Supplementary Information

Insertion, elimination and isomerisation of olefins at alkylaluminium hydride: an experimental and theoretical study

Nandita M. Weliange,[a] David S. McGuinness,*[a] Michael G. Gardiner[a] and Jim Patel[b]

[a] School of Physical Sciences – Chemistry, Private Bag 75, Hobart 7001, Australia. Email: david.mcguinness@utas.edu.au
[b] CSIRO Earth Science and Resource Engineering, 71 Normanby Rd, Clayton North 3168, Australia.

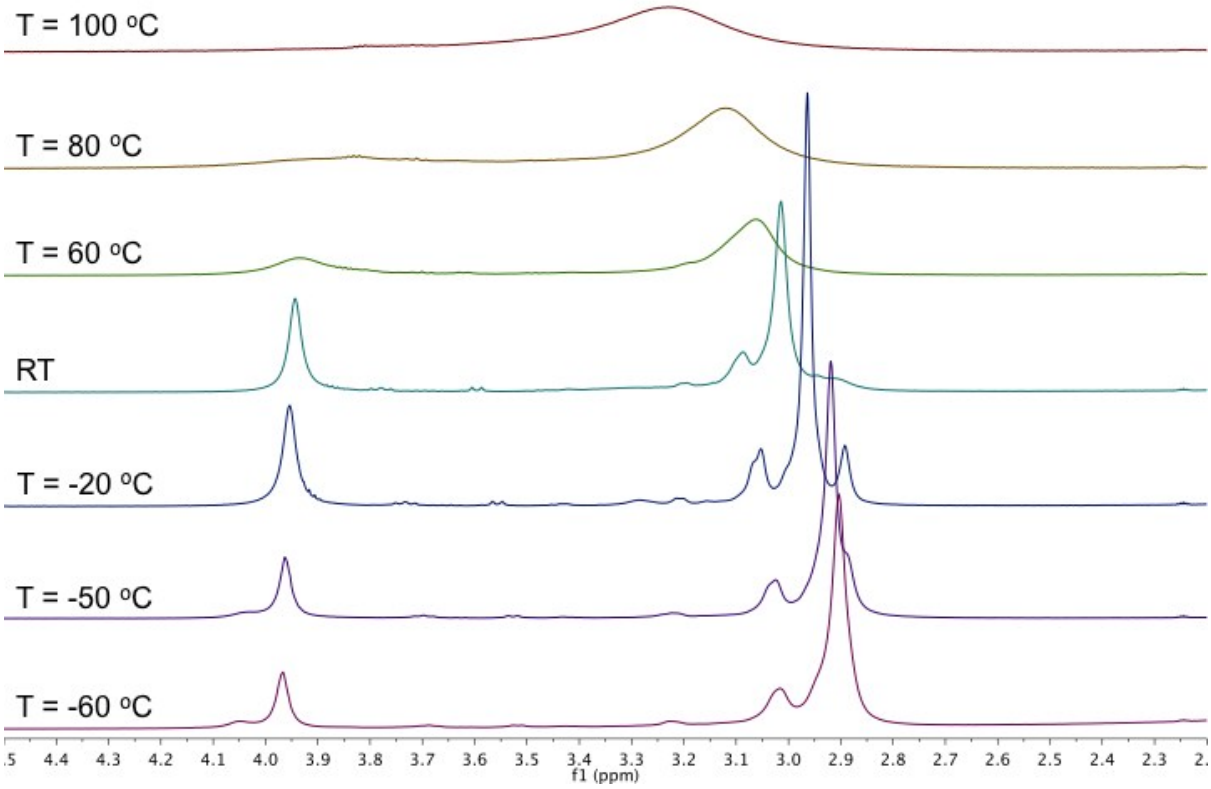

Figure S1. Variable temperature ^{1}H NMR spectra (toluene-d_8) of a mixture of $[(Oct)_2AlH]$ (60%) and $[Al(Oct)_3]$ (40%), showing Al-H signal convergence at higher temperatures.

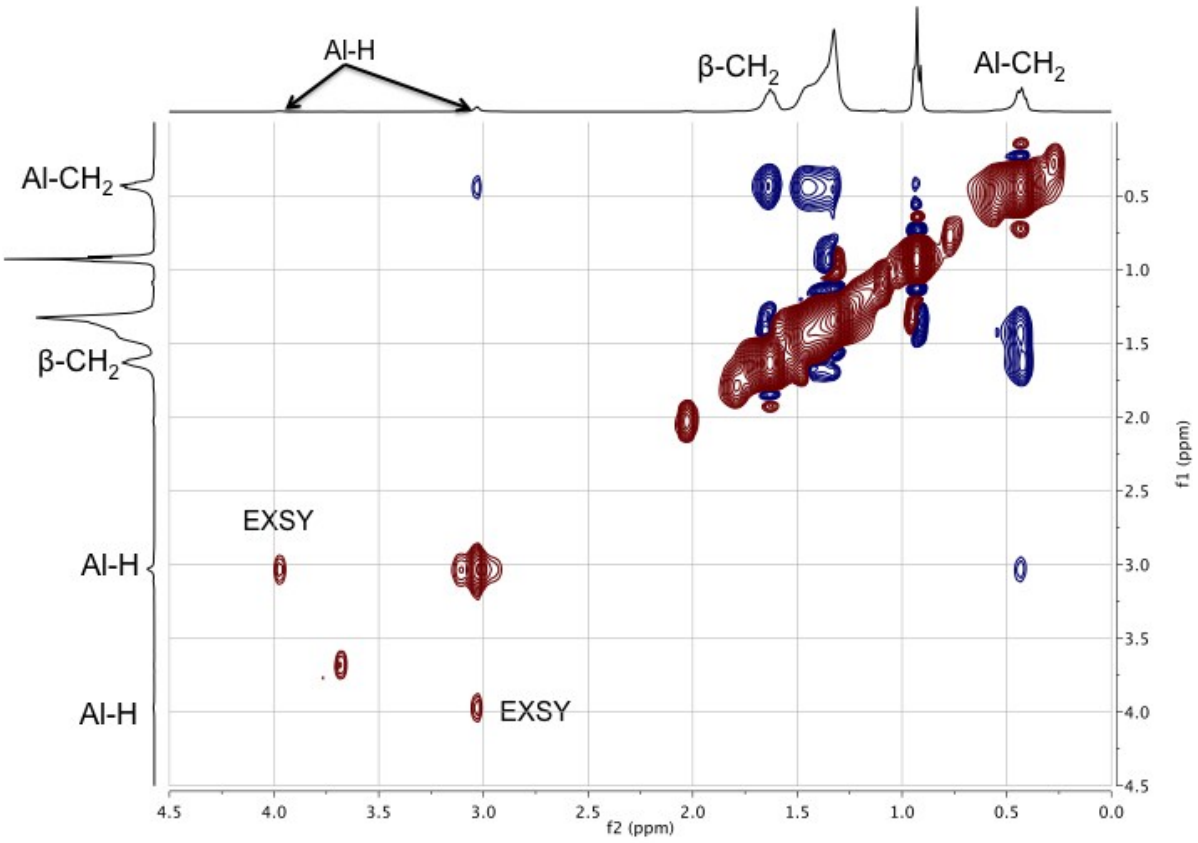

Figure S2. EXSY NMR spectrum (C_6D_6) of a mixture of [$(Oct)_2AlH$] (55%) and [$Al(Oct)_3$] (45%).

Reaction of [$Al(Oct)_3$] and [$(Oct)_2AlH$] with THF

The formation of THF adducts of [$Al(Oct)_3$] and [$(Oct)_2AlH$] was studied by NMR spectroscopy. When an equimolar amount of THF is added to [$Al(Oct)_3$] the major change observed in the ^1H NMR spectrum is an upfield shift in the α–C proton signal (from 0.53 ppm to 0.11 ppm, Figure S3). This is attributed to formation of [$Al(Oct)_3(THF)$]. In a mixture of [$Al(Oct)_3$] and [$(Oct)_2AlH$], the THF ligand preferentially coordinates to [$Al(Oct)_3$]. Thus, if the amount of THF added is equal only to the amount of [$Al(Oct)_3$] present, then only [$Al(Oct)_3(THF)$] forms. In this case the Al–H signal is observed at 3.00 ppm, which is consistent with hydride-bridged cyclic oligomers formed in the absence of [$Al(Oct)_3$] (see main article). When the amount of THF added is equal to the total amount of aluminium, then both [$Al(Oct)_3(THF)$] and [$(Oct)_2AlH(THF)$] are formed. In [$(Oct)_2AlH(THF)$] the hydride resonance appears as a sharp singlet at 4.07 ppm (Figure S4). The other significant change is an upfield shift in the α–C proton signal from 0.43 ppm to 0.05 ppm, Figure S3 top).

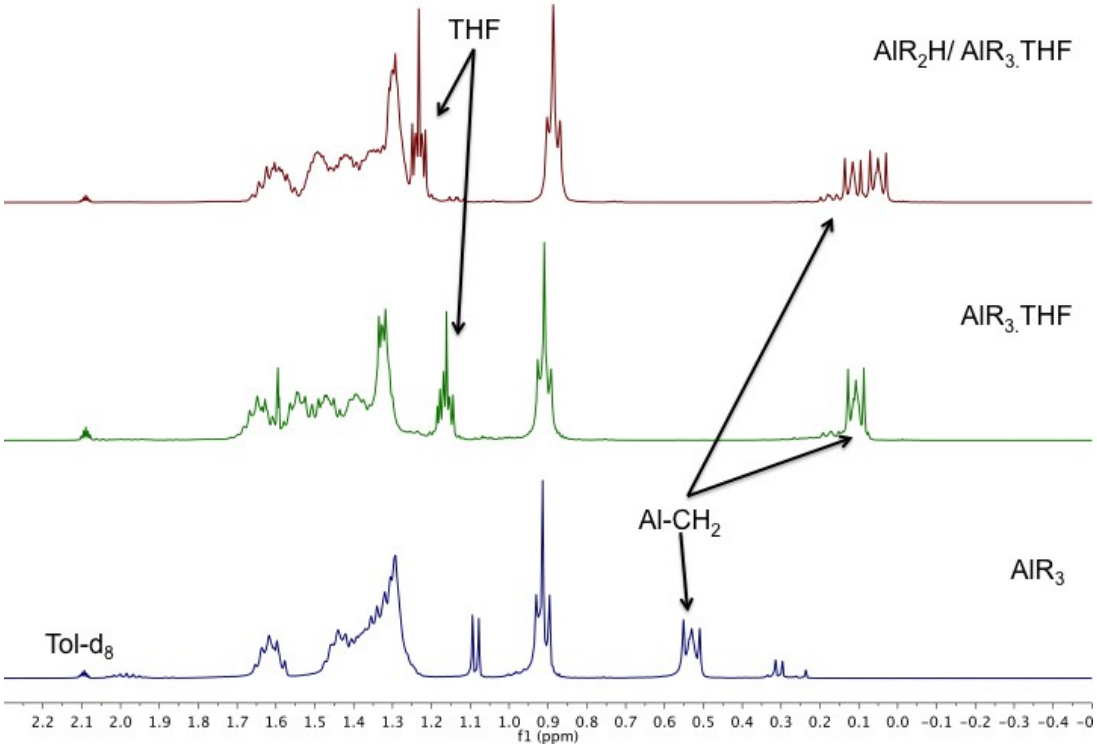

Figure S3. ^{1}H NMR spectra (toluene-d_8) of the alkyl region of [Al(Oct)$_3$], [Al(Oct)$_3$] and equimolar THF, and [(Oct)$_2$AlH] (70%) and [Al(Oct)$_3$] (30%) plus THF.

