Tetracarbalane Structures: Nido Polyhedra and Non-spherical Deltahedra

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Supporting Information

Complete Gaussian09 Reference (reference 23)

Gaussian 09, Revision E.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Table S1A. Initial $(CH_3)_6Al_2C_4$ structures, a total of 22 structures:

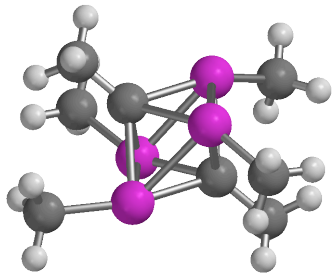
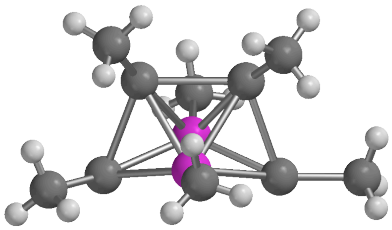
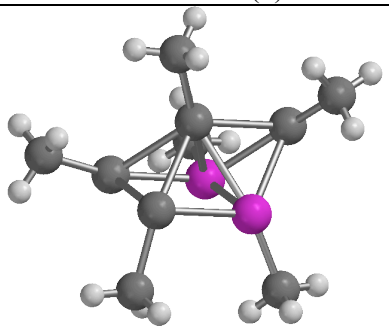
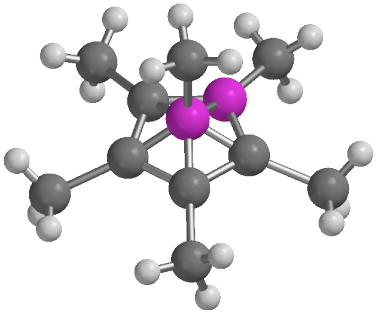
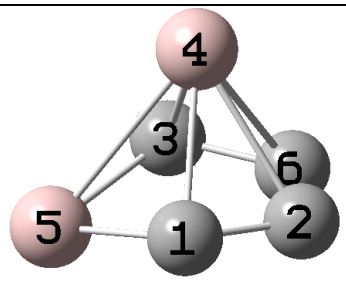
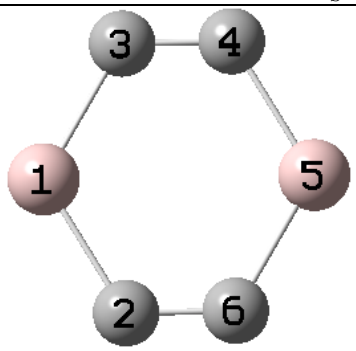
 Octahedron (2)	 Bicapped Tetrahedron (7)
 Capped tetragonal pyramid (9)	 Pentagonal pyramid (4)

Table 1B. Distance table for the lowest-lying $(CH_3)_6Al_2C_4$ structures after PBE0/Def2TZVPP optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry: For clarity, only the atoms forming the cluster framework are presented.



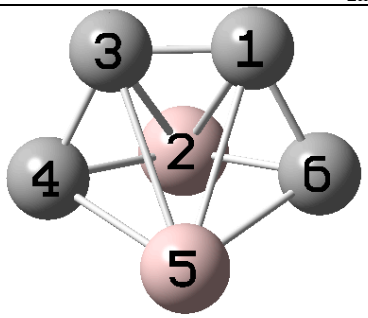
1. -875.8022003 0.0 C_S

		1	2	3	4	5
1	C	0.000000				
2	C	1.464018	0.000000			
3	C	2.690299	2.449180	0.000000		
4	Al	2.141121	2.200543	2.141141	0.000000	
5	Al	1.965056	2.796233	1.965079	2.613206	0.000000
6	C	2.449201	1.433009	1.463991	2.200577	2.796232



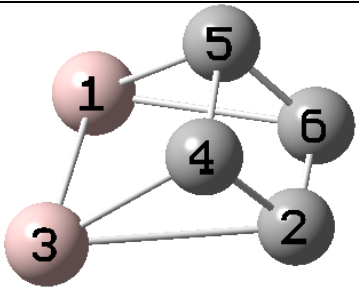
2. -875.7846969 +11.0 D_{2h}

		1	2	3	4	5
1	Al	0.000000				
2	C	1.972701	0.000000			
3	C	1.975051	3.400831	0.000000		
4	C	2.925915	3.679805	1.366343	0.000000	
5	Al	3.371074	2.925928	2.905732	1.972695	0.000000
6	C	2.905728	1.366350	3.650210	3.400815	1.975048



3. -875.7821209 +12.6 C_{2v}

		1	2	3	4	5
1	C	0.000000				
2	Al	2.361782	0.000000			
3	C	1.416652	2.361651	0.000000		
4	C	2.483955	1.995104	1.526675	0.000000	
5	Al	2.363084	2.833951	2.362867	1.994773	0.000000
6	C	1.526040	1.995564	2.483514	2.710030	1.995227



4. -875.7511818 +32.0 C_1

		1	2	3	4	5
1	Al	0.000000				
2	C	3.030421	0.000000			
3	Al	2.505087	2.678975	0.000000		
4	C	2.826251	1.520667	2.024823	0.000000	
5	C	2.055849	2.115946	2.871586	1.601112	0.000000
6	C	2.508946	1.381383	3.327774	2.125621	1.506113

Table 1C. Energy ranking for all of the $(CH_3)_6Al_2C_4$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	06v-04-PentPyr-a	-876.5284846	0.00
2	06v-03-CapTetrPyr-h	-876.5284819	0.00
3	06v-03-CapTetrPyr-e	-876.5284799	0.00
4	06v-02-BicappTd-b	-876.5173314	7.00
5	06v-03-CapTetrPyr-f	-876.5172640	7.04
6	06v-03-CapTetrPyr-c	-876.5171701	7.10
7	06v-03-CapTetrPyr-b	-876.5103238	11.40
8	06v-02-BicappTd-g	-876.5102530	11.44
9	06v-01-Oh-b	-876.4751512	33.47
10	06v-03-CapTetrPyr-i	-876.4750278	33.55
11	06v-03-CapTetrPyr-g	-876.4628336	41.20
12	06v-02-BicappTd-d	-876.4627205	41.27
13	06v-03-CapTetrPyr-a	-876.4627205	41.27
14	06v-03-CapTetrPyr-d	-876.4627205	41.27
15	06v-02-BicappTd-f	-876.4627195	41.27
16	06v-02-BicappTd-e	-876.4627183	41.27
17	06v-04-PentPyr-c	-876.4627064	41.28
18	06v-04-PentPyr-b	-876.4517512	48.15
19	06v-02-BicappTd-a	-876.4517438	48.16
20	06v-02-BicappTd-c	-876.4458464	51.86
21	06v-01-Oh-a	-876.3928864	85.09

Table 2A. Initial $(CH_3)_7Al_3C_4$ structures, a total of 51 structures:

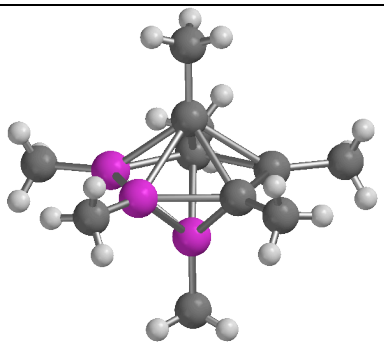
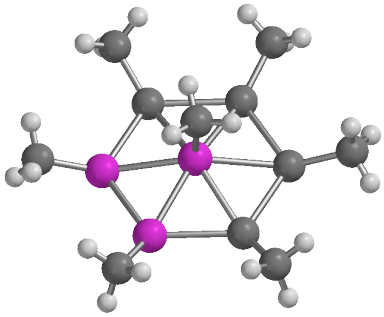
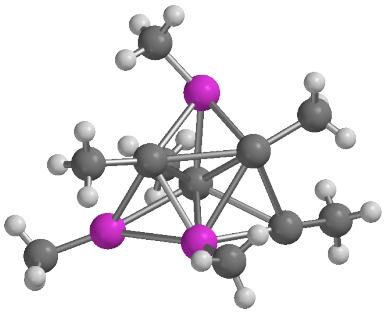
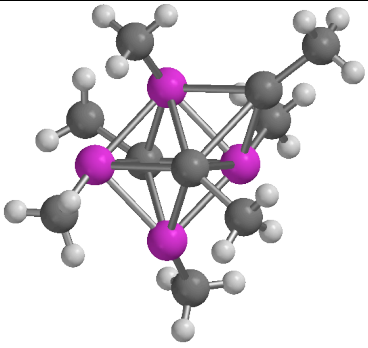
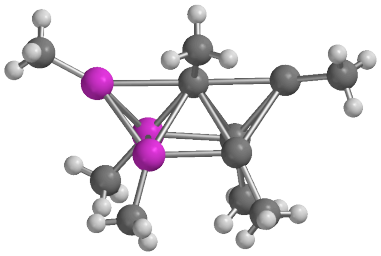
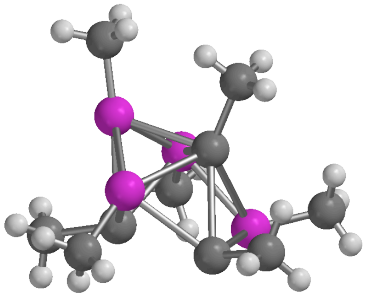
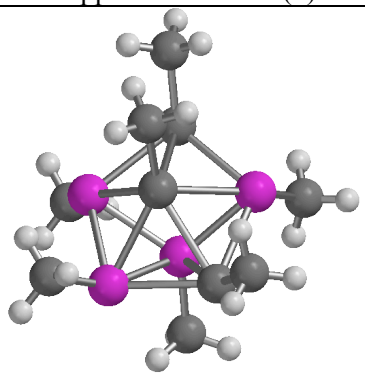
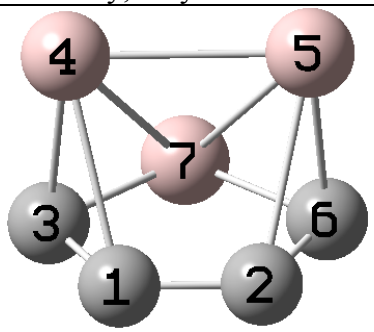
Initial	structures	 Pentagonal bipyramid (5)
 Hexagonal pyramid (6)	 Tricapped tetrahedron (12)	 Capped octahedron (8)
 Dicapped tetragonal pyr (11)	 Bisdisphenoid-1vxA (6)	 Bisdisphenoid-1vxAB (3)

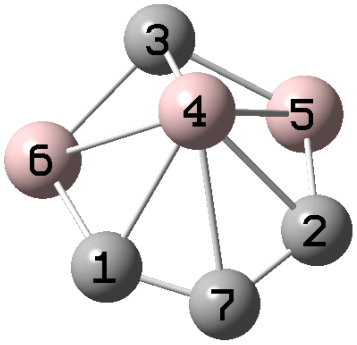
Table 2B. Distance table for the lowest-lying $(CH_3)_7Al_3C_4$ structures after PBE0/Def2TZVPP optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity, only the atoms forming the cluster framework are presented.



1. -1157.9701703 0.0 C_S

		1	2	3	4	5
1	C	0.000000				
2	C	1.439656	0.000000			
3	C	1.457508	2.482570	0.000000		
4	Al	2.380447	3.035914	2.129595	0.000000	
5	Al	3.035880	2.380431	3.384264	2.465993	0.000000
6	C	2.482566	1.457506	2.805404	3.384287	2.129614
7	Al	2.740018	2.740017	1.951818	2.999066	2.999074

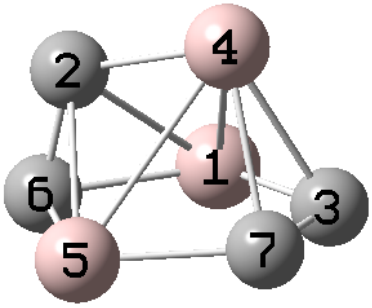
		6	7
6	C	0.000000	
7	Al	1.951814	0.000000



2. -1157.9670341 +2.0 C_S

		1	2	3	4	5
1	C	0.000000				
2	C	2.505414	0.000000			
3	C	3.033289	3.033212	0.000000		
4	Al	2.155889	2.156148	2.092697	0.000000	
5	Al	3.428181	1.984465	1.947662	2.650855	0.000000
6	Al	1.984564	3.427234	1.947597	2.651155	3.117602
7	C	1.436988	1.437063	3.464523	2.311549	3.042249

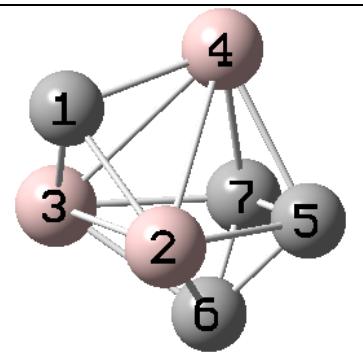
		6	7
6	Al	0.000000	
7	C	3.041573	0.000000



3. -1157.9520265 +11.4 C_S

		1	2	3	4	5
1	Al	0.000000				
2	C	2.312368	0.000000			
3	C	1.984005	3.091545	0.000000		
4	Al	2.737325	1.979819	2.183477	0.000000	
5	Al	3.112144	2.313932	2.894542	2.737254	0.000000
6	C	1.999060	1.479820	3.131121	3.012127	1.998706
7	C	2.894865	3.091778	1.427563	2.182560	1.984133

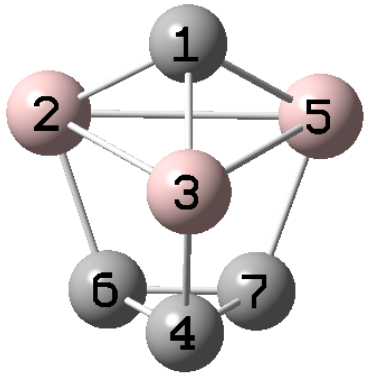
		6	7
6	C	0.000000	
7	C	3.131268	0.000000



4. -1157.9449099 +15.8 C_S

		1	2	3	4	5
1	C	0.000000				
2	Al	1.979714	0.000000			
3	Al	1.980306	2.666528	0.000000		
4	Al	1.980303	2.666571	2.665706	0.000000	
5	C	3.004857	2.100588	2.940227	2.100117	0.000000
6	C	3.004919	2.100505	2.100233	2.940326	1.588506
7	C	3.005754	2.939470	2.100765	2.100973	1.586284

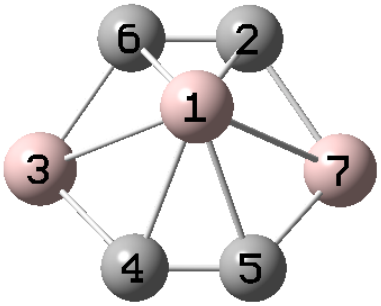
		6	7
6	C	0.000000	
7	C	1.586270	0.000000



5. -1157.9378768 +20.3 C_{3v}

		1	2	3	4	5
1	C	0.000000				
2	Al	1.980272	0.000000			
3	Al	1.980193	2.876465	0.000000		
4	C	3.044368	2.907155	1.975475	0.000000	
5	Al	1.979816	2.876598	2.877559	2.902345	0.000000
6	C	3.044161	1.975670	2.902097	1.576249	2.906055
7	C	3.043729	2.902491	2.906255	1.575373	1.975113

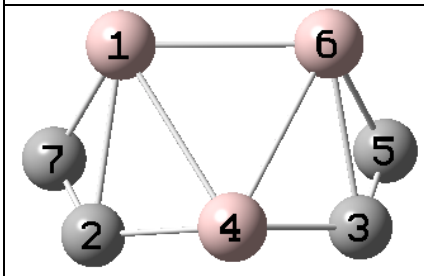
		6	7
6	C	0.000000	
7	C	1.575705	0.000000



6. -1157.9357916 +21.6 C_{2v}

		1	2	3	4	5
1	Al	0.000000				
2	C	2.213410	0.000000			
3	Al	2.670158	3.024444	0.000000		
4	C	2.212263	3.379951	1.959496	0.000000	
5	C	2.213941	3.055222	3.024424	1.444767	0.000000
6	C	2.212003	1.444988	1.959329	3.055993	3.380052
7	Al	2.672733	1.958945	3.675526	3.025084	1.959105

		6	7
6	C	0.000000	
7	Al	3.025120	0.000000



7. -1157.9233753 +29.4 C_S

		1	2	3	4	5
1	Al	0.000000				
2	C	2.479396	0.000000			
3	C	3.898669	3.453262	0.000000		
4	Al	2.865267	2.022201	2.031621	0.000000	
5	C	3.889675	4.083818	1.361341	3.024074	0.000000
6	Al	2.683846	3.912621	2.415830	2.826928	1.938015
7	C	1.937941	1.363401	4.077291	3.004991	4.284427

		6	7
6	Al	0.000000	
7	C	3.919774	0.000000

Table 2C. Energy ranking for all of the $(CH_3)_7Al_3C_4$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	07v-03-TricapTd-e2	-1158.8660676	0.00
2	07v-03-TricapTd-a5	-1158.8660622	0.00
3	07v-02-HexPyr-a2	-1158.8660585	0.01
4	07v-04-CapOh-i1	-1158.8660496	0.01
5	07v-04-CapOh-b4	-1158.8660460	0.01
6	07v-02-HexPyr-c1	-1158.8660448	0.01
7	07v-03-TricapTd-e1	-1158.8660445	0.01
8	07v-04-CapOh-k2	-1158.8660429	0.02
9	07v-04-CapOh-f2	-1158.8573216	5.49
10	07v-04-CapOh-e2	-1158.8573203	5.49
11	07v-07-BisdisphB-a2	-1158.8573180	5.49
12	07v-05-DicapTetrPyr-e1	-1158.8573174	5.49
13	07v-03-TricapTd-e4	-1158.8573168	5.49
14	07v-02-HexPyr-a1	-1158.8573151	5.49
15	07v-04-CapOh-a2	-1158.8500840	10.03
16	07v-01-PentBipyr-a3	-1158.8500741	10.04
17	07v-03-TricapTd-a4	-1158.8500391	10.06
18	07v-05-DicapTetrPyr-e3	-1158.8500081	10.08
19	07v-04-CapOh-e1	-1158.8390535	16.95
20	07v-03-TricapTd-c1	-1158.8390134	16.98
21	07v-02-HexPyr-a3	-1158.8368314	18.35
22	07v-06-BisdisphA-b1	-1158.8333649	20.52
23	07v-05-DicapTetrPyr-e2	-1158.8333533	20.53
24	07v-01-PentBipyr-c1	-1158.8333507	20.53
25	07v-04-CapOh-h1	-1158.8328112	20.87
26	07v-04-CapOh-c2	-1158.8327918	20.88
27	07v-05-DicapTetrPyr-a3	-1158.8327898	20.88
28	07v-06-BisdisphA-e2	-1158.8327877	20.88
29	07v-01-PentBipyr-c2	-1158.8327802	20.89
30	07v-04-CapOh-e3	-1158.8327702	20.89
31	07v-04-CapOh-c1	-1158.8327262	20.92
32	07v-07-BisdisphB-a1	-1158.8324530	21.09
33	07v-03-TricapTd-b1	-1158.8324491	21.10
34	07v-06-BisdisphA-a2	-1158.8324490	21.10
35	07v-03-TricapTd-a2	-1158.8300914	22.58
36	07v-04-CapOh-k1	-1158.8300072	22.63
37	07v-03-TricapTd-e3	-1158.8293811	23.02
38	07v-01-PentBipyr-a1	-1158.8212235	28.14
39	07v-03-TricapTd-b2	-1158.8212233	28.14
40	07v-06-BisdisphA-a3	-1158.8212206	28.14
41	07v-02-HexPyr-b2	-1158.8190474	29.51

42	07v-05-DicapTetrPyr-a2	-1158.8190466	29.51
43	07v-05-DicapTetrPyr-c1	-1158.8190453	29.51
44	07v-06-BisdisphA-a1	-1158.8190402	29.51
45	07v-04-CapOh-b2	-1158.8071192	36.99
46	07v-01-PentBipyr-a2	-1158.8071088	37.00
47	07v-04-CapOh-f1	-1158.8011557	40.73
48	07v-04-CapOh-a3	-1158.7988320	42.19
49	07v-05-DicapTetrPyr-c3	-1158.7951982	44.47
50	07v-03-TricapTd-a3	-1158.7922439	46.33
51	07v-07-BisdisphB-a3	-1158.7921788	46.37
52	07v-06-BisdisphA-e1	-1158.7892355	48.21
53	07v-04-CapOh-b1	-1158.7877174	49.17
54	07v-04-CapOh-a1	-1158.7877163	49.17
55	07v-02-HexPyr-b1	-1158.7844834	51.20
56	07v-05-DicapTetrPyr-a1	-1158.7844005	51.25
57	07v-05-DicapTetrPyr-f1	-1158.7830364	52.10
58	07v-03-TricapTd-a1	-1158.7815570	53.03
59	07v-05-DicapTetrPyr-c2	-1158.7815480	53.04
60	07v-04-CapOh-b3	-1158.7305348	85.05
61	07v-05-DicapTetrPyr-b1	-1158.6999975	104.21

Table 3A. Initial $(CH_3)_8Al_4C_4$ structures, a total of 105 structures:

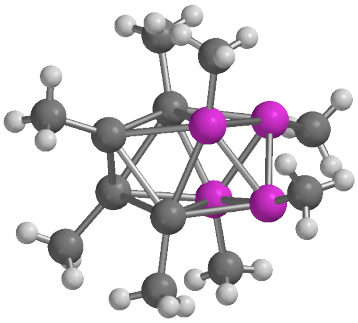
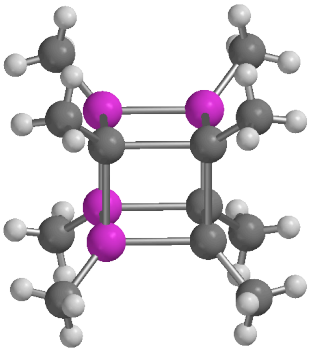
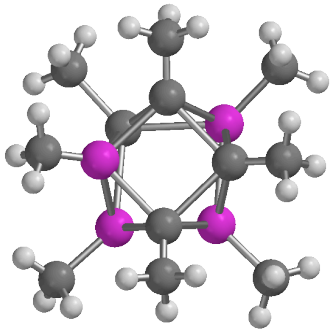
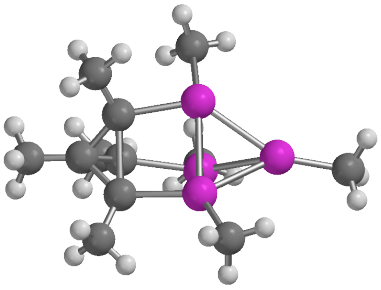
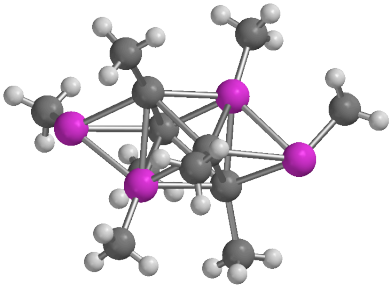
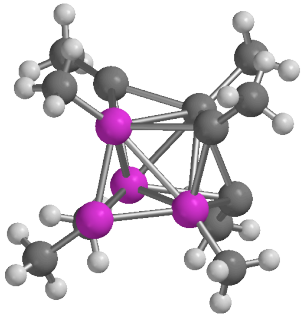
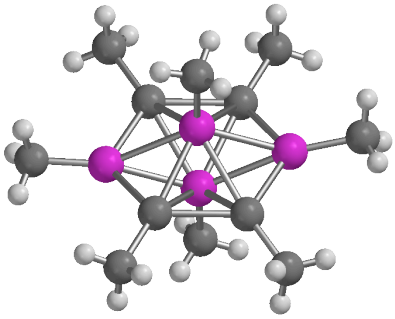
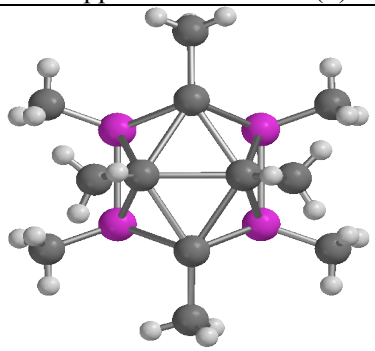
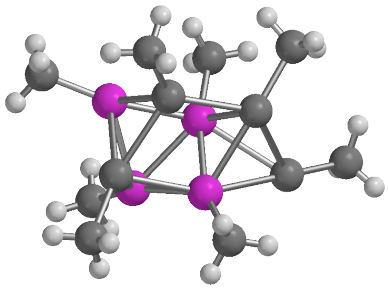
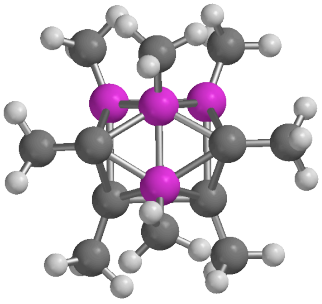
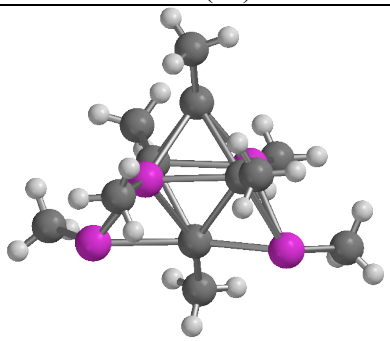
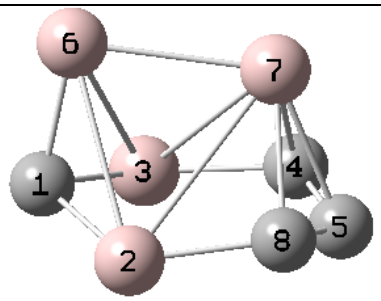
Initial structures	 Bisdisphenoid (21)	 Cube (4)
 Tetragonal antiprism (9)	 Dicapped trigonal prism (10)	 Bicapped octahedron A (8)
 All-capped Td (8)	 Hexagonal bipyramid (9)	 Nido (12)
 Dicapped trigonal prismA (12)	 Dicapped trigonal prismB (6)	 Bicapped octahedron B (6)

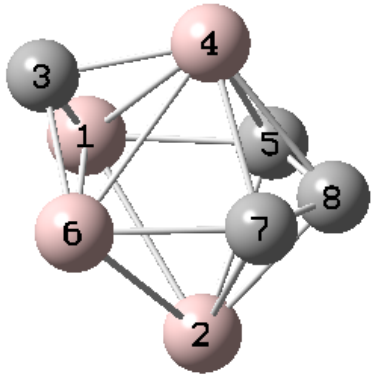
Table 3B. Distance table for the lowest-lying $(CH_3)_8Al_4C_4$ structures after PBE0/Def2TZVPP optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity, only the atoms forming the cluster framework are presented.



