Supporting information for:

$CAl_4Mg^{0/-}$: Global Minima with A Planar Tetracoordinate Carbon Atom

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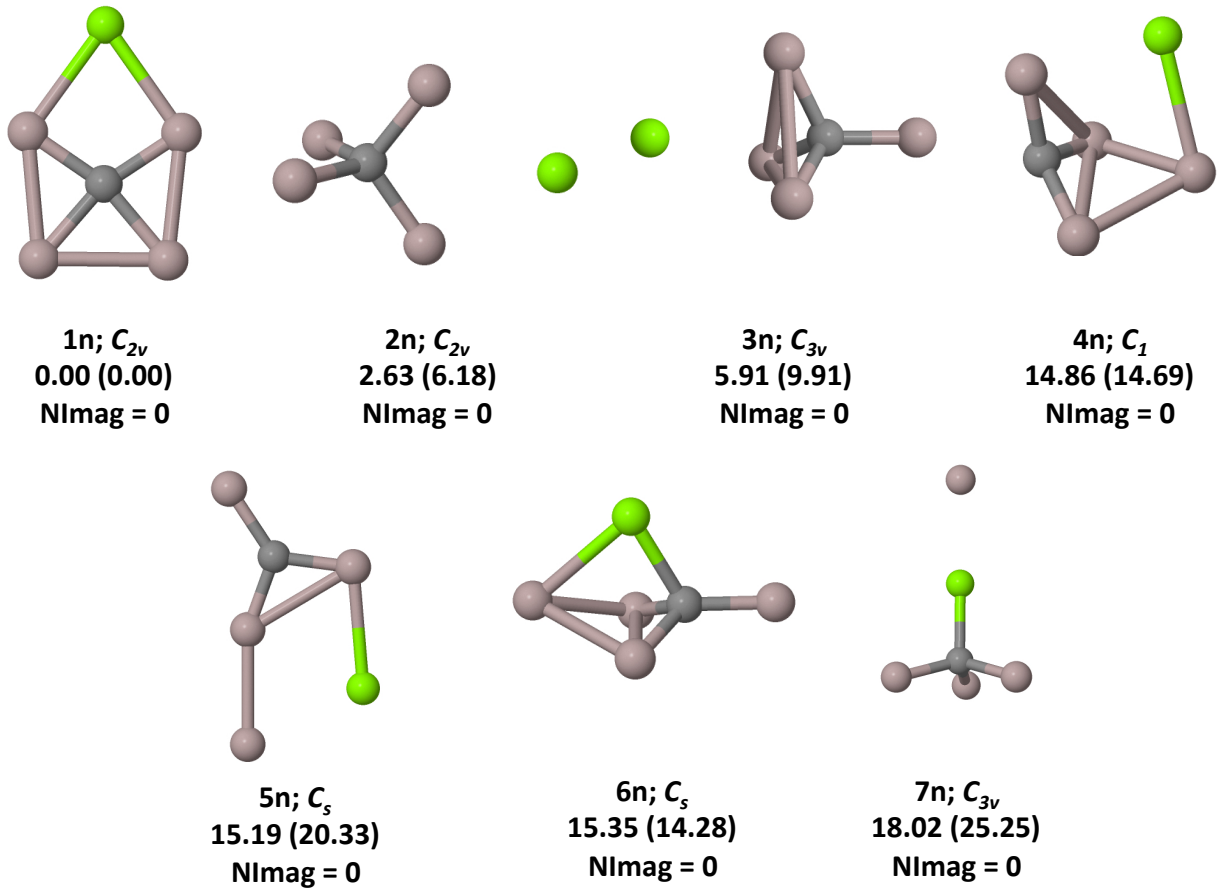

Figure S1: Isomers **1n**-**7n** of CAl_4Mg. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the ωB97XD/6-311++G(2d,2p) level of theory. Relative energies obtained at the CBS-QB3 level are shown in parentheses.

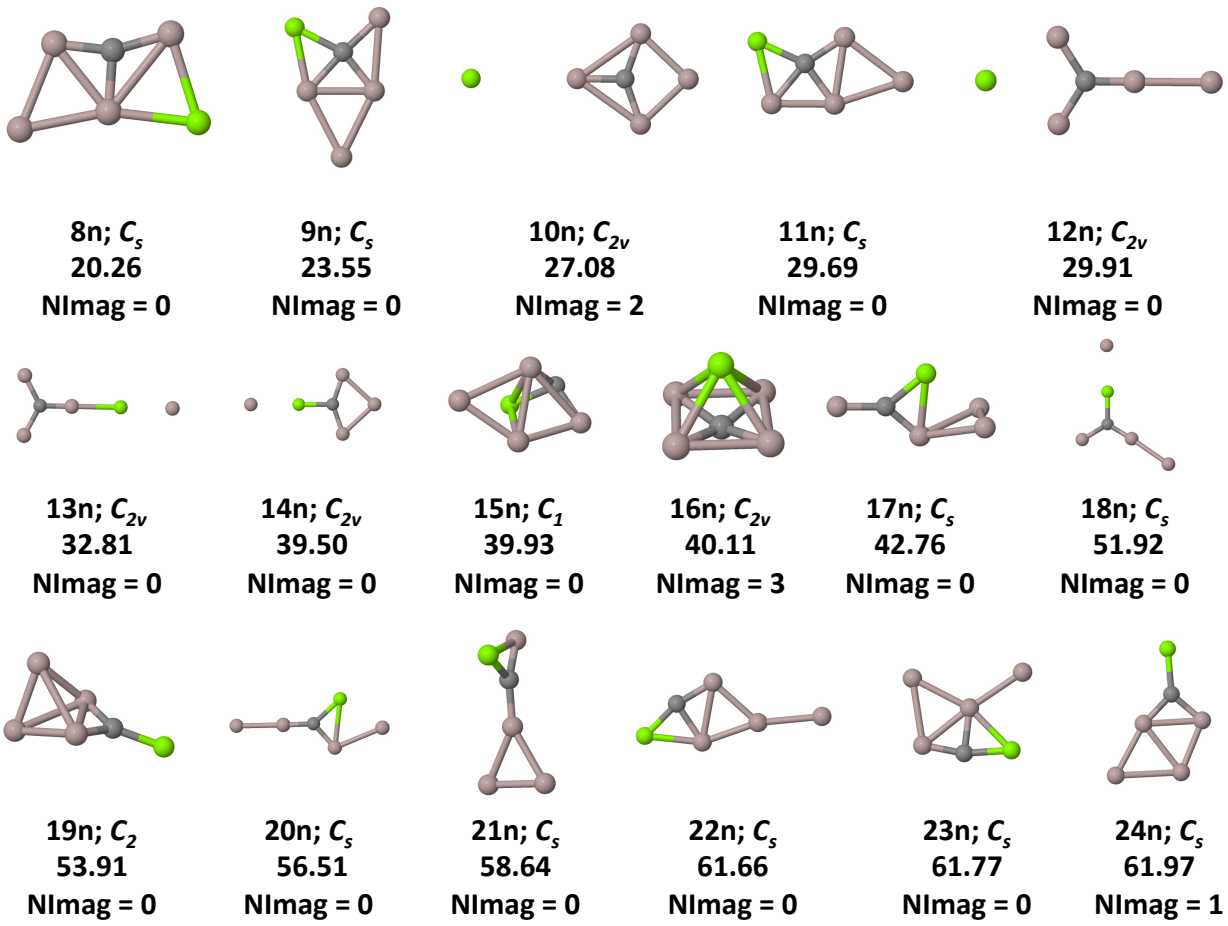

Figure S2: Isomers **8n-24n** of CAl_4Mg. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the ωB97XD/6-311++G(2d,2p) level of theory.

