SUPPORTING INFORMATION

Syntheses and Reductions of *C*-Dimesitylboryl-1,2-dicarba-*closo*-dodecaboranes

Jan Kahlert,[a] Lena Böhling,[a] Andreas Brockhinke,[a] Hans-Georg Stammler,[a] Beate Neumann,[a] Louis M. Rendina,[b] Paul J. Low,[c] Lothar Weber,*[,a] and Mark A. Fox*[,d]

[a] Fakultät für Chemie der Universität Bielefeld, 33615 Bielefeld, Germany.

E-mail: lothar.weber@uni-bielefeld.de

[b] School of Chemistry, The University of Sydney, Sydney, NSW 2006, Australia.

[c] School of Chemistry and Biochemistry, University of Western Australia, 35 Stirling Highway, Crawley, Perth 6009, Australia

[d] Department of Chemistry, Durham University, Durham DH1 3LE, United Kingdom.

E-mail: m.a.fox@durham.ac.uk

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Absorption spectra for **1** and **2,** detailed CV data for **1** and **2**, TD-DFT data for **1** and **2**, spectroelectrochemical data for **2**, computed GIAO-NMR data for **1-4**, NMR spectra for **1-4** and dianions $[\mathbf{2}]^{2-}$ and $[\mathbf{5}]^{2-}$, crystallographic data for **1** and **2** and Cartesian coordinates for eleven optimised geometries.

Figure S1. Absorption spectra of **1** and **2**.

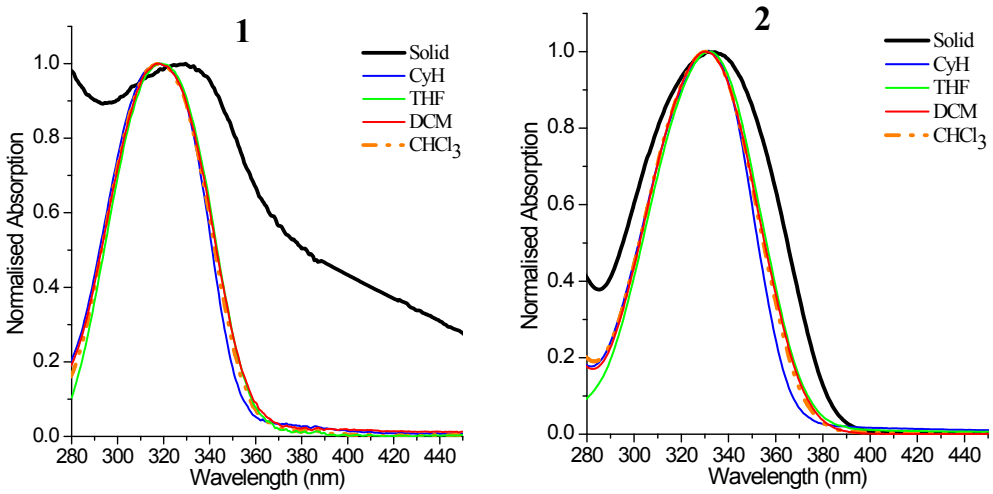

Figure S2. CV plots of **1** (left) and **2** with different solvents and working electrodes.

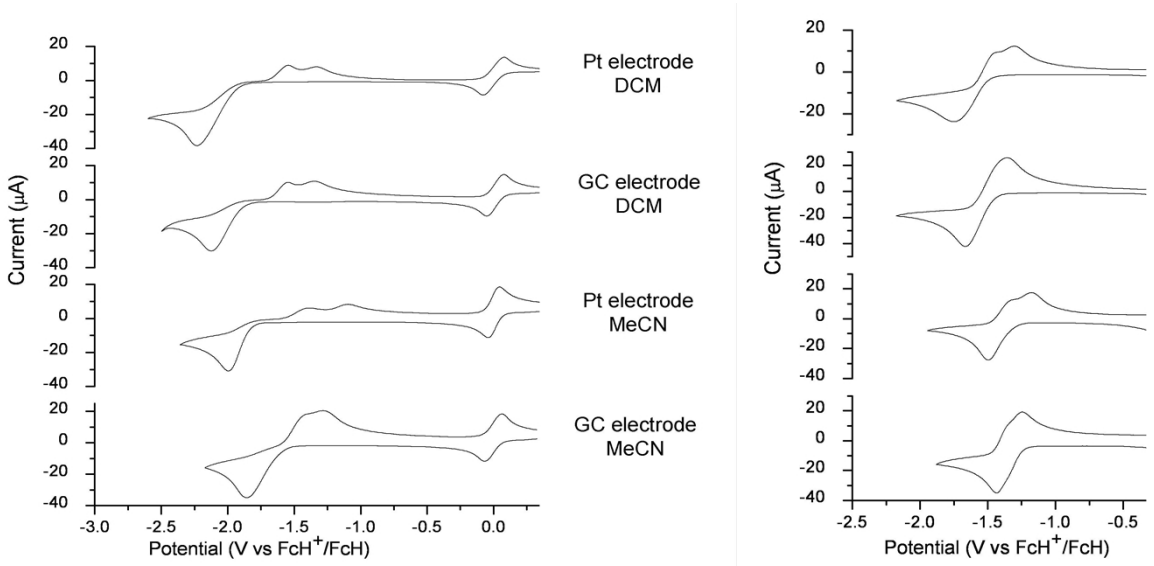

Table S1. Detailed CV data for **1** and **2**. Potentials are referenced to the internal ferrocenium/ferrocene couple at 0.0 V.

	Solvent	Working Electrode	E^{c}_{red1} (V)	E^{a}_{red1} (V)	$E^{½}_{red1}$ (V)	$E^{p\text{-}p}_{red1}$ (mV)	E^{c}_{red2} (V)	E^{a}_{red2} (V)	$E^{½}_{red2}$ (V)	$E^{p\text{-}p}_{red2}$ (mV)
1	DCM	Pt	-2.23	*-1.34*			-2.23	*-1.54*		
	DCM	GC	-2.12	*-1.35*			-2.12	*-1.55*		
	MeCN	Pt	-1.99	*-1.10*			-1.99	*-1.39*		
	MeCN	GC	-1.86	*-1.29*			-1.86	*-1.43*		
2	DCM	Pt	-1.75	-1.31	-1.53	440	-1.75	-1.45	-1.60	300
	DCM	GC	-1.66	-1.36	-1.51	300	-1.66	-1.36	-1.51	300
	MeCN	Pt	-1.50	-1.18	-1.34	320	-1.50	-1.33	-1.42	170
	MeCN	GC	-1.36	-1.25	-1.31	110	-1.44	-1.35	-1.39	90

DCM = dichloromethane, MeCN = acetonitrile, Pt = platinum, GC = glassy carbon

Descriptions for Table S1.
E^{c}_{red1} = cathodic wave on first one-electron reduction.
E^{a}_{red1}= anodic wave on first one-electron reduction.
E^{c}_{red2} = cathodic wave on second one-electron reduction – two-electron cathodic waves are usually observed so for these cathodic waves, $E^{c}_{red1} = E^{c}_{red2}$.
E^{a}_{red2} = anodic wave on second one-electron reduction – this would be at more negative potential than the anodic wave for the first one-electron reduction.
$E_{p\text{-}p}$ = peak separation between the cathodic and anodic waves.
$E^{½}$ = half step potential

Potentials reported in italics are those that are likely to be from rearranged / decomposed products after reductions to the dianions.

Figure S3. Observed and simulated square-wave voltammetry plots for **2** in MeCN with GC working electrode with the ferrocenium/ferrocene couple used as the reversible one-electron reference.

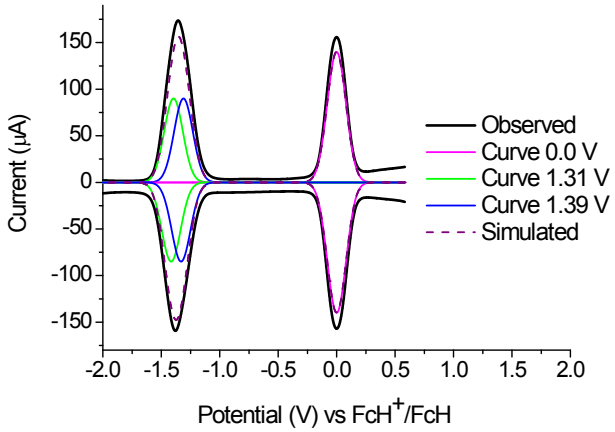

Figure S4. Absorption spectra of **2** and its reduced species in acetonitrile using a thin-layer spectroelectrochemical cell. The spectrum corresponding to the monoanion radical is not seen in the slow reduction of **2** to $[\mathbf{2}]^{2-}$.

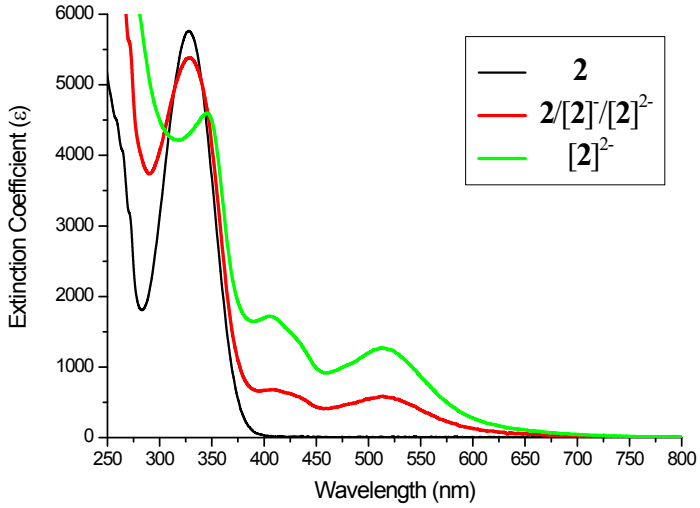

Table S2. Comparison between calculated and observed ^{11}B NMR data and assignment of boron peaks for **1**-**4**. The computed shifts are averaged for symmetry-equivalent boron atoms (3,6), (4,5), (7,11) and (8,10).

