ELECTRONIC SUPPLEMENTARY INFORMATION

Bimetallic Scorpionate-based Helical Organoaluminums for the Efficient Carbon Dioxide Fixation into a Variety of Cyclic Carbonates

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1.1. Computational Details

All the calculations reported in this paper were performed with the Gaussian 09 suite of programs.[1] Electron correlation was partially taken into account using the hybrid functional usually denoted as B3LYP[2] in conjunction with the D3 dispersion correction suggested by Grimme et al.[3] using the standard double-ζ quality 6-31G(d) basis set for all atoms. All species were characterized by frequency calculations,[4] and have positive definite Hessian matrices. The energetic diagrams are based on electronic energies corrected with zero-point vibrational energies. Solvent effects (solvent = toluene) were taken into account using the Polarizable Continuum Model (PCM)[5] during the geometry optimizations. This level is therefore denoted PCM-(toluene)-B3LYP-D3/6-31G(d).

1.2. Thermodynamic stability study of the different scorpionate arrangements in dinuclear aluminium complexes.

Herein we present the input coordinates for complexes **4** and **8** according the two different coordination arrangements of the scorpionate ligand, namely extended π-$C_2N_2(sp^2)$−Al_2 disposition and apical σ-$C(sp^3)$-Al mode. Gibbs free energies (ΔG) were also evaluated by frequency calculations (Table S1).

Table S1. *Gibbs free energies values calculated at 298.15 K of optimized structures at the B3LYP/6-31+G(d) level for the different ligand arrangements in dinuclear aluminium complexes.*

Complex	*Disposition*	ΔG (kcal/mol)	ΔΔG (kcal/mol)[a]
4	π-$C_2N_2(sp^2)$−Al_2	-1051408.256	-25.933712
	σ-$C(sp^3)$-Al	-1051382.323	
8	π-$C_2N_2(sp^2)$−Al_2	-1242696.896	-18.613814
	σ-$C(sp^3)$-Al	-1242678.282	

[a] ΔΔG = ΔG (π-$C_2N_2(sp^2)$−Al_2) – ΔG (σ-$C(sp^3)$-Al)

Input Coordinates.

[$AlMe_2$(pbpamd$^-$)$AlMe_2$], 4-π-C_2N_2(sp^2)−Al_2

ZPE at 298 K: -1051366.486 kcal/mol
Gibbs Energy at 298 K: -1051408.256 kcal/mol

Atomic Number	*X*	*Y*	*Z*
13	-2.600075000	0.643135000	0.952969000
13	2.600593000	0.643309000	-0.952207000
7	-2.363969000	-1.121925000	0.022587000
7	-1.096651000	-1.333891000	-0.463748000
7	2.363948000	-1.121999000	-0.022454000
7	1.096583000	-1.334123000	0.463663000
7	-1.210192000	1.489299000	-0.042931000
7	1.210205000	1.489399000	0.043189000
6	-1.090875000	-2.384118000	-1.327217000
6	-2.396782000	-2.861020000	-1.388669000
1	-2.749415000	-3.693250000	-1.980711000
6	-3.163991000	-2.036165000	-0.556923000
6	0.150780000	-2.855656000	-2.007139000
1	0.733395000	-2.011200000	-2.386587000
1	-0.111356000	-3.511214000	-2.841106000
1	0.797375000	-3.416131000	-1.320653000
6	-4.639622000	-2.070452000	-0.311104000
1	-4.869387000	-2.013946000	0.757697000
1	-5.062078000	-2.997368000	-0.707862000
1	-5.140124000	-1.227011000	-0.798479000
6	1.090687000	-2.384679000	1.326735000
6	2.396571000	-2.861634000	1.388141000
1	2.749089000	-3.694163000	1.979831000
6	3.163884000	-2.036524000	0.556746000
6	-0.150998000	-2.856278000	2.006566000
1	-0.732632000	-2.011908000	2.387741000
1	0.111072000	-3.513421000	2.839301000
1	-0.798527000	-3.415027000	1.319567000
6	4.639530000	-2.070832000	0.311027000
1	4.869435000	-2.012738000	-0.757649000
1	5.061687000	-2.998474000	0.706413000
1	5.140229000	-1.228292000	0.799765000
6	0.000006000	-0.561258000	0.000075000
6	0.000062000	0.842422000	0.000087000
6	-1.323191000	2.672336000	-0.922664000
1	-0.310513000	3.012583000	-1.158219000
6	-1.989773000	2.269581000	-2.248150000
1	-1.423760000	1.462432000	-2.726701000
1	-2.034701000	3.118801000	-2.941623000

1	-3.011966000	1.914381000	-2.074865000
6	-2.068830000	3.829998000	-0.250193000
1	-3.114245000	3.569327000	-0.055616000
1	-2.061855000	4.714411000	-0.898012000
1	-1.601371000	4.100371000	0.702823000
6	1.322720000	2.673204000	0.921970000
1	0.309884000	3.013081000	1.157364000
6	1.989688000	2.271842000	2.247670000
1	1.424209000	1.464719000	2.726892000
1	2.034209000	3.121621000	2.940483000
1	3.012073000	1.917138000	2.074517000
6	2.067675000	3.830748000	0.248529000
1	3.113259000	3.570544000	0.054198000
1	2.060178000	4.715696000	0.895609000
1	1.600089000	4.100071000	-0.704716000
6	-4.456811000	1.243597000	0.602520000
1	-4.653000000	2.222047000	1.062478000
1	-5.185711000	0.549834000	1.044450000
1	-4.711090000	1.336870000	-0.461862000
6	-2.064517000	0.409279000	2.848816000
1	-0.976833000	0.303110000	2.961565000
1	-2.527476000	-0.467006000	3.325857000
1	-2.358600000	1.281316000	3.451021000
6	2.065610000	0.410093000	-2.848283000
1	0.978091000	0.302472000	-2.961175000
1	2.529853000	-0.465210000	-3.325901000
1	2.358483000	1.282963000	-3.449865000
6	4.457278000	1.243029000	-0.600337000
1	4.653719000	2.222666000	-1.057630000
1	5.186148000	0.550317000	-1.043947000
1	4.711375000	1.333419000	0.464347000

[$AlMe_2$(pbpamd$^-$)$AlMe_2$], 4-σ-C(sp^3)-Al

ZPE at 298 K: -1051340.776 kcal/mol
Gibbs Energy at 298 K: -1051382.323 kcal/mol

Atomic Number	*X*	*Y*	*Z*
13	0.490402000	2.322363000	0.481038000
7	2.348825000	-1.213920000	0.735556000
7	1.018720000	-0.967398000	0.896258000
7	1.457416000	1.356274000	-0.937836000
7	1.135853000	0.047557000	-1.229638000
7	-1.150727000	1.268806000	0.259056000
7	-2.027798000	-0.965695000	-0.321913000
6	0.606490000	-1.242308000	2.173929000
6	1.738651000	-1.650605000	2.862124000
1	1.781915000	-1.916520000	3.909633000
6	2.793648000	-1.611693000	1.928670000
6	-0.784287000	-1.117450000	2.707256000
1	-1.186552000	-0.109336000	2.576305000
1	-0.771478000	-1.340818000	3.777503000
1	-1.469043000	-1.816875000	2.221281000
6	4.243808000	-1.933637000	2.128010000
1	4.709266000	-1.254422000	2.852863000
1	4.781629000	-1.842304000	1.179787000
1	4.378519000	-2.954536000	2.505479000
6	2.015821000	-0.445724000	-2.142249000
6	2.863295000	0.591397000	-2.497227000
1	3.671086000	0.544469000	-3.212671000
6	2.492915000	1.695012000	-1.720469000
6	2.077862000	-1.872922000	-2.567410000
1	1.189812000	-2.184174000	-3.121958000
1	2.193591000	-2.515935000	-1.688451000
1	2.948605000	-2.015395000	-3.212737000
6	3.106553000	3.060241000	-1.709315000
1	3.374755000	3.368571000	-0.693618000
1	2.418202000	3.810020000	-2.111339000
1	4.014004000	3.061021000	-2.318408000
6	0.256424000	-0.713502000	-0.361767000
6	-1.111177000	-0.013496000	-0.101816000
6	-2.437270000	1.962499000	0.503619000
1	-3.214264000	1.211830000	0.593657000
6	-2.403711000	2.714932000	1.840847000
1	-2.181620000	2.034119000	2.668860000
1	-3.378040000	3.179634000	2.028865000
1	-1.654189000	3.513084000	1.844598000
6	-2.807963000	2.883724000	-0.667482000
1	-2.774670000	2.336780000	-1.614654000

