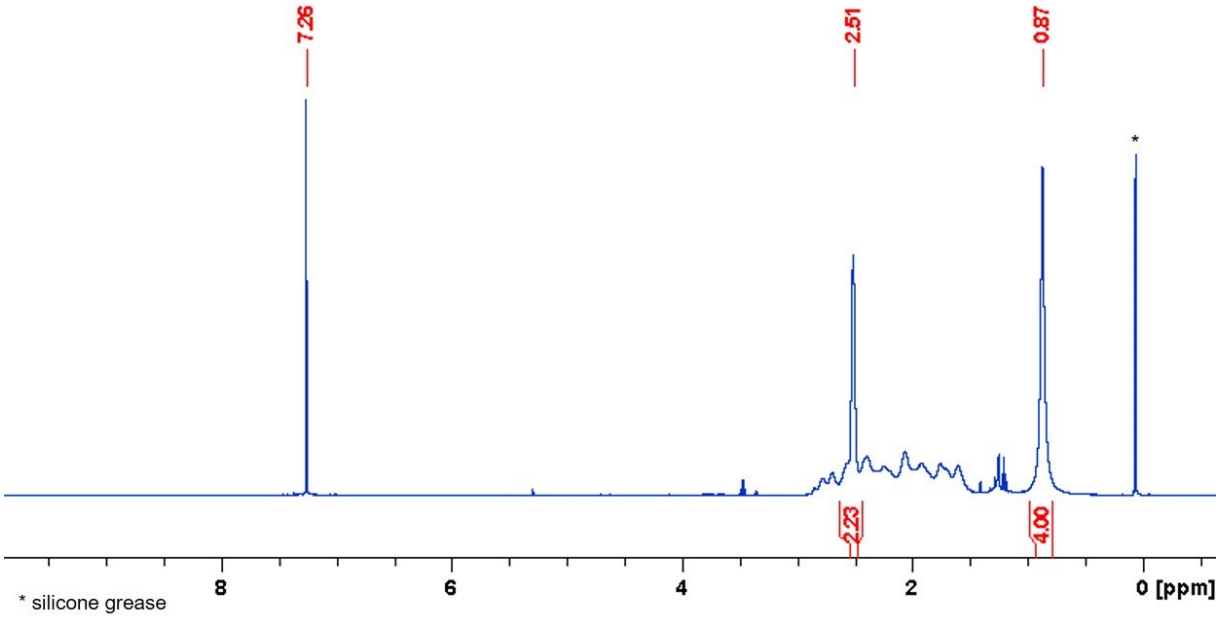


Figure S17. ^{1}H NMR spectra of **3** in $CDCl_3$

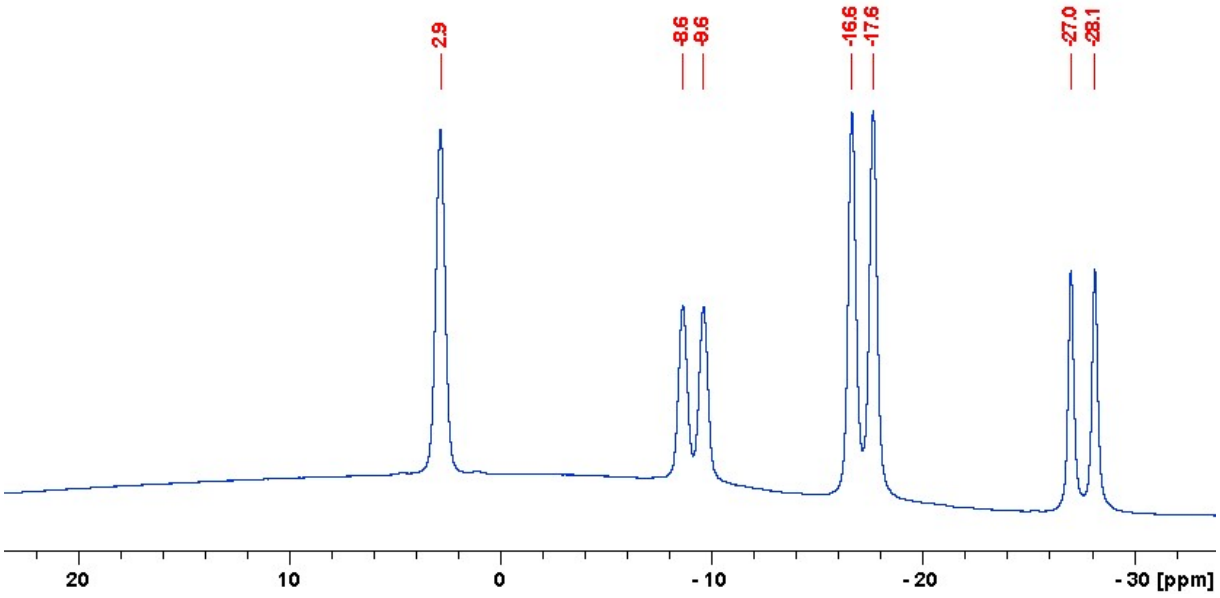


Figure S18. ^{11}B NMR spectra of **3** in $CDCl_3$

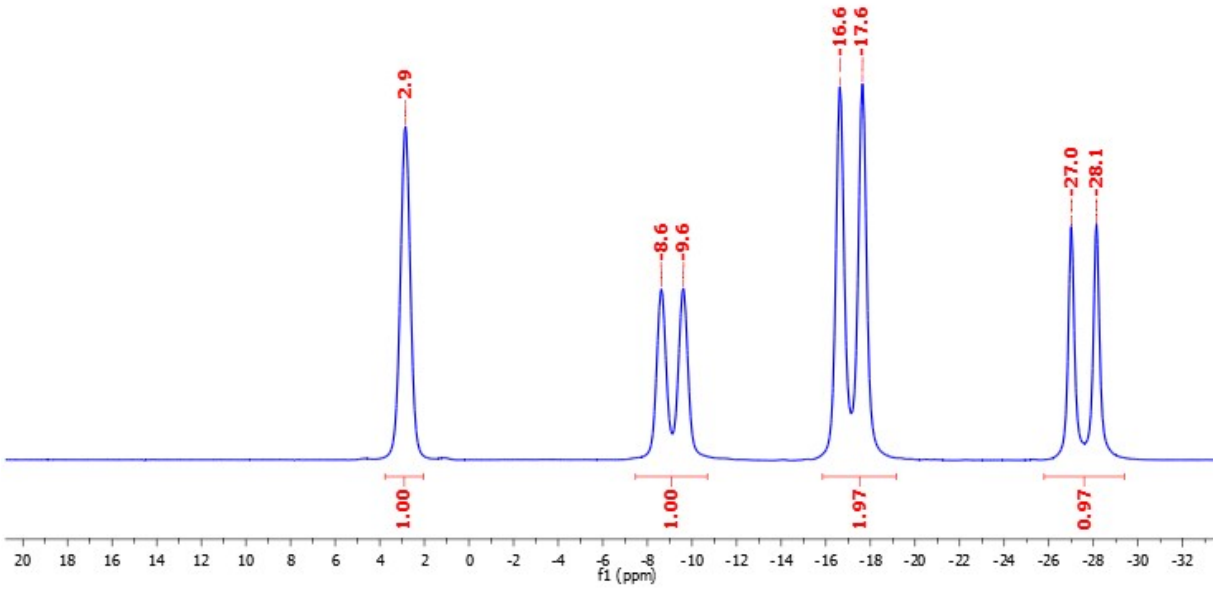


Figure S19. ^{11}B NMR spectra of **3** in $CDCl_3$ (MestReNova program was used for the baseline correction)

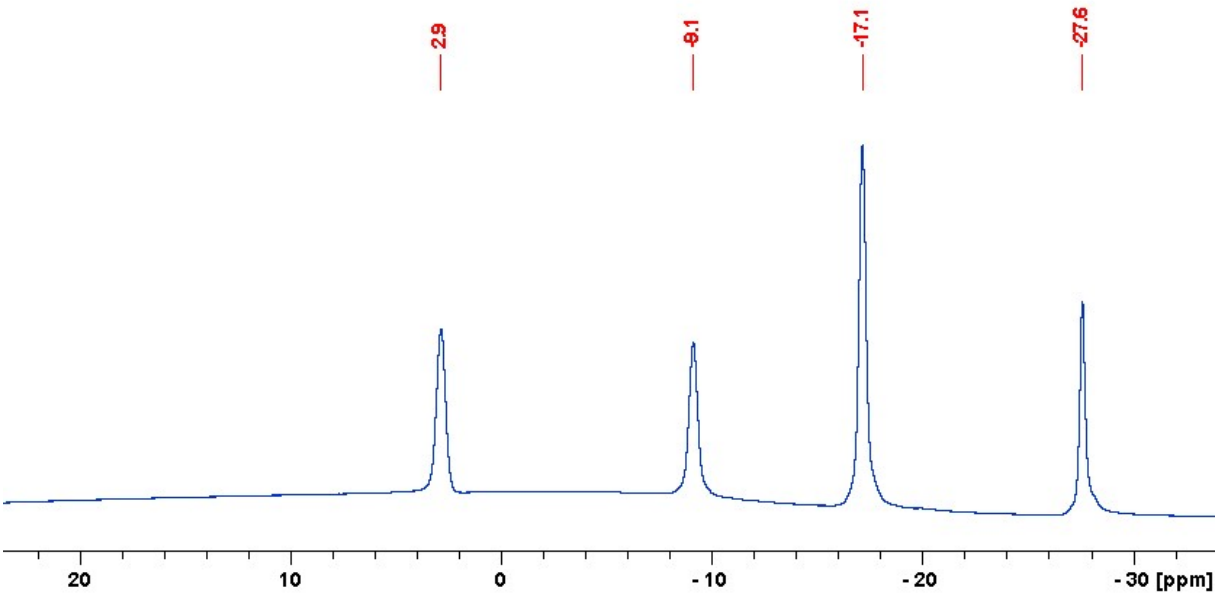


Figure S20. $^{11}B\{^1H\}$ NMR spectra of **3** in $CDCl_3$

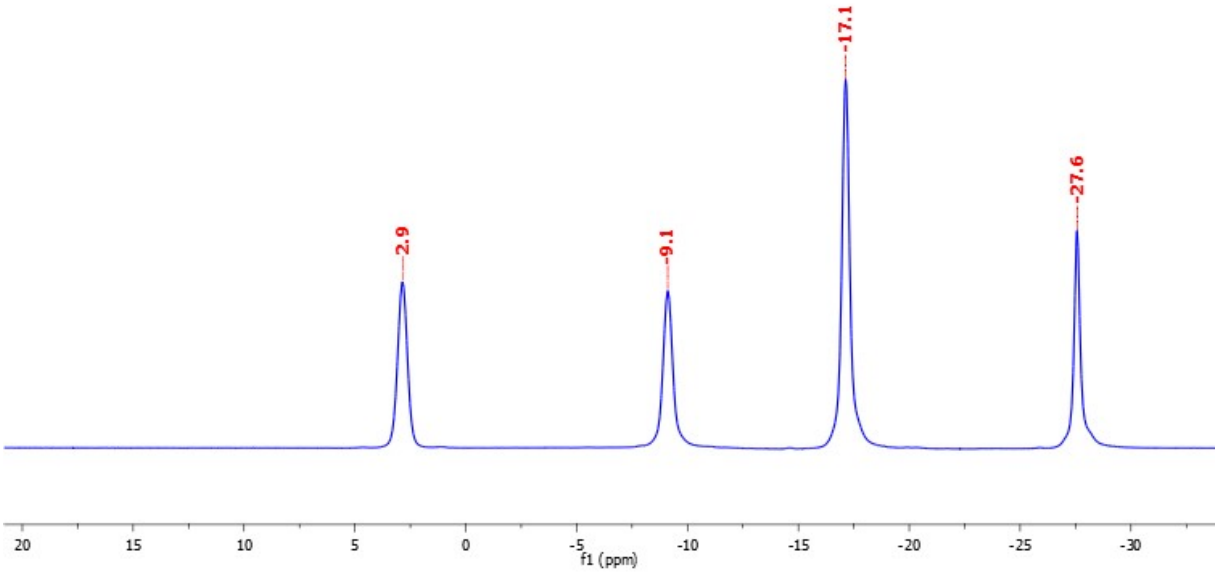


Figure S21. $^{11}B\{^{1}H\}$ NMR spectra of **3** in $CDCl_3$ (MestReNova program was used for the baseline correction)

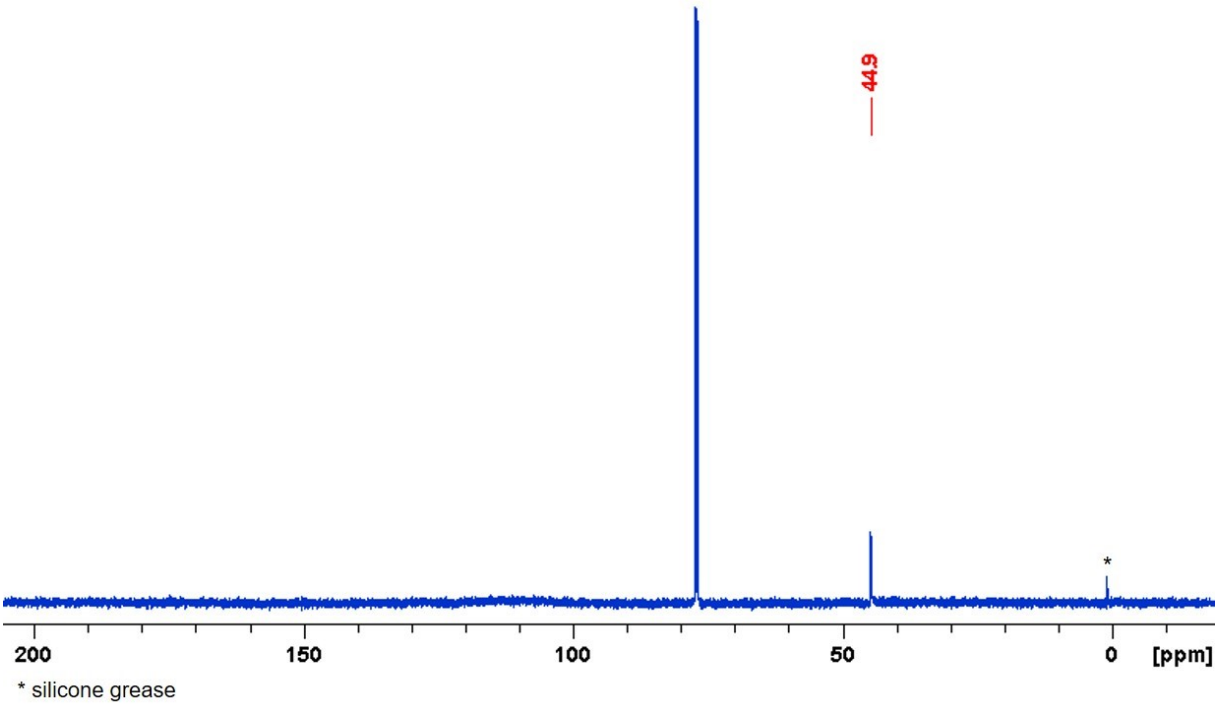


Figure S22. $^{13}C\{^{1}H\}$ NMR spectra of **3** in $CDCl_3$

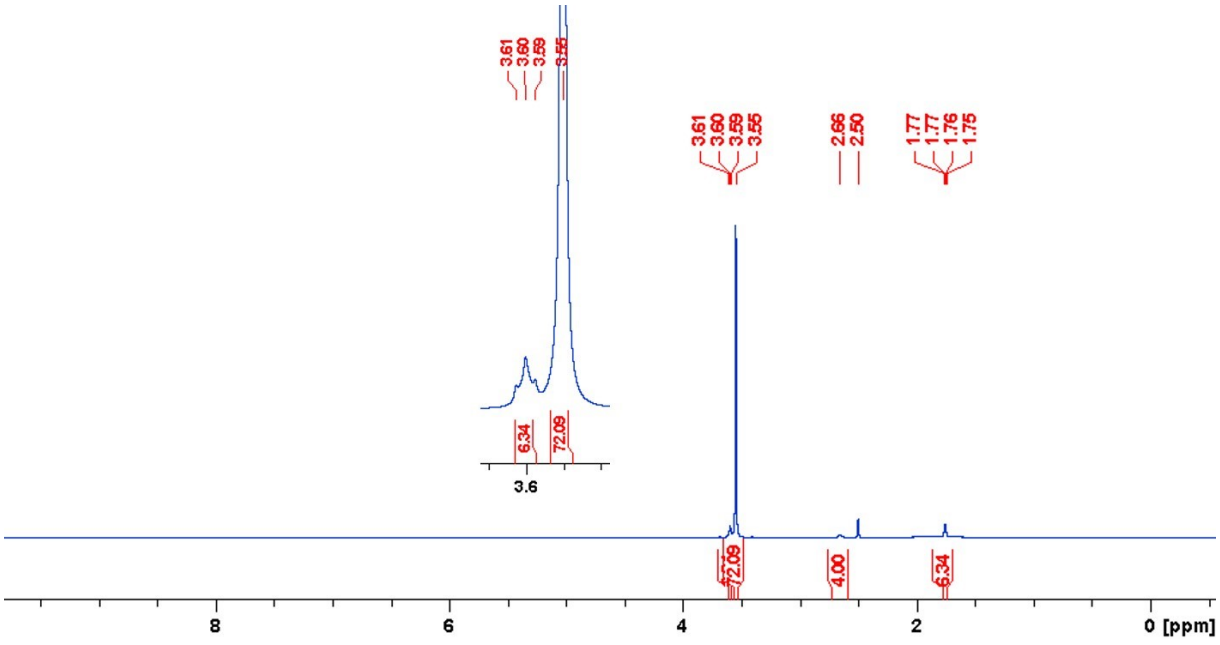


Figure S23. [1]H NMR spectra of **5** in DMSO-*d6*

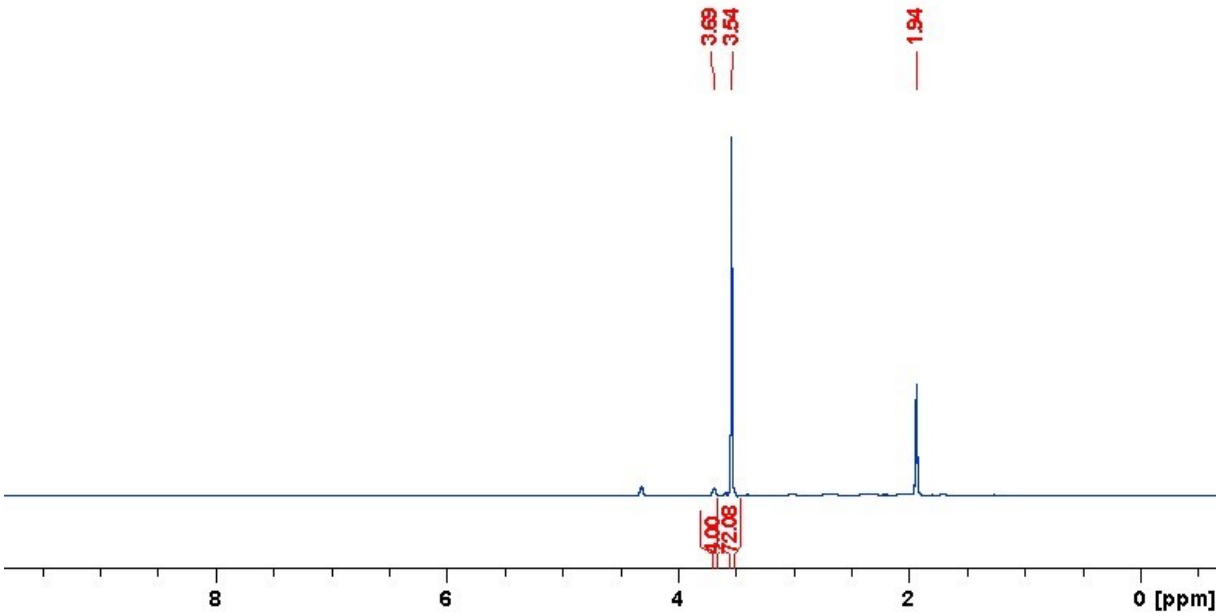


Figure S24. [1]H NMR spectra of **5** in CD_3CN

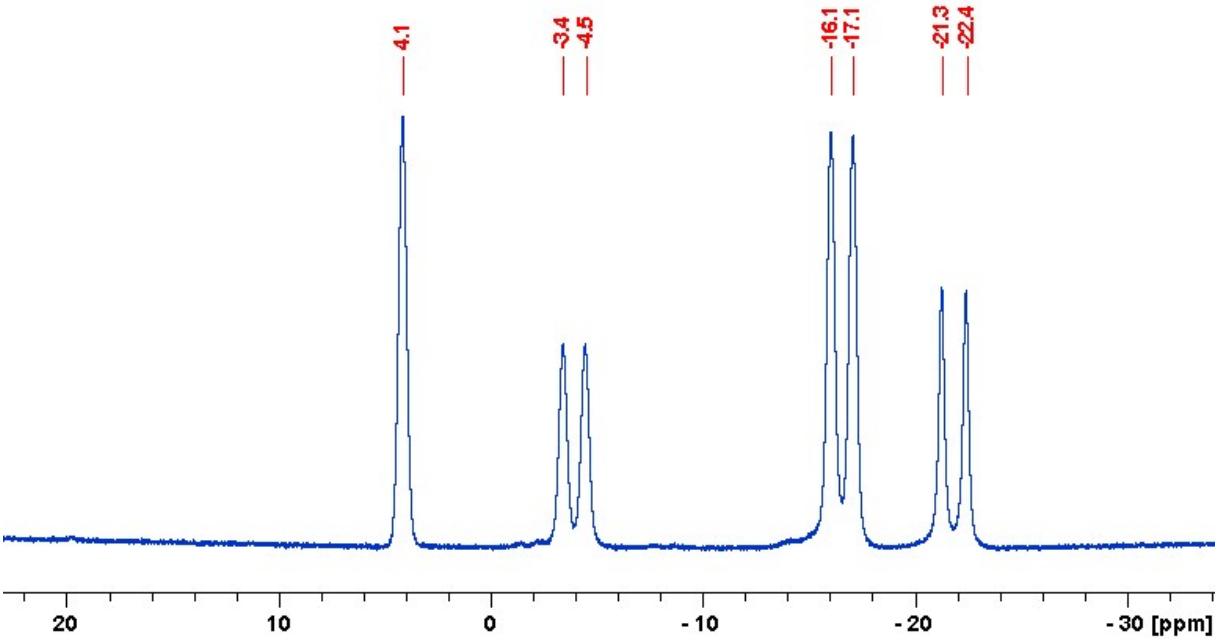


Figure S25. ^{11}B NMR spectra of **5** in CD_3CN

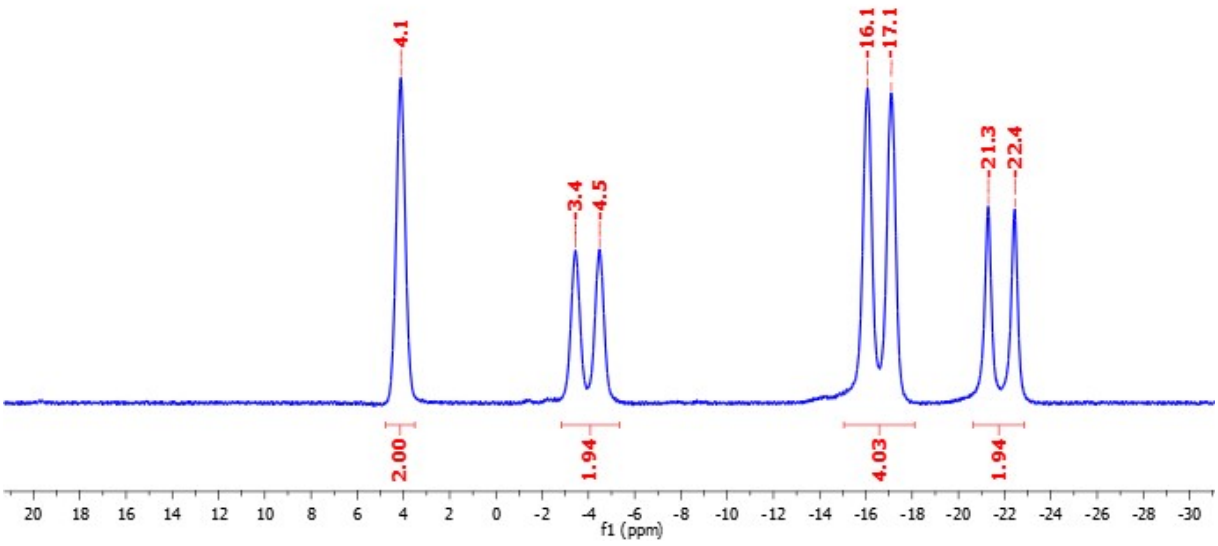


Figure S26. ^{11}B NMR spectra of **5** in CD_3CN (MestReNova program was used for the baseline correction)

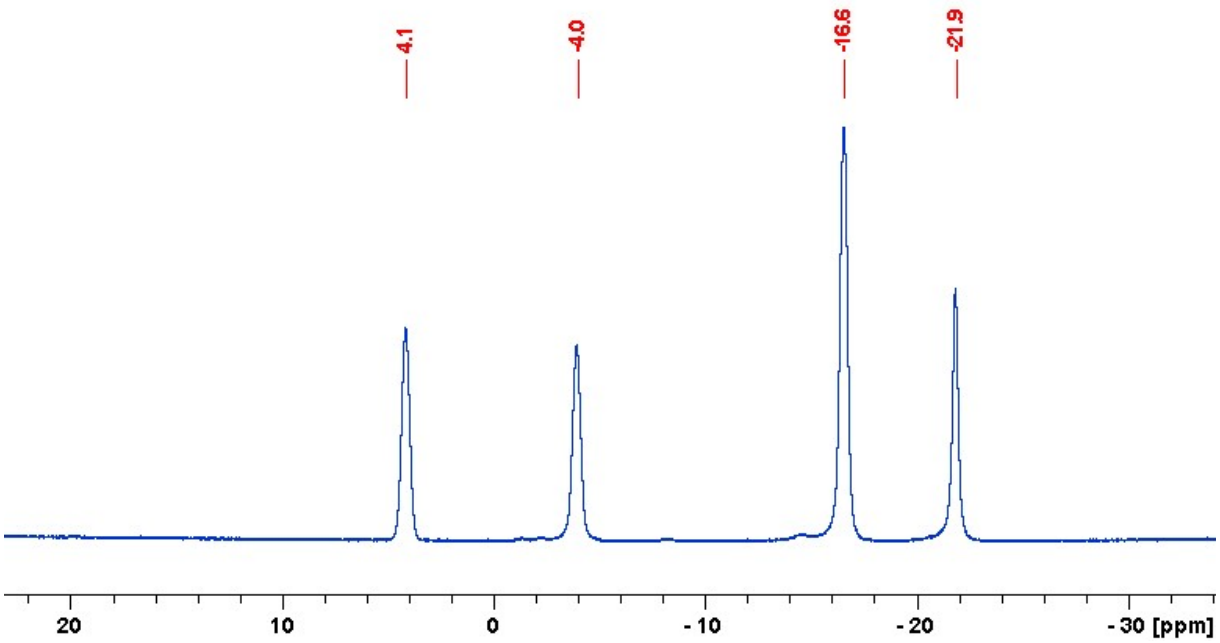


Figure S27. $^{11}B\{^{1}H\}$ NMR spectra of **5** in CD_3CN

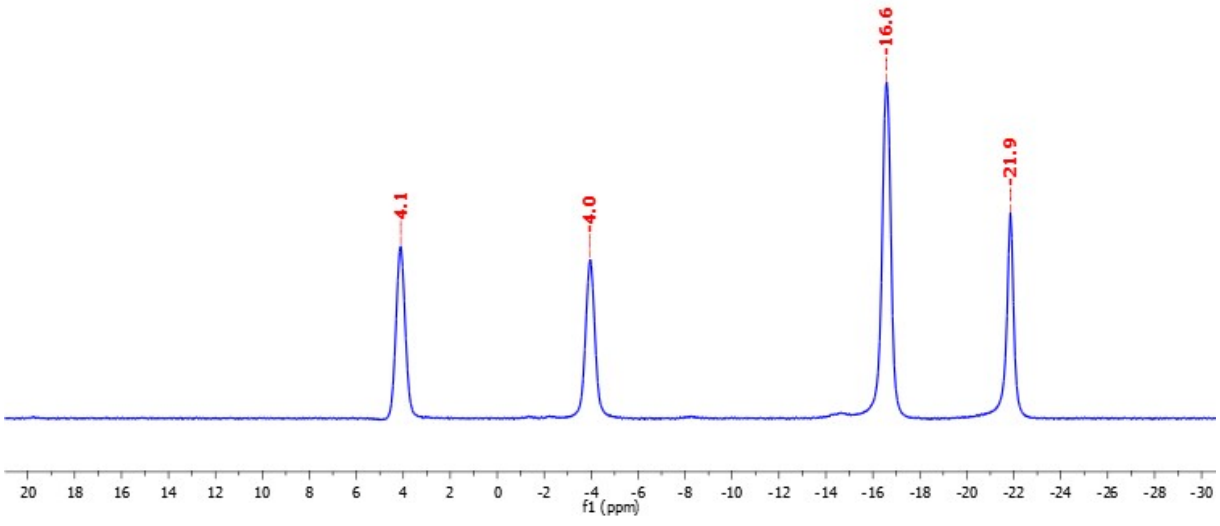


Figure S28. $^{11}B\{^{1}H\}$ NMR spectra of **5** in CD_3CN (MestReNova program was used for the baseline correction)

