Supplementary Materials

The reduction of the triple bond in $[B_{12}H_{11}NCR]^-$ anions by Lithium Aluminum Hydride: A novel approach to the synthesis of N-monoalkylammonio-substituted *closo*-dodecaborates.

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1. Spectral data for synthesised compounds.

Figure S1: $^{11}B\{^1H\}$ NMR spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH_3]$ 2a

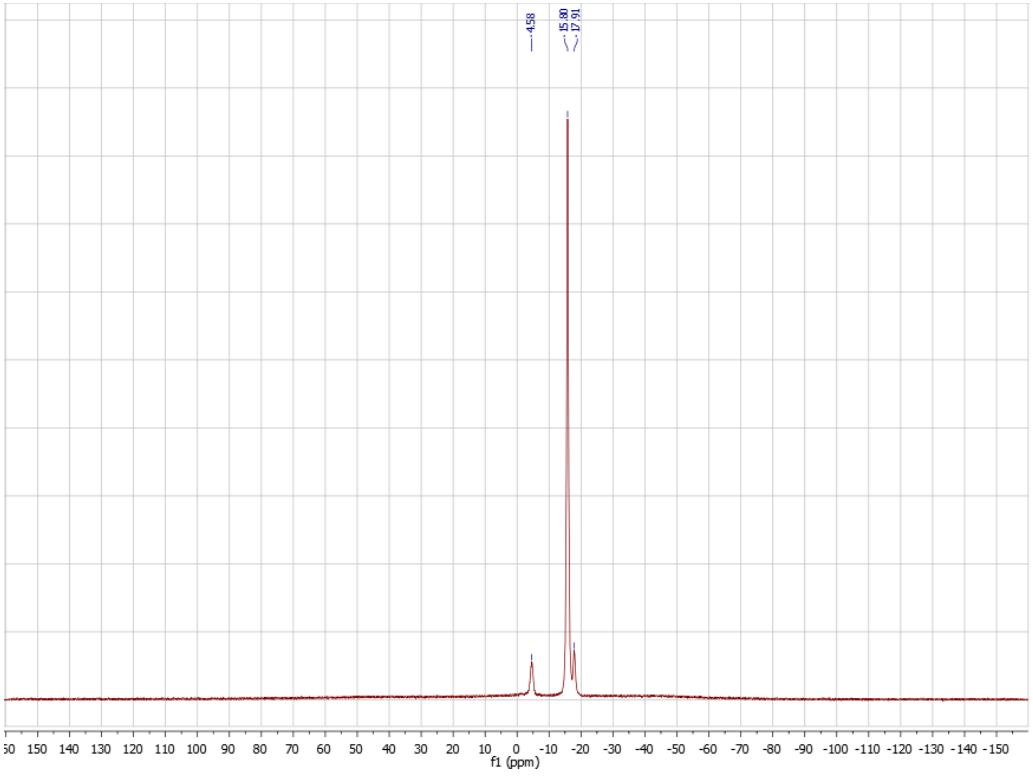

Figure S2: ^1H NMR spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH_3]$ 2a

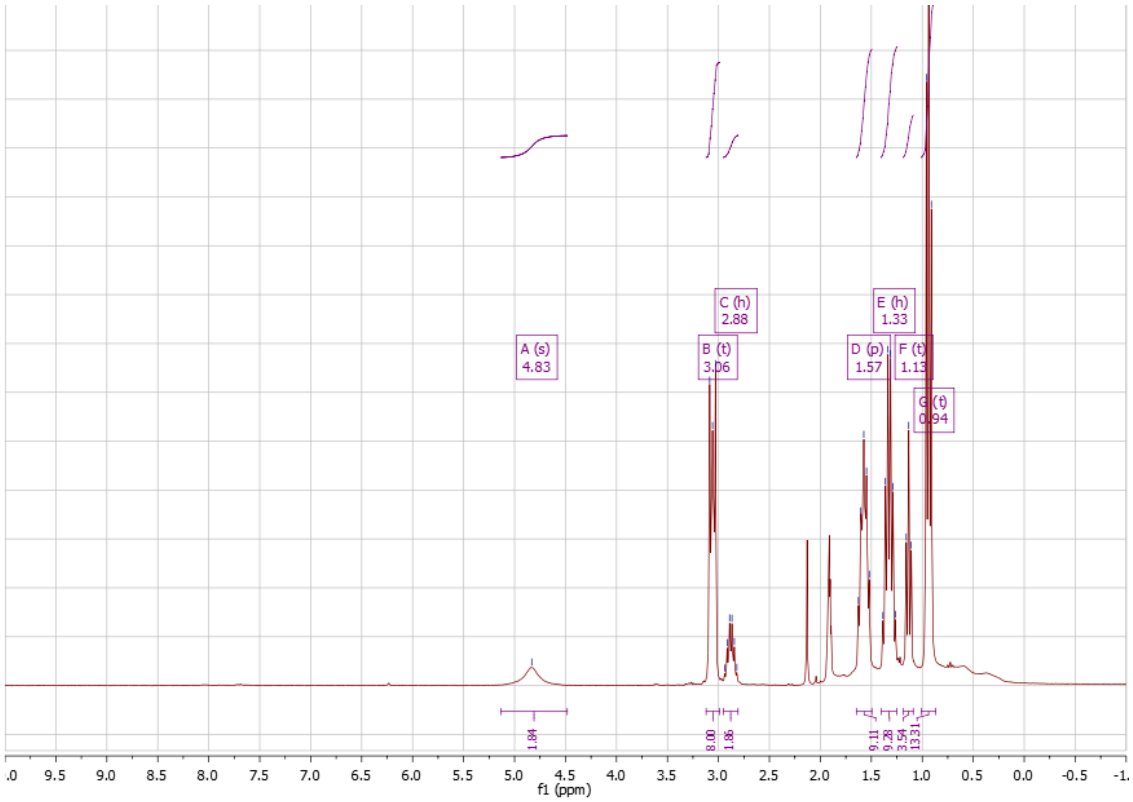

Figure S3: ^{13}C NMR spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH_3]$ 2a