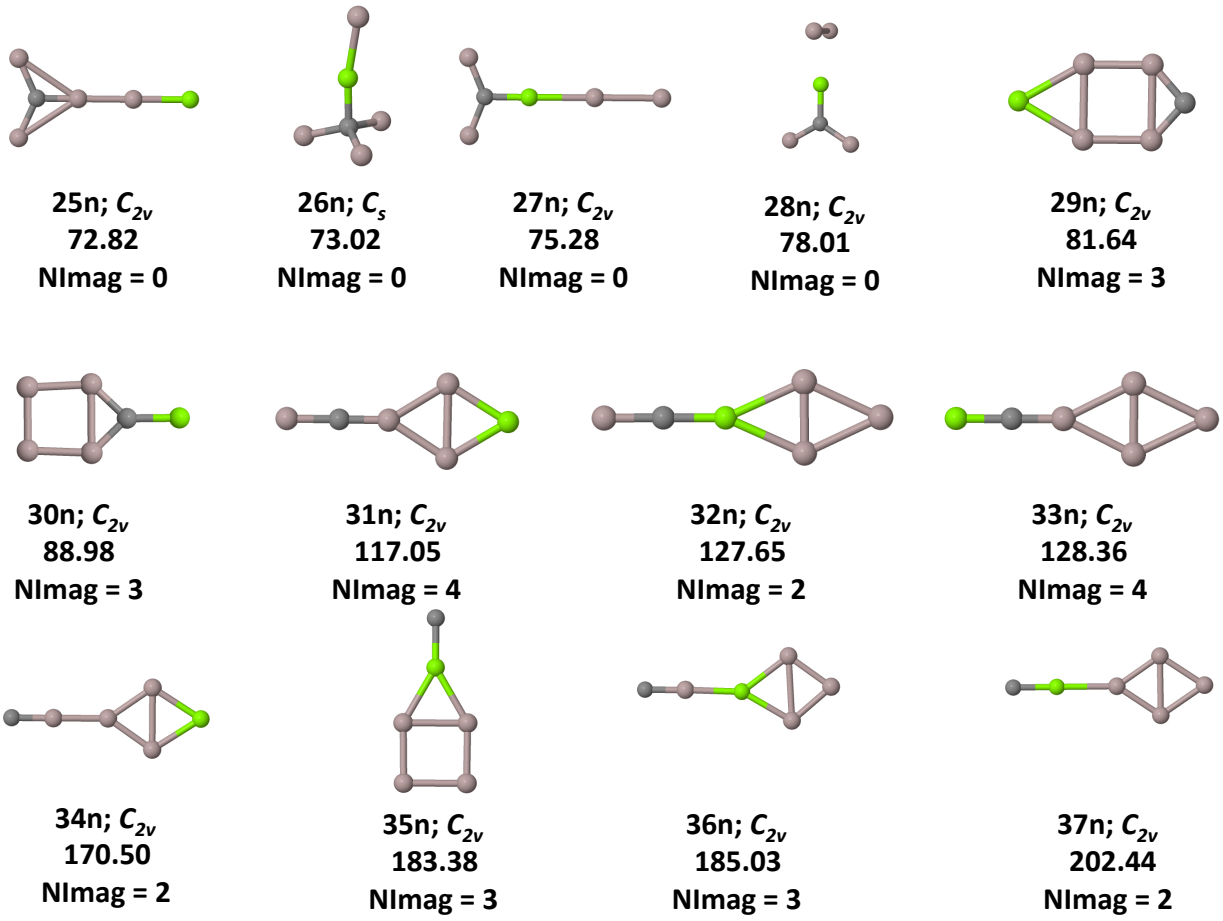

Figure S3: Isomers **25n-37n** of CAl_4Mg. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the ωB97XD/6-311++G(2d,2p) level of theory.

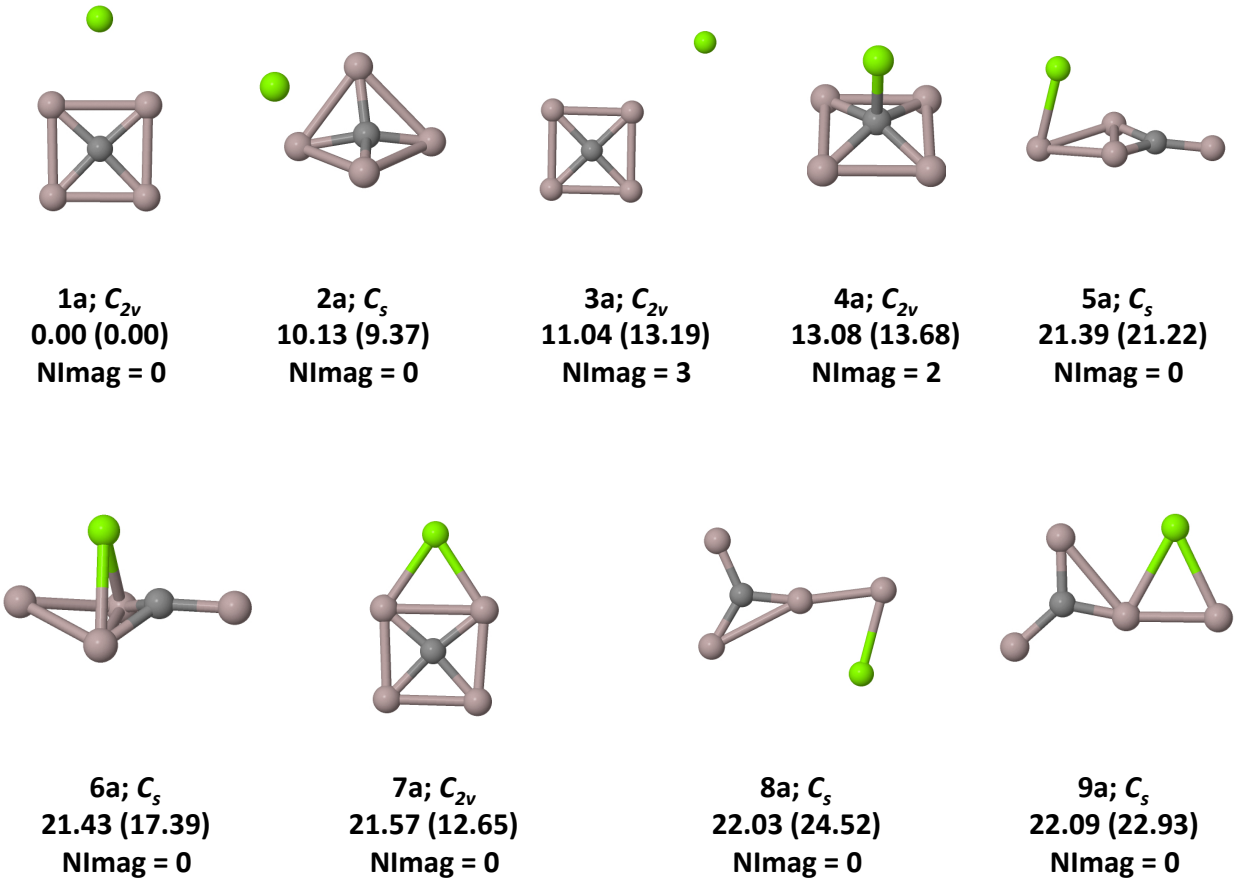

Figure S4: Isomers **1a**-**9a** of CAl_4Mg^-. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the UωB97XD/6-311++G(2d,2p) level of theory. Relative energies obtained at the CBS-QB3 level are shown in parentheses.