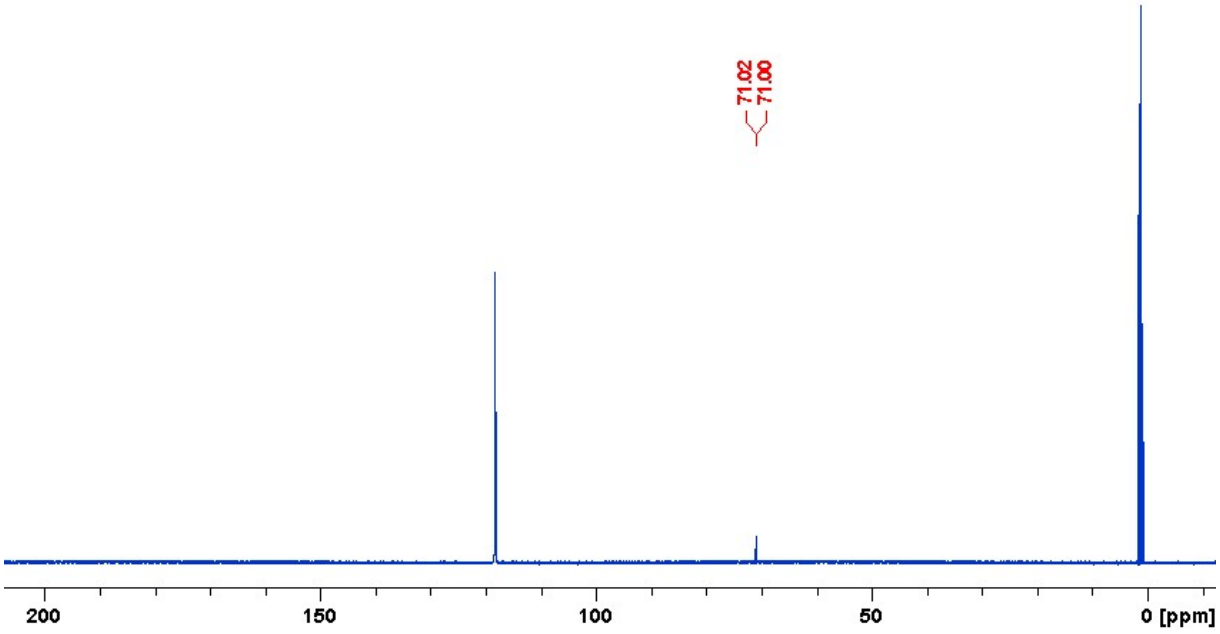


Figure S29. $^{13}C\{^{1}H\}$ NMR spectra of **5** in CD_3CN

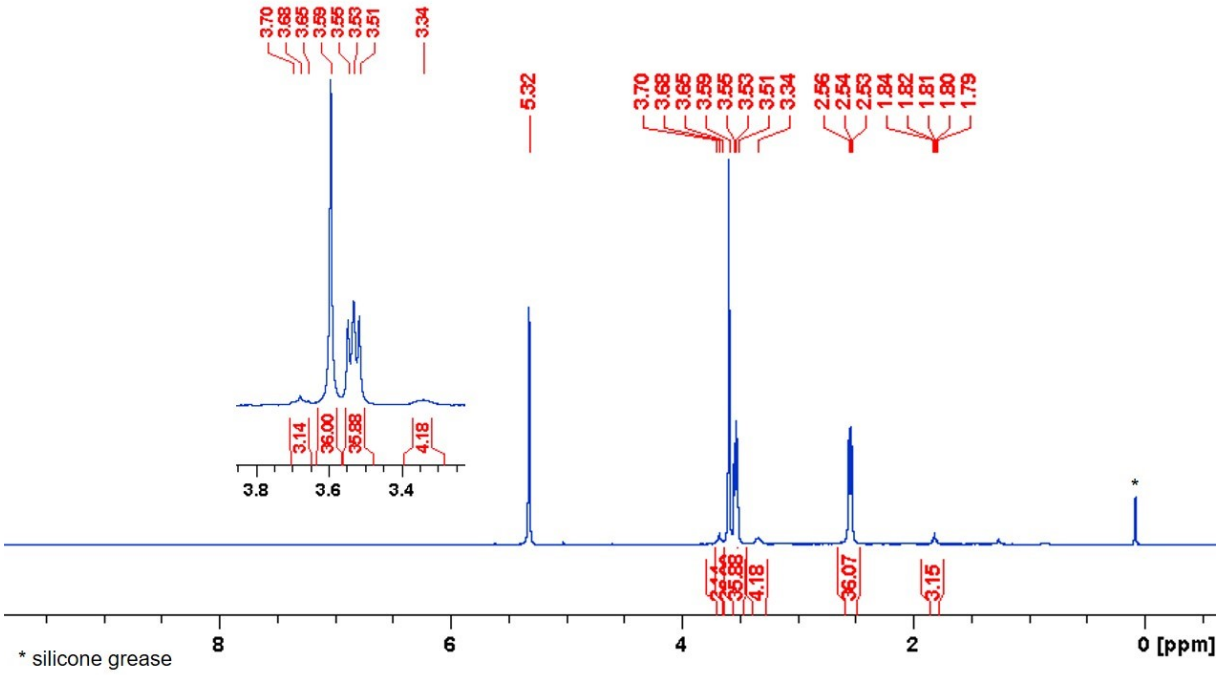


Figure S30. ^{1}H NMR spectra of **6** in CD_2Cl_2

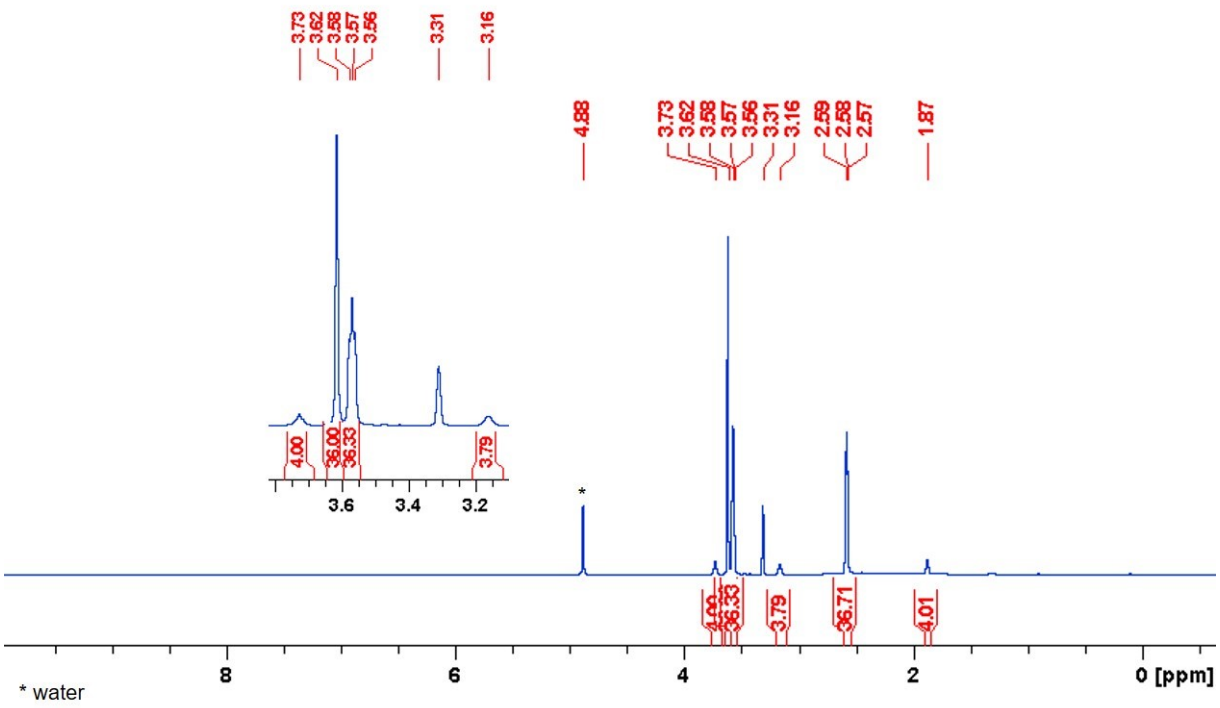


Figure S31. ^{1}H NMR spectra of **6** in CD_3OD

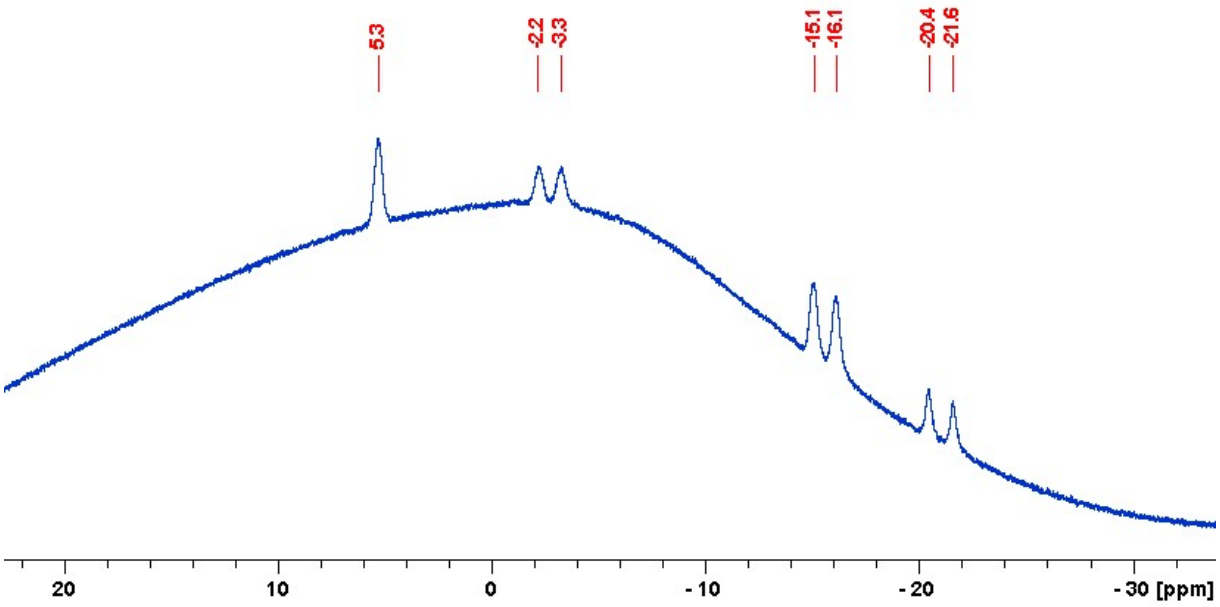


Figure S32. ^{11}B NMR spectra of **6** in CD_2Cl_2

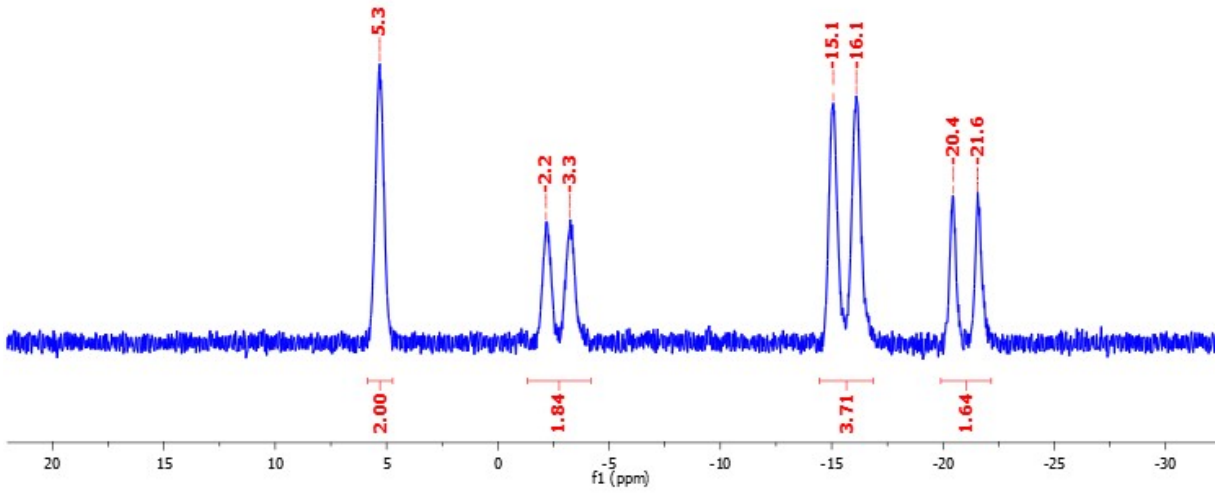


Figure S33. ^{11}B NMR spectra of **6** in CD_2Cl_2 (MestReNova program was used for the baseline correction)

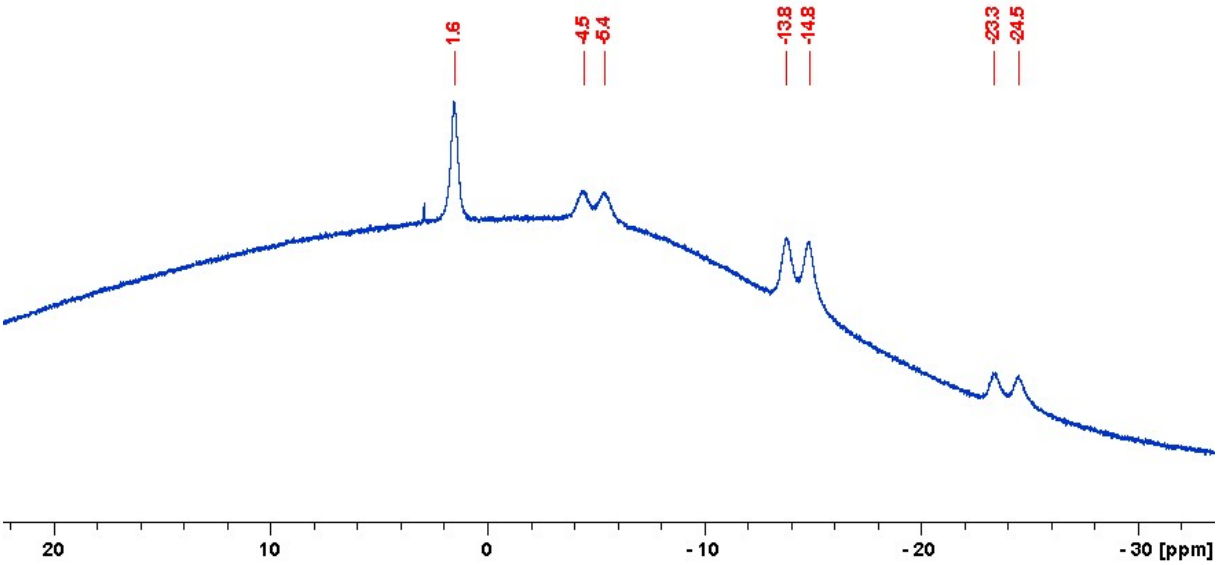


Figure S34. ^{11}B NMR spectra of **6** in CD_3OD. The signal around 2.9 ppm most likely belongs to the $[BOMe_4]^-$ anion as a product of the decomposition of the carborane cluster.

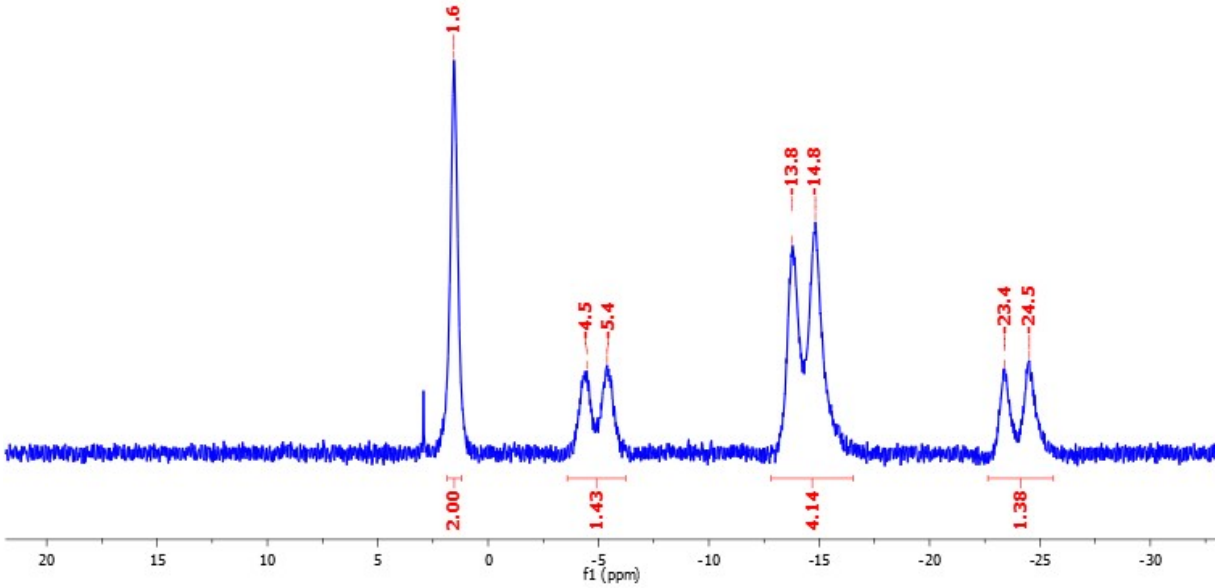


Figure S35. ^{11}B NMR spectra of **6** in CD_3OD The signal around 2.9 ppm most likely belongs to the $[BOMe_4]^-$ anion as a product of the decomposition of the carborane cluster. (MestReNova program was used for the baseline correction)

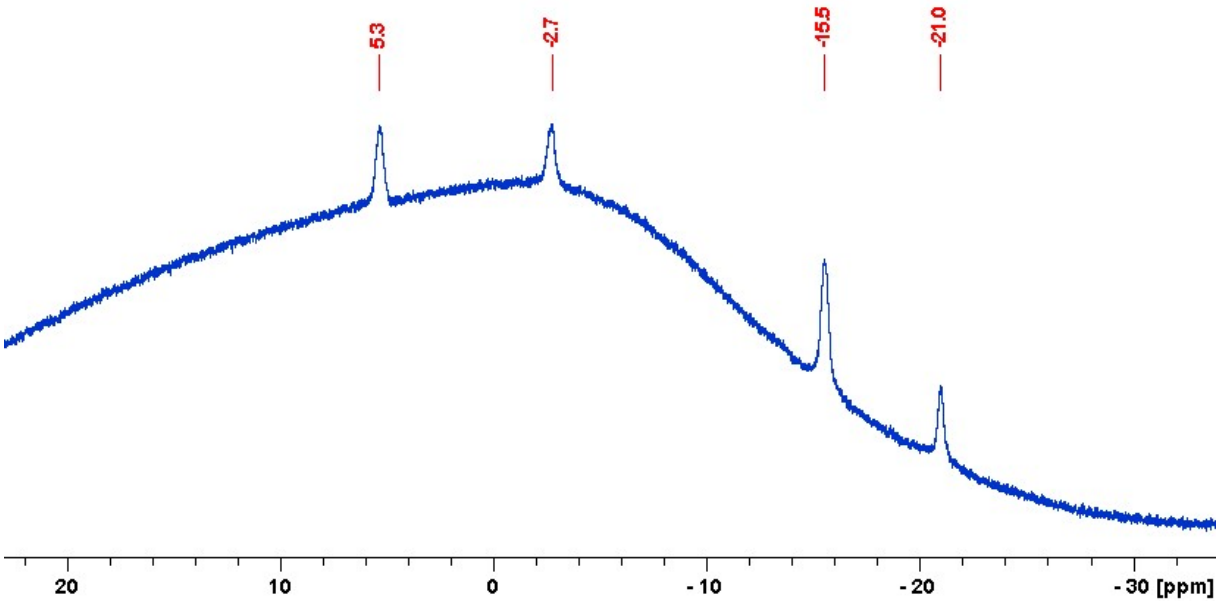


Figure S36. $^{11}B\{^1H\}$ NMR spectra of **6** in CD_2Cl_2

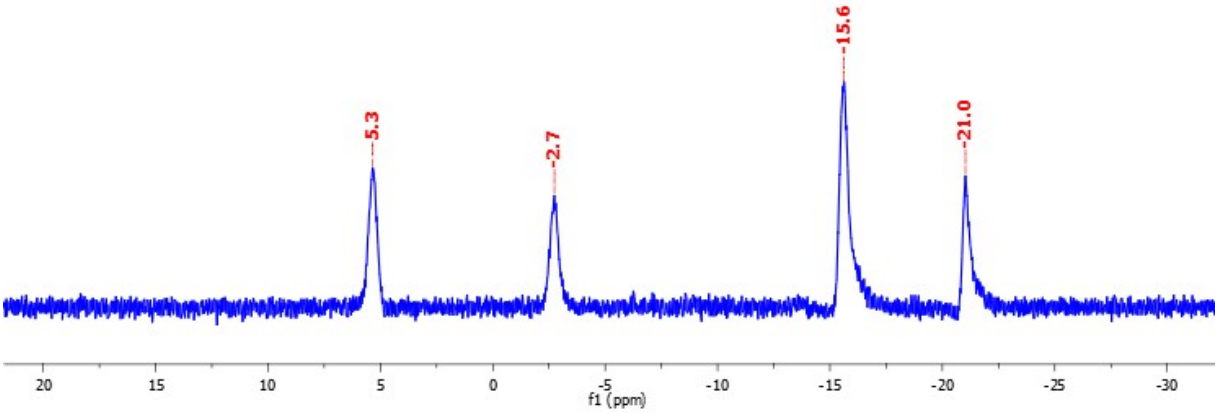


Figure S37. $^{11}B\{^{1}H\}$ NMR spectra of **6** in CD_2Cl_2 (MestReNova program was used for the baseline correction)

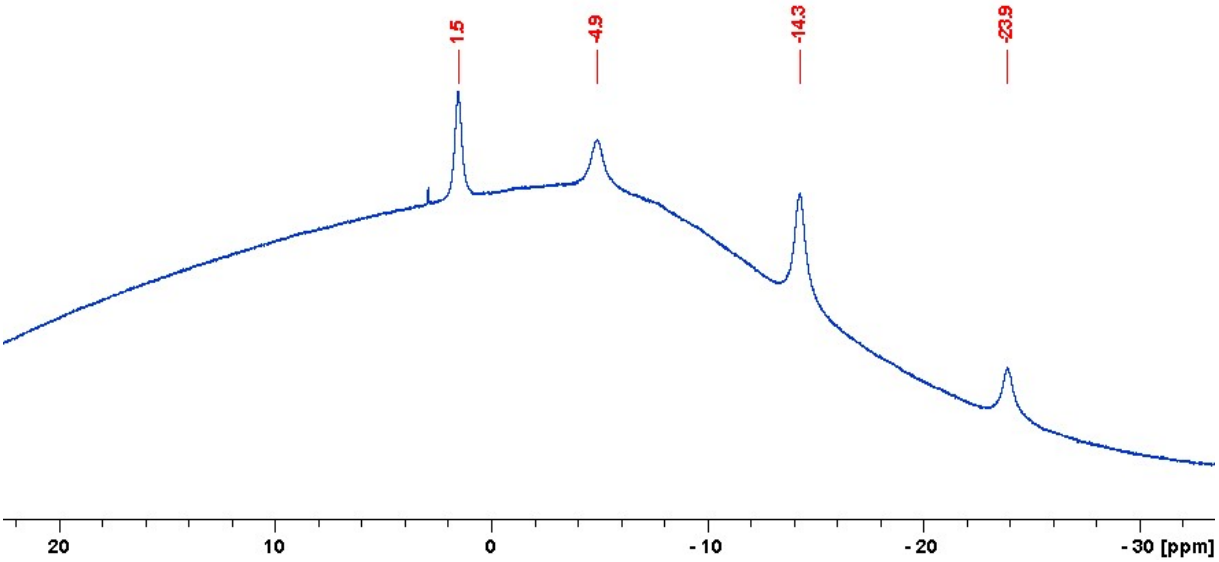


Figure S38. $^{11}B\{^{1}H\}$ NMR spectra of **6** in CD_3OD The signal around 2.9 ppm most likely belongs to the $[BOMe_4]^-$ anion as a product of the decomposition of the carborane cluster.

