

Supporting information
belonging to the manuscript

"Lewis Acid-Base Complexes of AlH_3 : Prediction of Structure and Stoichiometry"

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S1: DFT-calculated symmetries and ΔH_c for AlH_3 complexes.

Ligand	1:1 Monomer		1:1 Dimer		1:2	
	Highest Symmetry	ΔH_c	Highest Symmetry	ΔH_c	Highest Symmetry	ΔH_c
BDMA	C_1	---	C_1	-90.15	C_2	-123.47
DIOX	C_s	-84.44	---	---	C_{2v}	-116.82
Et_2O	C_1	-71.52	C_2	-52.14	C_2	-77.76
TEA	C_3	-89.05	C_2	-62.25	D_3	-90.29
DMEA	C_1	-102.2	C_2	-96.28	C_2	-128.10
TMA	C_{3v}	-108.13	C_{2h}	-112.58	C_{2v}	-145.90
QUIN	C_{3v}	-118.37	---	---	C_1	-156.04
TMEDA	C_1	-101.15	---	---	C_1	-125.57
TMPDA	C_i	-104.67	---	---	C_2	-136.47

$$\Delta H_c = (-1) [((E_{(\text{AlH}_3)} + E_{(\text{Lig})}) - (E_{(\text{comp})})) \times 627.5095 \times 4.184]$$

Where:

E = Lowest calculated optimized energy of formation + Zero point energy correction;

1 Hartree = 627.5095 kcal mol⁻¹; 1 Calorie = 4.184 Joules.

S2: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (D_3H symmetry) for AlH_3 .

13	0.000000000	0.000000000	0.000000000
1	0.000000000	1.583258000	0.000000000
1	1.371141000	-0.791629000	0.000000000
1	-1.371141000	-0.791629000	0.000000000

S3: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (D_2H symmetry) for AlH_3 (dimer).

13	-1.309152000	0.000000000	0.000000000
1	-1.999944000	1.415149000	0.000000000
1	0.000000000	0.000000000	1.145984000
1	-1.999944000	-1.415149000	0.000000000
13	1.309152000	0.000000000	0.000000000
1	1.999944000	1.415149000	0.000000000
1	1.999944000	-1.415149000	0.000000000
1	0.000000000	0.000000000	-1.145984000

S4: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_3 symmetry) for TEA (ligand).

7	0.000000000	0.000000000	0.027879000
6	0.329793000	1.366441000	0.449534000
1	1.415471000	1.479120000	0.409047000
1	0.043296000	1.536658000	1.504296000
6	-0.296721000	2.437857000	-0.443452000
1	0.030463000	2.305798000	-1.477323000
1	-1.388904000	2.398586000	-0.430118000
1	0.000000000	3.435910000	-0.107448000
6	1.018476000	-0.968829000	0.449534000
1	1.309137000	-0.805825000	1.504296000
1	0.573220000	-1.965394000	0.409047000
6	2.259606000	-0.961960000	-0.443452000
1	1.981648000	-1.179281000	-1.477323000
1	2.771688000	0.003533000	-0.430118000

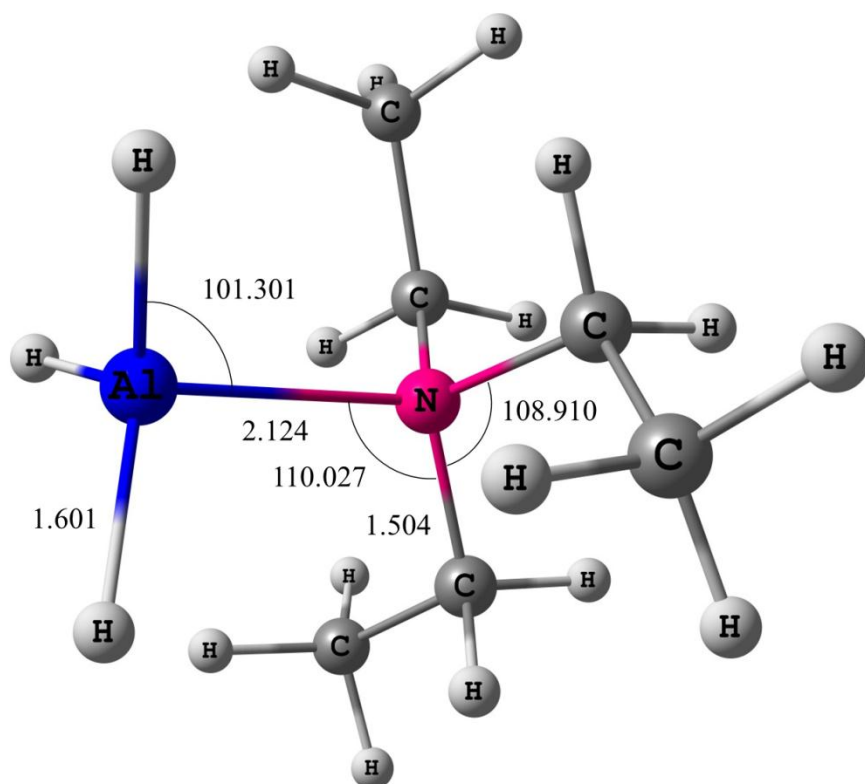
1	2.975586000	-1.717955000	-0.107448000
6	-1.348269000	-0.397612000	0.449534000
1	-1.988691000	0.486274000	0.409047000
1	-1.352433000	-0.730833000	1.504296000
6	-1.962885000	-1.475896000	-0.443452000
1	-2.012111000	-1.126517000	-1.477323000
1	-1.382784000	-2.402119000	-0.430118000
1	-2.975586000	-1.717955000	-0.107448000

S5: DFT Calculated Cartesian coordinates and Geometrical parameters for AlH₃·TEA (1:1).

- Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_3 symmetry):

13	0.000000000	0.000000000	1.883481000
1	-0.022921000	-1.570271000	2.197320000
1	1.371355000	0.765285000	2.197320000
1	-1.348434000	0.804986000	2.197320000
7	0.000000000	0.000000000	-0.240401000
6	-0.668928000	1.244896000	-0.755536000
1	-1.681237000	1.243412000	-0.356467000
1	-0.737623000	1.162463000	-1.849376000
6	0.000000000	2.561933000	-0.370722000
1	0.128450000	2.648626000	0.709435000
1	0.970180000	2.703975000	-0.849028000
1	-0.647282000	3.380669000	-0.695152000
6	-0.743647000	-1.201756000	-0.755536000
1	-0.637911000	-1.220031000	-1.849376000
1	-0.236208000	-2.077699000	-0.356467000
6	-2.218699000	-1.280966000	-0.370722000
1	-2.358002000	-1.213072000	0.709435000
1	-2.826801000	-0.511787000	-0.849028000
1	-2.604105000	-2.250898000	-0.695152000
6	1.412575000	-0.043139000	-0.755536000
1	1.917444000	0.834288000	-0.356467000
1	1.375533000	0.057569000	-1.849376000
6	2.218699000	-1.280966000	-0.370722000
1	2.229552000	-1.435554000	0.709435000
1	1.856621000	-2.192188000	-0.849028000
1	3.251387000	-1.129772000	-0.695152000

- Geometrical parameters for $\text{AlH}_3 \cdot \text{NEt}_3$ (C_3 symmetry; distances in Å; angles in deg):



S6: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_2 symmetry) for $\text{AlH}_3 \cdot \text{TEA}$ (1:1 dimer).

13	-0.545626000	1.303672000	0.015857000
1	-1.286603000	1.464313000	-1.388078000
1	0.959780000	0.638681000	0.019690000
1	-1.283523000	1.475214000	1.420117000
7	0.338976000	3.367969000	-0.001341000
6	0.545626000	3.849381000	1.401281000
1	-0.422187000	3.801250000	1.897397000
1	0.850161000	4.906568000	1.362033000
6	1.549441000	3.054136000	2.233262000
1	1.305208000	1.991121000	2.251996000
1	2.577031000	3.168205000	1.884650000
1	1.511075000	3.423007000	3.261669000
6	-0.598866000	4.296639000	-0.707930000
1	-0.099684000	5.270576000	-0.825273000
1	-0.759683000	3.884465000	-1.702641000
6	-1.961131000	4.492710000	-0.045353000
1	-2.460994000	3.540736000	0.139825000

1	-1.901952000	5.040890000	0.896235000
1	-2.592070000	5.074146000	-0.722767000
6	1.655601000	3.364804000	-0.715631000
1	2.292209000	2.647970000	-0.199721000
1	2.112257000	4.359869000	-0.600540000
6	1.609343000	2.986971000	-2.194568000
1	1.116145000	2.026779000	-2.350195000
1	1.110590000	3.737345000	-2.810204000
1	2.636600000	2.896876000	-2.557313000
13	0.545626000	-1.303672000	0.015857000
1	1.283523000	-1.475214000	1.420117000
1	1.286603000	-1.464313000	-1.388078000
1	-0.959780000	-0.638681000	0.019690000
7	-0.338976000	-3.367969000	-0.001341000
6	-1.655601000	-3.364804000	-0.715631000
1	-2.292209000	-2.647970000	-0.199721000
1	-2.112257000	-4.359869000	-0.600540000
6	-1.609343000	-2.986971000	-2.194568000
1	-1.116145000	-2.026779000	-2.350195000
1	-1.110590000	-3.737345000	-2.810204000
1	-2.636600000	-2.896876000	-2.557313000
6	-0.545626000	-3.849381000	1.401281000
1	-0.850161000	-4.906568000	1.362033000
1	0.422187000	-3.801250000	1.897397000
6	-1.549441000	-3.054136000	2.233262000
1	-1.305208000	-1.991121000	2.251996000
1	-2.577031000	-3.168205000	1.884650000
1	-1.511075000	-3.423007000	3.261669000
6	0.598866000	-4.296639000	-0.707930000
1	0.759683000	-3.884465000	-1.702641000
1	0.099684000	-5.270576000	-0.825273000
6	1.961131000	-4.492710000	-0.045353000
1	2.460994000	-3.540736000	0.139825000
1	1.901952000	-5.040890000	0.896235000
1	2.592070000	-5.074146000	-0.722767000

S7: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (D_3 symmetry) for $\text{AlH}_3 \cdot \text{TEA}$. (2:1).

13	0.000000000	0.000000000	0.000000000
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1	0.000000000	1.606242000	0.000000000
1	-1.391047000	-0.803121000	0.000000000
1	1.391047000	-0.803121000	0.000000000
7	0.000000000	0.000000000	2.368809000
6	-0.683990000	-1.227340000	2.869095000
1	-1.681046000	-1.233944000	2.431464000
1	-0.798930000	-1.149447000	3.962935000
6	-0.002923000	-2.549677000	2.521140000
1	0.196271000	-2.623658000	1.451535000
1	0.935531000	-2.698782000	3.057977000
1	-0.671908000	-3.368671000	2.798889000
6	-0.720913000	1.206023000	2.869095000
1	-0.595985000	1.266617000	3.962935000
1	-0.228104000	2.072801000	2.431464000
6	-2.206624000	1.277370000	2.521140000
1	-2.370290000	1.141853000	1.451535000
1	-2.804979000	0.539197000	3.057977000
1	-2.581401000	2.266225000	2.798889000
6	1.404903000	0.021318000	2.869095000
1	1.909150000	-0.838857000	2.431464000
1	1.394915000	-0.117170000	3.962935000
6	2.209547000	1.272307000	2.521140000
1	2.174019000	1.481805000	1.451535000
1	1.869448000	2.159584000	3.057977000
1	3.253309000	1.102446000	2.798889000
7	0.000000000	0.000000000	-2.368809000
6	-1.404903000	0.021318000	-2.869095000
1	-1.909150000	-0.838857000	-2.431464000
1	-1.394915000	-0.117170000	-3.962935000
6	-2.209547000	1.272307000	-2.521140000
1	-2.174019000	1.481805000	-1.451535000
1	-1.869448000	2.159584000	-3.057977000
1	-3.253309000	1.102446000	-2.798889000
6	0.683990000	-1.227340000	-2.869095000
1	0.798930000	-1.149447000	-3.962935000
1	1.681046000	-1.233944000	-2.431464000
6	0.002923000	-2.549677000	-2.521140000
1	-0.196271000	-2.623658000	-1.451535000
1	-0.935531000	-2.698782000	-3.057977000
1	0.671908000	-3.368671000	-2.798889000
6	0.720913000	1.206023000	-2.869095000

1	0.228104000	2.072801000	-2.431464000
1	0.595985000	1.266617000	-3.962935000
6	2.206624000	1.277370000	-2.521140000
1	2.370290000	1.141853000	-1.451535000
1	2.804979000	0.539197000	-3.057977000
1	2.581401000	2.266225000	-2.798889000

S8: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_1 symmetry) for BDMA (ligand).

6	-3.067991000	0.343108000	0.165693000
6	-2.641131000	-0.981925000	0.163769000
6	-2.147319000	1.362835000	-0.075847000
1	-3.347670000	-1.781588000	0.357588000
1	-2.471893000	2.397826000	-0.072624000
6	-1.301512000	-1.283723000	-0.079313000
6	-0.812182000	1.058202000	-0.322805000
1	-0.972797000	-2.318457000	-0.072057000
1	-0.088932000	1.846194000	-0.498429000
6	-0.374167000	-0.270567000	-0.330016000
1	-4.108215000	0.581215000	0.358079000
7	2.030034000	0.273456000	0.020882000
6	2.067467000	0.043828000	1.460159000
1	1.070209000	0.169091000	1.884785000
1	2.428391000	-0.969552000	1.719861000
1	2.731653000	0.772400000	1.931419000
6	3.358303000	0.173396000	-0.566808000
1	4.027983000	0.889259000	-0.083659000
1	3.806455000	-0.833290000	-0.462983000
1	3.314072000	0.416982000	-1.631245000
6	1.071222000	-0.600790000	-0.651527000
1	1.224715000	-0.482388000	-1.730315000
1	1.259663000	-1.668066000	-0.426438000

S9: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_1 symmetry) for AlH_3 ·BDMA (1:1 dimer).