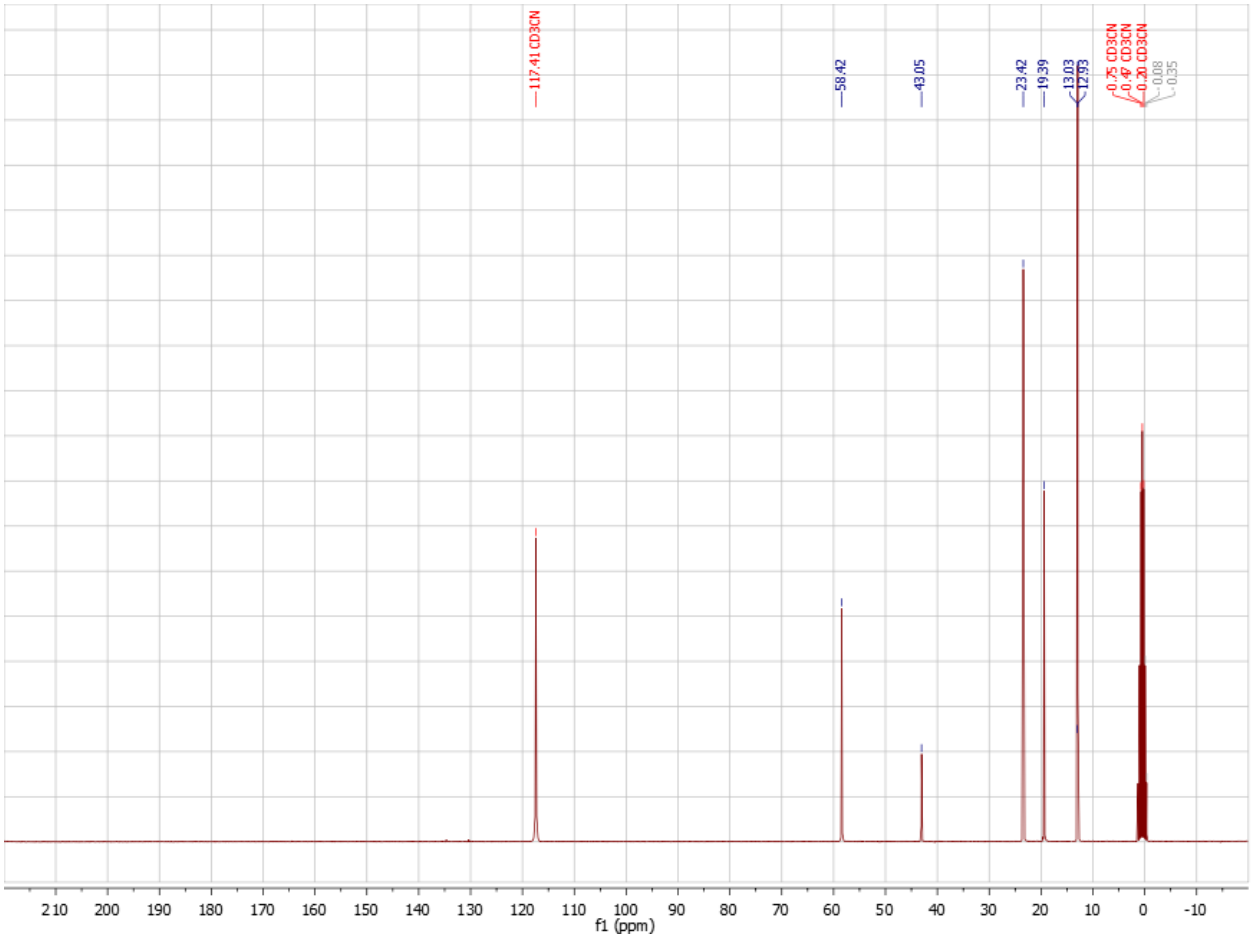

Figure S4: ESI-MS spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH_3]$ 2a (negative area) 1.

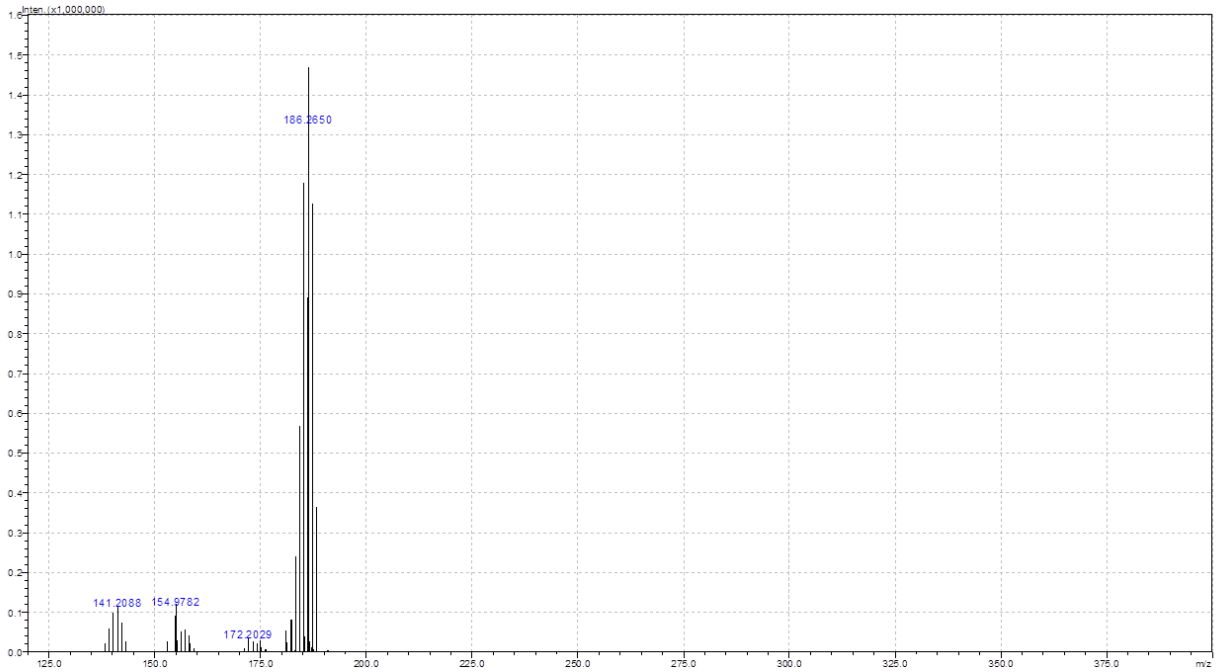

Figure S5: $^{11}B\{^1H\}$ NMR spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH_2CH_3]$ 2b

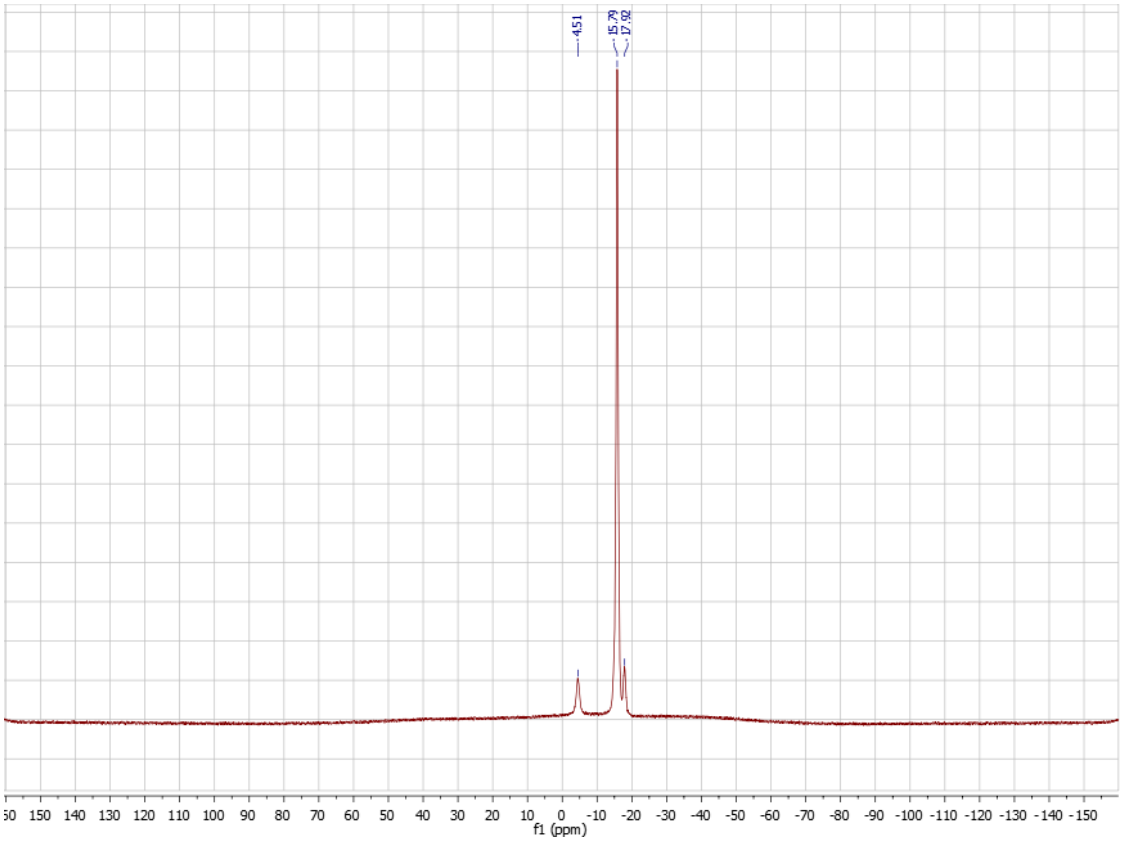

Figure S6: ^1H NMR spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH_2CH_3]$ 2b

