Supporting Information

Revisiting the Aufbau Reaction with Acetylene: Further Insights from Experiment and Theory

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Isolation and crystal structure of $Al_4Et_4(OPh)_8$. To a Schlenk flask under argon was added [{$AlEt_2(C_4H_7)$}$_2$] (**1**, 840 mg, 2.99 mmol). In a separate Schlenk, phenol (1.131g, 12.0 mmol) was dissolved in 3 mL of dry toluene. The flask containing **1** was cooled to -10 ºC in an ice bath before the phenol solution was added dropwise over 40 minutes. The solution was warmed to room temperature while gently stirring, then placed in a freezer at -20 ºC overnight. This yielded a colorless crystalline solid, which was suitable for the acquisition of an X-ray crystal structure.

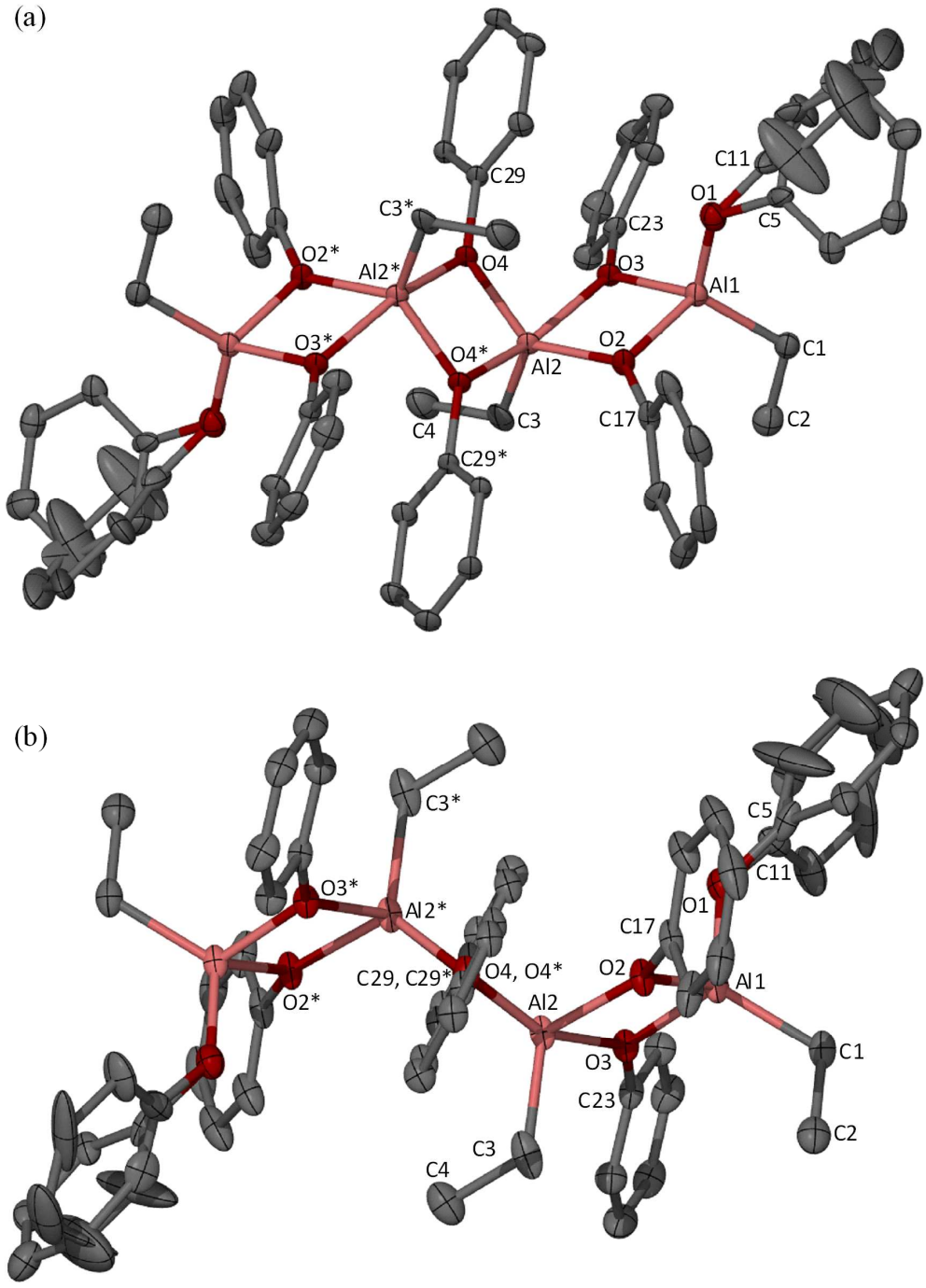


Figure S1. Crystal Structure of $Al_4Et_4(OPh)_8$ (ellipsoids drawn at 20% probability levels). (a) General view. (b) View along central O-O vector. The tetranuclear species is generated by a crystallographic inversion centre (symmetry operator = -x,-y,2-z). The terminal -OPh ligand is disordered over two orientations, both are shown (each restrained with AFIX 66 cards).

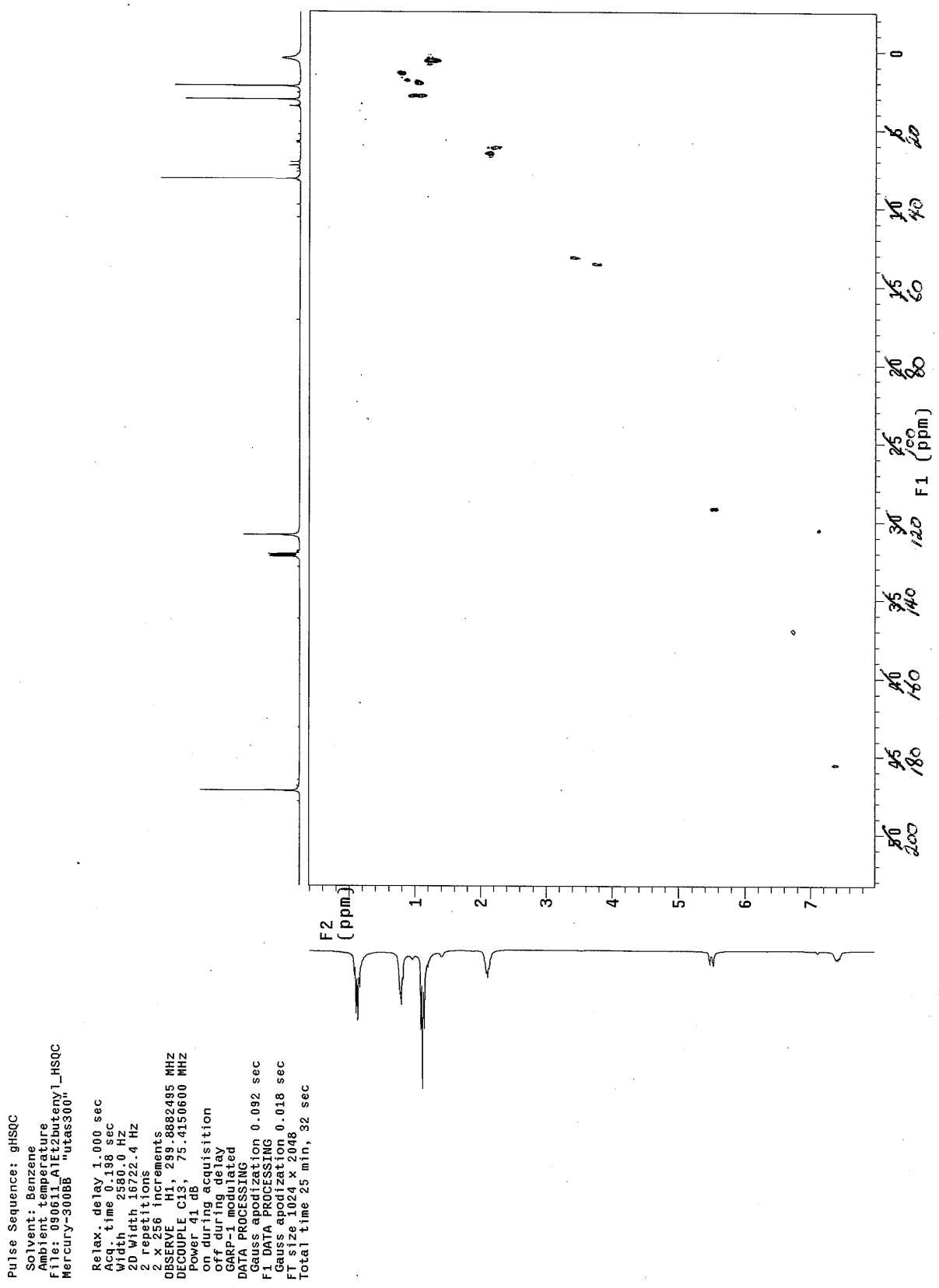
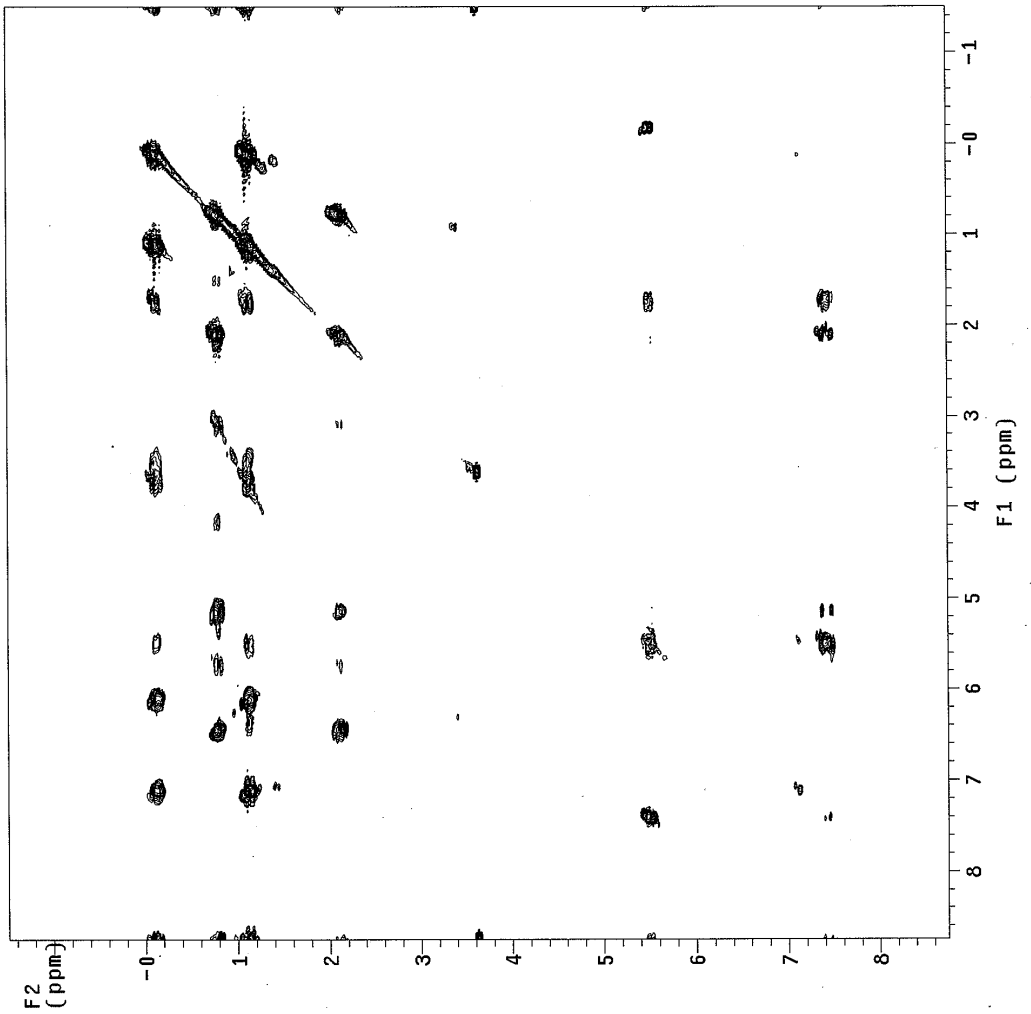


Figure S2. HSQC NMR spectrum of $[Et_2Al\text{-}CH{=}CHEt]_2$.



