

Supporting Information for:

Dialumination of Unsaturated Species with a Reactive Bis(cyclopentadienyl) Dialane

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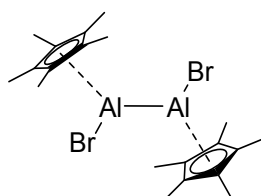
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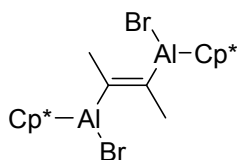
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Experimental Details

General experimental considerations: All syntheses were carried out in Argon-filled glovebox or with standard Schlenk techniques¹ unless otherwise stated. Cp*, KCp*, Cp*SiMe₃ and Cp*AlBr₂ were prepared as described previously.²⁻⁴ AlBr₃ was obtained from commercial sources and purified by sublimation. All solvents were dried by distillation over appropriate drying agents⁵ and stored over molecular sieves. All solution NMR spectra were acquired on a Bruker Avance 400 NMR spectrometer (¹H: 400.1 MHz, ²⁷Al: 104 MHz, ¹³C: 101 MHz) or a Bruker Avance I 500 spectrometer (¹H: 500.1 MHz, ²⁷Al: 130 MHz, ¹³C: 125.8 MHz). ¹H NMR and ¹³C NMR spectra were referenced to external TMS via residual protons of the solvent (¹H) or the solvent itself (¹³C). ²⁷Al NMR spectra were referenced to external Al(NO₃)₃. Elemental analyses were performed on a Elementar vario MICRO cube elemental analyzer. High-resolution mass spectrometry was obtained using a Thermo Scientific Exactive Plus spectrometer.

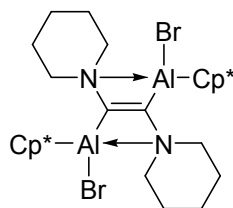


Preparation of [AlBr(η⁵-Cp*)]₂ (1): Cp*AlBr₂ (2.00 g, 6.21 mmol) was dissolved in 10 mL of benzene. KC₈ (0.840 g, 6.21 mmol) was added and the suspension was stirred for 12 h. The reaction mixture was filtered through a filter cannula and the residue was washed with benzene (2 x 3 mL). The solvent of the combined filtrates was removed under reduced pressure giving a beige solid (**1**; 960 mg, 1.98 mmol, 64%). The product can be crystallized out of a concentrated solution of toluene as colorless crystals. ¹H NMR (C₆D₆): δ 1.85 (s, 15 H, (C₅Me₅) ppm. ¹³C{¹H} NMR (C₆D₆): δ 116.5 (C₅Me₅), 11.0 (C₅Me₅) ppm. ²⁷Al NMR (C₆D₆): δ -10.9 (br). Anal. Found: C 49.77, H 6.36; Calcd. Data for C₂₀H₃₀Al₂Br₂: C 49.61; H, 6.24.

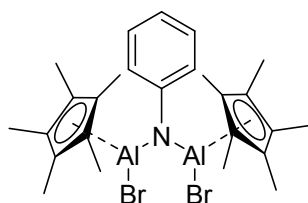


Preparation of E-[C₂Me₂{AlBr(η⁵-Cp*)}₂] (2): Dialane **1** (250 mg, 0.52 mmol) was dissolved in benzene and an excess of 2-butyne (0.2 mL) was added. The mixture was stirred for three days and the solvent was removed under reduced pressure to obtain a white solid (150 mg, 0.28 mmol, 54%). Colorless crystals of **2** were obtained by slow evaporation of a solution in benzene. ¹H NMR (C₆D₆): δ 1.83 (s, 15 H, C₅Me₅), 1.76 (s, 3 H, CH₃) ppm. ¹³C{¹H} NMR (C₆D₆): 152 (C=C), 116 (C₅Me₅), 30.4

(CH₃CCCH₃), 10.6 (C₅Me₅) ppm. ²⁷Al NMR (C₆D₆): δ –18 (s, br); Anal. Found: C 52.69, H 6.61; Calcd. Data for C₂₄H₃₆Al₂Br₂: C 53.55, H 6.74.



Preparation of *E*-[C₂pip₂{AlBr(η²-Cp^{*})₂]}₂ (3**):** Dialane **1** (30.0 mg, 0.062 mmol) was dissolved in C₆D₆ in a J. Young-style tube and 1,2-bis(piperidyl)acetylene (11.9 mg, 0.06 mmol) was added. Within 12 h, colorless crystals had precipitated. The crystals were washed with pentane (3 x 0.5 mL) and dried under reduced pressure to provide colorless crystals of **3** (yield: 32 mg, 0.047 mmol, 76%). Note: The ²⁷Al NMR spectrum of **3** showed only a weak signal at δ_{Al} 121. This signal is likely due to a very minor impurity, while the actual signal for **3** is presumably too broad to be observed. ¹H NMR (tol-*d*₈): δ 2.94-2.78 (m, 2H, axial 2,6-NC₅H₁₀), 2.53-2.32 (m, 2H, equatorial 2,6-NC₅H₁₀), 1.95 (s, 9H, C₅Me₅), 1.94 (s, 6H, C₅Me₅), 1.56-1.31 (m, 4H, 3,5-NC₅H₁₀), 1.22-1.15 (m, 2H, 4-NC₅H₁₀) ppm. ¹³C{¹H} NMR (tol-*d*₈): δ 153.0 (C_q), 119.1 (C₅Me₅), 118.8 (C₅Me₅), 57.0 (2,6-NC₅H₁₀), 56.9 (2,6-NC₅H₁₀), 57.0 (2,6-NC₅H₁₀), 25.3 (3,5-NC₅H₁₀), 25.0 (3,5-NC₅H₁₀), 23.2 (4-NC₅H₁₀), 12.5 (C₅Me₅), 12.4 (C₅Me₅) ppm. LIFDI-MS (*m/z*) calculated for [C₃₂H₅₀Al₂Br₂N₂] = 676.1946; found: 676.1946; calculated for [C₂₂H₃₅Al₂Br₂N₂ (C₃₂H₅₀Al₂Br₂N₂ – Cp^{*})] = 541.0774; found: 541.0772; calculated for [C₂₂H₃₆AlBrN₂ (C₃₂H₅₀Al₂Br₂N₂ – Cp^{*}AlBr)] = 434.1874; found: 434.1872.



Preparation of [PhN{AlBr(η⁵-Cp^{*})₂]}₂ (4**):** Dialane **1** (250 mg, 0.51 mmol) was dissolved in benzene and phenyl azide (61 mg, 0.51 mmol) was added at –78 °C. The orange reaction mixture was slowly warmed to room temperature, whereby the evolution of gaseous N₂ was observed. The solvent was removed under reduced pressure and the remaining white solid was washed with pentane (2 x 1 mL) to obtain **4** as a beige solid (180 mg, 0.30 mmol, 61%). Colorless crystals of **4** were obtained by slow evaporation of a solution in benzene. ¹H NMR (400.13 MHz, C₆D₆): δ = 7.09-7.05 (m, 2 H, C₆H₅), 6.99-6.97 (m, 2 H, C₆H₅), 6.90-6.86 (m, 1 H, C₆H₅), 1.74 (s, 30 H, C₅Me₅) ppm. ¹³C NMR (100.61 MHz, C₆D₆): δ = 153 (CN), 128.9 (C₆H₅), 128.5 (C₆H₅), 121 (C₆H₅), 116 (C₅Me₅), 11 (C₅Me₅) ppm. ²⁷Al NMR (104.26 MHz, C₆D₆): δ = –21 ppm. LIFDI-MS (*m/z*) calculated for [C₂₆H₃₅Al₂N₁Br₂] = 575.0741; found: 575.0742.

NMR Spectra

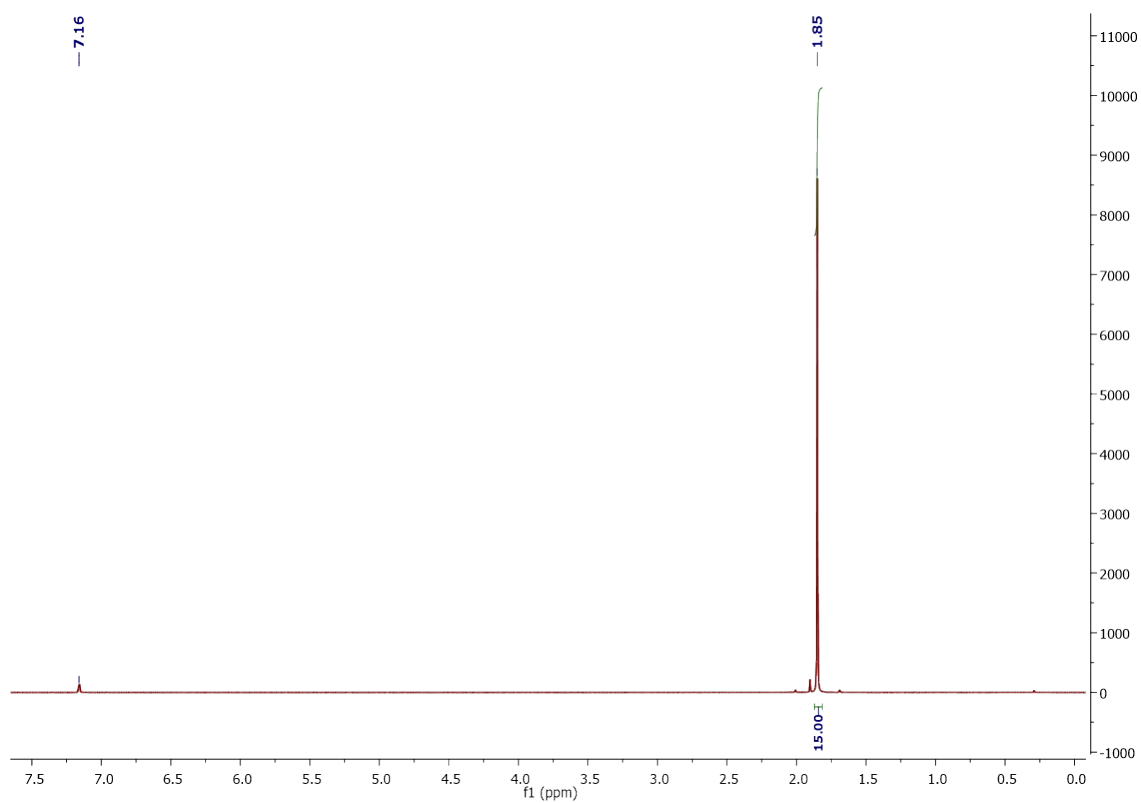


Figure S1. ^1H NMR (400 MHz, C_6D_6) spectrum of dialane **1**.