Compound	$\delta^{11}B$(exp.) [ppm]	$\delta^{11}B$(calcd.) [ppm]	Assignment
1	-12.9 (4)	-12.9	B7,11
		-12.7	B3,6
	-9.1 (2)	-8.6	B4,5
	-6.9 (2)	-6.1	B8,10
	-2.3 (1)	-1.1	B9
	1.9 (1)	3.7	B12
	78.9 (1)	78.1	$BMes_2$
2	-9.9 (4)	-10.3	B3,6
		-9.0	B4,5
	-8.0 (4)	-6.3	B8,10
		-6.2	B7,11
	-2.8 (1)	-1.1	B9
	3.7 (1)	5.3	B12
	80.4 (1)	79.4	$BMes_2$
3	-12.6 (6)	-12.9	B7,11
		-12.9	B3,6
		-10.8	B4,5
	-7.8 (2)	-6.9	B8,10
	-2.1 (1)	-0.5	B9
	-1.0 (1)	1.2	B12
	26.5 (1)	23.7	$B(OH)_2$
4	-11.7 (2)	-11.3	B3,6
	-10.6 (2)	-9.6	B7,11
	-8.3 (4)	-8.1	B4,5
		-7.4	B8,10
	-3.1 (1)	-1.2	B9
	0.9 (1)	2.5	B12
	26.5 (1)	22.3	$B(OH)_2$

Table S3. TD-DFT data for the S_0 geometry of **1**.

Excited state	Energy [eV]	Wavelength [nm]	Oscillator strength	MO contributions [%]	Transition type
1	3.55	349	0.0123	HOMO-2 →LUMO (43) HOMO-1 → LUMO (15) HOMO → LUMO (51)	π(Mes) → p(B) π(Mes) → p(B) π(Mes) → p(B)
2	3.60	345	0.0427	HOMO-2 → LUMO (53) HOMO → LUMO (43)	π(Mes) → p(B) π(Mes) → p(B)
3	3.61	344	0.0698	HOMO-1 → LUMO (66) HOMO → LUMO (19)	π(Mes) → p(B) π(Mes) → p(B)
4	3.74	331	0.0065	HOMO-3 → LUMO (69) HOMO-2 → LUMO (13)	π(Mes) → p(B) π(Mes) → p(B)
5	5.09	244	0.0012	HOMO-4 → LUMO (11) HOMO-3 →LUMO+1 (32) HOMO-3 → LUMO+2 (11) HOMO-3 → LUMO+3 (14) HOMO-2 → LUMO+1 (20) HOMO-2 → LUMO+2 (31) HOMO-2 → LUMO+4 (13) HOMO-1 → LUMO+2 (24) HOMO → LUMO+1 (33) HOMO → LUMO+2 (12)	Cage → p(B) π(Mes) → π*(Mes) π(Mes) → π*(Mes) π(Mes) → π*(Mes)/cage* π(Mes) → π*(Mes) π(Mes) → π*(Mes) π(Mes) → π*(Mes) π(Mes) → π*(Mes) π(Mes) → π*(Mes) π(Mes) → π*(Mes)
6	5.13	242	0.0025	HOMO-10 → LUMO (10) HOMO-9 → LUMO (16) HOMO-8 → LUMO (18) HOMO-7 → LUMO (16) HOMO-6 → LUMO (21) HOMO-5 → LUMO (28) HOMO-4 → LUMO (47) HOMO → LUMO+1 (13)	Cage/π(Mes) → p(B) Cage → p(B) Cage → p(B) Cage → p(B) Cage → p(B) Cage → p(B) Cage → p(B) π(Mes) → π*(Mes)
7	5.18	240	0.0016	HOMO-3 → LUMO+1 (31) HOMO-2 → LUMO+1 (13) HOMO-2 → LUMO+2 (21) HOMO-1 → LUMO+1 (14) HOMO-1 → LUMO+2 (11)	π(Mes) → π*(Mes) π(Mes) → π*(Mes) π(Mes) → π*(Mes) π(Mes) → π*(Mes) π(Mes) → π*(Mes)

				HOMO-1 → LUMO+3 (14) HOMO-1 → LUMO+4 (27) HOMO → LUMO+1 (37) HOMO → LUMO+3 (22)	π(Mes) → π*(Mes)/cage* π(Mes) → π*(Mes) π(Mes) → π*(Mes) π(Mes) → π*(Mes)/cage*
8	5.35	232	0.0014	HOMO-10 → LUMO (16) HOMO-6 → LUMO (35) HOMO-5 → LUMO (55) HOMO-4 → LUMO (11) HOMO-1 → LUMO+1 (13)	Cage/π(Mes) → p(B) Cage → p(B) Cage → p(B) Cage → p(B) π(Mes) → π*(Mes)
9	5.40	230	0.1248	HOMO-5 → LUMO (13) HOMO-1 → LUMO+1 (61) HOMO → LUMO+1 (20) HOMO → LUMO+2 (12)	Cage → p(B) π(Mes) → π*(Mes) π(Mes) → π*(Mes) π(Mes) → π*(Mes)
10	5.43	228	0.0082	HOMO-8 → LUMO (16) HOMO-7 → LUMO (12) HOMO-6 → LUMO (41) HOMO-5 → LUMO (21) HOMO-4 → LUMO (47)	Cage → p(B) Cage → p(B) Cage → p(B) Cage → p(B) Cage → p(B)

Table S4. TD-DFT data for the S_0 geometry of **2**.

Excited state	Energy [eV]	Wavelength [nm]	Oscillator strength	MO contributions [%]	Transition type
1	3.45	359	0.0297	HOMO-2 →LUMO (49) HOMO-1 → LUMO (33) HOMO → LUMO (36)	π(Mes) → p(B) π(Mes) → p(B) π(Mes) → p(B)
2	3.50	355	0.0237	HOMO-2 → LUMO (36) HOMO → LUMO (58)	π(Mes) → p(B) π(Mes) → p(B)
3	3.53	352	0.0683	HOMO-2 → LUMO (32) HOMO-1 → LUMO (59) HOMO → LUMO (12)	π(Mes) → p(B) π(Mes) → p(B) π(Mes) → p(B)
4	3.64	341	0.0068	HOMO-3 → LUMO (70)	π(Mes) → p(B)
5	4.34	286	0.0095	HOMO-4 → LUMO (70)	π(Ph) → p(B)
6	4.43	280	0.0003	HOMO-5 → LUMO (70)	π(Ph) → p(B)
7	4.68	265	0.0053	HOMO-2 → LUMO+1 (38) HOMO-1 → LUMO+1 (52) HOMO → LUMO+1 (27)	π(Mes) → π*(Ph) π(Mes) → π*(Ph) π(Mes) → π*(Ph)
8	4.71	263	0.0035	HOMO-3 → LUMO+1 (36) HOMO-2 → LUMO+1 (11) HOMO-1 → LUMO+1 (20) HOMO → LUMO+1 (55)	π(Mes) → π*(Ph) π(Mes) → π*(Ph) π(Mes) → π*(Ph) π(Mes) → π*(Ph)
9	4.82	257	0.0178	HOMO-3 → LUMO+1 (13) HOMO-2 → LUMO+1 (57) HOMO-1 → LUMO+1 (37)	π(Mes) → π*(Ph) π(Mes) → π*(Ph) π(Mes) → π*(Ph)
10	4.88	254	0.0005	HOMO-3 → LUMO+1 (58) HOMO-1 → LUMO+1 (21) HOMO → LUMO+1 (32)	π(Mes) → π*(Ph) π(Mes) → π*(Ph) π(Mes) → π*(Ph)

Figure S5: ^{1}H NMR spectrum of **1**.

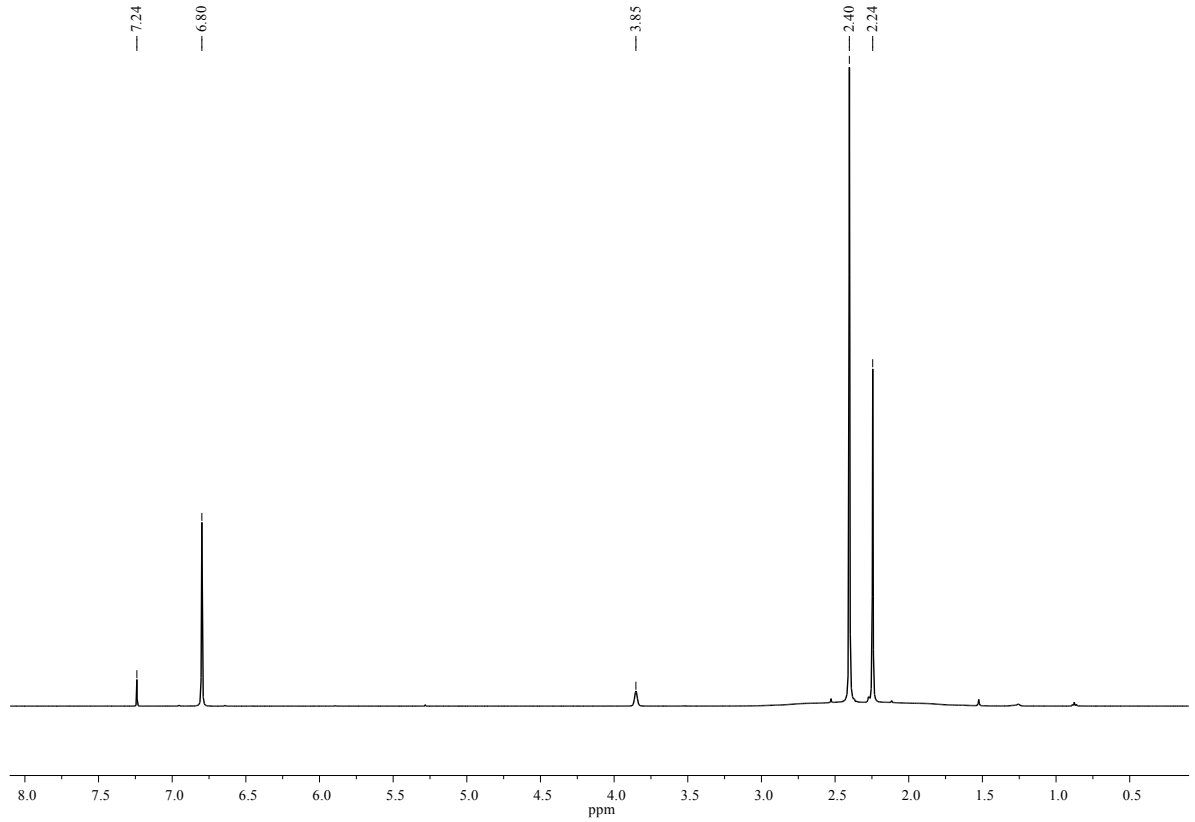

Figure S6: Baseline-corrected $^{11}B\{^{1}H\}$ NMR spectrum of **1**.