STANDARD 1H OBSERVE

Pulse Sequence: gCOSY
Solvent: Benzene
Ambient temperature
File: 090524_AlEt2but_COSY
Mercury-300BB "utas300"

Relax. delay 1.000 sec
Acq. time 0.166 sec
Width 3076.9 Hz
2D Width 3076.9 Hz
Single scan
256 increments
OBSERVE H1, 299.8882495 MHz
DATA PROCESSING
Sq. sine bell 0.083 sec
F1 DATA PROCESSING
Sq. sine bell 0.042 sec
FT size 1024 x 1024
Total time 6 min, 58 sec

Figure S3. COSY NMR spectrum of $[Et_2Al\text{-}CH{=}CHEt]_2$.

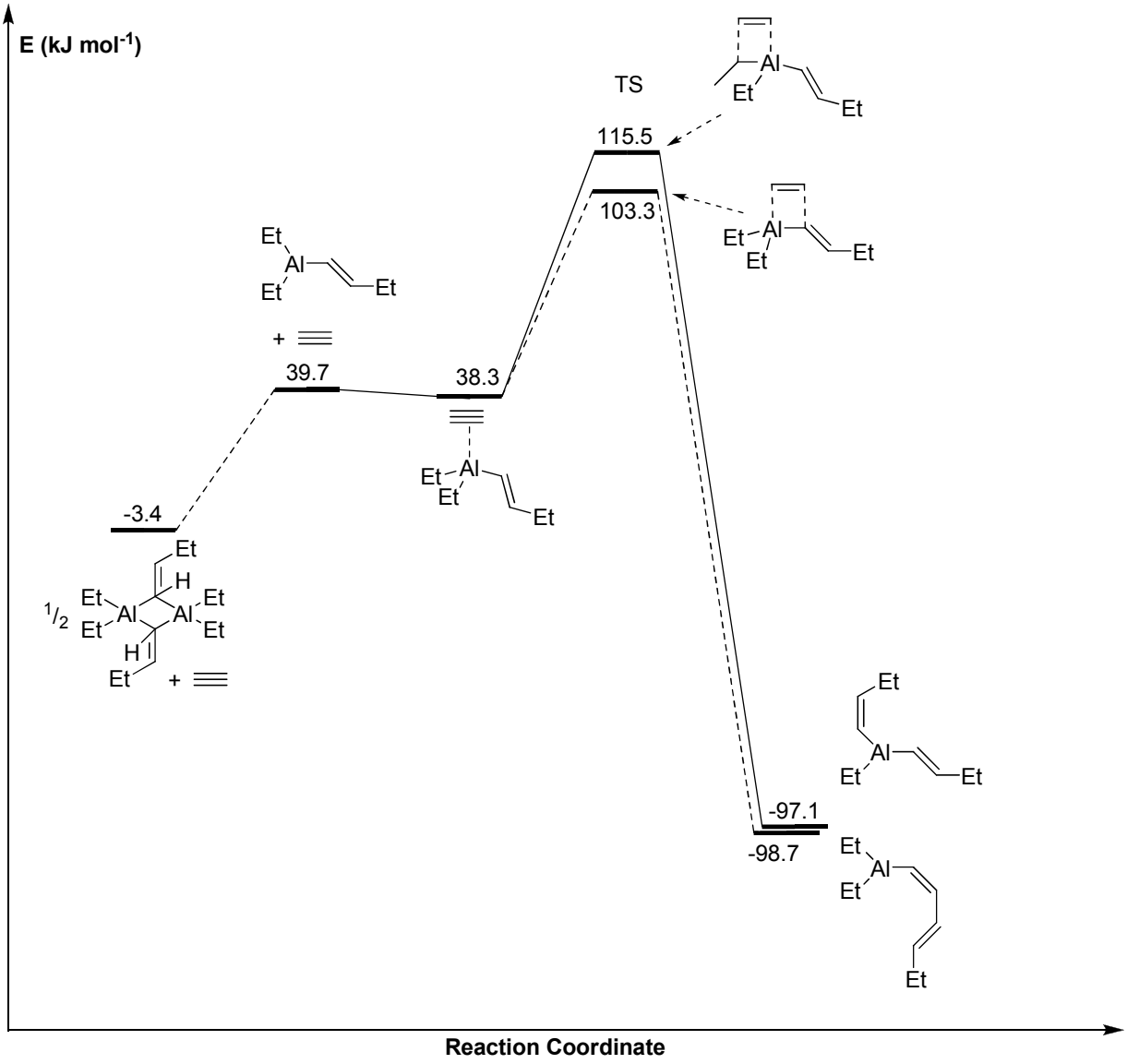


Figure S4. Relative energy surface for the two possible modes of acetylene insertion into *trans*-$AlEt_2$(butenyl). Energies in kJ/mol relative to *cis,cis*-[Al_2Et_4(μ-butenyl)$_2$].

Supporting Information

Optimized geometries and absolute energies (kJ/mol) of stationary points:

Acetylene Energy: -48542.6808410

C	0.00000	0.00000	0.60249
C	0.00000	0.00000	-0.60249
H	0.00000	0.00000	1.66914
H	0.00000	0.00000	-1.66914

$AlEt_3$ Energy: -301338.9454044

Al	-0.00135	-0.00492	-0.00581
C	-1.98630	0.05434	-0.00082
H	-2.29956	0.66826	0.85982
H	-2.30490	0.64679	-0.87463
C	0.95195	-1.74733	-0.03730
H	0.56307	-2.36430	0.78919
H	0.63128	-2.28879	-0.94278
C	1.03911	1.68664	0.01516
H	1.69646	1.66640	0.90001
H	1.74103	1.65888	-0.83450
C	0.25203	3.01061	-0.00928
H	-0.42014	3.09872	0.85326
H	0.91265	3.88828	0.00696
H	-0.37257	3.09567	-0.90711
C	-2.74656	-1.28506	0.01656
H	-3.83628	-1.14528	0.01520
H	-2.50149	-1.90273	-0.85641
H	-2.50079	-1.88046	0.90459
C	2.49107	-1.71420	0.02305
H	2.93027	-2.72091	-0.00247
H	2.91850	-1.15600	-0.81906
H	2.85222	-1.23067	0.93931

$AlEt_3$, Acetylene Coordinated Energy: -349883.9205874

Al	0.02491	-0.00195	-0.38519
C	-1.93387	-0.23073	-0.70740
H	-2.50396	0.56615	-0.20502
H	-2.06867	-0.01557	-1.78187
C	1.19447	-1.60289	-0.60630
H	0.79264	-2.43832	-0.01321
H	1.06699	-1.92672	-1.65387
C	0.81238	1.80938	-0.66184
H	1.74076	1.91360	-0.07869
H	1.15003	1.84546	-1.71197
C	-0.10159	3.01907	-0.38929
H	-0.41941	3.05728	0.66080
H	0.38970	3.97734	-0.60981
H	-1.01501	2.97936	-0.99594
C	-2.56700	-1.60100	-0.40196
H	-3.63420	-1.64046	-0.66170
H	-2.06995	-2.40518	-0.95785
H	-2.48962	-1.86684	0.66160
C	2.70030	-1.44779	-0.32278
H	3.26400	-2.37170	-0.51411
H	3.15186	-0.66186	-0.94095
H	2.89540	-1.17752	0.72470
C	-0.68759	-0.02323	2.25785
C	0.51577	0.09758	2.25008
H	-1.74941	-0.13539	2.28034
H	1.57781	0.20338	2.29487

$AlEt_3$, First Insertion, Transition State Energy: -349867.5175091

Al	-0.19263	-0.23633	-0.01769

C	1.16995	1.26350	-0.71687
H	2.23993	1.07113	-0.59498
H	0.91785	0.84431	-1.70825
C	-2.02774	0.41241	-0.43543
H	-2.17125	1.40375	0.01926
H	-2.09495	0.58111	-1.52265
C	0.49570	-1.99062	-0.66089
H	-0.15864	-2.78518	-0.27051
H	0.35235	-2.02248	-1.75381
C	1.95987	-2.33403	-0.33234
H	2.14065	-2.33794	0.74985
H	2.25416	-3.32280	-0.71181
H	2.65575	-1.60573	-0.76862
C	0.85042	2.75691	-0.72706
H	1.40728	3.28193	-1.51516
H	-0.21563	2.93829	-0.90145
H	1.11032	3.24823	0.22031
C	-3.17613	-0.51888	-0.00008
H	-4.16447	-0.12302	-0.27382
H	-3.09179	-1.51157	-0.46065
H	-3.18370	-0.67085	1.08718
C	0.99681	0.87688	1.55081
C	0.21452	0.00541	2.00754
H	1.72290	1.66909	1.57630
H	-0.11693	-0.41541	2.94460

cis-$AlEt_2$(butenyl) Energy: -349922.9371700

Al	-0.76701	0.00395	-0.05567
C	2.77427	-0.03630	-0.45949
H	3.29015	-0.06323	-1.43185
H	2.12851	0.84823	-0.47128
C	-0.37091	1.95075	-0.12426
H	0.38153	2.18288	0.64615
H	0.14083	2.16660	-1.07615
C	-2.65246	-0.58728	0.12526
H	-3.06785	-0.11197	1.02907
H	-3.22705	-0.13213	-0.69822
C	-2.92766	-2.10209	0.16832
H	-2.41649	-2.58360	1.01124
H	-3.99801	-2.32814	0.27040
H	-2.57943	-2.60395	-0.74299
C	3.83230	0.10332	0.64946
H	4.44998	0.99472	0.49272
H	3.35895	0.18560	1.63443
H	4.49933	-0.76687	0.67291
C	-1.57546	2.89935	0.03382
H	-1.28121	3.95630	-0.02174
H	-2.32840	2.73368	-0.74654
H	-2.08060	2.75687	0.99713
C	1.95215	-1.28884	-0.31384
C	0.61642	-1.38359	-0.15271
H	2.55553	-2.20433	-0.33658
H	0.25346	-2.41394	-0.06430

trans-$AlEt_2$(butenyl) Energy: -349924.7084227

Al	0.94727	-0.00354	-0.05433
C	1.23414	-1.96902	-0.07747
H	0.59508	-2.42191	0.69720
H	0.83007	-2.36198	-1.02447
C	2.47849	1.24539	0.11402
H	3.18123	1.03005	-0.70759
H	3.04141	0.97297	1.02158

