The Nature of Chemical Bonding in Lewis Adducts as Reflected by ^{27}Al NMR Quadrupolar Coupling Constant: Combined Solid-State NMR and Quantum Chemical Approach

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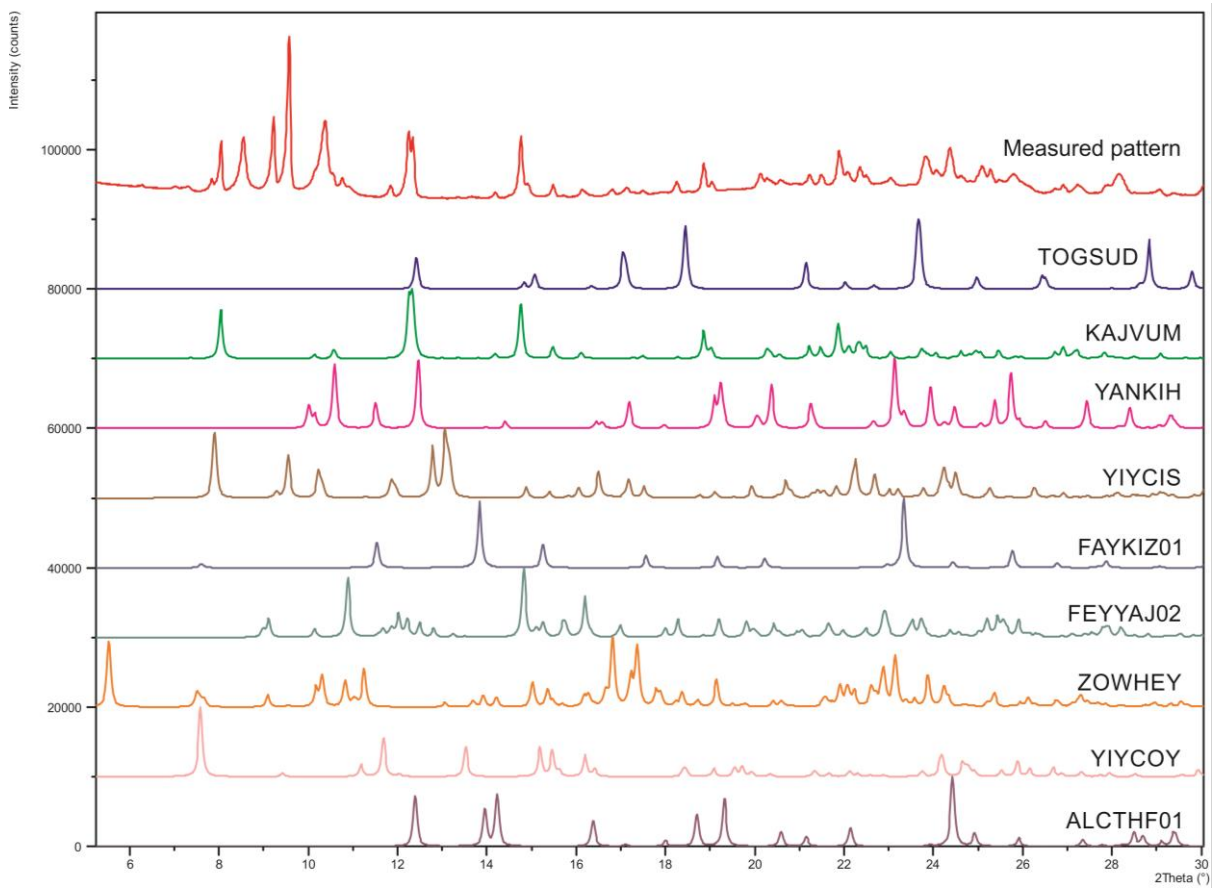


Figure S1. The measured PXRD pattern of as-prepared system compared with calculated PXRD patterns of selected CCDC entries. The comparison shows, that only crystalline phase represented by the powder diffraction pattern of CCDC's entry KAJVUM can be found in the sample.

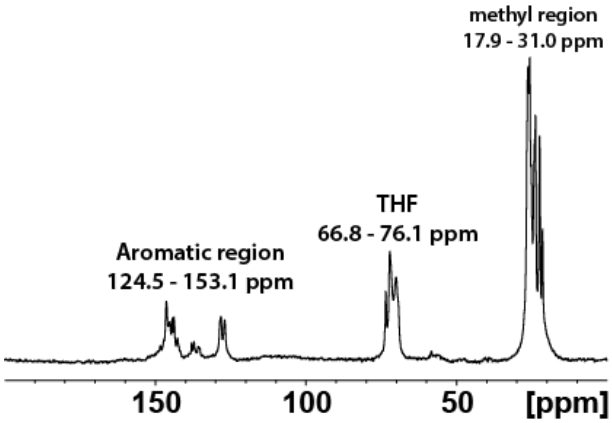


Figure S2 Experimental ^{13}C MAS NMR spectrum of multicomponent system investigated in this work.

The ^{13}C MAS NMR spectrum confirms presence of polycrystalline system, since all signals are well resolved and relatively narrow. On the other hand, complexity of the signals (splitting of signals is higher than predicted) indicate presence of several chemically identical entities in different crystalline forms. This spectrum clearly confirms presence of several independent structural units.

