Supplementary Materials

New aspects of the synthesis of *closo*-dodecaborate nitrilium derivatives $[B_{12}H_{11}NCR]^-$ (R = *n*-C_3H_7, *i*-C_3H_7, 4-$C_6H_4CH_3$, 1-$C_{10}H_7$): experimental and theoretical studies

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1. Spectral data for synthesised compounds.

Figure S1: $^{11}B\{^{1}H\}$ NMR spectrum $(Bu_4N)[B_{12}H_{11}(NC^nC_3H_7)]$ 1a

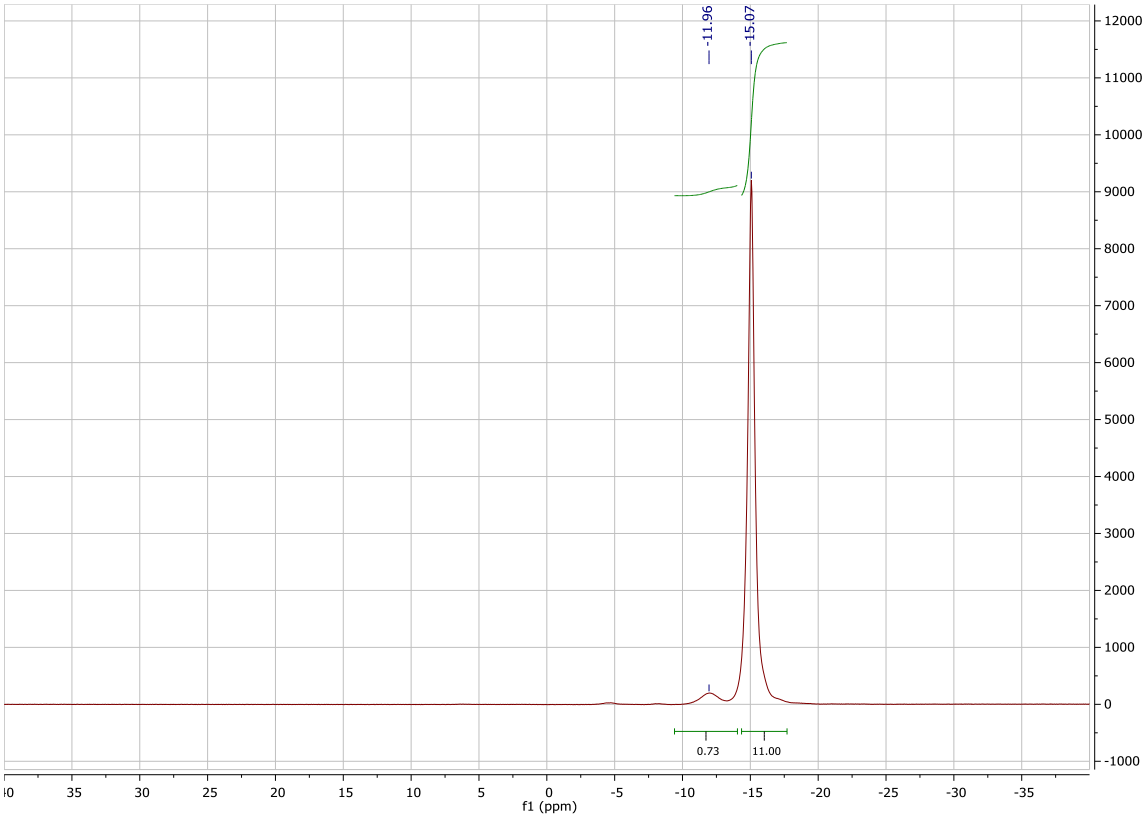


Figure S2: ^{1}H NMR spectrum $(Bu_4N)[B_{12}H_{11}(NC^nC_3H_7)]$ 1a

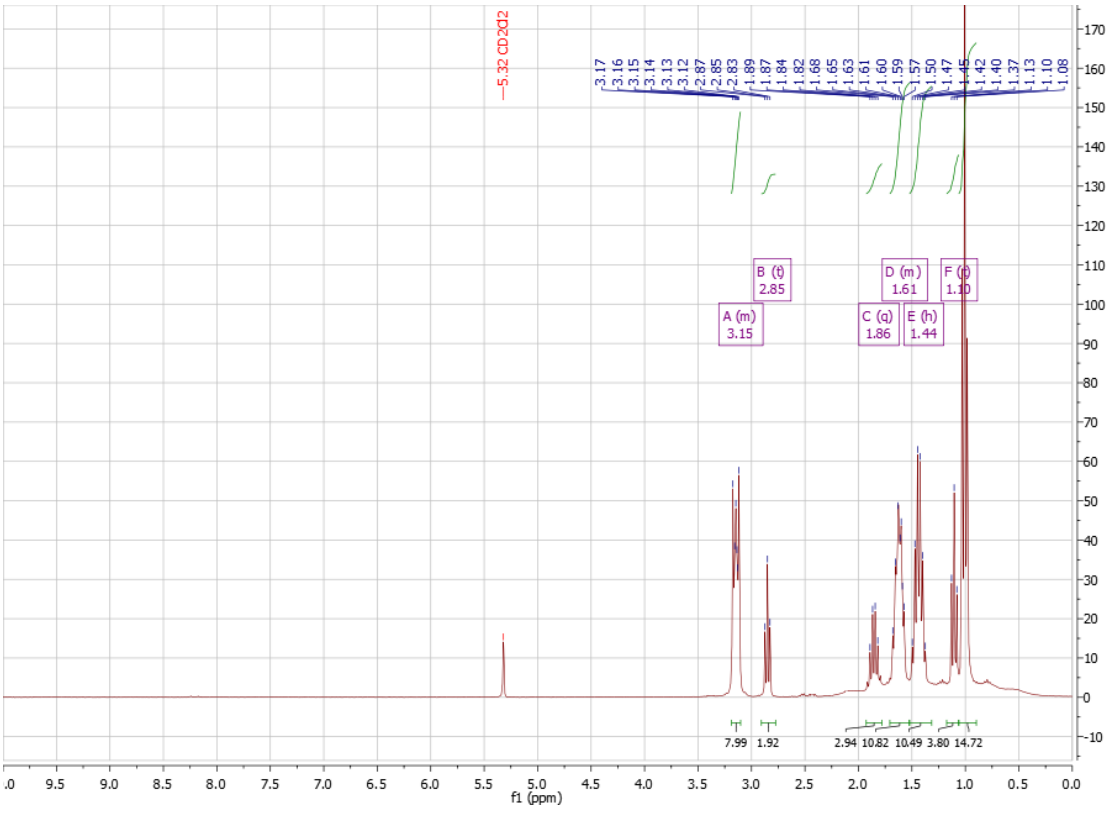


Figure S3: ^{13}C NMR spectrum $(Bu_4N)[B_{12}H_{11}(NC^nC_3H_7)]$ 1a

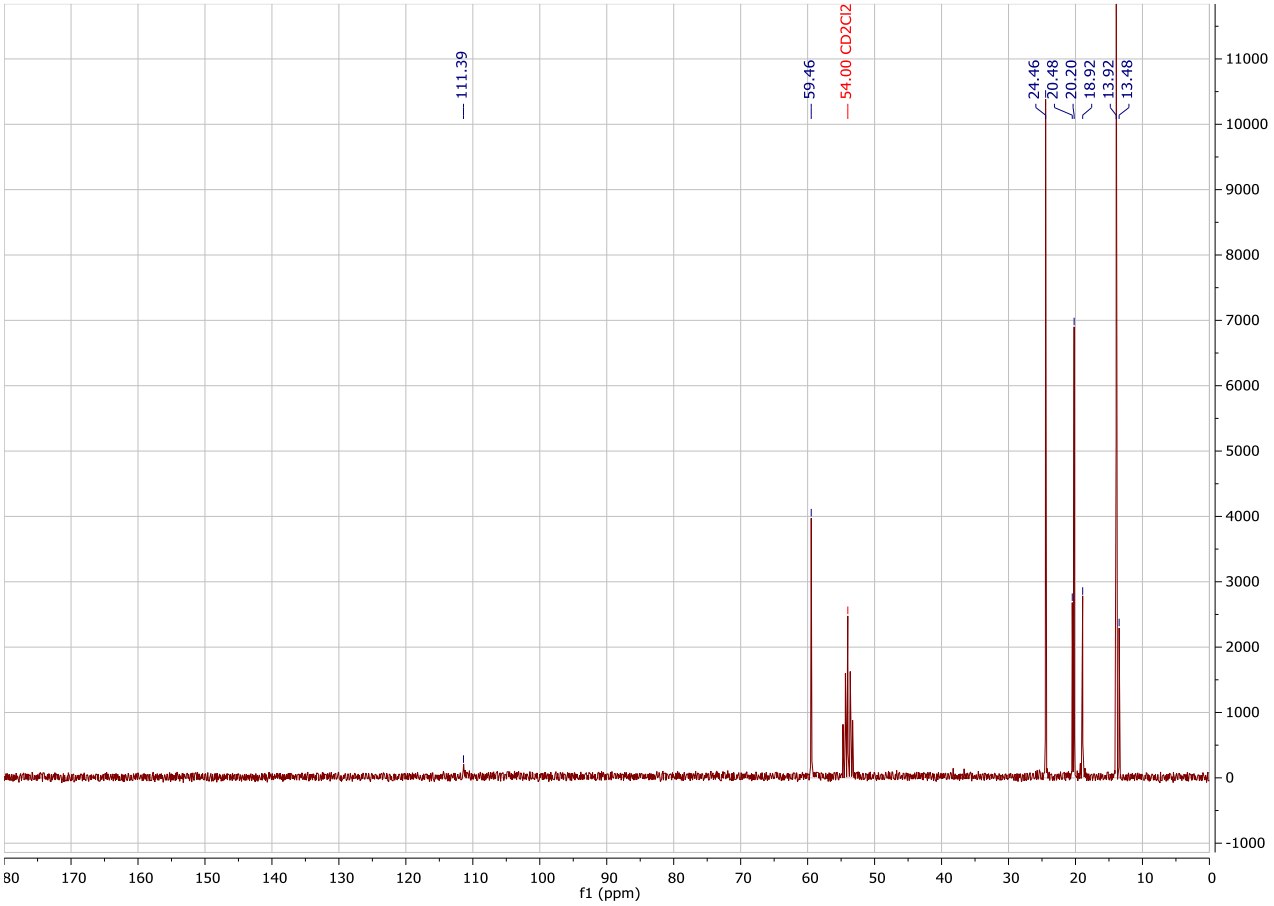


Figure S4: ESI-MS spectrum $(Bu_4N)[B_{12}H_{11}(NC^nC_3H_7)]$ (negative area) 1a.

