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Lewis Base Complexes of AlH_3: Structural Determination of Monomeric and Polymeric Adducts by X-Ray Crystallography and DFT Calculations

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S1: DFT-calculated symmetries for AlH_3 complexes at the B3LYP/6311G(d,p) level of theory.

Ligand	Highest Symmetry
BDMA (2:1)	C_2
DIOX (2:1)	C_{2v}
TEA(1:1)	C_3
TMEDA (2:1)	C_1
TMPDA (2:1)	C_2

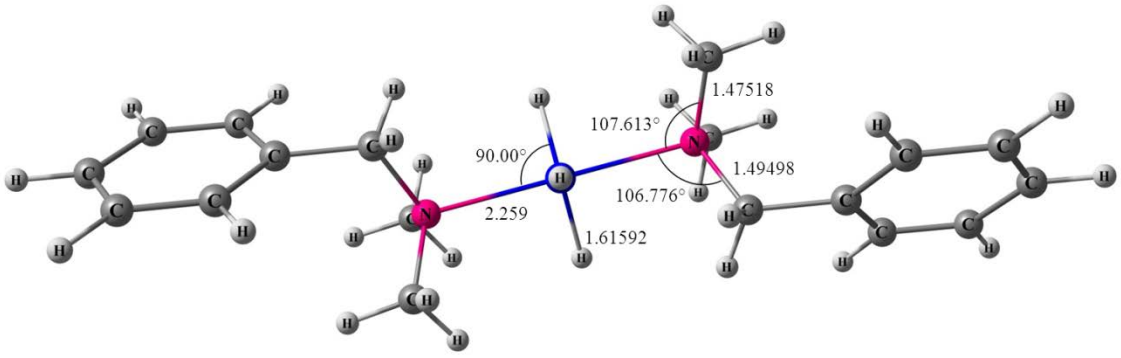
S2: Cartesian coordinates and Geometrical parameters for AlH_3·2BDMA

- 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 $AlH_3 \cdot 2BDMA$ (*C*2 symmetry; distances in Å; angles in deg):



S3: Cartesian coordinates and Geometrical parameters for $AlH_3 \cdot 2TMEDA$

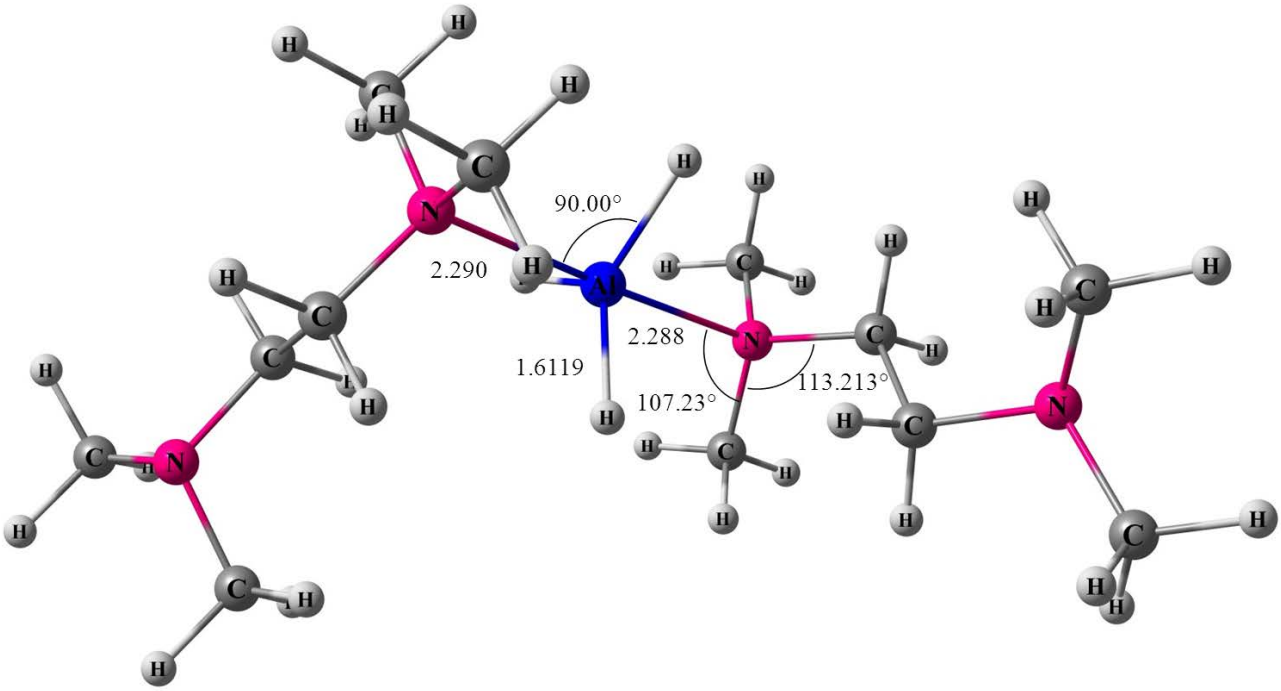
- Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_i symmetry):