6	3.532409000	1.739411000	-0.323774000
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6	-4.157951000	2.201686000	0.483712000
6	-7.494559000	-0.819178000	0.987858000
6	7.648180000	-0.035704000	-0.974562000
6	-6.179884000	-0.395872000	1.168298000
6	6.267432000	-0.023221000	-1.157540000
6	-7.843260000	-1.550884000	-0.145179000
6	8.205010000	-0.735561000	0.093622000
6	3.285044000	0.367192000	1.658282000
6	-3.542694000	1.151040000	-1.610783000
6	-5.192267000	-0.689251000	0.220713000
6	5.418311000	-0.702226000	-0.275829000
6	-3.760572000	-0.235540000	0.423961000
6	3.916491000	-0.695797000	-0.479820000
6	7.373784000	-1.428268000	0.971076000
6	-6.868431000	-1.863012000	-1.090173000
6	5.993685000	-1.412583000	0.784252000
6	-5.555168000	-1.437588000	-0.905269000
1	2.872198000	2.486081000	0.119375000
1	-3.779118000	3.151453000	0.103658000
1	-4.007515000	2.177101000	1.564104000
1	3.399679000	1.762691000	-1.406093000
1	4.570283000	1.985781000	-0.076507000
1	-5.227667000	2.127327000	0.262864000
1	-8.243850000	-0.585078000	1.735805000
1	8.288995000	0.493687000	-1.670802000
1	-5.914058000	0.156964000	2.063310000
1	5.844986000	0.508982000	-2.003366000
1	0.646980000	1.408235000	0.556821000
1	1.276159000	0.229658000	-1.892518000
1	2.624891000	1.120287000	2.090476000
1	-3.160645000	2.107450000	-1.969412000
1	-8.865047000	-1.884984000	-0.285270000
1	9.279776000	-0.749908000	0.234858000
1	4.313810000	0.566320000	1.975803000
1	-4.589053000	1.043120000	-1.914562000
1	-3.527874000	-0.190496000	1.489752000
1	3.682605000	-0.628311000	-1.544500000
1	2.974449000	-0.612432000	2.023549000
1	-2.950252000	0.353749000	-2.061747000
1	7.799784000	-1.987934000	1.796259000
1	-7.128068000	-2.445142000	-1.967324000

1	0.981719000	-1.358982000	0.423253000
1	-3.073144000	-0.955849000	-0.024764000
1	3.486533000	-1.630473000	-0.113074000
1	5.355631000	-1.969908000	1.462120000
1	-4.799457000	-1.701709000	-1.637652000
13	1.028643000	0.051692000	-0.324465000
7	3.148472000	0.406045000	0.186550000
7	-3.390302000	1.103543000	-0.140871000
13	-1.266719000	1.456539000	0.353578000
1	-1.224286000	2.864592000	-0.397674000
1	-1.507933000	1.275892000	1.922240000
1	-0.886073000	0.099857000	-0.530295000

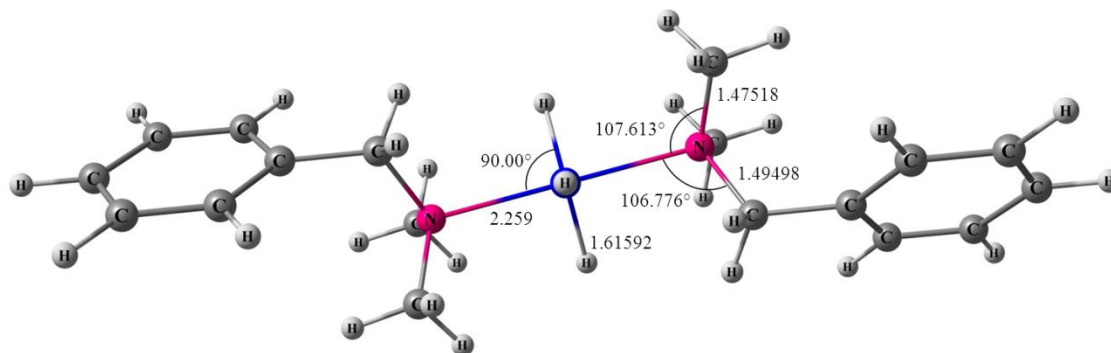
S10: DFT Calculated Cartesian coordinates and Geometrical parameters for $\text{AlH}_3\cdot 2\text{BDMA}$.

- Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_2 symmetry):

6	-1.104854000	2.460845000	1.863103000
6	1.104854000	-2.460845000	1.863103000
6	4.807583000	-4.664865000	0.512095000
6	-4.807583000	4.664865000	0.512095000
6	4.033152000	-3.510939000	0.605149000
6	-4.033152000	3.510939000	0.605149000
6	4.640010000	-5.533426000	-0.564166000
6	-4.640010000	5.533426000	-0.564166000
6	0.000000000	2.976554000	-0.225963000
6	0.000000000	-2.976554000	-0.225963000
6	3.074963000	-3.204369000	-0.368368000
6	-3.074963000	3.204369000	-0.368368000
6	2.238467000	-1.943467000	-0.264151000
6	-2.238467000	1.943467000	-0.264151000
6	-3.700286000	5.235499000	-1.548603000
6	3.700286000	-5.235499000	-1.548603000
6	-2.928400000	4.080020000	-1.450735000
6	2.928400000	-4.080020000	-1.450735000
1	-0.133399000	2.416264000	2.357196000
1	0.133399000	-2.416264000	2.357196000
1	1.774898000	-1.756844000	2.358706000
1	-1.774898000	1.756844000	2.358706000
1	-1.509674000	3.475239000	1.953839000

1	1.509674000	-3.475239000	1.953839000
1	5.546585000	-4.881594000	1.275520000
1	-5.546585000	4.881594000	1.275520000
1	4.183004000	-2.832219000	1.438416000
1	-4.183004000	2.832219000	1.438416000
1	1.274782000	0.580232000	1.250320000
1	-1.274782000	-0.580232000	1.250320000
1	0.963323000	2.932085000	0.283738000
1	-0.963323000	-2.932085000	0.283738000
1	5.244306000	-6.430328000	-0.640634000
1	-5.244306000	6.430328000	-0.640634000
1	-0.363598000	4.010481000	-0.220024000
1	0.363598000	-4.010481000	-0.220024000
1	2.801657000	-1.163536000	0.252731000
1	-2.801657000	1.163536000	0.252731000
1	0.141468000	2.646631000	-1.256250000
1	-0.141468000	-2.646631000	-1.256250000
1	-3.573347000	5.898397000	-2.397341000
1	3.573347000	-5.898397000	-2.397341000
1	0.000000000	0.000000000	-1.171506000
1	2.003974000	-1.564460000	-1.261105000
1	-2.003974000	1.564460000	-1.261105000
1	-2.211946000	3.847749000	-2.231789000
1	2.211946000	-3.847749000	-2.231789000
13	0.000000000	0.000000000	0.444844000
7	-0.932522000	2.058132000	0.454397000
7	0.932522000	-2.058132000	0.454397000

- Geometrical parameters for $\text{AlH}_3 \cdot 2\text{BDMA}$ (C_2 symmetry; distances in Å; angles in deg):



S11: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_{2h} symmetry) for DIOX (ligand).

8	0.228289000	1.395261000	0.000000000
6	-0.228289000	0.726581000	1.172645000
1	0.185675000	1.270030000	2.024816000
1	-1.326959000	0.767491000	1.224378000
6	0.228289000	-0.726581000	1.172645000
1	-0.185675000	-1.270030000	2.024816000
1	1.326959000	-0.767491000	1.224378000
6	-0.228289000	0.726581000	-1.172645000
1	-1.326959000	0.767491000	-1.224378000
1	0.185675000	1.270030000	-2.024816000
8	-0.228289000	-1.395261000	0.000000000
6	0.228289000	-0.726581000	-1.172645000
1	-0.185675000	-1.270030000	-2.024816000
1	1.326959000	-0.767491000	-1.224378000

S12: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_s symmetry) for $AlH_3 \cdot DIOX$ (1:1).

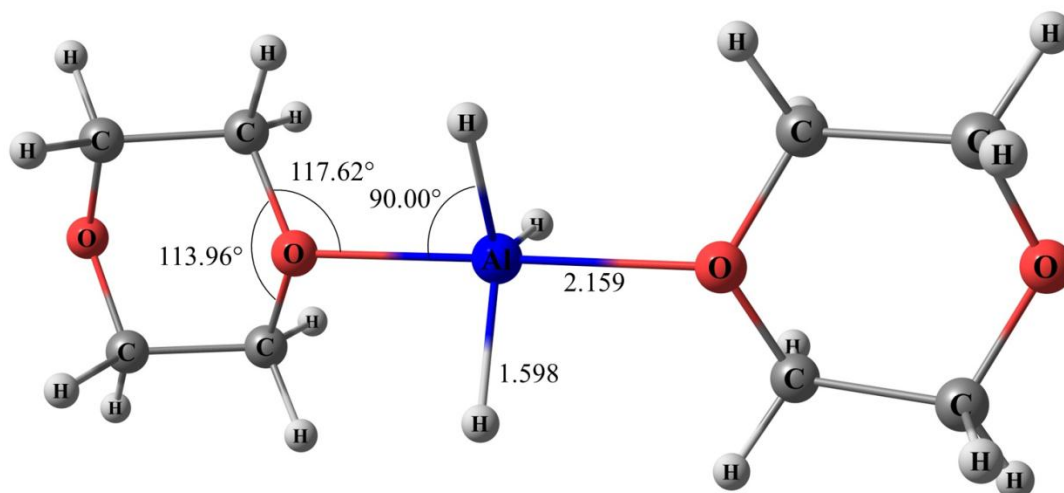
13	-1.119019000	2.298744000	0.000000000
1	-1.915712000	2.167040000	1.378096000
1	0.175055000	3.240146000	0.000000000
1	-1.915712000	2.167040000	-1.378096000
8	-0.259661000	0.475619000	0.000000000
6	0.379389000	-0.026074000	-1.206794000
1	-0.204613000	0.365334000	-2.039178000
1	1.398797000	0.370939000	-1.246042000
6	0.379389000	-1.543907000	-1.170756000
1	0.931526000	-1.938716000	-2.025250000
1	-0.654077000	-1.916132000	-1.212953000
6	0.379389000	-0.026074000	1.206794000
1	1.398797000	0.370939000	1.246042000
1	-0.204613000	0.365334000	2.039178000
8	1.029038000	-2.023242000	0.000000000
6	0.379389000	-1.543907000	1.170756000
1	0.931526000	-1.938716000	2.025250000
1	-0.654077000	-1.916132000	1.212953000

S13: DFT Calculated Cartesian coordinates and Geometrical parameters for $\text{AlH}_3 \cdot 2\text{DIOX}$.

- Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_{2v} symmetry):

13	0.000000000	0.000000000	0.130533000
1	-1.418893000	0.000000000	0.880958000
1	0.000000000	0.000000000	-1.483371000
1	1.418893000	0.000000000	0.880958000
8	0.000000000	2.158396000	0.180662000
6	1.192727000	2.838486000	-0.267105000
1	2.031156000	2.278762000	0.146919000
1	1.229733000	2.799640000	-1.362079000
6	1.170602000	4.275961000	0.224510000
1	2.024571000	4.826495000	-0.174748000
1	1.219846000	4.292629000	1.323141000
6	-1.192727000	2.838486000	-0.267105000
1	-1.229733000	2.799640000	-1.362079000
1	-2.031156000	2.278762000	0.146919000
8	0.000000000	4.950418000	-0.223544000
6	-1.170602000	4.275961000	0.224510000
1	-2.024571000	4.826495000	-0.174748000
1	-1.219846000	4.292629000	1.323141000
8	0.000000000	-2.158396000	0.180662000
6	-1.192727000	-2.838486000	-0.267105000
1	-2.031156000	-2.278762000	0.146919000
1	-1.229733000	-2.799640000	-1.362079000
6	-1.170602000	-4.275961000	0.224510000
1	-2.024571000	-4.826495000	-0.174748000
1	-1.219846000	-4.292629000	1.323141000
6	1.192727000	-2.838486000	-0.267105000
1	1.229733000	-2.799640000	-1.362079000
1	2.031156000	-2.278762000	0.146919000
8	0.000000000	-4.950418000	-0.223544000
6	1.170602000	-4.275961000	0.224510000
1	2.024571000	-4.826495000	-0.174748000
1	1.219846000	-4.292629000	1.323141000

Geometrical parameters for $\text{AlH}_3 \cdot 2\text{DIOX}$ (C_{2v} symmetry; distances in Å; angles in deg):



S14: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_{2v} symmetry) for Et_2O (ligand).

8	0.000000000	0.000000000	0.254885000
6	0.000000000	1.185485000	-0.522673000
1	-0.886681000	1.208040000	-1.175898000
1	0.886681000	1.208040000	-1.175898000
6	0.000000000	2.377771000	0.417080000
1	0.884910000	2.358249000	1.057181000
1	-0.884910000	2.358249000	1.057181000
1	0.000000000	3.313348000	-0.148547000
6	0.000000000	-1.185485000	-0.522673000
1	-0.886681000	-1.208040000	-1.175898000
1	0.886681000	-1.208040000	-1.175898000
6	0.000000000	-2.377771000	0.417080000
1	-0.884910000	-2.358249000	1.057181000
1	0.884910000	-2.358249000	1.057181000
1	0.000000000	-3.313348000	-0.148547000

S15: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_1 symmetry) for $\text{AlH}_3 \cdot \text{Et}_2\text{O}$ (1:1).

13	-1.383471000	-1.422994000	0.120820000
1	-0.504921000	-2.744414000	-0.073124000
1	-2.334381000	-0.978205000	-1.088508000
1	-1.910810000	-1.107361000	1.592845000
8	0.101596000	-0.065533000	-0.137278000

6	-0.227672000	1.285682000	-0.578947000
1	-0.650085000	1.208925000	-1.585089000
1	0.706945000	1.847605000	-0.628847000
6	-1.194277000	1.942996000	0.385190000
1	-0.770693000	1.993175000	1.389950000
1	-2.141446000	1.404376000	0.434558000
1	-1.400130000	2.960396000	0.040939000
6	1.445323000	-0.507390000	-0.492973000
1	1.383928000	-1.593284000	-0.539484000
1	1.670557000	-0.130790000	-1.495029000
6	2.464874000	-0.053978000	0.536139000
1	2.217450000	-0.454476000	1.520992000
1	2.521030000	1.035046000	0.607990000
1	3.455420000	-0.421675000	0.253915000

S16: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_2 symmetry) for $AlH_3 \cdot Et_2O$ (1:1 dimer).

13	-0.693827000	1.177052000	-0.141152000
1	-1.371444000	1.382772000	-1.566900000
1	-1.373406000	1.343173000	1.289801000
1	0.902860000	0.696256000	-0.161861000
8	-0.048698000	3.211380000	-0.089525000
6	0.048698000	3.942164000	1.159000000
1	-0.860597000	3.705856000	1.713695000
1	0.041187000	5.010312000	0.923834000
6	1.278135000	3.552566000	1.964122000
1	2.203114000	3.782983000	1.432689000
1	1.267273000	2.484933000	2.189252000
1	1.279435000	4.100792000	2.911264000
6	0.256096000	3.941283000	-1.298556000
1	-0.159462000	3.329178000	-2.098877000
1	-0.297035000	4.886577000	-1.273466000
6	1.745057000	4.172808000	-1.506506000
1	2.286948000	3.225168000	-1.495155000
1	2.170295000	4.828135000	-0.742692000
1	1.904303000	4.648499000	-2.478760000
13	0.693827000	-1.177052000	-0.141152000
1	1.371444000	-1.382772000	-1.566900000

1	1.373406000	-1.343173000	1.289801000
1	-0.902860000	-0.696256000	-0.161861000
8	0.048698000	-3.211380000	-0.089525000
6	-0.048698000	-3.942164000	1.159000000
1	0.860597000	-3.705856000	1.713695000
1	-0.041187000	-5.010312000	0.923834000
6	-1.278135000	-3.552566000	1.964122000
1	-2.203114000	-3.782983000	1.432689000
1	-1.267273000	-2.484933000	2.189252000
1	-1.279435000	-4.100792000	2.911264000
6	-0.256096000	-3.941283000	-1.298556000
1	0.159462000	-3.329178000	-2.098877000
1	0.297035000	-4.886577000	-1.273466000
6	-1.745057000	-4.172808000	-1.506506000
1	-2.286948000	-3.225168000	-1.495155000
1	-2.170295000	-4.828135000	-0.742692000
1	-1.904303000	-4.648499000	-2.478760000

S17: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_2 symmetry) for $AlH_3 \cdot Et_2O$ (2:1).

8	0.000000000	2.272402000	-0.004495000
6	0.521130000	2.863511000	-1.214916000
1	0.370147000	3.946337000	-1.151837000
1	-0.042381000	2.481018000	-2.073247000
6	1.998946000	2.548723000	-1.347940000
1	2.168253000	1.476143000	-1.443615000
1	2.549490000	2.911231000	-0.477401000
1	2.393910000	3.040264000	-2.241851000
6	-1.206493000	2.894286000	0.496926000
1	-1.245748000	3.918486000	0.113224000
1	-2.073549000	2.348203000	0.112439000
6	-1.186457000	2.896337000	2.013979000
1	-0.320719000	3.448358000	2.386892000
1	-1.148055000	1.877228000	2.399701000
1	-2.094795000	3.373976000	2.393175000
13	0.000000000	0.000000000	0.043998000
1	0.000000000	0.000000000	-1.562723000
1	1.390822000	-0.030334000	0.825556000

1	-1.390822000	0.030334000	0.825556000
8	0.000000000	-2.272402000	-0.004495000
6	1.206493000	-2.894286000	0.496926000
1	2.073549000	-2.348203000	0.112439000
1	1.245748000	-3.918486000	0.113224000
6	1.186457000	-2.896337000	2.013979000
1	0.320719000	-3.448358000	2.386892000
1	1.148055000	-1.877228000	2.399701000
1	2.094795000	-3.373976000	2.393175000
6	-0.521130000	-2.863511000	-1.214916000
1	-2.168253000	-1.476143000	-1.443615000
1	0.042381000	-2.481018000	-2.073247000
6	-1.998946000	-2.548723000	-1.347940000
1	-2.549490000	-2.911231000	-0.477401000
1	-0.370147000	-3.946337000	-1.151837000
1	-2.393910000	-3.040264000	-2.241851000

S18: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_1 symmetry) for DMEA (ligand).