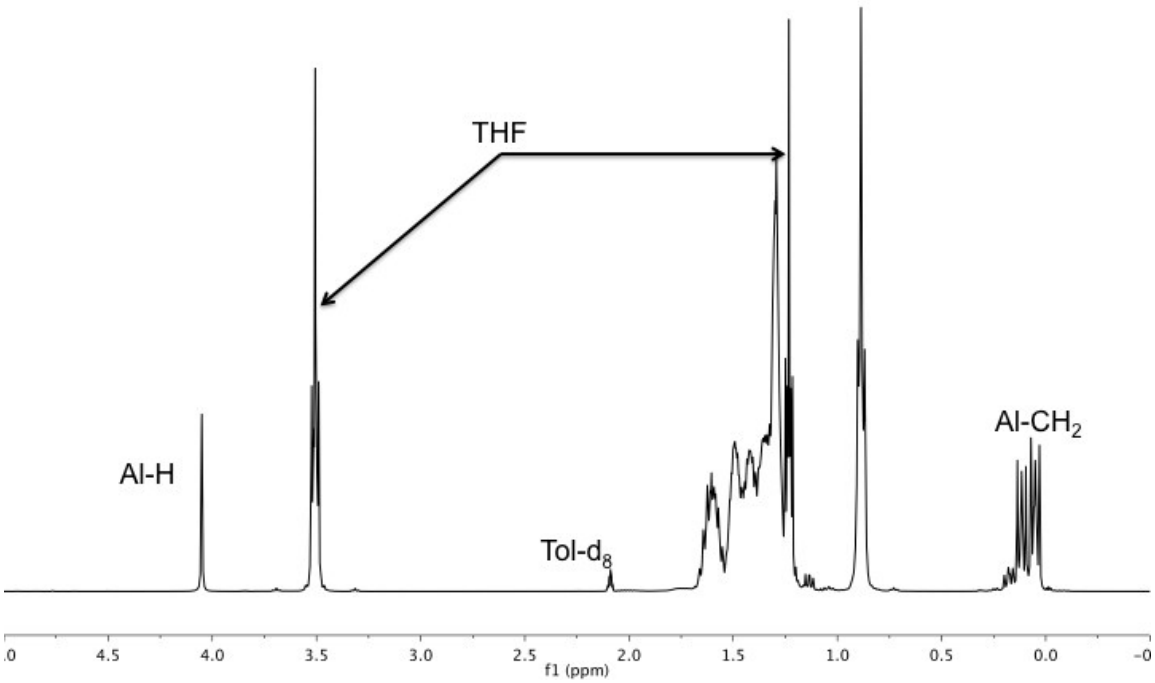

Figure S4. ^{1}H NMR spectrum (toluene-d_8) of [(Oct)$_2$AlH] (70%) and [Al(Oct)$_3$] (30%) plus THF.

Effect of aluminium hydride speciation on ^{13}C NMR spectrum.

The ^{13}C NMR spectrum of $[Al(Oct)_3]/[(Oct)_2AlH]$ as a function of the mole percentage of the hydride is shown in Figure S5. The signal of most interest is the α-C resonance numbered 1 in Figure S5. In pure $[Al(Oct)_3]$ this signal appears at 11.27 ppm and is attributed to $[(Oct)_2Al(\mu\text{-}Oct)_2Al(Oct)_2]$, complex **1** in the main article (it is known that fast exchange processes in alkyl aluminium dimers leads to equivalence of terminal and bridging alkyl groups).[1] As the amount of $[(Oct)_2AlH]$ is increased this signal moves upfield, and it is suggested that this most likely represents an average due to fast exchange between complex **1** and complex **2**, $[(Oct)_2Al(\mu\text{-}H)(\mu\text{-}Oct)Al(Oct)_2]$. When the amount of $[Al(Oct)_3]$ and $[(Oct)_2AlH]$ are approximately equal, an additional upfield signal begins to appear (highlighted in Figure S5). At high percentages of $[(Oct)_2AlH]$ this signal, at 8.53 ppm, is the only α–C resonance observed. It is proposed that this signal represents the hydride bridged cyclotrimer, complex **3**.

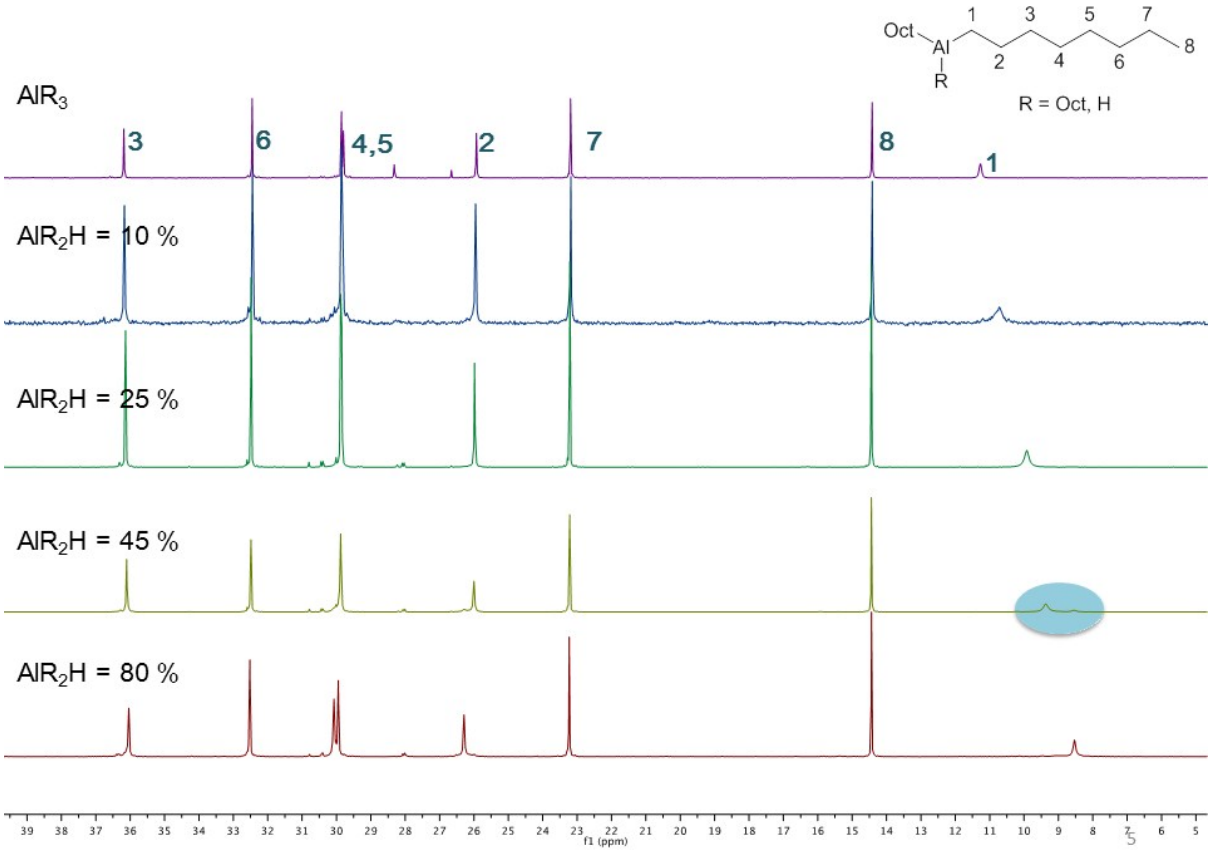

Figure S5. ^{13}C NMR spectra (C_6D_6) of $[Al(Oct)_3]/[(Oct)_2AlH]$ as a function of the mole percentage of the hydride.

Geometries and energies of all stationary points

[1] O. Yamamoto, K. Hayamizu, *J. Phys. Chem.* **1968**, *72*, 822.

$[(Bu)_2Al(\mu\text{-}Bu)(\mu\text{-}H)Al(Bu)_2]$ (complex **2**)