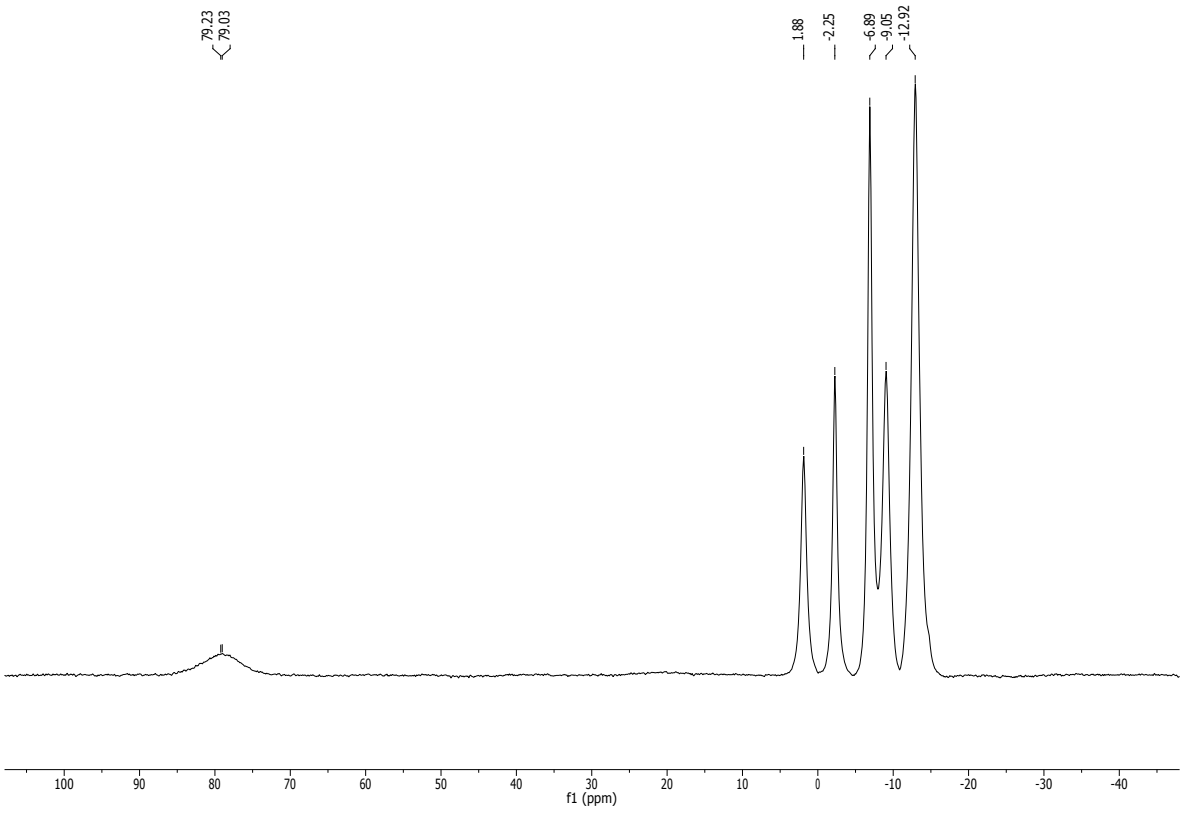

Figure S7: $^{13}C\{^{1}H\}$ NMR spectrum of **1**.

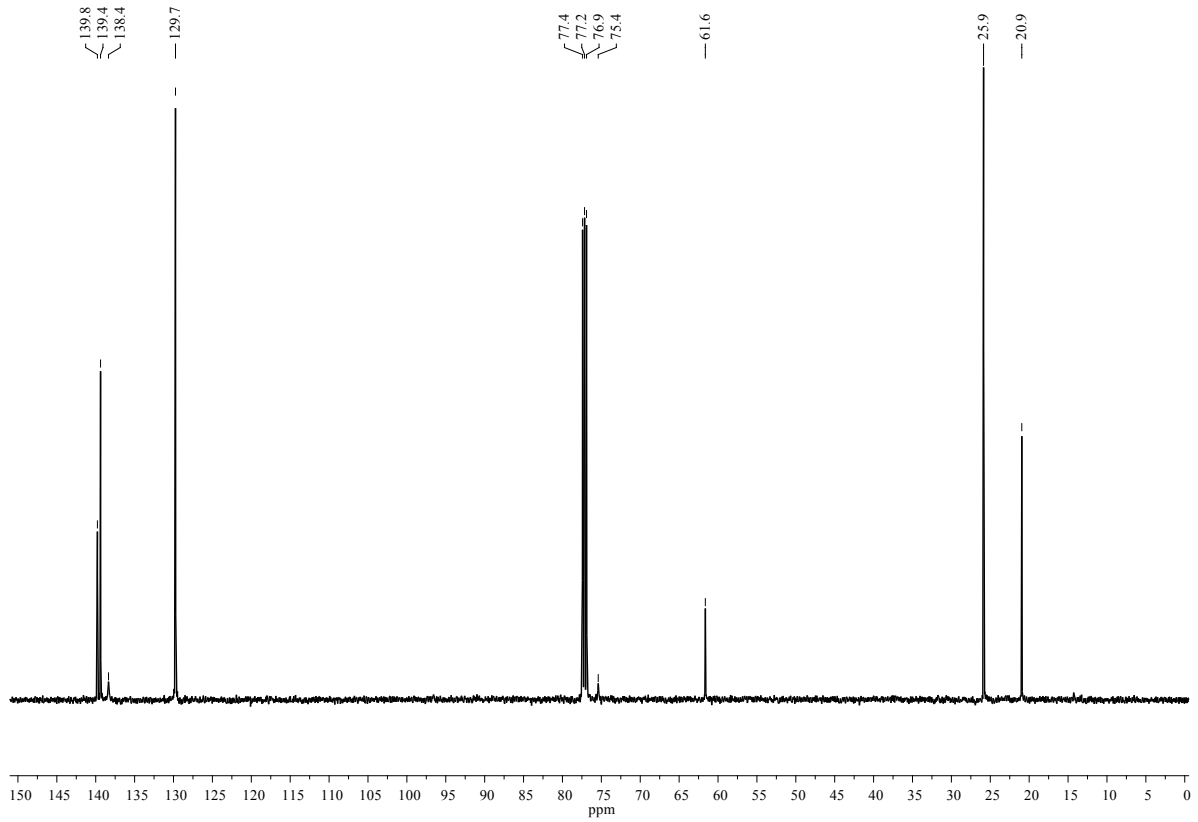

Figure S8: ^{1}H NMR spectrum of **2**.

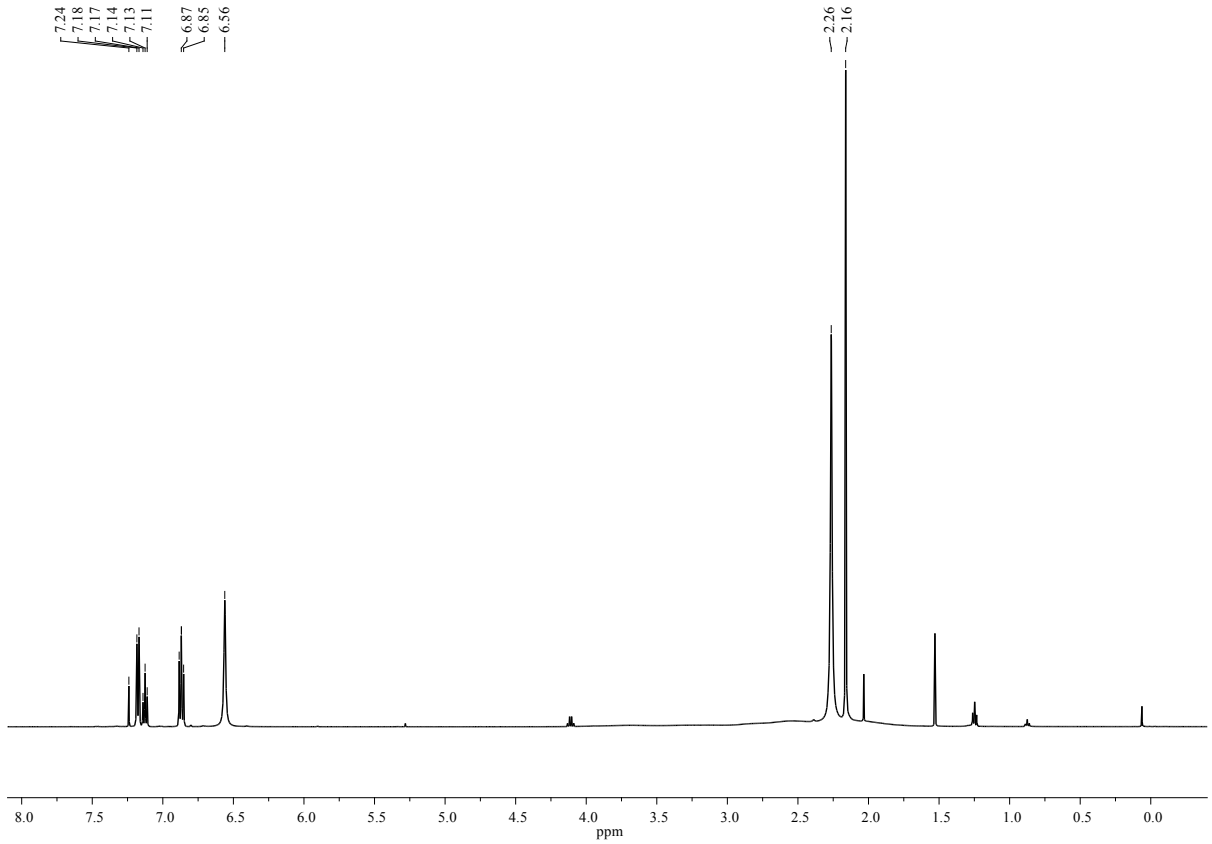

Figure S9: Baseline-corrected $^{11}B\{^{1}H\}$ NMR spectrum of **2**.

