Supporting Information

The Dynamic Equilibrium Between $(AlOMe)_n$ Cages and $(AlOMe)_n \cdot (AlMe_3)_m$ Nanotubes in Methylaluminoxane (MAO): A First-Principles Investigation

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What happens when we add more TMA to $(AlOMe)_{6,c} \cdot (AlMe_3)$?

There are three possibilities for the addition of the second $AlMe_3$ group, as illustrated in Fig. S1. The structures obtained via Branch B and Branch C have nearly the same free energy at ambient temperature, and they are preferred over the isomer in Branch A by over 10 kcal/mol. In fact, adding the second $AlMe_3$ via Branch A is calculated as being slightly endergonic, most likely because all of the O-$AlMe_2$ groups point towards the same side of the cage, resulting in unfavorable steric interactions. Branch B and C merge upon the addition of the third $AlMe_3$. This reaction is slightly exergonic, but the formation of $(AlOMe)_{6,c} \cdot (AlMe_3)_4$ from $(AlOMe)_{6,c} \cdot (AlMe_3)_3$ is endergonic due to unfavored sterics. Not only are Branches B and C favored over A because of the lower free energies of the isomers, but they also potentially allow for the addition of one more $AlMe_3$ (up to four groups) to the cage. In stark contrast to these results, the addition of three $AlMe_3$ groups to $(AlOMe)_{6,c}$ (via branch A) was calculated to have a ΔG of over +10 kcal/mol in Ref. 45 of the main text, again highlighting the importance of the appropriate treatment of dispersion in these types of systems.

Why is it that the two $(AlOMe)_{6,c} \cdot (AlMe_3)_2$ structures in Branch B and C are equally stable? One would suppose that the free energy of the former would be lower than that of the latter because the two $AlMe_3$ groups are on opposite sides of the cage, so the B-isomer is less crowded than the C-isomer. However, hitherto undiscussed interactions become important in stabilizing species where two $AlMe_3$ groups react with strained bonds belonging to two square faces that are adjacent to one another as in Branch C.

Let us consider $(AlOMe)_{6,c} \cdot (AlMe_3)$ in Fig. 8(a) of the main text. Adding the second $AlMe_3$ to this structure across the hexagonal face that results from the first addition of $AlMe_3$ (*i.e.* to O-$sp^{2.4}$ and Al-$sp^{3.0}$) yields a configuration where the aluminum in the O-$AlMe_2$ group lies close to the carbon in $AlMe_2$. Fig. 9(b) (see the main text) shows that this results in the formation of an Al-C bond measuring 2.268 A, and the initially three-coordinate aluminum increases its coordination by one. The average hybridization of this aluminum increases from $sp^{2.0}$ to $sp^{2.2}$. Because the carbon atom is now five-coordinate, the bond to the parent aluminum weakens and lengthens to 2.107 Å. Both of these Al-C bonds are somewhat longer than the other Al-C bonds within $(AlOMe)_{6,c} \cdot (AlMe_3)_2$ and the terminal Al-C bonds in $(AlMe_3)_2$, which all measure between 1.96-1.98 Å.

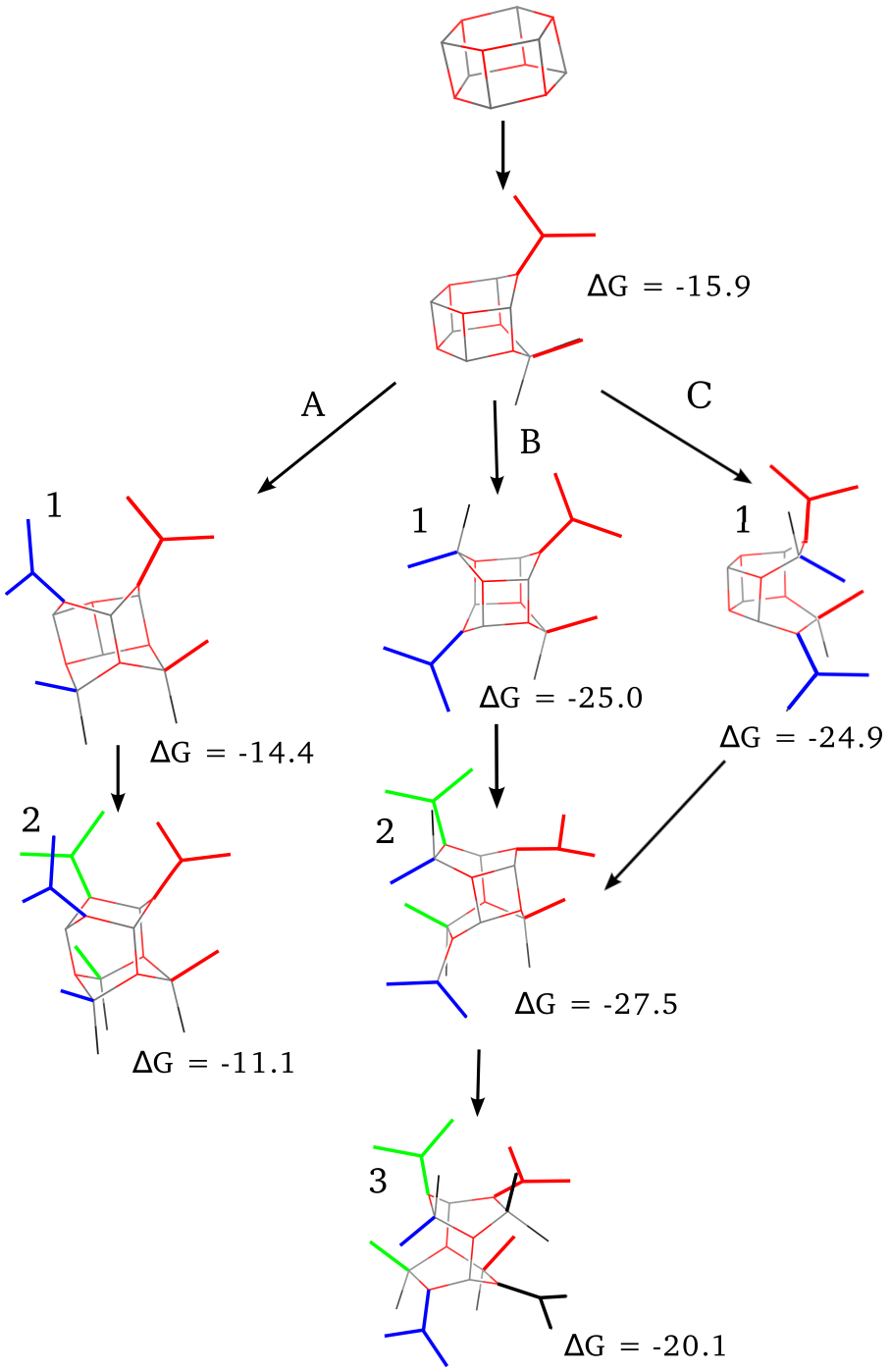

Figure S1: Possible pathways for the interaction of $(AlOMe)_{6,c}$ with $AlMe_3$ yielding $(AlOMe)_{6,c}\cdot(AlMe_3)_m$, (m = 1 − 4). The ΔG values given in kcal/mol are for Rxn. 2, from the main text, at 298 K and 1 atm.

In fact, they more closely resemble the 2.161 Å distance between the carbon atoms in the bridging methyl groups and aluminum in the TMA dimer (see Fig. 9(a) in the main text).

Interestingly, this newly formed motif is directly comparable to that seen in $(AlMe_3)_2$, where the dimerization occurs through the bridging of two methyl groups.[71] For example, the Al-C-Al and C-Al-C angles in the TMA dimer measure 73.9° and 104.8° , whereas in the O-Al-Me-O quadrilateral the angles are 97.7° (O-Al-C), 91.8° (O-Al-C), 93.7° (Al-O-Al) and 75.7° (Al-C-Al). However, the average hybridization of the bridging aluminum in the TMA dimer is significantly higher, $sp^{3.5}$. Based upon the electronic energy alone the $(AlOMe)_{6,c}\cdot(AlMe_3)_2$ isomer in Branch C is 2.3 kcal/mol more stable than the one in B, but the entropy favors B by 2.9 kcal/mol. The differences in the internal energy and zero point energy are less than 0.6 kcal/mol. So, the bridging methyl motif in the Branch C structure is a particularly stabilizing one.

The nanotubular structures (shown in Fig. 4 of manuscript) present yet another possible configuration which needs to be considered when more than one $AlMe_3$ is added to the same side of the tube. Instead of "bending in" to form an Al-μ-Me-Al bond with the methyl group that originated from addition of TMA as in Branch C discussed above, the O-$AlMe_2$ groups can "bend out". This leads to the formation of an Al-μ-Me-Al bond with a carbon atom on a methyl originating from the $(AlOMe)_{n,t}$ nanotube. (These two possibilities are illustrated in Fig. 9(c,d) of the manuscript). In the case of $(AlOMe)_{12,t}\cdot(AlMe_3)_4$, the Al-C bond for the "bending out" configuration is 0.15 Å longer than for the "bending in", and the ambient temperature free energy of the former is 11.2 kcal/mol larger than that of the latter. We have optimized the geometries of a few species where three or four TMA monomers have been added to an (AlOMe)n,t nanotube in these two configurations, and in all cases the "bending in" geometry was favored over "bending out" by 10 kcal/mol or more depending on the structure.

In the $(AlOMe_6)\cdot(AlMe_3)_2$ structure shown in Branch B in Fig. S1 a "bending out" Al-μ-Me-Al motif is not found. We attempted to force such an interaction by starting the geometry optimization from structures with a bridging bond, but in all cases the Al-C distance elongated during structural relaxation. The shortest Al–C measure was 2.7 Å, and these species were slightly less stable as compared to the minimum energy structure which had an Al–C distance of 3.3 Å. It may be that in the longer nanotubes the adjacent methyl groups along the tube interact via sterics, so that the methyls on the ends of the tube get pushed closer to the O-$AlMe_2$ group rendering such a "bending out" interaction possible. $(AlOMe_6)\cdot(AlMe_3)_2$ in Branch B does not have unfavorable steric interactions, so an Al-μ-Me-Al bond is not formed.

Consider adding the second $AlMe_3$ to $(AlOMe)_{n,t}\cdot(AlMe_3)_2$ either on the same side as the first (*i.e.* as in Branch C) or on the opposite side (like in Branch B). In general, we find the latter situation to yield the more stable isomer. For example, in the "opposite-side" $(AlOMe)_{12,t}\cdot(AlMe_3)_2$ a bridging Al-μ-Me-Al bond is formed via "bending out". The (free) energy of this species at 0/298 K is 3/2 kcal/mol lower than the "bending in" configuration that occurs when the TMA is added to the same side. When three or four TMAs are added, the "bending in" geometry is assumed on both sides of the tube.

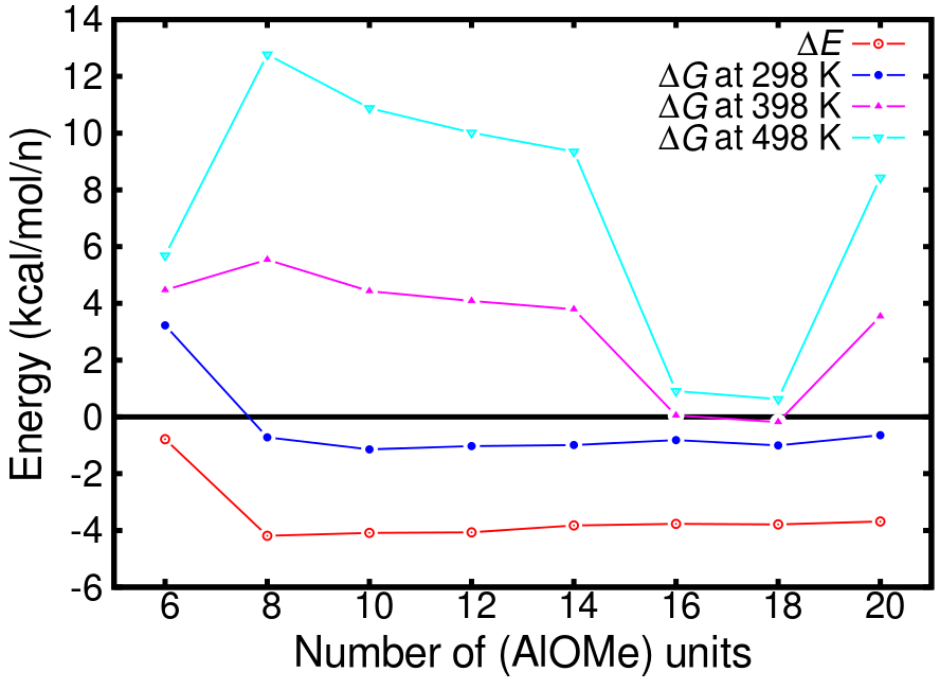

Figure S2: Changes in the electronic energy (0 K) and the Gibbs free energy for the reaction: $(AlOMe)_{12,c} + 2(AlMe_3)_2 \rightarrow (AlOMe)_{n,t} \cdot (AlMe_3)_4$ given in kcal/(mol *n*), at 298 K, 398 K and 498 K. Compare with Figure 2 of Ref. 32 in the main text.

Cartesian coordinates of geometries:

Optimized with M06

$(AlMe_3)$

C	0.000000	-1.955374	0.000000
Al	0.000000	0.000000	0.000000
C	-1.693404	0.977687	0.000000
H	-2.300632	0.713882	-0.874981
H	-1.570264	2.065332	0.000000
H	-2.300632	0.713882	0.874981
C	1.693404	0.977687	0.000000
H	2.573762	0.327223	0.000000
H	1.768556	1.635465	0.874981
H	1.768556	1.635465	-0.874981
H	-1.003498	-2.392555	0.000000
H	0.532076	-2.349347	0.874981
H	0.532076	-2.349347	-0.874981

$(AlMe_3)_2$

Al	0.000000	0.000000	1.305664
Al	0.000000	0.000000	-1.305664
C	1.691655	0.137198	0.000000
H	2.182343	-0.364681	0.848425

H	2.031166	1.178494	0.000000
H	2.182343	-0.364681	-0.848425
C	0.000000	1.743866	-2.186341
H	-0.814062	1.853047	-2.912404
H	-0.111093	2.551535	-1.451140
H	0.934920	1.931737	-2.727540
C	0.000000	-1.743866	-2.186341
H	-0.934920	-1.931737	-2.727540
H	0.814062	-1.853047	-2.912404
H	0.111093	-2.551535	-1.451140
C	-1.691655	-0.137198	0.000000
H	-2.182343	0.364681	-0.848425
H	-2.031166	-1.178494	0.000000
H	-2.182343	0.364681	0.848425
C	0.000000	-1.743866	2.186341
H	0.814062	-1.853047	2.912404
H	-0.934920	-1.931737	2.727540
H	0.111093	-2.551535	1.451140
C	0.000000	1.743866	2.186341
H	-0.814062	1.853047	2.912404
H	0.934920	1.931737	2.727540
H	-0.111093	2.551535	1.451140

(AlH_3)

Al	0.000000	0.000000	0.000000
H	0.000000	1.580695	0.000000
H	1.368922	-0.790348	0.000000
H	-1.368922	-0.790348	0.000000

$(AlH_3)_2$

Al	0.000013	1.295967	0.000000
Al	0.000013	-1.296009	0.000000
H	-1.413960	1.983630	0.000000
H	-0.000236	-0.000004	1.157880
H	-1.413886	-1.983701	0.000000
H	1.414160	-1.983191	0.000000
H	1.413832	1.983806	0.000000
H	-0.000236	-0.000004	-1.157880

$(AlOMe)_{4,c}$

Al	0.939349	0.939349	-0.939349
Al	0.939349	-0.939349	0.939349
Al	-0.939349	-0.939349	-0.939349
Al	-0.939349	0.939349	0.939349
O	0.913149	0.913149	0.913149
O	-0.913149	-0.913149	0.913149
O	-0.913149	0.913149	-0.913149
C	-2.048628	2.048628	2.048628
H	-3.111051	1.862564	1.862564
H	-1.862564	3.111051	1.862564
H	-1.862564	1.862564	3.111051
O	0.913149	-0.913149	-0.913149
C	-2.048628	-2.048628	-2.048628
H	-1.862564	-3.111051	-1.862564
H	-1.862564	-1.862564	-3.111051
H	-3.111051	-1.862564	-1.862564
C	2.048628	-2.048628	2.048628
H	1.862564	-3.111051	1.862564
H	1.862564	-1.862564	3.111051
H	3.111051	-1.862564	1.862564
C	2.048628	2.048628	-2.048628
H	1.862564	1.862564	-3.111051
H	3.111051	1.862564	-1.862564
H	1.862564	3.111051	-1.862564

$(AlOMe)_{4,c} \cdot (AlMe_3)$

Al	-0.517484	-2.259224	0.000000
Al	-0.998634	-0.037039	1.330012
Al	-0.998634	-0.037039	-1.330012
O	-1.844321	-1.016828	0.000000
O	-0.597352	1.182253	0.000000
Al	0.269005	2.711864	0.000000
C	0.464358	3.531607	1.749793
H	0.730834	2.803988	2.525306
H	1.230695	4.313597	1.756008
H	-0.475278	4.000050	2.067840
C	0.464358	3.531607	-1.749793
H	-0.475278	4.000050	-2.067840
H	1.230695	4.313597	-1.756008
H	0.730834	2.803988	-2.525306
O	0.378360	-1.224377	-1.261250
Al	1.738846	-0.908353	0.000000
O	0.378360	-1.224377	1.261250
C	2.448630	0.947034	0.000000
H	2.160940	1.503427	-0.905962
H	2.160940	1.503427	0.905962
H	3.544518	0.968265	0.000000
C	3.005676	-2.394086	0.000000
H	2.512763	-3.374294	0.000000
H	3.657283	-2.369951	-0.881530

H	3.657283	-2.369951	0.881530
C	-1.737026	0.625011	-2.983052
H	-2.517970	1.372334	-2.807269
H	-0.966520	1.096520	-3.602864
H	-2.179730	-0.178984	-3.579414
C	-1.737026	0.625011	2.983052
H	-0.966520	1.096520	3.602864
H	-2.517970	1.372334	2.807269
H	-2.179730	-0.178984	3.579414
C	-0.731406	-4.169824	0.000000
H	-1.284344	-4.508385	-0.881961
H	0.234849	-4.683390	0.000000
H	-1.284344	-4.508385	0.881961

$(AlOH)_{4,c}$

Al	0.936608	0.936608	-0.936608
Al	0.936608	-0.936608	0.936608
Al	-0.936608	-0.936608	-0.936608
Al	-0.936608	0.936608	0.936608
O	0.912177	0.912177	0.912177
O	-0.912177	-0.912177	0.912177
O	-0.912177	0.912177	-0.912177
H	-1.834633	1.834633	1.834633
O	0.912177	-0.912177	-0.912177
H	-1.834633	-1.834633	-1.834633
H	1.834633	-1.834633	1.834633
H	1.834633	1.834633	-1.834633

$(AlOH)_{4,c} \cdot (AlH_3)$

Al	1.792331	0.942352	0.000000
O	1.709881	-0.858272	0.000000
Al	0.408766	-0.872966	1.326460
O	-0.788867	-1.265202	0.000000
Al	0.408766	-0.872966	-1.326460
O	0.408766	0.968193	-1.256567
Al	-0.721419	1.700565	0.000000
O	0.408766	0.968193	1.256567
H	-2.199338	0.947661	0.000000
H	-0.878611	3.257090	0.000000
H	0.449325	-1.654240	-2.671450
Al	-2.533823	-0.833818	0.000000
H	-3.191403	-1.043211	1.417381
H	-3.191403	-1.043211	-1.417381
H	0.449325	-1.654240	2.671450
H	3.043657	1.865678	0.000000

$(AlOH)_{6,c}$

Al	0.171614	1.893698	-0.897401
Al	1.583797	0.825288	1.122179
Al	1.647453	-0.984056	-0.859998
Al	-0.171614	-1.893698	0.897401
Al	-1.583797	-0.825288	-1.122179
Al	-1.647453	0.984056	0.859998
O	-1.362104	0.957282	-1.025566
O	-1.611025	-0.815454	0.785458
O	0.007582	1.682796	0.989209
H	-2.848092	1.705169	1.541084
O	-0.007582	-1.682796	-0.989209
H	-2.726179	-1.424030	-1.994637
O	1.362104	-0.957282	1.025566
H	-0.293895	-3.275666	1.604743
O	1.611025	0.815454	-0.785458
H	2.848092	-1.705169	-1.541084
H	2.726179	1.424030	1.994637
H	0.293895	3.275666	-1.604743

$(AlOH)_{6,c} \cdot (AlH_3)$

Al	-1.151905	-1.201951	0.220163
Al	1.386259	-1.671977	0.775701
O	0.201680	-1.837922	-0.732476
Al	1.233437	-0.744850	-1.767309
Al	1.922390	1.328324	-0.204440
Al	-0.672280	1.698219	-0.740809
O	-1.808851	0.327453	-0.440087
Al	-3.553350	-0.165840	-0.354040
H	-4.327999	0.349450	0.907710
H	-4.158065	-0.654051	-1.716926
O	0.415817	1.695748	0.731552
Al	0.151065	0.803683	2.317794
O	-0.058078	-0.911150	1.592538
H	1.603008	0.726368	2.974435
H	-1.196366	1.243921	3.012869
O	0.734871	0.979648	-1.643588
H	-1.367176	3.002051	-1.246549
O	2.260702	-0.448260	-0.200533
H	3.102245	2.342322	-0.265712
H	1.807373	-1.315085	-3.097613
H	2.109481	-2.884549	1.429230
H	-2.644658	-1.847477	0.331503

Optimized with MP2

($AlMe_3$)

Al	-0.000002	-0.000002	0.000001
C	0.422637	1.926918	-0.000001
C	1.457450	-1.329468	0.000000
C	-1.880082	-0.597445	0.000000
H	2.101901	-1.199976	-0.873507
H	1.102621	-2.360478	-0.000027
H	2.101875	-1.200016	0.873531
H	-2.595557	0.225341	0.000008
H	-2.090167	-1.220298	0.873510
H	-2.090165	-1.220280	-0.873523
H	1.492929	2.135147	-0.000001
H	-0.011717	2.420274	0.873520
H	-0.011722	2.420285	-0.873512

($AlMe_3)_2$

Al	0.000000	1.307369	0.007816
Al	0.000000	-1.307369	0.007816
C	-1.689170	0.000000	-0.218578
H	-2.002890	0.000000	-1.263013
H	-2.187882	0.844720	0.272737
C	0.000000	2.403299	-1.628218
H	-0.877772	3.052419	-1.675888
H	0.877772	3.052419	-1.675888
H	0.000000	1.789321	-2.531740
C	0.000000	2.063871	1.829046
H	0.876766	2.693938	2.000244
H	-0.876766	2.693938	2.000244
H	0.000000	1.295629	2.605444
C	0.000000	-2.063871	1.829046
H	0.876766	-2.693938	2.000244
H	0.000000	-1.295629	2.605444
H	-0.876766	-2.693938	2.000244
C	0.000000	-2.403299	-1.628218
H	0.877772	-3.052419	-1.675888
H	-0.877772	-3.052419	-1.675888
H	0.000000	-1.789321	-2.531740
H	-2.187882	-0.844720	0.272737
C	1.689170	0.000000	-0.218578
H	2.187882	-0.844720	0.272737
H	2.002890	0.000000	-1.263013
H	2.187882	0.844720	0.272737

(AlH_3)

Al	0.000000	0.000000	-0.000002
H	1.301804	-0.893388	0.000011
H	0.122797	1.574088	0.000010
H	-1.424599	-0.680699	0.000011

($AlH_3)_2$

Al	-1.308576	0.000026	0.000001
Al	1.308615	-0.000031	-0.000001
H	-1.994219	1.413418	0.000006
H	0.000000	-0.000532	-1.142445
H	1.995365	1.412819	-0.000002
H	1.995168	-1.412997	0.000012
H	-1.996823	-1.412101	-0.000020
H	0.000001	-0.000546	1.142450

$(AlOMe)_{4,c}$

Al	0.944204	0.944204	-0.944204
Al	0.944204	-0.944204	0.944204
Al	-0.944204	-0.944204	-0.944204
Al	-0.944204	0.944204	0.944204
O	0.919128	0.919128	0.919128
O	-0.919128	-0.919128	0.919128
O	-0.919128	0.919128	-0.919128
C	-2.064744	2.064744	2.064744
H	-3.122870	1.877282	1.877282
H	-1.877282	3.122870	1.877282
H	-1.877282	1.877282	3.122870
O	0.919128	-0.919128	-0.919128
C	-2.064744	-2.064744	-2.064744
H	-1.877282	-3.122870	-1.877282
H	-1.877282	-1.877282	-3.122870
H	-3.122870	-1.877282	-1.877282
C	2.064744	-2.064744	2.064744
H	1.877282	-3.122870	1.877282
H	1.877282	-1.877282	3.122870
H	3.122870	-1.877282	1.877282
C	2.064744	2.064744	-2.064744
H	1.877282	1.877282	-3.122870
H	3.122870	1.877282	-1.877282
H	1.877282	3.122870	-1.877282

$(AlOMe)_{4,c} \cdot (AlMe_3)$

Al	2.699572	0.279654	-0.001788
Al	-0.066654	-1.023030	-1.329937
Al	-0.067182	-1.009517	1.340493
Al	-0.866506	1.761096	-0.008415
Al	-2.287611	-0.475721	0.002145
O	-1.228405	0.400678	-1.269320
O	-1.073951	-1.841995	0.009258
O	1.168622	-0.627497	0.003522
O	-1.229429	0.413131	1.265459
C	-4.222100	-0.636812	0.002214
C	1.049970	2.355320	-0.009139
C	-2.260248	3.148669	-0.016422
C	0.538333	-1.796077	3.013709
C	0.539138	-1.827797	-2.994290
C	3.592864	0.422522	-1.742221
C	3.596738	0.440427	1.734950
H	-4.569501	-1.177948	0.883479
H	-4.703529	0.341432	0.000963
H	-4.569395	-1.180113	-0.877764
H	1.568317	2.026039	0.901198
H	1.569946	2.018230	-0.915711
H	1.176247	3.439987	-0.013890
H	-3.271516	2.736361	-0.017456
H	-2.179321	3.795352	0.860671
H	-2.175128	3.789169	-0.897651
H	1.296163	-2.561765	2.841585
H	0.969527	-1.045127	3.677475
H	-0.290517	-2.263557	3.547766
H	0.993646	-1.088855	-3.655948
H	1.278481	-2.608914	-2.811289
H	-0.293860	-2.279349	-3.535506
H	2.899132	0.520192	-2.578816
H	4.264317	1.283276	-1.767505
H	4.202612	-0.464303	-1.933469
H	4.231242	-0.430054	1.920523
H	4.244939	1.318855	1.759892
H	2.904293	0.516772	2.574817

$(AlOH)_{4,c}$

Al	0.943407	0.943407	-0.943407
Al	0.943407	-0.943407	0.943407
Al	-0.943407	-0.943407	-0.943407
Al	-0.943407	0.943407	0.943407
O	0.917846	0.917846	0.917846
O	-0.917846	-0.917846	0.917846
O	-0.917846	0.917846	-0.917846
H	-1.841587	1.841587	1.841587
O	0.917846	-0.917846	-0.917846
H	-1.841587	-1.841587	-1.841587
H	1.841587	-1.841587	1.841587
H	1.841587	1.841587	-1.841587

$(AlOH)_{4,c} \cdot (AlH_3)$

Al	1.804215	0.942464	0.000000
O	1.719799	-0.868828	0.000000
Al	0.411859	-0.883881	1.333276
O	-0.796057	-1.280275	0.000000
Al	0.411859	-0.883881	-1.333276
O	0.411859	0.974012	-1.262042
Al	-0.724517	1.712714	0.000000
O	0.411859	0.974012	1.262042
H	-2.187519	0.930094	0.000000
H	-0.925539	3.264847	0.000000
H	0.463493	-1.665933	-2.677900
Al	-2.550943	-0.815447	0.000000
H	-3.217321	-1.025193	1.412646
H	-3.217321	-1.025193	-1.412646
H	0.463493	-1.665933	2.677900
H	3.058856	1.860342	0.000000

$(AlOH)_{6,c}$

Al	0.169446	1.911684	-0.895213
Al	1.592839	0.831122	1.121050
Al	-1.660321	0.996154	0.857709
Al	1.660321	-0.996154	-0.857709
Al	-0.169446	-1.911684	0.895213
Al	-1.592839	-0.831122	-1.121050
O	-1.377978	0.969987	-1.027703
O	1.377978	-0.969987	1.027703
O	-1.615457	-0.818130	0.785387
O	-0.006132	-1.705697	-0.993194
O	1.615457	0.818130	-0.785387
O	0.006132	1.705697	0.993194
H	-0.297099	-3.293426	1.606244
H	-2.864074	1.713265	1.541670
H	2.864074	-1.713265	-1.541670
H	2.737190	1.429113	1.995088
H	0.297099	3.293426	-1.606244

H	-2.737190	-1.429113	-1.995088

$(AlOH)_{6,c} \cdot (AlH_3)$

Al	1.378091	-1.662568	0.839597
Al	-1.170565	-1.146858	0.333897
Al	0.261161	0.942152	2.292674
Al	1.173207	-0.867931	-1.752868
Al	-3.584608	-0.188077	-0.322896
Al	-0.672043	1.689451	-0.808257
Al	1.943751	1.287794	-0.335149
O	0.142649	-1.887543	-0.619487
O	-0.028658	-0.812977	1.667745
O	-1.831942	0.350248	-0.406423
O	2.254592	-0.505703	-0.236286
O	0.469074	1.744676	0.636190
O	0.705293	0.885721	-1.717547
H	2.089548	-2.859358	1.536478
H	-2.693642	-1.739409	0.479795
H	1.742324	0.854815	2.876020
H	-4.414861	0.420114	0.858872
H	-1.024725	1.460423	3.046752
H	1.692606	-1.529429	-3.065146
H	-1.357030	2.981091	-1.363865
H	3.138472	2.275573	-0.497790
H	-4.137673	-0.760696	-1.675612

Optimized with revPBE+D3

$(AlMe_3)$

Al	-0.506625	-0.832326	0.000000
C	-0.004169	0.008255	1.724695
C	-1.484638	-2.558927	0.000000
H	-2.577154	-2.375048	0.000000
H	-1.270761	-3.168705	-0.894781
H	-1.270761	-3.168705	0.894781
C	-0.004169	0.008255	-1.724695
H	0.982416	-0.369122	-2.058700
H	-0.716090	-0.231444	-2.533994
H	0.086724	1.106539	-1.661622
H	0.086724	1.106539	1.661622
H	-0.716090	-0.231444	2.533994
H	0.982416	-0.369122	2.058700

$(AlMe_3)_2$

Al	0.000000	1.299259	0.018525
Al	0.000000	-1.299259	0.018525
C	-1.712601	0.000000	-0.202629
H	-2.016833	0.000000	-1.260955
H	-2.215986	0.856151	0.291132
C	0.000000	2.334899	-1.660958
H	-0.887928	2.985051	-1.751781
H	0.887928	2.985051	-1.751781
H	0.000000	1.658347	-2.532898
C	0.000000	2.031196	1.852684
H	0.886578	2.660323	2.049067
H	-0.886578	2.660323	2.049067
H	0.000000	1.228793	2.609397
C	0.000000	-2.031196	1.852684
H	0.886578	-2.660323	2.049067
H	0.000000	-1.228793	2.609397
H	-0.886578	-2.660323	2.049067
C	0.000000	-2.334899	-1.660958
H	0.887928	-2.985051	-1.751781
H	-0.887928	-2.985051	-1.751781
H	0.000000	-1.658347	-2.532898
H	-2.215986	-0.856151	0.291132
C	1.712601	0.000000	-0.202629
H	2.215986	-0.856151	0.291132
H	2.016833	0.000000	-1.260955
H	2.215986	0.856151	0.291132

(AlH_3)

AL	0.000000	0.000000	0.000000
H	0.800100	-1.385813	0.000000
H	0.800100	1.385813	0.000000
H	-1.600199	0.000000	0.000000

$(AlH_3)_2$

Al	0.000000	1.316303	-0.001844
Al	0.000000	-1.316303	-0.001844
H	-1.163961	0.000000	0.000001
H	0.000000	1.998271	-1.437601
H	0.000000	2.004245	1.431063
H	0.000000	-2.004245	1.431063
H	0.000000	-1.998271	-1.437601
H	1.163961	0.000000	0.000001

$(AlOH)_{4,c}$

Al	-0.939261	0.939261	0.939261
Al	0.939261	-0.939261	0.939261
Al	0.939261	0.939261	-0.939261
Al	-0.939261	-0.939261	-0.939261
O	-0.933805	-0.933805	0.933805
O	0.933805	-0.933805	-0.933805
O	0.933805	0.933805	0.933805
O	-0.933805	0.933805	-0.933805
H	-1.847699	1.847699	1.847699
H	1.847699	1.847699	-1.847699
H	1.847699	-1.847699	1.847699
H	-1.847699	-1.847699	-1.847699

$(AlOH)_{4,c} \cdot (AlH_3)$

Al	-4.007575	3.482357	0.550982
Al	-1.719463	1.453037	-0.042126
Al	-1.907114	3.924209	-0.972565
Al	-3.328720	1.990615	-2.092630
Al	-4.750519	0.447547	0.418391
O	-3.338588	0.801514	-0.671986
O	-1.514111	2.303915	-1.706919
O	-2.197726	3.097327	0.708102
O	-3.751855	3.621807	-1.282454
H	-4.957706	2.151198	0.933865
H	-6.096196	0.166946	-0.383792
H	-4.275542	-0.256062	1.766978
H	-4.549603	4.758290	1.311414
H	-0.676112	0.510823	0.661244
H	-3.943336	1.595729	-3.484918
H	-1.167414	5.293825	-1.192026

$(AlOH)_{6,c}$

Al	-1.622216	-0.936587	-0.962307
Al	-1.622216	0.936587	0.962307
Al	0.000000	-1.873174	0.962307
Al	0.000000	1.873174	-0.962307
Al	1.622216	0.936587	0.962307
Al	1.622216	-0.936587	-0.962307
O	0.000000	-1.765438	-0.955709
O	0.000000	1.765438	0.955709
O	1.528914	-0.882719	0.955709
O	1.528914	0.882719	-0.955709
O	-1.528914	0.882719	-0.955709
O	-1.528914	-0.882719	0.955709
H	-2.803804	1.618777	1.748117
H	2.803804	1.618777	1.748117
H	0.000000	-3.237554	1.748117
H	2.803804	-1.618777	-1.748117
H	-2.803804	-1.618777	-1.748117
H	0.000000	3.237554	-1.748117

$(AlOH)_{6,c} \cdot (AlH_3)$

Al	0.257322	-1.776175	-1.589092
Al	0.080505	0.849505	-1.318198
Al	-2.206336	-0.932637	0.071379
Al	2.256567	-0.925004	0.049782
Al	-0.252834	3.396060	-0.593227
Al	0.085467	0.806275	1.772186
Al	0.275658	-1.869442	1.603655
O	1.474687	-0.249236	-1.482041
O	-1.083351	-0.508835	-1.380630
O	0.037266	1.774826	0.224243
O	0.978176	-2.338937	-0.021749
O	-1.061760	-0.613542	1.491454
O	1.482551	-0.378744	1.606889
H	-1.765666	3.875025	-0.577614
H	1.037564	4.311428	-0.712562
H	3.815201	-1.150335	0.004250
H	0.243566	-2.943211	2.751692
H	-3.505939	-0.019383	0.083782
H	-2.179057	-2.552780	-0.023619
H	-0.139134	2.258591	-2.176602
H	0.223233	-2.722245	-2.843312
H	-0.053674	1.708798	3.059325

$(AlOH)_{6,c} \cdot (AlH_3)$ - perpendicular

Al	0.196200	-1.970967	-1.595182
Al	0.287879	0.704232	-1.605648
Al	2.234348	-1.326648	0.020312
Al	0.177477	-1.947570	1.620839
Al	0.264659	0.727674	1.586121
Al	-1.544371	2.585730	-0.035578
Al	-2.158013	-0.471099	-0.015248
O	0.036300	1.593735	-0.017836
O	1.537045	-0.619775	-1.505865
O	-1.062248	-0.603888	1.432518
O	-1.043170	-0.621024	-1.444654
O	1.518320	-0.597109	1.526308

O	0.770422	-2.584176	0.020378
H	-1.801969	3.215492	-1.471049
H	-1.817492	3.245871	1.382173
H	-3.405517	-1.444985	-0.014788
H	-2.618185	1.161932	-0.029077
H	0.269662	1.673883	2.842987
H	0.012352	-2.950607	2.821641
H	3.744587	-1.768575	0.030862
H	0.307559	1.630154	-2.877487
H	0.038745	-2.986223	-2.786727