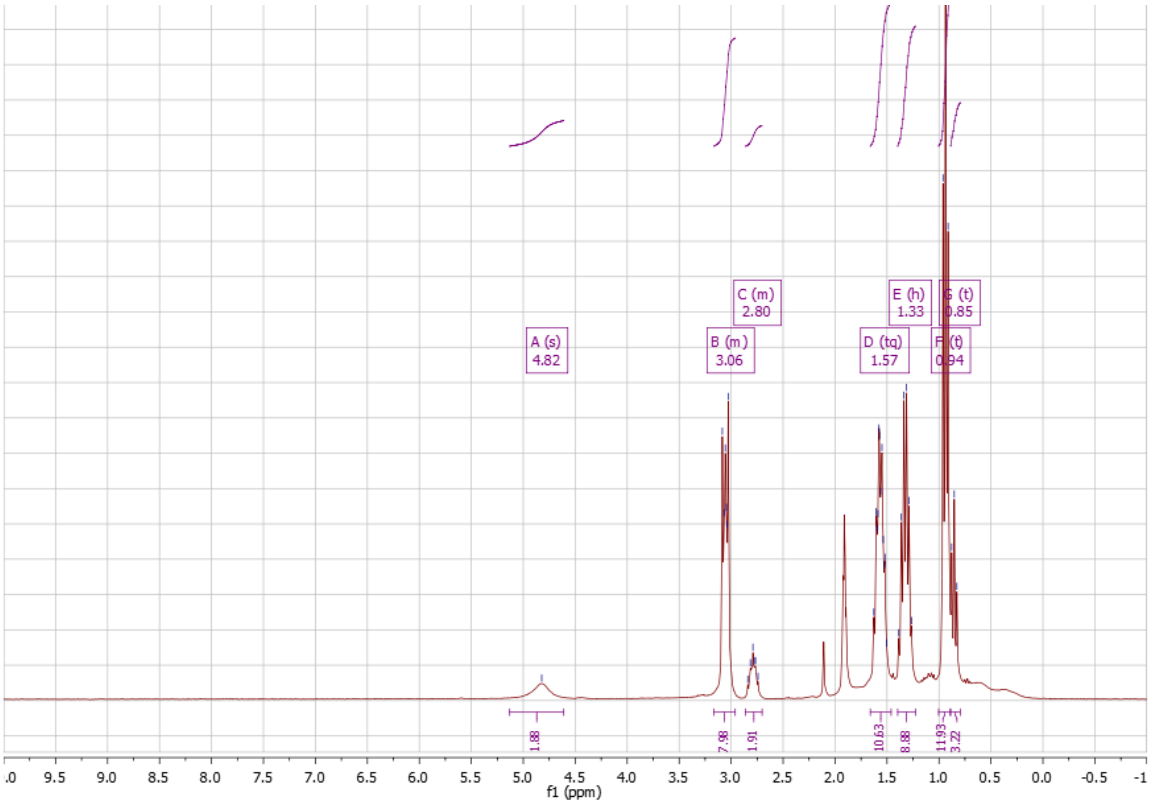

Figure S7: ^{13}C NMR spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH_2CH_3]$ 2b

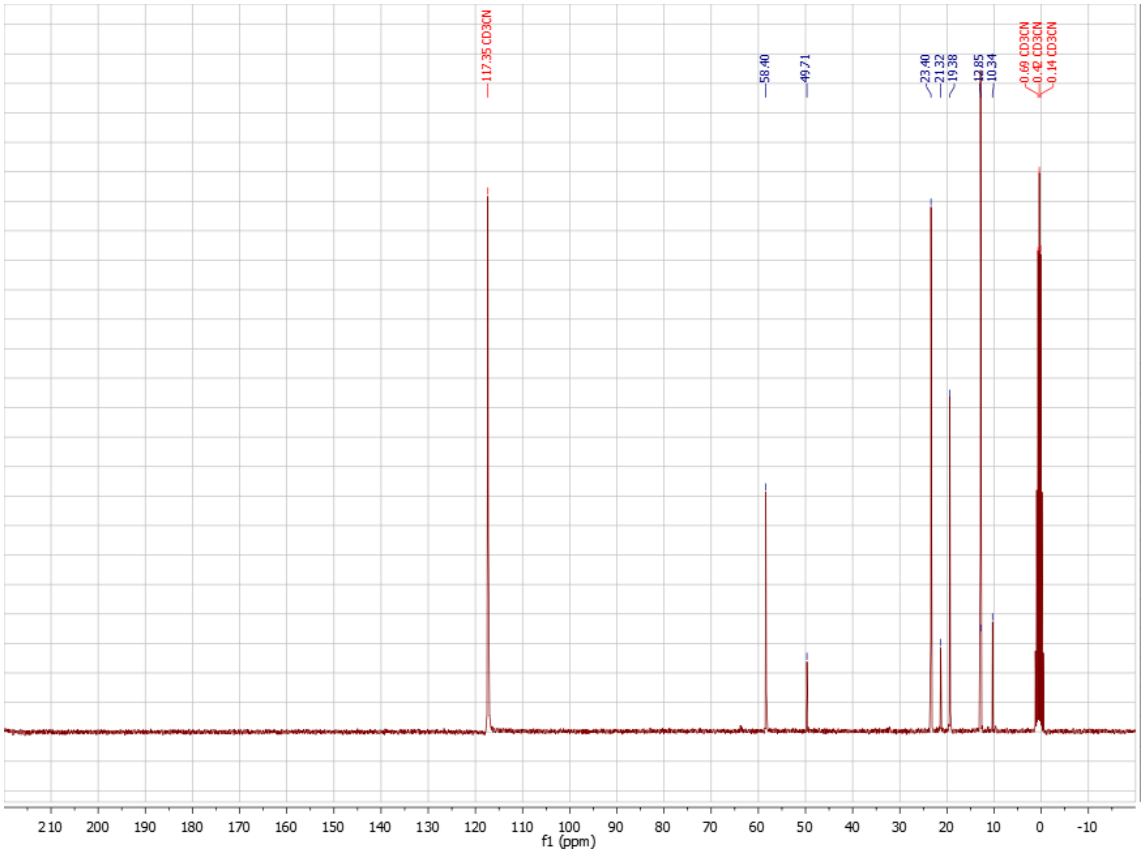

Figure S8: ESI-MS spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH_2CH_3]$ 2b (negative area).

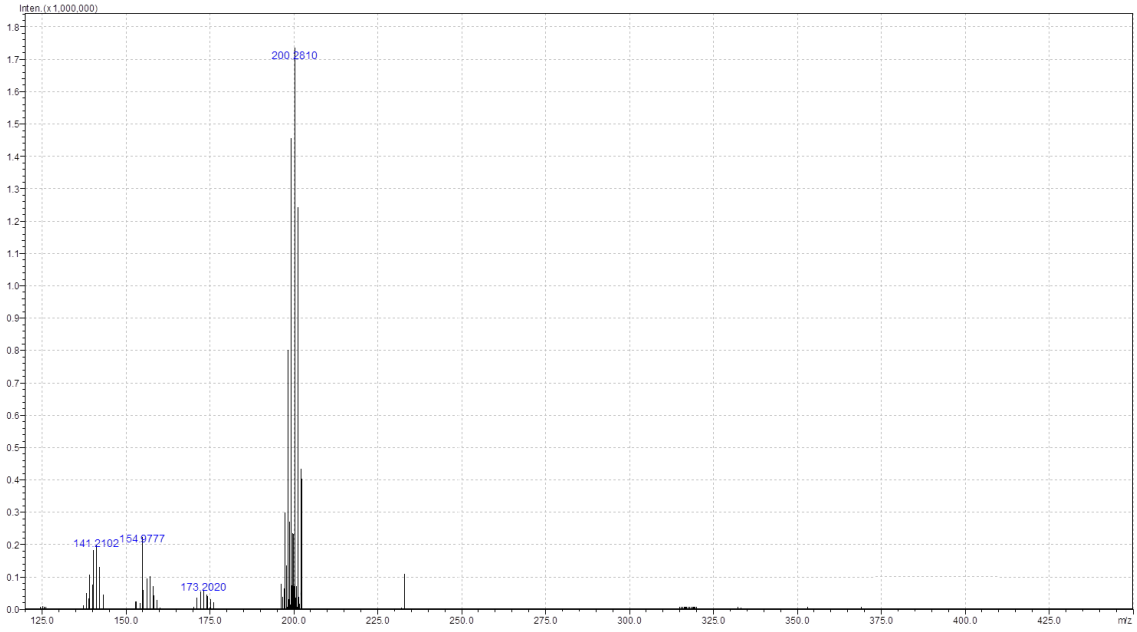

Figure S9: $^{11}B\{^1H\}$ NMR spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH_2CH_2CH_3]$ 2c