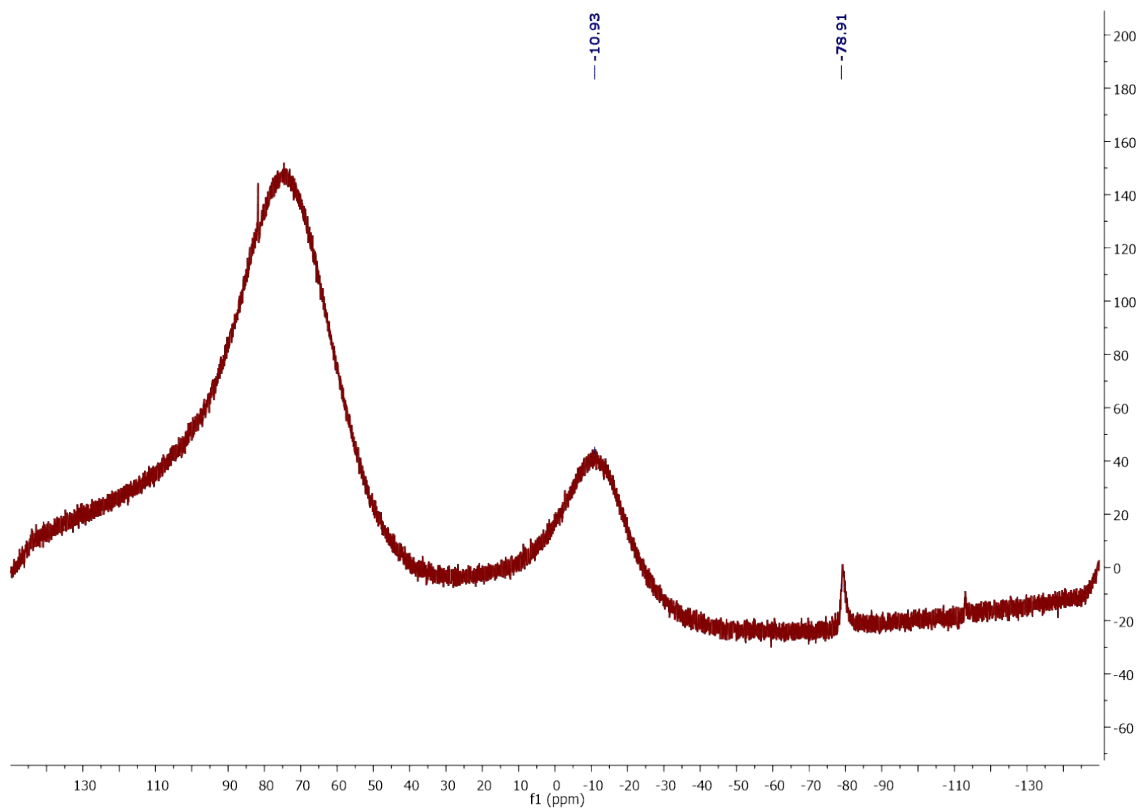


Figure S2. ^{27}Al NMR (104 MHz, C_6D_6) spectrum of dialane **1**.

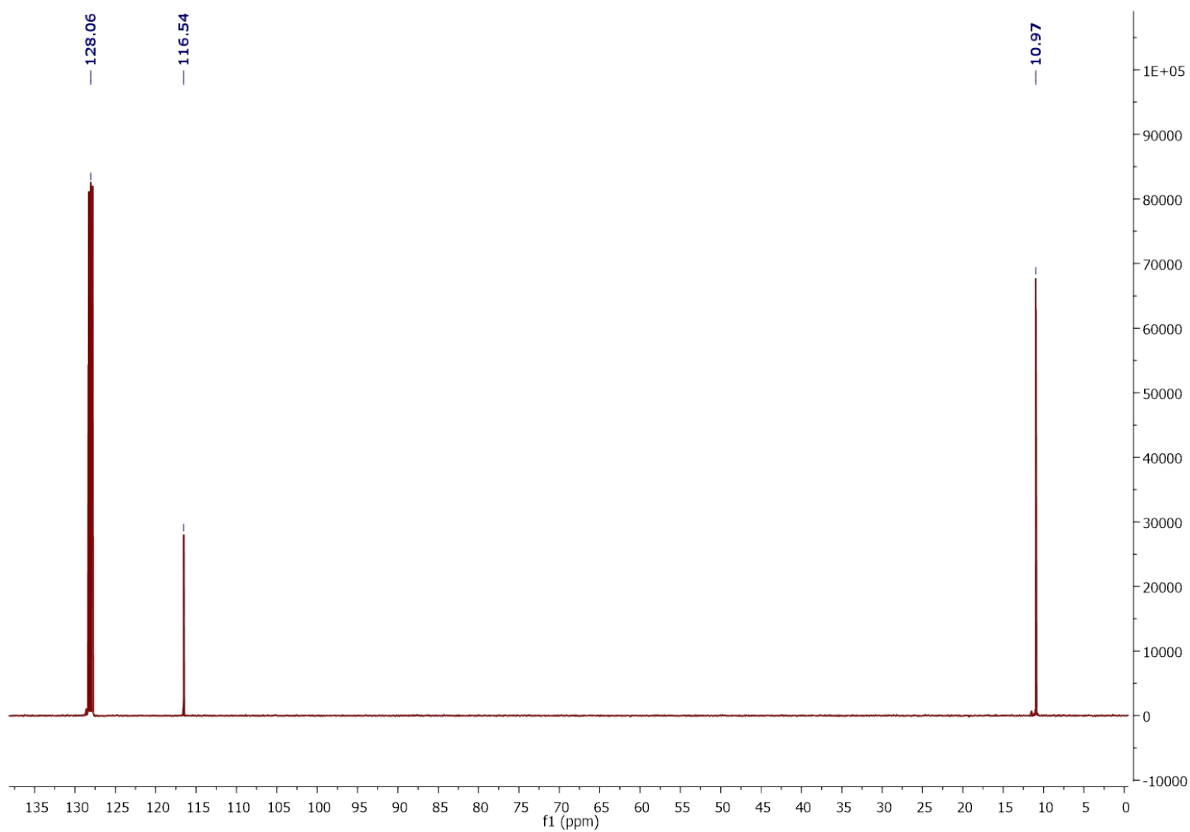


Figure S3. $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, C_6D_6) spectrum of dialane 1.

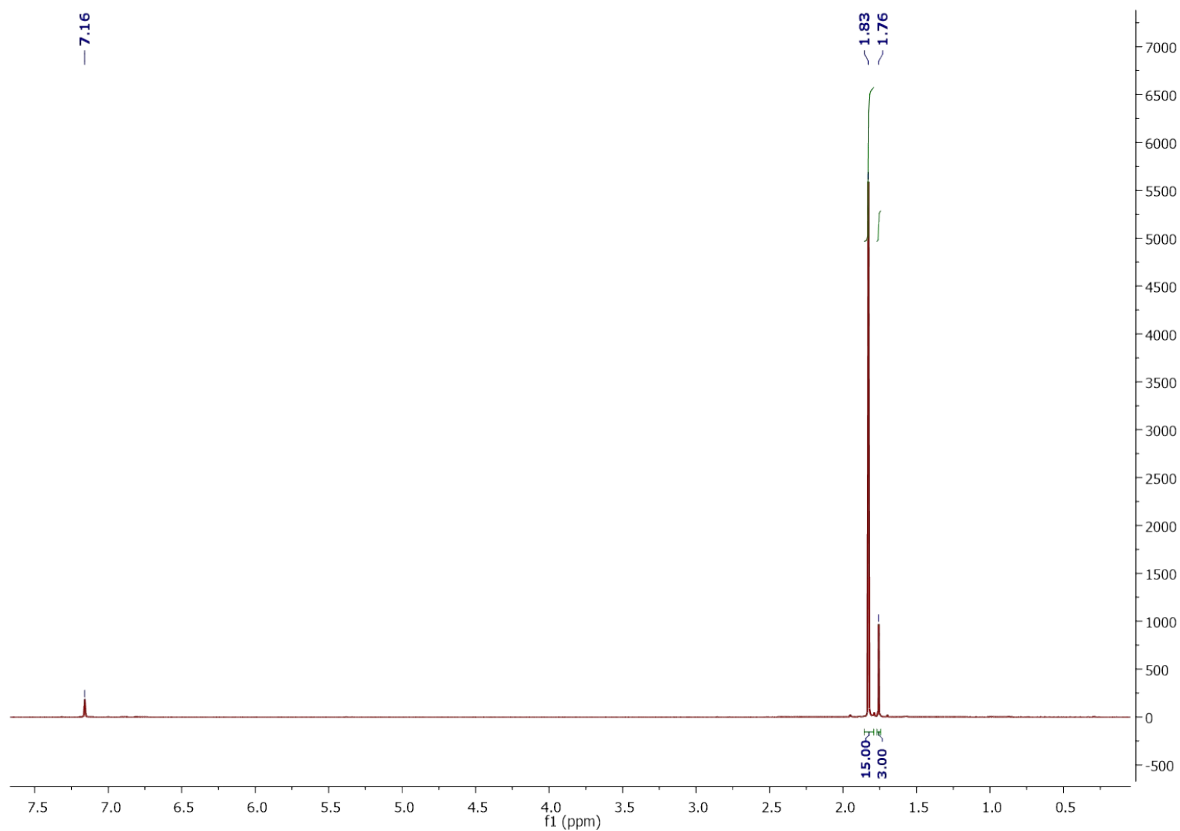


Figure S4. ^1H NMR (500 MHz, C_6D_6) spectrum of 2.

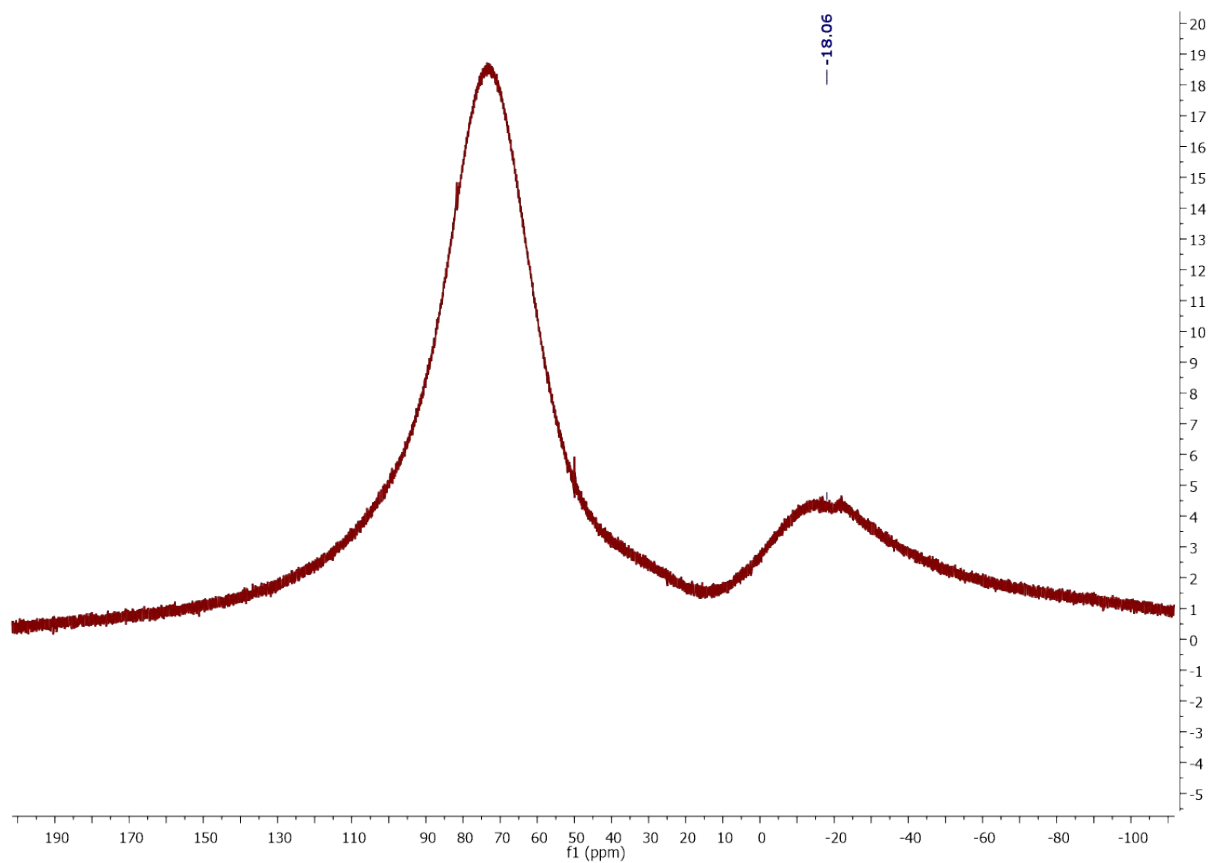


Figure S5. ^{27}Al NMR (130.3 MHz, C_6D_6) spectrum of **2**.