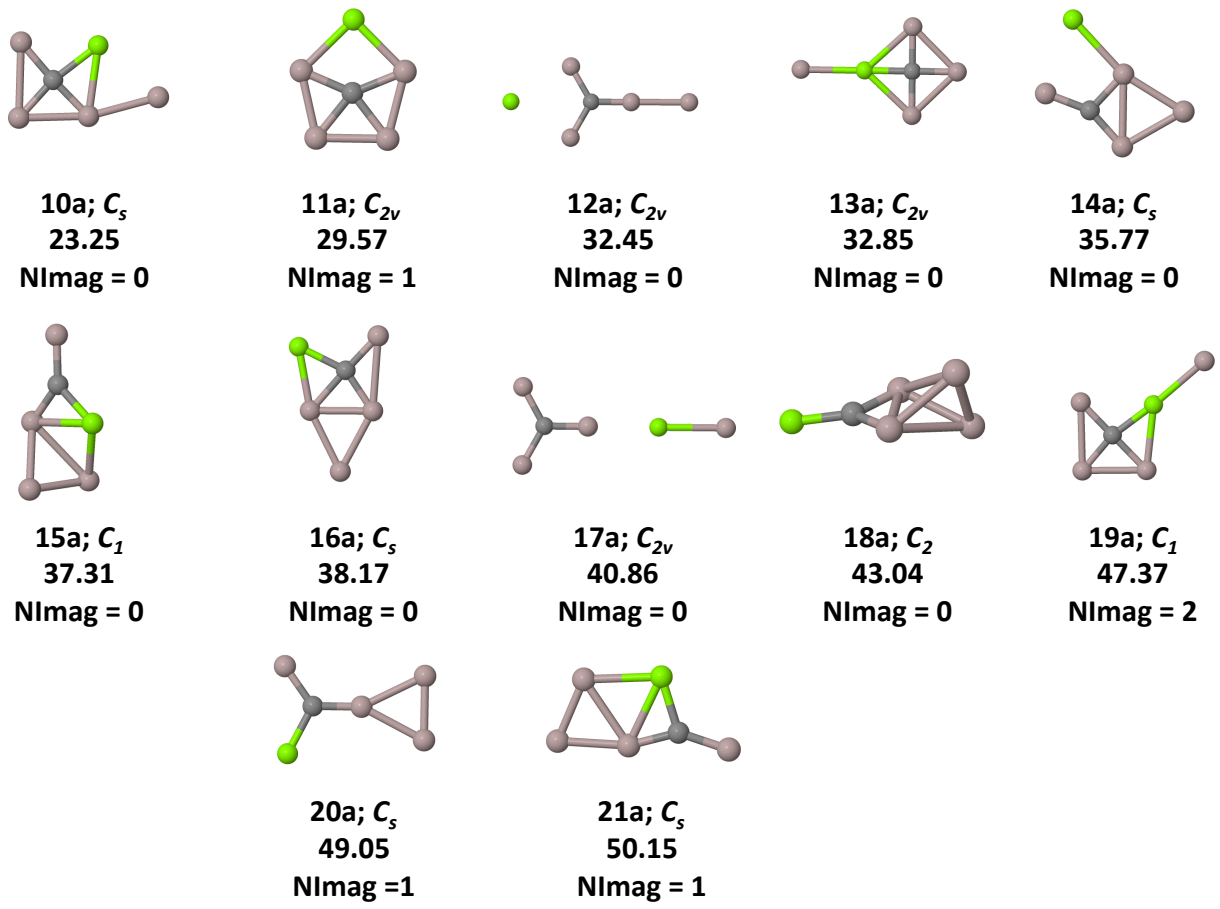

Figure S5: Isomers **10a-21a** of CAl_4Mg^-. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the UωB97XD/6-311++G(2d,2p) level of theory.

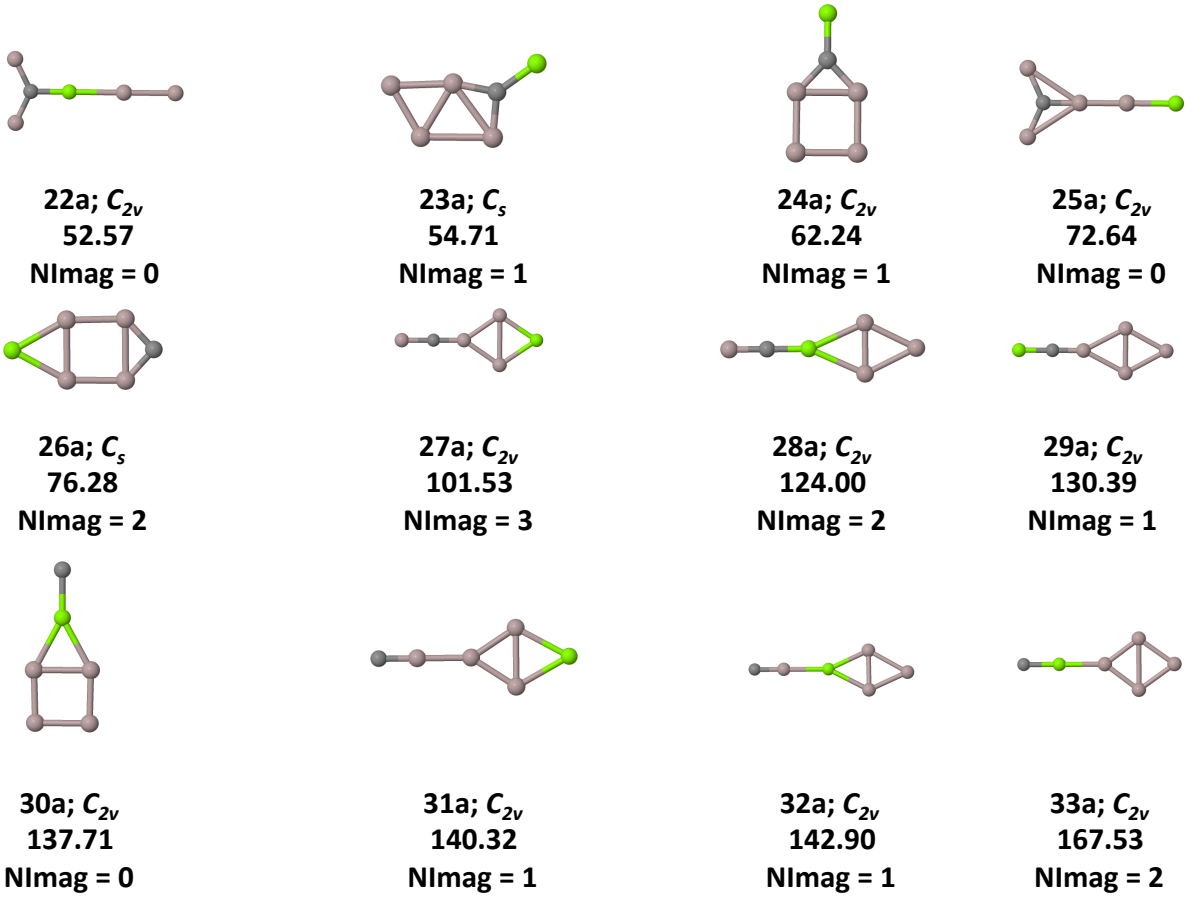

Figure S6: Isomers **22a-33a** of CAl_4Mg^-. ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the UωB97XD/6-311++G(2d,2p) level of theory.

Table S1: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$-corrected total energy (E+$ZPVE$), net dipole moment (μ), relative energy without ZPVE-correction (ΔE), ZPVE-corrected relative energy (ΔE+$ZPVE$), and number of imaginary frequencies of CAl_4Mg isomers in their respective singlet ground electronic state calculated at the ωB97XD/6-311++G(2d,2p) level of theory.

