Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Theoretical design of stable hydrides clusters: isoelectronic transformation in the $E_nAl_{4-n}H_{7+n}^-$ series

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First part, anionic systems: Cartesians coordinates and relative energies

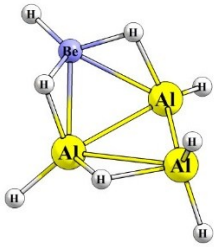
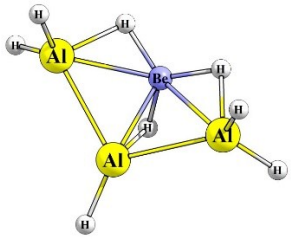
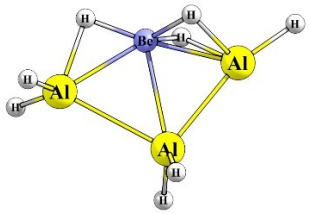
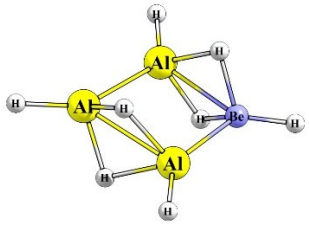
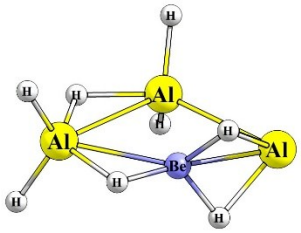
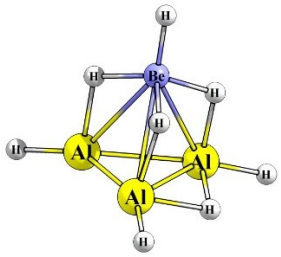
$Al_3BeH_8^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Be-1 C_1		H -1.288424000 1.398349000 1.113825000 H -1.488177000 -1.081419000 1.217202000 H -0.651656000 2.617785000 -1.198352000 H -3.506970000 0.275978000 0.917583000 H -1.087383000 -2.602412000 -1.058900000 H 0.883898000 -1.586398000 0.289711000 H 2.531401000 -0.153974000 1.670977000 H 2.781346000 -0.382367000 -1.017451000 Be -2.144839000 0.223793000 0.773509000 Al 1.812813000 -0.035076000 0.231280000 Al -0.321206000 1.326761000 -0.310243000 Al -0.691197000 -1.244048000 -0.307854000	CC -745.5122 G4 -746.4409	CC 0.0 G4 0.6
Be-2 C_s		H -0.934965000 -1.504322000 1.221691000 H -1.624168000 0.580686000 0.000000000 H -0.934965000 -1.504322000 -1.221691000 H -0.814287000 0.000887000 -3.352798000 H -0.814287000 0.000887000 3.352798000 H 1.385894000 -1.347347000 -2.547341000 H 1.385894000 -1.347347000 2.547341000 H 0.245495000 2.789471000 0.000000000 Be -0.953058000 -0.713577000 0.000000000 Al 0.151734000 -0.397878000 -2.121258000 Al 0.151734000 -0.397878000 2.121258000 Al 0.151734000 1.194657000 0.000000000	CC -745.5108 G4 -746.4418	CC 0.9 G4 0.0
Be-3 C_1		H -2.929529000 -0.485410000 1.356571000 H -2.929242000 -0.486062000 -1.356702000 H -1.176995000 -1.958269000 0.000361000 H -0.015958000 2.181937000 -1.368653000 H -0.014149000 2.182783000 1.368217000 H 3.510119000 -1.059253000 0.000385000 H 1.053475000 -1.413320000 -1.083203000 H 1.052708000 -1.411860000 1.084314000 Be 0.071764000 -1.229485000 0.000153000 Al -2.067384000 -0.382370000 -0.000002000 Al 2.053856000 -0.377955000 -0.000144000 Al 0.102952000 1.327047000 -0.000001000	CC -745.5099 G4 -746.4413	CC 1.5 G4 0.3
Be-4 C_s		H -3.277846000 -0.448653000 0.000000000 H -1.037967000 -1.517881000 -1.114903000 H -1.037967000 -1.517881000 1.114903000 H 3.268714000 -0.128896000 0.000000000 H 1.148833000 0.947454000 -1.131460000 H 1.148833000 0.947454000 1.131460000 H 0.089324000 3.191750000 0.000000000 H 0.014098000 -3.444478000 0.000000000 Be -0.077850000 -2.063682000 0.000000000 Al -1.662031000 -0.394472000 0.000000000 Al 1.661675000 -0.397637000 0.000000000 Al 0.000000000 1.578713000 0.000000000	CC -745.5049 G4 -746.4345	CC 4.6 G4 4.6
Be-5 C_s		H -2.967210000 0.013212000 -1.381809000 H -2.967210000 0.013212000 1.381809000 H -1.390400000 1.542403000 0.000000000 H -1.355767000 -1.536632000 0.000000000 H 0.840617000 1.649653000 -1.090182000 H 0.840617000 1.649653000 1.090182000 H 0.702580000 -2.079688000 -1.362216000 H 0.702580000 -2.079688000 1.362216000 Be 0.000000000 1.201348000 0.000000000 Al -2.158893000 -0.038105000 0.000000000 Al 2.173223000 0.996687000 0.000000000 Al 0.415993000 -1.264544000 0.000000000	CC -745.5042 G4 -746.4349	CC 5.0 G4 4.3
Be-6 C_s		H -0.712228000 3.015707000 0.000000000 H -0.690319000 -1.697900000 0.000000000 H -0.690193000 -1.581700000 -2.631587000 H -0.690193000 -1.581700000 2.631587000 H 3.251161000 -0.112922000 0.000000000 H 1.428453000 1.392191000 0.000000000 H 1.378689000 -0.875132000 -1.189023000 H 1.378689000 -0.875132000 1.189023000 Be 1.869998000 -0.064480000 0.000000000 Al -0.311130000 -0.635570000 -1.387886000 Al -0.311130000 -0.635570000 1.387886000 Al -0.311130000 1.469178000 0.000000000	CC -745.5028 G4 -746.4329	CC 5.9 G4 5.6

Figure SI-1. Lowest energy isomers for $Al_3BeH_8^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

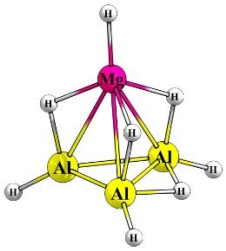
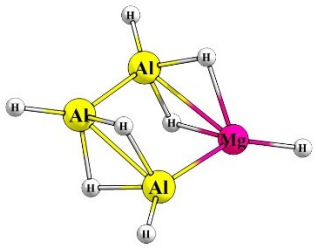
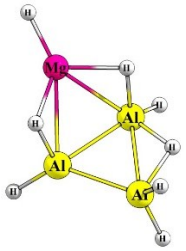
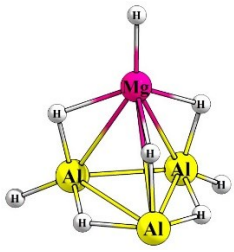
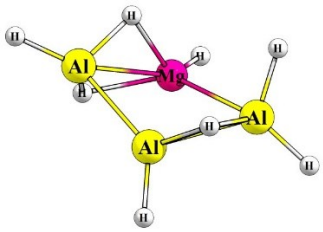
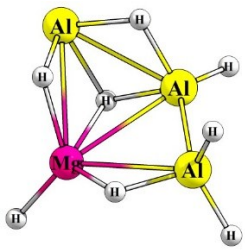
$Al_3MgH_8^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Mg-1 C_s		H	-1.398219082	2.845574663	0.000000000	CC -930.4794 G4 -931.6384	CC 0.0 G4 0.0
		H	-1.272712084	-1.524224578	-2.598945000		
		H	-1.272712084	-1.524224578	2.598945000		
		H	-0.914620064	-1.749967475	0.000000000		
		H	3.654666770	0.019132978	0.000000000		
		H	1.081093782	1.763849533	0.000000000		
		H	1.060409312	-1.084456285	-1.394679000		
		H	1.060409312	-1.084456285	1.394679000		
		Mg	1.912518334	0.005390110	0.000000000		
		Al	-0.593601257	1.463297006	0.000000000		
		Al	-0.590580136	-0.690364875	-1.405635000		
		Al	-0.590580136	-0.690364875	1.405635000		
Mg-2 C_s		H	-2.781840465	-1.998049370	0.000000000	CC -930.4768 G4 -931.6341	CC 1.6 G4 2.7
		H	-2.457952282	2.436239477	0.000000000		
		H	-1.700529327	0.203226716	-1.132838000		
		H	-1.700529327	0.203226716	1.132838000		
		H	3.101280108	2.218368253	0.000000000		
		H	1.950754703	-2.846189491	0.000000000		
		H	1.690605257	-0.427769124	-1.205080000		
		H	1.690605257	-0.427769124	1.205080000		
		Mg	1.649893360	1.228967947	0.000000000		
		Al	-1.443697173	-1.093819557	0.000000000		
		Al	-1.139470671	1.485880629	0.000000000		
		Al	1.124261413	-1.460685849	0.000000000		
Mg-3 C_1		H	-3.924537000	-0.043004000	0.909014000	CC -930.4745 G4 -931.6323	CC 3.1 G4 3.8
		H	-1.158225000	1.537482000	0.847334000		
		H	-1.093426000	-1.621157000	0.711472000		
		H	-0.179395000	2.619512000	-1.445050000		
		H	-0.136257000	-2.403041000	-1.669611000		
		H	3.348964000	0.129604000	-0.517657000		
		H	2.465811000	-0.040580000	2.053843000		
		H	1.370640000	1.555798000	0.355518000		
		Mg	-2.246390000	-0.091822000	0.470571000		
		Al	-0.116841000	1.331470000	-0.491012000		
		Al	2.099928000	-0.084680000	0.484042000		
		Al	0.037152000	-1.295463000	-0.523162000		
Mg-4 C_s		H	-1.211378741	-0.364634478	-1.399936000	CC -930.4711 G4 -931.6309	CC 5.3 G4 4.7
		H	-1.211378741	-0.364634478	1.399936000		
		H	-0.664253365	1.587203780	0.000000000		
		H	2.300479971	2.858763060	0.000000000		
		H	1.272408695	0.460485637	-1.695813000		
		H	1.272408695	0.460485637	1.695813000		
		H	0.594231303	-2.027199925	-2.434931000		
		H	0.594231303	-2.027199925	2.434931000		
		Mg	1.223001404	1.491339385	0.000000000		
		Al	-2.031968304	0.511161883	0.000000000		
		Al	0.417360852	-0.929331989	-1.280486000		
		Al	0.417360852	-0.929331989	1.280486000		
Mg-5 C_1		H	-3.490271000	-0.791800000	0.853886000	CC -930.4677 G4 -931.6259	CC 7.3 G4 7.8
		H	-2.087976000	0.661975000	-0.999377000		
		H	-1.377099000	0.921519000	1.261159000		
		H	-0.240993000	3.282161000	-0.791555000		
		H	3.591551000	-0.070884000	-0.313644000		
		H	2.081129000	0.985180000	1.691378000		
		H	1.506828000	-1.473661000	0.768431000		
		H	0.650617000	-2.345581000	-1.569103000		
		Mg	-0.370930000	1.589473000	-0.382963000		
		Al	-2.026635000	-0.351886000	0.364008000		
		Al	2.127639000	0.137227000	0.317814000		
		Al	0.192640000	-1.342463000	-0.397639000		
Mg-6 C_1		H	-3.443288000	-0.102537000	-0.764645000	CC -930.4676 G4 -931.6264	CC 7.4 G4 7.5
		H	-2.642548000	-0.670258000	1.782799000		
		H	-1.736797000	1.451437000	0.524764000		
		H	1.301989000	1.085217000	0.992238000		
		H	1.194965000	-1.333032000	0.853726000		
		H	1.188514000	-0.092511000	-1.041298000		
		H	0.323919000	-2.612489000	-1.290424000		
		H	0.221294000	2.978299000	-1.320349000		
		Mg	0.000557000	1.622405000	-0.255712000		
		Al	-2.234998000	-0.163725000	0.304356000		
		Al	2.461947000	-0.096042000	0.366608000		
		Al	0.048840000	-1.292001000	-0.414677000		

Figure SI-2. Lowest energy isomers for $Al_3MgH_8^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

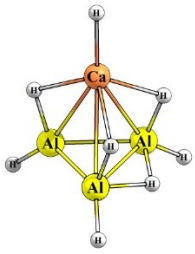
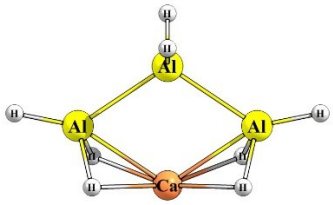
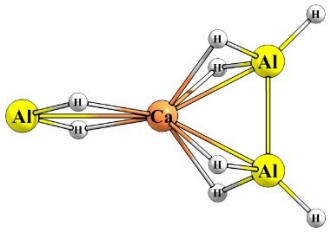
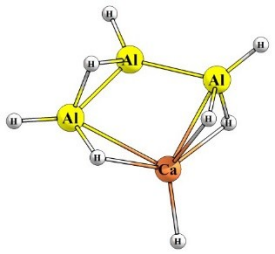
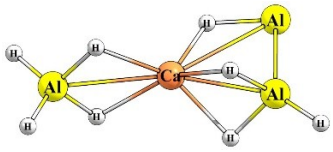
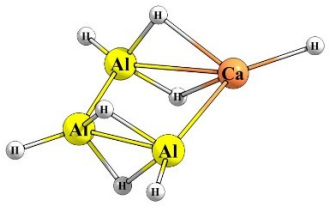
$Al_3CaH_8^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Ca-1 C_s		H	-1.952807031	2.649950906	0.000000000	CC -1407.6372 G4 -1409.1206	CC 0.0 G4 0.0
		H	-1.791196342	-1.434711461	-2.531909008		
		H	-1.791196342	-1.434711461	2.531909008		
		H	-1.198149540	-1.763406084	-0.000000000		
		H	3.853307092	0.115690735	0.000000000		
		H	0.718041776	-1.253586161	-1.554199501		
		H	0.718041776	-1.253586161	1.554199501		
		H	0.708559623	2.029240749	0.000000000		
		Ca	1.780660192	0.047854802	0.000000000		
		Al	-0.871643785	-0.727515346	-1.419617502		
		Al	-0.871643785	-0.727515346	1.419617502		
		Al	-0.866595550	1.471748339	0.000000000		
Ca-2 C_{2v}		H	-1.346306498	0.000000000	2.640818378	CC -1407.6286 G4 -1409.1129	CC 5.4 G4 4.8
		H	-1.187046504	-1.878438756	-1.055179619		
		H	-1.187046504	1.878438756	-1.055179619		
		H	1.346306498	0.000000000	2.640818378		
		H	1.187046504	-1.878438756	-1.055179619		
		H	1.187046504	1.878438756	-1.055179619		
		H	0.000000000	-3.803243008	0.479376883		
		H	0.000000000	3.803243008	0.479376883		
		Ca	0.000000000	0.000000000	-1.412900121		
		Al	0.000000000	-2.227858005	0.148718381		
		Al	0.000000000	2.227858005	0.148718381		
		Al	0.000000000	0.000000000	1.719782879		
Ca-3 C_{2v}		H	-1.199418971	-1.527891611	0.879197980	CC -1407.6278 G4 -1409.1113	CC 5.9 G4 5.8
		H	-1.199418971	1.527891611	0.879197980		
		H	-1.162620220	0.000000000	-2.374945311		
		H	1.199418971	-1.527891611	0.879197980		
		H	1.199418971	1.527891611	0.879197980		
		H	1.162620220	0.000000000	-2.374945311		
		H	0.000000000	-2.484958790	3.173816553		
		H	0.000000000	2.484958790	3.173816553		
		Ca	0.000000000	0.000000000	-0.416722164		
		Al	0.000000000	-1.330841870	2.054620127		
		Al	0.000000000	1.330841870	2.054620127		
		Al	0.000000000	0.000000000	-3.683069413		
Ca-4 C_1		H	-3.119318000	-1.952828000	0.630238000	CC -1407.6265 G4 -1409.1088	CC 6.7 G4 7.4
		H	-2.266321000	0.128284000	-0.937416000		
		H	-1.678877000	0.246453000	1.409271000		
		H	-0.898542000	3.539844000	-0.643934000		
		H	3.803528000	0.324833000	0.341756000		
		H	1.656657000	-1.277700000	1.043135000		
		H	1.427758000	1.377791000	1.070773000		
		H	1.158353000	-2.904947000	-1.042316000		
		Ca	-0.574633000	1.549848000	-0.159394000		
		Al	-1.898357000	-0.972094000	0.278200000		
		Al	2.211802000	0.184924000	0.215275000		
		Al	0.564203000	-1.557345000	-0.392216000		
Ca-5 C_s		H	-4.462760086	-1.047280746	-0.000000000	CC -1407.6250 G4 -1409.1059	CC 7.7 G4 9.2
		H	-4.311415518	1.695646341	0.000000000		
		H	-2.424505021	0.217123357	-1.231329990		
		H	-2.424505021	0.217123357	1.231329990		
		H	3.230300897	2.259548067	0.000000000		
		H	0.964421739	1.346843064	-1.203124987		
		H	0.964421739	1.346843064	1.203124987		
		H	0.613137668	-1.731625632	0.000000000		
		Ca	-0.478053933	0.135611756	0.000000000		
		Al	-3.556193000	0.278277730	0.000000000		
		Al	2.401185026	-1.696781136	0.000000000		
		Al	2.156308132	1.056874602	0.000000000		
Ca-6 C_s		H	-3.466299497	-1.124458199	0.000000000	CC -1407.6243 G4 -1409.1039	CC 8.1 G4 10.5
		H	-2.191346248	2.984678743	0.000000000		
		H	-1.822025932	0.694133223	-1.137044000		
		H	-1.822025932	0.694133223	1.137044000		
		H	3.837697588	1.199126274	0.000000000		
		H	1.234609245	-1.321012268	-1.218163000		
		H	1.234609245	-1.321012268	1.218163000		
		H	0.388510919	-3.591610610	0.000000000		
		Ca	1.867239718	0.533069744	0.000000000		
		Al	-1.937771126	-0.598955032	0.000000000		
		Al	-1.011352980	1.860977098	0.000000000		
		Al	0.280888814	-1.984844312	0.000000000		

Figure SI-3. Lowest energy isomers for $Al_3CaH_8^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