$(AlOMe)_1$

Al	0.327918	-0.283336	0.000000
O	1.905370	0.119073	0.000000
C	-1.581434	-0.774620	0.000000
H	-2.211962	0.128706	0.000000
H	-1.824341	-1.370561	0.893361
H	-1.824341	-1.370561	-0.893361

$(AlOMe)_{4,c}$

Al	-0.941187	0.941187	0.941187
Al	0.941187	-0.941187	0.941187
Al	0.941187	0.941187	-0.941187
Al	-0.941187	-0.941187	-0.941187
O	-0.934998	-0.934998	0.934998
O	0.934998	-0.934998	-0.934998
O	0.934998	0.934998	0.934998
O	-0.934998	0.934998	-0.934998
C	-2.068833	2.068833	2.068833
C	2.068833	2.068833	-2.068833
C	2.068833	-2.068833	2.068833
C	-2.068833	-2.068833	-2.068833
H	-1.881422	3.139222	1.881422
H	-1.881422	1.881422	3.139222
H	-3.139222	1.881422	1.881422
H	3.139222	1.881422	-1.881422
H	1.881422	3.139222	-1.881422
H	1.881422	1.881422	-3.139222
H	-1.881422	-1.881422	-3.139222
H	-3.139222	-1.881422	-1.881422
H	-1.881422	-3.139222	-1.881422
H	3.139222	-1.881422	1.881422
H	1.881422	-3.139222	1.881422
H	1.881422	-1.881422	3.139222

$(AlOMe)_{4,c} \cdot (AlMe_3)$

Al	-0.603009	2.020945	-0.024461
Al	0.328817	-0.668157	1.376328
Al	1.734637	0.833877	-0.276902
Al	-0.047583	-0.848499	-1.256941
Al	-2.877313	-1.023492	0.504125
O	-1.112946	-1.072114	0.258449
O	1.433884	-0.972000	-0.110409
O	0.214470	0.977434	-1.383514
O	0.579556	1.152223	1.179128
C	-2.551551	1.580690	0.283066
C	-3.433681	-1.258696	2.379974
C	-3.928146	-1.487713	-1.097258
C	-0.110229	3.929723	-0.218436
C	0.407766	-1.550023	3.122626
C	-0.437073	-1.958688	-2.822016
C	3.448876	1.723161	-0.577356
H	0.963267	4.067942	-0.438334
H	-0.323316	4.498421	0.704565
H	-0.670129	4.416120	-1.037021
H	-2.954961	0.963727	-0.549965
H	-3.224536	2.455014	0.321157
H	-2.695596	1.084138	1.267925
H	0.221073	-2.633763	3.033514
H	-0.348559	-1.142551	3.814366
H	1.392351	-1.420135	3.602239
H	0.378760	-1.921551	-3.563084
H	-1.357104	-1.628293	-3.332669
H	-0.580732	-3.015193	-2.538088
H	-2.760316	-0.742797	3.084166
H	-3.417861	-2.329582	2.653160
H	-4.457687	-0.891790	2.564529
H	-3.975382	-2.584899	-1.221040
H	-3.484629	-1.083647	-2.021783
H	-4.967542	-1.123055	-1.035568
H	4.161357	1.515798	0.238605
H	3.318074	2.815930	-0.636379
H	3.918084	1.392164	-1.519148

$(AlOMe)_{4,c} \cdot (AlMe_3)_2$

Al	-0.376934	1.068073	-0.078971
Al	0.219156	-1.811448	0.826189
Al	1.906433	0.067694	-0.944212
Al	-0.599927	-1.555513	-1.684523
Al	2.005926	-3.665874	-1.332635

Al	-3.117137	-1.422266	0.536227
O	-1.445815	-1.656997	-0.019261
O	0.690543	-2.592664	-0.807004
O	0.130426	0.118750	-1.679682
O	0.912863	-0.127578	0.698797
C	-2.329523	1.001393	0.493919
C	-3.423427	-1.855901	2.434734
C	-4.483850	-1.556883	-0.878803
C	0.152274	2.978794	0.030987
C	0.369563	-2.824344	2.496443
C	-1.476018	-2.248578	-3.293743
C	2.914290	1.762843	-1.177119
H	0.120327	3.471273	-0.956523
H	1.157303	3.151853	0.442951
H	-0.570783	3.508033	0.677461
H	-2.998074	0.598618	-0.299445
H	-2.738183	2.006040	0.698323
H	-2.464207	0.460651	1.458052
H	-0.155028	-3.792826	2.432759
H	-0.063120	-2.270347	3.346444
H	1.421220	-3.036104	2.752814
H	-0.800799	-2.222162	-4.165525
H	-2.367911	-1.656958	-3.560195
H	-1.802370	-3.294078	-3.161189
H	-4.284003	-1.308004	2.855463
H	-2.545800	-1.636804	3.065006
H	-3.641218	-2.932984	2.553017
H	-4.737755	-2.614735	-1.073136
H	-4.146997	-1.129378	-1.837952
H	-5.422258	-1.047653	-0.598365
H	3.782900	1.570392	-1.832357
H	3.312233	2.137293	-0.217843
H	2.333301	2.582566	-1.624663
C	3.197713	-1.417867	-1.466495
H	4.197025	-1.029722	-1.729010
H	2.871216	-1.950785	-2.388449
H	3.397918	-2.126389	-0.631848
C	1.851845	-4.309606	-3.189690
H	1.377454	-3.570021	-3.855570
H	1.229548	-5.222108	-3.230581
H	2.831744	-4.572001	-3.624107
C	2.900208	-4.651376	0.122043
H	2.990568	-4.056342	1.046050
H	3.914357	-4.980810	-0.162477
H	2.327802	-5.560718	0.382748

$(AlOMe)_{6,c}$

Al	-1.62995	-0.94105	-0.95712
Al	-1.62995	0.94105	0.95712
Al	0.00000	-1.88210	0.95712
Al	0.00000	1.88210	-0.95712
Al	1.62995	0.94105	0.95712
Al	1.62995	-0.94105	-0.95712
O	0.00000	-1.76231	-0.96374
O	0.00000	1.76231	0.96374
O	1.52621	-0.88116	0.96374
O	1.52621	0.88116	-0.96374
O	-1.52621	0.88116	-0.96374
O	-1.52621	-0.88116	0.96374
C	-3.12724	-1.80551	-1.87228
C	-3.12724	1.80551	1.87228
C	0.00000	3.61103	-1.87228
C	3.12724	1.80551	1.87228
C	3.12724	-1.80551	-1.87228
C	0.00000	-3.61103	1.87228
H	4.08786	-1.33163	-1.60869
H	4.08786	1.33163	1.60869
H	3.19715	-2.87438	-1.60869
H	3.19715	2.87438	1.60869
H	0.89071	4.20601	-1.60869
H	0.89071	-4.20601	1.60869
H	0.00000	-3.49404	2.96970
H	-0.89071	-4.20601	1.60869
H	-0.89071	4.20601	-1.60869
H	-3.19715	2.87438	1.60869
H	-3.19715	-2.87438	-1.60869
H	-3.02593	1.74702	2.96970
H	-4.08786	1.33163	1.60869
H	-4.08786	-1.33163	-1.60869
H	0.00000	3.49404	-2.96970
H	3.02593	1.74702	2.96970
H	3.02593	-1.74702	-2.96970
H	-3.02593	-1.74702	-2.96970

$(AlOMe)_{6,c} \cdot (AlMe_3)$

Al	0.56422	-1.93618	-1.50223
Al	0.14754	0.68863	-1.57859
Al	-2.04570	-1.03381	0.09014
Al	2.47252	-0.84461	0.05084
Al	-0.13961	3.43934	-0.10036

Al	0.17640	0.80478	1.60396	$(AlOMe)_{6,c} \cdot (AlMe_3)$ - perpendicular			
Al	0.58484	-1.81993	1.70563	Al	0.187840	-2.008827	-1.590548
O	1.64409	-0.35099	-1.51784	Al	-0.107040	0.635332	-1.601152
O	-0.88204	-0.80518	-1.35689	Al	2.127514	-1.062039	0.013463
O	0.06623	1.66474	-0.01642	Al	0.173650	-1.999843	1.606412
O	1.29977	-2.35982	0.11008	Al	-0.120994	0.643510	1.592842
O	-0.85542	-0.70114	1.51116	Al	0.967382	3.161339	0.001901
O	1.67535	-0.24559	1.58484	Al	-2.414864	-1.018743	-0.007778
C	-1.95492	4.11297	0.20389	O	0.056925	1.616731	-0.006706
C	1.51168	4.44513	-0.43997	O	1.348841	-0.483350	-1.549752
C	4.42804	-0.95457	-0.02262	O	-1.207902	-0.813308	1.397656
C	0.66764	-3.07497	3.20324	O	-1.195742	-0.820236	-1.403517
C	-3.40865	0.41100	0.09452	O	1.335104	-0.474096	1.566066
C	-2.46633	-2.98443	0.18000	O	0.893005	-2.524317	0.012503
C	-0.21471	1.97166	-3.03910	C	1.450753	3.989460	-1.713178
C	0.53926	-3.26997	-2.93262	H	2.043274	4.900580	-1.527752
C	-0.04371	2.16296	3.02143	H	2.059143	3.310814	-2.334503
H	-2.39025	3.66008	1.10958	H	0.574131	4.263053	-2.320189
H	-2.62359	3.84332	-0.63114	C	1.576663	3.880026	1.726706
H	-1.98443	5.20884	0.31856	H	2.126860	3.128021	2.316104
H	-1.21365	2.43710	-2.94117	H	2.249943	4.735525	1.550332
H	-0.21176	1.46625	-4.02026	H	0.743601	4.222971	2.360332
H	0.52907	2.78619	-3.11073	C	-3.001840	-2.924504	-0.005046
H	0.23173	-2.82443	-3.89400	H	-3.607962	-3.169788	-0.895840
H	-0.18554	-4.06902	-2.69945	H	-2.157669	-3.642334	0.000082
H	1.52097	-3.74923	-3.08176	H	-3.616056	-3.166190	0.881101
H	-1.06576	2.57544	3.06889	C	-3.632811	0.553373	-0.015593
H	0.65412	3.01617	2.91857	H	-4.286932	0.575786	-0.905587
H	0.16955	1.72223	4.01085	H	-3.063653	1.503463	-0.017853
H	-0.07243	-3.88404	3.08041	H	-4.289815	0.581849	0.872109
H	0.46351	-2.58727	4.17098	C	-0.570175	1.760288	3.148034
H	1.66206	-3.54863	3.26861	H	-1.200972	2.625035	2.881060
H	1.31993	5.43101	-0.89503	H	0.304029	2.147256	3.693505
H	2.19263	3.88576	-1.10251	H	-1.155941	1.145143	3.852934
H	2.05766	4.62427	0.50407	C	0.092400	-3.283452	3.081126
H	4.76098	-1.51046	-0.91553	H	1.042976	-3.827117	3.212173
H	4.86158	-1.44654	0.86335	H	-0.693636	-4.035832	2.896454
H	4.87451	0.05320	-0.08732	H	-0.147957	-2.789682	4.037834
H	-3.10284	-3.30800	-0.66316	C	4.085371	-1.247996	0.024006
H	-3.00784	-3.23689	1.10980	H	4.551815	-0.727799	-0.829588
H	-1.57297	-3.63967	0.15832	H	4.384493	-2.308467	-0.043861
H	-4.11731	0.34173	-0.74977	H	4.530384	-0.845081	0.949199
H	-2.93885	1.40878	0.03659	C	-0.537403	1.736928	-3.172003
H	-4.00981	0.39947	1.02202	H	-1.067310	1.099674	-3.900868
				H	0.338884	2.164732	-3.682139

H	-1.216225	2.570890	-2.925703
C	0.119364	-3.302625	-3.056971
H	-0.110115	-2.815095	-4.019513
H	-0.670147	-4.051833	-2.874600
H	1.070362	-3.848757	-3.173895

$(AlOMe)_{6,c} \cdot (AlMe_3)_2$

Al	0.528106	-1.802385	-1.542429
Al	0.114197	0.782076	-1.404384
Al	-2.156943	-0.989566	0.034620
Al	2.750863	-0.211815	0.157214
Al	-0.356096	3.389392	0.319532
Al	0.062039	0.604155	1.733040
Al	0.480852	-1.979096	1.597429
Al	0.936547	-4.588807	-0.110291
O	1.581410	-0.316502	-1.316572
O	-0.941860	-0.717678	-1.374320
O	-0.070578	1.630403	0.214901
O	0.656347	-2.828055	-0.023643
O	-0.989029	-0.884317	1.510777
O	1.533469	-0.477007	1.565932
C	-2.166399	3.965391	0.793066
C	1.179525	4.547813	-0.047157
C	4.006700	-1.759560	0.099504
C	0.711237	-3.339633	3.008368
C	-3.415236	0.555078	0.105366
C	-2.870403	-2.847886	-0.092568
C	-0.107361	2.144088	-2.815131
C	0.717524	-3.009590	-3.092116
C	-0.134766	1.817114	3.278335
H	-2.701454	3.200800	1.375373
H	-2.768114	4.148789	-0.114544
H	-2.152753	4.907100	1.367463
H	-1.075894	2.674857	-2.745658
H	-0.089289	1.679470	-3.816345
H	0.691164	2.906164	-2.804252
H	0.594303	-2.455399	-4.038968
H	-0.050138	-3.806423	-3.105603
H	1.706090	-3.498662	-3.136034
H	-1.131196	2.289657	3.328493
H	0.619641	2.626752	3.284192
H	0.004494	1.269600	4.226760
H	-0.080990	-4.107965	2.997148
H	0.688477	-2.873313	4.008735
H	1.684298	-3.862415	2.941273
H	0.864123	5.534625	-0.425873
H	1.872743	4.095114	-0.772566
H	1.762603	4.723946	0.874455
H	4.299399	-2.023192	-0.933450
H	3.592426	-2.675897	0.554288
H	4.941039	-1.532229	0.644191
H	-3.840436	-2.863694	-0.621641
H	-3.045384	-3.299665	0.900565
H	-2.203502	-3.534582	-0.640887
H	-4.374146	0.311008	-0.386289
H	-3.026538	1.459581	-0.393257
H	-3.658725	0.844557	1.143892
C	3.469144	1.643741	0.278641
H	3.683099	2.076860	-0.715951
H	4.418500	1.665671	0.844560
H	2.783652	2.343345	0.786623
C	2.726856	-5.170367	-0.651279
H	3.263296	-4.387021	-1.206346
H	2.684635	-6.082253	-1.270881
H	3.341084	-5.411287	0.235114
C	-0.576403	-5.743027	0.352400
H	-1.333462	-5.209629	0.945302
H	-0.244002	-6.632018	0.915684
H	-1.084119	-6.110481	-0.557713

$(AlOMe)_{6,c} \cdot (AlMe_3)_3$

Al	1.85349	-1.16478	-1.03161
Al	1.47156	0.96123	-2.58560
Al	-0.76625	-1.15183	-2.94305
Al	-1.32651	1.42662	-1.20762
Al	-1.15267	-1.32540	0.23383
Al	-0.15242	3.73018	0.68673
Al	-0.13483	3.58677	-3.28411
Al	1.35760	1.52914	0.62410
Al	0.34536	-3.50964	0.69981
O	-0.04963	1.99679	-2.46830
O	-0.39943	1.96031	0.27923
O	1.04236	-0.81117	-2.65829
O	0.62950	-1.77429	0.14827
O	-1.39362	-0.39127	-1.30700
O	2.01078	0.70048	-0.82924
C	1.79229	0.74214	2.36910
C	-1.87111	-3.31232	0.31564
H	-2.61960	-2.99055	-0.44066
H	-2.40753	-3.44383	1.26770

H	-1.63789	-4.32036	-0.08184	C	0.42197	-3.66291	2.66807
C	-3.10830	2.25177	-1.36062	H	-0.07598	-4.57564	3.03996
H	-3.60921	1.94763	-2.29494	H	-0.05706	-2.80298	3.16432
H	-3.13964	3.35137	-1.30944	H	1.46717	-3.70135	3.02406
H	-3.73212	1.87623	-0.52915	C	1.13766	-4.88939	-0.47570
C	-1.43377	-0.05021	-4.47959	H	2.11624	-5.20952	-0.07676
H	-1.98733	-0.68601	-5.19426	H	1.30482	-4.55694	-1.51143
H	-0.61021	0.41898	-5.05028	H	0.50446	-5.79268	-0.52431
H	-2.11573	0.76634	-4.18536	H	2.88152	0.70608	2.54742
C	3.55770	-2.14156	-0.97256	H	1.40799	-0.28801	2.45351
H	3.45086	-3.19588	-1.27616	H	1.34452	1.33227	3.18654
H	4.31227	-1.68112	-1.63329				
H	3.97714	-2.13876	0.04946	$(AlOMe)_{6,c} \cdot (AlMe_3)_4$			
C	-0.74547	5.01058	-0.74410	Al	1.71233	-1.32228	-1.35231
H	-1.23449	4.58247	-1.64830	Al	1.67003	1.32007	-3.00924
H	0.04959	5.69487	-1.08020	Al	-1.08505	-1.18491	-3.07134
H	-1.55210	5.64496	-0.33322	Al	-1.22532	1.48348	-1.46262
C	-0.57096	4.19118	2.55678	Al	-1.17091	-1.09463	0.15689
H	-0.17408	5.18028	2.84661	Al	-0.07232	3.17432	1.12477
H	-0.14862	3.45071	3.25667	Al	0.29045	-3.39774	-3.58352
H	-1.66131	4.21844	2.73089	Al	0.31836	3.51852	-3.64128
C	-1.92358	-0.48256	1.84147	Al	1.55878	1.27899	0.21998
H	-3.01214	-0.32875	1.72245	Al	0.41387	-2.96272	1.19129
H	-1.47886	0.49536	2.08082	O	-0.05689	1.92869	-2.80096
H	-1.78637	-1.14234	2.71473	O	-0.24709	1.65869	0.07616
C	-1.13745	-3.10182	-3.00299	O	0.62170	-1.79740	-2.74308
H	-0.79727	-3.49352	-3.97908	O	0.64396	-1.46429	0.13159
H	-2.21754	-3.32287	-2.93609	O	-1.48689	-0.37175	-1.49824
H	-0.63785	-3.70592	-2.23364	O	1.97400	0.53155	-1.40140
C	1.51094	4.66326	-3.26863	C	2.48314	0.43455	1.74783
H	1.26700	5.73844	-3.25865	C	-1.67311	-3.17949	0.35411
H	2.13591	4.47396	-4.15603	H	-2.44804	-2.89192	-0.39173
H	2.12916	4.44743	-2.38397	H	-2.24718	-3.44565	1.25598
C	-1.73799	3.88304	-4.37028	H	-1.28273	-4.10947	-0.10008
H	-1.79520	4.90670	-4.77353	C	-2.91609	2.48333	-1.59842
H	-2.65606	3.68281	-3.79793	H	-3.62403	1.94352	-2.25234
H	-1.73564	3.17770	-5.21927	H	-2.78399	3.49102	-2.02690
C	2.79428	1.60413	-3.89297	H	-3.41016	2.61121	-0.62033
H	2.35386	1.89757	-4.86172	C	-1.58811	-0.17961	-4.69106
H	3.49491	0.77689	-4.10336	H	-1.87874	-0.87404	-5.49746
H	3.39002	2.45742	-3.53289	H	-0.77736	0.46020	-5.07096
C	2.06278	3.55876	0.66068	H	-2.45248	0.48243	-4.50195
H	1.93416	4.54944	0.17999	C	2.30002	0.29110	-4.56820
H	2.89464	3.14777	0.04910	H	3.22615	-0.26135	-4.32500
H	2.46852	3.74590	1.66736	H	2.53676	0.96843	-5.40619

H	1.57263	-0.45128	-4.92874	C	0.17533	-2.50775	3.10044
C	3.41129	-2.31585	-1.36071	H	-0.31593	-3.33676	3.64148
H	3.31304	-3.33097	-1.78053	H	-0.42265	-1.60182	3.27943
H	4.15909	-1.78282	-1.97417	H	1.15926	-2.35358	3.57901
H	3.83932	-2.42588	-0.34990	C	1.50582	-4.54882	0.76794
C	-1.13809	4.75678	0.61892	H	2.29960	-4.63172	1.53132
H	-1.59232	4.71443	-0.37898	H	1.99831	-4.53130	-0.21251
H	-0.54992	5.68946	0.67314	H	0.91859	-5.48212	0.82356
H	-1.96071	4.86204	1.34904	H	3.24370	-0.28976	1.40573
C	0.04169	2.74325	3.05194	H	1.77419	-0.12068	2.38238
H	0.49771	3.57788	3.61465	H	2.98936	1.18084	2.38172
H	0.62459	1.83856	3.28165				
H	-0.97160	2.59612	3.46659	$(AlOMe)_{8,c}$			
C	-2.17973	-0.21886	1.61129	Al	1.159736	0.645678	2.335309
H	-2.91194	0.50660	1.21424	Al	1.495720	-1.482094	0.723701
H	-1.50633	0.33868	2.28130	Al	1.481733	1.495744	-0.723268
H	-2.73062	-0.95225	2.22290	Al	-0.645763	1.159777	-2.335220
C	-1.95533	-3.10223	-3.31180	Al	0.645763	-1.159777	-2.335220
H	-2.19900	-3.44937	-4.33049	Al	-1.481733	-1.495744	-0.723268
H	-2.87907	-2.56112	-3.00558	Al	-1.495720	1.482094	0.723701
H	-1.94844	-3.97121	-2.63207	Al	-1.159736	-0.645678	2.335309
C	-0.07020	5.21265	-2.71489	O	-1.167254	-0.588896	-2.290010
H	-1.14501	5.45754	-2.68387	O	-1.839711	-0.369785	0.643268
H	0.42583	6.03292	-3.26563	O	1.839711	0.369785	0.643268
H	0.29800	5.24592	-1.68064	O	-0.588794	1.167529	2.290193
C	0.12251	3.34357	-5.59638	O	0.588794	-1.167529	2.290193
H	0.56716	4.19684	-6.13795	O	-0.369986	1.839787	-0.643190
H	-0.94194	3.29353	-5.88678	O	0.369986	-1.839787	-0.643190
H	0.59829	2.42557	-5.97778	O	1.167254	0.588896	-2.290010
C	2.54554	3.23660	-3.22971	C	-2.370863	-1.399178	3.671737
H	2.84788	3.56682	-4.23831	H	-1.923138	-1.411239	4.679300
H	3.45250	2.70741	-2.85955	H	-3.311235	-0.824894	3.726104
H	2.49414	4.11763	-2.56772	H	-2.640765	-2.439726	3.420875
C	0.62140	-5.08090	-2.61641	C	-3.078510	2.638988	0.785948
H	1.69331	-5.31999	-2.51784	H	-3.777603	2.342310	1.586177
H	0.16339	-5.91108	-3.18405	H	-2.800216	3.691702	0.966277
H	0.19342	-5.10386	-1.60460	H	-3.641362	2.615760	-0.163888
C	0.60762	-3.23539	-5.52485	C	-2.638597	-3.078554	-0.785452
H	0.20125	-4.09349	-6.08883	H	-3.691275	-2.800271	-0.966149
H	1.68731	-3.17970	-5.75029	H	-2.341972	-3.777117	-1.586303
H	0.14982	-2.32141	-5.93784	H	-2.615392	-3.642052	0.163890
C	2.05760	3.37066	0.41288	C	1.399871	-2.371008	-3.671594
H	1.70438	4.29636	-0.07858	H	2.441164	-2.639598	-3.422457
H	2.86908	3.06125	-0.28406	H	1.410234	-1.923792	-4.679560
H	2.58457	3.64573	1.34035	H	0.826849	-3.312184	-3.725686

C	-1.399871	2.371008	-3.671594	H	-2.260839	-3.729844	-1.612062
H	-2.441164	2.639598	-3.422457	H	-2.588039	-3.619731	0.128490
H	-1.410234	1.923792	-4.679560	C	1.442347	-2.316789	-3.586062
H	-0.826849	3.312184	-3.725686	H	2.480906	-2.586788	-3.326835
C	2.638597	3.078554	-0.785452	H	1.466625	-1.866749	-4.592375
H	3.691275	2.800271	-0.966149	H	0.869965	-3.257600	-3.653231
H	2.615392	3.642052	0.163890	C	-1.241744	2.486881	-3.545272
H	2.341972	3.777117	-1.586303	H	-2.289288	2.755778	-3.323717
C	3.078510	-2.638988	0.785948	H	-1.223347	2.061066	-4.562200
H	3.777603	-2.342310	1.586177	H	-0.662589	3.425318	-3.560254
H	3.641362	-2.615760	-0.163888	C	2.853574	2.894487	-0.666265
H	2.800216	-3.691702	0.966277	H	3.255405	2.916865	-1.693269
C	2.370863	1.399178	3.671737	H	3.701593	2.754331	0.024154
H	1.923138	1.411239	4.679300	H	2.427636	3.887227	-0.449605
H	3.311235	0.824894	3.726104	C	2.703331	-2.694576	1.408178
H	2.640765	2.439726	3.420875	H	3.405661	-2.271283	2.143698
				H	3.248734	-2.787802	0.448668
$(AlOMe)_{8,c} \cdot (AlMe_3)$				H	2.567095	-3.764856	1.676106
Al	1.130087	1.281154	2.567654	C	1.894534	0.282363	4.109686
Al	1.232004	-1.394899	0.926296	H	1.166728	-0.392270	4.591082
Al	1.512680	1.469637	-0.489959	H	2.756903	-0.341437	3.814471
Al	-0.550195	1.239660	-2.206023	H	2.257532	0.975078	4.889743
Al	0.670929	-1.111478	-2.250760	C	-0.106997	-4.854613	1.806256
Al	-1.504333	-1.432454	-0.693837	H	-0.180799	-4.601152	0.735809
Al	-1.510200	1.509731	0.815838	H	-1.130666	-5.087649	2.150734
Al	-1.405501	-0.636442	2.406715	H	0.482568	-5.782329	1.899179
Al	0.656024	-3.349593	2.817510	C	1.459712	-3.398796	4.604824
O	-1.123353	-0.500657	-2.234649	H	2.224693	-2.617843	4.729748
O	-1.937329	-0.313903	0.653461	H	1.921775	-4.376710	4.821570
O	1.658876	0.351966	0.953648	H	0.694313	-3.221028	5.381401
O	-0.703743	1.057971	2.411385	C	1.470735	3.230311	2.370904
O	0.017294	-1.758787	2.243397	H	0.900957	3.728049	1.567114
O	-0.323607	1.882951	-0.499611	H	2.531126	3.489576	2.219974
O	0.366791	-1.807840	-0.585597	H	1.150108	3.705040	3.317600
O	1.237287	0.604230	-2.100458				
C	-2.721660	-1.245348	3.729248	$(AlOMe)_{8,c} \cdot (AlMe_3)_2$			
H	-2.283457	-1.335694	4.738789	Al	1.62008	1.37560	1.97383
H	-3.574798	-0.550121	3.807346	Al	1.75133	-0.79819	0.41804
H	-3.135598	-2.233913	3.461173	Al	1.85745	1.99332	-1.18638
C	-3.018123	2.764578	0.879692	Al	-0.91080	1.93514	-2.78565
H	-3.776814	2.463753	1.622342	Al	0.89017	-0.64157	-2.64596
H	-2.677013	3.778556	1.151736	Al	-1.21128	-0.70176	-1.01107
H	-3.530153	2.849035	-0.095116	Al	-0.88145	2.17978	0.28717
C	-2.609812	-3.049480	-0.816385	Al	-0.96739	-0.42995	2.04804
H	-3.666208	-2.810653	-1.027488	Al	3.62321	0.92942	-3.40476

Al	-0.37118	4.16066	2.14203	C	-0.96273	4.31858	4.00836
O	-0.77159	0.09867	-2.62913	H	-1.69169	3.53938	4.27939
O	-1.39138	0.45701	0.39101	H	-1.41083	5.30300	4.22625
O	2.25694	1.02028	0.27767	H	-0.09999	4.19849	4.68880
O	0.27615	2.54358	1.65564	C	0.00449	2.63305	-4.40679
O	0.88148	-0.30255	1.97191	H	0.05552	1.87230	-5.20705
O	0.07446	2.40294	-1.22910	H	1.04064	2.95948	-4.21618
O	0.59670	-1.21565	-0.91832	H	-0.53223	3.50124	-4.82993
O	2.08103	0.73822	-2.53342	C	1.51181	-1.91127	-4.01468
C	-1.73897	0.67371	3.51553	H	1.60835	-1.44070	-5.00945
H	-2.31525	0.04978	4.22187	H	0.82105	-2.76369	-4.12981
H	-0.97096	1.20127	4.10703	H	2.49761	-2.34042	-3.75609
H	-2.43191	1.44617	3.13731	C	3.52851	1.62233	-5.23294
C	-2.28786	3.58987	0.71252	H	3.58449	2.72490	-5.22518
H	-3.19927	2.96536	0.65600	H	2.56981	1.36164	-5.70737
H	-2.47262	4.12204	1.67486	H	4.35184	1.25678	-5.86850
H	-2.36153	4.34846	-0.08079	C	5.17408	0.29603	-2.38373
C	-2.61640	-2.05587	-1.23171	H	6.09641	0.85716	-2.60671
H	-2.94395	-2.10270	-2.28397	H	5.38242	-0.76697	-2.60079
H	-2.27041	-3.06077	-0.94053	H	4.97133	0.36924	-1.30320
H	-3.50307	-1.83304	-0.61504				
C	-2.81747	2.41273	-2.45341	$(AlOMe)_{8,c} \cdot (AlMe_3)_3$			
H	-2.98184	3.49582	-2.32183	Al	1.39917	1.00605	2.37172
H	-3.39357	2.11059	-3.34806	Al	1.26700	-1.52558	0.50219
H	-3.30434	1.90525	-1.60067	Al	1.48949	1.30651	-0.77175
C	3.11488	3.46376	-1.62736	Al	-1.22811	1.48830	-2.27005
H	4.18290	3.17275	-1.62343	Al	1.03878	-1.42085	-2.57735
H	3.03070	4.26001	-0.86464	Al	0.97436	-3.61971	2.33295
H	2.89547	3.94862	-2.59538	Al	3.50680	-0.35445	-2.66986
C	3.27998	-2.02949	0.51594	Al	-3.66867	0.41389	-2.54705
H	2.96545	-3.06372	0.73797	Al	-1.61764	-1.44285	-0.85747
H	4.00465	-1.73101	1.29299	Al	-1.35707	1.26067	0.82667
H	3.82858	-2.05718	-0.44255	Al	-1.13780	-0.91669	2.34108
C	-1.41256	-2.36117	1.90979	O	-1.97577	-0.17878	-2.13303
H	-0.82791	-2.91858	1.15756	O	-1.86913	-0.52974	0.69589
H	-2.47639	-2.56265	1.70344	O	1.74049	0.20536	0.67834
H	-1.17744	-2.82020	2.88875	O	-0.44205	0.78490	2.35340
C	2.83246	1.99619	3.38739	O	0.23685	-2.02496	1.92444
H	3.26760	2.98142	3.14123	O	-0.34199	1.63102	-0.67561
H	3.67500	1.30354	3.55319	O	0.23170	-1.77389	-0.98403
H	2.30745	2.10545	4.35257	O	1.82048	0.17882	-2.18072
C	0.36759	5.61251	1.03388	C	-2.83305	2.53263	1.09926
H	0.44966	5.29783	-0.02056	H	-3.69448	2.31620	0.44897
H	1.38285	5.89270	1.37100	H	-3.19010	2.46197	2.14141
H	-0.24685	6.52872	1.06489	H	-2.54200	3.58293	0.92686

C	-2.67428	-3.08611	-1.08265	C	-4.98188	0.02742	-1.12315
H	-2.50645	-3.54457	-2.07341	H	-4.50331	0.01235	-0.13053
H	-2.42152	-3.85139	-0.32727	H	-5.46087	-0.95633	-1.26933
H	-3.75606	-2.88580	-0.99270	H	-5.79383	0.77540	-1.08984
C	0.04489	-1.72560	-4.24163	C	3.88593	0.02286	-4.56751
C	-3.01472	2.59099	-2.35194	H	4.11325	1.09285	-4.72013
H	-2.56229	3.32444	-1.65284	H	3.01708	-0.21778	-5.20277
H	-3.05434	3.06717	-3.34391	H	4.74704	-0.54923	-4.95424
H	-4.05100	2.56649	-1.96083	C	4.82755	-0.17751	-1.20754
C	2.60457	2.90255	-1.05025	H	4.34669	-0.10689	-0.21762
H	3.63565	2.74494	-0.68904	H	5.42939	0.73926	-1.33596
H	2.21977	3.80268	-0.54698	H	5.53931	-1.02168	-1.17519
H	2.66573	3.12338	-2.13085	C	2.28414	-0.11033	3.76233
C	2.76873	-2.88004	0.68558	H	2.82983	0.51132	4.49432
H	3.11353	-3.25600	1.67649	H	3.02463	-0.80134	3.32054
H	3.64859	-2.28623	0.37480	H	1.57519	-0.73215	4.33554
H	2.71470	-3.74781	0.01145	H	-0.16818	-2.80007	-4.38614
C	-2.23874	-1.61815	3.80501	H	0.65921	-1.39960	-5.09875
H	-2.66120	-2.60626	3.54964	H	-0.91255	-1.18546	-4.28444
H	-3.08836	-0.95802	4.04763				
H	-1.65102	-1.74439	4.73115	$(AlOMe)_{8,c} \cdot (AlMe_3)_4$			
C	1.76734	2.95496	2.28181	Al	1.53777	1.16989	2.27724
H	1.08497	3.51761	1.62054	Al	1.30638	-1.54682	0.70144
H	2.79360	3.19383	1.95658	Al	1.52263	1.24541	-0.85166
H	1.63979	3.37815	3.29549	Al	-1.16867	1.39994	-2.46921
C	0.29169	-5.09490	1.22594	Al	1.10287	-1.56970	-2.43333
H	0.02383	-4.73856	0.21740	Al	-0.39016	-3.57823	2.61175
H	-0.61836	-5.54178	1.66515	Al	3.56224	-0.51942	-2.69774
H	1.02772	-5.90954	1.11563	Al	-3.63262	0.32670	-2.60664
C	1.75297	-3.77782	4.12835	Al	0.48174	3.64134	2.43224
H	2.49191	-2.98896	4.33534	Al	-1.53566	-1.33963	-0.74154
H	2.23415	-4.75704	4.29134	Al	-1.27054	1.52215	0.66903
H	0.95987	-3.67515	4.89142	Al	-1.44758	-1.11421	2.38030
C	-0.22340	2.04489	-3.86892	O	-1.94928	-0.22093	-2.12129
H	0.61790	1.38177	-4.11889	O	-1.69288	-0.28580	0.78053
H	0.18879	3.06301	-3.74421	O	1.72876	0.26400	0.71290
H	-0.90489	2.07293	-4.73714	O	-0.09351	1.95134	1.98938
C	2.81356	-2.54059	-2.78421	O	0.17376	-1.91013	2.07806
H	2.97252	-2.81779	-3.83748	O	-0.28500	1.66155	-0.90104
H	2.24896	-3.38129	-2.32948	O	0.26971	-1.75944	-0.82846
H	3.78218	-2.63428	-2.25618	O	1.89665	0.06121	-2.18596
C	-4.01212	0.29937	-4.48607	C	-1.82747	-0.05500	3.99146
H	-3.12818	0.62174	-5.06233	H	-1.48307	-0.60403	4.88522
H	-4.86291	0.92350	-4.81055	H	-1.34791	0.93524	3.99821
H	-4.23756	-0.73755	-4.79389	H	-2.91582	0.09918	4.10617