C	-0.88269	0.66608	-0.21198
H	-1.10515	1.73944	-0.20218
C	-1.95415	-0.14196	-0.34458
H	-1.81079	-1.22769	-0.35916
C	2.68335	-2.46160	0.10249
H	3.10579	-2.13876	1.06219
H	2.75694	-3.55734	0.07161
H	3.34497	-2.07315	-0.68167
C	2.15995	2.75247	0.13714
H	1.50639	3.01641	0.97792
H	3.06545	3.36794	0.22878
H	1.64545	3.07245	-0.77747
C	-3.39359	0.28670	-0.46606
H	-3.45190	1.38228	-0.47435
H	-3.79070	-0.05966	-1.43284
C	-4.27830	-0.28062	0.65815
H	-5.32420	0.01679	0.52244
H	-4.24188	-1.37651	0.67627
H	-3.94583	0.08012	1.63784

trans,trans-AlEt(butenyl)$_2$ Energy: -398509.5094741

Al	-0.77565	-1.11946	-0.12840
C	-1.91589	-2.73079	0.03650
H	-1.86762	-3.27328	-0.92202
H	-1.43777	-3.41488	0.75576
C	-1.51071	0.67460	0.11972
H	-2.45794	0.82296	0.65181
C	1.12209	-1.32746	-0.55245
H	1.49470	-2.24807	-1.01778
C	2.06993	-0.42057	-0.24057
H	1.77804	0.51679	0.24305
C	-3.38918	-2.51378	0.43041
H	-3.91290	-1.87713	-0.29324
H	-3.94693	-3.45831	0.49221
H	-3.47911	-2.02378	1.40803
C	-0.96411	1.79317	-0.39812
H	-0.02373	1.72409	-0.95370
C	3.55291	-0.56033	-0.47045
H	3.75609	-1.49833	-1.00228
H	3.89348	0.25605	-1.12603
C	4.36419	-0.50941	0.83624
H	5.43930	-0.57467	0.63424
H	4.18208	0.42564	1.37966
H	4.09093	-1.33806	1.49890
C	-1.51500	3.19178	-0.29028
C	-0.54010	4.16056	0.40193
H	-2.47069	3.17096	0.24845
H	-1.72932	3.57302	-1.30067
H	-0.95225	5.17537	0.43575
H	-0.33521	3.84159	1.42993
H	0.41765	4.20640	-0.13043

trans-AlEt$_2$(butenyl), Acetylene Coordinated Energy: -398469.5549338

Al	0.69260	0.03658	-0.32027
C	0.93703	1.99488	-0.57591
H	0.45687	2.25022	-1.53570
H	0.35425	2.54467	0.17877
C	1.95587	-1.23784	-1.18492
H	2.99531	-0.89268	-1.07137
H	1.76252	-1.15591	-2.26847
C	-1.12079	-0.59713	0.12711
H	-1.33605	-1.66806	0.23644

C	-2.19124	0.21150	0.24951
H	-2.06198	1.29429	0.14430
C	2.38216	2.52867	-0.59111
H	2.99108	2.03191	-1.35729
H	2.42998	3.60777	-0.79408
H	2.88422	2.36760	0.37235
C	1.85442	-2.71947	-0.77526
H	0.84256	-3.11194	-0.93547
H	2.54199	-3.36156	-1.34368
H	2.08529	-2.86408	0.28806
C	-3.61688	-0.21318	0.50038
H	-3.65648	-1.30059	0.64378
H	-3.97444	0.24346	1.43671
C	-4.56665	0.20047	-0.63749
H	-5.59993	-0.08940	-0.41464
H	-4.54941	1.28614	-0.79196
H	-4.27455	-0.27411	-1.58083
C	1.10283	-0.15622	2.38680
C	2.22397	-0.18401	1.93413
H	0.11303	-0.13639	2.78611
H	3.22768	-0.21289	1.57099

trans-$AlEt_2$(butenyl), Insertion at 2nd Ethyl, Transition State Energy: -398452.0632917

Al	-0.68665	-0.23403	0.24764
C	-1.09748	-2.02035	-0.52015
H	-0.55677	-2.10093	-1.47735
H	-0.65101	-2.79352	0.12319
C	-1.60029	1.21390	-1.04053
H	-2.64549	1.06023	-1.32542
H	-1.01279	0.69221	-1.81760
C	1.16115	0.34183	0.58405
H	1.38145	1.33776	0.98892
C	2.23645	-0.43339	0.35282
H	2.09759	-1.44365	-0.04746
C	-2.58418	-2.34727	-0.75038
H	-3.05584	-1.62950	-1.43394
H	-2.73114	-3.34629	-1.18444
H	-3.15408	-2.31646	0.18662
C	-1.20950	2.68953	-1.04137
H	-0.14646	2.81975	-0.81165
H	-1.39595	3.15524	-2.01862
H	-1.77480	3.27437	-0.30290
C	3.68028	-0.05590	0.57599
H	3.73218	0.94647	1.02028
H	4.12787	-0.74806	1.30610
C	4.51483	-0.10069	-0.71569
H	5.56531	0.14155	-0.51692
H	4.48250	-1.09708	-1.17300
H	4.13318	0.61506	-1.45254
C	-1.86582	0.15633	1.91355
C	-2.33175	1.02621	1.13530
H	-1.95037	-0.20320	2.92736
H	-2.94120	1.85715	0.82852

cis,trans-$AlEt(butenyl)_2$ Energy: -398508.2575365

Al	-0.08052	-0.08015	-0.21612
C	-0.37690	1.76601	0.45384
H	-1.06931	1.74397	1.30891
H	0.56880	2.15345	0.85983
C	-3.63717	-0.17211	0.02517
H	-4.31672	0.22959	-0.74246

H	-2.98319	0.65295	0.32796
C	1.74819	-0.72153	-0.45912
H	1.94801	-1.72230	-0.86058
C	2.84414	0.00324	-0.15631
H	2.72498	1.01167	0.25353
C	-0.91365	2.75741	-0.60330
H	-1.87786	2.43384	-1.01475
H	-1.06298	3.76327	-0.18780
H	-0.22266	2.86190	-1.44970
C	-4.47985	-0.63928	1.22520
H	-3.83929	-1.00447	2.03596
H	-5.09299	0.17977	1.61760
H	-5.15430	-1.45618	0.94131
C	4.27896	-0.43113	-0.30755
H	4.31518	-1.43291	-0.75355
H	4.78725	0.24747	-1.01001
C	5.04643	-0.41892	1.02641
H	6.09461	-0.70266	0.87923
H	5.03080	0.57798	1.48320
H	4.60061	-1.11974	1.74094
C	-1.48782	-1.34982	-0.71315
C	-2.82783	-1.28844	-0.57862
H	-1.12993	-2.27802	-1.17429
H	-3.44125	-2.13029	-0.92121

trans-$AlEt_2$(butenyl), Second Insertion, Transition State Energy: -398455.1489913

Al	0.92765	0.08767	-0.06820
C	0.87705	2.06583	-0.30759
H	0.33339	2.26780	-1.24511
H	0.25688	2.51155	0.48491
C	1.95389	-1.09752	-1.30539
H	2.99073	-0.73122	-1.35610
H	1.54378	-0.92914	-2.31449
C	-0.93661	-0.68345	0.29444
H	-1.11569	-1.74558	0.08979
C	-2.03399	0.09641	0.39669
H	-1.91464	1.15908	0.62763
C	2.24127	2.77941	-0.34830
H	2.88026	2.38852	-1.15069
H	2.14668	3.86207	-0.51515
H	2.79379	2.64915	0.59150
C	1.95785	-2.60585	-1.00485
H	0.94111	-3.01913	-0.99118
H	2.52528	-3.18051	-1.75095
H	2.40354	-2.82383	-0.02607
C	-3.46220	-0.34042	0.20027
H	-3.49549	-1.41721	-0.00753
H	-4.01462	-0.18137	1.14072
C	-4.17530	0.43587	-0.92071
H	-5.22218	0.12443	-1.00783
H	-4.16121	1.51469	-0.72562
H	-3.68671	0.26521	-1.88617
C	0.42724	-0.75186	2.07979
C	1.58618	-0.30795	1.90738
H	-0.40618	-1.21867	2.56572
H	2.52966	-0.17834	2.41295

cis,trans-$AlEt_2$(hexadienyl) Energy: -398505.7745769

Al	-1.04520	-0.18246	0.06377
C	-2.09661	1.47629	-0.25592
H	-1.93438	2.19123	0.56416

H	-1.73893	1.98117	-1.16570
C	-0.67573	-0.72469	1.93887
H	-1.66382	-0.88585	2.40405
H	-0.26541	0.14207	2.47947
C	1.70937	-0.89828	-1.16247
H	2.60872	-1.45887	-0.89655
C	1.69599	0.43038	-0.92819
H	0.86749	1.02501	-1.32505
C	-3.61401	1.21435	-0.40136
H	-4.03932	0.75860	0.50273
H	-4.17958	2.13826	-0.58504
H	-3.83258	0.53734	-1.23755
C	0.20761	-1.95998	2.18554
H	1.21927	-1.81475	1.78780
H	0.30961	-2.19126	3.25504
H	-0.19930	-2.85312	1.69683
C	2.79898	1.20948	-0.26200
H	3.59982	0.52440	0.04281
H	3.24028	1.90034	-0.99616
C	2.32169	2.02549	0.95125
H	3.14268	2.61745	1.37084
H	1.52023	2.71967	0.67078
H	1.93767	1.37038	1.74081
C	0.59970	-1.65450	-1.75956
C	-0.68952	-1.43379	-1.42060
H	0.88647	-2.42537	-2.48148
H	-1.43615	-2.01326	-1.97018

trans,trans-$AlEt_2$(hexadienyl) Energy: -398511.6838386

Al	2.00183	0.01747	-0.08478
C	2.22648	1.98282	-0.26357
H	2.16106	2.22609	-1.33733
H	1.35987	2.49134	0.18518
C	3.58132	-1.16379	0.12466
H	4.13197	-0.83327	1.02038
H	4.27628	-0.95758	-0.70558
C	0.20127	-0.73457	-0.14051
H	0.03695	-1.81747	-0.10314
C	-0.92794	0.01409	-0.22041
H	-0.85294	1.10446	-0.25962
C	3.52830	2.58024	0.30727
H	4.41730	2.12240	-0.14371
H	3.59994	3.66266	0.13341
H	3.60578	2.42511	1.39091
C	3.31870	-2.67931	0.21216
H	2.82003	-3.05740	-0.68901
H	4.24600	-3.25628	0.33220
H	2.67206	-2.93057	1.06207
C	-2.28696	-0.50551	-0.25943
C	-3.38765	0.26392	-0.33742
H	-2.39470	-1.59108	-0.22375
H	-3.26376	1.34899	-0.36846
C	-4.80236	-0.23716	-0.36930
C	-5.64624	0.28465	0.80790
H	-4.80686	-1.33435	-0.37359
H	-5.27841	0.08138	-1.30935
H	-6.67961	-0.07290	0.73668
H	-5.23312	-0.05152	1.76513
H	-5.67125	1.38080	0.82170

cis-$AlEt_2$(butenyl), Acetylene Coordinated Energy: -398467.8931086

Al	0.54170	0.02684	-0.27957

C	-2.98198	0.00581	0.40265
H	-3.45848	-0.02212	1.39532
H	-2.32463	0.88175	0.39399
C	0.12960	1.97684	-0.23552
H	-0.60176	2.16572	-1.03923
H	-0.40728	2.22845	0.69128
C	2.17176	-0.57481	-1.25325
H	1.96419	-0.40699	-2.32437
H	3.01374	0.10007	-1.03455
C	2.61985	-2.03572	-1.05915
H	1.82652	-2.74100	-1.33647
H	3.50049	-2.28984	-1.66589
H	2.88008	-2.24444	-0.01350
C	-4.08310	0.16974	-0.65965
H	-4.68471	1.06586	-0.46917
H	-3.64875	0.25731	-1.66193
H	-4.76000	-0.69334	-0.66552
C	1.31755	2.94176	-0.41335
H	1.00383	3.99471	-0.43605
H	2.04471	2.85019	0.40543
H	1.86373	2.74844	-1.34498
C	-2.17829	-1.25395	0.20859
C	-0.85581	-1.35275	-0.02970
H	-2.78746	-2.16505	0.25744
H	-0.50875	-2.38680	-0.15154
C	1.97003	0.14905	2.03547
C	1.05719	-0.57067	2.36928
H	2.79364	0.78131	1.78542
H	0.24802	-1.20492	2.65650

cis-$AlEt_2$(butenyl), Second Insertion, Transition State Energy: -398453.5910559