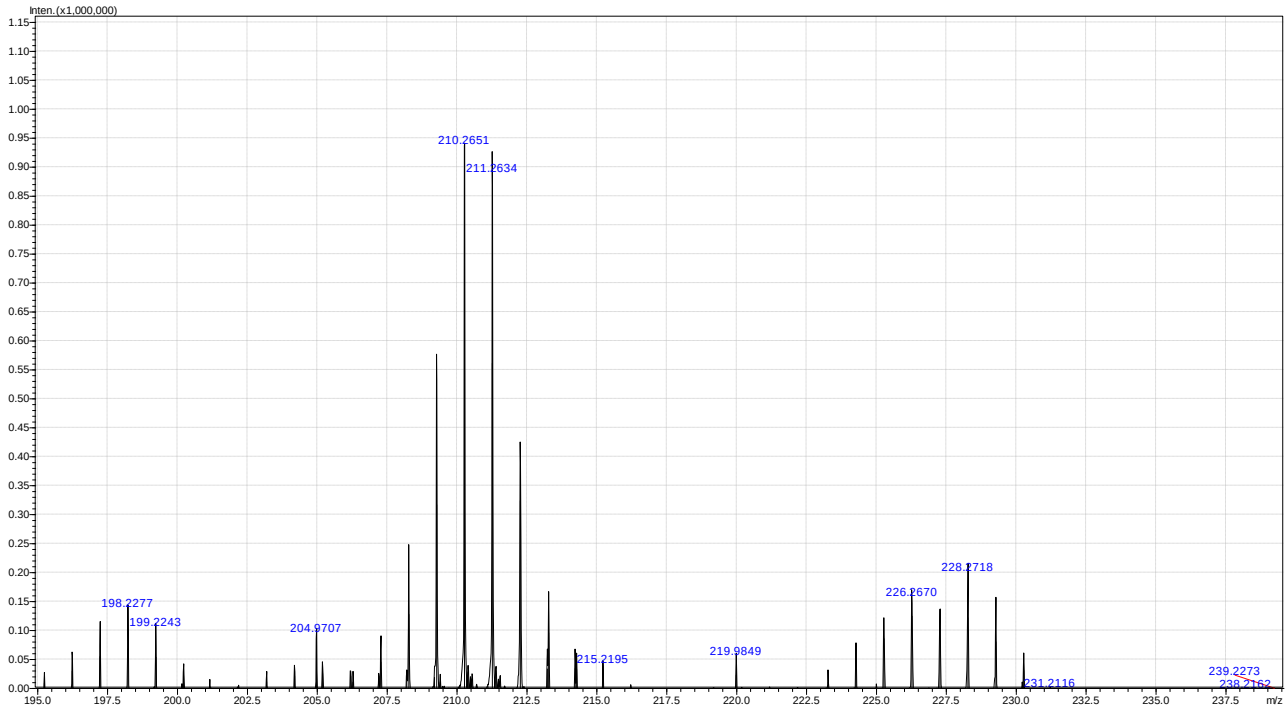


Figure S5: $^{11}B\{^{1}H\}$ NMR spectrum $(Bu_4N)[B_{12}H_{11}(NC^iC_3H_7)]$ 1b

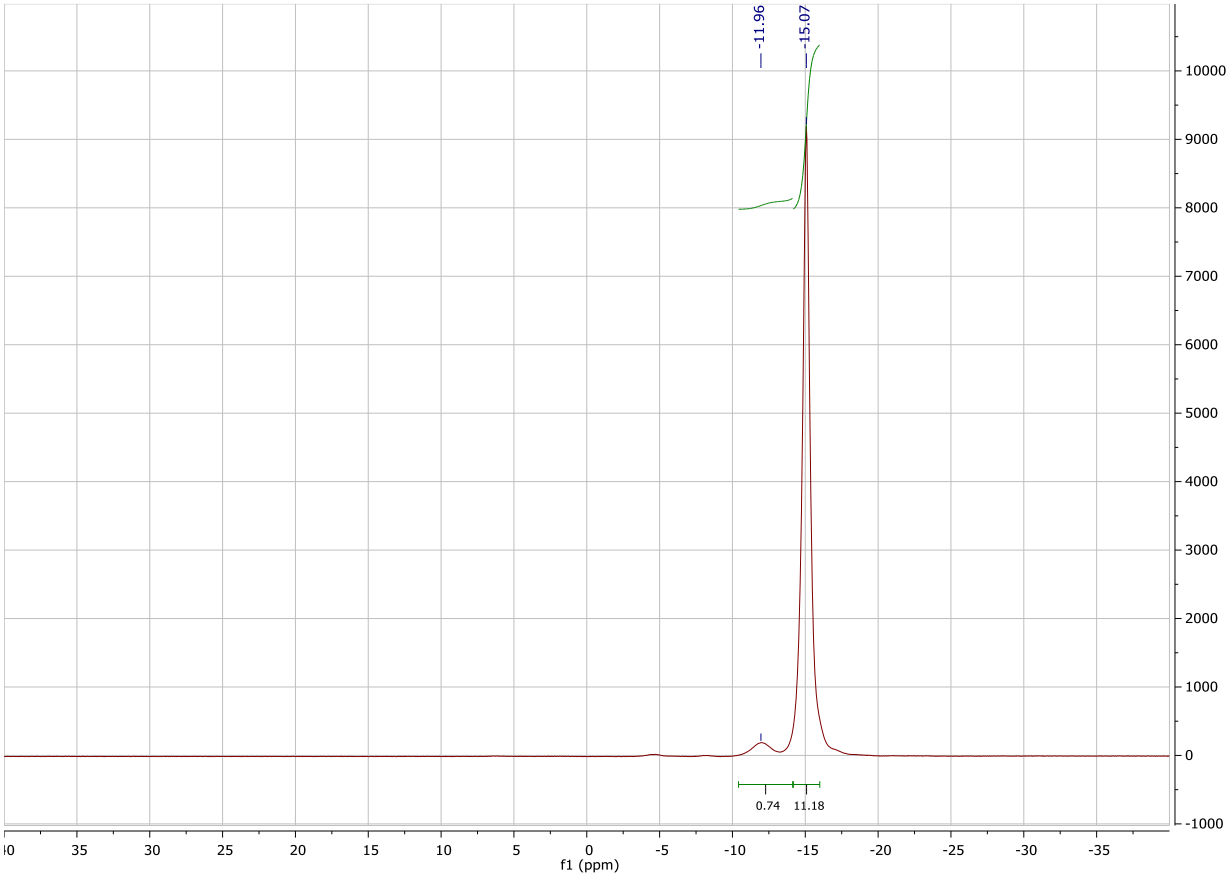


Figure S6: ^{1}H NMR spectrum $(Bu_4N)[B_{12}H_{11}(NC^iC_3H_7)]$ 1b.