1	-2.125750000	3.732602000	-0.740231000
1	-3.823353000	3.274410000	-0.530567000
6	-3.499846000	-1.091976000	-0.282053000
1	-3.646900000	-2.116730000	-0.647994000
6	-4.267273000	-0.211213000	-1.283139000
1	-3.735386000	-0.172157000	-2.239014000
1	-4.429160000	0.809894000	-0.934345000
1	-5.254007000	-0.654119000	-1.459950000
6	-4.106874000	-1.089803000	1.130427000
1	-3.632408000	-1.853600000	1.753018000
1	-5.175627000	-1.323284000	1.063351000
1	-4.007420000	-0.128992000	1.643926000
6	1.345624000	2.061132000	2.243164000
1	0.610896000	1.841219000	3.029780000
1	1.889612000	2.962439000	2.559490000
1	2.058518000	1.228437000	2.240322000
6	0.352961000	4.201275000	-0.146480000
1	1.324358000	4.697640000	-0.011538000
1	0.090262000	4.300951000	-1.208223000
1	-0.370421000	4.802184000	0.420269000
13	-0.855608000	-2.344344000	-1.029140000
6	-0.656119000	-3.955446000	0.105068000
1	-0.025824000	-4.717913000	-0.373996000
1	-1.625659000	-4.436410000	0.302816000
1	-0.202445000	-3.729664000	1.078565000
6	-1.334537000	-2.577308000	-2.944713000
1	-0.809272000	-3.401690000	-3.445838000
1	-1.171028000	-1.670524000	-3.543964000
1	-2.408823000	-2.806292000	-3.019901000

[$AlMe_2$(phbpamd$^-$)$AlMe_2$], 8-π-C_2N_2(sp^2)−Al_2

ZPE at 298 K: -1242649.786 kcal/mol
Gibbs Energy at 298 K: -1242696.896 kcal/mol

Atomic Number	*X*	*Y*	*Z*
13	0.370863000	-2.544609000	-1.188455000
13	0.348401000	2.543277000	1.189422000
7	2.137762000	-2.349802000	-0.259471000
7	2.360237000	-1.135160000	0.343532000
7	2.116335000	2.364431000	0.259024000
7	2.349946000	1.151392000	-0.342859000
7	-0.458028000	-1.206672000	-0.096441000
7	-0.469035000	1.197418000	0.098461000
6	3.415623000	-1.217210000	1.197328000
6	3.887888000	-2.524453000	1.127940000
1	4.722532000	-2.934989000	1.677591000
6	3.053348000	-3.205143000	0.233351000
6	3.891327000	-0.050606000	1.996992000
1	4.440761000	0.667410000	1.375942000
1	4.557268000	-0.395514000	2.791462000
1	3.049177000	0.485064000	2.445821000
6	3.072401000	-4.650379000	-0.154213000
1	4.006647000	-5.113163000	0.174214000
1	2.986035000	-4.775210000	-1.238497000
1	2.238933000	-5.191753000	0.306000000
6	3.404151000	1.242464000	-1.197232000
6	3.864177000	2.554158000	-1.129284000
1	4.694670000	2.971992000	-1.679738000
6	3.023638000	3.227864000	-0.235021000
6	3.890125000	0.079610000	-1.996167000
1	4.446411000	-0.632820000	-1.374800000
1	4.552416000	0.429922000	-2.791317000
1	3.052653000	-0.464092000	-2.444071000
6	3.028875000	4.673680000	0.150785000
1	2.191368000	5.206768000	-0.311761000
1	3.959456000	5.144587000	-0.176496000
1	2.939150000	4.799160000	1.234706000
6	1.590575000	0.004801000	0.000841000
6	0.191110000	-0.001638000	0.000804000
6	-1.712680000	-1.358667000	0.555246000
6	-1.871542000	-1.001691000	1.902843000
1	-1.023511000	-0.595850000	2.446492000
6	-3.104046000	-1.149801000	2.533248000
1	-3.205322000	-0.858989000	3.577086000
6	-4.213085000	-1.673279000	1.853683000
6	-4.038927000	-2.049617000	0.516462000
1	-4.881061000	-2.457567000	-0.038488000

6	-2.813390000	-1.889527000	-0.128174000
1	-2.715779000	-2.142439000	-1.179932000
6	-5.558401000	-1.791984000	2.531261000
1	-6.139457000	-0.865464000	2.426448000
1	-5.452766000	-1.987343000	3.604373000
1	-6.157225000	-2.600532000	2.097770000
6	-1.724420000	1.340480000	-0.553785000
6	-1.881862000	0.979883000	-1.900097000
1	-1.033381000	0.572677000	-2.442026000
6	-3.116917000	1.116034000	-2.529184000
1	-3.218253000	0.817015000	-3.570623000
6	-4.228480000	1.634135000	-1.850531000
6	-4.058111000	2.006121000	-0.511053000
1	-4.905677000	2.398417000	0.047087000
6	-2.830497000	1.858804000	0.131729000
1	-2.736090000	2.103515000	1.185719000
6	-5.558908000	1.807856000	-2.545376000
1	-6.394744000	1.668430000	-1.850524000
1	-5.679388000	1.091995000	-3.365998000
1	-5.659349000	2.814166000	-2.974737000
6	0.616284000	-1.921242000	-3.052503000
1	-0.290352000	-2.078964000	-3.654051000
1	1.431677000	-2.445338000	-3.571919000
1	0.842307000	-0.847156000	-3.103393000
6	-0.322107000	-4.356488000	-0.818980000
1	-0.291167000	-4.600977000	0.251681000
1	0.232201000	-5.142729000	-1.349262000
1	-1.371882000	-4.447230000	-1.128118000
6	0.601030000	1.922822000	3.053356000
1	-0.306407000	2.072530000	3.655727000
1	1.412275000	2.454176000	3.571893000
1	0.836627000	0.850785000	3.103999000
6	-0.361121000	4.348544000	0.818895000
1	-0.333155000	4.592096000	-0.252066000
1	0.186566000	5.140336000	1.347805000
1	-1.411471000	4.429957000	1.128714000

[$AlMe_2$(phbpamd$^-$)$AlMe_2$], 8-σ-C(sp^3)-Al

ZPE at 298 K: -1242629.892 kcal/mol
Gibbs Energy at 298 K: -1242678.282 kcal/mol

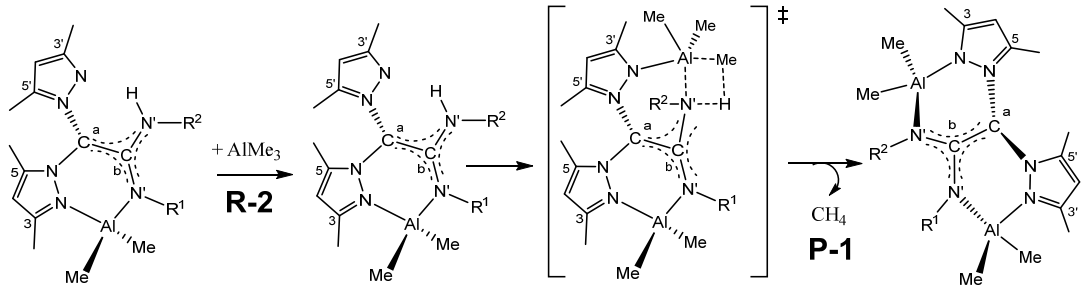
Atomic Number	*X*	*Y*	*Z*
13	0.890712000	2.462939000	0.691021000
7	3.575943000	-1.197990000	0.630003000
7	2.257100000	-0.923580000	0.841498000
7	2.288583000	1.799580000	-0.528540000
7	2.253671000	0.517822000	-1.039948000
7	-0.354575000	1.042153000	0.199981000
7	-0.672855000	-1.299473000	-0.377307000
6	1.877680000	-1.231038000	2.123100000
6	3.021434000	-1.688648000	2.759181000
1	3.088492000	-2.004314000	3.791416000
6	4.047942000	-1.643745000	1.793352000
6	0.500725000	-1.134742000	2.696721000
1	0.069973000	-0.136733000	2.582095000
1	0.551427000	-1.356308000	3.766156000
1	-0.179481000	-1.856993000	2.234856000
6	5.493494000	-2.011012000	1.938394000
1	5.998368000	-1.368399000	2.670246000
1	6.006824000	-1.905244000	0.978289000
1	5.608757000	-3.046614000	2.280031000
6	3.247239000	0.367793000	-1.957802000
6	3.889397000	1.591366000	-2.073578000
1	4.718897000	1.820105000	-2.726365000
6	3.267607000	2.457427000	-1.167771000
6	3.580837000	-0.914674000	-2.640160000
1	2.782642000	-1.239369000	-3.311659000
1	3.766417000	-1.694896000	-1.896088000
1	4.488697000	-0.777630000	-3.233481000
6	3.561798000	3.902069000	-0.907969000
1	3.589271000	4.118874000	0.164917000
1	2.799527000	4.546528000	-1.358475000
1	4.532071000	4.166094000	-1.336192000
6	1.504080000	-0.540689000	-0.379225000
6	0.037766000	-0.192988000	-0.124967000
6	1.518815000	2.353011000	2.558799000
1	0.689609000	2.405093000	3.279143000
1	2.185924000	3.194678000	2.794934000
1	2.075200000	1.432099000	2.771556000
6	0.213506000	4.174985000	-0.020821000
1	0.890219000	5.015355000	0.183599000
1	0.060021000	4.135984000	-1.108247000
1	-0.756703000	4.434705000	0.422438000