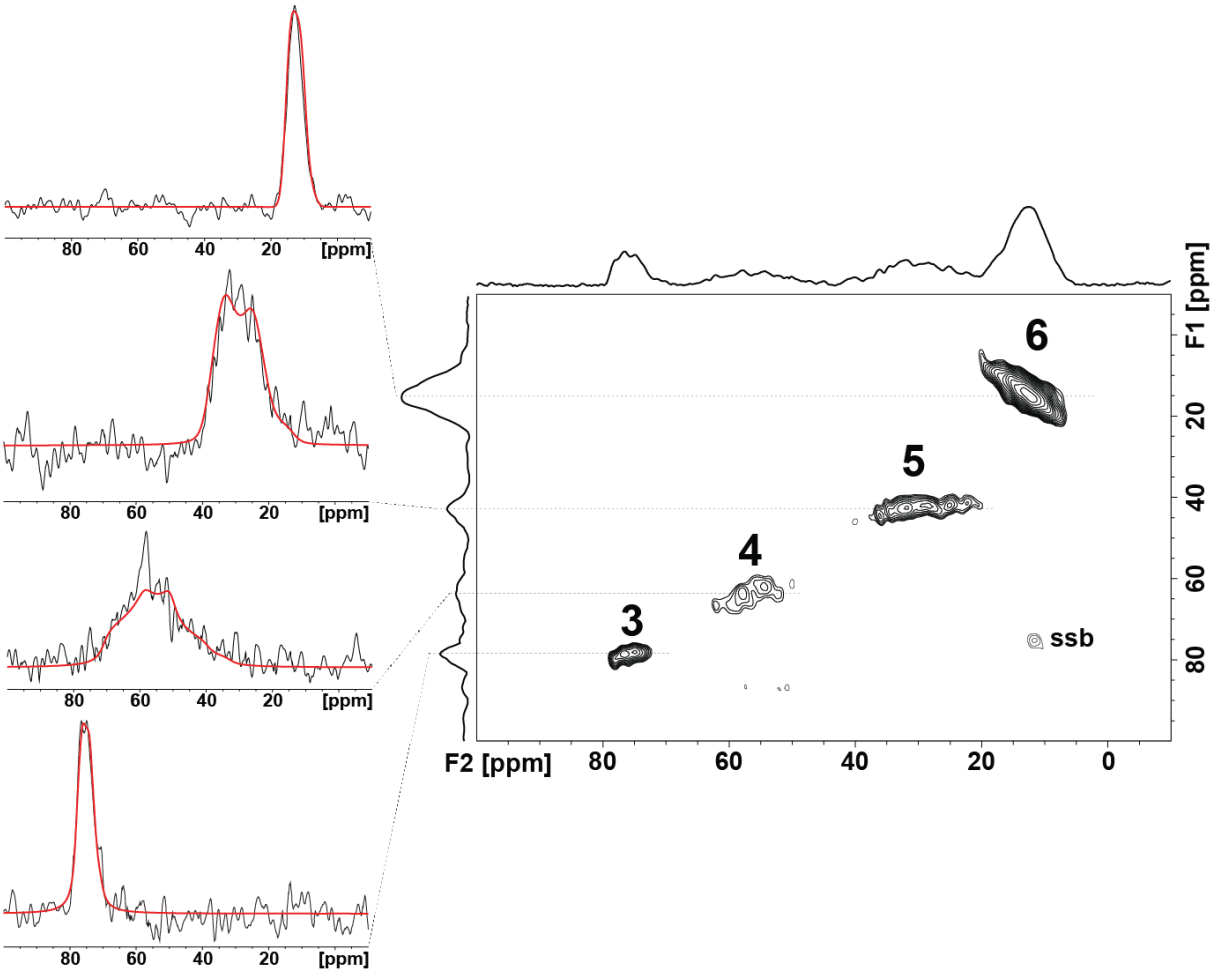


Figure S3: Experimental ^{27}Al 3Q/MAS NMR spectrum with slices and fitting (red lines) of individual signals. Fitting of individual slices was accomplished using data from Table 2 from main text.

From individual slices of ^{27}Al 3QMAS NMR spectrum follows that used calculated NMR parameters and experimental results in Figure 2b and c (from main text) are in mutual agreement.

Table S2. The DFT ^{27}Al NMR parameters for all possible structural units preselected based on PXRD pattern.

site	site	σ_{iso}^{cal} (ppm)	δ_{iso}^{cal} (ppm)[a]	C_Q (MHz)	η	Ω	κ	α (°)	β (°)	γ (°)
$AlCl_3$	Al^{VI}	523.0	-1.6*	0.32	0.33	1.38	0.56	180	83	180
FAYKIZ	Al^{III}	279.6	241.8	45.1	0.01	150.1	-0.97	218	0	205
FAYKIZ-01	Al^{III}	277.9	243.5	50.9	0.01	121.4	-0.98	184	0	102
ZOWHEY[b]	Al^{IV}	415.0	106.4	22.7	0.95	128.6	-0.53	271	8	86
YIYCOY[b]	Al^{IV}	400.2	121.2	33.3	0.55	191.3	-0.65	308	7	239
YIYCIS[b]	Al^{IV}	410.5	110.9	23.8	0.69	96.8	-0.49	217	9	84
YANKIH	Al^{IV}	423.4	98.0	17.7	0.65	76.1	-0.33	276	17	185
KAJVUM	Al^{IV}	405.9	115.5	28.3	0.13	42.4	0.03	207	77	201
ALCTHF	Al^{V}	476.2	45.2	6.14	0.06	150.5	0.87	1	89	360
ALCTHF-01	Al^{V}	475.5	45.9	6.74	0.12	152.0	0.89	182	89	0
TOGSUD	Al^{IV}	433.4	88.0	6.09	0.02	72.4	0.92	178	90	354
FEYYAJ[b,c]	Al^{IV}	427.4	94.0	2.25	0.70	19.1	0.13	79	82	170
	Al^{VI}	529.1	-7.7	6.55	0.16	62.9	-0.92	148	2	205
FEYYAJ-01[b,c]	Al^{IV}	426.3	95.1	1.16	0.63	13.7	-0.01	59	85	185
	Al^{VI}	528.1	-6.6	5.90	0.24	57.2	-0.95	204	2	226
FEYYAJ-02[b]	Al^{IV}	428.0	93.4	1.68	0.60	21.8	-0.19	187	5	241
	Al^{VI}	528.8	-8.4	6.28	0.16	57.7	-0.91	161	1	270