E (B3LYP/6-311+G(2d,p)) = -1275.05483138

C	2.43604200	-1.10252300	-0.91750600
H	2.74335100	-0.80311700	-1.92958800
H	1.85212400	-2.01989100	-1.06049200
C	1.96699800	2.13465900	0.25829200
H	1.13933100	2.75431100	0.62737800
H	2.64958700	2.03019100	1.11399000
C	-2.34888100	1.74659500	0.15746000
H	-1.66318700	2.53311200	0.49828200
H	-2.78042900	2.13167300	-0.77653200
C	-2.16292100	-1.52989100	-0.99107200
H	-1.38619000	-2.27234300	-1.21319300
H	-2.78847700	-1.99095200	-0.21428300
H	-0.03266000	0.56377600	-1.32017100
Al	1.28381500	0.34533900	-0.22818300
Al	-1.32692900	0.11033100	-0.27301500
C	3.69702200	-1.41295600	-0.08962600
H	4.28782600	-0.49871700	0.04707900
H	3.41648000	-1.73381400	0.92210200
C	2.69609400	2.88385600	-0.87288100
H	3.53496000	2.28022100	-1.24190500
H	2.02353900	3.00909700	-1.73094300
C	-3.47648900	1.57001400	1.19199000
H	-4.17300000	0.79048500	0.85847500
H	-3.06361500	1.20654500	2.14289700
C	-3.02086800	-1.30149000	-2.25067300
H	-3.81291000	-0.57259300	-2.03800600
H	-2.41032300	-0.85022800	-3.04313900
C	3.23099500	4.26341800	-0.46979100
H	2.39680800	4.87692200	-0.11109800
H	3.90902500	4.14611600	0.38327200
C	3.95402300	4.99125900	-1.60437400
H	4.32214800	5.96894900	-1.28365000
H	4.81268400	4.41439100	-1.95992900
H	3.28926200	5.15155100	-2.45812600
C	4.60055400	-2.48916000	-0.70421400
H	4.02009100	-3.40967500	-0.83335500
H	4.89327800	-2.17277900	-1.71172800
C	5.85115700	-2.78141900	0.12642700
H	6.47055200	-3.55178900	-0.33937300
H	6.46799000	-1.88543600	0.24122200
H	5.58805600	-3.13012200	1.12933600
C	-3.66794700	-2.57707000	-2.80348600
H	-2.88088800	-3.30625400	-3.02696400
H	-4.28606000	-3.02983200	-2.01983000
C	-4.51615900	-2.33833700	-4.05367800
H	-4.95892500	-3.26743600	-4.42109500
H	-5.33330200	-1.64005000	-3.85053600
H	-3.91566400	-1.91477200	-4.86394600
C	-4.27714200	2.84715400	1.47598900
H	-3.58913600	3.62995500	1.81454300
H	-4.70978200	3.21011300	0.53696200
C	-5.38564000	2.65216600	2.51174800
H	-5.93614100	3.57919200	2.68976400
H	-6.10584200	1.89738800	2.18281700
H	-4.97686100	2.32060900	3.47077500
C	0.00089600	-0.40338600	1.38306100
H	0.81368500	0.11312900	1.92392000
H	-0.84819700	0.03164900	1.93683700
C	0.08373400	-1.90876000	1.71071000
H	-0.78192800	-2.42806400	1.28989900
H	0.95458900	-2.34934600	1.21691700
C	0.15840100	-2.20729600	3.21260300
H	-0.71699000	-1.77337200	3.70936700

H	1.03075700	-1.69789000	3.63826700
C	0.23518200	-3.70244100	3.52507900
H	0.28594400	-3.88252400	4.60134300
H	-0.64128800	-4.23161500	3.14100300
H	1.11991600	-4.15683900	3.07064700

$[(Bu)_2Al(\mu\text{-}H)]_3$ (complex **3**)

E (B3LYP/6-311+G(2d,p)) = -1755.30149572

Al	0.61100200	1.79784100	-0.04248300
Al	-1.73835700	-0.35818300	0.51691500
C	-2.06598400	-0.54579100	2.45250500
C	-2.62388700	-1.91048200	2.89716800
H	-2.75980200	0.24782600	2.76224900
H	-1.13427500	-0.33781000	2.99403400
H	-3.56390900	-2.12064000	2.37159200
H	-1.93430800	-2.71107400	2.60067300
C	-3.05722400	-0.53920400	-0.93879400
C	-4.27693200	0.39679100	-0.85074900
H	-3.40270500	-1.58209000	-0.95775100
H	-2.55057100	-0.38907900	-1.90079900
H	-4.79905400	0.24453600	0.10213200
H	-3.94600100	1.44313500	-0.84203600
C	1.32037400	2.48416100	1.66503400
C	2.75674200	3.03794200	1.60595400
H	1.26491800	1.69284800	2.42343700
H	0.64372200	3.27148900	2.02468000
H	3.44371000	2.25738200	1.25508100
H	2.81721000	3.84099300	0.86097100
C	0.46609400	2.78456000	-1.74421100
C	-0.37659800	4.07219100	-1.68284600
H	0.06022200	2.11788900	-2.51557700
H	1.48098000	3.03171900	-2.08466000
H	-1.39796600	3.83532000	-1.35856500
H	0.02623400	4.74842500	-0.91840700
H	-0.92736800	1.12888200	0.28616800
H	-0.42661500	-1.38057700	0.12478500
H	1.41735500	0.32912500	-0.38149300
Al	1.18025000	-1.36221700	-0.45596000
C	2.29168900	-2.18716700	0.94922500
C	3.80879800	-2.17173300	0.68315600
H	2.08332000	-1.70011200	1.91021800
H	1.95780200	-3.22620900	1.07685200
H	4.02522100	-2.65762900	-0.27636600
H	4.15800900	-1.13702500	0.57536300
C	1.14072300	-1.85405300	-2.36556100
C	0.80730900	-3.32911200	-2.65788400
H	0.42689900	-1.20742400	-2.89160800
H	2.12007200	-1.61208700	-2.80093500
H	1.52012400	-3.98409200	-2.14133200
H	-0.17759800	-3.57977500	-2.24407300
C	-0.45335800	4.83241800	-3.01263700
H	-0.85880600	4.16425600	-3.78074300
H	0.56268500	5.08468800	-3.33648400
C	-1.30034600	6.10384000	-2.93770300
H	-1.33250700	6.62111700	-3.89971000
H	-2.33071600	5.87617700	-2.64972000
H	-0.89936700	6.80361500	-2.19876600
C	3.27340000	3.57498700	2.94588000
H	3.22312200	2.77499900	3.69468000
H	2.59657900	4.36232900	3.29987300
C	4.70132400	4.12321300	2.88431000
H	5.37537100	3.33503600	2.52960300
H	4.74922600	4.92159600	2.13489000
C	5.20376000	4.65552400	4.22743900

H	5.20028200	3.87082300	4.98926100
H	6.22436300	5.03825400	4.15039900
H	4.57064100	5.46972400	4.59121600
C	4.64027300	-2.85589100	1.77474200
H	4.43396000	-2.37209500	2.73735700
H	4.30356400	-3.89449000	1.88086000
C	6.14759900	-2.83589200	1.50928000
H	6.48212900	-1.79725000	1.40598000
H	6.35046400	-3.31597600	0.54504400
C	6.96445700	-3.52635700	2.60286500
H	8.03460000	-3.49393500	2.38423800
H	6.80960200	-3.04709700	3.57367600
H	6.67860200	-4.57700300	2.70559100
C	0.81213100	-3.68459700	-4.14962600
H	0.09589200	-3.03940700	-4.67067700
H	1.79600100	-3.44442000	-4.56804300
C	0.47895000	-5.15155900	-4.42686600
H	-0.51380800	-5.41007100	-4.04737200
H	0.49086900	-5.36982800	-5.49752900
H	1.19939000	-5.81879000	-3.94489200
C	-5.28398100	0.21459200	-1.99270500
H	-4.77004300	0.37290500	-2.94748600
H	-5.62532900	-0.82671300	-2.00189800
C	-6.49028000	1.15011400	-1.89662600
H	-6.18037100	2.19891700	-1.91789500
H	-7.18537000	0.99392000	-2.72520300
H	-7.04278800	0.98924000	-0.96639400
C	-2.87473000	-2.01995400	4.40612600
H	-1.93789500	-1.81682300	4.93704700
H	-3.57139300	-1.22994500	4.70848400
C	-3.42345300	-3.38162200	4.83507400
H	-2.73072200	-4.18708200	4.57462300
H	-3.58959800	-3.42450200	5.91426300
H	-4.37730500	-3.59673000	4.34468600

$[(Bu)_2Al(\mu\text{-}H)]_5$ (complex **4**)

E (B3LYP/6-311+G(2d,p)) = -2794.41691784

H	1.84158000	4.55248600	0.08451200
H	3.10892200	2.40716600	-0.04325200
H	-0.54301800	3.93392100	-0.16361000
H	1.31624100	0.68772300	0.07402600
H	-1.04245100	1.48335700	-0.06907400
Al	3.47359200	4.06919000	0.03027000
Al	0.33445400	5.28514300	0.38744200
Al	-1.71059600	2.86786800	-0.79514500
Al	-0.18281800	0.27777400	0.76696200
Al	2.92642900	0.76873000	-0.47035200
C	0.11505600	5.42991900	2.34191900
H	0.93365300	6.05432300	2.72602200
H	0.26948600	4.44453800	2.79964500
C	0.09080400	6.74295400	-0.91984900
H	-0.98000600	6.98234800	-0.97710900
H	0.35811700	6.37864800	-1.91989600
C	4.17987700	4.66343400	-1.71283400
H	4.09326200	5.75818000	-1.75414100
H	3.52331700	4.29508500	-2.51130700
C	4.29667700	4.38757000	1.79422300
H	5.21858300	3.79236300	1.85102300
H	3.64407400	3.97883700	2.57604900
C	2.92323300	0.64415400	-2.43861900
H	2.15917500	1.31922400	-2.84480700
H	3.87954500	1.04363300	-2.80391400
C	4.03634700	-0.29603800	0.76508900
H	3.79942400	-0.01179100	1.79826800

H	3.73303200	-1.34873900	0.67896500
C	-0.16436500	0.77265600	2.67695000
H	-1.20568000	0.91912400	2.99611500
H	0.31001600	1.75503000	2.79667600
C	-0.73416500	-1.46768200	0.03093000
H	-0.00011100	-2.22118200	0.34835800
H	-0.66526900	-1.44224000	-1.06393600
C	-1.42190000	2.69402600	-2.73872800
H	-0.35311000	2.53619400	-2.93253700
H	-1.91116600	1.76800900	-3.07144800
C	-3.42111900	3.26001900	0.10687000
H	-3.26418800	3.24396700	1.19303100
H	-3.70474400	4.29563600	-0.12651700
C	-2.14334200	-1.92905900	0.44710600
H	-2.22215500	-1.95168300	1.54125400
H	-2.89028500	-1.19730500	0.11336300
C	-1.92979600	3.86953000	-3.59464300
H	-3.00265000	4.02168100	-3.42274300
H	-1.44565100	4.80166000	-3.27782700
C	0.87909000	8.03095500	-0.61610100
H	0.60641000	8.41172100	0.37603900
H	1.95294000	7.81015500	-0.56213300
C	5.63480600	4.26231800	-2.01926800
H	6.30086800	4.63547800	-1.23134400
H	5.73642100	3.16967000	-1.99785000
C	2.71478700	-0.77018500	-3.01163900
H	3.47834200	-1.45116400	-2.61529100
H	1.75367500	-1.17532000	-2.67102900
C	0.51303300	-0.24207800	3.61736400
H	0.03886400	-1.22564200	3.51040000
H	1.55982400	-0.38707000	3.32238400
C	5.55645500	-0.18822500	0.54186000
H	5.87589300	0.85689600	0.64376100
H	5.80651800	-0.47434900	-0.48740100
C	4.62573800	5.85711500	2.11698700
H	5.28580300	6.27248200	1.34525200
H	3.71165000	6.46351600	2.08022900
C	-1.22907900	6.01205200	2.81765200
H	-1.38944100	7.00008700	2.36831200
H	-2.05657100	5.38754100	2.45878500
C	-4.58876500	2.32365700	-0.25621500
H	-4.76404700	2.34630800	-1.33895500
H	-4.32333000	1.28451500	-0.02271600
C	-1.34604900	6.14588000	4.34094100
H	-1.19377500	5.16110800	4.79662000
H	-0.52840800	6.77784900	4.70573300
C	-5.90405700	2.65965600	0.45715200
H	-5.73974400	2.62629700	1.54008700
H	-6.17919300	3.69457600	0.22460500
C	0.47551500	0.15748500	5.09748000
H	0.95794300	1.13433600	5.21496800
H	-0.56823500	0.29708000	5.40091800
C	6.39145900	-1.04491400	1.50145400
H	6.14918000	-0.76218600	2.53199800
H	6.08913600	-2.09288500	1.39576200
C	5.28814200	6.06093100	3.48512100
H	4.62941300	5.65738000	4.26221100
H	6.20598700	5.46362300	3.52606800
C	-7.05533000	1.72489200	0.08274000
H	-7.97552000	1.99285600	0.60759900
H	-7.26322200	1.76334100	-0.99046800
H	-6.82063900	0.68687900	0.33548200
C	1.14677100	-0.86173400	6.01951400
H	1.10092700	-0.54712400	7.06498000
H	0.66276000	-1.83994100	5.94661600
H	2.20078900	-0.99631200	5.76015400
C	7.89885100	-0.91920700	1.27476400
H	8.46201400	-1.54322600	1.97295800