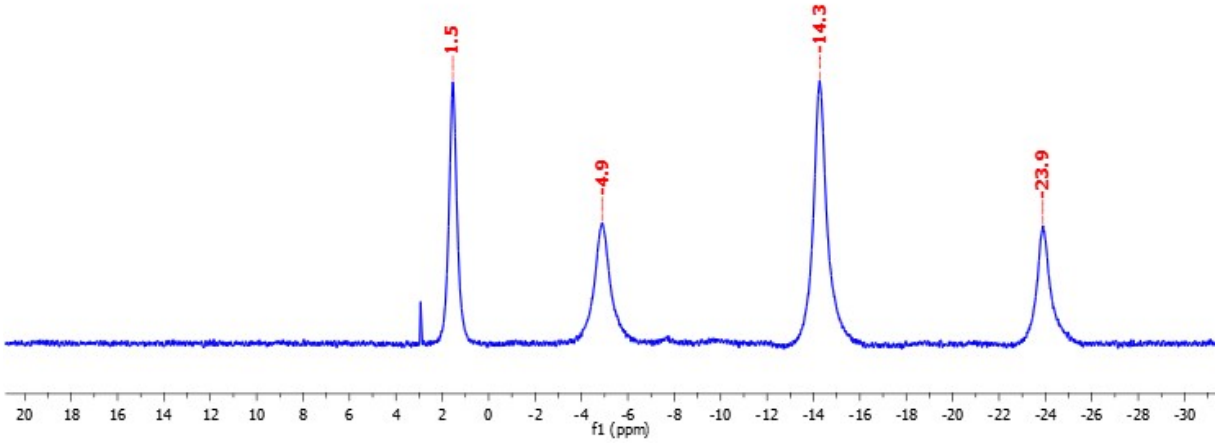


Figure S39. $^{11}B\{^{1}H\}$ NMR spectra of **6** in CD_3OD The signal around 2.9 ppm most likely belongs to the $[BOMe_4]^-$ anion as a product of the decomposition of the carborane cluster. (MestReNova program was used for the baseline correction)

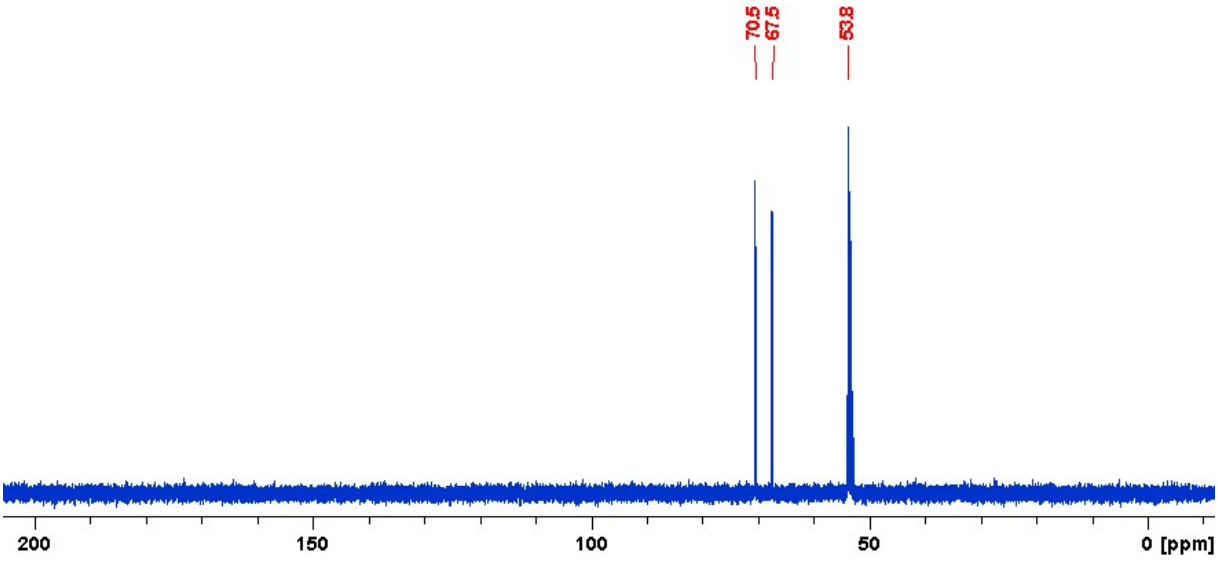


Figure S40. $^{13}C\{^{1}H\}$ NMR spectra of **6** in CD_2Cl_2

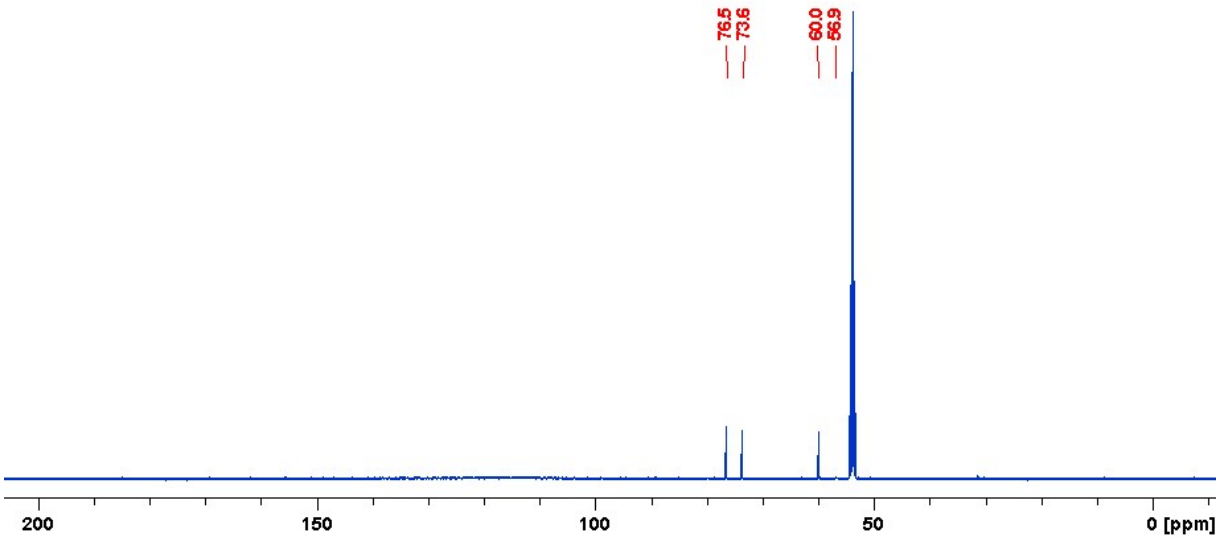


Figure S41. $^{13}C\{^{1}H\}$ NMR spectra of **6** in CD_3OD

IR and UV spectra of compound 4

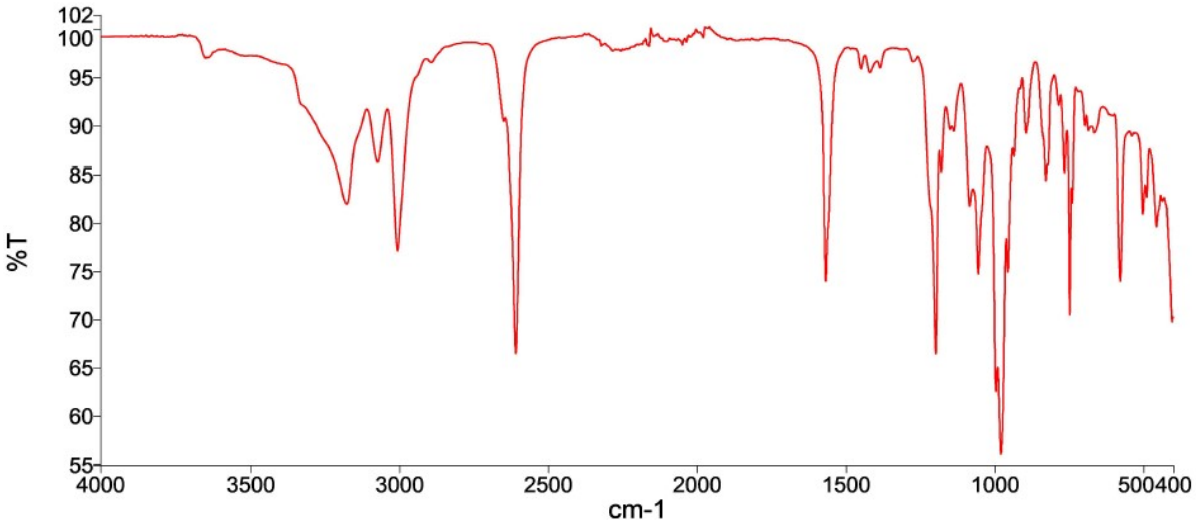


Figure S42. IR spectra of **4**

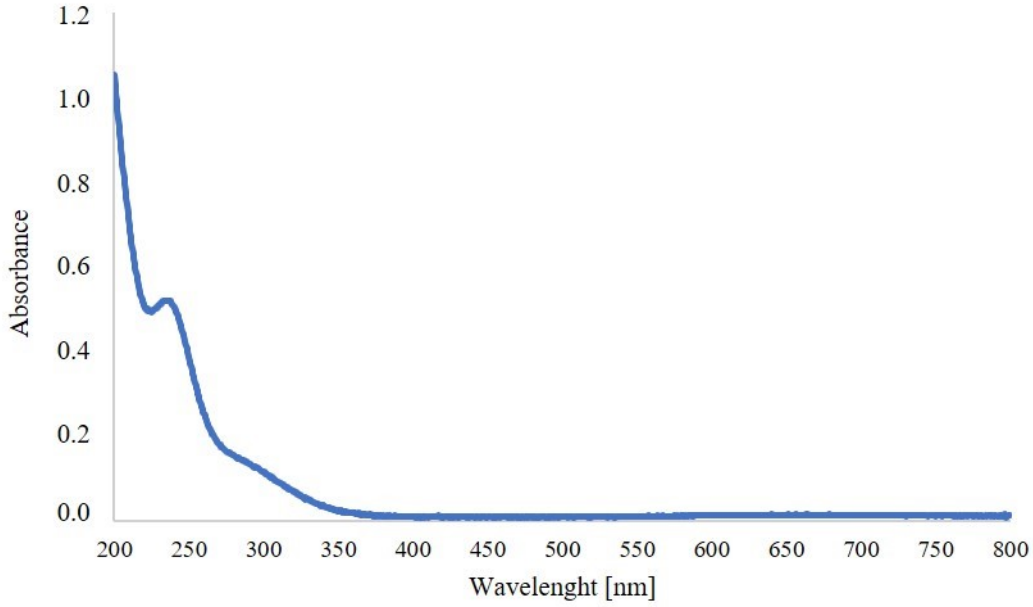


Figure S43. UV-Vis spectra of **4**

Single Crystal X-ray Diffraction (SC-XRD) studies

Compound **1**

Crystal data: $C_2H_{12}B_{10}S_2$, *Fwt.*: 208.34, colourless, block, size: 0.45 x 0.30 x 0.10 mm, monoclinic, space group $P\,2_1/n$, a = 7.3227(6)Å, b = 13.3818(10)Å, c = 11.5551(8)Å, $\alpha = 90°$, $\beta = 90.383(6)°$, $\gamma = 90°$, V = 1132.27(15)Å^3, T = 103(2)K, Z= 4, Z'=1, $F(000) = 424$, D_x = 1.222 Mg/m^3, μ 0.410mm^{-1}.

A crystal of **1** was mounted on a fiber. Cell parameters were determined by least-squares using 39031 ($3.045 \leq \theta \leq 27.475°$) reflections.

Intensity data were collected on a Rigaku RAXIS-RAPID II diffractometer (monochromator; Mo-$K\alpha$ radiation, λ = 0.71075Å) at 103(2) K in the range $3.045 \leq \theta \leq 25.341$. A total of 43625 reflections were collected of which 2062 were unique [R(int) = 0.1445, $R(\sigma)$ = 0.0434]; intensities of 1982 reflections were greater than $2\sigma(I)$. Completeness to θ = 0.998.

A numerical absorption correction was applied to the data (the minimum and maximum transmission factors were 0.987689 and 0.997209).

The structure was solved by direct methods (and subsequent difference syntheses).

Anisotropic full-matrix least-squares refinement on F^2 for all non-hydrogen atoms yielded R_1 = 0.0525 and wR^2 = 0.1190 for 1332 [$I>2\sigma(I)$] and R_1 = 0.0562 and wR^2 = 0.1212 for all (2062) intensity data, (number of parameters = 128, goodness-of-fit = 1.179, the maximum and mean shift/esd is 0.001 and 0.000).

The maximum and minimum residual electron density in the final difference map was 0.28 and -0.28e.Å^{-3}.

The weighting scheme applied was $w = 1/[\sigma^2(F_o^2)+(0.05260.7198P)^2+0.7198P]$ where$P = (F_o^2+2F_c^2)/3$.

Hydrogen atomic positions were calculated from assumed geometries. Hydrogen atoms were included in structure factor calculations but they were not refined. The isotropic displacement parameters of the hydrogen atoms were approximated from the U(eq) value of the atom they were bonded to.

Compound **2**

Crystal data: $C_2H_{12}B_{10}S_2$, *Fwt.*: 208.34, colourless, block, size: 0.30 x 0.20 x 0.15 mm, monoclinic, space group *C* 2/*c*, *a* = 10.8421(18)Å, *b* = 8.7020(13)Å, *c* = 12.067(2)Å, α = 90°, β = 105.688(7)°, γ = 90°, *V* = 1096.1(3)Å^3, *T* = 103(2)K, *Z*= 4, Z'=1, *F*(000) = 424, D_x = 1.262 Mg/m^3, μ 0.424mm^{-1}.

A crystal of **2** was mounted on a fiber. Cell parameters were determined by least-squares using 10595 (3.05 ≤ θ ≤ 27.46°) reflections.

Intensity data were collected on a(n) Rigaku RAXIS-RAPID II diffractometer (monochromator; Mo-*K*α radiation, λ = 0.71075Å) at 103(2) K in the range 3.048 ≤ θ ≤ 25.345. A total of 11065 reflections were collected of which 1009 were unique [*R*(int) = 0.0615, *R(*σ) = 0.0288]; intensities of 941 reflections were greater than 2σ(*I*). Completeness to θ = 0.996.

A numerical absorption correction was applied to the data (the minimum and maximum transmission factors were 0.958962 and 0.980800).

The structure was solved by direct methods (and subsequent difference syntheses).

Anisotropic full-matrix least-squares refinement on F^2 for all non-hydrogen atoms yielded R_1 = 0.0565 and wR^2 = 0.1317for 1332 [I>2σ(I)] and R_1 = 0.0621 and wR^2 = 0.1347 for all (1009) intensity data, (number of parameters = 66, goodness-of-fit = 1.220, the maximum and mean shift/esd is 0.001 and 0.000).

The maximum and minimum residual electron density in the final difference map was 0.34 and -0.27e.Å^{-3}.

The weighting scheme applied was $w = 1/[\sigma^2(F_o^2)+(0.05951.5983P)^2+1.5983P]$ where$P = (F_o^2+2F_c^2)/3$.

Hydrogen atomic positions were calculated from assumed geometries. Hydrogen atoms were included in structure factor calculations but they were not refined. The isotropic displacement parameters of the hydrogen atoms were approximated from the *U*(eq) value of the atom they were bonded to.

Compound **3**

Crystal data: $C_2H_{14}B_{10}N_2$, *Fwt.*: 174.25, colourless, block, size: 0.50 x 0.48 x 0.15 mm, monoclinic, space group *C* 2/*c*, *a* = 24.7966(6)Å, *b* = 6.9932(2)Å, *c* = 11.6138(3)Å, α = 90°, β = 98.493(7)°, γ = 90°, *V* = 1991.84(10)Å^3, *T* = 103(2)K, *Z*= 8, Z'=1, *F*(000) = 720, D_x = 1.162 Mg/m^3, μ 0.382mm^{-1}.

A crystal of **3** was mounted on a fiber. Cell parameters were determined by least-squares using 34070 (3.605 ≤ θ ≤ 71.98°) reflections.

Intensity data were collected on a(n) Rigaku RAXIS-RAPID II diffractometer (monochromator; Cu-*K*α radiation, λ = 1.54187Å) at 103(2) K in the range 3.605 ≤ θ ≤ 68.248. A total of 37471 reflections were collected of which 1828 were unique [*R*(int) = 0.0453, *R(*σ) = 0.0169]; intensities of 1732 reflections were greater than 2σ(*I*). Completeness to θ = 0.999.

A numerical absorption correction was applied to the data (the minimum and maximum transmission factors were 0.977126 and 0.991424).

The structure was solved by direct methods (and subsequent difference syntheses).

Anisotropic full-matrix least-squares refinement on F^2 for all non-hydrogen atoms yielded R_1 = 0.0509 and wR^2 = 0.1305for 1332 [I>2σ(I)] and R_1 = 0.0533 and wR^2 = 0.1323 for all (1828) intensity data, (number of parameters = 128, goodness-of-fit = 1.131, the maximum and mean shift/esd is 0.001 and 0.000).

The maximum and minimum residual electron density in the final difference map was 0.22 and -0.26e.Å^{-3}.

The weighting scheme applied was $w = 1/[\sigma^2(F_o^2)+(0.05811.9150P)^2+1.9150P]$ where$P = (F_o^2+2F_c^2)/3$.

Hydrogen atomic positions were calculated from assumed geometries. Hydrogen atoms were included in structure factor calculations but they were not refined. The isotropic displacement parameters of the hydrogen atoms were approximated from the *U*(eq) value of the atom they were bonded to.

Compound **4**

Crystal data: $C_4H_{30}B_{20}Cl_2CuN_4O_2$, *Fwt.*: 516.96, blue, block, size: 0.21×0.12×0.10 mm, monoclinic, space group *C* 2/*m*, *a* = 15.9986(11) Å, *b* = 12.1898(10) Å, *c* = 6.7272(5) Å, α = 90°, β = 105.470(3)°, γ = 90°, *V* = 1264.41(17)Å^3, *T* = 296(2)K, *Z*= 2, Z'=0.25, *F*(000) = 522, D_x = 1.358 Mg/m^3, μ 1.088 mm^{-1}.

A blue block-shaped crystal (**4**) with dimensions 0.21 × 0.12 × 0.10 mm was mounted on a Mitegen Loop. Intensity data were collected using a Bruker Venture D8 APEX-II CCD diffractometer operating at *T* = 296(2) K (monochromator; Mo-*K*α radiation, λ = 0.71073 Å) in the range 3.142 ≤ θ ≤ 25.741

The unit cell was refined using Bruker SAINT on 4621 reflections, 53% of the observed reflections.

A total of 8764 reflections were collected of which 1257 were unique [$R_{(int)}$ = 0.0535, *R(*σ) = 0.0308]; intensities of 1183 reflections were greater than 2σ(*I*). Completeness to θ = 0.989.

Multi-scan absorption correction was applied to the data, the Ratio of minimum to maximum transmission is 0.9121.

The structure was solved and the space group *C*2/*m* (# 12) determined by the ShelXT (Sheldrick, 2015) structure solution program using using geom methods and refined by full matrix least squares minimisation on $\boldsymbol{F^2}$ using version 2018/3 of ShelXL (Sheldrick, 2015), managed by Olex2 1.5 (Dolomanov et al., 2009) as the graphical interface. All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Most hydrogen atom positions were calculated geometrically and refined using the riding model, but some hydrogen atoms were refined freely.

Compound **5**

Crystal data: $C_{60}H_{132}B_{20}K_4O_{23}S_4$, *Fwt.*: 1721.58, colorless, plate, size: 0.260 x 0.157 x 0.090 mm, monoclinic, space group *C* 1 *c* 1, a = 18.4531(6)Å, b = 25.6027(7)Å, c = 19.2303(6)Å, α = 90°, β = 94.515(3)°, γ = 90°, V = 9057.1(5)Å^3, T = 100.15K, Z= 4, $F(000)$ = 3660, D_x = 1.263 Mg/m^3, μ= 3.126mm^{-1}.

A crystal of **5** was mounted on a glass fiber. Cell parameters were determined by least-squares using 43890 ($2.96 \leq \theta \leq 70.76°$) reflections.

Intensity data were collected on a STOE STADIVARI diffractometer (Graded multilayer mirror monochromator; Cu-$K\alpha$ radiation, λ = 1.54186Å) at 100(2) K in the range $2.958 \leq \theta \leq 70.204$. A total of 31158 reflections were collected of which 31158 were unique [R(int) = 0.0371, $R(\sigma)$ = 0.0529]; intensities of 22714 reflections were greater than $2\sigma(I)$. Completeness to θ = 0.966. A(n) multi-scan absorption correction was applied to the data (the minimum and maximum transmission factors were 0.4455 and 0.7559).

The structure was solved by direct methods (and subsequent difference syntheses).

Anisotropic full-matrix least-squares refinement on F^2 for all non-hydrogen atoms yielded R_1 = 0.0472 and wR^2 = 0.1090for 1332 [$I>2\sigma(I)$] and R_1 = 0.0763 and wR^2 = 0.1218 for all (31158) intensity data, (number of parameters = 1023, goodness-of-fit = 1.015, the maximum and mean shift/esd is 0.152 and 0.008). The absolute structure parameter is 0.03(4). (Friedel coverage: 0.998, Friedel fraction max.: 0.966, Friedel fraction full: 0.987).

The maximum and minimum residual electron density in the final difference map was 0.48 and -0.34e.Å^{-3}.

The weighting scheme applied was $w = 1/[\sigma^2(F_o^2)+(0.0685P)^2+0P]$ where $P = (F_o^2+2F_c^2)/3$.

Hydrogen atomic positions were calculated from assumed geometries. Hydrogen atoms were included in structure factor calculations but they were not refined. The isotropic displacement parameters of the hydrogen atoms were approximated from the U(eq) value of the atom they were bonded to.

Compound **5'**

Crystal data: $C_{40}H_{94}B_{20}K_4O_{19}S_4$, 4($CH_3CN$) , *Fwt.*: 1523.67, colourless, prism, size: 0.17 x 0.13 x 0.08 mm, monoclinic, space group *P* 1 21/n 1, *a* = 16.1368(6)Å, *b* = 25.8487(14)Å, *c* = 18.8254(8)Å, α = 90°, β = 90.405(3)°, γ = 90°, *V* = 7852.2(6)Å^3, *T* = 100.15K, *Z*= 4, Z'=1, *F*(000) = 3212, D_x = 1.289 Mg/m^3, μ 0.395mm^{-1}.

A crystal of **5'** was mounted on a glass fiber. Cell parameters were determined by least-squares using 40412 (2.676 ≤ θ ≤ 54.082°) reflections.

Intensity data were collected on a STOE STADIVARI diffractometer (Graded multilayer mirror monochromator; Cu-*K*α radiation, λ = 1.54186Å) at 100(2) K in the range 1.338 ≤ θ ≤ 27.041. A total of 40412 reflections were collected of which 16844were unique [*R*(int) = 0.0375, *R(*σ) = 0.0425]; intensities of 12693 reflections were greater than 2σ(*I*). Completeness to θ = 0.979. An integration absorption correction was applied to the data (the minimum and maximum transmission factors were 0.9380 and 0.9789).

The structure was solved by direct methods (and subsequent difference syntheses).

Anisotropic full-matrix least-squares refinemen on F^2 for all non-hydrogen atoms yielded R_1 = 0.0574 and wR^2 = 0.1314for 1332 [I>2σ(I)] and R_1 = 0.0841 and wR^2 = 0.1468 for all (16844) intensity data, (number of parameters = 980, goodness-of-fit = 1.165, the maximum and mean shift/esd is 3.227 and 0.052).

The maximum and minimum residual electron density in the final difference map was 1.130 and -0.603e.Å^{-3}.

The weighting scheme applied was $w = 1/[\sigma^2(F_o^2)+(0.033100P)^2+18.412601P]$ where $P = (F_o^2+2F_c^2)/3$.

Hydrogen atomic positions were calculated from assumed geometries. Hydrogen atoms were included in structure factor calculations but they were not refined. The isotropic displacement parameters of the hydrogen atoms were approximated from the *U*(eq) value of the atom they were bonded to.

Compound **6**

Crystal data: $C_{63.16}H_{141.34}B_{20}K_4N_7O_{20.84}S_4$, *Fwt.*: 1833.4, fluorescent yellow, prism-shaped, size: 0.37×0.10×0.05 mm, monoclinic, space group $P2_1$, a = 13.8220(16) Å, b = 26.063(3) Å, c = 14.3906(18) Å, α = 90°, β = 110.293(3)°, γ = 90°, V = 4864.1(10) Å^3, T = 150(2)K, Z= 2, Z'=1, F(000) = 1952, D_x = 1.252 Mg/m^3, μ 0.333 mm^{-1}.

Single fluorescent yellow prism-shaped crystals of **6** with dimensions 0.37 × 0.10 × 0.05 mm was mounted on a Mitegen Loop. Intensity data were collected using a Bruker Venture D8 APEX-II CCD diffractometer operating at T = 150(2) K (monochromator; Mo-$K\alpha$ radiation, λ = 0.71073 Å) in the range 1.699 ≤ θ ≤ 24.108

The unit cell was refined using Bruker SAINT on 3079 reflections, 11% of the observed reflections.

A total of 27994 reflections were collected of which 13527 were unique [R_{int} = 0.1367, R_{sigma} = 0.1845]; intensities of 7977 reflections were greater than 2σ(I). Completeness to θ = 0.997.

Multi-scan absorption correction was applied to the data, the and the minimum and maximum transmissions are 0.960 and 0.990.

The structure was solved and the space group $P2_1$ (# 4) determined by the ShelXT (Sheldrick, 2015) structure solution program using using iterative methods and refined by full matrix least squares minimisation on $\boldsymbol{F^2}$ using version 2018/3 of ShelXL (Sheldrick, 2015), managed by Olex2 1.5 (Dolomanov et al., 2009) as the graphical interface. All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Hydrogen atom positions were calculated geometrically and refined using the riding model and 83% of the solvent (THF) was modeled.

The Flack parameter was refined to 0.00(6). Determination of absolute structure using Bayesian statistics on Bijvoet differences using the Olex2 results in None. The chiral atoms in this structure are: N2(R), N3(R), N4(R), N5(S), N6(S), N8(R). Note: The Flack parameter is used to determine chirality of the crystal studied, the value should be near 0, a value of 1 means that the stereochemistry is wrong and the model should be inverted. A value of 0.5 means that the crystal consists of a racemic mixture of the two enantiomers.

Table S28. Summary of structure determinations and refinement for **1** and **2**

	1	**2**
CCDC number	2333791	2333790
Empirical formula	$C_2H_{12}B_{10}S_2$	$C_2H_{12}B_{10}S_2$
Formula weight	208.34	208.34
Temperature	103(2)	103(2)
Radiation and wavelength	Mo-Kα, λ =0.71075Å	Mo-Kα, λ =0.71075Å
Crystal system	monoclinic	monoclinic
Space group	*P* $2_1/n$	*C* 2/*c*
Unit cell dimensions	*a* =7.3227(6)Å	*a* =10.8421(18)Å
	b =13.3818(10)Å	*b* =8.7020(13)Å
	c =11.5551(8)Å	*c* =12.067(2)Å
	α =90°	α =90°
	β =90.383(6)°	β =105.688(7)°
	γ =90°	γ =90°
Volume	1132.27(15)Å^3	1096(1)Å^3
Z, Z'	4, 1	4, 1
Density (calculated)	1.222 Mg/m^3	1.262 Mg/m^3
Absorption coefficient, μ	0.410 mm^{-1}	0.424 mm^{-1}
F(000)	424	424
Crystal colour	colourless	colourless
Crystal description	block	block
Crystal size	0.450 x 0.300 x 0.100 mm	0.300 x 0.200 x 0.150 mm
Absorption correction	numerical	numerical
Max. and min. transmission	0.987689 and 0.997209	0.958962 and 0.980800
θ–range for data collection	3.045 ≤ θ ≤ 25.341°	3.048 ≤ θ ≤ 25.345°
Index ranges	-8 ≤ *h* ≤8; -16≤ *k* ≤16; -13 ≤ *l* ≤13	-13 ≤ *h* ≤13; -10≤ *k* ≤10; -14 ≤ *l* ≤14
Reflections collected	43625	11065
Completeness to 2θ	0.998	0.996
Independent reflections	2062 [*R*(int) =0.1445]	1009 [*R*(int) =0.0615]
Reflections *I*>2σ(*I*)	1982	941
Data / restraints / parameters	2062 /0 /128	1009 /0 /66
Goodness-of-fit on *F*2	1.179	1.220
Final *R* indices [*I*>2σ(*I*)]	R_1 =0.0525, wR^2 =0.1190	R_1 =0.0565, wR^2 =0.1317
R indices (all data)	R_1 =0.0562, wR^2 =0.1212	R_1 =0.0621, wR^2 =0.1347
Max. and mean shift/esd	0.001;0.000	0.001;0.000
Largest diff. peak and hole	0.28;-0.28 e.Å^{-3}	0.34;-0.27 e.Å^{-3}

Table S29. Summary of structure determinations and refinement for **3-5**

	3	**4**	**5**
CCDC number	2333792	2379108	2333793
Empirical formula	$C_2H_{14}B_{10}N_2$	$C_4H_{30}B_{20}Cl_2CuN_4O_2$	$C_{60}H_{132}B_{20}K_4O_{23}S_4$
Formula weight	174.25	516.96	1721.58
Temperature	103(2)	296(2)	100.15
Radiation and wavelength	Cu-Kα, λ =1.54187Å	MoK_α λ =0.71073 Å	Cu-Kα, λ =1.54186Å
Crystal system	monoclinic	monoclinic	monoclinic
Space group	*C* 2/*c*	$C2/m$	*C* 1 *c* 1
Unit cell dimensions	*a* =24.7966(6)Å	*a* =15.9986(11)	*a* =18.4531(6)Å
	b =6.9932(2)Å	*b* =12.1898(10)	*b* =25.6027(7)Å
	c =11.6138(3)Å	*c* =6.7272(5)	*c* =19.2303(6)Å
	α =90°	α =90°	α =90°
	β =98.493(7)°	β =105.470(3)°	β =94.515(3)°
	γ =90°	γ =90°	γ =90°
Volume	1991.84(10)Å^3	1264.41(17) Å^3	9057.1(5)Å^3
Z, Z'	8,1	2, 0.25	4, 1
Density (calculated)	1.162 Mg/m^3	1.358 Mg/m^3	1.263 Mg/m^3
Absorption coefficient, μ	0.382 mm^{-1}	1.088 mm^{-1}	3.126 mm^{-1}
F(000)	720	522	3660
Crystal colour	colourless	blue	colorless
Crystal description	block	block	plate
Crystal size	0.500 x 0.480 x 0.150 mm	0.21×0.12×0.10 mm	0.260 x 0.157 x 0.090 mm
Absorption correction	numerical	multi-scan	multi-scan
Max. and min. transmission	0.977126 and 0.991424	0.680 and 0.745	0.4455 and 0.7559
θ–range for data collection	3.605 ≤ θ ≤ 68.248°	3.142 ≤ θ ≤ 25.741	2.958 ≤ θ ≤ 70.204°
Index ranges	-29 ≤ *h* ≤29; -8≤ *k* ≤8; -13 ≤ *l* ≤13	-19 ≤ *h* ≤ 19, -14 ≤ *k* ≤ 14, -8 ≤ *l* ≤ 8	-22 ≤ *h* ≤22; -30≤ *k* ≤30; -22 ≤ *l* ≤22
Reflections collected	37471	8764	31158
Completeness to 2θ	0.999	0.989	0.987
Independent reflections	1828 [*R*(int) =0.0453]	1257 [R_{int} = 0.0535]	31158 [*R*(int) =0.0371]
Reflections *I*>2σ(*I*)	1732	1183	22714
Data / restraints / parameters	1828 /0 /128	1257/0/106	31158 /39 /1023
Goodness-of-fit on *F*2	1.131	1.105	1.015
Final *R* indices [*I*>2σ(*I*)]	R_1 =0.0509, wR^2 =0.1305	R_1 =0.0260, wR^2 =0.1305	R_1 =0.0472, wR^2 =0.1090
R indices (all data)	R_1 =0.0533, wR^2 =0.1323	R_1 =0.0293, wR^2 =0.1323	R_1 =0.0763, wR^2 =0.1218
Max. and mean shift/esd	0.001;0.000	0.000	0.152 ;0.008
Largest diff. peak and hole	0.22;-0.26 e.Å^{-3}	0.246;-0.167 e.Å^{-3}	0.48;-0.34 e.Å^{-3}