7	0.452657000	-0.004439000	-0.310704000
6	1.652600000	-0.794844000	-0.074929000
1	1.506621000	-1.812417000	-0.446017000
1	2.495778000	-0.357051000	-0.615585000
1	1.931091000	-0.856800000	0.995015000
6	0.656752000	1.379942000	0.093742000
1	0.832235000	1.488780000	1.181983000
1	1.523804000	1.789690000	-0.430225000
1	-0.207202000	1.990462000	-0.173255000
6	-0.719462000	-0.613258000	0.319333000
1	-0.699091000	-1.679374000	0.073588000
1	-0.662714000	-0.545296000	1.424247000
6	-2.044966000	-0.027091000	-0.165871000
1	-2.182834000	1.009046000	0.151887000
1	-2.094626000	-0.059324000	-1.257081000
1	-2.881207000	-0.605141000	0.236721000

S19: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_1 symmetry) for $AlH_3 \cdot DMEA$ (1:1).

7	-0.085389000	0.468464000	0.005159000
6	-0.772715000	1.541075000	-0.761665000
1	-0.945220000	1.199599000	-1.782708000
1	-1.734508000	1.756488000	-0.298396000
1	-0.161040000	2.450709000	-0.782408000
6	0.107905000	0.924361000	1.404534000
1	0.750033000	1.812868000	1.438139000
1	-0.864503000	1.168415000	1.832748000
1	0.553616000	0.128653000	1.997779000
6	1.226908000	0.190369000	-0.666529000
1	0.986438000	-0.097022000	-1.691815000
1	1.789283000	1.133400000	-0.709004000
6	2.077853000	-0.896344000	-0.018857000
1	2.422568000	-0.617968000	0.978942000
1	1.540293000	-1.842405000	0.054644000
1	2.964205000	-1.055829000	-0.637969000
13	-1.373919000	-1.200581000	-0.010569000
1	-2.726346000	-0.468958000	0.439247000
1	-0.713767000	-2.178592000	1.069529000
1	-1.242081000	-1.617829000	-1.552337000

S20: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_2 symmetry) for $AlH_3 \cdot DMEA$ (1:1 dimer).

7	0.483712000	3.270590000	0.130453000
6	1.430271000	3.209866000	1.267183000
1	0.876806000	3.020257000	2.187641000
1	2.134464000	2.392966000	1.111978000
1	1.982726000	4.153336000	1.366251000
6	1.238420000	3.487828000	-1.122011000
1	1.764896000	4.451619000	-1.105698000
1	1.968058000	2.685597000	-1.237439000
1	0.563673000	3.456137000	-1.975365000
6	-0.483712000	4.377383000	0.394528000
1	-0.987282000	4.122504000	1.329793000
1	0.087974000	5.301136000	0.569272000
6	-1.525084000	4.614649000	-0.694780000
1	-1.079849000	4.972244000	-1.625517000
1	-2.093989000	3.710796000	-0.913423000
1	-2.221483000	5.383106000	-0.349272000

13	-0.525866000	1.294093000	0.042851000
1	0.978326000	0.598264000	0.048842000
1	-1.201450000	1.499377000	-1.385952000
1	-1.266935000	1.528980000	1.439141000
7	-0.483712000	-3.270590000	0.130453000
6	-1.430271000	-3.209866000	1.267183000
1	-0.876806000	-3.020257000	2.187641000
1	-2.134464000	-2.392966000	1.111978000
1	-1.982726000	-4.153336000	1.366251000
6	-1.238420000	-3.487828000	-1.122011000
1	-1.764896000	-4.451619000	-1.105698000
1	-1.968058000	-2.685597000	-1.237439000
1	-0.563673000	-3.456137000	-1.975365000
6	0.483712000	-4.377383000	0.394528000
1	0.987282000	-4.122504000	1.329793000
1	-0.087974000	-5.301136000	0.569272000
6	1.525084000	-4.614649000	-0.694780000
1	1.079849000	-4.972244000	-1.625517000
1	2.093989000	-3.710796000	-0.913423000
1	2.221483000	-5.383106000	-0.349272000
13	0.525866000	-1.294093000	0.042851000
1	-0.978326000	-0.598264000	0.048842000
1	1.201450000	-1.499377000	-1.385952000
1	1.266935000	-1.528980000	1.439141000

S21: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_2 symmetry) for $AlH_3 \cdot DMEA$ (2:1).

7	0.000000000	2.287610000	0.080897000
6	-1.329802000	2.671545000	-0.432872000
1	-1.462676000	2.258705000	-1.434075000
1	-2.101538000	2.259062000	0.216453000
1	-1.436625000	3.764742000	-0.478789000
6	0.158048000	2.796969000	1.455521000
1	0.122862000	3.895844000	1.484271000
1	-0.649561000	2.399270000	2.071182000
1	1.102275000	2.453727000	1.874745000
6	1.028978000	2.843049000	-0.841133000
1	0.831576000	2.396680000	-1.818427000
1	0.867177000	3.928672000	-0.935841000

6	2.478061000	2.574304000	-0.446819000
1	2.763183000	3.096265000	0.469256000
1	2.660960000	1.509156000	-0.304193000
1	3.132009000	2.934998000	-1.245339000
13	0.000000000	0.000000000	0.137185000
1	-1.374659000	0.057480000	0.973579000
1	1.374659000	-0.057480000	0.973579000
1	0.000000000	0.000000000	-1.477979000
7	0.000000000	-2.287610000	0.080897000
6	1.329802000	-2.671545000	-0.432872000
1	1.462676000	-2.258705000	-1.434075000
1	2.101538000	-2.259062000	0.216453000
1	1.436625000	-3.764742000	-0.478789000
6	-0.158048000	-2.796969000	1.455521000
1	-0.122862000	-3.895844000	1.484271000
1	0.649561000	-2.399270000	2.071182000
1	-1.102275000	-2.453727000	1.874745000
6	-1.028978000	-2.843049000	-0.841133000
1	-0.831576000	-2.396680000	-1.818427000
1	-0.867177000	-3.928672000	-0.935841000
6	-2.478061000	-2.574304000	-0.446819000
1	-2.763183000	-3.096265000	0.469256000
1	-2.660960000	-1.509156000	-0.304193000
1	-3.132009000	-2.934998000	-1.245339000

S22: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_{3v} symmetry) for TMA (ligand).

7	0.000000000	0.000000000	0.369404000
6	0.000000000	1.389756000	-0.060422000
1	0.884122000	1.899212000	0.331397000
1	0.000000000	1.503830000	-1.162207000
1	-0.884122000	1.899212000	0.331397000
6	-1.203564000	-0.694878000	-0.060422000
1	-2.086827000	-0.183934000	0.331397000
1	-1.302355000	-0.751915000	-1.162207000
1	-1.202705000	-1.715278000	0.331397000
6	1.203564000	-0.694878000	-0.060422000
1	1.302355000	-0.751915000	-1.162207000
1	2.086827000	-0.183934000	0.331397000
1	1.202705000	-1.715278000	0.331397000

S23: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_{3v} symmetry) for $AlH_3 \cdot TMA$ (1:1).

13	0.000000000	0.000000000	1.693074000
1	-1.366797000	0.789121000	1.966601000
1	0.000000000	-1.578241000	1.966601000
1	1.366797000	0.789121000	1.966601000
7	0.000000000	0.000000000	-0.406254000
6	0.000000000	1.402621000	-0.890544000
1	0.886018000	1.912835000	-0.512798000
1	0.000000000	1.433544000	-1.986471000
1	-0.886018000	1.912835000	-0.512798000
6	-1.214705000	-0.701310000	-0.890544000
1	-2.099573000	-0.189103000	-0.512798000
1	-1.241485000	-0.716772000	-1.986471000
1	-1.213555000	-1.723732000	-0.512798000
6	1.214705000	-0.701310000	-0.890544000
1	1.241485000	-0.716772000	-1.986471000
1	2.099573000	-0.189103000	-0.512798000
1	1.213555000	-1.723732000	-0.512798000

S24: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_{2h} symmetry) for $AlH_3 \cdot TMA$ (1:1 dimer).

13	0.641908000	1.228768000	0.000000000
1	1.363773000	1.413503000	1.412878000
1	1.363773000	1.413503000	-1.412878000
7	-0.163306000	3.278022000	0.000000000
7	0.163306000	-3.278022000	0.000000000
6	0.983697000	-3.482384000	1.211812000
6	-0.983697000	3.482384000	1.211812000
6	-0.983697000	-4.208930000	0.000000000
6	0.983697000	4.208930000	0.000000000
1	1.593199000	4.028336000	0.886084000
1	0.644679000	5.252971000	0.000000000
1	1.593199000	4.028336000	-0.886084000
1	-1.384656000	4.503794000	1.248925000
1	-0.370961000	3.302378000	2.095475000
1	-1.593199000	-4.028336000	-0.886084000
1	-1.593199000	-4.028336000	0.886084000

1	-0.644679000	-5.252971000	0.000000000
1	1.384656000	-4.503794000	1.248925000
1	0.370961000	-3.302378000	2.095475000
1	-0.926474000	0.673279000	0.000000000
6	0.983697000	-3.482384000	-1.211812000
6	-0.983697000	3.482384000	-1.211812000
1	-1.811010000	2.771888000	-1.212775000
1	-1.384656000	4.503794000	-1.248925000
1	-0.370961000	3.302378000	-2.095475000
1	-1.811010000	2.771888000	1.212775000
1	0.370961000	-3.302378000	-2.095475000
1	1.811010000	-2.771888000	-1.212775000
1	1.384656000	-4.503794000	-1.248925000
1	1.811010000	-2.771888000	1.212775000
1	-1.363773000	-1.413503000	1.412878000
13	-0.641908000	-1.228768000	0.000000000
1	0.926474000	-0.673279000	0.000000000
1	-1.363773000	-1.413503000	-1.412878000

S25: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_{2v} symmetry) for $AlH_3 \cdot TMA$ (2:1).

13	0.000000000	0.000000000	0.000000000
1	0.000000000	1.616350000	0.000000000
1	-1.399800000	-0.808175000	0.000000000
1	1.399800000	-0.808175000	0.000000000
7	0.000000000	0.000000000	2.248291000
6	-1.209205000	0.698135000	2.720987000
1	-2.092319000	0.185780000	2.337666000
1	-1.252468000	0.723113000	3.818989000
1	-1.207050000	1.719111000	2.337666000
6	1.209205000	0.698135000	2.720987000
1	1.207050000	1.719111000	2.337666000
1	1.252468000	0.723113000	3.818989000
1	2.092319000	0.185780000	2.337666000
6	0.000000000	-1.396270000	2.720987000
1	0.000000000	-1.446226000	3.818989000
1	-0.885269000	-1.904892000	2.337666000
1	0.885269000	-1.904892000	2.337666000
7	0.000000000	0.000000000	-2.248291000

6	-1.209205000	0.698135000	-2.720987000
1	-1.207050000	1.719111000	-2.337666000
1	-1.252468000	0.723113000	-3.818989000
1	-2.092319000	0.185780000	-2.337666000
6	0.000000000	-1.396270000	-2.720987000
1	-0.885269000	-1.904892000	-2.337666000
1	0.000000000	-1.446226000	-3.818989000
1	0.885269000	-1.904892000	-2.337666000
6	1.209205000	0.698135000	-2.720987000
1	1.252468000	0.723113000	-3.818989000
1	1.207050000	1.719111000	-2.337666000
1	2.092319000	0.185780000	-2.337666000

S26: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_{3v} symmetry) for QUIN (ligand).

7	0.000000000	0.000000000	1.291649000
6	0.000000000	0.000000000	-1.294127000
6	0.000000000	1.447245000	-0.762630000
6	0.000000000	1.387073000	0.798695000
6	-1.253351000	-0.723622000	-0.762630000
6	-1.201241000	-0.693537000	0.798695000
6	1.201241000	-0.693537000	0.798695000
6	1.253351000	-0.723622000	-0.762630000
1	0.879513000	1.982135000	-1.134985000
1	-0.879513000	1.982135000	-1.134985000
1	0.879154000	1.889466000	1.211865000
1	-0.879154000	1.889466000	1.211865000
1	1.196749000	-1.706103000	1.211865000
1	2.075903000	-0.183364000	1.211865000
1	1.276822000	-1.752748000	-1.134985000
1	2.156336000	-0.229386000	-1.134985000
1	-1.276822000	-1.752748000	-1.134985000
1	-2.156336000	-0.229386000	-1.134985000
1	-2.075903000	-0.183364000	1.211865000
1	-1.196749000	-1.706103000	1.211865000
1	0.000000000	0.000000000	-2.387249000

S27: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_{3v} symmetry) for $AlH_3 \cdot QUIN$ (1:1).

13	0.000000000	0.000000000	2.676837000
1	0.000000000	-1.577223000	2.963781000
1	1.365915000	0.788612000	2.963781000
1	-1.365915000	0.788612000	2.963781000
7	0.000000000	0.000000000	0.596300000
6	0.000000000	0.000000000	-1.995439000
6	0.000000000	1.444659000	-1.465745000
6	0.000000000	1.409594000	0.086236000
6	-1.251111000	-0.722329000	-1.465745000
6	-1.220744000	-0.704797000	0.086236000
6	1.220744000	-0.704797000	0.086236000
6	1.251111000	-0.722329000	-1.465745000
1	0.878826000	1.979638000	-1.835677000
1	-0.878826000	1.979638000	-1.835677000
1	0.878910000	1.900009000	0.506895000
1	-0.878910000	1.900009000	0.506895000
1	1.206001000	-1.711163000	0.506895000
1	2.084911000	-0.188846000	0.506895000
1	1.275004000	-1.750904000	-1.835677000
1	2.153830000	-0.228734000	-1.835677000
1	-1.275004000	-1.750904000	-1.835677000
1	-2.153830000	-0.228734000	-1.835677000
1	-2.084911000	-0.188846000	0.506895000
1	-1.206001000	-1.711163000	0.506895000
1	0.000000000	0.000000000	-3.087837000

S28: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_1 symmetry) for $AlH_3 \cdot QUIN$ (2:1).