C	-2.86788	2.67304	0.79279	H	-0.11825	-4.51736	0.20863
H	-3.71230	2.32995	0.17654	H	-0.91164	-5.73371	1.23244
H	-3.21978	2.68386	1.84047	H	0.83813	-5.47801	1.35888
H	-2.65382	3.71868	0.51350	C	-0.06616	-3.85009	4.53920
C	-2.69072	-2.93669	-0.83112	H	-0.32825	-2.94600	5.11435
H	-2.67275	-3.32260	-1.86706	H	1.00104	-4.05835	4.73498
H	-2.37041	-3.76274	-0.17933	H	-0.64292	-4.68997	4.96364
H	-3.74334	-2.70877	-0.59146	C	-0.16716	1.76626	-4.12373
C	0.06136	-2.01669	-4.04171	H	0.79246	1.23298	-4.19418
H	0.61673	-1.69252	-4.93926	H	0.04421	2.84700	-4.21884
H	-0.93413	-1.55080	-4.07678	H	-0.77980	1.48012	-4.99655
H	-0.07481	-3.10969	-4.12456	C	2.87445	-2.69275	-2.62786
C	-2.94500	2.50722	-2.65993	H	2.87933	-3.11331	-3.64536
H	-2.48340	3.30830	-2.04650	H	2.42684	-3.45483	-1.95624
H	-2.99219	2.87379	-3.69731	H	3.92123	-2.71122	-2.26355
H	-3.97827	2.53361	-2.25840	C	-3.97323	0.00547	-4.52480
C	2.67215	2.83582	-1.05385	H	-3.08454	0.25242	-5.12997
H	3.73210	2.61954	-0.83564	H	-4.81416	0.60398	-4.91596
H	2.37071	3.69250	-0.43314	H	-4.21216	-1.05482	-4.72138
H	2.62129	3.17041	-2.10632	C	-4.96913	0.08187	-1.17027
C	2.90745	-2.69066	0.83346	H	-4.49593	0.06716	-0.17426
H	3.30742	-2.62440	1.86172	H	-5.51259	-0.87091	-1.29303
H	3.72309	-2.39777	0.15578	H	-5.72838	0.88364	-1.15971
H	2.67926	-3.75355	0.64459	C	3.84885	-0.28647	-4.63699
C	1.96883	0.18606	3.92380	H	4.06913	0.76603	-4.88953
H	1.63404	0.76714	4.80009	H	2.95067	-0.57482	-5.20901
H	1.50531	-0.81005	3.98267	H	4.68894	-0.89247	-5.01892
H	3.06158	0.05448	4.02231	C	4.94347	-0.20693	-1.31785
C	-2.56089	-2.88378	2.61723	H	4.50524	-0.16228	-0.30697
H	-2.58797	-3.93207	2.25648	H	5.46752	0.74899	-1.49309
H	-3.34508	-2.44361	1.96665	H	5.71540	-0.99676	-1.30611
H	-2.95069	-2.88664	3.64669				
C	2.65438	2.95026	2.39725	$(AlOMe)_{10,c}$			
H	2.66265	3.98324	1.99331	Al	-2.021421	0.768091	-2.208272
H	3.41876	2.48670	1.73945	Al	0.734799	2.366455	-2.028350
H	3.07897	2.99802	3.41176	Al	0.741192	-0.824681	-2.080331
C	0.16660	4.95757	0.99152	Al	2.517210	0.796010	0.148818
H	0.14522	4.47507	0.00027	Al	-1.760948	3.147311	-0.050704
H	0.93818	5.74667	0.95564	Al	-1.651606	-1.736734	-0.124850
H	-0.80358	5.46644	1.13037	Al	-3.180817	0.951090	0.181272
C	0.21826	3.99193	4.35633	Al	-0.403657	0.704557	1.879076
H	0.50375	3.11485	4.96115	Al	1.303250	3.102108	0.466440
H	-0.84333	4.20412	4.57744	Al	0.924752	-1.863877	0.364001
H	0.80321	4.85193	4.72566	O	-0.182737	0.769591	-2.087901
C	-0.12598	-4.95797	1.21937	O	-2.580674	-0.407240	-0.881768

O	-0.177319	-2.113527	-1.144437	H	1.463487	2.517292	-4.488138
O	1.903544	-0.690662	-0.636495	H	1.416584	4.148397	-3.779658
O	2.211274	2.236729	-0.940279	H	-0.090519	3.338226	-4.265651
O	-0.097103	3.340052	-0.681537				
O	-2.746806	2.136915	-1.217919	$(AlOMe)_{10,c} \cdot (AlMe_3)$			
O	-1.777495	1.675221	1.126180	Al	-1.802693	0.836323	-2.066345
O	1.169633	1.460153	1.286800	Al	0.890968	2.520447	-1.693131
O	-0.487549	-0.987888	1.154327	Al	0.968355	-0.665635	-2.043224
C	1.925397	4.619629	1.530573	Al	2.647390	0.759445	0.352214
H	1.181848	4.887337	2.301827	Al	-1.650102	3.083069	0.141715
H	2.094559	5.517997	0.914007	Al	-1.540750	-1.693364	-0.222987
H	2.866234	4.386316	2.056676	Al	-3.231044	0.564068	0.755983
C	-2.581801	4.776211	0.673027	Al	-0.341261	0.562192	1.942501
H	-2.691372	5.555281	-0.100674	Al	1.454317	3.040833	0.852266
H	-1.976788	5.211948	1.487368	Al	1.030611	-1.912076	0.293835
H	-3.586342	4.579938	1.085802	Al	-3.096320	3.710981	-2.595913
C	-4.902760	0.756744	1.086567	O	0.033512	0.904619	-1.923573
H	-5.701595	0.438375	0.396393	O	-2.478032	-0.252215	-0.782485
H	-5.219432	1.700897	1.560583	O	-0.034820	-1.979720	-1.259052
H	-4.840402	-0.001461	1.886938	O	2.079532	-0.676382	-0.552576
C	4.284502	0.637597	0.986988	O	2.369271	2.289717	-0.619773
H	5.066731	0.399986	0.245870	O	0.073161	3.405633	-0.266065
H	4.305931	-0.162438	1.747633	O	-2.244670	2.545558	-1.550013
H	4.583738	1.572187	1.491983	O	-1.698889	1.578399	1.155681
C	1.856579	-3.236323	1.398647	O	1.273143	1.332427	1.505597
H	2.594997	-3.785377	0.791109	O	-0.375154	-1.092804	1.136278
H	1.151800	-3.970986	1.822886	C	2.133997	4.431640	2.048271
H	2.401247	-2.784519	2.246334	H	1.404492	4.662018	2.844373
C	-2.722621	-3.243634	0.533244	H	2.345261	5.373529	1.514985
H	-3.264761	-3.746132	-0.286019	H	3.063844	4.110508	2.547106
H	-3.478553	-2.917362	1.268911	C	-2.686727	4.657781	0.720830
H	-2.096816	-4.005771	1.028748	H	-2.480395	5.541241	0.092413
C	-0.513766	0.672544	3.843881	H	-2.436508	4.945000	1.757390
H	-1.461724	0.228958	4.195449	H	-3.774834	4.473869	0.704413
H	-0.453012	1.686761	4.275920	C	-4.832223	1.677291	0.357692
H	0.304108	0.081862	4.292384	H	-4.780054	2.337561	-0.521043
C	-2.628902	0.466368	-4.045682	H	-5.089876	2.309590	1.226280
H	-2.234012	-0.482409	-4.449506	H	-5.693253	1.002234	0.195275
H	-2.275138	1.268452	-4.716154	C	4.398351	0.569982	1.220297
H	-3.727687	0.427771	-4.126367	H	5.202047	0.399554	0.483541
C	1.481054	-1.242654	-3.845013	H	4.418839	-0.280375	1.924232
H	0.678371	-1.351863	-4.594548	H	4.667663	1.472598	1.795760
H	2.066083	-2.177032	-3.847598	C	1.889395	-3.423590	1.190067
H	2.143994	-0.436251	-4.204783	H	2.625167	-3.927683	0.541760
C	0.899466	3.175101	-3.804627	H	1.147780	-4.175147	1.508674

H	2.424897	-3.092538	2.097102	Al	-1.806741	-3.137107	-2.588906
C	-2.508425	-3.375721	0.068808	Al	-3.474093	3.959550	-2.199231
H	-2.765471	-3.843787	-0.897406	O	-0.490170	0.901230	-1.904242
H	-3.440004	-3.249233	0.640822	O	-2.963479	-0.019238	-0.423193
H	-1.880896	-4.099789	0.617596	O	-1.121027	-1.802105	-1.620782
C	-0.548166	0.457591	3.896597	O	1.487398	-0.898047	-0.626225
H	-1.512307	0.009476	4.186603	O	2.058632	2.073796	-0.964476
H	-0.491074	1.452244	4.373414	O	-0.056719	3.430051	-0.345126
H	0.248704	-0.159222	4.348597	O	-2.579917	2.713124	-1.297333
C	-2.365783	0.477974	-3.922110	O	-1.784180	1.769164	1.345932
H	-1.974886	-0.495294	-4.270133	O	1.187492	1.313425	1.337258
H	-1.972018	1.231949	-4.628872	O	-0.673711	-0.996235	1.124552
H	-3.460597	0.447186	-4.045708	C	2.431845	4.312832	1.582945
C	1.778367	-0.933931	-3.807270	H	1.875213	4.645192	2.476422
H	1.006463	-0.970148	-4.595306	H	2.643331	5.209342	0.976531
H	2.357916	-1.869945	-3.868560	H	3.396719	3.911072	1.935399
H	2.461679	-0.106267	-4.067616	C	-2.584013	4.905351	0.909927
C	1.068144	3.503673	-3.382575	H	-2.302380	5.129020	1.954190
H	1.750985	2.983459	-4.076377	H	-3.687282	4.854186	0.901685
H	1.460600	4.523785	-3.236801	H	-2.278763	5.776799	0.306358
H	0.099195	3.600284	-3.902338	C	-4.964206	2.120930	0.994994
C	-3.556190	-0.783531	2.185834	H	-5.045538	2.659629	0.038539
H	-4.432831	-1.403403	1.928518	H	-4.954827	2.878528	1.798690
H	-3.823336	-0.215384	3.096355	H	-5.902387	1.547897	1.115507
H	-2.743659	-1.468548	2.472062	C	4.228659	0.373769	0.518734
C	-2.158219	5.416918	-2.856559	H	4.441517	-0.507852	1.142228
H	-2.775305	6.274158	-2.538301	H	4.576870	1.262291	1.074384
H	-1.906519	5.578738	-3.919025	H	4.850749	0.302443	-0.390498
H	-1.218653	5.437414	-2.283625	C	0.596560	-3.840709	0.263886
C	-4.795045	3.121635	-3.379712	H	0.800398	-3.996090	-0.807993
H	-4.696812	2.997513	-4.472193	H	-0.421553	-4.216295	0.460901
H	-5.598900	3.858067	-3.210261	H	1.286031	-4.501943	0.819234
H	-5.120726	2.157921	-2.961159	C	-3.057807	-3.145897	0.373083
				H	-2.745239	-4.058229	-0.172609
$(AlOMe)_{10,c} \cdot (AlMe_3)_2$				H	-4.124943	-2.992357	0.144400
Al	-2.335201	0.959081	-1.823002	H	-2.983248	-3.409120	1.441474
Al	0.493785	2.447432	-1.843593	C	-0.409906	0.552701	3.914244
Al	0.325683	-0.737650	-2.010448	H	-1.393181	0.274774	4.327234
Al	2.331592	0.549873	0.045303	H	-0.128545	1.523098	4.361196
Al	-1.732348	3.236071	0.281462	H	0.323798	-0.189437	4.270604
Al	-2.009410	-1.502730	0.005168	C	-3.173268	0.662690	-3.588798
Al	-3.427257	0.868203	1.168568	H	-2.808873	-0.267710	-4.057239
Al	-0.417160	0.654210	1.949993	H	-2.932924	1.473110	-4.303139
Al	1.434230	2.960809	0.579096	H	-4.271883	0.583350	-3.540979
Al	0.907173	-1.957167	0.831215	C	1.052888	-1.125570	-3.800711

H	0.258764	-1.231446	-4.562222	Al	-2.53405	-2.04518	-2.99688
H	1.659246	-2.045809	-3.828239	O	-0.83569	0.85819	-2.12123
H	1.703984	-0.304229	-4.150665	O	-3.05650	-0.23679	-0.21061
C	0.532900	3.412105	-3.553857	O	-1.28716	-1.74648	-1.69937
H	1.091791	2.846737	-4.319681	O	1.43033	-0.78304	-0.72428
H	1.010078	4.402357	-3.462963	O	1.69346	1.70544	-1.89251
H	-0.481665	3.578138	-3.955266	O	-0.32600	3.39810	-0.36949
C	-3.668959	-0.506867	2.591834	O	-2.75996	2.56132	-1.37105
H	-4.531371	-1.153624	2.349811	O	-1.89780	1.68161	1.35053
H	-3.923599	0.026412	3.526219	O	1.05880	1.49698	1.01919
H	-2.823789	-1.169355	2.836545	O	-0.58909	-0.98528	1.10372
C	-2.413583	5.545604	-2.666631	C	2.68724	4.12877	0.27171
H	-2.889430	6.472065	-2.303261	H	2.61737	5.23238	0.27510
H	-2.297826	5.650123	-3.759191	H	2.93982	3.82475	-0.75834
H	-1.405492	5.481546	-2.230151	H	3.55283	3.86096	0.90182
C	-5.353672	3.587593	-2.615974	C	-2.94695	4.68246	1.07372
H	-5.606267	3.859276	-3.654865	H	-2.37177	5.61828	0.98120
H	-6.021115	4.170958	-1.957834	H	-3.11099	4.50566	2.14984
H	-5.594089	2.524104	-2.467486	H	-3.93306	4.84877	0.61270
C	2.114739	-1.744289	2.400209	C	-5.05979	1.87555	1.03428
H	2.356558	-0.727324	2.744836	H	-5.05098	2.39866	0.06292
H	3.070397	-2.268042	2.224118	H	-5.16358	2.65262	1.81106
H	1.623163	-2.254797	3.249298	H	-5.98216	1.26632	1.06495
C	-0.563967	-4.523354	-3.211050	C	4.07303	0.90241	0.15794
H	-0.875025	-4.947641	-4.180298	H	4.60030	1.65737	-0.44590
H	-0.508279	-5.353883	-2.487170	H	4.57702	-0.06506	-0.00062
H	0.455835	-4.123496	-3.320634	H	4.21126	1.17212	1.21829
C	-3.703172	-2.938161	-3.063703	C	0.72663	-3.73397	0.18181
H	-4.157837	-2.090119	-2.528898	H	0.14366	-3.83943	-0.74892
H	-4.277870	-3.847443	-2.819386	H	0.20373	-4.32739	0.95151
H	-3.827777	-2.755964	-4.145489	H	1.70330	-4.22282	0.00865
				C	-2.71897	-3.33311	0.73876
$(AlOMe)_{10,c} \cdot (AlMe_3)_3$				H	-2.44698	-4.18807	0.10028
Al	-2.60516	0.74496	-1.65951	H	-3.81916	-3.29392	0.79538
Al	0.01139	2.46492	-1.88019	H	-2.34771	-3.54821	1.75468
Al	0.17501	-0.66671	-2.01951	C	-0.18714	0.62912	3.79191
Al	-2.66842	3.74187	-2.75854	H	-1.15812	0.51088	4.30069
Al	2.15854	0.82650	-0.25991	H	0.27966	1.54824	4.18299
Al	-2.01202	3.14849	0.28733	H	0.44921	-0.21837	4.09600
Al	-1.94230	-1.65185	0.09399	C	-3.85901	0.06628	-3.09698
Al	-3.48876	0.69622	1.35962	H	-4.42437	-0.88701	-3.05269
Al	-0.40141	0.70472	1.83918	H	-3.64874	0.30025	-4.14702
Al	0.98637	3.36633	0.97208	H	-4.66207	0.76567	-2.77917
Al	1.03298	-1.85476	0.76452	C	1.18178	-1.18092	-3.69896
Al	2.38655	0.98659	-3.41897	H	0.74205	-0.95774	-4.67794

H	1.00425	-2.26324	-3.51980	Al	2.676279	0.000000	-1.338393
H	2.28615	-1.19548	-3.80153	Al	0.000000	1.338479	-2.676621
C	-0.24505	3.83579	-3.34762	Al	1.338413	2.676986	0.000000
H	0.80132	4.19617	-3.24627	Al	2.676279	0.000000	1.338393
H	-0.77865	4.80137	-3.23224	Al	0.000000	-1.338479	-2.676621
H	-0.35220	3.49818	-4.38498	Al	1.338413	-2.676986	0.000000
C	-3.56474	-0.58038	2.87944	Al	-2.676279	0.000000	-1.338393
H	-4.39175	-1.29909	2.74219	Al	0.000000	1.338479	2.676621
H	-3.76843	-0.03078	3.81610	Al	-1.338413	-2.676986	0.000000
H	-2.65261	-1.17212	3.05631	Al	0.000000	-1.338479	2.676621
C	-3.04653	5.59884	-2.23069	Al	-2.676279	0.000000	1.338393
H	-4.06291	5.69887	-1.81418	O	0.000000	2.448540	1.269166
H	-2.97713	6.27373	-3.10159	O	1.269092	0.000000	-2.448437
H	-2.35262	5.97064	-1.46111	O	2.448006	1.269228	0.000000
C	-3.11365	3.00418	-4.53473	O	0.000000	2.448540	-1.269166
H	-2.47972	2.14536	-4.80587	O	2.448006	-1.269228	0.000000
H	-2.94140	3.78684	-5.29409	O	-1.269092	0.000000	-2.448437
H	-4.16492	2.68496	-4.62470	O	0.000000	-2.448540	-1.269166
C	2.37191	-1.51486	2.19177	O	-2.448006	1.269228	0.000000
H	2.46741	-0.46828	2.52188	O	1.269092	0.000000	2.448437
H	3.37582	-1.84227	1.86886	O	-2.448006	-1.269228	0.000000
H	2.11477	-2.10467	3.09005	O	0.000000	-2.448540	1.269166
C	-1.90916	-1.79001	-4.85209	O	-1.269092	0.000000	2.448437
H	-1.50573	-0.78012	-5.02619	C	-2.200449	-4.438598	0.000000
H	-2.76824	-1.91788	-5.53361	C	2.200449	-4.438598	0.000000
H	-1.13711	-2.51529	-5.15717	C	4.438054	0.000000	2.200161
C	-3.89279	-3.37217	-2.48412	C	0.000000	-2.200624	4.438159
H	-4.45018	-3.08100	-1.58050	C	-4.438054	0.000000	2.200161
H	-3.43582	-4.35307	-2.27077	C	0.000000	2.200624	4.438159
H	-4.62352	-3.51695	-3.29889	C	-2.200449	4.438598	0.000000
C	1.62528	1.67504	-5.10534	C	2.200449	4.438598	0.000000
H	1.84218	2.74169	-5.27968	C	4.438054	0.000000	-2.200161
H	0.53321	1.54334	-5.16001	C	0.000000	2.200624	-4.438159
H	2.06261	1.10874	-5.94611	C	0.000000	-2.200624	-4.438159
C	4.25736	0.40806	-3.23124	C	-4.438054	0.000000	-2.200161
H	4.38980	-0.35039	-2.44435	H	-1.451958	-5.249193	0.000000
H	4.91483	1.25374	-2.96849	H	-2.842053	-4.584864	0.886099
H	4.63000	-0.01999	-4.17818	H	-2.842053	-4.584864	-0.886099
C	0.23019	4.12421	2.64515	H	2.842053	-4.584864	-0.886099
H	-0.68038	3.63502	3.02592	H	2.842053	-4.584864	0.886099
H	-0.01157	5.19349	2.51276	H	1.451958	-5.249193	0.000000
H	0.98092	4.06192	3.45348	H	5.248564	0.000000	1.451583
				H	4.584430	0.886093	2.841765
$(AlOMe)_{12,c}$				H	4.584430	-0.886093	2.841765
Al	-1.338413	2.676986	0.000000	H	0.886097	-2.842253	4.584385

H	0.000000	-1.452250	5.248856
H	-0.886097	-2.842253	4.584385
H	-5.248564	0.000000	1.451583
H	-4.584430	-0.886093	2.841765
H	-4.584430	0.886093	2.841765
H	0.886097	2.842253	4.584385
H	-0.886097	2.842253	4.584385
H	0.000000	1.452250	5.248856
H	-1.451958	5.249193	0.000000
H	-2.842053	4.584864	-0.886099
H	-2.842053	4.584864	0.886099
H	2.842053	4.584864	0.886099
H	2.842053	4.584864	-0.886099
H	1.451958	5.249193	0.000000
H	5.248564	0.000000	-1.451583
H	4.584430	-0.886093	-2.841765
H	4.584430	0.886093	-2.841765
H	0.886097	2.842253	-4.584385
H	0.000000	1.452250	-5.248856
H	-0.886097	2.842253	-4.584385
H	-0.886097	-2.842253	-4.584385
H	0.000000	-1.452250	-5.248856
H	0.886097	-2.842253	-4.584385
H	-5.248564	0.000000	-1.451583
H	-4.584430	0.886093	-2.841765
H	-4.584430	-0.886093	-2.841765

$(AlOMe)_{14,c}$

Al	-2.558925	-2.993239	0.000000
Al	-2.935063	-0.917147	1.606371
Al	-2.935063	-0.917147	-1.606371
Al	0.804410	3.021798	-1.316781
Al	0.804410	3.021798	1.316781
Al	-0.735557	0.668538	-2.882844
Al	1.883743	0.278990	-2.775630
Al	-1.956951	1.694919	0.000000
Al	2.540475	-1.276220	0.000000
Al	3.273087	1.316531	0.000000
Al	1.883743	0.278990	2.775630
Al	-0.735557	0.668538	2.882844
Al	0.079566	-2.225382	1.669231
Al	0.079566	-2.225382	-1.669231
O	2.813640	0.040164	1.266570
O	0.383934	-0.796489	2.750561
O	0.793284	-1.795332	0.000000
O	0.383934	-0.796489	-2.750561
O	-1.727247	-2.342380	-1.490999
O	-1.727247	-2.342380	1.490999
O	2.813640	0.040164	-1.266570
O	-1.878419	0.573813	1.467588
O	-1.878419	0.573813	-1.467588
O	-0.483334	2.745586	0.000000
O	2.066617	2.654614	0.000000
O	0.731042	1.717628	2.530787
O	-3.626742	-1.420038	0.000000
O	0.731042	1.717628	-2.530787
C	0.906667	-3.876292	-2.355300
H	0.400281	-4.223769	-3.272052
H	1.971696	-3.736712	-2.610582
H	0.865858	-4.701601	-1.622881
C	0.906667	-3.876292	2.355300
H	0.865858	-4.701601	1.622881
H	1.971696	-3.736712	2.610582
H	0.400281	-4.223769	3.272052
C	0.911231	4.835041	2.057725
H	0.952719	5.598569	1.263387
H	0.048445	5.076350	2.702135
H	1.817451	4.957694	2.676473
C	0.911231	4.835041	-2.057725
H	1.817451	4.957694	-2.676473
H	0.048445	5.076350	-2.702135
H	0.952719	5.598569	-1.263387
C	-3.675052	2.657639	0.000000
H	-3.787852	3.303791	-0.887750
H	-4.534003	1.961720	0.000000
H	-3.787852	3.303791	0.887750
C	-1.550777	1.040668	4.632379
H	-0.858302	1.652321	5.236056
H	-2.503004	1.590374	4.554715
H	-1.752766	0.120271	5.204755
C	2.929907	0.297072	4.433117
H	2.292691	0.495172	5.311773
H	3.720918	1.066791	4.420384
H	3.429354	-0.672488	4.603164
C	5.155936	1.869485	0.000000
H	5.412401	2.475287	0.886088
H	5.822771	0.990325	0.000000
H	5.412401	2.475287	-0.886088
C	3.850123	-2.736586	0.000000
H	3.738049	-3.386171	-0.884265

H	4.883105	-2.349471	0.000000
H	3.738049	-3.386171	0.884265
C	2.929907	0.297072	-4.433117
H	2.292691	0.495172	-5.311773
H	3.720918	1.066791	-4.420384
H	3.429354	-0.672488	-4.603164
C	-1.550777	1.040668	-4.632379
H	-0.858302	1.652321	-5.236056
H	-2.503004	1.590374	-4.554715
H	-1.752766	0.120271	-5.204755
C	-4.177342	-0.886024	-3.119353
H	-3.666944	-0.895956	-4.095128
H	-4.797381	0.026562	-3.090378
H	-4.861574	-1.750779	-3.090782
C	-4.177342	-0.886024	3.119353
H	-3.666944	-0.895956	4.095128
H	-4.861574	-1.750779	3.090782
H	-4.797381	0.026562	3.090378
C	-3.270946	-4.812430	0.000000
H	-3.892419	-5.002322	-0.891171
H	-3.892419	-5.002322	0.891171
H	-2.461951	-5.563183	0.000000

$(AlOMe)_{10,t} \cdot (AlMe_3)$

Al	-1.93049	-3.92924	0.26822
Al	-2.76894	-1.38920	1.80354
Al	-3.01699	-1.42877	-1.28009
Al	0.38736	2.85003	-1.20148
Al	0.52278	2.88117	1.42562
Al	-1.03249	0.39894	-2.68628
Al	1.60829	0.19395	-2.71504
Al	-2.19845	1.30940	0.22012
Al	2.53997	-1.26723	0.02365
Al	3.04269	1.37744	-0.00967
Al	1.88292	0.23619	2.83865
Al	-0.74776	0.46112	3.06834
Al	-5.49893	-1.27348	1.10856
Al	0.27085	-2.39565	1.81589
Al	0.06298	-2.42913	-1.52081
O	2.74691	0.07393	1.28425
O	0.44229	-0.91967	2.87230
O	0.86255	-1.95966	0.10581
O	0.18855	-0.97166	-2.61013
O	-1.71179	-2.69766	-1.13442
O	-1.53164	-2.68184	1.64237
O	2.63089	0.06150	-1.24951
O	-1.98267	0.25333	1.74423
O	-2.09178	0.17616	-1.23729
O	-0.78249	2.44364	0.18250
O	1.74927	2.62888	0.05316
O	0.62450	1.60754	2.67530
O	-3.85716	-1.33846	0.34534
O	0.37952	1.55790	-2.42291
C	1.04099	-3.89226	-2.42211
H	0.38354	-4.75012	-2.63895
H	1.45089	-3.54409	-3.38628
H	1.88145	-4.28265	-1.82578
C	1.38744	-3.79082	2.64833
H	1.62848	-4.64125	1.99452
H	2.34538	-3.35120	2.98242
H	0.90025	-4.19446	3.55312
C	0.44796	4.70805	2.13959
H	0.36498	5.45674	1.33474
H	-0.41630	4.85264	2.81126
H	1.35109	4.95472	2.72459
C	0.23681	4.66293	-1.93320
H	-0.69553	4.78423	-2.51154
H	0.23665	5.43369	-1.14523
H	1.07038	4.89381	-2.61898
C	-3.86828	2.34421	0.08605
H	-3.72864	3.11154	-0.69731
H	-4.73512	1.73550	-0.21368
H	-4.14934	2.88096	1.00684
C	-1.59766	0.69468	4.82335
H	-0.83954	0.83293	5.61263
H	-2.25878	1.57850	4.84506
H	-2.21494	-0.17267	5.11364
C	2.98255	0.30406	4.45967
H	2.36326	0.44210	5.36269
H	3.71133	1.13237	4.43300
H	3.55869	-0.62686	4.59894
C	4.87068	2.08474	-0.10007
H	5.11503	2.72752	0.76333
H	5.61576	1.27132	-0.12496
H	5.02370	2.69701	-1.00552
C	3.97893	-2.59582	-0.03147
H	3.88505	-3.33245	0.78390
H	3.96858	-3.16202	-0.97797
H	4.97070	-2.12162	0.05777
C	2.58720	0.26371	-4.41136

H	1.90295	0.39029	-5.26724
H	3.31137	1.09625	-4.44326
H	3.15932	-0.66434	-4.58373
C	-1.95879	0.74628	-4.37857
H	-1.23378	0.80067	-5.20880
H	-2.49077	1.71338	-4.35006
H	-2.70287	-0.02443	-4.63291
C	-4.32531	-1.67115	-2.72875
H	-3.86393	-1.97596	-3.68268
H	-4.90565	-0.75367	-2.92851
H	-5.04313	-2.46463	-2.45534
C	-4.08789	-1.73748	3.28153
H	-3.54371	-2.44329	3.93665
H	-5.03552	-2.29357	3.09896
H	-4.34794	-0.85388	3.88095
C	-3.80220	-4.57907	0.42863
H	-4.23274	-4.36717	1.42275
H	-3.82155	-5.67689	0.30563
H	-4.49840	-4.16104	-0.31614
C	-0.53190	-5.33384	0.19959
H	-0.79461	-6.04066	-0.60856
H	-0.54573	-5.90186	1.14672
H	0.50845	-5.02939	0.02242
C	-6.76734	-2.70678	0.67147
H	-6.50374	-3.66821	1.13708
H	-6.79499	-2.88654	-0.41676
H	-7.78682	-2.43599	0.99299
C	-6.05499	0.43718	1.90535
H	-5.19769	1.03621	2.24464
H	-6.69621	0.23250	2.78030
H	-6.63993	1.06507	1.21313

$(AlOMe)_{16,c} - T_d$

Al	0.92657	0.92657	-3.14543
Al	-0.92657	-0.92657	-3.14543
Al	-2.00908	2.00908	-2.00908
Al	-0.92657	-3.14543	-0.92657
Al	0.92657	-3.14543	0.92657
Al	-2.00908	-2.00908	2.00908
Al	0.92657	3.14543	-0.92657
Al	-0.92657	3.14543	0.92657
Al	2.00908	2.00908	2.00908
Al	3.14543	0.92657	-0.92657
Al	-0.92657	0.92657	3.14543
Al	-3.14543	0.92657	0.92657
Al	-3.14543	-0.92657	-0.92657
Al	3.14543	-0.92657	0.92657
Al	0.92657	-0.92657	3.14543
Al	2.00908	-2.00908	-2.00908
O	0.90939	-0.90939	-2.97813
O	0.90939	-2.97813	-0.90939
O	2.97813	-0.90939	-0.90939
O	-0.90939	2.97813	-0.90939
O	2.97813	0.90939	0.90939
O	0.90939	2.97813	0.90939
O	-0.90939	0.90939	-2.97813
O	-0.90939	-2.97813	0.90939
O	-2.97813	-0.90939	0.90939
O	-1.64514	1.64514	1.64514
O	0.90939	0.90939	2.97813
O	-0.90939	-0.90939	2.97813
O	1.64514	-1.64514	1.64514
C	1.69248	-1.69248	4.78090
H	1.25238	-1.25238	5.69139
H	2.78333	-1.53127	4.83112
H	1.53127	-2.78333	4.83112
C	-1.69248	1.69248	4.78090
H	-1.25238	1.25238	5.69139
H	-2.78333	1.53127	4.83112
H	-1.53127	2.78333	4.83112
O	-2.97813	0.90939	-0.90939
C	-4.78090	1.69248	1.69248
H	-5.69139	1.25238	1.25238
H	-4.83112	2.78333	1.53127
H	-4.83112	1.53127	2.78333
O	-1.64514	-1.64514	-1.64514
C	-4.78090	-1.69248	-1.69248
H	-5.69139	-1.25238	-1.25238
H	-4.83112	-2.78333	-1.53127
H	-4.83112	-1.53127	-2.78333
C	-3.14396	-3.14396	3.14396
H	-2.54553	-3.79993	3.79993
H	-3.79993	-3.79993	2.54553
H	-3.79993	-2.54553	3.79993
C	1.69248	-4.78090	1.69248
H	1.25238	-5.69139	1.25238
H	1.53127	-4.83112	2.78333
H	2.78333	-4.83112	1.53127
C	-1.69248	-4.78090	-1.69248
H	-1.25238	-5.69139	-1.25238

H	-1.53127	-4.83112	-2.78333
H	-2.78333	-4.83112	-1.53127
C	3.14396	-3.14396	-3.14396
H	3.79993	-3.79993	-2.54553
H	3.79993	-2.54553	-3.79993
H	2.54553	-3.79993	-3.79993
C	4.78090	-1.69248	1.69248
H	5.69139	-1.25238	1.25238
H	4.83112	-2.78333	1.53127
H	4.83112	-1.53127	2.78333
O	1.64514	1.64514	-1.64514
C	4.78090	1.69248	-1.69248
H	5.69139	1.25238	-1.25238
H	4.83112	2.78333	-1.53127
H	4.83112	1.53127	-2.78333
C	3.14396	3.14396	3.14396
H	3.79993	2.54553	3.79993
H	2.54553	3.79993	3.79993
H	3.79993	3.79993	2.54553
C	-1.69248	4.78090	1.69248
H	-1.25238	5.69139	1.25238
H	-1.53127	4.83112	2.78333
H	-2.78333	4.83112	1.53127
C	1.69248	4.78090	-1.69248
H	1.25238	5.69139	-1.25238
H	1.53127	4.83112	-2.78333
H	2.78333	4.83112	-1.53127
C	-3.14396	3.14396	-3.14396
H	-2.54553	3.79993	-3.79993
H	-3.79993	3.79993	-2.54553
H	-3.79993	2.54553	-3.79993
C	-1.69248	-1.69248	-4.78090
H	-1.25238	-1.25238	-5.69139
H	-2.78333	-1.53127	-4.83112
H	-1.53127	-2.78333	-4.83112
C	1.69248	1.69248	-4.78090
H	1.25238	1.25238	-5.69139
H	2.78333	1.53127	-4.83112
H	1.53127	2.78333	-4.83112

$(AlOMe)_{16,c} - C_{3v}$

AL	2.521277	1.332032	1.811858
AL	2.521277	-1.332032	1.811858
AL	0.000000	0.000000	3.500452
AL	-0.107065	2.849506	1.811858
AL	-0.107065	-2.849506	1.811858
AL	-2.414212	1.517474	1.811858
AL	-2.414212	-1.517474	1.811858
AL	3.565046	0.000000	-0.953011
AL	1.802063	0.000000	-2.874009
AL	-0.901031	-1.560632	-2.874009
AL	-0.901031	1.560632	-2.874009
AL	-1.782523	-3.087421	-0.953011
AL	1.550515	-2.685571	-0.981490
AL	-1.782523	3.087421	-0.953011
AL	1.550515	2.685571	-0.981490
AL	-3.101030	0.000000	-0.981490
O	1.665339	0.000000	2.760334
O	-0.832670	1.442226	2.760334
O	-0.832670	-1.442226	2.760334
O	1.285830	-2.227123	0.806709
O	1.285830	2.227123	0.806709
O	3.314853	0.000000	0.813387
O	2.455834	1.288070	-1.730797
O	2.455834	-1.288070	-1.730797
O	0.000000	0.000000	-2.790034
O	-2.343418	1.482780	-1.730797
O	-2.343418	-1.482780	-1.730797
O	-2.571660	0.000000	0.806709
O	-1.657427	-2.870747	0.813387
O	-0.112416	-2.770850	-1.730797
O	-0.112416	2.770850	-1.730797
O	-1.657427	2.870747	0.813387
C	2.457450	0.000000	-4.720252
H	3.558783	0.000000	-4.774953
H	2.099754	0.885934	-5.273492
H	2.099754	-0.885934	-5.273492
C	5.419523	0.000000	-1.584369
H	5.973433	0.887998	-1.231901
H	5.467886	0.000000	-2.686429
H	5.973433	-0.887998	-1.231901
C	3.738707	-2.509271	2.798517
H	4.160780	-3.297574	2.150442
H	3.229298	-3.022201	3.632902
H	4.581034	-1.942103	3.230422
C	-1.228725	2.128214	-4.720252
H	-1.817118	1.375473	-5.273492
H	-0.282636	2.261407	-5.273492
H	-1.779391	3.081996	-4.774953
C	-1.228725	-2.128214	-4.720252

H	-1.817118	-1.375473	-5.273492
H	-1.779391	-3.081996	-4.774953
H	-0.282636	-2.261407	-5.273492
C	2.532571	-4.386542	-1.066878
H	2.201149	-5.355481	-0.649217
H	3.537408	-4.583991	-0.649217
H	2.563327	-4.439813	-2.167582
C	0.303739	-4.492451	2.798517
H	1.002654	-4.307755	3.632902
H	0.775393	-5.252128	2.150442
H	-0.608607	-4.938343	3.230422
C	-4.042446	-1.983179	2.798517
H	-4.231952	-1.285554	3.632902
H	-3.972427	-2.996241	3.230422
H	-4.936172	-1.954554	2.150442
C	-4.042446	1.983179	2.798517
H	-4.231952	1.285554	3.632902
H	-4.936172	1.954554	2.150442
H	-3.972427	2.996241	3.230422
C	-2.709761	4.693444	-1.584369
H	-2.733943	4.735328	-2.686429
H	-2.217688	5.617144	-1.231901
H	-3.755746	4.729146	-1.231901
C	-2.709761	-4.693444	-1.584369
H	-2.217688	-5.617144	-1.231901
H	-2.733943	-4.735328	-2.686429
H	-3.755746	-4.729146	-1.231901
C	-5.065142	0.000000	-1.066878
H	-5.126655	0.000000	-2.167582
H	-5.738557	0.771490	-0.649217
H	-5.738557	-0.771490	-0.649217
C	0.000000	0.000000	5.463968
H	0.512484	0.887648	5.873576
H	0.512484	-0.887648	5.873576
H	-1.024968	0.000000	5.873576
C	3.738707	2.509271	2.798517
H	4.160780	3.297574	2.150442
H	4.581034	1.942103	3.230422
H	3.229298	3.022201	3.632902
C	2.532571	4.386542	-1.066878
H	2.563327	4.439813	-2.167582
H	3.537408	4.583991	-0.649217
H	2.201149	5.355481	-0.649217
C	0.303739	4.492451	2.798517
H	-0.608607	4.938343	3.230422
H	0.775393	5.252128	2.150442
H	1.002654	4.307755	3.632902

