Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Exhaustive exploration of MgB_n (n = 10−20) clusters and their anions

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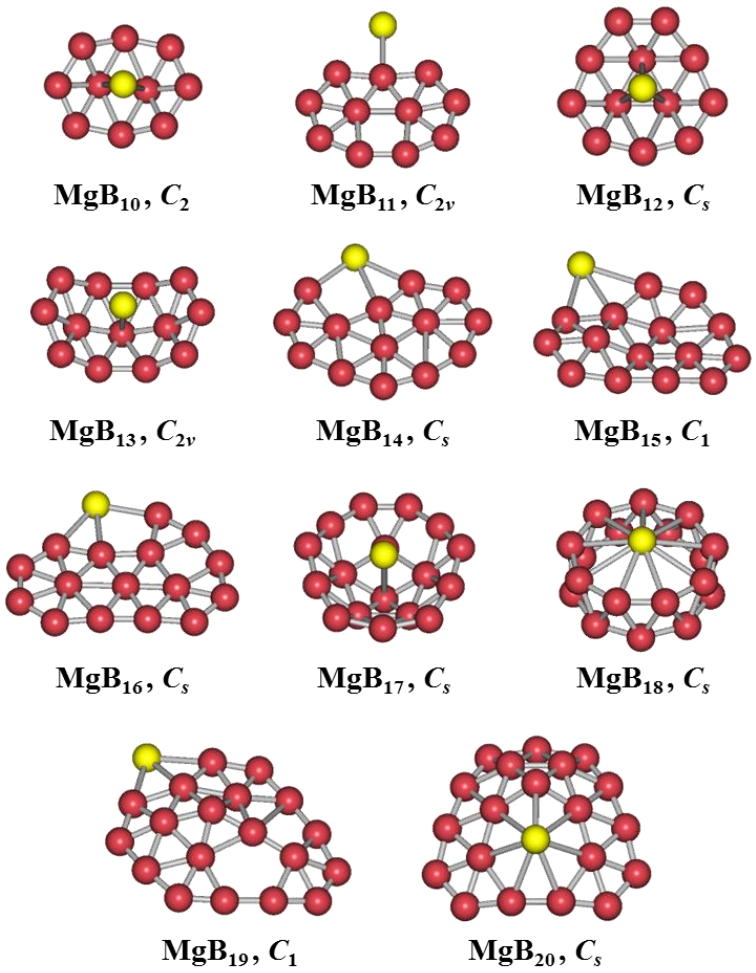

Figure S1. The lowest-energy structures of neutral MgB_n (n = 10−20) clusters, along with their point group symmetry.

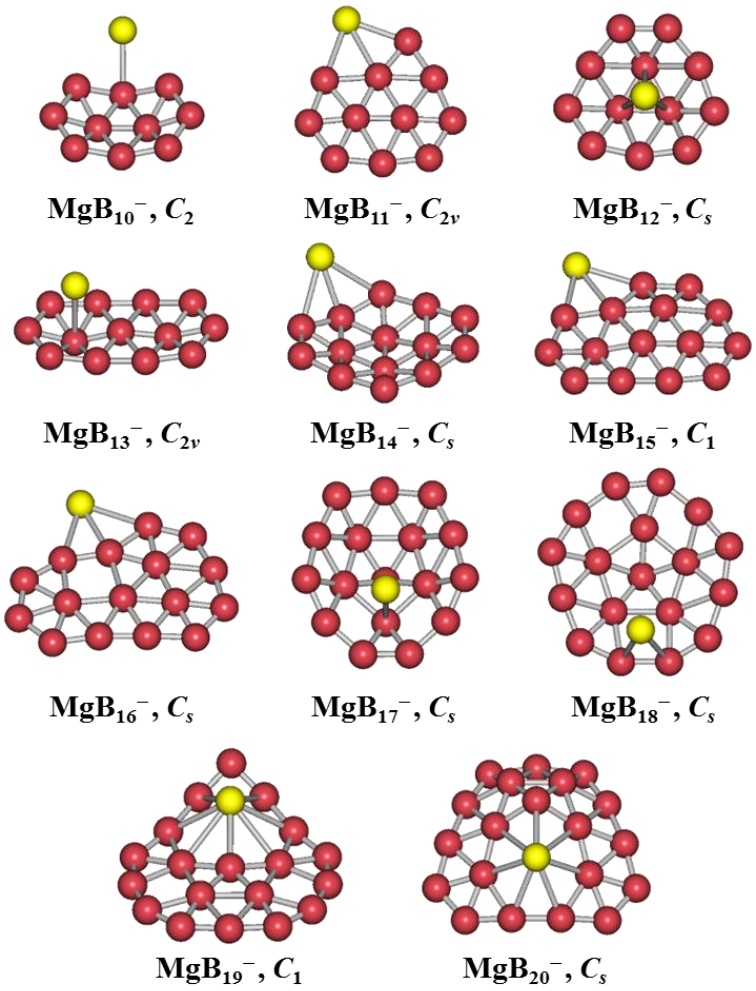

Figure S2. The lowest-energy structures of anionic MgB_n^- (n = 10−20) clusters, along with their point group symmetry.

Table S1. The Electronic States, Point Symmetry, Average Binding Energies (E_b, in eV), of the three typical structures of the $MgB_n^{0/-}$ (n = 10 – 20) Clusters.

