Supplementary materials

Theoretical insight on B–C chemical bonding in *closo*-borate $[B_nH_{n-1}CH_3]^{2-}$ (n = 6, 10, 12) and monocarborane $[CB_nH_nCH_3]^-$ (n = 5, 9, 11) anions

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Table S1. ΔH – relative enthalpy energies of carborane isomers, kJ/mol, ΔG – relative Gibbs energy of carborane isomers, kJ/mol.

Model species	ΔH	ΔG
[*ortho*-$CB_5H_5CH_3$]$^-$	0.0	0.0
[*meta*-$CB_5H_5CH_3$]$^-$	0.9	1.4
[*ortho*-$CB_9H_9CH_3$]$^-$	0.0	0.0
[*meta*-$CB_9H_9CH_3$]$^-$	3.1	2.5
[*para*-$CB_9H_9CH_3$]$^-$	2.2	1.5
[*ortho*-$CB_{11}H_{11}CH_3$]$^-$	0.0	0.0
[*meta*-$CB_{11}H_{11}CH_3$]$^-$	8.0	6.6
[*para*-$CB_{11}H_{11}CH_3$]$^-$	3.3	1.8

Table S2. B–C bond lengths and bond order descriptors. LBO - Laplacian bond order. FBO - fuzzy bond order, Mayer indices, Wiberg indices.

Model species	B–C length (Å)	LBO	FBO	Mayer Index	Wiberg Index
$(CH_3)BH_2$	1.56	1.251	1.195	1.014	0.95
$(CH_3)_2BH$	1.57	1.215	1.150	0.997	0.94
$(CH_3)_3B$	1.58	1.170	1.099	0.998	0.92
$[B_6H_5CH_3]^{2-}$	1.63	0.887	1.050	0.473	0.90
$[1\text{-}B_{10}H_9CH_3]^{2-}$	1.61	0.923	1.050	0.381	0.91
$[2\text{-}B_{10}H_9CH_3]^{2-}$	1.62	0.905	1.023	0.113	0.98
$[B_{12}H_{11}CH_3]^{2-}$	1.62	0.920	1.020	0.132	0.92
[*ortho*-$CB_5H_5CH_3$]$^-$	1.60	0.992	1.079	0.746	0.93
[*meta*-$CB_5H_5CH_3$]$^-$	1.60	0.987	1.078	0.899	0.93
[*ortho*-$CB_9H_9CH_3$]$^-$	1.60	1.010	1.053	0.757	0.93
[*meta*-$CB_9H_9CH_3$]$^-$	1.61	0.953	1.041	0.632	0.93
[*para*-$CB_9H_9CH_3$]$^-$	1.60	0.995	1.070	0.827	0.93
[*ortho*-$CB_{11}H_{11}CH_3$]$^-$	1.60	0.999	1.044	0.763	0.94
[*meta*-$CB_{11}H_{11}CH_3$]$^-$	1.61	0.969	1.039	0.869	0.94
[*para*-$CB_{11}H_{11}CH_3$]$^-$	1.61	0.972	1.038	0.902	0.94

Table S3. Main topological parameters of electron density for B–C interactions. $\rho(r)$ – electron density at the bcp, $\nabla^2\rho(r)$ – Laplacian of electron density at the bcp, G(r) – Lagrangian kinetic energy, V(r) – potential energy, H_b – total energy at the bcp, δ(B–C) – delocalization index, ε_b – ellipticity at the bcp, $\bar{N}$ – electron population in basins ELF.

Model species	$\rho(r)$ (e Å^{-3})	$\nabla^2\rho(r)$ (e Å^{-5})	G(r) (h e^{-1})	V(r) (h e^{-1})	H_b (h e^{-1})	ε	δ(B– C)	$\bar{N}$(e)
$(CH_3)BH_2$	0.186	-0.154	0.153	-0.344	-0.191	0.293	0.525	2.03
$(CH_3)_2BH$	0.183	-0.138	0.152	-0.339	-0.187	0.283	0.497	2.04
$(CH_3)_3B$	0.180	-0.136	0.149	-0.332	-0.183	0.284	0.474	2.04
$[B_6H_5CH_3]^{2-}$	0.149	0.039	0.143	-0.276	-0.133	0.002	0.637	1.96
$[1\text{-}B_{10}H_9CH_3]^{2-}$	0.156	0.020	0.147	-0.290	-0.142	0.001	0.647	1.97
$[2\text{-}B_{10}H_9CH_3]^{2-}$	0.156	-0.017	0.141	-0.285	-0.145	0.135	0.629	1.94
$[B_{12}H_{11}CH_3]^{2-}$	0.158	-0.035	0.140	-0.288	-0.148	0.002	0.628	1.95
[*ortho*-$CB_5H_5CH_3]^-$	0.164	-0.045	0.144	-0.299	-0.155	0.037	0.621	2.01
[*meta*-$CB_5H_5CH_3]^-$	0.163	-0.053	0.141	-0.295	-0.154	0.001	0.648	2.00
[*ortho*-$CB_9H_9CH_3]^-$	0.170	-0.104	0.143	-0.303	-0.166	0.001	0.594	2.00
[*meta*-$CB_9H_9CH_3]^-$	0.164	-0.085	0.137	-0.295	-0.158	0.119	0.650	1.96
[*para*-$CB_9H_9CH_3]^-$	0.167	-0.063	0.140	-0.306	-0.159	0.071	0.659	2.00
[*ortho*-$CB_{11}H_{11}CH_3]^-$	0.170	-0.122	0.137	-0.304	-0.167	0.052	0.621	1.99
[*meta*-$CB_{11}H_{11}CH_3]^-$	0.166	-0.102	0.136	-0.298	-0.162	0.002	0.647	1.97
[*para*-$CB_{11}H_{11}CH_3]^-$	0.166	-0.102	0.137	-0.298	-0.162	0.002	0.645	1.97

Table S4. Main parameters of molecular orbitals for B–C interactions obtained with the help of NBO formalism.