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 AlH_3·2TMEDA (C_i symmetry; distances in Å; angles in deg):



S4: Cartesian coordinates and Geometrical parameters for AlH_3·2TMPDA

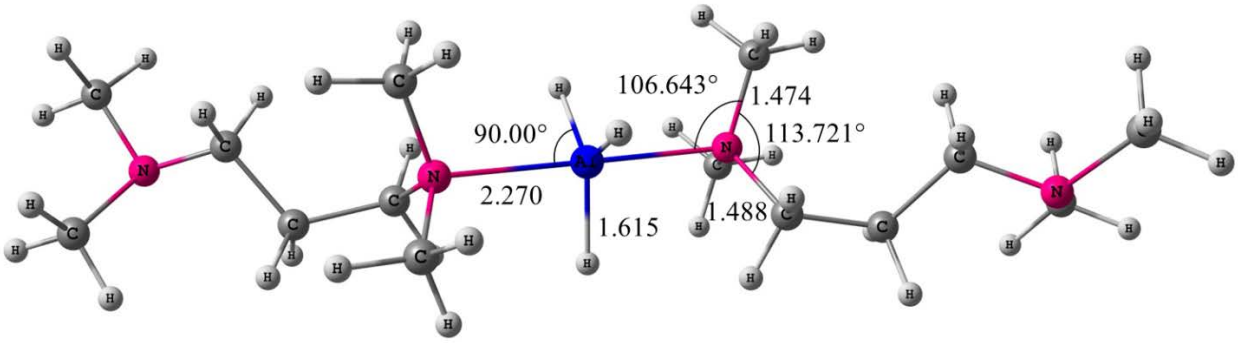
- Cartesian coordinates at the B3LYP/6311G(d,p) level of theory (C_2 symmetry):

6	0.216780000	5.415871000	0.258181000
1	-0.621712000	5.372065000	0.977656000
6	0.000000000	4.436495000	-0.904584000
1	0.708965000	4.727793000	-1.687306000
1	-0.995844000	4.558920000	-1.339844000
1	1.114646000	5.110479000	0.805201000
6	0.268449000	2.947205000	-0.612337000
1	1.200747000	2.838701000	-0.051070000
1	0.419560000	2.436633000	-1.566644000