$(AlOMe)_{18,c}$

Al	1.839609	-0.551399	3.833973
Al	-2.800121	0.243130	2.310026
Al	-2.889244	0.226552	-0.735171
Al	-1.839609	0.551399	-3.833973
Al	0.435960	-1.813715	-3.865945
Al	1.342168	1.345273	-3.859885
Al	-1.187515	2.588394	-2.259609
Al	-1.249201	2.598427	0.775184
Al	-0.435960	1.813715	3.865945
Al	-1.342168	-1.345273	3.859885
Al	-1.634516	-2.394018	0.752579
Al	-1.642375	-2.294945	-2.286124
Al	1.249201	-2.598427	-0.775184
Al	1.187515	-2.588394	2.259609
Al	1.642375	2.294945	2.286124
Al	1.634516	2.394018	-0.752579
Al	2.889244	-0.226552	0.735171
Al	2.800121	-0.243130	-2.310026
O	-2.242793	1.043574	0.779593
O	-2.397390	1.189354	-2.183331
O	-1.289474	-1.148420	-3.690184
O	-2.047803	-1.418027	-0.752779
O	-2.197558	-1.502905	2.218498
O	-1.627975	0.487879	3.714375
O	0.397905	-1.711837	3.683828
O	0.209362	-2.479264	0.740306
O	0.175127	-2.639416	-2.221814
O	1.627975	-0.487879	-3.714375
O	-0.397905	1.711837	-3.683828
O	-0.209362	2.479264	-0.740306
O	-0.175127	2.639416	2.221814
O	1.289474	1.148420	3.690184
O	2.397390	-1.189354	2.183331
O	2.242793	-1.043574	-0.779593
O	2.197558	1.502905	-2.218498
O	2.047803	1.418027	0.752779
C	1.797201	-4.368662	2.810826
H	0.934908	-5.043726	2.955102
H	2.321712	-4.306252	3.779861
H	2.472270	-4.856275	2.092036
C	2.501859	-4.120529	-0.712520

H	2.008408	-5.069153	-0.445026
H	3.325121	-3.966748	0.005586
H	2.971029	-4.266313	-1.702316
C	0.749575	-3.065514	-5.342186
H	1.722388	-3.574706	-5.224243
H	0.764482	-2.572517	-6.328880
H	-0.024866	-3.850325	-5.375765
C	2.268796	2.200747	-5.360667
H	3.336647	1.922898	-5.371726
H	2.217943	3.301689	-5.305816
H	1.844424	1.907165	-6.336126
C	-1.797201	4.368662	-2.810826
H	-2.472270	4.856275	-2.092036
H	-0.934908	5.043726	-2.955102
H	-2.321712	4.306252	-3.779861
C	2.336971	4.235967	-0.721445
H	2.241047	4.684996	-1.726954
H	3.404312	4.281480	-0.449874
H	1.792194	4.897299	-0.027162
C	-2.501859	4.120529	0.712520
H	-2.971029	4.266313	1.702316
H	-2.008408	5.069153	0.445026
H	-3.325121	3.966748	-0.005586
C	2.848472	3.746159	2.819744
H	3.873582	3.368977	2.981553
H	2.513750	4.192031	3.772127
H	2.916488	4.554698	2.076307
C	3.039186	-0.895378	5.345718
H	2.562475	-0.640117	6.308177
H	3.962649	-0.294567	5.278827
H	3.339454	-1.955202	5.399132
C	-2.268796	-2.200747	5.360667
H	-3.336647	-1.922898	5.371726
H	-1.844424	-1.907165	6.336126
H	-2.217943	-3.301689	5.305816
C	-4.657473	0.604627	2.826842
H	-4.891315	0.149954	3.804379
H	-4.827314	1.691619	2.925264
H	-5.392594	0.231959	2.097280
C	-4.835974	-0.082234	-0.716651
H	-5.410098	0.820963	-0.452858
H	-5.143498	-0.882560	-0.023044
H	-5.168637	-0.392685	-1.724206
C	4.657473	-0.604627	-2.826842
H	5.392594	-0.231959	-2.097280
H	4.891315	-0.149954	-3.804379
H	4.827314	-1.691619	-2.925264
C	-2.336971	-4.235967	0.721445
H	-2.241047	-4.684996	1.726954
H	-1.792194	-4.897299	0.027162
H	-3.404312	-4.281480	0.449874
C	-0.749575	3.065514	5.342186
H	-1.722388	3.574706	5.224243
H	0.024866	3.850325	5.375765
H	-0.764482	2.572517	6.328880
C	-3.039186	0.895378	-5.345718
H	-3.962649	0.294567	-5.278827
H	-2.562475	0.640117	-6.308177
H	-3.339454	1.955202	-5.399132
C	4.835974	0.082234	0.716651
H	5.410098	-0.820963	0.452858
H	5.168637	0.392685	1.724206
H	5.143498	0.882560	0.023044
C	-2.848472	-3.746159	-2.819744
H	-3.873582	-3.368977	-2.981553
H	-2.916488	-4.554698	-2.076307
H	-2.513750	-4.192031	-3.772127

$(AlOMe)_{20,c}$

Al	0.65396	1.99539	4.55398
Al	-1.17556	0.08224	4.47969
Al	1.68849	-0.57929	2.97903
Al	-2.54804	0.42923	1.62089
Al	-1.24713	2.96650	2.99713
Al	2.73183	-0.18532	0.00762
Al	1.70603	2.37834	-1.55685
Al	1.70033	2.36213	1.57742
Al	-1.24173	2.97160	-2.99357
Al	0.67261	2.01330	-4.54217
Al	-1.15192	0.09359	-4.48740
Al	-1.00583	2.86748	0.00156
Al	-2.53983	0.43017	-1.63734
Al	-1.00938	-4.15460	-0.00978
Al	1.77403	-3.09253	1.32074
Al	-1.02657	-2.33106	2.70052
Al	1.71070	-0.56125	-2.97350
Al	-0.99861	-2.32141	-2.71127
Al	-2.81262	-2.20335	-0.01519
Al	1.78753	-3.08158	-1.31146
O	-1.70422	-0.62318	2.88370

O	-1.66791	2.02861	1.48835	H	-2.18904	-3.49921	4.73604
O	-1.22811	1.90902	4.48509	H	-0.45329	-3.29108	5.06618
O	0.62003	2.88723	2.95746	C	-1.60047	-6.02377	-0.01196
O	0.69278	0.18489	4.29423	H	-1.19252	-6.58549	-0.87048
O	1.89616	0.52187	1.51654	H	-2.70038	-6.09481	-0.06709
O	1.91967	0.53876	-1.50826	H	-1.28397	-6.55752	0.90040
O	0.62710	2.89711	-2.94190	C	-4.73730	-2.57378	-0.03041
O	-1.68663	-0.61850	-2.89672	H	-5.22627	-2.14950	-0.92354
O	-1.66210	2.02913	-1.48810	H	-5.24421	-2.13560	0.84578
O	0.81686	2.69432	0.01011	H	-4.94123	-3.65805	-0.02435
O	-2.43555	-0.41426	-0.00838	C	-4.38708	0.76936	-2.23875
O	-1.80670	-3.06463	1.25818	H	-4.40707	1.36376	-3.17139
O	0.75997	-2.04334	2.37740	H	-4.96653	1.33457	-1.48781
O	2.48937	-1.99809	0.01092	H	-4.94330	-0.16141	-2.44326
O	0.76130	-3.89599	-0.00420	C	-1.90723	-0.65011	-6.13594
O	0.78286	-2.02484	-2.36989	H	-3.00330	-0.74621	-6.04539
O	0.71522	0.20153	-4.28916	H	-1.51693	-1.64179	-6.40687
O	-1.20968	1.92045	-4.48514	H	-1.71114	0.03355	-6.97988
O	-1.79497	-3.06140	-1.28208	C	1.74930	2.74091	-6.00130
C	-1.39156	4.80628	0.00188	H	1.55608	3.81247	-6.17267
H	-2.46708	5.04683	0.00232	H	1.56555	2.20753	-6.94865
H	-0.94780	5.29974	-0.87945	H	2.82510	2.63774	-5.77560
H	-0.94764	5.29749	0.88435	C	-2.18976	4.66136	-3.29553
C	3.50065	-1.07163	-3.63860	H	-2.94007	4.86288	-2.51585
H	3.45043	-1.85040	-4.41768	H	-2.71140	4.62469	-4.26691
H	4.17761	-1.43945	-2.84937	H	-1.51041	5.52941	-3.32078
H	3.99906	-0.19221	-4.08579	C	3.41527	3.33643	-1.77368
C	-1.12885	-3.49426	-4.29267	H	3.95051	2.97806	-2.67198
H	-0.92424	-4.53167	-3.96709	H	4.10797	3.23409	-0.92598
H	-0.39042	-3.25773	-5.07629	H	3.23111	4.41517	-1.91802
H	-2.12540	-3.49730	-4.76314	C	4.67989	0.13574	-0.00013
C	2.97412	-4.36563	-2.20131	H	5.10546	0.05163	1.01351
H	3.71140	-3.88835	-2.86481	H	4.97606	1.11623	-0.40233
H	2.39359	-5.07500	-2.81741	H	5.17490	-0.62916	-0.62206
H	3.52837	-4.96365	-1.45798	C	3.45075	3.23783	1.83052
C	2.95229	-4.38695	2.20767	H	4.28353	2.68479	1.36913
H	2.36714	-5.09691	2.81808	H	3.67234	3.30854	2.91164
H	3.69013	-3.91669	2.87518	H	3.47053	4.26631	1.43314
H	3.50553	-4.98311	1.46243	C	-2.17923	4.66404	3.30477
C	3.47671	-1.09131	3.64965	H	-2.92985	4.87679	2.52831
H	4.15386	-1.46922	2.86528	H	-1.48991	5.52418	3.33087
H	3.42076	-1.86391	4.43457	H	-2.69821	4.62995	4.27774
H	3.97704	-0.21027	4.09144	C	-4.40157	0.76387	2.20440
C	-1.18830	-3.51053	4.27457	H	-4.97400	1.33069	1.44930
H	-0.99886	-4.54924	3.94415	H	-4.43334	1.35400	3.13926

H	-4.95777	-0.16924	2.39821
C	-1.94352	-0.66782	6.11991
H	-3.03738	-0.77524	6.01633
H	-1.76418	0.01761	6.96605
H	-1.54689	-1.65576	6.39529
C	1.72237	2.71111	6.02522
H	1.54641	3.78659	6.19024
H	2.79926	2.58590	5.81672
H	1.51411	2.18458	6.97145

$(AlOMe)_{20,t} \cdot (AlMe_3)$

Al	2.01600	1.35423	4.34480
Al	-0.47037	-0.42280	4.14220
Al	2.20454	-1.14646	2.52312
Al	-2.09972	0.09835	1.49428
Al	-0.57035	2.45699	2.99290
Al	3.06387	-0.60818	-0.47352
Al	1.97466	2.06326	-1.79969
Al	2.18460	1.89487	1.31974
Al	-1.03690	2.84149	-3.02262
Al	0.76237	1.92952	-4.72560
Al	-1.10041	0.05328	-4.68743
Al	-0.61968	2.55938	-0.06297
Al	-2.29534	0.24291	-1.73920
Al	-0.82324	-4.46959	-0.48908
Al	2.06783	-3.55210	0.72472
Al	-0.61366	-2.79560	2.30854
Al	1.82331	-0.77016	-3.39160
Al	-0.91859	-2.47228	-3.07080
Al	-2.29521	1.03781	5.64252
Al	-2.54031	-2.45355	-0.25666
Al	1.92097	-3.39068	-1.89786
O	-1.24406	-1.10069	2.65270
O	-1.16494	1.67938	1.43398
O	-1.20409	1.24055	4.21169
O	1.24399	2.22137	2.87888
O	1.31859	-0.36065	3.92780
O	2.41852	0.05416	1.14066
O	2.14865	0.21772	-1.87641
O	0.82640	2.71028	-3.08109
O	-1.56103	-0.74830	-3.11349
O	-1.40385	1.82176	-1.55597
O	1.18797	2.30436	-0.17181
O	-2.07021	-0.69576	-0.17951
O	-1.51504	-3.45516	0.90346
O	1.15002	-2.52144	1.88841
O	2.75038	-2.41051	-0.56322
O	0.95198	-4.25229	-0.57778
O	0.89031	-2.25447	-2.84217
O	0.77207	0.10350	-4.59337
O	-1.11967	1.87250	-4.57156
O	-1.64421	-3.27405	-1.63363
C	-0.94844	4.50752	0.04058
H	-2.01511	4.77111	0.13113
H	-0.55562	5.04053	-0.84150
H	-0.43097	4.93768	0.91447
C	3.53770	-1.27238	-4.23650
H	3.39105	-1.97066	-5.07758
H	4.25979	-1.73782	-3.54566
H	4.03193	-0.37079	-4.64154
C	-1.22372	-3.56287	-4.68662
H	-1.06332	-4.62473	-4.42135
H	-0.53035	-3.33332	-5.51196
H	-2.24957	-3.48399	-5.08170
C	3.02001	-4.64747	-2.92985
H	3.71026	-4.14439	-3.62429
H	2.38872	-5.32405	-3.53235
H	3.62365	-5.28161	-2.25831
C	3.25309	-4.94506	1.44625
H	2.82438	-5.42595	2.34237
H	4.24111	-4.55613	1.73544
H	3.41234	-5.73596	0.69440
C	3.93082	-1.95859	3.05290
H	4.58565	-2.17722	2.19197
H	3.78169	-2.90829	3.59257
H	4.50172	-1.28826	3.71325
C	-0.67769	-3.95442	3.91009
H	-0.32953	-4.96689	3.63435
H	-1.69325	-4.06843	4.32531
H	-0.02146	-3.62014	4.73230
C	-1.44530	-6.32592	-0.59340
H	-1.14904	-6.80011	-1.54523
H	-2.54446	-6.38792	-0.52497
H	-1.03005	-6.95011	0.21666
C	-4.47816	-2.73571	-0.20959
H	-4.95923	-2.32561	-1.11319
H	-4.94705	-2.23380	0.65305
H	-4.73454	-3.80727	-0.15644
C	-4.17018	0.62763	-2.21179
H	-4.22163	1.26237	-3.11633

H	-4.70040	1.17142	-1.41189
H	-4.75469	-0.28183	-2.42853
C	-1.97833	-0.58847	-6.31870
H	-3.06543	-0.69188	-6.15330
H	-1.61349	-1.56200	-6.67802
H	-1.84310	0.14608	-7.13113
C	1.75203	2.70214	-6.22093
H	1.58001	3.78544	-6.32519
H	1.47668	2.22163	-7.17450
H	2.83692	2.55470	-6.08473
C	-1.96835	4.55768	-3.19616
H	-2.66450	4.73761	-2.36269
H	-2.54915	4.56868	-4.13413
H	-1.27523	5.41438	-3.22792
C	3.71386	2.90978	-2.18074
H	4.00549	2.68509	-3.22434
H	4.53696	2.56535	-1.53815
H	3.65876	4.00837	-2.09471
C	5.01071	-0.33443	-0.62228
H	5.33753	0.69137	-0.39499
H	5.36935	-0.56977	-1.63796
H	5.54394	-1.00429	0.07340
C	3.84142	2.97938	1.31378
H	4.75537	2.39276	1.12814
H	3.97444	3.47705	2.28812
H	3.79909	3.76724	0.54426
C	-1.19651	4.24965	3.51290
H	-2.12484	4.53832	2.99262
H	-0.45266	5.03518	3.30222
H	-1.39933	4.28590	4.59758
C	-3.96858	0.54674	1.94188
H	-4.02756	1.31315	2.73177
H	-4.59990	-0.29864	2.25845
H	-4.44010	0.97834	1.03989
C	-1.01616	-1.12375	5.96434
H	-1.74480	-1.94437	5.90076
H	-1.32058	-0.50670	6.84061
H	-0.06133	-1.54644	6.32746
C	1.29774	1.97633	6.09646
H	0.56390	2.79343	6.02160
H	2.12871	2.34825	6.72137
H	0.81301	1.16999	6.67155
C	3.99543	1.35098	4.25124
H	4.47079	1.04727	3.30841
H	4.39268	0.69630	5.04660
H	4.35468	2.37170	4.47052
C	-2.04161	2.27542	7.15126
H	-1.74547	3.27840	6.80233
H	-1.25085	1.94390	7.84256
H	-2.97380	2.38393	7.73157
C	-3.96132	0.05088	5.31012
H	-3.82519	-0.71437	4.53138
H	-4.78817	0.70118	4.98135
H	-4.29026	-0.45728	6.23311

$(AlOMe)_{20,t} \cdot 2(AlMe_3)$

Al	2.01261	1.37386	4.67564
Al	-2.37620	1.25966	5.68275
Al	-0.52311	-0.28827	4.34313
Al	2.21367	-1.19136	2.94932
Al	-1.92326	0.23184	1.56523
Al	-0.42463	2.55848	3.11158
Al	3.35384	-0.81215	0.03323
Al	2.48892	1.89117	-1.48202
Al	2.41130	1.80333	1.65225
Al	-0.26460	2.73250	-3.03741
Al	2.24179	1.62153	-4.54624
Al	-0.30803	-0.04258	-4.41202
Al	-0.22493	2.59635	0.04681
Al	-1.84292	0.33187	-1.68117
Al	-0.78163	-4.45005	-0.16568
Al	2.06536	-3.65138	1.23561
Al	-0.67344	-2.70194	2.57435
Al	2.36159	-1.02822	-2.95197
Al	-0.54376	-2.54772	-2.78897
Al	-2.09451	1.54445	-5.76423
Al	-2.37755	-2.31955	-0.14118
Al	2.12968	-3.57962	-1.38768
O	-1.22314	-0.96736	2.82360
O	-0.94262	1.78169	1.52796
O	-1.19363	1.39789	4.31883
O	1.37873	2.22298	3.14109
O	1.27212	-0.32316	4.26540
O	2.59420	-0.05463	1.55631
O	2.68066	0.03348	-1.48550
O	1.53681	2.38403	-2.99777
O	-1.07897	-0.79899	-2.96734
O	-0.86473	1.88140	-1.52028
O	1.56146	2.19875	0.07256
O	-1.78122	-0.59331	-0.08295

O	-1.51930	-3.33884	1.12564	H	-3.71649	1.65893	-2.86744
O	1.12606	-2.54007	2.29957	H	-4.18434	1.25711	-1.20850
O	2.91926	-2.60125	-0.02875	H	-4.33930	0.04370	-2.48912
O	0.99872	-4.32933	-0.12402	C	-0.89679	-0.57274	-6.28272
O	1.24169	-2.40455	-2.43021	H	-1.64217	-1.38015	-6.28314
O	1.48237	-0.09000	-4.26392	H	0.05544	-0.98871	-6.66056
O	-0.98203	1.64118	-4.33553	H	-1.17480	0.10753	-7.11899
O	-1.45925	-3.26568	-1.42350	C	1.51286	2.42099	-6.21855
C	-0.46807	4.56234	0.14215	H	0.76224	3.21053	-6.06687
H	-1.48244	4.85742	0.45980	H	1.04906	1.66228	-6.87127
H	-0.27370	5.05801	-0.82267	H	2.33869	2.86720	-6.79980
H	0.24019	5.00443	0.86457	C	-0.79976	4.57763	-3.46623
C	4.00083	-1.92328	-3.61175	H	-1.77552	4.84954	-3.02924
H	4.61909	-1.24567	-4.21885	H	-0.88607	4.68813	-4.56216
H	3.74621	-2.79291	-4.24017	H	-0.07097	5.33237	-3.12887
H	4.65032	-2.29385	-2.80057	C	4.17095	2.92850	-1.49698
C	-0.77446	-3.57308	-4.46371	H	4.57023	3.06338	-2.51190
H	-0.52686	-4.63291	-4.27004	H	4.97481	2.49745	-0.88062
H	-0.11870	-3.24909	-5.28945	H	3.96772	3.93612	-1.09476
H	-1.81249	-3.55389	-4.83830	C	5.31664	-0.67090	0.08027
C	3.15872	-5.00338	-2.27015	H	5.72858	-1.11506	1.00189
H	2.63087	-5.38543	-3.16143	H	5.67397	0.36995	0.03384
H	3.29076	-5.85408	-1.58064	H	5.76966	-1.20655	-0.77089
H	4.15670	-4.68177	-2.60168	C	4.11954	2.78111	1.84784
C	3.06292	-5.12666	2.06783	H	5.00435	2.17480	1.59366
H	2.48953	-5.58538	2.89263	H	4.25134	3.12328	2.88579
H	4.03387	-4.81981	2.48284	H	4.14184	3.67402	1.20448
H	3.24980	-5.91877	1.32316	C	-1.03912	4.35972	3.60245
C	3.82616	-2.11986	3.63189	H	-2.12562	4.46677	3.43419
H	4.51194	-2.44576	2.83129	H	-0.54788	5.17594	3.05236
H	3.54803	-3.02274	4.20111	H	-0.85774	4.53232	4.67835
H	4.41425	-1.47392	4.30066	C	-3.80023	0.71675	1.94517
C	-0.97377	-3.81404	4.18106	H	-4.27149	1.12701	1.03601
H	-0.70679	-4.86131	3.94898	H	-3.85677	1.50367	2.71545
H	-2.02765	-3.82017	4.50856	H	-4.43668	-0.11410	2.28813
H	-0.35936	-3.52490	5.05072	C	-1.19472	-0.90803	6.15486
C	-1.55360	-6.25093	-0.22724	H	-1.94804	-1.70551	6.08840
H	-1.23501	-6.81461	-1.12071	H	-1.50990	-0.25354	6.99916
H	-2.65620	-6.19830	-0.24962	H	-0.26869	-1.34962	6.56703
H	-1.27353	-6.85441	0.65315	C	1.20460	2.06449	6.35988
C	-4.33499	-2.42684	-0.18965	H	0.47484	2.87591	6.22479
H	-4.74221	-1.92933	-1.08553	H	2.00379	2.45343	7.01475
H	-4.78595	-1.91922	0.67889	H	0.69496	1.27113	6.93220
H	-4.69581	-3.46896	-0.19335	C	3.98273	1.19773	4.79214
C	-3.69649	0.85530	-2.11294	H	4.52553	0.85294	3.90184

H	4.21907	0.50112	5.61579
H	4.41477	2.17445	5.06971
C	-2.19991	2.54951	7.15564
H	-2.04600	3.56783	6.75967
H	-1.34343	2.33826	7.81344
H	-3.11156	2.56847	7.77654
C	-4.03919	0.27772	5.31106
H	-3.87734	-0.52415	4.57569
H	-4.85031	0.91486	4.92338
H	-4.40362	-0.18748	6.24376
C	4.21454	1.44385	-4.58423
H	4.71613	1.02951	-3.69935
H	4.66233	2.43461	-4.77341
H	4.48393	0.80645	-5.44483
C	-3.77486	0.55588	-5.49870
H	-3.64733	-0.26644	-4.77911
H	-4.09034	0.11610	-6.46128
H	-4.60585	1.18091	-5.13446
C	-1.85962	2.87481	-7.19384
H	-2.72270	2.86422	-7.88124
H	-1.78245	3.89402	-6.77781
H	-0.94823	2.71186	-7.78850

$(AlOMe)_{10,t}$

Al	0.148312	0.105854	-2.118162
Al	-0.149339	2.458213	-3.350516
Al	-2.286295	1.000904	-3.995804
Al	-3.068860	2.669257	-2.056077
Al	-0.448030	2.581950	-0.109511
Al	-0.307336	-0.539873	0.777185
Al	-2.926991	-0.461129	-1.171761
Al	-3.521291	2.006990	0.837184
Al	-3.223411	-0.340249	2.074303
Al	-1.089646	1.119735	2.720760
O	-1.926535	2.807498	-3.479144
O	-2.303695	2.647440	-0.382223
O	-0.170522	1.297205	1.147689
O	-1.071370	-0.525907	-0.895920
O	-3.633627	0.190681	0.371086
O	-2.847709	1.495621	2.459554
O	-0.528415	0.623486	-3.737021
O	-1.446521	-0.686498	2.202146
O	-3.207678	0.828755	-2.423549
O	0.261666	1.923179	-1.648739
C	-5.215606	2.982913	1.000735
H	-5.059711	4.063858	1.154637
H	-5.871595	2.872519	0.124182
H	-5.764740	2.601233	1.880044
C	-3.589949	-2.243284	-1.683428
H	-3.380960	-3.002434	-0.908425
H	-4.680981	-2.240927	-1.848502
H	-3.122117	-2.610508	-2.614496
C	1.297569	-1.649850	0.992760
H	1.466122	-1.829617	2.068944
H	1.187646	-2.634234	0.508385
H	2.209876	-1.189717	0.584098
C	0.223824	4.362043	0.396288
H	0.019746	5.120832	-0.380319
H	1.314940	4.351979	0.560621
H	-0.240883	4.734073	1.326956
C	-4.670948	3.787097	-2.272695
H	-4.622932	4.299764	-3.248699
H	-4.771218	4.556666	-1.491614
H	-5.598503	3.191182	-2.261187
C	-3.172570	0.485431	-5.660469
H	-3.333775	-0.605932	-5.697636
H	-2.579417	0.757783	-6.549273
H	-4.162159	0.962961	-5.756360
C	1.833806	-0.890626	-2.283876
H	1.734457	-1.954684	-2.016721
H	2.182905	-0.837582	-3.329485
H	2.631257	-0.471108	-1.649488
C	-4.522310	-1.412830	3.066569
H	-5.523874	-0.951189	3.045970
H	-4.232640	-1.540389	4.123011
H	-4.620673	-2.422265	2.631111
C	1.154001	3.528789	-4.338529
H	1.261149	4.534365	-3.896427
H	0.865118	3.665111	-5.393960
H	2.151657	3.058372	-4.321200
C	-0.198924	1.623995	4.385971
H	-0.063352	2.717582	4.446644
H	0.802849	1.168504	4.457858
H	-0.773789	1.316445	5.275756

$(AlOMe)_{10,t} \cdot (AlMe_3)$

Al	0.21337	-0.25820	-1.33995
Al	-0.18662	1.64177	-3.17531
Al	-2.43248	0.20139	-3.10262
Al	-2.88701	2.40517	-1.67162

Al	-0.02381	2.71325	-0.09328
Al	0.08678	-0.01465	1.66512
Al	-2.71963	-0.38518	0.04258
Al	-2.84270	2.45373	1.35541
Al	-2.66768	-0.03936	3.20241
Al	-0.32708	2.20065	3.09617
Al	-2.44600	4.66221	3.15086
O	-1.95900	2.05724	-3.20353
O	-1.91952	2.78548	-0.17414
O	0.39511	1.81865	1.43167
O	-0.85503	-0.45737	0.13556
O	-3.11993	0.68217	1.48422
O	-1.81959	3.14933	2.68588
O	-0.66652	-0.19506	-2.94787
O	-0.88264	0.44697	3.15842
O	-3.15251	0.57393	-1.45767
O	0.43759	1.60059	-1.45931
C	0.77345	2.98826	4.51556
H	1.66660	2.37618	4.72751
H	0.21338	3.08567	5.46202
H	1.13003	3.99665	4.24030
C	-2.71061	-2.02578	3.17092
H	-3.67537	-2.45319	2.85232
H	-2.51480	-2.38640	4.19792
H	-1.93348	-2.47833	2.52987
C	-4.53966	3.53411	1.67085
H	-5.13588	3.08253	2.48016
H	-4.68377	4.63320	1.72254
H	-5.06389	3.30640	0.72353
C	-3.53419	-2.17037	-0.12749
H	-2.98956	-2.95504	0.41839
H	-4.57406	-2.17842	0.24187
H	-3.57573	-2.47145	-1.19051
C	1.58284	-1.22683	2.06786
H	1.57474	-1.47499	3.14292
H	1.52779	-2.17116	1.50329
H	2.56271	-0.77268	1.84362
C	0.72179	4.52726	-0.25767
H	0.44366	5.16734	0.59707
H	0.36557	5.04538	-1.16637
H	1.82408	4.50607	-0.30888
C	-4.43768	3.59373	-1.91602
H	-4.53493	3.86457	-2.98088
H	-4.34124	4.53225	-1.34613
H	-5.39049	3.12406	-1.61938
C	-3.53851	-0.71846	-4.42568
H	-3.72224	-1.76371	-4.12300
H	-3.06192	-0.74495	-5.41973
H	-4.52351	-0.23465	-4.53664
C	0.99104	2.30046	-4.59046
H	1.18056	3.38171	-4.47476
H	0.56065	2.15022	-5.59451
H	1.97137	1.79544	-4.56534
C	1.84363	-1.34737	-1.38556
H	1.63022	-2.41509	-1.21013
H	2.31688	-1.26555	-2.37950
H	2.58817	-1.04009	-0.63494
C	-3.63373	4.62392	4.71366
H	-3.05453	4.50414	5.64657
H	-4.34002	3.78047	4.66788
H	-4.21916	5.55394	4.81091
C	-1.70189	6.25303	2.25874
H	-0.87136	6.70379	2.83005
H	-2.45763	7.04387	2.11049
H	-1.29783	5.98129	1.26946
C	-3.68604	0.98743	4.56743
H	-3.19568	1.93558	4.84122
H	-3.80090	0.40546	5.49917
H	-4.70542	1.24162	4.22623

$(AlOMe)_{10,t} \cdot (AlMe_3)_2$

Al	0.156896	-0.118592	-1.167220
Al	-0.035143	2.302524	-3.108368
Al	-2.318815	0.039953	-3.016979
Al	-2.846996	2.269336	-1.674508
Al	-0.096423	2.760871	0.048744
Al	0.055476	0.042656	1.865455
Al	-2.694369	-0.448661	0.142041
Al	-2.946703	2.430589	1.358260
Al	-2.756336	0.009559	3.299266
Al	-0.472068	2.272168	3.208249
Al	-2.965297	4.654404	2.972544
Al	0.172218	-2.343368	-2.782037
O	-1.824889	1.812540	-3.127200
O	-1.976102	2.757798	-0.137175
O	0.324554	1.861742	1.584831
O	-0.814783	-0.445737	0.327924
O	-3.160818	0.651934	1.544505
O	-1.981793	3.152630	2.721888
O	-0.809138	-0.840648	-2.530285

O	-0.966535	0.499481	3.318051
O	-3.115934	0.450395	-1.393890
O	0.369912	1.660167	-1.353691
C	0.531586	3.155399	4.643287
H	1.441414	2.594302	4.916637
H	-0.074870	3.258994	5.560091
H	0.854373	4.169249	4.347070
C	-2.784122	-1.975177	3.376450
H	-3.728202	-2.427999	3.031393
H	-2.638548	-2.280619	4.429413
H	-1.972038	-2.451785	2.799173
C	-4.633121	3.555290	1.524981
H	-5.013805	4.039304	2.452874
H	-4.763862	4.276770	0.706255
H	-5.395293	2.762765	1.391363
C	-3.421545	-2.276020	0.039242
H	-2.878046	-3.006539	0.656153
H	-4.480795	-2.311607	0.346926
H	-3.378696	-2.632502	-1.005797
C	1.593035	-1.127428	2.235429
H	1.910757	-1.031007	3.287464
H	1.341783	-2.188782	2.065584
H	2.470066	-0.895680	1.608278
C	0.630629	4.588255	0.151762
H	0.087528	5.318582	-0.465728
H	1.690112	4.623817	-0.155088
H	0.586866	4.944913	1.196700
C	-4.383827	3.440362	-2.044331
H	-4.702272	3.343602	-3.096114
H	-4.131434	4.501568	-1.875311
H	-5.260759	3.209934	-1.416557
C	-3.321480	-0.843742	-4.452461
H	-3.644125	-1.857736	-4.156553
H	-2.714552	-0.947014	-5.368990
H	-4.231398	-0.282982	-4.726244
C	1.049106	1.214871	-4.379755
H	1.623493	1.857311	-5.070482
H	0.425892	0.550786	-5.003091
H	1.783403	0.569277	-3.867042
C	1.843045	-1.242831	-1.334322
H	1.974307	-1.963100	-0.514586
H	2.220845	-1.729449	-2.262064
H	2.606570	-0.451140	-1.203849
C	-3.710762	4.873892	4.777104
H	-4.247871	3.972384	5.109641
H	-4.399261	5.732751	4.849483
H	-2.898854	5.049099	5.506153
C	-2.518740	6.071912	1.683163
H	-2.245257	5.628697	0.712323
H	-1.656528	6.676548	2.014022
H	-3.359766	6.766106	1.516987
C	-3.840960	1.097023	4.570464
H	-4.575238	1.742571	4.057655
H	-3.217995	1.761149	5.193998
H	-4.415453	0.454484	5.261023
C	0.916965	-2.563650	-4.586713
H	1.455087	-1.662580	-4.918855
H	0.104625	-2.737391	-5.315608
H	1.604326	-3.423350	-4.659498
C	-0.273185	-3.759175	-1.490361
H	-1.136886	-4.363027	-1.818748
H	-0.544220	-3.314417	-0.519547
H	0.567296	-4.454217	-1.325084
C	-0.007152	4.287240	-3.185406
H	-0.152502	4.592824	-4.238359
H	0.936925	4.739887	-2.840114
H	-0.819281	4.763912	-2.608232

$(AlOMe)_{10,t} \cdot (AlMe_3)_3$

Al	0.41364	-0.17002	-0.96410
Al	0.63112	2.41073	-2.71109
Al	-2.22147	-0.04161	-2.90808
Al	-2.35294	2.71090	-1.46780
Al	0.28141	2.74175	0.38986
Al	0.09845	-0.00639	2.09067
Al	-2.44807	4.87390	3.37306
Al	-2.54568	-0.05137	0.21284
Al	-2.62984	2.76170	1.60328
Al	-0.53714	4.76525	-3.24366
Al	-0.93232	-2.41266	-2.87698
Al	-2.78931	0.24150	3.38905
Al	-0.25976	2.21316	3.51777
O	-1.06466	3.09794	-2.68175
O	-1.56927	3.01081	0.17067
O	0.57139	1.79304	1.91562
O	-0.72754	-0.32841	0.49001
O	-3.02450	1.00576	1.64390
O	-1.63742	3.29154	3.03642
O	-0.58317	-0.67275	-2.39644
O	-0.96302	0.51978	3.50463

O	-2.66096	0.88666	-1.39492
O	0.72179	1.66325	-1.05303
C	0.76860	2.89455	5.04306
H	1.59751	2.21929	5.31512
H	0.13505	3.00900	5.94020
H	1.21380	3.88231	4.82890
C	-2.98234	-1.73255	3.48550
H	-4.01347	-2.10474	3.36563
H	-2.64772	-2.03098	4.49707
H	-2.34899	-2.28776	2.77189
C	-4.16852	4.07325	1.76103
H	-5.02527	3.39061	1.60197
H	-4.50760	4.60977	2.67597
H	-4.17585	4.80607	0.94121
C	-3.63990	-1.68769	0.06147
H	-3.11381	-2.51769	-0.43162
H	-3.95202	-2.05084	1.05085
H	-4.56180	-1.49253	-0.51319
C	1.40970	-1.36251	2.62567
H	1.89699	-1.07813	3.57416
H	0.89882	-2.32535	2.80387
H	2.19838	-1.54485	1.88060
C	1.20897	4.48226	0.46315
H	0.86930	5.20942	-0.28639
H	2.30250	4.38068	0.36034
H	1.02383	4.94123	1.45065
C	-3.98293	3.76761	-1.80052
H	-4.30132	3.63871	-2.85119
H	-3.81149	4.84630	-1.64475
H	-4.84026	3.47483	-1.17113
C	-2.52419	0.89547	-4.61555
H	-2.11903	0.28438	-5.44047
H	-2.05912	1.88992	-4.67429
H	-3.60470	1.02068	-4.80907
C	1.29378	1.33700	-4.21847
H	2.38156	1.16181	-4.13576
H	1.12563	1.88800	-5.15988
H	0.80732	0.35469	-4.30840
C	2.07972	-1.22100	-0.93770
H	1.91979	-2.25126	-0.57978
H	2.47620	-1.28741	-1.96744
H	2.87285	-0.77389	-0.31562
C	-3.26293	5.05472	5.15193
H	-3.98890	4.25357	5.35782
H	-3.77119	6.02472	5.28486
H	-2.48528	4.98704	5.93429
C	-1.76090	6.32463	2.23792
H	-0.88012	6.81528	2.68859
H	-2.51221	7.11198	2.05857
H	-1.44366	5.93364	1.25947
C	-3.82427	1.40404	4.63814
H	-4.44634	2.15347	4.11919
H	-3.17149	1.96129	5.33136
H	-4.51189	0.80278	5.25906
C	-3.11526	-1.92500	-3.23861
H	-3.29632	-2.02579	-4.31971
H	-4.04120	-1.50487	-2.79404
H	-3.14264	-2.94163	-2.79740
C	-0.60881	4.93517	-5.20947
H	0.20064	5.57114	-5.60735
H	-1.56094	5.37868	-5.55102
H	-0.51786	3.94870	-5.69497
C	-1.12377	6.18282	-1.99499
H	-1.32614	5.78209	-0.98968
H	-2.05517	6.65677	-2.34887
H	-0.37850	6.98869	-1.87741
C	1.63809	4.25979	-2.91271
H	2.15616	4.24694	-3.88310
H	2.35232	3.88035	-2.15263
H	1.56677	5.31739	-2.59074
C	-0.72754	-3.65214	-1.34727
H	-0.79845	-3.12459	-0.38220
H	0.25814	-4.14845	-1.37533
H	-1.48814	-4.45232	-1.33767
C	-0.32751	-2.78618	-4.71767
H	-0.78988	-3.69053	-5.14996
H	0.76683	-2.93031	-4.75995
H	-0.56828	-1.94243	-5.38668

