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

Supporting information for:

Global minimum and a heap of low-lying isomers with planar tetracoordinate carbon in $CAl_3MgH_2^-$ system

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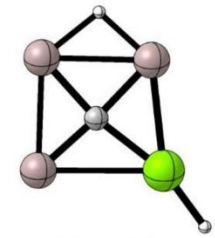
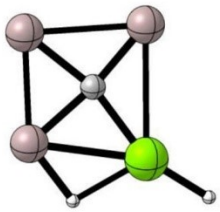
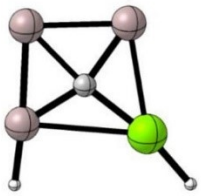


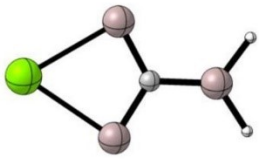
1*; C_s; 0.0
μ = 1.28; NImag = 0



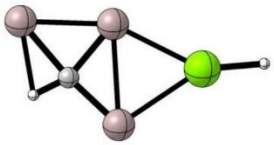
2*; C_s; 2.3
μ = 2.04; NImag = 0



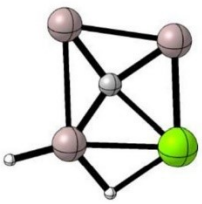
3*; C_s; 4.5
μ = 2.90; NImag = 0



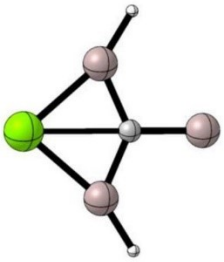
4; C_{2v}; 4.9
μ = 0.12; NImag = 0



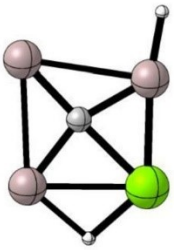
5*; C_s; 9.4
μ = 1.12; NImag = 0



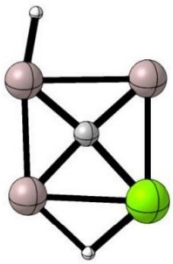
6*; C_s; 9.7
μ = 5.24; NImag = 0



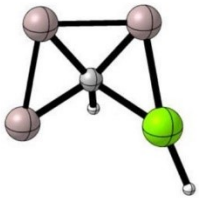
7*; C_{2v}; 12.2
μ = 2.13; NImag = 0



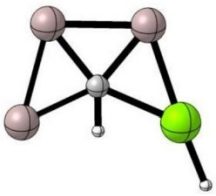
8*; C_s; 12.6
μ = 3.51; NImag = 0



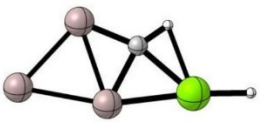
9*; C_s; 14.7
μ = 0.18; NImag = 0



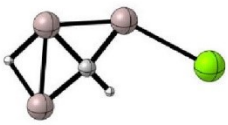
10; C_1; 16.9
μ = 1.27; NImag = 0



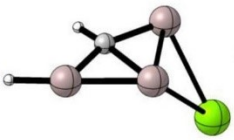
11*; C_s; 17.2
μ = 1.14; NImag = 1



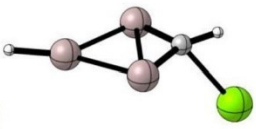
12*; C_s; 18.4