Table S30. Summary of structure determinations and refinement for **5'** and **6**

	5'	**6**
CCDC number	2371840	2379108
Empirical formula	$C_{40}H_{94}B_{20}K_4O_{19}S_4$, 4($CH_3CN$)	$C_{63.16}H_{141.34}B_{20}K_4N_7O_{20.84}S_4$
Formula weight	1523.67	1833.34
Temperature	100.15	150(2)
Radiation and wavelength	Mo-Kα, λ =0.71073Å	Mo-Kα, λ =0.71073Å
Crystal system	monoclinic	monoclinic
Space group	$P\ 1\ 2_1/n\ 1$	$P2_1$
Unit cell dimensions	a =16.1368(6)Å	a =13.8220(16)Å
	b =25.8487(14)Å	b =26.063(3)Å
	c =18.8254(8)Å	c =14.3906(18) Å
	α =90°	α =90°
	β =90.405(3)°	β =110.239(3) °
	γ =90°	γ =90°
Volume	7852.2(6)Å^3	4864.1(10)
Z, Z'	4, 1	2, 1
Density (calculated)	1.289 Mg/m^3	1.252 Mg/m^3
Absorption coefficient, μ	0.395 mm^{-1}	0.333 mm^{-1}
F(000)	3212	1952
Crystal colour	colourless	fluorescent yellow
Crystal description	prism	prism
Crystal size	0.17 x 0.13 x 0.08 mm	0.37×0.10×0.05 mm
Absorption correction	integration	multi-scan
Max. and min. transmission	0.9789 and 0.9380	0.960 and 0.990
θ–range for data collection	1.338 ≤ θ ≤ 27.041°	3.398 ≤ θ ≤ 48.216
Index ranges	-20 ≤ h ≤20; -32≤ k ≤28; -23 ≤ l ≤23	-15 ≤ h ≤ 15, -29 ≤ k ≤ 27, -16 ≤ l ≤ 16
Reflections collected	40412	27994
Completeness to 2θ	0.999	0.997
Independent reflections	16844 [R(int) =0.0375]	13527 [R_{int} = 0.1367]
Reflections I>2σ(I)	12693	7977
Data / restraints / parameters	16844 /3 /980	13527/66/1081
Goodness-of-fit on F2	1.165	1.002
Final R indices [I>2σ(I)]	R_1 =0.0574, wR^2 =0.1314	R_1 = 0.0792, wR_2 = 0.1484
R indices (all data)	R_1 =0.0841, wR^2 =0.1468	R_1 = 0.1448, wR_2 = 0.1812
Max. and mean shift/esd	0.006;0.001	0.001
Largest diff. peak and hole	0.84 and 0.57 e.Å^{-3}	0.52 and-0.377 e.Å^{-3}

XYZ Geometries and Energies

26

1-NH_2-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -387.573409

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.684615
B	1.490259	0.000000	0.860284
B	1.230963	1.039259	-0.558812
B	-0.469936	1.540936	-0.558819
B	-1.251728	0.808718	0.860251
B	1.213917	0.978825	2.320348
B	2.006530	1.685406	0.894260
B	0.782106	2.651780	0.026508
B	-0.770748	2.504540	0.894226
B	-0.488447	1.480921	2.320333
B	0.770949	2.613876	1.799536
N	-0.359547	-1.219042	-0.615063
H	3.156328	1.953250	0.904988
H	-1.591172	3.353470	0.904953
H	1.048409	3.554583	2.456853
H	1.066161	3.614819	-0.595717
H	-2.317011	0.308024	0.838289
H	-1.077321	1.567572	-1.570195
H	-1.117046	1.477212	3.317367
H	1.739892	0.634578	3.317380
H	2.113311	-0.998662	0.838310
H	1.755607	0.732010	-1.570175
H	-0.279412	-0.947336	2.114983
H	0.389446	-1.610818	-1.167006
H	-1.201408	-1.141714	-1.166798

26

1-PH_2-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -674.172571

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.650552

B	1.503639	0.000000	0.839266
B	1.229836	1.034097	-0.578203
B	-0.471500	1.536041	-0.578213
B	-1.262819	0.816193	0.839218
B	1.215665	0.978136	2.296417
B	2.008580	1.688412	0.875321
B	0.781229	2.647851	0.002533
B	-0.770375	2.508301	0.875288
B	-0.490046	1.481371	2.296390
B	0.771205	2.613921	1.778463
P	-0.480082	-1.627402	-0.791598
H	3.157766	1.958676	0.883625
H	-1.588772	3.359119	0.883588
H	1.048534	3.553954	2.437028
H	1.064946	3.609528	-0.621831
H	-2.329995	0.318597	0.830531
H	-1.076506	1.573756	-1.588956
H	-1.110826	1.469399	3.298186
H	1.730499	0.631123	3.298232
H	2.129777	-0.997206	0.830587
H	1.758420	0.737348	-1.588942
H	-0.276456	-0.937032	2.105762
H	0.589814	-1.666153	-1.718728
H	-1.399836	-1.079288	-1.718623

27

1-CH_3-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -371.529272

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.644643
B	1.506359	0.000000	0.841302
B	1.233494	1.026651	-0.573827
B	-0.465663	1.535759	-0.573750
B	-1.258190	0.828332	0.841426
B	1.220692	0.974535	2.296148
B	2.016562	1.684623	0.877923

B	0.792236	2.643970	0.001262
B	-0.757916	2.515982	0.877916
B	-0.483606	1.485297	2.296171
B	0.783169	2.613591	1.779054
C	-0.382742	-1.277285	-0.723494
H	3.166791	1.950780	0.886461
H	-1.572221	3.370838	0.886455
H	1.064247	3.551513	2.439170
H	1.079930	3.604221	-0.623544
H	-2.325584	0.331719	0.827686
H	-1.070101	1.568809	-1.585905
H	-1.102486	1.474400	3.299395
H	1.731736	0.625131	3.299310
H	2.124796	-1.001752	0.827639
H	1.756476	0.721925	-1.586006
H	-0.279781	-0.933625	2.104191
H	0.437705	-1.612175	-1.353605
H	-0.618024	-2.071917	-0.017444
H	-1.255257	-1.107277	-1.349695

27

1-SiH_3-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -622.923378

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.646219
B	1.506129	0.000000	0.838267
B	1.230753	1.032829	-0.576685
B	-0.468982	1.536771	-0.576722
B	-1.262763	0.820943	0.838281
B	1.217793	0.977097	2.294776
B	2.012067	1.688247	0.876024
B	0.785054	2.648042	0.000735
B	-0.766770	2.512098	0.876063
B	-0.488419	1.482888	2.294811
B	0.775338	2.615089	1.777020
Si	-0.474591	-1.600857	-0.916801

H	3.161112	1.958994	0.884575
H	-1.582597	3.365347	0.884649
H	1.053737	3.554116	2.436863
H	1.070310	3.610196	-0.622085
H	-2.333253	0.329343	0.832599
H	-1.074403	1.578694	-1.587912
H	-1.107552	1.470811	3.297762
H	1.730294	0.629457	3.297706
H	2.135739	-0.995592	0.832543
H	1.761160	0.738012	-1.587903
H	-0.276275	-0.931931	2.111223
H	-1.665564	-1.337143	-1.749485
H	0.668000	-2.029392	-1.748766
H	-0.778940	-2.625820	0.109022

25

1-OH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -407.441427

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.663080
B	1.503513	0.000000	0.861223
B	1.232899	1.008839	-0.577758
B	-0.472313	1.526606	-0.590869
B	-1.260485	0.814677	0.831059
B	1.216499	0.989174	2.302606
B	2.012699	1.678784	0.871023
B	0.788221	2.631889	-0.015954
B	-0.764145	2.506192	0.856070
B	-0.490429	1.486971	2.286749
B	0.774054	2.615831	1.760395
O	-0.388631	-1.165584	-0.607683
H	0.375715	-1.581989	-1.022480
H	3.162185	1.947217	0.875585
H	-1.579277	3.359632	0.860554
H	1.051116	3.562418	2.408877
H	1.079869	3.584715	-0.649634

H	-2.319624	0.305577	0.812254
H	-1.069691	1.539704	-1.605574
H	-1.117315	1.490547	3.284496
H	1.730043	0.654777	3.309247
H	2.110000	-1.010091	0.836428
H	1.753571	0.682666	-1.585686
H	-0.285472	-0.940130	2.105791

25

1-SH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -730.413177

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.661894
B	1.502699	0.000000	0.850032
B	1.229206	1.026245	-0.580038
B	-0.473427	1.535845	-0.583369
B	-1.262689	0.812625	0.836905
B	1.212999	0.984021	2.301442
B	2.005754	1.685392	0.874358
B	0.780734	2.644132	-0.001377
B	-0.772008	2.506121	0.868554
B	-0.491883	1.483320	2.295286
B	0.767921	2.616516	1.773374
S	-0.522573	-1.504343	-0.837051
H	3.155478	1.952836	0.879747
H	-1.592136	3.354895	0.876346
H	1.044700	3.558841	2.428405
H	1.067146	3.602112	-0.629632
H	-2.326983	0.311493	0.825485
H	-1.075852	1.561766	-1.594468
H	-1.118163	1.476764	3.293487
H	1.729844	0.639102	3.302864
H	2.128690	-0.996139	0.838606
H	1.756640	0.722312	-1.588721
H	-0.280976	-0.939462	2.108047
H	0.714673	-1.975792	-1.073744

24

1-Cl-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -791.814908

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.636158
B	1.517994	0.000000	0.825659
B	1.227099	1.005716	-0.612077
B	-0.487406	1.509868	-0.612084
B	-1.276400	0.821652	0.825664
B	1.219222	0.992323	2.265459
B	2.006398	1.687426	0.832908
B	0.772164	2.626112	-0.052804
B	-0.773710	2.504878	0.832914
B	-0.488058	1.494332	2.265446
B	0.770569	2.620657	1.725035
Cl	-0.441184	-1.500370	-0.800386
H	3.154466	1.960408	0.831934
H	-1.591296	3.355839	0.831934
H	1.049628	3.569774	2.368719
H	1.051451	3.575976	-0.696012
H	-2.333640	0.309872	0.815184
H	-1.090912	1.516860	-1.622505
H	-1.102653	1.492913	3.270693
H	1.735237	0.658476	3.270708
H	2.129955	-1.002585	0.815175
H	1.738344	0.684923	-1.622492
H	-0.275207	-0.935916	2.093347

24

1-O^--*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -406.932214

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.291862
B	1.402034	0.000000	1.413595
B	1.263473	1.044136	-0.041687
B	-0.543445	1.546366	-0.041695

B	-1.200961	0.723456	1.413591
B	1.193188	0.997330	2.889913
B	1.962938	1.681104	1.461785
B	0.732419	2.635247	0.574457
B	-0.813950	2.452892	1.461756
B	-0.507404	1.470004	2.889911
B	0.729367	2.624166	2.340020
O	-0.287051	-1.032743	-0.554897
H	3.109144	1.990938	1.442865
H	-1.635882	3.309754	1.442821
H	0.999273	3.595208	2.967324
H	1.005357	3.617227	-0.036454
H	-2.286683	0.247883	1.393477
H	-1.167060	1.780128	-1.022449
H	-1.151366	1.518286	3.885255
H	1.769706	0.706382	3.885254
H	2.086642	-0.967614	1.393469
H	1.918291	0.922566	-1.022427
H	-0.252343	-0.907869	2.818768

24

1-S$^-$-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -729.897833

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.748536
B	1.484794	0.000000	0.939672
B	1.263597	1.073645	-0.444316
B	-0.432146	1.600816	-0.444327
B	-1.223104	0.841797	0.939679
B	1.220020	0.942926	2.429570
B	2.030490	1.678373	1.043037
B	0.832113	2.676613	0.188299
B	-0.721088	2.533753	1.043070
B	-0.470404	1.468430	2.429570
B	0.808757	2.601583	1.963779
S	-0.452045	-1.454121	-0.854221

H	3.187774	1.935637	1.070748
H	-1.528547	3.401797	1.070790
H	1.095292	3.523266	2.653003
H	1.138000	3.660532	-0.400499
H	-2.313574	0.399374	0.924747
H	-1.029996	1.736484	-1.452070
H	-1.110683	1.449051	3.424791
H	1.736456	0.563962	3.424797
H	2.132230	-0.982697	0.924749
H	1.833007	0.846439	-1.452050
H	-0.296020	-0.952204	2.155335

26

3-NH_2-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -387.610358

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.595657
B	1.587527	0.000000	0.797957
B	1.213545	1.000120	-0.626337
B	-0.502655	1.476623	-0.636016
B	-1.293952	0.802472	0.797784
B	1.213424	1.000234	2.222112
B	1.987255	1.725461	0.797900
B	0.735887	2.628732	-0.091382
B	-0.807643	2.488020	0.797747
B	-0.502756	1.476667	2.231608
B	0.735781	2.628776	1.686945
N	2.333957	-1.235266	0.797958
H	-0.242460	-0.938333	2.066231
H	-1.630401	3.334296	0.797689
H	3.130973	2.022251	0.797941
H	0.998886	3.581292	-0.738274
H	0.998756	3.581413	2.333744
H	1.728553	0.687851	3.237544
H	1.728755	0.687710	-1.641711
H	-1.098958	1.477728	-1.652785

H	-2.349519	0.282477	0.797801
H	-1.099141	1.477806	3.248330
H	-0.242347	-0.938368	-0.470556
H	2.867507	-1.452050	1.624799
H	2.868821	-1.451239	-0.028245

26

3-PH_2-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -674.185601

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.613138
B	1.535017	0.000000	0.810898
B	1.210714	1.002159	-0.624205
B	-0.504619	1.484773	-0.631486
B	-1.289330	0.800572	0.803728
B	1.207622	1.008690	2.241112
B	1.984757	1.710727	0.808633
B	0.738349	2.627091	-0.084487
B	-0.807617	2.490768	0.802893
B	-0.507793	1.486867	2.240010
B	0.735074	2.631783	1.693934
P	2.540690	-1.672876	0.795970
H	-0.266215	-0.930240	2.088053
H	-1.632605	3.334853	0.800935
H	3.128464	2.003185	0.809439
H	1.008631	3.578994	-0.728822
H	1.002170	3.585602	2.336650
H	1.721033	0.698617	3.255846
H	1.728410	0.688948	-1.636014
H	-1.105109	1.481157	-1.645363
H	-2.342647	0.276865	0.803335
H	-1.112996	1.485323	3.251171
H	-0.259483	-0.932820	-0.473413
H	3.534786	-1.250509	-0.121115
H	3.326679	-1.400278	1.943634

27

3-CH_3-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -371.541045

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.616210
B	1.536158	0.000000	0.808246
B	1.193329	1.014562	-0.624171
B	-0.523043	1.482454	-0.627745
B	-1.295938	0.786178	0.808016
B	1.193150	1.014768	2.240475
B	1.966211	1.718413	0.808179
B	0.712437	2.632581	-0.081575
B	-0.832053	2.482385	0.807948
B	-0.523238	1.482592	2.243810
B	0.712277	2.632665	1.697684
C	2.428283	-1.301293	0.808449
H	-0.256568	-0.932354	2.091871
H	-1.664691	3.319181	0.807853
H	3.108130	2.021634	0.808169
H	0.974537	3.588733	-0.723414
H	0.974318	3.588893	2.339438
H	1.716770	0.703893	3.250436
H	1.717088	0.703622	-1.634055
H	-1.129331	1.475425	-1.638566
H	-2.345650	0.254372	0.808034
H	-1.129640	1.475598	3.254559
H	-0.256428	-0.932419	-0.475590
H	3.063613	-1.339498	1.693871
H	1.838895	-2.221118	0.793117
H	3.085058	-1.324262	-0.061689

27

3-SiH_3-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -622.920805

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.618331
B	1.527149	0.000000	0.809164

B	1.203949	1.008873	-0.623942
B	-0.512627	1.486755	-0.627010
B	-1.289797	0.793643	0.809164
B	1.203949	1.008873	2.242274
B	1.975974	1.713976	0.809163
B	0.727118	2.632108	-0.080605
B	-0.816711	2.489403	0.809140
B	-0.512628	1.486756	2.245342
B	0.727085	2.632138	1.698949
Si	2.686393	-1.647042	0.809257
H	-0.266426	-0.927428	2.098065
H	-1.646325	3.329224	0.809120
H	3.118803	2.010465	0.809159
H	0.993701	3.585873	-0.723699
H	0.993627	3.585893	2.342073
H	1.719703	0.701182	3.256981
H	1.719704	0.701180	-1.638653
H	-1.117711	1.482140	-1.638251
H	-2.341603	0.266533	0.809151
H	-1.117727	1.482141	3.256573
H	-0.266410	-0.927431	-0.479734
H	4.122871	-1.280083	0.808079
H	2.411936	-2.482260	2.009840
H	2.410330	-2.483557	-0.390063

25

3-OH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -407.4991174

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.625802
B	1.540042	0.000000	0.810633
B	1.189468	1.015076	-0.628199
B	-0.521833	1.487292	-0.623895
B	-1.289024	0.781337	0.814063
B	1.191209	1.013261	2.251525
B	1.973788	1.708510	0.811431

B	0.721067	2.627718	-0.077710
B	-0.824045	2.480962	0.813849
B	-0.520155	1.487230	2.250833
B	0.722814	2.626979	1.703268
O	2.246380	-1.190071	0.808113
H	3.198782	-1.078793	0.832338
H	-0.240660	-0.940578	2.094140
H	-1.652110	3.321651	0.814410
H	3.118495	2.005278	0.811108
H	0.988076	3.585268	-0.715122
H	0.991040	3.584006	2.340968
H	1.723703	0.693167	3.253760
H	1.720176	0.695065	-1.631282
H	-1.133218	1.485546	-1.631368
H	-2.341370	0.255400	0.813972
H	-1.129621	1.484997	3.259476
H	-0.242163	-0.940051	-0.468672

25

3-SH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -730.447542

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.609970
B	1.543841	0.000000	0.790738
B	1.211222	1.007542	-0.635648
B	-0.502108	1.488974	-0.626335
B	-1.285954	0.808461	0.813854
B	1.225231	0.994866	2.227917
B	1.996620	1.708164	0.793581
B	0.744631	2.629608	-0.084716
B	-0.793520	2.495155	0.812147
B	-0.489515	1.486245	2.244250
B	0.758312	2.623528	1.693040
S	2.553942	-1.551505	0.711685
H	-0.249656	-0.936039	2.081023
H	-1.613583	3.343605	0.817584

H	3.141850	1.991576	0.789213
H	1.012039	3.583052	-0.727551
H	1.033866	3.572224	2.339547
H	1.746263	0.677078	3.236820
H	1.721379	0.690295	-1.649289
H	-1.109290	1.491647	-1.636088
H	-2.341880	0.290255	0.814473
H	-1.081963	1.485398	3.262850
H	-0.262731	-0.931511	-0.473623
H	2.956556	-1.526463	1.994106

24

3-Cl-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -791.870117

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.624402
B	1.523905	0.000000	0.812186
B	1.214927	1.000405	-0.626420
B	-0.497262	1.488923	-0.624876
B	-1.281297	0.801981	0.812205
B	1.214926	1.000404	2.250821
B	2.000293	1.695680	0.812182
B	0.755064	2.621994	-0.077556
B	-0.790736	2.491640	0.812198
B	-0.497262	1.488924	2.249278
B	0.755053	2.622018	1.701948
Cl	2.500647	-1.492664	0.812178
H	-0.253413	-0.935683	2.095197
H	-1.609098	3.341506	0.812196
H	3.146967	1.972227	0.812164
H	1.030403	3.573949	-0.718921
H	1.030382	3.573976	2.343314
H	1.737884	0.673708	3.254042
H	1.737872	0.673717	-1.629650
H	-1.102766	1.491529	-1.635432
H	-2.337624	0.284963	0.812189

H	-1.102767	1.491530	3.259835
H	-0.253413	-0.935682	-0.470795

24

3-O^--*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -406.972848

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.556104
B	2.364818	0.000000	0.778042
B	1.204709	0.888902	-0.642609
B	-0.486296	1.494004	-0.646397
B	-1.278800	0.830431	0.778053
B	1.204709	0.888902	2.198713
B	2.066141	1.648372	0.778039
B	0.824005	2.542500	-0.131595
B	-0.716919	2.511427	0.778030
B	-0.486297	1.494005	2.202502
B	0.824005	2.542510	1.687686
O	2.975565	-1.070132	0.778039
H	-0.312514	-0.920110	2.026507
H	-1.472020	3.426490	0.778020
H	3.163469	2.114229	0.778043
H	1.154894	3.503312	-0.746035
H	1.154914	3.503325	2.302107
H	1.678137	0.630558	3.256295
H	1.678137	0.630558	-1.700191
H	-1.085872	1.552603	-1.667400
H	-2.377739	0.389584	0.778049
H	-1.085871	1.552604	3.223503
H	-0.312498	-0.920115	-0.470403

24

3-S^--*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -729.924111

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.553459
B	2.054834	0.000000	0.776756

B	1.213602	0.940586	-0.631258
B	-0.506298	1.470717	-0.645569
B	-1.303089	0.801999	0.776747
B	1.213601	0.940566	2.184742
B	2.017422	1.717512	0.776747
B	0.750510	2.589049	-0.119833
B	-0.793929	2.491140	0.776794
B	-0.506307	1.470657	2.199087
B	0.750518	2.589049	1.673341
S	2.952172	-1.441880	0.776718
H	-0.249276	-0.934773	2.028219
H	-1.591471	3.368101	0.776824
H	3.127333	2.135968	0.776754
H	1.030641	3.551499	-0.754938
H	1.030630	3.551487	2.308471
H	1.676890	0.700421	3.247051
H	1.676898	0.700471	-1.693571
H	-1.087818	1.497368	-1.676631
H	-2.380048	0.313637	0.776735
H	-1.087817	1.497274	3.230155
H	-0.249274	-0.934765	-0.474778

26

4-NH_2-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -387.607448

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.613963
B	1.505933	0.000000	0.784440
B	1.265196	1.022964	-0.675363
B	-0.467079	1.493464	-0.625242
B	-1.269326	0.812954	0.806267
B	1.228312	0.986953	2.235251
B	2.010614	1.688424	0.808802
B	0.776301	2.632405	-0.071206
B	-0.768624	2.501863	0.808294
B	-0.482898	1.490367	2.244895

B	0.773225	2.617255	1.705904
N	1.883434	0.616718	-1.922307
H	-0.264748	-0.929160	2.090453
H	-1.586078	3.353708	0.808698
H	3.159947	1.963829	0.814653
H	1.052307	3.588950	-0.708728
H	1.055332	3.564820	2.352146
H	2.131281	-0.997637	0.777558
H	1.746310	0.659770	3.242174
H	-1.071715	1.505327	-1.638549
H	-2.335198	0.314717	0.799743
H	-1.088040	1.496558	3.255924
H	-0.263451	-0.921797	-0.491819
H	1.642414	1.133326	-2.752283
H	2.867663	0.404691	-1.912354

26

4-PH_2-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -674.186305

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.617418
B	1.514713	0.000000	0.800544
B	1.229301	0.997851	-0.644109
B	-0.485866	1.489853	-0.629103
B	-1.278263	0.808897	0.808319
B	1.219096	0.994554	2.241991
B	2.000681	1.691361	0.807696
B	0.765511	2.623552	-0.078395
B	-0.781173	2.497643	0.806531
B	-0.491732	1.491836	2.243972
B	0.761327	2.621197	1.701225
P	2.040046	0.416491	-2.326006
H	-0.266615	-0.929736	2.091814
H	-1.598018	3.349548	0.803039
H	3.147281	1.971754	0.808230
H	1.040846	3.575734	-0.720139

H	1.039360	3.573371	2.341572
H	2.134726	-1.000326	0.801077
H	1.736949	0.672588	3.250297
H	-1.095297	1.497676	-1.638430
H	-2.338015	0.298590	0.804329
H	-1.098249	1.498044	3.254238
H	-0.264619	-0.927602	-0.480747
H	1.912904	1.651931	-3.009093
H	3.390554	0.637431	-1.954717

27

4-CH_3-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -371.539348

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.624110
B	1.504317	0.000000	0.807317
B	1.229275	0.993885	-0.655758
B	-0.495143	1.489062	-0.619971
B	-1.279876	0.806979	0.815882
B	1.217454	0.999174	2.245589
B	1.996048	1.686880	0.804706
B	0.754804	2.617082	-0.079305
B	-0.788142	2.494861	0.814186
B	-0.493123	1.492114	2.250943
B	0.760957	2.621720	1.698222
C	1.940917	0.603267	-2.017083
H	-0.266915	-0.929192	2.099274
H	-1.606707	3.345522	0.813475
H	3.143504	1.967687	0.802361
H	1.029872	3.569335	-0.722999
H	1.040238	3.575031	2.337014
H	2.130257	-0.997175	0.804940
H	1.738691	0.677460	3.252562
H	-1.105055	1.494154	-1.629527
H	-2.339436	0.295248	0.816132
H	-1.098949	1.496795	3.261813

H	-0.274990	-0.929004	-0.472246
H	2.258624	1.503078	-2.545472
H	2.830075	-0.008618	-1.859630
H	1.279681	0.056367	-2.692058

27

4-SiH_3-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -622.922011

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.622683
B	1.511369	0.000000	0.803372
B	1.222925	0.993703	-0.642314
B	-0.493285	1.487896	-0.626557
B	-1.279402	0.803968	0.813406
B	1.216789	0.997918	2.245073
B	1.995800	1.692917	0.807951
B	0.755892	2.620737	-0.076815
B	-0.789396	2.494593	0.811130
B	-0.495197	1.492268	2.249453
B	0.756280	2.623108	1.701603
Si	2.118352	0.495103	-2.376551
H	-0.264461	-0.930740	2.096508
H	-1.608757	3.344087	0.807442
H	3.142248	1.974991	0.809716
H	1.027513	3.573923	-0.719323
H	1.032904	3.576171	2.341356
H	2.133315	-0.999350	0.812753
H	1.737766	0.676107	3.251851
H	-1.111487	1.497074	-1.630759
H	-2.338227	0.291360	0.810002
H	-1.102697	1.496138	3.259348
H	-0.271534	-0.930079	-0.471876
H	1.968016	1.570898	-3.388581
H	3.567948	0.227249	-2.191761
H	1.501830	-0.742428	-2.934528

25

4-OH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -407.495411

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.613132
B	1.512598	0.000000	0.809892
B	1.256452	1.007004	-0.653930
B	-0.484578	1.489432	-0.618489
B	-1.280518	0.814806	0.810620
B	1.216137	0.996248	2.248940
B	2.009414	1.686393	0.823298
B	0.773333	2.619859	-0.078544
B	-0.777910	2.499670	0.805217
B	-0.491912	1.493261	2.243590
B	0.768155	2.619997	1.700983
O	1.891887	0.599883	-1.823084
H	-0.268233	-0.928039	2.089712
H	-1.590724	3.355667	0.801714
H	3.156460	1.965386	0.821704
H	1.053057	3.572213	-0.721915
H	1.044007	3.573706	2.340296
H	2.134411	-0.998434	0.798500
H	1.725385	0.671749	3.260872
H	-1.070915	1.495944	-1.642607
H	-2.342033	0.307673	0.809254
H	-1.098672	1.499597	3.253417
H	-0.262442	-0.925602	-0.485607
H	1.772582	1.202330	-2.559760

