Theoretical Study of *Closo*-Borate Anions $[B_nH_n]^{2-}$ (n = 5-12): Bonding, Atomic Charges and Reactivity Analysis

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Table S1. B–H bond lengths**,** Wiberg index, and 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, H_b – total energy at the bcp, δ(B–C) – delocalization index, ε_b – ellipticity at the bcp.

Anion	B position	B–H length (Å)	Wiberg Index	$\rho(r)$ (e Å^{-3})	$\nabla^2\rho(r)$ (e Å^{-5})	H_b (h e^{-1})	δ(B–H)	ε_b
$[B_5H_5]^{2-}$	B_{ap}	1.22	0.96	0.150	-0.060	-0.144	0.782	0.000
	B_{eq}	1.22	0.93	0.150	-0.075	-0.144	0.741	0.302
$[B_6H_6]^{2-}$		1.22	0.96	0.151	-0.085	-0.146	0.723	0.001
$[B_7H_7]^{2-}$	B_{ap}	1.22	0.96	0.155	-0.133	-0.154	0.687	0.001
	B_{eq}	1.22	0.95	0.151	-0.073	-0.146	0.728	0.210
$[B_8H_8]^{2-}$	B_{ap}	1.22	0.95	0.156	-0.132	-0.155	0.721	0.140
	B_{eq}	1.22	0.96	0.156	-0.121	-0.154	0.688	0.142
$[B_9H_9]^{2-}$	B_{ap}	1.21	0.95	0.156	-0.083	-0.152	0.724	0.114
	B_{eq}	1.22	0.95	0.158	-0.117	-0.156	0.692	0.163
	B_{eq}	1.21	0.95	0.156	-0.088	-0.153	0.725	0.110
$[B_{10}H_{10}]^{2-}$	B_{ap}	1.21	0.95	0.158	-0.096	-0.155	0.724	0.000
	B_{eq}	1.21	0.95	0.159	-0.127	-0.159	0.696	0.125
$[B_{11}H_{11}]^{2-}$	B11	1.21	0.95	0.163	-0.158	-0.166	0.681	0.232
	B6,7	1.21	0.95	0.159	-0.099	-0.157	0.713	0.156
	B4,5,8,9	1.21	0.95	0.161	-0.130	-0.161	0.691	0.111
	B2,3	1.21	0.95	0.162	-0.131	-0.162	0.696	0.058
	B10	1.21	0.96	0.161	-0.131	-0.161	0.686	0.021
$[B_{12}H_{12}]^{2-}$		1.21	0.96	0.162	-0.136	-0.162	0.691	0.002

Table S2. HOMO and LUMO energies, electronic chemical potential μ, electronegativity χ, chemical hardness η, softness S, and electrophilicity ω.

Anion	HOMO, eV	LUMO, eV	Gap, eV	μ, eV	χ, eV	η, eV	S, eV^{-1}	ω, eV
$[B_5H_5]^{2-}$	2.22	7.13	4.91	4.68	-4.68	4.91	0.20	2.23
$[B_6H_6]^{2-}$	1.13	7.11	5.98	4.12	-4.12	5.98	0.17	1.42
$[B_7H_7]^{2-}$	0.61	7.03	6.42	3.82	-3.82	6.42	0.16	1.14
$[B_8H_8]^{2-}$	1.37	6.94	5.57	4.16	-4.16	5.57	0.18	1.55
$[B_9H_9]^{2-}$	0.88	6.90	6.02	3.89	-3.89	6.02	0.17	1.26
$[B_{10}H_{10}]^{2-}$	-0.17	6.73	6.89	3.28	-3.28	6.89	0.15	0.78
$[B_{11}H_{11}]^{2-}$	0.15	6.61	6.46	3.38	-3.38	6.46	0.15	0.88
$[B_{12}H_{12}]^{2-}$	-1.72	6.54	8.26	2.41	-2.41	8.26	0.12	0.35