H	8.17401200	-1.22522700	0.26130100
H	8.23433100	0.11319500	1.40914700
C	5.61236900	7.52354500	3.79334700
H	4.70770600	8.13833600	3.79327300
H	6.08484300	7.63101800	4.77278000
H	6.29507900	7.94299400	3.04872000
C	-2.68606400	6.72327700	4.79961400
H	-3.51961800	6.09228800	4.47810700
H	-2.73477900	6.80645300	5.88811300
H	-2.85007200	7.72162700	4.38366600
C	-2.53871200	-3.30751200	-0.09733200
H	-2.47280200	-3.29028800	-1.19101400
H	-1.80234500	-4.04618000	0.23882500
C	-3.94032900	-3.74865700	0.32687800
H	-4.70007400	-3.04480500	-0.02487500
H	-4.18944400	-4.73309100	-0.07658300
H	-4.02420200	-3.80619900	1.41597100
C	2.75325200	-0.83349000	-4.54336300
H	1.98723400	-0.16139300	-4.94601000
H	3.71493900	-0.43930900	-4.89074200
C	2.54432300	-2.24304000	-5.09943000
H	1.57556500	-2.64896000	-4.79425100
H	2.57740300	-2.25170900	-6.19162700
H	3.31649400	-2.92900200	-4.73929400
C	6.14762300	4.77025600	-3.37218900
H	5.48994500	4.39530200	-4.16434300
H	6.05939900	5.86227100	-3.39707000
C	7.59226200	4.36375000	-3.66784400
H	7.70203000	3.27552300	-3.68143800
H	7.92415400	4.74150000	-4.63802200
H	8.27679100	4.75379600	-2.90902700
C	0.66662500	9.15048900	-1.64253000
H	0.95258800	8.78260400	-2.63425600
H	-0.40346300	9.37925200	-1.70119700
C	1.44816100	10.42547900	-1.32141100
H	1.27515700	11.20105100	-2.07148500
H	1.15627400	10.83367900	-0.34952400
H	2.52421300	10.23215100	-1.28738800
C	-1.69889300	3.68881900	-5.10003700
H	-0.62778500	3.54331300	-5.28003000
H	-2.18878900	2.76432600	-5.42603900
C	-2.20645800	4.86311000	-5.93838900
H	-1.70915700	5.79524300	-5.65538300
H	-2.02598000	4.70203400	-7.00402700
H	-3.28191900	5.00998800	-5.80330500

[$(Bu)_6Al_3(\mu\text{-}Bu)(\mu\text{-}H)_2$] (complex **5**)

E (B3LYP/6-311+G(2d,p)) = -1912.57871005

Al	0.96058500	1.95245100	-0.33179900
Al	-1.39434700	-0.07576900	-0.04373700
C	-2.19600700	0.21101000	1.73578900
C	-2.82200800	-1.03865800	2.38336300
H	-2.96633900	0.98853300	1.63629600
H	-1.44361000	0.63551600	2.41089400
H	-3.58033900	-1.46804900	1.71666900
H	-2.05972200	-1.81890000	2.50463300
C	-2.34002400	-0.83662600	-1.60083800
C	-3.67160500	-0.14461900	-1.94901000
H	-2.52901000	-1.90034600	-1.40089800
H	-1.68221200	-0.82311500	-2.47833600
H	-4.33670500	-0.14949700	-1.07637900
H	-3.49466400	0.91400700	-2.17854500
C	1.41182200	1.92707200	1.59465600
C	2.80539800	2.48968000	1.93555100
H	1.29901600	0.93728200	2.04901800

H	0.65020000	2.55176200	2.08327800
H	3.58364300	1.85001200	1.50031100
H	2.93784600	3.47484200	1.46995700
C	0.86554900	3.69925300	-1.26516700
C	0.01914100	4.74863500	-0.51971500
H	0.46788100	3.58111100	-2.28027300
H	1.88310800	4.09331700	-1.39938900
H	-1.00271100	4.37339500	-0.37772400
H	0.41825500	4.90386700	0.49016200
H	-0.62483800	1.34845900	-0.56439500
H	0.10254700	-0.85477100	0.17607600
Al	1.63273000	-1.07187600	-0.56196600
C	2.86575900	-1.51433100	0.92099700
C	4.27400600	-1.96387500	0.48604800
H	2.95378700	-0.68539100	1.63147900
H	2.39538500	-2.32819800	1.49058700
H	4.20054400	-2.78894000	-0.23347000
H	4.78033500	-1.14982100	-0.04988500
C	1.32395400	-2.39336500	-2.00427800
C	0.98983700	-3.80082400	-1.47292800
H	0.52000100	-2.06803400	-2.67505500
H	2.22037700	-2.45701300	-2.63740900
H	1.79072700	-4.15224900	-0.81056100
H	0.08829000	-3.76071200	-0.84803000
C	-0.05888200	6.10743000	-1.22670300
H	-0.46728700	5.96145700	-2.23317500
H	0.95704800	6.49433200	-1.36583700
C	-0.90247800	7.13819600	-0.47463000
H	-0.93946100	8.09170100	-1.00728700
H	-1.93155200	6.78992300	-0.34731700
H	-0.49528300	7.33136300	0.52203800
C	3.07344200	2.62451000	3.43939300
H	2.94845800	1.64345300	3.91379100
H	2.30657600	3.27266700	3.88081700
C	4.46025800	3.17821900	3.77529300
H	5.22496400	2.52819200	3.33462500
H	4.58371000	4.15708700	3.29742500
C	4.71146300	3.31189900	5.27824400
H	4.63110700	2.34348000	5.78005000
H	5.70806400	3.71013400	5.48400700
H	3.98361400	3.98379300	5.74180600
C	5.17485800	-2.40878400	1.64503800
H	5.25835100	-1.58852200	2.36836100
H	4.68556300	-3.23267100	2.17871400
C	6.57519400	-2.84721500	1.20940100
H	7.06508900	-2.02021300	0.68245200
H	6.48772300	-3.66076600	0.48000500
C	7.45721400	-3.30158800	2.37373400
H	8.44775300	-3.60941300	2.02991500
H	7.59423800	-2.49820200	3.10308600
H	7.00997100	-4.14992200	2.89939100
C	0.77177500	-4.84896200	-2.57107100
H	-0.03594200	-4.51093700	-3.22990400
H	1.67085500	-4.89987600	-3.19572100
C	0.44383500	-6.24107600	-2.02854400
H	-0.46877000	-6.22581000	-1.42570100
H	0.29412000	-6.96136000	-2.83666400
H	1.25066800	-6.61872700	-1.39376400
C	-4.41511500	-0.77998400	-3.13026900
H	-3.75976300	-0.77227600	-4.00861600
H	-4.60443600	-1.83528900	-2.90352900
C	-5.73393000	-0.08199900	-3.46632700
H	-5.57071600	0.96675400	-3.73095100
H	-6.23752900	-0.56110600	-4.30957300
H	-6.42065600	-0.10325200	-2.61517300
C	-3.46835900	-0.77521700	3.74878700
H	-2.71323200	-0.35845000	4.42457600
H	-4.23412200	0.00056200	3.63516300

C	-4.09074800	-2.02231500	4.37889200
H	-3.34100100	-2.80315300	4.53602300
H	-4.54249800	-1.79823700	5.34839200
H	-4.87241800	-2.44090300	3.73833200
C	2.28106000	0.74960800	-1.58253200
H	2.85184100	1.64912000	-1.28597700
H	3.13066700	0.04691800	-1.49996500
C	1.92256000	0.86927900	-3.07976400
H	1.52687200	-0.08578600	-3.43280100
H	1.11342600	1.59178200	-3.21672200
C	3.10555200	1.27834600	-3.96455300
H	3.91713700	0.55259800	-3.83661600
H	3.49910000	2.23997600	-3.61632200
C	2.73947200	1.38042000	-5.44590200
H	3.60197500	1.67251300	-6.04914700
H	2.37452100	0.42381900	-5.82966900
H	1.95411700	2.12355800	-5.60871300

$[(Bu)_2Al(\mu\text{-}H)]_2$ (complex **6**)