13	0.756371000	-2.278119000	-1.308639000
6	1.335682000	-3.933769000	-0.404347000
1	2.202702000	-4.392120000	-0.899918000
1	0.541210000	-4.693587000	-0.393353000
1	1.623236000	-3.746252000	0.638229000
6	0.391740000	-2.269891000	-3.260450000
1	1.178832000	-2.768512000	-3.842348000
1	0.271774000	-1.258355000	-3.673121000
1	-0.538130000	-2.812556000	-3.483783000
6	-1.721899000	1.444426000	0.064571000
6	-2.399308000	1.297785000	-1.151681000
6	-2.382539000	2.038723000	1.143860000
6	-3.728756000	1.692195000	-1.261781000
6	-3.711903000	2.440892000	1.019021000
6	-4.414136000	2.259838000	-0.177949000
1	-1.884971000	0.853003000	-1.998219000
1	-1.863257000	2.157387000	2.091607000
1	-4.246695000	1.554073000	-2.208003000
1	-4.213283000	2.890856000	1.872562000
6	-2.041401000	-1.551006000	-0.120349000
6	-2.780793000	-2.238563000	-1.092979000
6	-2.677814000	-1.202005000	1.079945000
6	-4.127799000	-2.527841000	-0.887117000
6	-4.024340000	-1.495220000	1.273415000
6	-4.780304000	-2.151334000	0.293304000
1	-2.299787000	-2.520059000	-2.024480000
1	-2.126831000	-0.682940000	1.852792000
1	-4.682515000	-3.050171000	-1.663259000
1	-4.498702000	-1.199693000	2.206452000
6	-5.872545000	2.633497000	-0.297429000
1	-6.097254000	3.066150000	-1.278754000
1	-6.514043000	1.749828000	-0.179163000
1	-6.167507000	3.357938000	0.468703000
6	-6.253537000	-2.414754000	0.494930000
1	-6.598364000	-3.258587000	-0.111948000
1	-6.482489000	-2.634374000	1.543616000
1	-6.853233000	-1.539823000	0.209126000

1.2. Reaction profile study for the synthesis of dinuclear scorpionate aluminium complexes.

For the transformation of the corresponding mononuclear scorpionate aluminium derivatives into binuclear counterparts, we obtained by DFT calculations the following input coordinates of optimized geometries for all reactants, products, intermediates and transition states involved in the reaction. Vibrational frequency calculations were performed to confirm all stationary points as either minima (no imaginary frequencies) or transition states (only one imaginary frequency). Calculated Gibbs free energies are presented in Table S2 for each specie involved in the reaction.

Table S2. Zero-Point vibrational energy and Gibbs free energy (in parenthesis) in kcal/mol obtained at 298.15 K and B3LYP/6-31+G(d) level for all reactants, intermediates, transition states and products for the reaction to form the dinuclear scorpionate complexes **4**, **6** and **8**.



R-1	R-2	I-1	TS	P-1	P-2
1-NH tautomer -849495.2834 (-849533.7485)		**2** -1076740.064 (-1076784.618)	**TS-pbamd** -1076704.413 (-1076747.261)		**4-π-$C_2N_2(sp^2)$−Al_2** -1051366.486 (-1051408.256)
NH-tautomer [$AlMe_2(\kappa^2$-tbpamd)][a] -849498.1015 (-849537.0768)	**$AlMe_3$** -227213.3084 (-227235.1897)	**3** -1076737.426 (-1076780.632)	**TS-tbamd** -1076699.252 (-1076742.619)	**CH_4** -25397.51474 (-25409.20712)	**6-π-$C_2N_2(sp^2)$−Al_2** -1051360.793 (-1051401.734)
CH tautomer [$AlMe_2(\kappa^2$-phbpamd)][a] -1040778.372 (-1040823.44)		**CH-adduct [$AlMe_2(\kappa^2$-phbpamd)$AlMe_3$][b]** -1268007.468 (-1268056.831)	**TS-CH-phbamd** -1267974.267 (-1268023.06)		**8-π-$C_2N_2(sp^2)$−Al_2** -1242649.786 (-1242696.896)
NH tautomer [$AlMe_2(\kappa^2$-phbpamd)] [a] -1040778.791 (-1040823.433)		**NH-adduct [$AlMe_2(\kappa^2$-phbpamd)$AlMe_3$][c]** -1268018.598 (-1268068.767)	**TS-NH-phbamd** -1267992.01 (-1268040.428)		

[a] Data obtained from calculations presented in ref. 6 at the same level of theory B3LYP/6-31+G(d). [b] Hypothetical complex; [c] *Not isolated product.*

Input Coordinates.

$AlMe_3$

ZPE at 298 K: -227213.3084 kcal/mol
Gibbs Energy at 298 K: -227235.1897 kcal/mol

Atomic Number	*X*	*Y*	*Z*
13	0.000644000	0.000365000	-0.000319000
6	1.950175000	0.311720000	-0.001300000
1	2.442434000	-0.227065000	-0.823252000
1	2.222603000	1.370629000	-0.089237000
1	2.406706000	-0.066039000	0.925413000
6	-0.705038000	-1.843529000	-0.000994000
1	-1.261672000	-2.051212000	0.924744000
1	-1.417075000	-1.998932000	-0.824027000
1	0.075347000	-2.609238000	-0.090596000
6	-1.245376000	1.531736000	0.002515000
1	-1.216139000	2.057431000	-0.963587000
1	-2.288670000	1.243360000	0.181165000
1	-0.970474000	2.276757000	0.762206000

CH_4

ZPE at 298 K: -25397.51474 kcal/mol
Gibbs Energy at 298 K: -25409.20712 kcal/mol

Atomic Number	*X*	*Y*	*Z*
1	0.000000000	0.000000000	1.093438000
6	0.000000000	0.000000000	-0.000014000
1	0.000000000	1.031073000	-0.364452000
1	0.892936000	-0.515537000	-0.364452000
1	-0.892936000	-0.515537000	-0.364452000

[$AlMe_2(\kappa^2$-pbpamd)], 1-NH tautomer

ZPE at 298 K: -849495.2834 kcal/mol
Gibbs Energy at 298 K: -849533.7485 kcal/mol

Atomic Number	*X*	*Y*	*Z*
6	-1.822752000	-2.909255000	-0.050492000
6	-0.838828000	-3.563804000	-0.798902000
1	-0.862673000	-4.585629000	-1.149268000
6	0.173660000	-2.636995000	-1.026045000
6	-3.140623000	-3.439744000	0.419182000
1	-3.332074000	-3.171644000	1.462912000
1	-3.152631000	-4.529596000	0.334276000
1	-3.965004000	-3.039698000	-0.180479000
6	1.454593000	-2.773322000	-1.780218000
1	1.649594000	-1.885551000	-2.388638000
1	1.404547000	-3.651814000	-2.428407000
1	2.308984000	-2.889655000	-1.103203000
6	2.409659000	-1.139743000	1.151839000
6	3.784754000	-1.118002000	1.012870000
1	4.507207000	-1.547387000	1.693412000
6	4.040078000	-0.407892000	-0.186647000
6	1.530743000	-1.742883000	2.198065000
1	0.747954000	-1.044377000	2.510010000
1	2.125423000	-2.017948000	3.072888000
1	1.027847000	-2.646228000	1.829925000
6	5.362541000	-0.062141000	-0.800630000
1	5.213112000	0.460740000	-1.749431000
1	5.959543000	-0.961939000	-0.991000000
1	5.951663000	0.584908000	-0.139308000
6	0.539361000	-0.281157000	-0.261215000
6	-0.023700000	0.972644000	-0.412096000
6	-1.933784000	2.158932000	-1.345451000
1	-1.140225000	2.878009000	-1.566867000
6	-2.330789000	1.464721000	-2.658073000
1	-1.468895000	0.943468000	-3.089643000
1	-2.699777000	2.190060000	-3.394341000
1	-3.121159000	0.726104000	-2.477293000
6	1.120407000	2.914776000	0.631230000
6	2.290253000	3.837693000	0.281883000
1	3.178340000	3.260274000	-0.002194000
1	2.553785000	4.464152000	1.140707000
1	2.021296000	4.491046000	-0.556370000
1	1.432267000	2.264710000	1.467589000
6	-1.755294000	0.397310000	2.669571000
1	-0.710385000	0.733074000	2.719993000
1	-1.844119000	-0.480463000	3.326140000