μ = 2.01; NImag = 0



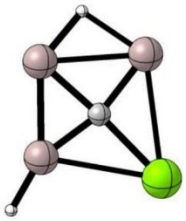
13*; C_s; 18.6
μ = 1.63; NImag = 0



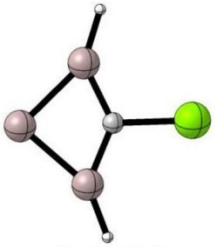
14; C_1; 20.6
μ = 4.05; NImag = 0



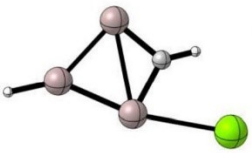
15; C_1; 21.6
μ = 6.97; NImag = 0



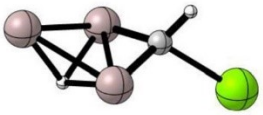
16*; C_s; 21.8
μ = 7.53; NImag = 0



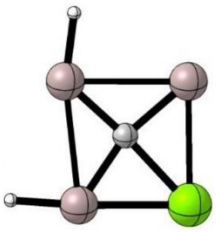
17; C_{2v}; 22.0
μ = 8.16; NImag = 0



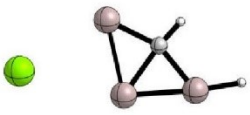
18*; C_s; 22.1
μ = 4.88; NImag = 1



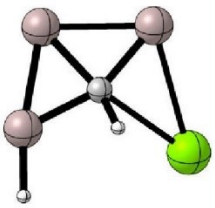
19; C_1; 22.4
μ = 6.78; NImag = 0



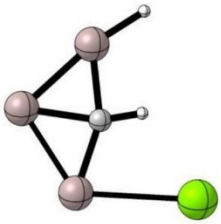
20*; C_s; 22.7
μ = 1.33; NImag = 0



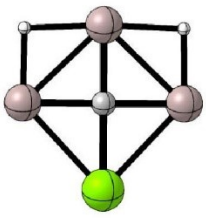
21*; C_s; 22.9
μ = 5.61; NImag = 1



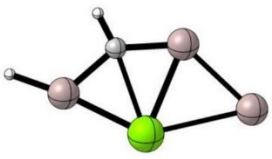
22; C_1; 23.3
μ = 3.09; NImag = 0



23*; C_s; 23.4
μ = 1.93; NImag = 1



24*; C_{2v}; 25.4
μ = 2.34; NImag = 1



25*; C_s; 30.9
μ = 1.36; NImag = 0

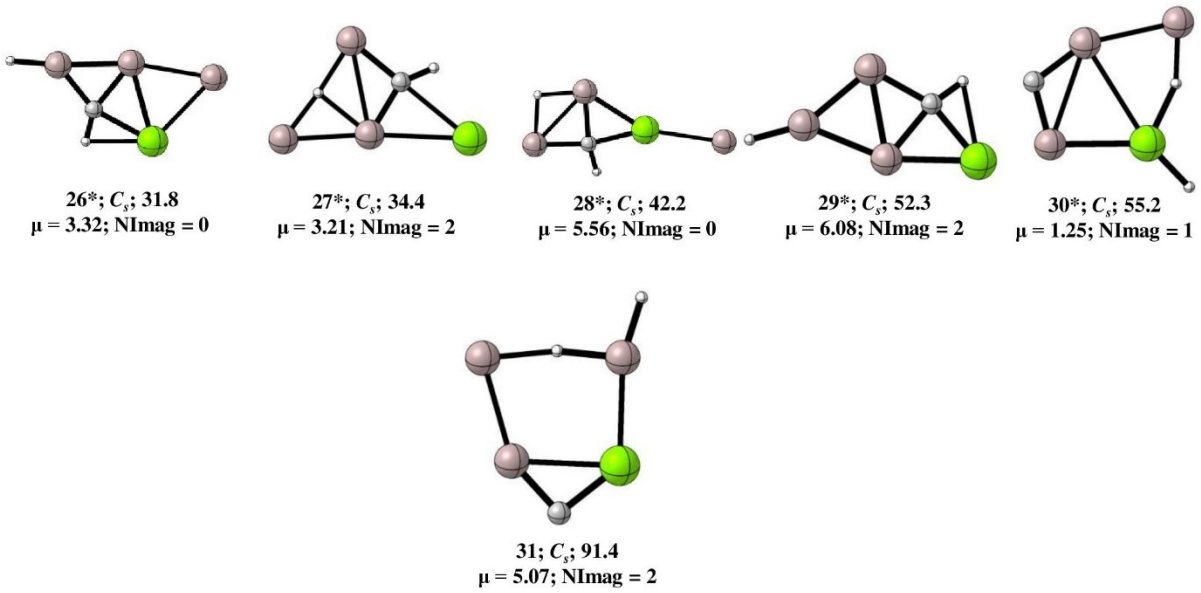


Figure S1. Isomers of $CAl_3MgH_2^-$ on the PES with their zero-point vibrational energy (ZPVE) corrected relative energies (in kcal mol^{-1}), dipole moments (in Debye), and the number of imaginary frequencies (NImag) calculated at MP2/aug-cc-pVTZ level. The ptCs, ppCs and ptAl are marked with asterisk.