E (B3LYP/6-311+G(2d,p)) = -1117.76177749

C	2.26737600	1.75760300	0.09149500
H	2.85307000	1.79751900	1.02013800
H	1.50753500	2.54168400	0.19697200
C	2.26737600	-1.75760100	-0.09149600
H	1.50753400	-2.54168200	-0.19697800
H	2.85307300	-1.79751600	-1.02013700
H	0.06133400	0.04963700	-1.14371700
C	-2.14964000	-1.75708400	-0.04567600
H	-1.39403900	-2.54789900	-0.12718400
H	-2.63052200	-1.91870300	0.92890100
C	-2.14964000	1.75708600	0.04567500
H	-1.39403900	2.54790100	0.12718400
H	-2.63052100	1.91870500	-0.92890200
H	0.06133400	-0.04963500	1.14371600
Al	1.37872600	0.00000100	0.00000000
Al	-1.25625100	0.00000100	-0.00000100
C	3.18642700	2.09012300	-1.09958100
H	3.95198000	1.31214600	-1.21268000
H	2.60898100	2.07411200	-2.03259200
C	3.18642100	-2.09012500	1.09958300
H	3.95197400	-1.31215000	1.21268700
H	2.60897100	-2.07411700	2.03259200
C	-3.19886700	-1.93021300	-1.16053200
H	-3.95505300	-1.13819400	-1.09134100
H	-2.72576100	-1.80141900	-2.14231700
C	-3.19886700	1.93021500	1.16053100
H	-3.95505200	1.13819700	1.09133900
H	-2.72576200	1.80142100	2.14231600
C	3.88733300	-3.44917500	0.98491400
H	3.12803800	-4.23143700	0.87341700
H	4.47809900	-3.46720600	0.06204500
C	4.78741900	-3.77275000	2.17831900
H	5.27137900	-4.74563100	2.06257900
H	5.57544200	-3.02307000	2.29505400
H	4.21552700	-3.79655300	3.11041700
C	3.88734000	3.44917200	-0.98491300
H	3.12804500	4.23143500	-0.87342100
H	4.47810200	3.46720500	-0.06204100
C	4.78743100	3.77274300	-2.17831500
H	5.27139100	4.74562400	-2.06257600
H	5.57545400	3.02306200	-2.29504500
H	4.21554400	3.79654300	-3.11041600
C	-3.91340900	3.28691700	1.13915800
H	-3.16566100	4.08403800	1.21786000

H	-4.39497700	3.41872400	0.16358100
C	-4.95255100	3.44408800	2.25047300
H	-5.44373200	4.41912600	2.20455000
H	-5.72970700	2.67798100	2.17612700
H	-4.49261200	3.35140500	3.23854600
C	-3.91340900	-3.28691400	-1.13915900
H	-3.16566100	-4.08403600	-1.21786000
H	-4.39497700	-3.41872100	-0.16358200
C	-4.95255100	-3.44408600	-2.25047400
H	-5.44373200	-4.41912400	-2.20455100
H	-5.72970700	-2.67797900	-2.17612800
H	-4.49261100	-3.35140400	-3.23854700

$[(Bu)_2Al(\mu\text{-}H)]_6$ (complex **7**)

E (B3LYP/6-311+G(2d,p)) = -3353.29786061

Al	-1.02233800	-1.82390600	0.22752600
Al	2.06462500	-0.72876700	1.13216900
H	0.52024200	-1.40959700	0.84503200
C	-0.76415200	-2.74151600	-1.50669500
H	-1.70094900	-3.26201300	-1.76449900
H	-0.01720900	-3.54135600	-1.38321000
C	-2.23400200	-0.30835100	0.61655500
H	-2.11184900	-0.01660300	1.67131900
H	-1.89706700	0.56672500	0.03720500
C	3.35648000	-1.71122700	0.00006000
H	3.24017100	-2.79319000	0.16827900
H	3.07347100	-1.55536800	-1.05409800
C	1.87060400	1.23632700	1.27297500
H	2.79050700	1.64368300	1.72372800
H	1.07047100	1.47416800	1.99121800
C	1.59436800	1.97562700	-0.05363200
H	2.39214800	1.75927500	-0.78022100
H	0.66627700	1.59660600	-0.50911400
C	1.47255900	3.49970600	0.10045900
H	0.67498200	3.72219200	0.82355300
H	2.40079400	3.88861400	0.54278900
C	1.18766900	4.22456400	-1.21915700
H	1.10681200	5.30787100	-1.07293500
H	1.98584300	4.04650400	-1.95064400
H	0.24753200	3.87848900	-1.66654700
C	4.83819500	-1.32218300	0.18506100
H	4.96948900	-0.24407500	0.00680600
H	5.14467500	-1.48959300	1.22919400
C	5.79947100	-2.09136700	-0.73480800
H	5.67778300	-3.16933500	-0.55674000
H	5.50504200	-1.92126200	-1.78033700
C	7.26863000	-1.70013300	-0.54427300
H	7.92525400	-2.26651600	-1.21477600
H	7.42474900	-0.63352700	-0.74871200
H	7.59986700	-1.89034900	0.48427100
C	-3.72942600	-0.55610200	0.32697100
H	-3.86984200	-0.81771500	-0.73294000
H	-4.08596700	-1.42813500	0.89745000
C	-0.35104600	-1.83765300	-2.68699900
H	-1.09599200	-1.04009200	-2.82956100
H	0.59440200	-1.32293100	-2.45479100
C	-4.63167200	0.64311900	0.65835100
H	-4.50254900	0.90419000	1.71840600
H	-4.28726800	1.51659000	0.08651500
C	-6.11455800	0.38954500	0.36781700
H	-6.72743500	1.26385300	0.61577700
H	-6.27773200	0.15924800	-0.69246100
H	-6.49395100	-0.45863200	0.95135600
C	-0.18068300	-2.59167300	-4.01526200

H	0.56911400	-3.38465900	-3.88155000
H	-1.12331400	-3.10279400	-4.25781700
C	0.22918100	-1.68709100	-5.18203500
H	0.34270400	-2.25717200	-6.11132200
H	-0.52030600	-0.90592000	-5.36062400
H	1.18471100	-1.18701000	-4.98015300
Al	0.99652900	-6.17497900	2.65579200
Al	2.80392000	-4.65608000	5.08508600
H	1.71225100	-5.36771800	3.98098100
C	0.15404500	-7.82656400	3.34949400
H	-0.54868200	-8.20532900	2.58943800
H	-0.47301200	-7.57660800	4.21973200
C	2.23191600	-6.01435900	1.11837200
H	2.56434100	-4.96746100	1.03626900
H	3.14587800	-6.58559700	1.34939900
C	1.93458300	-4.75498700	6.86056200
H	0.91242400	-4.35186700	6.78918200
H	1.80460600	-5.82015400	7.11333800
C	4.64011400	-5.23495400	4.62684700
H	5.35144400	-4.55359900	5.12137000
H	4.80731700	-5.08809700	3.54854400
C	4.99360400	-6.68916500	5.00466100
H	4.85285700	-6.84243800	6.08537800
H	4.29825000	-7.38827100	4.51386900
C	6.42978900	-7.09301700	4.63578200
H	6.57350100	-6.95279600	3.55494000
H	7.13088300	-6.40341100	5.12723000
C	6.77419700	-8.53626800	5.01835800
H	7.80380500	-8.79051000	4.74126900
H	6.67192000	-8.69522500	6.09914700
H	6.10894700	-9.24970300	4.51606600
C	2.68044900	-4.05530900	8.01621600
H	3.70030300	-4.45937300	8.10570300
H	2.80538800	-2.98410700	7.79313300
C	1.97908700	-4.18976200	9.37703600
H	0.96123800	-3.78246400	9.29540700
H	1.86076700	-5.25705200	9.61254200
C	2.72356800	-3.49031900	10.51907500
H	2.19732100	-3.60908900	11.47325400
H	3.73401400	-3.89937200	10.64355400
H	2.82502900	-2.41480400	10.32720200
C	1.67961500	-6.47868000	-0.24554100
H	1.36818200	-7.53272200	-0.18752500
H	0.76832300	-5.91336100	-0.49563600
C	1.13142100	-8.95677400	3.73555400
H	1.74804300	-9.23397000	2.86709300
H	1.83928100	-8.59917200	4.49984200
C	2.68083500	-6.32579400	-1.40140800
H	2.99608800	-5.27425700	-1.46293900
H	3.58761800	-6.90100900	-1.16562900
C	2.12308500	-6.77538300	-2.75576600
H	2.86448600	-6.65660500	-3.55434900
H	1.82600300	-7.83138800	-2.73254400
H	1.23772200	-6.18990200	-3.03426300
C	0.43742800	-10.22045300	4.26748700
H	-0.17512600	-9.95020500	5.13942200
H	-0.26490300	-10.58819200	3.50574300
C	1.41305300	-11.33817800	4.64996400
H	0.88364100	-12.22251400	5.02298800
H	2.01622600	-11.65084000	3.78838600
H	2.10548600	-11.00969100	5.43511100
Al	-1.81616100	-4.40035400	2.28909800
H	-1.30962500	-3.02375800	1.40967400
H	-0.22023100	-4.98900200	2.46663700
C	-2.77951700	-5.61935000	1.06282400
H	-2.83911300	-6.61268800	1.53688800
H	-2.17703000	-5.77165800	0.15352500
C	-2.43274800	-3.74930400	4.05317500

H	-3.36990000	-3.18848600	3.90424000
H	-1.71545100	-3.00787000	4.43830200
C	-4.20095500	-5.17024100	0.66253500
H	-4.81975900	-5.03724900	1.56292700
H	-4.16430500	-4.18085900	0.17995200
C	-2.66325600	-4.83676300	5.12373600
H	-3.39069400	-5.57784000	4.75886800
H	-1.73129400	-5.39652500	5.29831000
C	-3.15898500	-4.28581200	6.47012100
H	-2.43365100	-3.54822600	6.84227600
H	-4.09606500	-3.73449800	6.30693300
C	-3.37754700	-5.37219100	7.52831900
H	-3.73321400	-4.94616400	8.47357200
H	-4.12033800	-6.10754100	7.19460100
H	-2.44706900	-5.91449600	7.73743900
C	-4.91703100	-6.14618200	-0.28423200
H	-4.30883300	-6.27458900	-1.19099800
H	-4.96357800	-7.13563600	0.19264100
C	-6.32900000	-5.69429900	-0.67122700
H	-6.30969500	-4.72191100	-1.17911100
H	-6.80922900	-6.41197500	-1.34637500
H	-6.96920100	-5.59094500	0.21380900
Al	2.50938400	-1.36735800	4.39376900
H	2.15129600	-1.36378800	2.72034500
H	2.61071600	-3.07653700	4.45167700
C	0.88420300	-0.84548100	5.39596300
H	0.98614500	-1.22847700	6.42474700
H	0.01334200	-1.37702600	4.98104600
C	4.33119400	-0.62687400	4.62548200
H	4.32788300	0.41732900	4.27192200
H	5.02800600	-1.15360600	3.95480700
C	0.58050900	0.66611200	5.45175100
H	1.43941500	1.20655900	5.87770800
H	0.45641600	1.06387800	4.43285500
C	4.88413600	-0.66407500	6.06574900
H	4.20178400	-0.13046000	6.74467500
H	4.91444900	-1.70219900	6.43193900
C	6.28896400	-0.05695500	6.20705400
H	6.97736400	-0.59050600	5.53632400
H	6.26457900	0.98324200	5.85231200
C	6.82976000	-0.09947100	7.64000200
H	7.83263300	0.33828100	7.70377400
H	6.17971200	0.45744200	8.32638500
H	6.89278400	-1.13054500	8.00991500
C	-0.67296800	1.01641100	6.26885700
H	-1.53612800	0.48379100	5.84476500
H	-0.55135400	0.63102200	7.29125400
C	-0.96821700	2.51915200	6.31732300
H	-1.12648300	2.92527500	5.31038500
H	-1.86728000	2.73303200	6.90678100
H	-0.13538600	3.07295700	6.76851100