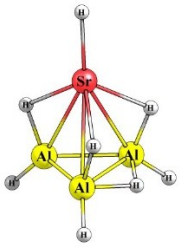
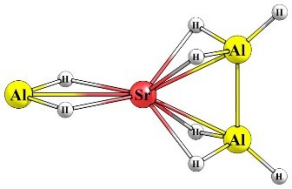
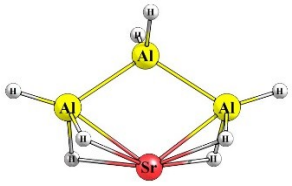
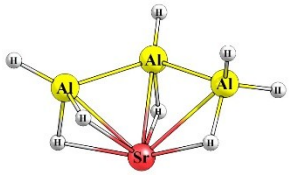
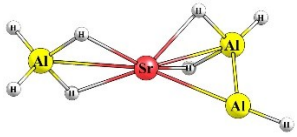
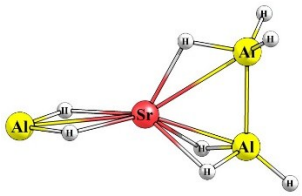
$Al_3SrH_8^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Sr-1 C_s		H	-3.588100516	0.361538630	0.000000000	-761.2296	0.0
		H	-0.233612711	-1.269908689	-1.672022500		
		H	-0.233612711	-1.269908689	1.672022500		
		H	2.725347785	2.420730972	0.000000000		
		H	2.323954469	-1.589743140	-2.478115000		
		H	2.323954469	-1.589743140	2.478115000		
		H	1.537281175	-1.889808640	0.000000000		
		H	0.016825457	2.096904536	0.000000000		
		Sr	-1.361637715	0.121638508	0.000000000		
		Al	1.368994684	-0.830041893	-1.430979000		
		Al	1.516232658	1.365756293	0.000000000		
		Al	1.368994684	-0.830041893	1.430979000		
Sr-2 C_{2v}		H	-2.442481011	0.000000000	3.467985087	-761.2240	3.5
		H	-1.589748514	-1.213224976	1.149433610		
		H	-1.589748514	1.213224976	1.149433610		
		H	2.442481011	0.000000000	3.467985087		
		H	1.589748514	-1.213224976	1.149433610		
		H	1.589748514	1.213224976	1.149433610		
		H	0.000000000	-1.172491444	-2.482728908		
		H	0.000000000	1.172491444	-2.482728908		
		Sr	0.000000000	0.000000000	-0.326039378		
		Al	-1.335509510	0.000000000	2.299360097		
		Al	1.335509510	0.000000000	2.299360097		
		Al	0.000000000	0.000000000	-3.781826420		
Sr-3 C_{2v}		H	-1.345540953	0.000000000	3.058860064	-761.2225	4.4
		H	-1.203211491	-2.032579250	-0.578537851		
		H	-1.203211491	2.032579250	-0.578537851		
		H	1.345540953	0.000000000	3.058860064		
		H	1.203211491	-2.032579250	-0.578537851		
		H	1.203211491	2.032579250	-0.578537851		
		H	0.000000000	-3.817823000	1.102203661		
		H	0.000000000	3.817823000	1.102203661		
		Sr	0.000000000	0.000000000	-1.107384887		
		Al	0.000000000	-2.278807500	0.624793147		
		Al	0.000000000	2.278807500	0.624793147		
		Al	0.000000000	0.000000000	2.133852098		
Sr-4 C_1		H	-3.179698000	1.956713000	1.179156000	-761.2223	4.6
		H	-2.604901000	-0.226441000	-0.397943000		
		H	-1.443352000	-0.113160000	1.691475000		
		H	3.704873000	0.028559000	-0.443728000		
		H	2.881595000	0.819847000	1.997808000		
		H	1.808602000	-1.304056000	0.797493000		
		H	0.614218000	3.030107000	-1.434762000		
		H	0.071454000	0.383171000	-1.905748000		
		Sr	-0.317604000	-1.132423000	-0.170519000		
		Al	-1.995085000	1.049195000	0.568439000		
		Al	2.421790000	0.302143000	0.528120000		
		Al	0.359154000	1.606919000	-0.712254000		
Sr-5 C_1		H	-3.858890584	2.256735214	0.000000000	-761.2216	5.0
		H	-3.435063464	-2.465585668	-0.000000000		
		H	-1.252162486	-1.376157123	-1.216278001		
		H	-1.252162486	-1.376157123	1.216278001		
		H	4.532979855	1.168080969	0.000000000		
		H	4.352209922	-1.567865154	0.000000000		
		H	2.488308612	-0.076545353	-1.243145991		
		H	2.488308612	-0.076545353	1.243145991		
		Sr	0.334347994	-0.009943948	0.000000000		
		Al	-2.434431072	-1.195562654	-0.000000000		
		Al	-2.407830579	1.503034825	0.000000000		
		Al	3.601176134	-0.143817046	0.000000000		
Sr-6 C_1		H	-2.526545188	0.175914275	-1.174790337	-761.2202	5.9
		H	-2.526545188	0.175914275	1.174790337		
		H	3.523830865	2.217621630	0.000000000		
		H	3.038059032	-2.254404377	-1.352006099		
		H	3.038059032	-2.254404377	1.352006099		
		H	1.196494151	1.445347762	-1.209367500		
		H	1.196494151	1.445347762	1.209367500		
		H	0.782721757	-1.940584904	0.000000000		
		Sr	-0.390251965	0.074000390	0.000000000		
		Al	-3.830856996	0.241263731	0.000000000		
		Al	2.463725374	-1.560903629	0.000000000		
		Al	2.350112772	1.115498032	0.000000000		

Figure SI-4. Lowest energy isomers for $Al_3SrH_8^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

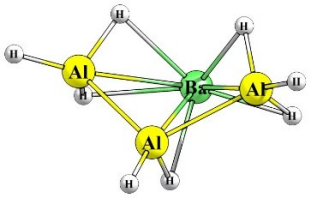
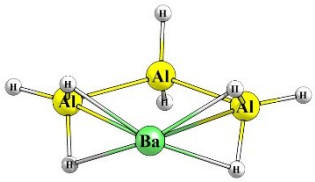
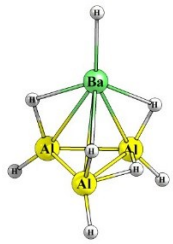
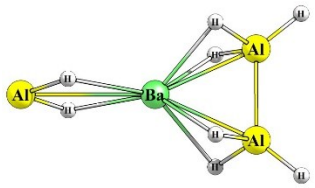
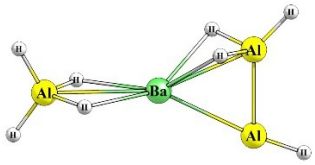
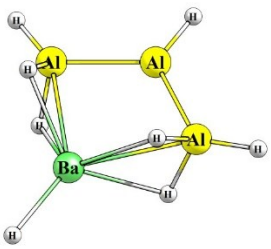
$Al_3BaH_8^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Ba-1 C_s		H	-3.512995732	-1.435662810	-0.000000000	-755.9845	0.0
		H	-1.892215807	0.992574768	-3.526867995		
		H	-1.892215807	0.992574768	3.526867995		
		H	-0.808716158	-1.949575957	-0.000000000		
		H	-0.130656722	1.759009713	-1.553083496		
		H	-0.130656722	1.759009713	1.553083496		
		H	0.306399362	-0.389322462	-2.617405998		
		H	0.306399362	-0.389322462	2.617405998		
		Ba	0.874162788	-0.064362177	0.000000000		
		Al	-2.040426387	-0.762646568	-0.000000000		
		Al	-1.068924370	0.520791165	-2.219863497		
		Al	-1.068924370	0.520791165	2.219863497		
Ba-2 C_{2v}		H	-3.811772000	0.000000000	1.628390847	-755.9777	4.2
		H	-2.189586000	-1.214901472	-0.209392365		
		H	-2.189586000	1.214901472	-0.209392365		
		H	3.811772000	0.000000000	1.628390847		
		H	2.189586000	-1.214901472	-0.209392365		
		H	2.189586000	1.214901472	-0.209392365		
		H	0.000000000	-1.346613803	3.340291014		
		H	0.000000000	1.346613803	3.340291014		
		Ba	0.000000000	0.000000000	-0.921729462		
		Al	-2.335688500	0.000000000	0.977938149		
		Al	2.335688500	0.000000000	0.977938149		
		Al	0.000000000	0.000000000	2.415272622		
Ba-3 C_s		H	-2.934426293	1.387661813	-2.253571000	-755.9767	4.9
		H	-2.934426293	1.387661813	2.253571000		
		H	-2.897134678	-2.688298245	-0.000000000		
		H	-1.557342532	1.669089465	0.000000000		
		H	-0.248732979	1.125413549	-1.991937000		
		H	-0.248732979	1.125413549	1.991937000		
		H	-0.215094304	-2.183916459	-0.000000000		
		H	3.489745293	-0.028497733	0.000000000		
		Ba	1.085652132	0.045476815	0.000000000		
		Al	-1.755772743	0.629371923	-1.464944000		
		Al	-1.755772743	0.629371923	1.464944000		
		Al	-1.755460538	-1.558210156	-0.000000000		
Ba-4 C_{2v}		H	-2.380219924	0.000000000	-3.739453361	-755.9761	5.2
		H	-1.651578568	-1.221046163	-1.385173871		
		H	-1.651578568	1.221046163	-1.385173871		
		H	2.380219924	0.000000000	-3.739453361		
		H	1.651578568	-1.221046163	-1.385173871		
		H	1.651578568	1.221046163	-1.385173871		
		H	0.000000000	-1.173630074	2.649607283		
		H	0.000000000	1.173630074	2.649607283		
		Ba	0.000000000	0.000000000	0.266295491		
		Al	-1.341633154	0.000000000	-2.507323444		
		Al	1.341633154	0.000000000	-2.507323444		
		Al	0.000000000	0.000000000	3.941960005		
Ba-5 C_s		H	-4.051469923	2.283983229	0.000000000	-755.9739	6.6
		H	-3.835592772	-2.226180196	-0.000000000		
		H	-1.529727381	-1.429821328	-1.225331004		
		H	-1.529727381	-1.429821328	1.225331004		
		H	4.719320931	1.045584423	0.000000000		
		H	4.428110259	-1.675794045	0.000000000		
		H	2.631788196	-0.117080379	-1.253792493		
		H	2.631788196	-0.117080379	1.253792493		
		Ba	0.265961072	-0.027941624	0.000000000		
		Al	-2.661385171	-1.117149964	-0.000000000		
		Al	-2.553181216	1.620480225	0.000000000		
		Al	3.725806685	-0.223576170	0.000000000		
Ba-6 C_{2v}		H	-3.752794007	0.000000000	-1.869684031	-755.9728	7.3
		H	-1.996588254	-1.236775002	-0.195115774		
		H	-1.996588254	1.236775002	-0.195115774		
		H	3.752794007	0.000000000	-1.869684031		
		H	1.996588254	-1.236775002	-0.195115774		
		H	1.996588254	1.236775002	-0.195115774		
		H	0.000000000	0.000000000	-4.289063023		
		H	0.000000000	0.000000000	3.467817932		
		Ba	0.000000000	0.000000000	1.068938977		
		Al	-2.247261005	0.000000000	-1.298760028		
		Al	2.247261005	0.000000000	-1.298760028		
		Al	0.000000000	0.000000000	-2.666428031		

Figure SI-5. Lowest energy isomers for $Al_3BaH_8^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

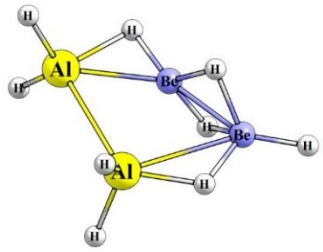
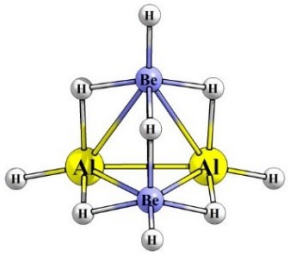
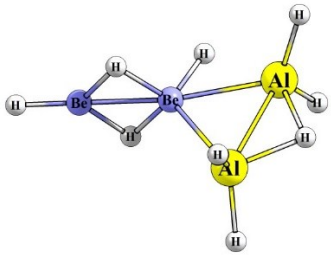
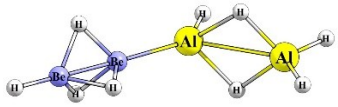
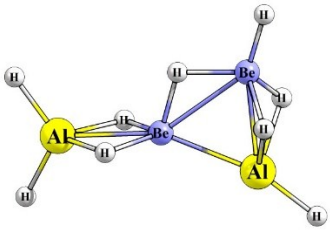
$Al_2Be_2H_9^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Be_2-1 C_s		Al 0.779247000 1.085916000 0.000000000 Be 0.231739000 -1.335133000 0.000000000 Be 2.191312000 -1.199577000 0.000000000 H 1.160990000 -1.537023000 1.080685000 H 3.412542000 -1.827663000 0.000000000 H 2.296994000 0.282358000 0.000000000 H 0.844865000 1.960306000 1.355842000 H 0.844865000 1.960306000 -1.355842000 H 1.160990000 -1.537023000 -1.080685000 H -1.107873000 -1.879264000 0.000000000 Al -1.698527000 -0.181918000 0.000000000 H -2.548177000 -0.033030000 1.356161000 H -2.548177000 -0.033030000 -1.356161000	CC -518.8110 G4 -519.4925	CC 0.0 G4 0.0
Be_2-2 C_{2v}		Al -0.887665000 -0.877479000 -0.596067000 Be -0.887665000 0.898735000 1.272717000 H 0.020622000 1.865262000 0.488964000 H 0.000000000 0.000000000 2.007626000 H 1.864645000 -0.001691000 0.489394000 H -0.020622000 -1.865262000 0.488964000 H -1.864645000 0.001691000 0.489394000 Be 0.887665000 -0.898735000 1.272717000 H -1.653560000 1.675712000 2.120162000 H 1.653560000 -1.675712000 2.120162000 H 1.852177000 1.830408000 -1.444332000 H -1.852177000 -1.830408000 -1.444332000 Al 0.887665000 0.877479000 -0.596067000	CC -518.8008 G4 -519.4828	CC 6.4 G4 6.1
Be_2-3 C_s		Al 0.386251000 1.448609000 0.000000000 H 1.714348000 -1.642288000 1.382578000 H 0.438577000 2.306389000 1.364068000 H 1.913708000 0.598002000 0.000000000 Be -1.110609000 -0.496630000 0.000000000 H -2.121102000 -0.450826000 -1.093937000 H -2.121102000 -0.450826000 1.093937000 Al 1.158871000 -1.046573000 0.000000000 Be -3.069693000 -0.427881000 0.000000000 H -4.426242000 -0.366501000 0.000000000 H 1.714348000 -1.642288000 -1.382578000 H 0.438577000 2.306389000 -1.364068000 H -0.551019000 -1.808733000 0.000000000	CC -518.7990 G4 -519.4790	CC 7.5 G4 8.5
Be_2-4 C_s		H 1.145111000 -0.146162000 1.161030000 H -2.808365000 -1.086316000 0.000000000 Al 0.076087000 0.771412000 0.000000000 H 2.062381000 -2.414257000 0.000000000 H 1.145111000 -0.146162000 -1.161030000 Be -2.176162000 0.252618000 0.000000000 Be -3.964899000 -0.079292000 0.000000000 H -3.138443000 0.690713000 -1.040439000 H -5.314431000 -0.329242000 0.000000000 H -3.138443000 0.690713000 1.040439000 H 1.005245000 2.097394000 0.000000000 Al 2.184449000 -0.821557000 0.000000000 H 3.643668000 -0.170350000 0.000000000	CC -518.7918 G4 -519.4740	CC 12.0 G4 11.6
Be_2-5 C_s		Al 2.377495000 0.670712000 0.000000000 H 1.175209000 0.304525000 -1.135259000 Al -2.039698000 0.128363000 0.000000000 H 3.615359000 -0.344562000 0.000000000 H -3.533350000 0.729954000 0.000000000 H -1.303466000 -3.376015000 0.000000000 Be 0.218124000 -0.080877000 0.000000000 H 1.175209000 0.304525000 1.135259000 H 2.723103000 2.233345000 0.000000000 H -2.035293000 -1.250531000 -1.086249000 Be -1.264184000 -1.994324000 0.000000000 H -2.035293000 -1.250531000 1.086249000 H 0.202986000 -1.528486000 0.000000000	CC -518.7917 G4 -519.4730	CC 12.1 G4 12.2

Figure SI-6. Lowest energy isomers for $Al_2Be_2H_9^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

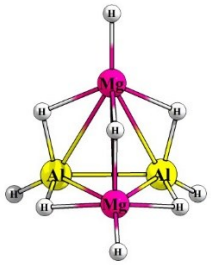
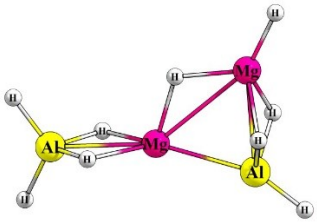
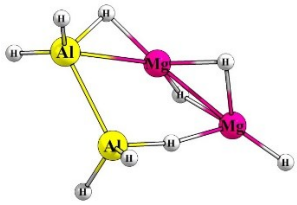
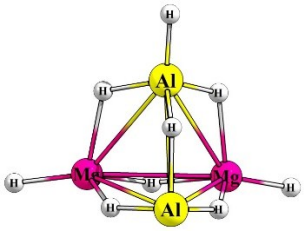
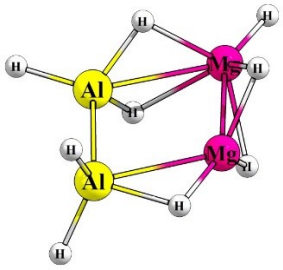
$Al_2Mg_2H_9^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Mg_2-1 C_{2v}		Al 1.028322000 -0.827174000 -0.992956000 Mg -1.028322000 -1.271138000 1.035605000 H -2.128084000 0.054112000 0.014156000 H 0.000000000 0.000000000 1.906333000 H -0.503852000 2.066658000 0.014520000 H 2.128084000 -0.054112000 0.014156000 H 0.503852000 -2.066658000 0.014520000 Mg 1.028322000 1.271138000 1.035605000 H -2.023877000 -2.504217000 1.763515000 H 2.023877000 2.504217000 1.763515000 H -1.789880000 1.441369000 -2.264180000 H 1.789880000 -1.441369000 -2.264180000 Al -1.028322000 0.827174000 -0.992956000	CC -888.7440 G4 -889.8848	CC 0.0 G4 0.0
Mg_2-2 C_s		Al 3.280020000 0.094070000 0.000000000 Mg 0.539233000 -0.203415000 0.000000000 H 4.210186000 -1.212169000 0.000000000 H 2.119837000 -0.020107000 -1.211199000 H 3.991817000 1.529561000 0.000000000 H 2.119837000 -0.020107000 1.211199000 Mg -2.182836000 1.400440000 0.000000000 H -2.974131000 -2.493525000 0.000000000 H -2.381107000 -0.148526000 1.187135000 H -0.297282000 1.495276000 0.000000000 Al -1.885775000 -1.304608000 0.000000000 H -3.205151000 2.819357000 0.000000000 H -2.381107000 -0.148526000 -1.187135000	CC -888.7301 G4 -889.8685	CC 8.7 G4 10.2
Mg_2-3 C_s		Al 0.564379000 -1.598439000 -0.001324000 Mg -0.348415000 1.093555000 -0.003637000 Mg -2.733848000 0.095809000 0.002625000 H -1.703453000 1.112145000 1.283669000 H -4.384862000 -0.424291000 -0.001949000 H -1.065894000 -0.985031000 -0.020815000 H 0.610829000 -2.459879000 1.362524000 H 0.638679000 -2.474626000 -1.354530000 H -1.713479000 1.136041000 -1.276336000 H 1.287354000 2.005325000 0.008732000 Al 2.286776000 0.550128000 0.001919000 H 3.128093000 0.717280000 1.366245000 H 3.124874000 0.728693000 -1.363133000	CC -888.7182 G4 -889.8597	CC 16.2 G4 15.8
Mg_2-4 C_s		H 1.334440000 -1.718200000 0.000000000 H 1.135955000 -1.635503000 3.156921000 Mg 0.695566000 -1.011273000 1.588093000 Mg 0.695566000 -1.011273000 -1.588093000 H 1.219322000 3.158112000 0.000000000 H -1.105027000 -0.575753000 1.228304000 Al -2.095863000 0.161099000 0.000000000 H -1.105027000 -0.575753000 -1.228304000 H 1.381611000 0.831860000 -1.312382000 Al 0.775732000 1.621830000 0.000000000 H -0.904838000 1.569359000 0.000000000 H 1.381611000 0.831860000 1.312382000 H 1.135955000 -1.635503000 -3.156921000	CC -888.7100 G4 -889.8580	CC 21.3 G4 16.8
Mg_2-5 C_s		Mg 2.323373000 0.238056000 0.000000000 H 1.336423000 1.559640000 1.286770000 H 1.143799000 -1.044302000 -1.197637000 H 1.336423000 1.559640000 -1.286770000 Mg 0.068533000 1.674943000 0.000000000 Al -2.221232000 0.173933000 0.000000000 H -3.080240000 0.085050000 1.362164000 H -1.758202000 1.895222000 0.000000000 H -3.080240000 0.085050000 -1.362164000 H 1.143799000 -1.044302000 1.197637000 Al 0.022950000 -1.366213000 0.000000000 H 4.058478000 0.103448000 0.000000000 H -0.369834000 -2.927070000 0.000000000	CC -888.7068 G4 -889.8494	CC 23.3 G4 22.2