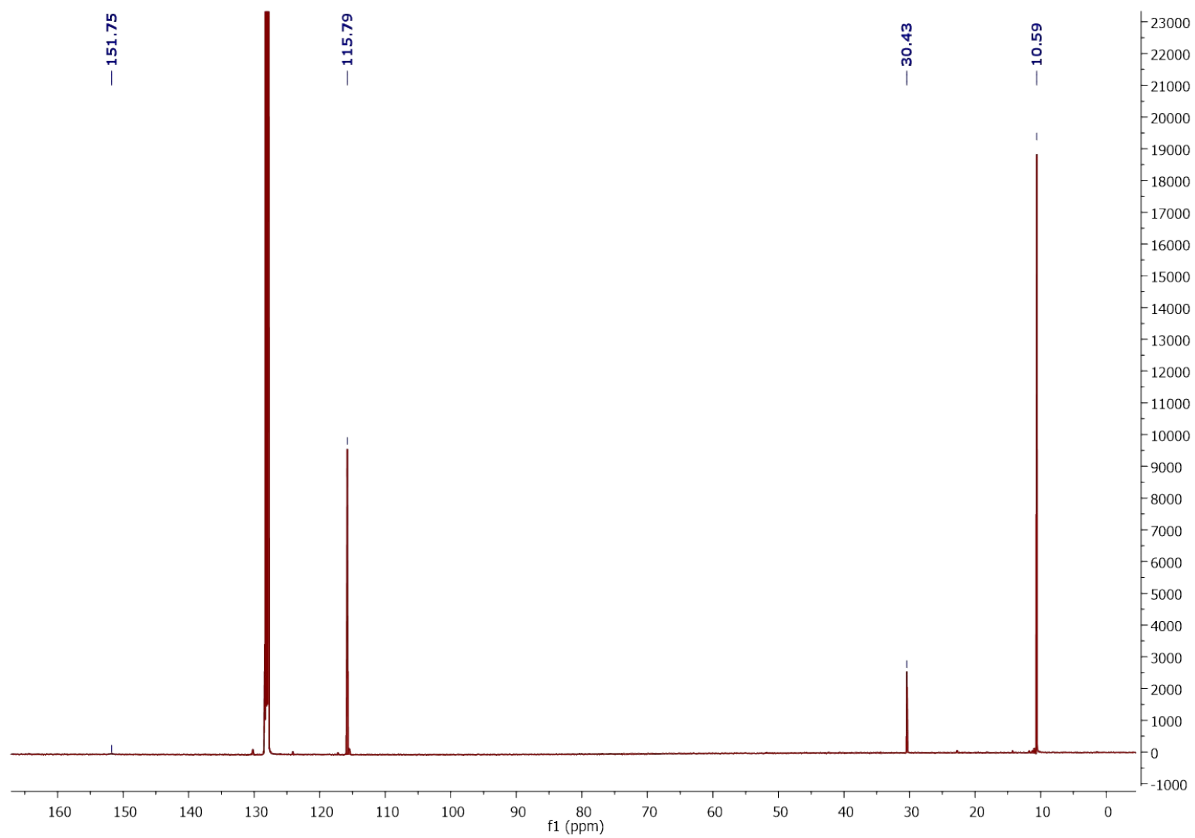


Figure S6. ^{13}C NMR (125.8 MHz, C_6D_6) spectrum of **2**.

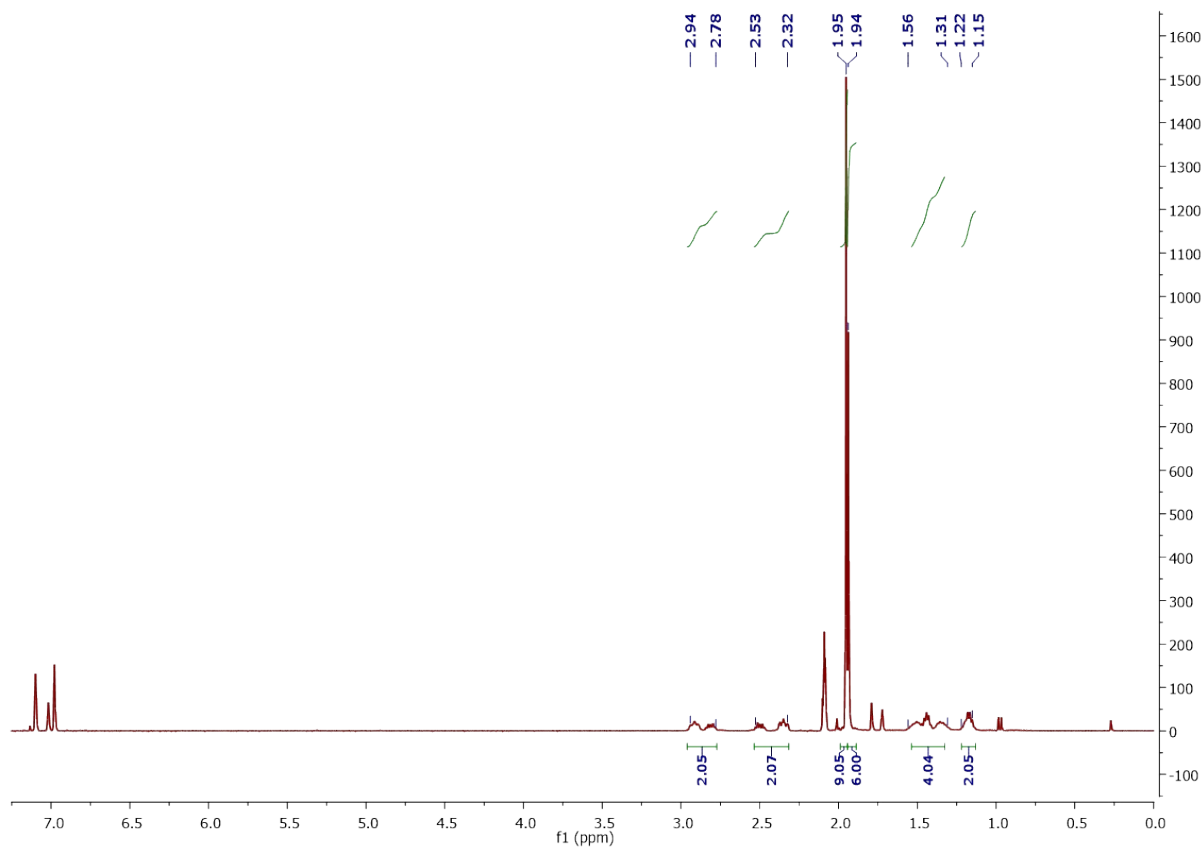


Figure S7. ^1H NMR (400 MHz, tol-d_8) spectrum of **3**.

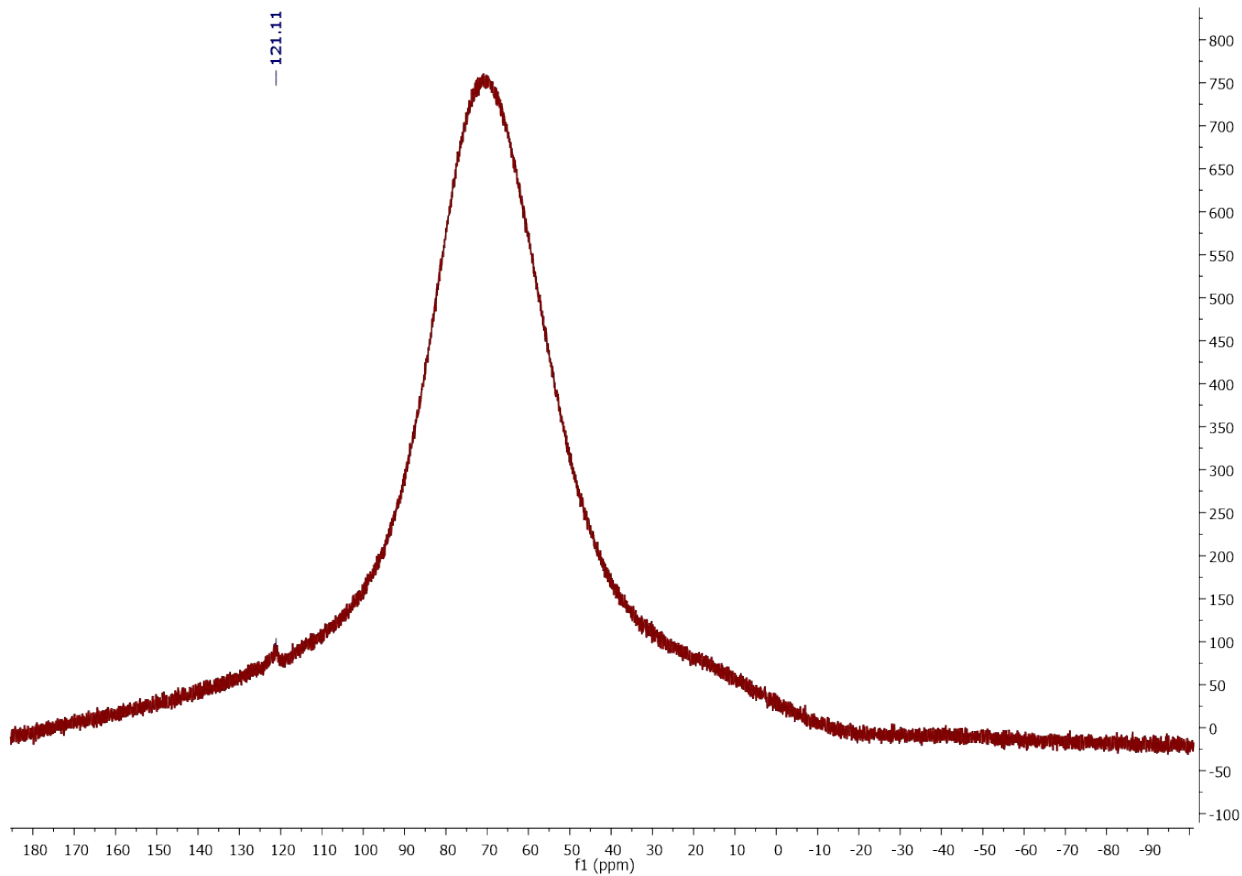


Figure S8. ^{27}Al NMR (104 MHz, tol-d_8) spectrum of **3**.