Al	0.73171	0.17978	0.00376
C	-2.85338	-0.35316	0.25301
H	-3.50001	-0.84557	0.99700
H	-2.28900	0.41835	0.78617
C	-0.06239	2.01297	0.02055
H	-0.68809	2.12360	-0.87943
H	-0.75284	2.12960	0.86836
C	2.35908	-0.17450	-1.10059
H	2.07525	0.02633	-2.14682
H	3.10765	0.59533	-0.85816
C	3.00985	-1.56478	-1.01103
H	2.30868	-2.36187	-1.29078
H	3.88138	-1.66265	-1.67418
H	3.35554	-1.78726	0.00643
C	-3.74961	0.29551	-0.81701
H	-4.45911	0.99471	-0.36069
H	-3.14773	0.84875	-1.54588
H	-4.32672	-0.46031	-1.36341
C	0.97689	3.15100	0.05524
H	0.51026	4.14618	0.02897
H	1.59174	3.11182	0.96421
H	1.66586	3.09884	-0.79734
C	-1.91738	-1.37993	-0.32183
C	-0.56872	-1.39013	-0.24796
H	-2.42830	-2.18953	-0.85671
H	-0.08564	-2.26736	-0.69164
C	1.17257	-0.36243	2.00319
C	0.31815	-1.26269	1.83116
H	1.85949	0.02445	2.73897
H	-0.30094	-2.11187	2.03757

cis,cis-$AlEt_2$(hexadienyl) Energy: -398501.5722878

Al	-0.99578	0.16984	0.20390
C	2.31144	-1.49777	-0.11284
H	3.29847	-1.94565	0.08212
H	1.71358	-1.66219	0.78894
C	-1.93603	-1.57826	0.07565
H	-1.83855	-1.97279	-0.94712
H	-1.44900	-2.31874	0.72569
C	-1.42886	1.54084	-1.16334
H	-1.32593	1.07894	-2.15802
H	-2.51414	1.71932	-1.06603
C	-0.68918	2.88996	-1.13698
H	0.38422	2.76109	-1.31822
H	-1.06659	3.58408	-1.90065
H	-0.79015	3.38941	-0.16592
C	1.68798	-2.22883	-1.31310
H	1.63506	-3.30753	-1.12925
H	0.66947	-1.87772	-1.51770
H	2.27880	-2.07207	-2.22359
C	-3.43937	-1.50163	0.43207
H	-3.93632	-2.47710	0.33982
H	-3.59978	-1.16297	1.46440
H	-3.97947	-0.80621	-0.22312
C	2.51986	-0.02382	-0.34702
C	2.17508	1.00468	0.44994
H	3.09609	0.21546	-1.24311
H	2.54317	1.99457	0.16995
C	0.10240	0.57982	1.78809
C	1.39657	0.94883	1.70632
H	-0.31672	0.57317	2.80023
H	1.94361	1.27614	2.59815

cis-$AlEt_2$(butenyl), Insertion at 2nd Ethyl, Transition State Energy: -398450.6802148

Al	0.48292	0.14371	0.30776
C	-3.06396	0.23134	0.37013
H	-3.65020	0.52895	1.25360
H	-2.38451	1.06358	0.15256
C	0.22076	2.01710	-0.30629
H	-0.42474	1.98665	-1.19943
H	-0.36701	2.55910	0.44994
C	1.75002	-0.78396	-1.15371
H	0.95919	-0.45367	-1.85145
H	2.64609	-0.23879	-1.46455
C	1.91618	-2.29553	-1.28688
H	0.99069	-2.82193	-1.03076
H	2.18612	-2.58161	-2.31252
H	2.70606	-2.69114	-0.63364
C	-4.03119	0.02742	-0.80884
H	-4.62404	0.93034	-0.99548
H	-3.48446	-0.21683	-1.72690
H	-4.72859	-0.79560	-0.60997
C	1.49334	2.82115	-0.62999
H	1.26801	3.84711	-0.95324
H	2.15643	2.89615	0.24082
H	2.07464	2.35354	-1.43490
C	-2.28037	-1.01389	0.69889
C	-0.94282	-1.15964	0.69957
H	-2.91716	-1.87106	0.94920
H	-0.60363	-2.16571	0.97565
C	2.53106	-0.51027	0.99449
C	1.85202	0.07935	1.87219

H	3.36648	-1.04693	0.58231
H	1.88251	0.37128	2.91044

cis,cis-AlEt(butenyl)$_2$ Energy: -398505.7412148

Al	0.07499	0.10529	-0.62987
C	3.47151	0.10733	0.44181
H	4.23632	0.83666	0.13354
H	2.64729	0.68168	0.87945
C	-0.01350	1.78552	0.42846
H	-0.35227	1.55946	1.45212
H	0.99926	2.19449	0.54577
C	-3.28266	-0.22275	0.47467
H	-2.50930	0.42495	0.90360
H	-4.11867	0.43307	0.18657
C	-3.78339	-1.21147	1.54290
H	-2.96776	-1.85306	1.89539
H	-4.19825	-0.68048	2.40707
H	-4.56848	-1.86357	1.14166
C	4.08298	-0.81921	1.50827
H	4.45942	-0.24255	2.36071
H	3.33910	-1.53285	1.88041
H	4.92044	-1.39623	1.09806
C	-0.92836	2.87481	-0.17439
H	-0.95981	3.77744	0.45076
H	-0.58365	3.18784	-1.16840
H	-1.96081	2.52461	-0.28997
C	2.99802	-0.64932	-0.77055
C	1.74184	-0.71755	-1.25497
H	3.79689	-1.21415	-1.26565
H	1.63895	-1.37132	-2.12951
C	-2.76041	-0.92068	-0.75360
C	-1.51326	-0.85794	-1.26080
H	-3.50882	-1.55757	-1.23983
H	-1.36135	-1.48961	-2.14425

cis,cis-AlEt$_2$(hexadienyl), Acetylene Coordinated Energy: -447047.0650893

Al	-0.78673	0.05583	-0.14225
C	2.91980	0.95202	-0.44243
H	3.90082	1.16142	-0.89750
H	2.18640	0.99993	-1.25344
C	-1.27045	1.89389	-0.75577
H	-0.30541	2.39479	-0.94010
H	-1.73787	1.84150	-1.75130
C	-0.73630	-0.33917	1.80601
H	0.12115	0.20911	2.22841
H	-1.61890	0.12258	2.27543
C	-0.63841	-1.81319	2.23842
H	0.25465	-2.29407	1.82188
H	-0.58970	-1.92732	3.33059
H	-1.50687	-2.39446	1.90012
C	2.63825	2.04511	0.60225
H	2.67365	3.04113	0.14646
H	1.65126	1.91958	1.06182
H	3.38037	2.02039	1.40949
C	-2.11423	2.78701	0.17220
H	-2.26421	3.79634	-0.23594
H	-3.11573	2.37200	0.35570
H	-1.64496	2.90391	1.15668
C	2.96593	-0.43502	0.14248
C	2.31786	-1.53547	-0.27569
H	3.66485	-0.55493	0.97288
H	2.57872	-2.47783	0.21283

C	0.13977	-1.07262	-1.48136
C	1.35281	-1.65615	-1.39016
H	-0.38494	-1.29577	-2.41884
H	1.69229	-2.32822	-2.18842
C	-3.41094	-0.53796	-0.64324
C	-2.89107	-1.62956	-0.64591
H	-3.90190	0.41039	-0.64130
H	-2.44434	-2.59941	-0.65700

cis,cis-$AlEt_2$(hexadienyl), Third Insertion, Transition State Energy: -447039.0257709

Al	-1.62517	-0.13080	-0.16051
C	4.39596	-0.45746	0.10854
H	5.03838	-0.42061	1.00165
H	4.05558	-1.49403	0.01787
C	-3.03306	-1.24288	-1.04139
H	-2.67307	-1.47557	-2.05692
H	-3.09971	-2.21416	-0.52929
C	-1.25071	1.72183	-0.81587
H	-0.34709	1.68716	-1.44337
H	-2.06880	1.96728	-1.51155
C	-1.11713	2.86243	0.20924
H	-0.30683	2.68081	0.92772
H	-0.91021	3.83179	-0.26635
H	-2.03499	2.98466	0.79849
C	5.24453	-0.08314	-1.12065
H	6.11002	-0.74859	-1.21479
H	4.65441	-0.15663	-2.04043
H	5.61793	0.94498	-1.04518
C	-4.43266	-0.60860	-1.13312
H	-5.14970	-1.24681	-1.66951
H	-4.85728	-0.41887	-0.13854
H	-4.40940	0.35478	-1.65889
C	3.23976	0.48222	0.30777
C	1.91882	0.20015	0.31271
H	3.52538	1.52603	0.44748
H	1.22824	1.02753	0.46400
C	-0.02711	-1.36279	0.18823
C	1.31025	-1.10676	0.14848
H	-0.28971	-2.42304	0.10942
H	2.00052	-1.93849	-0.01040
C	-2.12394	-0.03410	1.90301
C	-1.07764	-0.69882	2.08053
H	-2.94583	0.42116	2.43184
H	-0.29294	-1.22154	2.58844

cis,cis,cis-$AlEt_2$(octatrienyl) Energy: -447091.2770874

Al	-0.84930	-0.15172	-0.07405
C	2.87146	-0.81571	0.08688
H	3.88494	-0.54822	-0.25447
H	2.71098	-0.26601	1.02137
C	-0.50407	-0.66211	1.81902
H	-0.04194	-1.65919	1.87037
H	0.23071	0.02905	2.25742
C	-1.36634	-1.50645	-1.44227
H	-1.13226	-1.12932	-2.45008
H	-0.75771	-2.41514	-1.32162
C	-2.85998	-1.89742	-1.39472
H	-3.51346	-1.03030	-1.55772
H	-3.12318	-2.64147	-2.15978
H	-3.13752	-2.32987	-0.42433
C	2.82389	-2.32799	0.34700

H	3.59426	-2.62250	1.06740
H	1.85209	-2.63071	0.75038
H	2.99593	-2.89283	-0.57704
C	-1.77575	-0.65518	2.69631
H	-1.56360	-0.92149	3.74144
H	-2.25259	0.33306	2.70829
H	-2.52652	-1.37030	2.33420
C	1.89202	-0.35556	-0.95974
C	1.28359	0.85631	-1.01517
H	1.70363	-1.05202	-1.77687
H	0.63936	1.05833	-1.87315
C	0.55097	2.91728	0.17505
C	1.49668	1.99122	-0.11159
H	0.85430	3.78871	0.75541
H	2.48960	2.10644	0.31860
C	-1.54571	1.69385	-0.39181
C	-0.85525	2.84714	-0.21519
H	-2.58493	1.83671	-0.70925
H	-1.35015	3.81709	-0.32061