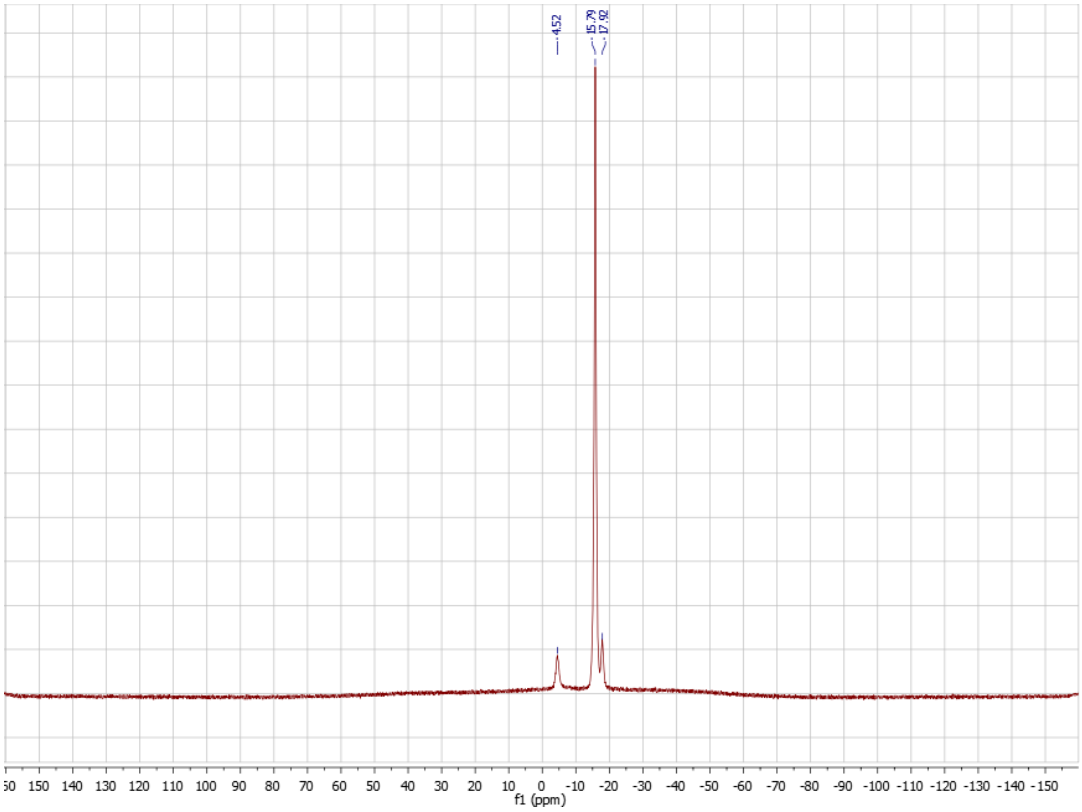

Figure S10: ^1H NMR spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH_2CH_2CH_3]$ 2c

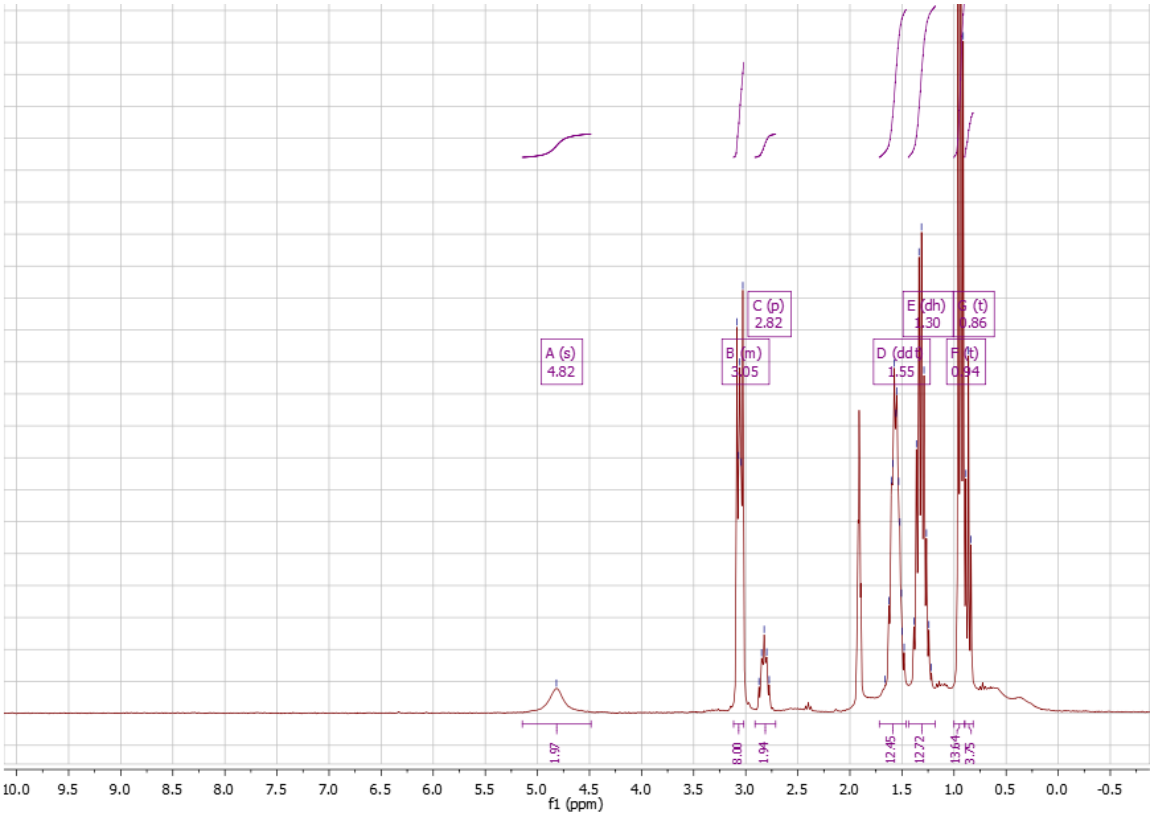

Figure S11: ^{13}C NMR spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH_2CH_2CH_3]$ 2c

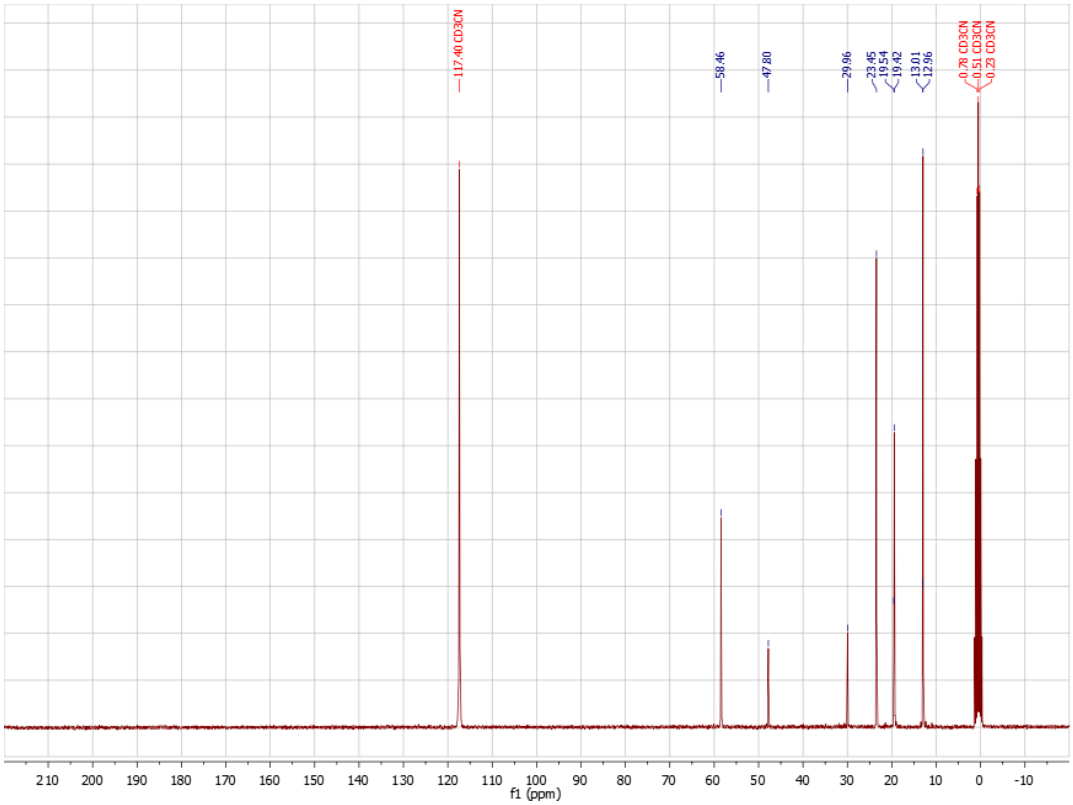

Figure S12: ESI-MS spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH_2CH_2CH_3]$ 2c (negative area).