[a]$\delta_{iso}^{cal} = \sigma_{iso}^{cal}(AlCl_3) - \sigma_{iso}^{cal}$-1.6(ppm). [b]Asymmetric units contain two crystalographically distinct Al atoms with very similar calculated NMR parameters, which were used as averaged value. [c]The structure of these CIF files were modified by adding of hydrogens using ADF program. *Usually, ^{27}Al NMR spectra are referenced to the Al $(NO_3)_3$ or $AlCl_3$ in D_2O at 0.00 ppm. The used correction ($\delta_{iso}(AlCl_3)$ = -1.6 ppm) employed to converting of the chemical shielding (σ_{iso}^{cal}) to the chemical shift (δ_{iso}^{cal}) origin from experimental chemical shift of solid $AlCl_3$ defined in literature data.[1]

Table S2. The comparison of the supermolecular and SAPT interaction energies for small complexes.

dimer	ΔE_{HF}	ΔE_{MP2}	$\Delta E_{CCSD(T)}$	E_{SAPT}
$C_2H_2 \cdot AlCl_3$	–51.9	–62.2	–56.8	–55.0
$C_2H_4 \cdot AlCl_3$	–58.0	–71.5	–63.9	–60.5

ΔE_{method} refers to the counterpoise-corrected value obtained using the given method applied together with the standard aug-cc-pVDZ basis set, and E_{SAPT} is the result of the SAPT-DFT treatment described in the main text; all values are in kJ/mol.

Table S3. The values (in kJ/mol) of the interaction energies described in the main text

term	C_2H_2 *$AlCl_3$	C_2H_4 *$AlCl_3$	$AlCl_3$ *HCN	$AlCl_2Mes$ *HCN	$AlClMes_2$ * HCN	$AlMes_3$ *HCN	$AlMes_3$ *THF
$E_{\text{pol.}}^{\text{SAPT (1)}}$	–104.5	–104.2	–189.5	–171.6	–153.7	–138.4	–200.2
$E_{\text{exch.}}^{\text{SAPT (1)}}$	155.7	154.7	237.5	232.4	218.1	203.3	270.2
$E_{\text{disp.}}^{\text{SAPT (2)}}$	–45.8	–50.1	–46.7	–56.1	–63.6	–72.0	–116.7
$E_{\text{disp.}-\text{exch.}}^{\text{SAPT (2)}}$	10.7	11.3	10.6	12.6	13.9	15.0	25.1
$E_{\text{ind.}}^{\text{SAPT (2)}}$	–198.1	–207.4	–323.0	–285.8	–242.4	–201.5	–288.9
$E_{\text{ind.}-\text{exch.}}^{\text{SAPT (2)}}$	139.6	147.2	213.2	196.6	171.0	143.8	221.5
$E_{\delta(\text{HF})}^{\text{SAPT}}$	–12.6	–11.9	–1.0	–7.1	–10.8	–12.2	–23.1
$E_{\text{total}}^{\text{SAPT}}$	–55.0	–60.5	–99.0	–79.0	–67.6	–62.0	–112.2
dE	–52.3	–54.4	–100.4	–76.4	–63.4	–52.8	–108.8

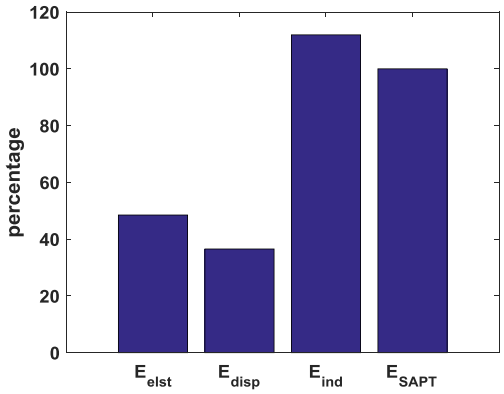
It should be noted that the order of the total interaction energies within this set is the same for the SAPT ($E_{\text{total}}^{\text{SAPT}}$) and supermolecular ($dE$) calculations. The respective SAPT contributions were grouped as

$$E_{\text{elst}} = E_{\text{pol.}}^{\text{SAPT (1)}} + E_{\text{exch.}}^{\text{SAPT (1)}}$$

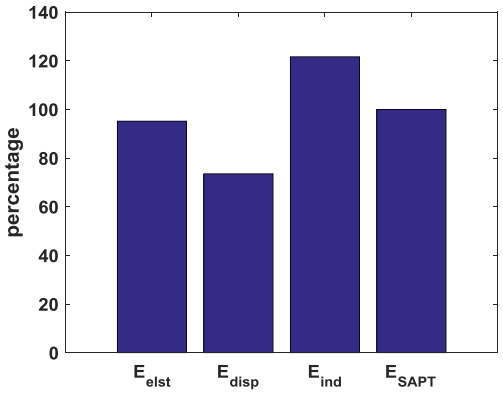
$$E_{\text{disp}} = E_{\text{disp.}}^{\text{SAPT (2)}} + E_{\text{disp.}-\text{exch.}}^{\text{SAPT (2)}}$$

$$E_{\text{ind}} = E_{\text{ind.}}^{\text{SAPT (2)}} + E_{\text{ind.}-\text{exch.}}^{\text{SAPT (2)}} + E_{\delta(\text{HF})}^{\text{SAPT}}$$