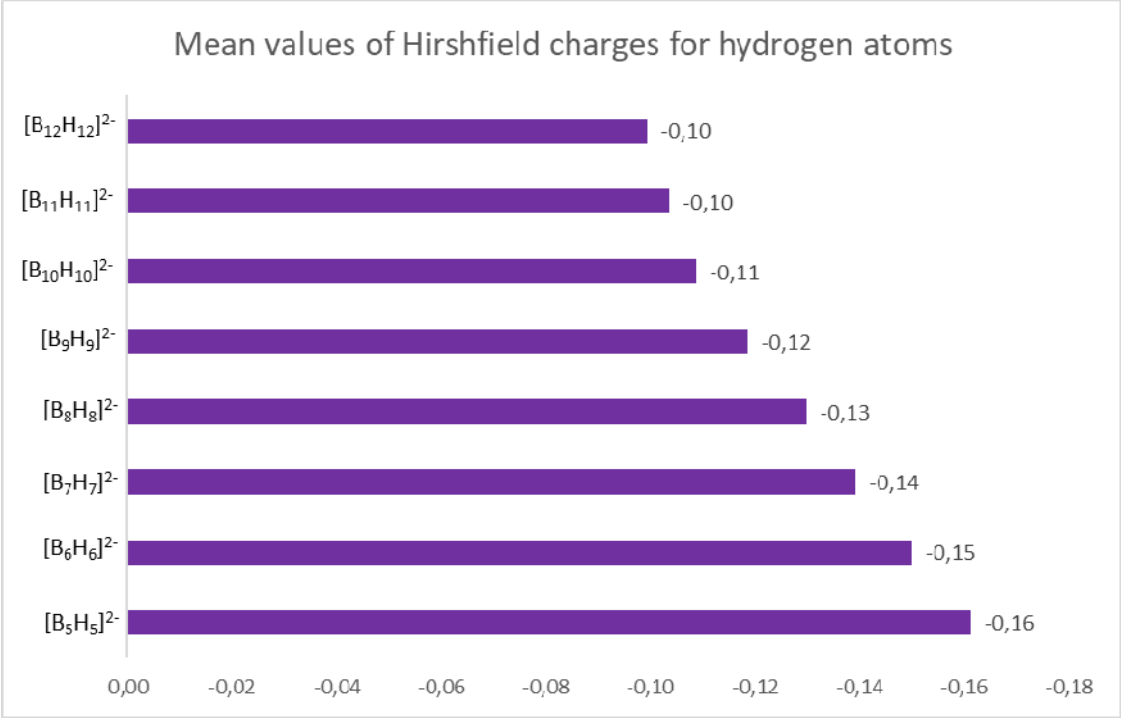

Figure S1. Mean values of Hirshfeld charges for hydrogen atoms for the closo-borate anions of general form $[B_nH_n]^{2-}$ (n = 5-12).

Table S3. NBO, QTAIM and Hirshfeld atomic charges of $[B_nH_n]^{2-}$ (n = 5 -12).

Compound	Atom	NBO	QTAIM	Hirshfeld
$[B_5H_5]^{2-}$				
	B (1)	-0.46	0.20	-0.29
	B (2)	-0.45	0.21	-0.29
	B (3)	-0.29	0.41	-0.20
	B (4)	-0.29	0.42	-0.20
	B (5)	-0.29	0.42	-0.20
	H (6)	-0.05	-0.76	-0.17
	H (7)	-0.04	-0.72	-0.16
	H (8)	-0.04	-0.72	-0.16
	H (9)	-0.04	-0.72	-0.16
	H (10)	-0.05	-0.76	-0.17
$[B_6H_6]^{2-}$				
	B (1)	-0.30	0.39	-0.18
	B (2)	-0.29	0.41	-0.18
	B (3)	-0.30	0.39	-0.18
	H (4)	-0.04	-0.73	-0.15
	H (5)	-0.04	-0.73	-0.15
	B (6)	-0.30	0.39	-0.18
	B (7)	-0.29	0.41	-0.18
	B (8)	-0.30	0.39	-0.18
	H (9)	-0.04	-0.73	-0.15
	H (10)	-0.04	-0.73	-0.15
	H (11)	-0.04	-0.73	-0.15
	H (12)	-0.04	-0.73	-0.15
$[B_7H_7]^{2-}$				
	B (1)	-0.14	0.75	-0.08
	B (2)	-0.14	0.75	-0.08
	B (3)	-0.31	0.27	-0.17
	B (4)	-0.30	0.31	-0.17
	B (5)	-0.30	0.31	-0.17
	B (6)	-0.30	0.28	-0.17
	B (7)	-0.30	0.28	-0.17
	H (8)	-0.04	-0.73	-0.14
	H (9)	-0.04	-0.73	-0.14
	H (10)	-0.03	-0.70	-0.14
	H (11)	-0.03	-0.70	-0.14
	H (12)	-0.02	-0.70	-0.14
	H (13)	-0.02	-0.70	-0.14
	H (14)	-0.02	-0.70	-0.14
$[B_8H_8]^{2-}$				
	B (1)	-0.19	0.58	-0.09
	B (2)	-0.19	0.58	-0.09