1	-2.360238000	1.192727000	3.129050000
6	-4.273849000	-0.203681000	0.476802000
1	-4.845073000	0.685039000	0.777520000
1	-4.681712000	-1.037614000	1.063928000
1	-4.521474000	-0.400467000	-0.575510000
7	-1.425200000	-1.645949000	0.199294000
7	-0.203737000	-1.486546000	-0.406929000
7	2.901881000	-0.037189000	-0.772501000
7	1.906003000	-0.478470000	0.060933000
7	-1.377326000	1.155623000	-0.408415000
7	0.845283000	2.073554000	-0.563515000
1	1.732801000	1.738480000	-0.934945000
13	-2.334913000	0.036294000	0.807389000
6	-0.101976000	3.710602000	1.085713000
1	-0.457716000	4.364560000	0.281720000
1	-0.916773000	3.046332000	1.379517000
1	0.162590000	4.333044000	1.948383000
6	-3.118532000	2.924724000	-0.749100000
1	-3.426761000	3.724116000	-1.433150000
1	-3.983373000	2.272001000	-0.595896000
1	-2.856878000	3.381477000	0.210128000

[$AlMe_2(\kappa^2$-pbpamd)$AlMe_3$], 2

ZPE at 298 K: -1076740.064 kcal/mol
Gibbs Energy at 298 K: -1076784.618 kcal/mol

Atomic Number	*X*	*Y*	*Z*
13	3.018557000	0.226815000	-1.617684000
13	-3.093257000	0.110185000	0.334505000
7	-0.749561000	-1.536953000	-0.255419000
7	2.476404000	-0.492296000	0.284388000
7	1.213536000	-0.708537000	0.807371000
7	-2.098705000	-1.589605000	0.009103000
7	0.486553000	1.946535000	0.183050000
1	1.455827000	1.651024000	0.182453000
6	-0.422151000	0.913997000	-0.028407000
6	0.018514000	-0.396667000	0.117669000
6	-0.315050000	-2.749332000	-0.701443000
6	1.298467000	-1.263076000	2.050125000
6	3.342737000	-0.892342000	1.231869000
6	-1.421933000	-3.591436000	-0.724067000
1	-1.428217000	-4.627426000	-1.030295000
6	-2.514148000	-2.834745000	-0.294321000
6	2.643500000	-1.395392000	2.342627000
1	3.073647000	-1.795039000	3.249682000
6	0.234417000	2.963619000	1.221999000
6	0.571694000	2.416315000	2.616691000
1	-0.019357000	1.519857000	2.831701000
1	0.362797000	3.160053000	3.394214000
1	1.633568000	2.145951000	2.678147000
6	1.032699000	4.224391000	0.888453000
1	0.862897000	5.000797000	1.642351000
1	0.744307000	4.616295000	-0.092188000
1	2.107360000	4.005596000	0.861683000
7	-1.704109000	1.214230000	-0.372708000
6	1.397108000	0.342426000	-2.775970000
1	1.727467000	0.485156000	-3.817271000
1	0.784108000	1.213970000	-2.516862000
1	0.726739000	-0.526199000	-2.778417000
6	1.101485000	-3.064957000	-1.052163000
1	1.531430000	-2.308867000	-1.711200000
1	1.135096000	-4.030994000	-1.561872000
1	1.738243000	-3.126894000	-0.162416000
6	-4.750816000	-0.012840000	-0.746030000
1	-5.234653000	0.960211000	-0.902740000
1	-5.498828000	-0.648996000	-0.252469000
1	-4.574741000	-0.440507000	-1.742552000
6	0.081586000	-1.638274000	2.826266000
1	-0.667673000	-0.842075000	2.798330000

1	0.348025000	-1.842953000	3.865633000
1	-0.389827000	-2.535732000	2.407328000
6	4.332938000	-1.161116000	-2.207955000
1	4.088301000	-2.172777000	-1.851517000
1	5.366103000	-0.956090000	-1.896401000
1	4.344167000	-1.217617000	-3.306735000
6	3.756639000	2.023489000	-1.107675000
1	4.657085000	2.266976000	-1.690653000
1	4.043594000	2.111435000	-0.048873000
1	3.032993000	2.827220000	-1.302413000
6	4.828818000	-0.812636000	1.069071000
1	5.193203000	-1.609358000	0.413392000
1	5.312096000	-0.920883000	2.043956000
1	5.136180000	0.139427000	0.628989000
6	-3.947406000	-3.248874000	-0.178375000
1	-4.402729000	-2.870365000	0.742273000
1	-4.017758000	-4.339848000	-0.175051000
1	-4.538208000	-2.869895000	-1.018734000
6	-3.297408000	0.354420000	2.292215000
1	-2.362228000	0.645111000	2.790411000
1	-3.662076000	-0.551254000	2.798689000
1	-4.025127000	1.148808000	2.513445000
6	-1.951649000	2.420710000	-1.201624000
1	-1.018162000	2.988545000	-1.251661000
6	-2.319015000	2.001882000	-2.633323000
1	-1.526976000	1.379282000	-3.061066000
1	-2.448751000	2.885059000	-3.271343000
1	-3.253459000	1.431032000	-2.646829000
1	-0.832508000	3.193859000	1.188549000
6	-3.030375000	3.326621000	-0.592460000
1	-3.142779000	4.236787000	-1.192679000
1	-4.005170000	2.827215000	-0.568384000
1	-2.777633000	3.622391000	0.431200000

TS-pbpamd

ZPE at 298 K: -1076704.413 kcal/mol
Gibbs Energy at 298 K: -1076747.261 kcal/mol
Imaginary frequency: -1089.4887 cm^{-1}

Atomic Number	*X*	*Y*	*Z*
13	2.875907000	0.361728000	-1.316034000
13	-2.951113000	0.198558000	0.581783000
7	-0.833766000	-1.498947000	-0.426648000
7	2.468355000	-0.832324000	0.208181000
7	1.184963000	-0.993637000	0.703821000
7	-2.155804000	-1.536275000	-0.037541000
7	0.674070000	1.781664000	0.408419000
1	2.127084000	1.794358000	0.014975000
6	-0.283897000	0.898580000	0.076622000
6	0.042390000	-0.480226000	0.046909000
6	-0.522125000	-2.641577000	-1.098302000
6	1.210510000	-1.789753000	1.800836000
6	3.292010000	-1.512586000	1.038372000
6	-1.673377000	-3.422353000	-1.140807000
1	-1.772162000	-4.394272000	-1.602555000
6	-2.674092000	-2.691473000	-0.493979000
6	2.535036000	-2.142198000	2.029186000
1	2.911094000	-2.762572000	2.829849000
6	0.293202000	2.960791000	1.195349000
6	0.946274000	2.858330000	2.587125000
1	0.643606000	1.925880000	3.076234000
1	0.652686000	3.699656000	3.228297000
1	2.040753000	2.855744000	2.513202000
6	0.642572000	4.305289000	0.532277000
1	0.284073000	5.137314000	1.150874000
1	0.182980000	4.396827000	-0.455787000
1	1.723192000	4.434374000	0.408265000
7	-1.597313000	1.242734000	-0.222687000
6	1.488100000	0.736417000	-2.662818000
1	1.945980000	0.844883000	-3.655934000
1	0.978274000	1.675880000	-2.423180000
1	0.705779000	-0.025454000	-2.738736000
6	0.840014000	-2.950230000	-1.626429000
1	1.249487000	-2.107209000	-2.188723000
1	0.782309000	-3.815499000	-2.291638000
1	1.545293000	-3.185925000	-0.821162000
6	-4.768489000	0.280296000	-0.219121000
1	-5.217894000	1.278891000	-0.131368000
1	-5.454422000	-0.406590000	0.297059000
1	-4.795038000	0.014855000	-1.284651000
6	-0.035666000	-2.164095000	2.526215000