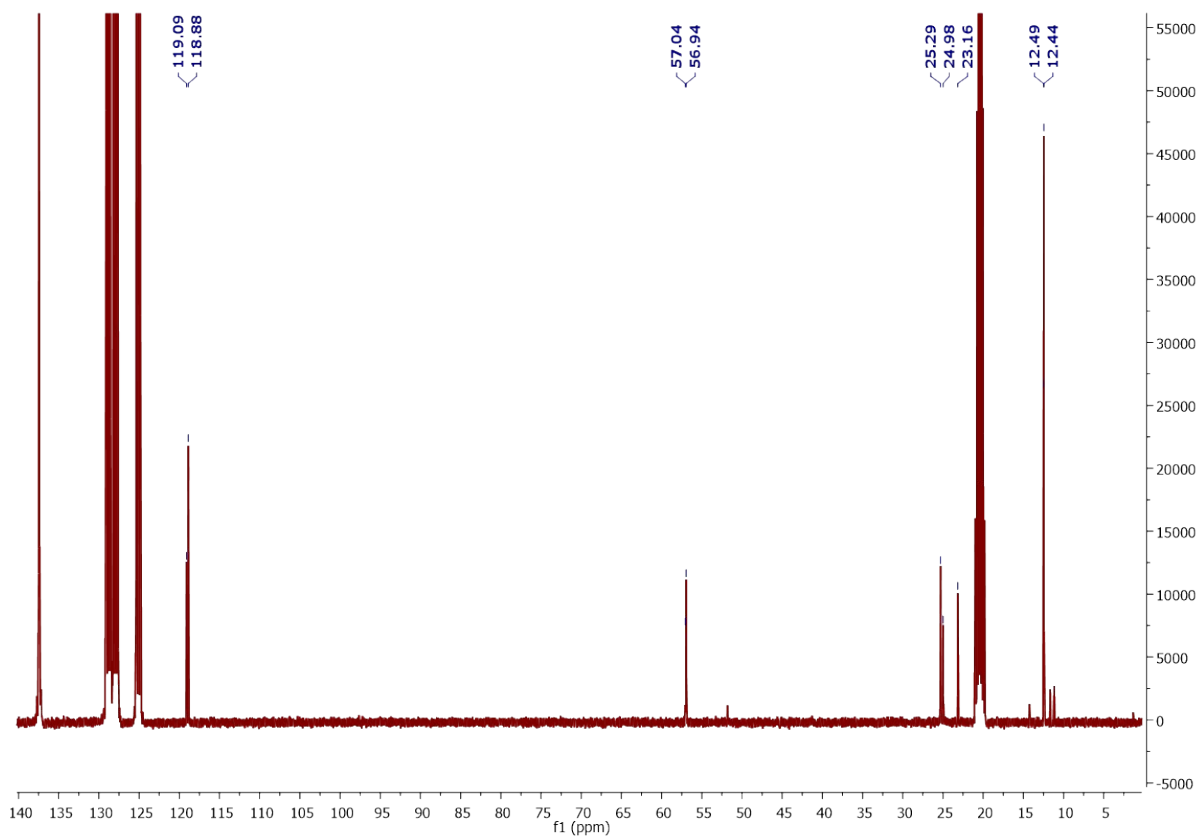


Figure S9. $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, tol-d_8) spectrum of **3**.

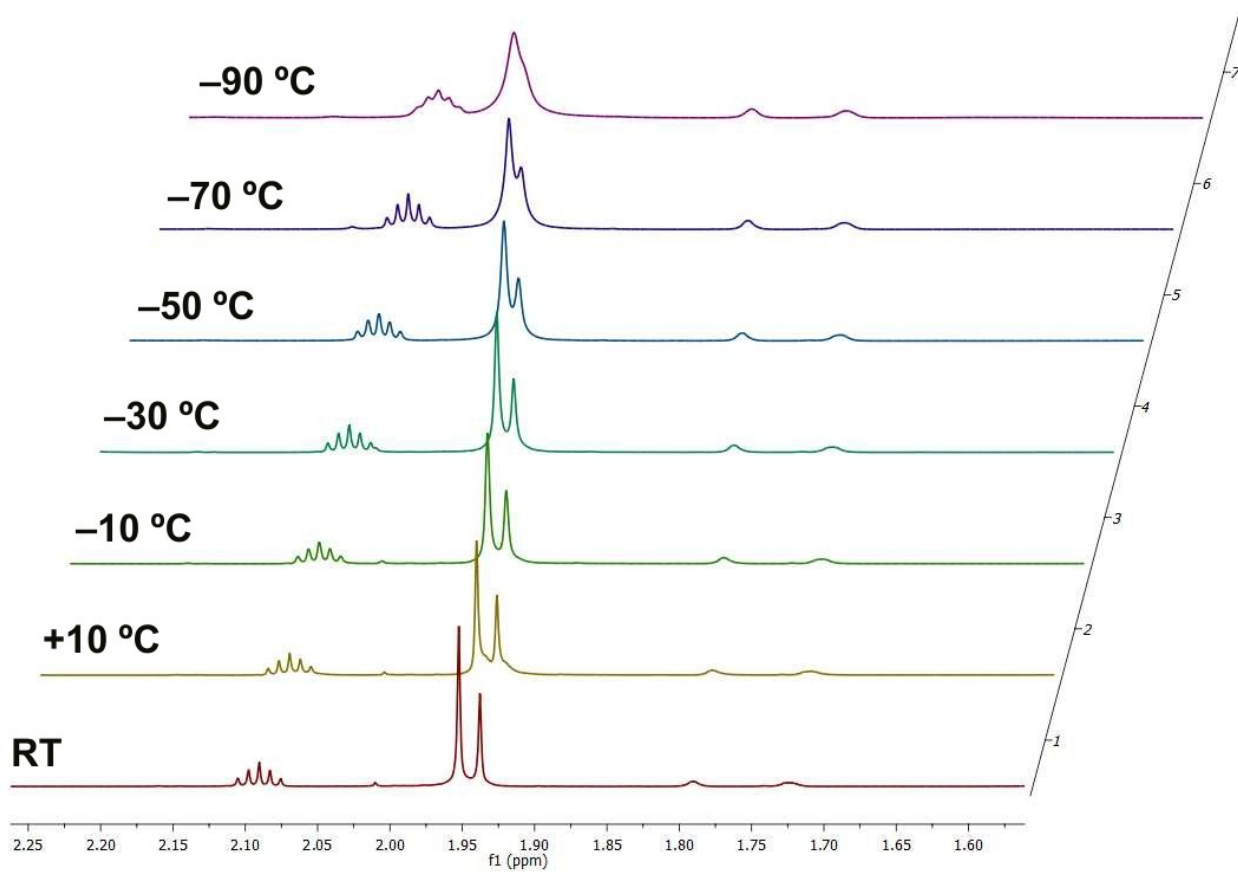


Figure S10. Variable temperature ^1H NMR (101 MHz, C_6D_6) spectra of **3** from RT to $-90\text{ }^\circ\text{C}$.

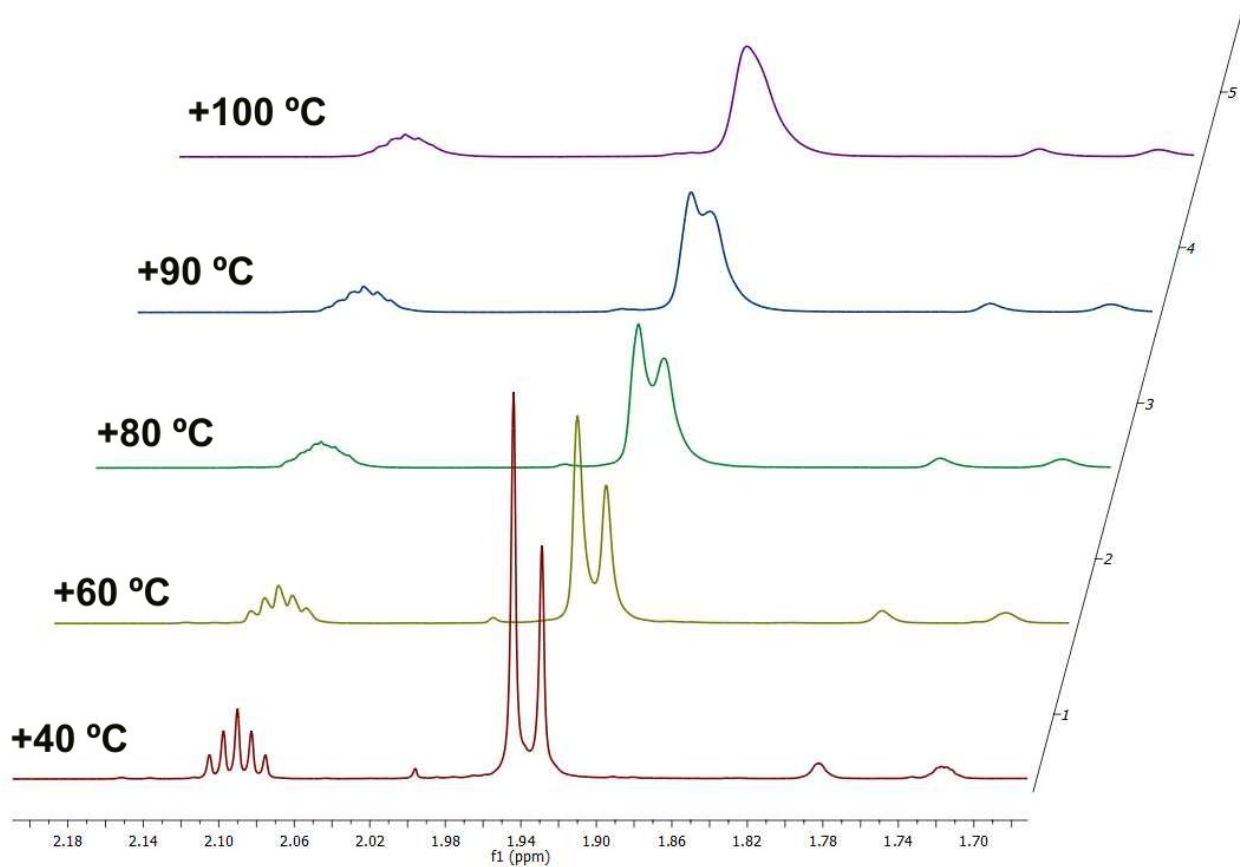


Figure S11. Variable temperature ^1H NMR (101 MHz, tol-d_8) spectra of **3** from $+40$ to $+100\text{ }^\circ\text{C}$.