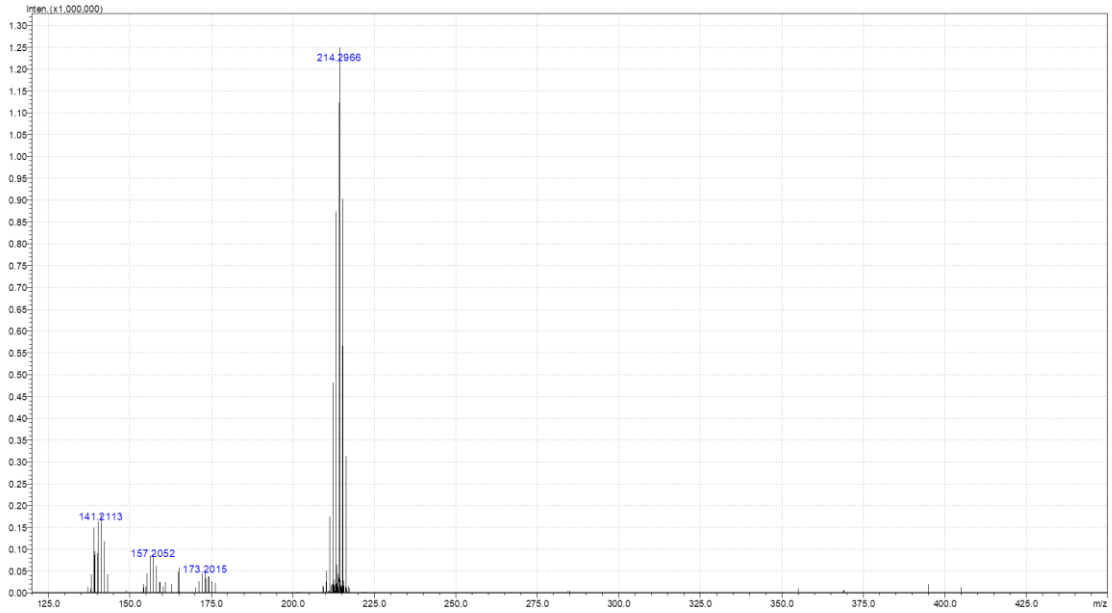

Figure S13: $^{11}B\{^{1}H\}$ NMR spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH(CH_3)_2]$ 2d

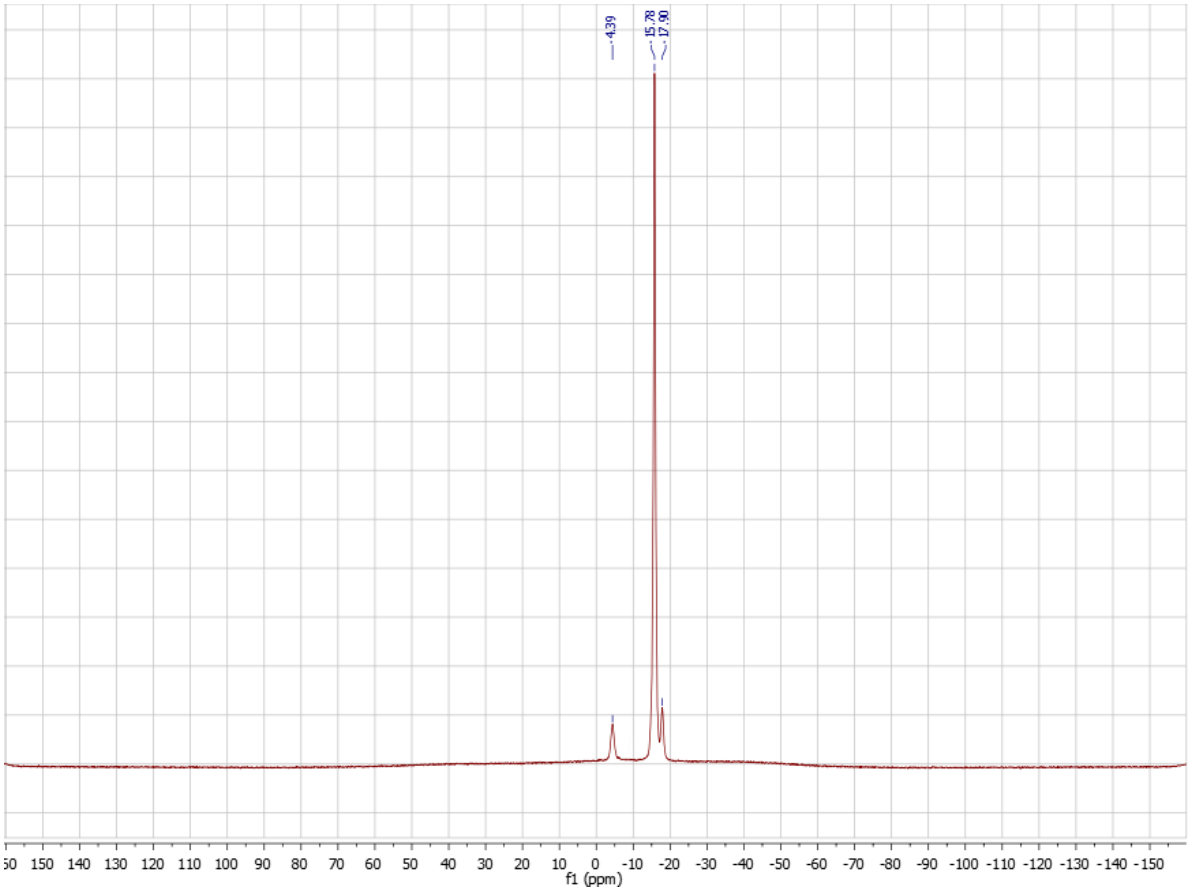

Figure S14: ^{1}H NMR spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH(CH_3)_2]$ 2d

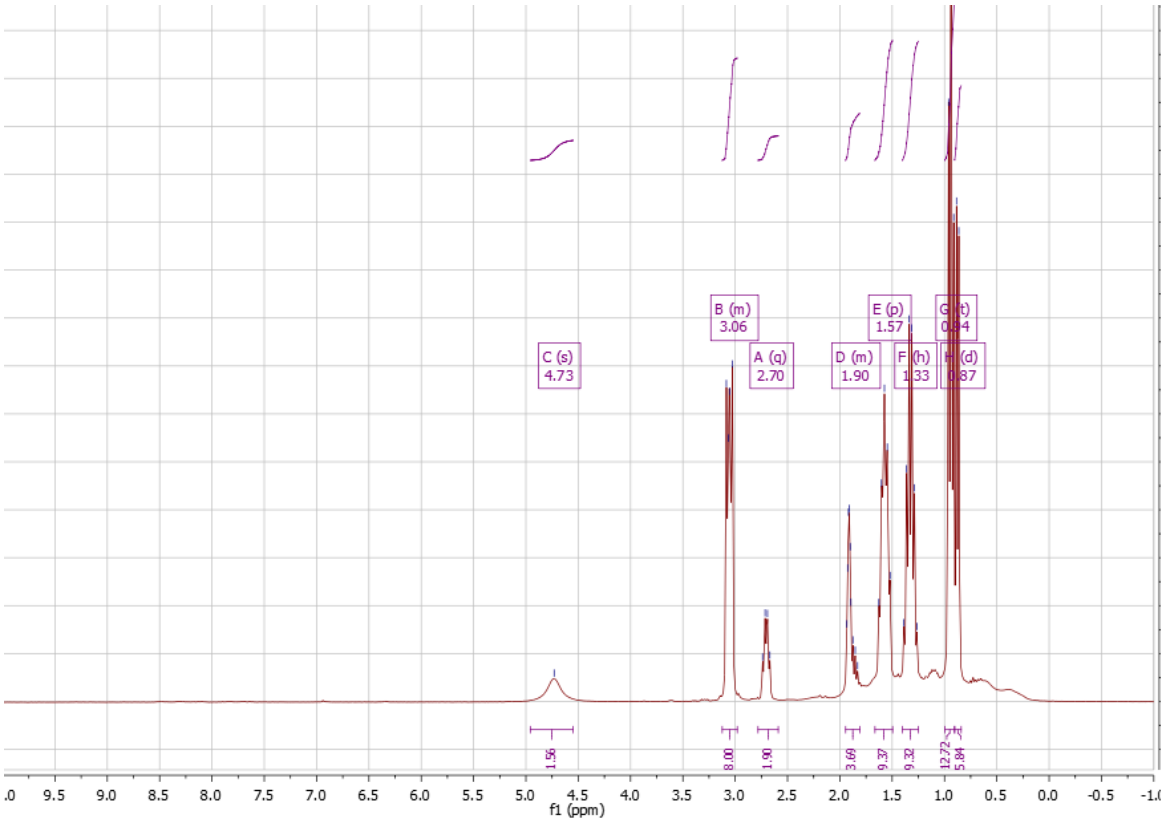

Figure S15: ^{13}C NMR spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH(CH_3)_2]$ 2d