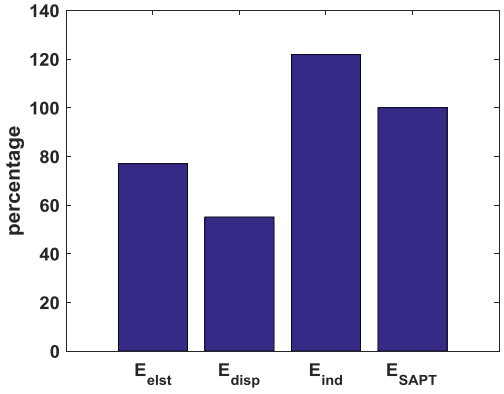
and the absolute values of E_{elst}, E_{disp} and E_{ind} were used to obtain the relative values shown below:



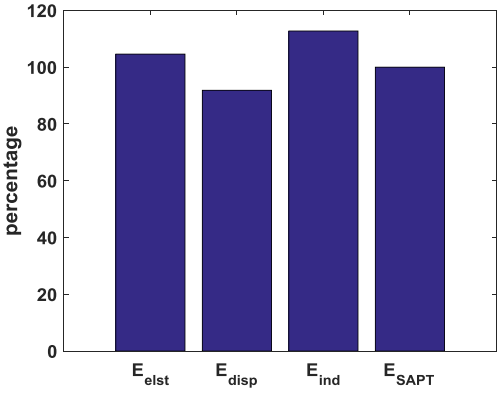
Relative contributions to the SAPT-DFT interaction energy of $AlCl_3 \cdot HCN$.



Relative contributions to the SAPT-DFT interaction energy of $AlClMes_2 \cdot HCN$.



Relative contributions to the SAPT-DFT interaction energy of $AlCl_2Mes \cdot HCN$.



Relative contributions to the SAPT-DFT interaction energy of $AlMes_3 \cdot HCN$.

Figure S4. Relative contributions to the SAPT-DFT interaction energy of $AlCl_3 \cdot HCN$, $AlClMes_2 \cdot HCN$, $AlCl_2Mes \cdot HCN$, $AlMes_3 \cdot HCN$.

Energetic parameters and final coordinates of all investigated systems

C_2H_2_monomer.xyz

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4 atoms: C2H2 monomer // HF/6-31G**
RI-MP2/CBS=-77.204291; ZPE=0.029336; asymp=0.13165 h
C 0.000000    0.000000    0.593075
C 0.000000    0.000000   -0.593075
H 0.000000    0.000000    1.649861
H 0.000000    0.000000   -1.649861
```

C_2H_4_monomer.xyz

```
6 atoms: C2H4 monomer // HF/6-31G**
RI-MP2/CBS=-78.449650; ZPE=0.054492; asymp=0.12044 h
C 0.000000    0.000000    0.658120
C 0.000000    0.000000   -0.658120
H 0.000000    0.915369    1.224591
H 0.000000   -0.915369    1.224591
H 0.000000   -0.915369   -1.224591
H 0.000000    0.915369   -1.224591
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HCN_monomer.xyz

```
3 atoms: HCN monomer // HF/6-31G**
RI-MP2/CBS=-93.302508; ZPE=0.017883; asymp=0.14763  h
C 0.000000    0.000000   -0.490784
H 0.000000    0.000000   -1.549448
N 0.000000    0.000000    0.642022
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$AlCl_3$_monomer.xyz

```
4 atoms: AlCl3 monomer // HF/6-31G**
RI-MP2/CBS=-1621.484862; ZPE=0.004873; asymp=0.08951 h
Al     0.000059    0.000021    0.000000
Cl    -0.000015    2.077280    0.000000
Cl    -0.000015   -1.038648    1.798954
Cl    -0.000015   -1.038648   -1.798954
```

THF_monomer.xyz

```
13 atoms: THF monomer // HF/6-31G**
RI-MP2/CBS=-232.124487; ZPE=0.133046; asymp=0.10863 h
O    -0.000113   -1.229289    0.000151
C     1.155933   -0.433768    0.130881
C     0.731150    0.990094   -0.223491
H     1.928614   -0.824544   -0.521402
H     1.518391   -0.489907    1.155220
H     0.796486    1.149170   -1.296095
H     1.337474    1.743602    0.265942
C    -1.155914   -0.433628   -0.131128
C    -0.731048    0.990154    0.223652
H    -1.518249   -0.489576   -1.155528
H    -1.928729   -0.824403    0.521031
H    -1.337008    1.743742   -0.266110
H    -0.796794    1.149112    1.296246
```

$AlMesCl_2$_monomer.xyz

```
23 atoms: AlCl2Mes // HF/6-31G**
RI-MP2/CBS=-1510.696610; ZPE=0.186748; asymp=0.07661 h
Al     1.627730    0.001159    0.001971
Cl     2.765920   -0.971567   -1.477639
Cl     2.760865    0.974677    1.484973
C     -0.316069    0.000281   -0.000675
C     -1.032291    1.146780   -0.376346
C     -2.418523    1.130568   -0.378616
C     -3.126726   -0.004527   -0.008345
C     -2.417119   -1.137695    0.362206
C     -1.030056   -1.148524    0.369260
C     -0.301846    2.411960   -0.778048
C     -4.636327    0.003795    0.016104
C     -0.298732   -2.414774    0.766100
H     -2.957820    2.014960   -0.673158
H     -2.954648   -2.026066    0.647660
H     -0.986302    3.170968   -1.136230
H      0.243228    2.836510    0.061123
H      0.408564    2.225336   -1.582141
H     -5.038542   -0.989909   -0.144608
H     -5.001685    0.356132    0.977154
H     -5.038544    0.659105   -0.748267
H     -0.978810   -3.163043    1.154034
H      0.218610   -2.854124   -0.082851
H      0.436252   -2.224980    1.547146
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AlMes$_2$Cl_monomer.xyz