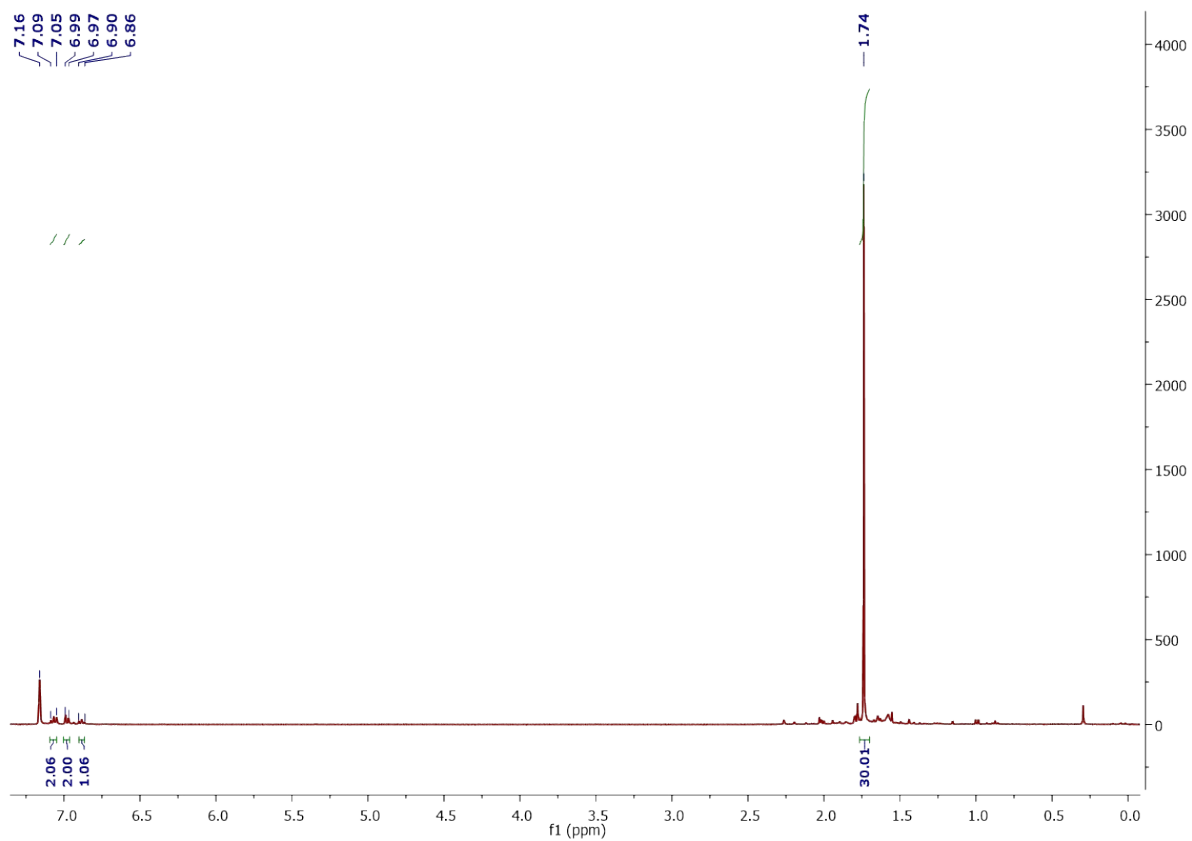


Figure S12. ^1H NMR (400 MHz, C_6D_6) spectrum of **4**.

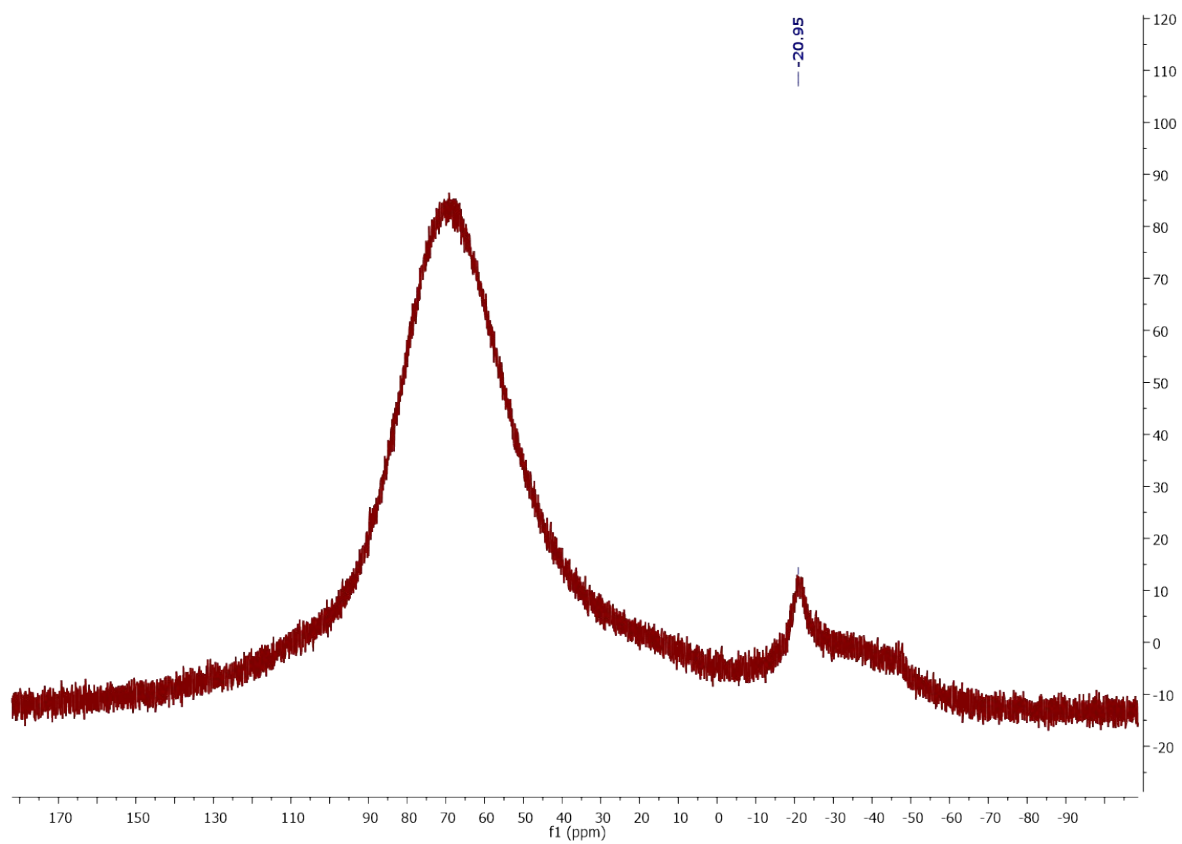


Figure S13. ^{27}Al NMR (104 MHz, C_6D_6) spectrum of **4**.

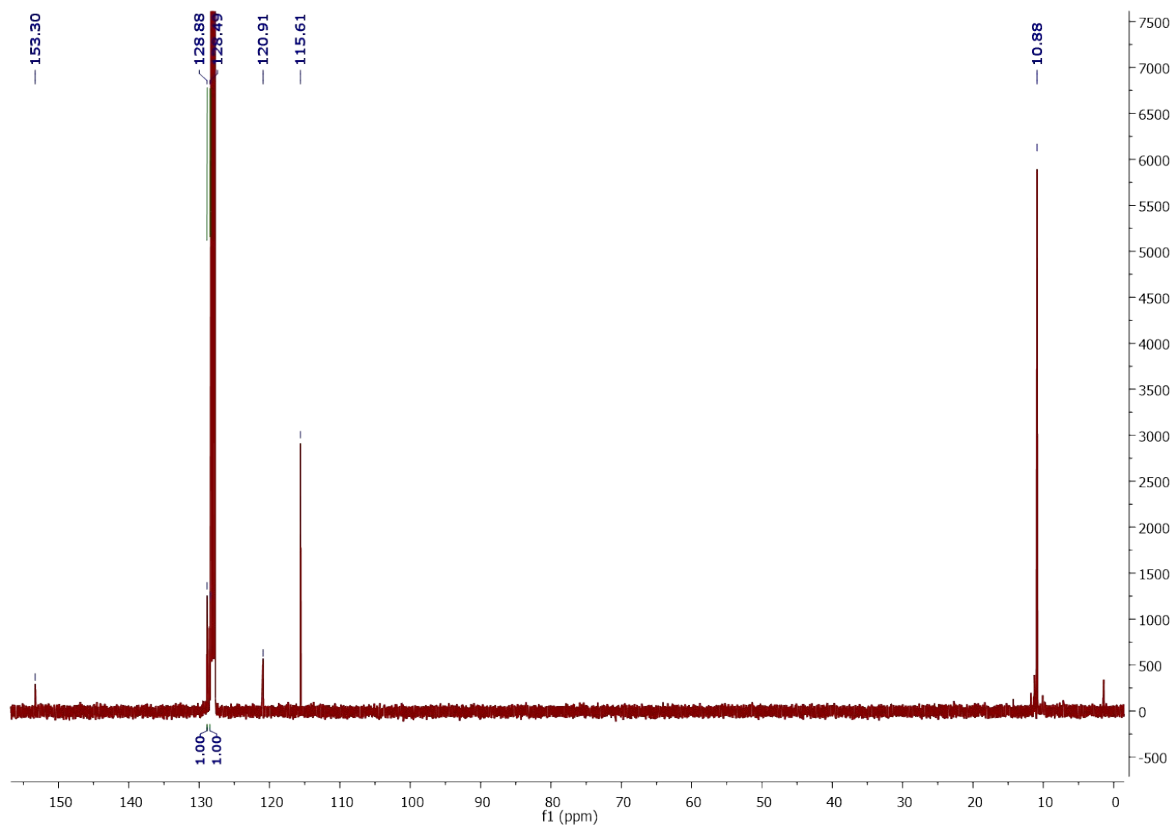


Figure S14. ^{13}C NMR (101 MHz, C_6D_6) spectrum of 4.

Crystallographic Details

The crystal data of **1** were collected on a Bruker X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated Mo $\kappa\alpha$ radiation. The structure was solved using the intrinsic phasing method,⁶ refined with the ShelXL program⁷ and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions. Crystal data for **1**: C₂₀H₃₀Al₂Br₂, $M_r = 484.22$, colourless block, 0.867×0.59×0.561 mm³, monoclinic space group $P2_1/n$, $a = 10.394(5)$ Å, $b = 14.012(8)$ Å, $c = 15.316(7)$ Å, $\beta = 97.53(4)^\circ$, $V = 2211(2)$ Å³, $Z = 4$, $\rho_{\text{calcd}} = 1.454$ g·cm⁻³, $\mu = 3.745$ mm⁻¹, $F(000) = 984$, $T = 100(2)$ K, $R_1 = 0.0618$, $wR^2 = 0.1115$, 4352 independent reflections [$2\theta \leq 52.04^\circ$] and 227 parameters. CCDC-1588296.

The crystal data of **2** were collected on a Bruker X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated Mo $\kappa\alpha$ radiation. The structure was solved using the intrinsic phasing method,⁶ refined with the ShelXL program⁷ and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions. The displacement parameters of atoms Al1, C1, C2, C3 and Br1 of the residue 1, Al1, C1, C2, C3 and Br1 of the residue 11, C1-C10 of the residue 2 and C1-C10 of the residue 22 were restrained to the same value with similarity restraint SIMU. The atomic displacement parameters of atoms all Atoms were restrained with the RIGU keyword in ShelXL input ('enhanced rigid bond' restraint for all bonds in the connectivity list. Standard values of 0.004 for both parameters s1 and s2 were used). Crystal data for **2**: C₂₄H₃₆Al₂Br₂, $M_r = 538.31$, colourless plate, 0.391×0.322×0.10 mm³, monoclinic space group $P2_1/n$, $a = 9.136(4)$ Å, $b = 8.291(3)$ Å, $c = 16.801(8)$ Å, $\beta = 101.961(15)^\circ$, $V = 1245.0(9)$ Å³, $Z = 2$, $\rho_{\text{calcd}} = 1.436$ g·cm⁻³, $\mu = 3.334$ mm⁻¹, $F(000) = 552$, $T = 100(2)$ K, $R_1 = 0.0440$, $wR^2 = 0.0896$, 2452 independent reflections [$2\theta \leq 52.044^\circ$] and 266 parameters. CCDC-1588297.