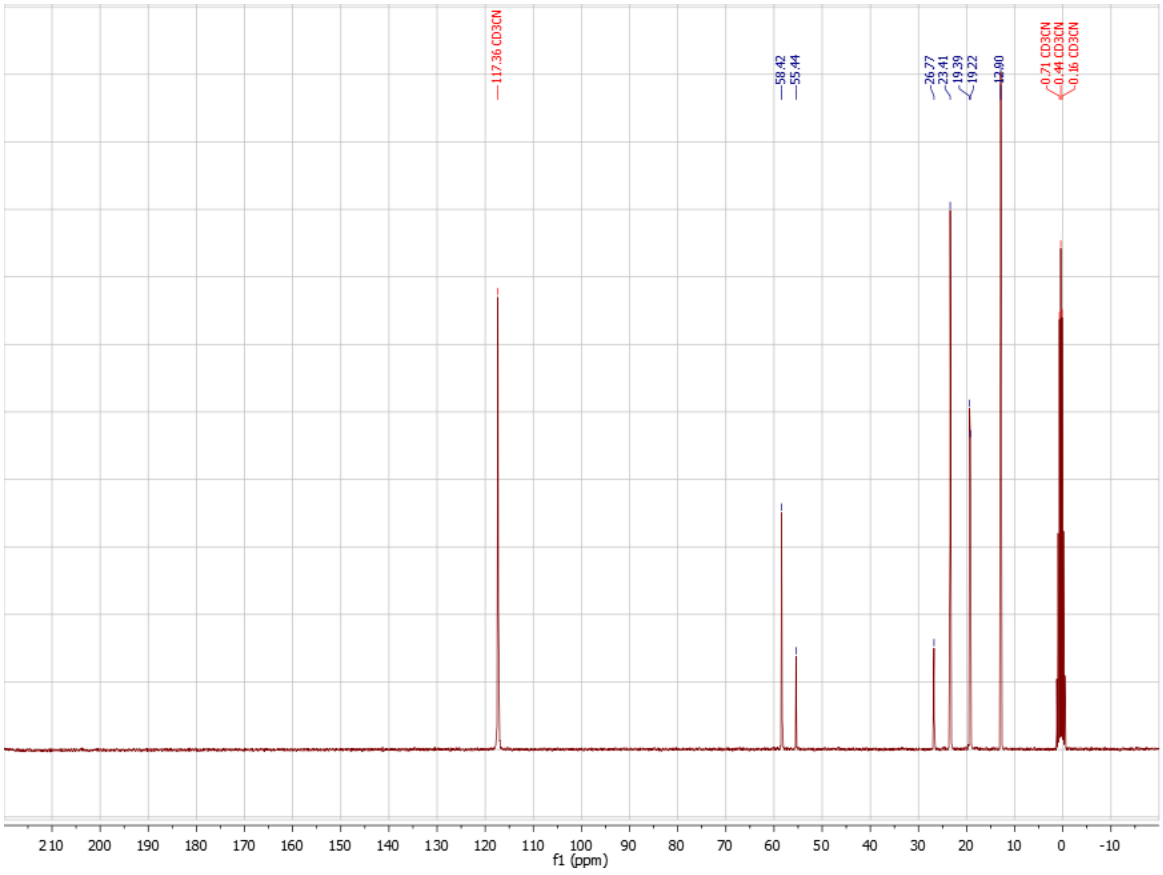

Figure S16: ESI-MS spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2CH(CH_3)_2]$ 2d (negative area).

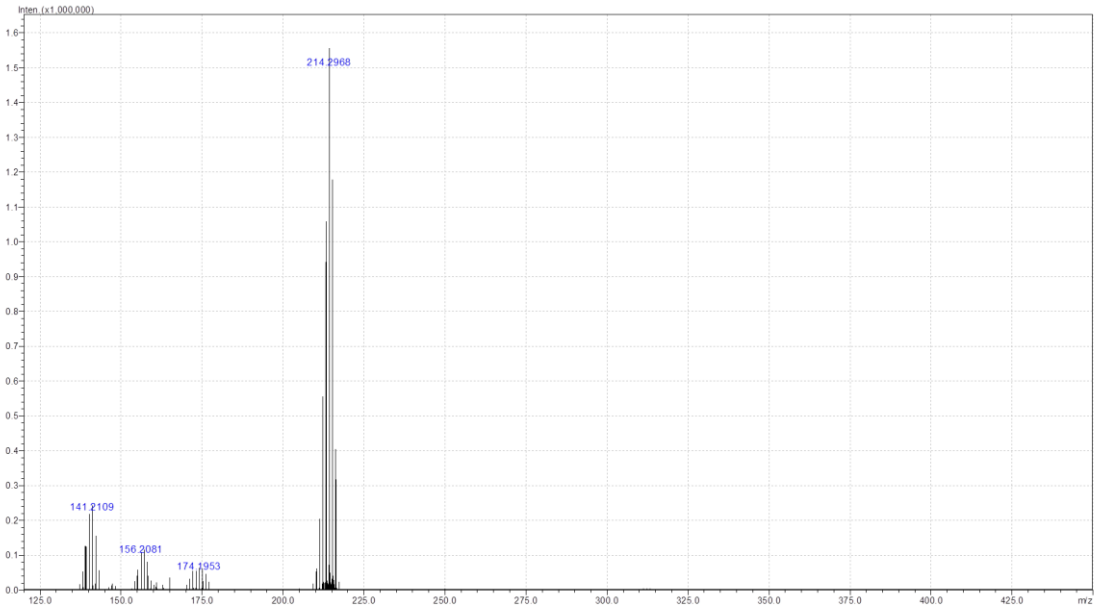

Figure S17: $^{11}B\{^{1}H\}$ NMR spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2C_6H_4CH_3]$ 2e

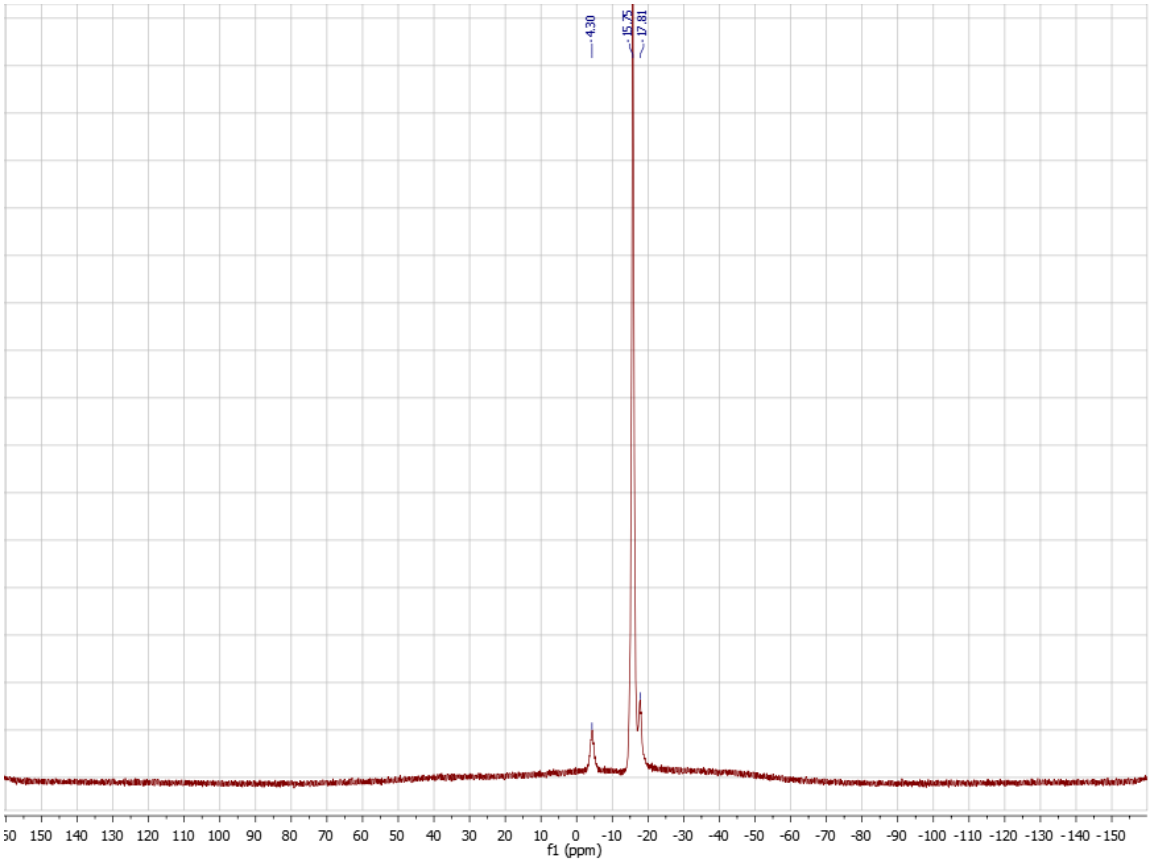

Figure S18: ^{1}H NMR spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2C_6H_4CH_3]$ 2e