Isomer	Point Group	E a.u	$ZPVE$ a.u	E+$ZPVE$ a.u	μ Debye	ΔE kcal mol^{-1}	ΔE+$ZPVE$ kcal mol^{-1}	NImag	T_1^a
1n	C_{2v}	-1207.821919	0.008554	-1207.813365	6.75	0.00	0.00	0	0.0247
2n	C_{2v}	-1207.816793	0.007601	-1207.809191	3.06	3.22	2.63	0	0.0261
3n	C_{3v}	-1207.811101	0.007151	-1207.803950	1.99	6.79	5.91	0	0.0252
4n	C_1	-1207.797796	0.008114	-1207.789682	2.94	15.14	14.86	0	0.0336
5n	C_s	-1207.797182	0.008021	-1207.789160	4.54	15.52	15.19	0	0.0297
6n	C_s	-1207.796844	0.007935	-1207.788909	1.56	15.74	15.35	0	0.0342
7n	C_{3v}	-1207.792274	0.007619	-1207.784655	2.78	18.60	18.02	0	0.0229
8n	C_s	-1207.789047	0.007966	-1207.781081	3.09	20.63	20.26	0	0.0362
9n	C_s	-1207.783961	0.008121	-1207.775839	4.05	23.82	23.55	0	0.0704
10n	C_{2v}	-1207.776951	0.006736	-1207.770215	2.15	28.22	27.08	2	0.0350
11n	C_s	-1207.774372	0.008298	-1207.766074	4.79	29.83	29.69	0	0.0373
12n	C_{2v}	-1207.773064	0.007361	-1207.765702	6.32	30.66	29.91	0	0.0307
13n	C_{2v}	-1207.768729	0.007644	-1207.761085	9.67	33.38	32.81	0	0.0274
14n	C_{2v}	-1207.757739	0.007329	-1207.750410	2.71	40.27	39.50	0	0.0372
15n	C_1	-1207.757867	0.008130	-1207.749737	2.13	40.19	39.93	0	0.0383
16n	C_{2v}	-1207.757019	0.007574	-1207.749446	2.74	40.73	40.11	3	0.0285
17n	C_s	-1207.753284	0.008056	-1207.745228	5.60	43.07	42.76	0	0.0272
18n	C_s	-1207.737983	0.007357	-1207.730625	5.65	52.67	51.92	0	0.0288
19n	C_2	-1207.735090	0.007642	-1207.727447	5.48	54.49	53.91	0	0.0509
20n	C_s	-1207.730588	0.007281	-1207.723307	6.98	57.31	56.51	0	0.0318
21n	C_s	-1207.727782	0.007869	-1207.719912	5.87	59.07	58.64	0	0.0314
22n	C_s	-1207.723406	0.008303	-1207.715103	0.79	61.82	61.66	0	0.0378
23n	C_s	-1207.722509	0.007588	-1207.714921	3.23	62.38	61.77	0	0.0380
24n	C_s	-1207.721990	0.007385	-1207.714605	0.23	62.71	61.97	1	0.0715
25n	C_{2v}	-1207.705747	0.008422	-1207.697325	13.27	72.90	72.82	0	0.0340
26n	C_s	-1207.704635	0.007629	-1207.697006	2.24	73.60	73.02	0	0.0237
27n	C_{2v}	-1207.700276	0.006883	-1207.693393	18.62	76.33	75.28	0	0.0499
28n	C_{2v}	-1207.696046	0.006994	-1207.689052	8.11	78.99	78.01	0	0.5027
29n	C_{2v}	-1207.690834	0.007569	-1207.683265	5.22	82.26	81.64	3	0.0504
30n	C_{2v}	-1207.679725	0.008152	-1207.671573	5.23	89.23	88.98	3	0.0363
31n	C_{2v}	-1207.633423	0.006596	-1207.626828	12.54	118.28	117.05	4	0.1009
32n	C_{2v}	-1207.615669	0.005730	-1207.609939	2.02	129.42	127.65	2	0.0249
33n	C_{2v}	-1207.615325	0.006509	-1207.608816	7.23	129.64	128.36	4	0.0438
34n	C_{2v}	-1207.547973	0.006319	-1207.541653	12.04	171.90	170.50	2	0.0433
35n	C_{2v}	-1207.526300	0.005167	-1207.521132	4.03	185.50	183.38	3	0.0723
36n	C_{2v}	-1207.523730	0.005228	-1207.518502	9.04	187.12	185.03	3	0.0677
37n	C_{2v}	-1207.495490	0.004741	-1207.490749	8.00	204.84	202.44	2	0.0451

[a] T_1 diagnostic values are calculated at the CCSD/6-311++g(2d,2p)//ωB97XD/6-311++G(2d,2p) level of theory.

Table S2: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$-corrected total energy (E+$ZPVE$), net dipole moment (μ), relative energy without ZPVE-correction (ΔE), ZPVE-corrected relative energy (ΔE+$ZPVE$), number of imaginary frequencies, and $< S^2 >$ of CAl_4Mg^- isomers in their respective doublet ground electronic state calculated at the UωB97XD/6-311++G(2d,2p) level of theory.

Isomer	Point Group	E a.u	$ZPVE$ a.u	E+$ZPVE$ a.u	μ Debye	ΔE kcal mol^{-1}	ΔE+$ZPVE$ kcal mol^{-1}	NImag	$< S^2 >$
1a	C_{2v}	-1207.897170	0.008601	-1207.888570	2.31	0.00	0.00	0	0.764771
2a	C_s	-1207.879680	0.007253	-1207.872427	0.89	10.98	10.13	0	0.777748
3a	C_{2v}	-1207.877771	0.006795	-1207.870976	0.74	12.17	11.04	1	0.768781
4a	C_{2v}	-1207.875520	0.007797	-1207.867723	3.37	13.59	13.08	2	0.753527
5a	C_s	-1207.862031	0.007543	-1207.854488	2.29	22.05	21.39	0	0.796411
6a	C_s	-1207.862045	0.007625	-1207.854420	1.03	22.04	21.43	0	0.971248
7a	C_{2v}	-1207.863088	0.008892	-1207.854196	3.79	21.39	21.57	0	0.760092
8a	C_s	-1207.861371	0.007912	-1207.853458	2.32	22.46	22.03	0	0.761474
9a	C_s	-1207.861212	0.007851	-1207.853361	2.08	22.56	22.09	0	0.758820
10a	C_s	-1207.859307	0.007793	-1207.851514	0.82	23.76	23.25	0	0.847274
11a	C_{2v}	-1207.849796	0.008345	-1207.841452	2.32	29.73	29.57	1	0.775357
12a	C_{2v}	-1207.844164	0.007312	-1207.836852	2.67	33.26	32.45	0	0.754200
13a	C_{2v}	-1207.843562	0.007337	-1207.836225	4.10	33.64	32.85	0	0.769523
14a	C_s	-1207.839054	0.007495	-1207.831559	2.05	36.47	35.77	0	1.219783
15a	C_1	-1207.837007	0.007891	-1207.829116	2.55	37.75	37.31	0	0.774617
16a	C_s	-1207.835768	0.008025	-1207.827743	5.03	38.53	38.17	0	0.757058
17a	C_{2v}	-1207.830794	0.007331	-1207.823463	4.22	41.65	40.86	0	0.753369
18a	C_2	-1207.827911	0.007923	-1207.819988	2.21	43.46	43.04	0	0.758284
19a	C_1	-1207.820046	0.006970	-1207.813076	0.86	48.40	47.37	2	0.977176
20a	C_s	-1207.818459	0.008048	-1207.810411	2.00	49.39	49.05	1	0.756766
21a	C_s	-1207.816892	0.008240	-1207.808652	3.34	50.38	50.15	1	0.795978
22a	C_{2v}	-1207.812259	0.007469	-1207.804790	6.93	53.28	52.57	0	0.753291
23a	C_s	-1207.809333	0.007953	-1207.801380	3.29	55.12	54.71	1	0.772189
24a	C_{2v}	-1207.797134	0.007753	-1207.789382	3.64	62.77	62.24	1	1.814065
25a	C_{2v}	-1207.781689	0.008878	-1207.772811	5.03	72.47	72.64	0	0.827230
26a	C_s	-1207.774373	0.007521	-1207.766852	1.64	77.06	76.38	2	1.164486
27a	C_{2v}	-1207.733336	0.006556	-1207.726780	10.90	102.81	101.52	3	0.778591
28a	C_{2v}	-1207.697925	0.006962	-1207.690963	2.78	125.03	124.00	2	1.049741
29a	C_{2v}	-1207.692694	0.011904	-1207.680789	7.90	128.31	130.38	1	0.783430
30a	C_{2v}	-1207.674998	0.005889	-1207.669109	1.33	139.42	137.71	0	0.756797
31a	C_{2v}	-1207.671277	0.006323	-1207.664953	3.47	141.75	140.32	1	2.854163
32a	C_{2v}	-1207.666442	0.005590	-1207.660851	1.87	144.78	142.90	1	1.787204
33a	C_{2v}	-1207.627162	0.005565	-1207.621597	0.70	169.43	167.53	2	1.683910

