Theoretical Study on the Small Clusters of LiH, NaH, BeH_2, and MgH_2

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1. Cartesian coordinates (angstroms) of lithium hydride clusters at QCISD/6-311G level.**

(a) LiH ($C_{\infty v}$)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	0.000000	0.000000	0.400047
2	1	0	0.000000	0.000000	-1.200141

(b) $(LiH)_2$ (D_{2h})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	0.000000	0.000000	1.133854
2	1	0	0.000000	1.343135	0.000000
3	3	0	0.000000	0.000000	-1.133853
4	1	0	0.000000	-1.343135	0.000000

(c) $(LiH)_3$ (D_{3h})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	-0.448444	1.541250	0.000000
2	1	0	1.259300	1.314227	0.000000
3	1	0	-1.767832	0.433477	0.000000
4	3	0	1.559019	-0.382271	0.000000
5	3	0	-1.110564	-1.158989	0.000000
6	1	0	0.508499	-1.747675	0.000000

(d) $(LiH)_4$ (D_{4h})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.637981	1.637889	0.000000
2	3	0	0.000000	2.106383	0.000000
3	3	0	2.106559	-0.000070	0.000000
4	1	0	1.638010	-1.638041	0.000000
5	1	0	-1.638053	1.638092	0.000000
6	3	0	-0.000003	-2.106439	0.000000
7	3	0	-2.106552	0.000095	0.000000
8	1	0	-1.637950	-1.637848	0.000000

(e) $(LiH)_4$ (T_d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	3	0	0.333045	1.416082	-0.452383
2	1	0	1.328841	0.555895	0.844230
3	1	0	-1.304474	0.999583	0.294462
4	3	0	-0.310817	0.003231	1.491387
5	3	0	-1.212510	-0.507231	-0.770322
6	3	0	1.190279	-0.912081	-0.268682
7	1	0	0.340636	-0.003539	-1.634472
8	1	0	-0.364997	-1.551942	0.495783

2. Cartesian coordinates (angstroms) of sodium hydride clusters at QCISD/6-311G level.**

(a) NaH(C_{∞})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	11	0	0.000000	0.000000	0.159391
2	1	0	0.000000	0.000000	-1.753306

(b)$(NaH)_2$ (D_{2h})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	11	0	0.000000	1.414403	0.000000
2	1	0	-1.577582	0.000000	0.000000
3	11	0	0.000000	-1.414403	0.000000
4	1	0	1.577582	0.000000	0.000000

(c) $(NaH)_3$ (D_{3h})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	11	0	0.000000	1.987922	0.000000
2	1	0	1.865869	1.077260	0.000000
3	1	0	-1.865869	1.077260	0.000000
4	11	0	1.721591	-0.993961	0.000000
5	11	0	-1.721591	-0.993961	0.000000
6	1	0	0.000000	-2.154520	0.000000

(d) $(NaH)_4$ (D_{4h})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	-2.766701	0.000000
2	11	0	1.833105	-1.833101	0.000000
3	11	0	-1.833105	-1.833104	0.000000
4	1	0	-2.766711	-0.000002	0.000000
5	1	0	2.766711	0.000002	0.000000
6	11	0	-1.833105	1.833101	0.000000
7	11	0	1.833105	1.833104	0.000000
8	1	0	0.000000	2.766701	0.000000

(e) $(NaH)_4$ (T_d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	11	0	1.182821	-0.900779	-1.169177
2	1	0	1.549796	1.154636	-0.384249
3	1	0	-0.935366	-0.424971	-1.681420
4	11	0	-0.593040	1.601172	-0.813631
5	11	0	-1.487628	-1.108318	0.368834
6	11	0	0.897846	0.407925	1.613974
7	1	0	0.617823	-1.668084	0.847632
8	1	0	-1.232251	0.938421	1.218039

3. Cartesian coordinates (angstroms) of beryllium hydride clusters at QCISD/6-311G level.**

(a) BeH_2 ($D_{\infty h}$)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	1.330347
2	4	0	0.000000	0.000000	0.000000
3	1	0	0.000000	0.000000	-1.330347

(b) $(BeH_2)_2$ (D_{2h})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	4	0	1.004950	0.000002	0.000000
2	1	0	2.333890	0.000004	0.000000
3	4	0	-1.004951	-0.000002	0.000000
4	1	0	0.000003	-1.077295	0.000000
5	1	0	0.000000	1.077295	0.000000
6	1	0	-2.333890	-0.000004	0.000000

(c) $(BeH_2)_3$ (chain C_{2v},)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	4	0	-0.000047	-0.000036	0.000000
2	4	0	-0.000158	-0.019922	-1.983027
3	1	0	0.785936	0.730760	-0.976278
4	1	0	-0.786154	-0.750253	-0.961299
5	1	0	-0.740445	0.795770	0.960957
6	1	0	0.740619	-0.776268	0.976621
7	4	0	0.000189	0.019974	1.983026
8	1	0	-0.000334	-0.033348	-3.312582
9	1	0	0.000446	0.033274	3.312583