25

4-SH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -730.447683

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.619327
B	1.509543	0.000000	0.797003
B	1.232778	1.010779	-0.646390
B	-0.483147	1.495940	-0.626793

B	-1.273944	0.808033	0.808357
B	1.222853	0.992546	2.239723
B	2.003304	1.693662	0.806789
B	0.764541	2.632606	-0.072833
B	-0.779726	2.499598	0.811512
B	-0.489059	1.490637	2.246522
B	0.763732	2.620987	1.704572
S	2.003244	0.569746	-2.281242
H	-0.264972	-0.930745	2.092804
H	-1.599365	3.348604	0.811053
H	3.150642	1.970731	0.805606
H	1.041656	3.582410	-0.715796
H	1.044417	3.570097	2.348095
H	2.135369	-0.996100	0.790599
H	1.744343	0.668612	3.245442
H	-1.088908	1.501886	-1.637750
H	-2.335720	0.302156	0.802078
H	-1.094958	1.495626	3.256892
H	-0.261089	-0.924024	-0.488804
H	3.156730	0.082088	-1.792001

24

4-Cl-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -791.869593

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.621085
B	1.511884	0.000000	0.818871
B	1.222788	1.003302	-0.629090
B	-0.496978	1.495104	-0.622910
B	-1.280543	0.806901	0.809867
B	1.213831	1.000712	2.250524
B	2.001401	1.691978	0.815769
B	0.758335	2.626022	-0.078664
B	-0.788717	2.496604	0.810720
B	-0.496642	1.491743	2.246662
B	0.758399	2.623690	1.699995

Cl	2.030912	0.544547	-2.164377
H	-0.267290	-0.930006	2.094611
H	-1.606596	3.347051	0.808376
H	3.147268	1.970915	0.806583
H	1.038530	3.572654	-0.724840
H	1.035307	3.577135	2.338367
H	2.137498	-0.994929	0.803304
H	1.729803	0.679828	3.259773
H	-1.087883	1.495987	-1.641339
H	-2.338825	0.294026	0.806173
H	-1.104796	1.496541	3.255392
H	-0.258670	-0.926390	-0.485853

24

4-O^--*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -406.943299

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.623289
B	1.481580	0.000000	0.692636
B	1.661485	1.385675	-0.943571
B	-0.419579	1.475388	-0.622567
B	-1.254052	0.836191	0.818585
B	1.242957	0.948904	2.196505
B	2.069613	1.657440	0.796653
B	0.798254	2.664334	-0.097315
B	-0.736636	2.491576	0.799105
B	-0.442369	1.506731	2.245279
B	0.839460	2.596863	1.676574
O	2.201145	1.047325	-2.016614
H	-0.274151	-0.915592	2.121290
H	-1.521183	3.382145	0.820888
H	3.210355	1.960502	0.934190
H	1.021042	3.708066	-0.621660
H	1.131454	3.543759	2.331133
H	2.097141	-1.013012	0.738922
H	1.786790	0.638993	3.202508

H	-1.070803	1.515297	-1.614262
H	-2.341008	0.368644	0.840489
H	-1.023521	1.554114	3.275284
H	-0.337315	-0.922454	-0.448170

24

4-S^--*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -729.906742

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.631191
B	1.494712	0.000000	0.752121
B	1.317264	1.035378	-0.775414
B	-0.482615	1.483091	-0.612156
B	-1.270826	0.811212	0.832237
B	1.227840	0.979603	2.223692
B	2.007199	1.678274	0.789487
B	0.760828	2.621367	-0.085704
B	-0.774832	2.488979	0.826816
B	-0.478233	1.486835	2.263809
B	0.782597	2.605865	1.695409
S	2.082608	0.549753	-2.286625
H	-0.255021	-0.930953	2.109653
H	-1.591734	3.348273	0.840254
H	3.153549	1.969011	0.829954
H	1.007024	3.609597	-0.689560
H	1.069512	3.558367	2.342066
H	2.114883	-1.002184	0.785041
H	1.765552	0.658598	3.227775
H	-1.133153	1.511867	-1.597059
H	-2.341910	0.313234	0.842015
H	-1.071059	1.501206	3.287309
H	-0.277251	-0.923195	-0.481508

26

8-NH_2-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -387.602118

C	0.000000	0.000000	0.000000

C	0.000000	0.000000	1.630271
B	1.510736	0.000000	0.807035
B	1.197140	1.000080	-0.634514
B	-0.517569	1.490777	-0.616310
B	-1.278580	0.801580	0.827191
B	1.219651	0.984507	2.243946
B	2.039042	1.701657	0.793919
B	0.739323	2.618262	-0.088869
B	-0.784736	2.495214	0.818670
B	-0.479711	1.490276	2.255396
B	0.776492	2.611372	1.691095
N	3.459839	2.044447	0.826152
H	-0.272260	-0.929251	-0.471567
H	-1.602066	3.347041	0.834464
H	1.061840	3.565306	2.329185
H	1.019545	3.571771	-0.728518
H	-2.337433	0.289301	0.834626
H	-1.135515	1.491313	-1.620145
H	-1.081466	1.503826	3.268718
H	1.754094	0.669685	3.245647
H	2.135169	-0.997914	0.796014
H	1.712033	0.679073	-1.646508
H	-0.264683	-0.931646	2.101676
H	3.693855	3.009130	0.996213
H	4.056898	1.665174	0.109420

26

8-PH_2-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -674.185284

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.624649
B	1.512790	0.000000	0.814076
B	1.214884	0.994052	-0.622360
B	-0.491279	1.492653	-0.625250
B	-1.278170	0.806746	0.808829
B	1.213070	0.998379	2.253450

B	2.015580	1.690393	0.817466
B	0.767377	2.617989	-0.074689
B	-0.782439	2.497386	0.811484
B	-0.499066	1.491465	2.247502
B	0.759491	2.619759	1.705413
P	3.921215	2.150676	0.714732
H	-0.266388	-0.929739	-0.474513
H	-1.597587	3.350865	0.808559
H	1.036698	3.572740	2.344816
H	1.047335	3.570077	-0.715347
H	-2.338164	0.296722	0.807303
H	-1.096211	1.501137	-1.636307
H	-1.107849	1.498126	3.256416
H	1.730674	0.675030	3.261507
H	2.135827	-0.998260	0.815607
H	1.739753	0.675356	-1.627829
H	-0.268873	-0.929339	2.098599
H	3.816003	3.440159	1.297524
H	4.326890	1.535050	1.929262

27

8-CH_3-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -371.537684

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.622647
B	1.511706	0.000000	0.811011
B	1.215667	0.994713	-0.621916
B	-0.492942	1.492734	-0.624727
B	-1.278709	0.806586	0.811255
B	1.215727	0.994990	2.245472
B	2.031988	1.696084	0.811704
B	0.763341	2.617712	-0.076085
B	-0.783002	2.495345	0.811810
B	-0.493509	1.491525	2.248103
B	0.762171	2.617122	1.700370
C	3.573089	2.092957	0.811502

H	-0.269009	-0.928996	-0.474271
H	-1.599809	3.347830	0.811691
H	1.041879	3.570022	2.340953
H	1.041647	3.570764	-0.717196
H	-2.338162	0.295050	0.811010
H	-1.100386	1.499204	-1.634746
H	-1.101429	1.496863	3.257845
H	1.734958	0.673406	3.254418
H	2.133291	-0.999967	0.811975
H	1.735358	0.675277	-1.631262
H	-0.268457	-0.929273	2.096721
H	3.709805	3.139368	1.087514
H	4.152997	1.496028	1.517811
H	4.027365	1.959387	-0.171866

27

8-SiH_3-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -622.922472

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.619334
B	1.515019	0.000000	0.809913
B	1.217876	0.996183	-0.625561
B	-0.492717	1.491673	-0.627187
B	-1.280089	0.808839	0.809754
B	1.217786	0.996329	2.244519
B	2.017303	1.689427	0.809461
B	0.762511	2.620639	-0.080046
B	-0.783581	2.496237	0.809368
B	-0.492577	1.492569	2.246087
B	0.763464	2.621294	1.697934
Si	3.969668	2.188724	0.813572
H	-0.267413	-0.929091	-0.475478
H	-1.599064	3.349620	0.809375
H	1.036433	3.574118	2.340460
H	1.036102	3.573148	-0.722161
H	-2.339507	0.297121	0.809808

H	-1.097733	1.497840	-1.638379
H	-1.097401	1.499386	3.257377
H	1.730867	0.674934	3.256049
H	2.132909	-1.001347	0.809331
H	1.730640	0.673582	-1.637008
H	-0.267570	-0.928935	2.094986
H	4.404785	2.665707	2.153945
H	4.833577	1.028639	0.456741
H	4.256026	3.271120	-0.164998

25

8-OH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -407.492442

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.628486
B	1.512380	0.000000	0.814221
B	1.203993	0.989745	-0.627717
B	-0.502867	1.488050	-0.621925
B	-1.281450	0.800055	0.814278
B	1.204011	0.989690	2.256195
B	2.026460	1.703693	0.814237
B	0.751693	2.614467	-0.077851
B	-0.788634	2.493118	0.814259
B	-0.502837	1.488048	2.250438
B	0.751736	2.614414	1.706356
O	3.397451	1.994001	0.814187
H	-0.267903	-0.931161	-0.470489
H	-1.606257	3.344728	0.814281
H	1.037826	3.569167	2.342892
H	1.037763	3.569232	-0.714370
H	-2.338352	0.284221	0.814271
H	-1.113204	1.494488	-1.630058
H	-1.113153	1.494482	3.258584
H	1.730884	0.675453	3.262297
H	2.139052	-0.995488	0.814234
H	1.730830	0.675485	-1.633833

H -0.267887 -0.931166 2.098975
H 3.591919 2.932869 0.814731

25

8-SH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -730.446733

C 0.000000 0.000000 0.000000
C 0.000000 0.000000 1.629188
B 1.511849 0.000000 0.812553
B 1.206476 0.995957 -0.629731
B -0.502280 1.490947 -0.621222
B -1.278453 0.803372 0.816759
B 1.211157 0.993369 2.255047
B 2.011931 1.692222 0.810761
B 0.757533 2.617230 -0.079158
B -0.782508 2.496581 0.815621
B -0.495822 1.489889 2.251994
B 0.763516 2.616067 1.704593
S 3.841426 2.085628 0.799827
H -0.267484 -0.930560 -0.472159
H -1.596550 3.350939 0.818025
H 1.047402 3.568971 2.341613
H 1.039319 3.569697 -0.717247
H -2.337778 0.292515 0.818322
H -1.112084 1.498399 -1.629296
H -1.102597 1.499703 3.261908
H 1.740599 0.674917 3.257370
H 2.140237 -0.994213 0.811620
H 1.732259 0.677206 -1.633975
H -0.265597 -0.930781 2.101992
H 3.710292 3.414710 0.946522

24

8-Cl-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -791.869813

C 0.000000 0.000000 0.000000
C 0.000000 0.000000 1.624388

B	1.508684	0.000000	0.812181
B	1.208647	0.998601	-0.627873
B	-0.500460	1.490700	-0.624965
B	-1.281539	0.801261	0.812210
B	1.208639	0.998594	2.252257
B	1.995860	1.699930	0.812209
B	0.747983	2.625900	-0.079213
B	-0.794327	2.492698	0.812197
B	-0.500458	1.490695	2.249383
B	0.747991	2.625882	1.703641
Cl	3.746278	2.137963	0.812211
H	-0.264573	-0.930024	-0.474822
H	-1.613674	3.341806	0.812188
H	1.033687	3.576342	2.341281
H	1.033679	3.576361	-0.716853
H	-2.338287	0.285637	0.812198
H	-1.107498	1.494962	-1.634522
H	-1.107491	1.494941	3.258944
H	1.740408	0.684561	3.254688
H	2.146178	-0.987531	0.812195
H	1.740391	0.684560	-1.630315
H	-0.264573	-0.930024	2.099210

24

8-O^--*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -406.915862

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.627533
B	1.527409	0.000000	0.813753
B	1.225365	0.979422	-0.617228
B	-0.481795	1.489887	-0.617405
B	-1.276331	0.795745	0.813776
B	1.225373	0.979429	2.244733
B	2.212405	1.761865	0.813750
B	0.770406	2.613683	-0.075052
B	-0.773716	2.488971	0.813772

B	-0.481769	1.489896	2.244938
B	0.770421	2.613664	1.702587
O	3.460806	2.061938	0.813741
H	-0.274015	-0.930063	-0.469156
H	-1.601706	3.339695	0.813781
H	1.005448	3.572685	2.361025
H	1.005413	3.572708	-0.733490
H	-2.341605	0.285574	0.813774
H	-1.099862	1.495348	-1.628251
H	-1.099836	1.495368	3.255784
H	1.700135	0.643921	3.276960
H	2.102423	-1.034196	0.813745
H	1.700113	0.643903	-1.649458
H	-0.273999	-0.930069	2.096689

24

8-S$^-$-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -729.891955

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.617349
B	1.536821	0.000000	0.808663
B	1.233912	0.982076	-0.619930
B	-0.476605	1.489250	-0.621814
B	-1.276948	0.804340	0.808666
B	1.233938	0.982088	2.237255
B	2.146312	1.705866	0.808655
B	0.786365	2.609260	-0.076992
B	-0.764672	2.490855	0.808631
B	-0.476588	1.489270	2.239140
B	0.786404	2.609257	1.694339
S	3.886220	2.092130	0.808649
H	-0.268680	-0.929797	2.090044
H	-1.582465	3.349444	0.808617
H	1.036635	3.564774	-0.728983
H	1.036676	3.564768	2.346333
H	2.116090	-1.027658	0.808667

H	1.717847	0.646997	3.261622
H	1.717811	0.646951	-1.644292
H	-1.086497	1.498432	-1.635974
H	-2.343251	0.297696	0.808670
H	-1.086476	1.498465	3.253303
H	-0.268669	-0.929806	-0.472684

26

9-NH_2-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -387.602931

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.628312
B	1.509011	0.000000	0.819736
B	1.210673	0.987255	-0.625986
B	-0.503592	1.487250	-0.621555
B	-1.284817	0.799863	0.822451
B	1.218085	1.013945	2.239331
B	1.992850	1.686937	0.800084
B	0.755695	2.654501	-0.115171
B	-0.809539	2.482808	0.814617
B	-0.501399	1.494259	2.245276
B	0.745638	2.630145	1.675357
N	1.134803	3.809483	-0.923784
H	-0.263593	-0.927971	2.106576
H	-1.626391	3.336018	0.805771
H	3.136079	1.980617	0.791731
H	1.020217	3.590316	2.309205
H	2.132997	-0.997733	0.820620
H	1.735079	0.708978	3.253726
H	1.722557	0.666952	-1.638353
H	-1.115583	1.488228	-1.630632
H	-2.339696	0.278100	0.819193
H	-1.095457	1.505155	3.263448
H	-0.270410	-0.929801	-0.471511
H	1.323049	4.674213	-0.443451
H	0.627700	3.984538	-1.775772

26

9-PH_2-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -674.185641

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.622576
B	1.513614	0.000000	0.811320
B	1.215197	0.999489	-0.625635
B	-0.496287	1.487817	-0.624113
B	-1.278988	0.805547	0.813363
B	1.216554	0.995844	2.247232
B	2.000724	1.689324	0.811761
B	0.764027	2.632875	-0.089779
B	-0.784917	2.495538	0.807257
B	-0.492106	1.496221	2.246381
B	0.763171	2.622239	1.696104
P	1.124347	4.209122	-1.202555
H	-0.268258	-0.928550	2.098039
H	-1.602427	3.347149	0.803964
H	3.146757	1.970875	0.809790
H	1.038420	3.576220	2.335149
H	2.136640	-0.997875	0.809043
H	1.733571	0.678798	3.257611
H	1.732043	0.679566	-1.635548
H	-1.101284	1.496976	-1.635071
H	-2.339273	0.296177	0.813910
H	-1.100298	1.505896	3.255572
H	-0.267394	-0.929084	-0.475283
H	1.576175	5.059976	-0.159983
H	2.438931	3.852157	-1.605418

27

9-CH_3-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -371.538091

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.623471
B	1.511794	0.000000	0.811495

B	1.213863	0.998205	-0.625705
B	-0.491767	1.492590	-0.625701
B	-1.277429	0.808520	0.811478
B	1.216638	1.000380	2.245733
B	1.995953	1.690216	0.807798
B	0.767771	2.648315	-0.099392
B	-0.782502	2.495625	0.807727
B	-0.493044	1.495982	2.245701
B	0.759674	2.620618	1.692874
C	1.140634	3.935584	-0.956502
H	-0.269023	-0.928139	2.099100
H	-1.601148	3.347455	0.805817
H	3.143288	1.972033	0.805891
H	1.036517	3.575940	2.331252
H	2.135573	-0.997732	0.810719
H	1.734953	0.682654	3.255536
H	1.733031	0.676138	-1.634518
H	-1.102601	1.498240	-1.634571
H	-2.338134	0.299135	0.810640
H	-1.100968	1.504726	3.255482
H	-0.269199	-0.928773	-0.474769
H	1.383923	4.782712	-0.313300
H	2.005556	3.761087	-1.599125
H	0.317755	4.248068	-1.602037

27

9-SiH_3-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -622.922488

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.622772
B	1.511872	0.000000	0.810863
B	1.215212	1.000853	-0.625189
B	-0.494235	1.495042	-0.625280
B	-1.279074	0.806412	0.810761
B	1.215117	0.999246	2.248098
B	1.996462	1.692793	0.810383

B	0.761133	2.635147	-0.087574
B	-0.786451	2.496732	0.810761
B	-0.495256	1.493056	2.248130
B	0.757126	2.621755	1.699413
Si	1.235831	4.265086	-1.172753
H	-0.268383	-0.928801	2.098245
H	-1.608396	3.344420	0.813693
H	3.143905	1.971741	0.813753
H	1.032438	3.573459	2.342078
H	2.137251	-0.996384	0.809406
H	1.733901	0.680761	3.257072
H	1.732295	0.678398	-1.634033
H	-1.104147	1.497427	-1.633950
H	-2.339375	0.296863	0.809126
H	-1.103859	1.500059	3.257164
H	-0.268287	-0.928164	-0.476856
H	1.713662	5.376963	-0.307906
H	2.315075	3.972394	-2.156174
H	0.067042	4.771385	-1.943600

25

9-OH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -407.493354

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.627230
B	1.511181	0.000000	0.817911
B	1.212644	0.991795	-0.626871
B	-0.504717	1.483020	-0.626894
B	-1.282675	0.799110	0.817736
B	1.215795	1.006079	2.243960
B	1.995377	1.683471	0.808688
B	0.757476	2.648030	-0.104654
B	-0.803373	2.483997	0.808602
B	-0.499941	1.496771	2.243854
B	0.750345	2.623318	1.683284
O	1.071028	3.743782	-0.919456

H	-0.265488	-0.927883	2.104703
H	-1.615563	3.341209	0.800933
H	3.138022	1.981489	0.801236
H	1.025788	3.586323	2.313597
H	2.133327	-0.998601	0.817454
H	1.730270	0.698702	3.258813
H	1.730168	0.674794	-1.636812
H	-1.111506	1.487538	-1.636891
H	-2.338709	0.280399	0.817454
H	-1.099155	1.508130	3.258700
H	-0.266143	-0.930664	-0.472404
H	1.295362	4.537772	-0.430819

25

9-SH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -730.447387

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.626008
B	1.511811	0.000000	0.818115
B	1.213322	0.994154	-0.624315
B	-0.505610	1.484541	-0.624253
B	-1.283047	0.797602	0.817578
B	1.214134	1.005633	2.244824
B	1.995983	1.687925	0.809708
B	0.751504	2.630764	-0.093558
B	-0.803813	2.487516	0.808151
B	-0.501245	1.496068	2.244120
B	0.750073	2.628376	1.686313
S	1.170679	4.096033	-1.178961
H	-0.265467	-0.928238	2.103311
H	-1.618263	3.340473	0.799097
H	3.138078	1.981908	0.801494
H	1.023616	3.587602	2.319007
H	2.136651	-0.996540	0.816905
H	1.730077	0.697813	3.258376
H	1.729119	0.679855	-1.635533

H	-1.109586	1.490151	-1.635465
H	-2.339870	0.281196	0.816437
H	-1.102659	1.507481	3.257276
H	-0.265330	-0.930030	-0.474257
H	1.390348	4.970098	-0.182003

24

9-Cl-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -791.870991

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.622834
B	1.512288	0.000000	0.812820
B	1.215281	0.993422	-0.626893
B	-0.499952	1.487897	-0.626892
B	-1.280212	0.805038	0.812822
B	1.215227	1.001186	2.246203
B	1.998736	1.688763	0.811413
B	0.756564	2.624498	-0.080365
B	-0.793068	2.493585	0.811458
B	-0.495776	1.494449	2.246206
B	0.756475	2.624000	1.699874
Cl	1.176228	4.080327	-1.063868
H	-0.267586	-0.928230	2.098934
H	-1.602651	3.350923	0.801117
H	3.140460	1.983581	0.801033
H	1.033013	3.583257	2.328390
H	2.136280	-0.996870	0.811805
H	1.733032	0.686074	3.256362
H	1.732238	0.686217	-1.639007
H	-1.101108	1.503028	-1.639004
H	-2.339105	0.293313	0.811781
H	-1.101843	1.503319	3.256373
H	-0.267661	-0.928428	-0.476350

24

9-O^--*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -406.914490

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.626881
B	1.512910	0.000000	0.804822
B	1.218037	0.985714	-0.645135
B	-0.471314	1.494363	-0.645137
B	-1.261406	0.835318	0.804822
B	1.232807	1.005775	2.225451
B	2.017564	1.671840	0.789315
B	0.842289	2.797498	-0.211007
B	-0.759107	2.507870	0.789283
B	-0.472552	1.519243	2.225452
B	0.791688	2.629406	1.666626
O	1.149633	3.818227	-0.925169
H	-0.280796	-0.932570	-0.461621
H	3.179976	1.909189	0.808211
H	-1.597231	3.347566	0.808174
H	1.073050	3.563855	2.343003
H	-2.328766	0.324805	0.810457
H	-1.114089	1.455965	-1.640120
H	-1.074145	1.536178	3.246771
H	1.743742	0.687740	3.246769
H	2.120957	-1.014967	0.810442
H	1.732770	0.598797	-1.640108
H	-0.277585	-0.921906	2.107120

24

9-S$^-$-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -729.889871

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.627585
B	1.508973	0.000000	0.802576
B	1.218933	0.994030	-0.645429
B	-0.473444	1.499929	-0.645424
B	-1.261417	0.828138	0.802571
B	1.228988	1.005885	2.225032
B	2.011066	1.680779	0.784882

B	0.814206	2.723878	-0.185141
B	-0.758738	2.508741	0.784862
B	-0.475310	1.515355	2.225036
B	0.786530	2.631129	1.659610
S	1.234723	4.130710	-1.189625
H	-0.277947	-0.929807	-0.468742
H	3.168073	1.928858	0.798347
H	-1.589796	3.351090	0.798327
H	1.067498	3.571050	2.322867
H	-2.329800	0.322964	0.805729
H	-1.104496	1.469161	-1.644147
H	-1.079390	1.536226	3.243139
H	1.745429	0.691794	3.243128
H	2.124840	-1.008637	0.805737
H	1.729570	0.621984	-1.644154
H	-0.275819	-0.922672	2.108149

26

1-NH_2-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -387.5928325

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.709131
B	1.516462	0.000000	0.792113
B	1.259927	0.941091	-0.679551
B	-0.404928	1.552245	-0.667286
B	-1.186343	0.943060	0.802227
C	1.244408	1.089069	2.053629
B	2.105810	1.655567	0.694946
B	0.919135	2.623444	-0.205803
B	-0.607471	2.624479	0.719796
B	-0.359410	1.655924	2.188053
B	0.948081	2.692570	1.564837
N	-0.387404	-1.217469	-0.642692
H	1.259012	3.529293	-0.882077
H	-0.827299	1.845509	3.252656
H	1.351350	3.578937	2.228360

H	-1.363411	3.531052	0.707585
H	-0.240961	-0.959390	2.343558
H	-2.304546	0.566150	0.779789
H	1.796045	0.925225	2.965300
H	3.265761	1.847191	0.772498
H	1.757412	0.565450	-1.681653
H	-1.015741	1.564397	-1.676705
H	2.189434	-0.959657	0.873766
H	-0.012320	-1.281216	-1.578540
H	-1.392073	-1.315825	-0.682098

26

1-PH_2-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -674.1961403

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.695764
B	1.522436	0.000000	0.773526
B	1.264310	0.932280	-0.695741
B	-0.409173	1.535186	-0.671060
B	-1.190603	0.951824	0.809303
C	1.257254	1.081004	2.037870
B	2.115298	1.654004	0.676861
B	0.922628	2.612104	-0.223479
B	-0.597832	2.622567	0.715200
B	-0.342715	1.660908	2.184445
B	0.963836	2.688716	1.548486
P	-0.444768	-1.608495	-0.861517
H	1.254498	3.516359	-0.905618
H	-0.798797	1.850724	3.254138
H	1.372337	3.574840	2.209514
H	-1.348219	3.533572	0.699224
H	-0.233149	-0.954585	2.343057
H	-2.312753	0.593192	0.804775
H	1.812110	0.913886	2.947013
H	3.276349	1.839750	0.750906
H	1.763156	0.564577	-1.698883

H	-1.023913	1.565590	-1.676236
H	2.195375	-0.959869	0.860748
H	-0.873743	-1.017488	-2.076154
H	-1.762424	-1.709795	-0.346693

27

1-CH_3-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -371.5531127

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.700314
B	1.516109	0.000000	0.769529
B	1.266505	0.946437	-0.688832
B	-0.407029	1.530555	-0.663123
B	-1.187321	0.946458	0.817608
C	1.254371	1.078477	2.043303
B	2.112225	1.657879	0.685767
B	0.919168	2.618599	-0.210464
B	-0.603590	2.618628	0.724345
B	-0.344412	1.657902	2.193836
B	0.957801	2.689066	1.560172
C	-0.444068	-1.264375	-0.723294
H	1.245984	3.527953	-0.888501
H	-0.800562	1.844289	3.264261
H	1.365641	3.573036	2.224645
H	-1.356127	3.527976	0.708952
H	-0.230073	-0.959516	2.341410
H	-2.307654	0.579713	0.804807
H	1.811354	0.908499	2.950570
H	3.273208	1.844170	0.763459
H	1.762118	0.579475	-1.693577
H	-1.024121	1.559269	-1.668137
H	2.192026	-0.959448	0.854475
H	-0.115971	-2.153177	-0.187655
H	-1.528143	-1.294589	-0.804928
H	-0.025301	-1.295223	-1.726529

27

1-SiH_3-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -622.9485025

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.700084
B	1.516381	0.000000	0.768805
B	1.260941	0.942417	-0.695932
B	-0.410579	1.538018	-0.668441
B	-1.190958	0.942432	0.809978
C	1.253078	1.080152	2.040254
B	2.109753	1.657595	0.679474
B	0.916483	2.619007	-0.216229
B	-0.607346	2.619030	0.719692
B	-0.348040	1.657644	2.188989
B	0.954604	2.689264	1.554288
Si	-0.556206	-1.579609	-0.905284
H	1.245634	3.527743	-0.893765
H	-0.804697	1.845650	3.258790
H	1.361887	3.574757	2.217284
H	-1.360473	3.527784	0.706891
H	-0.229482	-0.953188	2.350399
H	-2.314349	0.583049	0.805047
H	1.810488	0.912933	2.947852
H	3.270411	1.845712	0.755891
H	1.764497	0.583141	-1.700198
H	-1.027262	1.572677	-1.672555
H	2.200134	-0.953206	0.858269
H	-1.300925	-1.193995	-2.122270
H	-1.424523	-2.367388	-0.002259
H	0.641540	-2.369807	-1.267279

25

1-OH-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -407.4639864

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.700655
B	1.522794	0.000000	0.756850

B	1.268958	0.942150	-0.708359
B	-0.417777	1.508331	-0.674184
B	-1.199097	0.941989	0.821148
C	1.252585	1.082286	2.021434
B	2.105466	1.666018	0.658854
B	0.904292	2.609312	-0.241255
B	-0.618645	2.609281	0.702452
B	-0.347220	1.665933	2.178784
B	0.947705	2.692653	1.529537
O	-0.373988	-1.186360	-0.603841
H	1.218159	3.517427	-0.926500
H	-0.794653	1.860809	3.250935
H	1.354110	3.582910	2.185469
H	-1.372086	3.517295	0.678542
H	-0.225007	-0.961938	2.336326
H	-2.311677	0.555073	0.801361
H	1.814194	0.923178	2.927657
H	3.264700	1.860923	0.735492
H	1.746504	0.555246	-1.713429
H	-1.040462	1.499689	-1.678936
H	2.192360	-0.961827	0.838232
H	-0.871865	-0.988425	-1.404531