Figure SI-7. Lowest energy isomers for $Al_2Mg_2H_9^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

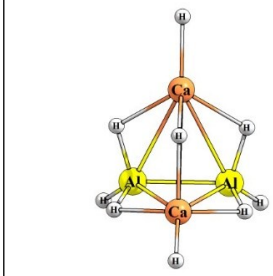
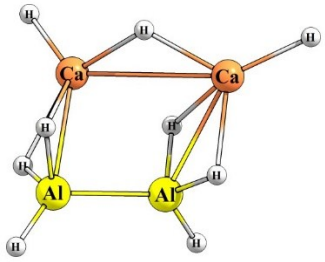
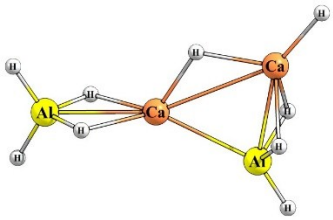
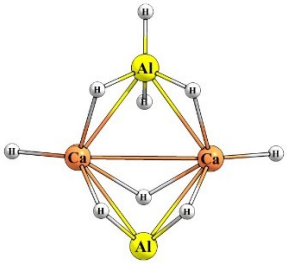
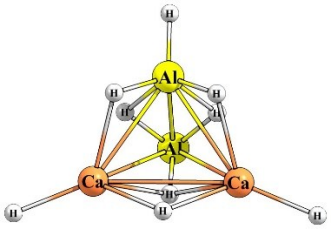
$Al_2Ca_2H_9^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Ca_2-1 C_{2v}		Al	1.098519000	-0.779718000	-1.314172000	CC -1843.0434 G4 -1844.8308	CC 0.0 G4 0.0
		Ca	-1.098519000	-1.546996000	0.890173000		
		H	-2.233881000	-0.013498000	-0.371116000		
		H	0.000000000	0.000000000	1.933610000		
		H	-0.723035000	2.113399000	-0.371620000		
		H	2.233881000	0.013498000	-0.371116000		
		H	0.723035000	-2.113399000	-0.371620000		
		Ca	1.098519000	1.546996000	0.890173000		
		H	-2.196970000	-3.091783000	1.741052000		
		H	2.196970000	3.091783000	1.741052000		
		H	-1.782915000	1.266060000	-2.684349000		
		H	1.782915000	-1.266060000	-2.684349000		
		Al	-1.098519000	0.779718000	-1.314172000		
Ca_2-2 C_s		Ca	-0.927369000	1.606459000	-0.237575000	CC -1843.0294 G4 -1844.8171	CC 8.8 G4 8.6
		H	1.056396000	1.706327000	0.715101000		
		H	1.383266000	-1.886536000	0.330813000		
		H	-1.670976000	0.326345000	1.605716000		
		H	-3.286173000	-1.854586000	1.236801000		
		Al	-2.162869000	-0.908472000	0.590764000		
		Ca	2.393962000	0.105265000	0.292442000		
		H	-2.743067000	0.151110000	-0.568654000		
		H	0.135026000	-2.708919000	-1.855215000		
		Al	0.022792000	-1.661623000	-0.637002000		
		H	0.629319000	-0.153752000	-1.237209000		
		H	4.460684000	0.192963000	0.392062000		
		H	-1.475332000	3.403792000	-1.115653000		
Ca_2-3 C_s		Al	-4.014195000	-0.118492000	0.000000000	CC -1843.0252 G4 -1844.8090	CC 11.4 G4 13.7
		Ca	-0.922838000	-0.113531000	0.000000000		
		H	-4.833870000	1.261583000	0.000000000		
		H	0.277913000	1.676949000	0.000000000		
		H	-2.873622000	-0.121824000	1.227176000		
		H	-2.873622000	-0.121824000	-1.227176000		
		H	-4.845674000	-1.490917000	0.000000000		
		H	3.821752000	2.840708000	0.000000000		
		Al	1.830589000	-1.600449000	0.000000000		
		Ca	2.462528000	1.260621000	0.000000000		
		H	2.593752000	-0.629175000	-1.203813000		
		H	2.593752000	-0.629175000	1.203813000		
		H	2.610929000	-3.018376000	0.000000000		
Ca_2-4 C_s		Al	2.501028000	0.217008000	0.000000000	CC -1843.0115 G4 -1844.8008	CC 20.0 G4 18.8
		Ca	-0.043379000	-0.329193000	-1.868351000		
		H	4.069122000	-0.064255000	0.000000000		
		H	0.082250000	-1.256455000	-3.714237000		
		H	1.507868000	-1.127196000	0.000000000		
		H	1.903293000	0.945913000	-1.340200000		
		H	1.903293000	0.945913000	1.340200000		
		Ca	-0.043379000	-0.329193000	1.868351000		
		H	-1.163667000	-0.869398000	0.000000000		
		H	-1.484878000	1.169992000	-1.207304000		
		H	-1.484878000	1.169992000	1.207304000		
		H	0.082250000	-1.256455000	3.714237000		
		Al	-2.493611000	0.418073000	0.000000000		
Ca_2-5 C_s		Ca	-0.562787000	-0.839892000	-1.766465000	CC -1843.0050 G4 -1844.7951	CC 24.1 G4 22.4
		H	0.866128000	1.147030000	1.118063000		
		H	-0.513164000	-1.636574000	-3.683343000		
		H	-1.512882000	-1.738265000	0.000000000		
		Al	-0.535966000	1.752677000	0.000000000		
		H	-0.411232000	3.342731000	0.000000000		
		H	-1.501286000	1.161005000	-1.240991000		
		Ca	-0.562787000	-0.839892000	1.766465000		
		H	-1.501286000	1.161005000	1.240991000		
		H	-0.513164000	-1.636574000	3.683343000		
		H	0.866128000	1.147030000	-1.118063000		
		H	0.936819000	-0.856981000	0.000000000		
		Al	2.056439000	0.499001000	0.000000000		

Figure SI-8. Lowest energy isomers for $Al_2Ca_2H_9^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

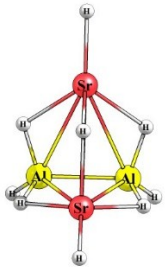
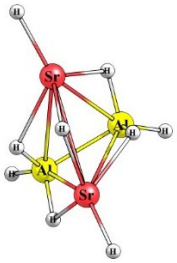
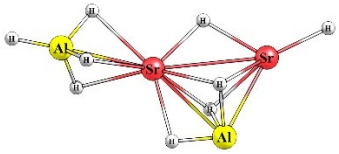
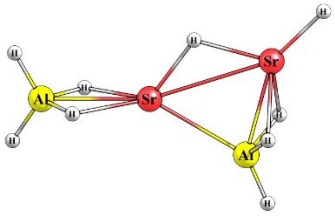
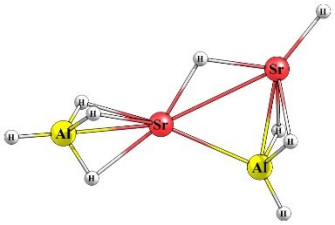
$Al_2Sr_2H_9^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Sr_2-1 C_2		Al	0.109610000	-1.344052000	-1.784108000	-550.2236	0.0
		Sr	2.009692000	0.164200000	0.567726000		
		H	0.177366000	-2.150975000	-3.174670000		
		H	1.446728000	-1.745859000	-0.854351000		
		H	1.146954000	1.955817000	-0.856684000		
		H	-1.146954000	-1.955817000	-0.856684000		
		H	4.046816000	0.334624000	1.487203000		
		Al	-0.109610000	1.344052000	-1.784108000		
		H	-0.177366000	2.150975000	-3.174670000		
		H	-1.446728000	1.745859000	-0.854351000		
		H	-4.046816000	-0.334624000	1.487203000		
		Sr	-2.009692000	-0.164200000	0.567726000		
		H	0.000000000	0.000000000	1.749090000		
Sr_2-2 C_2		Al	0.948114000	0.922753000	-1.811617000	-550.2184	3.2
		Sr	0.948114000	-1.610639000	0.672696000		
		H	-0.233210000	-2.359899000	-1.357004000		
		H	0.000000000	0.000000000	2.067305000		
		H	-1.647841000	-0.613879000	-0.295694000		
		H	0.233210000	2.359899000	-1.357004000		
		H	1.647841000	0.613879000	-0.295694000		
		Sr	-0.948114000	1.610639000	0.672696000		
		H	2.309636000	-3.161485000	1.522669000		
		H	-2.309636000	3.161485000	1.522669000		
		H	-2.091616000	-1.154088000	-2.915047000		
		H	2.091616000	1.154088000	-2.915047000		
		Al	-0.948114000	-0.922753000	-1.811617000		
Sr_2-3 C_s		Al	4.251317000	0.465959000	0.000000000	-550.2146	5.7
		H	5.835627000	0.672914000	0.000000000		
		H	3.578697000	-0.365783000	-1.259354000		
		H	3.578697000	-0.365783000	1.259354000		
		H	3.277427000	1.790784000	0.000000000		
		Sr	-2.374829000	0.580721000	0.000000000		
		H	-0.303158000	1.699280000	0.000000000		
		Al	-1.047377000	-2.201715000	0.000000000		
		Sr	1.281930000	-0.048518000	0.000000000		
		H	-0.724609000	-0.864019000	-1.151366000		
		H	-0.724609000	-0.864019000	1.151366000		
		H	0.634376000	-2.461577000	0.000000000		
		H	-4.339927000	1.708165000	0.000000000		
Sr_2-4 C_s		Al	-1.044084000	-2.149560000	0.000000000	-550,2079	9.8
		H	-0.345260000	1.633150000	0.000000000		
		H	-2.057554000	-1.480133000	1.215564000		
		H	-1.318636000	-3.747008000	0.000000000		
		H	-2.057554000	-1.480133000	-1.215564000		
		Sr	-2.484998000	0.553183000	0.000000000		
		H	-4.382326000	1.762131000	0.000000000		
		Sr	1.404560000	0.100885000	0.000000000		
		Al	4.611732000	0.727377000	0.000000000		
		H	5.058132000	2.273381000	0.000000000		
		H	3.525935000	0.453038000	1.242536000		
		H	5.776289000	-0.379700000	0.000000000		
		H	3.525935000	0.453038000	-1.242536000		
Sr_2-5 C_s		H	0.077647000	-1.573096000	0.000000000	-550.2076	10.0
		Al	1.276505000	2.067047000	0.000000000		
		H	1.745760000	3.619586000	0.000000000		
		H	2.199275000	1.278554000	1.215293000		
		Sr	2.331723000	-0.799045000	0.000000000		
		H	4.051381000	-2.257439000	0.000000000		
		Al	-4.472715000	-0.155501000	0.000000000		
		H	-6.056985000	-0.354271000	0.000000000		
		H	-3.600194000	-0.777108000	-1.258205000		
		H	-3.862802000	1.374182000	0.000000000		
		H	-3.600194000	-0.777108000	1.258205000		
		Sr	-1.476849000	0.170984000	0.000000000		
		H	2.199275000	1.278554000	-1.215293000		

Figure SI-9. Lowest energy isomers for $Al_2Sr_2H_9^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

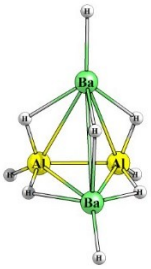
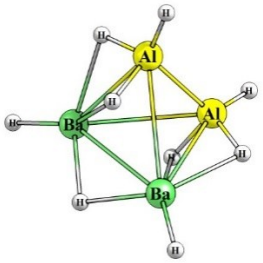
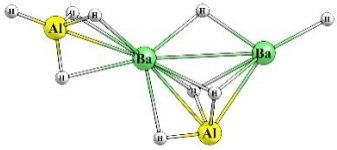
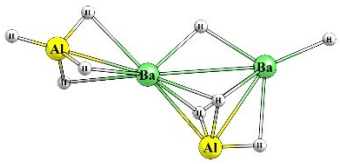
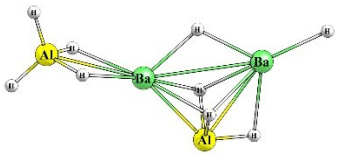
$Al_2Ba_2H_9^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Ba_2-1 C_{2v}		Al	2.136052000	1.107676000	0.000000000	-539.7122	0.0
		Ba	-0.246170000	-0.456222000	2.114618000		
		H	-0.689466000	-1.275199000	4.322642000		
		H	3.491393000	1.979520000	0.000000000		
		H	-0.891587000	-1.648774000	0.000000000		
		H	2.177222000	0.045861000	1.295952000		
		H	-1.155860000	1.846500000	1.296739000		
		H	-1.155860000	1.846500000	-1.296739000		
		H	2.177222000	0.045861000	-1.295952000		
		Al	-0.246170000	2.394325000	0.000000000		
		H	-0.689466000	-1.275199000	-4.322642000		
		H	-0.261078000	4.005823000	0.000000000		
		Ba	-0.246170000	-0.456222000	-2.114618000		
Ba_2-2 C_2		Al	-0.466115000	-1.251941000	2.120967000	-539,7116	0.3
		Ba	1.985539000	-0.254123000	-0.412569000		
		H	2.097426000	1.202700000	1.799221000		
		H	0.000000000	0.000000000	-1.896759000		
		H	-0.015001000	1.814614000	0.595109000		
		H	-2.097426000	-1.202700000	1.799221000		
		H	0.015001000	-1.814614000	0.595109000		
		Ba	-1.985539000	0.254123000	-0.412569000		
		H	4.065883000	-0.980491000	-1.349955000		
		H	-4.065883000	0.980491000	-1.349955000		
		H	0.111810000	2.343887000	3.249340000		
		H	-0.111810000	-2.343887000	3.249340000		
		Al	0.466115000	1.251941000	2.120967000		
Ba_2-3 C_s		H	-3.803634000	1.262713000	-1.272651000	-539.7114	0.5
		H	-3.803634000	1.262713000	1.272651000		
		Ba	-1.638002000	-0.070510000	0.000000000		
		H	0.262009000	1.590736000	0.000000000		
		H	4.569769000	1.540734000	0.000000000		
		Ba	2.443060000	0.324082000	0.000000000		
		H	-4.416164000	-0.846549000	0.000000000		
		Al	-4.731834000	0.768533000	0.000000000		
		H	-6.267790000	1.221522000	0.000000000		
		Al	0.749846000	-2.383316000	0.000000000		
		H	-0.933988000	-2.642546000	0.000000000		
		H	0.480396000	-1.059171000	-1.155394000		
		H	0.480396000	-1.059171000	1.155394000		
Ba_2-4 C_s		Ba	-2.495525000	-0.099547000	0.000000000	-539.7106	1.0
		H	-0.458384000	-1.615270000	0.000000000		
		H	-1.975188000	2.513830000	0.000000000		
		H	-4.839960000	-0.854352000	0.000000000		
		Ba	1.582016000	-0.141395000	0.000000000		
		H	4.102782000	-0.303870000	-1.272267000		
		Al	4.571859000	-1.244584000	0.000000000		
		H	3.366149000	-2.367493000	0.000000000		
		H	4.102782000	-0.303870000	1.272267000		
		H	6.080492000	-1.779592000	0.000000000		
		Al	-0.271652000	2.440903000	0.000000000		
		H	-0.389777000	1.084089000	1.153001000		
		H	-0.389777000	1.084089000	-1.153001000		
Ba_2-5 C_s		Ba	2.466182000	-0.442781000	0.000000000	-539.7096	1.6
		H	-3.867223000	-0.452144000	1.255873000		
		Al	-4.934012000	-0.711050000	0.000000000		
		H	0.580247000	1.043226000	-1.156613000		
		H	-6.081985000	0.421127000	0.000000000		
		H	-5.445702000	-2.239690000	0.000000000		
		H	2.346020000	2.242954000	0.000000000		
		Al	0.651816000	2.393610000	0.000000000		
		H	0.195618000	-1.608565000	0.000000000		
		H	0.580247000	1.043226000	1.156613000		
		H	4.666384000	-1.539340000	0.000000000		
		Ba	-1.573403000	0.150721000	0.000000000		
		H	-3.867223000	-0.452144000	-1.255873000		

Figure SI-10. Lowest energy isomers for $Al_2Ba_2H_9^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