13	-0.001209000	0.001025000	-0.012230000
1	-0.000853000	0.704784000	-1.469249000
1	0.003676000	-1.612677000	0.104576000
1	-0.001840000	0.916821000	1.323166000
7	-2.231730000	0.001269000	-0.004937000
6	-4.823675000	-0.000798000	0.009362000
6	-4.282806000	-0.705187000	1.265824000
6	-2.730916000	-0.617884000	1.253607000

6	-4.296577000	-0.740794000	-1.233576000
6	-2.743577000	-0.778209000	-1.165788000
6	-2.738718000	1.398114000	-0.094315000
6	-4.290992000	1.442649000	-0.016661000
1	-4.687273000	-0.232286000	2.165535000
1	-4.611491000	-1.748949000	1.278124000
1	-2.353525000	-0.011633000	2.079192000
1	-2.267615000	-1.602031000	1.336537000
1	-2.367825000	1.810765000	-1.034166000
1	-2.272298000	1.964362000	0.713075000
1	-4.703174000	1.981664000	-0.875025000
1	-4.618323000	1.976758000	0.880739000
1	-4.631994000	-0.229868000	-2.141142000
1	-4.704373000	-1.755144000	-1.267550000
1	-2.367806000	-1.796823000	-1.055079000
1	-2.286567000	-0.360817000	-2.064333000
1	-5.916756000	-0.002213000	0.014921000
7	2.231874000	0.001456000	-0.006761000
6	4.824191000	-0.001985000	0.009425000
6	4.293849000	1.436511000	-0.124694000
6	2.738724000	1.397830000	-0.094141000
6	4.297294000	-0.834777000	-1.172669000
6	2.743534000	-0.775887000	-1.168814000
6	2.729401000	-0.619757000	1.251726000
6	4.282447000	-0.605310000	1.317811000
1	4.680179000	2.056541000	0.689580000
1	4.650752000	1.879790000	-1.059258000
1	2.335805000	1.937805000	0.764087000
1	2.302887000	1.842749000	-0.990261000
1	2.331321000	-1.635359000	1.285566000
1	2.281113000	-0.069009000	2.080169000
1	4.671485000	-1.618512000	1.454411000
1	4.627092000	-0.013086000	2.170939000
1	4.644717000	-1.868331000	-1.084284000
1	4.693945000	-0.444237000	-2.114555000
1	2.354983000	-0.296830000	-2.068724000
1	2.298143000	-1.770247000	-1.113785000
1	5.917262000	-0.003475000	0.015093000

S29: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_i symmetry) for TMEDA (ligand).

6	1.006104000	-0.603982000	-2.834187000
6	1.226154000	-0.142942000	2.380807000
6	0.240358000	-0.484346000	-0.543828000
6	-0.240358000	0.484346000	0.543828000
6	-1.226154000	0.142942000	-2.380807000
6	-1.006104000	0.603982000	2.834187000
1	0.727997000	-1.665045000	-2.982533000
1	2.042413000	-0.569419000	-2.489555000
1	1.855378000	-0.735753000	1.715086000
1	-0.322855000	-1.430957000	-0.450937000
1	1.242548000	-0.624364000	3.361724000
1	1.291937000	-0.724745000	-0.369535000
1	0.958836000	-0.106698000	-3.806594000
1	-1.684097000	-0.859749000	-2.482557000
1	1.684097000	0.859749000	2.482557000
1	-0.958836000	0.106698000	3.806594000
1	-1.291937000	0.724745000	0.369535000
1	-1.242548000	0.624364000	-3.361724000
1	-2.042413000	0.569419000	2.489555000
1	0.322855000	1.430957000	0.450937000
1	-1.855378000	0.735753000	-1.715086000
1	-0.727997000	1.665045000	2.982533000
7	-0.143904000	-0.089229000	1.886443000
7	0.143904000	0.089229000	-1.886443000

S30: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_1 symmetry) for $\text{AlH}_3 \cdot \text{TMEDA}$ (1:1).

6	2.353843000	-0.650116000	1.334048000
6	-2.658848000	1.117326000	0.828924000
6	0.046325000	-0.447017000	0.661884000
6	-1.029969000	-0.205759000	-0.402040000
6	1.705959000	-1.471225000	-0.845940000
6	-3.407669000	-0.591185000	-0.684318000
1	2.130050000	-1.616994000	1.799380000
1	2.207381000	0.144581000	2.066085000
1	-1.883615000	1.412813000	1.537587000

1	-0.142241000	-1.418426000	1.135824000
1	-3.600774000	1.050243000	1.378446000
1	-0.023711000	0.318705000	1.434910000
1	3.391200000	-0.632345000	1.002737000
1	1.450875000	-2.459223000	-0.444547000
1	-2.752391000	1.920738000	0.076323000
1	-4.360400000	-0.621182000	-0.149898000
1	1.438725000	2.414490000	0.519524000
1	-1.021676000	-1.029160000	-1.119430000
1	2.760613000	-1.456609000	-1.121818000
1	-3.204665000	-1.595613000	-1.063378000
1	-0.818191000	0.714325000	-0.968485000
1	3.598292000	1.245875000	-0.687019000
1	1.117078000	-1.276028000	-1.739973000
1	-3.524674000	0.088582000	-1.548102000
1	1.260671000	1.483451000	-2.044830000
7	-2.349836000	-0.179591000	0.231913000
7	1.460299000	-0.414384000	0.168225000
13	2.011258000	1.458266000	-0.632281000

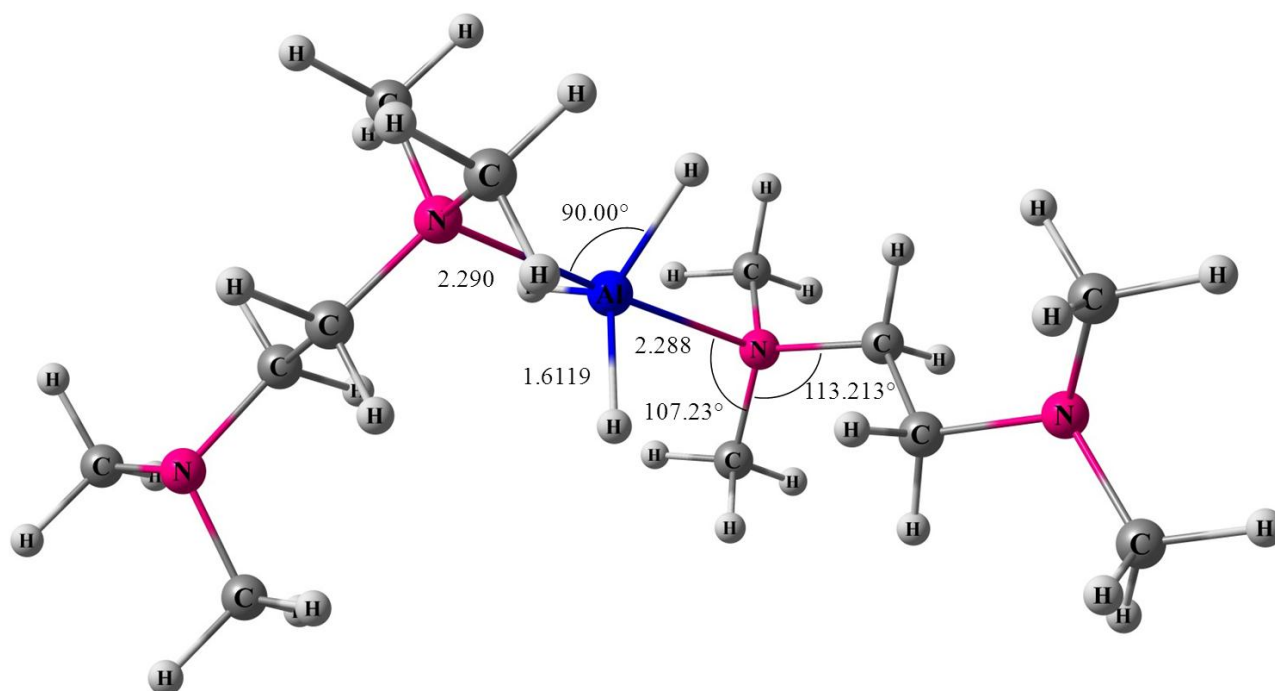
S31: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_1 symmetry) for $\text{AlH}_3 \cdot 2\text{TMEDA}$.

- Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_1 symmetry):

6	-1.770921000	-1.724897000	2.499633000
6	-4.496162000	1.738984000	-0.505142000
6	-3.061252000	-0.757860000	0.727645000
6	-3.235577000	-0.329719000	-0.732961000
6	-1.491172000	-2.588732000	0.270687000
6	-5.036028000	0.204966000	-2.268883000
1	-2.585469000	-2.428462000	2.721660000
1	-1.911966000	-0.818803000	3.090733000
1	-4.137451000	1.837236000	0.520504000
1	-3.872016000	-1.457362000	0.979159000
1	-5.505474000	2.156638000	-0.545399000
1	-3.165761000	0.112539000	1.377202000
1	-0.816651000	-2.171480000	2.776483000
1	-2.300762000	-3.323582000	0.386427000
1	-3.842197000	2.353356000	-1.151871000
1	-6.028440000	0.658650000	-2.335679000

1	-0.841802000	1.193408000	1.586304000
1	-3.231681000	-1.214743000	-1.373233000
1	-0.555315000	-3.035730000	0.608520000
1	-5.132609000	-0.851483000	-2.530463000
1	-2.392495000	0.300215000	-1.054252000
1	0.928259000	-0.949746000	1.660064000
1	-1.380284000	-2.333136000	-0.781889000
1	-4.390800000	0.690472000	-3.025332000
1	-0.026908000	-0.065542000	-0.796001000
7	-4.529471000	0.337531000	-0.909252000
7	-1.749578000	-1.372485000	1.064938000
13	0.013494000	0.065889000	0.809674000
1	6.144650000	-0.618410000	0.152244000
6	5.622653000	-1.201068000	-0.610664000
6	2.290751000	1.838262000	1.928915000
6	3.530717000	-0.121480000	-0.017446000
6	2.758791000	1.150915000	-0.381246000
6	3.816836000	-1.178956000	-2.190325000
6	1.097393000	2.814047000	0.081104000
1	5.364629000	-2.185650000	-0.176618000
1	2.669502000	0.914431000	2.363160000
1	2.836113000	-0.943259000	0.211213000
1	1.501410000	2.216495000	2.579789000
1	4.120065000	0.056159000	0.884905000
1	6.319051000	-1.372390000	-1.435890000
1	3.456231000	-2.180570000	-1.890440000
1	3.100289000	2.580629000	1.880495000
1	0.321293000	3.141817000	0.771856000
1	2.242369000	1.002992000	-1.330918000
1	4.522955000	-1.303378000	-3.015403000
1	0.636318000	2.611683000	-0.886845000
1	3.486626000	1.963351000	-0.523326000
1	2.961477000	-0.616126000	-2.566851000
1	1.843632000	3.611891000	-0.038879000
7	1.719621000	1.576025000	0.593982000
7	4.463946000	-0.463275000	-1.096110000

Geometrical parameters for $\text{AlH}_3 \cdot 2\text{TMEDA}$ (C_1 symmetry; distances in Å; angles in deg):



S32: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_i symmetry) for TMPDA (ligand).

6	0.879745000	0.359138000	0.175536000
1	0.573470000	0.600577000	-0.859575000
6	-0.076825000	-0.664562000	0.797825000
1	0.396395000	-1.028893000	1.717118000
1	-0.191165000	-1.535352000	0.144930000
1	0.810126000	1.290858000	0.747282000
6	-1.477224000	-0.128886000	1.180345000
1	-1.361114000	0.775718000	1.788464000
1	-1.941026000	-0.878388000	1.832733000
7	2.280690000	-0.068106000	0.217658000
7	-2.449038000	0.171804000	0.132155000
6	2.548797000	-1.200956000	-0.658996000
1	3.598132000	-1.492216000	-0.568839000
1	1.941726000	-2.060819000	-0.372082000
1	2.346590000	-0.976491000	-1.724652000
6	-2.247071000	1.402606000	-0.611448000
1	-1.441977000	1.356503000	-1.366381000
1	-3.171593000	1.664672000	-1.136359000
1	-2.014737000	2.217513000	0.079002000

6	3.181368000	1.037761000	-0.077405000
1	4.218027000	0.707309000	0.027747000
1	3.055870000	1.441942000	-1.100586000
1	3.014336000	1.852765000	0.631278000
6	-2.797000000	-0.952575000	-0.715911000
1	-2.005636000	-1.244288000	-1.431048000
1	-3.029754000	-1.824843000	-0.098349000
1	-3.689982000	-0.707613000	-1.299044000

S33: DFT Calculated Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_i symmetry) for $AlH_3 \cdot TMPDA$ (1:1).

6	1.681699000	-0.556372000	-0.020962000
1	1.427138000	-0.474846000	1.053387000
6	0.644005000	0.179746000	-0.880599000
1	0.988464000	0.125153000	-1.916813000
1	0.621141000	1.243781000	-0.631375000
1	1.629851000	-1.620766000	-0.270334000
6	-0.775527000	-0.421244000	-0.799262000
1	-0.730478000	-1.453862000	-0.442942000
1	-1.226133000	-0.453338000	-1.792133000
7	3.050056000	-0.115038000	-0.278900000
7	-1.777385000	0.279594000	0.071907000
6	3.325720000	1.215579000	0.248182000
1	4.349163000	1.503102000	-0.003034000
1	2.660197000	1.955166000	-0.200533000
1	3.215166000	1.272985000	1.348380000
6	-1.317566000	0.392425000	1.477738000
1	-0.436434000	1.036190000	1.559850000
1	-2.123952000	0.814251000	2.078477000
1	-1.080427000	-0.600299000	1.860052000
6	4.025922000	-1.080417000	0.212819000
1	5.032864000	-0.755447000	-0.059863000
1	3.995794000	-1.209236000	1.311272000
1	3.850357000	-2.054793000	-0.249001000
6	-2.117160000	1.623312000	-0.459517000
1	-1.255341000	2.297515000	-0.437903000
1	-2.473576000	1.523850000	-1.484922000
1	-2.915615000	2.049819000	0.148043000
13	-3.533436000	-0.875596000	0.056778000

1	-2.976625000	-2.242144000	0.680980000
1	-4.462266000	0.028268000	0.999138000
1	-3.865873000	-0.872673000	-1.510289000

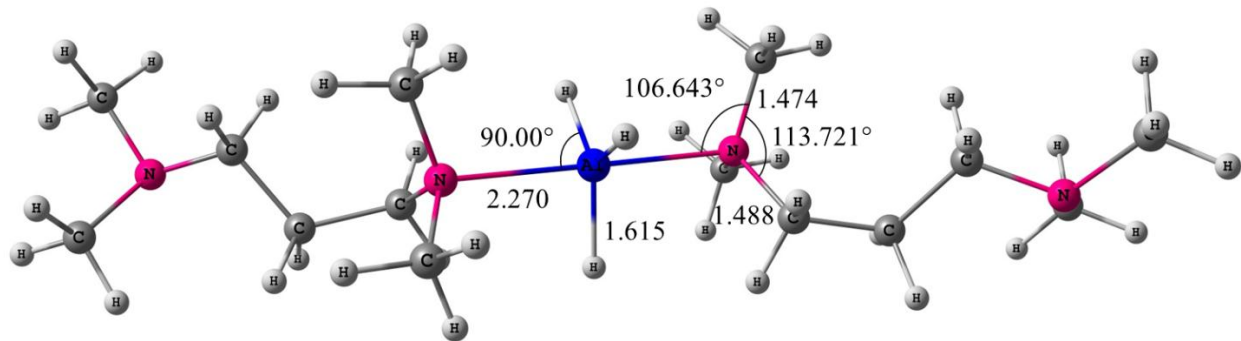
S34: DFT Calculated Cartesian coordinates and Geometrical parameters for $\text{AlH}_3\cdot 2\text{TMPDA}$.

- Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_2 symmetry):

6	-1.770921000	-1.724897000	2.499633000
6	-4.496162000	1.738984000	-0.505142000
6	-3.061252000	-0.757860000	0.727645000
6	-3.235577000	-0.329719000	-0.732961000
6	-1.491172000	-2.588732000	0.270687000
6	-5.036028000	0.204966000	-2.268883000
1	-2.585469000	-2.428462000	2.721660000
1	-1.911966000	-0.818803000	3.090733000
1	-4.137451000	1.837236000	0.520504000
1	-3.872016000	-1.457362000	0.979159000
1	-5.505474000	2.156638000	-0.545399000
1	-3.165761000	0.112539000	1.377202000
1	-0.816651000	-2.171480000	2.776483000
1	-2.300762000	-3.323582000	0.386427000
1	-3.842197000	2.353356000	-1.151871000
1	-6.028440000	0.658650000	-2.335679000
1	-0.841802000	1.193408000	1.586304000
1	-3.231681000	-1.214743000	-1.373233000
1	-0.555315000	-3.035730000	0.608520000
1	-5.132609000	-0.851483000	-2.530463000
1	-2.392495000	0.300215000	-1.054252000
1	0.928259000	-0.949746000	1.660064000
1	-1.380284000	-2.333136000	-0.781889000
1	-4.390800000	0.690472000	-3.025332000
1	-0.026908000	-0.065542000	-0.796001000
7	-4.529471000	0.337531000	-0.909252000
7	-1.749578000	-1.372485000	1.064938000
13	0.013494000	0.065889000	0.809674000
1	6.144650000	-0.618410000	0.152244000
6	5.622653000	-1.201068000	-0.610664000
6	2.290751000	1.838262000	1.928915000
6	3.530717000	-0.121480000	-0.017446000

6	2.758791000	1.150915000	-0.381246000
6	3.816836000	-1.178956000	-2.190325000
6	1.097393000	2.814047000	0.081104000
1	5.364629000	-2.185650000	-0.176618000
1	2.669502000	0.914431000	2.363160000
1	2.836113000	-0.943259000	0.211213000
1	1.501410000	2.216495000	2.579789000
1	4.120065000	0.056159000	0.884905000
1	6.319051000	-1.372390000	-1.435890000
1	3.456231000	-2.180570000	-1.890440000
1	3.100289000	2.580629000	1.880495000
1	0.321293000	3.141817000	0.771856000
1	2.242369000	1.002992000	-1.330918000
1	4.522955000	-1.303378000	-3.015403000
1	0.636318000	2.611683000	-0.886845000
1	3.486626000	1.963351000	-0.523326000
1	2.961477000	-0.616126000	-2.566851000
1	1.843632000	3.611891000	-0.038879000
7	1.719621000	1.576025000	0.593982000
7	4.463946000	-0.463275000	-1.096110000

Geometrical parameters for $\text{AlH}_3 \cdot 2\text{TMPDA}$ (C_2 symmetry; distances in Å; angles in deg):

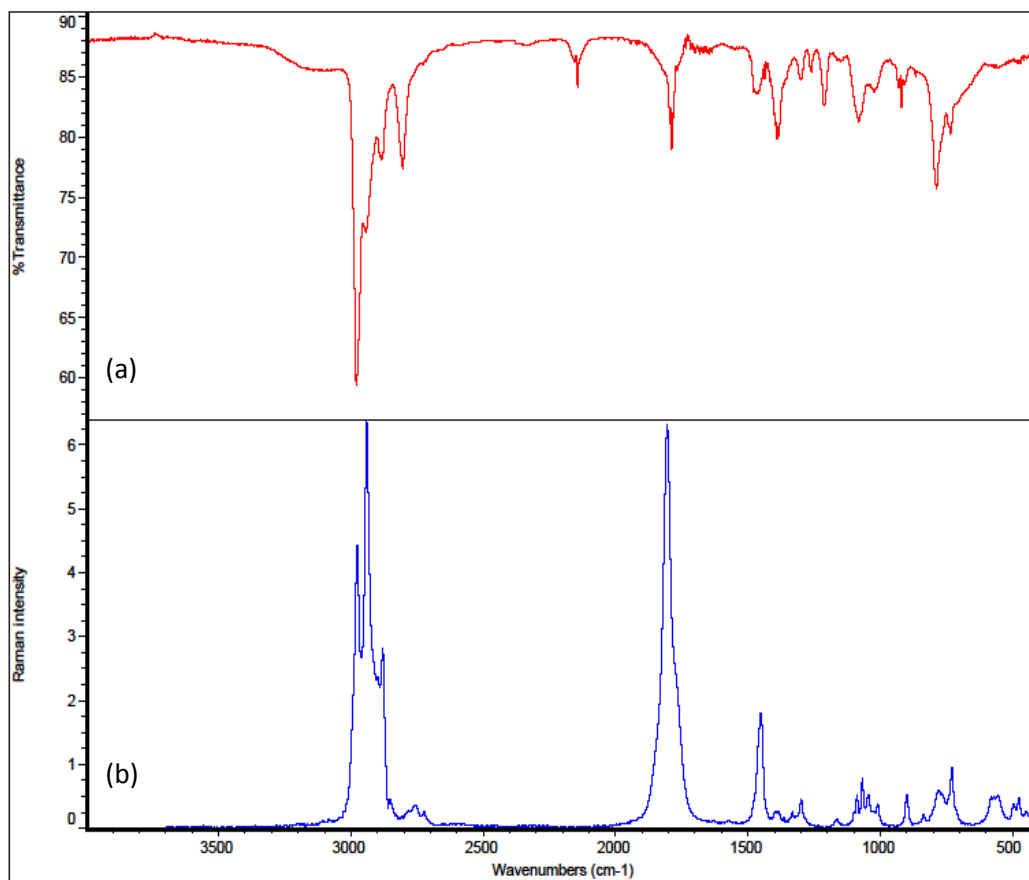


S35: Raman operating conditions for AlH_3 complexes.

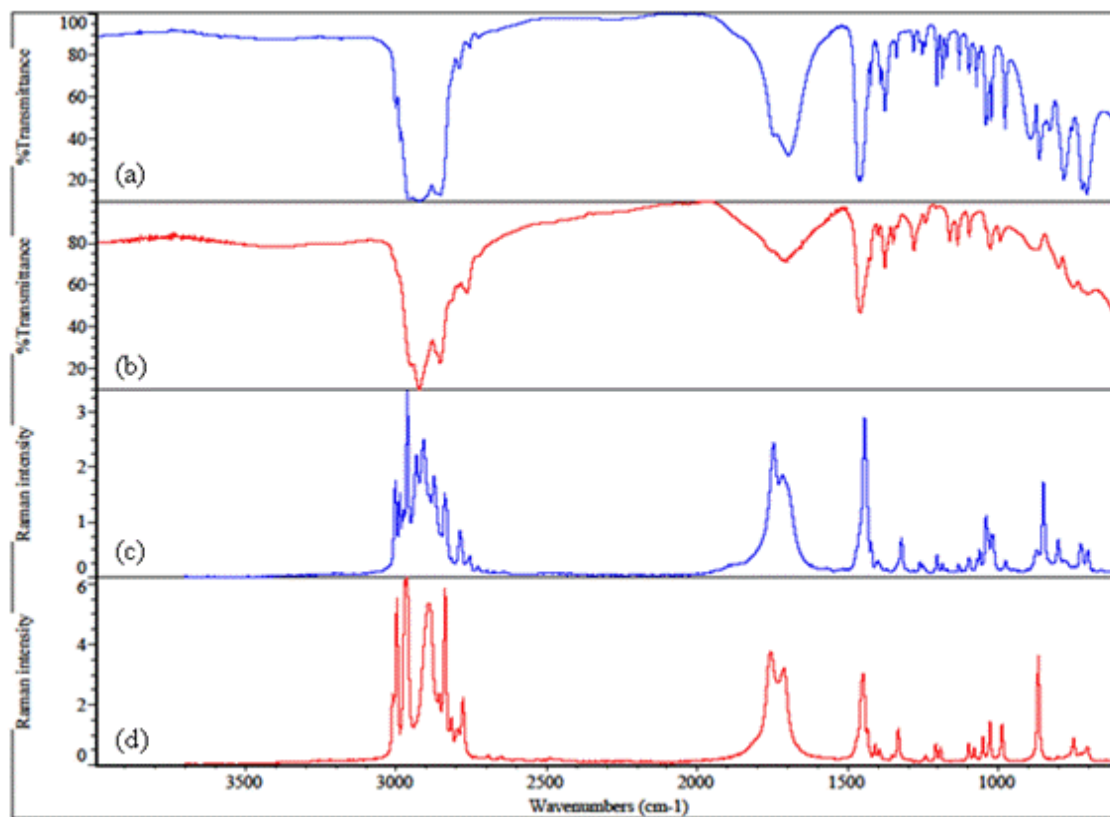
Complex	Number of scans	Laser power (W)
$\text{AlH}_3 \cdot \text{TMEDA}$	1024	0.105
$\text{AlH}_3 \cdot 2\text{BDMA}$	2048	0.303

$\text{AlH}_3 \cdot \text{TEA}$	2048	0.207
$\text{AlH}_3 \cdot \text{TMPDA}$	2048	0.105
$\text{AlH}_3 \cdot \text{DIOX}$	2048	0.303
$\text{AlH}_3 \cdot \text{DMEA}$	1024	0.0303
$\text{AlH}_3 \cdot 2\text{TMA}$	2048	0.303
$\text{AlH}_3 \cdot \text{TMA}$	2048	0.0303
$\text{AlH}_3 \cdot \text{Et}_2\text{O}$	2028	0.210

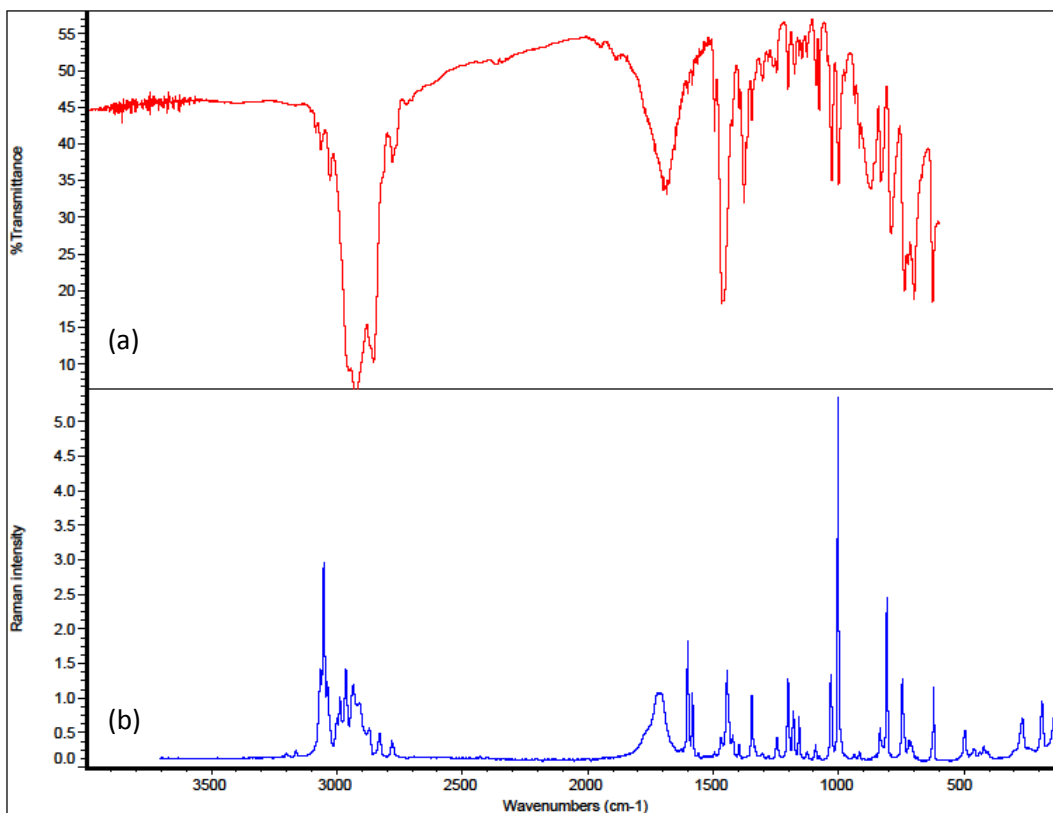
S36: Stacked FT-IR (a) and Raman spectra (b) of $\text{AlH}_3 \cdot \text{TEA}$. The FT-IR was conducted in the gas phase and the Raman spectrum was recorded for a neat liquid sample.



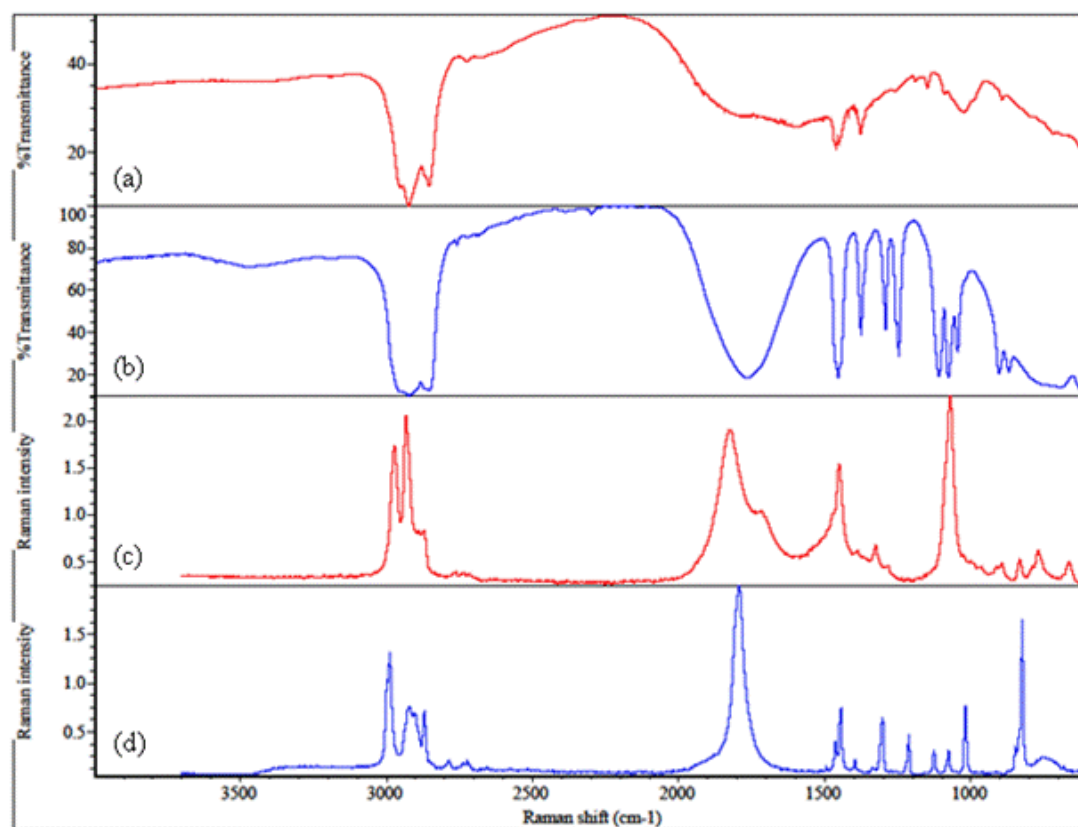
S37: Stacked Raman and FT-IR spectra of $\text{AlH}_3 \cdot \text{TMPDA}$ and $\text{AlH}_3 \cdot \text{TMEDA}$. (a) and (c) are FT-IR and Raman spectra of $\text{AlH}_3 \cdot \text{TMPDA}$, and (b) and (d) are FT-IR and Raman of $\text{AlH}_3 \cdot \text{TMEDA}$; respectively. FT-IR spectra were measured in a Nujol Mull, and Raman spectra were recorded for solid samples.