$(AlOMe)_{10,t} \cdot (AlMe_3)_4$

Al	1.81264	-1.29271	-1.45176
Al	1.62815	1.36614	-3.02690
Al	-1.04211	-1.29552	-3.08841
Al	-1.29509	1.35581	-1.50986
Al	1.43807	1.49392	0.11331
Al	1.73780	-1.30559	1.67606
Al	-0.98716	-1.43825	0.05544
Al	-1.35504	1.35503	1.61745
Al	-1.18583	-1.30195	3.19129
Al	0.04293	3.58790	3.54591

Al	0.43825	-3.51777	-3.39373	H	2.26037	1.00960	-5.48705
Al	0.15782	3.58636	-3.41145	H	1.61531	-0.51741	-4.83172
Al	1.50611	1.34924	3.25212	C	3.54126	-2.21382	-1.65268
Al	0.26398	-3.53655	3.56081	H	3.53224	-3.21542	-1.19190
O	-0.11281	1.87915	-2.79277	H	3.77651	-2.34737	-2.72420
O	-0.41423	1.64532	0.07242	H	4.38024	-1.65565	-1.20484
O	1.86997	0.54923	1.65404	C	-0.42496	4.92364	2.16673
O	0.86450	-1.58995	0.08988	H	-0.44189	4.47181	1.16353
O	-1.48258	-0.49930	1.58106	H	0.28060	5.77143	2.12441
O	-0.21910	1.87136	2.94702	H	-1.42690	5.34983	2.34822
O	0.68832	-1.80256	-2.79121	C	-0.38237	3.74593	5.46631
O	0.55206	-1.82312	2.95957	H	0.02162	4.66345	5.92803
O	-1.41220	-0.49994	-1.49033	H	0.02026	2.88839	6.03076
O	1.93056	0.56231	-1.41596	H	-1.47502	3.75576	5.62973
C	2.05268	0.35683	4.86355	C	-1.80366	-0.31152	4.77884
C	-1.98564	-3.23090	3.50784	H	-2.90784	-0.30361	4.82391
H	-2.82000	-2.95181	2.82941	H	-1.46017	0.73122	4.83292
H	-2.38592	-3.23626	4.53343	H	-1.45043	-0.83153	5.68661
H	-1.84480	-4.28964	3.20884	C	-1.81627	-3.23040	-3.43747
C	-3.07891	2.27260	1.84899	H	-2.16773	-3.23539	-4.48087
H	-3.42915	2.14827	2.88950	H	-2.68376	-2.96087	-2.79836
H	-2.99231	3.35566	1.66051	H	-1.67825	-4.28983	-3.13971
H	-3.87330	1.89148	1.18773	C	-0.41118	4.94808	-2.09949
C	-1.78828	-3.24699	0.04745	H	-1.44612	5.27650	-2.29822
H	-1.46178	-3.83424	0.91692	H	0.22035	5.85314	-2.11057
H	-2.89192	-3.23127	0.05545	H	-0.39117	4.55392	-1.07227
H	-1.47487	-3.82621	-0.83196	C	-0.13991	3.69197	-5.35937
C	3.44976	-2.22923	1.96147	H	0.29125	4.59891	-5.81736
H	3.77971	-2.09266	3.00669	H	-1.21827	3.68908	-5.59930
H	3.35697	-3.31418	1.78640	H	0.30515	2.82106	-5.86963
H	4.26038	-1.86426	1.31040	C	2.41229	3.30487	-3.33352
C	2.23123	3.30526	0.12386	H	2.81523	3.32507	-4.35772
H	1.89094	3.89221	-0.74069	H	3.24965	3.03280	-2.65611
H	3.33476	3.29776	0.10325	H	2.25587	4.35953	-3.02712
H	1.92358	3.88071	1.00747	C	0.92655	-4.84120	-2.01119
C	-3.01929	2.26360	-1.78807	H	1.96496	-5.19063	-2.14358
H	-3.24060	2.32441	-2.86880	H	0.28152	-5.73666	-2.01791
H	-3.01341	3.29441	-1.39625	H	0.85964	-4.40296	-1.00423
H	-3.86505	1.73946	-1.31362	C	0.81753	-3.68551	-5.32251
C	-1.60723	-0.31033	-4.69839	H	0.32552	-4.56147	-5.78075
H	-1.25157	-0.85098	-5.59311	H	1.90040	-3.78174	-5.51991
H	-1.23586	0.72249	-4.75911	H	0.46798	-2.79098	-5.86602
H	-2.70980	-0.27383	-4.76476	C	2.29281	3.27800	3.60700
C	2.24795	0.35243	-4.60030	H	2.16603	4.33833	3.30678
H	3.27698	-0.02583	-4.45887	H	3.16144	3.00217	2.97175

H	2.64030	3.28049	4.65174
C	0.59473	-3.67510	5.50037
H	0.16408	-4.58699	5.94940
H	0.16903	-2.81227	6.03901
H	1.67791	-3.68926	5.71723
C	0.80378	-4.89210	2.22858
H	1.79360	-5.31513	2.47251
H	0.87674	-4.46127	1.21845
H	0.10093	-5.74097	2.16537
H	3.15396	0.33856	4.95542
H	1.69779	-0.68284	4.90399
H	1.66595	0.88083	5.75529

$(AlOMe)_{12,t}$

Al	-1.195424	-0.539042	-4.039803
Al	0.233971	-2.144529	-2.456472
Al	1.251385	0.499014	-3.993852
Al	-0.201727	2.017199	-2.347199
Al	-0.205874	1.824795	0.694664
Al	1.976738	0.095689	-0.905963
Al	0.193658	-2.116726	0.591075
Al	-1.966036	-0.302799	-0.945507
Al	-2.098423	-0.403381	2.097858
Al	0.490877	-1.452496	3.704679
Al	-0.548235	0.993583	3.763151
Al	2.064649	0.031642	2.140006
O	-1.424276	-1.274550	-2.377362
O	0.597867	-1.195874	-3.982960
O	1.455525	1.143629	-2.290944
O	-0.542813	1.152539	-3.927893
O	-1.001129	1.288965	-0.880430
O	1.387159	0.860217	0.665146
O	1.011601	-1.496895	-0.941008
O	-1.399153	-1.151347	0.590432
O	-1.202677	-0.797812	3.648538
O	-1.226316	1.255531	2.081287
O	1.146217	0.342213	3.696457
O	1.193483	-1.623615	2.021196
C	-2.477430	-0.986737	-5.442531
H	-3.460976	-0.529515	-5.237230
H	-2.634401	-2.075987	-5.516678
H	-2.150253	-0.624809	-6.431660
C	0.292640	-4.082344	-2.746186
H	-0.472440	-4.628578	-2.173931
H	1.270562	-4.506384	-2.462716
H	0.135247	-4.304839	-3.815544
C	2.554138	1.020962	-5.351062
H	3.535308	0.554970	-5.154343
H	2.709928	2.112808	-5.365845
H	2.243282	0.710752	-6.362771
C	-0.256883	3.967875	-2.532473
H	-0.084100	4.247855	-3.585831
H	-1.238950	4.376397	-2.240663
H	0.499640	4.481990	-1.920470
C	0.195880	3.742736	0.882828
H	0.359742	3.982383	1.949883
H	-0.622649	4.390686	0.530333
H	1.109456	4.043501	0.345092
C	3.899978	-0.303735	-1.035986
H	4.176098	-0.446823	-2.097196
H	4.181996	-1.227930	-0.506286
H	4.535520	0.507207	-0.645436
C	-0.210007	-4.041884	0.669408
H	0.613799	-4.670148	0.294304
H	-1.115582	-4.312800	0.103024
H	-0.389225	-4.338774	1.719482
C	-3.887338	0.103833	-1.081673
H	-4.148047	0.304204	-2.137510
H	-4.177377	0.998156	-0.506936
H	-4.528198	-0.726769	-0.744816
C	-4.045049	-0.466559	2.319678
H	-4.571322	0.310284	1.744575
H	-4.304146	-0.330642	3.383728
H	-4.459121	-1.438267	2.002133
C	0.966213	-2.781520	5.053505
H	0.623757	-2.488728	6.060188
H	2.056726	-2.940096	5.100829
H	0.505140	-3.757797	4.823607
C	-1.043431	2.248479	5.174397
H	-2.134772	2.402940	5.216011
H	-0.713402	1.903138	6.168505
H	-0.581381	3.236154	5.002530
C	4.007795	0.081932	2.393302
H	4.542755	-0.662567	1.784428
H	4.251382	-0.111903	3.452027
H	4.425990	1.069379	2.135299

$(AlOMe)_{12,t} \cdot (AlMe_3)$

Al	0.24908	-2.17231	-2.24473
Al	0.15591	-1.99953	0.81410

Al	-0.39360	1.96332	-2.35503
Al	-0.48462	1.93446	0.69392
Al	-1.23379	-0.71565	-3.92319
Al	-2.06946	-0.38088	-0.84137
Al	1.16085	0.44282	-3.90958
Al	1.83963	0.23414	-0.78259
Al	0.05182	-1.71684	3.98253
Al	-0.86453	1.32687	3.78200
Al	-2.23311	-0.33769	2.21877
Al	1.70231	0.31064	2.29511
Al	2.31030	2.31579	4.26653
O	-1.45074	-1.37870	-2.22729
O	-1.49123	-1.13962	0.74170
O	1.31044	1.18077	-2.23806
O	1.16890	1.02799	0.72303
O	-0.66284	1.00919	-3.89912
O	-1.19459	1.26698	-0.87455
O	0.58641	-1.27439	-3.81393
O	0.97602	-1.40738	-0.75080
O	-1.28943	-0.44955	3.80338
O	0.93587	1.41117	3.54555
O	-1.54366	1.39656	2.06523
O	0.94476	-1.33171	2.33101
H	3.45874	0.54002	-5.04298
H	2.56925	2.04472	-5.35411
H	2.18064	0.56870	-6.27469
C	2.46087	0.94969	-5.27837
H	-3.49036	-0.89049	-5.13027
H	-2.58433	-2.40541	-5.31218
H	-2.17103	-0.99091	-6.31469
C	-2.48314	-1.30699	-5.30554
H	-1.61919	-3.61937	3.23019
H	-1.51304	-3.43029	4.98840
H	-0.25940	-4.33652	4.11759
C	-0.91143	-3.44886	4.05974
H	-1.10527	3.60709	4.96484
H	-1.02845	2.29827	6.16471
H	-2.53920	2.61536	5.28714
C	-1.44249	2.57660	5.17995
H	4.07947	-0.52777	2.66263
H	3.92362	0.71081	3.84721
H	4.20722	1.16389	2.14771
C	3.64066	0.47795	2.79433
H	-4.78877	-0.04127	1.81341
H	-4.43851	-0.42716	3.51743
H	-4.41089	-1.70741	2.28564
C	-4.15405	-0.65077	2.47507
H	0.05064	4.14427	1.85203
H	-0.94569	4.49507	0.42200
H	0.79133	4.16088	0.24570
C	-0.11900	3.86960	0.79495
H	0.19266	-4.36834	1.82450
H	0.87867	-4.40272	0.18901
H	-0.87922	-4.35656	0.41527
C	0.07633	-3.96925	0.80652
C	-4.01158	-0.08576	-0.99419
H	4.16735	-0.38412	-1.70372
H	4.13087	-0.72219	0.03234
H	4.32518	0.94681	-0.54482
C	3.79735	-0.00296	-0.73454
H	0.13024	4.49461	-2.03142
H	-1.58153	4.24899	-2.41374
H	-0.36509	4.13547	-3.70433
C	-0.56143	3.89742	-2.64484
H	-0.35041	-4.69124	-1.96106
H	1.37926	-4.50083	-2.29154
H	0.20595	-4.31658	-3.61216
C	0.37949	-4.10805	-2.54222
H	-4.28089	0.10682	-2.04932
H	-4.35347	0.78692	-0.41387
H	-4.60425	-0.95405	-0.66325
C	1.32525	-1.25441	5.44999
H	3.00787	1.08359	6.43019
C	2.57279	2.06749	6.19629
H	3.21628	2.84479	6.63948
H	1.59599	2.10566	6.70930
H	2.48021	4.72754	3.35204
C	2.98131	3.76907	3.12842
H	4.06470	3.93168	3.25911
H	2.79211	3.54679	2.06619
H	0.99199	-0.38621	6.04342
H	2.34366	-1.01985	5.09471
H	1.42737	-2.09899	6.15450

$(AlOMe)_{12,t} \cdot (AlMe_3)_2$

Al	0.56531	-2.24853	-2.05396
Al	0.41947	-2.01178	1.01736
Al	-0.57406	1.49809	-2.54562
Al	-0.63438	1.80049	0.50172
Al	-1.63195	-1.17092	-3.94134

Al	-1.95709	-0.83784	-0.78153	H	-0.25318	4.18695	1.32721
Al	1.27840	0.15321	-3.90943	H	-1.48462	4.22013	0.04497
Al	2.63282	-3.00680	-3.71613	H	0.24150	4.10334	-0.37024
Al	1.87818	0.28744	-0.80211	C	-0.52674	3.76315	0.34371
Al	0.28275	-1.46902	4.14508	H	0.19726	-4.40929	1.99369
Al	-0.90557	1.46405	3.67994	H	1.54596	-4.32912	0.84456
Al	-2.11223	-0.45984	2.28020	H	-0.12564	-4.43812	0.25847
Al	1.68324	0.55183	2.26020	C	0.51522	-3.98206	1.03288
Al	2.33262	2.69055	3.84135	C	-3.92189	-0.99605	-0.77629
O	-1.16863	-1.75820	-2.17565	H	4.24638	-0.14630	-1.70189
O	-1.29516	-1.33934	0.88224	H	4.28031	-0.32645	0.05526
O	1.23891	1.07721	-2.30998	H	4.26188	1.29845	-0.67065
O	1.10858	1.10352	0.64509	C	3.85151	0.27791	-0.76188
O	-0.54107	0.32097	-3.97155	H	-1.04096	4.07597	-2.41785
O	-1.29925	0.89411	-0.97485	H	-2.24089	3.22436	-3.41437
O	1.59366	-1.55522	-3.39910	H	-0.62963	3.55699	-4.07267
O	1.19300	-1.44522	-0.56543	C	-1.16843	3.26792	-3.15298
O	-1.14915	-0.34550	3.85733	H	-0.05272	-4.62950	-2.31486
O	0.87719	1.68252	3.44097	H	1.55512	-4.68743	-1.56098
O	-1.58958	1.30609	1.96522	H	1.31579	-4.67840	-3.32335
O	1.15368	-1.15880	2.46259	C	0.97389	-4.21866	-2.36655
H	3.48303	0.67427	-5.14751	H	-4.30602	-1.30380	-1.75948
H	2.20652	1.77730	-5.69757	H	-4.41809	-0.04517	-0.51815
H	2.25227	0.10583	-6.29579	H	-4.25545	-1.74468	-0.04017
C	2.40965	0.73420	-5.40152	C	1.53261	-0.77468	5.53477
H	-3.72890	0.34504	-3.43202	H	2.97257	1.72106	6.15102
H	-4.27059	-1.20348	-4.10861	C	2.81520	2.73263	5.74653
H	-3.51101	0.01096	-5.15770	H	3.72520	3.32563	5.93868
C	-3.46754	-0.44906	-4.15222	H	2.00049	3.18824	6.33779
H	-1.25337	-3.53616	3.58496	H	2.13393	5.01612	2.70088
H	-0.97880	-3.33514	5.32056	C	2.68875	4.08378	2.49701
H	0.26649	-4.10129	4.31376	H	3.75949	4.34717	2.45438
C	-0.48075	-3.29057	4.33401	H	2.38437	3.73900	1.49588
H	-1.55458	3.76180	4.67248	H	1.14889	0.12910	6.03659
H	-1.22507	2.59305	5.97147	H	2.52258	-0.51082	5.12513
H	-2.77155	2.54175	5.09917	H	1.71039	-1.52877	6.32133
C	-1.68796	2.70843	4.97569	C	-0.98365	-2.56543	-5.21572
H	4.00976	-0.08719	2.74751	H	-0.16616	-2.19166	-5.85556
H	4.04810	1.35655	3.65159	H	-1.79709	-2.88123	-5.89258
H	4.15348	1.45883	1.88000	H	-0.60857	-3.48134	-4.72975
C	3.62852	0.95225	2.70262	C	4.09856	-3.17672	-2.41232
H	-4.69896	-0.39372	1.96855	H	3.78472	-2.78607	-1.43070
H	-4.23928	-0.56584	3.68261	H	4.99393	-2.60605	-2.71543
H	-4.18284	-1.96975	2.59521	H	4.41378	-4.22520	-2.27483
C	-3.99218	-0.88438	2.65523	C	2.61240	-3.65414	-5.57310

H	1.59085	-3.86799	-5.92342
H	3.22079	-4.56399	-5.71074
H	3.02671	-2.88275	-6.24735

$(AlOMe)_{12,t} \cdot (AlMe_3)_3$

Al	0.74549	-2.47311	-2.03782
Al	0.49617	-2.13095	1.05214
Al	-0.49923	1.41467	-2.53878
Al	-0.67329	1.73939	0.56379
Al	-1.50751	-1.42493	-3.87943
Al	-1.80155	-0.91140	-0.80244
Al	1.96094	0.02135	-3.84531
Al	1.85022	0.18427	-0.73720
Al	0.25956	-1.55932	4.16236
Al	-1.05007	1.32669	3.68922
Al	3.49388	-2.19418	-3.75185
Al	-2.12204	-0.64982	2.24836
Al	1.62282	0.52006	2.32180
Al	2.11847	2.70354	3.90426
Al	-2.96787	0.72999	-4.54311
O	-1.00673	-1.86043	-2.18452
O	-1.23194	-1.47404	0.86809
O	1.25697	0.82648	-2.36960
O	1.07968	1.05082	0.68680
O	-1.32781	0.38663	-3.80069
O	-1.20907	0.84508	-0.94626
O	1.76597	-1.72687	-3.35795
O	1.25534	-1.55765	-0.52149
O	-1.21893	-0.48665	3.85646
O	0.72499	1.62755	3.46567
O	-1.68162	1.15148	1.95994
O	1.14859	-1.20801	2.50869
H	1.76770	1.70645	-5.78617
H	0.27352	0.74569	-5.72006
H	1.76439	0.03730	-6.38590
C	1.36385	0.69602	-5.59602
H	-4.49973	-0.88869	-4.17582
H	-3.69535	-2.26953	-3.60264
H	-3.64559	-1.91275	-5.34797
C	-3.56368	-1.45786	-4.34865
H	-1.11546	-3.69982	3.47741
H	-1.15346	-3.37911	5.21844
H	0.25461	-4.18321	4.49174
C	-0.49134	-3.38766	4.33231
H	-1.76381	3.61980	4.60949
H	-1.41423	2.50960	5.95223
H	-2.95761	2.39343	5.07835
C	-1.87725	2.57561	4.95226
H	3.94520	-0.03845	2.94133
H	3.86630	1.40214	3.84570
H	4.08774	1.51458	2.08534
C	3.52830	0.98513	2.86951
H	-4.68081	-0.33250	2.42618
H	-4.11634	-1.57319	3.56437
H	-4.32944	-1.96822	1.83822
C	-3.99164	-1.18794	2.53826
H	-0.54453	4.14649	1.46439
H	-1.54760	4.11941	-0.00375
H	0.22263	4.08016	-0.12965
C	-0.63374	3.70640	0.45530
H	0.95577	-4.38788	2.23430
H	1.44077	-4.47728	0.52782
H	-0.26860	-4.61237	0.97474
C	0.67206	-4.08861	1.21456
C	-3.77137	-0.95448	-0.94244
H	4.19374	1.30838	-0.52626
H	4.34815	-0.24761	-1.36666
H	4.15017	-0.22212	0.37403
C	3.81921	0.27054	-0.55631
H	-0.00571	3.98787	-2.56040
H	-1.69454	3.66840	-3.00399
H	-0.39655	3.36272	-4.17975
C	-0.66232	3.29256	-3.10803
H	0.16539	-4.98223	-1.59191
H	1.88310	-4.81358	-2.00601
H	0.64858	-4.68635	-3.27923
C	0.87322	-4.42814	-2.22827
H	-4.18359	-1.97655	-0.89442
H	-4.12891	-0.49500	-1.87398
H	-4.23749	-0.38343	-0.12273
C	1.41399	-0.80374	5.60421
H	2.53202	1.83056	6.30154
C	2.52077	2.82345	5.82579
H	3.49441	3.30573	6.01762
H	1.75502	3.42560	6.34722
H	1.89991	4.98310	2.66424
C	2.49875	4.06546	2.53206
H	3.56080	4.36627	2.54356
H	2.26940	3.67333	1.52838
H	2.39094	-0.44393	5.24103

H	1.62605	-1.55663	6.38323
H	0.93173	0.05021	6.10967
C	-0.71339	-2.49553	-5.33073
H	0.37515	-2.62844	-5.26396
H	-0.93353	-2.00626	-6.29512
H	-1.17046	-3.50033	-5.36858
C	4.44126	-2.95798	-2.19392
H	3.95046	-2.68099	-1.24719
H	5.49285	-2.62902	-2.12333
H	4.45510	-4.06079	-2.24629
C	3.65461	-2.84240	-5.60909
H	3.06913	-2.21463	-6.30098
H	3.26828	-3.87295	-5.70228
H	4.69603	-2.85420	-5.97416
C	4.06144	0.00663	-4.02952
H	4.27801	0.20389	-5.09118
H	4.96287	-0.48107	-3.60595
H	4.09917	0.98062	-3.49843
C	-2.84198	0.90820	-6.50478
H	-2.20470	0.11926	-6.93711
H	-2.39402	1.87702	-6.78988
H	-3.82311	0.84797	-7.00732
C	-4.09438	1.86526	-3.38096
H	-3.74208	1.84995	-2.33686
H	-5.15274	1.55203	-3.36915
H	-4.07562	2.91487	-3.72081

$(AlOMe)_{12,t} \cdot (AlMe_3)_4$

Al	0.55204	-2.50736	-2.15642
Al	0.15883	-2.18621	0.94035
Al	-0.36995	1.47436	-2.53581
Al	-0.58982	1.60155	0.59252
Al	-1.54381	-1.22857	-4.04939
Al	-1.95597	-0.79784	-1.00527
Al	3.35939	-2.37851	-3.79539
Al	2.03617	-0.03013	-3.78076
Al	1.84165	-0.01786	-0.68437
Al	0.06950	-1.85404	4.03378
Al	-1.11364	1.71337	3.65968
Al	-2.80512	1.07534	-4.65819
Al	-2.29497	-3.12172	4.23717
Al	-2.35186	-0.65911	2.10830
Al	1.62065	0.29239	2.43605
Al	1.18018	3.03333	4.13858
O	-1.15097	-1.78101	-2.36002
O	-1.51650	-1.43456	0.66120
O	1.33000	0.75132	-2.29622
O	1.09563	0.84274	0.75724
O	-1.23579	0.55859	-3.85812
O	-1.18993	0.89431	-0.99095
O	1.67160	-1.77589	-3.40078
O	1.06504	-1.70217	-0.58008
O	-1.66310	-1.54404	3.55380
O	0.67356	1.36308	3.57991
O	-1.61537	1.04605	2.03991
O	0.88982	-1.41685	2.46605
H	2.04349	1.80541	-5.58811
H	0.49212	0.94392	-5.66176
H	1.96294	0.19414	-6.32602
C	1.57063	0.81110	-5.49957
H	-4.46479	-0.43071	-4.42267
H	-3.80282	-1.89830	-3.89129
H	-3.65971	-1.47053	-5.61608
C	-3.57464	-1.07016	-4.59414
H	-0.76260	-4.78118	4.20231
H	0.06095	-4.00716	5.57123
H	0.77100	-4.10824	3.93934
C	-0.16352	-3.89606	4.49935
H	-3.29766	1.47967	5.01404
H	-1.90958	1.71977	6.09518
H	-2.23692	0.11205	5.40035
C	-2.24568	1.19003	5.18742
H	4.04697	-0.57819	2.86739
H	3.52820	0.56977	4.11390
H	4.07784	1.16744	2.53185
C	3.50268	0.36795	3.02728
H	-4.80225	0.23330	1.92308
H	-4.55367	-0.70724	3.40422
H	-4.79538	-1.54328	1.85337
C	-4.31462	-0.67068	2.32549
H	0.09078	4.00551	1.34245
H	-1.49005	4.04141	0.53458
H	-0.00174	3.90419	-0.41181
C	-0.49084	3.57271	0.51795
H	1.00956	-4.60092	1.40931
H	-0.25969	-4.61405	0.17709
H	-0.69873	-4.46436	1.87424
C	0.04270	-4.14854	1.12858
C	-3.91458	-0.71764	-1.24114
H	4.27951	0.88358	-0.66938

H	4.27543	-0.80584	-1.21769
H	4.09287	-0.43683	0.49254
C	3.80696	-0.10230	-0.51758
H	0.54241	3.91676	-2.71033
H	-1.23514	3.92822	-2.71990
H	-0.33530	3.43547	-4.17291
C	-0.34824	3.37403	-3.06927
H	-0.34554	-4.96084	-2.15804
H	1.39916	-4.95151	-1.81750
H	0.80875	-4.68098	-3.47343
C	0.60659	-4.46350	-2.40862
H	-4.36161	-1.72137	-1.34596
H	-4.22620	-0.12352	-2.10980
H	-4.38877	-0.25133	-0.36277
C	0.88339	-1.09581	5.66212
H	1.35175	4.14749	6.49464
C	1.33437	3.11475	6.10573
H	0.48777	2.59710	6.58703
H	2.25662	2.61982	6.45777
H	2.23690	4.98245	2.74939
C	2.41548	3.89915	2.86256
H	3.46114	3.77815	3.19513
H	2.33973	3.45069	1.85877
H	1.96313	-1.32435	5.71011
H	0.41601	-1.54385	6.55560
H	0.78176	-0.00412	5.73707
C	-0.76356	-2.29853	-5.50711
H	0.32311	-2.44226	-5.43245
H	-0.97354	-1.80763	-6.47276
H	-1.22792	-3.29992	-5.54798
C	4.16430	-3.35991	-2.28013
H	3.67544	-3.10072	-1.32702
H	5.24348	-3.16496	-2.15560
H	4.04758	-4.44859	-2.42098
C	3.49107	-2.90997	-5.69097
H	2.97390	-2.18417	-6.34049
H	3.01172	-3.89080	-5.85951
H	4.53059	-2.99256	-6.05191
C	4.13180	-0.23417	-3.88881
H	4.42073	0.01730	-4.92089
H	4.96234	-0.82929	-3.45686
H	4.22848	0.68928	-3.28075
C	-2.55500	1.32970	-6.59882
H	-2.03643	2.28246	-6.80748
H	-3.50255	1.34749	-7.16410
H	-1.93254	0.52535	-7.02504
C	-3.87742	2.25255	-3.48740
H	-3.58962	2.13970	-2.42957
H	-4.96282	2.06275	-3.55115
H	-3.71905	3.31125	-3.75716
C	-0.95208	3.80389	3.86649
H	-0.29177	4.64560	3.57292
H	-1.37986	4.06008	4.84784
H	-1.75521	3.92406	3.11014
C	-2.83241	-2.91866	6.12679
H	-2.09343	-2.31633	6.68148
H	-2.93172	-3.88319	6.65400
H	-3.80288	-2.39923	6.21629
C	-3.27260	-4.17864	2.88365
H	-2.99634	-3.87887	1.85972
H	-4.36083	-4.02306	2.98551
H	-3.09389	-5.26482	2.96433

$(AlOMe)_{14,t}$

Al	-1.190697	-0.581733	-4.637342
Al	0.238658	-2.131842	-2.996834
Al	1.259734	0.455153	-4.633432
Al	-0.193304	2.049109	-3.057030
Al	-0.119598	1.907068	-0.026928
Al	2.029431	0.138540	-1.555195
Al	0.119886	-1.906209	0.026968
Al	1.190641	0.580814	4.638053
Al	2.006116	0.181253	1.580854
Al	-2.005670	-0.181389	-1.580620
Al	-2.029548	-0.136486	1.555045
Al	0.192399	-2.048776	3.056884
Al	-0.237596	2.131946	2.997549
Al	-1.260299	-0.454753	4.633459
O	-1.417485	-1.244063	-2.940989
O	0.599612	-1.235854	-4.558867
O	-0.531367	1.110874	-4.599130
O	-1.002779	1.388778	-1.559498
O	1.461825	1.163457	-2.952653
O	1.442272	0.910443	-0.001671
O	1.025971	-1.430867	-1.505999
O	-1.442088	-0.909626	0.002052
O	-1.025364	1.432096	1.506299
O	-0.599291	1.236010	4.559442
O	0.530487	-1.111424	4.599480
O	-1.462183	-1.162051	2.952359

O	1.418001	1.243294	2.941782
O	1.003143	-1.388803	1.559792
C	-2.485906	-1.080705	-6.013341
H	-2.644956	-2.171701	-6.045164
H	-2.169121	-0.756648	-7.018630
H	-3.467061	-0.615480	-5.814836
C	0.311849	-4.076387	-3.269513
H	-0.695571	-4.525887	-3.282115
H	0.886697	-4.599495	-2.490070
H	0.779349	-4.296472	-4.244262
C	2.573596	0.917862	-6.004399
H	3.550566	0.453637	-5.784195
H	2.737151	2.007301	-6.058842
H	2.267181	0.572543	-7.005828
C	-0.261797	3.985677	-3.382403
H	0.745827	4.434766	-3.392412
H	-0.847675	4.529155	-2.625426
H	-0.715180	4.179803	-4.369255
C	0.392281	3.811270	-0.048470
H	1.001835	4.064610	0.834688
H	-0.465044	4.502935	-0.062437
H	1.013078	4.042615	-0.929790
C	3.952970	-0.246448	-1.732513
H	4.213804	-0.435146	-2.790336
H	4.267963	-1.133158	-1.159741
H	4.578088	0.598097	-1.397152
C	-0.392280	-3.810429	0.047585
H	-1.013614	-4.041840	0.928507
H	0.464905	-4.502269	0.061878
H	-1.001411	-4.063570	-0.835929
C	-3.926495	0.195907	-1.797936
H	-4.167273	0.374896	-2.862147
H	-4.256727	1.085553	-1.238725
H	-4.554323	-0.648880	-1.468310
C	-3.953129	0.248215	1.732112
H	-4.269201	1.132856	1.156868
H	-4.213497	0.439862	2.789461
H	-4.577681	-0.597859	1.399692
C	0.259403	-3.985556	3.381613
H	-0.748497	-4.434059	3.390550
H	0.711797	-4.180388	4.368783
H	0.845605	-4.529135	2.624953
C	3.926921	-0.196288	1.798714
H	4.257940	-1.084315	1.237327
H	4.166472	-0.378426	2.862696
H	4.555069	0.649562	1.472315
C	-0.308907	4.076546	3.269905
H	0.698933	4.525125	3.281410
H	-0.775271	4.297275	4.245046
H	-0.884046	4.599934	2.490866
C	-2.574760	-0.918166	6.003593
H	-2.738150	-2.007689	6.057067
H	-3.551693	-0.453987	5.783156
H	-2.268976	-0.573626	7.005470
C	2.486100	1.078179	6.014333
H	2.169066	0.753577	7.019364
H	2.646033	2.169007	6.046944
H	3.466867	0.612283	5.815457

$(AlOMe)_{14,t} \cdot (AlMe_3)$

Al	-1.455064	-0.453757	-4.547211
Al	0.454118	-2.037605	-2.703895
Al	1.650174	0.285492	-4.384248
Al	0.048676	1.874011	-2.969188
Al	0.019648	1.922715	0.074377
Al	2.247112	0.115176	-1.279103
Al	0.298609	-1.875033	0.353490
Al	1.209904	0.830861	4.856824
Al	2.125646	0.306512	1.843125
Al	-1.824249	-0.248705	-1.403221
Al	-1.904007	-0.064316	1.725470
Al	0.294750	-1.883751	3.376344
Al	2.367814	-3.074910	-4.424740
Al	-0.178242	2.282731	3.095777
Al	-1.229954	-0.239287	4.826061
O	-1.151892	-1.229529	-2.814771
O	1.617520	-1.481782	-3.997685
O	-0.104356	0.801912	-4.466368
O	-0.827996	1.317675	-1.445989
O	1.734092	1.102305	-2.723360
O	1.597061	0.956145	0.220866
O	1.214570	-1.457232	-1.169955
O	-1.273252	-0.918721	0.229369
O	-0.903192	1.506480	1.616144
O	-0.583380	1.457388	4.686449
O	0.569296	-0.873019	4.884518
O	-1.367225	-1.027293	3.179860
O	1.490530	1.414146	3.145357
O	1.144927	-1.284872	1.880052
C	-1.056281	-1.889483	-5.875149

H	-0.917143	-2.882260	-5.414469
H	-0.142906	-1.683824	-6.457866
H	-1.882285	-1.995201	-6.600180
C	0.514290	-4.035379	-3.072782
H	-0.564275	-4.281934	-3.048463
H	1.001189	-4.603592	-2.267445
H	0.805336	-4.526363	-4.030639
C	-0.193005	3.768918	-3.432706
H	0.769778	4.280755	-3.603873
H	-0.726497	4.334671	-2.653259
H	-0.773894	3.846421	-4.367681
C	0.493787	3.833483	-0.038348
H	1.103475	4.144417	0.826193
H	-0.379560	4.503931	-0.080927
H	1.101616	4.033193	-0.937020
C	4.175610	-0.289830	-1.352254
H	4.487990	-0.447828	-2.400346
H	4.449965	-1.201179	-0.797287
H	4.788696	0.534847	-0.951290
C	-0.110160	-3.807842	0.369110
H	-0.721995	-4.099055	1.237573
H	0.794557	-4.438570	0.383756
H	-0.694588	-4.093781	-0.523022
C	-3.789967	-0.092704	-1.454643
H	-4.194230	-0.522874	-2.383647
H	-4.139054	0.952020	-1.404861
H	-4.252437	-0.629156	-0.611037
C	-3.801901	0.417583	1.936350
H	-4.145815	1.135923	1.175746
H	-3.952840	0.896332	2.922813
H	-4.477630	-0.452868	1.899223
C	0.327327	-3.809004	3.772943
H	-0.680246	-4.252293	3.696696
H	0.677652	-3.975421	4.805858
H	0.981809	-4.379682	3.096243
C	4.037153	-0.045636	2.160868
H	4.422482	-0.901268	1.584009
H	4.210599	-0.272125	3.229838
H	4.667339	0.825658	1.915171
C	-0.229110	4.238796	3.271241
H	0.785920	4.670476	3.245080
H	-0.676863	4.518455	4.239837
H	-0.806442	4.730738	2.473778
C	-2.591072	-0.630690	6.173115
H	-2.335798	-0.212327	7.160876
H	-2.747650	-1.715331	6.296429
H	-3.561653	-0.195659	5.876742
C	2.444237	1.379928	6.269162
H	2.084107	1.080524	7.267797
H	2.602788	2.471082	6.281556
H	3.433217	0.909978	6.127425
C	2.896286	0.763087	-5.818318
H	3.936082	0.481098	-5.576274
H	2.892509	1.849232	-6.012398
H	2.632110	0.262245	-6.765915
C	-3.136828	0.586241	-4.694787
H	-3.095148	1.134587	-5.654415
H	-3.279022	1.342318	-3.904152
H	-4.049514	-0.032080	-4.713769
C	2.191800	-3.579446	-6.316572
H	1.145302	-3.769760	-6.600415
H	2.789376	-4.469018	-6.577320
H	2.543194	-2.748327	-6.955173
C	3.782561	-3.613476	-3.168137
H	4.761972	-3.184121	-3.442690
H	3.907018	-4.708942	-3.127205
H	3.550198	-3.257453	-2.151801