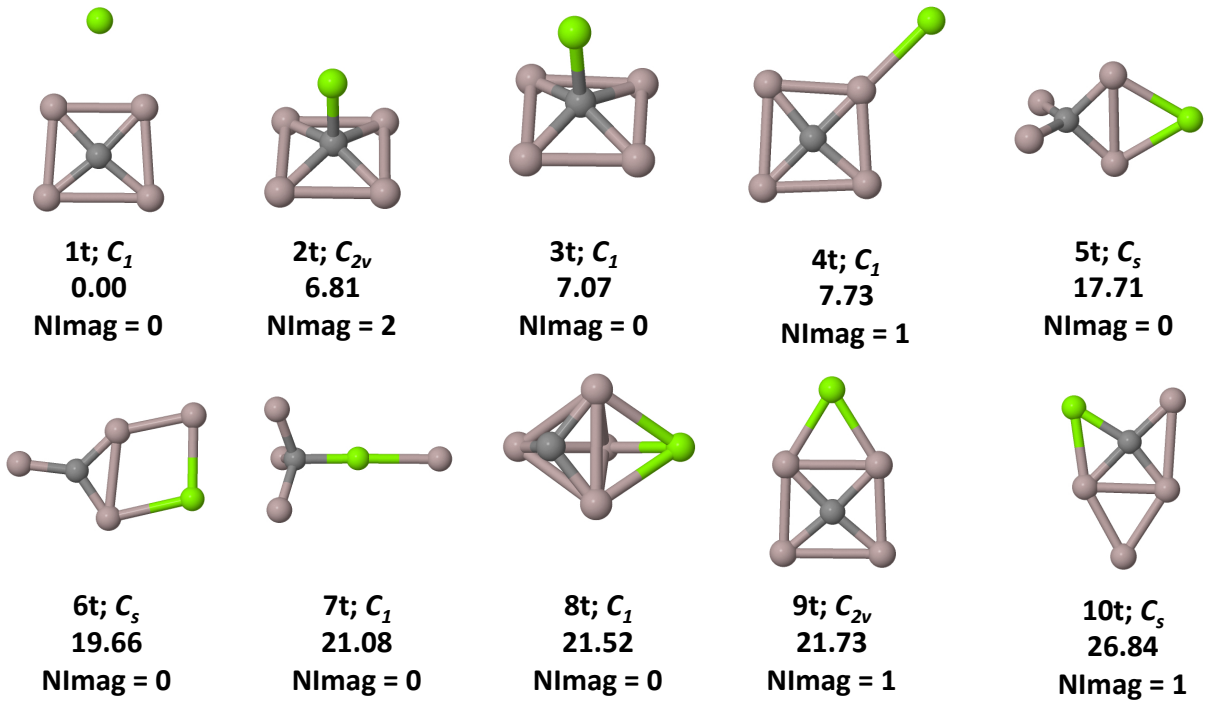

Figure S7: Isomers **1t-10t** of CAl_4Mg (triplet). ZPVE-corrected relative energies (in kcal mol^{-1}) are calculated at the UωB97XD/6-311++G(2d,2p) level of theory.

Table S3: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$-corrected total energy (E+$ZPVE$), net dipole moment (μ), relative energy without ZPVE-correction (ΔE), ZPVE-corrected relative energy (ΔE+$ZPVE$), number of imaginary frequencies, and $< S^2 >$ of CAl_4Mg isomers in their respective triplet ground electronic state calculated at the UωB97XD/6-311++G(2d,2p) level of theory.

Isomer	Point Group	E a.u	$ZPVE$ a.u	E+$ZPVE$ a.u	μ Debye	ΔE kcal mol^{-1}	ΔE+$ZPVE$ kcal mol^{-1}	NImag	$< S^2 >$
1t	C_1; ^3A	-1207.8049396	0.007881	-1207.797058	2.36	0.00	0.00	0	2.048387
2t	C_{2v}; $^3A_2$	-1207.7923899	0.006187	-1207.786203	2.90	7.88	6.81	2	2.025397
3t	C_1; ^3A	-1207.7925785	0.006787	-1207.785792	2.82	7.76	7.07	0	2.031360
4t	C_1; ^3A	-1207.7921357	0.007391	-1207.784745	5.70	8.03	7.73	1	2.042178
5t	C_s; ^3A"	-1207.7769739	0.008141	-1207.768833	4.10	17.55	17.71	0	2.048523
6t	C_s; ^3A"	-1207.7741820	0.008456	-1207.765726	4.66	19.30	19.66	0	2.034079
7t	C_1; ^3A	-1207.7710804	0.007617	-1207.763464	1.16	21.25	21.08	0	2.006889
8t	C_1; ^3A	-1207.7709241	0.008154	-1207.762770	2.91	21.35	21.52	0	2.098039
9t	C_{2v}; $^3B_1$	-1207.7707676	0.008336	-1207.762431	5.51	21.44	21.73	1	2.066218
10t	C_s; ^3A"	-1207.7622635	0.007982	-1207.754281	3.78	26.78	26.84	1	2.328429

Optimized geometries of CAl_4Mg (singlet) obtained at the wB97XD/6-311++G(2d,2p) level

```
    6
1n    scf done: -1207.821919
 C    -0.401152     0.000000     1.000000
Mg     2.908484    -0.000000     1.000000
Al     0.665381    -0.000000     2.585077
Al     0.665381    -0.000000    -0.585077
Al    -1.948487     0.000000     2.319726
Al    -1.948487     0.000000    -0.319726

    6
2n    scf done: -1207.816793
 C    -0.058630     0.000000     0.953180
Mg     3.671457    -0.000000     1.016827
Al     1.139992    -0.000000    -0.633404
Al     1.085452     0.000000     2.579840
Al    -1.216774    -1.601880     0.932782
Al    -1.216774     1.601880     0.932782

    6
3n    scf done: -1207.811101
Al     2.549559     0.000000     1.617000
 C     4.493769     0.000000     1.617000
Al     5.418970     0.000000    -0.147570
Al     5.418970     1.528163     2.499285
Al     5.418970    -1.528163     2.499285
Mg     8.119761    -0.000000     1.617000

    6
4n    scf done: -1207.797796
 C    -0.056250     0.553029     1.124817
Al     1.825150     0.750946     1.303472
Al     1.023192     0.642007     4.045791
Mg    -1.127542    -1.231137     3.906302
Al    -0.920695     1.453023     2.527781
Al    -0.863698    -1.166022     0.973378

    6
5n    scf done: -1207.797182
 C    -0.575044     0.000000    -0.166674
Al     0.148289     0.000000     1.554435
Mg     2.969146    -0.000000     1.015020
Al     3.548959    -0.000000    -1.978788
Al     0.919790    -0.000000    -1.238383
Al    -2.399093     0.000000    -0.752770

    6
6n    scf done: -1207.796844
 C     1.854420     0.405723     1.106547
Al     0.401911    -0.069386     2.298727
Al     2.077983     0.785400     4.292820
Mg     3.300299    -0.755573     2.336516
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```
Al     2.462042     2.066416     1.900088
Al     1.793333     0.105649    -0.780958

    6
7n    scf done: -1207.792274
Al    -0.191721     0.000000     1.617000
Mg     2.770544    -0.000000     1.617000
 C     4.913048    -0.000000     1.617000
Al     5.442888     0.000000    -0.256228
Al     5.442888     1.622263     2.553614
Al     5.442888    -1.622263     2.553614

    6
8n    scf done: -1207.789047
 C     0.011862     0.845574     0.000000
Al     1.169947     2.328719     0.000000
Al     1.042849    -0.763889    -0.000000
Al    -1.595188    -0.078612    -0.000000
Al    -0.871604    -2.860018    -0.000000
Mg     3.491190     0.625438     0.000000

    6
9n    scf done: -1207.783961
 C    -0.067657    -0.000000    -0.489978
Al     0.063423    -0.000000     1.432449
Al     1.835474     0.000000    -0.812153
Al     2.643192     0.000000    -3.528744
Al    -0.057189    -0.000000    -2.538591
Mg    -2.101514    -0.000000    -1.042633

    6
10n   scf done: -1207.776950
Al    -1.102556    -0.000000     1.000000
Mg     3.254757    -0.000000     1.000000
 C    -3.035300     0.000000     1.000000
Al    -3.668751     0.000000     2.796690
Al    -3.668751     0.000000    -0.796690
Al    -5.575168     0.000000     1.000000

    6
11n   scf done: -1207.774371
 C    -0.000000    -0.000000    -0.000000
Al    -0.000000     0.000000     2.066967
Mg     2.003707    -0.000000     0.528468
Al    -1.928053     0.000000     0.501249
Al    -3.443744     0.000000    -1.891069
Al    -0.560677    -0.000000    -1.783687

    6
12n   scf done: -1207.773064
Al    -0.620242    -0.000000     1.000000
Al     2.186066    -0.000000     1.000000
 C    -2.412353    -0.000000     1.000000
Al    -3.424036     0.000000     2.631500
Al    -3.424036    -0.000000    -0.631500
```