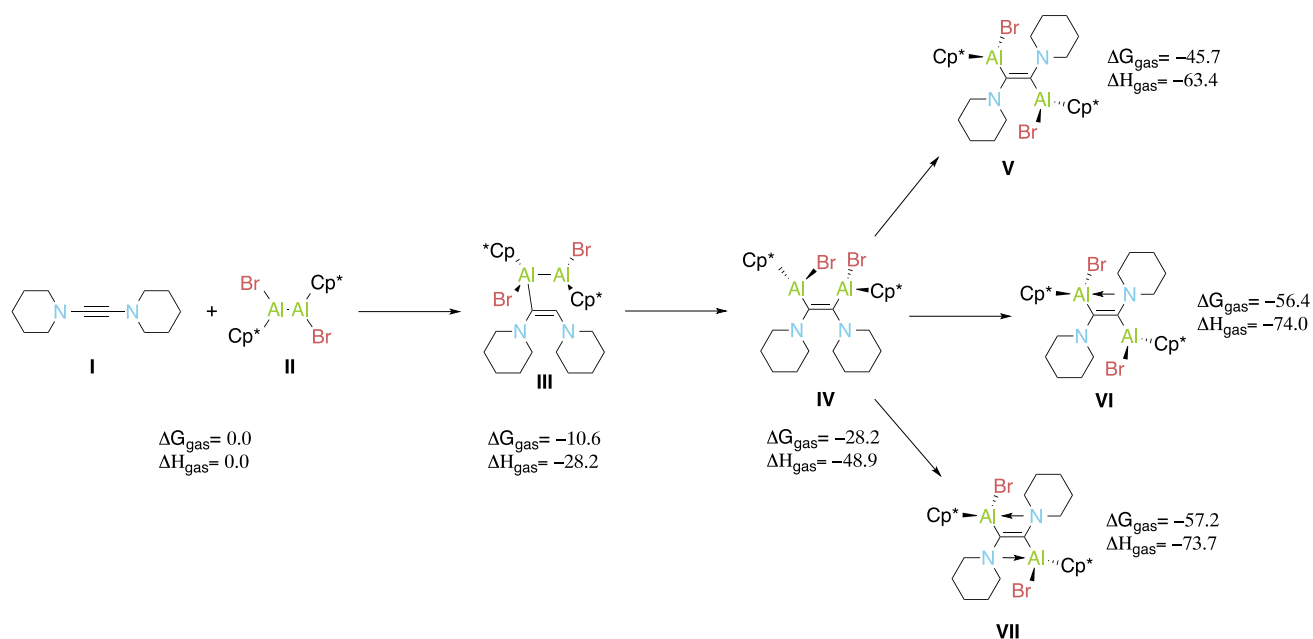
The crystal data of **3** were collected on a Bruker D8 Quest diffractometer with a CMOS area detector and multi-layer mirror monochromated Mo $\kappa\alpha$ radiation. The structure was solved using the intrinsic phasing method,⁶ refined with the ShelXL program⁷ and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions. The displacement parameters of atoms C1-C10 of the residue 1 and C1-C10 of the residue 2 were restrained to the same value with similarity restraint SIMU. The atomic displacement parameters of atoms C1-C10 of the residue 1 and C1-C10 of the residue 2 were restrained with the RIGU keyword in ShelXL input ('enhanced rigid bond' restraint for all bonds in the connectivity list. Standard values of 0.004 for both

parameters s_1 and s_2 were used). Crystal data for **3**: $C_{32}H_{50}Al_2Br_2N_2$, $M_r = 676.52$, colourless block, $0.428 \times 0.281 \times 0.155 \text{ mm}^3$, triclinic space group $P\bar{1}$, $a = 8.6234(20) \text{ \AA}$, $b = 11.477(5) \text{ \AA}$, $c = 18.064(7) \text{ \AA}$, $\alpha = 101.19(2)^\circ$, $\beta = 91.52(2)^\circ$, $\gamma = 110.23(2)^\circ$, $V = 1637.1(10) \text{ \AA}^3$, $Z = 2$, $\rho_{\text{calcd}} = 1.372 \text{ g}\cdot\text{cm}^{-3}$, $\mu = 2.553 \text{ mm}^{-1}$, $F(000) = 704$, $T = 100(2) \text{ K}$, $R_1 = 0.0613$, $wR^2 = 0.1213$, 6463 independent reflections [$2\theta \leq 52.044^\circ$] and 353 parameters. CCDC-1588298.

The crystal data of **4** were collected on a Bruker D8 Quest diffractometer with a CMOS area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structure was solved using the intrinsic phasing method,⁶ refined with the ShelXL program⁷ and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions. The structure was refined using the TWIN keyword (matrix: twin). The BASF parameter was refined to 0%. The displacement parameters of atoms C1-C6 of the residue 1, C1-C10 of the residue 2 and C1-C10 of the residue 3 were restrained to the same value with similarity restraint SIMU. The distances between atoms as well as C1_3 C2_3, C2_3 C3_3, C3_3 C4_3, C4_3 C5_3 and C5_3 C1_3 C1_2 C2_2, C2_2 C3_2 C3_2 C4_2 C4_2 C5_2 C5_2 C1_2 were restrained during refinement to the same value with the SADI restraint. The atomic displacement parameters of atoms C1-C6 of the residue 1, C1-C10 of the residue 2 and C1-C10 of the residue 3 were restrained with the RIGU keyword in ShelXL input ('enhanced rigid bond' restraint for all bonds in the connectivity list. Standard values of 0.004 for both parameters s_1 and s_2 were used). Crystal data for **4**: $C_{26}H_{35}Al_2Br_2N$, $M_r = 575.33$, colourless block, $0.367 \times 0.36 \times 0.129 \text{ mm}^3$, monoclinic space group $P2_1$, $a = 8.880(6) \text{ \AA}$, $b = 14.563(9) \text{ \AA}$, $c = 10.658(10) \text{ \AA}$, $\beta = 110.01(4)^\circ$, $V = 1295.1(17) \text{ \AA}^3$, $Z = 2$, $\rho_{\text{calcd}} = 1.475 \text{ g}\cdot\text{cm}^{-3}$, $\mu = 3.212 \text{ mm}^{-1}$, $F(000) = 588$, $T = 100(2) \text{ K}$, $R_1 = 0.0861$, $wR^2 = 0.1164$, 5026 independent reflections [$2\theta \leq 52.044^\circ$] and 291 parameters. CCDC-1588299.

Computational Methods

Geometry optimizations were performed in the gas phase using the hybrid PBE0 density functional which mixes 25% of HF exchange in its formulation.⁸ Grimme's D3 method⁹ for incorporating dispersion effects was explicitly included in the geometry optimizations. The electronic configurations of light atoms such as hydrogen, carbon, nitrogen, and aluminium were described with Pople's double- ζ 6-31G* basis set containing one polarization function. On the other hand, the pseudopotential LANL2DZ containing a polarization function was used for bromine.¹⁰ Single-point calculations of the PBE0-optimized geometries were performed using the M06 functional¹¹ with the same basis sets as specified for the geometry optimizations. This methodology was employed for estimating the solvent effect through Truhlar and coworkers' solvation model SMD¹² using toluene as the solvent. Thus, this level of theory to show the energy values can be written as (SMD:toluene)M06[6-31G(d),LANL2DZ(f)]/D3-PBE0/[6-31G(d),LANL2DZ(f)]. Aiming to compare two different methodologies, GIAO-NMR studies of ^{27}Al were carried out using the hybrid B3LYP¹³ and local M06-L¹⁴ functionals with the def2-TZVPP basis set¹⁵ for all atoms. AlH_4 ⁻¹⁶ was considered as the reference for obtaining ^{27}Al chemical shifts.



Scheme 1. Gas-phase reaction energies of each step of the alumination reaction (values are shown in kcal mol⁻¹).

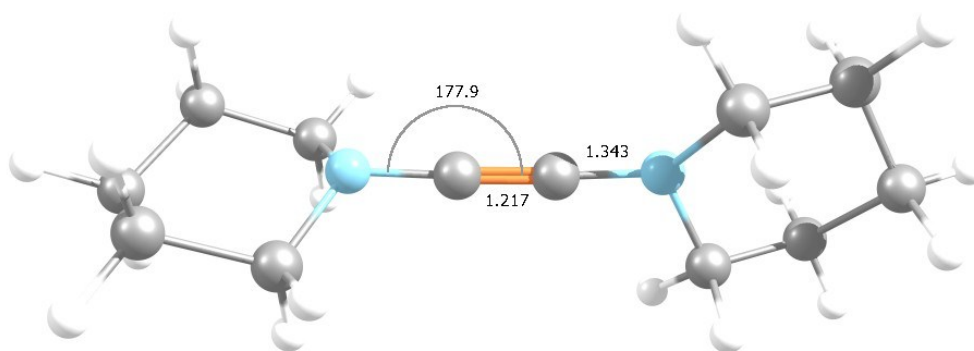


Figure S15. Optimized structure of species I.

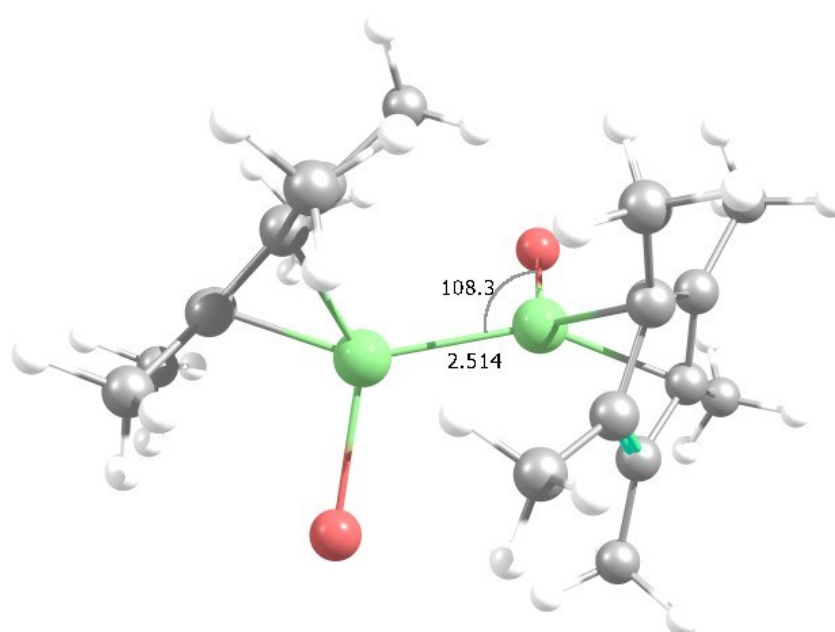


Figure S16. Optimized structure of species II.