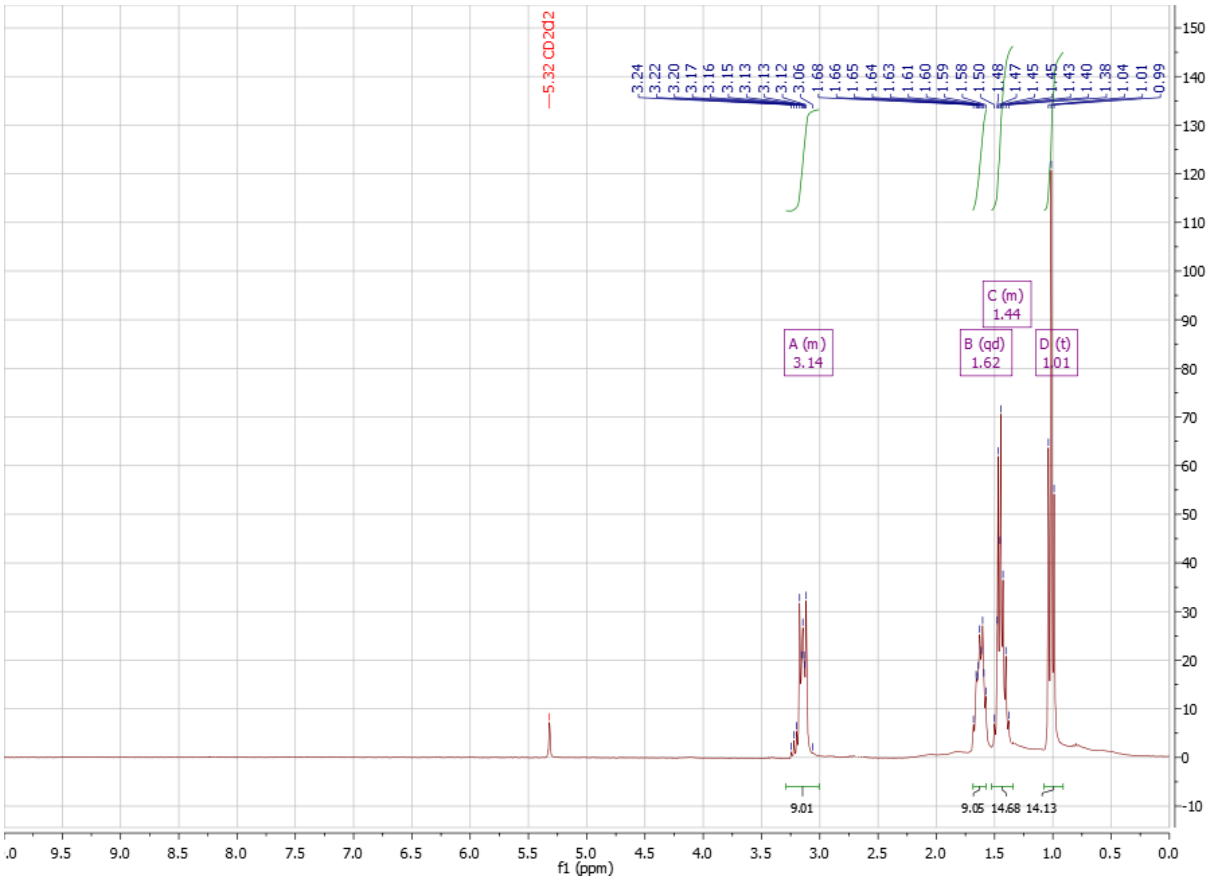


Figure S7: ^{13}C NMR spectrum $(Bu_4N)[B_{12}H_{11}(NC^iC_3H_7)]$ 1b

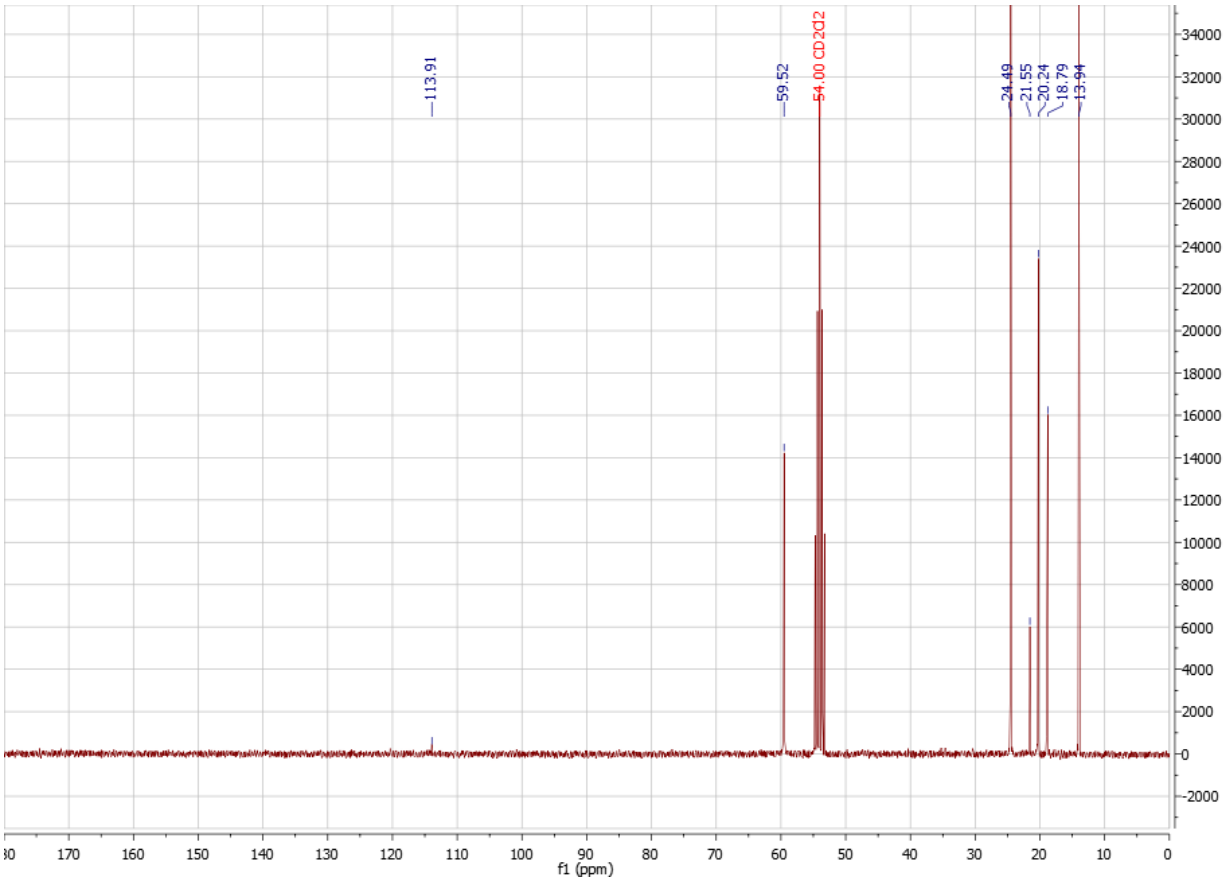


Figure S8: ESI-MS spectrum $(Bu_4N)[B_{12}H_{11}(NC^iC_3H_7)]$ (negative area) 1b.

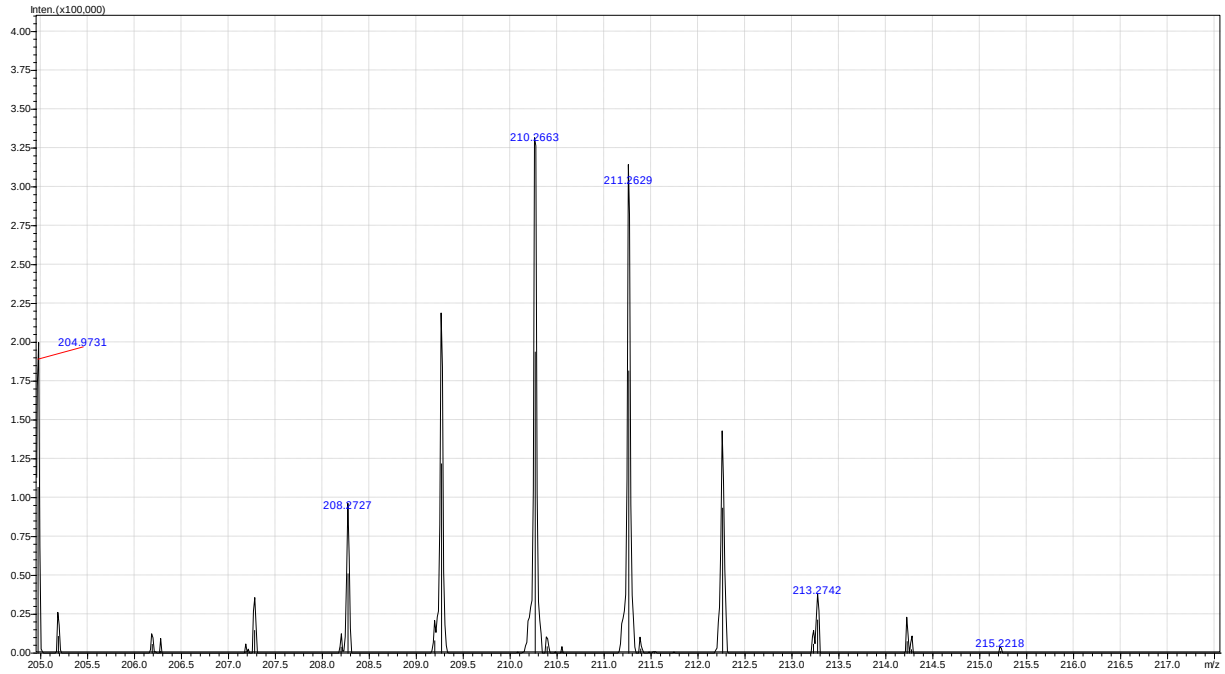


Figure S9: $^{11}B\{^{1}H\}$ NMR spectrum $(Bu_4N)[B_{12}H_{11}(NCC_6H_4CH_3)]$ 2a