Model species	Energy of B–C orbital	Coefficient of B atom	Coefficient of C atom
$(CH_3)BH_2$	-0.91	0.57	0.82
$(CH_3)_2BH$	-0.90	0.57	0.82
$(CH_3)_3B$	-0.90	0.56	0.83
$[B_6H_5CH_3]^{2-}$	-0.55	0.59	0.81
$[1\text{-}B_{10}H_9CH_3]^{2-}$	-0.59	0.60	0.80

$[2\text{-}B_{10}H_9CH_3]^{2-}$	-0.59	0.60	0.80
$[B_{12}H_{11}CH_3]^{2-}$	-0.60	0.61	0.79
[*ortho*-$CB_5H_5CH_3]^-$	-0.73	0.60	0.80
[*meta*-$CB_5H_5CH_3]^-$	-0.72	0.60	0.80
[*ortho*-$CB_9H_9CH_3]^-$	-0.76	0.61	0.79
[*meta*-$CB_9H_9CH_3]^-$	-0.73	0.62	0.79
[*para*-$CB_9H_9CH_3]^-$	-0.74	0.61	0.79
[*ortho*-$CB_{11}H_{11}CH_3]^-$	-0.77	0.62	0.79
[*meta*-$CB_{11}H_{11}CH_3]^-$	-0.74	0.62	0.78
[*para*-$CB_{11}H_{11}CH_3]^-$	-0.74	0.62	0.79

Table S5. Second order perturbation theory analysis of Fock matrix in NBO basis of *exo*-polyhedral B–C back bonding interactions. BD – bonding orbital of C–H bond, LV – boron lone valence orbital.

Model species	Donor	Acceptor	E(2)
BH_2CH_3			
	BD C2 - H3	LV B1	5.91
	BD C2-H4	LV B1	3.43
$BH(CH_3)_2$			
	BD C2 - H3	LV B1	7.23
	BD C2 - H5	LV B1	1.94
	BD C7 - H8	LV B1	1.73
	BD C7 - H10	LV B1	7.51
$B(CH_3)_3$			
	BD C2 - H3	LV B1	6.79
	BD C2- H4	LV B1	1.94
	BD C6 - H7	LV B1	2.67
	BD C6 - H9	LV B1	5.96
	BD C10 - H 11	LV B1	5.74
	BD C10 - H12	LV B1	2.85
$[B_6H_5CH_3]^{2-}$			
	BD C12 - H14	LV B1	0.15

	BD C12 - H13	LV B1	0.15
	BD C12 - H15	LV B7	0.12
	BD C12 - H14	LV B8	0.15
	BD C12 - H13	LV B8	0.08
$[1\text{-}B_{10}H_9CH_3]^{2-}$			
	BD C20 - H21	LV B5	0.07
	BD C20 - H23	LV B5	0.07
	BD C20 - H22	LV B3	0.06
	BD B1 - C20	LV B4	0.07
	BD C20 - H23	LV B4	0.13
$[2\text{-}B_{10}H_9CH_3]^{2-}$			
	BD C20 - H21	LV B1	0.06
	BD C20 - H23	LV B1	0.05
	BD C20 - H22	LV B3	0.08
	BD B1 - C20	LV B5	0.07
	BD C20 - H23	LV B5	0.08
$[B_{12}H_{11}CH_3]^{2-}$			
	BD C24 - H27	LV B3	0.08
	BD C24 - H26	LV B6	0.05
	BD C24 - H27	LV B14	0.06
	BD C24 - H25	LV B15	0.05
	BD C24 - H27	LV B18	0.07
[*ortho*-$CB_{11}H_{11}CH_3]^{1-}$			
	BD C24 - H25	LV B16	0.86
	BD C 24- H 26	LV B 16	0.69
	BD C24 - H 27	LV B 16	2.08

Table S6. NBO, QTAIM and Hirshfeld atomic charges of derivatives of *closo*-borate anions $[B_nH_{n-1}CH_3]^{2-}$ (n = 6, 10, 12), monocarboranes $[CB_nH_{n-1}CH_3]^-$ (n = 5, 9, 11) and $BH_{3-n}(CH_3)_n$ n=1-3.