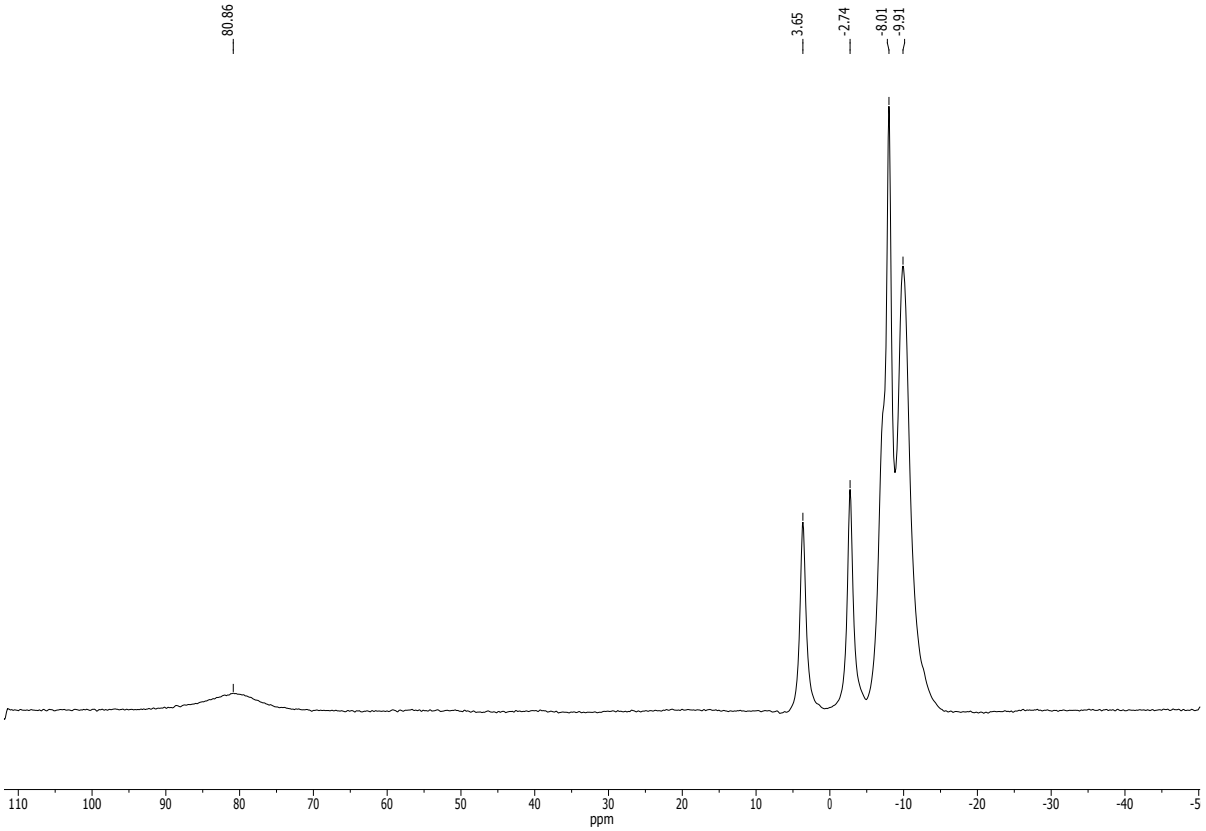

Figure S10: $^{13}C\{^{1}H\}$ NMR spectrum of **2**.

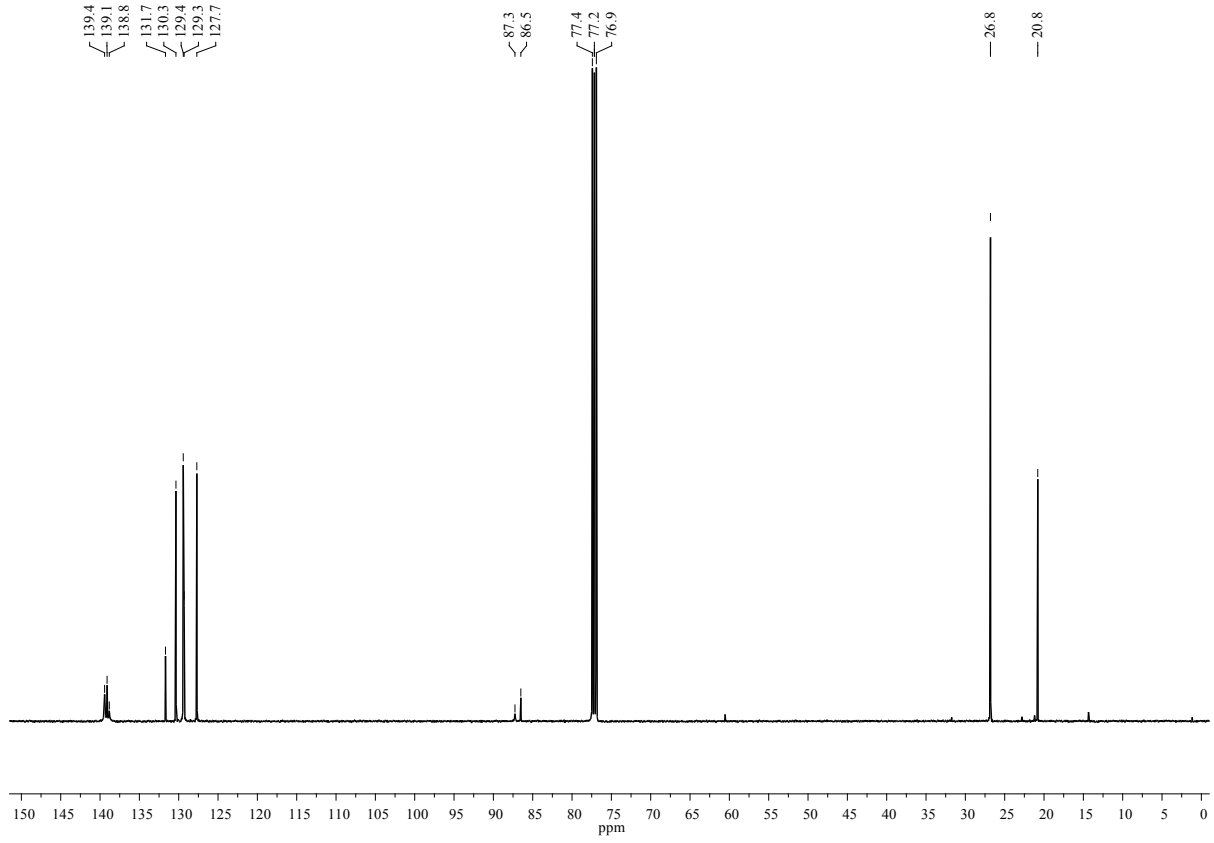

Figure S11: ^{11}B and $^{11}B\{^{1}H\}$ NMR spectra of **3**.

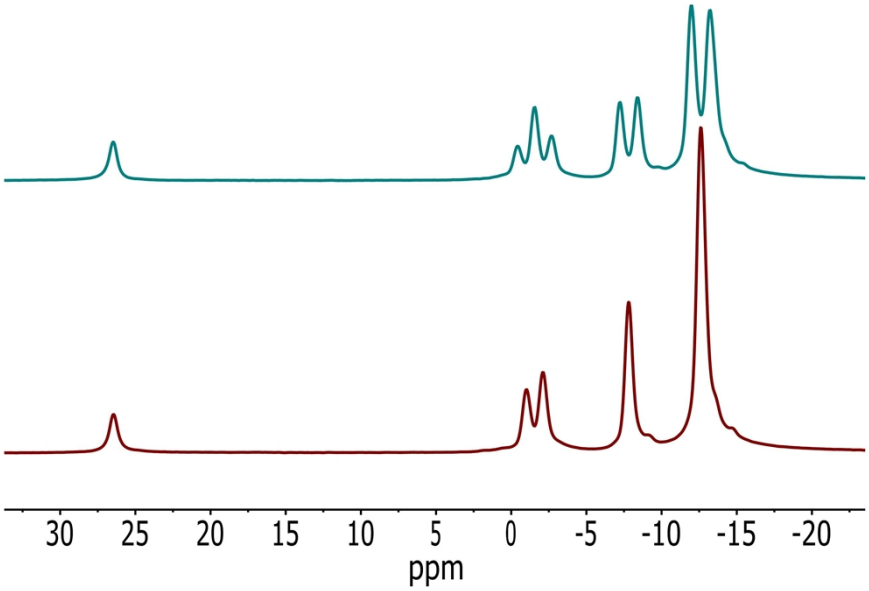

Figure S12: ^{11}B and $^{11}B\{^{1}H\}$ NMR spectra of **4**.

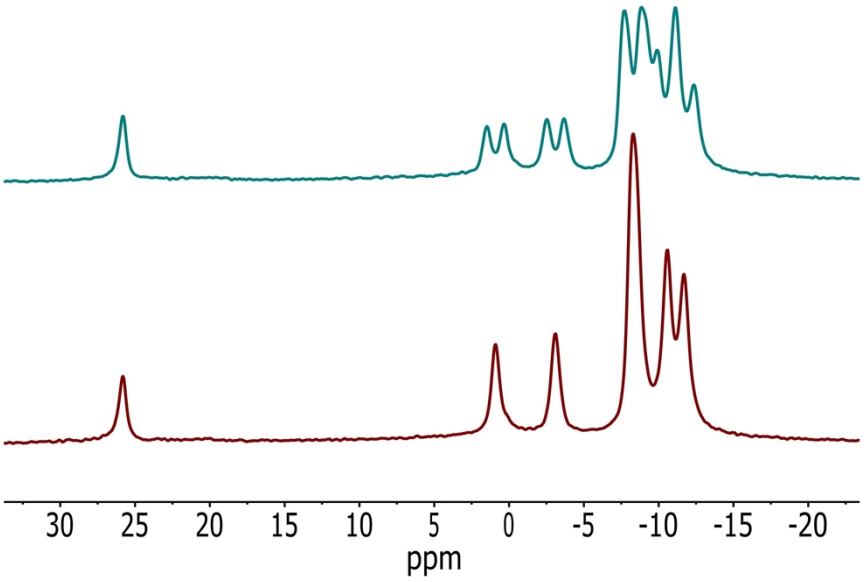

Figure S13. ^{19}F NMR spectra of products from 1:1 reactions of **1** and **2** with tetra-*n*-butylammonium fluoride hydrate (TBAFH) after 24 h. The fluoroborates with presumed formulae, $[(HO)_2BF_2]^-$ and $[(HO)BF_3]^-$, are typical products in deboronations of *ortho*-carboranes with fluorides. (See for example, M.A. Fox, J.A.H. MacBride and K. Wade, *Polyhedron*, 1997, **16**, 2449-2507.) The peak with the asterisk could be $[(HO)_3BF]^-$ (δ (^{11}B) = 8.8 ppm) but there are no observed J_{BF} couplings. The fluoride peak shift is sensitive to the environment. (See for example, M. Gerken, J.A. Boatz, A. Kornath, R. Haiges, S. Schneider, T. Schroer and K.O. Christe, *J. Fluorine Chem.*, 2002, **116**, 49-58.)