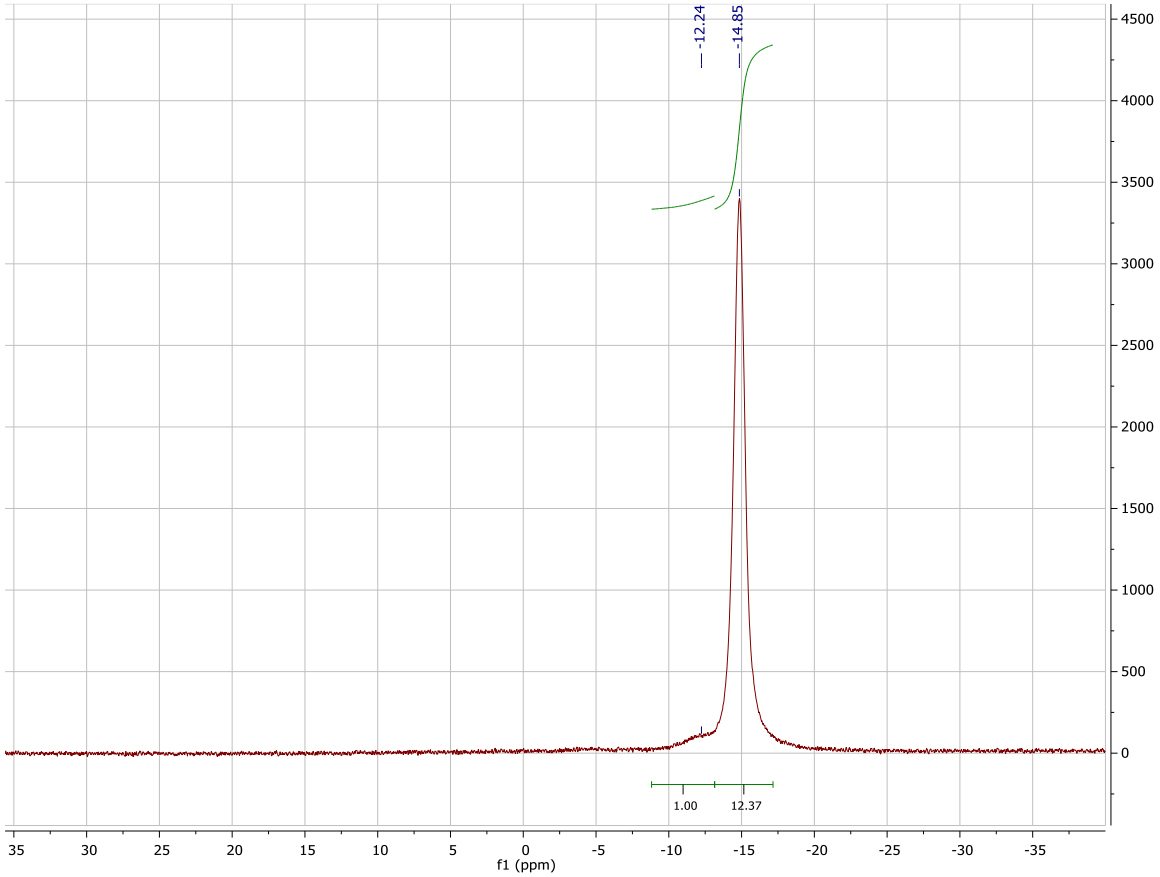


Figure S10: ^{1}H NMR spectrum $(Bu_4N)[B_{12}H_{11}(NCC_6H_4CH_3)]$ 2a

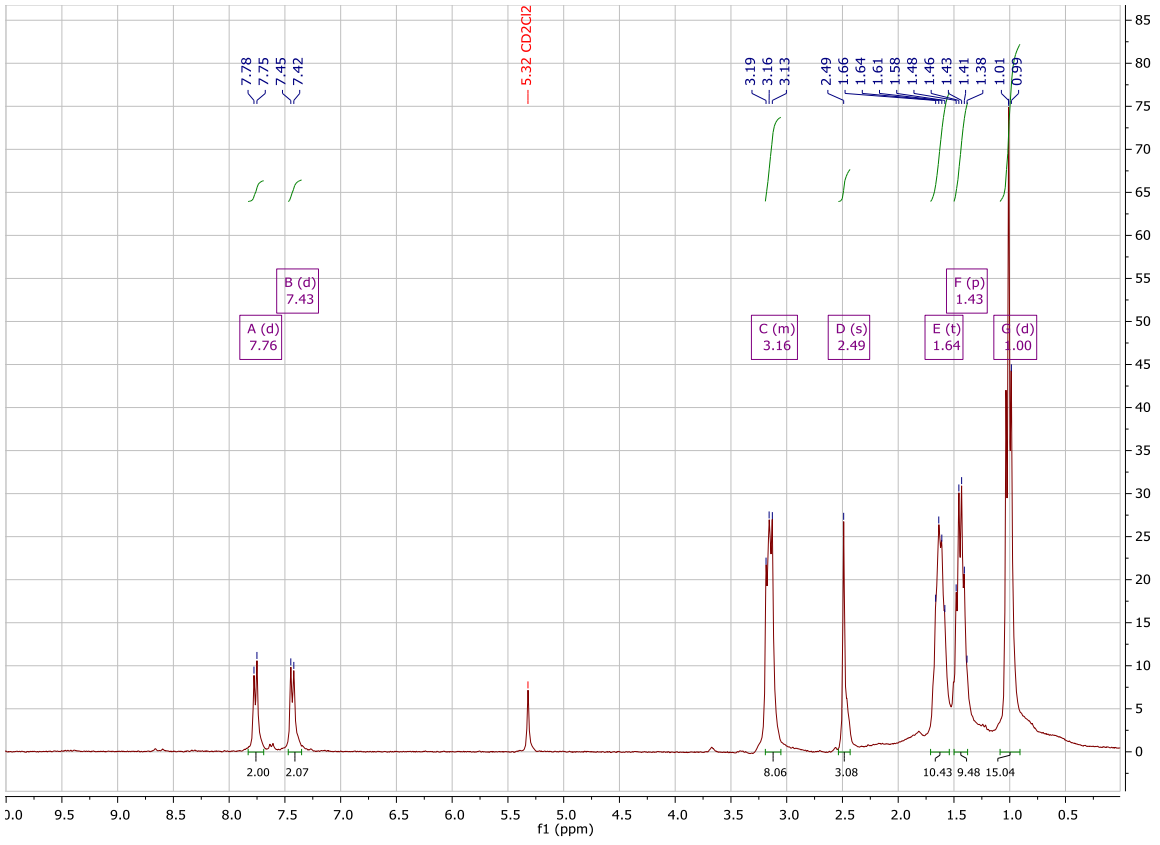


Figure S11: ^{13}C NMR spectrum $(Bu_4N)[B_{12}H_{11}(NCC_6H_4CH_3)]$ 2a

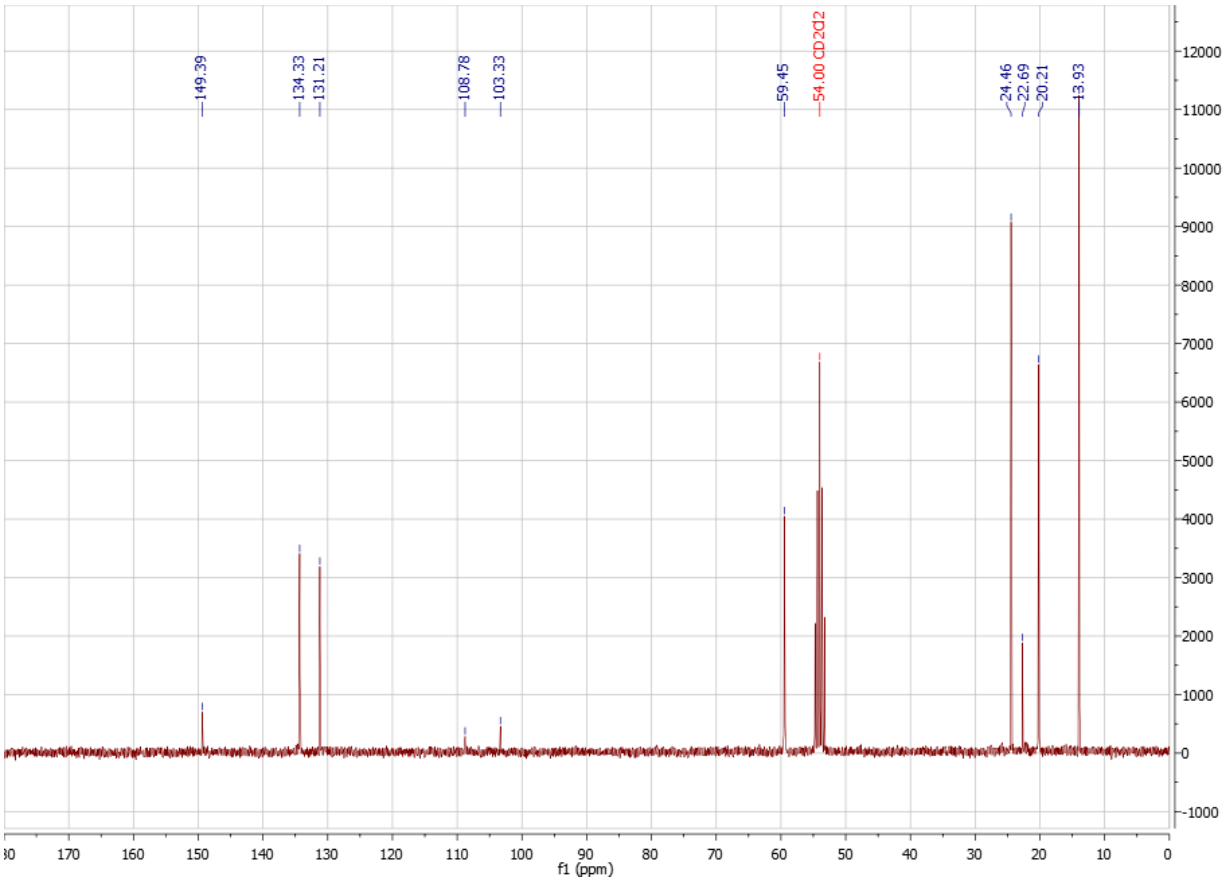


Figure S12: ESI-MS spectrum $(Bu_4N)[B_{12}H_{11}(NCC_6H_4CH_3)]$ (negative area) 2a.