$(AlOMe)_{14,t} \cdot (AlMe_3)_2$

Al	-1.52224	-0.37758	-4.44725
Al	0.42179	-2.00100	-2.66469
Al	1.59578	0.32254	-4.36102
Al	0.04853	1.91079	-2.88340
Al	0.12837	1.89988	0.15521
Al	2.28693	0.10172	-1.28186
Al	0.38728	-1.89959	0.40786
Al	2.01745	0.39809	5.00386
Al	2.29834	0.23726	1.84863
Al	-1.79051	-0.21857	-1.28302
Al	-1.77734	-0.11167	1.83991
Al	0.47027	-1.90692	3.44063
Al	-1.78677	3.05201	4.98290
Al	2.23687	-3.07623	-4.42408
Al	0.06582	2.01145	3.21995
Al	-1.08863	-0.32296	4.90950
O	-1.17731	-1.17492	-2.73962
O	1.54271	-1.45637	-4.00014
O	-0.15319	0.86362	-4.39390
O	-0.78653	1.34766	-1.34853
O	1.73490	1.11653	-2.69983

O	1.69485	0.93228	0.24799	C	4.26707	0.11079	1.85143
O	1.24056	-1.46604	-1.15281	H	4.63744	-0.92586	1.78684
O	-1.18517	-0.93281	0.30446	H	4.68612	0.54645	2.77146
O	-0.74142	1.46255	1.70441	H	4.69525	0.66034	0.99796
O	-1.06309	1.44863	4.54041	C	0.04555	4.00382	3.61391
O	0.66554	-0.85721	4.94740	H	1.12889	4.22440	3.56379
O	-1.21749	-1.12921	3.25011	H	-0.21149	4.49517	4.58100
O	1.66714	1.19642	3.29390	H	-0.44741	4.58704	2.82327
O	1.30728	-1.33449	1.90316	C	-2.28926	-0.81570	6.37414
C	-1.18801	-1.78114	-5.82630	H	-1.99848	-0.32427	7.31879
H	-1.07729	-2.79477	-5.40588	H	-2.27643	-1.90375	6.55648
H	-0.27412	-1.58255	-6.41107	H	-3.33636	-0.53477	6.16547
H	-2.02265	-1.83007	-6.54781	C	1.64744	1.80986	6.36322
C	0.38434	-3.99209	-3.07409	H	0.73156	1.60931	6.94296
H	-0.70842	-4.16539	-3.03512	H	1.52550	2.81326	5.92117
H	0.84525	-4.60176	-2.28445	H	2.47637	1.88558	7.08860
H	0.62752	-4.48753	-4.04203	C	2.81428	0.74663	-5.83826
C	-0.11304	3.82444	-3.30813	H	3.85022	0.43685	-5.61295
H	0.87749	4.30377	-3.39760	H	2.84240	1.82466	-6.06898
H	-0.67803	4.38835	-2.54977	H	2.51362	0.22392	-6.76355
H	-0.62389	3.95265	-4.27782	C	-3.17021	0.72191	-4.55913
C	0.54550	3.83125	0.13275	H	-3.10716	1.28575	-5.50913
H	1.18603	4.11699	0.98556	H	-3.27245	1.47042	-3.75509
H	-0.35729	4.46409	0.17275	H	-4.11141	0.14894	-4.58493
H	1.09947	4.11854	-0.77607	C	2.02781	-3.61389	-6.30456
C	4.17740	-0.39721	-1.53102	H	0.96930	-3.66201	-6.60370
H	4.30206	-0.83499	-2.53793	H	2.48771	-4.59448	-6.51436
H	4.53235	-1.14936	-0.80893	H	2.51179	-2.87832	-6.97191
H	4.85721	0.46897	-1.46729	C	3.62650	-3.67949	-3.16822
C	-0.04269	-3.82757	0.42104	H	4.63553	-3.32938	-3.44433
H	-0.58736	-4.12316	1.33258	H	3.66625	-4.78103	-3.11263
H	0.85162	-4.47000	0.35575	H	3.41749	-3.29561	-2.15721
H	-0.69948	-4.09016	-0.42711	C	-1.59745	3.50954	6.88470
C	-3.75369	-0.02520	-1.31561	H	-1.95954	2.66386	7.49747
H	-4.16726	-0.40021	-2.26444	H	-2.18130	4.39889	7.17411
H	-4.07807	1.02454	-1.21678	H	-0.54734	3.67683	7.17022
H	-4.22925	-0.58954	-0.49818	C	-3.19916	3.63159	3.74168
C	-3.67929	0.34572	2.07962	H	-3.00953	3.23372	2.73223
H	-4.04190	1.10976	1.37436	H	-3.25889	4.73109	3.67031
H	-3.83228	0.74715	3.09746	H	-4.19737	3.27215	4.04631
H	-4.33486	-0.53554	1.97675	C	3.70375	-0.64035	5.08558
C	0.71212	-3.81925	3.82929	H	3.82630	-1.37889	4.27544
H	-0.24826	-4.34437	3.96893	H	3.69299	-1.20830	6.03440
H	1.29085	-3.94369	4.76049	H	4.61452	-0.01908	5.08969
H	1.25263	-4.34110	3.02392				

$(AlOMe)_{14,t} \cdot (AlMe_3)_3$

Al	-1.47740	-0.40808	-4.45957
Al	0.44032	-2.04889	-2.67305
Al	1.62497	0.31917	-4.28138
Al	0.02440	1.86435	-2.81404
Al	0.08948	1.84424	0.21756
Al	2.31600	-3.06522	-4.40293
Al	2.24703	0.03798	-1.20266
Al	0.26910	-2.02388	0.37604
Al	2.83500	-2.11339	5.48259
Al	1.91367	0.37943	5.03487
Al	-2.68634	2.24421	5.26375
Al	2.09555	0.06072	1.94328
Al	-1.82345	-0.29950	-1.29992
Al	-1.80884	-0.11929	1.83724
Al	0.26810	-2.02840	3.47708
Al	-0.06206	2.04302	3.34501
Al	-1.79775	-0.27974	4.95121
O	-1.15800	-1.23205	-2.75929
O	1.59909	-1.46099	-3.95651
O	-0.12467	0.84117	-4.35197
O	-0.82548	1.27031	-1.29672
O	1.71140	1.08901	-2.60406
O	1.63453	0.82707	0.33977
O	1.20685	-1.53618	-1.12469
O	-1.26487	-1.00516	0.31515
O	-0.78036	1.42389	1.76861
O	-1.16903	1.41107	4.65550
O	1.32966	-1.33095	4.78631
O	-1.31400	-1.05212	3.37461
O	1.52297	1.07169	3.39692
O	1.09422	-1.50551	1.91863
C	-1.09418	-1.78896	-5.84899
H	-0.93993	-2.80044	-5.43846
H	-0.19464	-1.54910	-6.43977
H	-1.93314	-1.86626	-6.56250
C	0.45035	-4.03071	-3.13701
H	-0.64024	-4.21934	-3.13401
H	0.89487	-4.65121	-2.34657
H	0.72707	-4.50467	-4.10724
C	-0.22894	3.76104	-3.26328
H	0.72677	4.25728	-3.50556
H	-0.70017	4.33990	-2.45473
H	-0.87039	3.84005	-4.15797
C	0.55080	3.75675	0.10602
H	1.14406	4.05857	0.98473
H	-0.33932	4.40676	0.07698
H	1.15585	3.99565	-0.78404
C	4.16098	-0.37318	-1.47383
H	4.36809	-0.42574	-2.55877
H	4.47857	-1.33765	-1.04647
H	4.82006	0.40916	-1.06077
C	-0.14145	-3.95253	0.28511
H	-0.67078	-4.29359	1.18861
H	0.76762	-4.57146	0.19230
H	-0.79543	-4.20162	-0.56860
C	-3.78977	-0.21878	-1.44937
H	-4.11721	-0.69152	-2.38836
H	-4.19876	0.80490	-1.44661
H	-4.26684	-0.76425	-0.61941
C	-3.71680	0.38292	1.88369
H	-3.97118	0.97598	0.99108
H	-3.95817	1.01625	2.74648
H	-4.40213	-0.48082	1.90267
C	-0.01947	-3.94118	3.86181
H	-1.01146	-4.29642	3.53638
H	0.03728	-4.11165	4.95234
H	0.73462	-4.59101	3.38817
C	4.03571	-0.27993	2.09285
H	4.28558	-0.99469	2.88874
H	4.60055	0.64800	2.29064
H	4.43755	-0.70310	1.15925
C	0.16206	3.98430	3.61467
H	1.18859	4.32765	3.40209
H	-0.05362	4.25314	4.66462
H	-0.51743	4.57617	2.98040
C	-1.37191	-1.33245	6.56420
H	-0.31710	-1.62026	6.66296
H	-1.97076	-2.26052	6.58331
H	-1.65179	-0.75508	7.46190
C	1.32441	1.46392	6.57432
H	0.40046	1.04984	7.00717
H	1.10802	2.51204	6.31224
H	2.08895	1.46984	7.36906
C	2.84839	0.81717	-5.72765
H	3.89320	0.53615	-5.50814
H	2.83853	1.90315	-5.92117
H	2.56768	0.31760	-6.67161
C	-3.14414	0.65676	-4.60256
H	-3.07628	1.23150	-5.54518

H	-3.28711	1.39142	-3.79264
H	-4.06694	0.05615	-4.65407
C	2.16635	-3.51706	-6.31158
H	1.11816	-3.56029	-6.64469
H	2.64579	-4.47843	-6.56080
H	2.66064	-2.73956	-6.92171
C	3.70498	-3.65741	-3.14305
H	4.67610	-3.17230	-3.34183
H	3.86735	-4.74787	-3.18144
H	3.42179	-3.39149	-2.11232
C	-2.59886	2.59784	7.20370
H	-3.59641	2.64215	7.67469
H	-2.09388	3.55516	7.42331
H	-2.02740	1.80778	7.71879
C	-3.44347	3.47608	3.91990
H	-3.12160	3.21128	2.89992
H	-3.10404	4.50942	4.10941
H	-4.54687	3.49384	3.91785
C	3.92037	-0.11135	5.45824
H	4.68970	-0.85475	5.16515
H	4.13061	0.18185	6.49769
H	4.22657	0.73481	4.80821
C	-3.80622	0.24981	5.28136
H	-4.55347	1.01220	4.97981
H	-4.03796	-0.03227	6.31965
H	-4.12019	-0.59108	4.62827
C	2.62324	-2.39573	7.42409
H	2.17252	-1.50736	7.89790
H	3.57227	-2.60403	7.94685
H	1.94788	-3.24590	7.62709
C	3.65912	-3.38403	4.21464
H	3.37179	-3.15686	3.17523
H	3.32267	-4.41411	4.42674
H	4.76205	-3.39101	4.25431

$(AlOMe)_{14,t} \cdot (AlMe_3)_4$

Al	-1.63486	-0.54547	-4.39984
Al	0.35827	-2.20081	-2.75650
Al	2.04845	0.17038	-4.36884
Al	0.02087	1.88377	-2.85046
Al	0.12012	1.88170	0.24529
Al	2.11510	-0.05812	-1.25619
Al	0.16400	-2.04598	0.34539
Al	1.91105	0.35174	5.00857
Al	2.07090	0.02574	1.91001
Al	-1.78842	-0.20376	-1.31215
Al	-2.51633	1.95048	-4.88539
Al	-1.83244	-0.08342	1.84724
Al	2.78245	-2.16007	5.46008
Al	0.22658	-2.04058	3.44408
Al	-0.04856	2.04573	3.35429
Al	2.95460	-2.33913	-4.74865
Al	-2.63646	2.25249	5.31263
Al	-1.77594	-0.27922	4.97126
O	-1.22693	-1.23524	-2.76749
O	1.47002	-1.53084	-4.04560
O	-1.03219	1.15580	-4.15515
O	-0.76434	1.34806	-1.27497
O	1.61919	0.92498	-2.76543
O	1.61645	0.79126	0.29861
O	1.07742	-1.59756	-1.17875
O	-1.33295	-0.95793	0.30469
O	-0.78195	1.44485	1.78034
O	-1.14349	1.40207	4.66997
O	1.30524	-1.34767	4.74520
O	-1.34718	-1.04636	3.37395
O	1.52511	1.05627	3.37367
O	1.03142	-1.51761	1.87602
C	-1.14439	-1.67974	-5.93640
H	-1.76064	-2.59620	-5.94609
H	-0.09288	-1.99093	-5.96616
H	-1.36282	-1.13986	-6.87331
C	0.11576	-4.12192	-3.12820
H	-0.90439	-4.47014	-2.89658
H	0.81377	-4.76011	-2.56202
H	0.28379	-4.31908	-4.20248
C	0.24150	3.80258	-3.25518
H	1.28013	4.14534	-3.11152
H	-0.40081	4.44089	-2.62716
H	-0.02135	4.01007	-4.30831
C	0.63652	3.78006	0.19540
H	1.21563	4.05940	1.09058
H	-0.23347	4.45666	0.14979
H	1.26957	4.00837	-0.67712
C	4.02886	-0.54534	-1.35938
H	4.36112	-0.82130	-2.36672
H	4.22390	-1.42883	-0.72953
H	4.69033	0.26394	-1.00691
C	-0.31592	-3.95541	0.37905
H	-0.93863	-4.20761	1.25200

H	0.57368	-4.60696	0.41824
H	-0.88830	-4.24629	-0.51636
C	-3.72381	0.10407	-1.56483
H	-4.23197	-0.82805	-1.86861
H	-3.94102	0.86040	-2.33091
H	-4.21642	0.44483	-0.64419
C	-3.74100	0.41883	1.93954
H	-3.93623	1.27600	1.27456
H	-4.05892	0.74314	2.93734
H	-4.41270	-0.39997	1.63120
C	-0.07616	-3.93857	3.88569
H	-1.09600	-4.27436	3.63486
H	0.04976	-4.08828	4.97354
H	0.62593	-4.61792	3.37571
C	4.00176	-0.31668	2.15268
H	4.20376	-1.07519	2.92080
H	4.53189	0.60428	2.45226
H	4.48342	-0.67339	1.23241
C	0.18447	3.97973	3.67046
H	1.22496	4.30977	3.51151
H	-0.07619	4.23752	4.71307
H	-0.45416	4.59189	3.01320
C	-1.34023	-1.34749	6.57284
H	-0.29712	-1.67919	6.64644
H	-1.97780	-2.24838	6.61499
H	-1.57086	-0.75442	7.47441
C	1.33881	1.43482	6.55986
H	0.49704	0.94430	7.07401
H	0.99860	2.44781	6.29651
H	2.15599	1.53703	7.29277
C	4.04580	-0.33903	-4.84701
H	4.83366	-1.05459	-4.53545
H	4.36835	0.56292	-4.28447
H	4.20777	-0.12021	-5.91293
C	-3.62035	-0.03023	-4.89228
H	-3.78806	-0.31984	-5.94063
H	-4.40088	0.70956	-4.62296
H	-3.94946	-0.88208	-4.26193
C	2.69225	-2.68362	-6.67426
H	2.00896	-3.53517	-6.83908
H	3.62846	-2.91037	-7.21211
H	2.23534	-1.80671	-7.16282
C	3.83709	-3.54579	-3.46371
H	4.93065	-3.60431	-3.60107
H	3.44435	-4.57282	-3.56273
H	3.65479	-3.22363	-2.42638
C	-2.46499	2.65392	7.23825
H	-3.43607	2.82871	7.73239
H	-1.84816	3.55364	7.40994
H	-1.97110	1.82196	7.76712
C	-3.44138	3.43675	3.95635
H	-3.20861	3.08981	2.93727
H	-3.04548	4.46275	4.05137
H	-4.54021	3.50480	4.03440
C	3.89873	-0.18277	5.48762
H	4.66942	-0.92276	5.19093
H	4.08187	0.07874	6.54028
H	4.22941	0.68163	4.87471
C	-3.76629	0.27654	5.42536
H	-4.53869	1.01797	5.13595
H	-3.92565	0.04368	6.48925
H	-4.11293	-0.60551	4.84705
C	2.54833	-2.46012	7.39754
H	2.10694	-1.57147	7.87932
H	3.49412	-2.68241	7.92105
H	1.86518	-3.30562	7.59264
C	3.60508	-3.43991	4.20063
H	3.29285	-3.23854	3.16309
H	3.29295	-4.47164	4.43889
H	4.70844	-3.42464	4.21624
C	1.47285	1.19881	-5.95463
H	1.18105	2.23571	-5.72676
H	0.59818	0.72373	-6.42490
H	2.27424	1.23761	-6.71072
C	-2.29598	2.24127	-6.82446
H	-1.84208	1.35790	-7.30316
H	-1.62545	3.09483	-7.02700
H	-3.24801	2.44512	-7.34379
C	-3.35488	3.23013	-3.63527
H	-3.06719	3.02721	-2.59104
H	-4.45781	3.21976	-3.67646
H	-3.03307	4.26085	-3.86456

$(AlOMe)_{16,t}$

Al	0.615474	-1.174049	5.377831
Al	2.069694	0.383810	3.781187
Al	1.941867	0.193092	0.780156
Al	-1.941867	-0.193092	0.780156
Al	0.289529	-1.993433	2.337422
Al	0.193331	-1.941833	-0.779772

Al	-2.069694	-0.383810	3.781187	H	1.127288	-4.140235	-5.080793
Al	-0.615474	1.174049	5.377831	C	3.920843	0.023977	-2.661432
Al	-1.993381	-0.290321	-2.337015	H	4.153931	0.158444	-3.733779
Al	-0.289529	1.993433	2.337422	H	4.267481	-0.983562	-2.379189
Al	0.385055	-2.069569	-3.780571	H	4.544142	0.747505	-2.110026
Al	-1.173557	-0.616316	-5.377177	C	2.429845	1.196368	-6.754496
Al	-0.193331	1.941833	-0.779772	H	3.437413	0.790080	-6.558768
Al	1.993381	0.290321	-2.337015	H	2.523817	2.294756	-6.786995
Al	-0.385055	2.069569	-3.780571	H	2.131223	0.853640	-7.759181
Al	1.173557	0.616316	-5.377177	C	-0.613920	3.990508	-4.115749
O	-1.108256	1.346350	-2.274679	H	0.357227	4.510223	-4.179692
O	1.330678	1.316964	-3.694062	H	-1.198929	4.500640	-3.335545
O	-1.006133	1.400717	0.762553	H	-1.127288	4.140235	-5.080793
O	1.108256	-1.346350	-2.274679	C	0.183910	3.873572	-0.833697
O	-1.316177	1.331484	3.694751	H	0.786682	4.159371	0.043345
O	-1.330678	-1.316964	-3.694062	H	-0.725096	4.496996	-0.822141
O	-1.346759	-1.107620	2.275401	H	0.765723	4.162420	-1.723899
O	1.006133	-1.400717	0.762553	C	-0.022356	3.920913	2.660979
O	-1.400611	-1.006366	-0.761918	H	0.985076	4.267107	2.377827
O	1.346759	1.107620	2.275401	H	-0.155935	4.154354	3.733344
O	0.663010	-1.123533	-5.329353	H	-0.746150	4.544205	2.109891
O	-0.663010	1.123533	-5.329353	C	-1.194265	2.431275	6.754832
O	1.400611	1.006366	-0.761918	H	-2.292674	2.524303	6.789199
O	-1.124000	-0.662162	5.330097	H	-0.789250	3.438970	6.557145
O	1.124000	0.662162	5.330097	H	-0.849386	2.134060	7.759183
O	1.316177	-1.331484	3.694751	C	-3.990856	-0.611657	4.115743
C	-3.873577	0.184392	0.833147	H	-4.500808	-1.197099	3.335729
H	-4.158978	0.786911	-0.044220	H	-4.510312	0.359685	4.178703
H	-4.162696	0.766551	1.723021	H	-4.141156	-1.124296	5.081076
H	-4.497119	-0.724526	0.821589	C	0.022356	-3.920913	2.660979
C	-0.183910	-3.873572	-0.833697	H	-0.985076	-4.267107	2.377827
H	-0.786682	-4.159371	0.043345	H	0.155935	-4.154354	3.733344
H	0.725096	-4.496996	-0.822141	H	0.746150	-4.544205	2.109891
H	-0.765723	-4.162420	-1.723899	C	3.873577	-0.184392	0.833147
C	-3.920843	-0.023977	-2.661432	H	4.158978	-0.786911	-0.044220
H	-4.153931	-0.158444	-3.733779	H	4.162696	-0.766551	1.723021
H	-4.267481	0.983562	-2.379189	H	4.497119	0.724526	0.821589
H	-4.544142	-0.747505	-2.110026	C	3.990856	0.611657	4.115743
C	-2.429845	-1.196368	-6.754496	H	4.510312	-0.359685	4.178703
H	-3.437413	-0.790080	-6.558768	H	4.141156	1.124296	5.081076
H	-2.523817	-2.294756	-6.786995	H	4.500808	1.197099	3.335729
H	-2.131223	-0.853640	-7.759181	C	1.194265	-2.431275	6.754832
C	0.613920	-3.990508	-4.115749	H	0.789250	-3.438970	6.557145
H	-0.357227	-4.510223	-4.179692	H	0.849386	-2.134060	7.759183
H	1.198929	-4.500640	-3.335545	H	2.292674	-2.524303	6.789199

$(AlOMe)_{16,t} \cdot (AlMe_3)$

Al	0.05497	0.16778	0.02698
Al	1.82374	1.46369	1.54365
Al	1.95101	-1.72114	1.75218
Al	2.32340	1.98922	-1.52397
Al	5.27105	1.51474	1.77942
Al	0.17933	0.20255	-3.00412
Al	3.98379	-0.16136	0.02052
Al	1.87677	-2.06841	-1.39977
Al	4.04188	-0.37019	-3.02074
Al	1.82193	-2.05643	-4.51981
Al	4.12912	-0.38671	-6.12985
Al	2.39247	1.80111	-4.64551
Al	0.11666	0.02239	-6.14695
Al	0.84378	-0.60223	-9.17581
Al	1.99346	-2.34311	-7.51184
Al	3.42702	0.01877	-9.19404
Al	2.26658	1.87068	-7.66298
O	0.52429	-0.79266	-1.47244
O	2.87259	-1.57663	0.08051
O	3.57882	1.10296	1.27470
O	1.14485	1.67523	-0.16179
O	1.48019	1.52142	-3.09031
O	3.67817	0.67047	-1.55123
O	2.74563	-1.68230	-2.98567
O	2.86480	-1.74958	-6.02713
O	3.72709	0.51513	-4.58970
O	1.38036	1.39057	-6.14718
O	0.51452	-0.74448	-4.53699
O	0.51329	-1.18188	-7.47011
O	2.49930	-1.53786	-9.08788
O	1.77047	0.95931	-9.18158
O	3.74626	0.72143	-7.53353
O	0.98118	-0.15809	1.59846
C	6.16892	2.74377	0.53306
H	5.86788	3.79304	0.69534
H	7.26756	2.69807	0.62504
H	5.90480	2.49317	-0.50666
C	5.62988	1.30502	3.70192
H	5.44316	0.27638	4.04646
H	6.66517	1.57445	3.97056
H	4.96106	1.96228	4.28647
C	5.91301	-0.52050	0.56100
H	6.38802	-0.32421	1.55020
H	5.89533	-1.62725	0.57165
H	6.63808	-0.20885	-0.20362
C	2.51320	3.77313	-8.08320
H	2.04045	4.44302	-7.34951
H	3.58117	4.04615	-8.12393
H	2.08223	3.99154	-9.07488
C	4.80103	0.21555	-10.56777
H	4.44301	-0.09245	-11.56405
H	5.15700	1.25657	-10.64375
H	5.67852	-0.41021	-10.32938
C	1.78985	-4.27475	-7.80117
H	2.19865	-4.87789	-6.97676
H	0.73107	-4.56306	-7.91401
H	2.30858	-4.56612	-8.73012
C	-0.51005	-0.91181	-10.54925
H	-0.13322	-0.68627	-11.56070
H	-0.86072	-1.95746	-10.54593
H	-1.39377	-0.27253	-10.38072
C	-1.68934	0.74059	-6.48468
H	-1.78239	1.80389	-6.21013
H	-1.94845	0.65830	-7.55610
H	-2.46690	0.19270	-5.92720
C	3.19229	3.59621	-4.79066
H	2.43884	4.39921	-4.85060
H	3.81838	3.80296	-3.90768
H	3.84700	3.69871	-5.67164
C	5.93605	-1.13577	-6.39374
H	6.02814	-2.16699	-6.01586
H	6.19314	-1.16211	-7.46868
H	6.71561	-0.53445	-5.89718
C	0.87952	-3.78561	-4.61469
H	1.53160	-4.67264	-4.58743
H	0.18541	-3.86109	-3.76150
H	0.26247	-3.86154	-5.52579
C	5.84885	-1.14883	-2.84985
H	6.63562	-0.38034	-2.75782
H	5.93239	-1.80895	-1.96886
H	6.10334	-1.76894	-3.72325
C	3.32968	-1.58530	3.18875
H	3.23976	-0.64816	3.76299
H	3.22377	-2.41316	3.91162
H	4.36626	-1.62718	2.81564
C	0.58072	-3.15072	1.85562
H	0.98589	-4.17333	1.92449
H	0.00021	-2.96681	2.77915

H	-0.14256	-3.14947	1.02290
C	1.38750	-3.97603	-1.28084
H	1.75020	-4.40587	-0.33417
H	0.30067	-4.15598	-1.31836
H	1.84144	-4.55092	-2.10324
C	-1.61176	1.02597	-2.97396
H	-2.42664	0.28332	-2.98357
H	-1.76289	1.66114	-2.08541
H	-1.74956	1.67328	-3.85499
C	3.06766	3.80444	-1.29334
H	2.48727	4.56568	-1.84121
H	3.03478	4.08248	-0.22375
H	4.11772	3.89697	-1.61311
C	1.53338	2.78577	2.96043
H	2.02811	3.74689	2.73471
H	0.46325	3.00150	3.11810
H	1.93857	2.42992	3.92407
C	-1.86895	0.30440	0.40645
H	-2.10733	-0.28607	1.30785
H	-2.16864	1.34658	0.61393
H	-2.50340	-0.05846	-0.41641

$(AlOMe)_{16,t} \cdot (AlMe_3)_2$

Al	1.93187	0.06132	3.82428
Al	-2.01604	-0.00670	3.88487
Al	-0.36580	1.38823	5.44206
Al	0.09952	-1.76872	5.49587
Al	-1.70405	3.21282	-5.54903
Al	3.05442	1.80143	5.63370
Al	1.95650	-0.01824	0.78744
Al	2.06378	0.10763	-2.30800
Al	1.80657	0.20067	-5.46049
Al	-1.93315	0.17788	0.85456
Al	-2.02444	0.16834	-2.29227
Al	-1.36189	-0.22384	-5.35713
Al	0.03609	2.10272	2.40509
Al	0.10644	2.07057	-0.70367
Al	0.00905	2.04700	-3.75204
Al	-0.00526	-1.98170	2.32925
Al	-0.09675	-1.82524	-0.80871
Al	0.04790	-1.89044	-3.82917
O	0.97041	-1.46308	3.82248
O	-1.09232	1.61337	3.76118
O	1.40882	1.22140	5.13781
O	-1.03197	-0.31251	5.42702
O	0.78217	-1.43934	0.75331
O	0.91691	-1.35485	-2.30104
O	0.33338	-0.90481	-5.37435
O	-0.78378	1.63431	0.82981
O	-0.84199	1.63564	-2.22039
O	-1.16831	1.55089	-5.05801
O	1.51215	0.92957	2.30269
O	1.54884	0.91892	-0.73118
O	1.52865	1.08378	-3.78775
O	-1.47170	-0.84357	2.34407
O	-1.52705	-0.64822	-0.72726
O	-1.56204	-0.94854	-3.67056
C	-3.93161	-0.08789	4.31395
C	3.89499	-0.10080	4.35042
H	-4.07927	-0.71440	5.21039
H	4.36626	0.12931	5.33458
H	-4.33904	0.91135	4.54626
H	3.99467	-1.20282	4.34507
C	-3.80871	0.77457	0.97717
C	-3.89190	0.75244	-2.55584
C	3.77909	-0.75565	0.99148
C	4.01352	-0.20280	-2.34965
H	-4.51941	-0.06925	0.97478
H	-4.61055	0.07859	-2.05985
H	4.57480	0.00388	1.07188
H	4.50569	0.30318	-1.50400
H	-4.00578	1.35968	1.89119
H	-4.08970	1.77177	-2.18805
H	3.85177	-1.40424	1.88288
H	4.29295	-1.26783	-2.30088
H	-4.54320	-0.50571	3.50028
H	-4.06713	1.42099	0.12286
H	-4.13704	0.74928	-3.63374
H	4.57151	0.29499	3.58049
H	4.02795	-1.39844	0.13217
H	4.44972	0.20042	-3.27686
C	-0.31684	-3.92859	2.36080
C	-0.84614	-3.64213	-0.98680
C	0.13184	-3.80222	-4.27413
C	0.59671	3.97474	2.69391
C	0.67017	3.95925	-0.85091
C	0.21109	4.00879	-4.26282
H	0.09029	-4.37603	3.28056
H	-0.09267	-4.44609	-0.98845
H	0.48055	-4.42891	-3.43968

H	0.59733	4.20272	3.77576	H	-3.08892	5.06356	-4.37092
H	-0.18789	4.63756	-1.00411	H	-4.06548	3.58776	-4.54361
H	-1.38410	-4.20086	2.31664	H	-2.82016	3.67357	-3.28743
H	-1.53538	-3.83898	-0.14922	C	-1.46931	3.61675	-7.46019
H	-0.85180	-4.19357	-4.58674	H	-2.02098	2.88127	-8.07293
H	1.60974	4.19673	2.32328	H	-1.84731	4.61615	-7.73329
H	1.19190	4.30024	0.05701	H	-0.41389	3.55466	-7.76731
H	0.17797	-4.41534	1.50581	H	0.02452	4.47920	-5.25600
H	-1.43655	-3.74811	-1.91276	H	1.31470	4.08275	-4.22080
H	0.82224	-3.94687	-5.12298	H	-0.19272	4.69581	-3.50688
H	-0.09572	4.68848	2.21637				
H	1.37047	4.12294	-1.68895	$(AlOMe)_{16,t} \cdot (AlMe_3)_3$			
C	-0.76583	2.60263	6.92428	Al	1.96341	0.02938	3.83920
H	-1.84961	2.69928	7.10455	Al	-1.98556	-0.04177	3.87796
H	-0.30999	2.24579	7.86447	Al	-0.34571	1.39592	5.40991
H	-0.37616	3.61906	6.73913	Al	0.10833	-1.75571	5.55572
C	1.47648	-1.53558	6.92205	Al	2.80620	-2.25479	-5.74281
H	1.29369	-0.63402	7.52986	Al	-2.60297	2.27027	-5.82064
H	1.46750	-2.39433	7.61582	Al	3.06751	1.82922	5.61107
H	2.50754	-1.45299	6.54140	Al	1.98838	-0.10645	0.79102
C	-1.10387	-3.34261	5.56290	Al	2.02971	0.00505	-2.32322
H	-0.58686	-4.31578	5.57829	Al	1.95880	0.28375	-5.39938
H	-1.67882	-3.26391	6.50463	Al	-1.87010	0.08551	0.84432
H	-1.84189	-3.38603	4.74464	Al	-1.89475	0.00527	-2.31824
C	1.59727	1.58053	-6.88550	Al	-1.78854	-0.27223	-5.41158
H	0.68988	1.42111	-7.49103	Al	0.08428	2.04182	2.36493
H	1.53837	2.61034	-6.49632	Al	0.14490	1.98506	-0.75218
H	2.45370	1.55840	-7.58174	Al	-0.03238	2.05736	-3.83858
C	3.35759	-1.03314	-5.52573	Al	0.03727	-2.04878	2.38924
H	3.26301	-1.61776	-6.45973	Al	-0.03935	-1.98015	-0.74819
H	4.33931	-0.53293	-5.55309	Al	0.18149	-2.04416	-3.83239
H	3.39541	-1.76259	-4.69928	O	1.00220	-1.49059	3.87502
C	-2.59588	-0.62525	-6.82479	O	-1.06303	1.57665	3.72282
H	-2.24310	-0.18151	-7.77237	O	1.42985	1.22191	5.11990
H	-2.69832	-1.71048	-6.99367	O	-1.01820	-0.30443	5.43888
H	-3.60942	-0.22946	-6.63718	O	0.82898	-1.53586	0.80147
C	3.78163	3.17025	4.42346	O	0.94417	-1.50890	-2.24352
H	3.36491	4.17079	4.63147	O	1.31360	-1.39653	-5.11453
H	4.87997	3.24932	4.49444	O	-0.71494	1.53585	0.79816
H	3.52574	2.92935	3.37936	O	-0.81275	1.52057	-2.25954
C	3.44615	1.57591	7.54816	O	-1.13745	1.40742	-5.13989
H	4.44317	1.95757	7.82533	O	1.56106	0.86876	2.29498
H	2.70626	2.13143	8.15221	O	1.58548	0.81732	-0.74115
H	3.38381	0.52231	7.86099	O	1.51711	1.02814	-3.79945
C	-3.05035	3.96178	-4.32538	O	-1.42997	-0.91551	2.35656

O	-1.46093	-0.78214	-0.72149	H	-0.07658	4.61792	2.15071
O	-1.37196	-1.01042	-3.80077	H	1.34777	4.06381	-1.72479
C	-3.89879	-0.19374	4.29967	C	-0.77263	2.62114	6.87613
C	3.92544	-0.10053	4.37152	H	-1.86031	2.69190	7.04605
H	-4.02603	-0.91352	5.12697	H	-0.31896	2.27828	7.82250
H	4.39302	0.16403	5.34913	H	-0.40627	3.64564	6.69027
H	-4.33194	0.76404	4.63602	C	1.47914	-1.48431	6.98146
H	4.04473	-1.20016	4.39503	H	1.28648	-0.57609	7.57590
C	-3.69246	0.83212	1.00492	H	1.48429	-2.33311	7.68711
C	-3.82786	0.36568	-2.53057	H	2.50793	-1.39386	6.59661
C	3.80748	-0.85296	1.01712	C	-1.07841	-3.33849	5.63122
C	3.97972	-0.30284	-2.48679	H	-0.54596	-4.30310	5.65749
H	-4.50655	0.10131	0.86963	H	-1.66505	-3.26355	6.56546
H	-4.30172	0.60613	-1.56849	H	-1.80509	-3.39894	4.80415
H	4.62243	-0.10935	1.00971	C	1.50159	1.33935	-7.00083
H	4.45037	-0.38718	-1.49727	H	0.42613	1.52167	-7.12430
H	-3.85103	1.31445	1.98432	H	1.99749	2.32571	-6.98360
H	-4.04666	1.20386	-3.20705	H	1.86146	0.81326	-7.90112
H	3.89034	-1.41970	1.96162	C	3.95066	-0.29592	-5.80226
H	4.25647	-1.20524	-3.04973	H	4.17492	-0.13145	-6.86722
H	-4.50213	-0.54416	3.44849	H	4.26058	0.62752	-5.27088
H	-3.82356	1.62851	0.25218	H	4.70255	-1.00266	-5.39841
H	-4.35268	-0.52142	-2.92564	C	-1.31472	-1.32262	-7.01377
H	4.59480	0.28784	3.59124	H	-0.31276	-1.77059	-6.99754
H	4.01650	-1.58700	0.22072	H	-2.04255	-2.13594	-7.18026
H	4.46063	0.55725	-2.98374	H	-1.36930	-0.66170	-7.89597
C	-0.24390	-3.99861	2.45434	C	-3.76603	0.31797	-5.86140
C	-0.79394	-3.79365	-0.90250	H	-3.96308	0.09209	-6.92044
C	-0.15221	-3.93648	-4.28432	H	-4.10458	-0.56291	-5.27730
C	0.61407	3.92212	2.65631	H	-4.51876	1.06063	-5.52888
C	0.70552	3.87224	-0.84952	C	3.78709	3.17801	4.37464
C	0.32030	3.94712	-4.28448	H	3.33182	4.16955	4.54094
H	0.18088	-4.42460	3.37647	H	4.87980	3.29676	4.46874
H	-0.04671	-4.60230	-0.95180	H	3.56347	2.89808	3.33308
H	0.43104	-4.63837	-3.66669	C	3.43368	1.65030	7.53501
H	0.57615	4.16008	3.73534	H	4.41332	2.06377	7.82676
H	-0.15713	4.55642	-0.93130	H	2.66490	2.19679	8.11084
H	-1.30508	-4.29383	2.42128	H	3.39046	0.60164	7.86681
H	-1.45400	-4.00392	-0.04548	C	2.62419	-2.62910	-7.67315
H	-1.21419	-4.21078	-4.17004	H	3.58269	-2.86033	-8.16870
H	1.63236	4.16122	2.31312	H	1.95501	-3.49028	-7.84842
H	1.27978	4.17757	0.03905	H	2.18120	-1.76653	-8.19862
H	0.25528	-4.48515	1.60158	C	3.56114	-3.50432	-4.41297
H	-1.41761	-3.87350	-1.80872	H	3.24990	-4.53918	-4.63977
H	0.11354	-4.12311	-5.34067	H	4.66420	-3.49956	-4.37981