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42 atoms: AlClMes2 // HF/6-31G**
RI-MP2/CBS=-1399.904877; ZPE=0.369246; asymp=0.05523 h
Al     0.000002    1.036671   -0.000016
Cl     0.000006    3.172536   -0.000054
C    -1.754515    0.152599    0.092632
C    -2.058828   -0.722167    1.148707
C    -3.291366   -1.359798    1.204342
C    -4.253791   -1.155475    0.228871
C    -3.957831   -0.292463   -0.816923
C    -2.737175    0.360980   -0.892544
C    -1.065632   -0.970953    2.266696
C    -5.600056   -1.834420    0.309694
C    -2.495278    1.307013   -2.051510
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C     2.737168    0.361006    0.892531
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C     2.058827   -0.722233   -1.148672
C     2.495281    1.307086    2.051462
C     5.600079   -1.834385   -0.309701
C     1.065615   -0.971071   -2.266634
H    -3.502985   -2.029286    2.021110
H    -4.693148   -0.128638   -1.587046
H    -0.074905   -1.200044    1.885660
H    -1.371347   -1.803691    2.888714
H    -0.984129   -0.101938    2.916819
H    -5.961888   -2.108651   -0.675362
H    -6.337666   -1.173252    0.757107
H    -5.553387   -2.732949    0.914327
H    -1.528271    1.138528   -2.520653
H    -2.523190    2.341703   -1.725651
H    -3.244672    1.181933   -2.823949
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H     3.502964   -2.029415   -2.021000
H     1.528262    1.138651    2.520596
H     2.523234    2.341763    1.725568
H     3.244658    1.182007    2.823918
H     5.552999   -2.733931   -0.912791
H     5.962870   -2.106894    0.675472
H     6.337163   -1.173854   -0.758928
H     0.074926   -1.200276   -1.885567
H     1.371391   -1.803749   -2.888702
H     0.983998   -0.102037   -2.916717
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AlMes$_3$_monomer.xyz

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61 atoms: AlMes3 // HF/6-31G**
RI-MP2/CBS=-1289.112232; ZPE=0.55126; asymp=0.04880 h
Al    0.000013    0.000050   -0.000618
C    -1.625105    1.151578   -0.000520
C    -1.845550    2.106625   -1.009757
C    -2.985382    2.900067   -1.001947
C    -3.939219    2.786453   -0.003038
C    -3.730632    1.847810    0.995640
C    -2.601357    1.040365    1.007081
C    -2.438421    0.052135    2.145331
C    -0.861506    2.278134   -2.150416
C    -5.158123    3.677911    0.012802
C     1.809840    0.831648   -0.000517
C     2.201694    1.732643    1.007060
C     3.465685    2.306842    0.995627
C     4.382818    2.018126   -0.003016
C     4.004218    1.135287   -1.001980
C     2.747175    0.544981   -1.009794
C     2.403590   -0.392987   -2.150416
C     5.764421    2.627714    0.012711
C     1.264482    2.085694    2.145372
C    -0.184704   -1.983106   -0.000524
C    -0.901637   -2.651528   -1.009769
C    -1.018917   -4.035336   -1.001953
C    -0.443602   -4.804617   -0.003037
C     0.265011   -4.154694    0.995612
C     0.399705   -2.772965    1.007048
C     1.174093   -2.137810    2.145321
C    -0.606375   -6.305927    0.012742
C    -1.542192   -1.885019   -2.150386
H    -3.133067    3.619292   -1.790452
H    -4.462563    1.742914    1.779365
H    -2.256139   -0.953433    1.781277
H    -3.324134    0.019462    2.768884
H    -1.607128    0.328990    2.791130
H     0.150096    2.429017   -1.788751
H    -1.118770    3.130504   -2.768205
H    -0.856871    1.405630   -2.801171
H    -6.007457    3.175967    0.463257
H    -5.438523    3.980270   -0.990142
H    -4.968603    4.581323    0.587117
H     3.740824    2.993142    1.779355
H     4.700918    0.903579   -1.790503
H     2.028972   -1.344682   -1.788690
H     3.270220   -0.595959   -2.768586
H     1.645216    0.039009   -2.800815
H     6.164537    2.723496   -0.990633
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H     6.453059    2.009304    0.583032
H     5.755466    3.612310    0.467332
H     0.302157    2.429764    1.781411
H     1.678701    2.869721    2.768347
H     1.089378    1.227602    2.791727
H    -1.567957   -4.522838   -1.790458
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H     1.953496   -1.476788    1.781309
H     1.645642   -2.888547    2.768547
H     0.518612   -1.556746    2.791435
H    -0.725038   -6.700204   -0.990461
H    -1.485329   -6.593240    0.584421
H     0.251530   -6.790467    0.465970
H    -2.178976   -1.084661   -1.788664
H    -2.151405   -2.534050   -2.768447
H    -0.788908   -1.444365   -2.800888
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$AlCl_3$_C_2H_2.xyz

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8 atoms: AlCl3...C2H2 // HF/6-31G**
RI-MP2/CBS=-1698.710696; ZPE=0.035821 h
Al     0.002888    0.000000    0.203120
Cl     2.078618   -0.001144    0.581733
Cl    -1.038014    1.793918    0.572289
Cl    -1.040160   -1.792667    0.572460
C     -0.598531    0.000055   -2.248031
H     -1.659308    0.000333   -2.255734
C      0.592696   -0.000312   -2.308807
H      1.649209   -0.000627   -2.393983
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$AlCl_3$_C_2H_4.xyz