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Mg    -6.101167     0.000000     1.000000

    6
13n   scf done: -1207.768729
Mg     0.272839    -0.000000     1.000000
Al     3.250766    -0.000000     1.000000
Al    -2.528681     0.000000     1.000000
Al    -5.232065     0.000000     2.681150
Al    -5.232065    -0.000000    -0.681150
 C    -4.327225     0.000000     1.000000

    6
14n   scf done: -1207.757739
Mg    -0.787071    -0.000000     1.000000
Al     2.169675    -0.000000     1.000000
 C    -2.856919     0.000000     1.000000
Al    -3.465600     0.000000     2.783712
Al    -3.465600    -0.000000    -0.783712
Al    -5.390254     0.000000     1.000000

    6
15n   scf done: -1207.757867
 C     0.016740    -0.026422     0.004083
Mg    -0.027601     0.023308     2.122473
Al     2.734857     0.003324     1.433078
Al     2.043162     2.270267     2.698474
Al     0.867437     1.631033     0.064493
Al     1.269373    -1.300383    -0.468161

    6
16n   scf done: -1207.757019
 C     0.000000     0.000000    -0.650818
Mg    -0.000000    -0.000000     1.625327
Al     0.000000     1.971101    -0.300330
Al    -0.000000    -1.971101    -0.300330
Al     1.971059    -0.000000    -0.299632
Al    -1.971059     0.000000    -0.299632

    6
17n   scf done: -1207.753284
Al     0.087594    -0.815341     0.869239
Mg     0.743666     1.347711    -0.336713
 C    -0.940198     0.160395    -0.274383
Al    -2.684437     0.082061    -1.013430
Al     2.900034    -0.735466     0.483640
Al     2.031213     0.592440     2.387096

    6
18n   scf done: -1207.737983
 C    -0.487130     0.484265     0.556374
Al    -1.072206     2.188485     0.001773
Mg     0.704489    -0.635862    -0.670182
Al    -0.991112    -0.124270     2.161470
Al     2.423725    -2.207273    -2.484840
Al    -1.866555    -0.917955     4.685056
```

```
    6
19n   scf done: -1207.735090
 C    -0.034217     0.332780     0.307819
Al     0.267305    -0.758940     1.791331
Al     1.654634     0.643430     3.492768
Al     3.288482    -0.186113     1.640724
Al     1.519453     1.348746     0.501091
Mg    -1.521164     0.391698    -1.033987

    6
20n   scf done: -1207.730588
Al    -0.502374    -2.270066     0.787558
Mg     1.952849    -1.545091    -0.400973
Al    -0.606684     0.995521     0.284291
 C     0.150061    -0.625078     0.227532
Al    -1.743479     3.544565     0.350449
Al     1.528796    -4.401562     0.262794

    6
21n   scf done: -1207.727782
Al     0.271494    -2.646326     0.382364
Mg     2.135153    -0.964170    -0.834659
Al    -0.680148     0.754601    -0.263690
 C     0.266624    -0.862839    -0.146353
Al    -1.376220     3.073002     0.657171
Al    -2.211512     2.426553    -1.515493

    6
22n   scf done: -1207.723406
 C    -0.141043    -0.080785     2.298181
Mg    -1.959580    -0.349374     1.498425
Al     1.305015     0.082562     3.437213
Al     1.753990    -0.319908     8.341865
Al     0.457550    -0.323373     5.882904
Al    -1.242942    -0.455391     3.936965

    6
23n   scf done: -1207.722509
Al    -0.161531     0.000000    -0.590591
Al    -0.009762     0.000000     2.370459
Al     2.156512    -0.000000     0.531288
Mg     3.530022    -0.000000    -1.644704
Al     4.724964    -0.000000     1.522126
 C     1.525157     0.000000    -1.326933

    6
24n   scf done: -1207.720543
 C     0.013258    -0.000000     0.004192
Mg     0.065606    -0.000000     2.129340
Al     1.282830    -0.000000    -1.356817
Al    -1.433319     0.000000    -1.206406
Al    -2.981148     0.000000    -3.444497
Al     0.046442    -0.000000    -3.628100
```

```
    6
25n   scf done: -1207.705747
Al     0.063672    -0.000000     1.000000
Mg     2.554484    -0.000000     1.000000
Al    -2.362481     0.000000     1.000000
Al    -4.945853     0.000000     2.744879
Al    -4.945853    -0.000000    -0.744879
 C    -4.159736     0.000000     1.000000

    6
26n   scf done: -1207.704635
Mg    -0.166896    -0.001846     0.851611
Al     2.363302     0.003491     1.178172
 C    -2.229980    -0.000758     0.947525
Al    -2.882909    -0.000699    -0.897741
Al    -2.555607    -1.691812     1.899624
Al    -2.547911     1.691624     1.900809

    6
27n   scf done: -1207.700276
Al     0.338771    -0.000000     1.000000
Al     3.287346    -0.000000     1.000000
Mg    -2.537758     0.000000     1.000000
Al    -5.197144     0.000000     2.739864
Al    -5.197144    -0.000000    -0.739864
 C    -4.489841     0.000000     1.000000

    6
28n   scf done: -1207.696046
Al     1.203586    -1.608052     1.311487
Mg    -0.129775     1.122941    -0.083945
 C    -0.218158    -0.787956     0.432347
Al    -1.726573    -1.809095     0.049361
Al     0.526263     3.391775    -1.885060
Al    -0.487932     4.039437     0.348599

    6
29n   scf done: -1207.690834
 C     0.277693    -0.000000     1.000000
Al    -0.939787    -0.000000     2.369315
Al    -0.939787     0.000000    -0.369315
Al    -3.488363    -0.000000     2.383258
Al    -3.488363     0.000000    -0.383258
Mg    -5.960406     0.000000     1.000000

    6
30n   scf done: -1207.679725
 C     0.156702    -0.000000     1.000000
Mg     2.161593    -0.000000     1.000000
Al    -1.188509    -0.000000     2.276830
Al    -1.188509    -0.000000    -0.276830
Al    -3.593851     0.000000     2.171642
Al    -3.593851     0.000000    -0.171642

    6
```

```
31n   scf done: -1207.633424
 C     0.019136    -0.000000     1.000000
Al     1.941650    -0.000000     1.000000
Al    -1.784680    -0.000000     1.000000
Al    -3.922168     0.000000     2.329365
Al    -3.922168    -0.000000    -0.329365
Mg    -6.127538     0.000000     1.000000

    6
32n   scf done: -1207.615669
 C    -0.000000     0.000000     3.069531
Al    -0.000000     0.000000     5.042702
Mg    -0.000000     0.000000     0.990744
Al     0.000000     1.170933    -1.618688
Al    -0.000000    -1.170933    -1.618688
Al     0.000000    -0.000000    -4.136566

    6
33n   scf done: -1207.615325
 C     0.158851    -0.000000     1.000000
Mg     2.058514    -0.000000     1.000000
Al    -1.596728    -0.000000     1.000000
Al    -3.981925     0.000000     2.194737
Al    -3.981925     0.000000    -0.194737
Al    -6.452554     0.000000     1.000000