Isomer	State	ΔE (eV)	E_b	Isomer	State	ΔE (eV)	E_b
10-n1	^{1}A	0.00	4.56	**10-a1**	^{2}A’	0.00	4.80
10-n2	^{3}A"	0.40	4.52	10-a2	^{2}A	0.16	4.79
10-n3	1-A'	0.64	4.50	10-a3	^{2}A	1.35	4.68
11-n1	$^2A_1$	0.00	4.64	**11-a1**	^{1}A’	0.00	4.84
11-n2	^{2}A"	1.99	4.48	11-a2	^{1}A	0.06	4.83
11-n3	$^2A_1$	3.97	4.31	11-a3	^{1}A	0.14	4.83
12-n1	^{1}A’	0.00	4.70	**12-a1**	^{2}A	0.00	4.89
12-n2	^{1}A	0.17	4.69	12-a2	^{2}A	0.23	4.87
12-n3	$^1A_1$	0.83	4.64	12-a3	^{2}A"	0.33	4.86
13-n1	$^2A_2$	0.00	4.76	**13-a1**	^{3}A"	0.00	4.98
13-n2	^{2}A	0.73	4.71	13-a2	^{1}A'	0.57	4.93
13-n3	^{2}A"	0.97	4.69	13-a3	^{3}A	0.92	4.91
14-n1	^{1}A’	0.00	4.75	**14-a1**	^{4}A	0.00	4.94
14-n2	^{1}A’ '	0.37	4.73	14-a2	^{2}A"	0.06	4.94
14-n3	^{1}A	0.39	4.73	14-a3	^{2}A"	0.11	4.94
15-n1	^{2}A	0.00	4.83	**15-a1**	^{3}A	0.00	5.02
15-n2	^{2}A	0.20	4.82	15-a2	^{1}A'	0.21	5.06
15-n3	^{2}A"	0.74	4.78	15-a3	^{3}A	0.35	4.99
16-n1	^{1}A’	0.00	4.85	**16-a1**	^{2}A’	0.00	5.05
16-n2	^{1}A'	0.26	4.83	16-a2	^{2}A"	0.03	5.05
16-n3	^{3}A"	0.39	4.83	16-a3	^{2}A	0.34	5.03
17-n1	^{2}A”	0.00	4.94	**17-a1**	^{1}A’	0.00	5.12
17-n2	^{2}A'	0.15	4.93	17-a2	^{3}A'	0.13	5.11
17-n3	^{2}A	0.63	4.90	17-a3	^{3}A	0.20	5.11
18-n1	^{1}A’	0.00	5.02	**18-a1**	^{2}A	0.00	5.16
18-n2	^{1}A'	0.70	4.99	18-a2		0.16	5.15
18-n3	^{1}A	1.83	4.93	18-a3	^{2}A	1.21	5.10
19-n1	^{2}A	0.00	4.90	**19-a1**	^{1}A’	0.00	5.10
19-n2	^{2}A'	0.21	4.89	19-a2	^{1}A	0.04	5.10
19-n3	^{4}A	1.30	4.84	19-a3	^{3}A	1.12	5.04
20-n1	^{1}A’	0.00	5.01	**20-a1**	^{2}A"	0.00	5.15
20-n2	^{1}A	0.42	4.99	20-a2	^{2}A	0.56	5.13
20-n3	^{1}A	0.86	4.97	20-a3	^{2}A	0.72	5.12

Table S2. Cartesian coordinate of optimized MgB_{10} (C_2, ^1A) cluster.

Mg	0.00000000	0.00000000	1.44332300
B	-1.23874700	1.10240100	-0.39338900
B	1.95416200	0.20950700	0.09419600
B	1.23874700	-1.10240100	-0.39338900
B	1.45294200	1.71047200	-0.06830100
B	-1.45294200	-1.71047200	-0.06830100
B	0.59218700	0.57739700	-0.92313100
B	-1.95416200	-0.20950700	0.09419600
B	-0.59218700	-0.57739700	-0.92313100
B	0.00000000	-2.10615200	-0.44136200
B	0.00000000	2.10615200	-0.44136200

Table S3. Cartesian coordinate of optimized MgB_{12} (C_s, $^1A'$) cluster.

Mg	-0.07374500	1.46084100	0.00000000
B	-1.72817700	0.00015100	1.52232100
B	-2.09319600	0.09362400	0.00000000
B	-1.72817700	0.00015100	-1.52232100
B	-0.45248900	-0.26903200	-2.34444100
B	2.22245900	0.16353800	0.76696000
B	1.01771300	-0.74693800	0.00000000
B	1.00818500	-0.30542700	1.72881400
B	-0.42374200	-1.01558100	-0.82827800
B	-0.45248900	-0.26903200	2.34444100
B	-0.42374200	-1.01558100	0.82827800
B	2.22245900	0.16353800	-0.76696000
B	1.00818500	-0.30542700	-1.72881400

Table S4. Cartesian coordinate of optimized MgB_{18} (C_s, $^1A'$) cluster.

Mg	0.00098800	- 1.26224600	-0.00000000
B	1.77515200	0.58081700	1.53155900
B	-1.84487700	-0.89955900	-1.52248000
B	-1.17409500	0.55036500	-2.08465600
B	1.19247900	-0.93153900	2.02618500
B	-0.41104900	-0.95212400	-2.28213300
B	0.41109500	0.52818300	2.38745800
B	2.27922000	-0.87128700	0.81790200
B	-2.15456000	0.60424600	-0.80819700
B	2.27922000	-0.87128700	-0.81790200
B	-2.15456000	0.60424600	0.80819700
B	2.28206300	0.61239400	0.00000000
B	-2.43116600	-0.85998700	0.00000000
B	1.77515200	0.58081700	-1.53155900
B	-1.84487700	-0.89955900	1.52248000
B	1.19247900	-0.93153900	-2.02618500
B	-1.17409500	0.55036500	2.08465600
B	-0.41104900	-0.95212400	2.28213300
B	0.41109500	0.52818300	-2.38745800