Model species	Atom	Hirshfeld	NBO	QTAIM
$[B_6H_5CH_3]^{2-}$				
	1B	-0.18	-0.28	0.38
	2B	-0.18	-0.29	0.40
	3B	-0.19	-0.30	0.40
	4H	-0.15	-0.04	-0.73
	5H	-0.15	-0.04	-0.73
	6H	-0.15	-0.04	-0.73
	7B	-0.18	-0.29	0.38
	8B	-0.18	-0.28	0.39
	9B	-0.10	-0.05	0.49
	10H	-0.15	-0.04	-0.73
	11H	-0.15	-0.04	-0.73
	12C	-0.18	-0.92	-0.51
	13H	-0.02	0.20	-0.09
	14H	-0.02	0.20	-0.09
	15H	-0.02	0.20	-0.09
$[1\text{-}B_{10}H_9CH_3]^{2-}$				
	1B	-0.07	-0.04	0.44
	2B	-0.08	-0.19	0.50
	3B	-0.08	-0.19	0.49
	4B	-0.08	-0.19	0.49
	5B	-0.08	-0.19	0.49
	6H	-0.11	0.01	-0.67
	7H	-0.11	0.01	-0.67
	8H	-0.11	0.01	-0.67
	9B	-0.08	-0.19	0.52
	10B	-0.14	-0.27	0.32
	11B	-0.08	-0.19	0.51
	12B	-0.08	-0.19	0.52
	13B	-0.08	-0.19	0.52

	14H	-0.11	0.01	-0.67
	15H	-0.11	0.01	-0.67
	16H	-0.11	0.01	-0.67
	17H	-0.11	0.00	-0.68
	18H	-0.11	0.01	-0.67
	19H	-0.11	0.01	-0.67
	20C	-0.17	-0.90	-0.51
	21H	-0.01	0.21	-0.08
	22H	-0.01	0.21	-0.08
	23H	-0.01	0.21	-0.08
$[2\text{-}B_{10}H_9CH_3]^{2-}$				
	1B	-0.14	-0.26	0.31
	2B	-0.02	0.03	0.60
	3B	-0.08	-0.19	0.50
	4B	-0.08	-0.19	0.51
	5B	-0.08	-0.19	0.52
	6H	-0.11	0.00	-0.68
	7H	-0.11	0.02	-0.67
	8H	-0.11	0.01	-0.67
	9H	-0.11	0.02	-0.67
	10B	-0.08	-0.20	0.49
	11B	-0.13	-0.25	0.34
	12B	-0.08	-0.20	0.49
	13B	-0.08	-0.20	0.51
	14B	-0.08	-0.20	0.51
	15H	-0.11	0.02	-0.67
	16H	-0.11	0.01	-0.67
	17H	-0.11	0.01	-0.67
	18H	-0.11	0.00	-0.68
	19H	-0.11	0.02	-0.67
	20C	-0.17	-0.91	-0.51
	21H	-0.01	0.21	-0.07
	22H	-0.01	0.21	-0.08
	23H	-0.01	0.22	-0.07
$[B_{12}H_{11}CH_3]^{2-}$				

	1B	-0.07	-0.19	0.50
	2B	-0.07	-0.19	0.50
	3B	-0.07	-0.19	0.48
	4B	-0.07	-0.19	0.51
	5B	-0.07	-0.20	0.49
	6B	-0.07	-0.19	0.48
	7H	-0.10	0.03	-0.66
	8H	-0.10	0.03	-0.66
	9H	-0.10	0.03	-0.66
	10H	-0.10	0.03	-0.67
	11H	-0.10	0.03	-0.66
	12H	-0.10	0.03	-0.66
	13B	-0.07	-0.19	0.50
	14B	-0.07	-0.19	0.49
	15B	-0.07	-0.19	0.49
	16B	-0.01	0.03	0.59
	17B	-0.07	-0.19	0.50
	18B	-0.07	-0.19	0.49
	19H	-0.10	0.03	-0.67
	20H	-0.10	0.03	-0.66
	21H	-0.10	0.03	-0.66
	22H	-0.10	0.03	-0.67
	23H	-0.10	0.03	-0.66
	24C	-0.16	-0.90	-0.51
	25H	0.00	0.22	-0.07
	26H	0.00	0.22	-0.07
	27H	0.00	0.22	-0.07
[*ortho*-$CB_5H_5CH_3$]$^-$				
	1B	-0.09	-0.08	0.92
	2B	-0.09	-0.07	0.90
	3C	-0.12	-0.74	-1.89
	4H	-0.09	0.00	-0.68
	5H	-0.09	-0.01	-0.68
	6H	0.03	0.27	-0.02
	7B	-0.02	0.17	1.02

	8B	-0.09	-0.07	0.90
	9B	-0.11	-0.19	0.60
	10H	-0.09	0.00	-0.67
	11H	-0.10	0.00	-0.68
	12C	-0.17	-0.94	-0.57
	13H	0.01	0.23	-0.05
	14H	0.01	0.23	-0.05
	15H	0.01	0.22	-0.06
[*meta*-$CB_5H_5CH_3$]$^-$				
	1B	-0.09	-0.07	0.90
	2B	-0.09	-0.08	0.90
	3C	-0.12	-0.74	-1.90
	4H	-0.09	0.00	-0.67
	5H	-0.09	0.00	-0.68
	6H	0.03	0.27	-0.02
	7B	-0.09	-0.08	0.90
	8B	-0.09	-0.07	0.91
	9B	-0.04	0.05	0.72
	10H	-0.09	0.00	-0.67
	11H	-0.09	0.00	-0.67
	12C	-0.17	-0.94	-0.57
	13H	0.01	0.23	-0.05
	14H	0.01	0.23	-0.05
	15H	0.01	0.22	-0.06
[*ortho*-$CB_9H_9CH_3$]$^-$				
	1B	-0.08	-0.16	0.46
	2B	-0.05	-0.21	0.53
	3B	-0.05	-0.21	0.53
	4B	-0.05	-0.21	0.56
	5B	-0.05	-0.21	0.56
	6H	-0.07	0.03	-0.65
	7H	-0.07	0.05	-0.64
	8H	-0.07	0.05	-0.64
	9H	-0.07	0.05	-0.64
	10B	0.04	0.29	1.16