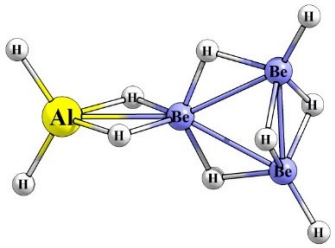
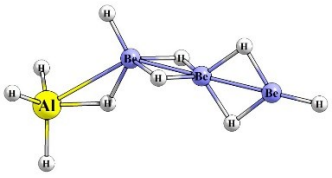
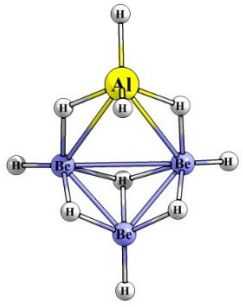
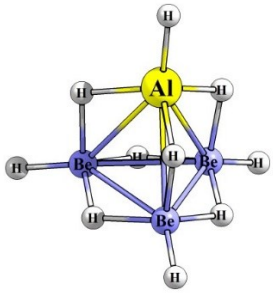
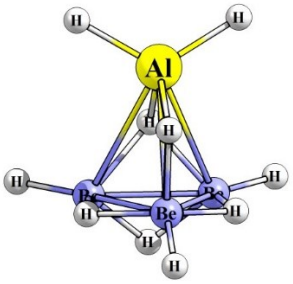
$AlBe_3H_{10}^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Be_3-1 C_s		Be -2.319093000 0.443832000 1.017498000 H -2.935468000 -0.444457000 0.000000000 Al 1.922523000 -0.341952000 0.000000000 H -0.954252000 -0.114798000 1.298561000 H 2.733758000 -0.424648000 1.373524000 H -2.964199000 0.731078000 2.201328000 Be -2.319093000 0.443832000 -1.017498000 H -0.954252000 -0.114798000 -1.298561000 H -2.964199000 0.731078000 -2.201328000 H -2.036611000 1.503984000 0.000000000 H 2.733758000 -0.424648000 -1.373524000 Be -0.375686000 -0.072099000 0.000000000 H 0.560869000 -1.331530000 0.000000000 H 0.804409000 0.922876000 0.000000000	CC -292.1042 G4 -292.5355	CC 0.0 G4 0.0
Be_3-2 C_s		Be 2.122450000 -0.336657000 0.000000000 H 1.256680000 -0.577550000 -1.093671000 H 2.848488000 0.980690000 0.000000000 H 1.256680000 -0.577550000 1.093671000 Be 0.177148000 -0.865643000 0.000000000 H -2.798161000 -0.318892000 -1.369970000 Al -2.300307000 0.371407000 0.000000000 H -2.472959000 1.985925000 0.000000000 H -0.581917000 0.358612000 0.000000000 H -2.798161000 -0.318892000 1.369970000 H 3.401278000 -1.131706000 0.000000000 Be 4.045478000 0.165267000 0.000000000 H -0.358318000 -2.124430000 0.000000000 H 5.353962000 0.505286000 0.000000000	CC -292.0955 G4 -292.5129	CC 5.4 G4 14.1
Be_3-3 C_s		Be -0.768476000 0.619671000 1.361135000 Be -2.207369000 -0.134418000 0.000000000 H 0.667572000 0.282895000 1.323900000 H -3.570959000 -0.001075000 0.000000000 H -0.962673000 1.483058000 2.409389000 Al 1.379163000 -0.428683000 0.000000000 H -1.534839000 -0.616794000 -1.217072000 H 2.869711000 0.167717000 0.000000000 Be -0.768476000 0.619671000 -1.361135000 H 0.667572000 0.282895000 -1.323900000 H -1.290463000 1.187788000 0.000000000 H -0.962673000 1.483058000 -2.409389000 H 1.222008000 -2.016584000 0.000000000 H -1.534839000 -0.616794000 1.217072000	CC -292.0956 G4 -292.5264	CC 5.4 G4 5.7
Be_3-4 C_{3v}		Be -1.036611000 0.636820000 1.217233000 Be -0.901517000 -1.464171000 0.000000000 Be -1.036611000 0.636820000 -1.217233000 H -1.539574000 1.255435000 2.342069000 H -1.274407000 -0.800000000 1.241576000 H -1.280683000 -2.789859000 0.000000000 H -1.413920000 1.343472000 0.000000000 H -1.539574000 1.255435000 -2.342069000 H -1.274407000 -0.800000000 -1.241576000 Al 1.103914000 0.070434000 0.000000000 H 0.641315000 -1.524675000 0.000000000 H 0.492713000 0.814249000 -1.351877000 H 2.697654000 0.172283000 0.000000000 H 0.492713000 0.814249000 1.351877000	CC -292.0952 G4 -292.5276	CC 5.6 G4 4.9
Be_3-5 C_s		Be -1.101988000 -1.274738000 0.000000000 Be -1.139865000 0.905092000 -1.060035000 H -1.214537000 -0.528067000 -1.260720000 H -1.000341000 1.661817000 -2.192885000 H -1.810204000 -2.455385000 0.000000000 H 0.063592000 1.117263000 0.000000000 H 2.012802000 -0.054573000 -1.372493000 H 0.369684000 -1.646779000 0.000000000 Al 1.212491000 -0.211668000 0.000000000 Be -1.139865000 0.905092000 1.060035000 H 2.012802000 -0.054573000 1.372493000 H -1.214537000 -0.528067000 1.260720000 H -1.000341000 1.661817000 2.192885000 H -2.030109000 1.358880000 0.000000000	CC -292.0906 G4 -292.5224	CC 8.5 G4 8.2

Figure SI-11. Lowest energy isomers for $AlBe_3H_{10}^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

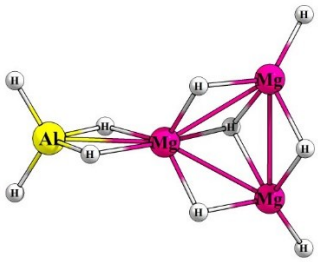
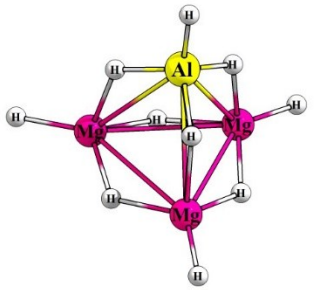
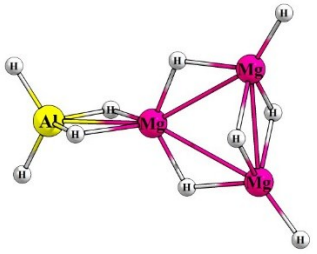
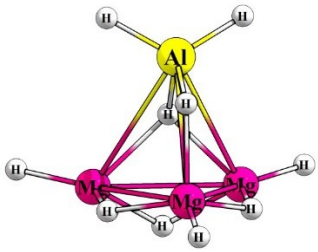
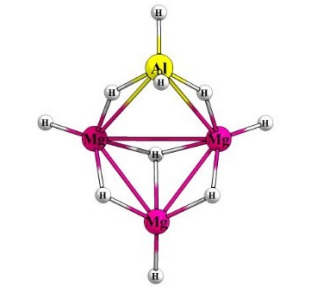
$AlMg_3H_{10}^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Mg_3-1 C_s		Mg	-2.034892000	-0.093888000	1.463181000	CC -846.9855 G4 -848.1078	CC 0.0 G4 0.0
		H	-0.377354000	0.826907000	1.546228000		
		H	-1.108192000	-1.105913000	0.000000000		
		H	-2.835642000	-0.747236000	2.868630000		
		H	1.870129000	-1.097509000	0.000000000		
		H	3.980183000	-0.149086000	1.378259000		
		H	2.169463000	1.306012000	0.000000000		
		H	3.980183000	-0.149086000	-1.378259000		
		Mg	-2.034892000	-0.093888000	-1.463181000		
		H	-2.835642000	-0.747236000	-2.868630000		
		H	-2.888678000	0.729120000	0.000000000		
		H	-0.377354000	0.826907000	-1.546228000		
		Al	3.173250000	-0.029246000	0.000000000		
		Mg	0.435467000	0.247102000	0.000000000		
Mg_3-2 C_{3v}		Al	0.000000000	0.000000000	1.868529000	CC -846.9836 G4 -848.1064	CC 1.2 G4 0.9
		Mg	-1.912682000	0.000000000	-0.715718000		
		H	0.761143000	-1.318339000	1.251762000		
		H	-3.638960000	0.000000000	-0.984549000		
		H	0.761143000	1.318339000	1.251762000		
		H	0.000000000	0.000000000	3.466579000		
		H	-1.522287000	0.000000000	1.251762000		
		Mg	0.956341000	-1.656431000	-0.715718000		
		Mg	0.956341000	1.656431000	-0.715718000		
		H	1.819480000	3.151432000	-0.984549000		
		H	1.680186000	0.000000000	-1.123089000		
		H	1.819480000	-3.151432000	-0.984549000		
		H	-0.840093000	-1.455084000	-1.123089000		
		H	-0.840093000	1.455084000	-1.123089000		
Mg_3-3 C_{2v}		Al	0.000000000	0.000000000	3.295501000	CC -846.9787 G4 -848.1023	CC 4.3 G4 3.5
		H	-1.210816000	0.000000000	2.125195000		
		H	0.000000000	1.379465000	4.105724000		
		H	1.210816000	0.000000000	2.125195000		
		Mg	0.000000000	-1.430874000	-2.128608000		
		H	0.000000000	-1.607043000	-0.223357000		
		H	1.272979000	0.000000000	-2.130581000		
		H	0.000000000	-2.871948000	-3.117002000		
		H	0.000000000	-1.379465000	4.105724000		
		H	-1.272979000	0.000000000	-2.130581000		
		Mg	0.000000000	1.430874000	-2.128608000		
		Mg	0.000000000	0.000000000	0.560426000		
		H	0.000000000	2.871948000	-3.117002000		
		H	0.000000000	1.607043000	-0.223357000		
Mg_3-4 C_s		Mg	0.522980000	-1.932779000	0.000000000	CC -846.9744 G4 -848.0968	CC 7.0 G4 6.9
		H	1.986806000	-0.631791000	0.000000000		
		H	-0.398369000	-1.227525000	1.460035000		
		H	1.104720000	-3.580326000	0.000000000		
		Mg	-1.266180000	0.388973000	1.505476000		
		H	-1.630991000	1.312274000	2.932662000		
		H	2.234195000	1.636440000	1.381074000		
		Mg	-1.266180000	0.388973000	-1.505476000		
		H	-1.630991000	1.312274000	-2.932662000		
		H	2.234195000	1.636440000	-1.381074000		
		H	-2.355808000	0.354438000	0.000000000		
		H	-0.398369000	-1.227525000	-1.460035000		
		Al	1.735508000	0.999170000	0.000000000		
		H	0.039606000	1.107916000	0.000000000		
Mg_3-5 C_s		Mg	0.196970000	0.581584000	-1.751643000	CC -846.9732 G4 -848.0953	CC 7.8 G4 7.8
		H	0.098212000	1.661809000	-3.109869000		
		H	1.381003000	-0.853175000	-1.540084000		
		H	-2.503998000	-2.266991000	0.000000000		
		Al	-2.375150000	-0.670281000	0.000000000		
		H	-1.465451000	-0.205380000	-1.303610000		
		H	-3.721072000	0.200509000	0.000000000		
		Mg	2.331214000	-0.405848000	0.000000000		
		H	1.381003000	-0.853175000	1.540084000		
		H	0.867283000	1.143607000	0.000000000		
		H	4.054502000	-0.157599000	0.000000000		
		Mg	0.196970000	0.581584000	1.751643000		
		H	0.098212000	1.661809000	3.109869000		
		H	-1.465451000	-0.205380000	1.303610000		

Figure SI-12. Lowest energy isomers for $AlMg_3H_{10}^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

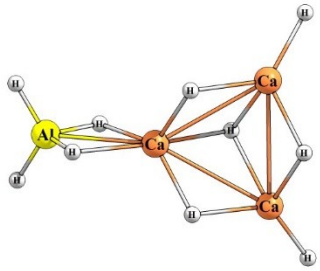
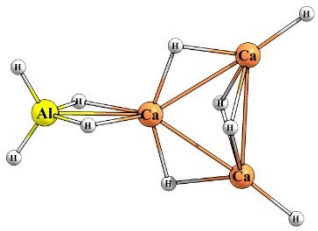
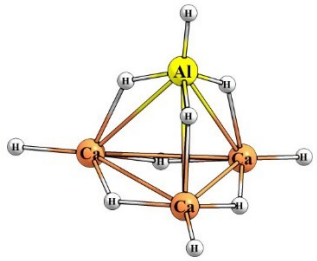
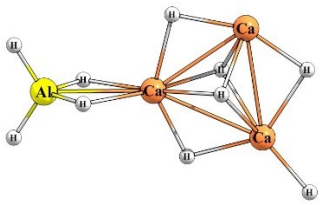
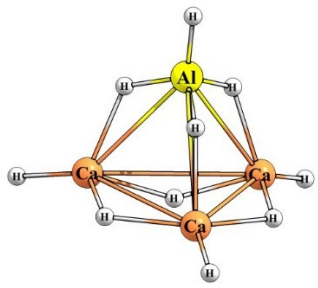
$AlCa_3H_{10}^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Ca_3-1 C_s		H	-2.892805000	0.931417000	0.000000000	CC -2278.4231 G4 -2280.5158	CC 0.0 G4 0.0
		H	-4.926773000	-0.178775000	-1.374758000		
		Al	-4.099336000	-0.229813000	0.000000000		
		H	-4.926773000	-0.178775000	1.374758000		
		H	-3.036111000	-1.520905000	0.000000000		
		H	2.807068000	1.112688000	3.492150000		
		Ca	1.963402000	0.267622000	1.783882000		
		Ca	1.963402000	0.267622000	-1.783882000		
		H	0.716441000	1.109418000	0.000000000		
		H	3.090373000	-0.329282000	0.000000000		
		H	0.110842000	-0.919581000	1.762033000		
		Ca	-1.019498000	-0.397377000	0.000000000		
		H	0.110842000	-0.919581000	-1.762033000		
		H	2.807068000	1.112688000	-3.492150000		
Ca_3-2 C_{3v}		Al	0.000000000	0.000000000	3.965915000	CC -2278.4158 G4 -2280.5110	CC 4.6 G4 3.0
		H	-1.231851000	0.000000000	2.834553000		
		H	0.000000000	1.369719000	4.806727000		
		H	1.231851000	0.000000000	2.834553000		
		Ca	0.000000000	-1.826841000	-1.882287000		
		H	0.000000000	-2.083940000	0.248389000		
		H	1.240540000	0.000000000	-1.314326000		
		H	0.000000000	-3.100586000	-3.537149000		
		H	0.000000000	-1.369719000	4.806727000		
		H	-1.240540000	0.000000000	-1.314326000		
		Ca	0.000000000	1.826841000	-1.882287000		
		Ca	0.000000000	0.000000000	0.882910000		
		H	0.000000000	3.100586000	-3.537149000		
		H	0.000000000	2.083940000	0.248389000		
Ca_3-3 C_{3v}		H	-0.573894000	-1.713723000	-1.313736000	CC -2278.4154 G4 -2280.5066	CC 4.8 G4 5.8
		H	1.692608000	-1.499063000	0.000000000		
		Al	0.240943000	-2.264905000	0.000000000		
		H	0.391846000	-3.854811000	0.000000000		
		H	-0.573894000	-1.713723000	1.313736000		
		Ca	-1.160452000	0.415110000	-1.972320000		
		H	-2.211937000	0.627705000	-3.751513000		
		Ca	2.241955000	0.737590000	0.000000000		
		Ca	-1.160452000	0.415110000	1.972320000		
		H	4.257231000	1.242989000	0.000000000		
		H	0.878344000	1.076034000	1.650030000		
		H	0.878344000	1.076034000	-1.650030000		
		H	-2.211937000	0.627705000	3.751513000		
		H	-1.969221000	0.806854000	0.000000000		
Ca_3-4 C_s		Ca	1.959267000	1.737551000	0.000000000	CC -2278.4114 G4 -2280.5092	CC 7.4 G4 4.1
		H	3.464792000	-0.083116000	0.000000000		
		H	-0.240027000	2.029086000	0.000000000		
		H	1.001521000	-0.027781000	1.272392000		
		H	1.001521000	-0.027781000	-1.272392000		
		H	3.092193000	3.515131000	0.000000000		
		Ca	-0.951027000	-0.019690000	0.000000000		
		H	-2.933285000	-0.231396000	1.237426000		
		H	-0.141478000	-2.179551000	0.000000000		
		Al	-4.043837000	-0.374819000	0.000000000		
		H	-4.713088000	-1.840128000	0.000000000		
		H	-5.066348000	0.868648000	0.000000000		
		Ca	1.892833000	-1.517385000	0.000000000		
		H	-2.933285000	-0.231396000	-1.237426000		
Ca_3-5 C_s		H	0.689986000	1.683446000	0.000000000	CC -2278.4108 G4 -2280.5066	CC 7.7 G4 5.8
		H	4.231532000	-0.036982000	0.000000000		
		H	-1.895310000	-1.644900000	-3.534656000		
		Ca	2.156159000	-0.149532000	0.000000000		
		H	1.405988000	-0.442415000	2.061419000		
		Ca	-0.721292000	-0.679691000	-2.117214000		
		H	-1.540992000	1.302357000	1.324614000		
		H	-0.318834000	-1.119851000	0.000000000		
		Al	-0.904908000	2.043685000	0.000000000		
		H	-1.208130000	3.612564000	0.000000000		
		H	1.405988000	-0.442415000	-2.061419000		
		H	-1.540992000	1.302357000	-1.324614000		
		Ca	-0.721292000	-0.679691000	2.117214000		
		H	-1.895310000	-1.644900000	3.534656000		

Figure SI-13. Lowest energy isomers for $AlCa_3H_{10}^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