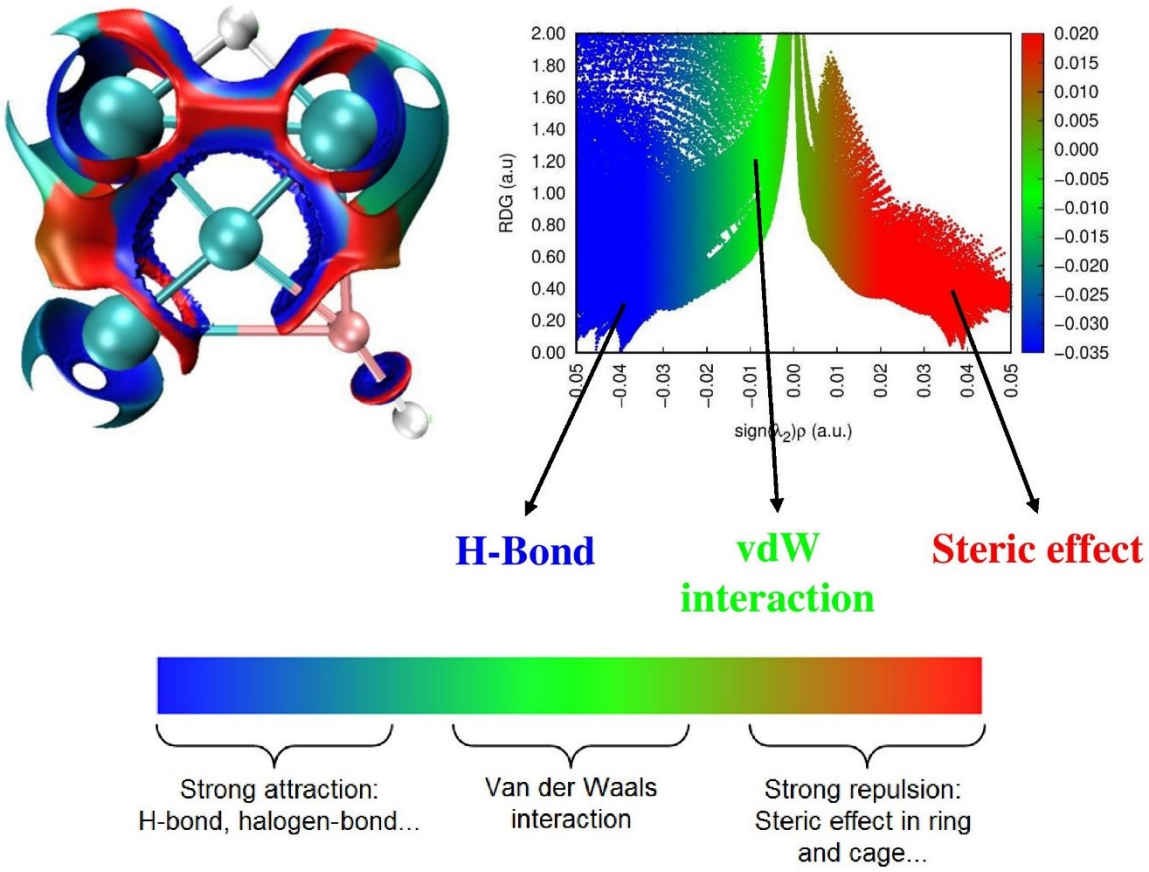


Figure S2. Noncovalent interaction (NCI) analysis of isomer **1** carried out at MP2/aug-cc-pVTZ level.

Table S1. Comparison of the relative energies (ΔE + ZPVE) of $CAl_3MgH_2^-$ isomers optimized at both the MP2/aug-cc-pVTZ, MP2/6-311++G(2d,2p) levels, and single point energy calculation at the CCSD(T)/aug-cc-pVTZ//MP2/aug-cc-pVTZ level.

ΔE+ZPVE (kcal mol^{-1})			
Isomers	**MP2/aug-cc-pVTZ**	**MP2/6-311++G(2d,2p)**	**CCSD(T)/aug-cc-pVTZ// MP2/aug-cc-pVTZ**
1	0	0	0
2	2.3	2.2	1.7
3	4.5	2.6	7.3
4	4.9	5.4	3.3
5	9.4	8.7	8.1
6	9.7	10.3	7.6
7	12.2	11.8	11.9
8	12.6	12.5	11.7
9	14.7	15.1	19.2
10	16.9	18.0	16.1
11	17.2	18.1	13.6
12	18.4	18.8	15.9
13	18.6	19.4	17.3
14	20.6	20.9	17.7
15	21.6	21.1	18.5
16	21.8	21.7	17.5
17	22.0	21.8	21.1
18	22.1	22.0	24.1
19	22.4	22.1	21.7
20	22.7	23.0	26.5
21	22.9	23.0	19.4
22	23.3	23.4	20.4
23	23.4	23.7	20.8
24	25.4	26.0	30.0

25	30.9	31.6	25.9
26	31.8	32.7	27.0
27	34.4	33.3	28.8
28	42.2	42.0	34.9
29	52.3	54.8	52.2
30	55.2	56.2	56.1
31	91.4	91.1	86.5

Table S2. Total energy (in a.u)**,** zero-point vibrational energy (ZPVE; in a.u), ZPVE corrected total energy (E+ZPVE; in a.u), relative energy (ΔE + ZPVE; in kcal mol^{-1}), dipole moment (in Debye) and the number of imaginary frequencies (NImag) of $CAl_3MgH_2^-$ isomers calculated at MP2/aug-cc-pVTZ level.

MP2/aug-cc-pVTZ						
Isomer	**Energy (a.u)**	**ZPVE (a.u)**	**E+ZPVE (a.u)**	**ΔE+ZPVE (kcal mol^{-1})**	**Dipole moment (Debye)**	**NImag**
1	-964.86246	0.018395	-964.84407	0	1.28	0
2	-964.85874	0.018301	-964.84044	2.3	2.04	0
3	-964.85484	0.018022	-964.83682	4.5	2.9	0
4	-964.85555	0.019246	-964.8363	4.9	0.12	0
5	-964.84993	0.02078	-964.82915	9.4	1.12	0
6	-964.84825	0.019649	-964.8286	9.7	5.24	0
7	-964.84381	0.019255	-964.82455	12.2	2.13	0
8	-964.84265	0.01865	-964.82399	12.6	3.51	0
9	-964.83925	0.018619	-964.82063	14.7	0.18	0
10	-964.83743	0.020278	-964.81715	16.9	1.27	0
11	-964.83703	0.020312	-964.81672	17.2	1.14	1
12	-964.83568	0.02097	-964.81471	18.4	2.01	0
13	-964.83621	0.021787	-964.81442	18.6	1.63	0
14	-964.83215	0.020916	-964.81123	20.6	4.05	0
15	-964.83188	0.022192	-964.80969	21.6	6.97	0
16	-964.828	0.018751	-964.80925	21.8	7.53	0
17	-964.82825	0.019306	-964.80894	22.0	8.16	0
18	-964.83103	0.02212	-964.80891	22.1	4.88	1
19	-964.8308	0.022437	-964.80836	22.4	6.78	0
20	-964.82682	0.018999	-964.80782	22.7	1.33	0
21	-964.82827	0.020709	-964.80756	22.9	5.61	1
22	-964.82788	0.021016	-964.80686	23.3	3.09	0
23	-964.82772	0.020986	-964.80673	23.4	1.93	1