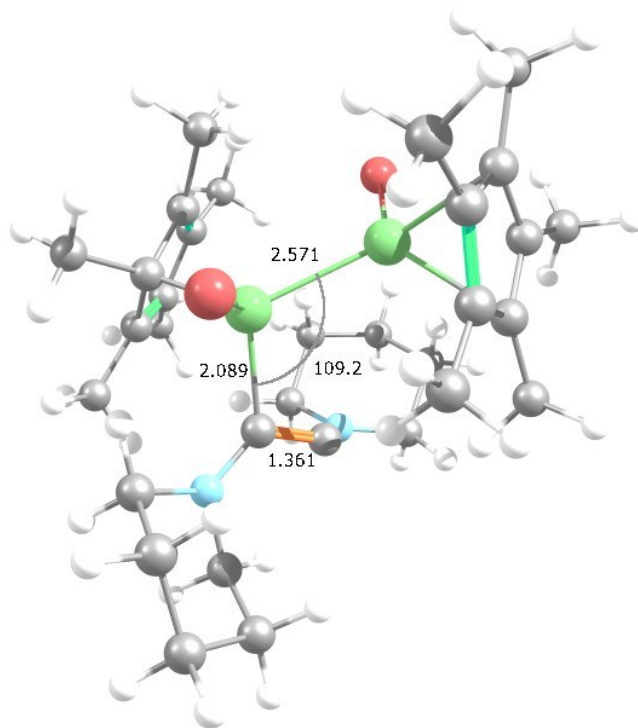


Figure S17. Optimized structure of species III.

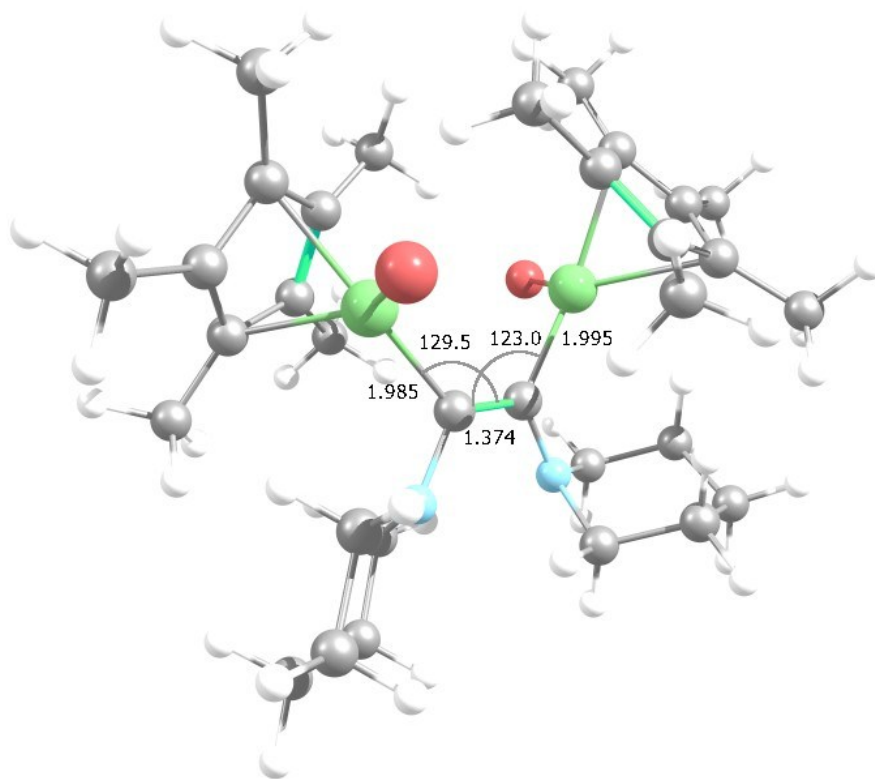


Figure S18. Optimized structure of species IV.

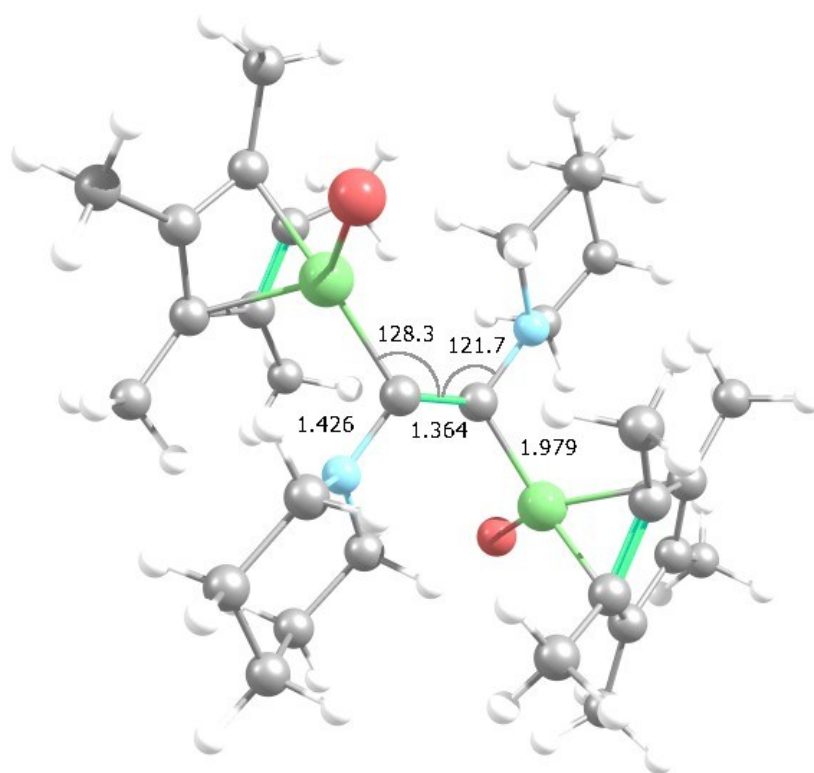


Figure S19. Optimized structure of species V.

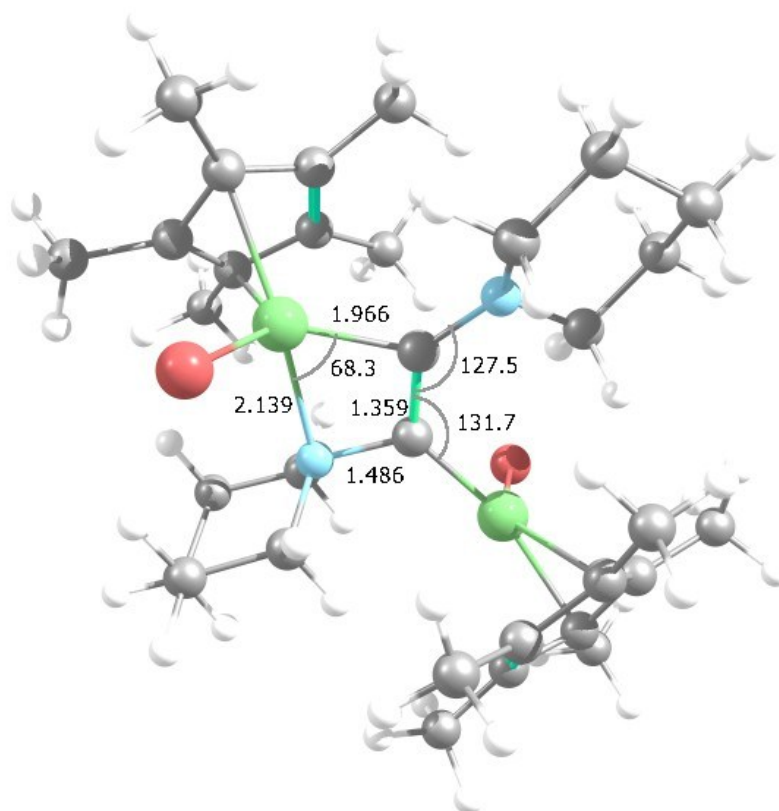


Figure S20. Optimized structure of species **VI**.

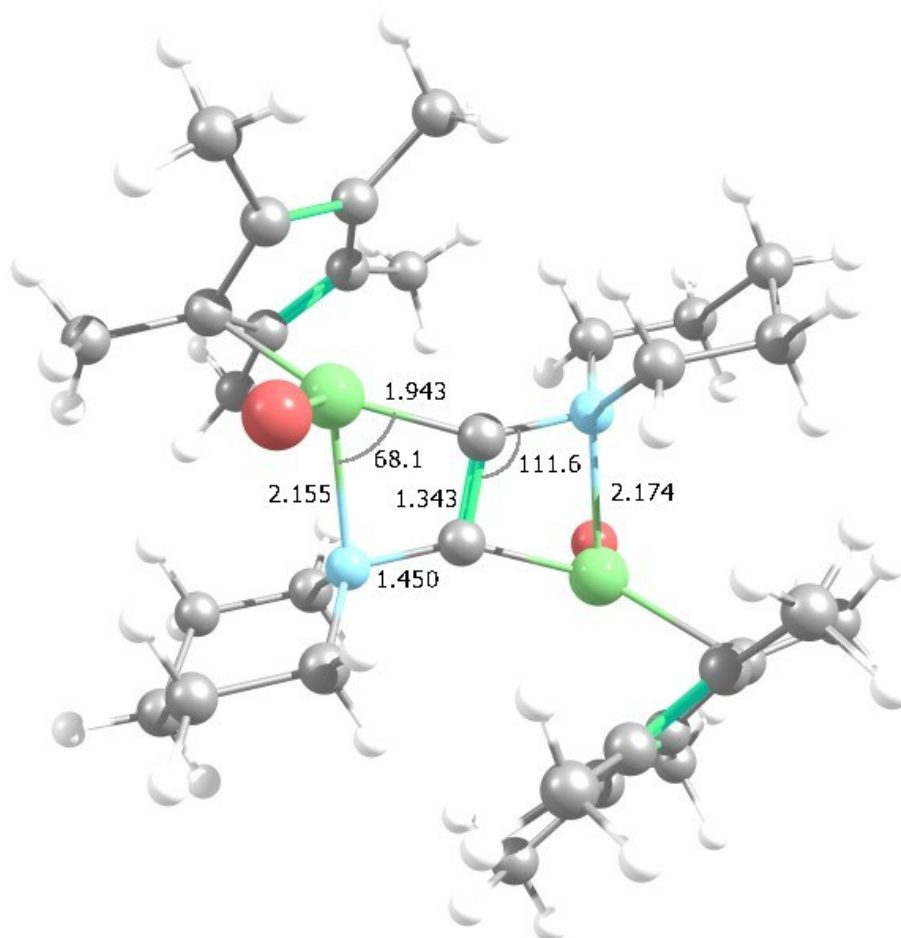


Figure S21. Optimized structure of species **VII**.

Table S1. Chemical shifts of ^{27}Al NMR calculations for species **V-VII** computed by using the B3LYP and M06-L functionals along with the def2-TZVPP basis set.

Compound	$\delta_{^{27}\text{Al}}$, B3LYP (ppm)	$\delta_{^{27}\text{Al}}$, M06-L (ppm)
V	-101.5	-99.8
VI	-101.2, -93.2	-105.3, -96.4
VII	-40.3, -26.3	-35.2, -47.9

Note: AlH_4^- was considered as the ^{27}Al reference reagent.