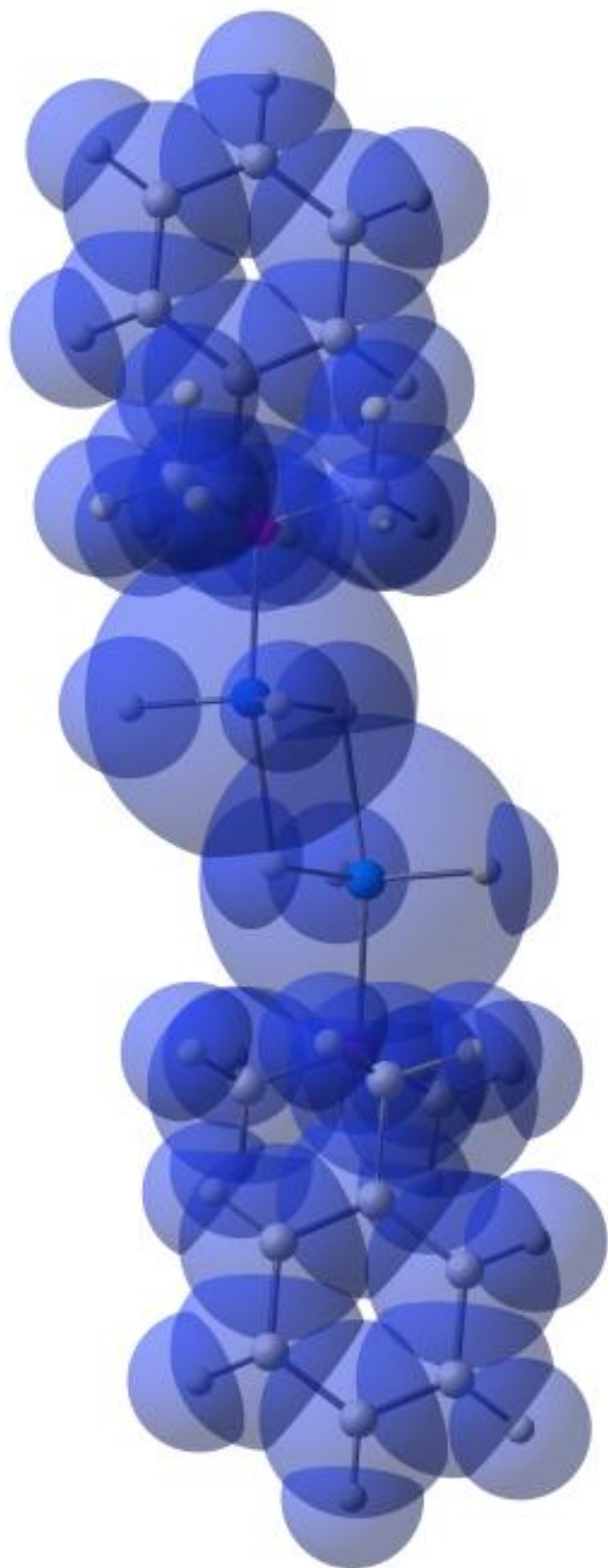
S38: Stacked FT-IR (a) and Raman spectra (b) of $\text{AlH}_3 \cdot 2\text{BDMA}$. The FT-IR spectrum was measured in a Nujol Mull, and the Raman spectrum was recorded for the solid.



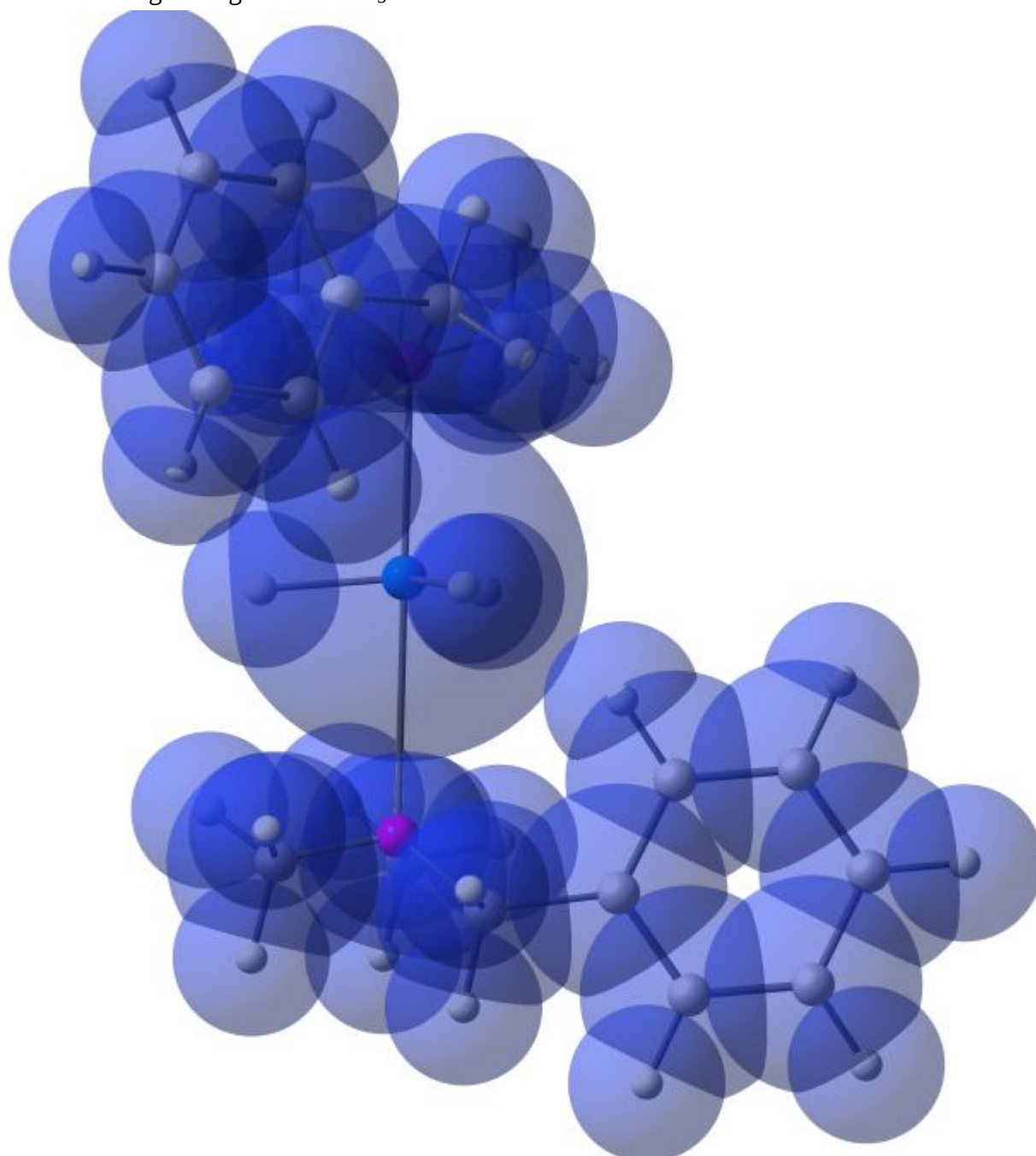
S39: Stacked Raman and FT-IR spectra of $\text{AlH}_3 \cdot n\text{Et}_2\text{O}$ and $\text{AlH}_3 \cdot \text{DIOX}$. (a) and (c) are FT-IR and Raman of $\text{AlH}_3 \cdot n\text{Et}_2\text{O}$, and (b) and (d) are FT-IR and Raman of $\text{AlH}_3 \cdot \text{DIOX}$; respectively. FT-IR spectra were measured in a Nujol Mull and the Raman spectra recorded as a solid.



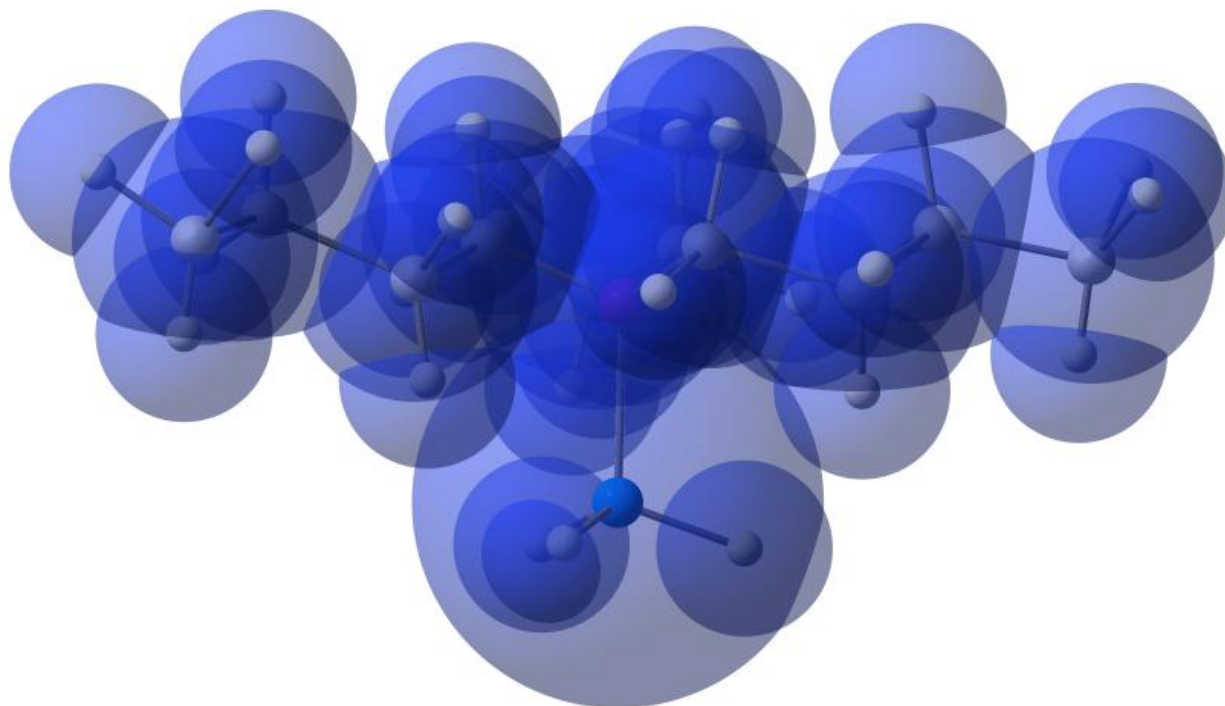
S40: Cone Angle Diagram for $\text{AlH}_3\cdot\text{BDMA}$ (dimer).



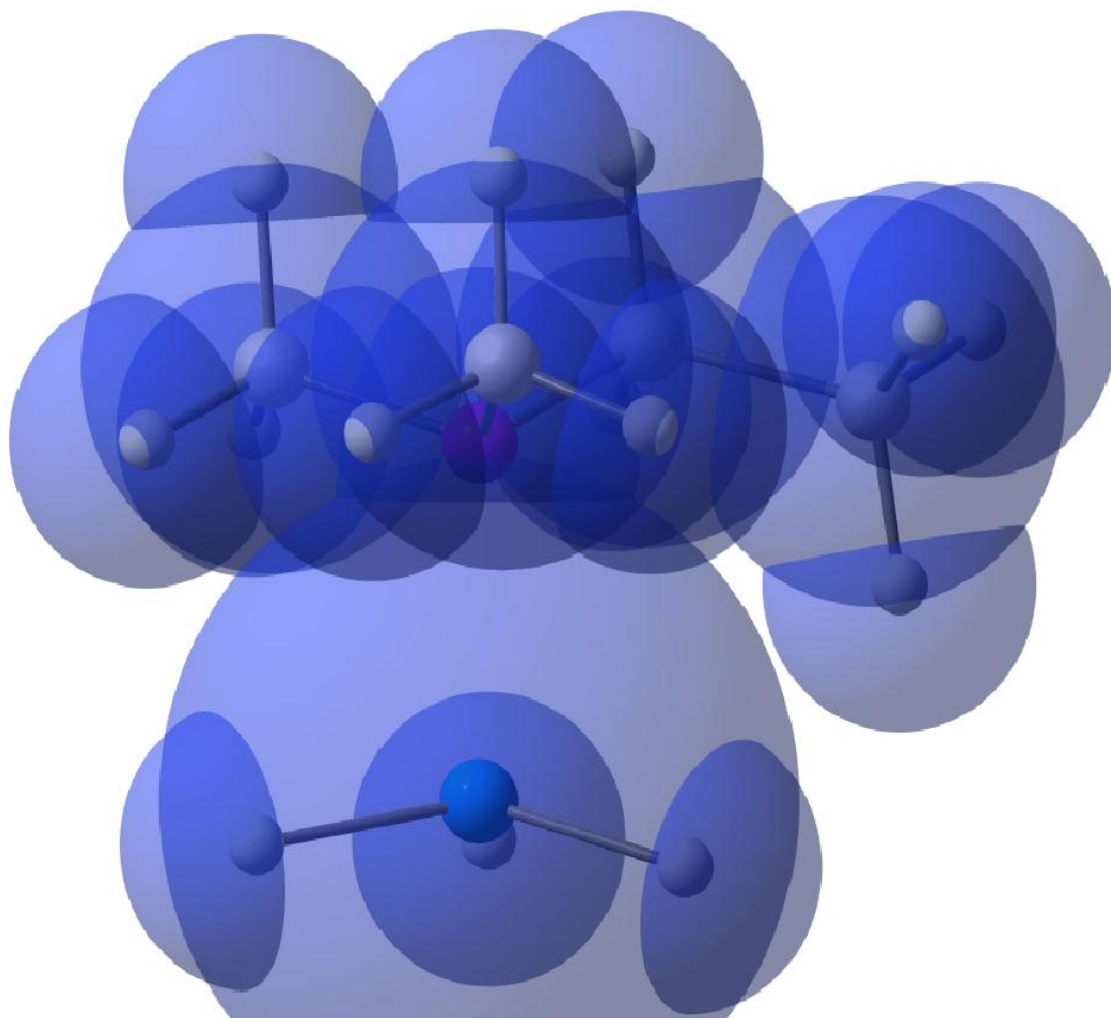
S41: Cone Angle Diagram for $\text{AlH}_3 \cdot 2\text{BDMA}$.



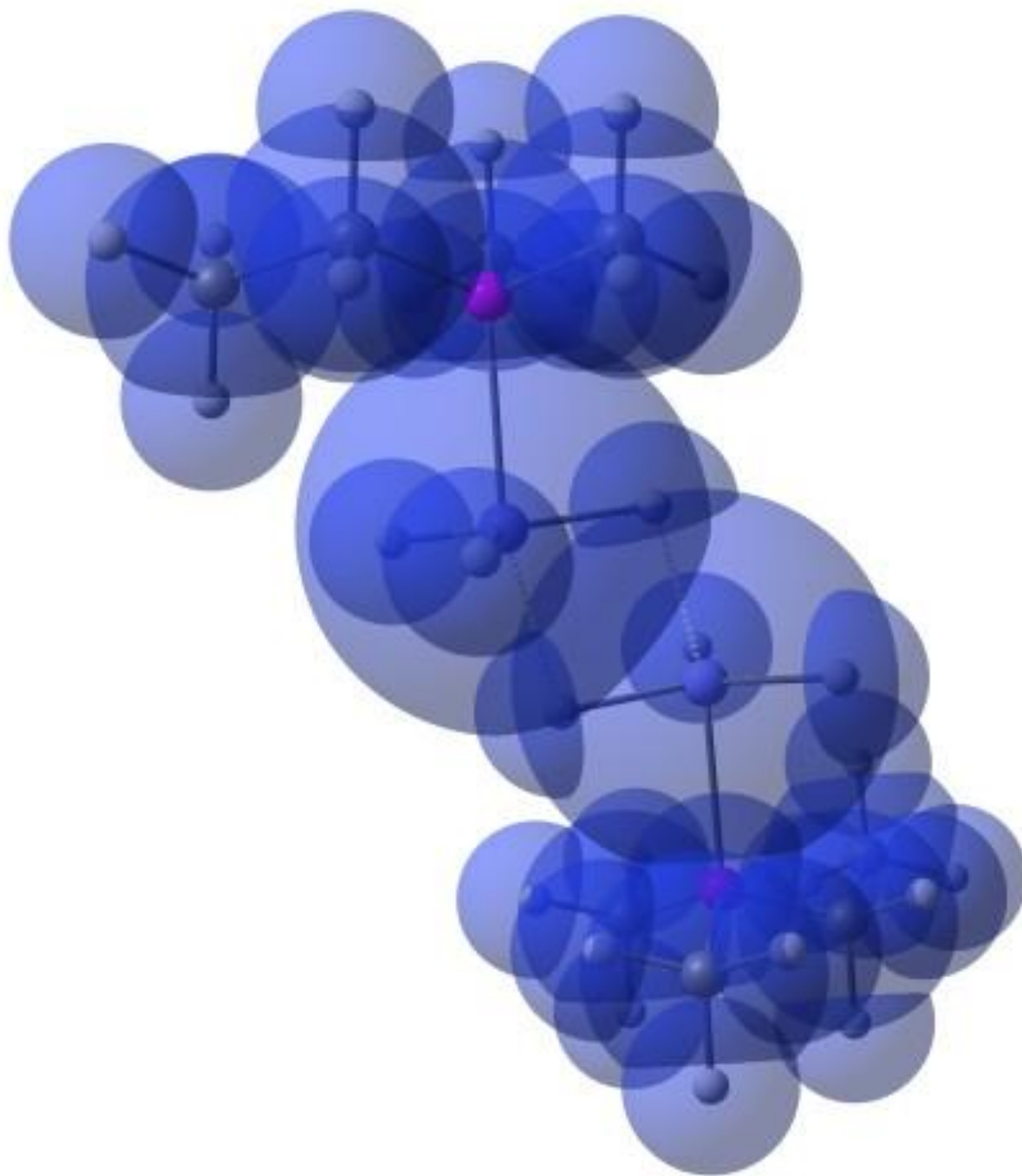
S42: Cone Angle Diagram for $\text{AlH}_3 \cdot n\text{-TBA}$.