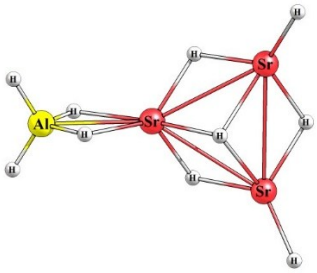
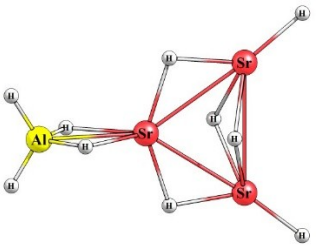
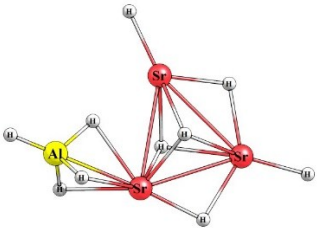
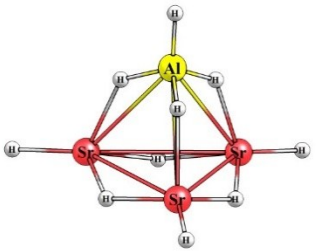
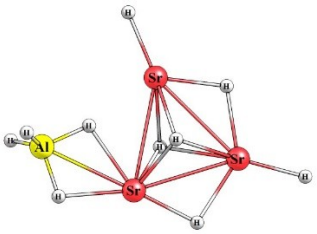
$AlSr_3H_{10}^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Sr_3-1 C_s		H	1.678193000	-3.288835000	0.000000000	-339.1918	0.0
		H	1.058182000	-5.519698000	1.373296000		
		Al	0.813264000	-4.720195000	0.000000000		
		H	1.058182000	-5.519698000	-1.373296000		
		H	-0.699429000	-4.010755000	0.000000000		
		H	0.637317000	2.788790000	-3.769202000		
		Sr	-0.115717000	1.739937000	-1.928582000		
		Sr	-0.115717000	1.739937000	1.928582000		
		H	1.021020000	0.603453000	0.000000000		
		H	-0.931159000	2.838201000	0.000000000		
		H	-0.920139000	-0.491999000	-1.880664000		
		Sr	-0.115717000	-1.593919000	0.000000000		
		H	-0.920139000	-0.491999000	1.880664000		
		H	0.637317000	2.788790000	3.769202000		
Sr_3-2 C_{2v}		Al	0.000000000	0.000000000	4.642753000	-339.1847	4.5
		H	-1.244241000	0.000000000	3.526804000		
		H	0.000000000	1.369388000	5.487333000		
		H	1.244241000	0.000000000	3.526804000		
		Sr	0.000000000	-1.981813000	-1.626413000		
		H	0.000000000	-2.244073000	0.669480000		
		H	1.309767000	0.000000000	-1.007716000		
		H	0.000000000	-3.387342000	-3.395708000		
		H	0.000000000	-1.369388000	5.487333000		
		H	-1.309767000	0.000000000	-1.007716000		
		Sr	0.000000000	1.981813000	-1.626413000		
		Sr	0.000000000	0.000000000	1.386611000		
		H	0.000000000	3.387342000	-3.395708000		
		H	0.000000000	2.244073000	0.669480000		
Sr_3-3 C_s		H	3.563411000	0.103669000	-1.252571000	-339.1834	5.3
		Sr	1.457227000	1.063880000	0.000000000		
		H	-0.098467000	2.734654000	0.000000000		
		H	2.079016000	-1.493642000	0.000000000		
		Al	3.655455000	-0.967910000	0.000000000		
		H	3.563411000	0.103669000	1.252571000		
		H	-3.941332000	2.616499000	0.000000000		
		Sr	-2.098792000	1.300060000	0.000000000		
		H	-0.166799000	0.022217000	-1.331871000		
		H	-2.644671000	-1.004157000	0.000000000		
		H	-0.454721000	-4.328238000	0.000000000		
		Sr	-0.578727000	-2.061814000	0.000000000		
		H	-0.166799000	0.022217000	1.331871000		
		H	4.822772000	-2.048603000	0.000000000		
Sr_3-4 C_{3v}		H	1.957769000	0.756205000	1.314686000	-339.1820	6.1
		H	1.959082000	-1.520531000	0.000000000		
		Al	2.585267000	-0.002228000	0.000000000		
		H	4.183796000	-0.001042000	0.000000000		
		H	1.957769000	0.756205000	-1.314686000		
		Sr	-0.342065000	1.223053000	2.117396000		
		H	-0.691550000	2.329126000	4.032027000		
		Sr	-0.342065000	-2.445220000	0.000000000		
		Sr	-0.342065000	1.223053000	-2.117396000		
		H	-0.691384000	-4.656417000	0.000000000		
		H	-0.866420000	-1.032157000	-1.788427000		
		H	-0.866420000	-1.032157000	1.788427000		
		H	-0.691550000	2.329126000	-4.032027000		
		H	-0.864168000	2.066954000	0.000000000		
Sr_3-5 C_s		H	-0.229767000	-0.042422000	1.345627000	-339.1814	6.5
		Sr	0.782007000	1.563799000	0.000000000		
		H	-0.229767000	-0.042422000	-1.345627000		
		Sr	-2.534873000	0.277994000	0.000000000		
		H	-4.760595000	0.672049000	0.000000000		
		H	-1.335529000	2.429969000	0.000000000		
		H	3.212895000	1.955225000	0.000000000		
		H	4.627776000	0.140775000	1.379981000		
		H	1.325241000	-4.128781000	0.000000000		
		Al	3.854869000	0.404023000	0.000000000		
		H	4.627776000	0.140775000	-1.379981000		
		H	-2.017779000	-2.025289000	0.000000000		
		Sr	0.301117000	-2.111121000	0.000000000		
		H	2.371797000	-0.391759000	0.000000000		

Figure SI-14. Lowest energy isomers for $AlSr_3H_{10}^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

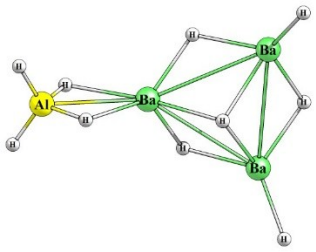
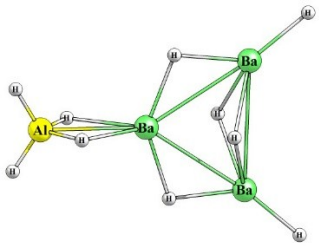
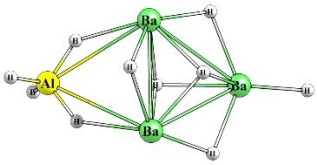
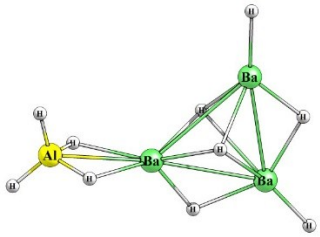
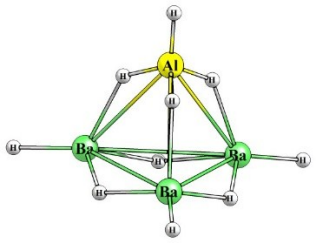
$AlBa_3H_{10}^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Ba_3-1 C_s		H	1.750127000	-3.847136000	0.000000000	-323.4221	0.0
		H	1.126720000	-6.077806000	1.370049000		
		Al	0.874916000	-5.268197000	0.000000000		
		H	1.126720000	-6.077806000	-1.370049000		
		H	-0.642743000	-4.579731000	0.000000000		
		H	0.985460000	2.703886000	-3.973032000		
		Ba	-0.090037000	1.704949000	-2.078561000		
		Ba	-0.090037000	1.704949000	2.078561000		
		H	1.023432000	0.455645000	0.000000000		
		H	-0.809372000	2.973193000	0.000000000		
		H	-0.896728000	-0.709602000	-1.995851000		
		Ba	-0.090037000	-1.951832000	0.000000000		
		H	-0.896728000	-0.709602000	1.995851000		
		H	0.985460000	2.703886000	3.973032000		
Ba_3-2 C_{2v}		Al	0.000000000	0.000000000	5.157692000	-323.4149	4.6
		H	-1.250589000	0.000000000	4.053236000		
		H	0.000000000	1.367347000	6.009950000		
		H	1.250589000	0.000000000	4.053236000		
		Ba	0.000000000	-2.152587000	-1.572305000		
		H	0.000000000	-2.393114000	0.879921000		
		H	1.362293000	0.000000000	-0.894555000		
		H	0.000000000	-3.711824000	-3.432484000		
		H	0.000000000	-1.367347000	6.009950000		
		H	-1.362293000	0.000000000	-0.894555000		
		Ba	0.000000000	2.152587000	-1.572305000		
		Ba	0.000000000	0.000000000	1.711001000		
		H	0.000000000	3.711824000	-3.432484000		
		H	0.000000000	2.393114000	0.879921000		
Ba_3-3 C_s		Ba	-0.894590000	-0.359606000	1.846623000	-323.4145	4.8
		H	0.568854000	-1.381133000	0.000000000		
		H	1.501514000	0.144958000	2.367454000		
		Ba	2.570829000	0.343531000	0.000000000		
		H	5.052939000	0.450357000	0.000000000		
		H	1.501514000	0.144958000	-2.367454000		
		Al	-3.603446000	1.882409000	0.000000000		
		H	-5.135647000	1.354739000	0.000000000		
		H	-3.465971000	3.494307000	0.000000000		
		H	-2.840832000	1.280222000	1.347600000		
		H	-2.840832000	1.280222000	-1.347600000		
		H	-2.094057000	-1.538911000	0.000000000		
		Ba	-0.894590000	-0.359606000	-1.846623000		
		H	-0.092516000	1.095055000	0.000000000		
Ba_3-4 C_s		Ba	1.994510000	0.513993000	0.000000000	-323.4139	5.2
		H	0.523931000	2.430619000	0.000000000		
		H	0.040191000	-0.474725000	1.375376000		
		Ba	-1.868774000	1.540463000	0.000000000		
		H	0.040191000	-0.474725000	-1.375376000		
		H	-3.048804000	-0.720569000	0.000000000		
		Al	5.414224000	0.037811000	0.000000000		
		Ba	-1.184013000	-2.346596000	0.000000000		
		H	6.629068000	1.093456000	0.000000000		
		H	4.356323000	0.332879000	1.254090000		
		H	4.356323000	0.332879000	-1.254090000		
		H	5.810831000	-1.526467000	0.000000000		
		H	-3.426242000	3.353268000	0.000000000		
		H	-1.143912000	-4.770537000	0.000000000		
Ba_3-5 C_{3v}		H	1.550645000	-1.716253000	1.315043000	-323.4123	6.2
		H	-0.543958000	-2.607262000	0.000000000		
		Al	1.099490000	-2.592964000	0.000000000		
		H	1.726193000	-4.065930000	0.000000000		
		H	1.550645000	-1.716253000	-1.315043000		
		Ba	1.099490000	0.745118000	2.257374000		
		H	2.013226000	1.602789000	4.287263000		
		Ba	-2.498715000	-0.783596000	0.000000000		
		Ba	1.099490000	0.745118000	-2.257374000		
		H	-4.826864000	-1.303481000	0.000000000		
		H	-1.355216000	0.347281000	-1.925521000		
		H	-1.355216000	0.347281000	1.925521000		
		H	2.013226000	1.602789000	-4.287263000		
		H	1.719134000	1.645725000	0.000000000		

Figure SI-15. Lowest energy isomers for $AlBa_3H_{10}^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

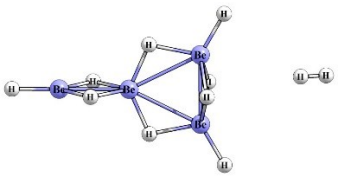
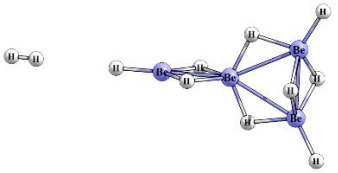
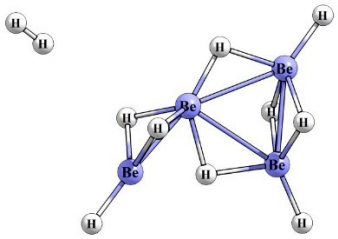
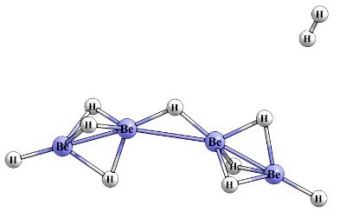
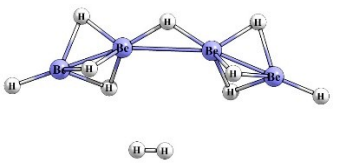
$Be_4H_{11}^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Be_4-1 C_s		Be	-1.286257000	0.218199000	1.011513000	-65.3534	0.0
		Be	-1.286257000	0.218199000	-1.011513000		
		Be	0.746177000	-0.006725000	0.000000000		
		H	0.176577000	0.065084000	1.301605000		
		H	1.692526000	-1.205395000	0.000000000		
		H	-1.388351000	1.304809000	0.000000000		
		H	-1.600917000	-0.829967000	0.000000000		
		H	0.176577000	0.065084000	-1.301605000		
		H	-1.972274000	0.283957000	-2.206718000		
		Be	2.743498000	-0.221715000	0.000000000		
		H	-4.300294000	-1.299235000	0.000000000		
		H	4.093346000	-0.375120000	0.000000000		
		H	-5.042070000	-1.394415000	0.000000000		
		H	1.930144000	0.962976000	0.000000000		
		H	-1.972274000	0.283957000	2.206718000		
Be_4-2 C_s		Be	1.800992000	-0.154685000	1.011701000	-65.3531	0.2
		Be	-0.232698000	-0.001637000	0.003558000		
		Be	1.796729000	-0.145156000	-1.014644000		
		Be	-2.214641000	0.325525000	0.007032000		
		H	2.031643000	-1.212320000	-0.006951000		
		H	-1.477890000	-0.904719000	0.001493000		
		H	2.486872000	-0.126610000	-2.209533000		
		H	0.328589000	-0.160824000	1.301614000		
		H	-1.113779000	1.246443000	0.010939000		
		H	0.322954000	-0.148655000	-1.298340000		
		H	-6.749527000	0.695746000	-0.012766000		
		H	1.973312000	0.932309000	0.003232000		
		H	-6.002038000	0.655228000	-0.009301000		
		H	-3.554027000	0.554466000	0.008174000		
		H	2.496172000	-0.147136000	2.203790000		
Be_4-3 C_s		H	-1.680212000	0.139556000	-1.077784000	-65.3489	2.9
		Be	-1.760627000	-0.885774000	0.000000000		
		H	1.490487000	-0.296482000	1.057948000		
		H	-1.680212000	0.139556000	1.077784000		
		H	-2.750840000	-1.840529000	0.000000000		
		Be	-1.301737000	1.089204000	0.000000000		
		H	-1.675209000	2.408591000	0.000000000		
		Be	0.453319000	-0.476392000	0.000000000		
		H	1.490487000	-0.296482000	-1.057948000		
		H	0.266578000	1.019435000	0.000000000		
		H	-0.420076000	-1.578551000	0.000000000		
		H	3.404339000	-2.330738000	0.000000000		
		H	2.894158000	1.601756000	0.000000000		
		H	3.926764000	-2.865260000	0.000000000		
		Be	1.901138000	0.673922000	0.000000000		
Be_4-4 C_s		Be	-2.991723000	-0.401787000	0.000000000	-65.3399	8.5
		Be	-1.316278000	0.246963000	0.000000000		
		H	3.532224000	3.866990000	0.000000000		
		H	-2.314537000	0.505241000	1.044258000		
		H	-1.643637000	-1.171198000	0.000000000		
		H	-0.093532000	0.951960000	0.000000000		
		H	3.260709000	3.169742000	0.000000000		
		H	-4.263194000	-0.899501000	0.000000000		
		Be	2.698908000	-0.602834000	0.000000000		
		Be	1.054237000	0.125138000	0.000000000		
		H	-2.314537000	0.505241000	-1.044258000		
		H	3.948835000	-1.152218000	0.000000000		
		H	1.576070000	-0.752821000	1.046873000		
		H	2.310797000	0.889430000	0.000000000		
		H	1.576070000	-0.752821000	-1.046873000		
Be_4-5 C_s		Be	0.042796000	-0.256884000	2.883698000	-65.3389	9.1
		Be	-0.367387000	0.231035000	-1.202957000		
		Be	0.042796000	-0.256884000	-2.883698000		
		Be	-0.367387000	0.231035000	1.202957000		
		H	3.523245000	0.495204000	-0.373158000		
		H	-0.836092000	0.801642000	0.000000000		
		H	0.350860000	-0.629662000	-4.161016000		
		H	-0.168846000	-1.147915000	-1.639668000		
		H	0.350860000	-0.629662000	4.161016000		
		H	-1.201546000	0.503428000	2.379914000		
		H	-0.168846000	-1.147915000	1.639668000		
		H	0.827742000	0.665583000	-1.934945000		
		H	3.523245000	0.495204000	0.373158000		
		H	0.827742000	0.665583000	1.934945000		
		H	-1.201546000	0.503428000	-2.379914000		

Figure SI-16. Lowest energy isomers for $Be_4H_{11}^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