24	-964.82265	0.01908	-964.80357	25.4	2.34	1
25	-964.81604	0.021312	-964.79473	30.9	1.36	0
26	-964.81488	0.021584	-964.7933	31.8	3.32	0
27	-964.81007	0.020816	-964.78925	34.4	3.21	2
28	-964.79868	0.02189	-964.77679	42.2	5.56	0
29	-964.78135	0.020601	-964.76075	52.3	6.08	2
30	-964.77278	0.016644	-964.75614	55.2	1.25	1
31	-964.71558	0.017187	-964.69839	91.4	5.07	1

Table S3. Total energy (in a.u)**,** zero-point vibrational energy (ZPVE; in a.u), ZPVE corrected total energy (E+ZPVE; in a.u), relative energy (ΔE + ZPVE; in kcal mol^{-1}), dipole moment (in Debye) and the number of imaginary frequencies (NImag) of $CAl_3MgH_2^-$ isomers calculated at MP2/6-311++G(2d,2p) level.

MP2/6-311++G(2d,2p)						
Isomer	**Energy (a.u)**	**ZPVE (a.u)**	**E+ZPVE (a.u)**	**ΔE+ZPVE (kcal mol^{-1})**	**Dipole moment (Debye)**	**NImag**
1	-964.79289	0.018504	-964.77438	0	1.27	0
2	-964.78922	0.018378	-964.77085	2.2	1.99	0
3	-964.78379	0.017941	-964.76585	2.6	2.91	0
4	-964.78951	0.019255	-964.77025	5.4	0.12	0
5	-964.77871	0.020739	-964.75797	8.7	1.06	0
6	-964.78025	0.019702	-964.76055	10.3	5.16	0
7	-964.7748	0.019269	-964.75553	11.8	2.11	0
8	-964.77313	0.018739	-964.75439	12.5	3.53	0
9	-964.769	0.018702	-964.7503	15.1	0.32	0
10	-964.76442	0.021009	-964.74341	18.0	1.93	0
11	-964.76721	0.021561	-964.74564	18.1	1.64	0
12	-964.76577	0.020271	-964.7455	18.8	1.3	0
13	-964.76464	0.020193	-964.74445	19.4	1.11	1
14	-964.76179	0.020769	-964.74102	20.9	3.91	0
15	-964.76304	0.022239	-964.7408	21.1	6.85	0
16	-964.76176	0.022445	-964.73931	21.7	6.63	0
17	-964.76204	0.022179	-964.73986	21.8	4.65	1
18	-964.75854	0.019347	-964.7392	22.0	8.16	0
19	-964.75847	0.018823	-964.73965	22.1	7.56	0
20	-964.75676	0.018984	-964.73777	23.0	1.48	0
21	-964.75829	0.02052	-964.73777	23.0	5.36	1

22	-964.75796	0.020929	-964.73703	23.4	3.16	0
23	-964.75753	0.020857	-964.73667	23.7	1.77	1
24	-964.75204	0.019094	-964.73295	26.0	2.56	1
25	-964.74517	0.021191	-964.72398	31.6	1.23	0
26	-964.74385	0.021587	-964.72226	32.7	3.17	0
27	-964.74208	0.020836	-964.72124	33.3	3.04	2
28	-964.7291	0.021671	-964.70743	42.0	5.72	0
29	-964.70537	0.020663	-964.68471	54.8	5.95	2
30	-964.70349	0.016538	-964.68695	56.2	1.45	1
31	-964.64614	0.017014	-964.62912	91.1	5.16	2

Table S4. Cartesian coordinates (in Angström units) for optimized geometries of $CAl_3MgH_2^-$ isomers obtained at MP2/aug-cc-pVTZ level.