7	0.435261000	6.790329000	-0.198180000
7	-0.754560000	2.140813000	0.106878000
6	-0.765131000	7.389611000	-0.767106000
1	-0.537967000	8.397986000	-1.121219000
1	-1.114462000	6.810571000	-1.623362000
1	-1.595352000	7.462039000	-0.037538000
6	-0.925114000	2.523503000	1.520423000
1	-1.410368000	3.499689000	1.631582000
1	-1.538962000	1.768049000	2.014044000
1	0.049808000	2.545707000	2.008542000
6	0.975029000	7.624627000	0.867297000
1	1.194758000	8.622105000	0.478144000
1	0.283717000	7.739320000	1.724305000
1	1.908352000	7.195270000	1.239554000
6	-2.055815000	2.140554000	-0.584640000
1	-2.543902000	3.122687000	-0.551254000
1	-1.912190000	1.843780000	-1.624565000
1	-2.707441000	1.409132000	-0.104278000
13	0.000000000	0.000000000	0.100186000
1	1.319609000	0.459160000	0.909488000
1	-1.319609000	-0.459160000	0.909488000
1	0.000000000	0.000000000	-1.513883000
6	-0.216780000	-5.415871000	0.258181000
1	0.621712000	-5.372065000	0.977656000
6	0.000000000	-4.436495000	-0.904584000
1	-0.708965000	-4.727793000	-1.687306000
1	0.995844000	-4.558920000	-1.339844000
1	-1.114646000	-5.110479000	0.805201000
6	-0.268449000	-2.947205000	-0.612337000
1	-1.200747000	-2.838701000	-0.051070000
1	-0.419560000	-2.436633000	-1.566644000
7	-0.435261000	-6.790329000	-0.198180000
7	0.754560000	-2.140813000	0.106878000
6	0.765131000	-7.389611000	-0.767106000
1	0.537967000	-8.397986000	-1.121219000
1	1.114462000	-6.810571000	-1.623362000
1	1.595352000	-7.462039000	-0.037538000
6	0.925114000	-2.523503000	1.520423000
1	1.410368000	-3.499689000	1.631582000
1	1.538962000	-1.768049000	2.014044000
1	-0.049808000	-2.545707000	2.008542000
6	-0.975029000	-7.624627000	0.867297000
1	-1.194758000	-8.622105000	0.478144000
1	-0.283717000	-7.739320000	1.724305000
1	-1.908352000	-7.195270000	1.239554000
6	2.055815000	-2.140554000	-0.584640000
1	2.543902000	-3.122687000	-0.551254000

1	1.912190000	-1.843780000	-1.624565000
1	2.707441000	-1.409132000	-0.104278000

Geometrical parameters for AlH_3·TMPDA (C_2 symmetry; distances in Å; angles in deg):



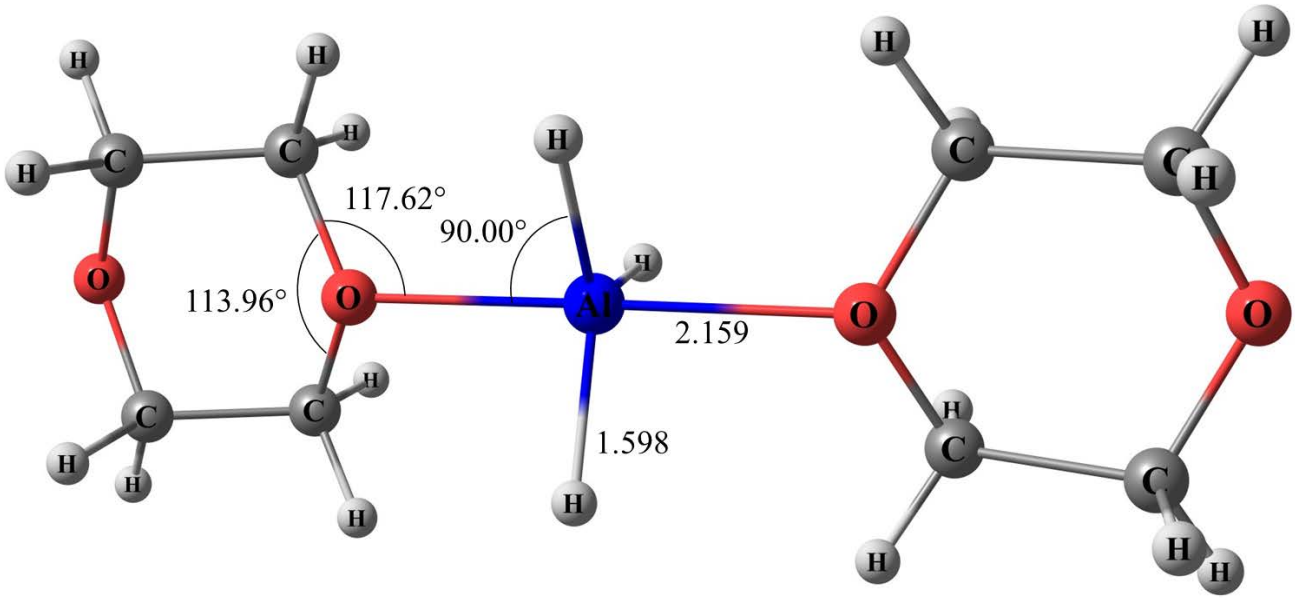
S5: Cartesian coordinates and Geometrical parameters for AlH_3·2DIOX