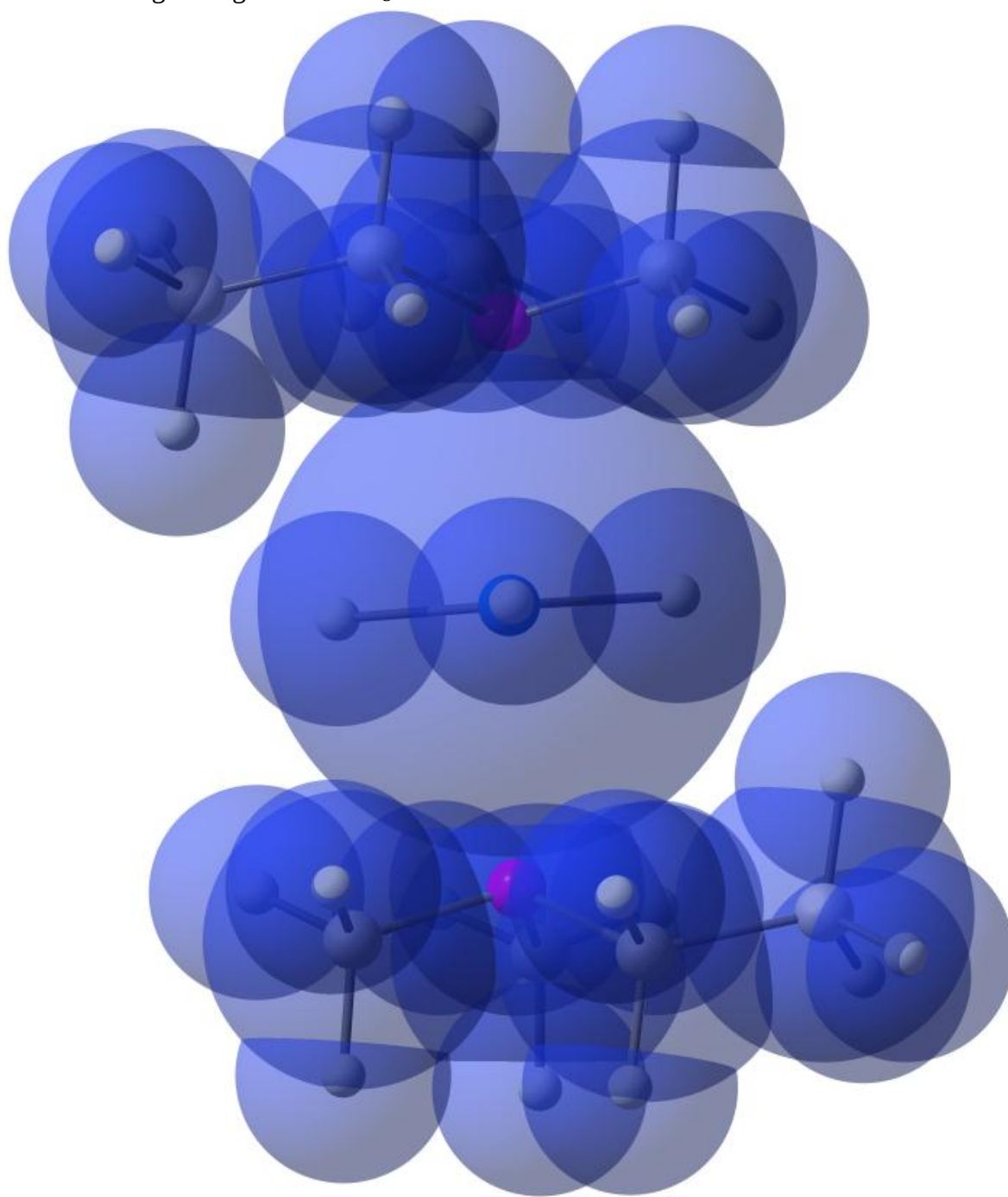
S43: Cone Angle Diagram for $\text{AlH}_3\cdot\text{DMEA}$.



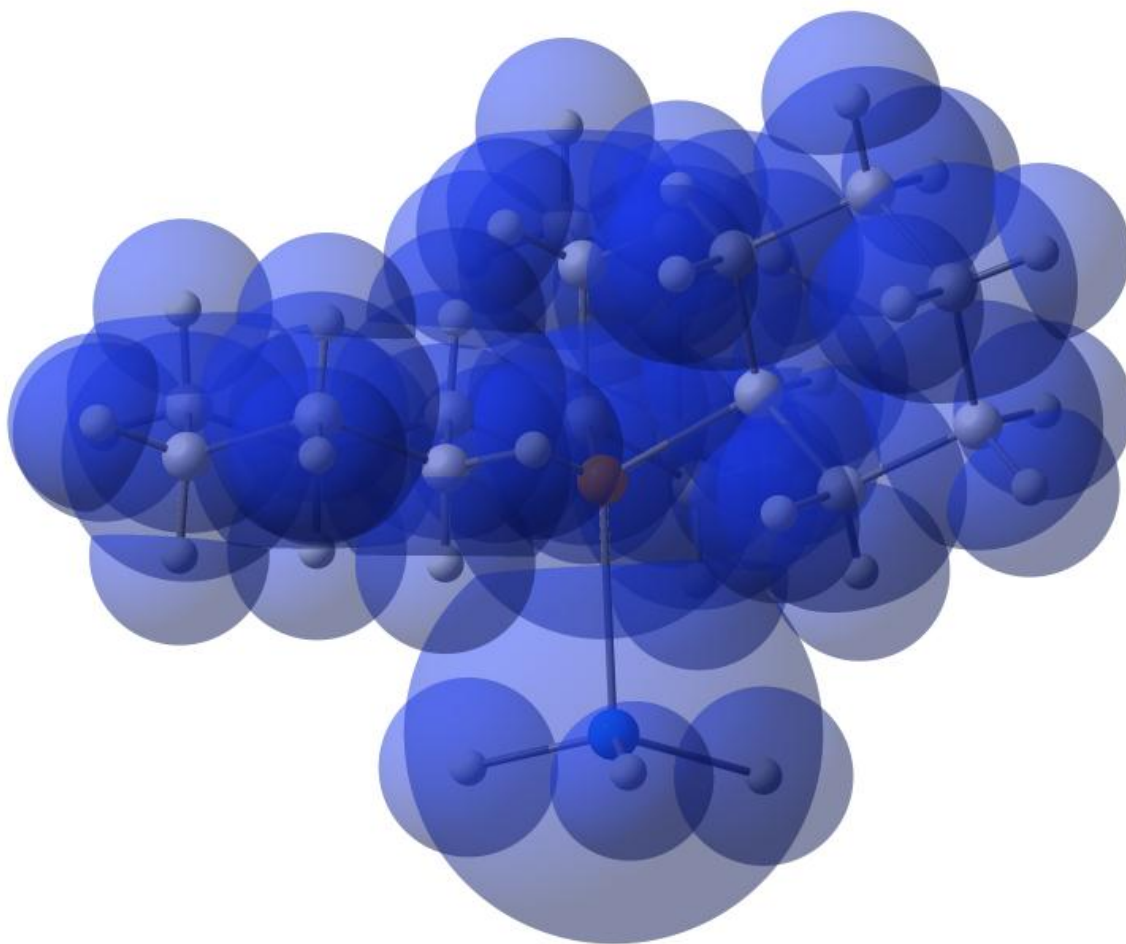
S44: Cone Angle Diagram for $\text{AlH}_3\cdot\text{DMEA}$ (dimer).



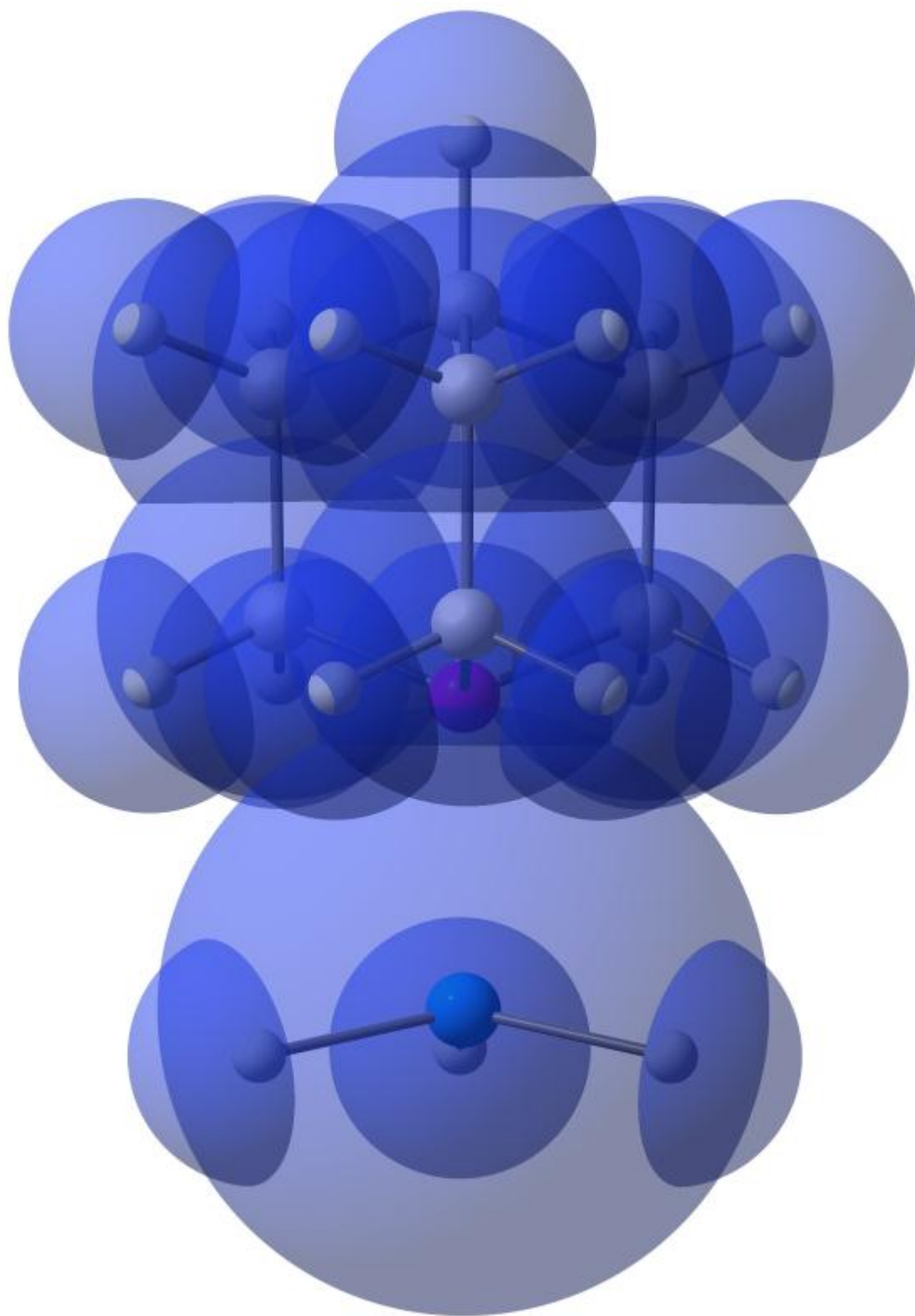
S45: Cone Angle Diagram for $\text{AlH}_3 \cdot 2\text{DMEA}$.



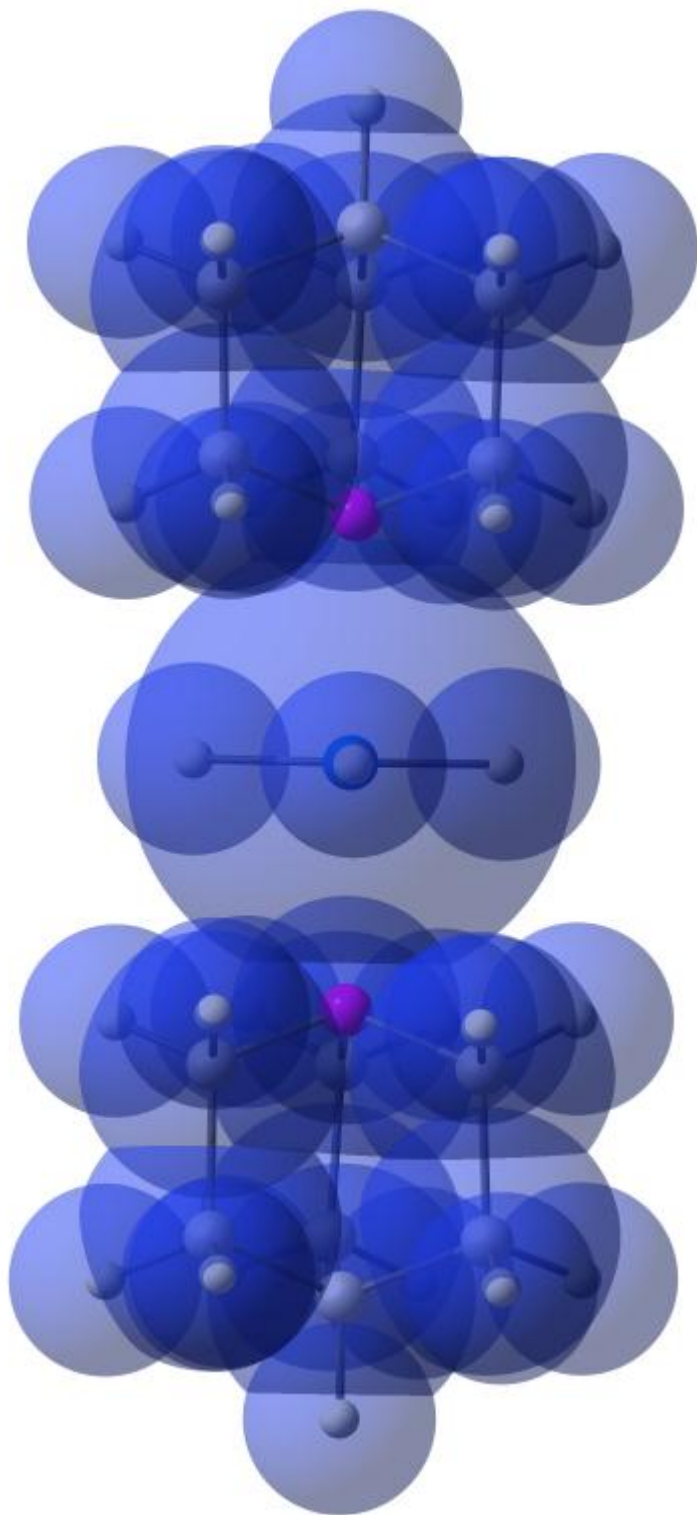
S46: Cone Angle Diagram for $\text{AlH}_3\cdot\text{PCy}_3$.