	11C	-0.11	-0.82	-2.19
	12B	0.00	0.04	1.06
	13B	0.00	0.04	1.07
	14B	0.00	0.04	1.06
	15H	-0.07	0.04	-0.64
	16H	-0.07	0.04	-0.64
	17H	-0.07	0.04	-0.64
	18H	0.06	0.30	0.01
	19H	-0.07	0.05	-0.64
	20C	-0.16	-0.94	-0.57
	21H	0.02	0.24	-0.04
	22H	0.02	0.23	-0.05
	23H	0.02	0.24	-0.03
[*meta*-$CB_9H_9CH_3$]$^-$				
	1B	-0.08	-0.18	0.43
	2B	0.00	0.03	0.66
	3B	-0.05	-0.20	0.55
	4B	-0.05	-0.21	0.56
	5B	-0.05	-0.20	0.56
	6H	-0.07	0.04	-0.64
	7H	-0.07	0.05	-0.64
	8H	-0.07	0.05	-0.64
	9H	-0.07	0.05	-0.63
	10B	0.00	0.03	1.04
	11C	-0.11	-0.80	-2.19
	12B	0.00	0.04	1.04
	13B	0.00	0.04	1.06
	14B	0.00	0.04	1.07
	15H	-0.07	0.04	-0.64
	16H	-0.07	0.03	-0.64
	17H	-0.07	0.03	-0.64
	18H	0.06	0.30	0.02
	19H	-0.07	0.04	-0.64
	20C	-0.16	-0.92	-0.55
	21H	0.02	0.24	-0.04

	22H	0.01	0.23	-0.05
	23H	0.02	0.24	-0.04
[*para*-$CB_9H_9CH_3$]$^-$				
	1B	-0.03	0.08	0.58
	2B	-0.06	-0.21	0.54
	3B	-0.05	-0.21	0.53
	4B	-0.05	-0.21	0.53
	5B	-0.05	-0.21	0.53
	6H	-0.07	0.05	-0.64
	7H	-0.07	0.05	-0.64
	8H	-0.07	0.05	-0.64
	9B	0.00	0.04	1.07
	10C	-0.11	-0.81	-2.18
	11B	0.00	0.04	1.07
	12B	0.00	0.04	1.07
	13B	0.00	0.04	1.06
	14H	-0.07	0.04	-0.64
	15H	-0.07	0.04	-0.64
	16H	-0.07	0.04	-0.64
	17H	0.06	0.30	0.02
	18H	-0.07	0.04	-0.64
	19H	-0.07	0.05	-0.64
	20C	-0.16	-0.92	-0.56
	21H	0.01	0.23	-0.05
	22H	0.01	0.23	-0.04
	23H	0.01	0.23	-0.04
[*ortho*-$CB_{11}H_{11}CH_3$]$^-$				
	1B	-0.04	-0.19	0.58
	2B	-0.04	-0.16	0.57
	3B	-0.01	-0.02	0.84
	4B	-0.01	-0.02	0.85
	5B	-0.05	-0.20	0.58
	6B	-0.05	-0.19	0.57
	7H	-0.07	0.06	-0.63
	8H	-0.07	0.06	-0.63

	9H	-0.06	0.05	-0.63
	10H	-0.06	0.05	-0.63
	11H	-0.07	0.06	-0.63
	12H	-0.07	0.06	-0.63
	13B	-0.04	-0.19	0.58
	14B	-0.05	-0.19	0.56
	15C	-0.03	-0.72	-1.78
	16B	0.03	0.23	0.94
	17B	-0.01	-0.02	0.85
	18B	-0.01	-0.03	0.83
	19H	-0.07	0.06	-0.63
	20H	-0.07	0.06	-0.63
	21H	0.06	0.32	0.03
	22H	-0.06	0.05	-0.63
	23H	-0.06	0.05	-0.63
	24C	-0.15	-0.93	-0.57
	25H	0.02	0.23	-0.04
	26H	0.02	0.24	-0.03
	27H	0.02	0.24	-0.03
[*meta*-$CB_{11}H_{11}CH_3$]$^-$				
	1B	-0.05	-0.19	0.58
	2B	-0.01	-0.02	0.84
	3B	-0.04	-0.16	0.55
	4B	-0.04	-0.19	0.59
	5B	-0.01	-0.02	0.85
	6B	-0.05	-0.19	0.56
	7H	-0.07	0.06	-0.63
	8H	-0.06	0.05	-0.63
	9H	-0.07	0.06	-0.64
	10H	-0.07	0.06	-0.63
	11H	-0.06	0.05	-0.63
	12H	-0.07	0.06	-0.63
	13C	-0.02	-0.72	-1.78
	14B	-0.01	-0.02	0.83
	15B	-0.05	-0.19	0.56