1. -1440.1427500 0.0 C_S

		1	2	3	4	5
1	C	0.000000				
2	Al	1.973848	0.000000			
3	Al	1.974193	3.028224	0.000000		
4	C	3.381104	3.377358	1.970211	0.000000	
5	C	3.820149	3.000451	2.999773	1.434077	0.000000
6	Al	1.977650	2.910825	2.909874	3.698354	4.186890
7	Al	3.384415	3.094404	3.095845	2.218196	2.287602
8	C	3.380263	1.969840	3.376162	2.483801	1.434176

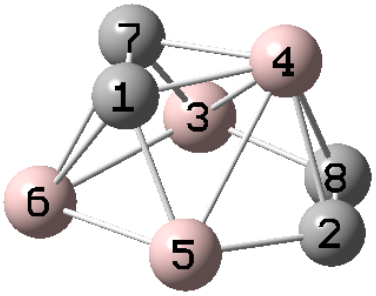
		6	7	8
6	Al	0.000000		
7	Al	2.597000	0.000000	
8	C	3.699106	2.217031	0.000000



2. -1440.1403677 +1.5 C_S

		1	2	3	4	5
1	Al	0.000000				
2	Al	2.677091	0.000000			
3	C	1.977311	3.620205	0.000000		
4	Al	2.694821	3.576807	1.953705	0.000000	
5	C	2.115562	2.325252	3.099853	2.216778	0.000000
6	Al	2.805412	2.670279	1.978267	2.698174	3.367155
7	C	3.378993	2.323845	3.109558	2.230213	2.457989
8	C	3.197892	2.266111	3.591150	2.327878	1.451259

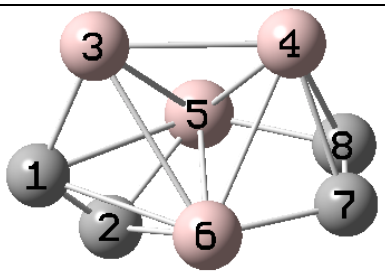
		6	7	8
6	Al	0.000000		
7	C	2.118586	0.000000	
8	C	3.192562	1.448746	0.000000



3. -1440.1245544 +11.4 C_S

		1	2	3	4	5
1	C	0.000000				
2	C	3.163167	0.000000			
3	Al	3.074706	3.002994	0.000000		
4	Al	2.078240	2.219621	2.746847	0.000000	
5	Al	2.088911	2.047747	3.461914	2.746326	0.000000
6	Al	2.345816	3.698916	2.570760	3.674767	2.570401
7	C	1.470448	3.471841	2.088487	2.078726	3.074514
8	C	3.472311	1.393889	2.047480	2.220568	3.003084

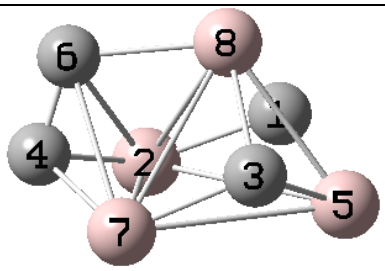
		6	7	8
6	Al	0.000000		
7	C	2.345493	0.000000	
8	C	3.698783	3.163182	0.000000



4. -1440.1201577 +14.2 C_S

		1	2	3	4	5
1	C	0.000000				
2	C	1.404759	0.000000			
3	Al	2.001288	2.856999	0.000000		
4	Al	3.745197	3.618172	2.557033	0.000000	
5	Al	2.784055	2.043132	2.977119	2.735491	0.000000
6	Al	2.499000	2.128188	2.845519	2.719367	3.020210
7	C	4.004929	3.185370	3.915339	2.259019	2.835597
8	C	4.126842	3.213400	3.969262	2.256436	2.004515

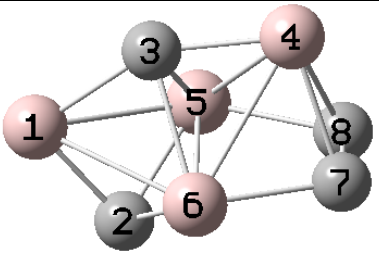
		6	7	8
6	Al	0.000000		
7	C	2.015843	0.000000	
8	C	2.913998	1.400088	0.000000



5. -1440.1188460 +15.0 C_S

		1	2	3	4	5
1	C	0.000000				
2	Al	1.914165	0.000000			
3	C	2.962092	3.600992	0.000000		
4	C	3.362984	2.083112	3.340546	0.000000	
5	Al	1.958683	3.195226	1.965742	4.059150	0.000000
6	C	3.210948	2.584894	3.196973	1.394317	4.100718
7	Al	3.605841	3.144014	1.919083	2.073385	3.183854
8	Al	2.097894	2.917970	2.080683	2.944966	2.656720

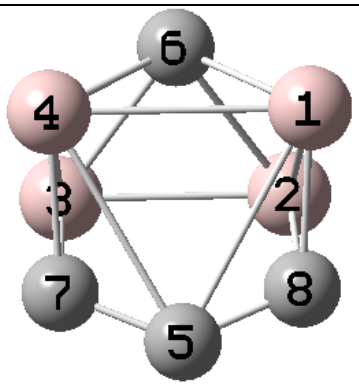
		6	7	8
6	C	0.000000		
7	Al	2.615845	0.000000	
8	Al	2.102691	2.939707	0.000000



6. -1440.1179821 +15.5 C_S

		1	2	3	4	5
1	Al	0.000000				
2	C	1.932779	0.000000			
3	C	2.033459	2.754330	0.000000		
4	Al	3.852538	3.771747	1.958858	0.000000	
5	Al	2.664398	2.036649	2.239376	2.691629	0.000000
6	Al	2.665434	2.035325	2.243825	2.691646	2.797201
7	C	4.323069	3.265503	3.196154	2.150722	2.900531
8	C	4.322265	3.264338	3.195176	2.152300	2.133598

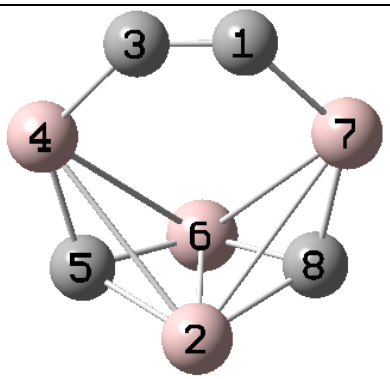
		6	7	8
6	Al	0.000000		
7	C	2.133601	0.000000	
8	C	2.899212	1.378884	0.000000



7. -1440.1165667 +16.4 C_S

		1	2	3	4	5
1	Al	0.000000				
2	Al	2.607262	0.000000			
3	Al	3.693310	2.439895	0.000000		
4	Al	2.793068	3.686510	2.608378	0.000000	
5	C	2.846567	2.944935	2.942244	2.848386	0.000000
6	C	2.000974	2.308907	2.318265	1.999474	3.294761
7	C	3.359604	3.272925	2.094721	2.014997	1.447268
8	C	2.014956	2.095964	3.270807	3.360174	1.446811

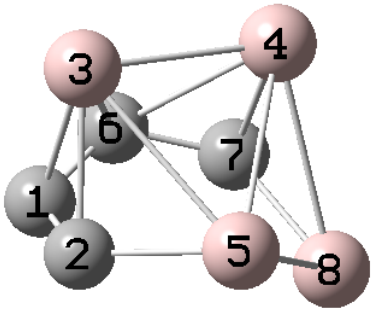
		6	7	8
6	C	0.000000		
7	C	2.970003	0.000000	
8	C	2.968159	2.588103	0.000000



8. -1440.1161435 +16.7 C_S

		1	2	3	4	5
1	C	0.000000				
2	Al	3.891848	0.000000			
3	C	1.366894	3.891327	0.000000		
4	Al	3.031742	3.182164	1.986199	0.000000	
5	C	4.060864	1.982116	3.532535	1.959921	0.000000
6	Al	4.141618	2.596625	4.141503	3.214696	1.980529
7	Al	1.986226	3.182364	3.031605	3.837902	3.886039
8	C	3.532573	1.981962	4.060316	3.885483	2.933261

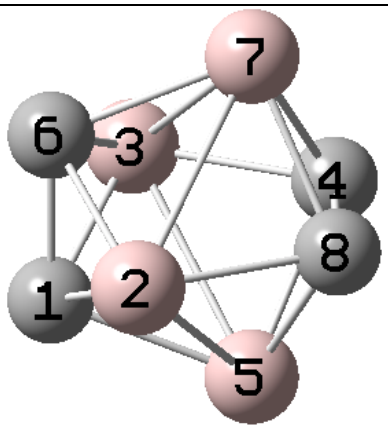
		6	7	8
6	Al	0.000000		
7	Al	3.215235	0.000000	
8	C	1.980654	1.960066	0.000000



9. -1440.1135879 +18.3 C_1

		1	2	3	4	5
1	C	0.000000				
2	C	1.414294	0.000000			
3	Al	2.260702	2.173237	0.000000		
4	Al	3.337568	3.413913	2.523770	0.000000	
5	Al	3.115904	2.032331	2.818131	2.859690	0.000000
6	C	1.472324	2.544072	2.561444	2.532561	3.513871
7	C	2.581820	3.169965	3.403164	2.154637	3.348074
8	Al	3.470809	3.266229	4.133602	2.788238	2.504816

		6	7	8
6	C	0.000000		
7	C	1.463004	0.000000	
8	Al	3.065325	1.956164	0.000000



10. -1440.1074182 +22.2 D_{2d}

		1	2	3	4	5
1	C	0.000000				
2	Al	2.032260	0.000000			
3	Al	2.035586	3.326367	0.000000		
4	C	2.971287	3.162056	2.078296	0.000000	
5	Al	2.078435	2.602056	2.602167	2.031062	0.000000
6	C	1.707271	2.035539	2.032290	2.972042	3.162025
7	Al	3.162115	2.602223	2.602153	2.036830	3.326419
8	C	2.972265	2.078432	3.162107	1.707331	2.036824
		6	7	8		
6	C	0.000000				
7	Al	2.078296	0.000000			
8	C	2.971256	2.031115	0.000000		

Table 3C. Energy ranking for all of the $(CH_3)_8Al_4C_4$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	08v-01-Bisdisph-b33	-1441.2052586	0.00
2	08v-01-Bisdisph-g21	-1441.2052398	0.01
3	08v-07-Bipirhex-a11	-1441.2051638	0.06
4	08v-09-DicapTrPrA-a111	-1441.2051550	0.07
5	08v-07-Bipirhex-a17	-1441.2051193	0.09
6	08v-03-Antipr-a21	-1441.2046661	0.37
7	08v-09-DicapTrPrA-a13	-1441.2045664	0.43
8	08v-11-DicapOh-a16	-1441.2045627	0.44
9	08v-01-Bisdisph-a22	-1441.1998207	3.41
10	08v-06-Tdallcap-a15	-1441.1998203	3.41
11	08v-01-Bisdisph-f23	-1441.1998200	3.41
12	08v-02-Cube-a13	-1441.1998082	3.42
13	08v-09-DicapTrPrA-a12	-1441.1985781	4.19
14	08v-09-DicapTrPrA-a18	-1441.1985720	4.20
15	08v-05-AntiprTrig-a13	-1441.1985712	4.20
16	08v-07-Bipirhex-a19	-1441.1985712	4.20
17	08v-04-TrigPyr-a21	-1441.1985671	4.20
18	08v-03-Antipr-a31	-1441.1985308	4.22
19	08v-05-AntiprTrig-a16	-1441.1867055	11.64
20	08v-06-Tdallcap-a17	-1441.1864292	11.82
21	08v-07-Bipirhex-a18	-1441.1863934	11.84
22	08v-08-Nido-a16	-1441.1863794	11.85
23	08v-06-Tdallcap-a13	-1441.1863764	11.85
24	08v-11-DicapOh-a15	-1441.1863645	11.86

25	08v-09-DicapTrPrA-a16	-1441.1863494	11.87
26	08v-07-Bipirhex-a15	-1441.1854090	12.46
27	08v-01-Bisdisph-a14	-1441.1840528	13.31
28	08v-01-Bisdisph-j11	-1441.1840513	13.31
29	08v-07-Bipirhex-a14	-1441.1840464	13.31
30	08v-01-Bisdisph-a13	-1441.1802554	15.69
31	08v-07-Bipirhex-a12	-1441.1799356	15.89
32	08v-04-TrigPyr-a22	-1441.1799305	15.89
33	08v-09-DicapTrPrA-a15	-1441.1799137	15.90
34	08v-11-DicapOh-a11	-1441.1756766	18.56
35	08v-01-Bisdisph-b21	-1441.1756764	18.56
36	08v-08-Nido-a13	-1441.1756760	18.56
37	08v-03-Antipr-a22	-1441.1756658	18.57
38	08v-05-AntiprTrig-a18	-1441.1756211	18.60
39	08v-10-DicapTrPrB-a12	-1441.1737659	19.76
40	08v-08-Nido-a14	-1441.1737532	19.77
41	08v-08-Nido-a110	-1441.1737502	19.77
42	08v-09-DicapTrPrA-a14	-1441.1737493	19.77
43	08v-02-Cube-a12	-1441.1737468	19.77
44	08v-05-AntiprTrig-a14	-1441.1737468	19.77
45	08v-01-Bisdisph-b41	-1441.1737464	19.77
46	08v-08-Nido-a11	-1441.1737437	19.78
47	08v-03-Antipr-a12	-1441.1737431	19.78
48	08v-06-Tdallcap-a14	-1441.1737429	19.78
49	08v-01-Bisdisph-a12	-1441.1737372	19.78
50	08v-05-AntiprTrig-a15	-1441.1685979	23.01
51	08v-08-Nido-a12	-1441.1683569	23.16
52	08v-04-TrigPyr-a11	-1441.1683422	23.17
53	08v-01-Bisdisph-c43	-1441.1667196	24.18
54	08v-07-Bipirhex-a16	-1441.1666501	24.23
55	08v-08-Nido-a18	-1441.1666398	24.23
56	08v-03-Antipr-c21	-1441.1666378	24.24
57	08v-01-Bisdisph-a31	-1441.1665708	24.28
58	08v-05-AntiprTrig-a17	-1441.1664897	24.33
59	08v-01-Bisdisph-b22	-1441.1664359	24.36
60	08v-01-Bisdisph-f21	-1441.1664240	24.37
61	08v-06-Tdallcap-a16	-1441.1664056	24.38
62	08v-08-Nido-a17	-1441.1624575	26.86
63	08v-04-TrigPyr-a41	-1441.1624546	26.86
64	08v-08-Nido-a15	-1441.1608250	27.88
65	08v-09-DicapTrPrA-a11	-1441.1608056	27.90
66	08v-04-TrigPyr-a13	-1441.1595093	28.71
67	08v-01-Bisdisph-b32	-1441.1555101	31.22
68	08v-05-AntiprTrig-a12	-1441.1554671	31.25
69	08v-04-TrigPyr-f21	-1441.1548153	31.65

70	08v-04-TrigPyr-a12	-1441.1519710	33.44
71	08v-04-TrigPyr-f22	-1441.1518705	33.50
72	08v-09-DicapTrPrA-a17	-1441.1483314	35.72
73	08v-11-DicapOh-a12	-1441.1483133	35.73
74	08v-08-Nido-a112	-1441.1482871	35.75
75	08v-01-Bisdisph-a11	-1441.1478608	36.02
76	08v-11-DicapOh-a13	-1441.1472838	36.38
77	08v-10-DicapTrPrB-a14	-1441.1441929	38.32
78	08v-01-Bisdisph-a21	-1441.1421803	39.58
79	08v-10-DicapTrPrB-a15	-1441.1421768	39.59
80	08v-01-Bisdisph-f22	-1441.1372088	42.70
81	08v-11-DicapOh-a14	-1441.1370768	42.79
82	08v-01-Bisdisph-b31	-1441.1369717	42.85
83	08v-01-Bisdisph-c42	-1441.1369703	42.85
84	08v-03-Antipr-a13	-1441.1369698	42.85
85	08v-03-Antipr-b11	-1441.1369696	42.85
86	08v-01-Bisdisph-c41	-1441.1369677	42.85
87	08v-07-Bipirhex-a13	-1441.1339209	44.77
88	08v-09-DicapTrPrA-a110	-1441.1290102	47.85
89	08v-10-DicapTrPrB-a13	-1441.1290061	47.85
90	08v-03-Antipr-a32	-1441.1277212	48.66
91	08v-08-Nido-a19	-1441.1277197	48.66
92	08v-04-TrigPyr-f11	-1441.1254813	50.06
93	08v-06-Tdallcap-a18	-1441.1120924	58.46
94	08v-04-TrigPyr-a31	-1441.1094832	60.10
95	08v-05-AntiprTrig-a11	-1441.1056840	62.49
96	08v-09-DicapTrPrA-a19	-1441.1056811	62.49
97	08v-06-Tdallcap-a12	-1441.1024330	64.53
98	08v-02-Cube-a11	-1441.1022245	64.66
99	08v-09-DicapTrPrA-a112	-1441.0999097	66.11
100	08v-08-Nido-a111	-1441.0999090	66.11
101	08v-03-Antipr-a11	-1441.0998971	66.12
102	08v-10-DicapTrPrB-a16	-1441.0998959	66.12
103	08v-06-Tdallcap-a11	-1441.0957958	68.69
104	08v-10-DicapTrPrB-a11	-1441.0903267	72.12
105	08v-02-Cube-a21	-1441.0693718	85.27

Table 4A. Initial $(CH_3)_9Al_5C_4$ structures, a total of 76 structures:

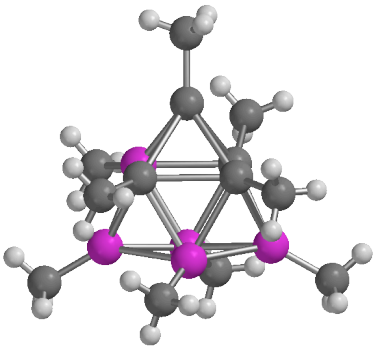
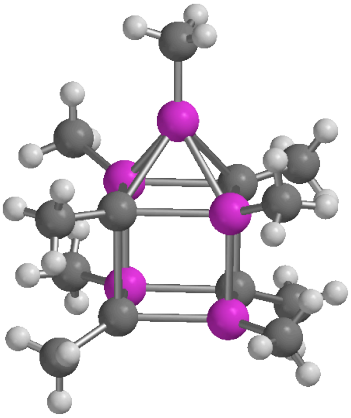
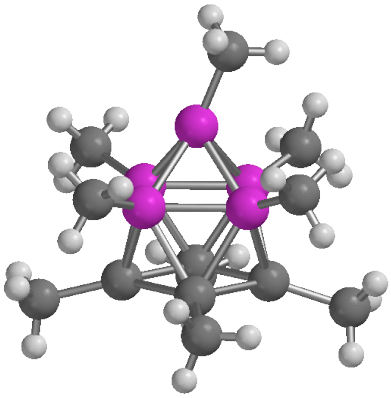
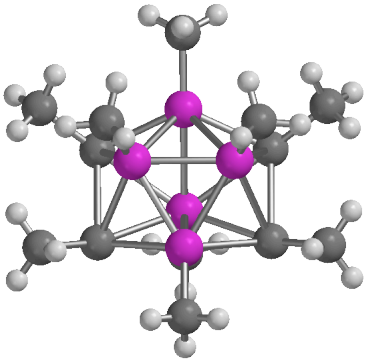
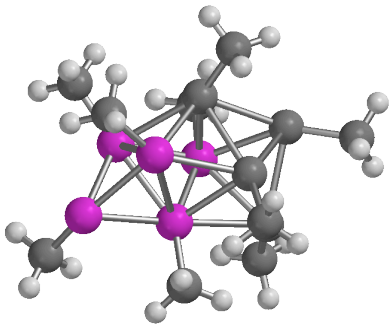
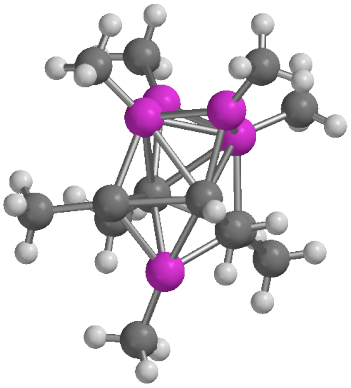
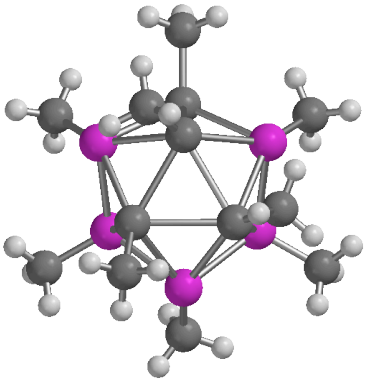
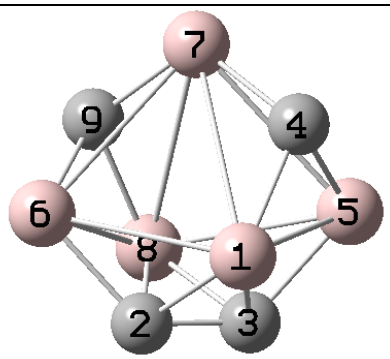
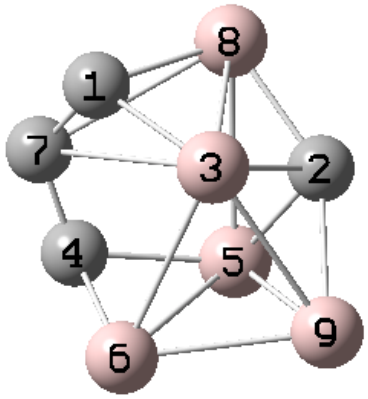
Initial	structures	 Tricapped trigonal prism (8)
 Capped cube (14)	 Capped square antiprism (10)	 Isocloso (10)
 Capped bisdisphenoid (12)	 Bicapped pentag bipyr (12)	 10vx-Isocloso-1vx (10)

Table 4B. Distance table for the lowest-lying $(CH_3)_9Al_5C_4$ structures after PBE0/Def2TZVPP optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity, only the atoms forming the cluster framework are presented.



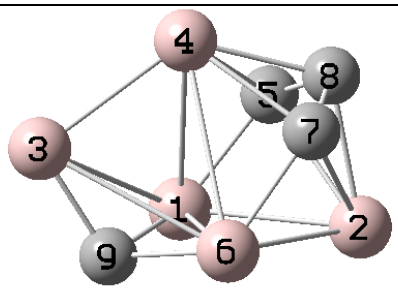
1. -1722.3032799 0.0 C_2

		1	2	3	4	5
1	Al	0.000000				
2	C	2.109613	0.000000			
3	C	2.161315	1.577926	0.000000		
4	C	2.018845	3.463156	3.028939	0.000000	
5	Al	2.587295	3.246849	1.997555	1.965175	0.000000
6	Al	2.983299	1.997444	3.247639	3.677458	4.229827
7	Al	3.280524	3.803943	3.803069	1.956801	3.083609
8	Al	3.490111	2.160429	2.109750	3.684911	2.983684
9	C	3.685236	3.029480	3.465310	3.319268	3.678753
		6	7	8	9	
7	Al	3.087922	0.000000			
8	Al	2.587582	3.277547	0.000000		
9	C	1.965434	1.955388	2.021046	0.000000	



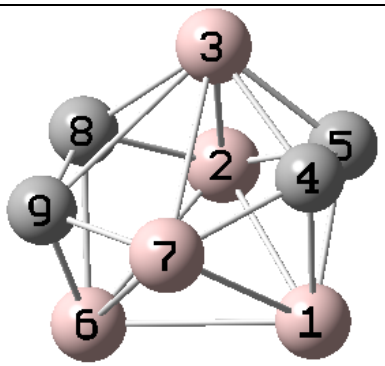
2. -1722.3029970 +0.2 C_1

		1	2	3	4	5
1	C	0.000000				
2	C	3.025032	0.000000			
3	Al	2.067517	2.185227	0.000000		
4	C	2.542028	3.317779	3.235273	0.000000	
5	Al	3.446542	2.106865	3.360753	2.076236	0.000000
6	Al	3.377392	3.461212	2.803387	2.060925	2.790177
7	C	1.443057	3.503426	2.983236	1.429870	2.986951
8	Al	2.016087	1.959505	2.618249	3.285205	2.918480
9	Al	4.174303	2.147645	2.677050	3.607897	2.567519
		6	7	8	9	
7	C	2.946657	0.000000			
8	Al	4.266846	2.722737	0.000000		
9	Al	2.555613	4.340416	3.937896	0.000000	



3. -1722.3008283 +1.5 C_S

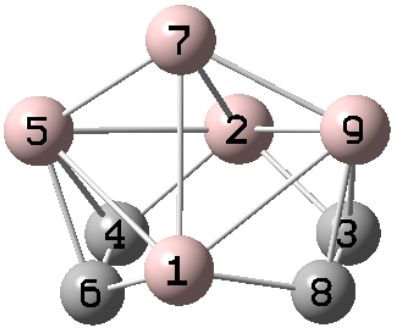
		1	2	3	4	5
1	Al	0.000000				
2	Al	2.684197	0.000000			
3	Al	3.079542	4.897807	0.000000		
4	Al	3.133013	3.842801	2.587178	0.000000	
5	C	2.074773	2.346199	3.883991	2.285837	0.000000
6	Al	2.790961	2.675157	3.079168	3.119864	3.336624
7	C	3.343166	2.344272	3.886165	2.267749	2.449158
8	C	3.167057	2.269080	4.350313	2.230697	1.453659
9	C	2.000521	3.693714	1.913584	3.290868	3.518315
		6	7	8	9	
7	C	2.081875	0.000000			
8	C	3.168609	1.455382	0.000000		
9	C	2.001344	3.525059	4.085025	0.000000	



4. -1722.2962195 +4.4 C_1

		1	2	3	4	5
1	Al	0.000000				
2	Al	2.664966	0.000000			
3	Al	3.529823	2.612395	0.000000		
4	C	2.149483	3.067721	2.051968	0.000000	
5	C	2.123931	2.020703	2.087425	1.569874	0.000000
6	Al	2.715990	2.679228	3.803000	3.650274	3.705601
7	Al	2.753389	3.787505	2.894176	2.046527	3.272172
8	C	3.550028	2.139081	2.048572	3.163252	3.082119
9	C	3.576368	3.281780	2.827049	3.229274	3.786963

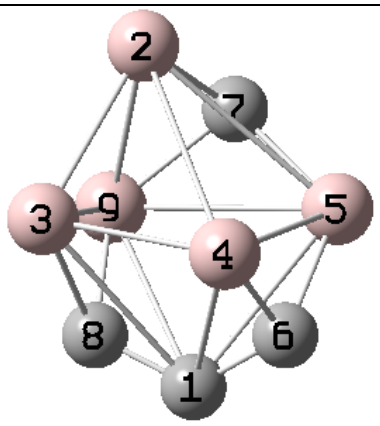
		6	7	8	9
6	Al	0.000000			
7	Al	2.822260	0.000000		
8	C	2.313047	2.883938	0.000000	
9	C	2.021074	1.946312	1.548690	0.000000



5. -1722.2953982 +5.0 C_{2V}

		1	2	3	4	5
1	Al	0.000000				
2	Al	3.331934	0.000000			
3	C	2.972097	2.056508	0.000000		
4	C	2.973151	2.057838	3.071992	0.000000	
5	Al	2.877989	2.878817	4.210827	2.204658	0.000000
6	C	2.058025	2.972847	3.368188	1.381673	2.204413
7	Al	2.949565	2.946554	3.782697	3.791381	2.514773
8	C	2.056518	2.971947	1.381681	3.368129	4.210476
9	Al	2.888477	2.888836	2.207162	4.224431	4.206522

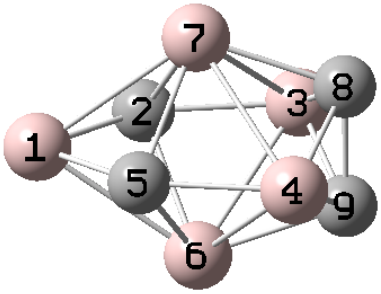
		6	7	8	9
6	C	0.000000			
7	Al	3.792477	0.000000		
8	C	3.071447	3.783906	0.000000	
9	Al	4.224252	2.511973	2.207432	0.000000



6. -1722.2945820 +5.4 C_1 ignored

		1	2	3	4	5
1	C	0.000000				
2	Al	4.303976	0.000000			
3	Al	3.044279	2.664640	0.000000		
4	Al	2.820436	3.443862	2.562448	0.000000	
5	Al	2.893982	3.237674	4.020496	3.090952	0.000000
6	C	1.454336	4.042617	3.405515	2.064384	2.011268
7	C	3.701092	1.982788	3.626760	3.884469	1.936082
8	C	1.420066	3.693804	2.150618	3.181098	3.420951
9	Al	2.910940	2.704002	2.831063	4.089159	3.038206

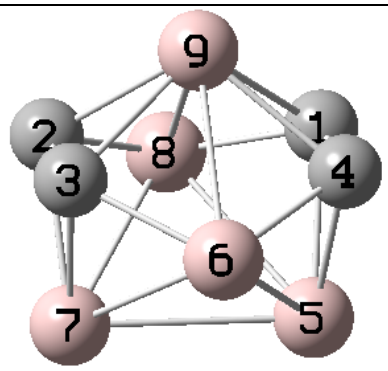
		6	7	8	9
6	C	0.000000			
7	C	3.410523	0.000000		
8	C	2.548579	3.439031	0.000000	
9	Al	3.461239	2.006610	2.037674	0.000000



7. -1722.2945624 +5.5 C_{2V}

		1	2	3	4	5
1	Al	0.000000				
2	C	1.963345	0.000000			
3	Al	3.828149	2.071415	0.000000		
4	Al	3.827488	3.737350	3.445681	0.000000	
5	C	1.963588	2.811339	3.740367	2.072071	0.000000
6	Al	2.597326	2.198758	2.647949	2.647099	2.195235
7	Al	2.596833	2.194361	2.646616	2.646691	2.201545
8	C	4.143811	3.147303	2.024473	2.013559	3.145701
9	C	4.143753	3.142789	2.013591	2.024359	3.148783

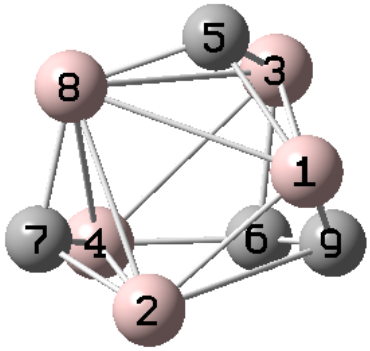
		6	7	8	9
6	Al	0.000000			
7	Al	3.042492	0.000000		
8	C	3.061848	2.070337	0.000000	
9	C	2.071012	3.060612	1.670865	0.000000



8. -1722.2931189 +6.4 C_{2V}

		1	2	3	4	5
1	C	0.000000				
2	C	3.105764	0.000000			
3	C	3.482070	1.575332	0.000000		
4	C	1.575112	3.483011	3.106084	0.000000	
5	Al	2.125229	3.617077	3.616508	2.123904	0.000000
6	Al	3.167167	3.168570	2.009462	2.007971	2.711765
7	Al	3.614973	2.125204	2.124057	3.614335	2.755875
8	Al	2.008949	2.009872	3.168336	3.167942	2.711481
9	Al	2.116685	2.115487	2.117058	2.119592	3.457470

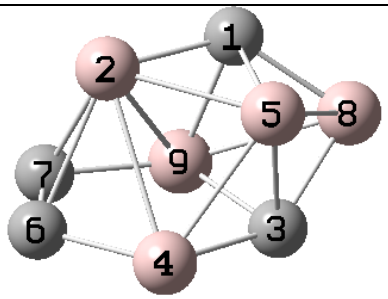
		6	7	8	9
6	Al	0.000000			
7	Al	2.710977	0.000000		
8	Al	3.808934	2.711223	0.000000	
9	Al	2.634279	3.455267	2.632348	0.000000



9. -1722.2885525 +9.2 C_1

		1	2	3	4	5
1	Al	0.000000				
2	Al	2.614434	0.000000			
3	Al	2.753866	4.363841	0.000000		
4	Al	3.754896	3.133553	3.070984	0.000000	
5	C	2.114487	3.618422	1.936074	3.482224	0.000000
6	C	3.116680	3.697061	2.142729	2.026599	3.392179
7	C	3.506074	1.992492	3.960749	1.940279	3.317264
8	Al	3.106425	2.982411	3.339315	3.021764	1.939049
9	C	2.109366	3.311977	2.299140	2.986283	3.153366

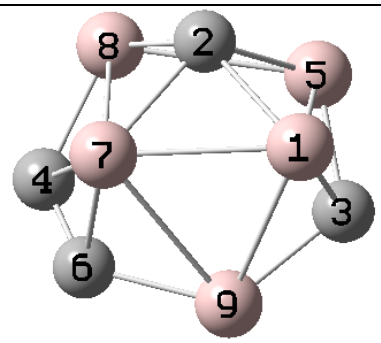
		6	7	8	9
6	C	0.000000			
7	C	3.479102	0.000000		
8	Al	4.003836	1.985270	0.000000	
9	C	1.398922	3.802144	4.097047	0.000000



10. -1722.2874637 +9.9 C_1

		1	2	3	4	5
1	C	0.000000				
2	Al	2.101505	0.000000			
3	C	2.755581	3.357187	0.000000		
4	Al	3.642421	2.869021	2.098483	0.000000	
5	Al	2.235784	2.540157	2.287539	2.585909	0.000000
6	C	3.917220	2.468295	3.394501	2.011542	3.838825
7	C	3.292147	2.238509	3.406143	2.855139	4.010127
8	Al	1.977865	3.734371	2.004338	3.851814	2.539360
9	Al	2.202755	2.715156	2.138370	3.019028	3.331238

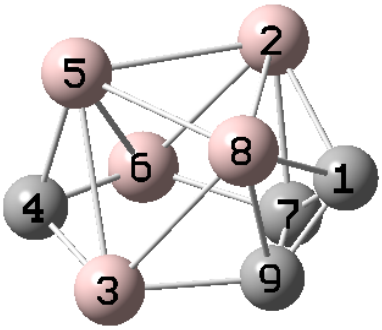
		6	7	8	9
6	C	0.000000			
7	C	1.381967	0.000000		
8	Al	4.790797	4.337710	0.000000	
9	Al	2.883917	2.032036	2.549557	0.000000