- 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 $AlH_3 \cdot 2DIOX$ (C_{2v} symmetry; distances in Å; angles in deg):



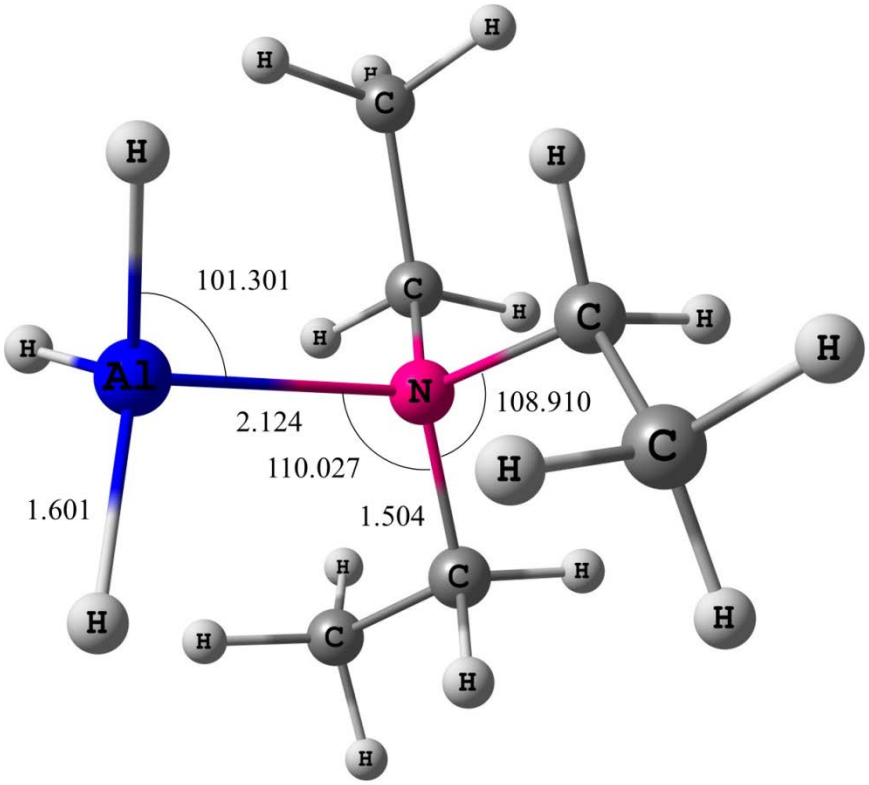
S6: Cartesian coordinates and Geometrical parameters for $AlH_3 \cdot TEA$