1				**2**			
Mg	2.129145	0.128233	0.000000	Mg	2.094570	-0.211349	0.000000
C	0.005034	0.120095	0.000000	C	0.008906	0.175146	0.000000
Al	-0.355035	2.028787	0.000000	Al	-0.111045	2.097210	0.000000
Al	0.202900	-1.864824	0.000000	H	1.479606	-2.136949	0.000000
Al	-1.986210	-0.230500	0.000000	Al	-2.049047	0.009880	0.000000
H	3.798379	0.607614	0.000000	H	3.805280	0.115327	0.000000
H	-1.571118	-2.003257	0.000000	Al	-0.195300	-1.819891	0.000000
3				**4**			
Mg	-0.655715	2.139788	0.000000	Mg	0.000000	0.000000	-2.887996
C	0.009701	0.175541	0.000000	C	0.000000	0.000000	0.624260
Al	-1.859751	-0.507539	0.000000	Al	0.000000	1.650622	-0.332614
Al	1.911697	0.050988	0.000000	H	0.000000	-1.325201	3.432292
Al	0.347610	-1.953296	0.000000	Al	0.000000	0.000000	2.515104
H	3.052318	1.183520	0.000000	H	0.000000	1.325201	3.432292
H	-0.820395	3.872118	0.000000	Al	0.000000	-1.650622	-0.332614
5				**6**			
Mg	2.646948	0.087721	0.000000	Mg	0.132726	-2.102566	0.000000
Al	0.002049	1.074479	0.000000	C	0.007335	0.231621	0.000000
Al	-2.594238	0.903470	0.000000	Al	-1.947054	-0.315669	0.000000
Al	0.476235	-1.724852	0.000000	H	3.182460	0.997405	0.000000
C	-1.093694	-0.555036	0.000000	Al	-0.491112	2.123460	0.000000
H	4.366298	0.426337	0.000000	Al	1.869276	0.094778	0.000000
H	-2.008342	-1.177366	0.000000	H	2.173795	-1.563601	0.000000
7				**8**			
C	0.000000	0.000000	0.480939	Al	-0.170627	2.161479	0.000000
Al	0.000000	0.000000	2.394721	C	0.001598	0.226166	0.000000
Al	0.000000	1.755998	-0.291357	Al	1.988113	0.084489	0.000000
Mg	0.000000	0.000000	-2.283863	Al	-1.836623	-0.374190	0.000000
Al	0.000000	-1.755998	-0.291357	Mg	0.112065	-2.029724	0.000000
H	0.000000	-3.130802	0.546559	H	1.943589	-1.839815	0.000000
H	0.000000	3.130802	0.546559	H	-3.189942	0.499890	0.000000
9				**10**			
Al	-1.851155	0.651717	0.000000	Mg	-2.015398	-0.939151	-0.171243
C	0.001214	0.082830	0.000000	C	0.029176	-0.154389	0.349298
Al	0.805975	1.868328	0.000000	Al	1.649467	-1.470744	0.076227
Al	-0.688607	-1.807399	0.000000	Al	-1.056501	1.566453	0.097664
Mg	1.956869	-0.789056	0.000000	Al	1.522151	1.157634	-0.198040
H	-2.237358	2.240833	0.000000	H	-0.157850	-1.022255	1.043020
H	1.177738	-2.484545	0.000000	H	-2.925734	-2.405249	-0.372095

11				**12**			
Mg	2.297491	0.659888	0.000000	Mg	2.630202	0.814962	0.000000
C	-0.000933	0.263549	0.000000	Al	-0.002647	0.951641	0.000000
Al	-1.706709	1.582135	0.000000	Al	-2.678506	0.282498	0.000000
Al	0.903679	-1.568575	0.000000	C	1.034202	-0.756526	0.000000
Al	-1.608403	-1.016188	0.000000	Al	-0.711568	-1.594713	0.000000
H	0.271673	1.365939	0.000000	H	4.371162	0.907674	0.000000
H	3.319518	2.069018	0.000000	H	1.974826	-1.335431	0.000000
13				**14**			
H	-1.102346	-0.461951	0.000000	C	-0.908079	0.823272	-0.359262
C	-0.004699	-0.545425	0.000000	Al	0.894208	1.539082	0.180841
Al	0.000281	-2.570307	0.000000	Al	-2.348140	-0.502009	-0.314240
Al	0.433418	1.426057	0.000000	Al	-0.222560	-0.681756	0.912676
Al	1.951995	-0.663464	0.000000	H	-1.266565	1.567502	-1.088538
H	1.880502	-2.392809	0.000000	Mg	2.680889	-0.892895	-0.485550
Mg	-2.615993	2.404684	0.000000	H	-3.724355	-0.368016	-1.132011
15				**16**			
Mg	2.917192	-0.001092	-0.587352	Mg	0.717293	2.349769	0.000000
Al	-0.314570	-1.519048	0.308390	C	-0.004040	0.143716	0.000000
C	0.805094	0.007849	0.779139	Al	-1.944928	0.474055	0.000000
Al	-2.264508	-0.005469	-0.479577	Al	1.689497	-0.668780	0.000000
Al	-0.324825	1.524848	0.300977	Al	-0.488865	-1.850615	0.000000
H	1.652336	0.012803	1.474054	H	-2.155819	-1.529590	0.000000
H	-3.846934	-0.012338	-0.814339	H	3.272904	-0.727429	0.000000
17				**18**			
Mg	0.000000	0.000000	-2.735746	Mg	3.059302	1.372954	0.000000
C	0.000000	0.000000	-0.484188	Al	-0.006468	1.003632	0.000000
Al	0.000000	1.724196	0.302626	C	0.844404	-0.736053	0.000000
Al	0.000000	-1.724196	0.302626	Al	-2.378582	0.033538	0.000000
Al	0.000000	0.000000	2.156138	Al	-0.686999	-1.928876	0.000000
H	0.000000	3.233984	-0.202452	H	1.896193	-1.041875	0.000000
H	0.000000	-3.233984	-0.202452	H	-3.942766	0.432321	0.000000
19				**20**			
C	-0.797041	-0.000182	0.554762	Mg	1.206048	-1.789598	0.000000
Al	0.325735	-1.476073	-0.088190	C	-0.000204	0.104872	0.000000
Al	0.325677	1.475662	-0.088385	Al	1.696844	1.100854	0.000000
Mg	-3.039748	-0.000308	-0.151228	Al	-1.374531	-1.310938	0.000000
H	-1.206146	-0.000144	1.576523	Al	-1.154112	1.646552	0.000000
Al	2.519815	-0.000176	0.046933	H	-0.668360	3.199585	0.000000
H	1.134128	-0.000405	-1.127337	H	-2.945989	-0.910984	0.000000
21				**22**			