$AlEt_3$ Dimer Energy: -602681.4732808

Al	1.30961	-0.08903	0.27508
Al	-1.30971	-0.08908	0.27500
C	-2.44434	1.35635	1.03746
C	-3.56958	1.92658	0.14954
H	-1.81288	2.18158	1.40053
H	-2.90458	0.93842	1.94881
H	-4.15691	2.69744	0.66708
H	-3.17985	2.38676	-0.76752
H	-4.27292	1.14440	-0.16148
C	-2.11312	-1.73066	-0.51469
C	-2.96536	-1.52883	-1.78509
H	-2.74074	-2.20975	0.25364
H	-1.32224	-2.46484	-0.72904
H	-3.38361	-2.47395	-2.15770
H	-3.81117	-0.85296	-1.60834
H	-2.38016	-1.09968	-2.60966
C	2.44425	1.35648	1.03736
C	3.56981	1.92618	0.14954
H	2.90416	0.93880	1.94899
H	1.81279	2.18191	1.39998
H	4.15715	2.69714	0.66694
H	4.27307	1.14375	-0.16099
H	3.18043	2.38607	-0.76781
C	2.11312	-1.73028	-0.51533
C	2.96416	-1.52819	-1.78648
H	1.32235	-2.46480	-0.72891
H	2.74163	-2.20907	0.25246
H	3.38258	-2.47315	-2.15932
H	2.37804	-1.09947	-2.61062
H	3.80979	-0.85186	-1.61056
C	0.00007	-0.75947	1.90750
H	0.83703	-0.30547	2.46456
C	-0.00003	2.37036	-1.26411
C	-0.00020	0.82627	-1.22461
H	0.87938	2.78697	-0.76572
H	-0.00059	2.74214	-2.29648
H	-0.87875	2.78722	-0.76468
H	-0.83839	0.46134	-1.84431
H	0.83768	0.46111	-1.84454
H	-0.83891	-0.30757	2.46325
C	0.00147	-2.28076	2.17868

H	0.00031	-2.49217	3.25534
H	-0.87641	-2.77049	1.74712
H	0.88154	-2.76856	1.74942

Dimer: 1 butenyl bridge (*trans*) Energy: -651274.8051715

Al	0.94939	-1.08968	0.25303
Al	-1.57056	-0.23364	0.20140
C	-2.11882	0.66939	1.88975
C	-2.63088	2.11922	1.78041
H	-1.29032	0.63436	2.61423
H	-2.91025	0.05273	2.34774
H	-2.91169	2.53846	2.75672
H	-1.87377	2.78942	1.35274
H	-3.51580	2.19028	1.13591
C	-2.82214	-0.51999	-1.31981
C	-3.40837	0.76743	-1.93452
H	-3.65027	-1.16365	-0.98313
H	-2.31483	-1.09543	-2.10827
H	-4.07437	0.55705	-2.78290
H	-3.99384	1.33808	-1.20301
H	-2.62090	1.43651	-2.30499
C	1.85718	-0.67544	1.97735
C	3.20177	0.07497	1.90299
H	2.02069	-1.63130	2.50237
H	1.16934	-0.11762	2.63200
H	3.62941	0.26599	2.89724
H	3.95114	-0.49204	1.33685
H	3.10160	1.04949	1.40750
C	1.82329	-2.11397	-1.21243
C	3.10085	-1.47364	-1.79321
H	1.10106	-2.27242	-2.02692
H	2.06611	-3.12355	-0.84453
H	3.53651	-2.07680	-2.60185
H	2.90375	-0.47709	-2.20979
H	3.87936	-1.35234	-1.02990
C	-0.85842	-2.22762	0.81063
H	-0.10663	-2.60052	1.52831
C	0.55253	1.86244	-0.22647
C	0.15570	0.64674	-0.67897
H	0.60992	2.03404	0.85206
H	0.13357	0.56106	-1.77310
H	-1.68892	-2.05537	1.51791
C	-1.25256	-3.39375	-0.12481
H	-1.55691	-4.27960	0.44728
H	-2.08811	-3.12466	-0.77796
H	-0.42353	-3.69377	-0.77285
C	0.94830	3.04557	-1.06465
C	2.39083	3.50902	-0.78858
H	0.26310	3.87611	-0.83683
H	0.82188	2.80756	-2.12732
H	2.62917	4.39811	-1.38200
H	2.53206	3.76280	0.26834
H	3.11110	2.72502	-1.04556

Dimer: 1 terminal butenyl (*trans*) Energy: -651266.5191160

Al	1.81680	-0.39018	0.22051
Al	-0.57602	0.64343	0.37119
C	-1.14935	2.46769	0.90418
C	-1.98875	3.25286	-0.12474
H	-0.28017	3.07212	1.20489
H	-1.74232	2.35761	1.82733
H	-2.30977	4.23066	0.25959

H	-1.43012	3.44269	-1.04990
H	-2.89485	2.70445	-0.40906
C	-1.93169	-0.70678	-0.06764
C	-3.25027	-0.52671	0.13874
H	-1.66064	-1.67721	-0.50238
H	-3.60528	0.41587	0.56913
C	3.55980	0.48476	0.61445
C	4.65864	0.37891	-0.46232
H	3.93534	0.01408	1.53880
H	3.40977	1.54144	0.88294
H	5.59867	0.85188	-0.14647
H	4.89098	-0.66678	-0.69897
H	4.36185	0.85996	-1.40329
C	1.75064	-2.29235	-0.36799
C	2.27915	-2.58918	-1.78695
H	0.72594	-2.68131	-0.27953
H	2.33819	-2.88356	0.35268
H	2.25079	-3.66173	-2.02373
H	1.68567	-2.08281	-2.55986
H	3.31859	-2.26211	-1.91593
C	0.61145	-0.19348	2.03382
H	1.57653	0.10723	2.47282
C	1.42016	2.24264	-1.51058
C	0.80113	0.84400	-1.29772
H	2.46013	2.27553	-1.17558
H	1.40659	2.52732	-2.57013
H	0.87913	3.01491	-0.95662
H	-0.18271	0.81596	-1.80066
H	1.33930	0.11904	-1.93221
H	-0.03897	0.57005	2.49534
C	0.19548	-1.56860	2.60217
H	0.14546	-1.54851	3.69805
H	-0.78834	-1.86784	2.22808
H	0.90068	-2.35743	2.32176
C	-4.35219	-1.50682	-0.17845
C	-5.38485	-0.94152	-1.16869
H	-4.87281	-1.77855	0.75288
H	-3.91682	-2.43207	-0.57698
H	-6.19154	-1.66083	-1.35040
H	-5.83899	-0.02037	-0.78376
H	-4.91646	-0.70454	-2.13050

$AlEt_2$(butenyl) Dimer (*trans,trans*) Energy: -699867.4259232

Al	0.29291	-1.21177	-0.06742
Al	0.17638	1.50730	-0.09794
C	-0.34333	2.43679	-1.78139
C	-1.54850	3.39305	-1.69302
H	-0.52964	1.68762	-2.56664
H	0.53492	2.99981	-2.13542
H	-1.78054	3.86556	-2.65806
H	-2.45834	2.87284	-1.36559
H	-1.37140	4.20352	-0.97475
C	0.66639	2.45146	1.58755
C	-0.44728	3.27544	2.26345
H	1.51982	3.11364	1.36982
H	1.05443	1.71509	2.30887
H	-0.10508	3.76348	3.18699
H	-0.82314	4.06814	1.60417
H	-1.30866	2.65092	2.53308
C	-0.12910	-2.20602	-1.74302
C	-1.16874	-3.33804	-1.63209
H	0.81471	-2.62534	-2.12661

H	-0.45070	-1.49071	-2.51621
H	-1.34535	-3.84028	-2.59394
H	-0.85074	-4.11143	-0.92172
H	-2.14134	-2.96688	-1.28358
C	0.88282	-2.08391	1.62456
C	-0.14777	-2.98857	2.32862
H	1.21791	-1.30709	2.33008
H	1.78635	-2.67427	1.40257
H	0.24557	-3.42942	3.25555
H	-1.05649	-2.43539	2.59910
H	-0.46182	-3.82221	1.68768
C	1.74997	0.20949	-0.73294
H	1.86224	0.19627	-1.82487
C	-2.46168	0.03540	-0.15468
C	-1.29381	0.08387	0.53442
H	-2.43247	0.00588	-1.24811
H	-1.42515	0.10315	1.62402
C	2.92693	0.27288	-0.06149
H	2.91460	0.28829	1.03234
C	-3.84942	0.01193	0.42357
C	-4.66172	-1.21508	-0.02916
H	-4.37580	0.92075	0.09356
H	-3.79696	0.05292	1.51795
H	-5.67872	-1.17432	0.37530
H	-4.73657	-1.26116	-1.12180
H	-4.19593	-2.14465	0.31519
C	4.30526	0.31490	-0.65968
C	5.18824	-0.85310	-0.18255
H	4.78426	1.26060	-0.36300
H	4.23675	0.31949	-1.75393
H	6.19686	-0.77036	-0.60125
H	5.27727	-0.86328	0.90991
H	4.76873	-1.81588	-0.49388

Dimer: 1 butenyl bridge, 1 terminal butenyl (*trans,trans*) Energy: -699859.6357441

Al	-0.63048	-0.54524	0.64467
Al	1.77405	-0.75080	-0.46221
C	1.67110	-0.51097	-2.43703
C	2.52826	0.61420	-3.05034
H	0.62127	-0.36571	-2.73584
H	1.96138	-1.46686	-2.90378
H	2.41718	0.67649	-4.14195
H	2.25944	1.59914	-2.64664
H	3.59622	0.46905	-2.84556
C	3.46529	-1.18442	0.49401
C	4.59459	-0.14837	0.32045
H	3.82646	-2.16740	0.15251
H	3.25768	-1.31310	1.56680
H	5.50099	-0.42384	0.87736
H	4.88686	-0.03806	-0.73116
H	4.29239	0.84601	0.67366
C	-1.99524	-0.16824	-0.72100
C	-3.31472	-0.08826	-0.46733
H	-1.72476	-0.02866	-1.77620
H	-3.67726	-0.22340	0.55739
C	-1.11444	-0.74830	2.56190
C	-1.75130	0.50209	3.20200
H	-0.21925	-1.02812	3.13620
H	-1.80366	-1.60020	2.67109
H	-1.99959	0.34605	4.26102
H	-1.07723	1.36729	3.15559

H	−2.67881	0.79338	2.69397
C	0.37252	−2.39274	0.01300
H	−0.67701	−2.60511	−0.25569
C	0.66677	2.04604	−0.05113
C	0.94168	0.88733	0.59772
H	0.16273	2.00255	−1.02051
H	1.43452	1.02014	1.56954
H	0.85589	−2.73793	−0.91831
C	0.78831	−3.34531	1.15647
H	0.61617	−4.39478	0.88549
H	1.84852	−3.24186	1.40550
H	0.22184	−3.14932	2.07189
C	0.95795	3.43888	0.43104
C	−0.31791	4.29259	0.55576
H	1.63463	3.92157	−0.29041
H	1.48651	3.39984	1.39076
H	−0.06869	5.31289	0.86596
H	−0.85152	4.35149	−0.39975
H	−1.00339	3.86809	1.29699
C	−4.40923	0.15921	−1.47589
C	−5.41978	−0.99835	−1.55444
H	−3.96393	0.33381	−2.46386
H	−4.95124	1.07906	−1.20653
H	−6.22161	−0.77553	−2.26784
H	−4.92856	−1.92489	−1.87234
H	−5.88364	−1.18599	−0.57843