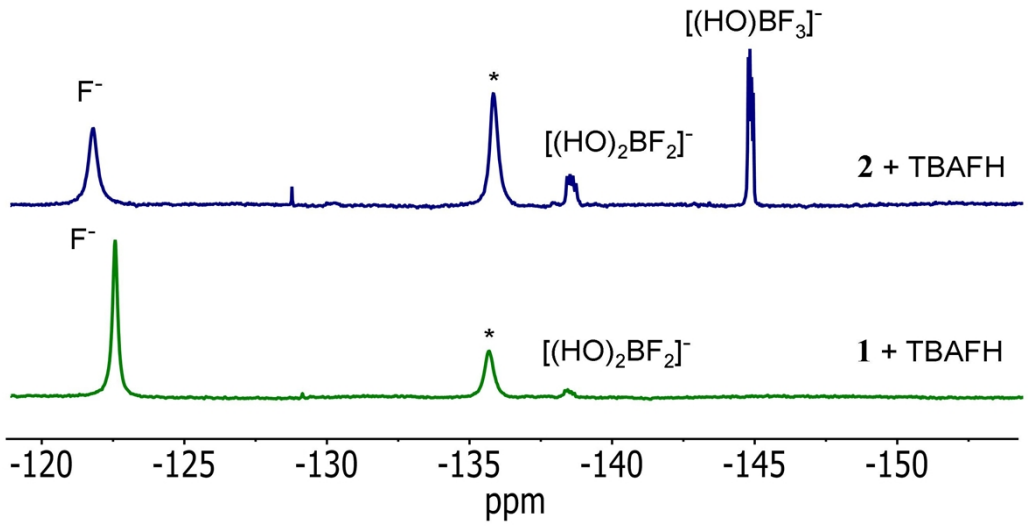

Table S5. Observed ^{11}B NMR data for M_2[**2**] in THF.

M	^{11}B
Li	68.0 (1), 0.0 (2), -11.0 (1), -12.8 (1), -15.5 (2), -18.8 (2), -28.5 (2)
Na	67.0 (1), 0.0 (2), -11.0 (2), -15.2 (2), -18.2 (2), -28.7 (2)
K	67.9 (1), -0.3 (2), -10.0 (2), -15.1 (2), -18.0 (2), -28.7 (2)

Figure S14: $^{1}H\{^{11}B\}$ NMR spectrum of $[\mathbf{2}]^{2-}$ in d_8-THF.

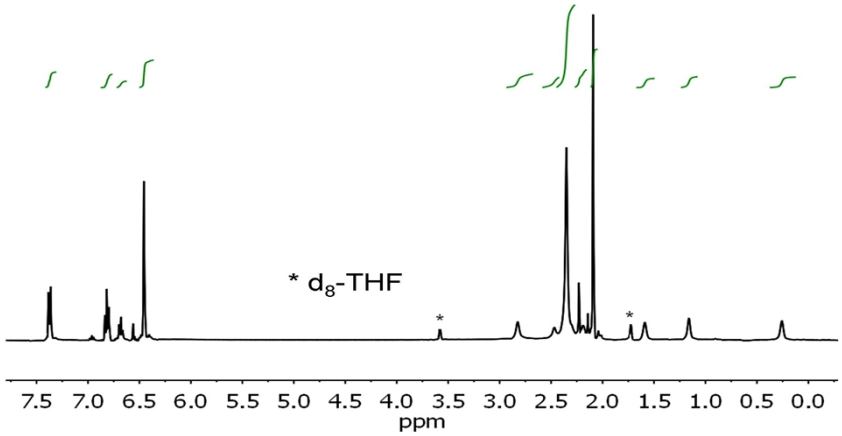

Figure S15: $^{13}C\{^{1}H\}$ NMR spectra of $[\mathbf{2}]^{2-}$ in CD_3CN and d_8-THF respectively.

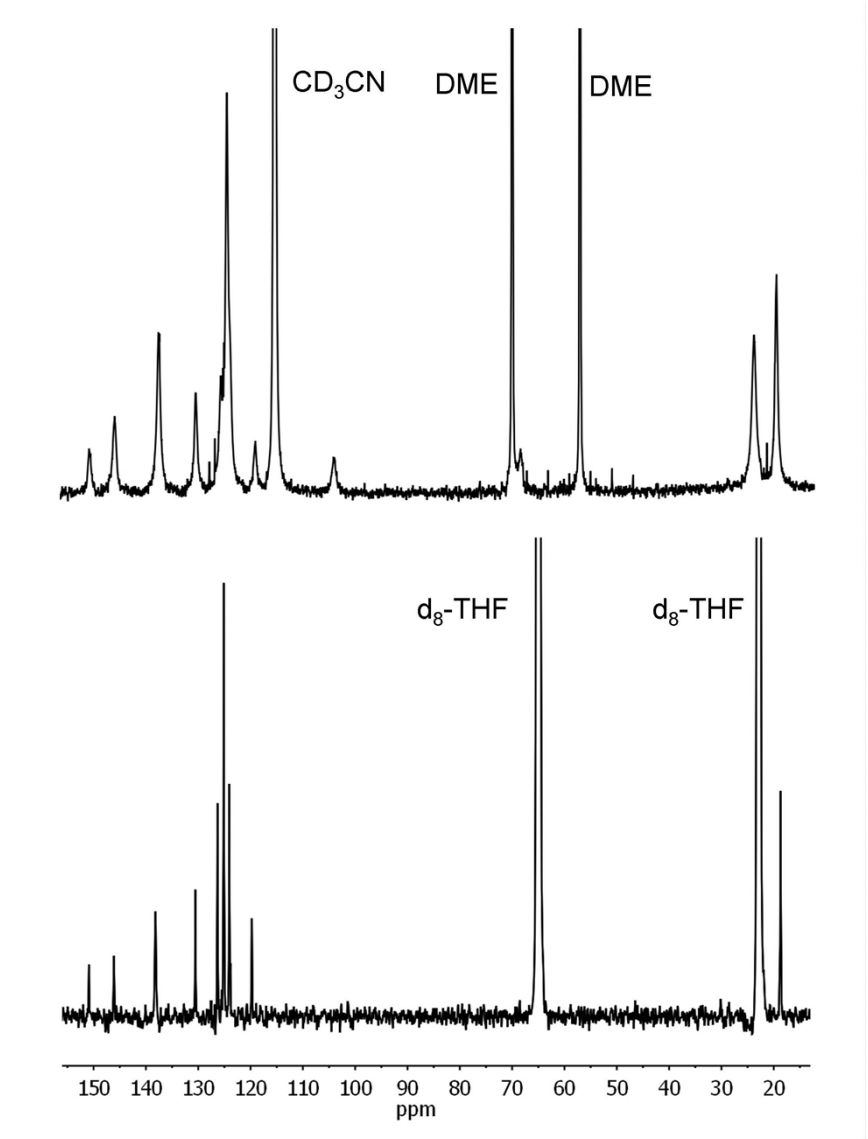

Table S6. Observed NMR data for M_2[**5**] in d_8-THF.

M	^{11}B	^{13}C	^{1}H
Li	4.5 (2), -10.8 (2), -17.6 (4), -29.8 (2)	156.2, 126.3, 124.5, 117.8, 82.2 (cage C)	7.58 (d, 4H), 7.00 (t, 4H), 6.75 (t, 2H), 3.48 (s, 2H, BH), 2.64 (s, 2H, BH), 1.32 (s, 4H, BH), 0.90 (s, 2H, BH)
Na	3.7 (2), -11.2 (2), -17.7 (4), -30.3 (2B)	154.7 (*ipso*), 126.9, 126.0, 120.0 (*para*), 81.2 (cage C)	7.33 (d, 4H), 6.90 (t, 4H), 6.67 (t, 2H), 3.38 (s, 2H, BH), 2.42 (s, 2H, BH), 1.28 (s, 4H, BH), 0.38 (s, 2H, BH)
K	7.0 (2), -9.3 (2), -17.3 (4), -27.5 (2)	155.4 (*ipso*), 126.4, 126.3, 119.9 (*para*), 90.8 (cage C)	7.37 (d, 4H), 6.94 (t, 4H), 6.68 (t, 2H), 3.55 (s, 2H, BH), 2.54 (s, 2H, BH), 1.29 (s, 4H, BH), 0.60 (s, 2H, BH)

Table S7. Crystallographic data for compounds **1** and **2**.

compound	**1** (CCDC-1048027)	**2** (CCDC-1048028)
diffractormeter	**Bruker ApexII**	
temperature [K]	100	100
formula	$C_{20}H_{33}B_{11}$	$C_{26}H_{37}B_{11}$
M_r [g mol^{-1}]	392.37	468.47
Crystal system, space group	Orthorhombic $Pna2_1$	Orthorhombic $P2_12_12_1$
Unit cell dimensions	a = 9.1171(8) Å b = 19.3834(13) Å c = 13.2464(9) Å	a = 9.6527(5)Å b = 13.7958(7)Å c = 20.2585(10)Å
Volume [Å^3]	2340.9(3)	2697.8(2)
Z, calc. density [Mg/m^3]	4, 1.113	4, 1.153
Absorption coefficient [mm^{-1}]	0.389	0.418
F(000)	832	992
Crystal size [mm^3], colour and habit	0.11 x 0.06 x 0.03, Colourless fragment	0.24 x 0.14 x 0.13, Colourless plate
θ range [°]	4.04 - 71.68	3.88 - 69.87
Reflections collected / unique	10855 / 2331 [R(int) = 0.0362]	17835 / 2858 [R(int) = 0.0258]
Data Completeness	97.2%	98.8%
Data / restraints / parameters	2331 / 1 / 330	2858 / 0 / 380
Goodness-of-fit (F^2)	1.052	1.055
Final *R1*, *wR2* [$I>2\sigma(I)$]	0.0358, 0.0927 [2238]	0.0306, 0.0818 [2816]
R1, *wR2* (all data)	0.0376, 0.0944	0.0310, 0.0826
Largest diff. peak and hole [eÅ^{-3}]	0.217 and -0.209	0.164 and -0.195