1	-0.678738000	-1.291578000	2.664804000
1	0.211727000	-2.592722000	3.500271000
1	-0.615029000	-2.902286000	1.958792000
6	4.647929000	-0.119435000	-2.051170000
1	5.509757000	0.060776000	-1.398812000
1	4.807741000	0.472254000	-2.964016000
1	4.691169000	-1.174029000	-2.359926000
6	3.370669000	2.146388000	-0.166149000
1	4.202661000	1.591355000	0.282932000
1	3.187295000	2.979417000	0.517126000
1	3.706396000	2.614397000	-1.102258000
6	4.781536000	-1.548088000	0.894943000
1	5.087502000	-1.979440000	-0.061968000
1	5.207045000	-2.153730000	1.699244000
1	5.218002000	-0.546087000	0.958368000
6	-4.117014000	-3.045053000	-0.312551000
1	-4.465298000	-2.804063000	0.696753000
1	-4.261229000	-4.115515000	-0.482784000
1	-4.750913000	-2.496950000	-1.017388000
6	-2.878202000	0.280292000	2.566998000
1	-1.891853000	0.593545000	2.937494000
1	-3.124167000	-0.670755000	3.061886000
1	-3.598164000	1.021274000	2.945481000
6	-1.805964000	2.369130000	-1.154711000
1	-0.836679000	2.852158000	-1.305964000
6	-2.267951000	1.845406000	-2.525523000
1	-1.545432000	1.120735000	-2.914228000
1	-2.358938000	2.665934000	-3.249290000
1	-3.242965000	1.352652000	-2.446259000
1	-0.791672000	2.944935000	1.350526000
6	-2.781506000	3.424071000	-0.615670000
1	-2.874892000	4.258375000	-1.321627000
1	-3.780868000	2.998568000	-0.473478000
1	-2.443125000	3.825887000	0.344154000

[$AlMe_2(\kappa^2$-tbpamd)$AlMe_3$], 3

ZPE at 298 K: -1076737.426 kcal/mol
Gibbs Energy at 298 K: -1076780.632 kcal/mol

Atomic Number	*X*	*Y*	*Z*
13	-2.962629000	-0.305959000	1.638027000
13	3.156151000	0.490079000	-0.171048000
7	0.987146000	-1.441729000	0.115370000
7	-2.328450000	-0.625323000	-0.344447000
7	-1.043985000	-0.674377000	-0.855404000
7	2.337709000	-1.325865000	-0.124116000
7	-0.573298000	1.956895000	0.186138000
1	-1.502988000	1.556345000	0.240104000
6	0.419692000	0.968755000	0.251148000
6	0.109290000	-0.337777000	-0.107513000
6	0.674679000	-2.742041000	0.382235000
6	-1.059388000	-1.096095000	-2.152153000
6	-3.141381000	-0.987412000	-1.353411000
6	1.861002000	-3.465449000	0.316162000
1	1.969321000	-4.527522000	0.481440000
6	2.874597000	-2.551880000	0.017078000
6	-2.383022000	-1.304554000	-2.493169000
1	-2.761816000	-1.634767000	-3.449644000
6	-0.576979000	3.017739000	-0.872521000
6	0.729013000	3.822112000	-0.896512000
1	1.591312000	3.186964000	-1.109882000
1	0.898282000	4.331999000	0.055300000
1	0.662927000	4.583113000	-1.681838000
6	-0.812826000	2.376776000	-2.254908000
1	0.011150000	1.702991000	-2.510362000
1	-0.877041000	3.143622000	-3.035444000
1	-1.743540000	1.798123000	-2.265142000
6	-1.747467000	3.949152000	-0.522926000
1	-1.826566000	4.753967000	-1.261834000
1	-1.600463000	4.394876000	0.466267000
1	-2.698950000	3.405074000	-0.511659000
7	1.664248000	1.294701000	0.688441000
6	-1.364192000	-0.170976000	2.825088000
1	-1.709047000	-0.228865000	3.869816000
1	-0.870210000	0.801542000	2.710938000
1	-0.586068000	-0.935847000	2.709897000
6	-0.704831000	-3.241733000	0.658297000
1	-1.209186000	-2.634945000	1.412120000
1	-0.644593000	-4.270034000	1.023096000
1	-1.329358000	-3.235791000	-0.242094000
6	4.800843000	0.482765000	0.929492000
1	5.041886000	1.496104000	1.282156000

1	5.676046000	0.134954000	0.363734000
1	4.722007000	-0.148870000	1.824380000
6	0.196243000	-1.288097000	-2.933236000
1	0.899298000	-0.468269000	-2.763321000
1	-0.031160000	-1.349361000	-3.999926000
1	0.704568000	-2.213537000	-2.635196000
6	-4.089320000	-1.927560000	1.956502000
1	-3.741850000	-2.817386000	1.411437000
1	-5.146171000	-1.786726000	1.691664000
1	-4.068749000	-2.193223000	3.023971000
6	-3.928874000	1.441001000	1.450013000
1	-4.795345000	1.477563000	2.127229000
1	-4.318191000	1.649129000	0.442798000
1	-3.291563000	2.294533000	1.719815000
6	-4.631160000	-1.057779000	-1.222895000
1	-4.936032000	-1.982128000	-0.722109000
1	-5.088277000	-1.040179000	-2.216210000
1	-5.026852000	-0.222950000	-0.640139000
6	4.346041000	-2.787805000	-0.119054000
1	4.754610000	-2.273296000	-0.995031000
1	4.544014000	-3.857658000	-0.223745000
1	4.887449000	-2.422142000	0.759904000
6	3.338682000	1.040613000	-2.068513000
1	2.379736000	1.203822000	-2.578420000
1	3.893852000	0.300792000	-2.663999000
1	3.895796000	1.985295000	-2.152083000
6	1.814277000	2.317467000	1.738849000
1	0.887475000	2.889136000	1.824087000
1	2.602473000	3.023842000	1.447802000
6	2.151982000	1.685952000	3.093613000
1	1.355017000	1.000710000	3.400316000
1	2.256803000	2.462728000	3.861695000
1	3.089221000	1.123539000	3.045509000

TS-tbpamd

ZPE at 298 K: -1076699.252 kcal/mol
Gibbs Energy at 298 K: -1076742.619 kcal/mol
Imaginary frequency: –845.7243 cm^{-1}

Atomic Number	*X*	*Y*	*Z*
13	2.630375000	-0.512341000	-1.532107000
13	-3.112614000	0.793532000	0.142749000
7	-1.194812000	-1.394979000	-0.245141000
7	2.183507000	-1.050008000	0.314081000
7	0.891296000	-0.977528000	0.802505000
7	-2.526282000	-1.096689000	-0.064510000
7	0.883657000	1.656769000	0.063090000
1	2.143381000	1.397595000	-0.808450000
6	-0.263293000	0.968433000	-0.112755000
6	-0.177105000	-0.439998000	0.051253000
6	-1.064175000	-2.716265000	-0.558132000
6	0.849524000	-1.430335000	2.077290000
6	2.949723000	-1.529542000	1.320974000
6	-2.345116000	-3.263653000	-0.580079000
1	-2.594949000	-4.291987000	-0.798218000
6	-3.228755000	-2.225062000	-0.292117000
6	2.141827000	-1.802388000	2.428524000
1	2.467759000	-2.197837000	3.379703000
6	1.028931000	2.765551000	1.027406000
6	2.184977000	2.346109000	1.972912000
1	1.919903000	1.427763000	2.508744000
1	2.411780000	3.129228000	2.709081000
1	3.096228000	2.145835000	1.398341000
6	1.436889000	4.096301000	0.351929000
1	1.521482000	4.897966000	1.096280000
1	0.709381000	4.410043000	-0.401409000
1	2.411106000	4.005828000	-0.138688000
7	-1.479595000	1.507141000	-0.467857000
6	1.259804000	-0.664246000	-2.939328000
1	1.529534000	0.020883000	-3.756791000
1	0.244571000	-0.408897000	-2.627431000
1	1.234477000	-1.669624000	-3.381680000
6	0.235403000	-3.413962000	-0.791513000
1	0.852190000	-2.879651000	-1.516537000
1	0.035280000	-4.414322000	-1.183862000
1	0.819399000	-3.521415000	0.129866000
6	-4.595756000	1.128017000	-1.134999000
1	-4.808105000	2.201701000	-1.242809000
1	-5.539556000	0.663253000	-0.818427000
1	-4.370416000	0.751122000	-2.142804000
6	-0.427770000	-1.461434000	2.843239000