Dimer: 1 terminal butenyl per Al (*trans,trans*) Energy: −699851.8247442

Al	1.30560	−0.67156	0.08291
Al	−1.30681	−0.67222	0.08007
C	−2.13941	1.07040	−0.27166
C	−3.46685	1.28683	−0.20711
H	−1.53849	1.95542	−0.51678
H	−4.13761	0.45512	0.03366
C	−2.42686	−2.27485	0.43314
C	−3.39412	−2.67508	−0.70088
H	−3.01006	−2.10194	1.35097
H	−1.77974	−3.13329	0.66832
H	−3.98513	−3.56554	−0.44656
H	−4.10443	−1.87277	−0.93504
H	−2.86140	−2.90813	−1.63300
C	2.13811	1.07109	−0.26910
C	3.46581	1.28672	−0.20719
H	1.53717	1.95668	−0.51219
H	4.13659	0.45440	0.03139
C	2.42748	−2.27344	0.43412
C	3.39183	−2.67446	−0.70210
H	1.78162	−3.13195	0.67240
H	3.01341	−2.09898	1.34993
H	3.98428	−3.56407	−0.44816
H	2.85671	−2.90934	−1.63239
H	4.10083	−1.87191	−0.93941
C	−0.00158	−0.45019	1.82869
H	0.83367	0.22678	2.07837
C	0.00148	−0.03690	−2.74229
C	0.00016	−1.09915	−1.62090
H	0.88336	0.60811	−2.68059
H	0.00256	−0.50723	−3.73362
H	−0.88045	0.60824	−2.68261
H	−0.83925	−1.79328	−1.79806
H	0.83968	−1.79355	−1.79607
H	−0.84622	0.21612	2.07583

C	0.00336	-1.63035	2.82462
H	-0.00683	-1.27244	3.86172
H	-0.86996	-2.27513	2.69191
H	0.89077	-2.25790	2.70346
C	-4.17511	2.60097	-0.42281
C	-4.99034	3.04544	0.80383
H	-4.85794	2.50690	-1.28138
H	-3.44218	3.37399	-0.68678
H	-5.52169	3.98333	0.60575
H	-5.73684	2.28995	1.07744
H	-4.33938	3.19937	1.67178
C	4.17441	2.60060	-0.42336
C	4.99297	3.04336	0.80168
H	3.44137	3.37437	-0.68482
H	4.85508	2.50689	-1.28369
H	5.52450	3.98106	0.60319
H	4.34425	3.19694	1.67138
H	5.73958	2.28708	1.07275

Dimer: 2 terminal butenyl on 1 Al (*trans,trans*) Energy: -699851.0700768

Al	-0.52081	-0.13189	0.39384
Al	2.07509	-0.42146	0.27089
C	2.85836	-2.24737	0.18599
C	3.84569	-2.55294	-0.95854
H	2.05571	-3.00086	0.18439
H	3.38048	-2.40340	1.14518
H	4.24843	-3.57346	-0.89889
H	3.37548	-2.45438	-1.94518
H	4.70385	-1.86982	-0.94528
C	3.20955	1.21387	0.21132
C	4.01593	1.43655	-1.08500
H	3.91465	1.16986	1.05665
H	2.59130	2.10217	0.40783
H	4.63147	2.34545	-1.03893
H	4.69485	0.60070	-1.29415
H	3.36430	1.54566	-1.96272
C	-1.73575	-1.66818	0.47225
C	-3.07620	-1.53853	0.46692
H	-1.36868	-2.70076	0.53060
H	-3.51873	-0.53891	0.40178
C	-1.28179	1.66832	0.58274
C	-1.09097	2.72869	-0.22336
H	-1.96270	1.85543	1.42396
H	-0.42887	2.64032	-1.09179
C	0.88478	-0.33405	2.08926
H	-0.08490	-0.73781	2.43033
C	0.30086	-1.55801	-2.21885
C	0.63418	-0.28001	-1.41659
H	-0.72428	-1.88915	-2.02978
H	0.40302	-1.38760	-3.29794
H	0.96316	-2.38631	-1.95057
H	1.59275	0.11850	-1.79159
H	-0.03616	0.53261	-1.74634
H	1.54064	-1.16210	2.40536
C	1.19694	0.92082	2.93449
H	1.04588	0.72699	4.00381
H	2.23195	1.25053	2.80498
H	0.55432	1.75966	2.65075
C	-4.08724	-2.65641	0.52227
C	-5.00593	-2.68640	-0.71160
H	-4.71166	-2.53562	1.42089
H	-3.56775	-3.61759	0.62638

H	-5.75239	-3.48465	-0.62866
H	-5.54278	-1.73720	-0.82815
H	-4.42692	-2.85506	-1.62654
C	-1.71891	4.09235	-0.07744
C	-2.57339	4.48717	-1.29442
H	-0.92504	4.84398	0.05221
H	-2.33011	4.11909	0.83367
H	-2.98617	5.49547	-1.17567
H	-1.97909	4.47626	-2.21620
H	-3.40825	3.79030	-1.42855

cis,trans-$AlEt_2$(hexadienyl) Dimer Energy: -797023.6880318

Al	-0.25361	1.36647	-0.01571
Al	0.06984	-1.37160	0.15283
C	1.48960	-2.55538	-0.60836
C	2.44156	-3.23154	0.39736
H	2.08017	-2.04198	-1.37999
H	0.93540	-3.33538	-1.15734
H	3.14889	-3.91460	-0.09499
H	3.03567	-2.49296	0.94831
H	1.89446	-3.82218	1.14193
C	-1.42770	-2.21502	1.17301
C	-0.98321	-3.23662	2.24018
H	-2.10267	-2.71396	0.46081
H	-2.04191	-1.44258	1.65902
H	-1.83508	-3.66565	2.78699
H	-0.43537	-4.07613	1.79474
H	-0.31953	-2.78406	2.98875
C	0.88715	2.70422	-0.96653
C	1.58350	3.77251	-0.10214
H	0.21241	3.20403	-1.68158
H	1.63665	2.20547	-1.59677
H	2.15966	4.48626	-0.70871
H	0.86349	4.35856	0.48103
H	2.28141	3.31823	0.61094
C	-1.89530	1.98915	0.94551
C	-1.66599	3.19543	1.87995
H	-2.32075	1.16489	1.53753
H	-2.67146	2.25225	0.21056
H	-2.57968	3.48374	2.41902
H	-0.90041	2.98559	2.63825
H	-1.33125	4.07990	1.32472
C	-0.51175	-0.14969	-1.50415
H	0.39898	-0.03871	-2.10844
C	2.02046	0.41324	1.89219
C	0.73576	0.18175	1.46997
H	0.05774	0.12638	2.33007
C	-1.57555	-0.40797	-2.33182
C	3.26666	0.57333	1.14694
C	3.46864	0.40852	-0.17423
H	2.64015	0.10189	-0.80846
C	-2.99087	-0.64017	-2.05926
C	-3.63924	-0.50727	-0.88703
H	-3.08936	-0.17923	-0.00990
C	4.78623	0.59722	-0.86523
C	5.27870	-0.67851	-1.57334
H	5.53869	0.94141	-0.14490
H	4.67979	1.39589	-1.61506
H	6.22446	-0.49058	-2.09331
H	5.43769	-1.48977	-0.85519
H	4.55086	-1.02717	-2.31499
C	-5.10406	-0.75720	-0.68889

C	-5.86287	0.50182	-0.22851
H	-5.22672	-1.53935	0.07534
H	-5.54763	-1.14626	-1.61393
H	-6.91829	0.27208	-0.04563
H	-5.43832	0.90312	0.69862
H	-5.81122	1.28964	-0.98776
H	-3.57367	-0.94624	-2.92886
H	-1.36051	-0.47393	-3.40271
H	4.12604	0.85634	1.75568
H	2.18003	0.51492	2.96997

cis,cis-$AlEt_2$(hexadienyl) Dimer Energy: -797021.1535606

Al	0.21658	1.44654	0.12799
Al	0.04872	-1.26518	0.55805
C	0.74020	-2.91407	-0.33717
C	1.94996	-3.60295	0.32369
H	0.93886	-2.76255	-1.40659
H	-0.12078	-3.60290	-0.30592
H	2.21930	-4.54363	-0.17732
H	2.84078	-2.96284	0.30932
H	1.75313	-3.84550	1.37509
C	-1.08826	-1.56663	2.17207
C	-0.48071	-2.50165	3.23822
H	-2.04648	-1.99383	1.83587
H	-1.35194	-0.61125	2.64901
H	-1.14531	-2.63664	4.10343
H	-0.27846	-3.50137	2.83371
H	0.47160	-2.11682	3.62718
C	1.03001	2.47635	-1.37365
C	1.83313	3.73626	-0.99596
H	0.18705	2.77204	-2.01955
H	1.65284	1.82606	-2.00093
H	2.21424	4.26514	-1.88162
H	1.22252	4.45468	-0.43549
H	2.70102	3.49315	-0.37104
C	-0.85391	2.39739	1.52225
C	-0.05695	3.38349	2.39985
H	-1.35980	1.67415	2.17722
H	-1.66499	2.94179	1.01301
H	-0.69082	3.88190	3.14702
H	0.74728	2.87759	2.94974
H	0.41430	4.17364	1.80271
C	-0.87326	-0.08410	-0.93775
H	-0.34486	-0.24305	-1.88591
C	2.85383	0.39734	1.24814
C	1.50060	0.17194	1.27489
H	1.17453	0.13081	2.32264
C	-2.22805	0.00621	-1.12079
C	3.83342	0.66790	0.19077
C	3.94608	0.26497	-1.09109
C	-3.22336	0.21516	-0.08680
C	-4.55692	0.30881	-0.28233
H	-2.85112	0.30244	0.92993
H	-2.62320	-0.08324	-2.13502
H	4.65779	1.28218	0.55611
H	3.33799	0.49079	2.22652
H	4.82453	0.63073	-1.62659
H	-5.17545	0.45818	0.60396
C	3.08550	-0.66507	-1.88646
C	3.89999	-1.80967	-2.51526
H	2.60543	-0.09412	-2.69571
H	2.28277	-1.06936	-1.26926

H	3.25676	-2.45367	-3.12443
H	4.69548	-1.42030	-3.16216
H	4.36759	-2.43115	-1.74442
C	-5.33057	0.21759	-1.56679
C	-6.32496	-0.95869	-1.56291
H	-4.66627	0.13517	-2.43279
H	-5.89401	1.15349	-1.69779
H	-6.91492	-0.97050	-2.48590
H	-5.79921	-1.91595	-1.48049
H	-7.02163	-0.88641	-0.71957

cis,trans-$AlEt_2$(hexadienyl)/*cis*-$AlEt_2$(butenyl) Dimer Energy: -748443.4021241

Al	0.78972	-1.22957	0.06450
Al	0.25131	1.46121	0.06462
C	-1.22490	2.47293	-0.82243
C	-2.26840	3.12380	0.10639
H	-1.73862	1.87050	-1.58483
H	-0.71313	3.26451	-1.39538
H	-3.00020	3.72845	-0.44836
H	-2.83145	2.37037	0.66986
H	-1.79826	3.78833	0.84164
C	1.66739	2.48108	1.03636
C	1.15175	3.40927	2.15501
H	2.22905	3.08505	0.30626
H	2.40604	1.78617	1.46300
H	1.96747	3.93698	2.66931
H	0.47257	4.17718	1.76390
H	0.59703	2.85456	2.92306
C	-0.22310	-2.69405	-0.83693
C	-0.78222	-3.80616	0.07079
H	0.48712	-3.13975	-1.55352
H	-1.03333	-2.29501	-1.46351
H	-1.27825	-4.60218	-0.50307
H	0.00834	-4.28498	0.66146
H	-1.52006	-3.41234	0.78003
C	2.48319	-1.63669	1.04385
C	2.34040	-2.61010	2.23161
H	2.94161	-0.70423	1.40537
H	3.20775	-2.05497	0.32709
H	3.29642	-2.78308	2.74582
H	1.63665	-2.23295	2.98492
H	1.96864	-3.59136	1.91180
C	1.01329	0.21366	-1.50873
H	0.20492	0.04763	-2.23263
C	-1.56264	-0.39261	1.90317
C	-0.30773	-0.04461	1.47194
H	0.35387	0.13060	2.32879
C	2.19679	0.48047	-2.12058
C	-2.77449	-0.73104	1.16166
C	-2.99119	-0.61063	-0.16184
H	-2.21072	-0.19346	-0.79424
C	-4.26401	-0.99332	-0.85628
C	-4.92684	0.18818	-1.58841
H	-4.96543	-1.42985	-0.13456
H	-4.03902	-1.78041	-1.59203
H	-5.82960	-0.14120	-2.11428
H	-5.20950	0.97776	-0.88424
H	-4.24787	0.62794	-2.32794
H	2.23398	0.50080	-3.21643
H	-3.58903	-1.11922	1.77397
H	-1.71801	-0.45812	2.98435
C	3.52740	0.76196	-1.48501