C	-1.350284	-0.595235	0.000000	C	0.053123	0.130576	0.413021
Al	0.371334	-1.597483	0.000000	Al	-0.835324	-1.669681	0.231715
Al	-2.464155	1.037128	0.000000	Al	1.536717	1.446195	0.124821
Al	-0.004835	0.987458	0.000000	Al	1.629000	-0.969454	-0.374933
H	-2.132489	-1.371936	0.000000	H	-0.499140	0.910063	0.971281
Mg	3.450171	-0.130112	0.000000	Mg	-2.665452	0.836275	-0.254616
H	-4.068438	0.937978	0.000000	H	1.231539	2.976576	0.523251
23				**24**			
C	0.014954	0.300050	0.000000	Mg	0.000000	0.000000	-2.166630
Al	-0.058725	-1.703242	0.000000	C	0.000000	0.000000	-0.058577
Al	-0.769035	2.135318	0.000000	Al	0.000000	1.969161	-0.052931
Al	-2.030249	0.015497	0.000000	Al	0.000000	-1.969161	-0.052931
H	1.021567	0.758645	0.000000	Al	0.000000	0.000000	1.858535
Mg	2.984845	-1.004432	0.000000	H	0.000000	1.947466	1.772212
H	0.255541	3.377201	0.000000	H	0.000000	-1.947466	1.772212
25				**26**			
Mg	-0.007752	1.274043	0.000000	Mg	0.751333	-1.747053	0.000000
C	-1.200358	-0.924915	0.000000	C	-1.232902	-0.716251	0.000000
Al	0.657884	-1.371093	0.000000	Al	0.002120	0.854655	0.000000
Al	-2.490057	0.562938	0.000000	H	-1.532851	-1.784353	0.000000
H	-1.859999	-1.815404	0.000000	Al	-2.449628	0.777726	0.000000
Al	2.842734	0.157354	0.000000	Al	2.767505	0.385351	0.000000
H	-4.074887	0.230844	0.000000	H	-4.053225	0.903822	0.000000
27				**28**			
C	-0.944990	-0.824163	0.000000	Mg	0.000951	1.073629	0.000000
Al	0.614528	-2.053955	0.000000	C	-0.597512	-0.999563	0.000000
Al	0.001429	0.789373	0.000000	H	-1.658398	-0.716867	0.000000
Mg	-3.025168	0.826878	0.000000	Al	1.343991	-1.211454	0.000000
H	-1.928736	-1.299580	0.000000	Al	-0.699107	-2.996101	0.000000
Al	2.639371	1.032951	0.000000	Al	-0.323849	3.986850	0.000000
H	1.617582	-0.448800	0.000000	H	1.168560	-2.948651	0.000000
29				**30**			
Mg	-2.605534	1.019967	0.000000	Mg	0.247443	-1.923027	0.000000
Al	0.003226	0.963837	0.000000	Al	-2.208870	-0.615497	0.000000
C	-1.282745	-0.599973	0.000000	C	-1.828711	1.199438	0.000000
Al	2.362017	0.028278	0.000000	Al	2.636816	0.750022	0.000000
Al	0.484682	-1.563450	0.000000	Al	-0.004601	1.424216	0.000000
H	-2.119711	-1.307734	0.000000	H	0.724748	-3.603119	0.000000
H	3.889658	0.473224	0.000000	H	1.782893	-0.796241	0.000000

31				
Mg	-1.983313	-0.294864	0.000000	
H	1.293842	-1.105670	0.000000	
Al	0.007233	1.657970	0.000000	
Al	0.017163	-2.252740	0.000000	
Al	2.475353	0.439853	0.000000	
C	-1.818789	1.689131	0.000000	
H	0.848995	-3.655286	0.000000	

Table S5. Cartesian coordinates (in Angström units) for optimized geometries of $CAl_3MgH_2^-$ isomers obtained at MP2/6-311++G(2d,2p) level.