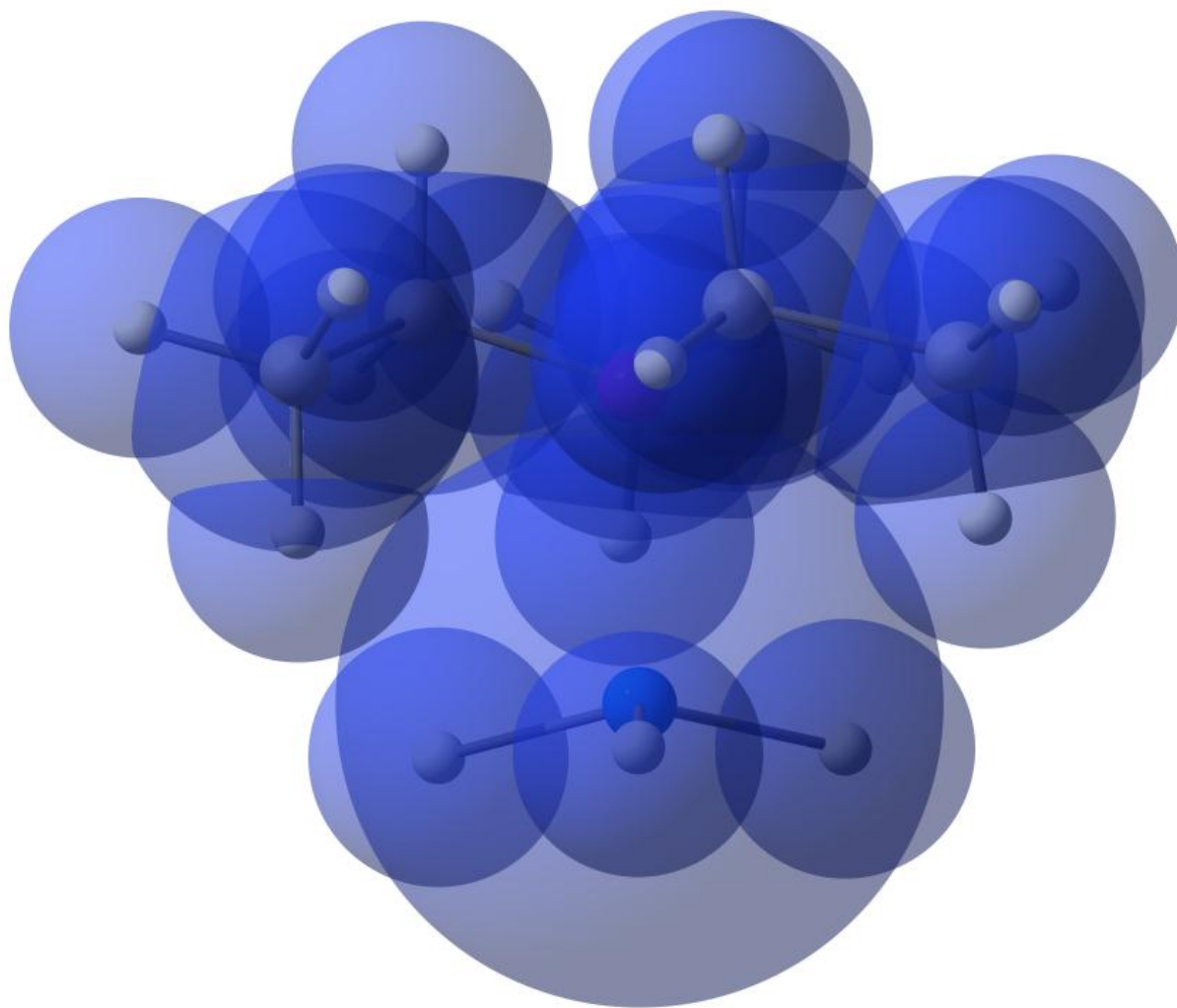
S47: Cone Angle Diagram for $\text{AlH}_3 \cdot \text{QUIN}$.



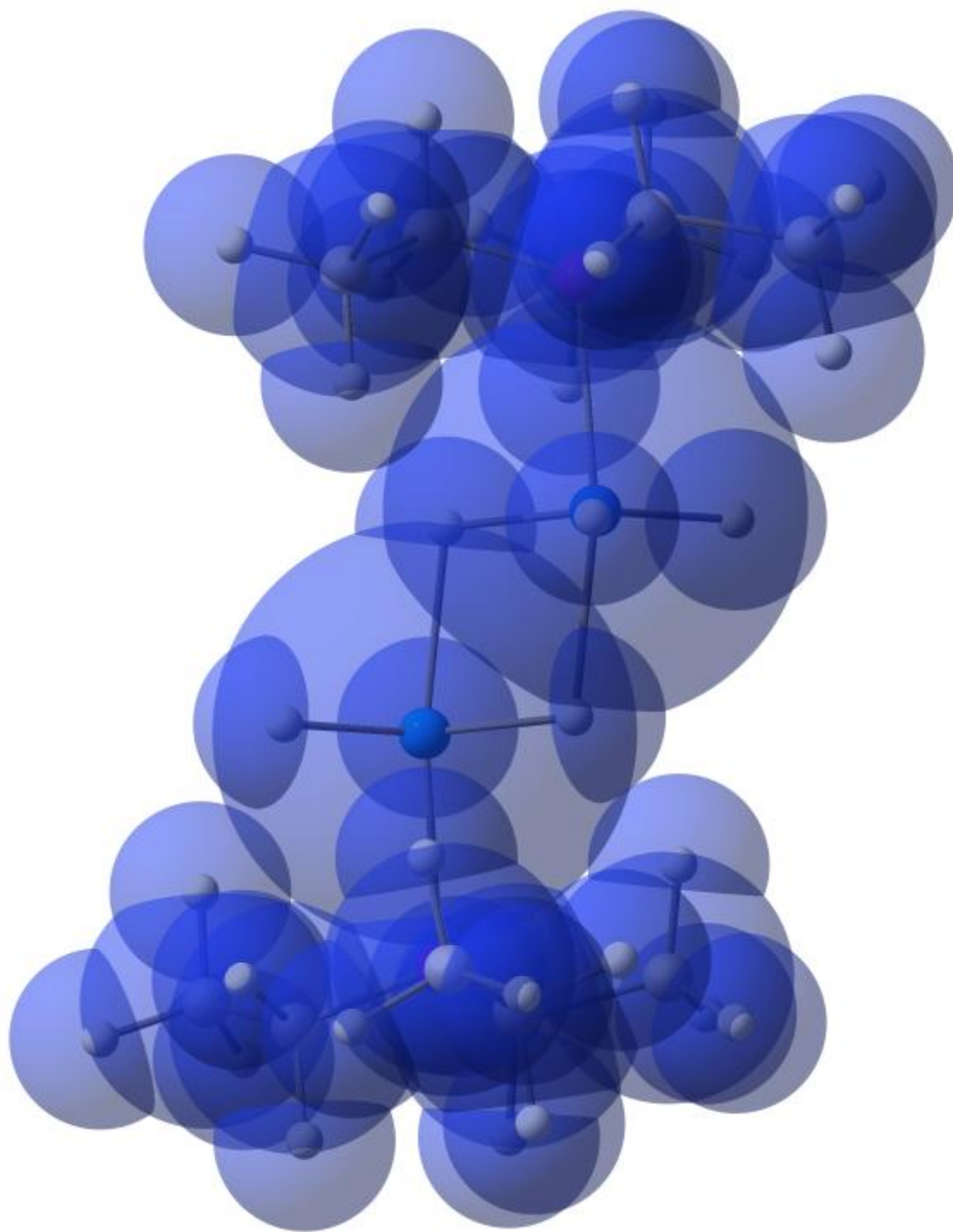
S48: Cone Angle Diagram for $\text{AlH}_3 \cdot 2\text{QUIN}$.



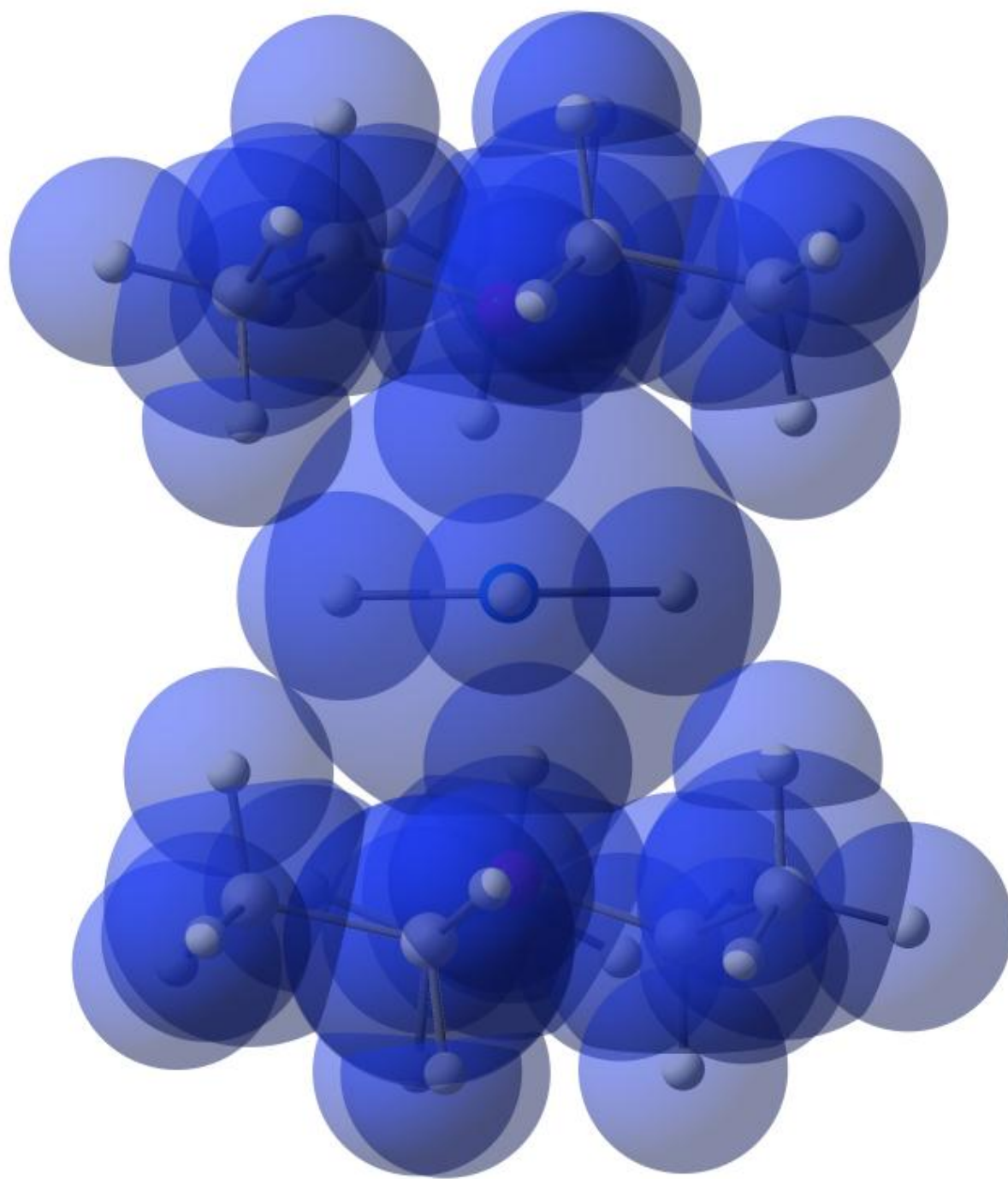
S49: Cone Angle Diagram for $\text{AlH}_3 \cdot \text{TEA}$.



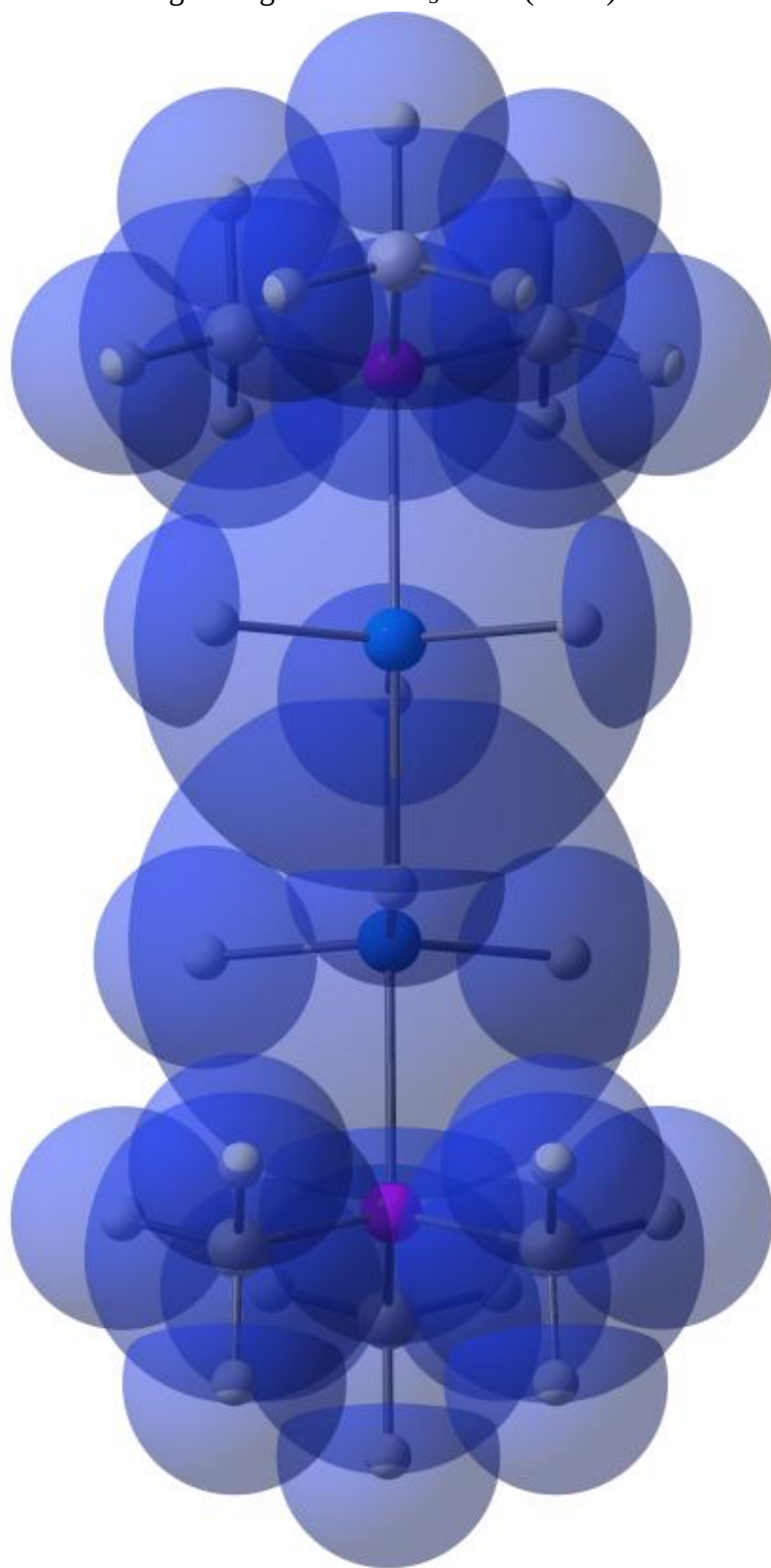
S50: Cone Angle Diagram for $\text{AlH}_3\cdot\text{TEA}$ (dimer).



S51: Cone Angle Diagram for $\text{AlH}_3 \cdot 2\text{TEA}$.



S52: Cone Angle Diagram for $\text{AlH}_3\cdot\text{TMA}$ (dimer).



S53: Cone Angle Diagram for $\text{AlH}_3 \cdot 2\text{TMA}$.