11. -1722.2861835 +10.7 C_1

		1	2	3	4	5
1	Al	0.000000				
2	C	2.131548	0.000000			
3	C	2.072961	3.016765	0.000000		
4	C	4.236931	3.185857	4.049611	0.000000	
5	Al	2.590858	2.101422	1.935431	3.887422	0.000000
6	C	3.806250	3.521356	3.516021	1.396550	4.038900
7	Al	2.620328	2.140900	3.610425	2.396444	3.708403
8	Al	3.839848	2.016076	3.864453	1.979595	2.781347
9	Al	2.775292	3.541215	1.964256	3.092448	3.359788

		6	7	8	9
6	C	0.000000			
7	Al	2.260094	0.000000		
8	Al	3.022709	2.728383	0.000000	
9	Al	2.009612	2.897907	3.892198	0.000000



12. -1722.2804876 +14.3 C_S

		1	2	3	4	5
1	C	0.000000				
2	Al	2.101887	0.000000			
3	Al	3.337397	3.959419	0.000000		
4	C	4.041413	3.682727	1.927435	0.000000	
5	Al	3.661172	2.706407	2.775871	2.083881	0.000000
6	Al	3.341328	2.690147	3.045502	1.927943	2.772740
7	C	1.565826	2.279007	3.045791	3.255249	3.583551
8	Al	2.095344	2.763374	2.699749	3.686237	2.706427
9	C	1.567843	3.098462	2.107834	3.253041	3.583726

		6	7	8	9
6	Al	0.000000			
7	C	2.114433	0.000000		
8	Al	3.959816	3.094528	0.000000	
9	C	3.049102	1.585963	2.284206	0.000000

Table 4C. Energy ranking for all of the $(CH_3)_9Al_5C_4$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	09v-07-Isocloso-6vx-a17	-1723.5346403	0.00
2	09v-05-CapBisdisph-a11	-1723.5261396	5.33
3	09v-06-BicapPentBipyr-a112	-1723.5261368	5.34
4	09v-06-BicapPentBipyr-a110	-1723.5261364	5.34
5	09v-02-CapCube-a18	-1723.5261344	5.34
6	09v-05-CapBisdisph-a16	-1723.5260750	5.37
7	09v-01-TricTrPrism-a16	-1723.5260713	5.38
8	09v-06-BicapPentBipyr-a12	-1723.5259762	5.44
9	09v-01-TricTrPrism-a13	-1723.5247824	6.19
10	09v-05-CapBisdisph-a13	-1723.5247822	6.19
11	09v-01-TricTrPrism-a17	-1723.5247520	6.21
12	09v-01-TricTrPrism-a11	-1723.5244237	6.41
13	09v-06-BicapPentBipyr-a15	-1723.5230532	7.27
14	09v-02-CapCube-a15	-1723.5229989	7.31
15	09v-06-BicapPentBipyr-a17	-1723.5227777	7.44
16	09v-02-CapCube-a113	-1723.5227219	7.48
17	09v-06-BicapPentBipyr-a18	-1723.5227165	7.48
18	09v-05-CapBisdisph-a112	-1723.5216840	8.13
19	09v-05-CapBisdisph-a18	-1723.5194308	9.54
20	09v-06-BicapPentBipyr-a11	-1723.5194087	9.56
21	09v-01-TricTrPrism-a12	-1723.5185078	10.12
22	09v-04-Tl99-a15	-1723.5182249	10.30
23	09v-07-Isocloso-6vx-a18	-1723.5180395	10.42
24	09v-07-Isocloso-6vx-a11	-1723.5178033	10.57
25	09v-01-TricTrPrism-a15	-1723.5177765	10.58
26	09v-05-CapBisdisph-a14	-1723.5177030	10.63
27	09v-07-Isocloso-6vx-a110	-1723.5176282	10.68
28	09v-02-CapCube-a112	-1723.5175325	10.74
29	09v-03-CapSqAntPr-a16	-1723.5170302	11.05
30	09v-04-Tl99-a11	-1723.5170238	11.05
31	09v-02-CapCube-a17	-1723.5155413	11.99
32	09v-04-Tl99-a110	-1723.5128587	13.67
33	09v-02-CapCube-a13	-1723.5028779	19.93
34	09v-04-Tl99-a18	-1723.5014824	20.81
35	09v-02-CapCube-a114	-1723.5009710	21.13
36	09v-05-CapBisdisph-a111	-1723.5009652	21.13
37	09v-04-Tl99-a12	-1723.4999935	21.74
38	09v-07-Isocloso-6vx-a14	-1723.4989780	22.38
39	09v-02-CapCube-a14	-1723.4985631	22.64
40	09v-03-CapSqAntPr-a15	-1723.4985266	22.66
41	09v-01-TricTrPrism-a14	-1723.4985227	22.66

42	09v-01-TricTrPrism-a18	-1723.4985151	22.67
43	09v-05-CapBisdisph-a17	-1723.4985089	22.67
44	09v-03-CapSqAntPr-a14	-1723.4985070	22.67
45	09v-06-BicapPentBipyr-a16	-1723.4937525	25.66
46	09v-07-Isocloso-6vx-a12	-1723.4916742	26.96
47	09v-07-Isocloso-6vx-a15	-1723.4915923	27.01
48	09v-07-Isocloso-6vx-a13	-1723.4915883	27.02
49	09v-02-CapCube-a111	-1723.4892328	28.49
50	09v-04-Tl99-a14	-1723.4890977	28.58
51	09v-06-BicapPentBipyr-a13	-1723.4890238	28.63
52	09v-02-CapCube-a110	-1723.4884699	28.97
53	09v-03-CapSqAntPr-a110	-1723.4884121	29.01
54	09v-06-BicapPentBipyr-a14	-1723.4827028	32.59
55	09v-06-BicapPentBipyr-a19	-1723.4822537	32.87
56	09v-04-Tl99-a17	-1723.4821890	32.91
57	09v-03-CapSqAntPr-a12	-1723.4754261	37.16
58	09v-05-CapBisdisph-a12	-1723.4752673	37.26
59	09v-02-CapCube-a11	-1723.4752572	37.26
60	09v-04-Tl99-a16	-1723.4738379	38.15
61	09v-02-CapCube-a12	-1723.4737058	38.24
62	09v-03-CapSqAntPr-a17	-1723.4687260	41.36
63	09v-07-Isocloso-6vx-a19	-1723.4670765	42.40
64	09v-05-CapBisdisph-a110	-1723.4653334	43.49
65	09v-07-Isocloso-6vx-a16	-1723.4592332	47.32
66	09v-02-CapCube-a19	-1723.4592297	47.32
67	09v-04-Tl99-a13	-1723.4556956	49.54
68	09v-03-CapSqAntPr-a19	-1723.4544415	50.33
69	09v-03-CapSqAntPr-a11	-1723.4527191	51.41
70	09v-03-CapSqAntPr-a13	-1723.4505852	52.75
71	09v-05-CapBisdisph-a15	-1723.4458673	55.71
72	09v-03-CapSqAntPr-a18	-1723.4412030	58.63
73	09v-05-CapBisdisph-a19	-1723.4303558	65.44
74	09v-06-BicapPentBipyr-a111	-1723.4289104	66.35
75	09v-04-Tl99-a19	-1723.4134340	76.06
76	09v-02-CapCube-a16	-1723.4018556	83.33

Table 5A. Initial $(CH_3)_{10}Al_6C_4$ structures, a total of 164 structures.

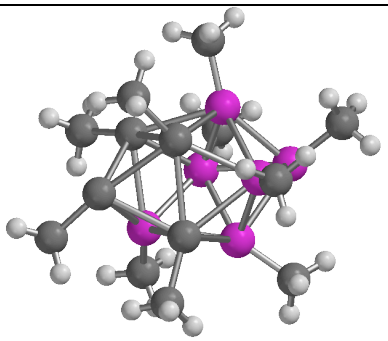
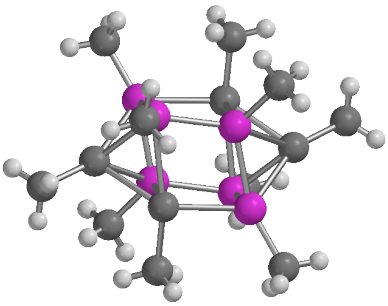
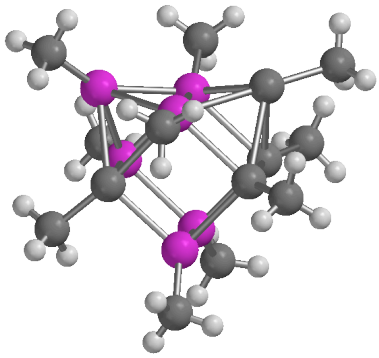
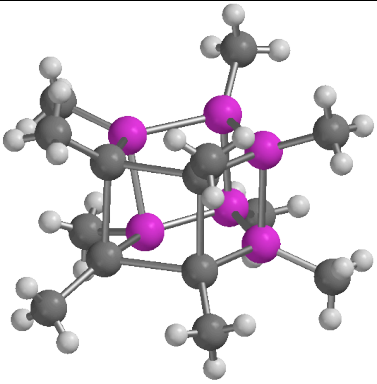
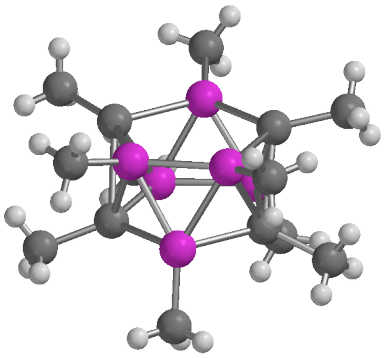
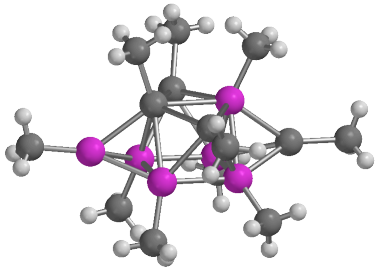
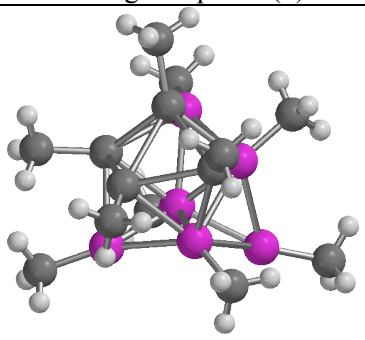
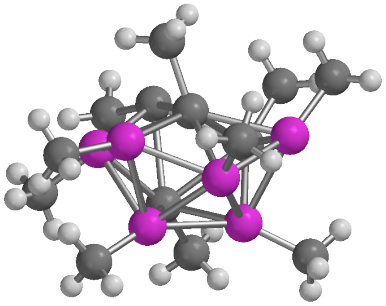
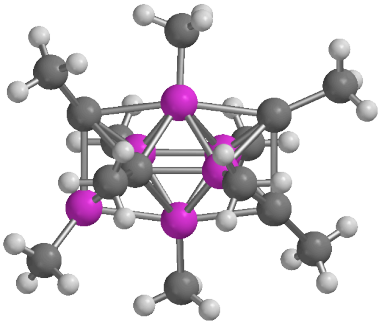
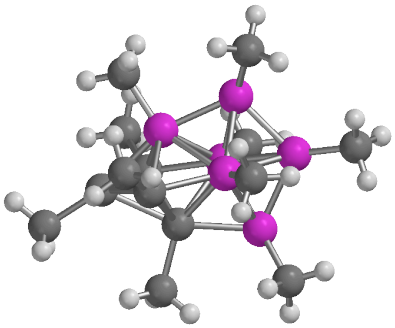
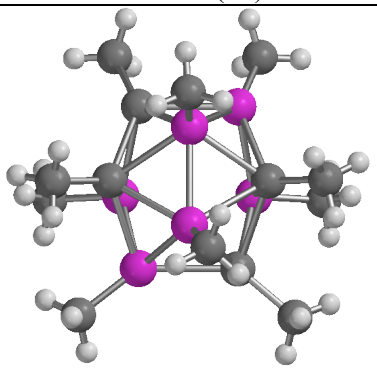
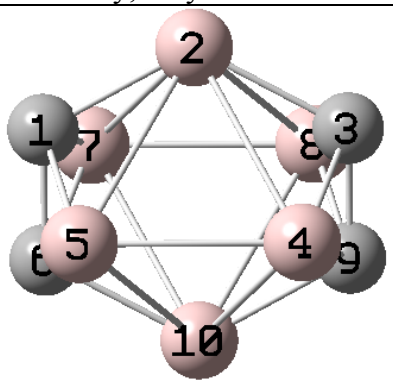
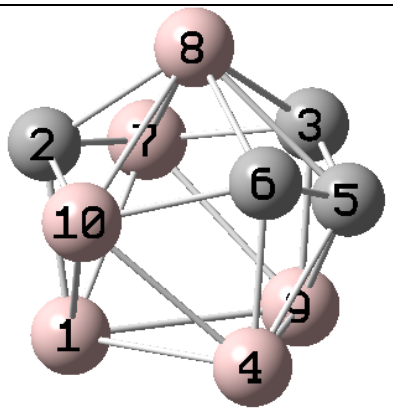
Initial structures	 Bicapped square antiprism (20)	 Bicapped cube A (8)
 Bicapped cube B (15)	 Pentagonal prism (8)	 Pentagonal antiprism (6)
 Tetracapped trig prism A (15)	 Tetracapped trig prism B (28)	 Isocloso (25)
 Tetracapped octahedron (14)	 Bisdisphenoid-like (15)	 Edge-coalesc icos -1vx (10)

Table 5B. Distance table for the lowest-lying $(CH_3)_{10}Al_6C_4$ structures after PBE0/Def2TZVPP optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity, only the atoms forming the cluster framework are presented.



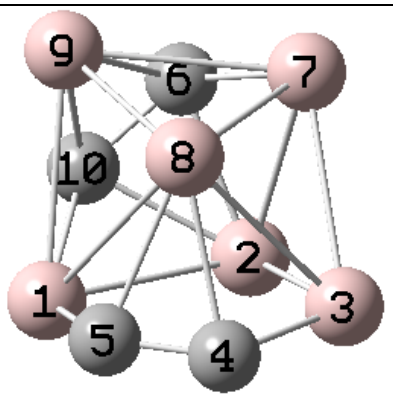
1. -2004.4892742 0.0 D_{2h}

	1	2	3	4	5
2 Al	2.023392	0.000000			
3 C	3.530687	2.022840	0.000000		
4 Al	3.673683	2.887964	2.082487	0.000000	
5 Al	2.095799	2.892595	3.670441	2.582942	0.000000
6 C	1.577057	3.115596	3.869175	3.670601	2.083730
7 Al	2.083386	2.886506	3.675636	4.554254	3.752212
8 Al	3.668853	2.886884	2.094658	3.750155	4.554923
9 C	3.864358	3.112032	1.576719	2.094345	3.673377
10 Al	3.112662	3.553110	3.114748	2.888936	2.885915
	6	7	8	9	10
7 Al	2.095607	0.000000			
8 Al	3.676455	2.583460	0.000000		
9 C	3.530646	3.667684	2.081882	0.000000	
10 Al	2.023567	2.889226	2.888292	2.022484	0.000000



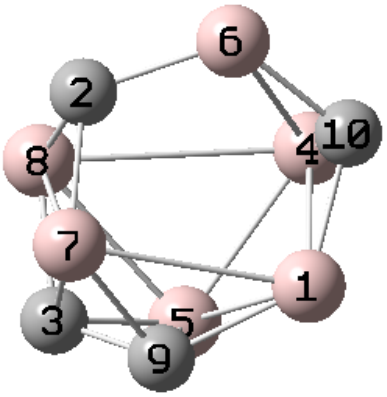
2. -2004.4824617 +4.3 C_S

	1	2	3	4	5
2 C	2.221269	0.000000			
3 C	3.604664	3.095665	0.000000		
4 Al	2.711292	3.639822	3.396975	0.000000	
5 C	3.630279	3.515811	1.554980	2.266586	0.000000
6 C	3.602809	3.095560	2.615704	2.136537	1.554856
7 Al	2.632981	2.042153	2.114776	4.053815	3.253459
8 Al	3.699109	2.105772	2.068870	3.691411	2.433462
9 Al	2.713061	3.638514	2.135198	2.665421	2.265210
10 Al	2.630407	2.041592	3.752225	2.575707	3.252447
	6	7	8	9	10
7 Al	3.753231	0.000000			
8 Al	2.069206	2.604276	0.000000		
9 Al	3.395339	2.574413	3.689549	0.000000	
10 Al	2.113511	3.675250	2.603045	4.052236	0.000000



3. -2004.4821264 +4.5 C_1

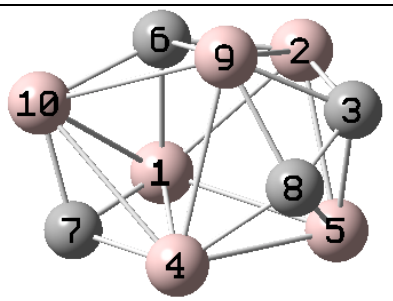
	1	2	3	4	5
2 Al	2.841347	0.000000			
3 Al	3.461436	2.631412	0.000000		
4 C	2.988163	3.872325	2.000894	0.000000	
5 C	1.998518	3.902914	2.942160	1.393854	0.000000
6 C	3.212530	2.180145	3.784607	4.664853	4.392582
7 Al	3.928327	2.786992	2.767844	3.892938	4.161381
8 Al	3.181685	4.054246	2.890351	2.303279	2.296693
9 Al	2.867858	3.704110	4.329930	4.293392	3.630644
10 C	2.025898	2.166967	3.932801	4.327677	3.691632
	6	7	8	9	10
7 Al	2.025654	0.000000			
8 Al	3.651971	2.695150	0.000000		
9 Al	2.151996	2.772344	2.627764	0.000000	
10 C	1.499988	3.108239	3.720415	2.134128	0.000000



4. -2004.4796005 +6.1 C_1

	1	2	3	4	5
2 C	3.641264	0.000000			
3 C	3.292534	3.078321	0.000000		
4 Al	2.873665	3.806212	3.984316	0.000000	
5 Al	2.875673	4.038251	2.108632	2.625880	0.000000
6 Al	3.162180	1.931178	4.282720	3.120726	4.450481
7 Al	3.077515	1.995526	2.097846	4.481596	3.671733
8 Al	3.937616	2.000013	2.035070	3.397026	2.800647
9 C	2.029233	3.439500	1.549774	3.731894	2.149927
10 C	1.986778	3.330502	4.297190	1.951330	3.637678

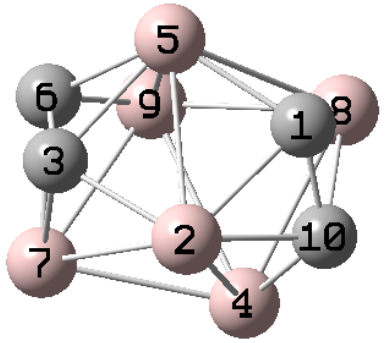
	6	7	8	9	10
7 Al	3.235750	0.000000			
8 Al	3.352128	2.626753	0.000000		
9 C	4.039621	2.131197	3.089655	0.000000	
10 C	1.966071	3.884457	3.936419	3.582387	0.000000



5. -2004.4793260 +6.2 C_1

	1	2	3	4	5
2 Al	2.721606	0.000000			
3 C	3.712229	2.015044	0.000000		
4 Al	2.900472	3.986434	3.329419	0.000000	
5 Al	2.813976	2.628119	2.175850	2.767706	0.000000
6 C	2.266816	2.063147	3.104743	3.473722	3.681836
7 C	2.010747	4.169306	4.441008	1.988628	3.744263
8 C	3.600850	3.061282	1.537096	2.052932	2.179937
9 Al	3.608567	2.613993	2.076529	3.073249	3.556629
10 Al	2.661633	3.932898	4.488029	3.124809	4.637754

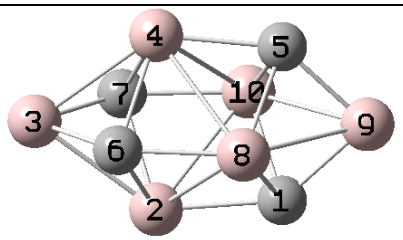
	6	7	8	9	10
7 C	2.985843	0.000000			
8 C	3.357646	3.632998	0.000000		
9 Al	2.062544	3.711037	2.095699	0.000000	
10 Al	2.018232	1.913899	4.028620	3.026358	0.000000



6. -2004.4783716 +6.8 C_2

	1	2	3	4	5
1 C	0.000000				
2 Al	2.119206	0.000000			
3 C	3.170073	2.031112	0.000000		
4 Al	3.218643	2.861255	3.610675	0.000000	
5 Al	2.031101	2.660076	2.119097	3.938843	0.000000
6 C	3.570082	3.190665	1.572411	3.664080	2.069885
7 Al	4.139332	2.919375	2.084972	2.640590	3.574264
8 Al	2.084920	3.574320	4.139394	2.747402	2.919490
9 Al	3.610574	3.938810	3.218679	2.918638	2.861295
10 C	1.572405	2.069861	3.570100	2.024365	3.190680

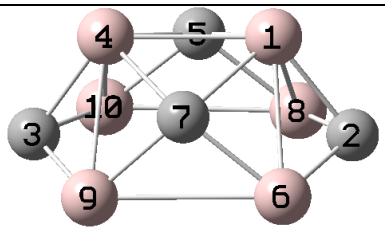
	6	7	8	9	10
6 C	0.000000				
7 Al	2.120813	0.000000			
8 Al	3.769347	4.278127	0.000000		
9 Al	2.024369	2.747404	2.640575	0.000000	
10 C	4.008398	3.769300	2.120868	3.664072	0.000000



7. -2004.4759304 +8.4 D_{2d}

		1	2	3	4	5
2	Al	2.115708	0.000000			
3	Al	4.361647	2.556488	0.000000		
4	Al	3.605385	3.103993	2.557534	0.000000	
5	C	2.743885	3.603975	4.361745	2.116004	0.000000
6	C	3.335809	2.152792	1.980157	2.162820	3.334649
7	C	3.334991	2.163288	1.980161	2.152234	3.334280
8	Al	2.163453	2.659890	3.861444	2.660907	2.152499
9	Al	1.980578	3.861509	5.568245	3.861884	1.979839
10	Al	2.152259	2.660497	3.861822	2.661319	2.162958

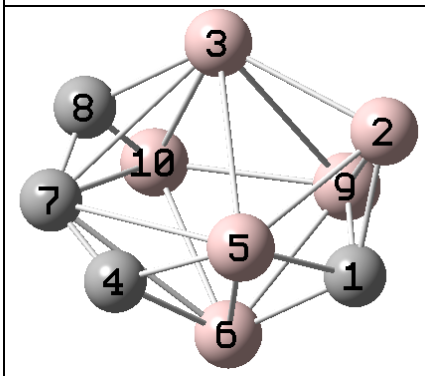
		6	7	8	9	10
7	C	2.743877	0.000000			
8	Al	2.115804	3.604298	0.000000		
9	Al	4.361793	4.361720	2.556859	0.000000	
10	Al	3.605060	2.115894	3.104007	2.557286	0.000000



8. -2004.4753040 +8.8 C_2

		1	2	3	4	5
2	C	2.077402	0.000000			
3	C	4.200226	5.029637	0.000000		
4	Al	2.650004	4.200815	2.077537	0.000000	
5	C	2.132024	3.119732	3.126633	2.143712	0.000000
6	Al	2.598912	1.936650	4.376919	3.853265	3.769700
7	C	2.143579	3.126775	3.119663	2.132566	3.075761
8	Al	2.612297	1.932457	4.356923	3.858494	2.044460
9	Al	3.858296	4.357716	1.932300	2.612423	3.763530
10	Al	3.852786	4.377577	1.936554	2.598750	2.034178

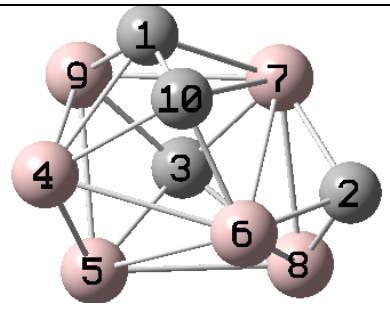
		6	7	8	9	10
7	C	2.034355	0.000000			
8	Al	3.260479	3.763276	0.000000		
9	Al	3.048600	2.044351	4.435774	0.000000	
10	Al	4.491144	3.769997	3.048493	3.261343	0.000000



9. -2004.4745299 +9.3 C_1

		1	2	3	4	5
1	C	0.000000				
2	Al	2.039395	0.000000			
3	Al	3.558452	2.581756	0.000000		
4	C	3.189503	4.074962	3.449417	0.000000	
5	Al	2.133171	2.576520	3.116981	2.034634	0.000000
6	Al	2.061120	3.713157	3.927843	2.087753	2.643218
7	C	4.143251	4.555521	3.030291	1.439184	3.011008
8	C	4.253578	4.172296	2.038754	2.545693	3.487688
9	Al	2.166536	2.594458	3.074566	3.960120	3.652725
10	Al	3.851994	4.279888	2.893584	3.188850	4.143048

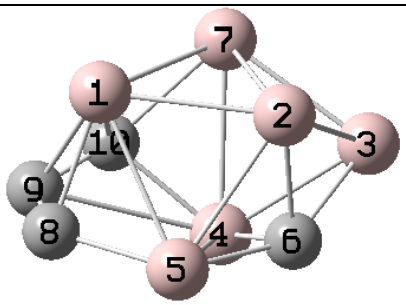
		6	7	8	9	10
6	Al	0.000000				
7	C	3.052551	0.000000			
8	C	3.546415	1.429986	0.000000		
9	Al	2.657224	4.283720	3.790621	0.000000	
10	Al	2.858043	2.707245	2.058466	2.619433	0.000000



10. -2004.4729329 +10.3 C_1

		1	2	3	4	5
2	C	3.539752	0.000000			
3	C	3.333443	2.978578	0.000000		
4	Al	2.350113	4.265564	3.665409	0.000000	
5	Al	3.675815	3.683587	2.096195	2.572661	0.000000
6	Al	2.997477	2.029346	3.489550	2.769916	3.034889
7	Al	2.460753	1.961746	2.118547	3.938234	3.581596
8	Al	4.390363	1.930517	2.073253	4.552483	2.823930
9	Al	2.122383	4.073070	2.081489	2.638328	2.633809
10	C	1.408156	3.185530	3.913376	2.183032	3.781416

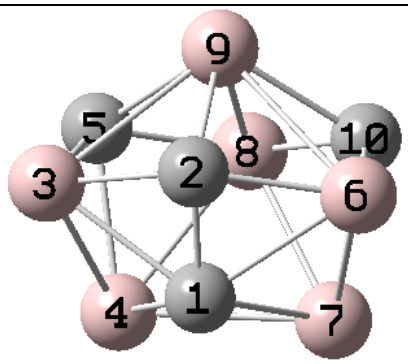
		6	7	8	9	10
7	Al	3.004252	0.000000			
8	Al	3.002145	2.627018	0.000000		
9	Al	3.846577	2.688324	3.928174	0.000000	
10	C	2.057752	2.955341	4.360602	3.188564	0.000000



11. -2004.4718637 +10.9 C_1

		1	2	3	4	5
2	Al	2.679050	0.000000			
3	Al	4.368548	2.663697	0.000000		
4	Al	3.676104	3.498425	2.543640	0.000000	
5	Al	2.795650	2.690796	3.999771	2.986328	0.000000
6	C	3.566096	2.131256	2.140948	2.073982	2.018890
7	Al	2.776630	2.738309	2.538285	2.847761	4.099465
8	C	2.142989	3.796921	4.978217	3.269639	2.009410
9	C	2.309601	4.208903	4.823672	2.886583	3.036746
10	C	2.436028	3.692250	3.703338	2.060333	3.371183

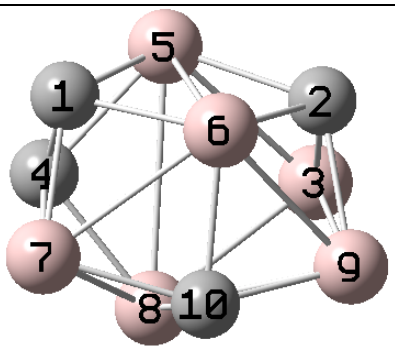
		6	7	8	9	10
7	Al	3.297258	0.000000			
8	C	3.487375	4.062463	0.000000		
9	C	3.858729	3.489106	1.408985	0.000000	
10	C	3.364832	2.232205	2.509279	1.468585	0.000000



12. -2004.4700425 +12.1 C_S

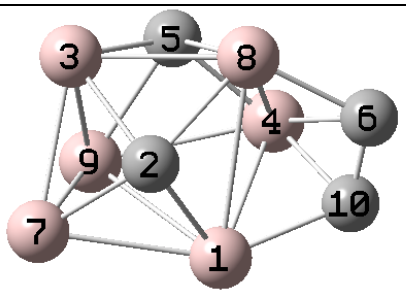
		1	2	3	4	5
1	C	0.000000				
2	C	1.663568	0.000000			
3	Al	2.231308	1.976262	0.000000		
4	Al	2.294463	3.419051	2.552852	0.000000	
5	C	3.061450	3.071933	2.020291	2.146841	0.000000
6	Al	2.231321	1.976242	3.678895	3.979416	3.971030
7	Al	2.294581	3.419149	3.979506	2.533055	3.557585
8	Al	3.541934	3.912542	3.726920	2.592441	2.071735
9	Al	2.993636	2.126268	2.611734	3.538414	2.129474
10	C	3.061467	3.071951	3.971050	3.557532	3.176917

		6	7	8	9	10
6	Al	0.000000				
7	Al	2.552936	0.000000			
8	Al	3.726941	2.592446	0.000000		
9	Al	2.611709	3.538466	2.620342	0.000000	
10	C	2.020313	2.146837	2.071751	2.129481	0.000000