1				**2**			
Mg	0.153270	-1.916000	0.000000	Mg	1.341600	1.550678	0.000000
C	0.255730	0.205310	0.000000	C	-0.261419	0.158449	0.000000
Al	2.177250	0.453930	0.000000	Al	-1.819199	1.285222	0.000000
Al	-1.736590	0.100920	0.000000	H	2.459757	-0.107302	0.000000
Al	-0.007500	2.212150	0.000000	Al	-1.413630	-1.547808	0.000000
H	0.549730	-3.605200	0.000000	H	2.136861	3.098361	0.000000
H	-1.792620	1.868060	0.000000	Al	1.186710	-1.238880	0.000000
3				**4**			
Mg	0.000000	0.000000	-2.941616	Mg	-1.286457	1.671886	0.000000
C	0.000000	0.000000	0.633439	C	0.012216	0.063225	0.000000
Al	0.000000	-1.647076	-0.311980	Al	-1.470042	-1.250614	0.000000
H	0.000000	1.321959	3.431867	Al	1.819219	0.671435	0.000000
Al	0.000000	0.000000	2.518660	Al	1.134073	-1.787245	0.000000
H	0.000000	-1.321959	3.431867	H	2.374177	2.179106	0.000000
Al	0.000000	1.647076	-0.311980	H	-2.091815	3.210757	0.000000
5				**6**			
Mg	1.031084	1.769158	0.000000	Mg	2.263842	-1.079385	0.000000
C	-0.187555	-0.286891	0.000000	Al	0.322451	0.977534	0.000000
Al	-1.649696	1.106235	0.000000	Al	-2.100472	1.946091	0.000000
H	2.257145	-2.422070	0.000000	Al	-0.492261	-1.761634	0.000000
Al	-1.463766	-1.760902	0.000000	C	-1.371021	-0.018262	0.000000
Al	1.535354	-1.003792	0.000000	H	3.955264	-1.536903	0.000000
H	2.570085	0.308062	0.000000	H	-2.469333	-0.141320	0.000000
7				**8**			
C	0.000000	0.000000	-0.476732	Al	1.608716	1.468830	0.000000
Al	0.000000	0.000000	-2.385569	C	0.175111	0.159763	0.000000
Al	0.000000	-1.752741	0.285825	Al	1.267472	-1.505811	0.000000
Mg	0.000000	0.000000	2.295454	Al	-1.421175	1.240455	0.000000
Al	0.000000	1.752741	0.285825	Mg	-1.552544	-1.315042	0.000000
H	0.000000	3.121509	-0.553696	H	-0.268615	-2.632811	0.000000
H	0.000000	-3.121509	-0.553696	H	-1.580625	2.839026	0.000000
9				**10**			
Al	0.209780	-2.109942	0.000000	H	-1.238350	0.013148	0.000000
C	0.008525	-0.182010	0.000000	C	-0.320181	-0.589045	0.000000
Al	1.912384	0.270661	0.000000	Al	-1.298478	-2.361885	0.000000
Al	-1.982364	-0.486689	0.000000	Al	0.998319	0.925477	0.000000
Mg	-0.477262	1.907259	0.000000	Al	1.334627	-1.651351	0.000000
H	1.695340	-2.786121	0.000000	H	0.415964	-3.113653	0.000000
H	-2.286574	1.452172	0.000000	Mg	-1.032572	3.465239	0.000000

11				**12**			
Mg	1.156677	-1.937256	-0.161867	Mg	2.159004	1.168698	0.000000
C	0.207748	0.041763	0.252377	C	0.017857	0.248124	0.000000
Al	1.441019	1.655126	-0.267680	Al	-1.927842	1.173688	0.000000
Al	-1.429892	-1.183924	0.207836	Al	1.314630	-1.323721	0.000000
Al	-1.213110	1.391579	-0.390788	Al	-1.264695	-1.352981	0.000000
H	1.078668	-0.011751	0.960893	H	0.035532	1.382176	0.000000
H	2.659630	-2.773607	-0.387500	H	2.812910	2.780388	0.000000
13				**14**			
Mg	0.338400	-2.725750	0.000000	C	-0.890355	1.073610	-0.114207
Al	0.938000	-0.159340	0.000000	Al	-1.586091	-0.744200	-0.586071
Al	0.742780	2.605160	0.000000	Al	0.495953	2.453829	-0.004748
C	-0.922580	-0.878280	0.000000	Al	0.813499	0.200711	-0.952994
Al	-1.458360	0.977540	0.000000	H	-1.730287	1.554955	0.406271
H	0.125260	-4.454100	0.000000	Mg	0.604397	-2.548100	0.800442
H	-1.641250	-1.713830	0.000000	H	0.228404	3.899685	0.636229
15				**16**			
Mg	2.929512	-0.001478	-0.601481	Mg	-3.406666	-0.162519	0.000000
Al	-0.310025	-1.520759	0.317216	Al	-0.369436	-0.912640	0.000000
C	0.798766	0.007907	0.788179	C	-0.491907	1.015765	0.000000
Al	-2.271372	-0.007089	-0.486167	Al	2.202954	-0.928537	0.000000
Al	-0.322123	1.525280	0.310126	Al	1.373348	1.538139	0.000000
H	1.650609	0.014009	1.473146	H	-1.352538	1.688033	0.000000
H	-3.851581	-0.010317	-0.819727	H	3.494721	-1.892901	0.000000
17				**18**			
Mg	-1.973376	1.530957	0.000000	C	-0.402372	0.835828	0.473203
C	-0.138397	0.095378	0.000000	Al	-1.529598	-0.480061	-0.435896
Al	-1.122272	-1.609715	0.000000	Al	1.298584	-0.119697	0.325892
Al	1.204671	1.400460	0.000000	Mg	-0.437869	3.025151	-0.431180
Al	1.565270	-1.057275	0.000000	H	-0.716154	1.330567	1.401053
H	0.666234	-2.495306	0.000000	Al	0.078402	-2.492220	0.260580
H	1.796019	2.867650	0.000000	H	0.237737	-1.172218	-0.959222
19				**20**			
Mg	0.000000	0.000000	2.727107	Mg	-1.972113	0.896525	0.000000
C	0.000000	0.000000	0.478031	C	0.105994	0.017793	0.000000
Al	-1.722321	0.000000	-0.300790	Al	0.803125	1.854737	0.000000
Al	1.722321	0.000000	-0.300790	Al	-1.063445	-1.570306	0.000000
Al	0.000000	0.000000	-2.169401	Al	1.811540	-0.875509	0.000000
H	-3.225125	0.000000	0.214645	H	3.257332	-0.137750	0.000000
H	3.225125	0.000000	0.214645	H	-0.393802	-3.043297	0.000000
21				**22**			