C	4.63755	-0.15501	-2.02870
H	3.46171	0.67973	-0.39741
H	3.79562	1.80599	-1.71022
H	5.60575	0.11244	-1.59262
H	4.43597	-1.20394	-1.78637
H	4.72514	-0.07194	-3.11868

$AlEt_2$(butenyl) Dimer (*cis*,*cis*) Energy: -699861.8062977

Al	0.34014	-1.22905	-0.06458
Al	-0.05571	1.48035	-0.13246
C	-1.21095	2.44138	-1.44501
C	-2.24252	3.43258	-0.87058
H	-1.72321	1.72159	-2.10050
H	-0.52804	2.99005	-2.11374
H	-2.83628	3.91915	-1.65744
H	-2.95211	2.94212	-0.19173
H	-1.75885	4.23193	-0.29623
C	1.00032	2.46261	1.24663
C	0.17200	3.29905	2.24344
H	1.71514	3.12557	0.73357
H	1.62319	1.75414	1.81263
H	0.80365	3.80601	2.98643
H	-0.41169	4.07705	1.73634
H	-0.54118	2.67867	2.80138
C	-0.47280	-2.55691	-1.31495
C	-0.99956	-3.86036	-0.68254
H	0.30609	-2.81178	-2.05154
H	-1.27296	-2.09062	-1.90863
H	-1.44470	-4.53556	-1.42719
H	-0.19783	-4.41904	-0.18438
H	-1.76874	-3.66856	0.07664
C	1.62988	-1.79350	1.35055
C	1.06362	-2.75355	2.41719
H	2.03730	-0.90612	1.85795
H	2.49697	-2.27080	0.86684
H	1.81315	-3.02366	3.17435
H	0.21449	-2.31016	2.95338
H	0.70525	-3.69027	1.97328
C	1.11173	0.23403	-1.42603
H	0.56144	0.13008	-2.36990
C	-2.40880	-0.15726	0.95078
C	-1.05800	-0.02744	1.02915
H	-0.70625	0.04086	2.06555
C	2.43646	0.45611	-1.62949
C	-3.25709	-0.26040	-0.28386
C	-4.25393	-1.43038	-0.22414
H	-2.62871	-0.33528	-1.17617
H	-3.82588	0.67738	-0.37789
H	-4.89635	-1.43380	-1.11098
H	-3.73444	-2.39282	-0.17938
H	-4.90124	-1.35499	0.65782
C	3.51459	0.65329	-0.60376
C	4.69816	-0.30831	-0.81219
H	3.11156	0.54902	0.40660
H	3.88351	1.68681	-0.69482
H	5.49364	-0.10293	-0.08822
H	4.38585	-1.35031	-0.68471
H	5.12348	-0.20461	-1.81763
H	2.81253	0.50362	-2.65855
H	-2.99494	-0.18523	1.87731

Dimer: 1 butenyl bridge, 1 terminal butenyl (*cis*,*cis*) Energy: -699854.8581667

Al	0.72998	-0.24517	0.09201
Al	-1.91737	-0.13531	-0.23171
C	-2.94550	-1.16882	-1.58674
C	-4.10344	-2.05042	-1.07740
H	-2.25497	-1.78340	-2.18357
H	-3.34825	-0.43065	-2.29906
H	-4.62153	-2.56834	-1.89659
H	-3.75551	-2.82443	-0.38145
H	-4.85863	-1.45949	-0.54520
C	-2.79563	1.08840	1.07403
C	-3.89720	0.46211	1.95486
H	-3.23072	1.93106	0.51379
H	-2.03933	1.54646	1.72924
H	-4.33455	1.18963	2.65272
H	-4.72189	0.06041	1.35370
H	-3.51516	-0.36704	2.56564
C	1.36925	0.89007	1.60151
C	2.13852	0.14217	2.71055
H	0.51029	1.40388	2.05941
H	2.00629	1.69791	1.20994
H	2.46945	0.81539	3.51339
H	1.52208	-0.63289	3.18541
H	3.03356	-0.35871	2.32172
C	-0.39890	0.80403	-1.38798
H	-0.31061	0.25008	-2.32995
C	-0.34225	2.14890	-1.56766
C	-0.41689	3.23253	-0.53180
C	0.76346	4.21511	-0.63368
H	-0.47306	2.80594	0.47269
H	-1.35170	3.79141	-0.69361
H	0.65476	5.02346	0.09686
H	1.71549	3.70951	-0.43976
H	0.82008	4.66784	-1.63072
H	-0.22129	2.53740	-2.58562
C	-0.76815	-1.60558	0.94891
C	-0.67679	-3.05855	0.42937
H	-1.73995	-1.49532	1.46482
H	-0.10581	-1.50475	1.82501
H	-0.99193	-3.77796	1.19591
H	-1.30942	-3.21767	-0.44933
H	0.34661	-3.31550	0.14192
C	1.87971	-1.38770	-1.03244
C	3.20766	-1.33988	-1.24836
H	1.36588	-2.15498	-1.62350
H	3.66418	-2.04700	-1.95131
C	4.20597	-0.40215	-0.62043
C	5.32988	-1.14388	0.12328
H	3.70063	0.29028	0.06231
H	4.66040	0.21408	-1.41204
H	6.07013	-0.44186	0.52394
H	4.92833	-1.72885	0.95860
H	5.85411	-1.83765	-0.54522

Dimer: 1 butenyl bridge (*cis*) Energy: -651271.9229160

Al	1.16347	-0.57019	-0.11571
Al	-1.39533	0.18450	-0.11756
C	-2.79613	-0.36695	-1.42216
C	-4.15351	-0.84640	-0.86988
H	-2.38812	-1.12852	-2.10311
H	-2.96903	0.51510	-2.05998
H	-4.86373	-1.09081	-1.67219
H	-4.05408	-1.74645	-0.24957

H	-4.62911	-0.08053	-0.24520
C	-1.78425	1.49189	1.33687
C	-2.88274	1.07648	2.33857
H	-2.07897	2.44448	0.86834
H	-0.86825	1.72629	1.89920
H	-3.05380	1.84187	3.10836
H	-3.84515	0.90191	1.84228
H	-2.62601	0.15011	2.87010
C	2.02611	-1.86724	-1.35695
C	2.75155	-3.07740	-0.73518
H	2.75174	-1.28649	-1.94931
H	1.28761	-2.22129	-2.09185
H	3.21898	-3.71687	-1.49697
H	3.54738	-2.76357	-0.04904
H	2.06888	-3.71583	-0.15991
C	2.16705	0.30524	1.36922
C	2.93740	-0.64110	2.31351
H	1.48259	0.92191	1.97101
H	2.88040	1.01989	0.92946
H	3.45712	-0.09703	3.11441
H	2.27240	-1.36375	2.80556
H	3.69651	-1.22270	1.77651
C	0.19412	0.79013	-1.42480
H	0.03662	0.28576	-2.38633
C	0.54304	2.09413	-1.57250
C	0.83808	3.10397	-0.50219
C	2.20026	3.79003	-0.70916
H	0.78763	2.64367	0.48750
H	0.05064	3.87271	-0.53730
H	2.36306	4.55934	0.05280
H	3.02054	3.06740	-0.64032
H	2.25865	4.27252	-1.69209
H	0.63437	2.50326	-2.58554
C	-0.55275	-1.61824	0.80420
C	-1.00072	-2.94083	0.14226
H	-1.29473	-1.33952	1.57326
H	0.29801	-1.84350	1.47334
H	-1.14563	-3.73456	0.88629
H	-1.94475	-2.82287	-0.39719
H	-0.26270	-3.30022	-0.58075

Dimer: 1 terminal butenyl (*cis*) Energy: -651265.6425047

Al	0.72144	0.17336	-0.23633
Al	-1.87101	-0.08492	-0.31136
C	-2.90730	-1.71216	0.15775
C	-4.05080	-1.50452	1.17298
H	-2.24084	-2.50990	0.51580
H	-3.33724	-2.10396	-0.77815
H	-4.60835	-2.43141	1.36509
H	-3.67945	-1.15019	2.14320
H	-4.77686	-0.76242	0.81833
C	-2.77552	1.56433	-0.96403
C	-3.62081	2.36547	0.04702
H	-3.42580	1.26285	-1.80245
H	-2.03332	2.23801	-1.41898
H	-4.10845	3.23539	-0.41403
H	-4.41544	1.75404	0.49285
H	-3.01093	2.75085	0.87508
C	1.32218	1.97232	-0.83763
C	2.01377	2.86887	0.20888
H	0.45514	2.51281	-1.24819
H	1.99933	1.84198	-1.69705

H	2.32782	3.83394	-0.21159
H	1.34990	3.09651	1.05349
H	2.91059	2.39529	0.62797
C	-0.65794	0.45207	1.43810
C	-0.51280	-0.59006	2.56950
H	-1.61279	0.98822	1.58612
H	0.03693	1.28604	1.63567
H	-0.72685	-0.14490	3.54928
H	-1.19601	-1.43457	2.43623
H	0.50181	-0.99629	2.60786
C	-0.47178	-0.65343	-1.89299
C	-0.30023	-2.16614	-2.15340
H	0.32561	-0.11250	-2.43190
H	-1.34361	-0.29392	-2.46823
H	-0.27535	-2.38328	-3.22875
H	0.63151	-2.53990	-1.71905
H	-1.11928	-2.74899	-1.72105
C	1.89664	-1.30935	0.30862
C	3.23389	-1.44420	0.22446
H	1.39416	-2.18376	0.73849
H	3.70292	-2.36818	0.58273
C	4.22582	-0.44744	-0.31521
C	5.28743	-0.04594	0.72338
H	3.70776	0.44550	-0.68205
H	4.73818	-0.89177	-1.18274
H	6.02656	0.63635	0.28837
H	4.82679	0.45445	1.58285
H	5.82463	-0.92485	1.10018