Cartesian coordinates of optimised geometries

1 (ground state, S_0)

C	-2.052779	-1.404762	-0.721021	C	1.759613	0.206487	0.000887
C	-0.601658	-1.322092	0.102210	C	2.388555	0.886408	-1.092864
B	-0.656160	-2.108014	-1.430822	C	2.634723	-0.351697	0.981139
B	-2.268260	-2.863427	-1.550815	C	3.780626	0.930307	-1.202055
B	-2.400640	-4.076358	-0.258879	C	4.023959	-0.252676	0.839914
B	-0.843356	-3.837478	-1.110982	C	4.627604	0.360298	-0.253021
B	-0.876959	-4.054854	0.660788	H	4.216618	1.440839	-2.058259
B	-2.313738	-3.203314	1.306500	H	4.651803	-0.672403	1.623614
B	-3.172200	-2.489271	-0.065674	C	-1.585783	1.340893	-2.424122
B	-2.123135	-1.477974	0.965246	H	-2.616902	1.126722	-2.733096
B	-0.710557	-2.452656	1.411217	H	-1.190159	2.063511	-3.147953
B	0.196473	-2.841879	-0.066149	H	-1.003823	0.427781	-2.542691
B	0.168958	0.126639	0.048308	C	1.629943	1.561352	-2.214669
H	-2.511101	-0.533799	1.560607	H	1.108720	0.838248	-2.850703
H	-0.186052	-2.213825	2.437727	H	0.891363	2.273159	-1.840743
H	1.379598	-2.835340	-0.085508	H	2.321955	2.109577	-2.860716
H	-0.135467	-1.568838	-2.346784	C	2.183420	-1.037321	2.253262
H	-4.320100	-2.199443	-0.127274	H	2.130765	-2.123284	2.122658
H	-2.881785	-3.550081	2.290379	H	2.902352	-0.843456	3.056533
H	-0.424965	-5.017912	1.190199	H	1.209735	-0.704468	2.603919
H	-0.379882	-4.631191	-1.863009	C	-0.002513	1.739994	2.493035
H	-2.808452	-2.827912	-2.605766	H	-0.349970	0.778180	2.891908
H	-3.055116	-5.057503	-0.401663	H	1.065200	1.645054	2.273240
H	-2.391194	-0.473604	-1.144687	H	-0.111454	2.473534	3.297610
C	-0.751096	1.436104	0.046003	C	6.127530	0.406679	-0.407726
C	-0.797131	2.163147	1.275595	H	6.484170	-0.424749	-1.030362
C	-1.550133	1.924954	-1.019877	H	6.452765	1.334481	-0.890885
C	-1.611713	3.287361	1.406562	H	6.633816	0.329125	0.559956
C	-2.347628	3.066543	-0.843447	C	-3.281307	4.978996	0.531715
C	-2.403991	3.762909	0.357806	H	-4.095958	4.783604	1.240744
H	-1.625801	3.810270	2.361064	H	-2.711973	5.829859	0.924700
H	-2.938952	3.418173	-1.687587	H	-3.733336	5.285320	-0.416816

1 (first excited state, S_1)

C	2.729637	0.891828	1.270075	C	-1.264085	1.408796	-0.226164
C	1.098232	-0.054790	-0.195793	C	-2.156616	1.627435	-1.313385
B	2.168876	-0.671463	1.183378	C	-1.174776	2.430710	0.755450
B	3.968066	-0.165166	1.331028	C	-2.917204	2.797774	-1.391283
B	4.606053	-0.263533	-0.329936	C	-1.968828	3.585608	0.658311
B	3.528354	-1.548646	0.324547	C	-2.836834	3.777739	-0.405143
B	3.430163	-1.024542	-1.388342	H	-3.578524	2.941586	-2.242640
B	3.566856	0.763720	-1.369571	H	-1.883114	4.345830	1.432174
B	3.946738	1.284922	0.277956	H	-3.438898	4.680000	-0.473099
B	2.164549	1.322438	-0.285996	C	-1.285424	-1.314761	0.209783
B	1.986604	0.017065	-1.561692	C	-1.927722	-1.536180	1.450287
B	1.956263	-1.426279	-0.460476	C	-1.448874	-2.332697	-0.747004
B	-0.422873	0.049702	-0.087945	C	-2.707583	-2.733277	1.712010
H	1.671663	2.391585	-0.447375	C	-2.245815	-3.518778	-0.461416
H	1.385085	0.161920	-2.582106	C	-2.870072	-3.719686	0.758227
H	1.346405	-2.434890	-0.609776	H	-3.162677	-2.837844	2.691583
H	1.600500	-1.146389	2.119245	H	-2.331124	-4.264391	-1.246391
H	4.532526	2.299356	0.483747	H	-3.452734	-4.611943	0.956596
H	4.000909	1.386432	-2.286601	C	-0.235522	2.377838	1.943084
H	3.764700	-1.708868	-2.305315	H	0.584743	3.091709	1.807779
H	3.906422	-2.639700	0.617177	H	-0.755551	2.655922	2.868404
H	4.564358	-0.277250	2.354344	H	0.218208	1.399008	2.088969
H	5.775447	-0.402713	-0.507318	C	-1.835334	-0.555367	2.572240
H	2.465400	1.518679	2.111032	H	-0.792316	-0.457925	2.895264

H	-2.151158	0.437399	2.234036
H	-2.438452	-0.851041	3.433875
C	-0.849691	-2.334011	-2.119128
H	-0.248480	-3.242609	-2.249559
H	-1.650505	-2.381338	-2.870754
H	-0.216738	-1.477614	-2.322972
C	-2.300376	0.635551	-2.446719
H	-1.334449	0.399267	-2.905336
H	-2.754677	-0.306090	-2.115344
H	-2.943898	1.038444	-3.234974

[**1** ·F]$^-$

C	-2.48722	-0.682870	-1.140841
C	-1.30036	-0.920602	0.019228
B	-1.70600	-2.184276	-1.125524
B	-3.45324	-2.035841	-1.464720
B	-4.33924	-2.309344	0.049736
B	-2.87107	-3.256622	-0.327664
B	-3.13452	-2.626279	1.320995
B	-3.87605	-1.008328	1.186183
B	-4.07048	-0.656619	-0.539720
B	-2.71013	0.045792	0.370664
B	-2.12939	-1.166793	1.505017
B	-1.51832	-2.547556	0.578360
B	0.17569	-0.017773	-0.423619
H	-2.57938	1.212763	0.484278
H	-1.62447	-0.808333	2.516014
H	-0.57939	-3.181085	0.907607
H	-0.93227	-2.459473	-1.972799
H	-4.85131	0.092249	-1.032447
H	-4.61603	-0.560829	2.005695
H	-3.34823	-3.341959	2.250418
H	-2.88837	-4.418696	-0.590542
H	-3.81893	-2.212828	-2.581995
H	-5.42822	-2.794825	0.050077
H	-2.17636	-0.037810	-1.946079
C	0.06197	1.614223	-0.024271
C	0.42370	2.122371	1.258658
C	-0.35013	2.605321	-0.972094
C	0.36786	3.488735	1.561357
C	-0.38403	3.967926	-0.628742
C	-0.03750	4.441217	0.631383
H	0.65761	3.813164	2.560773
H	-0.70118	4.685153	-1.385528
C	1.68286	-0.702872	-0.106237
C	2.70847	-0.370605	-1.058526
C	2.09286	-1.600824	0.916391
C	3.96780	-0.976236	-1.021913
C	3.36519	-2.204179	0.904245
C	4.31668	-1.930406	-0.065355
H	4.70558	-0.687930	-1.771120
H	3.60983	-2.903405	1.704895
C	-0.80173	2.332129	-2.402494
H	-1.75923	1.800042	-2.436225
H	-0.95937	3.282574	-2.925826
H	-0.08895	1.737851	-2.971647
C	2.54932	0.671421	-2.155319
H	2.00508	0.275525	-3.017101
H	2.00704	1.553068	-1.808455
H	3.53834	0.999154	-2.498825
C	1.29799	-1.953759	2.161390
H	1.21521	-3.040328	2.281940
H	1.82111	-1.573804	3.050334
H	0.29700	-1.544600	2.178290
C	0.89657	1.235872	2.389789
H	0.14314	0.495870	2.668990
H	1.80574	0.692184	2.122214
H	1.11060	1.834838	3.282575
C	5.66392	-2.614179	-0.084690
H	5.71143	-3.396825	-0.855480
H	6.47400	-1.905906	-0.301496
H	5.88424	-3.091973	0.877044
C	-0.11592	5.909396	0.980264
H	-1.00646	6.137086	1.583476
H	0.75488	6.234182	1.563885
H	-0.16660	6.531619	0.079150
F	0.04866	-0.132333	-1.854886

2 (ground state, S_0)

C	-1.639711	1.434911	-0.000875
C	0.117608	1.192211	0.286380
B	-1.048059	1.343772	1.585580
B	-2.276256	2.540359	1.145167
B	-1.447510	4.084354	0.855238
B	-0.915876	3.003587	2.178079
B	0.283120	3.854189	1.157120
B	-0.333097	3.847923	-0.518594
B	-1.910374	3.040981	-0.510413
B	-0.457355	2.148201	-1.026341
B	0.905519	2.687024	-0.023173
B	0.545823	2.152877	1.622093
B	0.917013	-0.237802	0.131406
H	-0.371750	1.752083	-2.127215
H	2.001303	2.633232	-0.461784
H	1.389117	1.733892	2.343909
H	-1.317999	0.403427	2.228021
H	-2.768907	3.203568	-1.310294
H	-0.084768	4.691558	-1.317327
H	0.987820	4.710622	1.582585
H	-1.072940	3.237654	3.332071
H	-3.389299	2.343266	1.500329
H	-2.013841	5.110586	1.049436
C	0.210022	-1.617576	0.523407
C	-0.090023	-2.521668	-0.542498
C	-0.136846	-2.026860	1.842738
C	-0.749695	-3.726848	-0.288969
C	-0.790405	-3.250751	2.052563
C	-1.110847	-4.096747	1.001991
H	-0.977607	-4.384526	-1.123995
H	-1.035939	-3.538797	3.072721
H	-1.619231	-5.039747	1.185418
C	2.444301	-0.211079	-0.362458
C	3.467809	-0.652016	0.535634
C	2.868303	0.211473	-1.658067
C	4.814251	-0.618436	0.157006
C	4.226044	0.198861	-2.005134
C	5.205029	-0.194594	-1.106037
H	5.565189	-0.943956	0.872231
H	4.507789	0.509802	-3.008401
H	6.254355	-0.186905	-1.388686
C	0.218287	-1.283090	3.119354
H	-0.669245	-1.146357	3.747211
H	0.934539	-1.870098	3.707708
H	0.659479	-0.302507	2.958330
C	3.196212	-1.147985	1.938173