    6
34n   scf done: -1207.547973
Al     0.416912    -0.000000     1.000000
 C     2.329437    -0.000000     1.000000
Al    -2.074495    -0.000000     1.000000
Al    -4.092031     0.000000     2.390724
Al    -4.092031    -0.000000    -0.390724
Mg    -6.283560     0.000000     1.000000

    6
35n   scf done: -1207.526300
Mg     0.870959    -0.000000     1.000000
 C     3.015150    -0.000000     1.000000
Al    -1.507593    -0.000000     2.349150
Al    -1.507593    -0.000000    -0.349150
Al    -4.058673     0.000000     2.311881
Al    -4.058673     0.000000    -0.311881

    6
36n   scf done: -1207.523730
Al     0.000000     0.030163    -3.418266
 C     0.000000     0.087314    -5.333707
Mg     0.000000    -0.104777    -0.731347
Al    -0.000000     1.486695     1.495659
Al    -0.000000    -1.493045     1.590911
Al     0.000000     0.030163     3.468497

    6
37n   scf done: -1207.495490
```

Mg	0.679442	-0.000000	1.000000
C	2.764698	-0.000000	1.000000
Al	-2.210935	0.000000	1.000000
Al	-4.304432	0.000000	2.411401
Al	-4.304432	0.000000	-0.411401
Al	-6.420109	0.000000	1.000000

Optimized geometries of CAl_4Mg^- (doublet) obtained at the UwB97XD/6-311++G(2d,2p) level

6

1a scf done: -1207.897171

C	-0.091810	0.000000	1.000000
Mg	3.736429	-0.000000	1.000000
Al	1.193383	-0.000000	2.423808
Al	1.193383	-0.000000	-0.423808
Al	-1.516768	0.000000	2.374569
Al	-1.516768	0.000000	-0.374569

6

2a scf done: -1207.879680

C	0.360811	0.564397	1.857642
Al	1.951968	0.671307	0.790632
Al	1.136123	0.555810	3.671058
Mg	-1.632710	-1.210134	4.077997
Al	-1.344479	1.327486	2.530437
Al	-0.591555	-0.907021	0.953775

6

3a scf done: -1207.877771

Al	-1.259989	0.000000	1.000000
Mg	2.282958	0.000000	1.000000
C	-3.211072	0.000000	1.000000
Al	-3.210827	-0.000000	2.974846
Al	-3.210827	0.000000	-0.974846
Al	-5.185641	-0.000000	1.000000

6

4a scf done: -1207.875520

C	0.000000	0.000000	-0.009219
Mg	0.000000	0.000000	2.088022
Al	0.000000	1.965482	-0.481146
Al	-0.000000	-1.965482	-0.481146
Al	1.965508	-0.000000	-0.480429
Al	-1.965508	0.000000	-0.480429

6

5a scf done: -1207.862031

Al	-1.540105	-2.112383	1.193520
C	-0.584016	-0.584715	0.693490
Al	1.237944	-0.102671	0.619612
Al	-1.036345	1.145497	0.093993
Mg	1.219740	1.484245	-2.203395
Al	1.304202	2.682826	0.288790

```
    6
6a    scf done: -1207.863088
 C    -0.513366    -0.000000     1.000000
Mg     2.945500    -0.000000     1.000000
Al     0.721610    -0.000000     2.482684
Al     0.721610    -0.000000    -0.482684
Al    -1.967118     0.000000     2.341015
Al    -1.967118    -0.000000    -0.341015

    6
7a    scf done: -1207.862045
 C     1.045792    -0.197868     0.315169
Mg    -0.092450     0.118250     2.265781
Al     2.624663     0.073710     1.437504
Al     1.738029     2.393231     2.672850
Al     0.841305     1.738399     0.132372
Al     0.746629    -1.524595    -0.969236

    6
8a    scf done: -1207.861371
 C     0.000000    -0.000000     0.000000
Al     0.000000     0.000000     1.874722
Al     1.532405    -0.000000    -1.083719
Al    -1.600899     0.000000    -0.918886
Al    -4.106477     0.000000    -1.685874
Mg    -2.406213    -0.000000    -3.799519

    6
9a    scf done: -1207.861212
 C    -0.613211    -0.000000    -0.144388
Al    -0.033998    -0.000000     1.644492
Mg     3.148464     0.000000     0.831728
Al     3.457207     0.000000    -1.960811
Al     0.995889     0.000000    -1.078499
Al    -2.342303    -0.000000    -0.859683

    6
10a   scf done: -1207.859307
Al     0.996017    -1.138850     2.531277
Mg     2.713624     0.226829     0.432486
 C     4.660518     0.265941     1.409908
Al     5.509413     1.132895    -0.065361
Al     6.246087     0.128338     2.556371
Al     3.694874    -0.615154     2.837320

    6
11a   scf done: -1207.849797
 C     0.000000     0.000000    -0.137135
Mg    -0.000000     0.000000     2.453944
Al    -0.000000     1.846695     0.631350
Al    -0.000000    -1.846695     0.631350
Al    -0.000000     1.270982    -1.732293
Al    -0.000000    -1.270982    -1.732293
```

```
    6
12a   scf done: -1207.844164
Al    -0.589173    -0.000000     1.000000
Al     2.075586    -0.000000     1.000000
 C    -2.436075     0.000000     1.000000
Al    -3.368859     0.000000     2.637716
Al    -3.368859    -0.000000    -0.637716
Mg    -6.108387     0.000000     1.000000

    6
13a   scf done: -1207.843562
Mg    -1.040411    -0.000000     1.000000
Al     1.840946    -0.000000     1.000000
 C    -3.151605     0.000000     1.000000
Al    -3.155800     0.000000     2.939855
Al    -3.155800    -0.000000    -0.939855
Al    -5.133099     0.000000     1.000000

    6
14a   scf done: -1207.839054
 C     0.028783     0.796485     0.000000
Al     1.067761     2.338124     0.000000
Al     1.062432    -0.814766    -0.000000
Al    -1.621783    -0.102176    -0.000000
Al    -0.869594    -2.725725    -0.000000
Mg     3.581457     0.605270     0.000000

    6
15a   scf done: -1207.837007
Al    -0.586719    -0.392191    -2.577561
Mg    -1.007116     0.309616     0.122031
Al     1.573479     0.218808     2.692357
Al     1.450074     0.995193    -0.670615
 C     0.864646     0.494130     0.993058
Al    -0.030323     2.075154    -2.626751

    6
16a   scf done: -1207.835768
 C    -0.040890     0.000000    -0.426157
Al    -0.030713     0.000000     1.450758
Al     1.847176    -0.000000    -0.877240
Al     2.566208    -0.000000    -3.526493
Al     0.028291     0.000000    -2.574805
Mg    -2.054343     0.000000    -1.025712

    6
17a   scf done: -1207.830794
Mg     0.434269    -0.000000     1.000000
Al     3.261956    -0.000000     1.000000
Al    -2.540458     0.000000     1.000000
Al    -5.290119     0.000000     2.648534
Al    -5.290119    -0.000000    -0.648534
 C    -4.371959     0.000000     1.000000

    6
```

```
18a   scf done: -1207.827911
 C    -0.099939     0.335291     0.248937
Al     0.308372    -0.683394     1.769627
Al     1.716682     0.622290     3.542362
Al     3.345076    -0.169296     1.699900
Al     1.499286     1.271002     0.538304
Mg    -1.594984     0.395707    -1.099384

    6
19a   scf done: -1207.820046
Al    -1.113336     1.503952    -0.167740
 C     0.213019    -0.023761    -0.022030
Al     0.779356     0.547020    -1.823392
Al     1.460783    -1.461553     0.115968
Mg    -0.707971    -0.279226     1.883226
Al    -1.788212    -0.760012     4.393877