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Cl 1.792079    1.234177    0.188215
Cl -1.789353    1.237993    0.189178
Cl -0.001295   -1.653662    1.372535
C  -0.668125   -0.965527   -2.042430
H  -1.230552   -1.764628   -1.591089
H  -1.228901   -0.195055   -2.539766
C  0.664826   -0.965970   -2.042870
H  1.226999   -1.765433   -1.591838
H  1.225774   -0.195901   -2.540634
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$AlCl_3$.HCN.xyz

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RI-MP2/CBS=-1714.828144; ZPE=0.025382 h
Al 0.224414    0.002139    0.009637
Cl 0.597322   -1.861947    0.934081
Cl 0.704045    0.153189   -2.043567
Cl 0.550993    1.727014    1.187048
C  -2.943757   -0.028454   -0.123468
H  -4.005937   -0.038145   -0.167718
N  -1.819862   -0.018468   -0.076473
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$AlCl_3$.THF.xyz

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17 atoms: AlCl3...THF // HF/6-31G**
RI-MP2/CBS=-1853.672683; ZPE=0.125142
O    -0.914919    0.045945   -0.217630
C    -1.741170    1.231038   -0.023792
C    -3.153294    0.733647   -0.277953
H    -1.394262    1.983024   -0.712277
H    -1.593380    1.564993    0.993857
H    -3.382469    0.776084   -1.337392
H    -3.885293    1.329185    0.252537
C    -1.720677   -1.168952   -0.263712
C    -3.093309   -0.716176    0.202661
H    -1.710893   -1.514628   -1.286488
H    -1.253334   -1.901352    0.375509
H    -3.878147   -1.336268   -0.211437
H    -3.156510   -0.761946    1.284423
Al    0.971056    0.000331    0.014835
Cl    1.584300    1.953704   -0.548134
Cl    1.562245   -1.572303   -1.284793
Cl    1.159372   -0.439536    2.089763
```

AlMesCl$_2$.HCN.xyz

```
26 atoms: AlCl2Mes...HCN // HF/6-31G**
RI-MP2/CBS=-1604.031602; ZPE=0.208031
Al    1.397004    0.164443   -0.160209
Cl    2.485720    1.806764    0.691621
Cl    2.384244   -0.606167   -1.899789
C    -0.575192    0.073998   -0.076757
C    -1.242498   -1.162693   -0.058560
C    -2.631484   -1.225381    0.021832
C    -3.404884   -0.083088    0.075282
C    -2.756398    1.144220    0.029785
C    -1.377190    1.238750   -0.048433
C    -0.508489   -2.489420   -0.117801
C    -4.910807   -0.151728    0.157744
C    -0.777864    2.629511   -0.116292
H    -3.112651   -2.189209    0.032210
H    -3.344344    2.046934    0.046157
H    -1.138742   -3.252676   -0.559150
H     0.393882   -2.441776   -0.714989
H    -0.239298   -2.835860    0.877491
H    -5.275904    0.364735    1.040649
H    -5.369042    0.319430   -0.706925
H    -5.258270   -1.177332    0.202357
H    -1.549896    3.368441   -0.295063
H    -0.272178    2.894574    0.805209
H    -0.053567    2.720494   -0.919080
C     2.595477   -1.870174    2.020997
H     3.057381   -2.489101    2.750449
N     2.106878   -1.214359    1.247927
```

AlMesCl$_2$.THF.xyz

```
36 atoms: AlCl2Mes...THF // HF/6-31G**
RI-MP2/CBS=-1742.877429; ZPE=0.315897 h
Al    -0.751440    0.828494    0.402851
Cl    -1.697681    2.292292   -0.876392
Cl    -1.468079    1.085805    2.416334
C     1.143263    0.291024    0.153976
C     1.623365   -0.863166    0.809464
```

```
C     2.933223   -1.293472    0.632933
C     3.821672   -0.601873   -0.171312
C     3.367318    0.545090   -0.801386
C     2.063257    0.997867   -0.649945
C     0.763451   -1.669942    1.765674
C     5.251758   -1.059369   -0.329956
C     1.690330    2.274080   -1.378571
O    -1.795391   -0.694787   -0.185756
C    -3.186491   -0.897416    0.189378
C    -3.781695   -1.671340   -0.976823
C    -2.579960   -2.439384   -1.527264
C    -1.456959   -1.427113   -1.390995
H     3.267277   -2.182030    1.142187
H     4.045954    1.103034   -1.424625
H     1.228333   -2.623209    1.988917
H     0.626252   -1.141766    2.703083
H    -0.224089   -1.876198    1.369266
H     5.621222   -0.857181   -1.329571
H     5.901543   -0.540709    0.370201
H     5.349260   -2.122899   -0.142472
H     2.567846    2.726591   -1.825026
H     0.973543    2.092779   -2.171552
H     1.249547    3.005669   -0.711475
H    -3.633286    0.070008    0.351728
H    -3.183803   -1.457357    1.112956
H    -4.166930   -0.985917   -1.723855
H    -4.591086   -2.315183   -0.656313
H    -2.709575   -2.758495   -2.553738
H    -2.373455   -3.315283   -0.920881
H    -0.475720   -1.850003   -1.248935
H    -1.438251   -0.721542   -2.210962
```

$AlMes_2Cl.HCN.xyz$