(d) $(BeH_2)_3$ (hat-like C_{2v})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.000658	-0.153665	0.000000
2	4	0	0.000116	-0.410827	1.222531
3	4	0	0.000116	-0.410827	-1.222531
4	1	0	-0.002124	1.155353	-1.390205
5	1	0	-0.002124	1.155353	1.390205
6	1	0	0.001130	-1.379156	2.131905
7	1	0	0.001130	-1.379156	-2.131905
8	4	0	0.000000	1.011015	0.000000
9	1	0	-0.999595	-0.156167	0.000000

(e) $(BeH_2)_3$ (D_{3h})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.382900	0.290955	0.000000
2	4	0	-0.969345	-1.081056	0.000000
3	4	0	-0.451549	1.380005	0.000000
4	1	0	0.943424	1.052147	0.000000
5	1	0	0.439474	-1.343103	0.000000
6	1	0	-1.858633	-2.072831	0.000000
7	1	0	-0.865806	2.646040	0.000000
8	4	0	1.420894	-0.298949	0.000000
9	1	0	2.724441	-0.573209	0.000000

(f) $(BeH_2)_4$ (D_{2h})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	4	0	0.983059	0.000299	0.000079
2	1	0	1.958021	-1.079670	0.000328
3	1	0	1.958628	1.079692	0.000329
4	1	0	-0.000012	0.000446	1.081751
5	1	0	0.000012	0.000445	-1.081535
6	4	0	2.968108	-0.000287	-0.000056
7	4	0	-0.983059	0.000368	0.000136
8	1	0	4.298352	-0.000611	-0.000690
9	1	0	-1.957985	-1.079647	-0.000053
10	1	0	-1.958665	1.079716	-0.000055
11	4	0	-2.968109	-0.000310	-0.000131
12	1	0	-4.298352	-0.000651	-0.000191

(g) $(BeH_2)_4$ (C_1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.531081	0.894652	-0.765874
2	4	0	-1.841294	-0.382623	-0.104827
3	4	0	-0.395391	1.278087	0.032522
4	1	0	0.813137	0.317300	-0.673806
5	1	0	-0.544331	0.047692	1.009148
6	1	0	-3.039779	-0.729288	0.369404
7	1	0	0.084894	2.464621	0.407958
8	4	0	2.111638	-0.182172	-0.061567
9	4	0	0.191259	-0.823262	0.098594
10	1	0	-0.853685	-1.442403	-0.587885
11	1	0	1.444426	-1.352281	0.547543
12	1	0	3.361569	0.239586	-0.165376

(h) $(BeH_2)_4$ (T_d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	4	0	-0.287671	1.334127	-0.119564
2	1	0	0.091402	0.362797	-1.284854
3	1	0	0.869587	0.710334	0.727322
4	4	0	1.272115	-0.235193	-0.451536
5	4	0	-0.093458	-0.371330	1.315268
6	4	0	-0.890947	-0.727614	-0.744284
7	1	0	-1.241871	0.229829	0.441198
8	1	0	-0.565361	2.624152	-0.234630
9	1	0	0.280638	-1.302454	0.116653
10	1	0	2.501853	-0.462912	-0.887852
11	1	0	-0.184516	-0.730647	2.586968
12	1	0	-1.751887	-1.431056	-1.464341

(i) $(BeH_2)_4$ (C_2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.932078	-0.567141	0.000000
2	4	0	0.000349	-0.000016	1.030224
3	4	0	-0.000797	-1.863544	0.000000
4	1	0	-0.559828	-1.260725	1.362036
5	1	0	-0.931667	0.566867	0.000000
6	1	0	0.559629	1.261077	1.362062
7	1	0	0.481774	-3.107602	0.000000
8	4	0	0.000349	-0.000016	-1.030224
9	4	0	0.000349	1.863528	0.000000
10	1	0	0.559629	1.261077	-1.362062
11	1	0	-0.559828	-1.260725	-1.362036
12	1	0	-0.482790	3.107367	0.000000

4. Cartesian coordinates (angstroms) of magnesium hydride clusters at QCISD/6-311G level.**

(a) MgH_2 ($D_{\infty h}$)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	1.707884
2	12	0	0.000000	0.000000	0.000000
3	1	0	0.000000	0.000000	-1.707884

(b) $(MgH_2)_2$ (D_{2h})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	12	0	-0.000009	-1.397712	0.000000
2	1	0	0.000230	-3.099329	0.000000
3	12	0	-0.000009	1.397712	0.000000
4	1	0	-0.000072	0.000000	1.257577
5	1	0	-0.000072	0.000000	-1.257577
6	1	0	0.000141	3.099330	0.000000