1	-0.969325000	-0.518541000	2.718882000
1	-0.230171000	-1.630160000	3.904187000
1	-1.087113000	-2.259268000	2.480389000
6	4.395923000	-1.280334000	-1.981247000
1	5.248090000	-0.863734000	-1.431741000
1	4.583873000	-1.094367000	-3.048854000
1	4.427275000	-2.370749000	-1.848846000
6	3.189507000	1.632110000	-1.483646000
1	4.078383000	1.679273000	-0.847427000
1	2.849817000	2.652156000	-1.682802000
1	3.487099000	1.267733000	-2.477523000
6	4.434836000	-1.693194000	1.238739000
1	4.723764000	-2.449176000	0.503453000
1	4.818409000	-1.998880000	2.215574000
1	4.923743000	-0.755447000	0.957313000
6	-4.724570000	-2.247190000	-0.246647000
1	-5.107525000	-1.746077000	0.648981000
1	-5.080861000	-3.280792000	-0.241348000
1	-5.154457000	-1.739340000	-1.116634000
6	-3.535570000	1.064786000	2.065064000
1	-3.924822000	2.077621000	2.246133000
1	-2.672029000	0.943446000	2.732484000
1	-4.310861000	0.367120000	2.416658000
6	-1.480745000	2.732117000	-1.278592000
1	-1.005187000	3.568438000	-0.758012000
6	-0.824013000	2.543677000	-2.649623000
1	0.229395000	2.272972000	-2.533807000
1	-0.883032000	3.467470000	-3.238880000
1	-1.323144000	1.742705000	-3.206378000
1	-2.527163000	3.023161000	-1.423518000
6	-0.214072000	2.997937000	1.910384000
1	-1.070736000	3.374942000	1.348555000
1	-0.521633000	2.064214000	2.393219000
1	0.021061000	3.724761000	2.697305000

[$AlMe_2$(tbpamd$^-$)$AlMe_2$], 6-π-C_2N_2(sp^2)−Al_2

ZPE at 298 K: -1051360.793 kcal/mol
Gibbs Energy at 298 K: -1051401.734 kcal/mol

Atomic Number	*X*	*Y*	*Z*
13	-2.705667000	1.097148000	-0.686792000
13	2.405465000	0.327647000	1.215315000
7	-2.567719000	-0.794024000	-0.050879000
7	-1.321297000	-1.208279000	0.350053000
7	2.125098000	-1.317243000	0.078429000
7	0.890402000	-1.323133000	-0.524094000
7	-1.132987000	1.651994000	0.225546000
7	1.282080000	1.398113000	0.103129000
6	-3.453065000	-1.698186000	0.409404000
6	-2.766164000	-2.713783000	1.081817000
1	-3.194459000	-3.585038000	1.556092000
6	-1.416434000	-2.373664000	1.047452000
6	-4.925839000	-1.531094000	0.202388000
1	-5.327280000	-0.737618000	0.841886000
1	-5.445772000	-2.462162000	0.442749000
1	-5.155698000	-1.263986000	-0.834415000
6	-0.234680000	-3.083563000	1.621030000
1	0.344356000	-3.599983000	0.845983000
1	-0.574486000	-3.827921000	2.345373000
1	0.440068000	-2.384530000	2.121841000
6	0.855840000	-2.237270000	-1.529330000
6	2.110226000	-2.837546000	-1.568371000
1	2.431980000	-3.614236000	-2.247136000
6	2.878935000	-2.221095000	-0.569718000
6	-0.375062000	-2.469428000	-2.338971000
1	-0.127852000	-3.024233000	-3.247077000
1	-0.843153000	-1.519194000	-2.615196000
1	-1.119900000	-3.044985000	-1.775444000
6	4.318176000	-2.441065000	-0.224927000
1	4.933580000	-1.596369000	-0.552603000
1	4.687245000	-3.346304000	-0.714017000
1	4.457808000	-2.546335000	0.855442000
6	-0.153651000	-0.494885000	-0.041454000
6	-0.006905000	0.895336000	0.082061000
6	-1.080680000	2.849926000	1.074332000
1	-1.708670000	3.631509000	0.628727000
1	-0.060228000	3.238902000	1.110136000
6	-1.558126000	2.555247000	2.500834000
1	-2.583695000	2.171440000	2.498453000
1	-1.531689000	3.463828000	3.115863000
1	-0.912092000	1.803965000	2.967546000
6	1.752266000	2.382556000	-0.922160000

6	0.627352000	3.062634000	-1.725896000
1	-0.011995000	2.332464000	-2.227669000
1	1.085532000	3.694109000	-2.496001000
1	-0.005180000	3.701717000	-1.107457000
6	2.595074000	3.469385000	-0.231237000
1	1.988396000	4.027859000	0.489843000
1	2.990529000	4.178955000	-0.967868000
1	3.444673000	3.034393000	0.303172000
6	2.627265000	1.607675000	-1.937600000
1	3.470629000	1.118862000	-1.442093000
1	3.029331000	2.277265000	-2.708208000
1	2.029892000	0.832274000	-2.431116000
6	-2.512756000	1.049275000	-2.659473000
1	-2.596573000	2.052710000	-3.100900000
1	-3.291619000	0.433269000	-3.132887000
1	-1.544907000	0.645296000	-2.986738000
6	-4.341996000	1.911629000	0.075354000
1	-4.519771000	1.625122000	1.120605000
1	-5.246572000	1.648045000	-0.489652000
1	-4.275720000	3.009329000	0.060197000
6	1.569998000	-0.001502000	2.984434000
1	1.740550000	0.850949000	3.658386000
1	1.990429000	-0.883135000	3.490940000
1	0.483383000	-0.147360000	2.931318000
6	4.357421000	0.682407000	1.270149000
1	4.853661000	0.830876000	0.302690000
1	4.876613000	-0.148936000	1.769033000
1	4.569084000	1.576907000	1.873395000

[$AlMe_2(\kappa^2$-phbpamd)$AlMe_3$], CH-adduct (Hypothetical**)**

ZPE at 298 K: -1268007.468 kcal/mol
Gibbs Energy at 298 K: -1268056.831 kcal/mol

Atomic Number	*X*	*Y*	*Z*
13	-1.646475000	-2.172527000	0.276172000
7	2.084849000	-1.536364000	-0.993676000
7	1.015571000	-0.666093000	-1.118624000
7	0.017205000	-1.882314000	1.383627000
7	0.656045000	-0.674171000	1.276290000
7	-1.823429000	-0.282269000	-0.126776000
7	-1.084139000	1.948984000	-0.109434000
6	0.479504000	-0.737266000	-2.379981000
6	1.188281000	-1.717515000	-3.049060000
1	1.000188000	-2.055717000	-4.057634000
6	2.142658000	-2.214492000	-2.154883000
6	-0.652172000	0.058958000	-2.949639000
1	-1.617693000	-0.342630000	-2.637290000
1	-0.589025000	0.002930000	-4.039266000
1	-0.631543000	1.108706000	-2.655869000
6	3.062346000	-3.373163000	-2.379991000
1	3.469242000	-3.749554000	-1.440317000
1	3.898957000	-3.104967000	-3.031029000
1	2.501160000	-4.179131000	-2.864531000
6	1.166959000	-0.282818000	2.476503000
6	0.900283000	-1.310918000	3.366928000
1	1.206231000	-1.352307000	4.401735000
6	0.197625000	-2.290301000	2.654322000
6	1.867237000	1.013612000	2.714974000
1	1.294917000	1.867120000	2.334755000
1	2.849393000	1.024014000	2.236721000
1	2.007704000	1.146523000	3.790055000
6	-0.316692000	-3.604451000	3.149380000
1	-0.446341000	-4.315963000	2.330000000
1	-1.283236000	-3.483059000	3.648912000
1	0.387908000	-4.029333000	3.870110000
6	0.576170000	0.115063000	0.051697000
1	1.269886000	0.938917000	0.190507000
6	-0.857169000	0.677694000	-0.091599000
6	-1.278603000	-3.378662000	-1.245124000
1	-1.620911000	-2.976722000	-2.207994000
1	-1.793739000	-4.338512000	-1.100738000
1	-0.210376000	-3.597539000	-1.361216000
6	-3.084003000	-2.670955000	1.536814000
1	-3.033069000	-3.718356000	1.861871000