```
45 atoms: AlClMes2...HCN // HF/6-31G**
RI-MP2/CBS=-1493.234896; ZPE=0.39050 h
Al    -0.040332    0.951477   -0.242586
Cl    -0.143845    2.717994   -1.508589
C    -1.777748   -0.030474   -0.156510
C    -2.953584    0.520150    0.382291
C    -4.137293   -0.212939    0.423559
C    -4.211481   -1.499709   -0.071827
C    -3.064569   -2.044971   -0.631874
C    -1.872802   -1.340041   -0.683194
C    -3.007540    1.925409    0.950509
C    -5.498960   -2.287872   -0.035250
C    -0.690112   -2.026858   -1.340082
C     1.731565    0.037876   -0.060751
C     2.747463    0.081449   -1.045572
C     3.967880   -0.537258   -0.834084
C     4.247988   -1.229271    0.338233
C     3.256335   -1.301109    1.293501
C     2.017379   -0.687709    1.107513
C     2.552157    0.787074   -2.373086
C     5.590515   -1.891146    0.537367
C     1.014577   -0.861690    2.235422
H    -5.019481    0.240312    0.844498
H    -3.105907   -3.039398   -1.045204
H    -2.665199    1.946921    1.982663
H    -4.024859    2.299764    0.945592
H    -2.406062    2.621024    0.379174
```

```
H    -5.356748   -3.245999    0.455920
H    -5.860906   -2.488588   -1.039762
H    -6.275885   -1.751205    0.497022
H     0.078437   -2.288858   -0.622010
H    -0.225152   -1.398545   -2.093638
H    -1.004284   -2.938033   -1.835680
H     4.720637   -0.489635   -1.603927
H     3.436298   -1.852364    2.202241
H     2.566718    1.864887   -2.260794
H     1.605478    0.530059   -2.835606
H     3.337412    0.513838   -3.068566
H     5.637559   -2.412065    1.486822
H     6.392793   -1.158860    0.517917
H     5.790978   -2.612118   -0.249822
H     1.200225   -0.156464    3.042584
H     1.093307   -1.856002    2.661637
H    -0.012289   -0.737224    1.915178
C     0.355442    2.839421    2.385496
H     0.568954    3.513905    3.177163
N     0.127772    2.125365    1.545181
```

AlMes$_2$Cl.THF.xyz

```
55 atoms: AlClMes2... THF // HF/6-31G**
RI-MP2/CBS=-1632.078052; ZPE=0.498872 h
Al     0.007759    0.305717    0.592668
Cl     0.088626    1.034460    2.663975
C      1.849098   -0.340240    0.104461
C      2.627695    0.101891   -0.983210
C      3.921010   -0.363376   -1.181481
C      4.499916   -1.290352   -0.330116
C      3.731947   -1.765544    0.716968
C      2.436116   -1.312442    0.939647
C      2.092336    1.075655   -2.015172
C      5.919022   -1.762293   -0.538934
C      1.691070   -1.932418    2.107860
C     -1.669263   -0.687690    0.088129
C     -2.931292   -0.324599    0.608227
C     -4.081375   -1.030658    0.269874
C     -4.043404   -2.120131   -0.580403
C     -2.814598   -2.483186   -1.105919
C     -1.649336   -1.796111   -0.790393
C     -3.120448    0.836073    1.567909
C     -5.292649   -2.900620   -0.911857
C     -0.373591   -2.299357   -1.439677
O     -0.307264    2.081476   -0.230814
C      0.297831    3.301858    0.273137
C     -0.055457    4.352352   -0.765416
C     -1.417510    3.871454   -1.264158
C     -1.239001    2.362633   -1.304841
H      4.485568   -0.004702   -2.026621
H      4.144460   -2.513564    1.374118
H      1.102793    0.791029   -2.355761
H      2.734488    1.103177   -2.887726
H      2.032522    2.088396   -1.630223
H      6.060960   -2.766723   -0.155351
H      6.622885   -1.112651   -0.024442
H      6.184207   -1.763311   -1.590875
H      0.628790   -2.042576    1.912647
H      1.792406   -1.334311    3.006086
H      2.076675   -2.923545    2.320252
```

```
H    -5.026663   -0.720752    0.683859
H    -2.762258   -3.320876   -1.781324
H    -2.521116    1.699005    1.305217
H    -2.840317    0.560737    2.578004
H    -4.158369    1.149987    1.583943
H    -5.271497   -3.263106   -1.934181
H    -6.182519   -2.293472   -0.787416
H    -5.391066   -3.765399   -0.260585
H     0.144241   -1.519232   -1.984951
H    -0.594238   -3.094715   -2.142161
H     0.325480   -2.690407   -0.710421
H    -0.140912    3.508478    1.236627
H     1.354291    3.120428    0.394829
H     0.667668    4.353282   -1.574328
H    -0.082575    5.345100   -0.333713
H    -2.197296    4.141127   -0.559471
H    -1.685685    4.268827   -2.235188
H    -2.136559    1.796266   -1.125681
H    -0.784467    2.034177   -2.228735
```

AlMes$_3$.HCN.xyz

```
64 atoms: AlMes3...HCN // HF/6-31G**
RI-MP2/CBS=-1382.438996; ZPE=0.573286 h
Al     0.000000    0.000000    0.225132
C      1.564416    1.258228   -0.046947
C      2.599333    0.962179   -0.969156
C      3.700227    1.791510   -1.103157
C      3.840258    2.951857   -0.351963
C      2.822560    3.273607    0.520213
C      1.700265    2.457889    0.671884
C      0.643811    2.970863    1.635203
C      2.549594   -0.256790   -1.871458
C      5.058479    3.830051   -0.510145
C      0.307449   -1.983937   -0.046947
C      1.278462   -2.701417    0.671884
C      1.423748   -4.081212    0.520212
C      0.636255   -4.801689   -0.351963
C     -0.298620   -4.100246   -1.103157
C     -0.466396   -2.732178   -0.969155
C     -1.497185   -2.079619   -1.871457
C      0.787683   -6.295797   -0.510145
C      2.250938   -2.042987    1.635203
C     -1.871865    0.725710   -0.046946
C     -2.132938    1.769999   -0.969155
C     -3.401608    2.308735   -1.103157
C     -4.476513    1.849831   -0.351963
C     -4.246308    0.807604    0.520213
C     -2.978727    0.243528    0.671884
C     -2.894748   -0.927875    1.635204
C     -5.846162    2.465744   -0.510145
C     -1.052411    2.336409   -1.871457
H      4.466290    1.536791   -1.817524
H      2.886265    4.185678    1.091810
H      0.915239    2.765456    2.668609
H     -0.333729    2.545588    1.453596
H      0.546022    4.047814    1.545335
H      1.576211   -0.382208   -2.333667
H      2.763033   -1.172091   -1.332335
H      3.275408   -0.166687   -2.671832
H      4.969124    4.738664    0.074448
```