	B (3)	-0.19	0.57	-0.09
	B (4)	-0.18	0.60	-0.08
	B (5)	-0.28	0.31	-0.16
	B (6)	-0.28	0.31	-0.16
	B (7)	-0.27	0.32	-0.15
	B (8)	-0.28	0.31	-0.16
	H (9)	-0.02	-0.70	-0.13
	H (10)	-0.02	-0.70	-0.13
	H (11)	-0.02	-0.70	-0.13
	H (12)	-0.02	-0.70	-0.13
	H (13)	-0.02	-0.70	-0.13
	H (14)	-0.02	-0.70	-0.13
	H (15)	-0.02	-0.70	-0.13
	H (16)	-0.02	-0.70	-0.13
$[B_9H_9]^{2-}$				
	B (1)	-0.17	0.57	-0.08
	B (2)	-0.17	0.57	-0.08
	B (3)	-0.17	0.57	-0.08
	B (4)	-0.17	0.57	-0.08
	B (5)	-0.17	0.57	-0.08
	B (6)	-0.17	0.57	-0.08
	B (7)	-0.32	0.26	-0.15
	B (8)	-0.32	0.25	-0.15
	B (9)	-0.32	0.25	-0.15
	H (10)	0.00	-0.69	-0.12
	H (11)	0.00	-0.69	-0.12
	H (12)	0.00	-0.69	-0.12
	H (13)	0.00	-0.69	-0.12
	H (14)	0.00	-0.69	-0.12
	H (15)	0.00	-0.68	-0.12
	H (16)	0.00	-0.68	-0.12
	H (17)	0.00	-0.68	-0.12
	H (18)	0.00	-0.69	-0.12
$[B_{10}H_{10}]^{2-}$				
	B (1)	-0.26	0.33	-0.14
	B (2)	-0.20	0.51	-0.08
	B (3)	-0.20	0.51	-0.08
	B (4)	-0.20	0.51	-0.08
	B (5)	-0.20	0.51	-0.08
	H (6)	0.00	-0.68	-0.11
	H (7)	0.01	-0.67	-0.11
	H (8)	0.01	-0.67	-0.11
	H (9)	0.01	-0.67	-0.11
	H (10)	0.01	-0.67	-0.11
	B (11)	-0.20	0.51	-0.08
	B (12)	-0.26	0.33	-0.14