	16B	0.00	0.05	0.69
	17B	-0.01	-0.02	0.85
	18B	-0.01	-0.02	0.83
	19H	0.06	0.32	0.04
	20H	-0.06	0.05	-0.63
	21H	-0.07	0.06	-0.63
	22H	-0.06	0.05	-0.63
	23H	-0.06	0.05	-0.63
	24C	-0.15	-0.92	-0.55
	25H	0.01	0.23	-0.04
	26H	0.02	0.23	-0.04
	27H	0.02	0.24	-0.04
[*para*-$CB_{11}H_{11}CH_3$]$^-$				
	1B	-0.01	-0.02	0.86
	2B	-0.01	-0.02	0.84
	3B	-0.05	-0.19	0.56
	4B	-0.01	-0.01	0.85
	5C	-0.03	-0.72	-1.78
	6B	-0.05	-0.19	0.56
	7H	-0.06	0.05	-0.63
	8H	-0.06	0.05	-0.63
	9H	-0.07	0.06	-0.63
	10H	-0.06	0.05	-0.63
	11H	0.06	0.32	0.04
	12H	-0.07	0.06	-0.63
	13B	-0.01	-0.02	0.84
	14B	-0.05	-0.19	0.57
	15B	-0.05	-0.19	0.56
	16B	0.00	0.08	0.68
	17B	-0.01	-0.01	0.85
	18B	-0.05	-0.19	0.57
	19H	-0.06	0.05	-0.63
	20H	-0.07	0.06	-0.63
	21H	-0.07	0.06	-0.63
	22H	-0.06	0.05	-0.63

	23H	-0.07	0.06	-0.63
	24C	-0.15	-0.92	-0.55
	25H	0.02	0.23	-0.04
	26H	0.02	0.23	-0.04
	27H	0.02	0.23	-0.04

Fig S1. Correlation matrix of main B–C bond descriptors and mean boron atomic charges in *closo*-borate anions of the general form $[B_nH_{n-1}CH_3]^{2-}$ (n = 6, 10, 12) and monocarboranes $[CB_nH_{n-1}CH_3]^-$ (n = 5, 9, 11).