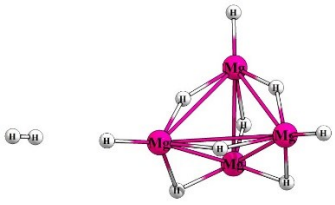
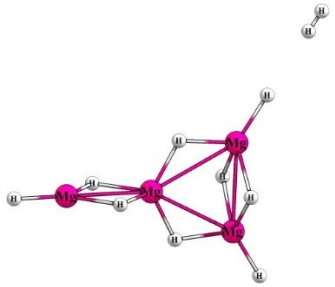
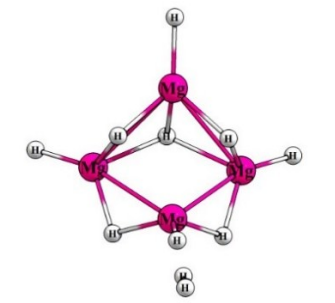
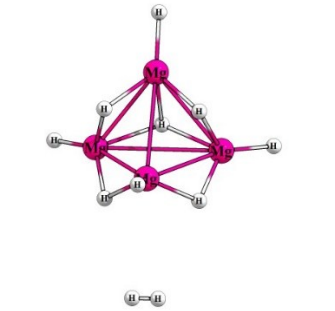
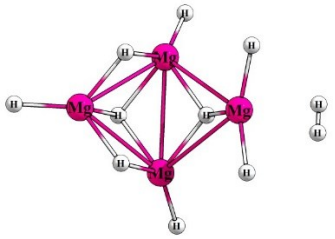
$Mg_4H_{11}^-$	Structure	Cartesian Coordinates	Energy (a.u)	ΔE
Mg_4-1 C_s		Mg -2.025420000 0.189532000 0.000000000 H -0.685080000 0.399552000 1.321745000 H -3.645089000 0.831180000 0.000000000 H 1.234881000 -1.372202000 -1.525492000 H -0.685080000 0.399552000 -1.321745000 Mg 1.162538000 0.559073000 -1.789172000 H 1.786303000 1.378299000 3.196498000 Mg 0.226999000 -1.384749000 0.000000000 H -1.571302000 -1.719705000 0.000000000 Mg 1.162538000 0.559073000 1.789172000 H 1.234881000 -1.372202000 1.525492000 H -6.537856000 2.018849000 0.000000000 H -5.842530000 1.736190000 0.000000000 H 1.688654000 0.869411000 0.000000000 H 1.786303000 1.378299000 -3.196498000	-805.1783	0.0
Mg_4-2 C_s		Mg 0.776516000 -0.027794000 0.000077000 H -4.856757000 4.066011000 -0.004257000 H 0.168357000 -1.719920000 -0.002466000 Mg -1.740967000 -1.840788000 0.000133000 H -2.460151000 -3.437573000 -0.000268000 H 2.234789000 0.188340000 1.286705000 H -2.021829000 -0.441594000 -1.276412000 H -5.350789000 4.632062000 -0.007227000 H -0.296842000 1.416104000 0.001634000 H 5.238560000 0.637249000 -0.001940000 H 2.233306000 0.191220000 -1.288060000 Mg 3.530759000 0.383213000 -0.001268000 H -3.308455000 2.291853000 0.006830000 Mg -2.155225000 0.970674000 0.004699000 H -2.015949000 -0.444125000 1.281820000	-805.1746	2.4
Mg_4-3 C_s		Mg 0.381462000 -0.884555000 -1.815399000 Mg 0.381462000 -0.884555000 1.815399000 H 2.550690000 2.408048000 0.000000000 H -1.349195000 -1.259671000 1.355049000 H -5.215422000 2.240817000 0.000000000 H -0.032568000 0.963377000 -1.353910000 H 1.266441000 -0.729825000 0.000000000 H 1.310026000 -1.464944000 -3.164884000 H -5.855650000 2.633171000 0.000000000 H -0.032568000 0.963377000 1.353910000 Mg 1.197843000 1.325064000 0.000000000 H 1.310026000 -1.464944000 3.164884000 H -1.349195000 -1.259671000 -1.355049000 Mg -1.790460000 -0.015260000 0.000000000 H -3.205964000 1.000283000 0.000000000	-805.1742	2.6
Mg_4-4 C_s		Mg 1.425169000 -0.809388000 0.000000000 H 2.209969000 -2.361424000 0.000000000 H 1.563169000 0.493092000 -1.359188000 H -0.703433000 1.890531000 -3.162289000 H 4.490854000 0.720689000 0.373285000 Mg -0.153589000 0.942048000 -1.812863000 H -0.703433000 1.890531000 3.162289000 Mg -1.881508000 -0.656294000 0.000000000 H -1.009046000 1.209955000 0.000000000 Mg -0.153589000 0.942048000 1.812863000 H 1.563169000 0.493092000 1.359188000 H -0.633213000 -0.887589000 1.364291000 H -0.633213000 -0.887589000 -1.364291000 H -3.580764000 -1.001294000 0.000000000 H 4.490854000 0.720689000 -0.373285000	-805.1740	2.7
Mg_4-5 C_s		Mg -0.764296000 0.314291000 1.525629000 H 0.137519000 1.126417000 0.000000000 H 2.550187000 1.075096000 1.673776000 H 1.776853000 3.575509000 0.375406000 H -1.465633000 1.240774000 2.811320000 H 0.083530000 -1.342794000 1.459511000 Mg -0.764296000 0.314291000 -1.525629000 H -1.465633000 1.240774000 -2.811320000 H 2.550187000 1.075096000 -1.673776000 Mg -0.764296000 -2.171544000 0.000000000 H 1.776853000 3.575509000 -0.375406000 H -1.828688000 -0.438763000 0.000000000 H 0.083530000 -1.342794000 -1.459511000 Mg 2.061965000 1.042643000 0.000000000 H -1.427631000 -3.780998000 0.000000000	-805.1601	11.4

Figure SI-17. Lowest energy isomers for $Mg_4H_{11}^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

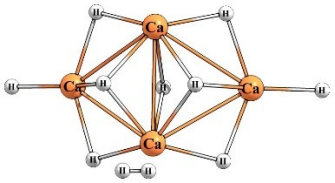
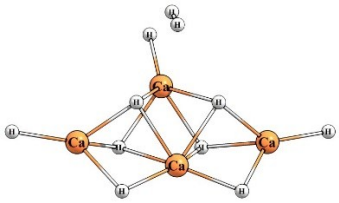
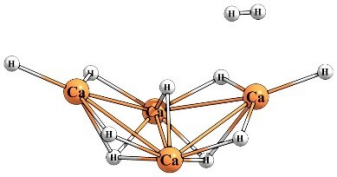
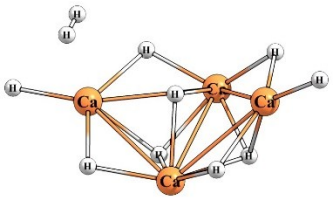
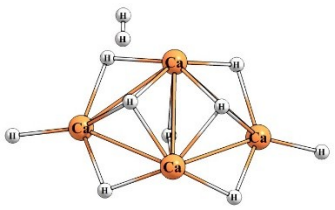
$Ca_4H_{11}^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Ca_4-1 C_s		Ca	1.781583000	0.577133000	0.000000000	-2713.7667	0.0
		H	0.129252000	1.343615000	-1.338388000		
		H	-2.400404000	3.334902000	0.374325000		
		H	0.080423000	-0.891333000	0.000000000		
		H	0.129252000	1.343615000	1.338388000		
		H	-2.400404000	3.334902000	-0.374325000		
		H	2.210147000	-0.363230000	-1.892823000		
		H	0.067816000	-1.459221000	4.542870000		
		Ca	-1.559110000	0.649644000	0.000000000		
		Ca	0.085760000	-0.662211000	-2.601006000		
		Ca	0.085760000	-0.662211000	2.601006000		
		H	-2.023410000	-0.266718000	-1.897823000		
		H	-2.023410000	-0.266718000	1.897823000		
		H	0.067816000	-1.459221000	-4.542870000		
		H	2.210147000	-0.363230000	1.892823000		
Ca_4-2 C_s		Ca	-1.744046000	-0.307256000	0.000000000	-2713.7663	0.2
		H	-2.358478000	-2.853106000	0.000000000		
		H	-0.576920000	1.209079000	1.348567000		
		H	-3.791533000	-0.670967000	0.000000000		
		H	-0.019708000	-1.152914000	-1.340548000		
		H	-0.025127000	0.073360000	-5.159042000		
		Ca	1.208957000	0.390724000	0.000000000		
		H	-0.019708000	-1.152914000	1.340548000		
		H	2.173660000	0.611124000	1.954257000		
		H	2.173660000	0.611124000	-1.954257000		
		Ca	0.351637000	0.176464000	-3.103800000		
		H	-0.576920000	1.209079000	-1.348567000		
		H	-0.025127000	0.073360000	5.159042000		
		Ca	0.351637000	0.176464000	3.103800000		
		H	-1.614108000	-2.973284000	0.000000000		
Ca_4-3 C_s		Ca	-2.612033000	-0.481284000	0.000000000	-2713.7659	0.5
		Ca	2.562237000	-0.735831000	0.000000000		
		H	1.885510000	-0.334992000	2.121403000		
		H	4.448417000	-1.663827000	0.000000000		
		H	-0.023594000	-0.824848000	0.000000000		
		H	-4.583967000	-1.199553000	0.000000000		
		H	-1.890338000	-0.164917000	2.116216000		
		H	-1.263550000	1.468100000	0.000000000		
		H	1.407746000	1.349042000	0.000000000		
		H	1.513550000	-3.247437000	0.000000000		
		H	2.257628000	-3.361740000	0.000000000		
		Ca	0.041589000	0.683403000	-1.670683000		
		H	1.885510000	-0.334992000	-2.121403000		
		H	-1.890338000	-0.164917000	-2.116216000		
		Ca	0.041589000	0.683403000	1.670683000		
Ca_4-4 C_s		Ca	-0.029995000	0.642526000	1.666753000	-2713.7653	0.9
		H	-1.671673000	-3.505189000	-0.373942000		
		H	1.948443000	-0.080919000	2.123412000		
		H	-1.671673000	-3.505189000	0.373942000		
		H	-1.429844000	1.271117000	0.000000000		
		H	-1.830158000	-0.474733000	-2.103922000		
		H	0.148814000	-0.829122000	0.000000000		
		H	-1.830158000	-0.474733000	2.103922000		
		Ca	-2.589043000	-0.767102000	0.000000000		
		Ca	-0.029995000	0.642526000	-1.666753000		
		Ca	2.679203000	-0.360801000	0.000000000		
		H	4.681904000	-0.994460000	0.000000000		
		H	-4.582718000	-1.419231000	0.000000000		
		H	1.948443000	-0.080919000	-2.123412000		
		H	1.228644000	1.515790000	0.000000000		
Ca_4-5 C_s		Ca	-0.106371000	0.231789000	1.669869000	-2713.7642	1.5
		H	2.325840000	5.943581000	-0.372988000		
		H	-2.061281000	-0.559012000	2.116900000		
		H	2.325840000	5.943581000	0.372988000		
		H	-1.385595000	1.056343000	0.000000000		
		H	1.709487000	-0.840411000	2.116787000		
		Ca	-2.789819000	-0.858354000	0.000000000		
		H	-4.780010000	-1.523781000	0.000000000		
		Ca	2.386583000	-1.243768000	0.000000000		
		H	1.282082000	0.856840000	0.000000000		
		H	-2.061281000	-0.559012000	-2.116900000		
		H	-0.219067000	-1.269631000	0.000000000		
		H	4.257974000	-2.193290000	0.000000000		
		Ca	-0.106371000	0.231789000	-1.669869000		
		H	1.709487000	-0.840411000	-2.116787000		

Figure SI-18. Lowest energy isomers for $Ca_4H_{11}^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory

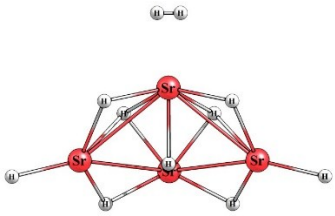
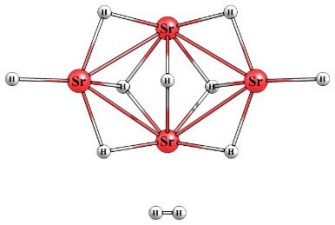
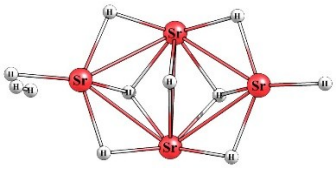
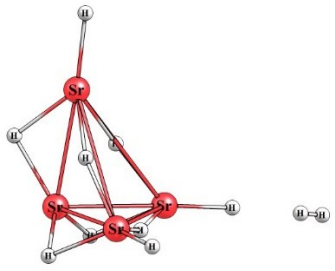
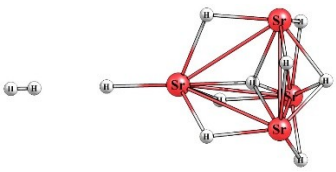
$Sr_4H_{11}^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Sr_4-1 C_s		Sr	0.601772000	-1.876690000	0.000000000	-128.1281	0.0
		H	-1.102959000	-0.891747000	1.438938000		
		H	-4.276029000	-0.535979000	-0.374095000		
		H	0.732521000	0.533812000	0.000000000		
		H	-1.102959000	-0.891747000	-1.438938000		
		H	-4.276029000	-0.535979000	0.374095000		
		H	1.703681000	-1.561695000	2.023279000		
		H	1.188873000	0.885960000	-4.969245000		
		Sr	-1.637883000	1.004697000	0.000000000		
		Sr	0.601772000	0.431966000	2.824725000		
		Sr	0.601772000	0.431966000	-2.824725000		
		H	-1.061075000	1.989711000	2.027481000		
		H	-1.061075000	1.989711000	-2.027481000		
		H	1.188873000	0.885960000	4.969245000		
		H	1.703681000	-1.561695000	-2.023279000		
Sr_4-2 C_s		H	1.132263000	0.787256000	5.003290000	-128.1273	0.5
		Sr	-1.635810000	0.985057000	0.000000000		
		Sr	0.563192000	-1.922041000	0.000000000		
		Sr	0.563192000	0.357992000	-2.849390000		
		Sr	0.563192000	0.357992000	2.849390000		
		H	-1.084359000	1.932740000	2.055556000		
		H	-1.134045000	-0.926196000	-1.433855000		
		H	-1.956709000	3.790839000	-0.376778000		
		H	-1.956709000	3.790839000	0.376778000		
		H	1.659424000	-1.630435000	-2.031405000		
		H	-1.134045000	-0.926196000	1.433855000		
		H	1.659424000	-1.630435000	2.031405000		
		H	0.723781000	0.489612000	0.000000000		
		H	1.132263000	0.787256000	-5.003290000		
		H	-1.084359000	1.932740000	-2.055556000		
Sr_4-3 C_s		H	-0.542884000	-1.920268000	2.252278000	-128.1270	0.7
		Sr	-0.601905000	0.364329000	-1.824039000		
		Sr	1.917071000	2.269362000	0.000000000		
		H	3.543885000	3.851510000	0.000000000		
		H	1.241913000	1.714482000	2.250818000		
		H	-0.636236000	1.979792000	0.000000000		
		H	1.241913000	1.714482000	-2.250818000		
		Sr	-0.601905000	0.364329000	1.824039000		
		Sr	-0.601905000	-2.791259000	0.000000000		
		H	0.819891000	-0.327413000	0.000000000		
		H	-0.542884000	-1.920268000	-2.252278000		
		H	-3.085338000	-3.978078000	0.000000000		
		H	-1.901338000	-0.600883000	0.000000000		
		H	-0.898459000	-5.042855000	0.000000000		
		H	-3.471970000	-3.327435000	0.000000000		
Sr_4-4 C_s		Sr	2.511702000	0.991008000	0.000000000	-128.1187	5.9
		H	0.822645000	0.140043000	1.481139000		
		H	4.771969000	0.902999000	0.000000000		
		H	-2.055558000	0.879158000	-2.056503000		
		H	0.822645000	0.140043000	-1.481139000		
		Sr	-0.967414000	-1.196227000	-2.373974000		
		H	-1.069361000	-2.777495000	3.985089000		
		Sr	-0.967414000	1.376558000	0.000000000		
		H	0.961284000	2.772823000	0.000000000		
		Sr	-0.967414000	-1.196227000	2.373974000		
		H	-2.055558000	0.879158000	2.056503000		
		H	7.907026000	1.019508000	0.000000000		
		H	7.154624000	0.990945000	0.000000000		
		H	-1.349810000	-1.223930000	0.000000000		
		H	-1.069361000	-2.777495000	-3.985089000		
Sr_4-5 C_s		H	-7.817691000	-0.006585000	0.029149000	-128.1183	6.1
		H	-7.061914000	-0.004090000	0.018030000		
		H	-1.363469000	0.436709000	-2.249859000		
		Sr	0.968068000	0.388783000	-2.003293000		
		H	1.368374000	2.467016000	-0.845995000		
		H	-1.375786000	1.727527000	1.493999000		
		Sr	-2.424542000	0.002447000	-0.009153000		
		H	-4.736637000	0.003821000	-0.017345000		
		Sr	0.956026000	-1.932927000	0.668467000		
		H	-1.377093000	-2.160152000	0.739296000		
		H	1.365557000	-1.971470000	-1.707670000		
		H	1.352121000	-0.498734000	2.566740000		
		H	2.328468000	-0.002129000	0.007565000		
		H	-0.032823000	0.000451000	-0.001302000		
		Sr	0.957050000	1.541898000	1.343121000		

Figure SI-19. Lowest energy isomers for $Sr_4H_{11}^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory

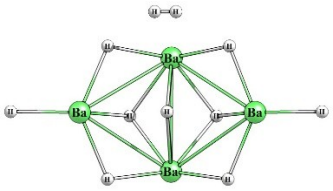
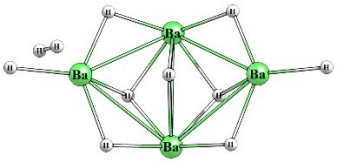
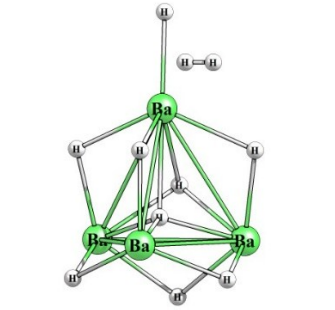
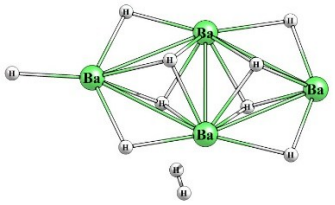
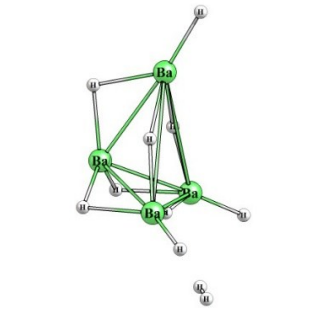
$Ba_4H_{11}^-$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
Ba_4-1 C_s		H	0.929510000	0.661270000	5.522805000	-107.1033	0.0
		Ba	-1.822263000	1.097624000	0.000000000		
		Ba	0.606135000	-2.092875000	0.000000000		
		Ba	0.606135000	0.421793000	-3.113803000		
		Ba	0.606135000	0.421793000	3.113803000		
		H	-1.085232000	2.091281000	2.163125000		
		H	-1.166221000	-0.929138000	-1.540474000		
		H	-0.704310000	3.800952000	-0.378120000		
		H	-0.704310000	3.800952000	0.378120000		
		H	1.794318000	-1.622398000	-2.139393000		
		H	-1.166221000	-0.929138000	1.540474000		
		H	1.794318000	-1.622398000	2.139393000		
		H	0.679836000	0.489299000	0.000000000		
		H	0.929510000	0.661270000	-5.522805000		
		H	-1.085232000	2.091281000	-2.163125000		
Ba_4-2 C_s		H	2.028286000	0.634338000	-2.353806000	-107.1028	0.3
		Ba	2.878068000	1.164484000	0.000000000		
		H	2.028286000	0.634338000	2.353806000		
		H	-0.107962000	0.754396000	0.000000000		
		H	1.714639000	-1.348753000	0.000000000		
		H	5.133751000	2.117066000	0.000000000		
		Ba	0.099559000	-0.892294000	2.009244000		
		Ba	-3.077896000	0.456109000	0.000000000		
		H	-1.348793000	-1.719595000	0.000000000		
		H	-2.148841000	0.101772000	2.357227000		
		H	-4.030857000	3.436865000	0.000000000		
		H	-2.148841000	0.101772000	-2.357227000		
		H	-4.590533000	2.916513000	0.000000000		
		H	-5.476722000	0.954368000	0.000000000		
		Ba	0.099559000	-0.892294000	-2.009244000		
Ba_4-3 C_s		Ba	1.145854000	0.503410000	-1.949948000	-107.0963	4.4
		Ba	-1.712173000	-1.678057000	0.000000000		
		H	1.116671000	-1.173787000	0.000000000		
		H	-0.727076000	-1.058519000	2.362309000		
		H	1.205768000	-5.053591000	-0.372930000		
		H	1.205768000	-5.053591000	0.372930000		
		H	-0.727076000	-1.058519000	-2.362309000		
		H	-2.914565000	-3.874765000	0.000000000		
		Ba	1.145854000	0.503410000	1.949948000		
		Ba	-1.815087000	2.613516000	0.000000000		
		H	-0.325736000	2.672399000	2.041954000		
		H	2.638150000	1.278209000	0.000000000		
		H	-0.328453000	0.775333000	0.000000000		
		H	-3.216284000	0.612188000	0.000000000		
		H	-0.325736000	2.672399000	-2.041954000		
Ba_4-4 C_s		Ba	-0.183937000	-0.668999000	-1.629516000	-107.0926	6.7
		Ba	-0.011636000	0.754061000	1.731470000		
		Ba	-3.522340000	0.511723000	0.029849000		
		Ba	3.407367000	-0.451810000	0.091008000		
		H	2.473835000	0.638767000	2.328037000		
		H	-2.857983000	-0.522128000	-2.195086000		
		H	0.067460000	-3.263494000	-0.153635000		
		H	1.300856000	1.079728000	-0.455325000		
		H	-0.263312000	-3.751847000	-0.626989000		
		H	-1.699848000	-0.953023000	0.556100000		
		H	0.942890000	-1.358328000	0.588594000		
		H	-2.628201000	1.344969000	2.262108000		
		H	-1.374859000	1.448140000	-0.469994000		
		H	5.894434000	-0.773849000	0.098435000		
		H	2.249082000	-1.256383000	-2.155055000		
Ba_4-5 C_s		Ba	2.751983000	1.025639000	0.000000000	-107.0917	7.3
		H	0.892111000	0.149489000	1.558368000		
		H	5.179987000	0.943459000	0.000000000		
		H	-2.150930000	0.937440000	-2.219768000		
		H	0.892111000	0.149489000	-1.558368000		
		Ba	-1.011865000	-1.284968000	-2.551439000		
		H	-1.153026000	-2.958875000	4.301845000		
		Ba	-1.011865000	1.523950000	0.000000000		
		H	1.124210000	2.944865000	0.000000000		
		Ba	-1.011865000	-1.284968000	2.551439000		
		H	-2.150930000	0.937440000	2.219768000		
		H	8.285205000	1.155912000	0.000000000		
		H	7.532953000	1.103144000	0.000000000		
		H	-1.416441000	-1.264109000	0.000000000		
		H	-1.153026000	-2.958875000	-4.301845000		

Figure SI-20. Lowest energy isomers for $Ba_4H_{11}^-$ and the relative energies in kcal.mol^{-1} at the CCSD(T)/def2-TZVP//PBE0//def2-TZVP level of theory.