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

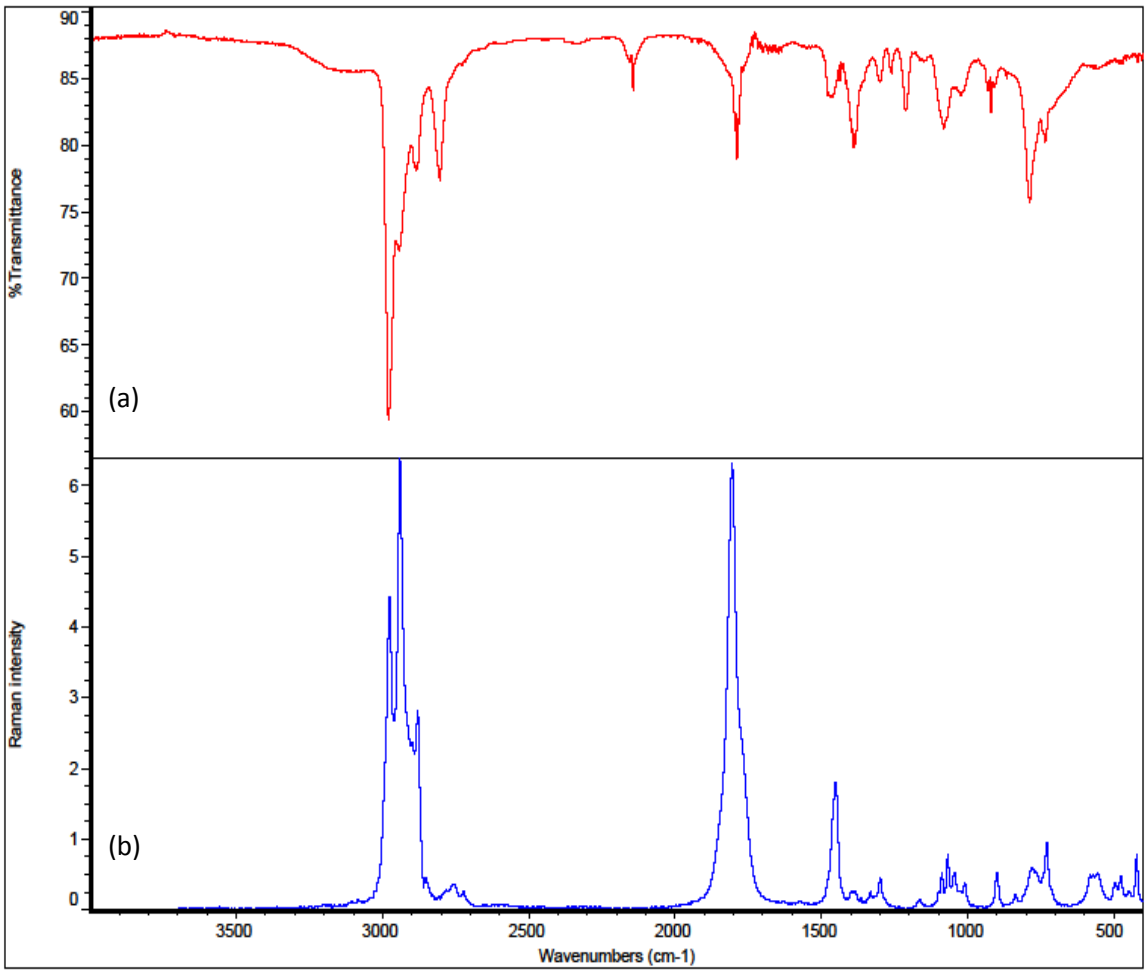
13	0.000000000	0.000000000	1.883481000
1	-0.022921000	-1.570271000	2.197320000
1	1.371355000	0.765285000	2.197320000
1	-1.348434000	0.804986000	2.197320000
7	0.000000000	0.000000000	-0.240401000
6	-0.668928000	1.244896000	-0.755536000
1	-1.681237000	1.243412000	-0.356467000
1	-0.737623000	1.162463000	-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