C	-0.858144	1.053710	0.000000	C	0.191666	0.098059	-0.263252
Al	-1.458218	-0.836843	0.000000	Al	-1.584966	-0.827699	-0.373554
Al	0.475620	2.513570	0.000000	Al	1.440382	1.582612	0.242700
Al	0.995223	0.104012	0.000000	Al	-1.029326	1.635898	0.437602
H	-1.772866	1.664527	0.000000	H	1.033602	-0.404668	-0.770302
Mg	0.702874	-3.540608	0.000000	Mg	0.989543	-2.521927	0.566456
H	-0.022779	4.039663	0.000000	H	3.004659	1.270504	0.036540
23				**24**			
C	-0.114202	0.509393	0.000000	Mg	0.000000	0.000000	-2.179972
Al	1.254310	-0.941363	0.000000	C	0.000000	0.000000	-0.070059
Al	-0.758076	2.401005	0.000000	Al	0.000000	-1.968039	-0.060902
Al	1.602276	1.664798	0.000000	Al	0.000000	1.968039	-0.060902
H	-1.175625	0.206466	0.000000	Al	0.000000	0.000000	1.845266
Mg	-1.528651	-2.447250	0.000000	H	0.000000	-1.938467	1.760424
H	-2.353791	2.600632	0.000000	H	0.000000	1.938467	1.760424
25				**26**			
Mg	-1.136160	-0.676341	0.000000	Mg	-1.372526	-1.660398	0.000000
C	0.174506	1.540585	0.000000	C	-1.311749	0.582306	0.000000
Al	1.484721	0.159391	0.000000	Al	0.639894	0.165954	0.000000
Al	-1.762843	1.842075	0.000000	H	-2.392877	0.339951	0.000000
H	0.601091	2.560291	0.000000	Al	-0.521877	2.331601	0.000000
Al	1.333223	-2.514456	0.000000	Al	1.460820	-2.525811	0.000000
H	-2.332388	3.354565	0.000000	H	-1.118364	3.822609	0.000000
27				**28**			
C	-0.373204	-0.780675	0.000000	Mg	0.108590	-1.121420	0.000000
Al	-1.956670	0.402836	0.000000	C	0.726430	0.946140	0.000000
Al	0.945379	0.546711	0.000000	H	1.766820	0.603400	0.000000
Mg	1.802294	-2.401031	0.000000	Al	-1.216680	1.169300	0.000000
H	-0.546339	-1.856841	0.000000	Al	0.848880	2.934060	0.000000
Al	0.451399	3.164476	0.000000	Al	0.416210	-4.052160	0.000000
H	-0.663713	1.771592	0.000000	H	-1.009610	2.895850	0.000000
29				**30**			
Mg	-1.805003	0.394870	0.000000	Mg	2.562486	1.074577	0.000000
Al	-0.891140	-2.244284	0.000000	Al	-0.044279	0.965878	0.000000
C	0.952220	-2.090837	0.000000	C	1.268329	-0.570383	0.000000
Al	1.167422	2.388363	0.000000	Al	-2.375644	-0.040087	0.000000
Al	1.499374	-0.338822	0.000000	Al	-0.457845	-1.583774	0.000000
H	-3.395222	1.113638	0.000000	H	2.167304	-1.193279	0.000000
H	-0.469800	1.742542	0.000000	H	-3.914951	0.347029	0.000000

31				
Mg	-0.793814	-2.001288	0.000000	
H	-0.347160	1.352277	0.000000	
Al	1.773145	-0.885120	0.000000	
Al	-1.869733	0.580215	0.000000	
Al	1.526055	1.877740	0.000000	
C	1.108496	-2.584616	0.000000	
H	-2.884108	1.851882	0.000000	