$[Me_2Al(\mu\text{-}Bu)]_2$

G (CBS-QB3) = -958.378582

Al	-0.00140600	1.31150400	0.05211500
Al	-0.00139100	-1.31156600	0.05200200
C	1.62212900	0.00000300	0.68693400
H	1.70105700	0.83469800	1.40398700
H	1.70111400	-0.83521300	1.40338500
C	2.88453800	0.00033200	-0.20364400
H	2.87276300	-0.87088000	-0.86517400
H	2.87293700	0.87224000	-0.86425700
C	4.19521800	-0.00021300	0.59640900
H	4.21526300	-0.87682100	1.25578600

H	4.21544100	0.87570700	1.25669400
C	5.44168400	0.00011900	-0.29337600
H	6.35809700	-0.00027600	0.30288900
H	5.46570900	-0.88237300	-0.94016500
H	5.46588500	0.88326700	-0.93926400
C	0.67646000	-2.37147100	-1.46228200
H	-0.09155100	-3.07793800	-1.80169100
H	0.96278200	-1.76955800	-2.33140800
H	1.54886800	-2.97538100	-1.18765800
C	-0.70306200	-2.22422900	1.64957600
H	-1.01764800	-1.54006400	2.44480900
H	-1.56093100	-2.86609300	1.41899300
H	0.06496600	-2.88073300	2.07782000
C	0.67617300	2.37171100	-1.46208500
H	0.96373400	1.76991300	-2.33087900
H	-0.09236400	3.07728300	-1.80215600
H	1.54776000	2.97661800	-1.18702300
C	-0.70320000	2.22392100	1.64979400
H	-1.56062100	2.86634100	1.41909400
H	-1.01852600	1.53953800	2.44454800
H	0.06497800	2.87979500	2.07872000
C	-1.57717900	-0.00005900	-0.69569100
H	-1.60812400	0.83461900	-1.41598000
H	-1.60820800	-0.83475400	-1.41596000
C	-2.89741400	-0.00000700	0.10673000
H	-2.93024000	-0.87116600	0.76760100
H	-2.93020800	0.87117100	0.76757400
C	-4.15032300	0.00000300	-0.78086400
H	-4.12539900	-0.87620500	-1.44057900
H	-4.12537900	0.87621100	-1.44057800
C	-5.45504400	0.00001900	0.02113600
H	-6.32810300	0.00012400	-0.63699000
H	-5.52384200	-0.88284200	0.66419200
H	-5.52373100	0.88279300	0.66432500

[Me_2AlBu]

G (CBS-QB3) = -479.184586

C	0.11707000	-0.80979500	0.00875700
H	0.17122300	-1.47234000	0.88719300
H	0.16972700	-1.50252100	-0.84590700
C	1.34284300	0.12239300	-0.00794400
H	1.30487900	0.80488100	0.85114300
H	1.30802300	0.76897500	-0.89454300
C	2.69097700	-0.61210700	0.00935100
H	2.73891100	-1.28856700	-0.85286400
H	2.73569400	-1.25300100	0.89851300
C	3.89931400	0.32878100	-0.00741200
H	3.89442600	0.99442300	0.86169700
H	4.84130000	-0.22665400	0.00622000
H	3.89851500	0.95795800	-0.90330500
C	-3.26893800	-1.14926200	-0.00606100
H	-3.94128600	-0.90905900	0.82674500
H	-3.85903800	-1.00067400	-0.91942600
H	-3.03241200	-2.21564200	0.05843900
C	-1.88850500	1.96686700	0.00312800
H	-1.49371000	2.40297900	0.92962900
H	-1.32433100	2.43585900	-0.81189700
H	-2.93029200	2.28888300	-0.08815500
Al	-1.67986100	0.01024900	-0.00018500

[Me_2AlBu] Elimination Transition Structure

G (CBS-QB3) = -479.135609

C	-3.37868600	-0.08773300	0.03020700
H	-3.66017500	-1.08443500	-0.32171800
H	-4.16072500	0.60869300	-0.28225000
H	-3.35810500	-0.11018600	1.12180500
C	-2.02050300	0.34604400	-0.54822800
H	-1.76830900	1.34649600	-0.18566000
H	-2.08164000	0.40419000	-1.63722700
C	-0.93520700	-0.62624700	-0.14336700
H	-0.97932900	-1.59288000	-0.63784800
C	-0.31090300	-0.57143600	1.11673600
H	-0.56402200	0.24647000	1.78423100
H	0.01260600	-1.49405800	1.58543200
C	2.66018800	-1.33039900	-0.25136800
H	3.24568000	-1.39146400	0.67270100
H	2.22306200	-2.31938600	-0.42547500
H	3.36553700	-1.14194900	-1.06784100
C	1.61317000	2.00514200	0.14119300
H	2.12951800	2.18335200	1.09092400
H	2.24347700	2.42264000	-0.65130400
H	0.68854000	2.59137100	0.15905100
H	0.17746100	-0.12820600	-1.37888300
Al	1.28600600	0.08054800	-0.14592100

Me_2AlH---1-butene Pie Complex

G (CBS-QB3) = -479.159013

C	-3.56519400	-0.04600900	-0.23435200
H	-3.72373100	-0.86645900	-0.93986800
H	-4.22515300	0.77492500	-0.52426900
H	-3.86804100	-0.39178600	0.75720400
C	-2.09762900	0.41644100	-0.23832900
H	-1.96446200	1.25072900	0.45651000
H	-1.84051200	0.78437400	-1.23741000
C	-1.16018100	-0.69918700	0.12070700
H	-1.17585500	-1.56197900	-0.54330300
C	-0.36510800	-0.73308900	1.20041800
H	-0.34327800	0.08763900	1.91030300
H	0.22589600	-1.60891900	1.44162700
C	2.71098800	-1.31415100	-0.16633000
H	3.01538500	-1.37329000	0.88414700
H	2.30474900	-2.29058700	-0.45277600
H	3.62980100	-1.17992700	-0.75220300
C	1.65911300	1.90898600	0.37154400
H	1.97848000	1.81852300	1.41521000
H	2.42405600	2.50800300	-0.13984400
H	0.73995200	2.50460900	0.35379400
H	0.70342800	0.15162100	-1.94029800
Al	1.46364200	0.16881300	-0.53929100

1-Butene

G (CBS-QB3) = -156.898797

C	1.72755100	-0.24697800	-0.29428800
H	1.92843300	-1.16647600	0.26379800
H	2.63683500	0.35980500	-0.27446900
H	1.52649300	-0.52527500	-1.33210700
C	0.53905600	0.52010900	0.30804400
H	0.36545800	1.44205800	-0.25623900
H	0.79682200	0.82244200	1.33134000
C	-0.72416900	-0.29384500	0.34072500
H	-0.67695000	-1.21601500	0.91972600

C	-1.85769400	0.01708900	-0.28094100
H	-1.95147700	0.92385100	-0.87164800
H	-2.73408400	-0.61863600	-0.22164300

Me_2AlH

G (CBS-QB3) = -322.263073

C	1.72695600	-0.42437400	-0.00033400
H	1.64069100	-1.51384200	-0.04435200
H	2.34599800	-0.10411100	-0.84723100
H	2.30129900	-0.17412200	0.90047600
C	-1.72695200	-0.42438100	-0.00030200
H	-2.30216500	-0.17269300	0.89954200
H	-2.34517300	-0.10544200	-0.84831100
H	-1.64066100	-1.51391300	-0.04259800
Al	0.00000000	0.50626200	-0.00145000
H	-0.00001500	2.09524200	0.00514400

$[(Me)_2Al(\mu\text{-}H)(\mu\text{-}Bu)AlMe_2]$

G (CBS-QB3) = -801.471237

H	-2.08347300	-0.00045700	0.85723900
Al	-1.16443700	-1.31049400	0.22075500
Al	-1.16488900	1.30968500	0.21980900
C	0.35312800	0.00002800	-0.65398000
H	0.32634300	-0.83513000	-1.37652000
H	0.32472500	0.83016300	-1.38207200
C	1.73517600	0.00307800	0.03691100
H	1.82142400	0.87770300	0.68934400
H	1.82094800	-0.86504000	0.69804000
C	2.91256000	-0.00204600	-0.94834200
H	2.83388900	0.87072100	-1.60848600
H	2.83375800	-0.88152000	-1.59951300
C	4.27867300	0.00135900	-0.25652700
H	5.09395300	-0.00235500	-0.98492700
H	4.40095000	0.88744400	0.37395900
H	4.40085900	-0.87833100	0.38286900
C	-0.37334100	2.31686800	1.70713800
H	-1.14395300	2.91291000	2.20973600
H	0.08718900	1.67831600	2.46701000
H	0.39256400	3.02213700	1.36474200
C	-2.22580600	2.14865500	-1.20485900
H	-2.57338800	1.43317900	-1.95724100
H	-3.11560700	2.64074600	-0.79585000
H	-1.65532200	2.92217400	-1.73281100
C	-0.37021500	-2.31605200	1.70769000
H	0.08730000	-1.67653200	2.46855700
H	-1.13885400	-2.91561500	2.20911900
H	0.39864600	-3.01798500	1.36505300
C	-2.22499700	-2.15035400	-1.20360200
H	-3.11512900	-2.64191300	-0.79470300
H	-2.57206200	-1.43504500	-1.95639700
H	-1.65458800	-2.92426100	-1.73104900