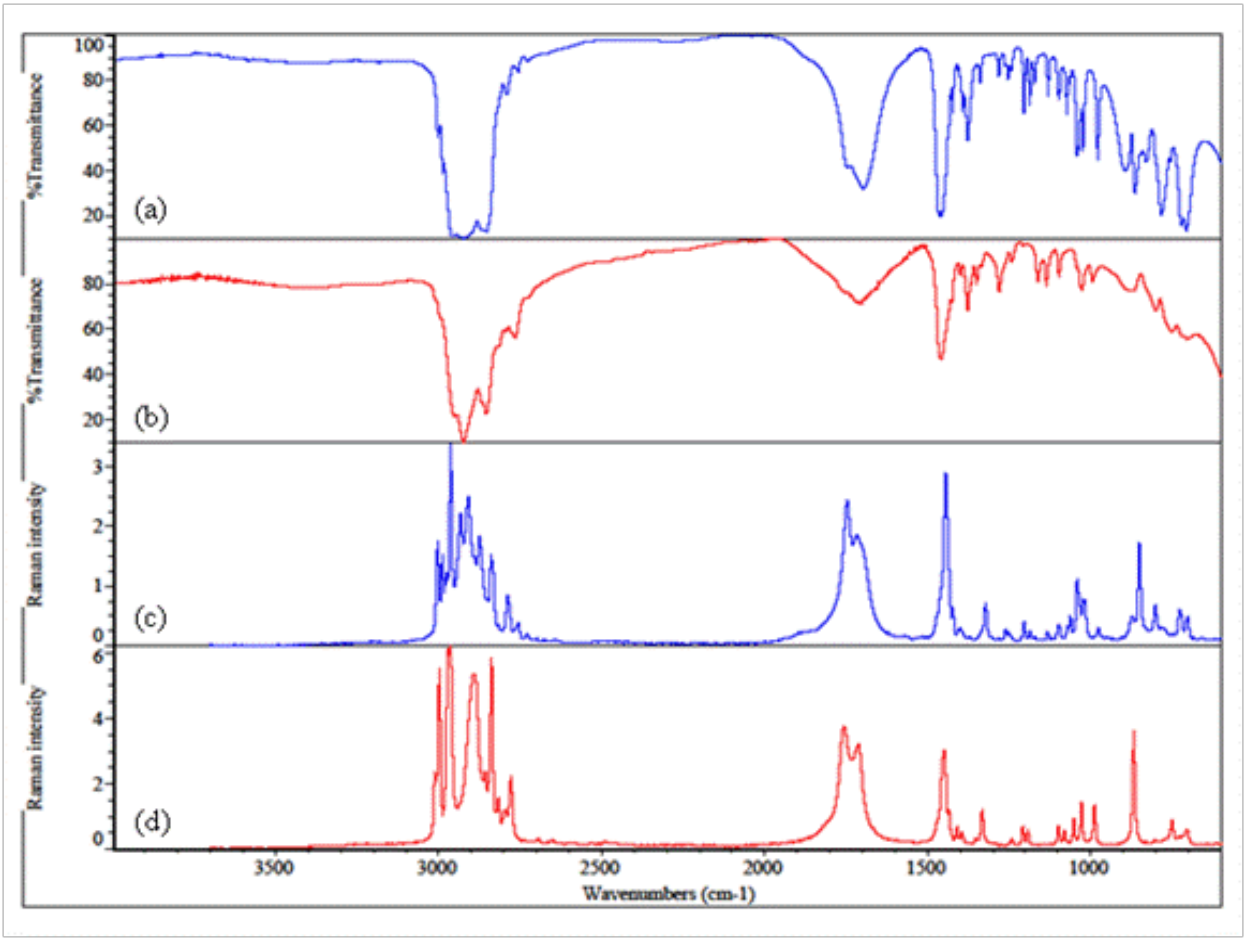
Geometrical parameters for $AlH_3 \cdot TEA$ (C_3 symmetry; distances in Å; angles in deg):