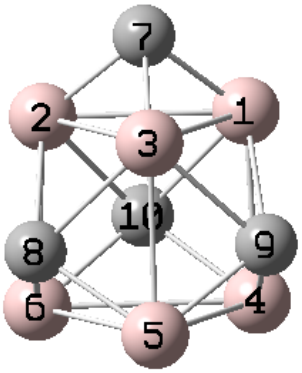
13. -2004.4675022 +13.7 C_1

	1	2	3	4	5
2 C	3.234166	0.000000			
3 Al	4.231757	2.085612	0.000000		
4 C	1.611092	3.468845	3.587482	0.000000	
5 Al	2.026401	2.078082	2.741729	2.117251	0.000000
6 Al	2.088850	2.182664	3.841934	3.040720	2.640303
7 Al	2.013340	4.105727	4.726749	2.050125	3.549569
8 Al	3.217889	3.298839	2.719590	2.101010	3.143759
9 Al	4.033179	2.072735	2.553745	3.934820	3.611750
10 C	3.043284	3.122867	3.757051	3.013861	3.674156
	6	7	8	9	10
7 Al	2.639547	0.000000			
8 Al	3.383704	2.606543	0.000000		
9 Al	2.618205	3.832873	2.714200	0.000000	
10 C	2.132656	2.034520	2.174738	2.015626	0.000000



14. -2004.4670011 +14.0 C_1

	1	2	3	4	5
2 C	2.102596	0.000000			
3 Al	3.601846	2.160456	0.000000		
4 Al	2.796635	3.635647	3.710164	0.000000	
5 C	3.388514	2.980527	2.009996	2.011724	0.000000
6 C	2.923614	3.378647	4.356618	2.446498	3.281185
7 Al	2.660153	2.089127	2.552447	4.320253	3.659737
8 Al	2.997121	2.129595	2.584674	2.802107	2.166964
9 Al	2.995072	3.289445	2.665035	2.674267	2.266293
10 C	2.056716	3.366590	4.572722	2.166548	3.534889
	6	7	8	9	10
7 Al	5.008672	0.000000			
8 Al	2.024815	3.927490	0.000000		
9 Al	4.534173	2.580554	3.803393	0.000000	
10 C	1.381269	4.551705	2.813349	4.050817	0.000000



15. -2004.4651666 +15.1 C_{3v}

	1	2	3	4	5
2 Al	2.694877	0.000000			
3 Al	2.706367	2.707049	0.000000		
4 Al	2.560060	3.779880	3.796209	0.000000	
5 Al	3.804339	3.811700	2.563114	2.911927	0.000000
6 Al	3.815821	2.561979	3.790999	2.918829	2.912731
7 C	1.953918	1.957456	1.958103	4.091906	4.104724
8 C	3.672596	2.287301	2.258167	3.600006	2.015081
9 C	2.262240	3.657530	2.268403	2.011503	2.013164
10 C	2.279220	2.242075	3.658958	2.009415	3.602801
	6	7	8	9	10
7 C	4.103575	0.000000			
8 C	2.006242	3.240241	0.000000		
9 C	3.605655	3.229121	3.064531	0.000000	
10 C	2.018108	3.232486	3.063602	3.065073	0.000000

Table 5C. Energy ranking for all of the $(CH_3)_{10}Al_6C_4$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	10v-11-EdgeCoalsced-1vx-a15	-2005.87866240	0.00
2	10v-06-TetrcTriPri1-a18	-2005.87843300	0.14
3	10v-03-BicapCubB-a15	-2005.87823760	0.27
4	10v-02-BicapCubA-a15	-2005.87823590	0.27
5	10v-09-DistTetracapOh-a11	-2005.87677940	1.18
6	10v-05-PentAntiPr-a14	-2005.87664710	1.26
7	10v-10-BisDisphenoid-Like-a17	-2005.87652760	1.34
8	10v-03-BicapCubB-a14	-2005.87435290	2.70
9	10v-07-TetrcTriPri2-a124	-2005.87430510	2.73
10	10v-07-TetrcTriPri2-a118	-2005.87427450	2.75
11	10v-06-TetrcTriPri1-a114	-2005.87390140	2.99
12	10v-08-Isocloso-a110	-2005.87177190	4.32
13	10v-11-EdgeCoalsced-1vx-a18	-2005.87177190	4.32
14	10v-10-BisDisphenoid-Like-a111	-2005.87052060	5.11
15	10v-10-BisDisphenoid-Like-a112	-2005.87048170	5.13
16	10v-07-TetrcTriPri2-a119	-2005.87044680	5.16
17	10v-04-PentagPrism-a17	-2005.87010480	5.37
18	10v-07-TetrcTriPri2-a113	-2005.87007720	5.39
19	10v-03-BicapCubB-a113	-2005.86989320	5.50
20	10v-07-TetrcTriPri2-a128	-2005.86714330	7.23
21	10v-01-BicapSqAntipr-a111	-2005.86630960	7.75
22	10v-04-PentagPrism-a15	-2005.86630350	7.76
23	10v-03-BicapCubB-a112	-2005.86630050	7.76
24	10v-04-PentagPrism-a16	-2005.86629360	7.76
25	10v-01-BicapSqAntipr-a118	-2005.86629150	7.76
26	10v-09-DistTetracapOh-a13	-2005.86628940	7.76
27	10v-08-Isocloso-a12	-2005.86625810	7.78
28	10v-08-Isocloso-a121	-2005.86619120	7.83
29	10v-11-EdgeCoalsced-1vx-a11	-2005.86618150	7.83
30	10v-06-TetrcTriPri1-a112	-2005.86607300	7.90
31	10v-03-BicapCubB-a12	-2005.86535300	8.35
32	10v-07-TetrcTriPri2-a115	-2005.86515970	8.47
33	10v-01-BicapSqAntipr-a17	-2005.86515480	8.48
34	10v-06-TetrcTriPri1-a110	-2005.86514880	8.48
35	10v-03-BicapCubB-a17	-2005.86514670	8.48
36	10v-11-EdgeCoalsced-1vx-a110	-2005.86513200	8.49
37	10v-08-Isocloso-a116	-2005.86513160	8.49
38	10v-07-TetrcTriPri2-a125	-2005.86399330	9.21
39	10v-08-Isocloso-a17	-2005.86385250	9.29
40	10v-05-PentAntiPr-a16	-2005.86383920	9.30

41	10v-01-BicapSqAntipr-a15	-2005.86383590	9.30
42	10v-07-TetrcTriPri2-a110	-2005.86383550	9.30
43	10v-02-BicapCubA-a16	-2005.86356820	9.47
44	10v-07-TetrcTriPri2-a13	-2005.86061560	11.32
45	10v-08-Isocloso-a13	-2005.86040600	11.46
46	10v-06-TetrcTriPri1-a115	-2005.86040210	11.46
47	10v-08-Isocloso-a123	-2005.85966060	11.92
48	10v-08-Isocloso-a18	-2005.85964260	11.94
49	10v-07-TetrcTriPri2-a116	-2005.85953600	12.00
50	10v-02-BicapCubA-a14	-2005.85951580	12.01
51	10v-08-Isocloso-a122	-2005.85899030	12.34
52	10v-06-TetrcTriPri1-a17	-2005.85889570	12.40
53	10v-01-BicapSqAntipr-a112	-2005.85878780	12.47
54	10v-07-TetrcTriPri2-a112	-2005.85752530	13.26
55	10v-01-BicapSqAntipr-a13	-2005.85750380	13.28
56	10v-08-Isocloso-a14	-2005.85739950	13.34
57	10v-10-BisDisphenoid-Like-a12	-2005.85612510	14.14
58	10v-07-TetrcTriPri2-a123	-2005.85609270	14.16
59	10v-04-PentagPrism-a13	-2005.85607970	14.17
60	10v-03-BicapCubB-a13	-2005.85607860	14.17
61	10v-08-Isocloso-a11	-2005.85588110	14.30
62	10v-09-DistTetracapOh-a17	-2005.85585590	14.31
63	10v-10-BisDisphenoid-Like-a11	-2005.85584600	14.32
64	10v-07-TetrcTriPri2-a14	-2005.85581550	14.34
65	10v-08-Isocloso-a125	-2005.85576620	14.37
66	10v-07-TetrcTriPri2-a17	-2005.85576080	14.37
67	10v-08-Isocloso-a111	-2005.85574680	14.38
68	10v-10-BisDisphenoid-Like-a110	-2005.85573240	14.39
69	10v-07-TetrcTriPri2-a120	-2005.85572560	14.39
70	10v-01-BicapSqAntipr-a18	-2005.85515060	14.75
71	10v-04-PentagPrism-a18	-2005.85506750	14.81
72	10v-07-TetrcTriPri2-a121	-2005.85504560	14.82
73	10v-09-DistTetracapOh-a114	-2005.85483150	14.95
74	10v-07-TetrcTriPri2-a16	-2005.85482250	14.96
75	10v-09-DistTetracapOh-a19	-2005.85320750	15.97
76	10v-07-TetrcTriPri2-a19	-2005.85305790	16.07
77	10v-07-TetrcTriPri2-a122	-2005.85297560	16.12
78	10v-10-BisDisphenoid-Like-a113	-2005.85284120	16.20
79	10v-01-BicapSqAntipr-a119	-2005.85265480	16.32
80	10v-06-TetrcTriPri1-a13	-2005.85201050	16.72
81	10v-08-Isocloso-a119	-2005.85192780	16.78
82	10v-02-BicapCubA-a17	-2005.85191790	16.78
83	10v-02-BicapCubA-a11	-2005.85117670	17.25
84	10v-07-TetrcTriPri2-a126	-2005.85117100	17.25
85	10v-01-BicapSqAntipr-a19	-2005.85116770	17.25

86	10v-08-Isocloso-a15	-2005.85116450	17.26
87	10v-05-PentAntiPr-a12	-2005.84907490	18.57
88	10v-06-TetrcTriPri1-a14	-2005.84822050	19.10
89	10v-08-Isocloso-a118	-2005.84819290	19.12
90	10v-08-Isocloso-a19	-2005.84814470	19.15
91	10v-01-BicapSqAntipr-a110	-2005.84814140	19.15
92	10v-08-Isocloso-a112	-2005.84811050	19.17
93	10v-09-DistTetracapOh-a18	-2005.84797780	19.26
94	10v-10-BisDisphenoid-Like-a16	-2005.84519390	21.00
95	10v-01-BicapSqAntipr-a11	-2005.84488500	21.20
96	10v-01-BicapSqAntipr-a120	-2005.84488330	21.20
97	10v-07-TetrcTriPri2-a18	-2005.84487950	21.20
98	10v-03-BicapCubB-a11	-2005.84487860	21.20
99	10v-03-BicapCubB-a115	-2005.84487510	21.20
100	10v-02-BicapCubA-a18	-2005.84081640	23.75
101	10v-01-BicapSqAntipr-a117	-2005.84070700	23.82
102	10v-06-TetrcTriPri1-a11	-2005.84068770	23.83
103	10v-07-TetrcTriPri2-a117	-2005.84059730	23.89
104	10v-05-PentAntiPr-a11	-2005.83996220	24.29
105	10v-10-BisDisphenoid-Like-a14	-2005.83732780	25.94
106	10v-09-DistTetracapOh-a12	-2005.83716720	26.04
107	10v-03-BicapCubB-a18	-2005.83703270	26.12
108	10v-08-Isocloso-a114	-2005.83441150	27.77
109	10v-04-PentagPrism-a14	-2005.83437940	27.79
110	10v-02-BicapCubA-a13	-2005.83320470	28.53
111	10v-07-TetrcTriPri2-a15	-2005.83315420	28.56
112	10v-07-TetrcTriPri2-a114	-2005.83314510	28.56
113	10v-11-EdgeCoalsced-1vx-a16	-2005.83248400	28.98
114	10v-11-EdgeCoalsced-1vx-a17	-2005.83245940	28.99
115	10v-01-BicapSqAntipr-a115	-2005.83245910	28.99
116	10v-07-TetrcTriPri2-a11	-2005.83245770	28.99
117	10v-10-BisDisphenoid-Like-a115	-2005.83215800	29.18
118	10v-10-BisDisphenoid-Like-a13	-2005.83146030	29.62
119	10v-05-PentAntiPr-a15	-2005.83090410	29.97
120	10v-01-BicapSqAntipr-a114	-2005.82986670	30.62
121	10v-06-TetrcTriPri1-a12	-2005.82777140	31.94
122	10v-03-BicapCubB-a110	-2005.82777130	31.94
123	10v-11-EdgeCoalsced-1vx-a14	-2005.82776540	31.94
124	10v-05-PentAntiPr-a13	-2005.82611910	32.97
125	10v-10-BisDisphenoid-Like-a18	-2005.82582240	33.16
126	10v-06-TetrcTriPri1-a16	-2005.82386570	34.39
127	10v-09-DistTetracapOh-a15	-2005.82295930	34.95
128	10v-10-BisDisphenoid-Like-a114	-2005.82269730	35.12
129	10v-09-DistTetracapOh-a113	-2005.82141850	35.92
130	10v-07-TetrcTriPri2-a111	-2005.82108250	36.13

131	10v-09-DistTetracapOh-a110	-2005.82107260	36.14
132	10v-01-BicapSqAntipr-a14	-2005.82107130	36.14
133	10v-03-BicapCubB-a16	-2005.82106460	36.14
134	10v-01-BicapSqAntipr-a16	-2005.81753170	38.36
135	10v-11-EdgeCoalsced-1vx-a13	-2005.81734310	38.48
136	10v-08-Isocloso-a113	-2005.81718190	38.58
137	10v-03-BicapCubB-a111	-2005.81644140	39.04
138	10v-11-EdgeCoalsced-1vx-a12	-2005.81638650	39.08
139	10v-03-BicapCubB-a114	-2005.81638580	39.08
140	10v-09-DistTetracapOh-a111	-2005.81428110	40.40
141	10v-08-Isocloso-a124	-2005.81264470	41.43
142	10v-04-PentagPrism-a11	-2005.81227020	41.66
143	10v-08-Isocloso-a115	-2005.81169830	42.02
144	10v-01-BicapSqAntipr-a12	-2005.81168530	42.03
145	10v-09-DistTetracapOh-a14	-2005.81111470	42.39
146	10v-07-TetrcTriPri2-a127	-2005.81050610	42.77
147	10v-10-BisDisphenoid-Like-a19	-2005.81035510	42.86
148	10v-08-Isocloso-a117	-2005.80920840	43.58
149	10v-01-BicapSqAntipr-a113	-2005.80767850	44.54
150	10v-07-TetrcTriPri2-a12	-2005.80379020	46.98
151	10v-06-TetrcTriPri1-a113	-2005.80333900	47.27
152	10v-06-TetrcTriPri1-a19	-2005.80323310	47.33
153	10v-08-Isocloso-a120	-2005.80267990	47.68
154	10v-11-EdgeCoalsced-1vx-a19	-2005.80267670	47.68
155	10v-10-BisDisphenoid-Like-a15	-2005.80203880	48.08
156	10v-02-BicapCubA-a12	-2005.79822080	50.48
157	10v-01-BicapSqAntipr-a116	-2005.79572150	52.05
158	10v-04-PentagPrism-a12	-2005.79336500	53.53
159	10v-03-BicapCubB-a19	-2005.78480360	58.90
160	10v-09-DistTetracapOh-a16	-2005.78368430	59.60
161	10v-09-DistTetracapOh-a112	-2005.76053500	74.13
162	10v-06-TetrcTriPri1-a111	-2005.72439250	96.81

Table S6A. Initial $(CH_3)_{11}Al_7C_7$ structures, a total of 155 structures:

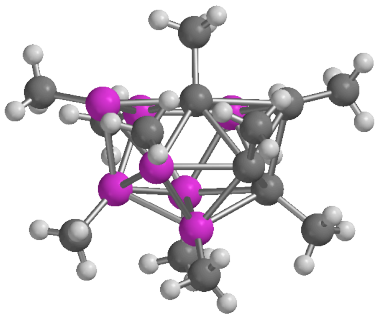
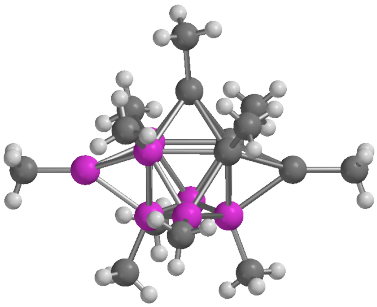
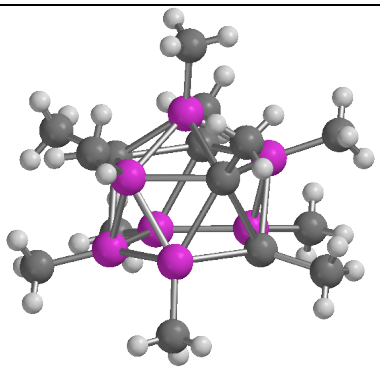
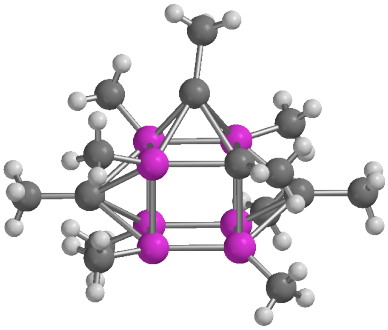
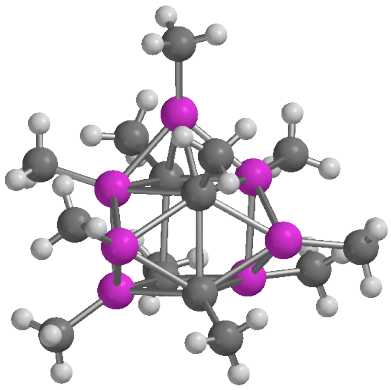
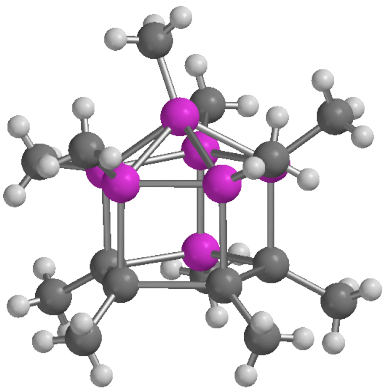
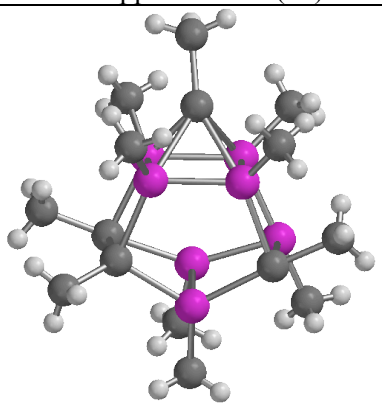
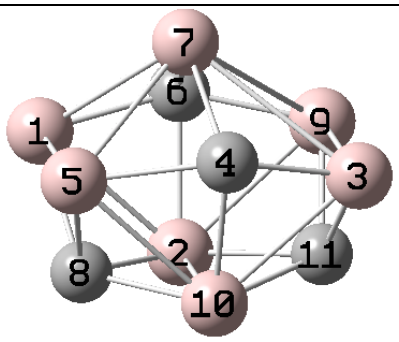
Initial	structures	 Edge-coalesced icos (32)
 Pentacapped trig prism (31)	 Capped pentag antiprism (29)	 Tricapped cube A (28)
 Tricapped cube B (22)	 Capped pentag prism A (5)	 Capped pentag prism B (8)

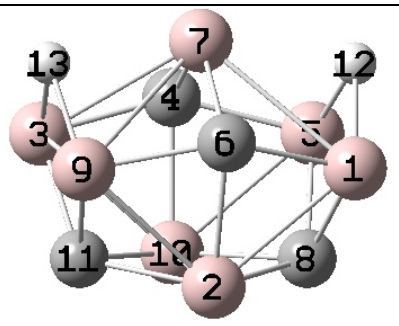
Table 6B. Distance table for the lowest-lying $(CH_3)_{11}Al_7C_4$ structures after PBE0/Def2TZVPP optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity, only the atoms forming the cluster framework are presented.



1. -2286.6722305 0.0 C_S

	1	2	3	4	5
1 Al	0.000000				
2 Al	2.615505	0.000000			
3 Al	4.703199	3.748873	0.000000		
4 C	3.703264	3.770653	1.956542	0.000000	
5 Al	2.564334	3.684116	3.865215	2.087860	0.000000
6 C	2.087854	2.154881	3.747774	3.648406	3.703457
7 Al	2.635977	3.536807	2.985689	2.191170	2.636301
8 C	2.100291	2.059260	4.099629	3.135597	2.100164
9 Al	3.864920	2.589309	2.799183	3.746466	4.702498
10 Al	3.684436	2.625390	2.589672	2.154808	2.615753
11 C	4.128418	2.159717	2.035524	3.057813	4.128373

	6	7	8	9	10
6 C	0.000000				
7 Al	2.190518	0.000000			
8 C	3.136149	3.432546	0.000000		
9 Al	1.956693	2.984460	4.099436	0.000000	
10 Al	3.771719	3.537684	2.059128	3.748969	0.000000
11 C	3.058509	3.559381	3.277797	2.035476	2.160003

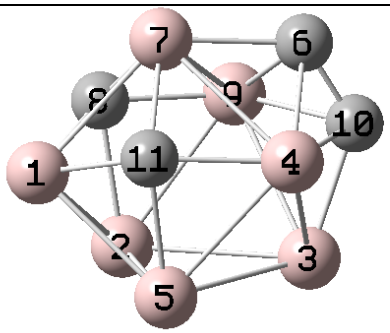
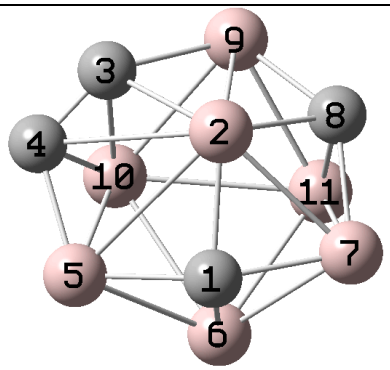


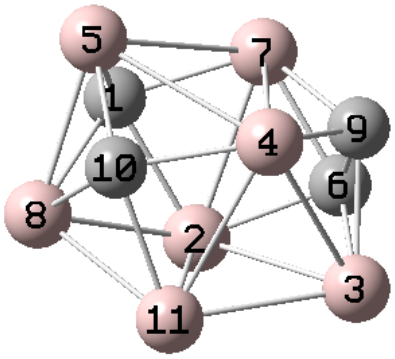
$C_4Al_7Me_{11}(\mu\text{-}H)_2$ optimized C2v

	1	2	3	4	5
1 Al	0.000000				
2 Al	2.598587	0.000000			
3 Al	4.751670	3.698110	0.000000		
4 C	3.653228	3.695644	2.050131	0.000000	
5 Al	2.662206	3.695257	3.931475	2.051905	0.000000
6 C	2.052069	2.181608	3.657753	3.431190	3.652986
7 Al	2.869933	3.527652	2.840455	2.059791	2.869826
8 C	2.062911	2.101046	4.147453	3.097536	2.062631
9 Al	3.931687	2.596081	2.674986	3.658321	4.751739
10 Al	3.695608	2.593259	2.596130	2.181684	2.598501
11 C	4.148702	2.104196	2.060560	3.096226	4.148501
12 H	1.845373	3.916638	4.575002	2.925074	1.845981
13 H	4.557347	3.914091	1.857424	2.911906	4.557156

	6	7	8	9	10
6 C	0.000000				
7 Al	2.059699	0.000000			
8 C	3.097566	3.543229	0.000000		
9 Al	2.050039	2.840831	4.147575	0.000000	
10 Al	3.695580	3.527698	2.101101	3.698294	0.000000
11 C	3.096041	3.518198	3.295349	2.060592	2.104178
12 H	2.924591	2.274206	2.854362	4.574999	3.917025
13 H	2.911844	2.203975	4.765287	1.857989	3.914015

	11	12	13
11 C	0.000000		

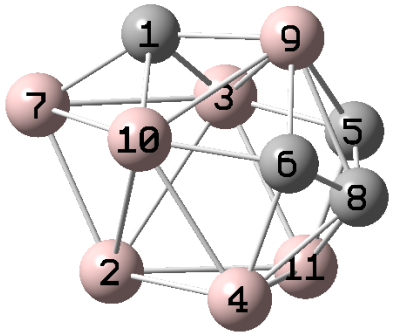
	12 H 4.775303 0.000000 13 H 2.856677 4.431020 0.000000
 2. -2286.6696386 +1.6 C_S	1 2 3 4 5 1 Al 0.000000 2 Al 2.590499 0.000000 3 Al 4.267869 2.769969 0.000000 4 Al 3.784471 4.106617 2.741683 0.000000 5 Al 2.591921 2.689478 2.771845 2.704594 0.000000 6 C 4.249518 4.216187 3.199069 2.244653 4.222886 7 Al 2.594629 3.692568 4.029863 2.726402 3.695978 8 C 2.068512 2.154988 3.743774 3.882025 3.587594 9 Al 3.785239 2.705909 2.748712 3.561090 4.114293 10 C 4.668692 3.912038 2.064685 2.228416 3.916646 11 C 2.067017 3.583691 3.743252 2.051627 2.155976 6 7 8 9 10 6 C 0.000000 7 Al 2.109757 0.000000 8 C 3.234275 2.074980 0.000000 9 Al 2.235749 2.723729 2.049131 0.000000 10 C 1.447564 3.184407 3.701843 2.228210 0.000000 11 C 3.240184 2.076253 3.052910 3.883470 3.704263
 3. -2286.6571368 +9.5 C_1	1 2 3 4 5 1 C 0.000000 2 Al 2.087025 0.000000 3 C 3.448069 2.185523 0.000000 4 C 3.258838 2.828555 1.420838 0.000000 5 Al 2.021255 2.983638 2.959095 1.968700 0.000000 6 Al 2.202263 3.633186 4.170007 3.860470 2.646291 7 Al 2.065278 2.623961 4.307903 4.678616 3.892839 8 C 3.114795 2.122697 3.296781 4.230400 4.360742 9 Al 4.005820 2.668135 2.169148 3.357876 4.315162 10 Al 3.568555 3.535217 2.440840 2.306939 2.819959 11 Al 3.596340 3.601683 3.987935 4.521613 4.392097 6 7 8 9 10 6 Al 0.000000 7 Al 2.620124 0.000000 8 C 3.621144 2.029197 0.000000 9 Al 4.163714 3.745225 2.031298 0.000000 10 Al 2.818136 4.212742 3.709467 2.698463 0.000000 11 Al 2.644878 2.608421 2.174325 2.607937 2.898157



4. -2286.6523421 +12.5 C_1

		1	2	3	4	5
1	C	0.000000				
2	Al	2.201195	0.000000			
3	Al	4.309614	2.906419	0.000000		
4	Al	3.614396	3.747061	2.711562	0.000000	
5	Al	2.000870	3.750121	4.815688	2.917699	0.000000
6	C	3.202613	2.059986	2.055573	3.224240	4.263348
7	Al	2.057560	2.658196	3.639859	3.149852	2.901375
8	Al	2.133024	2.619761	4.346856	3.715975	2.549752
9	C	3.496180	3.129670	2.126206	2.031821	3.747847
10	C	2.983428	3.601563	3.843829	2.066444	1.998359
11	Al	3.751349	2.923351	2.636752	2.779369	3.862978

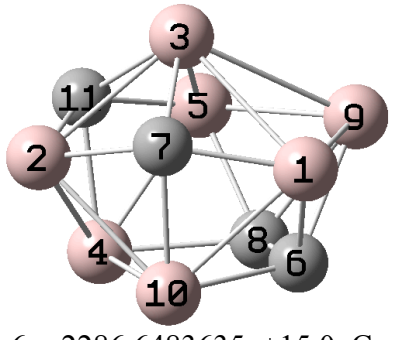
		6	7	8	9	10
6	C	0.000000				
7	Al	2.034530	0.000000			
8	Al	4.192978	3.828618	0.000000		
9	C	1.600987	2.054231	4.408919	0.000000	
10	C	4.196337	3.765466	2.150003	3.615342	0.000000
11	Al	3.705017	4.354895	2.518434	3.684800	2.220262



5. -2286.6523329 +12.5 C_S

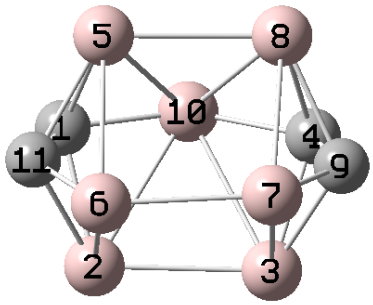
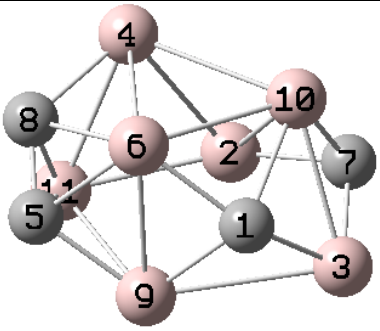
		1	2	3	4	5
1	C	0.000000				
2	Al	3.457634	0.000000			
3	Al	2.103886	3.006241	0.000000		
4	Al	4.072623	2.731015	3.976138	0.000000	
5	C	3.195263	3.920379	2.128646	3.339823	0.000000
6	C	3.195344	3.920444	3.646143	2.101575	2.590049
7	Al	2.026799	2.538866	2.744001	4.380811	4.438011
8	C	3.745985	3.908273	3.264926	2.243051	1.559918
9	Al	2.107003	4.408292	2.659917	3.735275	2.043451
10	Al	2.103945	3.006172	3.383244	2.647178	3.646014
11	Al	4.072568	2.731009	2.647221	2.601522	2.101511

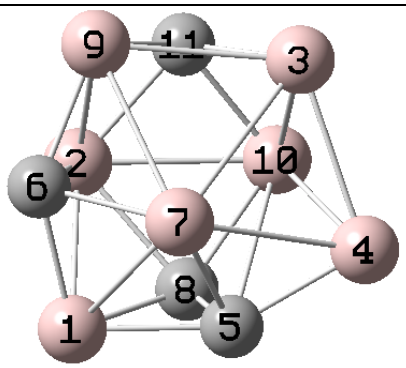
		6	7	8	9	10
6	C	0.000000				
7	Al	4.438049	0.000000			
8	C	1.559900	4.887574	0.000000		
9	Al	2.043440	3.980690	2.403479	0.000000	
10	Al	2.128639	2.743941	3.264829	2.659860	0.000000
11	Al	3.339864	4.380811	2.243070	3.735264	3.976031



6. -2286.6483635 +15.0 C_S

		1	2	3	4	5
1	Al	0.000000				
2	Al	3.766646	0.000000			
3	Al	2.758667	2.615208	0.000000		
4	Al	4.196855	2.612826	3.623048	0.000000	
5	Al	4.093547	3.767355	2.760870	2.593580	0.000000
6	C	2.135155	3.977887	3.566354	2.986912	3.272589
7	C	2.021355	2.033275	2.123870	3.610889	4.109641
8	C	3.273563	3.978380	3.567224	2.219074	2.134456
9	Al	2.558503	4.691671	2.915492	4.031233	2.557428