H	2.793307	-0.361207	2.583740	C	-2.509299	0.331915	-0.553630
H	2.491608	-1.982418	1.944822	C	-3.163891	-0.568816	0.299577
H	4.124154	-1.495794	2.401658	C	-2.760717	0.247916	-1.932747
C	1.946926	0.674815	-2.767794	C	-4.022731	-1.539005	-0.212858
H	1.883450	1.768410	-2.796669	H	-3.005598	-0.515125	1.369041
H	2.338348	0.349344	-3.737948	C	-3.621802	-0.722706	-2.443417
H	0.934393	0.289562	-2.683914	H	-2.298488	0.954491	-2.611909
C	0.249526	-2.225176	-1.987313	C	-4.252939	-1.623713	-1.585985
H	-0.347947	-1.395723	-2.384217	H	-4.512455	-2.229211	0.467844
H	1.306297	-1.976177	-2.117068	H	-3.803247	-0.765538	-3.513762
H	0.035531	-3.095392	-2.615401	H	-4.924638	-2.379552	-1.983540

2 (first excited state, S_1)

C	2.492446	-1.373420	0.073636	H	-5.689517	0.286486	0.608576
C	0.113124	-1.218527	0.590324	H	-4.205737	-1.772934	-2.824482
B	1.544427	-0.864605	1.445152	C	-0.085382	1.497923	-2.045238
B	3.043617	-1.950599	1.490511	H	0.637378	0.676918	-2.026950
B	2.401012	-3.611784	1.673383	H	-1.058523	1.091557	-2.335207
B	1.742956	-2.259943	2.643645	H	0.234658	2.203808	-2.816444
B	0.678212	-3.559797	1.994071	C	-0.516886	1.473971	3.100074
B	1.234751	-3.844128	0.315748	H	-0.844417	0.441939	3.041123
B	2.752231	-2.986404	0.043199	H	0.484502	1.463288	3.546602
B	1.150654	-2.227121	-0.518623	H	-1.171813	2.028289	3.781034
B	-0.191886	-2.836895	0.608213	C	0.263699	5.723103	0.615872
B	0.110714	-1.885649	2.091313	H	0.234076	6.140471	1.624469
B	-0.935777	-0.122309	0.281930	H	1.239517	5.951526	0.167160
H	0.940024	-2.153710	-1.680678	H	-0.484946	6.240088	-0.000325
H	-1.259009	-3.196789	0.229504	C	-1.661977	-1.684633	-2.358996
H	-0.717747	-1.533365	2.870759	H	-1.405839	-2.691674	-2.014854
H	1.700435	0.258537	1.811220	H	-2.041379	-1.772725	-3.382550
H	3.578081	-3.383706	-0.714649	H	-0.730090	-1.125250	-2.395865
H	1.066944	-4.889112	-0.229815	C	-3.439974	0.859820	1.790916
H	0.152722	-4.385158	2.673065	H	-4.431778	1.104082	2.182891
H	1.979533	-2.134026	3.804609	H	-2.937022	0.252589	2.549437
H	4.100865	-1.553572	1.863666	H	-2.897878	1.808305	1.702225
H	3.087454	-4.474191	2.124275	C	-6.545022	-1.012824	-1.634380
C	-0.500218	1.433980	0.490729	H	-6.997481	-1.857639	-1.098350
C	-0.161641	2.175231	-0.702996	H	-7.180674	-0.138775	-1.452320
C	-0.441593	2.160578	1.765946	H	-6.583488	-1.245714	-2.703365
C	0.057413	3.532525	-0.630116	C	3.228634	-0.394352	-0.759881
C	-0.231395	3.531936	1.779595	C	3.862838	0.723812	-0.184979
C	0.014234	4.250705	0.605550	C	3.346263	-0.569881	-2.152534
H	0.264569	4.088346	-1.540328	C	4.577462	1.627726	-0.968528
H	-0.211777	4.053729	2.732132	H	3.806349	0.868953	0.889015
C	-2.429442	-0.357267	-0.257277	C	4.060428	0.336361	-2.935081
C	-3.557411	0.132773	0.469246	H	2.887536	-1.436363	-2.617273
C	-2.710915	-1.065726	-1.462608	C	4.678808	1.442957	-2.349482
C	-4.858633	-0.088467	0.013950	H	5.068517	2.474989	-0.495568
C	-4.034928	-1.240738	-1.890765	H	4.142434	0.169575	-4.006336
C	-5.128719	-0.773839	-1.171334	H	5.241677	2.145041	-2.958954

[**2** ·F]$^-$

C	-1.800920	1.734918	-0.05769800	H	-0.497485	1.817089	-2.16887700
C	-0.032890	1.553441	0.32295500	H	1.804402	3.004162	-0.52842900
B	-1.237068	1.851301	1.54449400	H	1.114401	2.504236	2.34940600
B	-2.509002	2.942569	0.91929300	H	-1.509373	1.006447	2.31683100
B	-1.735770	4.471674	0.44939800	H	-2.950326	3.286492	-1.61450600
B	-1.216853	3.596926	1.91735200	H	-0.308064	4.834290	-1.73939900
B	-0.015272	4.343553	0.83380200	H	0.648980	5.278961	1.15668100
B	-0.560291	4.090966	-0.84272400	H	-1.435563	3.983392	3.02293400
B	-2.109783	3.253255	-0.77676000	H	-3.631752	2.758709	1.26036000
B	-0.618838	2.330427	-1.11377500	H	-2.346213	5.495227	0.48499300
B	0.687898	3.033917	-0.14454600	C	-0.086368	-1.378205	0.38267900
B	0.290405	2.742686	1.53899200	C	-0.290095	-1.983752	-0.89133500
B	0.857174	-0.014530	0.58963800	C	-0.658425	-2.077242	1.49243100

C	-1.008166	-3.174707	-1.04140000
C	-1.368914	-3.275082	1.29692800
C	-1.563288	-3.846476	0.04480400
H	-1.134848	-3.586491	-2.04264700
H	-1.787737	-3.776726	2.16939900
C	2.433649	-0.172561	-0.03584400
C	3.312888	-0.983065	0.76889700
C	3.054080	0.395264	-1.18212600
C	4.675370	-1.103242	0.47958700
C	4.434686	0.261236	-1.42833200
C	5.278169	-0.462569	-0.60305800
H	5.289679	-1.727676	1.12840400
H	4.845488	0.743114	-2.31662300
C	0.259991	-1.387913	-2.16737900
H	-0.088210	-0.363624	-2.32114400
H	1.352828	-1.361563	-2.15872000
H	-0.059139	-1.974375	-3.03683100
C	-0.557279	-1.659677	2.95533300
H	-0.771067	-0.606188	3.12087900
H	-1.260537	-2.252968	3.55314500
H	0.444933	-1.832806	3.35856700
C	-2.361545	-5.116214	-0.13738900
H	-2.544145	-5.615038	0.82148000
H	-3.341018	-4.914446	-0.59426600
H	-1.846268	-5.829823	-0.79345300
C	2.349171	1.139524	-2.30035600
H	2.766331	2.144738	-2.43467900
H	2.493800	0.604647	-3.24985000
H	1.285811	1.243026	-2.14949800
C	2.866188	-1.806054	1.96638900
H	3.640933	-2.539542	2.22079000
H	2.682375	-1.182899	2.84429300
H	1.945474	-2.354774	1.75981300
C	6.763222	-0.566894	-0.85999900
H	7.340227	0.070680	-0.17485300
H	7.126587	-1.593224	-0.71997300
H	7.015077	-0.257777	-1.88119400
C	-2.680151	0.586000	-0.49542900
C	-3.356276	-0.206760	0.44146300
C	-2.948923	0.377711	-1.85674600
C	-4.261194	-1.183630	0.03065200
H	-3.174295	-0.059639	1.49851400
C	-3.854071	-0.599047	-2.26802100
H	-2.457287	0.992548	-2.60098600
C	-4.515776	-1.385505	-1.32567600
H	-4.764273	-1.790937	0.77828800
H	-4.042299	-0.739843	-3.32958500
H	-5.222955	-2.147608	-1.64445200
F	1.079303	0.161055	1.98793400