	B (13)	-0.20	0.51	-0.08
	B (14)	-0.20	0.51	-0.08
	B (15)	-0.20	0.51	-0.08
	H (16)	0.02	-0.67	-0.11
	H (17)	0.02	-0.67	-0.11
	H (18)	0.02	-0.67	-0.11
	H (19)	0.02	-0.67	-0.11
	H (20)	0.00	-0.68	-0.11
$[B_{11}H_{11}]^{2-}$				
	B (1)	-0.19	0.61	-0.07
	B (2)	-0.19	0.61	-0.07
	B (3)	-0.22	0.46	-0.08
	B (4)	-0.23	0.45	-0.08
	B (5)	-0.18	0.48	-0.08
	B (6)	-0.18	0.48	-0.08
	B (7)	-0.28	0.32	-0.13
	B (8)	-0.28	0.32	-0.13
	B (9)	-0.18	0.48	-0.08
	B (10)	-0.18	0.48	-0.08
	B (11)	-0.10	0.67	-0.01
	H (12)	0.01	-0.67	-0.11
	H (13)	0.01	-0.67	-0.11
	H (14)	0.02	-0.68	-0.11
	H (15)	0.02	-0.68	-0.11
	H (16)	0.01	-0.67	-0.11
	H (17)	0.01	-0.67	-0.11
	H (18)	0.02	-0.67	-0.11
	H (19)	0.02	-0.67	-0.11
	H (20)	0.03	-0.67	-0.10
	H (21)	0.04	-0.64	-0.09
	H (22)	0.03	-0.66	-0.10
$[B_{12}H_{12}]^{2-}$				
	B (1)	-0.19	0.50	-0.07
	B (2)	-0.19	0.50	-0.07
	B (3)	-0.19	0.50	-0.07
	B (4)	-0.19	0.50	-0.07
	B (5)	-0.19	0.50	-0.07
	B (6)	-0.19	0.50	-0.07
	H (7)	0.03	-0.67	-0.10
	H (8)	0.03	-0.67	-0.10
	H (9)	0.03	-0.67	-0.10
	H (10)	0.03	-0.67	-0.10
	H (11)	0.03	-0.67	-0.10
	B (12)	-0.19	0.50	-0.07
	B (13)	-0.19	0.50	-0.07
	B (14)	-0.19	0.50	-0.07

	B (15)	-0.19	0.50	-0.07
	B (16)	-0.19	0.50	-0.07
	B (17)	-0.19	0.50	-0.07
	H (18)	0.03	-0.67	-0.10
	H (19)	0.03	-0.67	-0.10
	H (20)	0.03	-0.67	-0.10
	H (21)	0.03	-0.67	-0.10
	H (22)	0.03	-0.67	-0.10
	H (23)	0.03	-0.67	-0.10
	H (24)	0.03	-0.67	-0.10

Table S4. Fukui function values based on the NBO, QTAIM and Hirshfeld atomic charges in $[B_nH_n]^{2-}$ (n = 5-12).

Compound	Atom	F-NBO	F-QTAIM	F-Hirshfeld
$[B_5H_5]^{2-}$				
	B (1)	0.27	-0.03	0.17
	B (2)	0.27	-0.03	0.17
	B (3)	0.23	0.27	0.15
	B (4)	0.03	0.20	0.08
	B (5)	0.03	0.20	0.08
	H (6)	0.03	0.09	0.07
	H (7)	0.03	0.07	0.07
	H (8)	0.04	0.07	0.06
	H (9)	0.04	0.07	0.06
	H (10)	0.03	0.09	0.07
$[B_6H_6]^{2-}$				
	B (1)	0.15	0.10	0.11
	B (2)	0.22	0.04	0.13
	B (3)	0.03	0.15	0.08
	H (4)	0.04	0.07	0.06
	H (5)	0.04	0.07	0.05
	B (6)	0.15	0.10	0.11
	B (7)	0.22	0.04	0.13
	B (8)	0.03	0.15	0.08
	H (9)	0.04	0.07	0.06
	H (10)	0.03	0.07	0.06
	H (11)	0.04	0.07	0.05
	H (12)	0.03	0.07	0.06
$[B_7H_7]^{2-}$				
	B (1)	-0.03	0.07	0.03
	B (2)	-0.03	0.07	0.03
	B (3)	0.03	0.19	0.06
	B (4)	0.10	0.13	0.09
	B (5)	0.10	0.13	0.09
	B (6)	0.22	-0.06	0.13