$[(Me)_2Al(\mu\text{-}Bu)_2AlMe(2\text{-}Bu)]$

G (CBS-QB3) = -1076.052873

Al	-0.06594700	0.47240400	0.66883400
Al	-0.10418200	-1.96991100	-0.29304900
C	-1.59411500	-0.37407100	-0.60508200
H	-1.49775600	0.51240000	-1.24887500
H	-1.69923400	-1.14440300	-1.38972700
C	-2.94383100	-0.32847100	0.14779600
H	-3.01189000	-1.18222200	0.82960700
H	-2.98553900	0.55971900	0.78690900
C	-4.16538100	-0.32436700	-0.78169000
H	-4.14055600	-1.22251600	-1.41149300
H	-4.09444100	0.52879400	-1.46729700
C	-5.49627600	-0.26673100	-0.02631400
H	-6.34575200	-0.26909800	-0.71456600
H	-5.60856300	-1.12518600	0.64306300
H	-5.56605200	0.63906400	0.58389500
C	-0.94145800	-3.24829800	0.94670100
H	-0.27371200	-4.09884600	1.13206800
H	-1.19142300	-2.82068700	1.92291900
H	-1.86596400	-3.66775200	0.53287600
C	0.48963600	-2.56474100	-2.07434400
H	0.80030000	-1.74739400	-2.73395000
H	1.32952900	-3.26669000	-2.01682900
H	-0.32180700	-3.09801400	-2.58525300
C	-0.70833400	0.55443000	2.53360000
H	-1.09524700	-0.39935400	2.90660100
H	0.10413300	0.85422500	3.20710800
H	-1.50542600	1.29469200	2.66460900
C	0.64436400	2.14160700	-0.16373200
H	1.07033000	1.88852800	-1.14689000
C	1.57523100	-1.00424600	0.65075400
H	1.72671700	-0.42565200	1.57744500
H	1.67531000	-2.01746400	1.07849100
C	2.77825000	-0.74238000	-0.28282800
H	2.73142700	-1.41262100	-1.14545400
H	2.71766400	0.26975100	-0.69386200
C	4.13791800	-0.91857200	0.40854100
H	4.20848200	-1.93723600	0.80952100
H	4.19254900	-0.24809500	1.27518300
C	5.32464600	-0.64982900	-0.52124700
H	6.27703800	-0.78249100	-0.00099500
H	5.31756800	-1.32934000	-1.37916700
H	5.29839900	0.37289000	-0.90989400
C	-0.48598600	3.17219500	-0.41074000
H	-0.89842400	3.49582300	0.55439600
H	-1.31950700	2.69540600	-0.94293500
C	1.77258900	2.74384900	0.70267600
H	2.58372500	2.03019300	0.87977500
H	2.23236900	3.62827800	0.24725900
H	1.39432700	3.04986600	1.68481100
C	-0.07354600	4.41553800	-1.21406500
H	-0.93048100	5.07334000	-1.38879900
H	0.68813400	5.00298200	-0.69586500
H	0.33320300	4.13121300	-2.19004300

[BuAlMe(2-Bu)]

G (CBS-QB3) = -596.859236

C	-3.79284200	-1.96457200	-0.22540000
H	-4.69502700	-1.34806000	-0.23291500
H	-3.94759500	-2.78046300	-0.93808700
C	-2.53848200	-1.15164000	-0.57971500
H	-1.69146800	-1.84635000	-0.64157400
C	-2.20009200	-0.00331100	0.40653800

H	-2.14403300	-0.45981100	1.40953000
C	1.16741000	-0.48367200	0.35947600
H	1.17971000	-0.74236700	1.43073600
H	0.95883500	-1.44089700	-0.14120400
C	-0.09284000	2.59825600	-0.45331600
H	0.14366400	3.21121000	0.42697200
H	0.75220700	2.71317300	-1.14040400
H	-0.97237100	3.05078500	-0.92138100
H	-2.66125300	-0.73837100	-1.59060500
Al	-0.37494600	0.72275900	0.07638800
H	-3.69962500	-2.40599500	0.77209700
C	-3.29626500	1.08065400	0.44572200
H	-4.27300700	0.68411900	0.74503600
H	-3.05233500	1.88210100	1.15059400
H	-3.42702000	1.55020700	-0.53588200
C	2.56221100	0.02168700	-0.05590900
H	2.78123200	0.97156500	0.44890500
H	2.57035100	0.25359600	-1.12910700
C	3.70096400	-0.96488000	0.23924800
H	3.70513400	-1.19264600	1.31229600
H	3.49120700	-1.91354300	-0.26994000
C	5.08042200	-0.44965900	-0.18194000
H	5.33126100	0.48048700	0.33800000
H	5.86617700	-1.17646400	0.04252800
H	5.11533400	-0.24531800	-1.25686400

[BuAlMe(2-Bu)] Transition Structure (*cis*-2-butene)

G (CBS-QB3) = -596.811882

C	-3.29500000	-1.17248600	-1.25586200
H	-3.59431100	-0.15013500	-1.48710600
H	-3.02119700	-1.67196300	-2.18581000
C	-2.17507400	-1.22616500	-0.24679600
H	-1.66389200	-2.18277200	-0.19625500
C	-2.15055500	-0.44013200	0.93438600
H	-1.68469500	-0.92679800	1.78895700
C	1.20360800	-0.25083700	0.64712500
H	1.31231300	0.21478000	1.63750400
H	1.12666900	-1.32969100	0.84354500
C	-0.90702500	2.20324600	-0.76233900
H	-0.95814400	2.90613300	0.07653200
H	-0.12894300	2.56778000	-1.44155600
H	-1.85726600	2.26938200	-1.30129600
H	-0.98275900	-0.71787100	-1.33448500
Al	-0.50150400	0.37043800	-0.15110900
H	-4.16700300	-1.68229100	-0.82885200
C	-3.25078000	0.55292500	1.28106000
H	-4.16189700	0.04751500	1.62606800
H	-2.92822500	1.21952400	2.08430500
H	-3.53107800	1.18775500	0.43764500
C	2.47351800	0.02648100	-0.18103400
H	2.55963800	1.10243300	-0.38381600
H	2.38837300	-0.45375000	-1.16486100
C	3.77326600	-0.44795700	0.48518200
H	3.86435400	0.03057700	1.46807500
H	3.70112100	-1.52534100	0.67874900
C	5.02699000	-0.15790900	-0.34555800
H	5.14206100	0.91579500	-0.52579600
H	5.93288700	-0.50821900	0.15744400
H	4.97785600	-0.65152600	-1.32155700

[BuAlMe(2-Bu)] Transition Structure (*trans*-2-butene)

G (CBS-QB3) = -596.813332

C	-2.33318900	-1.00051900	-0.53510600
C	-2.36476400	-0.28149800	0.68209200
H	-1.98971900	-0.82553000	1.54829500
C	1.01306400	-0.14353300	0.62074300
H	1.07969300	0.31190400	1.61959400
H	0.91095100	-1.22189100	0.80392900
C	-0.95164800	2.41628800	-0.78590700
H	-1.01438200	3.07844400	0.08475100
H	-0.13808800	2.79047900	-1.41658200
H	-1.87906500	2.53624600	-1.35445800
H	-1.05961900	-0.46573900	-1.52506300
Al	-0.62879300	0.54250700	-0.25666000
C	-3.45830500	0.73821300	0.96724100
H	-4.36180600	0.25514700	1.35968600
H	-3.14163400	1.48066900	1.70398700
H	-3.74582100	1.28312100	0.06417400
C	2.32792900	0.11947700	-0.14000400
H	2.43890800	1.19448000	-0.33544600
H	2.28698400	-0.35784700	-1.12790600
C	3.58480700	-0.37320900	0.59216300
H	3.63307200	0.10614300	1.57760400
H	3.48651200	-1.44895800	0.78335500
C	4.88346300	-0.10419100	-0.17420600
H	5.02431400	0.96719200	-0.34968200
H	5.75703900	-0.46750500	0.37463900
H	4.87610500	-0.59903300	-1.15072000
C	-1.93632100	-2.45440700	-0.59612100
H	-2.79484600	-3.05535500	-0.27419900
H	-1.65279200	-2.76194900	-1.60369600
H	-1.10952900	-2.67107600	0.08252000
H	-3.02219600	-0.68125600	-1.31357100

BuMeAlH---*cis*-2-butene Pie Complex

G (CBS-QB3) = -596.840645

C	-3.76394500	0.33140200	-1.04585800
H	-4.13125700	0.61276900	-0.05911100
H	-3.48036100	1.24108600	-1.58207300
C	-2.61338400	-0.63082500	-0.99500200
H	-2.17153400	-0.86984600	-1.95912900
C	-2.12871300	-1.28096500	0.08030100
H	-1.33269600	-2.00063600	-0.09536700
C	1.14213000	-0.44296000	-0.10182700
H	1.05220100	-0.98247600	0.85165500
H	1.10004000	-1.21384700	-0.88482600
C	-1.00371800	1.93014200	1.16997200
H	-0.95528000	1.43207000	2.14367800
H	-0.36764200	2.82236400	1.24345000
H	-2.02660300	2.29752900	1.03341800
H	-0.64370300	1.37063300	-1.80621600
Al	-0.37507700	0.81704100	-0.33443000
H	-4.59473700	-0.11903900	-1.60054700
C	-2.62815700	-1.21678700	1.49466300
H	-3.11162400	-2.16534800	1.75485400
H	-1.80111700	-1.08193100	2.19679400
H	-3.34706700	-0.41491000	1.65886800
C	2.52608000	0.24027500	-0.15817500
H	2.60267800	0.99810900	0.63354500
H	2.63467900	0.78668500	-1.10497000
C	3.71048400	-0.72801800	-0.01811500
H	3.61395600	-1.27207700	0.92947100
H	3.64475200	-1.48391700	-0.81017400
C	5.07623600	-0.03746900	-0.07818600

H	5.18135700	0.70221500	0.72204600
H	5.89468100	-0.75568900	0.02545000
H	5.21318700	0.48594500	-1.02987000

BuMeAlH---*trans*-2-butene Pie Complex

G (CBS-QB3) = -596.840792

C	2.77148600	0.90925400	-0.22485700
C	2.37857800	0.40582500	0.95763500
H	1.70908500	1.00548700	1.57271800
C	-0.95378700	0.22219300	0.28833000
H	-0.85798400	-0.16670600	1.31185000
H	-0.82245400	1.31033600	0.37021400
C	0.94316400	-2.45118900	-0.76945400
H	0.80972700	-2.90023900	0.21958400
H	0.29508500	-3.00918500	-1.45868300
H	1.97058500	-2.65182100	-1.09217800
H	0.75479500	0.18788400	-2.26082300
Al	0.46445500	-0.53950900	-0.87310100
C	2.89002600	-0.85971900	1.58346800
H	3.51132900	-0.61067100	2.45143700
H	2.07755300	-1.49307300	1.94877500
H	3.49546700	-1.44331300	0.88793200
C	-2.38239200	-0.06688900	-0.22317400
H	-2.54229600	-1.15137100	-0.29758400
H	-2.49913200	0.32144000	-1.24416100
C	-3.49620000	0.52671300	0.65240700
H	-3.38918500	0.13968300	1.67318400
H	-3.35147300	1.61172600	0.72258700
C	-4.90630500	0.22793200	0.13464000
H	-5.08967300	-0.85027100	0.08619000
H	-5.67275900	0.66527000	0.78090900
H	-5.05224900	0.63176800	-0.87240200
C	2.43331400	2.28051200	-0.73482900
H	3.33253500	2.90710300	-0.72533000
H	2.07094200	2.24582900	-1.76431300
H	1.67702900	2.76657800	-0.11485600
H	3.46784700	0.32936700	-0.82972900