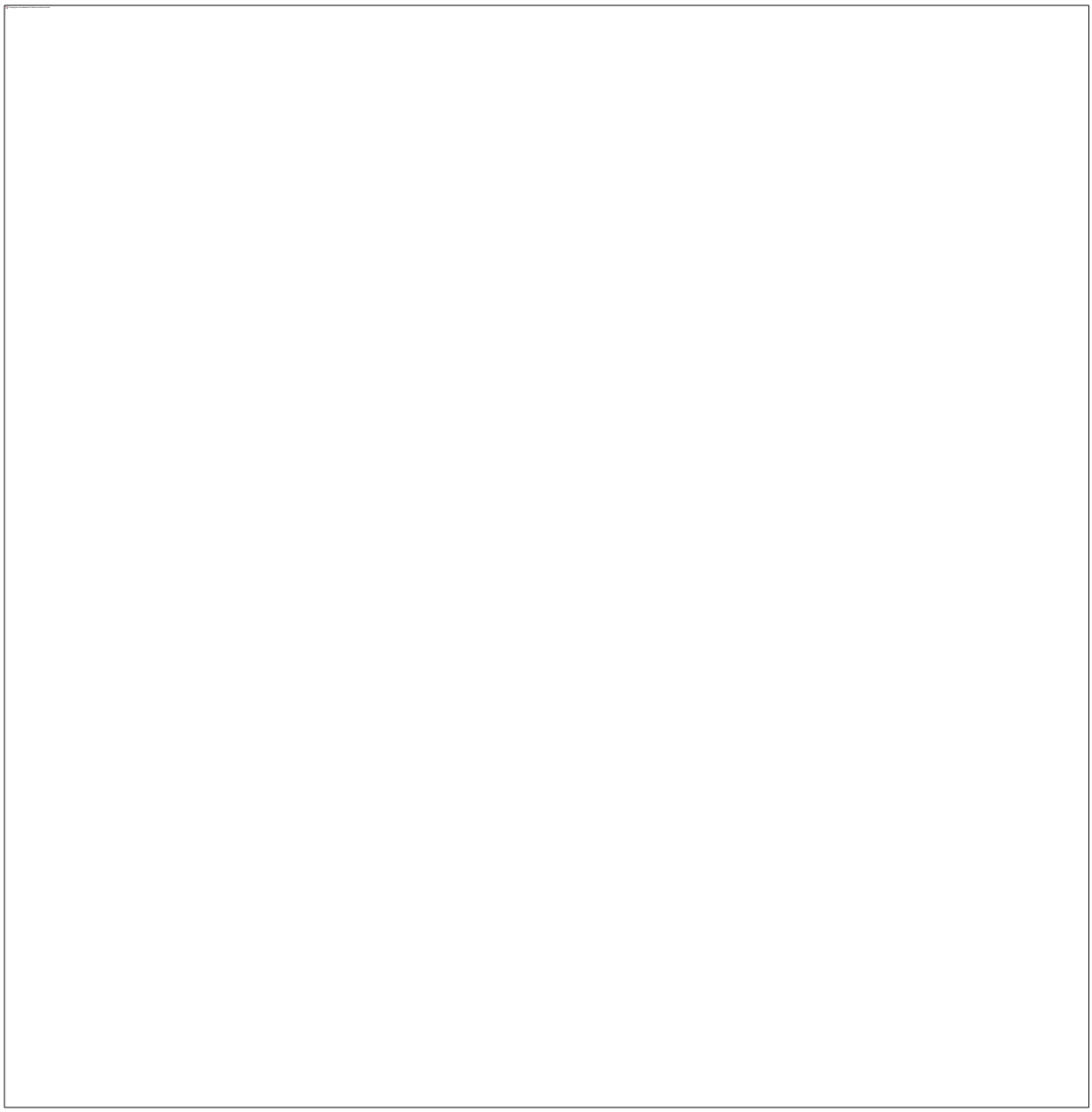

Table S7. Cartesian atomic coordinates of the calculated optimized equilibrium model structures. All coordinates are given in Angstrom units.

Model species	Atom	x	y	z
$(CH_3)BH_2$				
	B	-5.704145	1.748821	-0.013440
	C	-6.720228	0.561017	-0.036367
	H	-7.139583	0.461197	0.976747
	H	-6.206740	-0.392115	-0.215734
	H	-7.550766	0.661624	-0.739015
	H	-4.706366	1.662871	0.650355
	H	-5.890151	2.766665	-0.622537
$(CH_3)_2BH$				
	B	-5.814752	1.739815	0.298448
	C	-6.672670	0.512097	-0.169343
	H	-7.403641	0.321360	0.633543
	H	-6.107573	-0.413942	-0.315361
	H	-7.272357	0.721164	-1.061713
	H	-6.300870	2.840920	0.215997
	C	-4.357150	1.609120	0.864088
	H	-4.133457	2.322550	1.664060
	H	-4.077883	0.599189	1.180985
	H	-3.684956	1.880329	0.033135
$(CH_3)_3B$				
	B	-5.826495	1.769766	0.303636
	C	-6.680747	0.521978	-0.149222
	H	-7.083629	0.060514	0.766064
	H	-6.073655	-0.256828	-0.625838
	H	-7.535202	0.757038	-0.792058

	C	-4.383066	1.566928	0.910420
	H	-4.235641	2.163902	1.818558
	H	-4.111573	0.527479	1.120236
	H	-3.653599	1.959116	0.185579
	C	-6.421496	3.223289	0.135876
	H	-6.454288	3.457487	-0.938782
	H	-7.465741	3.268990	0.470049
	H	-5.857385	4.019281	0.631497
$[B_6H_5CH_3]^{2-}$				
	B	-0.683190	9.087749	4.779275
	B	-0.023884	10.036003	6.074066
	B	0.589995	10.224086	4.460968
	H	-1.805994	8.881741	4.341807
	H	-0.485184	10.787435	6.921866
	H	0.738532	11.166348	3.698493
	B	1.567932	9.466013	5.679177
	B	0.906272	8.519699	4.384001
	B	0.295444	8.333003	5.999462
	H	2.687545	9.650132	6.134472
	H	1.364964	7.749505	3.551868
	C	0.095531	7.076481	7.011804
	H	-0.946153	6.713957	7.022965
	H	0.728607	6.216394	6.735274
	H	0.352306	7.337848	8.052682
$[1\text{-}B_{10}H_9CH_3]^{2-}$				
	B	-0.273965	1.813916	-0.518151
	B	-0.422452	0.537862	-1.639481
	B	1.133356	0.877935	-0.736888

	B	0.210818	0.905589	0.841518
	B	-1.343665	0.566431	-0.059411
	H	2.161905	1.422550	-1.080596
	H	0.427912	1.482131	1.886968
	H	-2.498335	0.844685	0.192408
	B	0.781123	-0.792776	-1.355198
	B	0.296872	-1.859723	-0.118570
	B	-0.975277	-1.013802	-0.874678
	B	-0.526046	-0.752622	0.885087
	B	1.229514	-0.532234	0.404475
	H	-1.885776	-1.620832	-1.397139
	H	-1.040146	-1.129992	1.916609
	H	2.262700	-0.709239	1.013840
	H	0.478299	-3.047098	0.008945
	H	1.418505	-1.200850	-2.302468
	H	-0.761870	0.783537	-2.778698
	C	-0.519131	3.397005	-0.689973
	H	-0.120611	3.770174	-1.646044
	H	-1.590771	3.648507	-0.666211
	H	-0.033526	3.975123	0.111405
$[2\text{-}B_{10}H_9CH_3]^{2-}$				
	B	0.070969	1.929535	0.210223
	B	-0.294315	0.973255	-1.154610
	B	1.319431	0.883957	-0.278730
	B	0.448442	0.700920	1.324229
	B	-1.163317	0.784370	0.455398
	H	0.056392	3.133192	0.323774
	H	2.412755	1.324263	-0.566119