[**2**]$^{2-}$ Geometry C

C	2.808111	-0.945145	0.067627
C	0.173833	-0.452422	1.132605
B	1.382415	0.002231	1.986707
B	3.056039	-0.995174	1.697238
B	2.620353	-2.711014	2.241502
B	1.855074	-1.320568	3.032304
B	0.895722	-2.753675	2.493309
B	1.525920	-3.202500	0.886061
B	3.116213	-2.461622	0.573112
B	1.618749	-1.916843	-0.305230
B	0.112952	-2.065861	0.968272
B	0.124044	-1.181078	2.588676
H	1.276016	-2.112328	-1.438365
H	-0.913703	-2.560983	0.582498
H	-0.793523	-1.034328	3.351367
H	1.565577	1.142146	2.324433
H	4.064067	-3.095911	0.186302
H	1.289679	-4.335419	0.556403
H	0.434096	-3.604964	3.206198
H	2.231594	-1.106904	4.155136
H	4.068733	-0.511461	2.123020
H	3.317192	-3.459218	2.874663
C	-0.896307	0.429725	0.631376
C	-1.871017	-0.007295	-0.297559
C	-1.002656	1.780516	1.046221
C	-2.877909	0.835733	-0.766105
H	-1.819544	-1.031758	-0.649979
C	-2.008367	2.622601	0.578484
H	-0.273674	2.157489	1.756418
C	-2.963636	2.161997	-0.333980
H	-3.603930	0.450194	-1.482689
H	-2.047104	3.653652	0.931675
H	-3.749024	2.821043	-0.702015
B	3.635998	-0.124633	-0.892170
C	4.777493	0.926848	-0.397781
C	5.998730	0.525199	0.198528
C	4.586374	2.329876	-0.558897
H	2.024133	0.182552	-7.182080
C	6.971446	1.472743	0.560550
C	5.567370	3.246695	-0.172195
C	6.782121	2.839189	0.386567
H	7.901722	1.117868	1.008006
H	5.374108	4.312009	-0.307837
C	3.414598	-0.199357	-2.500816
C	4.440706	-0.688453	-3.360613
C	2.211519	0.210744	-3.128346
C	4.266953	-0.736336	-4.746079
C	2.074581	0.161002	-4.526204
C	3.085739	-0.306691	-5.358636
H	5.077240	-1.125582	-5.365058
H	1.133949	0.494630	-4.967692
C	7.826721	3.845748	0.814206
H	7.527952	4.385771	1.724853
H	8.785656	3.357500	1.027020
H	8.003879	4.605604	0.040309
C	6.345358	-0.921845	0.490573
H	6.543906	-1.053939	1.561002
H	5.541178	-1.608615	0.234275
H	7.253044	-1.227307	-0.051596
C	3.298508	2.886460	-1.126429
H	3.140104	2.564539	-2.161107
H	2.430396	2.549739	-0.549715
H	3.306213	3.983647	-1.110216
C	1.016746	0.729199	-2.356432
H	1.156991	0.668694	-1.279800
H	0.794927	1.773153	-2.620314
H	0.121296	0.142689	-2.589643
C	5.750481	-1.207223	-2.806602
H	6.316812	-0.418887	-2.299263
H	5.583616	-2.002279	-2.072182
H	6.379833	-1.615545	-3.607907
C	2.909701	-0.378042	-6.859092
H	3.777786	0.033854	-7.392633
H	2.785098	-1.413147	-7.210702

[**2**]$^{2-}$ Geometry D

C	2.745332	-1.073237	0.110714	H	-5.673778	-0.990542	0.367227
C	0.198678	-0.904016	0.881764	H	-3.451835	-2.568138	-2.933677
B	1.622672	-0.348374	1.429630	C	-0.898350	1.643164	-2.119133
B	3.276505	-1.166733	1.664688	H	0.032509	1.074163	-2.222304
B	2.973187	-2.846446	2.216920	H	-1.724009	0.944685	-2.287181
B	2.043286	-1.486278	2.876683	H	-0.918371	2.393843	-2.919504
B	1.240624	-3.018191	2.432559	C	-0.802163	1.637125	3.014154
B	1.953453	-3.524616	0.875110	H	-1.281478	0.661221	3.068237
B	3.412516	-2.555724	0.533264	H	0.253744	1.461243	3.248344
B	1.885930	-2.322810	-0.354956	H	-1.221688	2.282908	3.798131
B	0.389133	-2.573601	0.841422	C	-1.182722	5.930780	0.466000
B	0.331205	-1.519144	2.346999	H	-0.774012	6.357154	1.390747
B	-0.954797	-0.093580	0.388253	H	-0.641003	6.380180	-0.376470
H	1.727401	-2.577057	-1.514879	H	-2.227565	6.270478	0.390020
H	-0.560110	-3.240680	0.525590	C	-1.034857	-1.832498	-2.219222
H	-0.540640	-1.408310	3.172756	H	-0.659540	-2.818200	-1.924873
H	1.749289	0.828742	1.632241	H	-1.218731	-1.846764	-3.302961
H	4.450836	-2.915470	0.053876	H	-0.225240	-1.136590	-2.007458
H	1.874855	-4.693210	0.603370	C	-3.688163	0.109855	1.718696
H	0.838193	-3.826980	3.225968	H	-4.732530	0.121379	2.057055
H	2.267085	-1.123601	4.001863	H	-3.092595	-0.392820	2.489166
H	4.231284	-0.504378	1.962441	H	-3.335989	1.144789	1.665827
H	3.736154	-3.480340	2.895647	C	-5.998033	-2.427368	-1.939923
C	-0.953930	1.540593	0.442736	H	-6.275209	-3.373880	-1.451208
C	-0.981286	2.304014	-0.759394	H	-6.851016	-1.746177	-1.816407
C	-0.938693	2.287105	1.653244	H	-5.892240	-2.638788	-3.011364
C	-1.037173	3.702555	-0.737182	C	3.419067	-0.159524	-0.845670
C	-1.012897	3.689075	1.639657	C	3.799257	1.152454	-0.488475
C	-1.070275	4.422635	0.457279	C	3.711561	-0.557341	-2.169755
H	-1.049762	4.243388	-1.684762	C	4.428480	2.007786	-1.392193
H	-1.013256	4.220244	2.592925	H	3.582852	1.497909	0.516283
C	-2.296914	-0.756899	-0.253596	C	4.341883	0.296113	-3.073159
C	-3.560253	-0.601812	0.388274	H	3.438926	-1.560929	-2.479271
C	-2.301033	-1.507302	-1.459029	C	4.709218	1.591387	-2.695843
C	-4.730408	-1.134385	-0.162579	H	4.698843	3.014004	-1.072319
C	-3.496445	-2.013791	-1.994535	H	4.550373	-0.056343	-4.083639
C	-4.726532	-1.843112	-1.366201	H	5.199594	2.260214	-3.402063

3

C	0.137293	-1.321181	0.000499	H	-0.442143	2.091292	1.482305
C	-0.682976	0.100216	-0.000254	H	-0.441697	2.090122	-1.484161
B	0.108134	-0.408387	-1.448974	H	-0.570814	-0.795533	-2.337577
B	1.578344	-1.241884	-0.890342	H	1.920552	-2.210078	1.482479
B	2.571194	-0.066269	0.000136	H	2.166868	0.736201	2.483315
B	1.652346	0.446247	-1.452893	H	2.269770	2.539176	-0.001067
B	1.708008	1.492362	-0.000527	H	2.167365	0.734168	-2.483574
B	1.652170	0.447345	1.452732	H	1.921049	-2.211050	-1.480688
B	1.577965	-1.241352	0.891345	H	3.756490	-0.146161	0.000262
B	0.108049	-0.407127	1.449246	O	-2.807113	-1.237049	0.000020
B	0.183334	1.280308	0.887661	H	-3.774185	-1.276695	0.000181
B	0.183405	1.279524	-0.888577	O	-2.944743	1.194391	-0.000132
B	-2.266237	0.017609	0.000008	H	-3.910028	1.123041	0.000187
H	-0.571204	-0.793738	2.337857	H	-0.486641	-2.205562	0.000816

4

C	0.096475	-0.585376	-0.088839	B	2.477259	-0.772964	-1.526483
C	0.924945	0.878319	0.080393	B	3.376259	-0.418957	-0.020391
B	0.937335	0.081150	-1.446200	B	2.433638	-1.074913	1.351586
B	0.998617	-1.653758	-1.083972	B	0.974583	-1.835441	0.685825
B	2.510809	-1.964978	-0.197123	B	0.895106	-0.212407	1.406894

B	2.373455	0.659670	0.971475
B	2.394478	0.846366	-0.792385
B	0.081338	2.225822	0.208931
H	0.223481	0.064679	2.336423
H	2.717843	1.547260	1.676881
H	2.754748	1.859673	-1.291485
H	0.324873	0.556687	-2.332880
H	0.349600	-2.709225	1.185405
H	2.925728	-1.469331	2.358236
H	4.561317	-0.338220	0.003944
H	3.000263	-0.944687	-2.578980
H	0.380297	-2.394492	-1.772059
H	3.062543	-3.012646	-0.296528
C	-1.417369	-0.583328	-0.073154
C	-2.166783	-0.172545	-1.185736
C	-2.103082	-1.036836	1.064915
C	-3.561038	-0.206765	-1.155301
H	-1.664953	0.171283	-2.080970
C	-3.495971	-1.072592	1.091472
H	-1.545870	-1.370400	1.932194
C	-4.231953	-0.655520	-0.018077
H	-4.120461	0.113436	-2.029953
H	-4.003701	-1.430614	1.982669
H	-5.317910	-0.685066	0.001967
O	-0.336702	2.809431	-0.949321
H	-0.831923	3.634069	-0.839053
O	-0.130039	2.700805	1.466929
H	-0.617660	3.535606	1.518492

[**5**]$^{2-}$ Geometry C

C	-1.449270	0.619730	-0.155806
C	1.449354	0.619732	0.155763
B	0.607780	0.955801	1.408111
B	-1.220780	1.684830	1.033118
B	-0.852321	3.294113	0.182752
B	0.276310	2.670535	1.412091
B	0.852627	3.294071	-0.183149
B	-0.276096	2.670378	-1.412399
B	-1.820140	2.107445	-0.683886
B	-0.607679	0.955726	-1.408170
B	1.221068	1.684678	-1.033288
B	1.820300	2.107476	0.683704
H	-0.665297	0.325004	-2.433234
H	2.015044	1.688298	-1.941670
H	2.920388	2.434392	1.052113
H	0.665525	0.325242	2.433258
H	-2.920170	2.434640	-1.052191
H	-0.265682	3.294194	-2.443649
H	1.395139	4.352218	-0.371219
H	0.265892	3.294386	2.443321
H	-2.014765	1.688739	1.941506
H	-1.394842	4.352282	0.370680
C	-2.373621	-0.513273	-0.042662
C	-2.731227	-1.068036	1.210055
C	-2.943781	-1.140099	-1.179729
C	-3.594354	-2.157574	1.318467
H	-2.305822	-0.622478	2.103519
C	-3.804127	-2.229147	-1.071869
H	-2.693509	-0.745767	-2.160278
C	-4.145693	-2.754035	0.180499
H	-3.835597	-2.549874	2.307475
H	-4.218919	-2.673951	-1.977814
H	-4.819446	-3.606307	0.265065
C	2.373578	-0.513389	0.042697
C	2.944325	-1.139619	1.179798
C	2.730466	-1.068819	-1.209910
C	3.804562	-2.228766	1.072060
H	2.694615	-0.744726	2.160264
C	3.593468	-2.158476	-1.318206
H	2.304595	-0.623723	-2.103382
C	4.145391	-2.754349	-0.180217
H	4.219840	-2.673099	1.978012
H	3.834154	-2.551326	-2.307129
H	4.819074	-3.606686	-0.264705