25

1-SH-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -730.4366368

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.701970
B	1.521870	0.000000	0.755628
B	1.267607	0.945017	-0.707793
B	-0.417443	1.517956	-0.674051
B	-1.197247	0.941362	0.821053
C	1.255495	1.078036	2.026796
B	2.108029	1.663403	0.664856
B	0.908425	2.612070	-0.230470
B	-0.612858	2.609802	0.711852

B	-0.342756	1.662428	2.185045
B	0.953272	2.689713	1.539848
S	-0.487795	-1.553008	-0.796516
H	1.225516	3.520141	-0.914325
H	-0.792714	1.852138	3.257092
H	1.361162	3.577120	2.199081
H	-1.368174	3.516402	0.691572
H	-0.223773	-0.959637	2.342355
H	-2.313645	0.568436	0.811027
H	1.817610	0.912648	2.931873
H	3.268301	1.852776	0.739940
H	1.756166	0.571507	-1.711293
H	-1.039510	1.536797	-1.675994
H	2.196613	-0.958628	0.839298
H	-1.214548	-0.980118	-1.771194

24

1-Cl-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -791.8408191

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.699574
B	1.522192	0.000000	0.755848
B	1.253872	0.926851	-0.725219
B	-0.433725	1.503285	-0.699725
B	-1.207100	0.926869	0.800497
C	1.247306	1.094002	2.011903
B	2.094593	1.663327	0.641161
B	0.889047	2.600511	-0.262864
B	-0.630771	2.600527	0.679335
B	-0.357226	1.663349	2.161157
B	0.933817	2.694511	1.506190
Cl	-0.498669	-1.490919	-0.804343
H	1.204947	3.501456	-0.956054
H	-0.811102	1.860248	3.229998
H	1.336483	3.591054	2.155743
H	-1.392126	3.501471	0.654010

H	-0.220652	-0.957874	2.342080
H	-2.318352	0.540697	0.792498
H	1.809782	0.942554	2.919137
H	3.253777	1.860165	0.710004
H	1.740896	0.540508	-1.724026
H	-1.053951	1.500172	-1.700028
H	2.195851	-0.957839	0.843931

24

1-O^--*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -406.925801

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.773242
B	1.531635	0.000000	0.891075
B	1.366924	1.042678	-0.518198
B	-0.289790	1.679029	-0.504996
B	-1.134121	1.042630	0.920507
C	1.274746	1.021600	2.215728
B	2.185196	1.644327	0.917572
B	1.059814	2.691131	0.051479
B	-0.487457	2.691512	0.941422
B	-0.305056	1.645017	2.349913
B	1.050706	2.666544	1.825007
O	-0.379031	-0.999374	-0.660036
H	1.439811	3.639234	-0.553485
H	-0.778389	1.796572	3.425170
H	1.470026	3.498822	2.555224
H	-1.201105	3.639834	0.965803
H	-0.275739	-0.961548	2.400745
H	-2.280907	0.754763	0.886887
H	1.799997	0.786388	3.127597
H	3.352827	1.794181	1.049554
H	1.914049	0.752621	-1.525961
H	-0.875043	1.841502	-1.520898
H	2.213928	-0.960540	0.967996

24

1-S^--*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -729.9073225

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.719815
B	1.515406	0.000000	0.812758
B	1.304543	0.993904	-0.617684
B	-0.354601	1.603238	-0.593472
B	-1.160394	0.993633	0.857278
C	1.266893	1.061356	2.116721
B	2.143057	1.656444	0.787839
B	0.984909	2.659749	-0.089951
B	-0.544403	2.659928	0.825169
B	-0.318411	1.656572	2.260708
B	1.006389	2.688648	1.681058
S	-0.519017	-1.455396	-0.868202
H	1.338121	3.588468	-0.736801
H	-0.782519	1.824077	3.336126
H	1.422891	3.549763	2.377771
H	-1.281202	3.588765	0.830715
H	-0.244101	-0.950587	2.369630
H	-2.296585	0.679033	0.845786
H	1.810510	0.853838	3.024574
H	3.310218	1.823374	0.887159
H	1.831179	0.678162	-1.624141
H	-0.958311	1.710317	-1.601363
H	2.204173	-0.950038	0.904265

26

2-NH_2-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -387.6347941

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.736567
B	1.505697	0.000000	0.750929
B	1.244536	0.876925	-0.758560
B	-0.425222	1.478407	-0.733529
B	-1.177506	0.937425	0.788528

C	1.285900	1.136062	1.972041
B	2.115679	1.647252	0.578597
B	0.909884	2.572797	-0.343832
B	-0.601041	2.606895	0.620568
B	-0.309874	1.707291	2.121136
B	0.977083	2.718407	1.418955
N	-0.273874	-1.108090	2.606470
H	-0.321443	-0.919159	-0.463251
H	1.228072	3.455088	-1.060167
H	-0.747979	1.947523	3.188992
H	1.388047	3.633472	2.038394
H	-1.352544	3.516805	0.586200
H	-2.299144	0.572616	0.808494
H	1.853126	1.001833	2.879010
H	3.278512	1.833208	0.623075
H	1.731466	0.464622	-1.749419
H	-1.064214	1.464113	-1.724286
H	2.177083	-0.961235	0.865706
H	-1.182359	-1.211915	3.022148
H	0.224007	-1.977163	2.530843

26

2-PH_2-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -674.2117703

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.703080
B	1.512806	0.000000	0.752185
B	1.246299	0.899191	-0.744210
B	-0.431347	1.485167	-0.726182
B	-1.197178	0.927059	0.780355
C	1.256058	1.119429	1.986684
B	2.098379	1.659534	0.604903
B	0.892745	2.586485	-0.312021
B	-0.626196	2.601629	0.636339
B	-0.344787	1.683014	2.131721
B	0.942998	2.709856	1.453825

P	-0.325111	-1.491332	2.914565
H	-0.308972	-0.914395	-0.480089
H	1.211217	3.478710	-1.015700
H	-0.793413	1.906796	3.198368
H	1.345839	3.616716	2.089615
H	-1.384612	3.505343	0.607275
H	-2.315658	0.557265	0.787644
H	1.819402	0.982721	2.896020
H	3.258375	1.854796	0.668653
H	1.739164	0.499654	-1.736891
H	-1.057884	1.472701	-1.724402
H	2.201127	-0.948837	0.852973
H	-1.737811	-1.506107	2.793259
H	-0.124694	-2.536265	1.974759

27

2-CH_3-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -371.5662895

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.705772
B	1.516238	0.000000	0.731966
B	1.246457	0.894625	-0.760185
B	-0.429104	1.485643	-0.730149
B	-1.187893	0.942946	0.781677
C	1.268099	1.110478	1.972044
B	2.109724	1.650509	0.582510
B	0.904716	2.583238	-0.329503
B	-0.605381	2.611912	0.625153
B	-0.327886	1.695098	2.119955
B	0.964826	2.706151	1.438416
C	-0.326717	-1.246687	2.618159
H	-0.317376	-0.911007	-0.482080
H	1.224809	3.472841	-1.036056
H	-0.767853	1.922698	3.189916
H	1.378432	3.611138	2.070710
H	-1.357412	3.521458	0.596830

H	-2.307784	0.574527	0.794541
H	1.841154	0.979757	2.876228
H	3.271001	1.841608	0.642299
H	1.728678	0.490955	-1.756762
H	-1.061027	1.474627	-1.725352
H	2.192456	-0.957002	0.835965
H	-0.310076	-0.971337	3.673905
H	-1.325913	-1.631512	2.409352
H	0.378411	-2.067253	2.482232

27

2-SiH_3-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -622.9465387

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.701454
B	1.513887	0.000000	0.747651
B	1.246249	0.901178	-0.747691
B	-0.432421	1.485282	-0.729035
B	-1.197725	0.929050	0.778388
C	1.251927	1.117648	1.985381
B	2.097159	1.660702	0.602201
B	0.891367	2.587884	-0.316305
B	-0.626050	2.604339	0.630912
B	-0.347618	1.686861	2.127076
B	0.941213	2.711510	1.450138
Si	-0.440249	-1.575983	2.876811
H	-0.307203	-0.910866	-0.488643
H	1.211061	3.479949	-1.020029
H	-0.798981	1.917911	3.190943
H	1.344643	3.617751	2.086709
H	-1.385641	3.507195	0.601719
H	-2.317634	0.562622	0.782046
H	1.822109	0.991284	2.891860
H	3.257029	1.856476	0.668572
H	1.738449	0.501018	-1.740482
H	-1.058951	1.471383	-1.727307

H	2.209995	-0.943427	0.839900
H	-0.368589	-1.176553	4.306308
H	-1.813134	-2.066480	2.592717
H	0.505496	-2.703261	2.665387

25

2-OH-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -407.5231531

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.717288
B	1.515441	0.000000	0.735592
B	1.242127	0.893791	-0.756469
B	-0.432903	1.486491	-0.720856
B	-1.185330	0.941060	0.792789
C	1.280915	1.113772	1.977486
B	2.111639	1.649838	0.586012
B	0.901458	2.582577	-0.321196
B	-0.606224	2.609936	0.639993
B	-0.318414	1.694940	2.131153
B	0.970359	2.706714	1.445565
O	-0.222077	-1.124164	2.494447
H	-1.070479	1.480244	-1.712271
H	-0.756238	1.910900	3.205468
H	1.723669	0.495735	-1.755297
H	-1.357962	3.519638	0.614520
H	1.217105	3.473501	-1.027457
H	-2.303709	0.565360	0.816402
H	1.383074	3.613587	2.075400
H	3.272790	1.842684	0.636289
H	2.174925	-0.966172	0.852598
H	-0.321135	-0.916423	-0.469204
H	1.849936	0.971308	2.882487
H	-1.034974	-1.093333	3.003230

25

2-SH-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -730.4740978

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.708201
B	1.511534	0.000000	0.752021
B	1.243170	0.899100	-0.742739
B	-0.433517	1.484750	-0.720127
B	-1.196882	0.924072	0.787677
C	1.259881	1.118116	1.991674
B	2.098563	1.658265	0.609519
B	0.891063	2.586035	-0.307299
B	-0.625686	2.598317	0.645254
B	-0.342173	1.682595	2.138841
B	0.944968	2.708138	1.459074
S	-0.307322	-1.501824	2.745747
H	-1.064031	1.475296	-1.715685
H	-0.790433	1.900911	3.206208
H	1.736536	0.502642	-1.736171
H	-1.385184	3.501253	0.618781
H	1.206992	3.480251	-1.009170
H	-2.313648	0.549115	0.798222
H	1.346825	3.614877	2.095555
H	3.258615	1.853491	0.670028
H	2.190568	-0.954463	0.858322
H	-0.311368	-0.918443	-0.470971
H	1.821445	0.974392	2.900679
H	-1.480554	-1.089977	3.256634

24

2-Cl-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -791.894728

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.695178
B	1.520682	0.000000	0.736371
B	1.243612	0.913989	-0.741515
B	-0.437073	1.493128	-0.707250
B	-1.203134	0.928919	0.794306
C	1.259156	1.094140	1.996945

B	2.099131	1.657481	0.615403
B	0.888505	2.592797	-0.285647
B	-0.624475	2.601222	0.663622
B	-0.348667	1.671512	2.149520
B	0.944341	2.693686	1.483797
Cl	-0.354545	-1.430003	2.702239
H	-0.313208	-0.912324	-0.481878
H	1.203771	3.494172	-0.978299
H	-0.793055	1.869278	3.221579
H	1.349167	3.591436	2.130656
H	-1.380908	3.506496	0.644534
H	-2.316158	0.545617	0.805892
H	1.821895	0.942942	2.904197
H	3.258504	1.854154	0.680983
H	1.731264	0.526959	-1.741281
H	-1.067681	1.491115	-1.702537
H	2.190513	-0.959449	0.839650

24

2-O^--*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -406.9818005

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	2.583495
B	1.602218	0.000000	0.276175
B	0.917872	0.877461	-1.128648
B	-0.615264	1.465921	-0.491339
B	-0.748157	0.859314	1.210472
C	1.997757	1.118879	1.387453
B	2.219140	1.606277	-0.224909
B	0.748020	2.573275	-0.569134
B	-0.260779	2.545007	0.906110
B	0.610511	1.620290	2.154151
B	1.533321	2.669263	1.000916
O	0.011181	-0.958999	3.340552
H	-0.474480	-0.892296	-0.381897
H	0.735161	3.506261	-1.303020

H	0.582238	2.066261	3.261325
H	2.095785	3.615620	1.441856
H	-0.964915	3.459982	1.182157
H	-1.879292	0.687397	1.551758
H	2.903475	0.999618	1.964187
H	3.309954	1.812086	-0.644715
H	0.990358	0.512838	-2.255709
H	-1.610347	1.539898	-1.132222
H	2.252387	-0.986612	0.135637

24

2-S^--*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -729.943177

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.798197
B	1.513208	0.000000	0.698948
B	1.240129	0.831651	-0.837415
B	-0.416773	1.456862	-0.778285
B	-1.130730	0.994084	0.785723
C	1.363521	1.170987	1.875583
B	2.161400	1.622983	0.429575
B	0.953173	2.545579	-0.483607
B	-0.518160	2.645004	0.523961
B	-0.210239	1.784333	2.051672
B	1.076500	2.739603	1.275833
S	-0.333334	-1.341817	2.878013
H	-0.354209	-0.925148	-0.424118
H	1.265290	3.399594	-1.243572
H	-0.606518	2.122116	3.110866
H	1.526952	3.674104	1.846104
H	-1.251511	3.575207	0.476446
H	-2.271263	0.692565	0.821206
H	1.963623	1.065726	2.764403
H	3.332797	1.788972	0.430542
H	1.686812	0.375258	-1.833353
H	-1.088756	1.427058	-1.752417

H 2.193708 -0.954666 0.800269

26

4-NH_2-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -387.6333104

C 0.000000 0.000000 0.000000
B 0.000000 0.000000 1.679205
B 1.513246 0.000000 0.724539
B 1.301323 0.931163 -0.783444
B -0.402309 1.487221 -0.715656
B -1.193886 0.922239 0.778397
C 1.259483 1.091404 1.988148
B 2.106017 1.661228 0.626576
B 0.904209 2.603727 -0.276299
B -0.614806 2.600697 0.651975
B -0.349043 1.662945 2.140995
B 0.940229 2.693814 1.490054
N 1.893399 0.450070 -2.012570
H -0.293861 -0.903080 -0.510255
H 1.224706 3.507152 -0.966882
H -0.796726 1.869619 3.210897
H 1.345670 3.589851 2.140153
H -1.374136 3.504242 0.626686
H -0.212701 -0.949652 2.339508
H -2.315095 0.559766 0.770435
H 1.821561 0.940225 2.895321
H 3.266145 1.859919 0.702373
H -1.020586 1.492427 -1.721111
H 2.196801 -0.953939 0.816222
H 1.675110 0.930378 -2.869294
H 2.849419 0.136761 -2.004162

26

4-PH_2-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -674.2119879

C 0.000000 0.000000 0.000000
B 0.000000 0.000000 1.687001

B	1.514404	0.000000	0.738932
B	1.259225	0.914886	-0.752291
B	-0.430726	1.485870	-0.712727
B	-1.205204	0.916521	0.786126
C	1.247634	1.098545	1.995822
B	2.090174	1.665093	0.622844
B	0.883871	2.595754	-0.281460
B	-0.635889	2.595297	0.657301
B	-0.360702	1.662610	2.145841
B	0.926287	2.696232	1.487670
P	2.030177	0.236998	-2.414863
H	-0.301321	-0.909658	-0.494818
H	1.198362	3.497897	-0.974308
H	-0.811550	1.868741	3.214461
H	1.328102	3.597519	2.132071
H	-1.395482	3.498008	0.630460
H	-0.213564	-0.951485	2.343680
H	-2.320881	0.538529	0.783480
H	1.813172	0.953651	2.902201
H	3.249163	1.865313	0.692308
H	-1.054473	1.486114	-1.713562
H	2.199973	-0.951285	0.836916
H	1.886837	1.429634	-3.168122
H	3.389835	0.479420	-2.089148

27

4-CH_3-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -371.5653312

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.689790
B	1.512238	0.000000	0.743982
B	1.256912	0.906510	-0.763313
B	-0.436874	1.489878	-0.703210
B	-1.205903	0.919998	0.793110
C	1.248222	1.096225	1.998728
B	2.089052	1.654628	0.619691

B	0.881052	2.589352	-0.282978
B	-0.634180	2.596510	0.665248
B	-0.355998	1.663646	2.150944
B	0.932996	2.693360	1.484632
C	1.929967	0.420241	-2.112791
H	-0.311195	-0.910771	-0.486764
H	1.199064	3.491449	-0.975939
H	-0.802682	1.870278	3.221390
H	1.338967	3.594478	2.127142
H	-1.392427	3.500887	0.641913
H	-0.216287	-0.950749	2.347335
H	-2.321599	0.540763	0.794619
H	1.814931	0.952716	2.904380
H	3.248110	1.860271	0.686165
H	-1.060430	1.489050	-1.704388
H	2.196982	-0.952316	0.837071
H	1.220489	0.414378	-2.941328
H	2.744736	1.088834	-2.394872
H	2.353433	-0.582595	-2.033016

27

4-SiH_3-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -622.9478243

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.688986
B	1.514320	0.000000	0.741116
B	1.253384	0.913112	-0.749015
B	-0.436937	1.486786	-0.709228
B	-1.208206	0.915285	0.789427
C	1.243107	1.098765	2.000826
B	2.084890	1.664094	0.626155
B	0.879232	2.594316	-0.278778
B	-0.641808	2.594242	0.662423
B	-0.364280	1.662516	2.149670
B	0.922941	2.696178	1.490889
Si	2.113202	0.304961	-2.465948

H	-1.065655	1.489721	-1.707019
H	-0.815883	1.865558	3.218796
H	-0.214636	-0.952363	2.344259
H	-1.402186	3.496285	0.635357
H	1.191163	3.499168	-0.970000
H	-2.322591	0.533260	0.786511
H	1.324716	3.597741	2.134924
H	3.243328	1.867816	0.697615
H	2.199690	-0.950358	0.846283
H	-0.307939	-0.911179	-0.487425
H	1.809408	0.954101	2.906789
H	3.591232	0.222028	-2.332489
H	1.619078	-1.049878	-2.840343
H	1.800839	1.225974	-3.588204

25

4-OH-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -407.5216812

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.681365
B	1.516890	0.000000	0.738362
B	1.285362	0.924409	-0.769196
B	-0.419065	1.487482	-0.707403
B	-1.201584	0.922474	0.785021
C	1.253638	1.095238	1.994194
B	2.105027	1.658269	0.629987
B	0.896480	2.597182	-0.280894
B	-0.623922	2.599630	0.654846
B	-0.351449	1.664575	2.142506
B	0.938473	2.694551	1.484768
O	1.903237	0.451388	-1.921967
H	1.341544	3.595041	2.129600
H	2.198840	-0.953963	0.823647
H	-0.799769	1.872952	3.211530
H	1.216950	3.496822	-0.976707
H	-1.380326	3.505244	0.628505

H	3.263480	1.860973	0.698317
H	-1.027708	1.487314	-1.719571
H	-2.320091	0.552235	0.781821
H	-0.215642	-0.948845	2.341377
H	1.814142	0.948428	2.903059
H	-0.296029	-0.907151	-0.502619
H	1.612084	0.885778	-2.726096

25

4-SH-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -730.4739205

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.683546
B	1.517596	0.000000	0.738149
B	1.269511	0.921947	-0.751553
B	-0.421687	1.488526	-0.712995
B	-1.200722	0.919749	0.784846
C	1.252993	1.096333	1.995096
B	2.099396	1.665970	0.628142
B	0.894761	2.599860	-0.280064
B	-0.626546	2.598538	0.655166
B	-0.354562	1.663086	2.144277
B	0.932759	2.696310	1.489862
S	2.120456	0.314889	-2.288223
H	1.335776	3.595906	2.135555
H	2.201295	-0.952178	0.828521
H	-0.804523	1.868913	3.213129
H	1.213694	3.499508	-0.973585
H	-1.384931	3.502089	0.626995
H	3.258190	1.863425	0.694779
H	-1.039718	1.490896	-1.716902
H	-2.318158	0.547327	0.778021
H	-0.214375	-0.951255	2.340129
H	1.815630	0.947881	2.902548
H	-0.294736	-0.906029	-0.504441
H	1.369258	1.003514	-3.164698

24

4-Cl-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -791.8957601

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.689728
B	1.516221	0.000000	0.751425
B	1.247809	0.918792	-0.740579
B	-0.440019	1.493671	-0.707210
B	-1.205458	0.917282	0.789582
C	1.248312	1.098015	1.999180
B	2.094687	1.662945	0.624698
B	0.880657	2.598607	-0.282848
B	-0.636532	2.596854	0.663071
B	-0.357172	1.663230	2.148016
B	0.930666	2.696416	1.484402
Cl	2.013825	0.358768	-2.262827
H	-0.297188	-0.907632	-0.500666
H	1.201175	3.493526	-0.980695
H	-0.805241	1.869901	3.217217
H	1.334816	3.597399	2.127134
H	-1.395201	3.499945	0.638991
H	-0.214941	-0.951901	2.345002
H	-2.320461	0.538158	0.786469
H	1.813431	0.955017	2.905952
H	3.253146	1.863300	0.683469
H	-1.051212	1.489343	-1.713751
H	2.205162	-0.948222	0.831149

24

4-O^--*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -406.9643259

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.666815
B	1.510022	0.000000	0.672273
B	1.634203	1.131522	-1.008285
B	-0.324054	1.466978	-0.727962

B	-1.173970	0.941675	0.764675
C	1.263924	1.059437	1.981012
B	2.170877	1.620650	0.640389
B	0.958121	2.617759	-0.292083
B	-0.567950	2.592519	0.630741
B	-0.319965	1.670742	2.129304
B	0.995911	2.668767	1.468810
O	2.172579	0.717000	-2.067823
H	-0.323857	-0.903016	-0.494386
H	1.252376	3.597937	-0.893263
H	-0.759885	1.910205	3.201528
H	1.399913	3.563898	2.131918
H	-1.297411	3.528748	0.611909
H	-0.227238	-0.936791	2.351501
H	-2.314647	0.619445	0.766076
H	1.824278	0.910506	2.889912
H	3.318548	1.849568	0.826591
H	-0.971741	1.503688	-1.721342
H	2.166720	-0.975420	0.813410

24

4-S$^-$-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -729.9316774

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.681854
B	1.512930	0.000000	0.709159
B	1.372389	0.925955	-0.872028
B	-0.393728	1.476797	-0.712855
B	-1.194206	0.922522	0.786233
C	1.246411	1.083207	1.995560
B	2.111029	1.638442	0.617888
B	0.905146	2.589568	-0.284399
B	-0.613359	2.589544	0.660386
B	-0.352448	1.659331	2.151385
B	0.947653	2.677375	1.482403
S	2.129416	0.353522	-2.357072

H	-0.300019	-0.903432	-0.505133
H	1.207488	3.527484	-0.939125
H	-0.799479	1.874361	3.224944
H	1.354148	3.577763	2.134853
H	-1.368352	3.503334	0.637764
H	-0.215325	-0.950761	2.347387
H	-2.321522	0.563328	0.784007
H	1.814005	0.932031	2.899507
H	3.265794	1.854523	0.741888
H	-1.046712	1.499381	-1.696733
H	2.183325	-0.959480	0.846854

26

5-NH_2-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -387.6337762

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.679714
B	1.509229	0.000000	0.737340
B	1.218417	0.925266	-0.738375
B	-0.470260	1.538130	-0.753122
B	-1.198266	0.925264	0.770627
C	1.246038	1.095762	1.995565
B	2.083526	1.664792	0.613281
B	0.879603	2.608477	-0.276114
B	-0.634203	2.608473	0.669134
B	-0.363586	1.664772	2.141264
B	0.931978	2.693593	1.492602
N	-1.237406	1.520035	-1.981744
H	-0.317155	-0.896599	-0.507914
H	1.200399	3.513532	-0.964582
H	-0.815582	1.863383	3.211274
H	1.336406	3.591925	2.140326
H	-1.393619	3.513523	0.655156
H	-0.228017	-0.945234	2.341374
H	-2.316544	0.549943	0.768523
H	1.811528	0.950286	2.901227

H	3.243342	1.863415	0.676870
H	1.707409	0.549961	-1.744084
H	2.203818	-0.945239	0.822919
H	-2.195203	1.827878	-1.950142
H	-0.788570	1.827922	-2.828439

26

5-PH_2-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -674.212252

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.686058
B	1.513272	0.000000	0.743396
B	1.233453	0.918357	-0.737917
B	-0.452229	1.499307	-0.726161
B	-1.206091	0.918340	0.781714
C	1.244512	1.098035	1.997865
B	2.085581	1.664307	0.619062
B	0.875858	2.598888	-0.281103
B	-0.638453	2.598909	0.662191
B	-0.363802	1.664296	2.144797
B	0.927198	2.695240	1.488384
P	-1.485589	1.426573	-2.384093
H	-0.309042	-0.906348	-0.496272
H	1.192160	3.500241	-0.974146
H	-0.816884	1.867777	3.213053
H	1.328694	3.596509	2.133125
H	-1.399979	3.500239	0.640547
H	-0.222001	-0.949237	2.343230
H	-2.321477	0.537151	0.785062
H	1.809445	0.955083	2.904687
H	3.244197	1.867573	0.683438
H	1.728290	0.536892	-1.737430
H	2.201207	-0.949166	0.833774
H	-2.479412	2.367766	-2.012239
H	-0.714658	2.368435	-3.112384

27

5-CH_3-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -371.5654948

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.691314
B	1.515407	0.000000	0.749817
B	1.238981	0.914992	-0.728816
B	-0.459136	1.493652	-0.736749
B	-1.203635	0.915265	0.788418
C	1.243521	1.098885	2.002653
B	2.085665	1.662244	0.626435
B	0.874328	2.590295	-0.283352
B	-0.642755	2.589688	0.661075
B	-0.363325	1.661800	2.148911
B	0.921396	2.694997	1.484909
C	-1.299316	1.526790	-2.079744
H	-0.302842	-0.913978	-0.486262
H	1.190211	3.494457	-0.974632
H	-0.815071	1.867347	3.217612
H	1.321083	3.598635	2.127874
H	-1.402819	3.493445	0.636924
H	-0.218373	-0.951060	2.347713
H	-2.318871	0.532655	0.788066
H	1.807717	0.958449	2.910264
H	3.243583	1.869622	0.694722
H	1.732412	0.534783	-1.729831
H	2.201176	-0.950618	0.845163
H	-2.142742	0.834155	-2.058484
H	-1.711658	2.523689	-2.243239
H	-0.693335	1.282929	-2.953521

27

5-SiH_3-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -622.9477011

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.688722
B	1.514941	0.000000	0.746068

B	1.236722	0.916505	-0.736927
B	-0.451103	1.493925	-0.724973
B	-1.207469	0.916512	0.783950
C	1.243983	1.098558	1.999263
B	2.086920	1.662801	0.622388
B	0.876214	2.595563	-0.280880
B	-0.639111	2.595530	0.662005
B	-0.363636	1.662830	2.147198
B	0.925973	2.694593	1.488148
Si	-1.515222	1.534167	-2.434981
H	1.327301	3.595671	2.133166
H	1.738445	0.533967	-1.732744
H	2.200900	-0.950469	0.837979
H	-0.815779	1.867608	3.215583
H	1.195004	3.497691	-0.972272
H	-1.400231	3.497645	0.642549
H	3.245133	1.867622	0.688753
H	-2.322499	0.533993	0.794068
H	-0.220556	-0.950505	2.344676
H	1.808603	0.956069	2.906666
H	-0.303868	-0.912114	-0.488323
H	-1.802303	0.146557	-2.897867
H	-2.818754	2.223813	-2.252561
H	-0.776455	2.225248	-3.523428