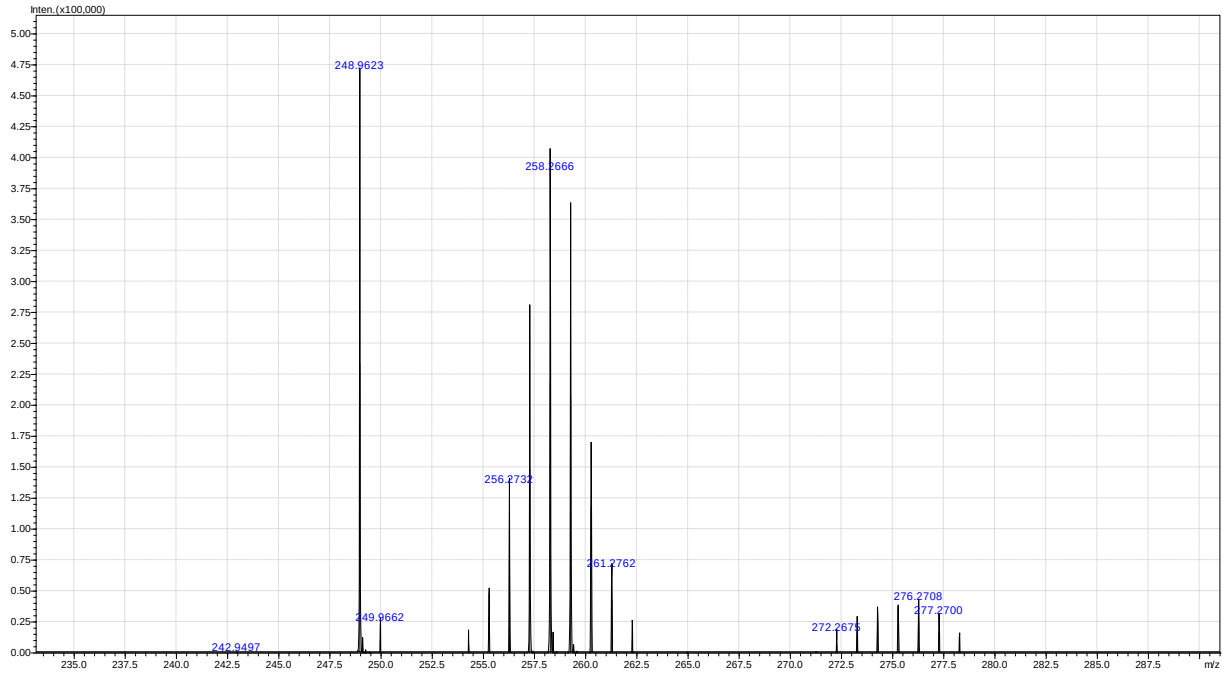


Figure S13: $^{11}B\{^{1}H\}$ NMR spectrum $(Bu_4N)[B_{12}H_{11}(NCC_{10}H_7)]$ 2b