H	3.20385	-3.27583	-3.39570
C	-3.37636	3.55022	-4.52985
H	-3.02832	4.57343	-4.75642
H	-4.47953	3.57601	-4.54176
H	-3.06659	3.32630	-3.49614
C	-2.38557	2.62553	-7.75045
H	-3.32555	2.91465	-8.25103
H	-1.66620	3.44715	-7.91702
H	-1.99043	1.74231	-8.27869
H	0.14712	4.11151	-5.36379
H	1.36645	4.23317	-4.08438
H	-0.31989	4.65571	-3.73478

$(AlOMe)_{16,t} \cdot (AlMe_3)_4$

Al	0.98228	-1.58069	7.04894
Al	1.88597	0.86952	5.46659
Al	1.85668	0.68154	2.35311
Al	0.72929	-1.79973	3.95616
Al	-1.82516	-0.67538	2.34908
Al	-0.69365	1.81796	3.94063
Al	-1.85375	-0.83732	5.46155
Al	-0.95412	1.63038	7.03655
Al	0.73006	-1.85301	0.81303
Al	-0.70364	1.86468	0.80234
Al	-1.76573	-0.77548	-0.78919
Al	0.94785	-1.84008	-2.28344
Al	1.82260	0.78949	-0.77035
Al	-0.86459	1.83965	-2.30575
Al	1.66770	0.97342	-3.86394
Al	-1.55482	-0.98377	-3.87981
Al	1.09268	3.30921	7.48120
Al	3.45076	-1.01852	-4.21813
Al	-3.33032	1.00499	-4.28096
Al	-1.04393	-3.29283	7.46960
O	1.10580	1.37889	3.88584
O	1.31492	-1.08461	2.37137
O	-1.07404	-1.36468	3.88597
O	-1.29207	1.09564	2.36261
O	-1.48135	0.98345	5.41879
O	-0.81220	-1.62681	6.74716
O	0.84462	1.63873	6.76688
O	-1.05810	-1.34355	0.80634
O	1.08962	1.36229	0.81287
O	-1.37380	1.04603	-0.72133
O	-0.88023	-1.49572	-2.27341
O	1.43333	-1.03667	-0.69608
O	0.96206	1.49499	-2.27321
O	-1.64115	0.81021	-3.59987
O	1.75014	-0.81684	-3.56655
O	1.52373	-0.95518	5.42793
C	-1.16166	3.67290	7.49365
H	-2.05547	3.70364	6.83499
H	-0.71444	4.65882	7.25470
H	-1.52005	3.72673	8.53290
C	-3.71736	-1.26806	5.94788
H	-4.12003	-2.12285	5.37999
H	-4.40658	-0.42163	5.79302
H	-3.77090	-1.52869	7.02039
C	-0.91038	3.77488	4.08087
H	-0.52396	4.19030	5.01924
H	-1.96217	4.09485	3.98644
H	-0.34813	4.27302	3.27669
C	-3.67721	-1.22653	-1.01860
H	-4.21293	-1.21861	-0.06001
H	-3.78657	-2.24529	-1.42946
H	-4.21778	-0.54242	-1.68714
C	3.73361	1.25972	-0.97778
H	4.24855	1.30471	-0.00891
H	3.83363	2.26178	-1.43008
H	4.30123	0.55803	-1.60476
C	-1.20219	3.70573	-2.85246
H	-2.22089	4.06333	-2.62695
H	-1.07427	3.75647	-3.94949
H	-0.49335	4.42515	-2.41217
C	-3.59772	-1.24604	-4.34349
H	-4.58972	-0.87992	-4.01113
H	-3.54866	-2.19111	-3.76356
H	-3.68182	-1.52747	-5.40413
C	3.71805	1.23023	-4.30117
H	4.70320	0.86932	-3.94332
H	3.66095	2.18678	-3.74155
H	3.82179	1.49188	-5.36523
C	1.31096	-3.70574	-2.81899
H	2.30315	-4.07540	-2.51052
H	1.27507	-3.74930	-3.92316
H	0.56016	-4.42102	-2.44633
C	-1.02550	3.81204	0.68715
H	-0.11882	4.40016	0.91134
H	-1.79805	4.11885	1.41146
H	-1.37776	4.12908	-0.30461

C	0.99219	-3.80952	0.71938
H	0.08828	-4.35422	1.04279
H	1.81565	-4.12618	1.38106
H	1.23901	-4.16935	-0.28908
C	-3.79428	-0.72499	2.46742
H	-4.24437	-0.04103	1.72767
H	-4.13391	-0.37192	3.45465
H	-4.23646	-1.72399	2.31551
C	0.99470	-3.74940	4.10424
H	0.70483	-4.16581	5.07578
H	2.04679	-4.03184	3.92778
H	0.38967	-4.27813	3.35288
C	3.82531	0.70068	2.48520
H	4.27466	0.04500	1.72005
H	4.14279	0.29280	3.45929
H	4.28720	1.69768	2.38976
C	3.75263	1.34436	5.90376
H	4.43559	0.48050	5.83927
H	3.82567	1.73087	6.93660
H	4.15368	2.12435	5.23616
C	1.21276	-3.61425	7.55551
H	2.16998	-3.59243	6.99071
H	0.82966	-4.60874	7.25223
H	1.47850	-3.67583	8.62134
C	1.74964	-0.65097	8.61501
H	0.99777	0.00468	9.08001
H	2.61307	-0.01299	8.37213
H	2.07574	-1.37310	9.38135
C	1.43447	3.21092	9.42280
H	0.74696	2.49740	9.90584
H	1.31449	4.18128	9.93409
H	2.45929	2.85713	9.63085
C	1.98752	4.53262	6.21882
H	1.86266	4.19536	5.17734
H	3.07164	4.57602	6.42087
H	1.60612	5.56692	6.27262
C	4.66385	-1.84816	-2.89853
H	4.24627	-1.79959	-1.87959
H	5.66158	-1.37803	-2.86192
H	4.82076	-2.91535	-3.13474
C	3.40892	-1.46729	-6.14075
H	4.37850	-1.31874	-6.64614
H	2.66229	-0.85809	-6.67614
H	3.12724	-2.52499	-6.28928
C	-0.69649	-1.74710	-5.48208
H	-1.04721	-1.19280	-6.36863
H	-0.99998	-2.79889	-5.62278
H	0.39998	-1.71676	-5.48127
C	-3.25643	1.43160	-6.20745
H	-4.21745	1.27836	-6.72746
H	-2.50181	0.81505	-6.72279
H	-2.97035	2.48698	-6.36362
C	-4.56372	1.85051	-2.98957
H	-4.15993	1.81850	-1.96436
H	-5.56036	1.37754	-2.95894
H	-4.72118	2.91347	-3.24385
C	0.83566	1.72369	-5.48583
H	1.19601	1.15909	-6.36199
H	1.14546	2.77270	-5.63338
H	-0.26084	1.69761	-5.49948
C	-1.43513	-3.14347	9.39919
H	-2.47064	-2.80364	9.57517
H	-0.76883	-2.40044	9.86867
H	-1.30739	-4.09229	9.94745
C	-1.88167	-4.55354	6.20750
H	-1.71845	-4.23737	5.16475
H	-2.97231	-4.60184	6.37040
H	-1.49489	-5.58303	6.29945
C	-1.83622	0.79647	8.59081
H	-2.91587	1.02856	8.58296
H	-1.42571	1.22609	9.52004
H	-1.73835	-0.29383	8.65314

$(AlOMe)_{18,t}$

Al	0.62914	-1.17217	0.05258
Al	2.07344	0.40083	-1.54647
Al	1.92052	0.20292	-4.55372
Al	0.30680	-2.00289	-2.99182
Al	-1.92052	-0.20292	-4.55372
Al	-0.30680	2.00289	-2.99182
Al	-2.07344	-0.40083	-1.54647
Al	-0.62914	1.17217	0.05258
Al	0.20637	-1.98412	-6.12776
Al	-0.20637	1.98412	-6.12776
Al	-1.94033	-0.29017	-7.67649
Al	0.43075	-1.97083	-9.22845
Al	1.94033	0.29017	-7.67649
Al	-0.43075	1.97083	-9.22845
Al	-2.04411	-0.54111	-10.67087
Al	0.70705	-1.12468	-12.26231

Al	-0.70705	1.12468	-12.26231	H	4.64564	0.26977	-10.72798
Al	2.04411	0.54111	-10.67087	H	4.18603	1.97479	-10.63505
O	1.33567	1.11321	-3.04835	H	4.02226	1.10420	-12.17487
O	0.99522	-1.40667	-4.57701	C	-1.42812	2.29787	-13.64648
O	-1.33567	-1.11321	-3.04835	H	-2.53088	2.26398	-13.65736
O	-0.99522	1.40667	-4.57701	H	-1.07433	2.02302	-14.65387
O	-1.32825	1.32923	-1.63125	H	-1.13802	3.34779	-13.47154
O	-1.11820	-0.66407	0.00300	C	-0.31347	3.90668	-9.60506
O	1.11820	0.66407	0.00300	H	0.69143	4.32074	-9.42284
O	-1.09232	1.35896	-7.62520	H	-1.01675	4.48842	-8.98625
O	-1.25065	-1.18379	-9.15638	H	-0.56958	4.11754	-10.65947
O	1.09232	-1.35896	-7.62520	C	3.89900	0.18131	-7.89175
O	-1.38600	-1.02788	-6.09818	H	4.31265	1.11229	-8.31104
O	1.25065	1.18379	-9.15638	H	4.20911	-0.63978	-8.55996
O	-1.43036	1.22739	-10.58038	H	4.39924	0.01229	-6.92844
O	-1.06160	-0.75066	-12.21219	C	0.31347	-3.90668	-9.60506
O	1.06160	0.75066	-12.21219	H	-0.69143	-4.32074	-9.42284
O	1.43036	-1.22739	-10.58038	H	1.01675	-4.48842	-8.98625
O	1.38600	1.02788	-6.09818	H	0.56958	-4.11754	-10.65947
O	1.32825	-1.32923	-1.63125	C	-3.89900	-0.18131	-7.89175
C	-1.17770	2.44331	1.43126	H	-4.31265	-1.11229	-8.31104
H	-2.27336	2.55090	1.48839	H	-4.20911	0.63978	-8.55996
H	-0.76323	3.44330	1.21508	H	-4.39924	-0.01229	-6.92844
H	-0.81330	2.15055	2.42994	C	0.13249	3.92466	-6.19586
C	-3.98899	-0.63484	-1.17739	H	0.66353	4.26729	-5.29404
H	-4.52995	-1.15765	-1.98013	H	-0.79155	4.52136	-6.27752
H	-4.48805	0.33962	-1.03707	H	0.76427	4.19046	-7.05869
H	-4.12334	-1.20484	-0.24267	C	-3.81854	0.31578	-4.40347
C	-0.00005	3.92348	-2.65949	H	-4.03630	1.06996	-5.17873
H	0.99892	4.24723	-2.99516	H	-4.02274	0.81394	-3.44103
H	-0.06212	4.14450	-1.57775	H	-4.55085	-0.50029	-4.50816
H	-0.73847	4.57173	-3.15885	C	0.00005	-3.92348	-2.65949
C	-0.13249	-3.92466	-6.19586	H	-0.99892	-4.24723	-2.99516
H	-0.66353	-4.26729	-5.29404	H	0.06212	-4.14450	-1.57775
H	0.79155	-4.52136	-6.27752	H	0.73847	-4.57173	-3.15885
H	-0.76427	-4.19046	-7.05869	C	3.81854	-0.31578	-4.40347
C	-3.90865	-1.00524	-11.08209	H	4.03630	-1.06996	-5.17873
H	-4.64564	-0.26977	-10.72798	H	4.02274	-0.81394	-3.44103
H	-4.18603	-1.97479	-10.63505	H	4.55085	0.50029	-4.50816
H	-4.02226	-1.10420	-12.17487	C	3.98899	0.63484	-1.17739
C	1.42812	-2.29787	-13.64648	H	4.48805	-0.33962	-1.03707
H	2.53088	-2.26398	-13.65736	H	4.12334	1.20484	-0.24267
H	1.07433	-2.02302	-14.65387	H	4.52995	1.15765	-1.98013
H	1.13802	-3.34779	-13.47154	C	1.17770	-2.44331	1.43126
C	3.90865	1.00524	-11.08209	H	0.76323	-3.44330	1.21508

H	0.81330	-2.15055	2.42994
H	2.27336	-2.55090	1.48839

$(AlOMe)_{18,t} \cdot (AlMe_3)$

Al	0.66276	-1.08312	0.16905
Al	2.11447	0.46993	-1.44782
Al	1.99945	0.18257	-4.44598
Al	-2.49419	-2.43194	-12.36910
Al	0.36714	-1.97773	-2.85311
Al	-1.85570	-0.19564	-4.46881
Al	-0.25414	2.02348	-2.93835
Al	-2.03312	-0.37582	-1.47077
Al	-0.61365	1.24454	0.10265
Al	0.26623	-2.02274	-5.97918
Al	-0.06628	1.95710	-6.05440
Al	-1.83388	-0.28526	-7.56970
Al	0.48463	-2.09022	-9.08458
Al	2.03798	0.18375	-7.59181
Al	-0.23743	1.94073	-9.16364
Al	-1.72600	-0.47579	-10.60053
Al	0.79819	-1.41220	-12.13592
Al	-0.23776	1.61025	-12.31762
Al	2.13554	0.31900	-10.61991
O	1.39140	1.14399	-2.97299
O	1.06524	-1.41503	-4.44039
O	-1.27733	-1.10256	-2.95210
O	-0.91821	1.40178	-4.51781
O	-1.30104	1.35307	-1.58643
O	-1.08373	-0.60096	0.09053
O	1.13836	0.75675	0.08461
O	-0.93560	1.33115	-7.55835
O	-1.17773	-1.18740	-9.03817
O	1.15038	-1.44663	-7.49184
O	-1.32094	-1.04891	-5.99181
O	1.40603	1.07715	-9.10789
O	-1.07599	1.20432	-10.64937
O	-0.97949	-1.57191	-11.86076
O	1.13167	0.38316	-12.17965
O	1.53312	-1.44034	-10.44167
O	1.49932	0.96176	-6.01930
O	1.38277	-1.26222	-1.50669
C	-1.21812	2.50497	1.46425
C	-3.94084	-0.65951	-1.10154
H	-4.46586	-1.18814	-1.91118
H	-4.47006	0.29648	-0.94649
H	-4.05687	-1.24699	-0.17503
C	-0.00840	3.94764	-2.57423
H	1.02291	4.28563	-2.76594
H	-0.23851	4.18148	-1.51883
H	-0.67126	4.57594	-3.19114
C	-0.09282	-3.96016	-5.92564
H	-0.71794	-4.21798	-5.05537
H	0.82621	-4.56691	-5.85777
H	-0.63882	-4.29759	-6.82113
C	-3.66925	-0.65944	-11.20492
H	-3.93909	0.41389	-11.20695
H	-4.32129	-1.15991	-10.47726
H	-4.03839	-0.94764	-12.21757
C	1.46081	-2.57507	-13.56493
H	2.54722	-2.46332	-13.71875
H	0.97008	-2.34607	-14.52688
H	1.27210	-3.64090	-13.34783
C	3.99868	0.76575	-11.06561
H	4.73386	0.06078	-10.64849
H	4.26992	1.76837	-10.69331
H	4.12074	0.77833	-12.16184
C	-1.50802	1.08655	-13.76591
H	-2.51656	0.82264	-13.40953
H	-1.14044	0.22025	-14.34024
H	-1.63753	1.91307	-14.48610
C	-0.29963	3.90999	-9.29056
H	0.69434	4.38605	-9.29854
H	-0.85767	4.33820	-8.44295
H	-0.81005	4.22048	-10.21589
C	3.99538	0.01177	-7.78746
H	4.42734	0.90963	-8.25844
H	4.27536	-0.84874	-8.41896
H	4.49970	-0.12182	-6.82050
C	0.27468	-4.03369	-9.37780
H	-0.72910	-4.41021	-9.12623
H	1.00269	-4.62230	-8.79514
H	0.44798	-4.26872	-10.44431
C	-3.78370	-0.11021	-7.86200
H	-4.23660	-1.09001	-8.09435
H	-4.03105	0.56733	-8.69837
H	-4.31327	0.28466	-6.98362
C	0.41064	3.86929	-5.99841
H	1.03449	4.07487	-5.11318
H	-0.45361	4.55228	-5.95336
H	1.00635	4.15360	-6.88040

C	-3.76389	0.30179	-4.34532
H	-3.96281	1.08438	-5.09672
H	-4.02347	0.75238	-3.37352
H	-4.47358	-0.52219	-4.52235
C	0.08602	-3.88881	-2.45100
H	-0.92479	-4.22899	-2.72946
H	0.20810	-4.08720	-1.37044
H	0.80128	-4.54143	-2.97729
C	3.89433	-0.32931	-4.24880
H	4.11442	-1.10613	-5.00060
H	4.09800	-0.79463	-3.27044
H	4.62319	0.48539	-4.38172
C	4.01754	0.77228	-1.07181
H	4.54461	-0.17413	-0.86189
H	4.12439	1.40812	-0.17705
H	4.55010	1.25676	-1.90359
C	1.24710	-2.31656	1.56528
H	0.85808	-3.33091	1.37026
H	0.89054	-2.01925	2.56504
H	2.34616	-2.39556	1.60865
H	-0.83149	3.51769	1.25855
H	-0.86712	2.22143	2.47028
H	-2.31768	2.57683	1.49871
C	0.66434	3.37062	-12.43281
H	1.25638	3.36473	-13.36710
H	1.37155	3.57427	-11.61164
H	-0.01865	4.23397	-12.48601
C	-2.83723	-2.36729	-14.30504
H	-1.99884	-2.83771	-14.85015
H	-2.91752	-1.33450	-14.67707
H	-3.75420	-2.90770	-14.59364
C	-3.02943	-3.85565	-11.12132
H	-2.86962	-3.53108	-10.08089
H	-2.43613	-4.77506	-11.26400
H	-4.09295	-4.12769	-11.23201

$(AlOMe)_{18,t} \cdot (AlMe_3)_2$

Al	0.27556	-1.83878	0.25534
Al	1.94217	0.16169	-1.41102
Al	2.04307	0.00836	-4.45184
Al	0.27740	-2.11792	-2.89993
Al	-1.82580	-0.15163	-4.44272
Al	-0.11376	1.96214	-2.90016
Al	-1.97935	-0.36499	-1.43542
Al	-0.53948	1.24170	0.12077
Al	0.16745	-2.05191	-6.01677
Al	0.09076	1.93516	-6.01325
Al	-1.79428	-0.15377	-7.57161
Al	0.40198	-2.09404	-9.11502
Al	2.09502	0.05714	-7.58085
Al	-0.04261	1.98564	-9.13138
Al	2.78826	2.05152	0.41816
Al	-1.67798	-0.30448	-10.61109
Al	-2.58923	-2.14178	-12.41676
Al	0.78437	-1.38995	-12.15314
Al	-0.03885	1.69925	-12.29353
Al	2.22756	0.22660	-10.60263
O	1.48276	0.95282	-2.96373
O	1.01952	-1.51823	-4.47521
O	-1.30338	-1.15123	-2.95379
O	-0.79859	1.39116	-4.49899
O	-1.23905	1.34370	-1.58183
O	-1.00894	-0.52490	0.13684
O	1.24578	1.28030	-0.13991
O	-0.78838	1.39478	-7.55030
O	-1.19977	-1.08002	-9.05912
O	1.09824	-1.50943	-7.51961
O	-1.34500	-0.97287	-6.00872
O	1.54278	1.01530	-9.09277
O	-0.90941	1.32622	-10.63841
O	-1.00866	-1.42118	-11.89397
O	1.24153	0.37522	-12.17364
O	1.49805	-1.48958	-10.45802
O	1.60500	0.85752	-6.01023
O	1.15389	-1.45491	-1.40021
C	-1.15329	2.39861	1.57367
C	-3.87043	-0.73256	-1.04971
H	-4.40988	-1.15109	-1.91330
H	-4.41602	0.17196	-0.72982
H	-3.93535	-1.45965	-0.22176
C	0.17694	3.88509	-2.54964
H	1.20492	4.22501	-2.74709
H	-0.04503	4.11770	-1.49185
H	-0.49485	4.50840	-3.16362
C	-0.43769	-3.92693	-6.10780
H	-1.05729	-4.17420	-5.23017
H	0.37272	-4.67285	-6.16071
H	-1.07417	-4.07504	-6.99633
C	-3.62564	-0.30698	-11.22782
H	-3.78841	0.78786	-11.21770

H	-4.32031	-0.74927	-10.50178
H	-4.02536	-0.54860	-12.24013
C	1.32727	-2.58436	-13.60763
H	2.41526	-2.57721	-13.78621
H	0.84075	-2.29589	-14.55626
H	1.04003	-3.63116	-13.40421
C	4.12152	0.49945	-11.05467
H	4.78430	-0.27512	-10.63886
H	4.49595	1.47087	-10.69022
H	4.23775	0.49303	-12.15203
C	-1.32903	1.30038	-13.76296
H	-2.36449	1.13294	-13.42567
H	-1.03621	0.40421	-14.33477
H	-1.36594	2.13657	-14.48293
C	0.05318	3.95199	-9.26264
H	1.08507	4.33922	-9.24691
H	-0.48467	4.42945	-8.42905
H	-0.40473	4.30218	-10.20100
C	4.03237	-0.28518	-7.77655
H	4.55465	0.57243	-8.23119
H	4.23277	-1.16065	-8.41826
H	4.51658	-0.48117	-6.80946
C	0.07033	-4.00914	-9.47976
H	-0.97004	-4.31832	-9.29454
H	0.71668	-4.66542	-8.87375
H	0.28891	-4.23082	-10.54090
C	-3.71476	0.21082	-7.86991
H	-4.27758	-0.71153	-8.09595
H	-3.88731	0.91109	-8.70635
H	-4.18944	0.66645	-6.98905
C	0.66980	3.81901	-5.95587
H	1.28599	3.99904	-5.05919
H	-0.15550	4.55033	-5.93553
H	1.29992	4.06060	-6.82752
C	-3.71486	0.41772	-4.31224
H	-3.87254	1.26398	-5.00163
H	-3.98409	0.79057	-3.31062
H	-4.44241	-0.36803	-4.57343
C	0.24843	-4.08799	-2.81883
H	-0.76407	-4.52201	-2.82609
H	0.74692	-4.44681	-1.90489
H	0.78781	-4.50966	-3.68139
C	3.92500	-0.53665	-4.17546
H	4.20834	-1.28218	-4.93644
H	4.07286	-1.04496	-3.20681
H	4.65666	0.28717	-4.22771
C	3.88973	0.24086	-0.81838
H	4.12961	-0.83879	-0.79622
H	4.29303	0.54663	0.17611
H	4.53726	0.70966	-1.57259
C	1.58479	-1.42668	1.70333
H	1.67716	-2.27743	2.40035
H	1.27820	-0.55432	2.30321
H	2.60177	-1.21342	1.33630
H	-0.88955	3.45748	1.40891
H	-0.70878	2.09517	2.53735
H	-2.24887	2.35102	1.69229
C	1.01939	3.37171	-12.39588
H	1.61442	3.30302	-13.32615
H	1.73894	3.50493	-11.57084
H	0.42752	4.29907	-12.45597
C	-2.95128	-2.00739	-14.34678
H	-2.15533	-2.51066	-14.92433
H	-2.97838	-0.96176	-14.69024
H	-3.90555	-2.48295	-14.62999
C	-3.24076	-3.53335	-11.18797
H	-3.05165	-3.23677	-10.14408
H	-2.73266	-4.50003	-11.34380
H	-4.32479	-3.70720	-11.29831
C	-0.72213	-3.54805	0.31482
H	-1.43047	-3.69082	-0.51791
H	-1.32048	-3.54281	1.24463
H	-0.08132	-4.44403	0.34385
C	3.41563	3.48194	-0.77533
H	3.27194	3.19209	-1.82836
H	4.48463	3.71216	-0.62901
H	2.85270	4.41884	-0.62322
C	3.07702	1.89281	2.35649
H	2.19088	2.28198	2.88976
H	3.95023	2.46357	2.71246
H	3.19835	0.84525	2.67139

$(AlOMe)_{18,t} \cdot (AlMe_3)_3$

Al	0.53581	-1.70007	0.18906
Al	2.02815	0.46219	-1.42890
Al	2.08815	0.18640	-4.51940
Al	0.38152	-1.93549	-2.91646
Al	-1.87890	-0.26520	-4.58437
Al	-0.25033	1.94035	-3.02548
Al	-1.98360	-0.38758	-1.50187

Al	-0.57437	1.86471	0.06519	C	-3.61415	-0.61999	-11.23289
Al	0.31923	-2.03816	-6.04410	H	-3.87591	0.45459	-11.26546
Al	-0.01151	1.90672	-6.12685	H	-4.22332	-1.08310	-10.44453
Al	-1.76130	-0.26461	-7.66383	H	-4.04833	-0.95323	-12.20429
Al	0.48633	-2.14267	-9.16503	C	1.47424	-2.66231	-13.62372
Al	2.08816	0.09795	-7.66328	H	2.56496	-2.58888	-13.76945
Al	-0.10494	1.92492	-9.25028	H	0.99987	-2.42153	-14.59086
Al	-1.65824	-0.45590	-10.68329	H	1.24726	-3.71982	-13.40311
Al	0.84430	-1.47139	-12.20647	C	4.10027	0.64361	-11.07901
Al	-2.47973	-2.40193	-12.42481	H	4.65670	-0.24686	-11.41923
Al	1.77991	3.10059	0.49100	H	4.64128	1.05602	-10.21430
Al	-0.08511	1.57148	-12.40641	H	4.14618	1.38488	-11.89556
Al	-1.83892	-2.91213	0.57845	C	-1.38577	1.07666	-13.83553
Al	2.22261	0.22852	-10.68382	H	-2.39533	0.85842	-13.45111
O	1.41899	1.10246	-3.04463	H	-1.06724	0.18487	-14.39910
O	1.15365	-1.41910	-4.50030	H	-1.50169	1.89395	-14.56790
O	-1.28094	-1.11052	-3.04393	C	-0.16301	3.89190	-9.37833
O	-0.94062	1.34168	-4.61742	H	0.82779	4.37249	-9.40540
O	-1.19983	1.29355	-1.54115	H	-0.70051	4.30801	-8.51168
O	-1.21290	-1.35878	-0.15746	H	-0.70023	4.20662	-10.28700
O	1.19114	1.50379	-0.17963	C	4.01291	-0.32823	-7.77001
O	-0.82901	1.32008	-7.66862	H	4.67338	0.55234	-7.71449
O	-1.15119	-1.20746	-9.12849	H	4.27200	-0.87249	-8.69359
O	1.16962	-1.50858	-7.58852	H	4.27851	-0.99174	-6.93087
O	-1.25901	-1.07213	-6.10571	C	0.27846	-4.08121	-9.48851
O	1.51707	1.02401	-9.18490	H	-0.71872	-4.47490	-9.23899
O	-0.94698	1.19243	-10.73911	H	1.01498	-4.66380	-8.90967
O	-0.93956	-1.56611	-11.94579	H	0.45675	-4.30885	-10.55569
O	1.24674	0.30961	-12.26387	C	-3.67281	0.17494	-7.91983
O	1.56380	-1.50673	-10.51009	H	-4.34659	-0.69821	-7.95155
O	1.54094	0.89647	-6.11120	H	-3.84481	0.75952	-8.84095
O	1.24881	-1.22048	-1.41203	H	-4.01343	0.81880	-7.09292
C	-1.55095	1.26962	1.67374	C	0.63512	3.77317	-6.12621
C	-3.88959	-0.24493	-1.01067	H	1.30539	3.92572	-5.26175
H	-4.46831	-1.16847	-1.18127	H	-0.13137	4.56450	-6.10297
H	-4.41461	0.57476	-1.52617	H	1.24940	3.93894	-7.02730
H	-3.93331	-0.02905	0.07315	C	-3.85506	-0.12889	-4.52305
C	-0.27555	3.90855	-2.79856	H	-4.22119	0.90756	-4.62125
H	0.55177	4.30232	-2.19082	H	-4.27689	-0.53425	-3.59123
H	-1.21732	4.21676	-2.31217	H	-4.29877	-0.70859	-5.34862
H	-0.23834	4.43268	-3.76266	C	0.35961	-3.88565	-2.57894
C	-0.12019	-3.96248	-6.02941	H	-0.47031	-4.20712	-1.93356
H	-0.88281	-4.17072	-5.25831	H	1.29751	-4.19483	-2.08528
H	0.74071	-4.62587	-5.83753	H	0.28491	-4.47256	-3.50331
H	-0.56141	-4.27245	-6.98994	C	4.05372	0.03145	-4.35553

H	4.40270	-1.01370	-4.41705	H	-2.71839	-5.05081	-0.64491
H	4.43867	0.44617	-3.41249	C	-0.32677	3.91610	0.52204
H	4.54689	0.58401	-5.17123	H	0.25735	4.78713	0.16457
C	3.90889	0.35392	-0.83976	H	-0.56098	4.07638	1.58557
H	4.45507	-0.50059	-1.26935	H	-1.27088	4.08517	-0.03584
H	3.90114	0.21540	0.25722				
H	4.49787	1.26290	-1.04751	$(AlOMe)_{18,t} \cdot (AlMe_3)_4$			
C	1.41660	-1.01467	1.81553	Al	0.56855	-1.68384	0.17509
H	0.71700	-1.12996	2.66043	Al	2.09664	0.44791	-1.40881
H	1.72408	0.03719	1.78125	Al	2.13981	0.12710	-4.47505
H	2.30852	-1.61708	2.05991	Al	0.37910	-1.93603	-2.91053
H	-0.91963	1.46294	2.55710	Al	-1.78248	-0.15531	-4.59558
H	-1.83095	0.21008	1.69112	Al	-0.12005	1.98573	-3.02650
H	-2.47330	1.86039	1.80867	Al	-1.94585	-0.32487	-1.52462
C	0.85854	3.31000	-12.48631	Al	-0.52228	1.88657	0.04520
H	1.45780	3.31835	-13.41519	Al	0.35454	-2.01362	-6.04927
H	1.56277	3.47520	-11.65416	Al	0.11069	1.89461	-6.16335
H	0.19444	4.18841	-12.51660	Al	-1.71262	-0.30934	-7.71074
C	-2.83986	-2.30837	-14.35541	Al	0.65332	-2.09290	-9.14818
H	-1.96924	-2.69749	-14.91354	Al	2.26880	0.11074	-7.59736
H	-2.99321	-1.27224	-14.69408	Al	0.00939	1.79448	-9.28223
H	-3.71616	-2.90314	-14.66170	Al	-1.62515	-0.62507	-10.76891
C	-2.99673	-3.81981	-11.16408	Al	0.98402	-2.03246	-12.23016
H	-2.82325	-3.48551	-10.12877	Al	-0.12227	1.54817	-12.37531
H	-2.40096	-4.73763	-11.30580	Al	2.24894	2.79674	-12.68497
H	-4.06019	-4.09861	-11.25593	Al	-1.36068	-3.29700	-12.62267
C	0.26482	-3.72387	0.74810	Al	-1.83440	-2.82424	0.55710
H	-0.31384	-4.61435	0.43098	Al	1.84020	3.09844	0.48032
H	0.46793	-3.81958	1.82569	Al	2.38295	0.23750	-10.67061
H	1.22209	-3.93023	0.22583	O	1.52239	1.10980	-3.02460
C	2.92591	4.07966	-0.78497	O	1.14516	-1.43483	-4.48825
H	3.98955	3.97824	-0.50647	O	-1.26104	-1.06268	-3.05770
H	2.70782	5.16072	-0.82594	O	-0.78224	1.39969	-4.62426
H	2.81932	3.68930	-1.81013	O	-1.13968	1.34934	-1.57467
C	2.14634	2.96266	2.42771	O	-1.16958	-1.27750	-0.15962
H	3.09772	2.43482	2.61746	O	1.24145	1.50201	-0.18053
H	1.35573	2.39587	2.94626	O	-0.75450	1.28460	-7.69658
H	2.22132	3.94649	2.92256	O	-1.01396	-1.25725	-9.15516
C	-2.30561	-2.65116	2.47995	O	1.31878	-1.48612	-7.55161
H	-1.53395	-2.07221	3.01273	O	-1.20404	-1.00336	-6.10564
H	-2.43927	-3.60045	3.02689	O	1.66952	0.96670	-9.13732
H	-3.25207	-2.09002	2.57676	O	-0.84945	1.06174	-10.78628
C	-2.92887	-3.96812	-0.68487	O	-0.78131	-1.67365	-12.00917
H	-2.77312	-3.64671	-1.72765	O	1.62591	1.20903	-12.01998
H	-4.00348	-3.84295	-0.46339	O	1.60910	-1.44818	-10.63066

O	1.66251	0.89301	-6.06408	H	-3.94942	0.83269	-8.43260
O	1.28719	-1.22259	-1.42805	H	-4.21218	-0.22649	-7.03623
C	-1.51156	1.23749	1.62781	C	0.74986	3.76457	-6.21885
C	-3.88051	-0.28300	-1.12000	H	1.37766	3.94933	-5.32902
H	-4.47538	-0.91187	-1.80191	H	-0.02271	4.55126	-6.25179
H	-4.29282	0.73860	-1.18201	H	1.41046	3.90786	-7.09229
H	-4.07323	-0.64079	-0.09170	C	-3.68433	0.37044	-4.49486
C	-0.13974	3.95800	-2.84364	H	-3.91488	1.07747	-5.30919
H	0.72022	4.39166	-2.31390	H	-3.90515	0.90299	-3.55485
H	-1.05267	4.28271	-2.31588	H	-4.39948	-0.46619	-4.56537
H	-0.17468	4.42981	-3.83596	C	0.34041	-3.89258	-2.61620
C	-0.33842	-3.86610	-6.05580	H	-0.50122	-4.24951	-2.00591
H	-1.05291	-3.96550	-5.21869	H	1.27130	-4.22262	-2.12299
H	0.39301	-4.68715	-5.97383	H	0.28850	-4.43055	-3.57284
H	-0.92886	-4.03299	-6.97451	C	4.02139	-0.41179	-4.21914
C	-3.50750	-0.54906	-11.34724	H	4.30349	-1.13573	-5.00169
H	-4.08336	0.25503	-10.86467	H	4.15147	-0.93390	-3.25637
H	-4.05333	-1.49156	-11.17100	H	4.75503	0.41064	-4.24201
H	-3.52325	-0.36132	-12.43682	C	3.99574	0.40337	-0.87272
C	1.96104	-1.43828	-13.83587	H	4.40804	-0.61924	-0.89542
H	2.25967	-0.38337	-13.83713	H	4.11257	0.77134	0.16280
H	1.32497	-1.60673	-14.72054	H	4.63812	1.02281	-1.51951
H	2.87285	-2.04290	-13.97993	C	1.55510	-1.04403	1.76018
C	4.30148	0.12321	-11.10185	H	1.01208	-1.33624	2.67439
H	4.83243	-0.64660	-10.52123	H	1.72073	0.03895	1.79890
H	4.83868	1.07477	-10.94954	H	2.54630	-1.52758	1.81180
H	4.39870	-0.14037	-12.17113	H	-1.64999	2.04570	2.36445
C	-0.98076	0.84952	-14.00717	H	-0.95181	0.43229	2.12645
H	-1.86867	1.44920	-14.27060	H	-2.50520	0.82795	1.39108
H	-1.29217	-0.20049	-13.95755	C	0.13788	3.57848	-12.89592
H	-0.27108	0.94721	-14.84553	H	-0.01010	3.70365	-13.97939
C	-0.05121	3.75203	-9.58722	H	0.68109	4.46629	-12.51654
H	0.82321	4.17199	-10.10448	H	-0.85067	3.75385	-12.42395
H	-0.14557	4.28914	-8.63307	C	-2.48087	-4.24437	-11.30164
H	-0.94459	4.01443	-10.17976	H	-3.54827	-4.17873	-11.57576
C	4.23782	-0.04047	-7.70747	H	-2.37559	-3.80293	-10.29727
H	4.65619	0.67984	-8.42885	H	-2.23949	-5.31715	-11.20987
H	4.58126	-1.04322	-8.01496	C	-1.72888	-3.19395	-14.55915
H	4.70187	0.17706	-6.73421	H	-1.80723	-4.18026	-15.04719
C	0.71561	-4.06614	-9.32476	H	-0.93574	-2.63223	-15.07941
H	-0.14025	-4.51262	-9.85133	H	-2.67785	-2.66259	-14.75045
H	0.75990	-4.53779	-8.33308	C	0.25895	-3.70135	0.68601
H	1.63149	-4.37586	-9.85626	H	-0.35004	-4.56198	0.34767
C	-3.66480	-0.13569	-7.98553	H	0.46742	-3.83447	1.75817
H	-4.05007	-0.92350	-8.65332	H	1.20508	-3.92131	0.14966