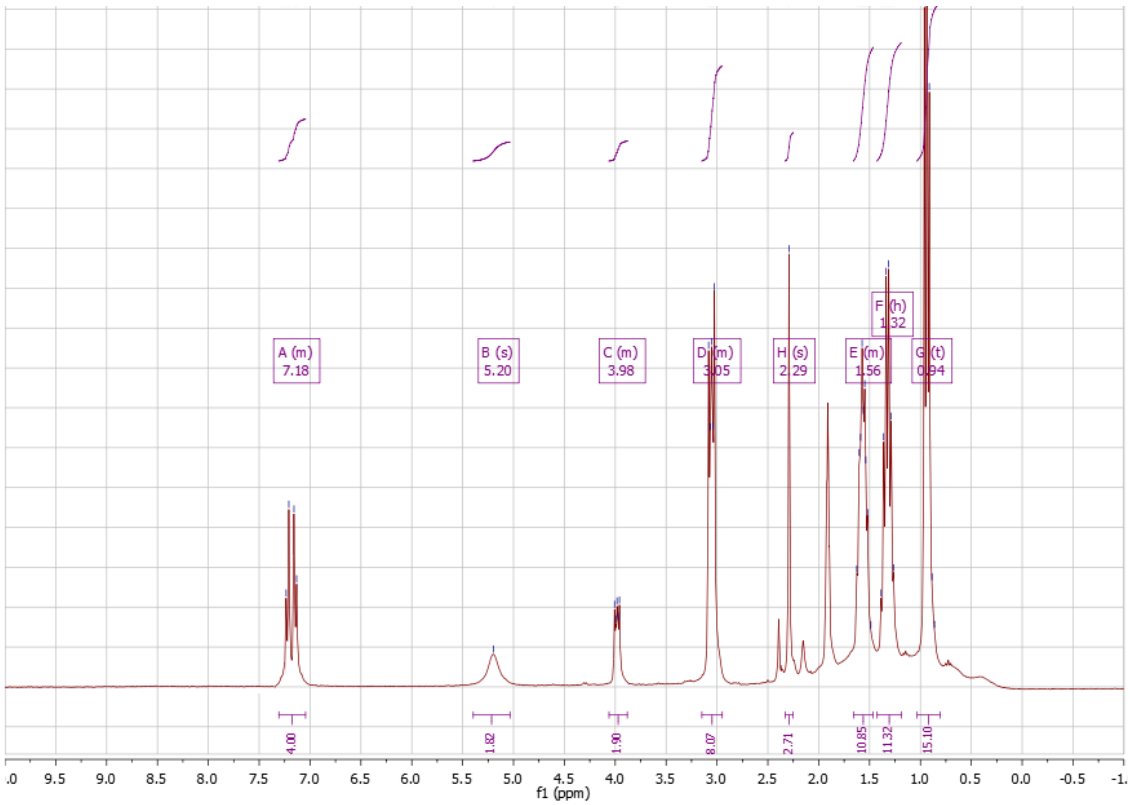

Figure S19: ^{13}C NMR spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2C_6H_4CH_3]$ 2e

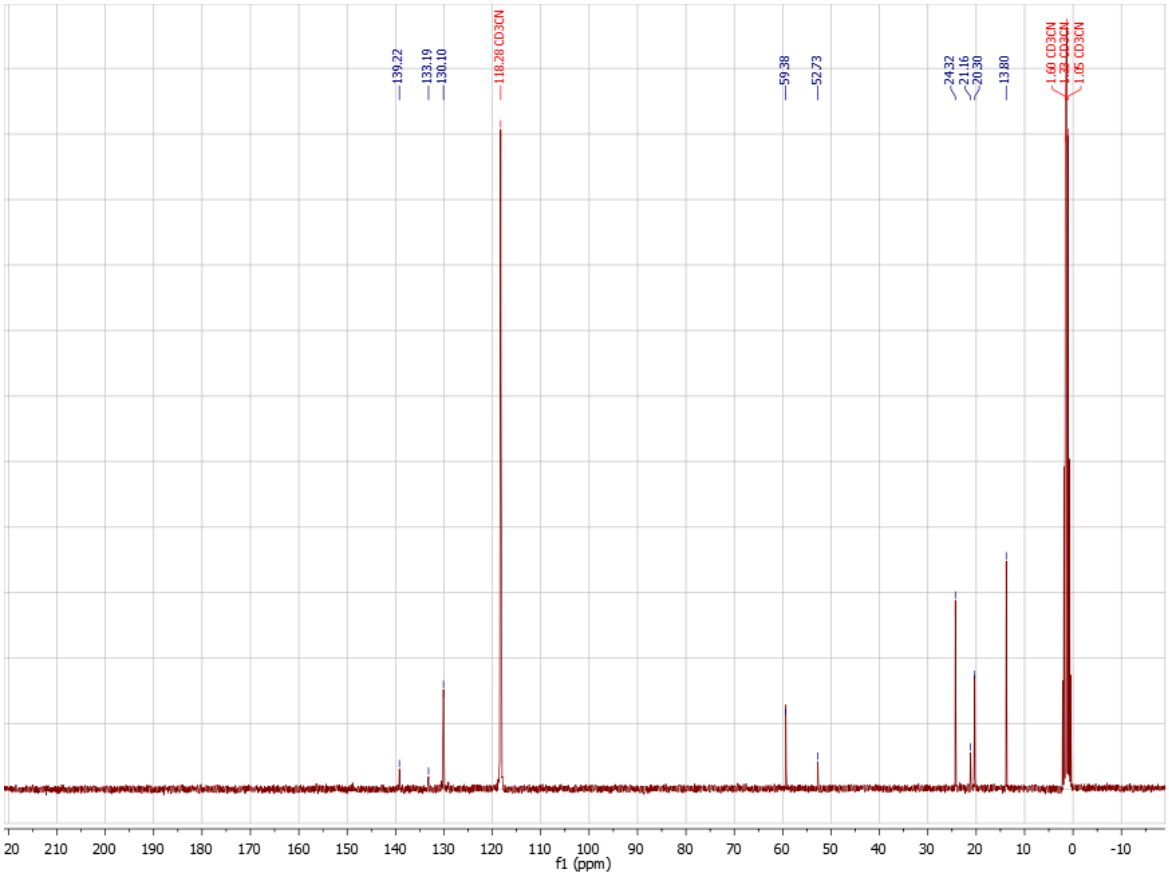

Figure S20: ESI-MS spectrum $(Bu_4N)[B_{12}H_{11}NH_2CH_2C_6H_4CH_3]$ 2e (negative area).