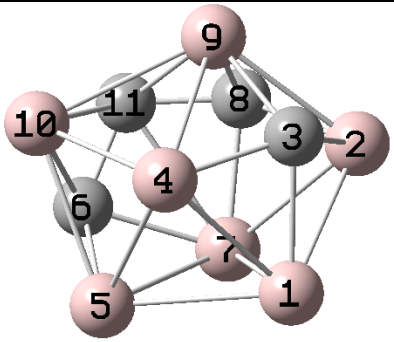
	10 Al 2.593475 2.612770 3.622389 2.660086 4.197327 11 C 4.108142 2.033451 2.124428 2.173028 2.021451 6 7 8 9 10 6 C 0.000000 7 C 3.184521 0.000000 8 C 1.503741 3.853080 0.000000 9 Al 2.269623 3.795762 2.269523 0.000000 10 Al 2.219263 2.172899 2.987966 4.031811 0.000000 11 C 3.851513 3.126121 3.183937 3.794234 3.610612
 7. -2286.6475654 +15.5 C_2	1 2 3 4 5 1 C 0.000000 2 Al 2.120227 0.000000 3 Al 3.767909 2.633719 0.000000 4 C 3.711061 3.785135 2.119804 0.000000 5 Al 2.130332 3.630116 4.437757 3.780372 0.000000 6 Al 3.259395 2.873490 3.802719 4.491746 2.896939 7 Al 4.460577 3.954583 2.911510 3.260651 3.763258 8 Al 3.800721 4.543580 3.636554 2.129907 2.651279 9 C 4.391633 4.099549 2.123293 1.542969 4.025189 10 Al 2.020933 2.876703 2.886069 2.019962 2.834563 11 C 1.541060 2.127320 4.037276 4.404470 2.117455 6 7 8 9 10 6 Al 0.000000 7 Al 2.544357 0.000000 8 Al 3.986525 2.864469 0.000000 9 C 3.962225 2.004272 2.116883 0.000000 10 Al 4.210178 4.189728 2.820351 3.223353 0.000000 11 C 2.003543 3.941993 4.121784 4.571944 3.231897
 8. -2286.6470836 +15.8 C_1	1 2 3 4 5 1 C 0.000000 2 Al 3.511219 0.000000 3 Al 2.034966 3.124928 0.000000 4 Al 3.709292 2.899116 4.716355 0.000000 5 C 3.190594 4.134567 4.695806 3.222420 0.000000 6 Al 2.073585 4.103335 3.989604 2.705547 2.152416 7 C 3.001975 1.993478 1.907323 3.881201 5.088034 8 C 3.687870 3.907412 5.164087 2.070032 1.484450 9 Al 2.050615 3.455825 2.993473 3.956411 2.049422 10 Al 2.181337 2.827943 2.641827 2.799216 4.271658 11 Al 3.889732 2.671985 4.561481 2.757495 2.204841 6 7 8 9 10 6 Al 0.000000 7 C 4.307330 0.000000 8 C 2.162015 5.032821 0.000000 9 Al 2.670570 3.914953 3.136626 0.000000 10 Al 2.796694 2.019612 3.977381 3.696565 0.000000 11 Al 3.486157 4.320903 2.163597 2.671500 4.213134



9. -2286.6465128 +16.1 C_1

	1	2	3	4	5
1 Al	0.000000				
2 Al	2.565033	0.000000			
3 Al	4.641821	3.705917	0.000000		
4 Al	3.975054	4.296571	2.626556	0.000000	
5 C	2.084186	3.301652	3.622290	2.022627	0.000000
6 C	2.032908	2.116678	3.793470	4.333485	3.151366
7 Al	2.619906	3.427398	2.898325	2.757684	2.178996
8 C	2.044790	2.184746	3.806335	2.932146	1.638267
9 Al	3.810575	2.582520	2.681293	4.430521	4.136211
10 Al	3.886161	2.627459	2.635570	2.727217	2.958912
11 C	4.115286	2.102611	2.149063	3.847154	3.913804

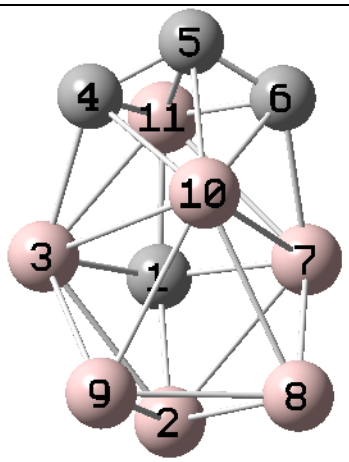
	6	7	8	9	10
6 C	0.000000				
7 Al	2.153777	0.000000			
8 C	3.068815	3.132911	0.000000		
9 Al	2.008849	2.765707	3.960358	0.000000	
10 Al	3.955722	3.774716	2.111803	3.723012	0.000000
11 C	3.122396	3.554708	3.218762	2.028161	2.087486



10. -2286.6450863 +17.0 C_1

	1	2	3	4	5
1 Al	0.000000				
2 Al	2.584121	0.000000			
3 C	2.232287	2.028231	0.000000		
4 Al	2.705809	3.769679	2.042628	0.000000	
5 Al	2.678661	4.215559	3.711015	2.759127	0.000000
6 C	3.781114	3.978186	4.094983	3.716127	2.082587
7 Al	2.815884	2.663754	3.644896	4.175941	2.758750
8 C	3.688277	2.076611	3.125173	4.098468	3.894262
9 Al	3.737172	2.569247	2.093530	2.842138	4.012175
10 Al	4.240556	4.500917	3.692358	2.654428	2.672163
11 C	4.110885	3.368239	3.629517	3.755809	3.234432

	6	7	8	9	10
6 C	0.000000				
7 Al	2.126520	0.000000			
8 C	2.655420	2.094478	0.000000		
9 Al	3.357368	3.578561	2.089688	0.000000	
10 Al	2.149842	3.817221	3.459417	2.717232	0.000000
11 C	1.551734	2.493412	1.605788	2.225406	2.150424



11. -2286.6446624 +17.3 C_S

		1	2	3	4	5
1	C	0.000000				
2	Al	2.073338	0.000000			
3	Al	2.101590	2.674300	0.000000		
4	C	3.219120	4.373187	2.187155	0.000000	
5	C	3.713733	4.952499	3.357069	1.450475	0.000000
6	C	3.214197	4.380666	3.618619	2.463464	1.449936
7	Al	2.102979	2.672059	3.351679	3.598169	3.340718
8	Al	3.913056	2.743513	4.017844	4.713205	4.755482
9	Al	3.916037	2.752546	2.785014	4.013351	4.763730
10	Al	3.606914	3.797791	2.895337	2.288082	2.254155
11	Al	2.020176	3.916560	2.655705	2.142351	2.252923

		6	7	8	9	10
6	C	0.000000				
7	Al	2.178583	0.000000			
8	Al	4.039601	2.788503	0.000000		
9	Al	4.750875	4.025824	2.508937	0.000000	
10	Al	2.315570	2.876104	2.824462	2.840814	0.000000
11	Al	2.127336	2.654500	4.899305	4.900820	3.386426

Table 6C. Energy ranking for all of the $(CH_3)_{11}Al_7C_4$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	11v-01-EdgeCoalscedIh-a112	-2288.2313757	0.00
2	11v-05-TricapCubeB-a15	-2288.2310618	0.20
3	11v-02-PentaCapTriPri-a28	-2288.2310495	0.20
4	11v-03-CapPentAnPr-a38	-2288.2220444	5.86
5	11v-07-CapPentPrB-a12	-2288.2219033	5.94
6	11v-06-CapPentPrA-a34	-2288.2092924	13.86
7	11v-07-CapPentPrB-a23	-2288.2091537	13.94
8	11v-06-CapPentPrA-a19	-2288.2090503	14.01
9	11v-03-CapPentAnPr-a20	-2288.2082076	14.54
10	11v-03-CapPentAnPr-a29	-2288.2078026	14.79
11	11v-03-CapPentAnPr-a33	-2288.2076699	14.88
12	11v-02-PentaCapTriPri-a32	-2288.2076179	14.91
13	11v-01-EdgeCoalscedIh-a131	-2288.2057636	16.07
14	11v-07-CapPentPrB-a28	-2288.2043423	16.96
15	11v-04-TricapCubeA-a26	-2288.2026971	18.00
16	11v-02-PentaCapTriPri-a35	-2288.2023850	18.19
17	11v-07-CapPentPrB-a32	-2288.2023775	18.20
18	11v-07-CapPentPrB-a36	-2288.2013193	18.86
19	11v-04-TricapCubeA-a18	-2288.2011891	18.94
20	11v-06-CapPentPrA-a22	-2288.2009439	19.10
21	11v-05-TricapCubeB-a28	-2288.2008318	19.17
22	11v-07-CapPentPrB-a20	-2288.2007841	19.20
23	11v-02-PentaCapTriPri-a29	-2288.2006436	19.29
24	11v-03-CapPentAnPr-a35	-2288.2005330	19.35
25	11v-06-CapPentPrA-a21	-2288.2005136	19.37
26	11v-04-TricapCubeA-a12	-2288.2004959	19.38
27	11v-03-CapPentAnPr-a26	-2288.2004802	19.39
28	11v-04-TricapCubeA-a31	-2288.2003715	19.46
29	11v-01-EdgeCoalscedIh-a19	-2288.1998505	19.78
30	11v-03-CapPentAnPr-a28	-2288.1998383	19.79
31	11v-01-EdgeCoalscedIh-a115	-2288.1980705	20.90
32	11v-06-CapPentPrA-a28	-2288.1974503	21.29
33	11v-07-CapPentPrB-a22	-2288.1973613	21.34
34	11v-02-PentaCapTriPri-a36	-2288.1971024	21.51
35	11v-05-TricapCubeB-a13	-2288.1971017	21.51
36	11v-05-TricapCubeB-a20	-2288.1971017	21.51
37	11v-02-PentaCapTriPri-a13	-2288.1971014	21.51
38	11v-05-TricapCubeB-a29	-2288.1967840	21.71
39	11v-06-CapPentPrA-a20	-2288.1965208	21.87

40	11v-01-EdgeCoalscedIh-a120	-2288.1958012	22.32
41	11v-06-CapPentPrA-a18	-2288.1948666	22.91
42	11v-04-TricapCubeA-a33	-2288.1935305	23.75
43	11v-01-EdgeCoalscedIh-a125	-2288.1934893	23.77
44	11v-06-CapPentPrA-a17	-2288.1922464	24.55
45	11v-02-PentaCapTriPri-a27	-2288.1922356	24.56
46	11v-01-EdgeCoalscedIh-a113	-2288.1922319	24.56
47	11v-02-PentaCapTriPri-a26	-2288.1922317	24.56
48	11v-04-TricapCubeA-a11	-2288.1922240	24.57
49	11v-03-CapPentAnPr-a15	-2288.1922050	24.58
50	11v-07-CapPentPrB-a25	-2288.1917406	24.87
51	11v-01-EdgeCoalscedIh-a129	-2288.1916390	24.94
52	11v-04-TricapCubeA-a36	-2288.1914919	25.03
53	11v-02-PentaCapTriPri-a11	-2288.1913123	25.14
54	11v-02-PentaCapTriPri-a33	-2288.1912998	25.15
55	11v-01-EdgeCoalscedIh-a14	-2288.1909255	25.38
56	11v-06-CapPentPrA-a15	-2288.1906304	25.57
57	11v-01-EdgeCoalscedIh-a130	-2288.1906050	25.58
58	11v-05-TricapCubeB-a14	-2288.1905349	25.63
59	11v-02-PentaCapTriPri-a39	-2288.1900879	25.91
60	11v-05-TricapCubeB-a26	-2288.1896081	26.21
61	11v-05-TricapCubeB-a32	-2288.1884462	26.94
62	11v-04-TricapCubeA-a29	-2288.1866497	28.07
63	11v-05-TricapCubeB-a21	-2288.1860424	28.45
64	11v-03-CapPentAnPr-a18	-2288.1850555	29.07
65	11v-04-TricapCubeA-a28	-2288.1848880	29.17
66	11v-06-CapPentPrA-a33	-2288.1848283	29.21
67	11v-07-CapPentPrB-a29	-2288.1847924	29.23
68	11v-05-TricapCubeB-a12	-2288.1847737	29.24
69	11v-04-TricapCubeA-a20	-2288.1845548	29.38
70	11v-03-CapPentAnPr-a34	-2288.1840561	29.69
71	11v-07-CapPentPrB-a26	-2288.1831489	30.26
72	11v-07-CapPentPrB-a19	-2288.1820953	30.92
73	11v-03-CapPentAnPr-a16	-2288.1813637	31.38
74	11v-01-EdgeCoalscedIh-a18	-2288.1807644	31.76
75	11v-05-TricapCubeB-a18	-2288.1782681	33.33
76	11v-06-CapPentPrA-a29	-2288.1781789	33.38
77	11v-03-CapPentAnPr-a27	-2288.1780379	33.47
78	11v-05-TricapCubeB-a30	-2288.1780253	33.48
79	11v-01-EdgeCoalscedIh-a116	-2288.1779200	33.54
80	11v-01-EdgeCoalscedIh-a118	-2288.1765876	34.38
81	11v-04-TricapCubeA-a21	-2288.1763228	34.55
82	11v-07-CapPentPrB-a11	-2288.1761077	34.68

83	11v-02-PentaCapTriPri-a22	-2288.1760747	34.70
84	11v-04-TricapCubeA-a22	-2288.1759188	34.80
85	11v-01-EdgeCoalscedIh-a119	-2288.1754504	35.09
86	11v-01-EdgeCoalscedIh-a114	-2288.1751468	35.28
87	11v-03-CapPentAnPr-a30	-2288.1747279	35.55
88	11v-06-CapPentPrA-a31	-2288.1745582	35.65
89	11v-03-CapPentAnPr-a24	-2288.1743283	35.80
90	11v-02-PentaCapTriPri-a17	-2288.1741769	35.89
91	11v-05-TricapCubeB-a23	-2288.1741475	35.91
92	11v-04-TricapCubeA-a37	-2288.1741356	35.92
93	11v-04-TricapCubeA-a25	-2288.1741284	35.92
94	11v-06-CapPentPrA-a14	-2288.1741275	35.92
95	11v-07-CapPentPrB-a38	-2288.1741024	35.94
96	11v-06-CapPentPrA-a13	-2288.1741011	35.94
97	11v-03-CapPentAnPr-a12	-2288.1739670	36.03
98	11v-04-TricapCubeA-a34	-2288.1739316	36.05
99	11v-07-CapPentPrB-a17	-2288.1739252	36.05
100	11v-07-CapPentPrB-a27	-2288.1737341	36.17
101	11v-02-PentaCapTriPri-a16	-2288.1735419	36.29
102	11v-03-CapPentAnPr-a39	-2288.1732950	36.45
103	11v-07-CapPentPrB-a33	-2288.1732215	36.49
104	11v-06-CapPentPrA-a35	-2288.1730891	36.58
105	11v-01-EdgeCoalscedIh-a11	-2288.1729869	36.64
106	11v-01-EdgeCoalscedIh-a16	-2288.1729842	36.64
107	11v-03-CapPentAnPr-a23	-2288.1693894	38.90
108	11v-06-CapPentPrA-a26	-2288.1688405	39.24
109	11v-04-TricapCubeA-a27	-2288.1687377	39.31
110	11v-01-EdgeCoalscedIh-a12	-2288.1669793	40.41
111	11v-05-TricapCubeB-a17	-2288.1667793	40.54
112	11v-07-CapPentPrB-a30	-2288.1667152	40.58
113	11v-06-CapPentPrA-a16	-2288.1661614	40.92
114	11v-03-CapPentAnPr-a19	-2288.1658595	41.11
115	11v-06-CapPentPrA-a27	-2288.1656871	41.22
116	11v-01-EdgeCoalscedIh-a110	-2288.1652685	41.48
117	11v-03-CapPentAnPr-a31	-2288.1652452	41.50
118	11v-04-TricapCubeA-a17	-2288.1630398	42.88
119	11v-07-CapPentPrB-a21	-2288.1626580	43.12
120	11v-05-TricapCubeB-a16	-2288.1621656	43.43
121	11v-07-CapPentPrB-a31	-2288.1621453	43.44
122	11v-05-TricapCubeB-a22	-2288.1620618	43.50
123	11v-01-EdgeCoalscedIh-a122	-2288.1598909	44.86
124	11v-04-TricapCubeA-a23	-2288.1593505	45.20
125	11v-01-EdgeCoalscedIh-a124	-2288.1590980	45.36

126	11v-02-PentaCapTriPri-a30	-2288.1587970	45.54
127	11v-06-CapPentPrA-a32	-2288.1587188	45.59
128	11v-06-CapPentPrA-a11	-2288.1579494	46.08
129	11v-05-TricapCubeB-a24	-2288.1574400	46.40
130	11v-01-EdgeCoalscedIh-a121	-2288.1573215	46.47
131	11v-03-CapPentAnPr-a36	-2288.1572490	46.52
132	11v-05-TricapCubeB-a27	-2288.1572225	46.53
133	11v-03-CapPentAnPr-a25	-2288.1566225	46.91
134	11v-03-CapPentAnPr-a17	-2288.1561989	47.17
135	11v-05-TricapCubeB-a25	-2288.1561783	47.19
136	11v-03-CapPentAnPr-a11	-2288.1561711	47.19
137	11v-03-CapPentAnPr-a21	-2288.1560870	47.25
138	11v-07-CapPentPrB-a18	-2288.1547891	48.06
139	11v-03-CapPentAnPr-a13	-2288.1547081	48.11
140	11v-03-CapPentAnPr-a22	-2288.1538440	48.65
141	11v-01-EdgeCoalscedIh-a15	-2288.1531545	49.09
142	11v-04-TricapCubeA-a38	-2288.1524339	49.54
143	11v-07-CapPentPrB-a35	-2288.1519887	49.82
144	11v-01-EdgeCoalscedIh-a132	-2288.1484798	52.02
145	11v-03-CapPentAnPr-a14	-2288.1480296	52.30
146	11v-07-CapPentPrB-a16	-2288.1478851	52.39
147	11v-01-EdgeCoalscedIh-a123	-2288.1471461	52.86
148	11v-02-PentaCapTriPri-a18	-2288.1471093	52.88
149	11v-04-TricapCubeA-a19	-2288.1469579	52.97
150	11v-04-TricapCubeA-a16	-2288.1465906	53.20
151	11v-07-CapPentPrB-a13	-2288.1425019	55.77
152	11v-07-CapPentPrB-a14	-2288.1425019	55.77
153	11v-07-CapPentPrB-a37	-2288.1418306	56.19
154	11v-03-CapPentAnPr-a32	-2288.1413929	56.47
155	11v-05-TricapCubeB-a19	-2288.1406234	56.95
156	11v-02-PentaCapTriPri-a20	-2288.1402222	57.20
157	11v-01-EdgeCoalscedIh-a128	-2288.1398085	57.46
158	11v-02-PentaCapTriPri-a31	-2288.1394860	57.66
159	11v-07-CapPentPrB-a24	-2288.1378982	58.66
160	11v-06-CapPentPrA-a23	-2288.1352141	60.34
161	11v-06-CapPentPrA-a12	-2288.1352100	60.35
162	11v-02-PentaCapTriPri-a19	-2288.1346975	60.67
163	11v-05-TricapCubeB-a31	-2288.1345511	60.76
164	11v-04-TricapCubeA-a35	-2288.1343682	60.87
165	11v-04-TricapCubeA-a24	-2288.1342788	60.93
166	11v-06-CapPentPrA-a30	-2288.1341948	60.98
167	11v-04-TricapCubeA-a13	-2288.1317838	62.50
168	11v-04-TricapCubeA-a15	-2288.1315534	62.64

169	11v-02-PentaCapTriPri-a21	-2288.1314750	62.69
170	11v-01-EdgeCoalscedIh-a127	-2288.1314207	62.72
171	11v-02-PentaCapTriPri-a23	-2288.1293703	64.01
172	11v-03-CapPentAnPr-a37	-2288.1290550	64.21
173	11v-02-PentaCapTriPri-a34	-2288.1289667	64.26
174	11v-07-CapPentPrB-a15	-2288.1287678	64.39
175	11v-06-CapPentPrA-a25	-2288.1285172	64.55
176	11v-06-CapPentPrA-a24	-2288.1273113	65.30
177	11v-05-TricapCubeB-a11	-2288.1271702	65.39
178	11v-04-TricapCubeA-a14	-2288.1253852	66.51
179	11v-02-PentaCapTriPri-a14	-2288.1246598	66.97
180	11v-07-CapPentPrB-a34	-2288.1241061	67.31
181	11v-01-EdgeCoalscedIh-a126	-2288.1098006	76.29
182	11v-04-TricapCubeA-a32	-2288.1080602	77.38
183	11v-02-PentaCapTriPri-a25	-2288.1064718	78.38
184	11v-02-PentaCapTriPri-a40	-2288.1055064	78.99
185	11v-01-EdgeCoalscedIh-a13	-2288.1028329	80.66
186	11v-01-EdgeCoalscedIh-a17	-2288.0999612	82.47
187	11v-02-PentaCapTriPri-a24	-2288.0980037	83.69
188	11v-01-EdgeCoalscedIh-a111	-2288.0907758	88.23
189	11v-02-PentaCapTriPri-a15	-2288.0849158	91.91
190	11v-01-EdgeCoalscedIh-a117	-2288.0829882	93.12
191	11v-02-PentaCapTriPri-a37	-2288.0781367	96.16
192	11v-02-PentaCapTriPri-a41	-2288.0781199	96.17
193	11v-02-PentaCapTriPri-a12	-2288.0755444	97.79
194	11v-02-PentaCapTriPri-a38	-2288.0571177	109.35

Table 7A. Initial $(CH_3)_{12}Al_8C_4$ structures, a total of 191 structures:

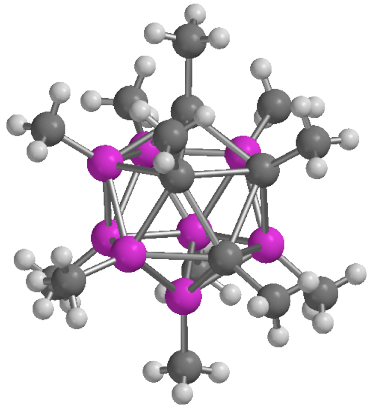
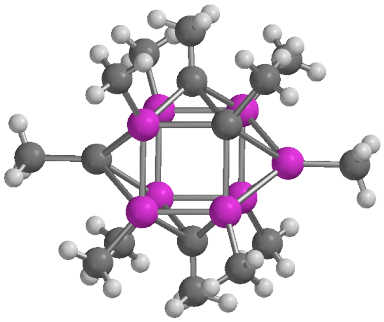
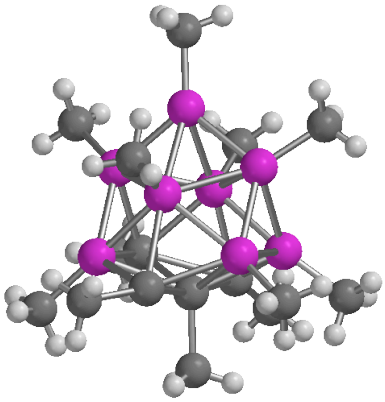
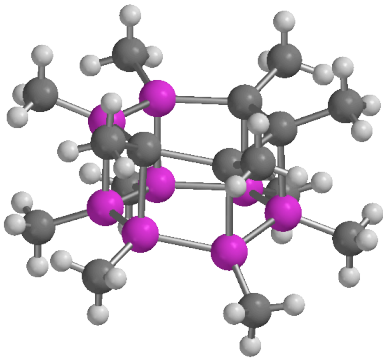
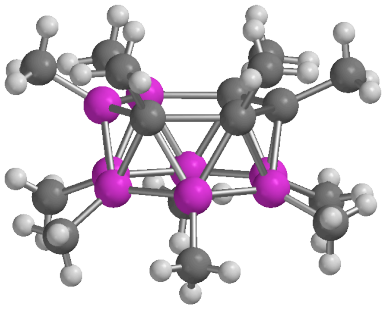
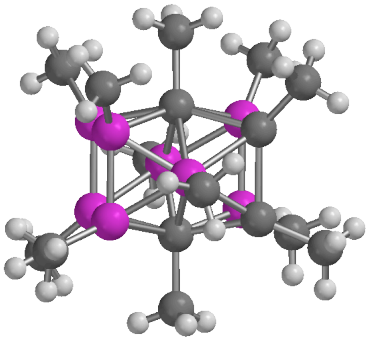
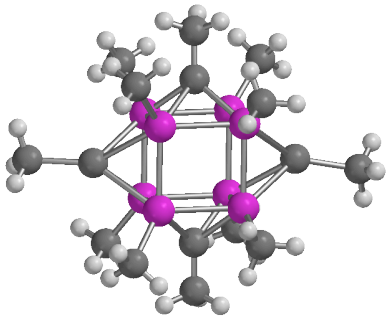
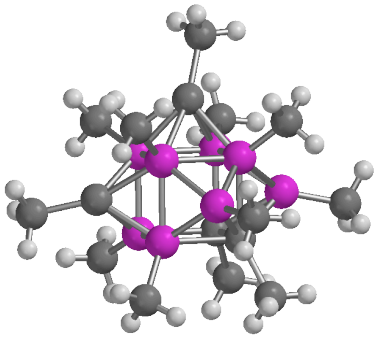
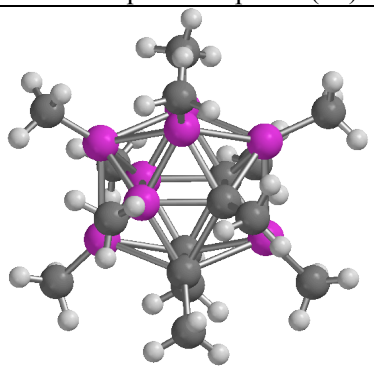
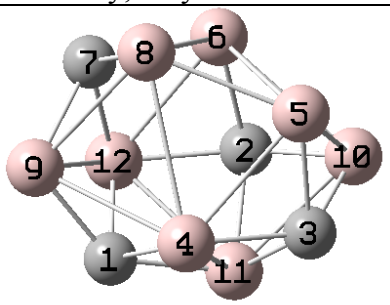
 Icosahedron (6)	 Cube octahedron (26)	 Anticube octahedron (28)
 Hexagonal prism (16)	 Hexagonal antiprism (15)	 Double square antiprism (18)
 Tetracapped cube A (26)	 Tetracapped cube B (40)	 2v6 structure (16)

Table 7B. Distance table for the lowest-lying $(CH_3)_{12}Al_8C_4$ structures after PBE0/Def2TZVPP optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity, only the atoms forming the cluster framework are presented.