	B (7)	0.22	-0.06	0.13
	H (8)	0.04	0.06	0.04
	H (9)	0.04	0.06	0.04
	H (10)	0.07	0.09	0.07
	H (11)	0.07	0.09	0.07
	H (12)	0.04	0.07	0.07
	H (13)	0.04	0.07	0.07
	H (14)	0.08	0.11	0.07
$[B_8H_8]^{2-}$				
	B (1)	-0.01	0.02	0.04
	B (2)	-0.01	0.02	0.04
	B (3)	-0.01	0.03	0.04
	B (4)	-0.01	0.02	0.04
	B (5)	0.16	0.10	0.10
	B (6)	0.16	0.10	0.10
	B (7)	0.16	0.11	0.10
	B (8)	0.16	0.10	0.10
	H (9)	0.04	0.05	0.05
	H (10)	0.04	0.05	0.05
	H (11)	0.04	0.05	0.05
	H (12)	0.06	0.07	0.05
	H (13)	0.06	0.07	0.05
	H (14)	0.06	0.07	0.05
	H (15)	0.06	0.07	0.05
	H (16)	0.04	0.05	0.06
$[B_9H_9]^{2-}$				
	B (1)	0.02	0.05	0.05
	B (2)	0.02	0.05	0.05
	B (3)	0.02	0.05	0.05
	B (4)	0.02	0.05	0.05
	B (5)	0.02	0.05	0.05
	B (6)	0.02	0.05	0.05
	B (7)	0.17	0.09	0.10
	B (8)	0.17	0.09	0.10
	B (9)	0.17	0.09	0.10
	H (10)	0.04	0.05	0.04
	H (11)	0.04	0.05	0.04
	H (12)	0.04	0.05	0.04
	H (13)	0.04	0.05	0.04
	H (14)	0.04	0.05	0.04
	H (15)	0.04	0.05	0.05
	H (16)	0.04	0.05	0.05
	H (17)	0.04	0.05	0.05
	H (18)	0.04	0.05	0.04
$[B_{10}H_{10}]^{2-}$				
	B (1)	0.17	-0.05	0.10

	B (2)	0.06	0.09	0.05
	B (3)	0.01	0.07	0.04
	B (4)	0.06	0.09	0.05
	B (5)	0.01	0.07	0.04
	H (6)	0.03	0.05	0.05
	H (7)	0.04	0.05	0.04
	H (8)	0.04	0.05	0.04
	H (9)	0.04	0.05	0.04
	H (10)	0.04	0.05	0.04
	B (11)	0.11	0.10	0.07
	B (12)	0.18	-0.02	0.10
	B (13)	-0.04	0.04	0.02
	B (14)	0.11	0.10	0.07
	B (15)	-0.04	0.04	0.02
	H (16)	0.04	0.05	0.05
	H (17)	0.04	0.05	0.04
	H (18)	0.04	0.05	0.05
	H (19)	0.04	0.05	0.04
	H (20)	0.03	0.06	0.05
$[B_{11}H_{11}]^{2-}$				
	B (1)	-0.01	0.04	0.03
	B (2)	-0.01	0.04	0.03
	B (3)	0.05	0.09	0.04
	B (4)	0.04	0.09	0.04
	B (5)	0.06	0.04	0.05
	B (6)	0.06	0.04	0.05
	B (7)	0.16	0.06	0.09
	B (8)	0.16	0.06	0.09
	B (9)	0.06	0.03	0.06
	B (10)	0.06	0.03	0.06
	B (11)	-0.09	-0.06	0.01
	H (12)	0.03	0.05	0.05
	H (13)	0.03	0.05	0.05
	H (14)	0.04	0.04	0.04
	H (15)	0.04	0.04	0.04
	H (16)	0.05	0.06	0.05
	H (17)	0.05	0.06	0.05
	H (18)	0.05	0.06	0.05
	H (19)	0.05	0.06	0.05
	H (20)	0.03	0.04	0.04
	H (21)	0.04	0.04	0.03
	H (22)	0.03	0.04	0.04
$[B_{12}H_{12}]^{2-}$				
	B (1)	-0.03	0.05	0.02
	B (2)	0.14	0.03	0.07
	B (3)	-0.03	0.04	0.02