(c) $(MgH_2)_3$ (chain C_{2v})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	12	0	0.000000	0.000106	-0.000174
2	12	0	-2.771310	-0.000089	0.000084
3	1	0	-1.374773	-0.895702	0.894741
4	1	0	-1.374968	0.895900	-0.894657
5	1	0	1.374898	-0.894825	-0.895668
6	1	0	1.374843	0.894826	0.895682
7	12	0	2.771310	-0.000016	0.000031
8	1	0	-4.473027	0.000109	0.000112
9	1	0	4.473026	-0.000325	0.000501

(d) $(MgH_2)_3$ (hat-like C_{2v})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	1.178658	0.000000
2	12	0	0.645470	0.127994	1.592519
3	12	0	0.645470	0.127994	-1.592519
4	1	0	-1.320625	-0.253842	-1.768139
5	1	0	-1.320625	-0.253842	1.768139
6	1	0	1.867042	0.360816	2.755087
7	1	0	1.867042	0.360816	-2.755087
8	12	0	-1.418444	-0.280766	0.000000
9	1	0	0.437212	-1.095261	0.000000

(e) $(MgH_2)_3$ (D_{3h})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000154	-1.525289	0.562950
2	12	0	0.000068	-1.525289	-1.268209
3	12	0	0.000068	-0.335657	1.955043
4	1	0	-0.000054	1.250173	1.039463
5	1	0	-0.000054	0.275115	-1.602414
6	1	0	0.000109	-2.836534	-2.358452
7	1	0	0.000109	-0.624212	3.635737
8	12	0	-0.000138	1.860946	-0.686834
9	1	0	-0.000234	3.460747	-1.277285

(f) $(MgH_2)_4$ (D_{2h})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	12	0	-1.373864	0.000249	0.000030
2	1	0	-2.749453	1.266096	0.000329
3	1	0	-2.748990	-1.266083	0.000335
4	1	0	-0.000034	0.000574	1.274974
5	1	0	0.000034	0.000571	-1.274736
6	12	0	-4.145064	-0.000240	-0.000103
7	12	0	1.373864	0.000224	0.000204
8	1	0	-5.847186	-0.000590	-0.000496
9	1	0	2.749443	1.266089	0.000012
10	1	0	2.749001	-1.266092	0.000010
11	12	0	4.145064	-0.000231	-0.000127
12	1	0	5.847186	-0.000587	-0.000468

(g) $(MgH_2)_4$ (C_1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.785684	1.139452	-0.937701
2	12	0	-2.559513	-0.386888	-0.197207
3	12	0	-0.365476	1.698702	0.089444
4	1	0	1.009319	0.361248	-0.624899
5	1	0	-0.817123	0.054927	1.173130
6	1	0	-4.144368	-0.724640	0.345317
7	1	0	0.423869	3.091942	0.695076
8	12	0	2.779616	-0.151481	-0.157420
9	12	0	0.169994	-1.230878	0.252501
10	1	0	-1.264966	-1.754685	-0.673902
11	1	0	1.904729	-1.657098	0.605162
12	1	0	4.378779	0.335393	-0.429984

(h) $(MgH_2)_4$ (T_d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	12	0	1.533532	-0.868988	-0.612856
2	1	0	-0.352580	-1.444449	-0.395974
3	1	0	1.059625	-0.018098	1.115528
4	12	0	-0.676061	-0.904865	1.485464
5	12	0	0.427669	1.751816	0.480306
6	12	0	-1.285137	0.022039	-1.352916
7	1	0	0.557431	0.746046	-1.224837
8	1	0	2.927366	-1.658733	-1.169629
9	1	0	-1.264447	0.716494	0.505270
10	1	0	-1.290501	-1.727107	2.835592
11	1	0	0.816195	3.344046	0.916559
12	1	0	-2.453129	0.041777	-2.582497

(i) $(MgH_2)_4$ (C_2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.056040	0.771552	0.000000
2	12	0	0.000749	0.000041	1.422392
3	12	0	0.000749	2.556609	0.000000
4	1	0	0.696402	1.655763	1.609139
5	1	0	1.057074	-0.771664	0.000000
6	1	0	-0.696424	-1.655189	1.608749
7	1	0	-0.596404	4.158985	0.000000
8	12	0	0.000749	0.000041	-1.422392
9	12	0	-0.002207	-2.556762	0.000000
10	1	0	-0.696424	-1.655189	-1.608749
11	1	0	0.696402	1.655763	-1.609139
12	1	0	0.594921	-4.159155	0.000000

(j) $(MgH_2)_4$ (C_{2v})

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.054325	0.769087	0.000000
2	12	0	0.001547	0.000013	1.422330
3	12	0	0.001547	2.555241	0.000000
4	1	0	0.694751	1.655035	1.608055
5	1	0	1.056295	-0.769873	0.000000
6	1	0	-0.695240	-1.653660	1.607700
7	1	0	-0.598493	4.154653	0.000000
8	12	0	0.001547	0.000013	-1.422330
9	12	0	-0.004357	-2.555372	0.000000
10	1	0	-0.695240	-1.653660	-1.607700
11	1	0	0.694751	1.655035	-1.608055
12	1	0	0.594089	-4.155375	0.000000