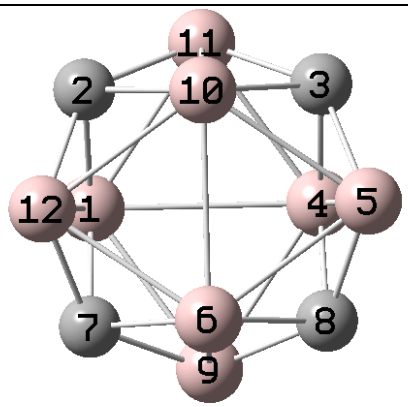


1. -2568.8635137 0.0 C1

	1	2	3	4	5
1 C	0.000000				
2 C	3.212603	0.000000			
3 C	3.246721	3.073982	0.000000		
4 Al	2.120065	3.883058	2.114591	0.000000	
5 Al	4.156600	3.724710	2.094770	2.692632	0.000000
6 Al	3.881796	2.121354	3.667613	4.009551	3.016919
7 C	3.074729	3.248027	4.432607	3.672549	3.888197
8 Al	3.729483	4.162620	3.897604	3.030972	2.583738
9 Al	1.997563	4.146660	4.387734	2.794251	4.347158
10 Al	4.146302	1.996935	2.037949	3.773529	2.697298
11 Al	2.083837	2.119210	2.118843	2.668761	3.739311
12 Al	2.118587	2.084118	4.010795	3.646303	4.482287

	6	7	8	9	10
6 Al	0.000000				
7 C	2.115872	0.000000			
8 Al	2.691816	2.092404	0.000000		
9 Al	3.772053	2.037715	2.695477	0.000000	
10 Al	2.792438	4.389404	4.356932	5.149088	0.000000
11 Al	3.646024	4.012586	4.491222	3.821373	2.575736
12 Al	2.669973	2.118403	3.740258	2.575301	3.820820

	11	12
12 Al	2.629794	0.000000

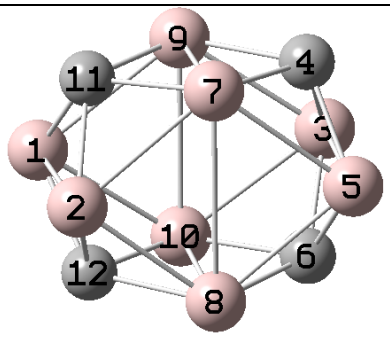


2. -2568.8424038 +13.3 C2v

	1	2	3	4	5
1 Al	0.000000				
2 C	2.159791	0.000000			
3 C	3.785823	3.168841	0.000000		
4 Al	3.056583	3.789238	2.157416	0.000000	
5 Al	4.493496	4.223457	2.010782	2.627302	0.000000
6 Al	3.635278	3.793046	3.792380	3.638155	2.689215
7 C	2.158272	3.177312	4.486179	3.789421	4.224417
8 C	3.783629	4.484893	3.170825	2.153719	2.011546
9 Al	2.701060	4.239581	4.235576	2.700588	3.767710
10 Al	3.634063	2.150781	2.155550	3.637858	2.692608
11 Al	2.695684	2.010139	2.007279	2.694467	3.767015
12 Al	2.611733	2.005936	4.229224	4.495499	4.363931

	6	7	8	9	10
7 C	2.155841	0.000000			
8 C	2.159786	3.170033	0.000000		
9 Al	2.619360	2.009288	2.005035	0.000000	
10 Al	3.071655	3.795457	3.795817	4.508884	0.000000
11 Al	4.504724	4.234985	4.228902	4.379690	2.618347
12 Al	2.700065	2.005961	4.229854	3.766368	2.701049

	11	12
12 Al	3.765786	0.000000

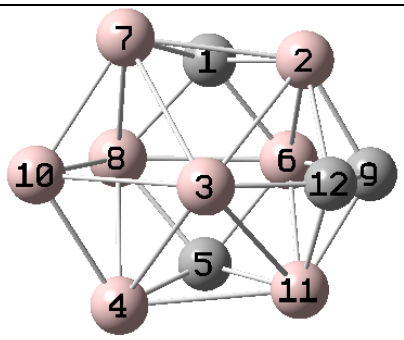


3. -2568.8398245 +14.9 D2h

	1	2	3	4	5
1 Al	0.000000				
2 Al	2.574065	0.000000			
3 Al	4.330558	4.962937	0.000000		
4 C	4.304859	4.246090	2.039475	0.000000	
5 Al	4.964503	4.163792	2.566751	2.057106	0.000000
6 C	4.294122	4.238530	2.039967	3.050018	2.056549
7 Al	3.731298	2.656067	3.729786	2.106409	2.661715
8 Al	3.734235	2.658787	3.733975	3.814533	2.660258
9 Al	2.673159	3.721657	2.668576	2.134250	3.718823
10 Al	2.666521	3.721812	2.667521	3.749881	3.718866
11 C	2.039059	2.059911	4.299458	3.313653	4.247382
12 C	2.039982	2.060094	4.297723	4.501377	4.241968

	6	7	8	9	10
6 C	0.000000				
7 Al	3.806789	0.000000			
8 Al	2.103043	3.308621	0.000000		
9 Al	3.745966	2.639545	4.162310	0.000000	
10 Al	2.129539	4.155965	2.648489	3.115385	0.000000
11 C	4.495716	2.106179	3.813579	2.132783	3.746101
12 C	3.300605	3.807712	2.104586	3.750171	2.133069

	11	12
11 C	0.000000	
12 C	3.049124	0.000000

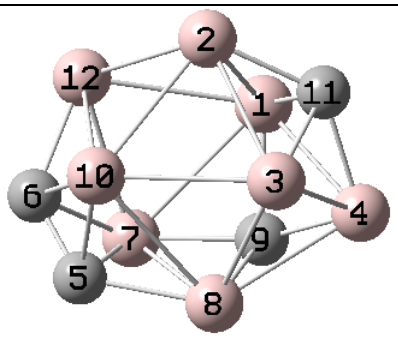


4. -2568.8395445 +15.0 CS

	1	2	3	4	5
1 C	0.000000				
2 Al	2.060074	0.000000			
3 Al	3.620689	2.952853	0.000000		
4 Al	4.156929	4.744508	2.998770	0.000000	
5 C	3.148452	3.929543	3.620602	2.059568	0.000000
6 Al	2.084488	2.658285	4.002701	3.878680	2.083881
7 Al	2.062092	2.789039	2.997864	4.143292	4.159794
8 Al	2.111354	3.771787	3.803603	2.749947	2.114990
9 C	3.172646	2.086001	3.316584	4.365102	3.174300
10 Al	3.783694	4.537634	2.815316	2.559253	3.785010
11 Al	3.928256	3.552876	2.947942	2.790310	2.063127
12 C	3.532174	2.132324	2.051934	3.949107	3.534345

	6	7	8	9	10
6 Al	0.000000				
7 Al	3.881485	0.000000			
8 Al	2.647765	2.750263	0.000000		
9 C	2.080039	4.363981	4.144439	0.000000	
10 Al	4.763861	2.557953	2.803381	5.264516	0.000000
11 Al	2.658716	4.742927	3.774732	2.086261	4.537010
12 C	3.129686	3.945936	4.325010	1.537274	4.542703

	11	12
12 C	2.130977	0.000000

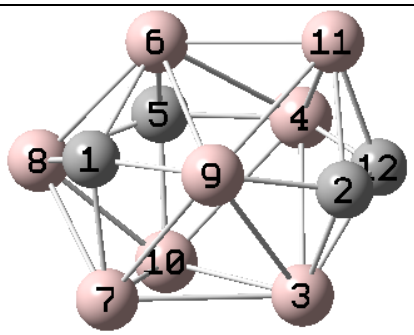


5. -2568.8357784 +17.4 C1

	1	2	3	4	5
1 Al	0.000000				
2 Al	2.719788	0.000000			
3 Al	3.690926	2.675312	0.000000		
4 Al	2.603910	3.715674	2.568485	0.000000	
5 C	4.154601	4.266327	3.920383	4.425201	0.000000
6 C	3.932292	3.826436	4.443697	5.019614	1.501927
7 Al	2.921612	4.295596	4.560173	3.937682	2.113091
8 Al	3.607722	4.127541	2.742937	2.675316	2.117989
9 C	2.078153	3.981727	3.609651	2.055638	3.211315
10 Al	4.080139	2.782213	2.815446	4.417139	2.182706
11 C	2.119904	2.019008	2.218048	2.023778	4.724274
12 Al	2.878355	2.685483	4.446974	4.811081	3.206296

	6	7	8	9	10
6 C	0.000000				
7 Al	2.172301	0.000000			
8 Al	3.292590	2.679900	0.000000		
9 C	3.704953	2.042429	2.129697	0.000000	
10 Al	2.156202	3.535721	2.945060	4.029107	0.000000
11 C	4.788590	4.359862	3.661346	3.101383	3.871450
12 Al	2.015133	2.769604	4.187396	3.763104	2.820718

	11	12
11 C	0.000000	
12 Al	3.933703	0.000000

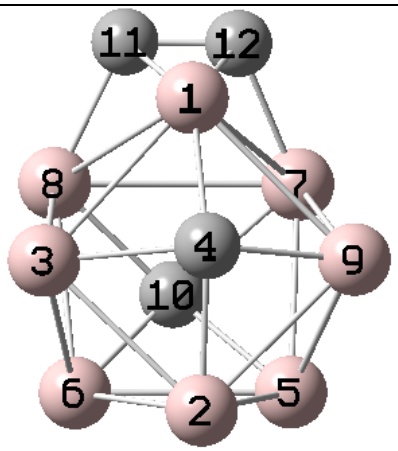


6. -2568.8336026 +18.8 CS

	1	2	3	4	5
1 C	0.000000				
2 C	3.671487	0.000000			
3 Al	3.756618	2.134007	0.000000		
4 Al	4.020636	3.165499	2.979632	0.000000	
5 C	3.055117	4.247299	3.744337	2.032209	0.000000
6 Al	2.147792	3.653781	4.195067	2.863389	2.144265
7 Al	2.124782	3.868130	2.835548	4.296069	3.531725
8 Al	2.064773	4.939366	4.329486	3.865198	2.062704
9 Al	2.032713	2.026789	2.993367	3.929100	4.012977
10 Al	3.529752	4.334607	2.812087	2.862346	2.130318
11 Al	3.847781	2.165939	3.794747	2.800372	3.846369
12 C	4.255017	1.506002	2.133891	2.026619	3.669190

	6	7	8	9	10
6 Al	0.000000				
7 Al	3.783254	0.000000			
8 Al	2.594553	2.572459	0.000000		
9 Al	2.860157	2.863336	3.863951	0.000000	
10 Al	3.782875	2.598816	2.575080	4.284550	0.000000
11 Al	2.667661	4.945553	4.907632	2.793278	4.941731
12 C	3.653479	4.351541	4.942299	3.166858	3.864558

	11	12
12 C	2.163880	0.000000

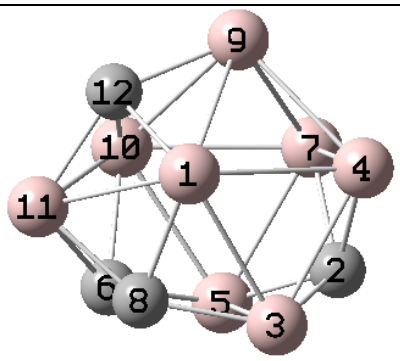


7. -2568.8305871 +20.7 CS

	1	2	3	4	5
1 Al	0.000000				
2 Al	3.887464	0.000000			
3 Al	2.739824	2.687554	0.000000		
4 C	2.056093	2.096625	2.110642	0.000000	
5 Al	4.346638	2.702764	4.185475	3.621343	0.000000
6 Al	4.308636	2.701062	2.686126	3.639086	2.679662
7 Al	3.211300	4.374798	4.476734	3.895964	2.662977
8 Al	3.138387	4.380760	2.901052	3.908872	3.914326
9 Al	2.830455	2.699312	3.854702	2.082656	2.674172
10 C	3.875067	3.728752	3.710695	3.996743	2.128442
11 C	2.290920	5.252863	3.713257	4.004368	4.793817
12 C	2.274502	5.204823	4.338420	3.937871	4.359470

	6	7	8	9	10
6 Al	0.000000				
7 Al	3.891978	0.000000			
8 Al	2.680729	3.021349	0.000000		
9 Al	4.184091	2.896144	4.478255	0.000000	
10 C	2.109938	2.080004	2.087613	3.715090	0.000000
11 C	4.392492	2.860988	1.994768	4.363970	3.330278
12 C	4.780501	1.992916	2.874007	3.638862	3.335386

	11	12
11 C	0.000000	
12 C	1.407543	0.000000

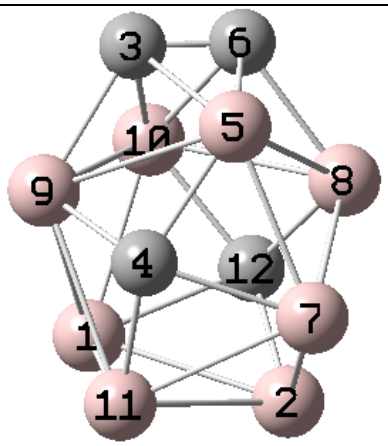


8. -2568.8283594 +22.0 CS

	1	2	3	4	5
1 Al	0.000000				
2 C	3.702758	0.000000			
3 Al	2.750265	2.040607	0.000000		
4 Al	2.802861	2.132043	2.634306	0.000000	
5 Al	4.174799	2.041441	2.826756	3.805127	0.000000
6 C	3.263120	3.365117	2.959121	4.339462	2.035263
7 Al	4.153709	2.133395	3.809622	2.677770	2.629434
8 C	2.221436	3.360031	2.030910	3.799236	2.956801
9 Al	2.779189	3.774553	4.309661	2.704811	4.298675
10 Al	3.502377	3.707284	4.179438	4.155097	2.744465
11 Al	2.586322	4.703601	3.914282	4.796960	3.912284
12 C	2.132416	4.384953	4.192019	3.821746	4.186138

	6	7	8	9	10
6 C	0.000000				
7 Al	3.806015	0.000000			
8 C	1.633009	4.339881	0.000000		
9 Al	4.170042	2.700967	4.172257	0.000000	
10 Al	2.219375	2.811594	3.263624	2.775215	0.000000
11 Al	2.045598	4.801395	2.049497	3.872633	2.585152
12 C	3.108222	3.825266	3.110615	2.027732	2.132613

	11	12
12 C	2.029371	0.000000



9. -2568.8233239 +25.2 C2

		1	2	3	4	5
1	Al	0.000000				
2	Al	2.690066	0.000000			
3	C	3.999674	4.903046	0.000000		
4	C	3.696115	3.744900	3.259050	0.000000	
5	Al	4.579881	4.338798	2.301489	2.034663	0.000000
6	C	4.294249	4.520200	1.416928	3.736475	2.296723
7	Al	4.207484	2.685163	4.298099	2.215804	2.553933
8	Al	3.831273	2.842105	3.180316	3.688755	2.777980
9	Al	2.797300	4.220162	2.137031	2.107301	2.788281
10	Al	2.555117	3.805297	2.305587	4.112368	3.776577
11	Al	2.681930	2.757188	4.519890	2.041689	3.806216
12	C	2.217417	2.041502	3.753038	4.142816	4.119566

		6	7	8	9	10
6	C	0.000000				
7	Al	3.992801	0.000000			
8	Al	2.143388	2.794997	0.000000		
9	Al	3.166893	3.834321	3.875548	0.000000	
10	Al	2.298603	4.576586	2.784426	2.775256	0.000000
11	Al	4.892143	2.690732	4.215393	2.844726	4.334598
12	C	3.265234	3.699162	2.106700	3.694401	2.036715

		11	12
11	Al	0.000000	
12	C	3.745209	0.000000

Table S7C. Energy ranking for all of the $(CH_3)_{12}Al_8C_4$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	12v-08-TetraCappedCube-C2v-37	-2570.5854318	0.00
2	12v-08-TetraCappedCube-C2v-1	-2570.5852367	0.12
3	12v-08-TetraCappedCube-C2v-40	-2570.5646595	13.04
4	12v-08-TetraCappedCube-C2v-35	-2570.5643837	13.21
5	12v-09-2v6-Dh-9	-2570.5602266	15.82
6	12v-02-CubeOh-26	-2570.5601365	15.87
7	12v-07-TetraCappedCube-D4h-26	-2570.5601346	15.87
8	12v-01-Icos-6	-2570.5598276	16.07
9	12v-07-TetraCappedCube-D4h-1	-2570.5597960	16.09
10	12v-02-CubeOh-1	-2570.5597948	16.09
11	12v-09-2v6-Dh-13	-2570.5594100	16.33
12	12v-01-Icos-4	-2570.5562262	18.33
13	12v-09-2v6-Dh-6	-2570.5560112	18.46
14	12v-08-TetraCappedCube-C2v-18	-2570.5535295	20.02
15	12v-02-CubeOh-23	-2570.5531277	20.27
16	12v-07-TetraCappedCube-D4h-23	-2570.5531277	20.27
17	12v-08-TetraCappedCube-C2v-9	-2570.5530187	20.34
18	12v-03-AnticubeOh-4	-2570.5517636	21.13
19	12v-01-Icos-5	-2570.5516835	21.18
20	12v-03-AnticubeOh-22	-2570.5516454	21.20
21	12v-03-AnticubeOh-25	-2570.5475283	23.79
22	12v-08-TetraCappedCube-C2v-7	-2570.5473120	23.92
23	12v-09-2v6-Dh-12	-2570.5471815	24.00
24	12v-03-AnticubeOh-20	-2570.5470801	24.07
25	12v-03-AnticubeOh-13	-2570.5449117	25.43
26	12v-08-TetraCappedCube-C2v-13	-2570.5446399	25.60
27	12v-03-AnticubeOh-23	-2570.5446050	25.62
28	12v-04-HexPr-11	-2570.5441890	25.88
29	12v-03-AnticubeOh-14	-2570.5427733	26.77
30	12v-09-2v6-Dh-3	-2570.5426793	26.83
31	12v-07-TetraCappedCube-D4h-25	-2570.5426173	26.87
32	12v-02-CubeOh-25	-2570.5426149	26.87
33	12v-09-2v6-Dh-11	-2570.5422544	27.09
34	12v-09-2v6-Dh-7	-2570.5405154	28.19
35	12v-08-TetraCappedCube-C2v-36	-2570.5389889	29.14
36	12v-03-AnticubeOh-3	-2570.5383319	29.56
37	12v-09-2v6-Dh-16	-2570.5382995	29.58
38	12v-07-TetraCappedCube-D4h-2	-2570.5368429	30.49
39	12v-02-CubeOh-2	-2570.5368419	30.49

40	12v-07-TetraCappedCube-D4h-24	-2570.5367528	30.55
41	12v-02-CubeOh-24	-2570.5367499	30.55
42	12v-08-TetraCappedCube-C2v-38	-2570.5367314	30.56
43	12v-05-HexAnPr-15	-2570.5348366	31.75
44	12v-06-DsqAnPr-13	-2570.5323374	33.32
45	12v-03-AnticubeOh-12	-2570.5322745	33.36
46	12v-03-AnticubeOh-1	-2570.5322553	33.37
47	12v-08-TetraCappedCube-C2v-4	-2570.5321851	33.41
48	12v-03-AnticubeOh-16	-2570.5320595	33.49
49	12v-08-TetraCappedCube-C2v-25	-2570.5320047	33.53
50	12v-08-TetraCappedCube-C2v-3	-2570.5317194	33.71
51	12v-04-HexPr-8	-2570.5305292	34.45
52	12v-08-TetraCappedCube-C2v-15	-2570.5303116	34.59
53	12v-04-HexPr-3	-2570.5301407	34.70
54	12v-06-DsqAnPr-7	-2570.5300117	34.78
55	12v-05-HexAnPr-14	-2570.5300085	34.78
56	12v-04-HexPr-1	-2570.5299977	34.79
57	12v-09-2v6-Dh-10	-2570.5298234	34.90
58	12v-02-CubeOh-6	-2570.5293100	35.22
59	12v-07-TetraCappedCube-D4h-6	-2570.5292948	35.23
60	12v-08-TetraCappedCube-C2v-32	-2570.5287575	35.56
61	12v-08-TetraCappedCube-C2v-24	-2570.5285462	35.70
62	12v-06-DsqAnPr-11	-2570.5282335	35.89
63	12v-03-AnticubeOh-15	-2570.5280214	36.03
64	12v-02-CubeOh-13	-2570.5279902	36.05
65	12v-07-TetraCappedCube-D4h-13	-2570.5279902	36.05
66	12v-05-HexAnPr-1	-2570.5276127	36.28
67	12v-03-AnticubeOh-18	-2570.5271324	36.58
68	12v-09-2v6-Dh-15	-2570.5233811	38.94
69	12v-03-AnticubeOh-26	-2570.5226911	39.37
70	12v-08-TetraCappedCube-C2v-14	-2570.5226750	39.38
71	12v-04-HexPr-15	-2570.5224495	39.52
72	12v-04-HexPr-9	-2570.5218813	39.88
73	12v-08-TetraCappedCube-C2v-6	-2570.5216642	40.02
74	12v-08-TetraCappedCube-C2v-5	-2570.5215787	40.07
75	12v-07-TetraCappedCube-D4h-19	-2570.5215716	40.07
76	12v-02-CubeOh-19	-2570.5215656	40.08
77	12v-03-AnticubeOh-21	-2570.5207651	40.58
78	12v-02-CubeOh-20	-2570.5204369	40.79
79	12v-07-TetraCappedCube-D4h-20	-2570.5204349	40.79
80	12v-02-CubeOh-3	-2570.5200729	41.01
81	12v-07-TetraCappedCube-D4h-3	-2570.5200729	41.01
82	12v-08-TetraCappedCube-C2v-12	-2570.5200528	41.03

83	12v-05-HexAnPr-8	-2570.5199496	41.09
84	12v-08-TetraCappedCube-C2v-23	-2570.5199480	41.09
85	12v-04-HexPr-10	-2570.5199049	41.12
86	12v-03-AnticubeOh-17	-2570.5194779	41.39
87	12v-08-TetraCappedCube-C2v-16	-2570.5191773	41.58
88	12v-08-TetraCappedCube-C2v-34	-2570.5191497	41.59
89	12v-08-TetraCappedCube-C2v-8	-2570.5188732	41.77
90	12v-02-CubeOh-9	-2570.5186732	41.89
91	12v-07-TetraCappedCube-D4h-9	-2570.5186732	41.89
92	12v-06-DsqAnPr-8	-2570.5184124	42.06
93	12v-02-CubeOh-5	-2570.5184082	42.06
94	12v-07-TetraCappedCube-D4h-5	-2570.5184082	42.06
95	12v-03-AnticubeOh-9	-2570.5173060	42.75
96	12v-04-HexPr-12	-2570.5154816	43.90
97	12v-08-TetraCappedCube-C2v-31	-2570.5153967	43.95
98	12v-03-AnticubeOh-6	-2570.5146128	44.44
99	12v-06-DsqAnPr-12	-2570.5139310	44.87
100	12v-04-HexPr-2	-2570.5136090	45.07
101	12v-02-CubeOh-10	-2570.5133784	45.21
102	12v-07-TetraCappedCube-D4h-10	-2570.5133784	45.21
103	12v-02-CubeOh-16	-2570.5132598	45.29
104	12v-07-TetraCappedCube-D4h-16	-2570.5132598	45.29
105	12v-04-HexPr-5	-2570.5118627	46.17
106	12v-08-TetraCappedCube-C2v-33	-2570.5105434	46.99
107	12v-03-AnticubeOh-7	-2570.5089053	48.02
108	12v-02-CubeOh-8	-2570.5084400	48.31
109	12v-07-TetraCappedCube-D4h-8	-2570.5084400	48.31
110	12v-04-HexPr-13	-2570.5076088	48.84
111	12v-03-AnticubeOh-5	-2570.5075250	48.89
112	12v-02-CubeOh-18	-2570.5071991	49.09
113	12v-07-TetraCappedCube-D4h-18	-2570.5071991	49.09
114	12v-06-DsqAnPr-5	-2570.5071955	49.09
115	12v-08-TetraCappedCube-C2v-19	-2570.5069509	49.25
116	12v-09-2v6-Dh-1	-2570.5069243	49.27
117	12v-02-CubeOh-7	-2570.5069177	49.27
118	12v-07-TetraCappedCube-D4h-7	-2570.5069177	49.27
119	12v-08-TetraCappedCube-C2v-11	-2570.5067439	49.38
120	12v-01-Icos-1	-2570.5066564	49.43
121	12v-09-2v6-Dh-5	-2570.5060184	49.83
122	12v-06-DsqAnPr-1	-2570.5057653	49.99
123	12v-01-Icos-2	-2570.5057549	50.00
124	12v-06-DsqAnPr-14	-2570.5054990	50.16
125	12v-08-TetraCappedCube-C2v-17	-2570.5054952	50.16

126	12v-09-2v6-Dh-8	-2570.5053796	50.23
127	12v-02-CubeOh-11	-2570.5052480	50.32
128	12v-07-TetraCappedCube-D4h-11	-2570.5052480	50.32
129	12v-03-AnticubeOh-24	-2570.5050583	50.44
130	12v-08-TetraCappedCube-C2v-39	-2570.5045403	50.76
131	12v-09-2v6-Dh-2	-2570.5033808	51.49
132	12v-09-2v6-Dh-14	-2570.5017673	52.50
133	12v-09-2v6-Dh-4	-2570.5017083	52.54
134	12v-01-Icos-3	-2570.5009163	53.04
135	12v-02-CubeOh-12	-2570.5008752	53.06
136	12v-07-TetraCappedCube-D4h-12	-2570.5008752	53.06
137	12v-05-HexAnPr-13	-2570.4994576	53.95
138	12v-03-AnticubeOh-8	-2570.4988826	54.31
139	12v-03-AnticubeOh-2	-2570.4984656	54.57
140	12v-05-HexAnPr-11	-2570.4970114	55.49
141	12v-06-DsqAnPr-10	-2570.4966006	55.74
142	12v-04-HexPr-6	-2570.4950902	56.69
143	12v-03-AnticubeOh-11	-2570.4938051	57.50
144	12v-02-CubeOh-21	-2570.4935989	57.63
145	12v-07-TetraCappedCube-D4h-21	-2570.4935989	57.63
146	12v-06-DsqAnPr-17	-2570.4926296	58.24
147	12v-04-HexPr-7	-2570.4920317	58.61
148	12v-03-AnticubeOh-10	-2570.4872823	61.59
149	12v-06-DsqAnPr-16	-2570.4868074	61.89
150	12v-05-HexAnPr-10	-2570.4857265	62.57
151	12v-05-HexAnPr-12	-2570.4833113	64.08
152	12v-05-HexAnPr-7	-2570.4830661	64.24
153	12v-04-HexPr-14	-2570.4829455	64.31
154	12v-08-TetraCappedCube-C2v-21	-2570.4818419	65.00
155	12v-02-CubeOh-17	-2570.4802310	66.02
156	12v-07-TetraCappedCube-D4h-17	-2570.4802310	66.02
157	12v-04-HexPr-4	-2570.4798279	66.27
158	12v-05-HexAnPr-9	-2570.4793472	66.57
159	12v-08-TetraCappedCube-C2v-30	-2570.4792312	66.64
160	12v-06-DsqAnPr-3	-2570.4790136	66.78
161	12v-08-TetraCappedCube-C2v-2	-2570.4785721	67.06
162	12v-06-DsqAnPr-6	-2570.4774215	67.78
163	12v-02-CubeOh-14	-2570.4768586	68.13
164	12v-07-TetraCappedCube-D4h-14	-2570.4768586	68.13
165	12v-06-DsqAnPr-9	-2570.4760365	68.65
166	12v-03-AnticubeOh-19	-2570.4742537	69.77
167	12v-08-TetraCappedCube-C2v-29	-2570.4711972	71.68
168	12v-07-TetraCappedCube-D4h-22	-2570.4707547	71.96

169	12v-02-CubeOh-22	-2570.4707481	71.97
170	12v-08-TetraCappedCube-C2v-26	-2570.4696570	72.65
171	12v-05-HexAnPr-6	-2570.4696197	72.67
172	12v-06-DsqAnPr-2	-2570.4665920	74.57
173	12v-08-TetraCappedCube-C2v-28	-2570.4654780	75.27
174	12v-08-TetraCappedCube-C2v-20	-2570.4647200	75.75
175	12v-08-TetraCappedCube-C2v-22	-2570.4616758	77.66
176	12v-08-TetraCappedCube-C2v-10	-2570.4615796	77.72
177	12v-05-HexAnPr-5	-2570.4597173	78.89
178	12v-05-HexAnPr-2	-2570.4590741	79.29
179	12v-02-CubeOh-4	-2570.4573398	80.38
180	12v-07-TetraCappedCube-D4h-4	-2570.4573398	80.38
181	12v-06-DsqAnPr-18	-2570.4570615	80.55
182	12v-05-HexAnPr-4	-2570.4553122	81.65
183	12v-06-DsqAnPr-4	-2570.4531042	83.04
184	12v-06-DsqAnPr-15	-2570.4501779	84.87
185	12v-07-TetraCappedCube-D4h-15	-2570.4456333	87.73
186	12v-02-CubeOh-15	-2570.4456272	87.73
187	12v-04-HexPr-16	-2570.4448418	88.22
188	12v-05-HexAnPr-3	-2570.4435002	89.06
189	12v-08-TetraCappedCube-C2v-27	-2570.4222703	102.39

Table S8A. Initial $(CH_3)_{13}Al_9C_4$ structures, a total of 240 structures:

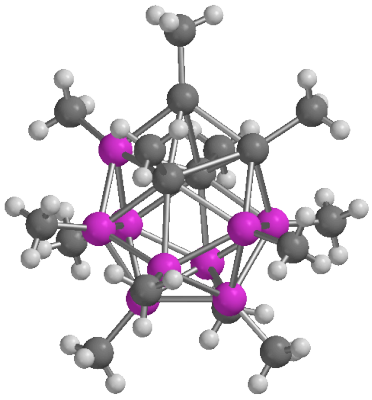
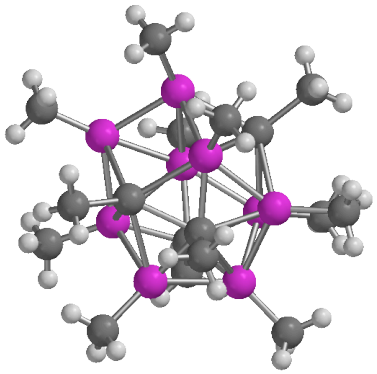
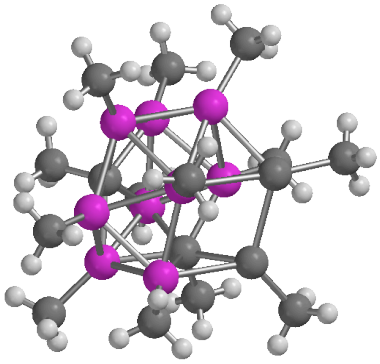
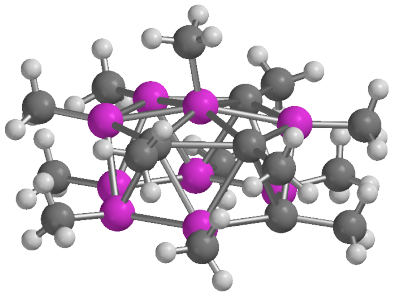
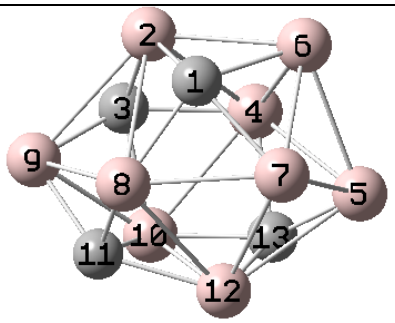
 Docosahedron (64)	 Henicosahedron (64)
 Ditrapezoidal icos (66)	 Capped hexag antiprism (46)

Table S8B. Distance table for the lowest-lying $(CH_3)_{13}Al_{11}C_2$ structures after PBE0/Def2TZVPP optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity, only the atoms forming the cluster framework are presented.