	B (4)	0.04	0.05	0.04
	B (5)	0.12	0.04	0.07
	B (6)	0.07	0.04	0.05
	H (7)	0.04	0.04	0.03
	H (8)	0.03	0.04	0.04
	H (9)	0.04	0.04	0.03
	H (10)	0.03	0.04	0.04
	H (11)	0.03	0.04	0.04
	B (12)	-0.03	0.04	0.02
	B (13)	0.04	0.05	0.04
	B (14)	0.14	0.03	0.07
	B (15)	0.12	0.03	0.07
	B (16)	0.07	0.04	0.05
	B (17)	-0.03	0.05	0.02
	H (18)	0.04	0.04	0.03
	H (19)	0.03	0.04	0.04
	H (20)	0.03	0.04	0.04
	H (21)	0.03	0.04	0.04
	H (22)	0.03	0.04	0.04
	H (23)	0.04	0.04	0.03
	H (24)	0.03	0.04	0.04

Table S5. Cartesian atomic coordinates of the calculated optimized equilibrium model structures. All coordinates are given in Angstrom units.

Compound	Atom	x	y	z
$[B_5H_5]^{2-}$				
	B	-2.349023	-0.000208	0.000000
	B	0.277019	-0.000165	0.000000
	B	-1.036308	1.047904	0.000000
	B	-1.036357	-0.524420	-0.908104
	B	-1.036357	-0.524420	0.908104
	H	-3.566759	0.000248	0.000000
	H	-1.036148	2.272399	0.000000
	H	-1.035973	-1.135702	-1.969368
	H	-1.035973	-1.135702	1.969368
	H	1.494583	0.000066	0.000000
$[B_6H_6]^{2-}$				
	B	-0.724456	9.557357	5.084812
	B	0.419420	9.873490	6.353719
	B	0.708843	10.477979	4.751076
	H	-1.923790	9.742974	4.941074
	H	0.936941	11.579707	4.274607
	B	1.684936	9.187314	5.380759
	B	0.541141	8.871294	4.112097
	B	0.251588	8.266707	5.714493
	H	2.884031	9.004017	5.529418
	H	0.602461	8.373502	2.998403
	H	0.023512	7.167181	6.196033
	H	0.358192	10.370983	7.466840
$[B_7H_7]^{2-}$				
	B	-0.824477	0.000000	1.162093
	B	-0.824477	0.000000	-1.162093
	B	0.585930	0.000000	0.000000
	B	-0.387230	-1.343597	0.000000
	B	-0.387230	1.343597	0.000000
	B	-1.965389	-0.829815	0.000000
	B	-1.965389	0.829815	0.000000
	H	-0.826511	0.000000	2.386749
	H	-0.826511	0.000000	-2.386749
	H	-0.007349	-2.503949	0.000000
	H	-0.007349	2.503949	0.000000
	H	-2.956795	-1.541714	0.000000
	H	-2.956795	1.541714	0.000000
	H	1.807073	0.000000	0.000000
$[B_8H_8]^{2-}$				
	B	-0.141249	1.260992	0.505090