25

5-OH-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -407.5219047

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.682350
B	1.516733	0.000000	0.744609
B	1.232366	0.916647	-0.729545
B	-0.467574	1.518674	-0.736179
B	-1.203990	0.924301	0.787842
C	1.248453	1.098285	1.997602
B	2.086473	1.663553	0.616746

B	0.875471	2.598971	-0.282052
B	-0.641471	2.603599	0.673294
B	-0.357107	1.664444	2.148963
B	0.927854	2.697061	1.486660
O	-1.245575	1.511847	-1.890275
H	-0.804937	1.864022	3.220232
H	-0.221583	-0.947508	2.342424
H	1.709915	0.543874	-1.741942
H	-1.399569	3.507734	0.650276
H	1.190155	3.501347	-0.977490
H	-2.319335	0.545422	0.778854
H	1.333816	3.598868	2.127966
H	3.244767	1.870214	0.678823
H	2.205627	-0.948481	0.837581
H	-0.314694	-0.902297	-0.499992
H	1.813904	0.955216	2.903613
H	-0.790903	1.832937	-2.671255

25

5-SH-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -730.4741848

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.682656
B	1.513214	0.000000	0.742557
B	1.230673	0.919920	-0.737529
B	-0.453098	1.512013	-0.724626
B	-1.205539	0.923824	0.780638
C	1.245356	1.096854	1.996682
B	2.085908	1.664083	0.615993
B	0.877898	2.603986	-0.280009
B	-0.636265	2.606571	0.668748
B	-0.361002	1.664878	2.145519
B	0.930717	2.694005	1.490960
S	-1.503371	1.543287	-2.259682
H	-0.812351	1.865457	3.214828
H	-0.226700	-0.947505	2.340527

H	1.720300	0.543068	-1.740816
H	-1.395899	3.508242	0.645218
H	1.194336	3.505364	-0.972534
H	-2.321204	0.545560	0.778111
H	1.336151	3.593767	2.135025
H	3.244753	1.865921	0.678644
H	2.201279	-0.949255	0.829776
H	-0.315814	-0.899464	-0.503584
H	1.810771	0.952501	2.902892
H	-0.498100	1.683989	-3.140906

24

5-Cl-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -791.8966493

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.689655
B	1.515718	0.000000	0.746791
B	1.246717	0.918454	-0.731346
B	-0.442863	1.497961	-0.711935
B	-1.207061	0.918470	0.795069
C	1.244616	1.097958	2.000708
B	2.088468	1.662947	0.626567
B	0.881775	2.598994	-0.281424
B	-0.642092	2.599039	0.666560
B	-0.360934	1.662958	2.150299
B	0.924772	2.695610	1.486534
Cl	-1.390921	1.524131	-2.235993
H	-0.311525	-0.902719	-0.500813
H	1.190711	3.499428	-0.977209
H	-0.811649	1.868441	3.218758
H	1.324806	3.598246	2.129498
H	-1.402738	3.499499	0.636173
H	-0.221258	-0.950925	2.344157
H	-2.322513	0.543129	0.780933
H	1.808962	0.956273	2.907909
H	3.246124	1.868337	0.694488

H	1.726969	0.543079	-1.738206
H	2.200531	-0.950983	0.837602

24

5-O^--*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -406.962792

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.669913
B	1.506483	0.000000	0.720459
B	1.157818	0.936780	-0.749119
B	-0.614628	1.969203	-0.975458
B	-1.175287	0.936810	0.721318
C	1.251765	1.100049	1.986147
B	2.070814	1.644903	0.588970
B	0.900076	2.637638	-0.299025
B	-0.658032	2.637655	0.682933
B	-0.362023	1.644926	2.122240
B	0.923061	2.696558	1.464539
O	-1.283428	1.978188	-2.036571
H	-0.306451	-0.913814	-0.486253
H	1.311598	3.577592	-0.897378
H	-0.798127	1.873284	3.200282
H	1.338006	3.590250	2.122949
H	-1.375363	3.577619	0.796031
H	-0.213825	-0.936341	2.361676
H	-2.298747	0.557027	0.762156
H	1.822023	0.972995	2.890972
H	3.231532	1.873158	0.660672
H	1.679391	0.556910	-1.744974
H	2.222820	-0.936339	0.825946

24

5-S^--*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -729.9285172

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.683898
B	1.510420	0.000000	0.744431

B	1.210549	0.920117	-0.734722
B	-0.526752	1.577014	-0.846146
B	-1.194717	0.919790	0.760916
C	1.249392	1.090201	2.009290
B	2.077210	1.654171	0.621771
B	0.876164	2.596764	-0.286865
B	-0.645353	2.596262	0.659427
B	-0.361555	1.653921	2.138306
B	0.920489	2.688808	1.481148
S	-1.456589	1.585260	-2.342008
H	-0.312372	-0.901163	-0.502113
H	1.232568	3.515634	-0.942075
H	-0.813301	1.861672	3.212460
H	1.325564	3.591509	2.131952
H	-1.390936	3.514921	0.689372
H	-0.222159	-0.946900	2.353909
H	-2.310057	0.534384	0.800061
H	1.813422	0.951117	2.916534
H	3.240227	1.862947	0.691389
H	1.738695	0.535695	-1.718255
H	2.209229	-0.947055	0.841719

26

9-NH_2-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -387.6272971

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.687260
B	1.518531	0.000000	0.742352
B	1.243255	0.916488	-0.736534
B	-0.433934	1.482732	-0.714283
B	-1.201578	0.923090	0.783405
C	1.245670	1.089778	2.004197
B	2.092016	1.658846	0.631064
B	0.900079	2.627303	-0.308553
B	-0.619424	2.596780	0.652195
B	-0.354651	1.667711	2.143942

B	0.941755	2.686338	1.492732
N	1.251769	3.731894	-1.201846
H	-0.304336	-0.910738	-0.489958
H	-0.810890	1.878410	3.209784
H	1.342737	3.590861	2.135277
H	-1.371888	3.507849	0.627007
H	-0.221920	-0.949925	2.343348
H	-2.319555	0.550897	0.786457
H	1.808269	0.940824	2.911684
H	3.252626	1.859742	0.694882
H	1.744438	0.535149	-1.733201
H	-1.053777	1.489033	-1.716420
H	2.201456	-0.952768	0.836605
H	0.894685	4.645210	-0.972311
H	2.206447	3.803417	-1.514590

26

9-PH_2-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -674.2113242

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.689265
B	1.516601	0.000000	0.745888
B	1.243333	0.918719	-0.734889
B	-0.439620	1.486599	-0.707833
B	-1.206291	0.917239	0.789887
C	1.245683	1.095225	2.001357
B	2.090231	1.662168	0.626305
B	0.886717	2.605325	-0.292679
B	-0.634328	2.595427	0.657488
B	-0.358249	1.666262	2.146627
B	0.932075	2.694298	1.484284
P	1.318794	4.086259	-1.505307
H	-0.304452	-0.909624	-0.492043
H	-0.809428	1.877165	3.214185
H	1.333572	3.596731	2.127332
H	-1.392742	3.499911	0.633134

H	-0.218618	-0.950094	2.346317
H	-2.322348	0.540475	0.790245
H	1.810204	0.953656	2.908904
H	3.248468	1.866349	0.694418
H	1.737312	0.536788	-1.734374
H	-1.058171	1.489807	-1.710704
H	2.202641	-0.950291	0.838578
H	1.494752	5.083705	-0.509789
H	2.711423	3.830150	-1.623171

27

9-CH_3-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -371.5636369

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.689464
B	1.514750	0.000000	0.745221
B	1.239299	0.916960	-0.734924
B	-0.438044	1.489880	-0.707381
B	-1.207237	0.917829	0.790320
C	1.245607	1.098810	1.998255
B	2.085432	1.663396	0.622483
B	0.885892	2.619520	-0.303189
B	-0.636972	2.592513	0.660962
B	-0.361604	1.663801	2.146924
B	0.926386	2.693522	1.481495
C	1.302315	3.840642	-1.234249
H	-0.305474	-0.909912	-0.490811
H	-0.810423	1.872015	3.216339
H	1.326594	3.597777	2.124667
H	-1.396925	3.496645	0.637533
H	-0.216024	-0.950660	2.346858
H	-2.322672	0.538033	0.790333
H	1.811281	0.957416	2.904989
H	3.244722	1.868042	0.688313
H	1.734288	0.535598	-1.734782
H	-1.062574	1.490147	-1.708117

H	2.201860	-0.949737	0.839157
H	2.256834	3.668278	-1.734502
H	0.559448	4.022752	-2.012583
H	1.400912	4.765013	-0.662729

27

9-SiH_3-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -622.9484866

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.688728
B	1.516827	0.000000	0.741977
B	1.241774	0.918898	-0.738615
B	-0.439781	1.491076	-0.709019
B	-1.207079	0.918749	0.789461
C	1.246647	1.096595	1.997259
B	2.089056	1.664193	0.618773
B	0.883818	2.606634	-0.294111
B	-0.635508	2.595950	0.660108
B	-0.359411	1.664369	2.147531
B	0.928574	2.694694	1.483188
Si	1.401293	4.157671	-1.468710
H	-1.063899	1.488522	-1.708817
H	-0.806619	1.874890	3.216669
H	-0.215793	-0.951009	2.345585
H	1.730521	0.533713	-1.739172
H	-1.397766	3.497335	0.641008
H	-2.322799	0.541207	0.787579
H	1.331082	3.595249	2.128263
H	3.247338	1.867975	0.690885
H	2.203070	-0.950012	0.835218
H	-0.306514	-0.908062	-0.493353
H	1.813625	0.956894	2.903318
H	0.385530	4.395545	-2.528558
H	1.528470	5.412991	-0.681549
H	2.704729	3.927084	-2.148235

25

9-OH-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= !!!!!!!!!

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.687118
B	1.515484	0.000000	0.741969
B	1.240220	0.909667	-0.736950
B	-0.436934	1.486106	-0.709158
B	-1.206310	0.923407	0.789763
C	1.246550	1.097398	1.998763
B	2.090309	1.660806	0.623129
B	0.889598	2.623737	-0.300001
B	-0.630497	2.593524	0.667056
B	-0.359348	1.661386	2.150604
B	0.933102	2.689984	1.496202
O	1.320616	3.679573	-1.116342
H	1.333790	3.596158	2.134742
H	1.735788	0.537394	-1.738653
H	2.199045	-0.951663	0.839503
H	-0.810751	1.866573	3.219368
H	-1.382391	3.505581	0.633332
H	3.248379	1.867096	0.685132
H	-1.061587	1.497329	-1.709778
H	-2.322400	0.545804	0.790171
H	-0.216434	-0.951025	2.343089
H	1.812792	0.950984	2.904341
H	-0.307969	-0.909704	-0.489610
H	0.624812	4.289024	-1.367641

25

9-SH-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -730.4721696

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.689557
B	1.518128	0.000000	0.747966
B	1.245275	0.915841	-0.733782
B	-0.440949	1.482733	-0.711550

B	-1.205908	0.915417	0.788002
C	1.243787	1.095393	2.003124
B	2.091835	1.659283	0.631508
B	0.885567	2.603706	-0.293411
B	-0.633826	2.593252	0.653595
B	-0.359609	1.668048	2.144098
B	0.933045	2.694004	1.485443
S	1.422784	3.991245	-1.430074
H	1.332761	3.600475	2.123053
H	1.742624	0.539882	-1.733074
H	2.203039	-0.950787	0.841667
H	-0.814074	1.881140	3.209701
H	-1.388345	3.500577	0.624867
H	3.248493	1.869700	0.694184
H	-1.055392	1.487192	-1.716154
H	-2.322474	0.540486	0.788757
H	-0.220124	-0.948851	2.347403
H	1.806318	0.954952	2.912038
H	-0.302144	-0.910468	-0.491920
H	0.664406	4.951798	-0.875376

24

9-Cl-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -791.8956091

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.689964
B	1.515131	0.000000	0.747135
B	1.239682	0.912344	-0.734879
B	-0.447180	1.486255	-0.708740
B	-1.210606	0.914536	0.791912
C	1.243966	1.101331	1.999116
B	2.086784	1.662333	0.626473
B	0.872562	2.599259	-0.284948
B	-0.648070	2.591448	0.665555
B	-0.365952	1.662360	2.149360
B	0.920575	2.697203	1.489364

Cl	1.351351	3.979685	-1.343368
H	-0.304244	-0.909697	-0.492044
H	-0.814607	1.870142	3.218223
H	1.321849	3.605790	2.121926
H	-1.399304	3.499717	0.632641
H	-0.214267	-0.950594	2.346985
H	-2.324813	0.533123	0.791207
H	1.810167	0.962285	2.905926
H	3.241860	1.881217	0.683880
H	1.734675	0.546814	-1.738264
H	-1.063779	1.493671	-1.711954
H	2.203922	-0.947799	0.840675

24

9-O^--*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -406.9409445

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.691449
B	1.508644	0.000000	0.740118
B	1.238088	0.908258	-0.744425
B	-0.423255	1.498702	-0.719641
B	-1.196368	0.935027	0.790950
C	1.255025	1.093895	1.990266
B	2.095797	1.655821	0.615732
B	0.946667	2.758305	-0.421526
B	-0.626884	2.597337	0.659177
B	-0.349755	1.672938	2.133513
B	0.952581	2.697899	1.462185
O	1.299313	3.733340	-1.179807
H	-0.315534	-0.910726	-0.483343
H	-0.793264	1.879083	3.212334
H	1.348936	3.576825	2.151418
H	-1.405633	3.491744	0.658637
H	-0.221460	-0.951321	2.353979
H	-2.316907	0.551076	0.796124
H	1.817161	0.948156	2.898761

H	3.266531	1.810699	0.706141
H	1.730805	0.472176	-1.729231
H	-1.082205	1.457839	-1.703901
H	2.188049	-0.961531	0.840188

24

9-S^--*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -729.9172863

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.689932
B	1.508950	0.000000	0.737105
B	1.240877	0.915126	-0.748898
B	-0.420269	1.504236	-0.722722
B	-1.193520	0.933191	0.786299
C	1.254237	1.092938	1.986615
B	2.095864	1.659973	0.605420
B	0.933781	2.689839	-0.379172
B	-0.618969	2.601168	0.649713
B	-0.344705	1.672925	2.130955
B	0.953152	2.700991	1.452686
S	1.435488	4.034799	-1.435952
H	-0.313961	-0.907797	-0.489651
H	-0.789169	1.886904	3.206416
H	1.356263	3.583881	2.126941
H	-1.390149	3.497899	0.643256
H	-0.222397	-0.950137	2.352922
H	-2.315393	0.557207	0.789020
H	1.821496	0.952844	2.892716
H	3.261630	1.827955	0.692903
H	1.726846	0.490657	-1.738111
H	-1.067090	1.472451	-1.711270
H	2.192082	-0.957912	0.832973

26

1-NH_2-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -387.5973511

C	0.000000	0.000000	0.000000

B	0.000000	0.000000	1.713713
B	1.526156	0.000000	0.786460
B	1.280990	0.945486	-0.689006
B	-0.409390	1.506562	-0.680764
B	-1.196324	0.950359	0.815762
B	1.325903	1.067736	2.167435
B	2.109577	1.663161	0.683780
B	0.910270	2.596858	-0.236767
B	-0.612690	2.600346	0.690695
B	-0.350061	1.667213	2.179053
C	0.904831	2.567874	1.467746
N	-0.458234	-1.184906	-0.653154
H	2.186961	-0.977097	0.755461
H	-0.841288	2.012812	3.192265
H	1.233759	3.565151	-0.824369
H	-1.277796	3.572250	0.707782
H	1.218500	3.462694	1.979901
H	1.769502	0.589540	-1.701228
H	3.237384	2.002445	0.710221
H	-1.019809	1.541083	-1.689259
H	-2.320379	0.604124	0.788466
H	-0.329578	-0.970572	2.293821
H	1.937519	1.021852	3.172996
H	-0.553016	-1.056177	-1.650423
H	0.144327	-1.975053	-0.471938

26

1-PH_2-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -371.5578679

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.717743
B	1.519198	0.000000	0.787881
B	1.261191	0.941227	-0.698778
B	-0.422631	1.506989	-0.696481
B	-1.201033	0.931913	0.799105
B	1.313879	1.083664	2.164674

B	2.091640	1.664947	0.671861
B	0.888333	2.600155	-0.246561
B	-0.634349	2.593801	0.675556
B	-0.367414	1.663012	2.168784
C	0.881522	2.570854	1.454223
P	-0.481437	-1.530426	-0.975392
H	-2.327539	0.588681	0.781399
H	1.214889	3.567101	-0.834267
H	1.927541	1.048118	3.169387
H	3.216845	2.012128	0.693727
H	1.189073	3.469777	1.963873
H	-0.326842	-0.964071	2.310072
H	-0.869168	2.010284	3.176299
H	2.198271	-0.962921	0.767510
H	1.761153	0.594263	-1.706815
H	-1.033900	1.541918	-1.703537
H	-1.310703	3.557827	0.696094
H	-0.106361	-2.475191	0.013809
H	-1.846198	-1.544221	-0.589570

27

1-CH_3-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -371.5578679

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.713324
B	1.520507	0.000000	0.797404
B	1.262919	0.932068	-0.689781
B	-0.415125	1.514600	-0.689588
B	-1.194740	0.940632	0.796639
B	1.315551	1.080629	2.171370
B	2.097994	1.658628	0.681379
B	0.900330	2.597133	-0.240518
B	-0.622085	2.601535	0.681342
B	-0.365606	1.662733	2.171470
C	0.890336	2.569451	1.462674
C	-0.439388	-1.266804	-0.720848

H	2.191067	-0.969127	0.774892
H	-0.867339	2.009839	3.179095
H	1.234434	3.562192	-0.827529
H	-1.293456	3.569166	0.703133
H	1.201223	3.466391	1.973274
H	1.763692	0.584027	-1.698400
H	3.224240	2.003082	0.703767
H	-1.023901	1.551492	-1.698125
H	-2.321134	0.594757	0.773865
H	-0.334741	-0.966019	2.299908
H	1.924428	1.042857	3.179048
H	-0.465467	-1.105569	-1.796458
H	0.249366	-2.083091	-0.513407
H	-1.433418	-1.566388	-0.395424

27

1-SiH_3-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -622.9525986

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.715092
B	1.521272	0.000000	0.792667
B	1.262465	0.935606	-0.696705
B	-0.421594	1.507349	-0.695877
B	-1.200645	0.935662	0.797026
B	1.314545	1.084543	2.166951
B	2.093650	1.663141	0.674627
B	0.891169	2.597473	-0.247960
B	-0.631109	2.597616	0.675159
B	-0.368933	1.663413	2.168105
C	0.882595	2.569866	1.454518
Si	-0.544488	-1.588391	-0.897817
H	-1.032605	1.549366	-1.703549
H	3.218738	2.011139	0.696301
H	-0.869670	2.011742	3.175730
H	1.924979	1.051266	3.173746
H	1.191309	3.468900	1.963528

H	-2.328589	0.596231	0.781087
H	-1.304703	3.563632	0.695771
H	-0.328262	-0.962329	2.311464
H	2.201412	-0.962578	0.777136
H	1.769325	0.595577	-1.704295
H	1.220878	3.563398	-0.835868
H	-2.021318	-1.609549	-0.982656
H	0.040332	-1.596373	-2.256784
H	-0.063933	-2.760026	-0.132753

25

1-OH-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -407.4685537

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.704981
B	1.530873	0.000000	0.789825
B	1.262690	0.923340	-0.703895
B	-0.428792	1.498369	-0.701774
B	-1.208644	0.939821	0.796272
B	1.315852	1.080567	2.159097
B	2.092988	1.660836	0.667620
B	0.887205	2.583355	-0.260002
B	-0.631224	2.593203	0.669651
B	-0.370035	1.661652	2.161798
C	0.882599	2.566543	1.446970
O	-0.396089	-1.128803	-0.695552
H	-2.327891	0.575294	0.770966
H	1.215192	3.547748	-0.850748
H	1.922177	1.045362	3.168089
H	3.217036	2.011655	0.686014
H	1.191805	3.466491	1.952948
H	-0.333192	-0.979026	2.274694
H	-0.866211	2.006396	3.172690
H	2.189604	-0.976287	0.764863
H	1.752365	0.561982	-1.710809
H	-1.039157	1.516158	-1.707466

H -1.301516 3.561330 0.686309
H -0.517403 -1.858377 -0.078535

25

1-SH-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -730.4413275

C 0.000000 0.000000 0.000000
B 0.000000 0.000000 1.726646
B 1.515191 0.000000 0.786072
B 1.259116 0.944299 -0.706734
B -0.427193 1.503478 -0.704100
B -1.204828 0.918863 0.796858
B 1.307833 1.088541 2.161853
B 2.082695 1.667619 0.665400
B 0.877747 2.600207 -0.250131
B -0.646511 2.584581 0.668118
B -0.374669 1.661102 2.165667
C 0.869488 2.571770 1.449470
S -0.444455 -1.544714 -0.837603
H 1.757677 0.591479 -1.711708
H 1.926239 1.057449 3.163505
H -1.330334 3.543221 0.686087
H -0.880822 2.010134 3.170120
H 1.174261 3.473040 1.956667
H -1.041681 1.529425 -1.708210
H 1.199053 3.568017 -0.839209
H -2.327655 0.564040 0.773028
H -0.324135 -0.969624 2.308234
H 2.191722 -0.963703 0.762758
H 3.207235 2.016195 0.689421
H -1.683005 -1.163330 -1.194669

24

1-Cl-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -791.8462717

C 0.000000 0.000000 0.000000
B 0.000000 0.000000 1.712768

B	1.523339	0.000000	0.780136
B	1.249551	0.918370	-0.727180
B	-0.444251	1.485073	-0.726876
B	-1.216364	0.917584	0.780798
B	1.307266	1.100986	2.138477
B	2.076649	1.666451	0.636135
B	0.864668	2.581108	-0.292520
B	-0.653914	2.580945	0.636541
B	-0.380537	1.665921	2.138986
C	0.862608	2.574603	1.410809
Cl	-0.498377	-1.487120	-0.814982
H	2.195104	-0.965029	0.760925
H	-0.882943	2.020950	3.142828
H	1.184826	3.540691	-0.894896
H	-1.337185	3.539688	0.647484
H	1.166373	3.481722	1.907808
H	1.741585	0.550952	-1.730131
H	3.199617	2.019974	0.648325
H	-1.059006	1.489488	-1.729404
H	-2.334039	0.552362	0.760303
H	-0.322613	-0.966150	2.300543
H	1.922488	1.081337	3.142120

24

1-O^--*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -406.9276741

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.787240
B	1.540974	0.000000	0.904265
B	1.356463	1.038900	-0.524332
B	-0.299531	1.681384	-0.524538
B	-1.137768	1.039386	0.903918
B	1.339127	1.001024	2.338080
B	2.175777	1.641823	0.912331
B	1.040323	2.679214	0.030432
B	-0.498063	2.679498	0.911991

B	-0.313835	1.642068	2.338061
C	0.992343	2.556828	1.731466
O	-0.383255	-0.989528	-0.669639
H	2.218402	-0.969220	0.866177
H	-0.823798	1.954028	3.360916
H	1.427402	3.678202	-0.475341
H	-1.130475	3.678317	0.989797
H	1.321705	3.406329	2.306532
H	1.907051	0.778759	-1.538470
H	3.316480	1.951997	0.991342
H	-0.881160	1.861607	-1.538723
H	-2.291567	0.781391	0.864777
H	-0.375594	-0.969494	2.351426
H	1.925956	0.886981	3.360959

24

1-S$^-$-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -729.9080955

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.743026
B	1.524752	0.000000	0.843063
B	1.302397	0.983248	-0.612472
B	-0.360624	1.591019	-0.612341
B	-1.165421	0.983433	0.843207
B	1.326535	1.048336	2.249035
B	2.131997	1.656422	0.792288
B	0.965841	2.640583	-0.108464
B	-0.560393	2.640880	0.792535
B	-0.337862	1.656353	2.249352
C	0.941112	2.573053	1.594397
S	-0.524908	-1.436385	-0.889801
H	2.210439	-0.958859	0.821949
H	-0.845111	1.986702	3.265905
H	1.324706	3.624796	-0.658325
H	-1.215956	3.624622	0.840697
H	1.260896	3.448128	2.136482

H	1.836511	0.691028	-1.622146
H	3.267633	1.984661	0.841653
H	-0.957383	1.713479	-1.621808
H	-2.308109	0.693744	0.821097
H	-0.349841	-0.959564	2.332060
H	1.927498	0.972922	3.265402

26

2-NH_2-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -387.6369566

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.762017
B	1.504323	0.000000	0.777736
B	1.237799	0.880981	-0.750191
B	-0.444781	1.452406	-0.750181
B	-1.193226	0.916287	0.777772
B	1.323890	1.138677	2.113259
B	2.083219	1.654321	0.592190
B	0.869094	2.558260	-0.351833
B	-0.644527	2.580888	0.592072
B	-0.356462	1.709480	2.113128
C	0.880585	2.592302	1.346864
N	-0.401745	-1.183471	2.495476
H	-1.322355	3.544285	0.587814
H	3.207665	2.005340	0.587955
H	1.191007	3.505689	-0.972678
H	1.192430	3.510342	1.818689
H	2.178744	-0.967248	0.786555
H	1.950551	1.144792	3.111727
H	1.738168	0.497361	-1.745200
H	-1.075343	1.452933	-1.745163
H	-2.317250	0.559959	0.786313
H	-0.849803	2.096259	3.111481
H	-0.314185	-0.925363	-0.455950
H	0.299189	-1.699814	2.999960
H	-1.272872	-1.167193	2.998735

26

2-PH_2-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -674.216683

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.720877
B	1.513142	0.000000	0.772549
B	1.237704	0.896646	-0.744485
B	-0.450786	1.460344	-0.744511
B	-1.209743	0.908987	0.772500
B	1.310345	1.121568	2.118758
B	2.074504	1.664005	0.605354
B	0.857204	2.567662	-0.332868
B	-0.658875	2.576509	0.605270
B	-0.373950	1.683854	2.118661
C	0.862639	2.584149	1.368346
P	-0.541551	-1.622823	2.664159
H	-1.342024	3.535696	0.611064
H	3.196851	2.020475	0.611175
H	1.175840	3.521984	-0.944755
H	1.167717	3.498174	1.852396
H	2.195417	-0.960697	0.766357
H	1.929741	1.120298	3.120420
H	1.735335	0.522154	-1.743819
H	-1.073540	1.459858	-1.743877
H	-2.332306	0.550820	0.766237
H	-0.870010	2.054971	3.120249
H	-0.306148	-0.917076	-0.478419
H	0.540242	-1.665935	3.581185
H	-1.432435	-1.007721	3.581237

27

2-CH_3-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -371.5696614

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.719392
B	1.519701	0.000000	0.760943

B	1.244619	0.885336	-0.756930
B	-0.439826	1.462695	-0.756908
B	-1.200143	0.932253	0.760978
B	1.324307	1.121082	2.100497
B	2.089624	1.655759	0.582937
B	0.878222	2.562243	-0.355327
B	-0.634510	2.589482	0.582971
B	-0.358081	1.697744	2.100494
C	0.885630	2.583785	1.348362
C	-0.433637	-1.265166	2.569388
H	-1.307642	3.556099	0.584760
H	3.214189	2.006199	0.584704
H	1.203413	3.511011	-0.972655
H	1.198718	3.497220	1.828142
H	2.190569	-0.968832	0.763318
H	1.944923	1.123288	3.102427
H	1.733773	0.502988	-1.757966
H	-1.060702	1.460820	-1.757930
H	-2.324278	0.578674	0.763380
H	-0.846842	2.080200	3.102430
H	-0.312903	-0.912890	-0.482205
H	-0.361919	-1.055760	3.637852
H	-1.465061	-1.560146	2.371280
H	0.200028	-2.130814	2.371345

27

2-SiH_3-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -622.95188

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.715168
B	1.517280	0.000000	0.768562
B	1.239904	0.897840	-0.747287
B	-0.447779	1.463882	-0.747302
B	-1.210448	0.914869	0.768538
B	1.312762	1.119795	2.113108
B	2.077970	1.664585	0.600795

B	0.861874	2.569715	-0.336018
B	-0.654062	2.580898	0.600773
B	-0.372089	1.684881	2.113103
C	0.866859	2.584571	1.365529
Si	-0.537819	-1.603564	2.811028
H	-1.335248	3.541513	0.607108
H	3.200616	2.020202	0.607145
H	1.181673	3.523187	-0.948957
H	1.173101	3.497650	1.850590
H	2.204266	-0.956632	0.757262
H	1.932641	1.121043	3.114855
H	1.734686	0.521659	-1.747523
H	-1.069309	1.462108	-1.747547
H	-2.335320	0.565936	0.757208
H	-0.865854	2.059649	3.114850
H	-0.305136	-0.909794	-0.492574
H	-0.435896	-1.299594	4.261967
H	-1.939362	-2.011132	2.525499
H	0.334582	-2.773766	2.525534