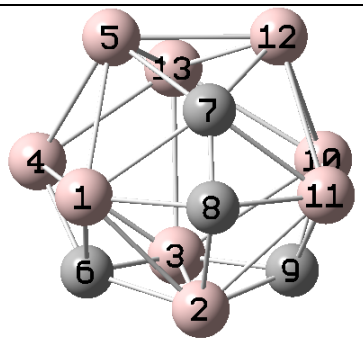


1. -2851.0367974 0.0 C_1

	1	2	3	4	5
1 C	0.000000				
2 Al	2.067847	0.000000			
3 C	3.631919	2.082659	0.000000		
4 Al	3.689517	2.785105	2.156417	0.000000	
5 Al	3.718517	4.322333	4.398810	2.763171	0.000000
6 Al	2.136354	2.638863	3.902180	2.805201	2.695017
7 Al	2.135971	3.898420	4.824946	4.205972	2.690345
8 Al	2.068034	3.081256	3.686887	4.362648	4.311972
9 Al	3.770879	2.841204	1.995036	3.889499	5.383010
10 Al	4.396999	3.724866	2.117338	2.644420	3.881969
11 C	3.630808	3.682716	3.000195	3.956952	4.395640
12 Al	3.705046	4.380100	3.969425	3.684659	2.771385
13 C	4.191777	4.101874	3.231719	2.114101	2.033197

	6	7	8	9	10
6 Al	0.000000				
7 Al	2.671025	0.000000			
8 Al	3.895566	2.636165	0.000000		
9 Al	4.964661	4.970110	2.848930	0.000000	
10 Al	4.685174	4.689595	3.723063	2.559827	0.000000
11 C	4.821446	3.907978	2.080726	1.996631	2.116867
12 Al	4.223582	2.824235	2.784707	3.897369	2.648592
13 C	3.760357	3.756838	4.089347	4.169775	2.044326

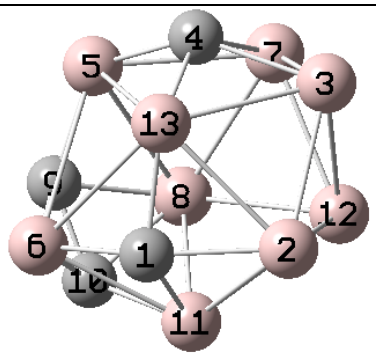
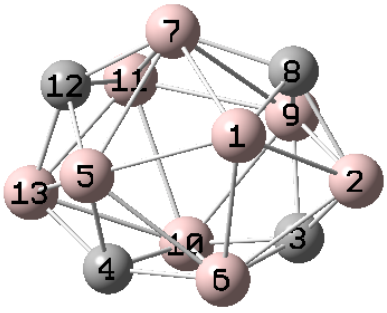
	11	12	13
11 C	0.000000		
12 Al	2.157403	0.000000	
13 C	3.223151	2.107743	0.000000

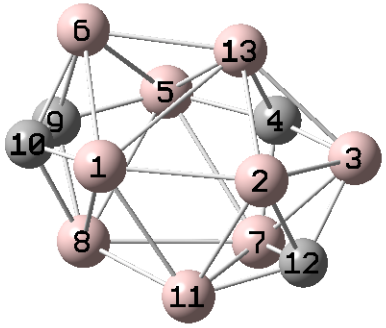


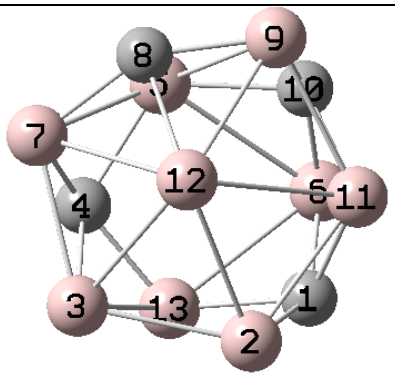
2. -2851.0142062 +14.2 C_S

	1	2	3	4	5
1 Al	0.000000				
2 Al	2.642307	0.000000			
3 Al	3.726185	2.645034	0.000000		
4 Al	2.701113	3.820917	2.722655	0.000000	
5 Al	2.712709	4.440100	4.211692	2.704062	0.000000
6 C	2.089267	2.064475	2.119636	2.045391	3.724885
7 C	2.377031	3.262852	4.225173	3.922616	2.266878
8 C	2.081756	2.107626	3.982879	4.187504	3.456528
9 C	4.072524	2.065051	2.122811	4.315319	4.725897
10 Al	4.933655	3.820021	2.721487	4.484961	4.375144
11 Al	3.794421	2.643660	3.728635	4.930253	4.160655
12 Al	4.163372	4.437877	4.205501	4.364831	2.627588
13 Al	4.270699	4.616241	2.914184	2.735276	2.709009

	6	7	8	9	10
6 C	0.000000				
7 C	3.705598	0.000000			

	8 C 3.173561 1.548807 0.000000 9 C 3.219349 3.701658 3.174959 0.000000 10 Al 4.313719 3.923097 4.192179 2.041878 0.000000 11 Al 4.072212 2.366945 2.082923 2.090981 2.704956 12 Al 4.721715 2.265884 3.459796 3.719650 2.704161 13 Al 3.863181 3.826849 4.645127 3.864883 2.741108 11 12 13 11 Al 0.000000 12 Al 2.710305 0.000000 13 Al 4.270971 2.702317 0.000000
 3. -2851.0079176 +18.1 C_1	1 2 3 4 5 1 C 0.000000 2 Al 2.141511 0.000000 3 Al 3.743720 2.600560 0.000000 4 C 3.502829 3.677812 2.197883 0.000000 5 Al 3.729987 4.724425 4.028108 2.033012 0.000000 6 Al 2.019514 4.004774 5.040939 3.923224 3.025558 7 Al 4.522661 4.170724 2.599749 2.099874 2.773105 8 Al 4.090454 4.516509 4.556999 3.774735 2.903476 9 C 3.522603 4.889348 5.140053 3.656583 2.004441 10 C 3.149779 4.403513 5.347533 4.439598 3.296958 11 Al 2.130356 2.669387 4.355269 4.326432 4.146464 12 Al 3.794138 2.730654 2.843951 3.665956 4.316789 13 Al 2.034216 2.698983 2.676235 2.050233 3.057691 6 7 8 9 10 6 Al 0.000000 7 Al 4.836768 0.000000 8 Al 3.595198 2.819661 0.000000 9 C 2.102382 3.850778 2.138859 0.000000 10 C 2.043964 4.402486 2.108161 1.553462 0.000000 11 Al 2.628509 4.336200 2.900518 3.201434 2.069562 12 Al 4.700208 2.629372 2.850824 4.361312 3.932692 13 Al 3.076995 3.796087 4.565436 3.965953 4.326203 11 12 13 11 Al 0.000000 12 Al 2.819380 0.000000 13 Al 3.737331 4.132044 0.000000
 4. -2851.0067415 +18.9 C_1	1 2 3 4 5 1 Al 0.000000 2 Al 2.580338 0.000000 3 C 3.658778 2.035007 0.000000 4 C 3.943834 4.405462 3.214853 0.000000 5 Al 2.778008 4.426685 4.140019 2.116061 0.000000 6 Al 2.833924 2.712417 2.095109 2.104640 2.833431 7 Al 2.705366 3.879193 4.167840 4.087741 2.844663 8 C 2.161654 2.070350 3.083954 4.506795 3.826989 9 Al 3.748247 2.564224 2.093739 4.090842 4.337766 10 Al 4.548023 3.901754 2.090290 2.094633 3.617859

	11 Al 4.806467 4.930248 3.987521 3.637558 3.729476 12 C 3.909280 5.101902 4.587174 3.083802 2.139507 13 Al 4.929485 5.648390 4.455741 2.010332 2.564576 6 7 8 9 10 6 Al 0.000000 7 Al 4.148797 0.000000 8 C 3.597323 2.081287 0.000000 9 Al 3.589096 2.999975 2.086112 0.000000 10 Al 2.676300 4.176151 4.117378 2.774610 0.000000 11 Al 4.571250 2.779517 3.801438 2.806278 2.852091 12 C 4.208723 2.105096 3.836028 3.880769 3.604098 13 Al 3.927097 3.882227 5.053800 4.466680 2.760192 11 12 13 11 Al 0.000000 12 C 2.093341 0.000000 13 Al 2.634584 2.046924 0.000000
 5. -2851.0045927 +20.2 C_1	1 2 3 4 5 1 Al 0.000000 2 Al 2.766199 0.000000 3 Al 4.559677 2.584280 0.000000 4 C 4.291839 3.618648 2.054505 0.000000 5 Al 4.019361 4.662687 3.960686 2.023652 0.000000 6 Al 2.794836 4.423778 5.052841 3.865702 2.714181 7 Al 4.215372 3.627472 2.595773 2.067657 3.028599 8 Al 2.925572 4.425590 4.893995 3.854459 3.054597 9 C 3.185366 4.997026 5.265164 3.709824 2.027944 10 C 2.031871 4.464498 5.482963 4.410106 3.210647 11 Al 2.763559 2.629339 3.717235 3.979963 4.488930 12 C 3.934775 2.193896 2.018266 3.100076 4.489733 13 Al 3.294301 2.782630 2.660752 2.213750 2.815884 6 7 8 9 10 6 Al 0.000000 7 Al 4.842846 0.000000 8 Al 3.705542 2.969064 0.000000 9 C 2.153507 3.956398 2.097362 0.000000 10 C 2.120006 4.423173 2.135341 1.523195 0.000000 11 Al 4.881840 2.671074 2.708224 4.299054 3.796475 12 C 5.410596 2.098646 4.022173 5.156826 5.050865 13 Al 2.691912 3.692125 4.384822 3.770637 3.902955 11 12 13 11 Al 0.000000 12 C 2.031797 0.000000 13 Al 4.247787 3.723933 0.000000

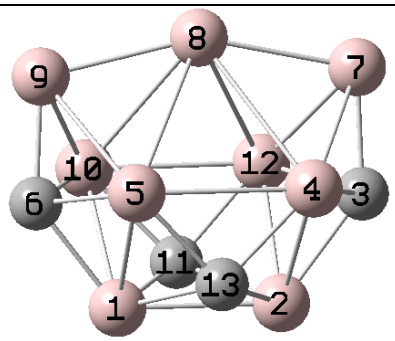


6. -2851.0045705 +20.2 C_1

	1	2	3	4	5
1 C	0.000000				
2 Al	2.112348	0.000000			
3 Al	3.814746	2.594107	0.000000		
4 C	3.573208	3.638941	2.266364	0.000000	
5 Al	3.824227	4.407536	3.897912	2.112480	0.000000
6 Al	1.968462	3.860756	4.900997	3.679101	3.052139
7 Al	4.944190	4.345204	2.562311	2.087711	2.615164
8 C	4.788855	4.483579	3.819737	3.158730	2.176037
9 Al	4.296915	4.461355	4.886140	4.188953	2.654673
10 C	3.070803	4.173886	4.904277	3.671325	2.123098
11 Al	2.117386	2.667378	4.412300	4.221011	3.593154
12 Al	4.030705	2.874180	2.824971	3.510612	3.509344
13 Al	2.105257	2.664492	2.627557	2.038154	3.330248

	6	7	8	9	10
6 Al	0.000000				
7 Al	5.119997	0.000000			
8 C	4.625003	2.001170	0.000000		
9 Al	3.879397	3.779866	1.949377	0.000000	
10 C	1.963489	4.309883	3.151784	2.039288	0.000000
11 Al	2.575471	4.784194	3.824521	2.683397	2.172138
12 Al	4.770368	2.707449	2.208971	2.759095	3.797507
13 Al	2.872515	3.885350	4.551399	4.896132	3.821378

	11	12	13
11 Al	0.000000		
12 Al	3.104458	0.000000	
13 Al	3.685094	4.135522	0.000000



7. -2851.0018334 +21.9 C_1

	1	2	3	4	5
1 Al	0.000000				
2 Al	2.610500	0.000000			
3 C	4.249162	2.110319	0.000000		
4 Al	3.789374	2.644847	2.152691	0.000000	
5 Al	2.656375	3.800096	4.404099	2.824873	0.000000
6 C	2.109509	4.247286	5.208086	4.389977	2.147012
7 Al	5.281110	3.834682	1.974672	2.656683	4.619041
8 Al	4.368009	4.365471	3.610951	3.140226	3.144149
9 Al	3.832392	5.276142	5.490666	4.615164	2.660692
10 Al	2.646427	3.788996	4.389511	4.503756	3.520176
11 C	2.093501	2.086326	3.238476	3.883832	3.899094
12 Al	3.802144	2.658397	2.145568	3.518859	4.521366
13 C	2.086432	2.092731	3.255626	2.054237	2.056829

	6	7	8	9	10
6 C	0.000000				
7 Al	5.494418	0.000000			
8 Al	3.614739	2.576667	0.000000		
9 Al	1.973793	5.044221	2.578478	0.000000	
10 Al	2.150876	4.619179	3.143877	2.654826	0.000000
11 C	3.251645	4.311488	3.979355	4.309398	2.052062

	12 Al 4.401515 2.661487 3.139699 4.613081 2.823649 13 C 3.240343 4.315386 3.981714 4.310223 3.886383 11 12 13 11 C 0.000000 12 Al 2.056827 0.000000 13 C 3.105744 3.901733 0.000000

Table S8C. Energy ranking for all of the $(CH_3)_{13}Al_9C_4$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	13v-01-Doc-37	-2852.9219412	0.00
2	13v-01-Doc-59	-2852.9218947	0.03
3	13v-03-DitrapIcos-37	-2852.9218734	0.04
4	13v-03-DitrapIcos-59	-2852.9218050	0.09
5	13v-01-Doc-53	-2852.9216944	0.15
6	13v-03-DitrapIcos-53	-2852.9216047	0.21
7	13v-02-Hen-29	-2852.9211301	0.51
8	13v-02-Hen-6	-2852.9194997	1.53
9	13v-01-Doc-61	-2852.8924995	18.48
10	13v-03-DitrapIcos-61	-2852.8924098	18.53
11	13v-04-CapHexAnPr-24	-2852.8920421	18.76
12	13v-01-Doc-45	-2852.8917050	18.97
13	13v-03-DitrapIcos-45	-2852.8916153	19.03
14	13v-01-Doc-39	-2852.8915080	19.10
15	13v-01-Doc-22	-2852.8914939	19.11
16	13v-01-Doc-46	-2852.8914813	19.11
17	13v-03-DitrapIcos-39	-2852.8914402	19.14
18	13v-03-DitrapIcos-22	-2852.8914261	19.15
19	13v-03-DitrapIcos-46	-2852.8913916	19.17
20	13v-02-Hen-15	-2852.8912335	19.27
21	13v-02-Hen-8	-2852.8910965	19.36
22	13v-02-Hen-50	-2852.8902585	19.88
23	13v-02-Hen-31	-2852.8901829	19.93
24	13v-04-CapHexAnPr-37	-2852.8894043	20.42
25	13v-02-Hen-16	-2852.8889998	20.67
26	13v-04-CapHexAnPr-38	-2852.8886809	20.87
27	13v-01-Doc-20	-2852.8885814	20.93
28	13v-03-DitrapIcos-20	-2852.8885247	20.97
29	13v-02-Hen-49	-2852.8875481	21.58
30	13v-04-CapHexAnPr-39	-2852.8871359	21.84
31	13v-04-CapHexAnPr-12	-2852.8869395	21.96
32	13v-04-CapHexAnPr-43	-2852.8860314	22.53

33	13v-02-Hen-39	-2852.8859405	22.59
34	13v-04-CapHexAnPr-10	-2852.8852203	23.04
35	13v-02-Hen-35	-2852.8850790	23.13
36	13v-04-CapHexAnPr-15	-2852.8829527	24.47
37	13v-04-CapHexAnPr-34	-2852.8827408	24.60
38	13v-01-Doc-6	-2852.8824796	24.76
39	13v-01-Doc-4	-2852.8824325	24.79
40	13v-03-DitrapIcos-6	-2852.8823899	24.82
41	13v-03-DitrapIcos-4	-2852.8823428	24.85
42	13v-01-Doc-10	-2852.8822868	24.88
43	13v-03-DitrapIcos-10	-2852.8822301	24.92
44	13v-02-Hen-1	-2852.8815440	25.35
45	13v-04-CapHexAnPr-17	-2852.8811535	25.60
46	13v-01-Doc-56	-2852.8805861	25.95
47	13v-03-DitrapIcos-56	-2852.8804964	26.01
48	13v-04-CapHexAnPr-41	-2852.8796125	26.56
49	13v-02-Hen-26	-2852.8795565	26.60
50	13v-01-Doc-34	-2852.8793409	26.73
51	13v-03-DitrapIcos-34	-2852.8792731	26.78
52	13v-04-CapHexAnPr-3	-2852.8792029	26.82
53	13v-02-Hen-57	-2852.8791496	26.85
54	13v-04-CapHexAnPr-30	-2852.8789924	26.95
55	13v-02-Hen-62	-2852.8788474	27.04
56	13v-01-Doc-29	-2852.8785920	27.20
57	13v-03-DitrapIcos-29	-2852.8785242	27.25
58	13v-04-CapHexAnPr-33	-2852.8784358	27.30
59	13v-04-CapHexAnPr-35	-2852.8783710	27.34
60	13v-01-Doc-36	-2852.8783478	27.36
61	13v-03-DitrapIcos-36	-2852.8782800	27.40
62	13v-02-Hen-22	-2852.8772652	28.04
63	13v-01-Doc-52	-2852.8772648	28.04
64	13v-03-DitrapIcos-52	-2852.8771751	28.09
65	13v-04-CapHexAnPr-29	-2852.8767282	28.37
66	13v-04-CapHexAnPr-11	-2852.8763703	28.60
67	13v-02-Hen-9	-2852.8757640	28.98
68	13v-02-Hen-54	-2852.8738302	30.19
69	13v-01-Doc-3	-2852.8736195	30.32
70	13v-03-DitrapIcos-3	-2852.8735517	30.37
71	13v-02-Hen-64	-2852.8732863	30.53
72	13v-04-CapHexAnPr-8	-2852.8727695	30.86
73	13v-01-Doc-26	-2852.8721626	31.24
74	13v-03-DitrapIcos-26	-2852.8720948	31.28
75	13v-01-Doc-5	-2852.8719231	31.39

76	13v-04-CapHexAnPr-16	-2852.8718493	31.43
77	13v-03-DitrapIcos-5	-2852.8718334	31.44
78	13v-02-Hen-56	-2852.8715310	31.63
79	13v-04-CapHexAnPr-14	-2852.8707108	32.15
80	13v-01-Doc-28	-2852.8706764	32.17
81	13v-03-DitrapIcos-28	-2852.8706086	32.21
82	13v-01-Doc-23	-2852.8689069	33.28
83	13v-03-DitrapIcos-23	-2852.8688391	33.32
84	13v-01-Doc-25	-2852.8687076	33.41
85	13v-02-Hen-51	-2852.8687075	33.41
86	13v-03-DitrapIcos-25	-2852.8686398	33.45
87	13v-02-Hen-53	-2852.8685682	33.49
88	13v-01-Doc-44	-2852.8684071	33.59
89	13v-03-DitrapIcos-44	-2852.8683174	33.65
90	13v-02-Hen-19	-2852.8679790	33.86
91	13v-02-Hen-14	-2852.8678566	33.94
92	13v-02-Hen-7	-2852.8676476	34.07
93	13v-02-Hen-43	-2852.8676408	34.07
94	13v-02-Hen-2	-2852.8672685	34.31
95	13v-01-Doc-38	-2852.8670991	34.41
96	13v-03-DitrapIcos-38	-2852.8670313	34.46
97	13v-01-Doc-15	-2852.8665211	34.78
98	13v-03-DitrapIcos-15	-2852.8664644	34.81
99	13v-04-CapHexAnPr-28	-2852.8654657	35.44
100	13v-01-Doc-40	-2852.8653659	35.50
101	13v-03-DitrapIcos-40	-2852.8652981	35.54
102	13v-01-Doc-49	-2852.8651445	35.64
103	13v-03-DitrapIcos-49	-2852.8650548	35.70
104	13v-01-Doc-48	-2852.8649738	35.75
105	13v-03-DitrapIcos-48	-2852.8648841	35.80
106	13v-02-Hen-36	-2852.8648828	35.81
107	13v-04-CapHexAnPr-9	-2852.8641002	36.30
108	13v-02-Hen-55	-2852.8636452	36.58
109	13v-02-Hen-18	-2852.8631093	36.92
110	13v-02-Hen-10	-2852.8629894	36.99
111	13v-01-Doc-7	-2852.8628764	37.06
112	13v-03-DitrapIcos-7	-2852.8627867	37.12
113	13v-01-Doc-27	-2852.8624056	37.36
114	13v-03-DitrapIcos-27	-2852.8623378	37.40
115	13v-04-CapHexAnPr-36	-2852.8610561	38.21
116	13v-01-Doc-43	-2852.8583846	39.88
117	13v-02-Hen-61	-2852.8583571	39.90
118	13v-03-DitrapIcos-43	-2852.8582949	39.94

119	13v-02-Hen-45	-2852.8577357	40.29
120	13v-01-Doc-33	-2852.8576016	40.37
121	13v-03-DitrapIcos-33	-2852.8575338	40.42
122	13v-04-CapHexAnPr-7	-2852.8574311	40.48
123	13v-02-Hen-46	-2852.8572484	40.60
124	13v-02-Hen-58	-2852.8572252	40.61
125	13v-02-Hen-44	-2852.8568883	40.82
126	13v-02-Hen-21	-2852.8567380	40.92
127	13v-01-Doc-9	-2852.8564327	41.11
128	13v-02-Hen-3	-2852.8563863	41.14
129	13v-03-DitrapIcos-9	-2852.8563430	41.16
130	13v-04-CapHexAnPr-32	-2852.8563352	41.17
131	13v-01-Doc-18	-2852.8562497	41.22
132	13v-03-DitrapIcos-18	-2852.8561930	41.26
133	13v-02-Hen-38	-2852.8561221	41.30
134	13v-01-Doc-35	-2852.8558075	41.50
135	13v-03-DitrapIcos-35	-2852.8557397	41.54
136	13v-01-Doc-16	-2852.8556776	41.58
137	13v-01-Doc-51	-2852.8556526	41.60
138	13v-03-DitrapIcos-16	-2852.8556209	41.62
139	13v-03-DitrapIcos-51	-2852.8555629	41.65
140	13v-01-Doc-17	-2852.8547810	42.14
141	13v-02-Hen-13	-2852.8547741	42.15
142	13v-03-DitrapIcos-17	-2852.8547243	42.18
143	13v-02-Hen-63	-2852.8543470	42.42
144	13v-01-Doc-11	-2852.8542046	42.51
145	13v-01-Doc-2	-2852.8542046	42.51
146	13v-03-DitrapIcos-11	-2852.8541479	42.54
147	13v-03-DitrapIcos-2	-2852.8541368	42.55
148	13v-02-Hen-47	-2852.8538248	42.74
149	13v-01-Doc-24	-2852.8524087	43.63
150	13v-03-DitrapIcos-24	-2852.8523409	43.68
151	13v-01-Doc-8	-2852.8519587	43.92
152	13v-03-DitrapIcos-8	-2852.8518690	43.97
153	13v-01-Doc-19	-2852.8516681	44.10
154	13v-02-Hen-52	-2852.8516593	44.10
155	13v-03-DitrapIcos-19	-2852.8516114	44.13
156	13v-02-Hen-37	-2852.8511451	44.43
157	13v-04-CapHexAnPr-20	-2852.8508125	44.63
158	13v-01-Doc-30	-2852.8501885	45.03
159	13v-03-DitrapIcos-30	-2852.8501207	45.07
160	13v-01-Doc-21	-2852.8500557	45.11
161	13v-03-DitrapIcos-21	-2852.8499879	45.15

162	13v-02-Hen-60	-2852.8489736	45.79
163	13v-02-Hen-59	-2852.8488731	45.85
164	13v-01-Doc-32	-2852.8485601	46.05
165	13v-03-DitrapIcos-32	-2852.8484923	46.09
166	13v-04-CapHexAnPr-22	-2852.8473136	46.83
167	13v-02-Hen-4	-2852.8467243	47.20
168	13v-02-Hen-30	-2852.8464622	47.36
169	13v-01-Doc-55	-2852.8459114	47.71
170	13v-03-DitrapIcos-55	-2852.8458217	47.77
171	13v-02-Hen-33	-2852.8453977	48.03
172	13v-04-CapHexAnPr-42	-2852.8453580	48.06
173	13v-01-Doc-60	-2852.8443808	48.67
174	13v-03-DitrapIcos-60	-2852.8442911	48.73
175	13v-01-Doc-63	-2852.8441833	48.79
176	13v-02-Hen-25	-2852.8441708	48.80
177	13v-03-DitrapIcos-63	-2852.8440936	48.85
178	13v-04-CapHexAnPr-25	-2852.8440302	48.89
179	13v-01-Doc-54	-2852.8438598	49.00
180	13v-03-DitrapIcos-54	-2852.8437701	49.05
181	13v-02-Hen-23	-2852.8423852	49.92
182	13v-02-Hen-24	-2852.8423852	49.92
183	13v-02-Hen-5	-2852.8394402	51.77
184	13v-01-Doc-47	-2852.8377416	52.84
185	13v-03-DitrapIcos-47	-2852.8376519	52.89
186	13v-01-Doc-31	-2852.8375427	52.96
187	13v-03-DitrapIcos-31	-2852.8374749	53.00
188	13v-04-CapHexAnPr-26	-2852.8367828	53.44
189	13v-04-CapHexAnPr-6	-2852.8363701	53.70
190	13v-04-CapHexAnPr-27	-2852.8349591	54.58
191	13v-01-Doc-13	-2852.8343648	54.96
192	13v-03-DitrapIcos-13	-2852.8343081	54.99
193	13v-02-Hen-41	-2852.8342765	55.01
194	13v-02-Hen-17	-2852.8336491	55.41
195	13v-04-CapHexAnPr-19	-2852.8334297	55.54
196	13v-01-Doc-50	-2852.8308265	57.18
197	13v-02-Hen-20	-2852.8307670	57.21
198	13v-03-DitrapIcos-50	-2852.8307368	57.23
199	13v-04-CapHexAnPr-31	-2852.8298179	57.81
200	13v-04-CapHexAnPr-45	-2852.8298048	57.82
201	13v-01-Doc-42	-2852.8276602	59.16
202	13v-03-DitrapIcos-42	-2852.8275705	59.22
203	13v-04-CapHexAnPr-2	-2852.8272718	59.41
204	13v-02-Hen-12	-2852.8270707	59.53

205	13v-04-CapHexAnPr-21	-2852.8245050	61.14
206	13v-01-Doc-14	-2852.8239091	61.52
207	13v-03-DitrapIcos-14	-2852.8238524	61.55
208	13v-02-Hen-42	-2852.8230398	62.06
209	13v-02-Hen-27	-2852.8205263	63.64
210	13v-02-Hen-34	-2852.8204800	63.67
211	13v-01-Doc-57	-2852.8201739	63.86
212	13v-01-Doc-62	-2852.8201126	63.90
213	13v-03-DitrapIcos-57	-2852.8200842	63.92
214	13v-03-DitrapIcos-62	-2852.8200229	63.96
215	13v-02-Hen-32	-2852.8189260	64.64
216	13v-01-Doc-64	-2852.8177816	65.36
217	13v-03-DitrapIcos-64	-2852.8176919	65.42
218	13v-02-Hen-28	-2852.8139611	67.76
219	13v-01-Doc-41	-2852.8134025	68.11
220	13v-03-DitrapIcos-41	-2852.8133128	68.17
221	13v-04-CapHexAnPr-1	-2852.8132891	68.18
222	13v-01-Doc-58	-2852.8126657	68.57
223	13v-03-DitrapIcos-58	-2852.8125760	68.63
224	13v-04-CapHexAnPr-40	-2852.8115327	69.28
225	13v-04-CapHexAnPr-46	-2852.8109126	69.67
226	13v-02-Hen-11	-2852.8107750	69.76
227	13v-04-CapHexAnPr-5	-2852.8098228	70.36
228	13v-02-Hen-48	-2852.8086305	71.10
229	13v-04-CapHexAnPr-13	-2852.8085300	71.17
230	13v-04-CapHexAnPr-23	-2852.8067017	72.32
231	13v-04-CapHexAnPr-4	-2852.8051200	73.31
232	13v-01-Doc-1	-2852.8035998	74.26
233	13v-03-DitrapIcos-1	-2852.8035431	74.30
234	13v-02-Hen-40	-2852.7969836	78.41
235	13v-01-Doc-12	-2852.7952299	79.51
236	13v-03-DitrapIcos-12	-2852.7951732	79.55
237	13v-04-CapHexAnPr-44	-2852.7763671	91.35

Table S9A. Initial $(CH_3)_{14}Al_{10}C_4$ structures, a total of 120 structures:

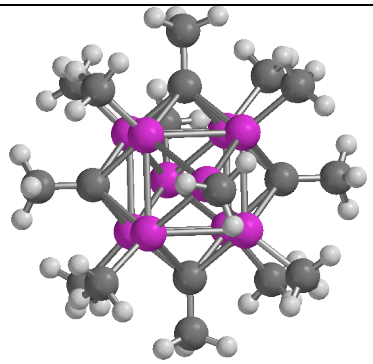
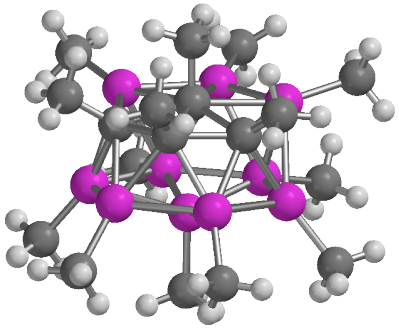
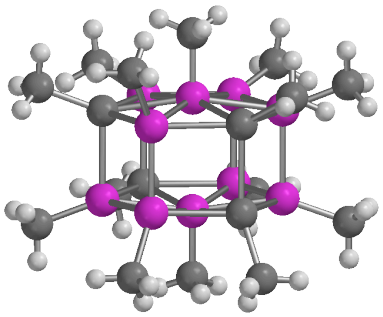
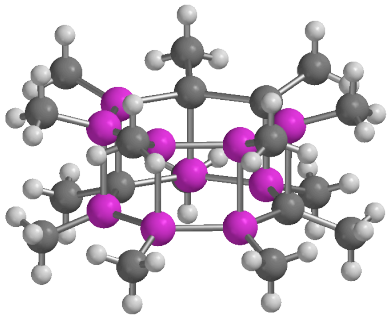
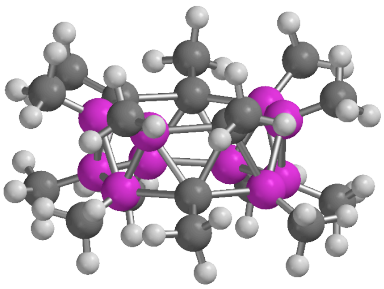
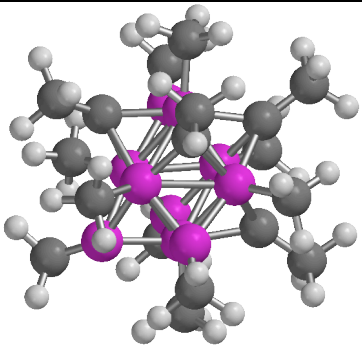
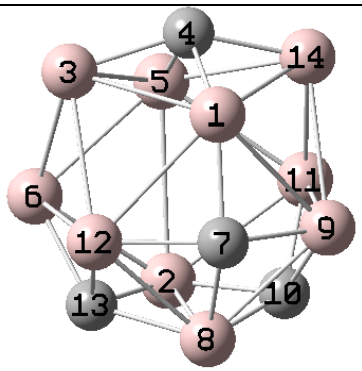
 Omnicapped cube (26)	 Bicapped hexag antiprism (28)	 Bicapped hexagonal prism (20)
 Heptagonal prism (18)	 Heptagonal antiprism (19)	 Omnicapped octahedron (9)

Table S9B. Distance table for the lowest-lying $(CH_3)_{14}Al_{10}C_4$ structures after PBE0/Def2TZVPP optimization. Included are the ZPcorrected E (a.u.), relative energy (kcal/mol) and symmetry. For clarity, only the atoms forming the cluster framework are presented.