	B	-0.141249	-1.260992	0.505090
	B	-0.915664	0.000000	1.681084
	B	1.264661	0.000000	0.411434
	B	0.692696	0.808380	1.936272
	B	0.692696	-0.808380	1.936272
	B	-1.357706	0.000000	0.020727
	B	0.040263	0.000000	-0.791440
	H	1.150779	1.613658	2.724880
	H	1.150779	-1.613658	2.724880
	H	-2.512310	0.000000	-0.363193
	H	-0.287991	2.448361	0.254466
	H	-0.287991	-2.448361	0.254466
	H	-1.794922	0.000000	2.530084
	H	2.436504	0.000000	0.066534
	H	0.277265	0.000000	-1.985128
$[B_9H_9]^{2-}$				
	B	0.000000	0.078425	-0.756803
	B	-0.983404	1.048214	0.645746
	B	0.983404	1.048214	0.645746
	B	0.000000	-1.397125	0.257705
	B	0.987945	-0.422603	1.665551
	B	-0.987945	-0.422603	1.665551
	B	0.000000	0.923945	2.043849
	B	1.426494	-0.481468	0.010735
	B	-1.426494	-0.481468	0.010735
	H	-1.721879	2.004515	0.503042
	H	1.721879	2.004515	0.503042
	H	0.000000	-2.595617	0.049991
	H	1.728996	-0.890392	2.508558
	H	-1.728996	-0.890392	2.508558
	H	0.000000	1.613349	3.039841
	H	2.476229	-0.822619	-0.487673
	H	-2.476229	-0.822619	-0.487673
	H	0.000000	0.305448	-1.951717
$[B_{10}H_{10}]^{2-}$				
	B	0.000203	1.877685	0.000031
	B	-0.495164	0.773187	-1.194532
	B	1.194646	0.773004	-0.495217
	B	0.495331	0.773079	1.194593
	B	-1.194479	0.773262	0.495278
	H	0.000333	3.085416	0.000032
	H	-0.932524	1.174824	-2.252287
	H	2.252445	1.174479	-0.932620
	H	0.932778	1.174621	2.252348
	H	-2.252191	1.174966	0.932682
	B	0.49511	-0.745941	-1.194405

	B	-0.000201	-1.850650	0.000029
	B	-1.194516	-0.745758	-0.495161
	B	-0.495273	-0.745834	1.194465
	B	1.194354	-0.746017	0.495221
	H	0.932463	-1.147745	-2.252118
	H	-2.252272	-1.147401	-0.932558
	H	-0.932712	-1.147547	2.252177
	H	2.252023	-1.147890	0.932617
	H	-0.000330	-3.058358	0.000030
$[B_{11}H_{11}]^{2-}$				
	B	1.485741	0.511091	0.064393
	B	-1.485741	0.511091	0.064393
	B	0.000000	1.477191	-0.168865
	B	0.000000	0.031194	0.933431
	B	0.931059	0.927227	-1.587439
	B	-0.931059	0.927227	-1.587439
	B	-1.673864	-0.549664	-1.324855
	B	1.673864	-0.549664	-1.324855
	B	-0.933948	-1.191094	0.029845
	B	0.933948	-1.191094	0.029846
	B	0.000000	-0.843768	-1.725778
	H	-2.647789	-0.979964	-1.893965
	H	2.647789	-0.979964	-1.893965
	H	2.432118	0.967759	0.666722
	H	-2.432118	0.967759	0.666722
	H	1.366698	-2.174190	0.590448
	H	-1.366698	-2.174190	0.590448
	H	1.365268	1.720488	-2.393966
	H	-1.365269	1.720488	-2.393966
	H	0.000000	2.637349	0.174088
	H	0.000000	-1.573688	-2.691225
	H	0.000000	0.049909	2.141942
$[B_{12}H_{12}]^{2-}$				
	B	2.937354	6.719692	2.867786
	B	1.505298	5.656369	2.844440
	B	4.089637	6.065790	4.062981
	B	3.051830	7.453134	4.489569
	B	1.454857	7.200393	3.736068
	B	3.133704	4.955515	3.046796
	H	3.312599	7.303452	1.877885
	H	0.859612	5.480660	1.837114
	H	5.284877	6.186924	3.923126
	H	3.507257	8.560468	4.655794
	H	0.774219	8.127963	3.364779
	B	0.734669	5.733981	4.451866
	B	1.772408	4.346671	4.025336

	B	3.318993	6.143375	5.670380
	B	3.369388	4.599394	4.778797
	B	1.690482	6.844547	5.468203
	B	1.886869	5.080307	5.647064
	H	-0.460596	5.612978	4.591648
	H	1.316548	3.239450	3.859659
	H	3.964678	6.319137	6.677706
	H	4.049836	3.671906	5.150596
	H	1.175812	7.517163	6.331013
	H	1.511596	4.496874	6.637134
	H	3.648225	4.283301	2.184183