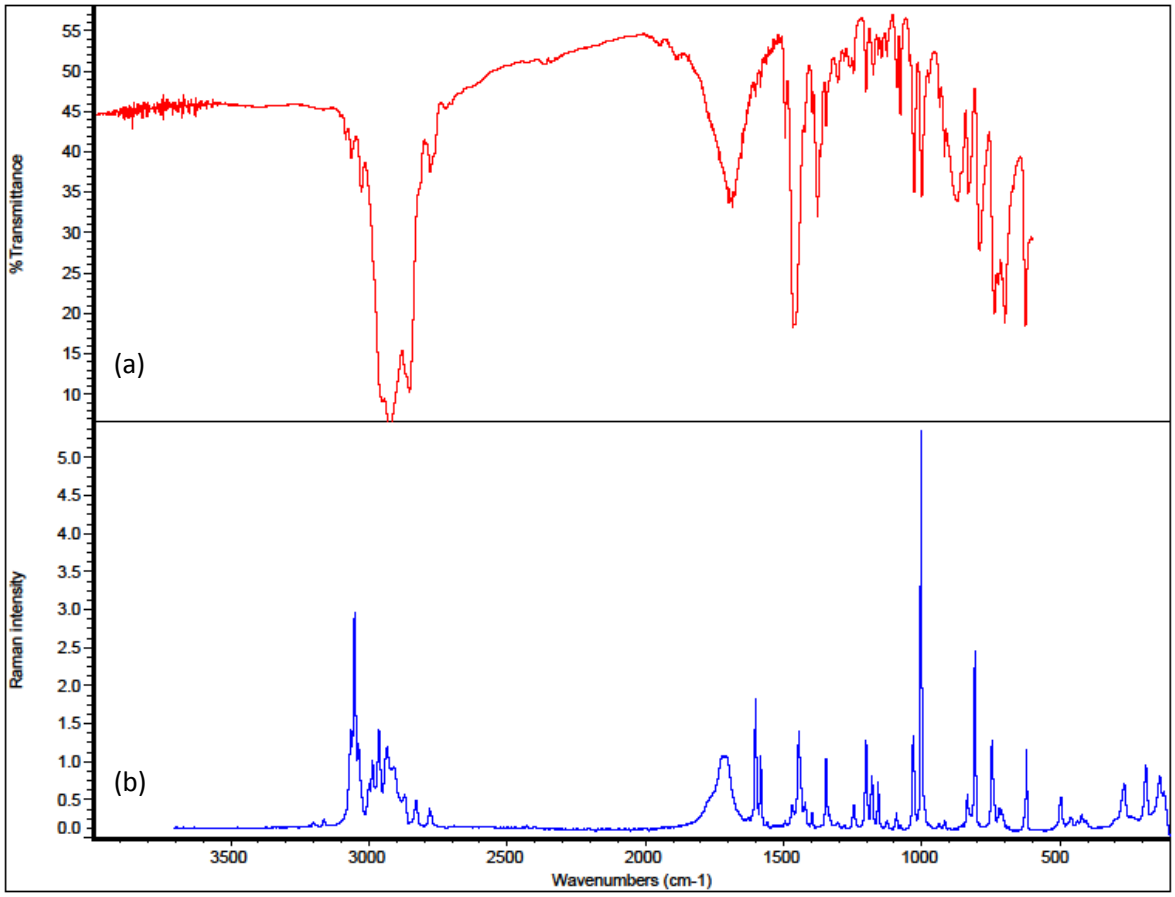
S7: Stacked FT-IR (a) and Raman spectra (b) of AlH_3·TEA. The FT-IR spectrum was measured for a sample in the gas phase and the Raman spectrum was recorded for a neat liquid sample.



S8: Stacked Raman and FT-IR spectra of AlH_3·TMPDA and AlH_3·TMEDA. (a) and (c) are FT-IR and Raman spectra of AlH_3·TMPDA, and (b) and (d) are FT-IR and Raman spectra of AlH_3·TMEDA; respectively. FT-IR spectra were measured in a Nujol Mull, and Raman spectra were recorded for solid samples.



S9: Stacked FT-IR spectra (a) and Raman spectra (b) of AlH_3·2BDMA. The FT-IR spectrum was measured in a Nujol Mull, and the Raman spectrum was recorded for the solid.



S10: Stacked Raman and FT-IR spectra of $AlH_3 \cdot nEt_2O$ and $AlH_3 \cdot DIOX$. (a) and (c) are FT-IR and Raman of $AlH_3 \cdot nEt_2O$, and (b) and (d) are FT-IR and Raman of $AlH_3 \cdot DIOX$; respectively. FT-IR spectra were measured in a Nujol Mull and the Raman spectra recorded as a solid.