C	3.00148	4.06112	-0.79022
H	4.06389	3.95065	-0.51206
H	2.79249	5.14334	-0.84095
H	2.89078	3.66149	-1.81127
C	2.15041	2.92737	2.42306
H	2.26004	3.89352	2.94413
H	3.06507	2.34367	2.62780
H	1.31341	2.38952	2.89924
C	-2.22621	-2.59961	2.47857
H	-1.42259	-2.03100	2.97463
H	-2.32970	-3.55828	3.01502
H	-3.16183	-2.03577	2.63714
C	-2.93603	-3.84046	-0.72545
H	-2.74539	-3.52118	-1.76277
H	-4.01067	-3.68194	-0.53019
H	-2.75804	-4.92881	-0.68336
C	-0.26023	3.94148	0.46038
H	0.30494	4.78706	0.02441
H	-0.45372	4.16086	1.52110
H	-1.23126	4.07697	-0.06028
C	0.75930	-4.09082	-12.63436
H	0.96998	-4.29127	-13.69587
H	0.19641	-4.95129	-12.22290
H	1.72126	-4.22534	-12.09803
C	3.26907	3.82407	-11.34249
H	3.03542	4.90247	-11.34285
H	4.35435	3.73149	-11.52258
H	3.07655	3.45267	-10.32296
C	2.77124	2.56344	-14.57376
H	2.01488	1.97765	-15.12141
H	3.72111	2.00362	-14.64209
H	2.91510	3.51048	-15.12061

$(AlOMe)_{20,t}$

Al	0.47339	-0.60827	7.02796
Al	1.81135	1.01247	5.38217
Al	1.75139	0.64982	2.37926
Al	-2.24700	-0.20309	5.32271
Al	-1.00688	1.58937	6.86493
Al	-0.66691	2.28193	3.80166
Al	-2.03186	-0.13864	2.32071
Al	0.32639	-1.62140	4.02893
Al	-0.49801	2.13696	0.68021
Al	-1.99593	-0.34468	-0.79772
Al	0.52288	-1.87493	-2.19640
Al	0.27770	-1.77125	0.90186
Al	1.92992	0.51924	-0.70129
Al	-0.42574	1.90158	-2.39082
Al	-1.88000	-0.62880	-3.86419
Al	0.71986	-2.09458	-5.23386
Al	1.96084	0.51988	-3.85945
Al	-0.64028	1.90822	-5.37951
Al	1.15370	0.65026	-6.90593
Al	-0.98915	-0.92110	-6.89859
O	0.98813	-1.03660	2.42630
O	-1.39597	-0.92229	3.88496
O	-1.25754	1.53686	2.24601
O	-1.67430	1.57894	5.16547
O	1.04865	1.56905	3.82834
O	-1.30708	-0.29225	6.90601
O	0.78138	1.26556	6.88748
O	1.23861	-0.77423	5.37173
O	-1.22466	1.35403	-0.83774
O	-1.21134	-1.20194	-2.24871
O	1.15259	-1.16590	-0.61347
O	-1.38245	-0.95053	0.81894
O	1.26196	1.16240	-2.29418
O	-1.24493	1.11913	-3.85871
O	1.17365	1.42414	-5.25015
O	-1.07850	-1.59107	-5.19907
O	1.30969	-1.21545	-3.75159
O	1.18736	1.35224	0.77371
O	-0.73819	0.87190	-6.90143
O	0.90587	-1.14348	-6.79680
C	-1.74850	2.82081	8.18468
H	-2.84946	2.77121	8.22047
H	-1.47685	3.86344	7.94696
H	-1.36929	2.60826	9.19829
C	-4.12766	-0.64708	5.67146
H	-4.57932	-1.27030	4.88544
H	-4.74922	0.26045	5.75752
H	-4.20873	-1.18892	6.62904
C	-0.53143	4.22248	4.12006
H	0.22309	4.70812	3.48166
H	-0.22649	4.40383	5.16904
H	-1.48573	4.75583	3.97477
C	-0.07054	-3.70487	1.07322
H	-0.68457	-3.87959	1.97209
H	0.82096	-4.34705	1.15976
H	-0.66332	-4.06841	0.21723

C	-3.79673	-0.55991	-4.32759	H	-4.28974	0.76552	1.54470
H	-4.35640	0.19330	-3.75285	H	-4.26109	0.74735	3.30769
H	-4.31427	-1.52605	-4.20655	H	-4.59757	-0.75080	2.42080
H	-3.89317	-0.28509	-5.39642	C	0.27047	-3.54092	4.48842
C	3.89731	0.43981	-4.22011	H	-0.71798	-3.99254	4.30457
H	4.42086	-0.26722	-3.55760	H	0.50640	-3.69359	5.55716
H	4.39887	1.41744	-4.12587	H	1.00300	-4.13017	3.91308
H	4.07097	0.09509	-5.25757	C	3.68751	0.34395	2.60842
C	-1.20079	3.73105	-5.84495	H	4.04086	-0.33980	1.81928
H	-1.80699	4.21475	-5.06520	H	3.89505	-0.16137	3.56699
H	-1.79171	3.70682	-6.77622	H	4.31799	1.24619	2.57299
H	-0.33197	4.38598	-6.02805	C	3.67935	1.46997	5.77415
C	-2.06420	-1.76403	-8.29189	H	4.28431	0.56625	5.96044
H	-3.13850	-1.55781	-8.14923	H	3.73207	2.09111	6.68410
H	-1.94000	-2.86010	-8.27720	H	4.16939	2.01813	4.95576
H	-1.79268	-1.40939	-9.29993	C	1.15371	-1.74419	8.46381
C	2.34099	1.34557	-8.29086	H	2.25569	-1.72706	8.50651
H	3.39246	1.11819	-8.04321	H	0.85387	-2.79338	8.29672
H	2.26255	2.44044	-8.39463	H	0.77290	-1.45110	9.45587
H	2.13550	0.89719	-9.27701				
C	1.14069	-3.98030	-5.57245	$(AlOMe)_{20,t} \cdot (AlMe_3)$			
H	2.18327	-4.23264	-5.31635	Al	0.17602	-1.37375	7.12447
H	1.01038	-4.18870	-6.64850	Al	1.59204	0.76610	5.39659
H	0.49476	-4.67345	-5.01300	Al	2.22376	2.76462	7.15191
C	-0.15827	3.83719	-2.68237	Al	1.71994	0.57462	2.35314
H	0.38530	4.03543	-3.62181	Al	-2.22530	-0.25671	5.34905
H	0.47486	4.23702	-1.87364	Al	-1.01512	1.56820	6.87475
H	-1.08080	4.43838	-2.70876	Al	-0.67147	2.22277	3.81478
C	3.90383	0.64461	-0.74710	Al	-2.07482	-0.17031	2.33107
H	4.23869	1.16205	-1.65901	Al	0.27055	-1.75079	3.97434
H	4.41270	-0.33389	-0.72274	Al	-0.52257	2.11447	0.69232
H	4.28104	1.22638	0.10779	Al	-2.04053	-0.31173	-0.81775
C	0.74843	-3.83993	-2.24072	Al	0.46431	-1.88399	-2.21449
H	-0.14659	-4.38916	-2.57868	Al	0.19470	-1.80192	0.86363
H	1.00546	-4.22223	-1.24304	Al	1.90004	0.48643	-0.70206
H	1.57530	-4.12239	-2.91084	Al	-0.42778	1.90849	-2.39222
C	-3.96629	-0.47888	-0.94933	Al	-1.89048	-0.60534	-3.89315
H	-4.26309	-1.15180	-1.76813	Al	0.72968	-2.08379	-5.23691
H	-4.46532	0.48883	-1.12840	Al	1.96616	0.51331	-3.84223
H	-4.39124	-0.89673	-0.02402	Al	-0.60431	1.93001	-5.37988
C	-0.61482	4.11346	0.63349	Al	1.20074	0.66708	-6.89056
H	-1.12567	4.49271	1.53177	Al	-0.94901	-0.89175	-6.91713
H	-1.20021	4.45383	-0.23461	O	0.92980	-1.09274	2.38671
H	0.36544	4.61691	0.58155	O	-1.44064	-1.01410	3.87715
C	-3.98153	0.16244	2.41514	O	-1.27618	1.49383	2.25263

O	-1.70378	1.53275	5.16788	C	-1.98290	-1.74139	-8.33712
O	1.04392	1.44772	3.82483	H	-3.06268	-1.54379	-8.22939
O	-1.26181	-0.23807	6.94269	H	-1.84935	-2.83620	-8.31080
O	0.76468	1.81520	6.64139	H	-1.68181	-1.39148	-9.33835
O	1.02021	-0.93673	5.46428	C	2.43584	1.35350	-8.23536
O	-1.23583	1.36264	-0.85064	H	3.47357	1.11478	-7.94365
O	-1.25946	-1.18629	-2.27091	H	2.37486	2.44907	-8.34119
O	1.09784	-1.18943	-0.63610	H	2.26777	0.90704	-9.22915
O	-1.45140	-0.93799	0.79237	C	1.18411	-3.95788	-5.59224
O	1.25595	1.16613	-2.28935	H	2.21695	-4.19543	-5.28687
O	-1.23897	1.13598	-3.87537	H	1.11305	-4.14811	-6.67687
O	1.20209	1.43542	-5.23346	H	0.52536	-4.67244	-5.07730
O	-1.07034	-1.56898	-5.22318	C	-0.16984	3.84652	-2.66929
O	1.29124	-1.21083	-3.74344	H	0.39442	4.06246	-3.59206
O	1.16501	1.33060	0.77030	H	0.43698	4.24299	-1.83915
O	-0.68999	0.90002	-6.91033	H	-1.09858	4.43711	-2.71010
O	0.94418	-1.12254	-6.79077	C	3.87877	0.58401	-0.70942
C	-1.71805	2.69809	8.31082	H	4.24325	1.10665	-1.60721
H	-2.79472	2.54102	8.48908	H	4.37582	-0.40041	-0.68060
H	-1.57441	3.77337	8.10661	H	4.24027	1.15474	0.15982
H	-1.19749	2.47618	9.25949	C	0.65728	-3.84918	-2.30591
C	-4.06771	-0.78491	5.78147	H	-0.21257	-4.36814	-2.74247
H	-4.60988	-1.24833	4.94411	H	0.81125	-4.26872	-1.30264
H	-4.66421	0.08052	6.12003	H	1.53801	-4.12717	-2.90589
H	-4.04663	-1.50569	6.61737	C	-4.01042	-0.35250	-1.00716
C	-0.52478	4.16860	4.10229	H	-4.33009	-1.08489	-1.76486
H	0.22590	4.65612	3.46064	H	-4.43833	0.62181	-1.29948
H	-0.22086	4.35719	5.14804	H	-4.48691	-0.64553	-0.05997
H	-1.48429	4.69059	3.94722	C	-0.69863	4.08832	0.64109
C	-0.32489	-3.70616	0.93707	H	-1.22956	4.44669	1.53672
H	-0.96006	-3.85247	1.82754	H	-1.29207	4.40228	-0.23208
H	0.48109	-4.45467	0.98616	H	0.26047	4.63215	0.59509
H	-0.95593	-3.94558	0.06344	C	-4.02404	0.13639	2.45842
C	-3.80259	-0.54314	-4.37451	H	-4.34094	0.79757	1.63453
H	-4.36791	0.21903	-3.81809	H	-4.29477	0.65895	3.39182
H	-4.31600	-1.50861	-4.23164	H	-4.63996	-0.77638	2.41049
H	-3.89723	-0.29464	-5.44958	C	0.48725	-3.70381	4.15109
C	3.90387	0.40229	-4.17965	H	-0.46684	-4.25409	4.17616
H	4.40254	-0.31412	-3.50808	H	1.02510	-3.95005	5.08011
H	4.42022	1.37096	-4.07380	H	1.07072	-4.10788	3.30958
H	4.09076	0.05519	-5.21394	C	3.64854	0.24494	2.65143
C	-1.14305	3.75848	-5.84944	H	4.04789	-0.40409	1.85556
H	-1.76347	4.24336	-5.08180	H	3.80240	-0.31502	3.59201
H	-1.71216	3.74266	-6.79427	H	4.28618	1.14364	2.69553
H	-0.26556	4.40799	-6.00882	C	3.52060	1.08078	5.97384

H	3.85544	0.02668	6.01620
H	3.91423	1.44861	6.94921
H	4.10757	1.58218	5.19199
C	-0.61698	-3.18488	7.24625
H	0.11925	-4.00232	7.30832
H	-1.30486	-3.43721	6.42248
H	-1.21300	-3.21034	8.17752
C	1.41604	-0.77751	8.56849
H	2.41266	-0.48498	8.19957
H	1.58157	-1.58951	9.29791
H	1.02617	0.08430	9.13395
C	2.61257	2.69271	9.07911
H	2.82610	1.66647	9.41549
H	1.74263	3.04299	9.66258
H	3.46940	3.32834	9.35934
C	2.67241	4.21883	5.90561
H	2.40537	3.93152	4.87617
H	3.75216	4.44719	5.92408
H	2.13606	5.15704	6.12721

$(AlOMe)_{20,t} \cdot (AlMe_3)_2$

Al	0.84713	-1.11574	6.90373
Al	1.78771	0.85882	5.37793
Al	1.81581	0.63164	2.35749
Al	0.79505	-1.91424	3.85511
Al	-1.81400	-0.69918	2.25263
Al	-0.83577	1.87254	3.83750
Al	-1.77497	-0.81505	5.27792
Al	-0.86247	1.58208	6.99749
Al	-0.61774	1.83944	0.74037
Al	-1.85858	-0.72688	-0.83527
Al	0.76580	-1.80690	-2.42319
Al	0.69610	-1.86949	0.69983
Al	1.92514	0.69888	-0.79741
Al	-0.68255	1.84391	-2.31528
Al	-1.84862	-0.73471	-3.91318
Al	0.75361	-1.79612	-5.50691
Al	1.90027	0.78919	-3.93031
Al	-0.66948	1.79616	-5.37415
Al	1.63875	0.77922	-7.14327
Al	-1.20070	-0.74578	-6.99578
Al	-2.74783	2.41104	-6.95349
Al	-2.15800	-2.82381	7.10188
O	0.96609	1.40877	3.83826
O	1.32759	-1.15383	2.27898
O	-1.03394	-1.42601	3.75886
O	-1.32510	1.08030	2.25978
O	-1.51788	0.96957	5.31559
O	-0.84720	-1.67408	6.59815
O	0.75926	0.70496	6.92205
O	-1.33429	1.06208	-0.79072
O	-1.03198	-1.34859	-2.37310
O	1.39619	-1.08602	-0.83887
O	-1.07422	-1.33246	0.71167
O	1.11038	1.36954	-2.33843
O	-1.29487	1.05714	-3.85596
O	-1.08167	-1.56231	-5.34368
O	1.37603	-0.98065	-3.97869
O	1.09588	1.49734	-5.44434
O	-1.66441	0.96407	-6.65783
O	0.62908	-0.75357	-7.03739
O	1.13181	1.23621	0.77632
O	1.60514	-1.00066	5.23026
C	-0.37027	3.49458	7.15126
H	-1.22077	4.19371	7.18164
H	0.31372	3.85501	6.36588
H	0.16927	3.59475	8.11201
C	-3.65087	-1.39943	5.83714
H	-4.15328	-2.00393	5.07008
H	-4.13354	-0.40375	5.84528
H	-4.00302	-1.78845	6.82150
C	-1.32278	3.77838	3.98118
H	-0.44878	4.44768	4.03248
H	-1.92119	3.96255	4.88744
H	-1.92199	4.09612	3.11439
C	0.70103	-3.84305	0.77345
H	0.21571	-4.17218	1.70767
H	1.69781	-4.31456	0.74570
H	0.10628	-4.26897	-0.05188
C	-3.80560	-0.79330	-4.14964
H	-4.35868	-0.15092	-3.44731
H	-4.21621	-1.81283	-4.05953
H	-4.04502	-0.43492	-5.16766
C	3.85078	1.04246	-3.98372
H	4.37246	0.37085	-3.28472
H	4.13003	2.07304	-3.70790
H	4.25917	0.85489	-4.98467
C	-1.09056	3.72413	-5.91020
H	-2.02494	4.31025	-5.81963
H	-0.57141	4.02259	-6.83503

H	-0.49543	4.15483	-5.08192
C	-2.19861	-1.56052	-8.46413
H	-3.28194	-1.59585	-8.25641
H	-1.87072	-2.59556	-8.65680
H	-2.06357	-0.99500	-9.40243
C	3.50660	0.14569	-7.32396
H	3.78680	-0.64702	-6.61021
H	4.27442	0.93374	-7.25983
H	3.58512	-0.29943	-8.33344
C	1.49872	-3.54315	-6.00179
H	2.58304	-3.59129	-5.80319
H	1.35731	-3.70859	-7.08345
H	1.03529	-4.38505	-5.46482
C	-1.20706	3.75452	-2.48525
H	-0.38505	4.45958	-2.69531
H	-1.68034	4.09596	-1.55325
H	-1.96444	3.87361	-3.27760
C	3.84786	1.15304	-0.69047
H	4.13350	1.87462	-1.46889
H	4.52860	0.28998	-0.77947
H	4.05637	1.63222	0.27722
C	1.22478	-3.72337	-2.59829
H	0.37571	-4.36121	-2.89721
H	1.61645	-4.12565	-1.65408
H	2.01424	-3.85807	-3.35397
C	-3.78114	-1.22277	-0.83168
H	-4.03273	-1.84561	-1.70353
H	-4.47739	-0.36651	-0.83315
H	-4.00528	-1.82153	0.06535
C	-0.44639	3.81366	0.76411
H	0.11216	4.10472	1.67033
H	-1.38473	4.39119	0.76195
H	0.15603	4.15393	-0.09536
C	-3.77705	-0.70940	2.51583
H	-4.26199	-0.17869	1.68038
H	-4.05599	-0.14139	3.42236
H	-4.24911	-1.70313	2.59209
C	1.01090	-3.84028	4.24496
H	0.11375	-4.43258	4.00462
H	1.20927	-3.98478	5.32327
H	1.85576	-4.29113	3.69867
C	3.76820	0.62542	2.67520
H	4.26090	0.02872	1.88996
H	4.00891	0.13108	3.63290
H	4.25017	1.61562	2.69492
C	3.48125	1.70331	5.90520
H	4.18584	0.94789	6.29638
H	3.29194	2.41820	6.72440
H	3.99523	2.23730	5.09297
C	1.66319	-2.08119	8.40034
H	2.69971	-1.76698	8.60554
H	1.68281	-3.17084	8.22256
H	1.08454	-1.91684	9.32678
C	-2.75252	3.01216	-8.82574
H	-2.81730	2.14256	-9.50377
H	-1.83093	3.55278	-9.09269
H	-3.60657	3.67124	-9.05490
C	-4.23550	2.50294	-5.66793
H	-3.88764	2.20761	-4.66491
H	-5.06962	1.82855	-5.92631
H	-4.65267	3.52255	-5.59386
C	0.94153	2.00582	-8.54359
H	1.42104	1.78197	-9.51244
H	1.16513	3.06356	-8.32143
H	-0.14357	1.93530	-8.70318
C	-2.59354	-2.77206	9.02166
H	-3.00147	-1.79733	9.32974
H	-1.68491	-2.94067	9.62679
H	-3.32182	-3.54997	9.30664
C	-2.34272	-4.37324	5.90347
H	-2.22695	-4.06155	4.85332
H	-3.33291	-4.85020	6.00558
H	-1.58183	-5.14866	6.09473
C	-2.03399	0.81334	8.41627
H	-2.96130	0.35360	8.03986
H	-2.34143	1.59922	9.12789
H	-1.51675	0.03906	9.00560

$(AlOMe)_{20,t} \cdot (AlMe_3)_3$

Al	0.00000000	0.00000000	0.00000000
Al	0.94701200	1.96901700	-1.52128200
Al	0.94848300	1.77883300	-4.54671500
Al	-0.06345300	-0.78604100	-3.04522900
Al	-2.66229800	0.43139700	-4.64846800
Al	-1.68816400	2.99782200	-3.05318700
Al	-2.62306200	0.30950900	-1.61891300
Al	-1.69287600	2.69742800	0.10234200
Al	-1.51138400	2.95495100	-6.17265000
Al	-2.69027200	0.35321000	-7.73145200
Al	-0.03790800	-0.72404800	-9.26406600

Al	-0.12106000	-0.73329100	-6.18068500
Al	1.03791000	1.86656600	-7.69721600
Al	-1.60213300	2.97654600	-9.24028600
Al	-2.59951000	0.36513400	-10.8248490
Al	0.01390300	-0.70720900	-12.3711380
Al	0.94498500	1.90625100	-10.8130790
Al	-1.67441100	2.99972800	-12.3451720
Al	0.80542800	2.10937100	-13.9317800
Al	-2.47376400	0.20414600	-13.9408700
Al	2.45942500	0.02921300	-14.3568680
Al	-4.12497300	2.28833500	-14.3505210
Al	-2.98183200	-1.72350700	0.19459300
O	0.11016300	2.53797200	-3.04880700
O	0.49504400	-0.00948000	-4.60024600
O	-1.88126000	-0.29766300	-3.13674300
O	-2.19024300	2.20730100	-4.62879300
O	-2.36641200	2.08810900	-1.57146200
O	-1.68798700	-0.55339400	-0.30301800
O	-0.07576500	1.82329600	0.02527600
O	-2.21942600	2.16317300	-7.70340600
O	-1.83854100	-0.26042700	-9.26740100
O	0.58024900	0.06098800	-7.71111200
O	-1.89323900	-0.20581800	-6.17135200
O	0.19891400	2.50473500	-9.23578100
O	-2.17661800	2.16830300	-10.7947530
O	-1.81098100	-0.35720300	-12.3503430
O	0.53180300	0.09977100	-10.8112500
O	0.15296600	2.64893000	-12.3289420
O	-2.44774700	2.00375300	-13.6721190
O	0.77774100	0.30543600	-13.6864920
O	0.24292800	2.37715600	-6.12055100
O	0.76031800	0.12005000	-1.66996300
C	-1.22472500	4.61742200	0.21988900
H	-2.08885700	5.30033800	0.24070000
H	-0.55908100	4.97163300	-0.58401400
H	-0.67639700	4.75423700	1.17035200
C	-4.48727700	-0.31559700	-1.07262600
H	-4.96453700	-0.93531000	-1.84347800
H	-4.99948200	0.66464200	-1.06978500
H	-4.83565100	-0.71351500	-0.09009300
C	-2.23256400	4.88901500	-2.92778600
H	-1.38937900	5.59658700	-2.88809400
H	-2.84165500	5.06166300	-2.02634800
H	-2.84417300	5.16439300	-3.80089500
C	-0.07479100	-2.70785300	-6.12288300
H	-0.57884000	-3.06172100	-5.20791600
H	0.93784500	-3.14605700	-6.12445200
H	-0.62562300	-3.14531100	-6.97144400
C	-4.56564700	0.24168800	-10.9846880
H	-5.04465900	0.77080500	-10.1468690
H	-4.96303300	-0.78660800	-10.9878680
H	-4.92697700	0.73760500	-11.8943390
C	2.91016200	2.04628600	-10.9723750
H	3.39351400	1.50315500	-10.1460880
H	3.29890300	3.07749900	-10.9545110
H	3.27343000	1.57212200	-11.8926120
C	-1.97906500	4.88526900	-12.8255280
H	-3.02927600	5.20691300	-12.7340350
H	-1.68594500	5.01635300	-13.8833930
H	-1.37121100	5.58202600	-12.2273680
C	-4.52976100	0.05321300	-14.3859660
H	-5.50439400	0.50959400	-14.1179820
H	-4.56748100	-0.85083500	-13.7422720
H	-4.60621700	-0.28353000	-15.4308510
C	2.86283100	2.26398100	-14.3810410
H	3.84144500	1.80998400	-14.1237070
H	2.89777300	3.16326900	-13.7305950
H	2.93271800	2.61059800	-15.4233710
C	0.31555400	-2.58644800	-12.8777820
H	1.36571100	-2.91183700	-12.7961460
H	0.01843100	-2.70043400	-13.9364690
H	-0.29224100	-3.29201700	-12.2893590
C	-2.09433400	4.89080300	-9.38832500
H	-1.23145300	5.56736200	-9.50770900
H	-2.64281800	5.22375300	-8.49504200
H	-2.75756400	5.05705100	-10.2516930
C	2.93071000	2.45219400	-7.65455300
H	3.15219200	3.12401200	-8.49838700
H	3.67424900	1.63733200	-7.67949900
H	3.11067900	3.02539300	-6.73185000
C	0.44989100	-2.63716400	-9.41845300
H	-0.41781900	-3.31653300	-9.46720600
H	1.05729000	-2.95258400	-8.55715200
H	1.05431600	-2.81982200	-10.3202470
C	-4.58415600	-0.24762300	-7.69386300
H	-4.79664000	-0.90721300	-8.55039600
H	-5.33970300	0.55646700	-7.70410000
H	-4.75706500	-0.84286500	-6.78324600
C	-1.37591900	4.92936700	-6.15388000
H	-0.82437000	5.23367600	-5.24806200

H	-2.32525400	5.48809000	-6.16164500
H	-0.78079600	5.27635100	-7.01492100
C	-4.62468400	0.37923700	-4.38711400
H	-5.12315800	0.88065100	-5.23239100
H	-4.92283000	0.94962600	-3.48833800
H	-5.06496500	-0.62846600	-4.29987600
C	0.19432800	-2.70729000	-2.66779600
H	-0.67706000	-3.33073400	-2.92023700
H	0.39692900	-2.85687800	-1.59079100
H	1.05834300	-3.11708400	-3.21709900
C	2.90768400	1.85748800	-4.31079700
H	3.39266700	1.30930600	-5.13498500
H	3.22318000	1.36058800	-3.37710400
H	3.33143000	2.87440100	-4.29587400
C	2.63879900	2.83607600	-1.03119200
H	3.37155600	2.10394100	-0.64949400
H	2.45299600	3.55874200	-0.21770200
H	3.11825600	3.37361500	-1.86230200
C	0.85642200	-0.94422700	1.48311500
H	1.88851400	-0.59618700	1.65589600
H	0.90573200	-2.03315800	1.31097300
H	0.30017400	-0.78777100	2.42373900
C	3.64847300	-0.88714700	-13.0723920
H	3.26006400	-0.82896700	-12.0430970
H	4.66931700	-0.46797400	-13.0539170
H	3.74658200	-1.95693100	-13.3255030
C	2.37165600	-0.37418600	-16.2858620
H	3.34427900	-0.28753600	-16.7993050
H	1.66571900	0.29649400	-16.8024680
H	2.01125800	-1.40524800	-16.4509060
C	-1.67734700	-0.60706200	-15.5485210
H	-2.02865500	-0.05616200	-16.4370000
H	-2.01684300	-1.65036700	-15.6680660
H	-0.58100900	-0.61097900	-15.5710320
C	-4.03445000	2.69148000	-16.2796950
H	-5.00723000	2.59390200	-16.7910330
H	-3.32327200	2.02644400	-16.7958270
H	-3.68554800	3.72595500	-16.4469900
C	-5.31707400	3.20350400	-13.0696080
H	-4.95539500	3.10890200	-12.0332950
H	-6.34977000	2.81483200	-13.0864570
H	-5.37736800	4.28161600	-13.2976020
C	0.00596300	2.93324700	-15.5313220
H	0.34147300	2.37443700	-16.4211570
H	0.36046500	3.97093700	-15.6560320
H	-1.09034900	2.95352400	-15.5450150
C	-3.38382200	-1.67549600	2.12024600
H	-3.82613400	-0.71646600	2.42984100
H	-2.44948400	-1.79286400	2.69826200
H	-4.06469800	-2.48363400	2.43498800
C	-3.10676900	-3.26922500	-1.01315200
H	-2.98527700	-2.94412700	-2.05869400
H	-4.07602300	-3.78955500	-0.93093500
H	-2.31518900	-4.01254000	-0.81666400
C	-2.85921400	1.91624800	1.51989700
H	-3.77595700	1.44342300	1.13322700
H	-3.18630700	2.69626400	2.22883500
H	-2.33672300	1.14799300	2.11211600

$(AlOMe)_{20,t} \cdot (AlMe_3)_4$

Al	0.93778	-1.59986	6.99601
Al	1.85890	0.87040	5.40065
Al	1.84337	0.67531	2.32012
Al	0.74537	-1.82134	3.90180
Al	-1.84977	-0.64831	2.33177
Al	-0.75301	1.85239	3.89420
Al	-1.86630	-0.83530	5.40475
Al	-0.94690	1.63873	6.98961
Al	-0.69437	1.83976	0.74882
Al	-1.87241	-0.77938	-0.78488
Al	0.80722	-1.83468	-2.32012
Al	0.67623	-1.81970	0.75933
Al	1.84845	0.78195	-0.80026
Al	-0.83860	1.82902	-2.32842
Al	-1.77306	-0.82665	-3.88461
Al	0.86914	-1.84116	-5.42857
Al	1.72623	0.80708	-3.90727
Al	-0.93055	1.80704	-5.43755
Al	1.56345	0.98445	-7.02172
Al	-1.64235	-1.03622	-6.99502
Al	1.12484	3.31746	7.36256
Al	3.28075	-1.03405	-7.45485
Al	-3.35643	0.97836	-7.44410
Al	-1.12239	-3.30212	7.35636
O	1.05614	1.40722	3.84138
O	1.32545	-1.09933	2.33251
O	-1.06224	-1.37845	3.84729
O	-1.33468	1.12857	2.32839
O	-1.48525	0.98170	5.38825
O	-0.85748	-1.60971	6.71829

O	0.84857	1.62151	6.73198	H	-3.74804	-1.63579	-8.47593
O	-1.42456	1.03410	-0.77005	C	3.60430	1.21067	-7.49679
O	-1.00331	-1.41312	-2.31415	H	4.60177	0.79553	-7.24791
O	1.40173	-1.02964	-0.77082	H	3.61212	2.11068	-6.84597
O	-1.08546	-1.27374	0.79781	H	3.64912	1.55984	-8.53948
O	0.97248	1.40306	-2.33187	C	1.26491	-3.70829	-5.90476
O	-1.40027	0.98318	-3.87246	H	2.33365	-3.96580	-5.82302
O	-0.96377	-1.56064	-5.39857	H	0.96734	-3.86801	-6.95700
O	1.35733	-1.00235	-3.87673	H	0.70875	-4.43276	-5.28986
O	0.90249	1.52596	-5.42310	C	-1.42632	3.71506	-2.50456
O	-1.67341	0.76372	-6.74634	H	-0.61121	4.43226	-2.69949
O	1.59917	-0.81145	-6.75427	H	-1.93203	4.04581	-1.58509
O	1.06911	1.28640	0.78397	H	-2.15290	3.81892	-3.32644
O	1.48277	-0.94825	5.39260	C	3.73175	1.41072	-0.79620
C	-1.10430	3.69394	7.43874	H	3.91327	2.11018	-1.62785
H	-2.06660	3.68227	6.88771	H	4.49798	0.61894	-0.85836
H	-0.70008	4.66118	7.08025	H	3.91912	1.96585	0.13644
H	-1.35292	3.80709	8.50471	C	1.40498	-3.71812	-2.48584
C	-3.74678	-1.19853	5.88232	H	0.59379	-4.44467	-2.66036
H	-4.20496	-2.00213	5.28444	H	1.92743	-4.03337	-1.57024
H	-4.37848	-0.30375	5.75557	H	2.12036	-3.82494	-3.31715
H	-3.81864	-1.49077	6.94585	C	-3.75529	-1.40490	-0.75926
C	-1.19609	3.76724	4.13124	H	-3.94775	-2.10858	-1.58473
H	-0.46884	4.33633	4.72834	H	-4.52024	-0.61169	-0.81671
H	-2.18120	3.87517	4.61784	H	-3.93232	-1.95407	0.17901
H	-1.27444	4.27437	3.16011	C	-0.53715	3.81437	0.69628
C	0.54483	-3.79583	0.72471	H	0.11894	4.12237	1.53030
H	-0.09009	-4.11209	1.57164	H	-1.46875	4.39977	0.76371
H	1.48898	-4.36245	0.78030	H	-0.01894	4.12713	-0.22610
H	0.01945	-4.12408	-0.18811	C	-3.81572	-0.64105	2.52014
C	-3.73532	-1.00177	-4.05318	H	-4.26926	-0.13938	1.64977
H	-4.22677	-0.47133	-3.22389	H	-4.11111	-0.05254	3.40572
H	-4.10940	-2.03861	-4.03998	H	-4.29016	-1.63123	2.61600
H	-4.10726	-0.52771	-4.96993	C	1.19844	-3.73461	4.14061
C	3.68476	1.00134	-4.09628	H	0.42119	-4.33261	4.63851
H	4.19279	0.48130	-3.27056	H	2.12742	-3.84512	4.72552
H	4.04211	2.04431	-4.08943	H	1.38975	-4.20830	3.16795
H	4.05499	0.53195	-5.01607	C	3.81091	0.68605	2.49610
C	-1.33912	3.66899	-5.92506	H	4.26506	0.17608	1.63084
H	-2.40803	3.92096	-5.82689	H	4.11990	0.11776	3.39018
H	-1.06106	3.82168	-6.98365	H	4.27383	1.68372	2.57131
H	-0.77662	4.40180	-5.32602	C	3.74180	1.26486	5.85123
C	-3.68722	-1.26748	-7.44074	H	4.37155	0.36179	5.78029
H	-4.68003	-0.84688	-7.18374	H	3.82646	1.63054	6.89101
H	-3.68556	-2.15530	-6.77326	H	4.19597	2.02523	5.19689

C	1.11070	-3.65726	7.44525	H	-1.16021	-2.90050	-8.69535
H	2.11437	-3.59218	6.97668	H	0.28132	-1.87166	-8.58173
H	0.76029	-4.60991	7.00315	C	-3.22693	1.35559	-9.37607
H	1.28946	-3.81688	8.51918	H	-4.17308	1.19952	-9.92126
C	1.70198	-0.72954	8.59551	H	-2.46331	0.71936	-9.85226
H	0.96400	-0.05467	9.05437	H	-2.92249	2.40308	-9.54858
H	2.59290	-0.12057	8.37957	C	-4.60147	1.87129	-6.19995
H	1.98309	-1.47548	9.35685	H	-4.22927	1.84898	-5.16331
C	1.54743	3.29841	9.29025	H	-5.60429	1.41059	-6.19042
H	0.89711	2.58712	9.82583	H	-4.73776	2.93081	-6.47716
H	1.42760	4.28314	9.77354	C	0.71947	1.78423	-8.61098
H	2.58855	2.97581	9.46673	H	1.00425	1.19917	-9.50102
C	1.99851	4.46182	6.01165	H	1.09643	2.80904	-8.77114
H	1.85539	4.06456	4.99375	H	-0.37495	1.83384	-8.58432
H	3.08716	4.50680	6.18914	C	-1.55835	-3.22505	9.28086
H	1.62826	5.50129	6.00948	H	-2.59077	-2.86585	9.43746
C	4.52425	-1.89997	-6.18937	H	-0.88948	-2.51755	9.79932
H	4.14545	-1.85414	-5.15585	H	-1.47342	-4.19687	9.79610
H	5.52668	-1.43887	-6.18343	C	-1.98772	-4.47272	6.02483
H	4.66139	-2.96543	-6.44182	H	-1.88299	-4.06453	5.00657
C	3.13919	-1.45359	-9.37716	H	-3.06933	-4.55766	6.22881
H	4.08898	-1.35163	-9.92835	H	-1.58084	-5.49806	6.00718
H	2.40020	-0.80111	-9.86976	C	-1.79597	0.84474	8.58278
H	2.79231	-2.49253	-9.51915	H	-2.86929	1.09984	8.61850
C	-0.81455	-1.85861	-8.58102	H	-1.33854	1.27057	9.49165
H	-1.14336	-1.31511	-9.48193	H	-1.71856	-0.24729	8.64676