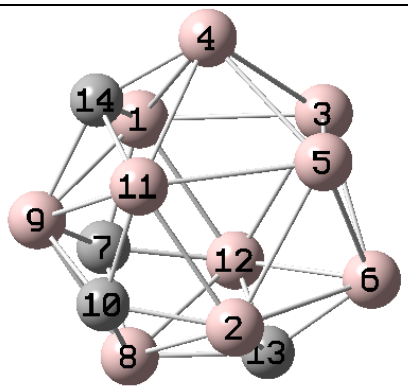


1. -3133.2133300 0.0 C_S

		1	2	3	4	5
1	Al	0.000000				
2	Al	4.797645	0.000000			
3	Al	2.770600	4.563844	0.000000		
4	C	2.100992	4.608539	2.040063	0.000000	
5	Al	3.702185	3.204869	2.748093	2.163438	0.000000
6	Al	4.317315	2.730765	2.641912	3.822771	2.818789
7	C	2.055921	3.903721	3.836214	3.680972	4.370028
8	Al	3.911279	2.615645	4.823180	4.898714	4.631173
9	Al	2.876254	3.706063	4.839506	3.834510	4.159973
10	C	4.321531	2.061824	5.268818	4.673445	3.943531
11	Al	4.316761	2.729612	4.963827	3.821674	2.818282
12	Al	2.876445	3.707679	2.860801	3.835125	4.160452
13	C	4.321465	2.061621	3.892417	4.673282	3.942662
14	Al	2.771293	4.564015	3.946277	2.039553	2.748413

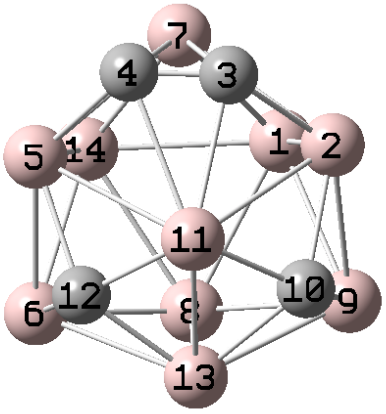
		6	7	8	9	10
6	Al	0.000000				
7	C	4.132730	0.000000			
8	Al	3.826878	2.089461	0.000000		
9	Al	4.961630	2.085526	2.627549	0.000000	
10	C	4.297881	3.169759	2.082983	2.104307	0.000000
11	Al	4.476710	4.132502	3.826802	2.707371	2.040884
12	Al	2.707833	2.085943	2.628474	3.862018	4.095778
13	C	2.040468	3.169719	2.082764	4.094204	3.194686
14	Al	4.965092	3.837293	4.824183	2.861893	3.893269

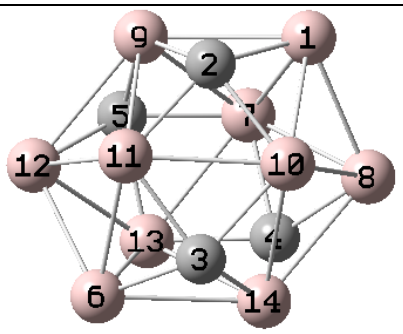
		11	12	13	14
11	Al	0.000000			
12	Al	4.962128	0.000000		
13	C	4.296545	2.105690	0.000000	
14	Al	2.641844	4.840969	5.268988	0.000000



2. -3133.2036292 +6.1 C_{2v}

		1	2	3	4	5
1	Al	0.000000				
2	Al	4.591750	0.000000			
3	Al	2.891161	4.290043	0.000000		
4	Al	2.819287	4.521106	2.746033	0.000000	
5	Al	4.286694	2.896083	2.695781	2.745933	0.000000
6	Al	4.513898	2.815327	2.745369	4.618940	2.742422
7	C	2.068264	4.003057	4.056930	4.430923	4.999034
8	Al	3.758017	2.660905	4.797530	5.242563	4.797043
9	Al	2.661641	3.756254	4.793914	3.924977	4.793613
10	C	4.003677	2.066090	4.998445	4.428737	4.055949
11	Al	3.718229	2.699385	4.289535	2.820642	2.893092
12	Al	2.698733	3.723118	2.898467	4.525385	4.296203
13	C	4.190949	2.146081	3.791719	5.121411	3.795672

	14 C 2.144323 4.195930 3.791352 1.980172 3.790295 6 7 8 9 10 6 Al 0.000000 7 C 4.425584 0.000000 8 Al 3.925011 2.081692 0.000000 9 Al 5.235418 2.083655 2.606975 0.000000 10 C 4.424269 3.165204 2.082608 2.081541 0.000000 11 Al 4.514227 4.007116 3.759282 2.662100 2.066588 12 Al 2.824107 2.066309 2.666744 3.760873 4.010330 13 C 1.981530 3.223738 2.126864 4.133074 3.231037 14 C 5.115589 3.232399 4.136461 2.127032 3.228572 11 12 13 14 11 Al 0.000000 12 Al 4.601357 0.000000 13 C 4.198586 2.142114 0.000000 14 C 2.142930 4.201493 4.822606 0.000000
 3. -3133.2017573 +7.3 C_S	1 2 3 4 5 1 Al 0.000000 2 Al 2.837940 0.000000 3 C 4.091747 2.118527 0.000000 4 C 4.515055 3.236870 1.401042 0.000000 5 Al 4.429066 4.178915 3.166277 2.083923 0.000000 6 Al 4.391801 5.030326 5.085664 4.492875 2.690780 7 Al 2.713811 2.826885 2.329248 2.272401 2.834478 8 Al 2.724741 4.346787 5.426724 5.450639 4.379671 9 Al 2.723709 2.704864 4.527755 5.208899 5.108550 10 C 3.777461 2.095163 3.295905 3.997964 4.242563 11 Al 4.611628 2.793374 2.388375 2.540745 2.887054 12 C 4.760079 4.138007 3.804743 3.284087 2.091804 13 Al 4.279929 3.804336 4.537353 4.625949 3.850017 14 Al 2.735701 4.411131 4.515501 4.048850 2.855990 6 7 8 9 10 6 Al 0.000000 7 Al 4.440987 0.000000 8 Al 2.692879 4.419078 0.000000 9 Al 4.408468 4.480041 2.695824 0.000000 10 C 4.255444 4.216120 3.839118 2.050439 0.000000 11 Al 3.859889 3.784481 4.672716 3.851025 2.047339 12 C 2.060906 4.158423 3.846284 4.260074 3.153835 13 Al 2.692784 4.863633 2.909668 2.703433 2.107745 14 Al 2.710783 2.717140 2.731813 4.427016 4.807354 11 12 13 14 11 Al 0.000000 12 C 2.042616 0.000000 13 Al 2.653106 2.119928 0.000000 14 Al 4.646430 3.774503 4.293553 0.000000

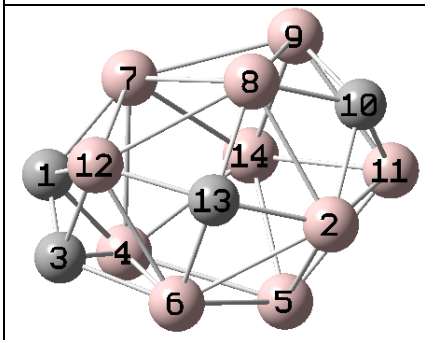


4. -3133.1945204 +11.8 C_2

	1	2	3	4	5
1 Al	0.000000				
2 C	2.087590	0.000000			
3 C	4.330581	3.230918	0.000000		
4 C	3.798965	4.309397	3.537617	0.000000	
5 C	3.831459	3.540326	4.312658	3.223502	0.000000
6 Al	5.526636	4.329599	2.087304	3.821254	3.796166
7 Al	2.813826	3.688423	4.541969	2.121233	2.127307
8 Al	2.617399	3.786423	3.831159	2.099481	4.324507
9 Al	2.797013	2.020457	4.225980	4.233972	2.018923
10 Al	2.695170	2.126665	2.134432	3.693148	4.548206
11 Al	4.014420	2.135556	2.124509	4.545163	3.698334
12 Al	5.039754	3.826067	3.784623	4.327331	2.105183
13 Al	4.764505	4.542545	3.698855	2.127260	2.113367
14 Al	4.409250	4.222935	2.020416	2.018433	4.241186

	6	7	8	9	10
6 Al	0.000000				
7 Al	4.760574	0.000000			
8 Al	5.035205	2.690252	0.000000		
9 Al	4.412316	2.926656	4.427020	0.000000	
10 Al	4.011886	4.106080	2.806874	3.796294	0.000000
11 Al	2.697042	4.592991	4.765622	2.908690	2.684415
12 Al	2.617055	4.017193	5.526139	2.769238	4.762954
13 Al	2.818017	2.669400	4.013410	3.781639	4.596757
14 Al	2.799191	3.786500	2.764967	4.816406	2.898917

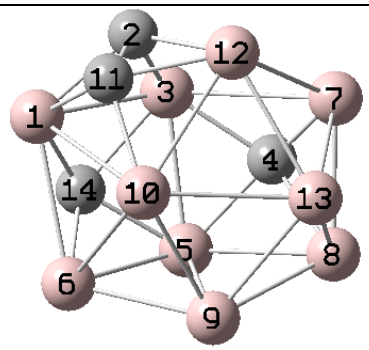
	11	12	13	14
11 Al	0.000000			
12 Al	2.802189	0.000000		
13 Al	4.112817	2.699158	0.000000	
14 Al	3.796194	4.436421	2.944787	0.000000

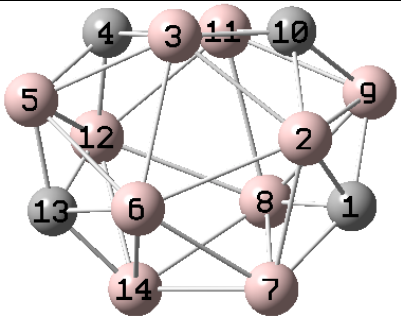


5. -3133.1907498 +14.2 C_1

	1	2	3	4	5
1 C	0.000000				
2 Al	4.845915	0.000000			
3 C	1.478919	4.453897	0.000000		
4 Al	2.184338	4.403055	2.208031	0.000000	
5 Al	4.382764	2.815102	3.959589	2.725711	0.000000
6 Al	3.179520	2.781443	2.104667	2.856025	2.765412
7 Al	2.065802	4.445761	3.252059	2.927108	4.370067
8 Al	4.048394	2.630673	4.339614	4.684616	4.499830
9 Al	4.568390	3.743808	5.303806	4.464682	4.246313
10 C	5.191860	2.093110	5.391843	4.961249	3.783686
11 Al	5.548628	2.734666	5.666190	4.486274	2.689918
12 Al	2.169525	3.908788	2.105875	3.656904	4.724742
13 C	3.610532	2.096492	3.168731	4.090615	3.836687
14 Al	3.995833	4.220758	4.543461	2.738453	2.795871

	6	7	8	9	10
6 Al	0.000000				
7 Al	4.059085	0.000000			

	8 Al 3.789030 3.036996 0.000000 9 Al 5.037079 2.736868 2.693266 0.000000 10 C 4.349737 3.934577 2.062044 2.100393 0.000000 11 Al 4.563590 4.452225 3.813591 2.646306 2.066921 12 Al 2.669373 2.875788 2.831978 4.620134 4.502325 13 C 2.085912 3.707930 2.056906 4.206265 3.207973 14 Al 4.466552 2.972437 4.371017 2.655944 3.712438 11 12 13 14 11 Al 0.000000 12 Al 5.534518 0.000000 13 C 4.355560 2.011985 0.000000 14 Al 2.682585 5.004149 4.823197 0.000000
 6. -3133.1851417 +17.7 C_1	1 2 3 4 5 1 Al 0.000000 2 C 2.109997 0.000000 3 Al 2.689302 2.106927 0.000000 4 C 4.370687 3.740552 2.089444 0.000000 5 Al 3.851507 4.287946 2.669049 2.067326 0.000000 6 Al 2.811772 4.273677 3.835604 4.297825 2.725466 7 Al 4.978159 3.583970 3.007278 2.039850 3.847999 8 Al 5.474476 5.034440 3.915507 2.133146 2.704572 9 Al 4.479279 4.887647 4.425425 3.777805 2.930627 10 Al 3.039593 3.227581 4.059391 4.549759 4.269674 11 C 2.061453 1.555611 3.264002 4.557553 4.706236 12 Al 3.733920 2.103455 3.314736 3.862131 4.838839 13 Al 5.082288 4.288919 4.393513 3.624352 4.292111 14 C 2.023541 3.202125 2.170097 3.236128 2.075950 6 7 8 9 10 6 Al 0.000000 7 Al 5.389280 0.000000 8 Al 4.466961 2.603607 0.000000 9 Al 2.604240 4.303771 2.712965 0.000000 10 Al 2.997992 4.373983 4.430758 2.768204 0.000000 11 C 3.852752 4.268837 5.286947 4.401561 2.053203 12 Al 4.972791 2.699442 4.397097 4.467579 2.812045 13 Al 4.686857 2.666971 2.645230 2.772335 2.895436 14 C 2.039174 4.605304 4.371347 3.734586 3.735362 11 12 13 14 11 C 0.000000 12 Al 2.098170 0.000000 13 Al 3.957436 2.769385 0.000000 14 C 3.562746 4.508802 4.979135 0.000000

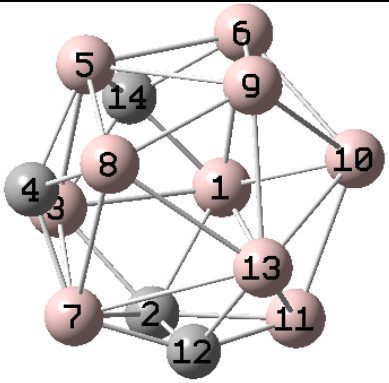


7. -3133.1838944 +18.5 C_2

	1	2	3	4	5
1 C	0.000000				
2 Al	2.122225	0.000000			
3 Al	4.283940	2.769673	0.000000		
4 C	4.992661	4.260657	2.093817	0.000000	
5 Al	5.645887	4.688046	2.683063	2.023178	0.000000
6 Al	3.942692	3.009887	2.946648	3.657617	2.725871
7 Al	2.011078	2.737096	4.537119	5.153268	5.067762
8 Al	2.237247	3.569551	4.371203	4.048074	4.880453
9 Al	1.994338	2.586282	3.881900	4.468871	5.761501
10 C	3.113956	2.071874	2.082331	3.226520	4.468865
11 Al	3.780272	3.593145	2.650928	2.082324	3.881894
12 Al	4.662387	4.718696	3.593146	2.071878	2.586291
13 C	4.970927	4.662386	3.780268	3.113960	1.994344
14 Al	3.913502	4.431837	4.702287	4.272469	3.834283

	6	7	8	9	10
6 Al	0.000000				
7 Al	2.802430	0.000000			
8 Al	4.046679	2.768399	0.000000		
9 Al	4.880471	3.834283	2.725887	0.000000	
10 C	4.048083	4.272457	3.657613	2.023177	0.000000
11 Al	4.371214	4.702290	2.946655	2.683078	2.093818
12 Al	3.569563	4.431840	3.009872	4.688053	4.260658
13 C	2.237247	3.913493	3.942669	5.645891	4.992660
14 Al	2.768399	2.633623	2.802430	5.067780	5.153275

	11	12	13	14
11 Al	0.000000			
12 Al	2.769672	0.000000		
13 C	4.283940	2.122228	0.000000	
14 Al	4.537140	2.737116	2.011070	0.000000



8. -3133.1814247 +20.0 C_1

	1	2	3	4	5
1 Al	0.000000				
2 C	2.453598	0.000000			
3 Al	2.725835	2.147051	0.000000		
4 C	4.251500	3.289442	2.109772	0.000000	
5 Al	3.763521	4.139373	2.651122	2.136705	0.000000
6 Al	2.679393	4.456933	3.862653	4.390557	2.742901
7 Al	4.329254	2.340604	2.660277	2.022647	3.855387
8 Al	5.064893	4.316943	3.824540	2.047696	2.697469
9 Al	4.243474	4.685020	4.499210	3.776460	2.889777
10 Al	2.822471	3.932748	4.635911	5.051809	4.351126
11 Al	2.626878	2.177198	3.979826	4.801557	5.129415
12 C	3.568517	1.631864	3.325966	3.513838	4.629630
13 Al	4.091120	3.267137	4.266395	3.762148	4.277169
14 C	2.054734	3.327212	2.045749	3.220743	2.082413

	6	7	8	9	10
6 Al	0.000000				
7 Al	5.329951	0.000000			

	8 Al 4.487161 2.856186 0.000000 9 Al 2.767674 4.478093 2.602479 0.000000 10 Al 2.620652 5.017550 4.660744 2.754321 0.000000 11 Al 4.385181 3.824252 5.022876 4.433325 2.647275 12 C 5.028952 1.982935 3.819782 4.348228 3.845022 13 Al 4.394846 3.030072 2.937809 2.760127 2.888571 14 C 2.077599 4.248097 4.258475 3.785408 3.763382 11 12 13 14 11 Al 0.000000 12 C 2.029479 0.000000 13 Al 2.702428 2.112149 0.000000 14 C 4.241715 4.396063 4.595081 0.000000

Table S9C. Energy ranking for all of the $(CH_3)_{14}Al_{10}C_4$ optimized structures after B3LYP/6-31G(d) optimizations:

No	Initial structure	Final energy (a.u.)	ΔE (kcal/mol)
1	14v-01-OmnicapCube-a43	-3135.2628999	0.00
2	14v-01-OmnicapCube-a41	-3135.2548229	5.07
3	14v-01-OmnicapCube-a44	-3135.2548214	5.07
4	14v-01-OmnicapCube-a14	-3135.2548182	5.07
5	14v-02-BicapHexAnPr-a32	-3135.2544759	5.29
6	14v-03-BicapHexPr-a18	-3135.2541918	5.46
7	14v-06-OmnicapOh-a12	-3135.2441401	11.77
8	14v-02-BicapHexAnPr-a43	-3135.2441185	11.79
9	14v-01-OmnicapCube-g12	-3135.2439530	11.89
10	14v-04-HepPr-a17	-3135.2425533	12.77
11	14v-01-OmnicapCube-a42	-3135.2424857	12.81
12	14v-01-OmnicapCube-e31	-3135.2404574	14.08
13	14v-01-OmnicapCube-a13	-3135.2326851	18.96
14	14v-05-HepAnPr-a119	-3135.2310828	19.97
15	14v-04-HepPr-a117	-3135.2310779	19.97
16	14v-02-BicapHexAnPr-a62	-3135.2298444	20.74
17	14v-02-BicapHexAnPr-a24	-3135.2290198	21.26
18	14v-02-BicapHexAnPr-a25	-3135.2260469	23.13
19	14v-02-BicapHexAnPr-a63	-3135.2259861	23.16
20	14v-02-BicapHexAnPr-a23	-3135.2231072	24.97
21	14v-03-BicapHexPr-a116	-3135.2158573	29.52
22	14v-03-BicapHexPr-a110	-3135.2147147	30.24
23	14v-02-BicapHexAnPr-a22	-3135.2146212	30.30
24	14v-02-BicapHexAnPr-g11	-3135.2146142	30.30
25	14v-04-HepPr-a14	-3135.2131819	31.20
26	14v-02-BicapHexAnPr-a16	-3135.2117217	32.12

27	14v-02-BicapHexAnPr-a31	-3135.2114748	32.27
28	14v-04-HepPr-a110	-3135.2111603	32.47
29	14v-04-HepPr-a18	-3135.2083669	34.22
30	14v-03-BicapHexPr-a120	-3135.2073457	34.86
31	14v-02-BicapHexAnPr-h11	-3135.2066113	35.32
32	14v-01-OmnicapCube-a11	-3135.2065862	35.34
33	14v-02-BicapHexAnPr-a17	-3135.2061047	35.64
34	14v-03-BicapHexPr-a114	-3135.2057099	35.89
35	14v-05-HepAnPr-a117	-3135.2043186	36.76
36	14v-03-BicapHexPr-a14	-3135.2042781	36.79
37	14v-02-BicapHexAnPr-d51	-3135.2039856	36.97
38	14v-03-BicapHexPr-a15	-3135.2032302	37.44
39	14v-03-BicapHexPr-a12	-3135.2032245	37.45
40	14v-03-BicapHexPr-a115	-3135.2014931	38.53
41	14v-03-BicapHexPr-a118	-3135.2001435	39.38
42	14v-04-HepPr-a19	-3135.1997903	39.60
43	14v-04-HepPr-a111	-3135.1977502	40.88
44	14v-02-BicapHexAnPr-a13	-3135.1973063	41.16
45	14v-02-BicapHexAnPr-a61	-3135.1973001	41.17
46	14v-02-BicapHexAnPr-a42	-3135.1968147	41.47
47	14v-04-HepPr-a118	-3135.1949108	42.66
48	14v-03-BicapHexPr-a16	-3135.1929861	43.87
49	14v-06-OmnicapOh-a17	-3135.1926151	44.11
50	14v-01-OmnicapCube-g11	-3135.1923510	44.27
51	14v-02-BicapHexAnPr-a21	-3135.1891581	46.27
52	14v-01-OmnicapCube-e41	-3135.1888143	46.49
53	14v-04-HepPr-a116	-3135.1859342	48.30
54	14v-06-OmnicapOh-a11	-3135.1822290	50.62
55	14v-05-HepAnPr-a17	-3135.1821709	50.66
56	14v-05-HepAnPr-a110	-3135.1803552	51.80
57	14v-02-BicapHexAnPr-a14	-3135.1802697	51.85
58	14v-05-HepAnPr-a113	-3135.1796745	52.23
59	14v-02-BicapHexAnPr-d12	-3135.1795190	52.32
60	14v-02-BicapHexAnPr-d11	-3135.1789298	52.69
61	14v-03-BicapHexPr-a119	-3135.1786827	52.85
62	14v-03-BicapHexPr-a11	-3135.1775946	53.53
63	14v-04-HepPr-a12	-3135.1770775	53.86
64	14v-03-BicapHexPr-a117	-3135.1768040	54.03
65	14v-01-OmnicapCube-b13	-3135.1763781	54.29
66	14v-05-HepAnPr-a12	-3135.1758497	54.63
67	14v-01-OmnicapCube-a23	-3135.1756099	54.78
68	14v-05-HepAnPr-a118	-3135.1749346	55.20
69	14v-05-HepAnPr-a112	-3135.1745817	55.42

70	14v-01-OmnicapCube-c12	-3135.1714574	57.38
71	14v-04-HepPr-a13	-3135.1702495	58.14
72	14v-06-OmnicapOh-a13	-3135.1698185	58.41
73	14v-05-HepAnPr-a116	-3135.1689577	58.95
74	14v-01-OmnicapCube-a27	-3135.1685704	59.19
75	14v-02-BicapHexAnPr-a12	-3135.1677623	59.70
76	14v-04-HepPr-a15	-3135.1659861	60.82
77	14v-05-HepAnPr-a111	-3135.1652261	61.29
78	14v-01-OmnicapCube-c13	-3135.1649495	61.47
79	14v-04-HepPr-a112	-3135.1642856	61.88
80	14v-05-HepAnPr-a16	-3135.1638961	62.13
81	14v-03-BicapHexPr-a19	-3135.1637252	62.23
82	14v-02-BicapHexAnPr-a15	-3135.1606999	64.13
83	14v-01-OmnicapCube-a26	-3135.1600639	64.53
84	14v-06-OmnicapOh-a15	-3135.1590589	65.16
85	14v-03-BicapHexPr-a17	-3135.1586258	65.43
86	14v-01-OmnicapCube-a21	-3135.1585483	65.48
87	14v-01-OmnicapCube-c11	-3135.1584363	65.55
88	14v-04-HepPr-a113	-3135.1565631	66.73
89	14v-02-BicapHexAnPr-a33	-3135.1556694	67.29
90	14v-02-BicapHexAnPr-d31	-3135.1547025	67.90
91	14v-06-OmnicapOh-a18	-3135.1544206	68.07
92	14v-06-OmnicapOh-a19	-3135.1541489	68.24
93	14v-05-HepAnPr-a19	-3135.1485972	71.73
94	14v-01-OmnicapCube-a25	-3135.1472341	72.58
95	14v-05-HepAnPr-a11	-3135.1470143	72.72
96	14v-03-BicapHexPr-a111	-3135.1458314	73.46
97	14v-05-HepAnPr-a114	-3135.1452216	73.85
98	14v-02-BicapHexAnPr-a11	-3135.1449924	73.99
99	14v-05-HepAnPr-a15	-3135.1447944	74.11
100	14v-05-HepAnPr-a115	-3135.1399972	77.12
101	14v-01-OmnicapCube-b11	-3135.1384875	78.07
102	14v-01-OmnicapCube-a24	-3135.1374458	78.72
103	14v-03-BicapHexPr-a113	-3135.1338759	80.97
104	14v-06-OmnicapOh-a14	-3135.1330027	81.51
105	14v-04-HepPr-a115	-3135.1329957	81.52
106	14v-03-BicapHexPr-a13	-3135.1298101	83.52
107	14v-04-HepPr-a11	-3135.1255157	86.21
108	14v-04-HepPr-a16	-3135.1242311	87.02
109	14v-01-OmnicapCube-a31	-3135.1231238	87.71
110	14v-04-HepPr-a114	-3135.1220931	88.36
111	14v-01-OmnicapCube-a12	-3135.1197110	89.85
112	14v-01-OmnicapCube-b12	-3135.1189090	90.36

113	14v-05-HepAnPr-a13	-3135.1132938	93.88
114	14v-06-OmnicapOh-a16	-3135.1120545	94.66
115	14v-01-OmnicapCube-a22	-3135.1120533	94.66
116	14v-03-BicapHexPr-a112	-3135.1036899	99.91
117	14v-05-HepAnPr-a18	-3135.1024398	100.69
118	14v-05-HepAnPr-a14	-3135.0956947	104.92
119	14v-02-BicapHexAnPr-a41	-3135.0889087	109.18
120	14v-02-BicapHexAnPr-d41	-3135.0859002	111.07

Table S10. Orbital energies and HOMO-LUMO gaps.

Structure	HOMO energy (Hartree)	LUMO energy (Hartree)	HOMO/LUMO gap (eV)
Al2C4-1	-0.179527	-0.024535	4.22
Al2C4-2	-0.232707	-0.061538	4.66
Al2C4-3	-0.170799	-0.023776	4.00
Al2C4-4	-0.195749	-0.046640	4.06
Al3C4-1	-0.183166	-0.032905	4.09
Al3C4-2	-0.192031	-0.038073	4.19
Al3C4-3	-0.168502	-0.045745	3.34
Al3C4-4	-0.195019	-0.011759	4.99
Al3C4-5	-0.213611	-0.030073	4.99
Al3C4-6	-0.229959	-0.069267	4.37
Al4C4-1	-0.206335	-0.055681	4.10
Al4C4-2	-0.185033	-0.030080	4.22
Al4C4-3	-0.197233	-0.053958	3.90
Al4C4-4	-0.174418	-0.054128	3.27
Al4C4-5	-0.203665	-0.052406	4.12
Al4C4-6	-0.206074	-0.059914	3.98
Al4C4-7	-0.192099	-0.064273	3.48
Al4C4-8	-0.220111	-0.040673	4.88
Al4C4-9	-0.187483	-0.053410	3.65
Al4C4-10	-0.147577	-0.012495	3.68
Al5C4-1	-0.187717	-0.040576	4.00
Al5C4-2	-0.189304	-0.043751	3.96
Al5C4-3	-0.194268	-0.046179	4.03
Al5C4-4	-0.164544	-0.047596	3.18
Al5C4-5	-0.187450	-0.060377	3.46
Al5C4-6	-0.184190	-0.078278	2.88
Al5C4-7	-0.167643	-0.025233	3.88
Al5C4-8	-0.147009	-0.046526	2.73
Al5C4-9	-0.193456	-0.076777	3.17
Al5C4-10	-0.190782	-0.042887	4.02
Al5C4-11	-0.185633	-0.071849	3.10
Al5C4-12	-0.181872	-0.053343	3.50
Al6C4-1	-0.184297	-0.055446	3.51
Al6C4-2	-0.182922	-0.049429	3.63
Al6C4-3	-0.190005	-0.052656	3.74
Al6C4-4	-0.199972	-0.073378	3.44
Al6C4-5	-0.191428	-0.047533	3.92
Al6C4-6	-0.165690	-0.061588	2.83
Al6C4-7	-0.192504	-0.023268	4.61
Al6C4-8	-0.211812	-0.060484	4.12

Al6C4-9	-0.195139	-0.075120	3.27
Al6C4-10	-0.186406	-0.074069	3.06
Al6C4-11	-0.179980	-0.055222	3.39
Al6C4-12	-0.191855	-0.025209	4.53
Al6C4-13	-0.178152	-0.070374	2.93
Al6C4-14	-0.185908	-0.069688	3.16
Al6C4-15	-0.200303	-0.092861	2.92
Al7C4-1	-0.182971	-0.073370	2.98
Al7C4-2	-0.186582	-0.075150	3.03
Al7C4-3	-0.189525	-0.066432	3.35
Al7C4-4	-0.172776	-0.061569	3.03
Al7C4-5	-0.192636	-0.057873	3.67
Al7C4-6	-0.189517	-0.066193	3.36
Al7C4-7	-0.191972	-0.050525	3.85
Al7C4-8	-0.189809	-0.069221	3.28
Al7C4-9	-0.187855	-0.072909	3.13
Al7C4-10	-0.177398	-0.068794	2.96
Al7C4-11	-0.184802	-0.071272	3.09
Al8C4-1	-0.196374	-0.088731	2.93
Al8C4-2	-0.176738	-0.054208	3.33
Al8C4-3	-0.176541	-0.067890	2.96
Al8C4-4	-0.200255	-0.077473	3.34
Al8C4-5	-0.177634	-0.074442	2.81
Al8C4-6	-0.182714	-0.070059	3.07
Al8C4-7	-0.194944	-0.076257	3.23
Al8C4-8	-0.191154	-0.074285	3.18
Al8C4-9	-0.174281	-0.094409	2.17
Al9C4-1	-0.203882	-0.073495	3.55
Al9C4-2	-0.205738	-0.093909	3.04
Al9C4-3	-0.181173	-0.077513	2.82
Al9C4-4	-0.187366	-0.104843	2.25
Al9C4-5	-0.190690	-0.067303	3.36
Al9C4-6	-0.189057	-0.067999	3.29
Al9C4-7	-0.194157	-0.084069	3.00
Al10C4-1	-0.205546	-0.092339	3.08
Al10C4-2	-0.204857	-0.129021	2.06
Al10C4-3	-0.206986	-0.092523	3.11
Al10C4-4	-0.185966	-0.103198	2.25
Al10C4-5	-0.189791	-0.093053	2.63
Al10C4-6	-0.192914	-0.084268	2.96
Al10C4-7	-0.183999	-0.086166	2.66
Al10C4-8	-0.188333	-0.087722	2.74