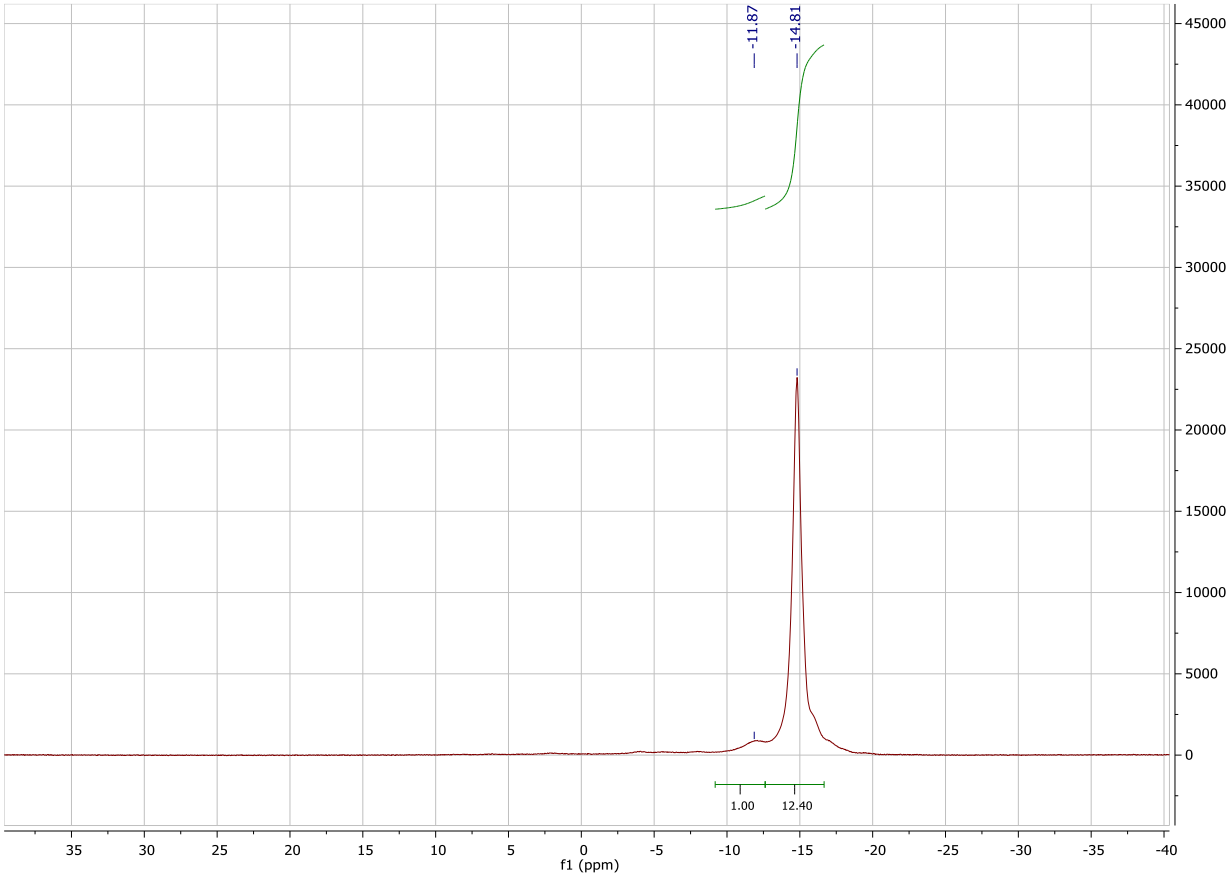


Figure S14: ^{1}H NMR spectrum $(Bu_4N)[B_{12}H_{11}(NCC_{10}H_7)]$ 2b

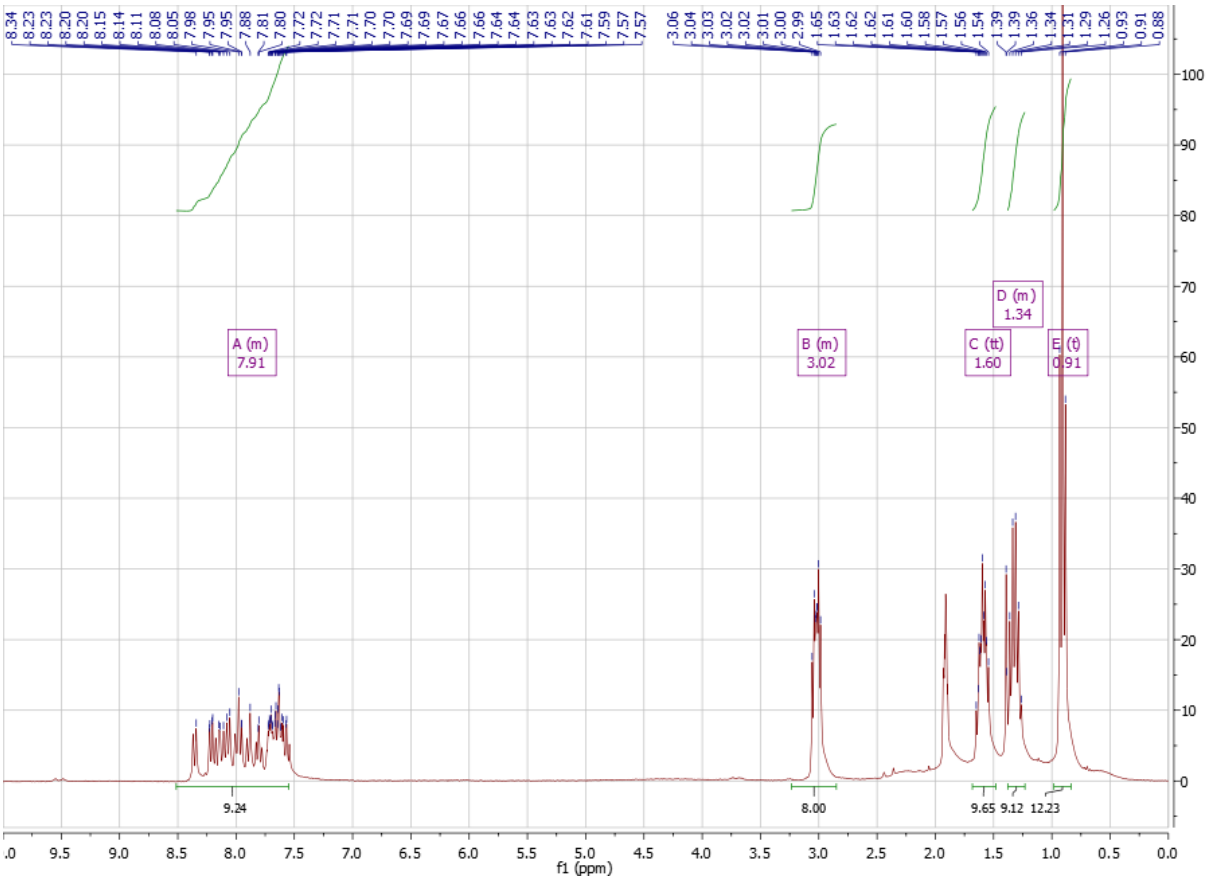


Figure S15: ^{13}C NMR spectrum $(Bu_4N)[B_{12}H_{11}(NCC_{10}H_7)]$ 2b

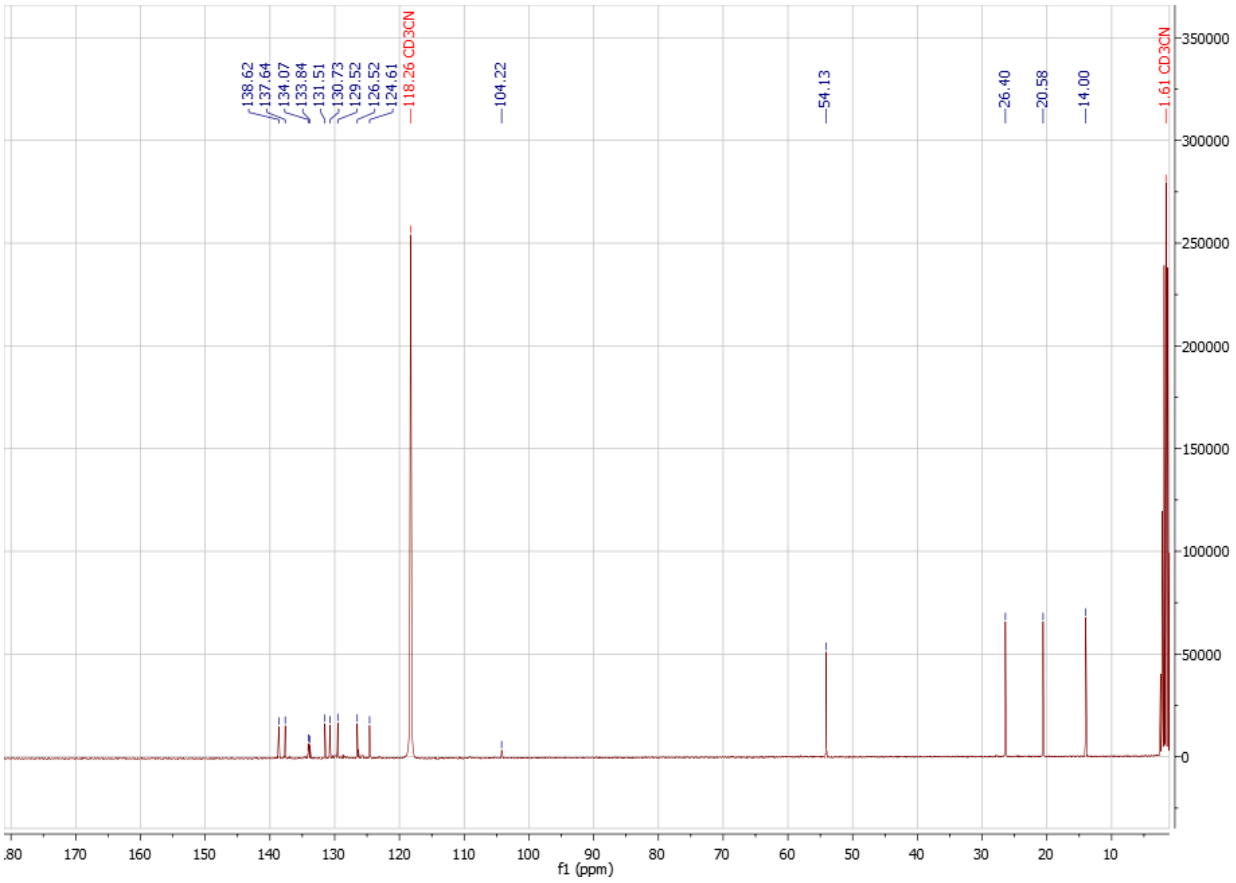
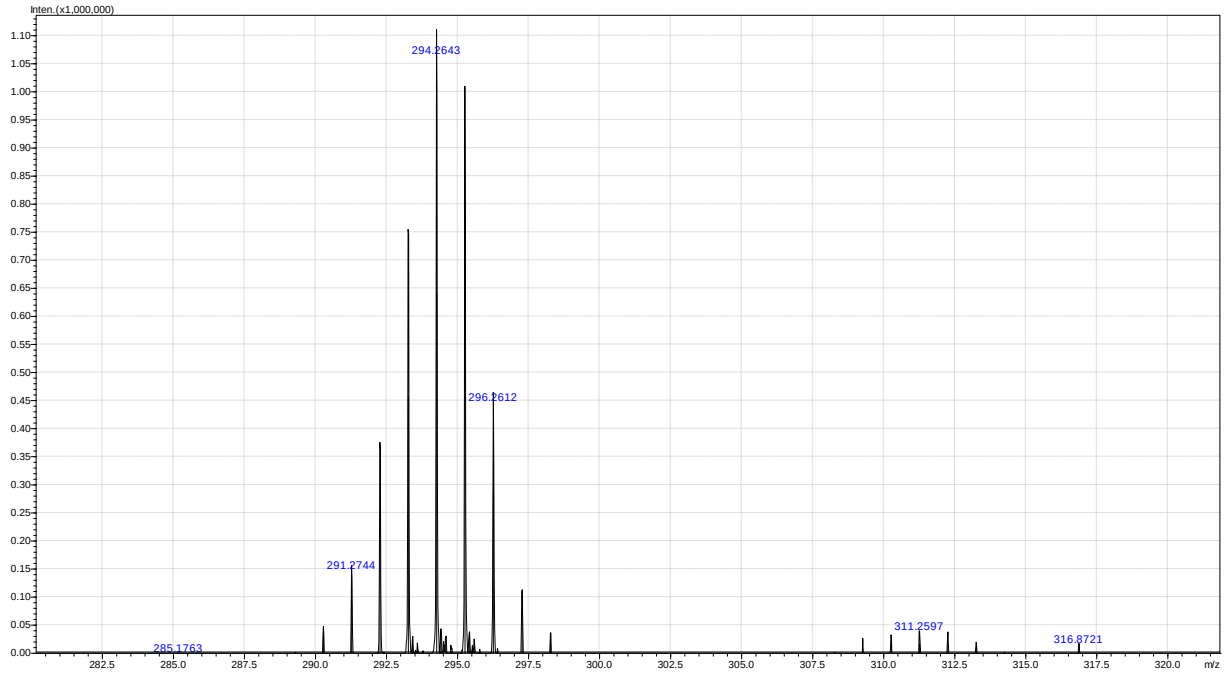


Figure S16: ESI-MS spectrum $(Bu_4N)[B_{12}H_{11}(NCC_{10}H_7)]$ (negative area) 2b.



2. Computational details

Table S1. Cartesian atomic coordinates of the calculated optimized equilibrium model structures. All coordinates are given in Angstrom units.

Optimized equilibrium model structures in gas phase

Structure	Atom	X	Y	Z
CH_3CN				
	C	3.630562	8.675135	11.07631
	N	3.629907	8.675135	9.929943
	C	3.630418	8.675135	12.53245
	H	4.653647	8.675135	12.90432
	H	3.118817	7.78878	12.90337
	H	3.118816	9.561489	12.90337
C_3H_7CN				
	C	-1.16182	0.392019	0.167032
	N	-0.18923	0.455499	0.77186
	C	-2.40726	0.286027	-0.59183
	H	-2.16021	0.365413	-1.65277
	H	-3.02744	1.147895	-0.34104
	C	-3.15512	-1.02233	-0.30942
	H	-3.40385	-1.06583	0.752698
	H	-4.10188	-0.98475	-0.85166
	C	-2.36746	-2.25997	-0.71423
	H	-1.42266	-2.32163	-0.17185
	H	-2.14021	-2.25065	-1.7819
	H	-2.93331	-3.16684	-0.50222
$CH_3C_6H_4CN$				
	N	4.277441	13.89055	2.012378
	C	3.195365	13.63237	1.726994
	C	1.84418	13.30139	1.373594
	C	1.512399	13.03962	0.048194
	C	0.858919	13.2439	2.357545
	C	0.207187	12.72166	-0.28431
	C	-0.43893	12.92415	2.009973
	C	-0.78664	12.65523	0.687225
	H	2.276966	13.08847	-0.71565
	H	1.11679	13.45029	3.387726
	H	-0.0426	12.52302	-1.31942
	H	-1.19965	12.88197	2.780285
	C	-2.19861	12.28403	0.333886
	H	-2.36429	12.31997	-0.74181
	H	-2.42329	11.27072	0.67254
	H	-2.91312	12.95428	0.81238
$[B_{12}H_{11}NCCH_3]^-$				
	N	4.325912	13.83306	2.011305