1	-3.089706000	-2.044970000	2.439690000
1	-4.062593000	-2.535084000	1.057656000
6	-0.085302000	2.929116000	-0.090343000
6	0.917808000	3.053445000	-1.068665000
6	-0.118884000	3.890807000	0.938635000
6	1.861685000	4.078646000	-0.998523000
6	0.833821000	4.903053000	1.002483000
6	1.843859000	5.020532000	0.035195000
1	0.971189000	2.335798000	-1.881738000
1	-0.900555000	3.817300000	1.689625000
1	2.635432000	4.134349000	-1.760721000
1	0.792509000	5.620132000	1.819856000
6	-3.193557000	0.117210000	-0.249141000
6	-3.993770000	-0.499354000	-1.218806000
6	-3.795418000	1.031344000	0.629935000
6	-5.356959000	-0.207763000	-1.312519000
6	-5.151594000	1.319855000	0.523872000
6	-5.959953000	0.710803000	-0.449456000
1	-3.552079000	-1.222127000	-1.900491000
1	-3.191164000	1.510612000	1.390631000
1	-5.955329000	-0.704663000	-2.072711000
1	-5.598224000	2.029548000	1.217317000
6	2.854888000	6.141445000	0.092100000
1	3.802181000	5.850108000	-0.374413000
1	2.492617000	7.033900000	-0.436005000
1	3.064286000	6.439948000	1.125302000
6	-7.425777000	1.057499000	-0.563606000
1	-7.967731000	0.320289000	-1.165039000
1	-7.903204000	1.106940000	0.422033000
1	-7.566213000	2.037660000	-1.038415000
13	3.927827000	-0.952972000	-0.066616000
6	3.851661000	1.030734000	-0.330508000
1	3.639139000	1.237480000	-1.390494000
1	4.870875000	1.409127000	-0.154296000
1	3.188382000	1.686560000	0.241747000
6	5.406164000	-1.599388000	-1.242095000
1	5.623300000	-2.674226000	-1.204763000
1	6.316806000	-1.089676000	-0.887512000
1	5.299669000	-1.321730000	-2.300253000
6	3.930995000	-1.834580000	1.723260000
1	4.833510000	-2.456217000	1.814883000
1	3.071466000	-2.504033000	1.858152000
1	3.932961000	-1.153484000	2.584164000

[$AlMe_2(\kappa^2$-phbpamd)$AlMe_3$], NH-adduct (not isolated**)**

ZPE at 298 K: -1268018.598 kcal/mol
Gibbs Energy at 298 K: -1268068.767 kcal/mol

Atomic Number	*X*	*Y*	*Z*
13	2.119176000	-2.062783000	2.053798000
13	-0.344721000	2.948080000	-0.606395000
7	2.161525000	1.423030000	-0.176097000
7	2.401963000	-1.941286000	-0.030158000
7	2.081008000	-0.869555000	-0.845286000
7	1.606128000	2.668426000	-0.347649000
7	-0.561651000	-1.103628000	-0.293888000
1	-0.035466000	-1.892007000	0.054490000
6	0.007750000	0.157916000	-0.165572000
6	1.375240000	0.251714000	-0.372494000
6	3.501235000	1.541430000	0.065295000
6	2.417493000	-1.128809000	-2.139484000
6	2.942025000	-2.867525000	-0.837968000
6	3.790165000	2.902576000	0.056450000
1	4.762965000	3.343969000	0.216445000
6	2.593511000	3.572635000	-0.188866000
6	2.984413000	-2.388737000	-2.161763000
1	3.363144000	-2.915363000	-3.025765000
7	-0.785926000	1.232380000	0.111067000
6	1.910718000	-0.231472000	2.822129000
1	1.648944000	-0.362154000	3.884895000
1	1.127176000	0.399375000	2.388405000
1	2.833164000	0.364896000	2.815545000
6	4.468714000	0.419140000	0.268006000
1	4.171022000	-0.238206000	1.086194000
1	5.444334000	0.847141000	0.511614000
1	4.583245000	-0.196610000	-0.630165000
6	-0.933585000	4.414540000	0.576087000
1	-2.013212000	4.353262000	0.765355000
1	-0.738812000	5.412692000	0.161899000
1	-0.442503000	4.365350000	1.557724000
6	2.134839000	-0.143784000	-3.222624000
1	1.065124000	0.090348000	-3.257255000
1	2.439390000	-0.549945000	-4.189536000
1	2.669053000	0.798271000	-3.054173000
6	3.821188000	-2.916387000	2.658914000
1	4.710245000	-2.539971000	2.130946000
1	3.840630000	-4.010945000	2.575795000
1	3.977280000	-2.681492000	3.722712000
6	0.480020000	-3.217693000	2.141257000
1	0.508488000	-3.821669000	3.060503000
1	0.391891000	-3.937632000	1.312517000

1	-0.461300000	-2.651749000	2.178570000
6	3.407628000	-4.203321000	-0.349514000
1	4.360123000	-4.118950000	0.181842000
1	3.543313000	-4.878690000	-1.198424000
1	2.685384000	-4.647701000	0.340847000
6	2.340689000	5.045183000	-0.272152000
1	1.759629000	5.304943000	-1.163610000
1	3.291976000	5.581708000	-0.314642000
1	1.782826000	5.401006000	0.600201000
6	-0.667672000	3.038041000	-2.558657000
1	-0.275074000	2.158979000	-3.089371000
1	-0.202317000	3.920154000	-3.021786000
1	-1.740729000	3.094387000	-2.792454000
6	-1.799990000	-1.400221000	-0.891878000
6	-2.467438000	-2.573511000	-0.516317000
6	-2.363456000	-0.583526000	-1.882149000
6	-3.674066000	-2.917355000	-1.120980000
6	-3.580491000	-0.933287000	-2.461379000
6	-4.262246000	-2.101469000	-2.096239000
1	-2.038575000	-3.207952000	0.255287000
1	-1.853909000	0.323841000	-2.188056000
1	-4.174689000	-3.834031000	-0.817002000
1	-4.005383000	-0.283481000	-3.223597000
6	-1.971263000	1.035447000	0.876822000
6	-1.965569000	0.275071000	2.056738000
6	-3.170707000	1.637690000	0.478004000
6	-3.132347000	0.115794000	2.797976000
6	-4.329728000	1.487843000	1.239188000
6	-4.337515000	0.717480000	2.406820000
1	-1.042196000	-0.187190000	2.388985000
1	-3.204392000	2.204271000	-0.448793000
1	-3.103302000	-0.480542000	3.707615000
1	-5.247956000	1.966489000	0.906115000
6	-5.598269000	-2.451078000	-2.708724000
1	-5.758855000	-3.534611000	-2.732190000
1	-6.426607000	-2.012602000	-2.135685000
1	-5.680252000	-2.075055000	-3.734696000
6	-5.602816000	0.511937000	3.206344000
1	-5.401896000	0.517759000	4.283863000
1	-6.342510000	1.291866000	2.996312000
1	-6.069459000	-0.454166000	2.970757000

TS-phbpamd-CH

ZPE at 298 K: -1267974.267 kcal/mol
Gibbs Energy at 298 K: -1268023.06 kcal/mol
Imaginary frequency: −1158.4742 cm^{-1}

Atomic Number	*X*	*Y*	*Z*
13	2.831813000	-1.613439000	0.359356000
7	-2.560846000	-0.967964000	0.663790000
7	-1.205536000	-0.882557000	0.902676000
7	1.055806000	-2.663282000	0.257674000
7	0.295894000	-1.917692000	-0.641253000
7	2.028148000	0.080842000	0.054491000
7	0.393439000	1.681135000	0.309589000
6	-0.978639000	-1.000197000	2.241199000
6	-2.210801000	-1.179264000	2.856957000
1	-2.384669000	-1.303156000	3.915960000
6	-3.172843000	-1.157137000	1.846408000
6	0.354957000	-0.916517000	2.900823000
1	0.953106000	-1.803927000	2.687423000
1	0.211099000	-0.844216000	3.981801000
1	0.916837000	-0.042313000	2.563591000
6	-4.658240000	-1.290376000	1.979264000
1	-5.064722000	-2.024612000	1.275508000
1	-5.157892000	-0.334985000	1.789620000
1	-4.909741000	-1.614811000	2.992101000
6	0.076501000	-2.646155000	-1.769235000
6	0.612221000	-3.912638000	-1.559488000
1	0.610633000	-4.729990000	-2.266312000
6	1.212401000	-3.883976000	-0.298260000
6	-0.477775000	-2.107573000	-3.047381000
1	-1.559002000	-1.985641000	-3.031051000
1	-0.232575000	-2.802687000	-3.854394000
1	-0.024756000	-1.140035000	-3.278388000
6	2.020628000	-4.945201000	0.379193000
1	1.584351000	-5.931690000	0.196074000
1	2.066770000	-4.773128000	1.457438000
1	3.045901000	-4.955729000	-0.009197000
6	-0.299862000	-0.652001000	-0.219379000
1	-1.382347000	-0.119585000	-1.322156000
6	0.698607000	0.442675000	0.071105000
6	3.682000000	-1.930102000	2.120280000
1	3.625074000	-2.988466000	2.414002000
1	3.260093000	-1.345424000	2.946796000
1	4.751039000	-1.680488000	2.067552000
6	3.840124000	-2.183367000	-1.244621000
1	4.403571000	-3.116549000	-1.106673000
1	3.180466000	-2.327170000	-2.111331000