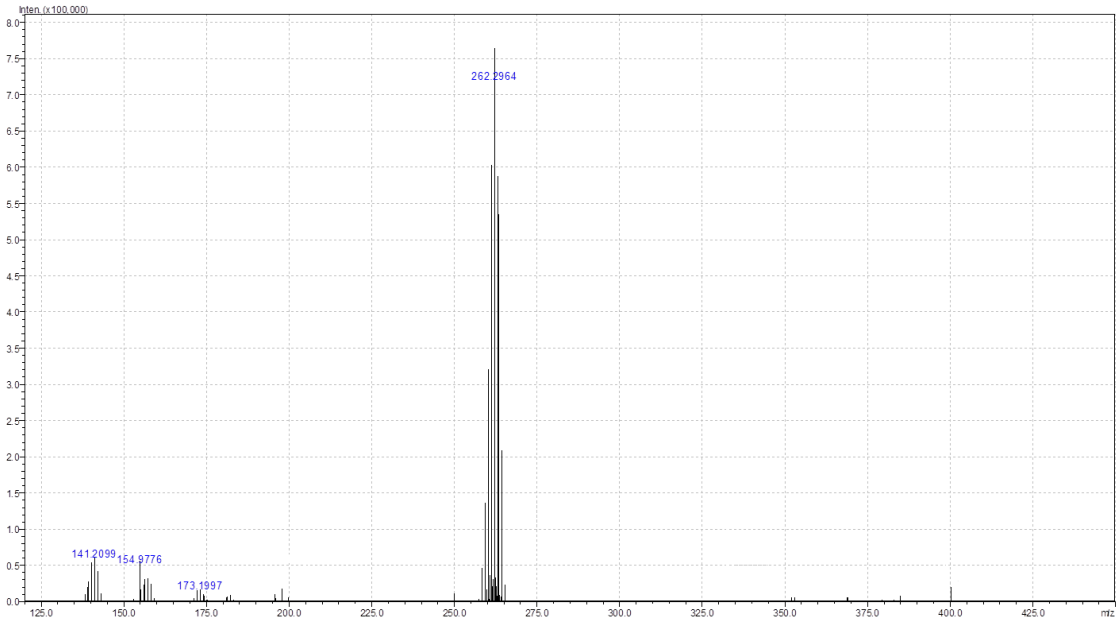

Figure S21: Molecular graph showing the results of the topological analysis of the electron density distribution in the model structure of the trimer of $[B_{12}H_{11}NH_2CH_2CH_3]^-$.

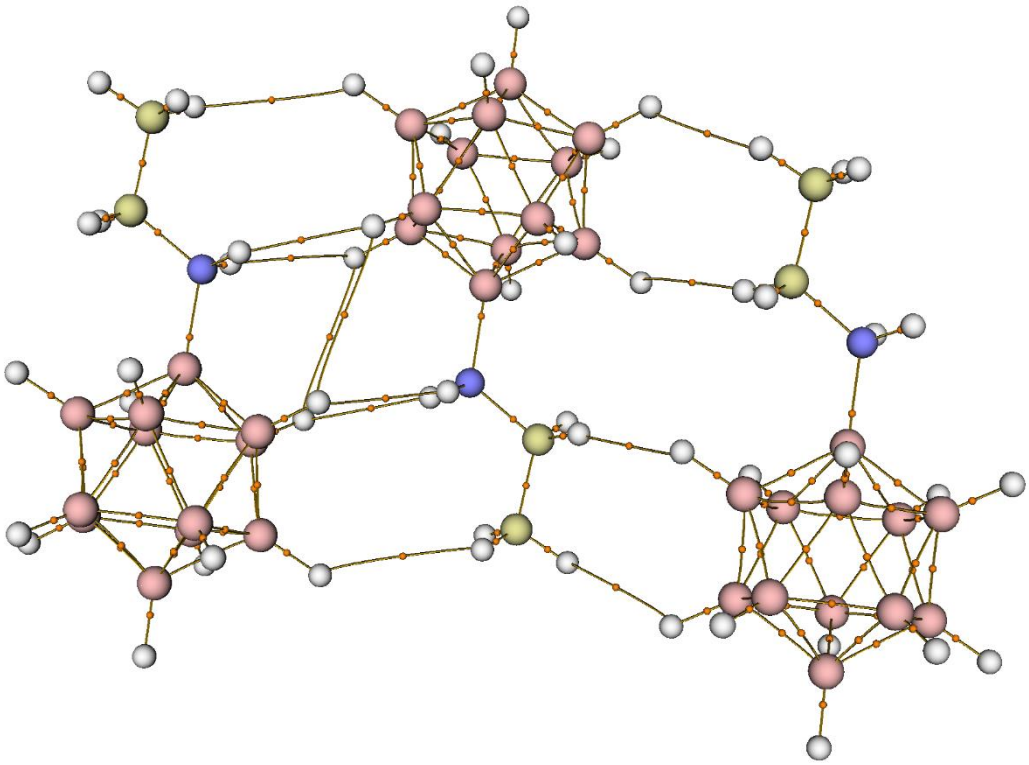

Table S1. Cartesian atomic coordinates of the calculated structure of $[B_{12}H_{11}NH_2Et]^-$ trimer.

	x	y	z
N	2.994833	6.460332	9.881283
H	3.188835	7.229974	10.3263
H	3.693763	6.293056	9.32291
C	1.845291	6.712234	9.0666
H	1.135773	7.093647	9.643411
H	1.512406	5.845363	8.724674
C	2.040783	7.624363	7.908723
H	2.642937	7.20384	7.260049
H	2.432353	8.467533	8.218973
H	1.175896	7.803011	7.48363
B	2.949834	5.289054	10.95148
B	4.389147	4.29671	11.15693
H	5.325994	4.46951	10.56832
B	3.876315	5.424903	12.44718
H	4.47612	6.335674	12.70362
B	2.088457	5.437841	12.49983
H	1.507744	6.352713	12.78565
B	1.51026	4.300591	11.2388
H	0.543468	4.473042	10.70117
B	2.930702	3.59547	10.39661

H	2.904863	3.309696	9.314164
B	4.428939	3.784365	12.86172
H	5.395793	3.607114	13.39916
B	3.016744	4.494661	13.69854
H	3.050781	4.786892	14.77916
B	1.544885	3.796009	12.95198
H	0.610114	3.626599	13.54564
B	2.06601	2.669109	11.63873
H	1.466629	1.761509	11.36978
B	3.840455	2.653584	11.59919
H	4.414743	1.736461	11.31041
B	2.996534	2.784258	13.16258
H	3.014201	1.944931	13.9034
N	-3.05109	6.477668	11.60864
H	-3.2451	5.708026	11.16363
H	-3.75002	6.644944	12.16702
C	-1.90155	6.225766	12.42333
H	-1.19203	5.844353	11.84652
H	-1.56867	7.092637	12.76525
C	-2.09704	5.313637	13.5812
H	-2.6992	5.73416	14.22988
H	-2.48861	4.470467	13.27095
H	-1.23216	5.134989	14.0063
B	-3.00609	7.648946	10.53845
B	-4.44541	8.64129	10.333
H	-5.38225	8.46849	10.92161
B	-3.93258	7.513097	9.042746
H	-4.53238	6.602326	8.786307
B	-2.14472	7.500159	8.990096
H	-1.56401	6.585287	8.70428
B	-1.56652	8.637409	10.25113
H	-0.59973	8.464958	10.78876
B	-2.98696	9.34253	11.09332
H	-2.96112	9.628304	12.17576
B	-4.4852	9.153635	8.628205
H	-5.45205	9.330886	8.090764
B	-3.07301	8.443339	7.791388
H	-3.10704	8.151108	6.710767
B	-1.60115	9.141991	8.537948
H	-0.66637	9.311401	7.944289
B	-2.12227	10.26889	9.851197
H	-1.52289	11.17649	10.12014
B	-3.89672	10.28442	9.890739
H	-4.471	11.20154	10.17952
B	-3.0528	10.15374	8.327346
H	-3.07046	10.99307	7.586524

N	7.240907	6.477668	11.60864
H	7.046904	5.708026	11.16363
H	6.541976	6.644944	12.16702
C	8.390449	6.225766	12.42333
H	9.099966	5.844353	11.84652
H	8.723333	7.092637	12.76525
C	8.194957	5.313637	13.5812
H	7.592803	5.73416	14.22988
H	7.803387	4.470467	13.27095
H	9.059844	5.134989	14.0063
B	7.285906	7.648946	10.53845
B	5.846593	8.64129	10.333
H	4.909746	8.46849	10.92161
B	6.359424	7.513097	9.042746
H	5.759619	6.602326	8.786307
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H	8.727995	6.585287	8.70428
B	8.725479	8.637409	10.25113
H	9.692271	8.464958	10.78876
B	7.305037	9.34253	11.09332
H	7.330877	9.628304	12.17576
B	5.8068	9.153635	8.628205
H	4.839946	9.330886	8.090764
B	7.218995	8.443339	7.791388
H	7.184958	8.151108	6.710767
B	8.690855	9.141991	8.537948
H	9.625626	9.311401	7.944289
B	8.169729	10.26889	9.851197
H	8.76911	11.17649	10.12014
B	6.395285	10.28442	9.890739
H	5.820997	11.20154	10.17952
B	7.239205	10.15374	8.327346
H	7.221538	10.99307	7.586524