	C	3.253626	13.57322	1.735547
	C	1.883957	13.24213	1.401799
	H	1.858921	12.68455	0.466858
	H	1.303513	14.1569	1.294105
	H	1.454917	12.63299	2.195851
	B	6.867204	14.70563	1.166121
	H	6.519046	14.85488	0.029281
	B	5.747202	14.14661	2.388537
	B	7.021129	13.06433	1.870918
	H	6.775108	12.09078	1.216802
	B	8.451896	14.08335	1.653831
	H	9.285307	13.81264	0.839485
	B	8.00168	15.76892	2.012542
	H	8.516115	16.69272	1.453074
	B	6.287885	15.80933	2.454173
	H	5.54331	16.71209	2.196705
	B	6.083671	14.8501	3.954984
	H	5.198478	15.09635	4.724295
	B	6.537081	13.15397	3.594338
	H	5.960666	12.24174	4.115938
	B	8.248816	13.13027	3.145429
	H	8.937527	12.18313	3.389144
	B	8.85507	14.7967	3.229246
	H	9.987121	15.03421	3.533543
	B	7.520939	15.85808	3.725013
	H	7.695803	16.84443	4.37886
	B	7.672953	14.2273	4.425238
	H	7.951046	14.05727	5.576188
$[B_{12}H_{11}NCC_3H_7]^-$				
	N	0.068438	7.192772	13.45591
	C	1.124834	6.984769	13.82334
	C	2.479593	6.858705	14.33311
	H	3.1568	6.881742	13.47637
	H	2.581208	5.882947	14.81011
	C	2.792743	8.001467	15.31122
	H	2.124659	7.918754	16.17024
	H	3.808439	7.842071	15.67912
	C	2.659341	9.378904	14.67712
	H	3.318153	9.480664	13.81235
	H	2.923624	10.15619	15.39352
	H	1.637599	9.57135	14.34463
	B	-1.3063	7.594179	13.00327
	B	-2.08307	6.807872	11.64992
	H	-1.54858	5.908926	11.06606
	B	-2.69504	6.583001	13.32125
	H	-2.5778	5.529855	13.87983

	B	-2.46092	8.122929	14.20851
	H	-2.17983	8.124076	15.37386
	B	-1.70537	9.297792	13.0872
	H	-0.90596	10.09808	13.4889
	B	-1.4711	8.487024	11.50666
	H	-0.51436	8.735581	10.82889
	B	-3.81924	6.889395	11.98772
	H	-4.5652	6.038709	11.60008
	B	-4.05149	7.69621	13.5589
	H	-4.9599	7.415972	14.28479
	B	-3.44263	9.364794	13.41623
	H	-3.91818	10.26689	14.04191
	B	-2.8348	9.58844	11.75592
	H	-2.88078	10.64952	11.20532
	B	-3.06712	8.0587	10.87315
	H	-3.27559	8.035186	9.695623
	B	-4.28225	8.603032	12.04928
	H	-5.36629	8.970596	11.70229
$[B_{12}H_{11}NCC_6H_4CH_3]^-$				
	N	4.261241	13.87133	1.998186
	C	3.18226	13.6249	1.724682
	B	6.80437	14.73655	1.162821
	H	6.454142	14.9151	0.030891
	B	5.680054	14.16465	2.376849
	B	6.94142	13.07844	1.83019
	H	6.680897	12.12351	1.155249
	B	8.383602	14.08462	1.629909
	H	9.210067	13.82205	0.805961
	B	7.95534	15.76726	2.027859
	H	8.478665	16.69687	1.486753
	B	6.243803	15.81977	2.477385
	H	5.510673	16.73734	2.243114
	B	6.033035	14.82872	3.957651
	H	5.154867	15.06864	4.736882
	B	6.464707	13.1353	3.557955
	H	5.879047	12.21937	4.061523
	B	8.174431	13.10067	3.101105
	H	8.851725	12.13956	3.320772
	B	8.801405	14.75775	3.219428
	H	9.937529	14.97437	3.523916
	B	7.482098	15.82418	3.744301
	H	7.671121	16.79316	4.41963
	B	7.616771	14.17633	4.407458
	H	7.897088	13.97731	5.553171
	C	1.838329	13.30521	1.374224
	C	1.513714	13.04523	0.045842

	C	0.85691	13.24798	2.362976
	C	0.209273	12.72592	-0.28477
	C	-0.43902	12.92746	2.012245
	C	-0.78312	12.65818	0.688402
	H	2.282403	13.09515	-0.71354
	H	1.119468	13.45332	3.392017
	H	-0.04044	12.52587	-1.31953
	H	-1.20078	12.8833	2.781325
	C	-2.19389	12.28214	0.334557
	H	-2.35738	12.31283	-0.74174
	H	-2.41625	11.26972	0.677701
	H	-2.91061	12.9531	0.808963

Table S2. Cartesian atomic coordinates of the calculated optimized equilibrium model structures. All coordinates are given in Angstrom units.

Optimized equilibrium model structures in dichloromethane

Structure	Atom	X	Y	Z
CH_3CN				
	C	3.630907	8.674766	11.08262
	N	3.629215	8.675509	9.935158
	C	3.630845	8.675065	12.53356
	H	4.655861	8.675154	12.90093
	H	3.117673	7.787039	12.89898
	H	3.117667	9.563277	12.89851
C_3H_7CN				
	C	-1.16558	0.401083	0.166245
	N	-0.19276	0.477471	0.77098
	C	-2.40677	0.284795	-0.5923
	H	-2.15263	0.364654	-1.65115
	H	-3.02629	1.146264	-0.33979
	C	-3.15024	-1.02472	-0.30544
	H	-3.3988	-1.06866	0.756692
	H	-4.09505	-0.98072	-0.84936
	C	-2.37019	-2.26382	-0.7162
	H	-1.42657	-2.34379	-0.17171
	H	-2.14069	-2.25025	-1.78377
	H	-2.94488	-3.16744	-0.50954
$CH_3C_6H_4CN$				
	N	4.271856	13.88835	2.011885
	C	3.189268	13.63002	1.725518
	C	1.840578	13.30058	1.372561
	C	1.513756	13.03972	0.044248
	C	0.857827	13.24436	2.36124
	C	0.208235	12.72222	-0.28725
	C	-0.43956	12.9248	2.012091

	C	-0.78556	12.65617	0.686936
	H	2.277556	13.0883	-0.72056
	H	1.114584	13.45021	3.391937
	H	-0.04141	12.52365	-1.32237
	H	-1.20032	12.88202	2.782246
	C	-2.19571	12.28532	0.334104
	H	-2.36059	12.31852	-0.74216
	H	-2.4186	11.27227	0.676456
	H	-2.9098	12.95514	0.814652
$[B_{12}H_{11}NCCH_3]^-$				
	N	4.297232	13.82544	2.00802
	C	3.223949	13.56685	1.731883
	C	1.864256	13.241	1.3922
	H	1.855165	12.68515	0.455707
	H	1.295144	14.16315	1.284746
	H	1.439596	12.63189	2.189041
	B	6.862616	14.70124	1.174707
	H	6.533315	14.85581	0.035577
	B	5.72116	14.13855	2.384968
	B	7.018197	13.06915	1.876748
	H	6.794067	12.09203	1.224997
	B	8.449814	14.08513	1.657818
	H	9.28689	13.81658	0.845884
	B	7.999859	15.76505	2.014874
	H	8.517522	16.68864	1.457073
	B	6.286911	15.79941	2.45624
	H	5.558327	16.71334	2.20382
	B	6.086943	14.846	3.950335
	H	5.219282	15.099	4.733329
	B	6.53904	13.1588	3.591822
	H	5.983263	12.24402	4.125192
	B	8.250645	13.13602	3.145293
	H	8.945731	12.19318	3.389595
	B	8.858328	14.79871	3.228142
	H	9.991182	15.03795	3.530784
	B	7.523155	15.8541	3.722472
	H	7.703876	16.84024	4.375866
	B	7.677216	14.22935	4.421096
	H	7.963217	14.06188	5.57092
$[B_{12}H_{11}NCC_3H_7]^-$				
	N	0.049664	7.497433	13.47797
	C	1.111652	7.317123	13.84642
	C	2.46569	7.155164	14.32843
	H	3.117095	7.199077	13.45296
	H	2.542561	6.15438	14.75543
	C	2.826068	8.241201	15.35269

	H	2.19072	8.124613	16.23168
	H	3.850079	8.03775	15.66685
	C	2.711157	9.651327	14.79638
	H	3.32832	9.776989	13.90454
	H	3.038861	10.38094	15.53721
	H	1.68085	9.898246	14.53015
	B	-1.34905	7.782691	13.00268
	B	-2.05754	6.864926	11.6852
	H	-1.45074	5.990738	11.13997
	B	-2.65824	6.668031	13.35352
	H	-2.46472	5.657418	13.96267
	B	-2.58272	8.258581	14.15765
	H	-2.33684	8.34966	15.32433
	B	-1.93527	9.437668	12.98654
	H	-1.23847	10.34146	13.34428
	B	-1.61084	8.576914	11.45911
	H	-0.6926	8.886153	10.75839
	B	-3.79668	6.793979	12.00469
	H	-4.45639	5.858481	11.65639
	B	-4.11954	7.651091	13.52563
	H	-5.00748	7.324538	14.25829
	B	-3.67464	9.355287	13.3004
	H	-4.24606	10.2372	13.87294
	B	-3.07725	9.551359	11.63968
	H	-3.22723	10.57238	11.03376
	B	-3.15171	7.968384	10.8387
	H	-3.35017	7.865485	9.663193
	B	-4.42563	8.450804	11.97358
	H	-5.53752	8.692192	11.60244
$[B_{12}H_{11}NCC_6H_4CH_3]^-$				
	N	4.237555	13.86037	1.992333
	C	3.158563	13.61514	1.713848
	B	6.804739	14.73088	1.172133
	H	6.473326	14.91287	0.037769
	B	5.661489	14.15327	2.373293
	B	6.946991	13.08198	1.838423
	H	6.710654	12.12244	1.165379
	B	8.387316	14.08857	1.636629
	H	9.218745	13.82939	0.815897
	B	7.955491	15.76498	2.03163
	H	8.480721	16.69515	1.492131
	B	6.244551	15.80733	2.478674
	H	5.524703	16.73369	2.248146
	B	6.038245	14.82302	3.952167
	H	5.175498	15.06923	4.742538
	B	6.473599	13.13895	3.556118