1	4.570082000	-1.411630000	-1.526522000
6	-0.849215000	2.300812000	0.249339000
6	-1.869482000	2.127435000	1.205629000
6	-1.057682000	3.288768000	-0.736411000
6	-3.058027000	2.851407000	1.128206000
6	-2.254084000	3.996993000	-0.811760000
6	-3.290009000	3.783684000	0.109033000
1	-1.721845000	1.434155000	2.025226000
1	-0.260233000	3.474255000	-1.450974000
1	-3.826513000	2.682186000	1.881067000
1	-2.385643000	4.734487000	-1.601613000
6	2.981551000	1.145395000	-0.032136000
6	3.807780000	1.469176000	1.047827000
6	3.161561000	1.835867000	-1.241923000
6	4.795707000	2.451435000	0.918478000
6	4.135399000	2.820172000	-1.358589000
6	4.975466000	3.145703000	-0.279942000
1	3.670626000	0.956529000	1.995211000
1	2.523548000	1.585247000	-2.084855000
1	5.429504000	2.682812000	1.771886000
1	4.257906000	3.342280000	-2.305756000
6	-4.611514000	4.506611000	-0.003443000
1	-5.358593000	3.890646000	-0.523541000
1	-5.024595000	4.747471000	0.983083000
1	-4.512798000	5.442347000	-0.564512000
6	6.029718000	4.218747000	-0.424369000
1	6.688704000	4.020300000	-1.278893000
1	5.575781000	5.204040000	-0.592431000
1	6.655450000	4.290501000	0.471228000
13	-3.425354000	-0.726570000	-1.077288000
6	-2.095903000	0.545087000	-2.218352000
1	-1.131997000	0.861549000	-2.629972000
1	-2.633436000	0.122459000	-3.081625000
1	-2.581132000	1.461337000	-1.875682000
6	-5.005399000	0.440381000	-0.938147000
1	-5.896297000	-0.093425000	-0.583736000
1	-5.255360000	0.854659000	-1.925213000
1	-4.831367000	1.292795000	-0.271320000
6	-3.655428000	-2.539070000	-1.828462000
1	-4.547359000	-2.977576000	-1.355667000
1	-2.824733000	-3.224413000	-1.619954000
1	-3.843515000	-2.562302000	-2.910515000

TS-phbpamd-NH

ZPE at 298 K: -1267992.01 kcal/mol
Gibbs Energy at 298 K: -1268040.428 kcal/mol
Imaginary frequency: −1237.8272 cm^{-1}

Atomic Number	*X*	*Y*	*Z*
13	1.911238000	-2.595074000	1.458656000
13	-0.428123000	2.824507000	-0.653369000
7	2.011699000	1.570173000	0.335215000
7	2.750348000	-1.767359000	-0.142543000
7	2.351354000	-0.552019000	-0.680506000
7	1.485512000	2.770081000	-0.092254000
7	-0.377235000	-1.202573000	-0.204635000
1	0.208083000	-2.447420000	0.261456000
6	0.052565000	0.065780000	-0.039011000
6	1.438247000	0.325758000	-0.050047000
6	3.194471000	1.789344000	0.972491000
6	3.041596000	-0.303146000	-1.822464000
6	3.671848000	-2.277326000	-0.991629000
6	3.427394000	3.161328000	0.948669000
1	4.279505000	3.673698000	1.371353000
6	2.331816000	3.740162000	0.303113000
6	3.895492000	-1.376058000	-2.035632000
1	4.580198000	-1.504804000	-2.861297000
7	-0.811714000	1.132713000	0.131713000
6	3.074986000	-4.032043000	2.158006000
1	2.640881000	-4.375859000	3.108481000
1	4.085465000	-3.672097000	2.398646000
1	3.188644000	-4.916611000	1.521399000
6	4.037646000	0.698256000	1.543294000
1	3.434699000	0.006821000	2.137457000
1	4.806613000	1.133508000	2.186368000
1	4.537293000	0.116339000	0.760219000
6	-1.293147000	4.308320000	0.328599000
1	-2.383078000	4.175485000	0.350137000
1	-1.102243000	5.293222000	-0.119235000
1	-0.964721000	4.356814000	1.376249000
6	2.837201000	0.947663000	-2.605624000
1	1.772045000	1.172150000	-2.706458000
1	3.281202000	0.844512000	-3.598433000
1	3.299924000	1.807238000	-2.106252000
6	0.379615000	-3.748385000	0.469355000
1	0.176762000	-4.243434000	1.429118000
1	1.136672000	-4.318051000	-0.081914000
1	-0.546586000	-3.866471000	-0.105551000
6	1.233633000	-1.385671000	2.858420000
1	1.951255000	-1.332619000	3.689667000

1	0.305193000	-1.799711000	3.277246000
1	1.016048000	-0.364314000	2.538726000
6	4.315436000	-3.618678000	-0.824773000
1	4.871577000	-3.691935000	0.113428000
1	5.008885000	-3.789615000	-1.652170000
1	3.574448000	-4.424467000	-0.832044000
6	2.037205000	5.188888000	0.070559000
1	1.662283000	5.364714000	-0.943091000
1	2.945539000	5.781131000	0.210094000
1	1.277556000	5.553669000	0.770037000
6	-0.513067000	2.847929000	-2.636056000
1	-0.304422000	1.874093000	-3.099415000
1	0.188704000	3.569622000	-3.079814000
1	-1.517199000	3.141192000	-2.975532000
6	-2.062783000	0.906559000	0.771859000
6	-2.129651000	0.326413000	2.046529000
6	-3.261708000	1.288435000	0.154179000
6	-3.359099000	0.113390000	2.665710000
6	-4.486186000	1.088036000	0.788373000
6	-4.561476000	0.491054000	2.052813000
1	-1.210250000	0.028753000	2.538892000
1	-3.234341000	1.695102000	-0.852955000
1	-3.384522000	-0.350122000	3.650318000
1	-5.402088000	1.381054000	0.279152000
6	-1.626055000	-1.435028000	-0.814073000
6	-1.917984000	-0.924512000	-2.092182000
6	-2.595945000	-2.235394000	-0.190163000
6	-3.144085000	-1.177677000	-2.699190000
6	-3.815226000	-2.497799000	-0.814014000
6	-4.120081000	-1.966970000	-2.072703000
1	-1.171773000	-0.316273000	-2.595273000
1	-2.406303000	-2.604767000	0.813064000
1	-3.347467000	-0.759182000	-3.683449000
1	-4.553823000	-3.109198000	-0.299189000
6	-5.465780000	-2.202018000	-2.718647000
1	-6.170601000	-1.394196000	-2.477663000
1	-5.386515000	-2.244766000	-3.811043000
1	-5.918548000	-3.139219000	-2.376312000
6	-5.890776000	0.285397000	2.741254000
1	-6.688793000	0.081193000	2.018326000
1	-5.852214000	-0.552507000	3.446276000
1	-6.190850000	1.175547000	3.311229000

[$AlMe_2(\kappa^2$-tbpamd)], NH-tautomer

ZPE at 298 K: -849498.1015 kcal/mol
Gibbs Energy at 298 K: -849537.0768 kcal/mol
(See reference 6 for more details)

[$AlMe_2(\kappa^2$-phbpamd)], CH-tautomer

ZPE at 298 K: -1040778.372 kcal/mol
Gibbs Energy at 298 K: -1040823.44 kcal/mol
(See reference 6 for more details)

[$AlMe_2(\kappa^2$-phbpamd)], NH-tautomer

ZPE at 298 K: -1040778.791 kcal/mol
Gibbs Energy at 298 K: -1040823.433 kcal/mol
(See reference 6 for more details)

[$AlMe_2$(pbpamd$^-$)$AlMe_2$], 4-π-$C_2N_2(sp^2)$−Al_2
(See section 1.2)

[$AlMe_2$(phbpamd$^-$)$AlMe_2$], 8-π-$C_2N_2(sp^2)$−Al_2
(See section 1.2)

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