	H	0.771351	0.978060	2.460128
	H	-2.264679	1.143679	0.816726
	B	0.704724	-0.546867	-1.208130
	B	0.095360	-1.779196	-0.201355
	B	-1.048921	-0.616764	-0.691604
	B	-0.530782	-0.809050	1.052926
	B	1.229301	-0.738590	0.533130
	H	-2.051502	-0.948321	-1.289651
	H	-1.071754	-1.326089	2.007595
	H	2.237892	-1.194713	1.029136
	H	0.103247	-2.979909	-0.334833
	H	1.246250	-0.818500	-2.259533
	C	-0.737958	1.674634	-2.548870
	H	0.037589	2.370787	-2.903376
	H	-0.924352	0.948898	-3.354709
	H	-1.659438	2.261177	-2.412306
$[B_{12}H_{11}CH_3]^{2-}$				
	B	2.946179	6.333901	2.866168
	B	1.362753	5.523982	3.014458
	B	4.046730	5.608254	4.066152
	B	3.278268	7.180644	4.401364
	B	1.617022	7.128587	3.752350
	B	2.865611	4.586489	3.211577
	H	3.345853	6.754781	1.805354
	H	0.636231	5.370307	2.060335
	H	5.235691	5.496603	3.869593
	H	3.915199	8.207281	4.438543
	H	1.070719	8.118595	3.324934

	H	3.214070	3.754243	2.405891
	B	0.715101	5.871168	4.640281
	B	1.489670	4.300281	4.305392
	B	3.401878	5.951944	5.689257
	B	3.154080	4.340220	4.957861
	B	1.899975	6.893895	5.497383
	B	1.820485	5.145767	5.836013
	H	-0.473103	5.967250	4.842949
	H	0.862844	3.265942	4.273004
	H	4.131471	6.093086	6.644273
	H	1.556511	7.717279	6.312720
	H	1.431881	4.712851	6.897285
	C	3.886041	3.013393	5.531276
	H	3.615351	2.828161	6.580847
	H	3.606438	2.119173	4.955545
	H	4.981086	3.107017	5.483562
[*ortho*-$CB_5H_5CH_3$]$^-$				
	B	-0.710688	9.138762	4.791212
	B	0.109613	9.969960	6.047885
	C	0.685379	9.934939	4.523685
	H	-1.784402	9.252682	4.270333
	H	-0.148909	10.900239	6.760596
	H	0.938595	10.727906	3.828485
	B	1.572055	9.150635	5.642535
	B	0.738126	8.312283	4.388022
	B	0.141422	8.247522	6.003470
	H	1.092470	7.619781	3.474390
	H	-0.137068	7.369350	6.776584

	C	3.103911	9.296523	6.074843
	H	3.337059	8.646102	6.927513
	H	3.791564	9.022925	5.263434
	H	3.349483	10.323091	6.379239
[*meta*-$CB_5H_5CH_3$]$^-$				
	B	-0.674545	9.072114	4.799513
	B	-0.020288	10.010137	6.080307
	C	0.569580	10.094606	4.564866
	H	-1.747074	9.006887	4.266401
	H	-0.448970	10.869513	6.799889
	H	0.699687	10.929402	3.886788
	B	1.554131	9.447328	5.688831
	B	0.899448	8.509016	4.406855
	B	0.292126	8.308704	6.016149
	H	2.662998	9.758231	6.024188
	H	1.368007	7.894449	3.489087
	C	0.094780	7.072401	7.015551
	H	-0.943573	6.715367	7.020726
	H	0.727590	6.218675	6.738803
	H	0.348826	7.339565	8.050226
[*ortho*-$CB_9H_9CH_3$]$^-$				
	B	0.039156	1.946161	0.248048
	B	-0.294381	0.987072	-1.117755
	B	1.315203	0.931874	-0.238686
	B	0.438099	0.716739	1.358152
	B	-1.175228	0.771784	0.476697
	H	0.004116	3.132740	0.388124
	H	2.390444	1.389430	-0.516079

	H	0.742167	0.995489	2.485667
	H	-2.272620	1.099604	0.836656
	B	0.748390	-0.493277	-1.203151
	C	0.147173	-1.569510	-0.174557
	B	-1.023246	-0.600971	-0.683949
	B	-0.505133	-0.798030	1.068870
	B	1.257504	-0.679749	0.563035
	H	-1.954776	-1.072515	-1.269146
	H	-1.008547	-1.430431	1.950742
	H	2.225887	-1.217283	1.017456
	H	0.180555	-2.642478	-0.303825
	H	-0.617708	1.496443	-2.156447
	C	1.471627	-0.974176	-2.543532
	H	2.357959	-1.580842	-2.316425
	H	0.800761	-1.587159	-3.160104
	H	1.799484	-0.126552	-3.154583
[*meta*-$CB_9H_9CH_3$]$^-$				
	B	0.071433	1.915873	0.207456
	B	-0.296791	0.969672	-1.165115
	B	1.321503	0.876687	-0.281686
	B	0.449539	0.692818	1.324504
	B	-1.165509	0.778028	0.454156
	H	0.058904	3.106578	0.322924
	H	2.405310	1.310172	-0.563530
	H	0.769203	0.967102	2.448566
	H	-2.255083	1.131469	0.815657
	B	0.705998	-0.540277	-1.211680
	C	0.093513	-1.603671	-0.180691