Second part, systems with a counterion: Cartesians coordinates and relative energies

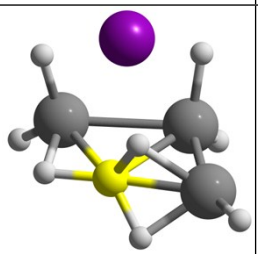
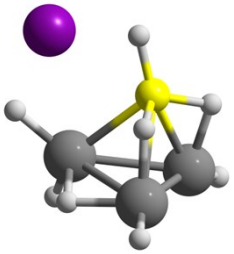
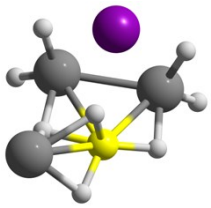
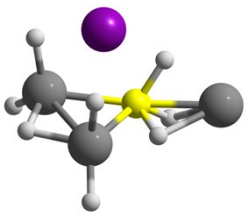
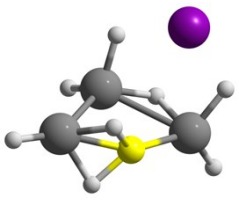
$NaBeAl_3H_8$	Structure	Cartesian Coordinates	Energy (a.u)	ΔE
NaBe-1 C_1		Al -0.310028000 -0.434698000 1.321280000 Al 1.864225000 -0.782967000 -0.369329000 H 2.859851000 -2.012480000 -0.341341000 H 0.059553000 1.115820000 1.777640000 H 0.987109000 -0.836830000 -1.924949000 H -1.480502000 -1.261635000 -1.523622000 H -3.575406000 0.361405000 -1.042419000 H 2.530012000 0.708116000 -0.566831000 Na 0.835591000 1.994728000 -0.005610000 H -0.294235000 -1.514089000 2.489376000 Al -2.205038000 -0.093966000 -0.383399000 H -0.825456000 0.800549000 -1.307504000 Be -0.247874000 -0.562917000 -1.222454000	CC -907.355722 G4 -908.551417	CC 0.0 G4 0.0
NaBe-2 C_1		Al -0.420916000 0.069104000 1.281204000 Be -0.330514000 -0.498147000 -1.217293000 H 0.131030000 -0.397500000 2.703023000 H -1.579438000 -0.726615000 -1.833358000 H 0.705764000 -1.469785000 -1.589764000 H -2.032494000 0.461134000 1.345772000 H 0.068296000 0.917665000 -1.491864000 Na -2.964175000 -0.072117000 -0.469379000 Al 1.566300000 -1.187248000 -0.121059000 Al 1.340140000 1.285710000 -0.368802000 H 0.266367000 1.636406000 0.982786000 H 2.190134000 -2.545554000 0.396370000 H 1.866527000 2.731761000 -0.768080000	CC -907.354717 G4 -908.547378	CC 0.6 G4 2.5
NaBe-3 C_1		Al 1.913267000 -0.372910000 0.781161000 Al -2.672992000 -0.044469000 0.360072000 Al 0.331180000 -0.886404000 -1.266410000 Be -0.516258000 -0.455839000 1.109993000 H 0.255302000 -2.183695000 -2.176903000 H 3.109124000 -1.243878000 1.353023000 H -1.009950000 0.877109000 0.734951000 H -1.756545000 -0.868340000 1.737758000 H 0.651292000 -0.511794000 1.989094000 H -0.054662000 0.532321000 -2.009272000 H 2.121392000 1.263708000 0.829602000 H -1.128287000 -1.057116000 -0.256525000 Na 0.495314000 1.996748000 -0.455854000	CC -907.345685 G4 -908.541472	CC 6.3 G4 6.2
NaBe-4 C_1		Al 0.654105000 -1.127054000 -1.021236000 H 0.710158000 0.158061000 -2.025326000 H 2.309130000 -0.967850000 -0.336553000 H -1.322723000 1.051676000 0.344943000 H 0.578297000 -2.608491000 -1.560263000 Na 0.479038000 1.937613000 -0.720549000 H 2.438423000 -0.716907000 2.371580000 Al -2.918406000 -0.077760000 0.306850000 Al 1.764302000 -0.117647000 1.071087000 Be -0.683610000 -0.218329000 0.700061000 H 2.161410000 1.410264000 0.619693000 H -1.701461000 -0.697126000 1.580554000 H -1.208227000 -0.878056000 -0.505951000	CC -907.343788 G4 -908.539587	CC 7.5 G4 7.4
NaBe-5 C_1		Al -0.213413000 -0.892412000 0.763301000 H -0.380736000 -1.524437000 2.221556000 Al -2.580272000 -0.146296000 -0.316651000 Be -1.000880000 1.214430000 -0.492924000 H -4.080511000 -0.570797000 -0.589084000 H -2.269636000 1.488299000 0.238491000 H -1.669925000 0.566501000 -1.649501000 H 0.552821000 -1.920622000 -0.287873000 Al 1.200759000 1.484573000 0.173884000 H 1.326918000 -0.022030000 1.105855000 H 2.341905000 0.977382000 -0.916775000 H 1.792387000 2.548663000 1.201548000 Na 2.463486000 -1.108811000 -0.674496000	CC -907.343446 G4 -908.535789	CC 7.7 G4 9.8

Figure SI-21. The most stable structures for $NaBeAl_3H_8$ calculated at CCSD(T)/def2-TZVP//PBE0/def2-TZVP level of theory. The relative energy values are expressed in kcal.mol^{-1}.

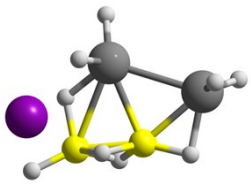
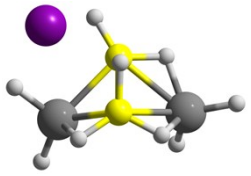
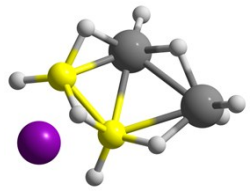
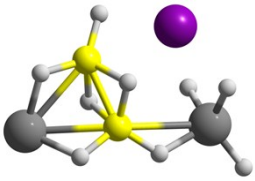
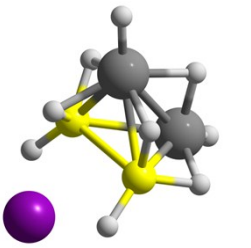
$NaBe_2Al_2H_9$	Structure	Cartesian Coordinates			Energy (a.u)	ΔE
NaBe2-1 C_1		Al	2.368407000	0.069467000	-0.355398000	CC -680.648523 G4 -681.593178	CC 0.0 G4 0.0
		Be	-1.272748000	1.334393000	0.833308000		
		H	-2.602111000	1.725952000	0.743912000		
		H	-1.304086000	-0.086238000	1.257040000		
		H	-1.016144000	-1.490837000	-0.760291000		
		H	2.568375000	-0.423546000	-1.856641000		
		Na	-2.706649000	-0.100749000	-0.686941000		
		Be	0.554423000	1.342323000	0.137372000		
		H	3.568087000	0.093910000	0.684999000		
		H	-0.030569000	1.947950000	1.345948000		
		H	-0.720590000	1.287644000	-0.576885000		
		H	1.771974000	1.761822000	-0.474844000		
		H	0.192445000	-2.166027000	1.563218000		
		Al	-0.043865000	-1.011717000	0.489796000		
NaBe2-2 C_1		H	0.921561000	-1.500961000	-1.360737000	CC -680.647215 G4 -681.591941	CC 0.8 G4 0.8
		Na	2.476451000	-1.142727000	0.047234000		
		H	-1.386195000	-1.374113000	-0.877108000		
		H	2.454102000	0.993094000	-0.103792000		
		Al	-2.460880000	-0.271768000	-0.093537000		
		H	-3.566217000	-1.276368000	0.451862000		
		H	0.491335000	1.175330000	1.614863000		
		Al	0.857698000	1.418284000	-0.166228000		
		Be	-0.335784000	0.096381000	1.160208000		
		H	0.626991000	2.922855000	-0.607868000		
		H	-1.723280000	0.164825000	1.441691000		
		H	-2.860046000	0.988218000	-0.969462000		
		Be	-0.057806000	-0.895034000	-0.577494000		
		H	0.216507000	-1.232984000	0.937069000		
NaBe2-3 C_1		Al	0.292026000	1.291254000	-0.270209000	CC -680.645213 G4 -681.588675	CC 2.1 G4 2.8
		H	0.378268000	2.447141000	-1.348536000		
		Be	-1.230305000	0.683043000	1.256732000		
		H	3.521807000	-0.964845000	0.791492000		
		H	-0.345810000	1.873655000	1.263404000		
		H	-1.186656000	-1.982355000	-0.100117000		
		Al	2.226658000	-0.659557000	-0.067787000		
		Be	-0.312509000	-1.020173000	0.426804000		
		H	-2.598298000	0.860607000	1.066994000		
		H	2.154547000	-0.728049000	-1.657624000		
		H	-0.717331000	-0.549427000	1.799644000		
		H	1.892934000	1.010868000	0.296037000		
		H	1.008281000	-1.603587000	0.633579000		
		Na	-2.789034000	-0.657050000	-0.462279000		
NaBe2-4 C_1		Be	-0.579657000	-0.673545000	0.505447000	CC -680.644044 G4 -681.587654	CC 2.8 G4 3.5
		H	-1.814137000	-1.256932000	0.904246000		
		H	-1.065260000	0.053837000	-0.734434000		
		H	0.471261000	-1.634250000	0.350631000		
		Al	-3.044315000	-0.378713000	-0.201391000		
		H	-0.180900000	0.555090000	1.172711000		
		Al	2.067543000	-1.145214000	-0.068387000		
		H	1.842409000	-0.155390000	-1.344534000		
		H	2.826013000	-2.518089000	-0.274289000		
		Na	1.593671000	1.712131000	-0.079894000		
		H	-0.429465000	2.427697000	-0.247615000		
		H	2.545418000	-0.119432000	1.103578000		
		Be	-1.064689000	1.280655000	0.215723000		
		H	-2.450308000	1.196644000	0.570968000		
NaBe2-5 C_1		Al	1.180473000	-1.283625000	-0.139254000	CC -680.641778 G4 -681.588210	CC 4.2 G4 3.1
		Al	1.039022000	1.277482000	0.071430000		
		Be	-0.462959000	0.302120000	-1.142307000		
		Be	-0.265131000	-0.332536000	1.281404000		
		H	-1.578437000	-0.442082000	1.732002000		
		H	-1.582686000	-0.108988000	-1.850195000		
		H	0.783916000	0.821806000	-1.696406000		
		H	-0.727658000	1.495737000	-0.324037000		
		H	1.826890000	2.635862000	0.189926000		
		H	0.553675000	0.795433000	1.711157000		
		H	1.711044000	-2.527573000	-0.948718000		
		H	0.683790000	-1.504256000	1.491275000		
		H	2.332398000	-0.060088000	0.134515000		
		Na	-2.722182000	-0.082212000	-0.010381000		

Figure SI-22. The most stable structures for $NaBe_2Al_2H_9$ calculated at CCSD(T)/def2-TZVP //PBE0/def2-TZVP level of theory. The relative energy values are expressed in kcal.mol^{-1}

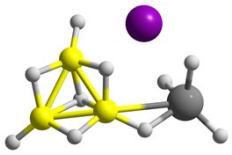
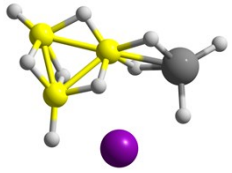
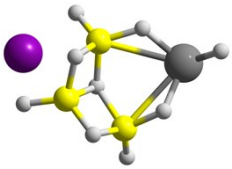
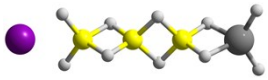
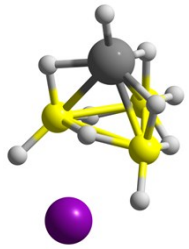
$NaBe_3AlH_{10}$	Structure	Cartesian Coordiantes			Energy (a.u)	ΔE
NaBe3-1 C_1		H	0.881404000	0.295212000	-1.122307000	CC -453.949578 G4 -454.643246	CC 0.0 G4 0.0
		H	2.172970000	-1.712553000	-0.688264000		
		H	3.175181000	0.534307000	-0.387439000		
		Be	1.814792000	0.906577000	-0.134962000		
		Be	1.000715000	-0.958177000	-0.400908000		
		H	-1.919395000	0.130306000	-1.148158000		
		H	-0.196464000	-1.723018000	-0.291326000		
		Al	-1.694533000	-0.940679000	0.058463000		
		H	-2.695447000	-2.149053000	0.246590000		
		Na	-0.745280000	1.802699000	0.046433000		
		Be	2.997220000	-0.824827000	0.212213000		
		H	1.563645000	-0.279750000	0.843977000		
		H	3.955667000	-1.367270000	0.990730000		
		H	-1.329218000	0.017791000	1.324560000		
		H	1.367751000	2.158877000	0.255478000		
NaBe3-2 C_1		H	0.701322000	0.243856000	0.936963000	CC -453.943874 G4 -454.638425	CC 3.6 G4 3.0
		Be	2.001034000	0.539871000	0.268856000		
		H	2.008227000	1.927202000	0.089125000		
		H	-2.056909000	0.870891000	0.267929000		
		Na	-0.142132000	2.009500000	-0.122068000		
		H	2.987979000	-0.342843000	0.825431000		
		H	-3.073218000	-1.606592000	-0.477653000		
		H	1.776521000	-0.253331000	-0.952765000		
		Al	-1.860647000	-0.723591000	0.002718000		
		Be	0.434835000	-0.978492000	0.202552000		
		Be	2.556287000	-1.366444000	-0.209185000		
		H	-0.497039000	-0.717343000	-1.001981000		
		H	3.449623000	-2.158566000	-0.847071000		
		H	1.311251000	-2.092056000	0.269955000		
		H	-0.824512000	-1.348764000	1.148580000		
NaBe3-3 C_1		H	0.414143000	0.389080000	-0.387904000	CC -453.943663 G4 -454.635519	CC 3.7 G4 4.8
		Be	0.276466000	-0.764635000	0.629413000		
		H	-1.074652000	-1.187806000	0.830748000		
		H	1.180417000	-1.746475000	0.209321000		
		Na	2.814219000	-0.529909000	-0.362950000		
		Be	1.060275000	1.167512000	0.808828000		
		H	0.725067000	0.084207000	1.735135000		
		H	0.118870000	2.242661000	0.738370000		
		H	-0.507369000	2.224519000	-1.668916000		
		H	2.420895000	1.335394000	0.551263000		
		H	-3.585169000	-0.612356000	0.783456000		
		H	-1.861857000	1.195473000	0.089271000		
		Al	-2.283883000	-0.419071000	-0.099417000		
		Be	-0.579355000	1.662175000	-0.437662000		
		H	-2.125814000	-0.907970000	-1.598195000		
NaBe3-4 C_1		Be	1.619022000	-0.000153000	0.000923000	CC -453.940509 G4 -454.635108	CC 5.7 G4 5.1
		H	4.621695000	-1.402295000	-0.001889000		
		H	-1.293765000	0.002803000	-1.085274000		
		H	0.671949000	-1.090502000	0.002088000		
		H	-3.114784000	1.203081000	0.003649000		
		H	2.577116000	-0.000400000	1.126156000		
		Na	-4.835454000	-0.001436000	-0.002970000		
		Be	-0.352563000	0.001577000	0.003559000		
		Be	-2.339226000	0.002438000	0.004361000		
		H	-3.111438000	-1.200560000	0.003779000		
		H	4.621252000	1.401469000	-0.002697000		
		H	-1.292991000	0.002649000	1.093017000		
		H	2.574689000	-0.000848000	-1.126245000		
		H	0.673824000	1.091829000	0.002817000		
		Al	3.888732000	-0.000529000	-0.001393000		
NaBe3-5 C_1		Be	-0.195401000	0.019683000	-1.332773000	CC -453.934644 G4 -454.628195	CC 9.4 G4 9.4
		Be	0.699725000	1.798036000	-0.000005000		
		H	-0.045973000	1.434525000	-1.226435000		
		H	-1.411289000	-0.402357000	-1.873658000		
		H	2.033169000	1.059831000	-0.000010000		
		H	-0.045960000	1.434532000	1.226430000		
		H	0.982852000	3.126928000	-0.000021000		
		Be	-0.195398000	0.019695000	1.332788000		
		H	1.053707000	-0.664401000	-1.646400000		
		H	-1.411278000	-0.402351000	1.873678000		
		Na	-2.538860000	-0.247300000	-0.000002000		
		Al	1.684251000	-0.562533000	0.000000000		
		H	1.053728000	-0.664384000	1.646394000		
		H	2.865406000	-1.605088000	-0.000012000		
		H	-0.277863000	-0.633659000	0.000012000		