	H	5.909805	12.2188	4.071192
	B	8.183722	13.10958	3.104195
	H	8.870023	12.15474	3.325936
	B	8.807397	14.76401	3.220929
	H	9.943497	14.98525	3.525168
	B	7.484387	15.82166	3.741977
	H	7.676329	16.79119	4.416653
	B	7.623891	14.18042	4.404788
	H	7.911346	13.98544	5.549928
	C	1.821181	13.29986	1.36572
	C	1.502129	13.04294	0.032758
	C	0.844608	13.24467	2.362998
	C	0.197924	12.72628	-0.2946
	C	-0.44996	12.92655	2.011557
	C	-0.79306	12.65935	0.684051
	H	2.268135	13.09281	-0.72912
	H	1.106622	13.4478	3.392425
	H	-0.05458	12.52782	-1.32856
	H	-1.21189	12.88196	2.779848
	C	-2.20178	12.28712	0.333076
	H	-2.36683	12.31231	-0.74303
	H	-2.42123	11.27642	0.684546
	H	-2.91471	12.95912	0.811979

Table S3. Cartesian atomic coordinates of the calculated optimized equilibrium model structures. All coordinates are given in Angstrom units.

Optimized equilibrium model structures in acetonitrile

Structure	Atom	X	Y	Z
CH_3CN				
	C	3.630907	8.674766	11.08346
	N	3.629215	8.675509	9.935744
	C	3.630841	8.675065	12.53377
	H	4.656107	8.675153	12.90039
	H	3.117552	7.786816	12.89843
	H	3.117544	9.5635	12.89797
C_3H_7CN				
	C	-1.16615	0.400522	0.165426
	N	-0.1929	0.476764	0.769899
	C	-2.40721	0.284623	-0.59247
	H	-2.15291	0.3649	-1.6512
	H	-3.02608	1.146248	-0.33906
	C	-3.15019	-1.02486	-0.30515
	H	-3.39936	-1.06852	0.75683
	H	-4.09442	-0.98051	-0.8498
	C	-2.36992	-2.26366	-0.71589

	H	-1.42656	-2.34419	-0.17073
	H	-2.13985	-2.24919	-1.78331
	H	-2.9449	-3.16727	-0.50987
$CH_3C_6H_4CN$				
	N	4.27106	13.88775	2.011749
	C	3.188257	13.62957	1.72529
	C	1.839997	13.30049	1.372412
	C	1.513777	13.03978	0.043777
	C	0.857554	13.24448	2.361611
	C	0.208294	12.72232	-0.28759
	C	-0.43971	12.92497	2.012301
	C	-0.7854	12.65627	0.686919
	H	2.27745	13.08828	-0.72118
	H	1.114093	13.45028	3.392392
	H	-0.04136	12.52373	-1.32269
	H	-1.20049	12.88219	2.782411
	C	-2.19519	12.28547	0.334119
	H	-2.35976	12.31851	-0.74218
	H	-2.41746	11.27242	0.676907
	H	-2.90899	12.95512	0.815281
$[B_{12}H_{11}NCCH_3]^-$				
	N	4.294097	13.82437	2.007367
	C	3.220364	13.56585	1.730961
	C	1.861732	13.24108	1.391191
	H	1.854329	12.68539	0.454547
	H	1.294614	14.16455	1.284054
	H	1.438206	12.63217	2.188848
	B	6.862111	14.70063	1.175553
	H	6.534479	14.85557	0.036318
	B	5.717554	14.13727	2.384278
	B	7.018006	13.06949	1.877335
	H	6.795841	12.09225	1.225702
	B	8.449491	14.08555	1.658811
	H	9.287879	13.81767	0.847821
	B	7.999548	15.76419	2.015502
	H	8.518464	16.68767	1.45841
	B	6.286617	15.7982	2.456364
	H	5.559413	16.71294	2.204359
	B	6.087122	14.84539	3.949788
	H	5.221038	15.09891	4.733871
	B	6.539269	13.15913	3.591535
	H	5.98546	12.24417	4.125929
	B	8.25085	13.13723	3.145264
	H	8.947615	12.19556	3.389916
	B	8.858238	14.79895	3.227966
	H	9.991224	15.03855	3.530493

	B	7.523372	15.85316	3.721898
	H	7.705684	16.83916	4.375289
	B	7.677718	14.22971	4.420095
	H	7.965562	14.06291	5.569688
$[B_{12}H_{11}NCC_3H_7]^-$				
	N	0.054424	7.488018	13.4713
	C	1.114816	7.309481	13.84644
	C	2.459533	7.151076	14.35125
	H	3.125391	7.171015	13.4859
	H	2.522244	6.160322	14.80335
	C	2.805923	8.259857	15.35573
	H	2.146429	8.173256	16.22027
	H	3.818752	8.053092	15.70166
	C	2.722706	9.655369	14.75918
	H	3.378432	9.75423	13.89193
	H	3.022296	10.40235	15.49455
	H	1.705936	9.90003	14.44227
	B	-1.34243	7.777797	12.99586
	B	-2.05482	6.873521	11.67037
	H	-1.45162	6.002454	11.11696
	B	-2.65622	6.664181	13.3362
	H	-2.46712	5.647987	13.93672
	B	-2.57757	8.247256	14.15315
	H	-2.33346	8.328665	15.32053
	B	-1.9274	9.434098	12.99258
	H	-1.22972	10.33376	13.35781
	B	-1.60458	8.58575	11.45865
	H	-0.68691	8.899352	10.75973
	B	-3.79423	6.803882	11.98859
	H	-4.45647	5.873083	11.63226
	B	-4.11551	7.648746	13.51597
	H	-5.00469	7.318235	14.24549
	B	-3.66698	9.353243	13.30505
	H	-4.23696	10.23164	13.88461
	B	-3.06893	9.56167	11.64671
	H	-3.21714	10.58795	11.04911
	B	-3.14665	7.986067	10.83295
	H	-3.3457	7.893321	9.656601
	B	-4.41979	8.461827	11.97097
	H	-5.53124	8.708775	11.60154
$[B_{12}H_{11}NCC_6H_4CH_3]^-$				
	N	4.235715	13.85911	1.991368
	C	3.156171	13.61408	1.712826
	B	6.804941	14.72893	1.1726
	H	6.476019	14.91051	0.037721
	B	5.658282	14.15172	2.372325

	B	6.947304	13.08149	1.840151
	H	6.713705	12.12094	1.168061
	B	8.387545	14.08779	1.637931
	H	9.220118	13.82837	0.818323
	B	7.955543	15.76379	2.031108
	H	8.481783	16.6934	1.491458
	B	6.244615	15.80592	2.477311
	H	5.526558	16.73324	2.246237
	B	6.038148	14.82352	3.950853
	H	5.177268	15.06936	4.742965
	B	6.473742	13.13996	3.556675
	H	5.91205	12.21989	4.073601
	B	8.183961	13.1106	3.105707
	H	8.87143	12.15681	3.328734
	B	8.807623	14.76464	3.221147
	H	9.943718	14.98642	3.525483
	B	7.484246	15.8219	3.740521
	H	7.677049	16.79191	4.41441
	B	7.623761	14.18202	4.404574
	H	7.912105	13.98851	5.549822
	C	1.819829	13.29957	1.365106
	C	1.500469	13.04586	0.03128
	C	0.844133	13.24147	2.363501
	C	0.196353	12.72967	-0.29577
	C	-0.45018	12.9235	2.012015
	C	-0.79376	12.65967	0.683778
	H	2.265716	13.09804	-0.73117
	H	1.106355	13.44251	3.393253
	H	-0.05714	12.53391	-1.32997
	H	-1.21172	12.8763	2.78047
	C	-2.20217	12.28794	0.332933
	H	-2.36796	12.31605	-0.74291
	H	-2.41976	11.27609	0.682267
	H	-2.91457	12.95774	0.815596

Table S4. Crystal data and structure refinement for **1a** and **1b**.

entification code	**1a**	**1b**
Empirical formula	$C_{10}H_{34}B_{12}N_2$	$C_{28}H_{38}B_{12}NP$
Formula weight	312.11	549.28
Temperature/K	100	100
Crystal system	orthorhombic	triclinic
Space group	Pbcn	P-1
a/Å	13.711(6)	10.076(2)
b/Å	17.515(3)	11.413(3)
c/Å	17.391(5)	15.720(4)
α/°	90	103.483(12)

β/°	90	95.907(10)
γ/°	90	113.512(9)
Volume/Å^3	4177(2)	1572.6(7)
Z	8	2
ρ_{calc}g/cm^3	0.993	1.160
μ/mm^{-1}	0.049	0.109
F(000)	1344.0	576.0
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
Reflections collected	12508	20048
Independent reflections	4079 [R_{int} = 0.0450, R_{sigma} = 0.0565]	8269 [R_{int} = 0.0279, R_{sigma} = 0.0393]
Data/restraints/parameters	4079/0/223	8269/0/380
Goodness-of-fit on F^2	1.033	1.061
Final R indexes [I>=2σ (I)]	R_1 = 0.0886, wR_2 = 0.2524	R_1 = 0.0488, wR_2 = 0.1279
Final R indexes [all data]	R_1 = 0.1095, wR_2 = 0.2738	R_1 = 0.0585, wR_2 = 0.1336