	B	-1.052637	-0.608766	-0.694709
	B	-0.533217	-0.800767	1.057527
	B	1.233150	-0.731264	0.535649
	H	-1.999778	-1.054684	-1.274806
	H	-1.045019	-1.414245	1.947901
	H	2.188762	-1.287439	0.992470
	H	0.100562	-2.677250	-0.299144
	H	1.218711	-0.928463	-2.220936
	C	-0.737313	1.670199	-2.546912
	H	0.032125	2.372481	-2.891681
	H	-0.918064	0.954340	-3.358522
	H	-1.658617	2.250134	-2.407961
[*para*-$CB_9H_9CH_3$]$^-$				
	B	-0.275199	1.810931	-0.518799
	B	-0.422384	0.532624	-1.641726
	B	1.135163	0.874277	-0.737399
	B	0.211153	0.902428	0.842879
	B	-1.346163	0.562036	-0.059232
	H	2.154994	1.409729	-1.076858
	H	0.427907	1.467154	1.880102
	H	-2.490357	0.828770	0.191120
	B	0.781569	-0.780824	-1.360355
	C	0.269533	-1.683299	-0.137303
	B	-0.980223	-1.003306	-0.877608
	B	-0.529468	-0.741150	0.886414
	B	1.230276	-0.519332	0.404967
	H	-1.824305	-1.701359	-1.358256
	H	-0.998295	-1.220837	1.876876

	H	2.228703	-0.809354	0.995923
	H	0.433133	-2.744521	-0.021742
	H	1.405143	-1.291562	-2.243959
	H	-0.758044	0.769898	-2.770357
	C	-0.515328	3.379226	-0.687445
	H	-0.117703	3.747466	-1.641505
	H	-1.583709	3.627903	-0.660830
[*ortho*-$CB_{11}H_{11}CH_3$]$^-$				
	B	2.896691	6.409654	2.815356
	B	1.228199	5.787932	2.892398
	B	3.887019	5.408304	3.891270
	B	3.321970	7.001508	4.432792
	B	1.676759	7.243775	3.818593
	B	2.600848	4.653905	2.937405
	H	3.366539	6.911287	1.834724
	H	0.491284	5.847403	1.949356
	H	5.060469	5.193438	3.807352
	H	4.121042	7.847019	4.703287
	H	1.277419	8.340325	3.552451
	H	2.863996	3.895298	2.048374
	B	0.626558	6.002465	4.556390
	B	1.199555	4.403473	4.011546
	C	3.203251	5.628132	5.430365
	B	2.851680	4.156441	4.627664
	B	1.925981	6.750130	5.503388
	B	1.635367	5.003145	5.618781
	H	-0.522856	6.215499	4.816450
	H	0.465009	3.464517	3.887768

	H	3.868420	5.571140	6.285020
	H	1.805709	7.431801	6.476811
	H	1.329681	4.523966	6.670656
	C	3.483976	2.776170	5.134674
	H	4.023935	2.898260	6.082414
	H	2.704086	2.023757	5.298415
	H	4.191600	2.368525	4.403583
[*meta*-$CB_{11}H_{11}CH_3$]$^-$				
	B	2.954994	6.334956	2.862410
	B	1.385216	5.522725	3.016266
	B	4.051517	5.609398	4.063796
	B	3.287156	7.182307	4.399174
	B	1.636087	7.120579	3.751979
	B	2.876446	4.585974	3.207625
	H	3.319235	6.760378	1.804093
	H	0.556735	5.394815	2.165195
	H	5.229965	5.505378	3.867858
	H	3.888463	8.216411	4.442358
	H	0.971463	8.043675	3.388531
	H	3.191325	3.756711	2.402666
	C	0.887407	5.855017	4.612104
	B	1.512966	4.303794	4.302467
	B	3.413195	5.952517	5.687575
	B	3.170233	4.333737	4.957258
	B	1.920432	6.887661	5.489777
	B	1.843035	5.145423	5.827520
	H	-0.177256	5.938486	4.795820
	H	0.772795	3.364986	4.298997

	H	4.109383	6.101601	6.651394
	H	1.445269	7.657573	6.268927
	H	1.322649	4.761768	6.832781
	C	3.876563	3.010612	5.534525
	H	3.604356	2.829362	6.581602
	H	3.595320	2.118387	4.961940
	H	4.969087	3.096864	5.489727
[*para*-$CB_{11}H_{11}CH_3$]$^-$				
	B	2.951216	6.317054	2.877956
	B	1.374743	5.510494	3.026158
	B	4.052912	5.599165	4.068773
	B	3.282827	7.160760	4.407103
	C	1.695532	6.986588	3.813533
	B	2.870625	4.576920	3.213953
	H	3.246945	6.836872	1.844075
	H	0.631364	5.498449	2.091085
	H	5.230033	5.524231	3.857308
	H	3.797294	8.237947	4.383873
	H	1.206713	7.873776	3.429230
	H	3.201800	3.774363	2.388753
	B	0.729977	5.856936	4.645066
	B	1.493632	4.291559	4.309322
	B	3.407224	5.944967	5.693388
	B	3.159696	4.330468	4.962346
	B	1.909389	6.875673	5.499015
	B	1.824562	5.137799	5.841364
	H	-0.437273	6.074603	4.776140
	H	0.842720	3.286816	4.260938

	H	4.121066	6.122956	6.639141
	H	1.521770	7.764644	6.195312
	H	1.413976	4.738837	6.894040
	C	3.885567	3.013556	5.530405
	H	3.611543	2.824852	6.575594
	H	3.610233	2.122825	4.952509
	H	4.977950	3.107984	5.487988