Figure SI-23. The most stable structures for $NaBe_3AlH_{10}$ calculated at CCSD(T)/def2-TZVP//PBE0/def2-TZVP level of theory. The relative energy values are expressed in $kcal.mol^{-1}$

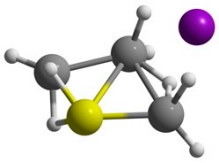
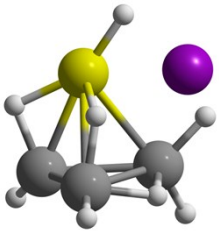
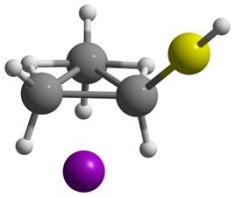
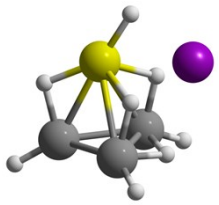
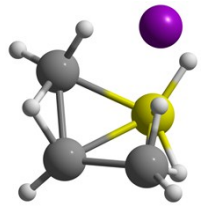
$NaMgAl_3H_8$	Structure	Cartesian Coordinates	Energy (a.u)	ΔE
NaMg-1 C_1		Na 2.734008000 -0.969469000 -0.749008000 H 0.251048000 -2.302608000 1.854884000 H 0.902445000 -1.973542000 -0.703723000 H 2.021845000 2.178479000 1.668761000 H 2.454756000 1.127049000 -0.755500000 Al 1.334151000 1.465834000 0.416580000 H 1.279733000 -0.201773000 0.986196000 Al 0.007616000 -1.380560000 0.566186000 Al -2.419189000 -0.636653000 -0.150789000 Mg -1.212433000 1.610960000 -0.375899000 H -2.605517000 0.823885000 0.720364000 H -2.057391000 0.318619000 -1.532881000 H -3.765319000 -1.469537000 -0.303933000	CC -1092.314850 G4 -1093.734529	CC 0.0 G4 0.7
NaMg-2 C_1		H -1.682752000 -0.528692000 1.581468000 H 1.413317000 1.990914000 -0.547045000 Al -0.044601000 -0.766417000 1.427658000 H -0.232820000 -1.882993000 0.070369000 Mg -0.378361000 1.621474000 -0.173840000 H -2.093094000 2.059862000 -0.242581000 Al 2.015396000 0.516428000 0.102980000 H 3.334822000 0.791921000 0.934850000 H 0.550883000 -1.653630000 2.605668000 Na -2.750520000 -0.057077000 -0.198589000 Al 0.619928000 -1.094780000 -1.247026000 H -0.650781000 0.056084000 -1.413164000 H 0.477086000 -2.181295000 -2.405970000	CC -1092.312924 G4 -1093.735648	CC 1.2 G4 0.0
NaMg-3 C_1		H 0.316551000 0.562749000 -1.636182000 Na -1.997610000 -1.709375000 -0.330845000 Al -0.940405000 0.420695000 1.555243000 H -0.474687000 1.124630000 2.898362000 H -2.081651000 -0.756825000 1.672679000 Al 0.810948000 -0.427163000 -0.313730000 H -1.858458000 1.581218000 0.663762000 H -1.153386000 2.707584000 -1.578511000 H -2.316547000 0.164775000 -1.451112000 Al -1.202986000 1.249604000 -0.964489000 H 0.138267000 -1.838919000 -0.850087000 Mg 3.464552000 -0.086760000 0.006499000 H 5.150753000 0.138266000 0.241082000	CC -1092.310198 G4 -1093.730103	CC 2.9 G4 3.5
NaMg-4 C_1		Mg 0.820620000 1.536401000 -0.000169000 H -0.633169000 2.084161000 1.170779000 H -0.633591000 2.083085000 -1.171823000 H -0.650485000 -2.029678000 1.266426000 Al 0.241423000 -1.495696000 -0.001283000 H 4.110005000 -0.776461000 0.001251000 H -0.650303000 -2.027482000 -1.269758000 H 2.161817000 0.773504000 -1.184522000 Na -2.577238000 -1.359907000 0.001154000 Al 2.573293000 -0.389162000 0.000750000 H -0.576068000 0.087657000 0.000259000 H 2.160671000 0.773016000 1.185793000 Al -1.798308000 1.542886000 -0.000165000	CC -1092.308542 G4 -1093.731000	CC 4.0 G4 2.9
NaMg-5 C_1		H 3.597645000 0.730630000 -0.032744000 H 0.116099000 -1.733278000 2.725943000 H 0.111931000 -2.092009000 -2.460984000 H -0.279957000 -1.765746000 0.122009000 H -2.208309000 2.061566000 -0.142795000 H 1.248364000 2.041853000 -0.151589000 H -1.028620000 0.215685000 1.353348000 H -1.010996000 0.030465000 -1.367539000 Mg -0.517617000 1.533926000 -0.103788000 Al 2.033372000 0.495524000 -0.033377000 Al 0.364946000 -0.774226000 1.478621000 Al 0.376824000 -0.974290000 -1.356754000 Na -2.764692000 -0.146126000 0.004495000	CC -1092.308383 G4 -1093.735647	CC 4.1 G4 0.0
NaMg-6 C_1		Al -1.093476000 1.721297000 -0.086260000 H 0.234117000 1.969073000 -1.216972000 H -1.799115000 3.098329000 0.277116000 H -2.071060000 0.716649000 -0.954483000 Na -2.231409000 -1.402319000 -0.643358000 H 0.029013000 -1.570158000 -0.636121000 H 2.619976000 -2.380387000 -1.073074000 H 1.448877000 -1.580268000 1.276232000 Al 1.690079000 -1.276504000 -0.410758000 H -1.799363000 -1.490522000 1.491995000 Mg -0.225259000 -0.655853000 1.330329000 Al 1.431700000 1.250381000 -0.156790000 H 2.218234000 2.495761000 0.447803000	CC -1092.307834 G4 -1093.730291	CC 4.4 G4 3.4

Figure SI-24. The most stable structures for $NaMgAl_3H_8$ calculated at CCSD(T)/def2-TZVP//PBE0/def2-TZVP level of theory. The relative energy values are expressed in $kcal.mol^{-1}$.

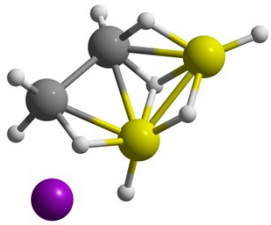
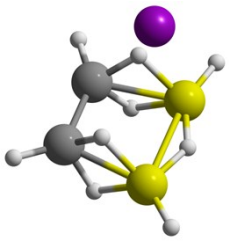
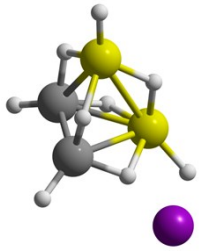
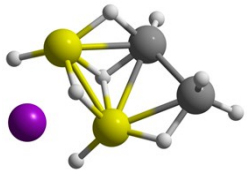
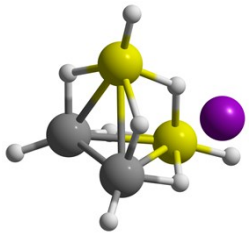
$NaMg_2Al_2H_9$	Structure	Cartesian Coordinates	Energy (a.u)	ΔE
NaMg2-1 C_1		Al 0.968892000 1.276159000 -0.677483000 H 2.256244000 1.168405000 0.400110000 H 1.333956000 2.184717000 -1.928957000 Al -1.313167000 1.262954000 0.660285000 H -2.618096000 1.086416000 -0.344776000 H -1.558268000 2.299102000 1.842652000 Mg -0.053566000 -1.272264000 0.213181000 Mg 2.866179000 -0.657867000 0.223772000 H -1.385109000 -0.322397000 1.312713000 H 1.487611000 -1.596832000 1.104459000 H 4.472286000 -1.177665000 -0.037827000 H 1.265864000 -0.378640000 -1.129003000 H -1.296417000 -2.181153000 -0.691029000 Na -3.021260000 -0.993532000 -0.504382000	CC -1050.574380 G4 -1051.977469	CC 0.0 G4 0.0
NaMg2-2 C_1		Na 3.401328000 0.005326000 -0.000255000 H 1.161952000 -0.029767000 -1.174830000 H 1.161188000 -0.029554000 1.175359000 H 2.207168000 -1.983207000 0.000581000 Al 0.757268000 -1.217149000 0.000265000 H -2.210532000 -0.299032000 1.202269000 Mg -2.514240000 1.238196000 0.000003000 H -2.751377000 -2.688968000 -0.000680000 H -3.862223000 2.296984000 -0.000069000 H -0.777708000 2.030510000 0.000012000 H -2.210307000 -0.298791000 -1.202391000 Al -1.804545000 -1.414033000 -0.000132000 Mg 0.918974000 1.519932000 0.000063000 H 2.625031000 2.051075000 0.000039000	CC -1050.570366 G4 -1051.974061	CC 2.5 G4 2.1
NaMg2-3 C_1		Al -1.364429000 -1.510535000 0.232590000 Mg 0.674980000 -0.377556000 -1.254390000 H 1.397633000 0.690237000 0.497547000 H -0.449274000 0.960118000 -1.681919000 H -0.828119000 1.752631000 1.080809000 H -2.541980000 -0.556366000 -0.461992000 H -0.477622000 -1.896593000 -1.167340000 Mg -1.927709000 1.336018000 -0.557777000 H 2.414155000 -0.625778000 -1.629829000 H -3.146477000 2.504664000 -0.866098000 H 0.558326000 0.365859000 2.980651000 H -1.917841000 -2.834345000 0.910942000 Al 0.036583000 0.386206000 1.473227000 Na 3.389631000 0.250392000 -0.008398000	CC -1050,569726 G4 -1051.972814	CC 2.9 G4 2.9
NaMg2-4 C_1		Na -3.094640000 -0.786500000 -0.607390000 Al 0.945020000 1.306230000 -0.670260000 H 0.907080000 2.273410000 -1.938750000 H -0.602410000 0.434850000 -0.796940000 H 0.184930000 2.228250000 0.593570000 Al 2.685210000 -0.549650000 0.106250000 Mg -0.074470000 -1.331780000 0.234690000 H 3.336410000 -0.287790000 1.542200000 H 1.649750000 -1.924250000 0.379800000 H -1.509550000 -2.157230000 -0.466920000 H 3.588290000 -1.034750000 -1.121240000 Mg -1.334580000 1.209720000 0.901260000 H -0.730980000 -0.332700000 1.680230000 H -3.066820000 1.080680000 0.509930000	CC -1050.567276 G4 -1051.970626	CC 4.5 G4 4.3
NaMg2-5 C_s		Al 1.548119000 0.482783000 0.000000000 Mg -0.823374000 -0.193255000 1.679641000 H -0.457311000 -2.028953000 1.277076000 H -1.529116000 0.361521000 0.000000000 H -0.457311000 -2.028953000 -1.277076000 H 0.656181000 1.226329000 -1.239670000 H 0.656181000 1.226329000 1.239670000 Mg -0.823374000 -0.193255000 -1.679641000 H -1.576744000 0.518706000 3.053670000 H -1.576744000 0.518706000 -3.053670000 H 1.540757000 -3.319195000 0.000000000 H 3.044966000 1.015074000 0.000000000 Al 0.645513000 -2.013067000 0.000000000 Na -0.823374000 2.458386000 0.000000000	CC -1050.566009 G4 -1051.971076	CC 5.3 G4 4.0

Figure SI-25. The most stable structures for $NaMg_2Al_2H_9$ calculated at CCSD(T)/def2-TZVP //PBE0/def2-TZVP level of theory. The relative energy values are expressed in kcal.mol^{-1}

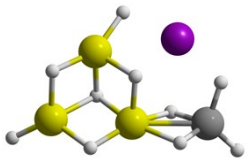
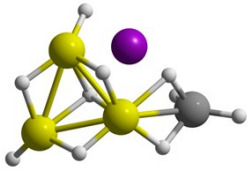
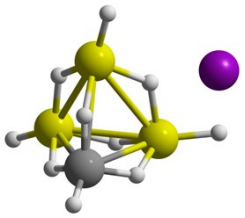
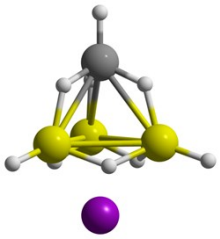
$NaMg_3AlH_9$	Structure	Cartesian Coordinates	Energy (a.u)	ΔE
NaMg3-1 C_1		Al -2.660340000 -1.084960000 0.113770000 Mg 0.051930000 -1.015760000 -0.257200000 H -1.643970000 -1.708310000 -1.052160000 H -3.143480000 0.395170000 -0.373130000 H 1.285440000 -0.090300000 1.034080000 H -0.069740000 0.677180000 -1.015830000 H -1.383770000 -0.711110000 1.134460000 H -3.734270000 -2.086110000 0.698940000 Na -1.617850000 1.953170000 0.015950000 Mg 1.338920000 1.538520000 -0.016910000 Mg 2.941450000 -0.874560000 0.109100000 H 0.314860000 2.898760000 0.512960000 H 2.888180000 0.887090000 -0.697390000 H 1.560590000 -1.864830000 -0.785710000 H 4.319320000 -1.556300000 0.869480000	CC -1008.823717 G4 -1010.209252	CC 0.0 G4 0.0
NaMg3-2 C_1		H -2.505150000 0.249660000 1.451210000 Na -0.932060000 1.817430000 0.841120000 Al -2.685580000 -0.614670000 0.083410000 Mg -0.076790000 -1.030140000 -0.816680000 H -1.773960000 0.290220000 -0.980020000 H -1.584440000 -1.876160000 0.084430000 H -4.129820000 -1.030620000 -0.408820000 Mg 1.542010000 1.290080000 -0.830150000 Mg 2.354670000 -1.049490000 0.787520000 H 0.688420000 2.765200000 -0.311460000 H 3.020000000 0.378850000 -0.305990000 H 1.344260000 -2.115620000 -0.420490000 H 2.998640000 -1.494300000 2.315520000 H 0.667130000 0.170890000 -2.029800000 H 0.601440000 0.135530000 0.580580000	CC -1008.819650 G4 -1010.205627	CC 2.6 G4 2.3
NaMg3-3 C_1		Al -1.302612000 0.966070000 1.487614000 Mg 0.692638000 -1.282716000 0.661696000 H -0.570739000 1.944560000 0.382879000 H 2.385207000 -1.706097000 1.121702000 H -2.384044000 0.054490000 0.668422000 H -1.861931000 1.739654000 2.749897000 H -0.109452000 -0.112080000 1.935801000 Mg 0.203384000 1.362230000 -1.332954000 Mg -2.091667000 -1.063338000 -0.968997000 H -3.510369000 -1.847287000 -1.538524000 H -1.155974000 0.277639000 -1.868220000 H 1.280599000 2.515791000 -2.055008000 H 1.295584000 0.055888000 -0.520670000 H -0.689065000 -2.070176000 -0.151383000 Na 3.327444000 -0.145946000 -0.034620000	CC -1008.810077 G4 -1010.194337	CC 8.6 G4 9.4
NaMg3-4 C_1		Al -2.331890000 -0.001260000 0.002640000 Mg 0.185380000 -0.380550000 1.945880000 H -1.668260000 1.424010000 -0.485030000 H 0.723210000 -0.692900000 3.546460000 H -1.666400000 -1.136410000 -0.986330000 H -3.909080000 -0.002280000 0.001250000 H -1.670120000 -0.290300000 1.482380000 Mg 0.183600000 1.877630000 -0.645650000 Mg 0.185260000 -1.495800000 -1.305390000 H 0.713470000 -2.726900000 -2.379310000 H 0.855410000 0.295060000 -1.506120000 H 0.709510000 3.423310000 -1.176760000 H 0.856840000 1.157350000 1.006470000 H 0.857910000 -1.451290000 0.496350000 Na 2.532830000 0.000130000 0.002570000	CC -1008.798140 G4 -1010.184603	CC 16.0 G4 15.5

Figure SI-26. The most stable structures for $NaMg_3AlH_9$ calculated at CCSD(T)/def2-TZVP //PBE0/def2-TZVP level of theory. The relative energy values are expressed in $kcal.mol^{-1}$

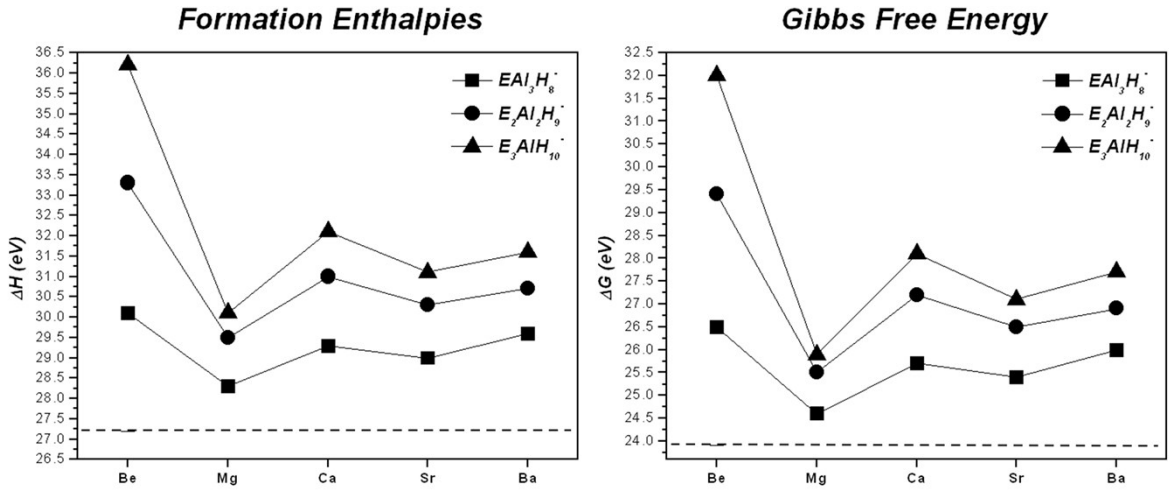


Figure SI-27. Change in the enthalpies (ΔH) and the Gibbs free energy (ΔG) calculated to PBE0/def2-TZVP level of theory. The formula used for these calculations were:

$$\Delta H = \left[nH(E^0) + (4-n-1)H(Al^0) + 1H(Al^-) + (7-n)H(H^0)\right] - \left[H(E_nAl_{4-n}H_{7+n})^-\right]$$

$$\Delta G = \left[nG(E^0) + (4-n-1)G(Al^0) + 1G(Al^-) + (7-n)G(H^0)\right] - \left[G(E_nAl_{4-n}H_{7+n})^-\right]$$