```
H     5.205372    4.113264   -1.548270
H     5.957155    3.312433   -0.185477
H     2.181773   -4.592417    1.091808
H    -0.902245   -4.636317   -1.817524
H    -1.119110   -1.173935   -2.333664
H    -2.396579   -1.806814   -1.332333
H    -1.782060   -2.753243   -2.671831
H     0.959495   -6.564617   -1.548271
H    -0.109921   -6.815264   -0.185467
H     1.619248   -6.672717    0.074440
H     2.371409   -0.983775    1.453595
H     3.232500   -2.496775    1.545334
H     1.937336   -2.175347    2.668609
H    -3.564046    3.099525   -1.817524
H    -5.068037    0.406738    1.091809
H    -2.037679   -1.561812    1.453596
H    -3.778521   -1.551038    1.545336
H    -2.852574   -0.590107    2.668610
H    -5.847231    3.502827   -0.185468
H    -6.588368    1.934048    0.074440
H    -6.164873    2.451361   -1.548271
H    -0.366457    2.978904   -1.332334
H    -1.493349    2.919931   -2.671831
H    -0.457103    1.556144   -2.333665
C     0.000001    0.000000    3.537176
H     0.000001   -0.000001    4.598469
N     0.000000    0.000000    2.411014
```

$AlMes_3$.THF.xyz

```
74 atoms: AlMes3...THF // HF/6-31G**
RI-MP2/CBS=-1521.276076; ZPE=0.682226 h
C     2.606863    0.593476    3.254771
C     1.626901   -0.440537    2.724506
O     0.635755    0.331052    2.027982
C     0.391737    1.508133    2.817795
C     1.728613    1.837061    3.496696
H     3.096533    0.245521    4.156297
H     3.369540    0.792513    2.514768
H     2.055434   -1.141867    2.029053
H     1.133508   -0.970949    3.529031
H    -0.374774    1.267603    3.543458
H     0.026592    2.276249    2.158332
H     2.176245    2.724568    3.069614
H     1.576216    2.024073    4.552950
Al    0.009649   -0.078753    0.073766
C    -1.316799   -1.627323    0.024591
C    -1.966440   -1.817737   -1.209936
C    -2.965069   -2.776007   -1.369458
C    -3.367983   -3.585739   -0.326851
C    -2.724026   -3.425358    0.890990
C    -1.724165   -2.480911    1.071598
C    -1.071179   -2.438999    2.437228
C    -1.619464   -0.998573   -2.439817
C    -4.470491   -4.604073   -0.494648
C    -1.020958    1.631113   -0.365415
C    -2.136693    2.003295    0.425470
C    -2.844794    3.171110    0.182514
C    -2.522349    4.015081   -0.869397
C    -1.482455    3.633476   -1.692133
C    -0.750581    2.468716   -1.465827
```

C	0.285085	2.146464	-2.526509
C	-3.285084	5.297759	-1.099582
C	-2.683580	1.125336	1.536405
C	1.928388	-0.415750	-0.564465
C	2.401231	-1.688699	-0.987648
C	3.726583	-1.883229	-1.341054
C	4.660931	-0.855569	-1.302342
C	4.222268	0.382837	-0.891834
C	2.892174	0.609653	-0.530355
C	2.587672	2.040960	-0.122366
C	6.095266	-1.100688	-1.704941
C	1.503108	-2.908292	-1.074161
H	-3.431702	-2.888855	-2.334474
H	-3.004479	-4.058603	1.717150
H	-1.124038	-1.453287	2.884805
H	-0.024336	-2.721922	2.378577
H	-1.550947	-3.130962	3.119813
H	-0.560915	-0.766611	-2.499964
H	-2.160298	-0.058517	-2.455991
H	-1.870490	-1.541684	-3.344508
H	-4.212331	-5.546202	-0.021151
H	-4.670343	-4.799605	-1.542236
H	-5.395545	-4.255503	-0.042099
H	-3.678082	3.421057	0.819958
H	-1.230605	4.247351	-2.542213
H	0.931192	1.325453	-2.261323
H	0.909972	3.008798	-2.738431
H	-0.213250	1.880544	-3.455521
H	-3.128480	5.674979	-2.103919
H	-2.966663	6.070281	-0.403841
H	-4.351240	5.152447	-0.957657
H	-1.945403	0.467840	1.967245
H	-3.476013	0.488810	1.155249
H	-3.101372	1.727021	2.338048
H	4.045633	-2.863076	-1.656352
H	4.919421	1.204809	-0.851386
H	1.564237	2.196710	0.179802
H	2.781538	2.717634	-0.948456
H	3.233077	2.354090	0.693350
H	6.525521	-1.923600	-1.141539
H	6.708576	-0.222811	-1.536313
H	6.165095	-1.358116	-2.758178
H	1.033239	-3.140041	-0.126461
H	2.075563	-3.777147	-1.378389
H	0.704445	-2.775520	-1.792855

References

[1] Zissi, G. D.; Bessada, C., Al-27 NMR spectra of the RECl3-AlCl3 (RE = Y, La) glasses and melts. *Zeitschrift Fur Naturforschung Section A-A Journal of Physical Sciences* **2001,** *56* (9-10), 697-701.