    6
20a   scf done: -1207.818459
Al    -1.821591    -2.434573     0.000000
Al    -0.902458     2.786078     0.000000
Al    -0.000000     0.297624     0.000000
Mg     1.464866    -2.647101    -0.000000
Al     1.468605     2.498071     0.000000
 C    -0.209604    -1.524731    -0.000000

    6
21a   scf done: -1207.816892
Al    -0.441463     0.000000     0.124528
Al    -0.196367     0.000000     2.510947
Al     2.093909     0.000000     1.336376
 C     3.409981    -0.000000     0.037703
Al     5.221605    -0.000000    -0.355609
Mg     1.913961    -0.000000    -1.347566

    6
22a   scf done: -1207.812259
Al     0.385761    -0.000000     1.000000
Al     3.033903    -0.000000     1.000000
Mg    -2.414734     0.000000     1.000000
Al    -5.198350     0.000000     2.681622
Al    -5.198350    -0.000000    -0.681622
 C    -4.403999     0.000000     1.000000

    6
23a   scf done: -1207.809333
 C     0.007729    -0.000000     0.019173
Mg     0.020597    -0.000000     2.017521
Al     1.412109     0.000000    -1.199100
Al    -1.334193    -0.000000    -1.263943
Al    -2.777423    -0.000000    -3.443882
Al    -0.335150     0.000000    -3.632057

    6
24a   scf done: -1207.797134
```

```
 C     0.000000    -0.000000     1.614880
Mg     0.000000    -0.000000     3.631797
Al     0.000000     1.273179     0.241005
Al    -0.000000    -1.273179     0.241005
Al     0.000000     1.270842    -2.289884
Al    -0.000000    -1.270842    -2.289884

    6
25a   scf done: -1207.781689
Al     0.049194    -0.000000     1.000000
Mg     2.487291    -0.000000     1.000000
Al    -2.314827    -0.000000     1.000000
Al    -4.935388     0.000000     2.709019
Al    -4.935388    -0.000000    -0.709019
 C    -4.146648     0.000000     1.000000

    6
26a   scf done: -1207.774373
 C     0.298298    -0.000000     1.000000
Al    -0.946244     0.000000     2.347246
Al    -0.946244     0.000000    -0.347246
Al    -3.516319     0.000000     2.323373
Al    -3.516319     0.000000    -0.323373
Mg    -5.912185    -0.000000     1.000000

    6
27a   scf done: -1207.733336
 C    -0.000852    -0.000000     1.000000
Al     1.868356    -0.000000     1.000000
Al    -1.790514    -0.000000     1.000000
Al    -3.899296     0.000000     2.440762
Al    -3.899296    -0.000000    -0.440762
Mg    -6.074167     0.000000     1.000000

    6
28a   scf done: -1207.697925
 C    -0.000000     0.000000     3.012976
Al    -0.000000     0.000000     4.808676
Mg    -0.000000     0.000000     1.048267
Al     0.000000     1.178571    -1.587794
Al    -0.000000    -1.178571    -1.587794
Al     0.000000    -0.000000    -3.965296

    6
29a   scf done: -1207.692694
 C     0.147979    -0.000000     1.000000
Mg     2.050571    -0.000000     1.000000
Al    -1.622533    -0.000000     1.000000
Al    -4.016250     0.000000     2.255934
Al    -4.016250     0.000000    -0.255934
Al    -6.339284     0.000000     1.000000

    6
30a   scf done: -1207.674998
Mg     0.854876    -0.000000     1.000000
```

```
 C     3.072838    -0.000000     1.000000
Al    -1.568113    -0.000000     2.306546
Al    -1.568113    -0.000000    -0.306546
Al    -4.018956     0.000000     2.246219
Al    -4.018956     0.000000    -0.246219

    6
31a   scf done: -1207.671277
Al     0.521336    -0.000000     1.000000
 C     2.328193    -0.000000     1.000000
Al    -1.990002    -0.000000     1.000000
Al    -4.067099     0.000000     2.364682
Al    -4.067099    -0.000000    -0.364682
Mg    -6.521097     0.000000     1.000000

    6
32a   scf done: -1207.666442
Al     0.182429     3.698065    -0.000000
 C     0.306078     5.537703    -0.000000
Mg     0.000000     0.914290     0.000000
Al    -1.325733    -1.465438     0.000000
Al     1.123740    -1.680048    -0.000000
Al    -0.121703    -3.952403     0.000000

    6
33a   scf done: -1207.627162
Mg     0.474227    -0.000000     1.000000
 C     2.592893    -0.000000     1.000000
Al    -2.210693    -0.000000     1.000000
Al    -4.194638     0.000000     2.480983
Al    -4.194638     0.000000    -0.480983
Al    -6.262919     0.000000     1.000000
```

Optimized geometries of CAl_4Mg (triplet) obtained at the UwB97XD/6-311++G(2d,2p) level

```
    6
1t    scf done: -1207.804940
Al     2.915797     0.902180     1.750838
 C     4.585852    -0.004985     1.268950
Al     4.079792    -0.934517    -0.381360
Al     5.335608     0.814803     2.887461
Al     6.360160    -0.802821     1.003519
Mg     8.142791     0.025341     3.172591

    6
2t    scf done: -1207.792390
 C    -0.000000     0.000000    -0.053722
Mg    -0.000000     0.000000     2.099126
Al     0.000000     1.990612    -0.568779
Al    -0.000000    -1.990612    -0.568779
Al     1.990672    -0.000000    -0.565958
Al    -1.990672     0.000000    -0.565958
```

```
    6
3t    scf done: -1207.792579
 C     1.974648     0.440130     1.917267
Al     0.246033    -0.653877     1.945371
Al     1.648144     1.108644     3.786522
Mg     3.534571    -1.003262     2.246717
Al     2.958620     2.163910     1.417312
Al     1.527972     0.482685    -0.159449

    6
4t    scf done: -1207.792136
Al    -1.210389    -0.001988     0.999467
Mg     1.552209     0.001900     1.000618
 C    -3.127148    -0.001266     0.999902
Al    -2.954125     0.002356     2.976671
Al    -2.954796     0.002344    -0.976916
Al    -5.101430    -0.003346     1.000257

    6
5t    scf done: -1207.776974
 C    -0.219069     0.000000     0.950298
Mg     3.503939    -0.000000     1.013952
Al     1.241895    -0.000000    -0.410781
Al     1.194387    -0.000000     2.360568
Al    -1.158214    -1.711801     0.933985
Al    -1.158214     1.711801     0.933985

    6
6t    scf done: -1207.774182
 C    -0.578615    -0.000000    -0.250300
Al     0.312474    -0.000000     1.365522
Mg     3.073250     0.000000     1.008543
Al     3.374121     0.000000    -1.643090
Al     0.880499    -0.000000    -1.387856
Al    -2.449682    -0.000000    -0.659978

    6
7t    scf done: -1207.771080
Al     0.050131    -0.001125     1.642545
Mg     2.770840     0.000665     1.602583
 C     4.870457     0.000282     1.613211
Al     5.411001     0.000265    -0.264505
Al     5.360307     1.644693     2.553900
Al     5.357800    -1.644781     2.554266

    6
8t    scf done: -1207.770924
 C    -0.090262     0.648551     1.068062
Al     1.718468     1.024453     1.390486
Al     1.192414    -0.045647     3.682862
Mg    -1.346700    -0.884882     4.008624
Al    -1.171560     1.469981     2.405531
Al    -0.422203    -1.210610     1.325975

    6
```

```
9t    scf done: -1207.770768
 C    -0.000000     0.000000    -0.680112
Mg     0.000000    -0.000000     2.961430
Al    -0.000000     1.378691     0.732771
Al    -0.000000    -1.378691     0.732771
Al    -0.000000     1.483191    -1.942636
Al    -0.000000    -1.483191    -1.942636

    6
10t   scf done: -1207.762263
 C    -0.009231    -0.000000    -0.562207
Al     0.044419    -0.000000     1.355503
Al     1.911161     0.000000    -0.816858
Al     2.439826     0.000000    -3.340892
Al    -0.013065    -0.000000    -2.597289
Mg    -2.057382    -0.000000    -1.017908
```