[BuMeAlH]

G (CBS-QB3) = -439.940606

C	-3.63582300	-0.39154400	0.00003900
H	-4.22744000	-0.09583600	0.87522100
H	-4.22760400	-0.09565500	-0.87497000
C	-0.20355600	-0.50789400	0.00008300
H	-0.22104300	-1.18612500	0.86747700
H	-0.22108300	-1.18637700	-0.86711200
Al	-1.89158900	0.50865600	-0.00000700
H	-1.85513100	2.09832600	-0.00009100
C	1.10870900	0.29887200	-0.00005900
H	1.13695900	0.96420600	0.87251700
H	1.13692700	0.96395800	-0.87282700
C	2.37586300	-0.56770900	0.00004100
H	2.35620100	-1.22763300	0.87607800
H	2.35617400	-1.22787600	-0.87581200
C	3.67210700	0.24800200	-0.00009300
H	3.73392700	0.89254000	0.88252700
H	4.55349300	-0.39938900	-0.00001700
H	3.73389900	0.89229600	-0.88289300
H	-3.56841500	-1.48333000	-0.00007300

Cis-2-Butene

G (CBS-QB3) = -156.901113

C	-0.00001500	0.66718200	0.66371100
H	-0.00002500	1.16517300	1.63142200
C	0.00001500	-0.66718200	0.66371100
H	0.00002500	-1.16517300	1.63142200
C	0.00001500	1.58947500	-0.52189600
H	0.00010600	1.05873300	-1.47486400
H	-0.87806900	2.24496200	-0.50378000
H	0.87807900	2.24499400	-0.50366800
C	-0.00001500	-1.58947500	-0.52189600
H	-0.00010600	-1.05873300	-1.47486400
H	0.87806900	-2.24496200	-0.50378000
H	-0.87807900	-2.24499400	-0.50366800

Trans-2-Butene

G (CBS-QB3) = -156.902551

C	0.32394200	0.58154700	-0.00024400
H	1.41390400	0.57142500	0.00044900
C	-0.32394200	-0.58154700	-0.00024400
H	-1.41390400	-0.57142500	0.00044900
C	-0.32394200	1.93555400	0.00011100
H	-1.41396200	1.85804100	-0.00048700
H	-0.02594700	2.51845200	0.87901100
H	-0.02505900	2.51920700	-0.87817900
C	0.32394200	-1.93555400	0.00011100
H	1.41396200	-1.85804100	-0.00048700
H	0.02594700	-2.51845200	0.87901100
H	0.02505900	-2.51920700	-0.87817900

$[(Me)_2Al(\mu\text{-}H)(\mu\text{-}Bu)AlMeBu]$

G (CBS-QB3) = -919.149762

H	-0.40961300	1.34630000	1.07425500
Al	-0.42210300	-0.31371700	0.60143100
Al	0.94003500	1.88001200	0.15302400
C	1.37406100	-0.12729900	-0.62261300
H	0.79945600	-0.84406200	-1.23514900
H	1.69918500	0.54356800	-1.43856600
C	2.62302100	-0.84392300	-0.06281400
H	3.23733200	-0.13249300	0.49821100
H	2.31910100	-1.60455000	0.66327500
C	3.48667600	-1.50559600	-1.14625800
H	3.80336500	-0.74359200	-1.86926700
H	2.87323200	-2.22003100	-1.70909500
C	4.71807900	-2.22063300	-0.58293200
H	5.30987500	-2.68191900	-1.37803700
H	5.36910200	-1.52399200	-0.04575100
H	4.43018200	-3.01041300	0.11779000
C	2.38235900	2.41503300	1.37145300
H	2.14220500	3.37671600	1.83966500
H	2.55606600	1.69796400	2.17946200
H	3.33447300	2.55289400	0.84625300
C	0.27308100	3.02596400	-1.29581800
H	-0.51050400	2.54950000	-1.89390000
H	-0.14864900	3.95624300	-0.89831000
H	1.07527400	3.31581400	-1.98502000
C	-0.03372700	-1.41230300	2.18339600
H	0.83235800	-1.05651500	2.74975200

H	-0.88978900	-1.41046000	2.86786900
H	0.15556000	-2.45983100	1.92205300
C	-1.99616600	-0.58370900	-0.55986600
H	-1.94675300	0.11126500	-1.40982300
H	-1.93349600	-1.58762200	-1.00689600
C	-3.36405400	-0.43295800	0.13729600
H	-3.43582800	-1.13770300	0.97643000
H	-3.44701300	0.56761600	0.58248400
C	-4.56853300	-0.65418600	-0.78919200
H	-4.49909500	-1.65647300	-1.22938800
H	-4.50549800	0.05016200	-1.62757500
C	-5.91831300	-0.49433200	-0.08343000
H	-6.75292900	-0.65986200	-0.77050300
H	-6.02094500	-1.20760500	0.74073100
H	-6.02867800	0.51090100	0.33581100

$[(Me)_2Al(\mu\text{-}Pr)AlMe(2\text{-}Bu)]$

G (CBS-QB3) = -997.596743

Al	-0.39102700	-0.15110500	0.65523700
Al	1.95620300	0.44821800	-0.35835900
C	0.88273000	-1.47021200	-0.49386400
H	-0.01261800	-1.71955200	-1.08311300
H	1.61208500	-1.40634900	-1.32062700
C	1.28958200	-2.69108900	0.36416700
H	2.15936300	-2.43422900	0.97534700
H	0.49246700	-2.92840800	1.07431400
C	1.60152300	-3.93815500	-0.47100500
H	2.43260800	-3.75514000	-1.15989200
H	0.73678400	-4.24031100	-1.07010900
C	3.43219100	0.15320200	0.90916900
H	4.03990600	1.06133000	1.00800500
H	3.10047600	-0.11939500	1.91625100
H	4.11236500	-0.63635200	0.56906100
C	2.34092600	1.02565500	-2.20110700
H	1.46339600	1.02989900	-2.85649100
H	2.77555600	2.03103900	-2.24015800
H	3.07885200	0.35473700	-2.65871200
C	-0.29582700	-0.64238600	2.56440400
H	0.72789700	-0.70453900	2.94764400
H	-0.82276800	0.09674100	3.18040500
H	-0.77139000	-1.60809800	2.76879500
C	-2.18307300	-0.01891200	-0.21391800
H	-2.04734400	0.39680400	-1.22438000
C	0.53986200	1.84171400	0.48276200
H	-0.07011800	1.88674000	1.40089200
H	1.47479900	2.26158800	0.89344000
C	-0.04785000	2.84916900	-0.53168100
H	0.61516700	2.93335900	-1.39593300
H	-0.99518600	2.46996400	-0.92394000
C	-0.26939400	4.24411800	0.06528900
H	0.66967400	4.66997400	0.43300500
H	-0.96784800	4.21081500	0.90753200
C	-2.84376500	-1.41009800	-0.38184800
H	-3.05996900	-1.83126600	0.60911200
H	-2.13838900	-2.10792300	-0.85142500
C	-3.10098300	0.94229000	0.57455400
H	-2.65860000	1.93670700	0.69274300
H	-4.07262700	1.09164500	0.09059800
H	-3.30097700	0.55844900	1.58154500
C	-4.13344600	-1.42281900	-1.21719800
H	-4.52066900	-2.44027500	-1.32857800
H	-4.92301400	-0.82162100	-0.75976900
H	-3.95098900	-1.02363600	-2.22026600
H	-0.67875100	4.93375200	-0.67873300

H	1.87771200	-4.78379500	0.16567000

[$(Me)_2Al(\mu\text{-}Pr)AlMeBu$]

G (CBS-QB3) = -997.600812

Al	0.16436800	-0.10256000	0.74913200
Al	-2.07565100	0.27052800	-0.56404500
C	-0.39649700	1.65024200	-0.43340200
H	0.69708400	1.57472000	-0.56479300
H	-0.67596400	1.78538500	-1.49122800
C	-0.69228600	2.96250000	0.32769800
H	-1.77071300	3.13743100	0.35520800
H	-0.38331900	2.86176300	1.37128900
C	-0.00023600	4.18332400	-0.29010300
H	-0.31668900	4.33563500	-1.32697400
H	1.08798600	4.06372000	-0.29186700
C	-3.60867600	1.10259800	0.35006200
H	-4.46782100	0.41986700	0.34383000
H	-3.41295300	1.36002400	1.39643100
H	-3.94266900	2.01911600	-0.14946500
C	-2.24601700	-0.29354000	-2.44269000
H	-1.31970600	-0.69322700	-2.86937600
H	-3.02024500	-1.05673900	-2.58120100
H	-2.54190800	0.56022800	-3.06549400
C	0.27914400	0.49608700	2.62185300
H	-0.66874100	0.87309500	3.02061800
H	0.58701500	-0.33711800	3.26622500
H	1.02438600	1.28666700	2.76466700
C	1.72421900	-0.97196800	-0.10649700
H	1.51711600	-1.17834800	-1.16589600
C	-1.49905200	-1.49917600	0.58499000
H	-1.15679000	-1.66954100	1.62000800
H	-2.58155300	-1.42733300	0.78467500
C	-1.24158900	-2.78749800	-0.22918400
H	-1.64382500	-2.67342900	-1.23886400
H	-0.16647200	-2.93695300	-0.35530800
C	-1.85066900	-4.03673000	0.41862300
H	-2.93643900	-3.94086600	0.52084600
H	-1.43934400	-4.20517500	1.41912000
C	3.05235500	-0.19529800	0.00742800
H	3.28172100	-0.00116300	1.06350300
H	2.95534200	0.79539100	-0.45943900
C	4.25370700	-0.90902400	-0.62997400
H	4.36578500	-1.89614700	-0.16518900
H	4.03606800	-1.09600200	-1.68856900
H	-1.65062200	-4.93137300	-0.17832900
H	-0.23327100	5.09587600	0.26642200
H	1.86247600	-1.96139300	0.35381700
C	5.56608200	-0.12987400	-0.50391300
H	5.82490500	0.04235000	0.54572500
H	6.39830700	-0.66844500	-0.96587400
H	5.49461000	0.84855200	-0.99000900