25

2-OH-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -407.523931

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.710867
B	1.532558	0.000000	0.749466
B	1.252346	0.880485	-0.760188
B	-0.433204	1.468317	-0.760197
B	-1.200195	0.953037	0.749453
B	1.336431	1.113404	2.094405
B	2.101459	1.650148	0.574956
B	0.892927	2.560368	-0.357152
B	-0.619557	2.599093	0.574941
B	-0.354235	1.703023	2.094400
C	0.898560	2.576561	1.351621
O	-0.402349	-1.153697	2.381748

H	-1.283690	3.571725	0.579222
H	3.226397	1.998862	0.579239
H	1.223905	3.509365	-0.970386
H	1.216098	3.487094	1.833799
H	2.184511	-0.980464	0.765671
H	1.950712	1.108027	3.100951
H	1.734978	0.499610	-1.764693
H	-1.048009	1.470169	-1.764707
H	-2.320467	0.590631	0.765651
H	-0.838638	2.080823	3.100939
H	-0.319278	-0.915508	-0.473248
H	-0.378782	-1.085610	3.337521

25

2-SH-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -730.475101

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.703363
B	1.529287	0.000000	0.756751
B	1.249010	0.894727	-0.749820
B	-0.439111	1.472335	-0.749801
B	-1.208721	0.936838	0.756780
B	1.323490	1.105917	2.107953
B	2.089823	1.658225	0.594730
B	0.878924	2.568746	-0.336069
B	-0.635945	2.590893	0.594741
B	-0.368586	1.684871	2.107975
C	0.880571	2.573545	1.371402
S	-0.523335	-1.529472	2.638548
H	-1.308627	3.557253	0.605124
H	3.213499	2.009943	0.605114
H	1.205359	3.522813	-0.943800
H	1.191345	3.481810	1.862414
H	2.195087	-0.969975	0.758967
H	1.935852	1.095670	3.113941
H	1.737066	0.518910	-1.753291

H	-1.055112	1.474282	-1.753260
H	-2.329171	0.578044	0.759020
H	-0.858864	2.051901	3.113967
H	-0.311060	-0.909075	-0.490800
H	-0.345102	-1.008506	3.863827

24

2-Cl-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -791.9001247

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.709297
B	1.522052	0.000000	0.769678
B	1.244511	0.903494	-0.736339
B	-0.445245	1.472029	-0.736339
B	-1.212506	0.920042	0.769678
B	1.314733	1.104718	2.127884
B	2.079131	1.661703	0.618239
B	0.865523	2.572478	-0.312746
B	-0.651797	2.580560	0.618254
B	-0.379546	1.674774	2.127884
C	0.865414	2.572111	1.392465
Cl	-0.486868	-1.447033	2.650687
H	-1.330546	3.542424	0.629634
H	3.201267	2.017640	0.629621
H	1.187947	3.530777	-0.915490
H	1.171026	3.480443	1.886523
H	2.189140	-0.969264	0.772374
H	1.924484	1.087859	3.134170
H	1.741015	0.534620	-1.738040
H	-1.063746	1.478309	-1.738041
H	-2.329818	0.551139	0.772374
H	-0.875474	2.029930	3.134170
H	-0.307700	-0.914524	-0.481797

24

2-O^--*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -406.966424

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	2.194734
B	1.463806	0.000000	0.792864
B	1.233381	0.866140	-0.761646
B	-0.449572	1.438517	-0.761655
B	-1.160274	0.892449	0.792856
B	1.357637	1.159137	2.119338
B	2.077344	1.635977	0.557105
B	0.866817	2.548649	-0.372156
B	-0.649131	2.563262	0.557063
B	-0.369401	1.746525	2.119327
C	0.879524	2.586046	1.330848
O	-0.341913	-1.005249	2.872202
H	-1.311523	3.544670	0.556173
H	3.200727	2.010051	0.556183
H	1.192959	3.507591	-0.983736
H	1.194817	3.513122	1.782298
H	2.165974	-0.954882	0.791180
H	2.046294	1.270285	3.076652
H	1.749842	0.492432	-1.760680
H	-1.086774	1.457170	-1.760696
H	-2.299023	0.563683	0.791177
H	-0.847505	2.254505	3.076629
H	-0.314109	-0.923581	-0.462434

24

2-S$^-$-*para*-carborane, E(B3LYP/aug-cc-pVTZ)= -729.9350111

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.838961
B	1.508087	0.000000	0.748063
B	1.245975	0.839163	-0.803442
B	-0.426230	1.440554	-0.803504
B	-1.162870	0.960184	0.748089
B	1.364934	1.170005	2.049264
B	2.111915	1.637382	0.494030

B	0.911709	2.535449	-0.465486
B	-0.585667	2.607094	0.494033
B	-0.307319	1.771280	2.049142
C	0.939444	2.612712	1.239941
S	-0.491512	-1.366977	2.840932
H	-1.245754	3.588114	0.470696
H	3.245568	1.973459	0.470647
H	1.245216	3.462979	-1.118020
H	1.272212	3.538444	1.681912
H	2.190848	-0.962000	0.756042
H	2.026647	1.239562	3.024734
H	1.728695	0.418714	-1.797949
H	-1.066078	1.423839	-1.798052
H	-2.301900	0.653229	0.756132
H	-0.773295	2.246403	3.024522
H	-0.334429	-0.930372	-0.429967

28

1,2-NH_2-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -442.948093

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.895371
B	1.428144	0.000000	0.947700
B	1.221341	1.032184	-0.504544
B	-0.482651	1.524523	-0.504550
B	-1.208094	0.761643	0.947669
B	1.221324	1.032219	2.399920
B	1.987800	1.684002	0.947677
B	0.765119	2.648281	0.066270
B	-0.783426	2.484655	0.947688
B	-0.482683	1.524501	2.399914
B	0.765115	2.648309	1.829083
N	-0.348302	-1.205545	2.482167
N	-0.348272	-1.205553	-0.586801
H	-2.281072	0.271387	0.947684
H	1.784317	0.723262	-1.494992
H	1.041346	3.604454	2.465174

H	3.139260	1.946752	0.947658
H	1.041368	3.604412	-0.569837
H	-1.123664	1.563419	3.390363
H	-1.617340	3.321007	0.947688
H	1.784296	0.723317	3.390375
H	2.074343	-0.986942	0.947701
H	-1.123614	1.563446	-1.495008
H	0.391490	-1.678998	2.974375
H	-1.226588	-1.211495	2.974403
H	-1.226615	-1.211556	-1.078937
H	0.391498	-1.678922	-1.079125

26

1,2-OH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -482.683302

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.776301
B	1.466976	0.000000	0.888817
B	1.221492	1.017765	-0.557437
B	-0.488257	1.515016	-0.559933
B	-1.234605	0.798134	0.887450
B	1.221049	1.018242	2.334512
B	1.989401	1.690490	0.888645
B	0.761427	2.637511	0.002332
B	-0.786369	2.495652	0.887817
B	-0.489007	1.514537	2.335642
B	0.760914	2.637561	1.774268
O	-0.292761	-1.187032	-0.596732
O	-0.293835	-1.187196	2.372384
H	2.084325	-0.999357	0.888894
H	-1.118540	1.525134	3.333679
H	1.035841	3.591255	-0.636673
H	-1.616335	3.334990	0.887788
H	1.034750	3.591395	2.413388
H	1.758195	0.697786	-1.555467
H	3.137651	1.962515	0.888805

H	-1.117049	1.525695	-1.558381
H	-2.291833	0.269467	0.887308
H	1.757055	0.698368	3.332961
H	-1.218110	-1.200688	-0.867493
H	-1.216513	-1.195951	2.652322

26

1,2-SH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -1128.626200

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.827995
B	1.453113	0.000000	0.914018
B	1.218687	1.028557	-0.536259
B	-0.487075	1.522873	-0.534577
B	-1.232578	0.772033	0.913993
B	1.218681	1.028574	2.364265
B	1.987903	1.689632	0.913987
B	0.761861	2.646105	0.031329
B	-0.784208	2.491580	0.913977
B	-0.487081	1.522886	2.362556
B	0.761844	2.646143	1.796608
S	-0.508880	-1.482299	2.670176
S	-0.508871	-1.482317	-0.842157
H	-2.305985	0.289060	0.913991
H	1.774975	0.717471	-1.527306
H	1.038349	3.598496	2.437259
H	3.139315	1.950251	0.913977
H	1.038384	3.598437	-0.609346
H	-1.122356	1.554714	3.353384
H	-1.617327	3.327537	0.913962
H	1.774956	0.717475	3.355316
H	2.108291	-0.978882	0.914028
H	-1.122328	1.554699	-1.525419
H	0.724618	-1.993110	2.835049
H	0.724635	-1.993096	-1.007069

25

1-O^-,2-OH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -482.178423

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.905754
B	1.479704	0.000000	1.064333
B	1.297146	1.049210	-0.341404
B	-0.418099	1.615062	-0.341261
B	-1.189145	0.880594	1.064576
B	1.243559	0.923813	2.556688
B	2.058937	1.645971	1.154394
B	0.876428	2.656276	0.287699
B	-0.675057	2.548083	1.154517
B	-0.449493	1.482574	2.556796
B	0.853320	2.585914	2.072127
O	-0.358204	-1.085447	-0.492259
O	-0.405114	-1.227989	2.376622
H	2.083942	-1.014320	1.048013
H	-1.086021	1.500826	3.554225
H	1.200203	3.637763	-0.296090
H	-1.455947	3.441397	1.176152
H	1.158879	3.511686	2.748205
H	1.882149	0.834124	-1.347054
H	3.218120	1.899138	1.176104
H	-1.016294	1.790538	-1.346844
H	-2.278413	0.425142	1.048130
H	1.766223	0.559661	3.553974
H	-0.577754	-1.750794	1.567080

25

1-S^-,2-SH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -1128.118379

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.151952
B	1.377774	0.000000	1.185030
B	1.239146	1.065498	-0.249814
B	-0.497533	1.556283	-0.254763

B	-1.179989	0.719516	1.176630
B	1.203427	1.016128	2.684053
B	1.962143	1.688288	1.246234
B	0.750106	2.662917	0.373036
B	-0.797097	2.463137	1.239238
B	-0.504997	1.492590	2.678375
B	0.738528	2.637429	2.135853
S	-0.396141	-1.432770	-0.794084
S	-0.497856	-1.512994	2.938292
H	2.069076	-0.957616	1.183393
H	-1.168553	1.540155	3.656729
H	1.028536	3.644897	-0.232273
H	-1.636216	3.301391	1.240709
H	1.005444	3.595525	2.782427
H	1.887594	0.880522	-1.219748
H	3.116048	1.963231	1.250959
H	-1.140192	1.735430	-1.229550
H	-2.267972	0.263074	1.173579
H	1.790026	0.711894	3.665875
H	0.712350	-2.099590	2.946727

24

1,2-O^--*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -481.503108

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.124603
B	1.438290	0.000000	1.063346
B	1.299987	1.025304	-0.387692
B	-0.390648	1.608873	-0.387928
B	-1.131781	0.886469	1.063060
B	1.299832	1.025982	2.513827
B	2.087974	1.651121	1.063038
B	0.920504	2.667210	0.176652
B	-0.625214	2.587265	1.062805
B	-0.390569	1.609261	2.513715
B	0.920467	2.667609	1.948813

O	-0.357525	-1.036721	-0.614638
O	-0.357642	-1.036578	2.739892
H	2.086847	-0.994485	1.063225
H	-1.012415	1.767508	3.516736
H	1.251393	3.625652	-0.456131
H	-1.400301	3.497856	1.062327
H	1.251320	3.626368	2.581141
H	1.887263	0.767055	-1.390810
H	3.259601	1.890328	1.062646
H	-1.012105	1.767582	-1.391129
H	-2.255799	0.504066	1.062871
H	1.886752	0.767270	3.517020

24

1,2-S^--*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -1127.474042

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.192474
B	1.368788	0.000000	1.095279
B	1.237453	1.048988	-0.366534
B	-0.475082	1.551159	-0.366698
B	-1.152198	0.739223	1.095045
B	1.237507	1.048953	2.557207
B	1.984443	1.692799	1.095335
B	0.782214	2.668066	0.213344
B	-0.756364	2.496347	1.095198
B	-0.475400	1.551025	2.557132
B	0.782095	2.667944	1.977404
S	-0.422883	-1.442069	3.040296
S	-0.422751	-1.442116	-0.848937
H	-2.257617	0.324532	1.095465
H	1.863876	0.822539	-1.347602
H	1.067172	3.640205	2.607903
H	3.146613	1.961683	1.095608
H	1.067387	3.640332	-0.417099
H	-1.124806	1.699344	3.538207

H	-1.589404	3.350153	1.095503
H	1.864061	0.823198	3.538382
H	2.075483	-0.945782	1.095642
H	-1.124487	1.698636	-1.347867

28

9,12-NH_2-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -443.007131

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.624641
B	1.514844	0.000000	0.827464
B	1.220045	0.993218	-0.625335
B	-0.492286	1.481690	-0.631252
B	-1.270018	0.815875	0.822088
B	1.214986	0.998406	2.247572
B	2.002830	1.677744	0.816015
B	0.778524	2.644200	-0.133300
B	-0.769289	2.496615	0.794288
B	-0.480072	1.510860	2.238949
B	0.788297	2.665360	1.687567
N	1.146225	3.901280	2.391275
N	1.077760	3.842015	-0.908276
H	2.135223	-1.000170	0.822624
H	-1.087375	1.539097	3.250167
H	-1.578572	3.357836	0.790231
H	1.747895	0.657937	-1.626341
H	3.150771	1.962933	0.811786
H	-1.106268	1.482502	-1.637563
H	-2.334800	0.314619	0.823543
H	-0.274895	-0.925183	2.102554
H	1.730177	0.693838	3.264547
H	-0.267078	-0.931060	-0.470038
H	1.319981	4.655741	-0.362051
H	1.692533	3.755496	-1.701297
H	0.434049	4.352372	2.942788
H	2.028430	3.925935	2.876965

26

9,12-OH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -482.787112

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.627053
B	1.513659	0.000000	0.811895
B	1.216419	1.001549	-0.616768
B	-0.494420	1.493485	-0.620976
B	-1.276743	0.806470	0.806320
B	1.214029	0.990753	2.257427
B	1.999202	1.675639	0.823790
B	0.771762	2.650397	-0.069786
B	-0.789058	2.487244	0.813461
B	-0.499013	1.489270	2.251677
B	0.767124	2.643950	1.737932
O	1.092885	3.762488	2.510642
O	1.056251	3.847386	-0.753521
H	-2.336651	0.295943	0.807414
H	1.741523	0.697622	-1.628843
H	3.142297	1.977640	0.822654
H	-1.112946	1.497954	3.257291
H	-1.591327	3.353632	0.813852
H	1.732468	0.669403	3.265665
H	2.134769	-0.999200	0.810624
H	-0.264913	-0.928995	-0.475659
H	-1.092758	1.513093	-1.636201
H	-0.269592	-0.929766	2.098208
H	1.225607	4.551229	1.978247
H	1.870171	3.829170	-1.260038

26

9,12-SH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -1128.696108

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.624619
B	1.511046	0.000000	0.820534

B	1.214896	0.990802	-0.626899
B	-0.499332	1.489371	-0.625488
B	-1.278210	0.806348	0.821458
B	1.217208	1.004905	2.244270
B	1.997947	1.687480	0.805007
B	0.759961	2.629151	-0.108237
B	-0.789821	2.493008	0.810115
B	-0.493341	1.495715	2.246564
B	0.761288	2.640063	1.690604
S	1.273745	4.138789	2.688327
S	1.182072	4.103642	-1.165181
H	2.137612	-0.995085	0.819786
H	-1.090758	1.516988	3.261243
H	-1.599060	3.351387	0.806826
H	1.734177	0.672382	-1.634657
H	3.139601	1.982879	0.801609
H	-1.111296	1.497680	-1.631737
H	-2.339335	0.299433	0.820417
H	-0.266810	-0.926447	2.105050
H	1.735752	0.705280	3.258070
H	-0.269706	-0.928386	-0.474610
H	1.546179	4.893194	-0.135310
H	0.071799	4.740799	2.701992

25

9-O^-,12-OH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -482.215023

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.633185
B	1.509016	0.000000	0.805503
B	1.215743	0.997699	-0.636919
B	-0.478104	1.498279	-0.636918
B	-1.266623	0.820231	0.805500
B	1.227579	1.001796	2.238774
B	2.008958	1.663066	0.800509
B	0.824667	2.790448	-0.162050

B	-0.782244	2.487902	0.800513
B	-0.485891	1.508125	2.238772
B	0.781877	2.645669	1.694932
O	1.125758	3.809273	2.422131
O	1.148530	3.886445	-0.763984
H	2.116304	-1.015203	0.809447
H	-1.094433	1.517731	3.255217
H	-1.607523	3.339383	0.825246
H	1.734592	0.622326	-1.634358
H	3.164509	1.929166	0.825263
H	-1.117650	1.465247	-1.634357
H	-2.328184	0.298191	0.809444
H	-0.273757	-0.926444	2.106863
H	1.743601	0.679064	3.255211
H	-0.275884	-0.933641	-0.461318
H	1.326485	4.488485	1.764662

25

9-S^-,12-SH-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -1128.149407

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.637949
B	1.503835	0.000000	0.806755
B	1.217523	1.003006	-0.632601
B	-0.485184	1.500994	-0.632601
B	-1.266837	0.810332	0.806754
B	1.225972	1.003375	2.237558
B	2.001783	1.677724	0.798880
B	0.794135	2.715253	-0.154682
B	-0.782284	2.491971	0.798888
B	-0.492103	1.505858	2.237558
B	0.769934	2.632642	1.689750
S	1.219750	4.170691	2.647651
S	1.223240	4.182432	-1.069983
H	2.122131	-1.006506	0.809873
H	-1.098226	1.519372	3.252815

H	-1.606455	3.338382	0.817059
H	1.731663	0.645931	-1.634764
H	3.152150	1.946656	0.817038
H	-1.110706	1.477233	-1.634763
H	-2.330046	0.295618	0.809898
H	-0.270631	-0.925307	2.116455
H	1.743856	0.688154	3.252815
H	-0.272107	-0.930352	-0.470388
H	1.420641	4.858234	1.484722

24

9,12-O^{-}-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -481.490207

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.614744
B	1.517086	0.000000	0.807362
B	1.235591	0.997897	-0.623603
B	-0.436569	1.527065	-0.623599
B	-1.240919	0.872919	0.807384
B	1.235590	0.997921	2.238339
B	2.047465	1.666230	0.807364
B	0.891745	2.817751	-0.180683
B	-0.715997	2.540889	0.807354
B	-0.436540	1.527127	2.238344
B	0.891769	2.817854	1.795358
O	1.201469	3.796178	2.592696
O	1.201430	3.796021	-0.978111
H	2.111204	-1.033694	0.807393
H	-1.068073	1.512724	3.249894
H	-1.583994	3.361183	0.807253
H	1.743911	0.622955	-1.635182
H	3.229329	1.837932	0.807287
H	-1.068050	1.512799	-1.635178
H	-2.321530	0.369154	0.807398
H	-0.293366	-0.926771	2.081370
H	1.743952	0.622897	3.249871

H -0.293386 -0.926781 -0.466595

24

9,12-S$^-$-*ortho*-carborane, E(B3LYP/aug-cc-pVTZ)= -1127.463462

C 0.000000 0.000000 0.000000
C 0.000000 0.000000 1.629994
B 1.503831 0.000000 0.815053
B 1.231998 1.000646 -0.618589
B -0.455211 1.520480 -0.618680
B -1.243100 0.846301 0.814954
B 1.231977 1.000701 2.248686
B 2.021398 1.682946 0.815044
B 0.837532 2.718432 -0.154058
B -0.723829 2.528727 0.814987
B -0.455287 1.520443 2.248605
B 0.837472 2.718399 1.784071
S 1.249835 4.057123 2.925703
S 1.249963 4.057145 -1.295663
H 2.115268 -1.018074 0.815050
H -1.082752 1.506475 3.254748
H -1.568887 3.360543 0.815006
H 1.742843 0.635997 -1.624719
H 3.188048 1.895007 0.815051
H -1.082650 1.506469 -1.624840
H -2.321450 0.348814 0.814993
H -0.284502 -0.923298 2.107656
H 1.742708 0.635972 3.254846
H -0.284403 -0.923320 -0.477680

28

9,10-NH_2-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -443.0314439

C 0.000000 0.000000 0.000000
B 0.000000 0.000000 1.691008
B 1.509798 0.000000 0.745895
B 1.224119 0.925011 -0.734158

B	-0.466977	1.487258	-0.691930
B	-1.219046	0.895572	0.800858
C	1.248711	1.110431	1.988106
B	2.078294	1.658142	0.615582
B	0.858703	2.627921	-0.299790
B	-0.704271	2.611897	0.680212
B	-0.376793	1.663283	2.144550
B	0.914852	2.692739	1.475599
N	-1.645174	3.725890	0.593708
N	1.153682	3.786754	-1.145321
H	-0.200730	-0.950850	2.352831
H	1.309846	3.604054	2.115070
H	-2.329275	0.501345	0.806207
H	-1.090006	1.489159	-1.694266
H	-0.302606	-0.909357	-0.493240
H	-0.811950	1.862722	3.222871
H	3.235350	1.880179	0.670204
H	1.712037	0.556917	-1.743096
H	2.198407	-0.948396	0.839270
H	1.810875	0.974506	2.897690
H	1.236768	3.638231	-2.137938
H	1.858751	4.432878	-0.829561
H	-1.400852	4.432735	-0.085432
H	-1.929809	4.162977	1.455737

26

9,10-OH-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -482.8104761

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.690358
B	1.517335	0.000000	0.752552
B	1.259174	0.907711	-0.733013
B	-0.425269	1.471741	-0.715435
B	-1.202748	0.915619	0.786726
C	1.236328	1.101799	2.004977
B	2.095564	1.658033	0.629807

B	0.907887	2.608526	-0.311585
B	-0.646151	2.612919	0.644691
B	-0.363436	1.663077	2.145600
B	0.929813	2.689449	1.485996
O	-1.462880	3.758210	0.598654
O	1.273637	3.676415	-1.138546
H	2.195097	-0.954406	0.857892
H	-1.049173	1.486910	-1.717592
H	3.253196	1.862279	0.704386
H	1.319655	3.605931	2.117210
H	1.798792	0.962221	2.913831
H	1.755995	0.520001	-1.728200
H	-2.323857	0.549059	0.782200
H	-0.827646	1.883252	3.205728
H	-0.218744	-0.950816	2.345674
H	-0.302234	-0.912259	-0.488166
H	-2.281452	3.638531	0.113862
H	0.703175	4.441705	-1.027790

26

9,10-SH-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -1128.7206425

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.692762
B	1.512167	0.000000	0.744603
B	1.230661	0.913602	-0.734819
B	-0.454015	1.486240	-0.701790
B	-1.214727	0.912365	0.799929
C	1.249572	1.101144	1.993922
B	2.077227	1.667404	0.619207
B	0.858920	2.605994	-0.287606
B	-0.674712	2.599846	0.680661
B	-0.363667	1.656469	2.158937
B	0.911917	2.695424	1.491428
S	-1.897986	4.005458	0.655301
S	1.388650	4.070240	-1.321268

H	2.203171	-0.946160	0.835142
H	-1.082043	1.494739	-1.698562
H	3.231690	1.891229	0.672965
H	1.308507	3.605352	2.125156
H	1.819118	0.964276	2.898924
H	1.720320	0.550373	-1.741896
H	-2.327938	0.528755	0.801592
H	-0.808430	1.863366	3.228984
H	-0.210855	-0.951877	2.348915
H	-0.309608	-0.908571	-0.490779
H	-1.099040	4.851437	-0.025537
H	0.623707	3.795973	-2.392224

25

9-O^--10-OH-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -482.2410195

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.691304
B	1.510415	0.000000	0.734724
B	1.239982	-0.918297	-0.747563
B	-0.429528	-1.478534	-0.707458
B	-1.205152	-0.931190	0.800390
C	1.259946	-1.088090	1.989599
B	2.097850	-1.659063	0.607113
B	0.909494	-2.743184	-0.383600
B	-0.643910	-2.612561	0.670611
B	-0.352569	-1.667574	2.147324
B	0.957708	-2.676570	1.483629
O	1.117802	-3.804381	-1.096063
O	-1.484480	-3.744474	0.583249
H	2.182339	0.965720	0.837676
H	1.348218	-3.570106	2.156490
H	1.725868	-0.486226	-1.737575
H	-1.088361	-1.466043	-1.692045
H	-0.311746	0.913077	-0.481277
H	3.268108	-1.817607	0.697993

H	-0.789681	-1.866111	3.229306
H	-2.323186	-0.542406	0.807760
H	-0.208430	0.958504	2.347450
H	1.825565	-0.932955	2.894320
H	-1.041581	-4.350774	-0.029613

25

9-S$^-$-10-SH-*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -1128.1775459

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.688581
B	1.512007	0.000000	0.729013
B	1.234185	0.922269	-0.750472
B	-0.429020	1.497483	-0.709793
B	-1.199673	0.930796	0.793260
C	1.261157	1.082337	1.987295
B	2.095715	1.661670	0.607209
B	0.921788	2.678065	-0.354888
B	-0.633880	2.605263	0.671897
B	-0.340960	1.667717	2.146333
B	0.956463	2.686574	1.473466
S	-1.761076	4.083850	0.581917
S	1.320708	4.087216	-1.375324
H	2.192377	-0.959609	0.819902
H	-1.078992	1.485182	-1.694985
H	3.260998	1.835122	0.687586
H	1.355284	3.574345	2.141313
H	1.830568	0.933987	2.890624
H	1.716589	0.509754	-1.746238
H	-2.318993	0.552021	0.798481
H	-0.779599	1.873143	3.224190
H	-0.216076	-0.955052	2.345974
H	-0.314764	-0.907203	-0.490046
H	-0.901016	4.695020	-0.296443

24

9,10-O^--*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -481.5165725

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.680025
B	1.510815	0.000000	0.734786
B	1.227790	0.926988	-0.743012
B	-0.444880	1.524575	-0.711114
B	-1.205168	0.927006	0.779151
C	1.240621	1.091601	1.982927
B	2.072957	1.670685	0.607934
B	0.929474	2.679207	-0.376412
B	-0.745026	2.679213	0.671202
B	-0.359963	1.670683	2.130101
B	0.906590	2.713762	1.449071
O	1.565267	3.961704	-1.480227
O	-2.015743	3.961715	0.760160
H	2.207170	-0.954175	0.824387
H	-1.072385	1.462400	-1.714115
H	3.240208	1.851258	0.700965
H	1.334938	3.580628	2.133687
H	1.808642	0.960167	2.890813
H	1.713649	0.508014	-1.739072
H	-2.313411	0.508043	0.780428
H	-0.786817	1.851268	3.220476
H	-0.223993	-0.954174	2.345434
H	-0.311412	-0.905236	-0.497743

24

9,10-S^--*meta*-carborane, E(B3LYP/aug-cc-pVTZ)= -1127.4930208

C	0.000000	0.000000	0.000000
B	0.000000	0.000000	1.680025
B	1.510818	0.000000	0.734787
B	1.227790	0.926988	-0.743012
B	-0.444898	1.524593	-0.711093
B	-1.205169	0.926999	0.779157
C	1.240621	1.091601	1.982927

B	2.072996	1.670670	0.607909
B	0.929479	2.679211	-0.376404
B	-0.745003	2.679212	0.671225
B	-0.359961	1.670675	2.130098
B	0.906606	2.713760	1.449061
S	-2.015707	3.961724	0.760211
S	1.565284	3.961717	-1.480201
H	2.207176	-0.954174	0.824382
H	-1.072415	1.462428	-1.714087
H	3.240247	1.851241	0.700940
H	1.334947	3.580627	2.133681
H	1.808642	0.960167	2.890812
H	1.713649	0.508014	-1.739072
H	-2.313411	0.508034	0.780435
H	-0.786815	1.851260	3.220474
H	-0.223993	-0.954174	2.345434
H	-0.311414	-0.905234	-0.497746