Dimer: 2 terminal butenyl on 1 Al (*cis,cis*) Energy: -699847.0724240

Al	-0.42985	-0.17672	-0.16952
Al	2.15641	0.16039	-0.31644
C	2.85774	1.25750	1.18708
C	3.64342	0.49062	2.27154
H	2.03208	1.80890	1.65972
H	3.51231	2.03749	0.76741
H	4.02613	1.15793	3.05607
H	3.02149	-0.26192	2.77353
H	4.50977	-0.03776	1.85361
C	3.33160	-0.72289	-1.65359
C	4.50190	-1.56754	-1.11219
H	3.73823	0.06503	-2.30880
H	2.71319	-1.34546	-2.31954
H	5.10490	-2.01032	-1.91684
H	5.18294	-0.96801	-0.49526
H	4.15186	-2.39942	-0.48669
C	1.04199	-1.55151	0.58658
C	0.35443	-1.91768	1.92771
H	2.12215	-1.62161	0.80650
H	0.88647	-2.36090	-0.13888
H	0.71327	-2.88498	2.30013
H	0.55430	-1.16591	2.69715
H	-0.73546	-1.99885	1.83219
C	0.69619	1.24777	-1.47636
C	0.92789	2.74356	-1.15987
H	-0.35105	1.16366	-1.81620
H	1.22616	0.97043	-2.40052
H	0.59477	3.38170	-1.98795
H	0.37750	3.04004	-0.26201
H	1.98471	2.97230	-0.98312
C	-1.46398	-1.26557	-1.44212
C	-2.67001	-1.84915	-1.30975

H	-0.98184	-1.45830	-2.40963
H	-3.07392	-2.44603	-2.13589
C	-3.57633	-1.80433	-0.10674
C	-3.85092	-3.20174	0.47636
H	-4.53771	-1.35493	-0.39993
H	-3.15049	-1.15342	0.66599
H	-4.55310	-3.14734	1.31612
H	-4.28383	-3.86866	-0.27922
H	-2.92565	-3.66658	0.83611
C	-1.13814	0.96525	1.27084
C	-2.22233	1.76346	1.26607
H	-0.57494	0.98750	2.21042
H	-2.46132	2.35505	2.15765
C	-3.19565	1.97056	0.13407
C	-3.27809	3.43989	-0.31521
H	-4.19696	1.65033	0.46118
H	-2.93211	1.33110	-0.71764
H	-4.02837	3.56979	-1.10349
H	-3.55501	4.09335	0.52101
H	-2.31408	3.78892	-0.70234

Dimer: 1 terminal butenyl per Al (*cis,cis*) Energy: -699848.7092185

Al	1.30603	0.21458	-0.25992
Al	-1.30616	0.21508	-0.25908
C	-2.13453	1.89447	-0.93206
C	-2.98205	2.71830	0.05755
H	-2.75428	1.64646	-1.80898
H	-1.33471	2.53718	-1.33357
H	-3.40240	3.62156	-0.40526
H	-3.82549	2.13942	0.45438
H	-2.39235	3.05421	0.92104
C	2.13466	1.89363	-0.93353
C	2.98179	2.71820	0.05578
H	1.33508	2.53608	-1.33592
H	2.75477	1.64487	-1.80999
H	3.40263	3.62092	-0.40763
H	2.39162	3.05507	0.91858
H	3.82486	2.13953	0.45370
C	0.00053	0.76906	1.41124
C	0.00021	-0.17185	2.63630
H	-0.83754	1.47915	1.51948
H	0.83966	1.47796	1.51916
H	0.00103	0.40057	3.57244
H	-0.88278	-0.81778	2.64684
H	0.88216	-0.81921	2.64617
C	-0.00052	-0.47877	-1.88110
C	-0.00021	-1.99852	-2.15595
H	0.83854	-0.02226	-2.43472
H	-0.84075	-0.02299	-2.43354
H	-0.00106	-2.20491	-3.23372
H	0.88323	-2.48136	-1.72755
H	-0.88261	-2.48193	-1.72604
C	-2.25885	-1.39335	0.35271
C	-3.56634	-1.71141	0.30534
H	-1.63038	-2.17732	0.79209
H	-3.89736	-2.67940	0.69957
C	-4.69638	-0.87294	-0.23280
C	-5.77235	-0.58153	0.82756
H	-5.16891	-1.40930	-1.07033
H	-4.31201	0.06832	-0.64155
H	-6.60875	-0.01906	0.39728
H	-6.17502	-1.51122	1.24777

H	-5.35827	0.00432	1.65614
C	2.25899	-1.39375	0.35172
C	3.56659	-1.71146	0.30511
H	1.63048	-2.17801	0.79055
H	3.89760	-2.67944	0.69935
C	4.69674	-0.87264	-0.23224
C	5.77202	-0.58113	0.82879
H	4.31239	0.06858	-0.64109
H	5.16990	-1.40878	-1.06956
H	6.60866	-0.01861	0.39902
H	5.35739	0.00470	1.65710
H	6.17450	-1.51079	1.24927

Hydrogen Energy: -740.1906289

H	0.00000	0.00000	0.37139
H	0.00000	0.00000	-0.37139

AlEt2H Energy: -251978.8552910

Al	0.03741	0.82738	-0.01272
C	-1.91540	0.50741	0.01113
H	-2.32590	1.03967	0.88493
H	-2.34782	1.04276	-0.85014
C	1.35413	-0.65091	-0.04854
H	1.10458	-1.35533	0.76111
H	1.17987	-1.23317	-0.96852
C	-2.40439	-0.95328	0.01476
H	-3.50040	-1.02352	0.02887
H	-2.05842	-1.49923	-0.87151
H	-2.03563	-1.50224	0.88993
C	2.84073	-0.25701	0.04051
H	3.50403	-1.13166	0.00069
H	3.13338	0.40865	-0.78052
H	3.06383	0.27481	0.97352
H	0.54569	2.34606	-0.01023

AlEt2H Dimer Energy: -503987.1322063

Al	1.33242	-0.02727	-0.43002
Al	-1.33245	-0.02728	-0.43004
C	-2.20760	-1.80261	-0.40167
C	-3.23475	-2.02490	0.72848
H	-1.43459	-2.58281	-0.35240
H	-2.70319	-1.95137	-1.37365
H	-3.69396	-3.02122	0.67552
H	-2.77409	-1.93687	1.72046
H	-4.05154	-1.29363	0.68684
C	-2.20063	1.75100	-0.48760
C	-3.06045	2.11343	0.74181
H	-2.82618	1.79803	-1.39245
H	-1.42860	2.52028	-0.63258
H	-3.52105	3.10552	0.64216
H	-3.87613	1.39616	0.89611
H	-2.46542	2.12750	1.66353
C	2.20757	-1.80260	-0.40165
C	3.23491	-2.02481	0.72836
H	2.70301	-1.95143	-1.37369
H	1.43457	-2.58280	-0.35220
H	3.69411	-3.02113	0.67540
H	4.05168	-1.29353	0.68654
H	2.77440	-1.93669	1.72041
C	2.20058	1.75101	-0.48756
C	3.06041	2.11345	0.74184
H	1.42853	2.52029	-0.63252

H	2.82612	1.79807	-1.39242
H	3.52100	3.10555	0.64219
H	2.46539	2.12749	1.66356
H	3.87610	1.39619	0.89612
H	-0.00003	0.00566	0.72091
H	-0.00001	-0.06394	-1.57907

AlEt2H Trimer Energy: -755986.7800758

Al	0.59442	1.77969	-0.04120
Al	-1.77161	-0.38843	0.51283
C	-2.15325	-0.65915	2.43580
C	-2.68695	-2.06014	2.79971
H	-2.88105	0.10205	2.75685
H	-1.24431	-0.44983	3.01846
H	-2.89360	-2.15644	3.87412
H	-3.62167	-2.29023	2.27260
H	-1.96883	-2.84857	2.54055
C	-3.04400	-0.48071	-1.00090
C	-4.20999	0.52738	-0.93444
H	-3.44960	-1.50276	-1.05378
H	-2.49436	-0.34216	-1.94350
H	-4.88880	0.43042	-1.79247
H	-4.81623	0.39017	-0.03010
H	-3.85096	1.56458	-0.92711
C	1.41963	2.41636	1.64127
C	2.88857	2.87055	1.51420
H	1.34533	1.62670	2.40332
H	0.81410	3.24856	2.03220
H	3.29490	3.22509	2.47101
H	3.53840	2.05382	1.17447
H	3.00129	3.69185	0.79505
C	0.34426	2.79434	-1.72243
C	-0.50043	4.07837	-1.58500
H	-0.10917	2.13732	-2.47874
H	1.33587	3.05304	-2.12431
H	-0.60067	4.61028	-2.54074
H	-1.51703	3.86064	-1.23331
H	-0.05720	4.78445	-0.87134
H	-0.92672	1.10030	0.37319
H	-0.44927	-1.41026	0.11709
H	1.36477	0.30617	-0.46635
Al	1.16692	-1.39820	-0.46052
C	2.30322	-2.11801	0.99188
C	3.82112	-1.94501	0.77601
H	2.01372	-1.65213	1.94516
H	2.07398	-3.18782	1.11475
H	4.16084	-2.43504	-0.14535
H	4.40609	-2.37359	1.60090
H	4.10280	-0.88685	0.70078
C	1.11702	-1.97148	-2.35441
C	0.71529	-3.44399	-2.57897
H	0.43099	-1.31614	-2.91104
H	2.10796	-1.79249	-2.79956
H	1.40289	-4.13556	-2.07572
H	0.71303	-3.71325	-3.64379
H	-0.29093	-3.65336	-2.19406

AlEt2(butenyl) + H2 Cleavage, Transition State Energy: -350639.6519514

Al	0.84814	0.11800	0.13631
C	-2.77418	-0.43796	0.54279
H	-3.41573	-0.89147	1.31349
H	-2.19022	0.34703	1.03479

C	0.10680	1.94738	-0.06744
H	-0.35180	2.02400	-1.06537
H	-0.71813	2.10132	0.64175
C	2.63068	-0.48679	-0.48519
H	2.62372	-0.49971	-1.58655
H	3.36124	0.29118	-0.21731
C	3.12205	-1.84847	0.03889
H	2.44795	-2.66465	-0.24990
H	4.11755	-2.10528	-0.34863
H	3.18739	-1.85944	1.13365
C	-3.67387	0.18318	-0.54172
H	-4.36376	0.91233	-0.10321
H	-3.07295	0.69553	-1.30052
H	-4.27223	-0.58366	-1.04793
C	1.14365	3.07706	0.10259
H	0.70044	4.06999	-0.05465
H	1.58270	3.07672	1.10807
H	1.97268	2.98018	-0.60962
C	-1.86695	-1.50166	-0.00920
C	-0.51618	-1.48323	-0.01921
H	-2.39725	-2.35949	-0.43693
H	-0.03224	-2.38224	-0.41368
H	0.06424	-0.98565	1.21890
H	0.69865	-0.39779	1.84268

AlEt2H + 1-Butene, Endpoint Energy: -350673.1641041

Al	-0.72239	0.16277	-0.35421
C	2.82701	-0.74196	-0.13018
H	3.71753	-1.12630	0.39213
H	2.51262	-1.52644	-0.82806
C	-0.59891	1.96098	0.49973
H	-0.72014	1.87216	1.59070
H	0.40654	2.38203	0.35009
C	-2.32934	-0.95696	0.02506
H	-2.53945	-0.98260	1.10481
H	-3.16897	-0.38211	-0.40347
C	-2.36885	-2.38342	-0.55082
H	-1.60506	-3.02914	-0.09746
H	-3.33689	-2.87677	-0.38443
H	-2.18609	-2.38671	-1.63250
C	3.21466	0.53475	-0.89106
H	4.04712	0.33450	-1.57365
H	2.37352	0.91005	-1.48099
H	3.53077	1.32611	-0.20094
C	-1.64417	2.96447	-0.03459
H	-1.56082	3.95068	0.44346
H	-1.53786	3.12623	-1.11548
H	-2.66960	2.61289	0.13797
C	1.76542	-0.53521	0.91408
C	0.72874	-1.36016	1.15506
H	1.89145	0.33994	1.55382
H	0.07043	-1.21039	2.00675
H	0.58482	-2.27267	0.58015
H	0.01385	-0.07237	-1.76179