Table S2. Cartesian coordinates (xyz) of the optimized geometries for all the species involved in the reaction mechanism of 1,2-dialumination calculated at the D3-PBE0/[6-31G(d)], LANL2DZ(f) level. Coordinates are given in Å.

I				II			
7	1.948627000	0.109008000	-0.091114000	35	1.901256000	2.034609000	-1.357395000
6	0.607613000	0.059951000	-0.031796000	13	1.254999000	0.066870000	-0.165032000
6	4.048073000	-0.686845000	-1.074784000	6	3.116246000	-0.292563000	0.907587000
1	3.998644000	0.059567000	-1.878670000	6	3.109097000	-1.053736000	-0.302127000
1	4.551959000	-1.577445000	-1.470511000	6	2.080136000	-2.048696000	-0.187861000
6	2.627787000	-1.051957000	-0.661392000	6	2.091901000	-0.819411000	1.755774000
1	2.042261000	-1.394549000	-1.519528000	6	1.478634000	-1.912914000	1.089881000
1	2.661314000	-1.873754000	0.078508000	6	4.071110000	0.804762000	1.245579000
6	2.637873000	0.680387000	1.064098000	1	5.008046000	0.394130000	1.646467000
1	2.671262000	-0.056713000	1.888280000	1	3.648088000	1.476423000	2.000845000
1	2.058835000	1.542927000	1.406257000	1	4.309053000	1.401651000	0.358738000
6	4.816717000	-0.107980000	0.110849000	6	1.753292000	-3.077089000	-1.222559000
1	4.916554000	-0.881737000	0.887064000	1	0.691870000	-3.341874000	-1.201862000
1	5.829907000	0.185318000	-0.189653000	1	2.342735000	-3.989167000	-1.057842000
6	4.058317000	1.084240000	0.689447000	1	1.983551000	-2.711616000	-2.229092000
1	4.009501000	1.885810000	-0.059489000	6	4.064490000	-0.876060000	-1.437140000
1	4.569412000	1.480262000	1.575800000	1	3.660478000	-1.294469000	-2.364671000
7	-1.948631000	0.108956000	0.091288000	1	5.016354000	-1.381615000	-1.224844000
6	-0.607616000	0.059895000	0.032013000	1	4.269597000	0.186452000	-1.607702000
6	-4.058232000	1.084679000	-0.688863000	6	0.290945000	-2.659061000	1.600206000
1	-4.009461000	1.885777000	0.060579000	1	-0.517054000	-1.964760000	1.881683000
1	-4.569247000	1.481264000	-1.575010000	1	0.537853000	-3.247931000	2.493533000
6	-2.637764000	0.681040000	-1.063643000	1	-0.113406000	-3.331401000	0.838790000
1	-2.058686000	1.543782000	-1.405222000	6	1.787055000	-0.359246000	3.144212000
1	-2.671081000	-0.055559000	-1.888270000	1	0.801357000	-0.712276000	3.461447000
6	-2.627868000	-1.052346000	0.660800000	1	1.805854000	0.734178000	3.229584000
1	-2.661345000	-1.873685000	-0.079611000	1	2.527750000	-0.753530000	3.853267000
1	-2.042422000	-1.395479000	1.518775000	35	-1.902340000	-2.035000000	-1.356925000
6	-4.816709000	-0.107878000	-0.111070000	13	-1.255053000	-0.067260000	-0.165289000
1	-4.916483000	-0.881160000	-0.887767000	6	-3.109013000	1.053644000	-0.301540000
1	-5.829924000	0.185257000	0.189508000	6	-3.115690000	0.292979000	0.908494000
6	-4.048191000	-0.687479000	1.074288000	6	-2.090913000	0.820059000	1.755981000
1	-3.998835000	0.058432000	1.878643000	6	-2.079763000	2.048448000	-0.188200000
1	-4.552124000	-1.578320000	1.469417000	6	-1.477790000	1.913158000	1.089418000
				6	-4.064915000	0.875807000	-1.436098000
				1	-5.016331000	1.382237000	-1.223864000
				1	-3.660893000	1.293223000	-2.364068000
				1	-4.270882000	-0.186675000	-1.605799000
				6	-1.785588000	0.360409000	3.144490000

1	-0.799788000	0.713567000	3.461274000
1	-2.526050000	0.754966000	3.853635000
1	-1.804348000	-0.732976000	3.230293000
6	-4.070555000	-0.804127000	1.247236000
1	-3.647581000	-1.475198000	2.003062000
1	-5.007553000	-0.393250000	1.647721000
1	-4.308392000	-1.401698000	0.360819000
6	-0.289984000	2.659483000	1.599179000
1	0.113954000	3.331848000	0.837589000
1	-0.536643000	3.248294000	2.492613000
1	0.518272000	1.965380000	1.880412000
6	-1.753415000	3.076517000	-1.223358000
1	-0.692169000	3.341979000	-1.202600000
1	-1.983228000	2.710392000	-2.229766000
1	-2.343513000	3.988271000	-1.059207000

I+II-III

35	-1.732556000	2.274139000	1.349918000
13	-0.302622000	1.458532000	-0.438929000
7	-0.457822000	-3.534490000	-1.128082000
6	-1.242780000	-2.739429000	-0.427577000
6	1.050087000	-2.513125000	-2.731297000
1	0.929308000	-1.557719000	-2.202779000
1	1.227295000	-2.294411000	-3.792331000
6	-0.241318000	-3.301646000	-2.556163000
1	-1.107952000	-2.764726000	-2.948723000
1	-0.165372000	-4.276913000	-3.060350000
6	0.611239000	-4.318471000	-0.520046000
1	0.665714000	-5.278993000	-1.053943000
1	0.348884000	-4.516146000	0.520138000
6	2.229172000	-3.268514000	-2.121163000
1	2.388063000	-4.206882000	-2.674247000
1	3.141732000	-2.668827000	-2.201529000
6	1.941462000	-3.583891000	-0.655086000
1	1.877379000	-2.639181000	-0.098107000
1	2.752046000	-4.177691000	-0.212228000
6	0.748794000	2.834932000	-2.015870000
6	-0.548772000	3.285740000	-1.625808000
6	-1.495588000	2.297823000	-2.041454000
6	0.604749000	1.613518000	-2.720898000
6	-0.764366000	1.243679000	-2.688112000
6	2.037188000	3.551377000	-1.769249000
1	2.344512000	4.129032000	-2.651907000
1	2.837367000	2.839882000	-1.533717000
1	1.940615000	4.253327000	-0.933179000
6	-2.982422000	2.437795000	-2.000747000
1	-3.467928000	1.489054000	-2.249745000
1	-3.308726000	3.188173000	-2.733932000
1	-3.330791000	2.754737000	-1.010559000
6	-0.878729000	4.605209000	-1.007870000

III

35	1.525380000	-1.963978000	-2.090079000
13	0.713375000	-0.109668000	-0.828781000
7	0.509647000	1.012318000	2.629489000
6	1.104388000	0.063868000	1.994973000
6	-0.840488000	2.809248000	1.698915000
1	-1.025727000	2.243981000	0.778803000
1	-0.837269000	3.867833000	1.422508000
6	0.539170000	2.427881000	2.215754000
1	1.291580000	2.533570000	1.431173000
1	0.817631000	3.023835000	3.096042000
6	-0.449783000	0.764670000	3.710523000
1	-0.189502000	1.440715000	4.536615000
1	-0.333591000	-0.266298000	4.040424000
6	-1.937848000	2.515198000	2.717816000
1	-1.838021000	3.192475000	3.579566000
1	-2.914718000	2.693332000	2.256004000
6	-1.853325000	1.070713000	3.204597000
1	-2.081972000	0.390210000	2.373322000
1	-2.581713000	0.876068000	4.001553000
6	-0.168263000	1.990955000	-2.254291000
6	1.213954000	1.533490000	-1.979347000
6	1.789041000	2.600149000	-1.133976000
6	-0.395479000	3.158773000	-1.573707000
6	0.826386000	3.543525000	-0.898544000
6	-1.081288000	1.275774000	-3.194872000
1	-0.683434000	1.297168000	-4.220170000
1	-2.082365000	1.715736000	-3.193996000
1	-1.201433000	0.212289000	-2.926939000
6	3.221195000	2.710031000	-0.723620000
1	3.399062000	2.390345000	0.314879000
1	3.563820000	3.750816000	-0.803529000
1	3.863778000	2.092066000	-1.361547000
6	2.036298000	1.162738000	-3.209732000

1	-1.833873000	4.557860000	-0.477166000	1	3.019001000	0.754366000	-2.944835000
1	-0.946958000	5.380750000	-1.783737000	1	2.191224000	2.059318000	-3.827743000
1	-0.113003000	4.916598000	-0.288581000	1	1.530067000	0.404225000	-3.814539000
6	-1.378439000	0.058717000	-3.361410000	6	1.025095000	4.816026000	-0.134314000
1	-2.085202000	-0.460168000	-2.702788000	1	1.858734000	5.398288000	-0.552555000
1	-0.602690000	-0.654508000	-3.655590000	1	1.267104000	4.645173000	0.924758000
1	-1.919384000	0.365706000	-4.267468000	1	0.127528000	5.443890000	-0.169181000
6	1.673891000	0.961463000	-3.533562000	6	-1.652572000	3.960366000	-1.521362000
1	1.475321000	1.147321000	-4.599487000	1	-1.471350000	4.999956000	-1.829752000
1	1.738336000	-0.117826000	-3.389167000	1	-2.069894000	3.985166000	-0.504699000
1	2.653696000	1.381116000	-3.292649000	1	-2.424119000	3.538221000	-2.171025000
7	-3.357285000	-1.505649000	-0.458274000	7	3.223353000	0.012560000	0.941931000
6	-2.047548000	-1.746900000	-0.459050000	6	1.895861000	0.025816000	0.887905000
6	-4.346627000	-0.232054000	1.398300000	6	4.495351000	-1.862797000	0.050956000
1	-3.452488000	-0.339248000	2.023376000	1	3.598358000	-2.494763000	0.028140000
1	-4.802029000	0.732745000	1.651884000	1	5.141835000	-2.180513000	-0.775425000
6	-3.906186000	-0.217851000	-0.061397000	6	4.053008000	-0.421490000	-0.174229000
1	-3.148213000	0.545261000	-0.228675000	1	3.489776000	-0.312401000	-1.101507000
1	-4.770986000	-0.003216000	-0.708314000	1	4.921860000	0.249705000	-0.214321000
6	-4.307621000	-2.603957000	-0.283787000	6	3.943588000	0.002449000	2.212736000
1	-5.197551000	-2.389965000	-0.895453000	1	4.830003000	0.642454000	2.104691000
1	-3.842201000	-3.521531000	-0.652758000	1	3.306704000	0.430108000	2.991809000
6	-5.311789000	-1.388824000	1.658026000	6	5.214819000	-1.995469000	1.394059000
1	-6.247827000	-1.209685000	1.106517000	1	6.162189000	-1.436835000	1.353674000
1	-5.570097000	-1.442223000	2.722628000	1	5.466122000	-3.043905000	1.592399000
6	-4.708716000	-2.712843000	1.185123000	6	4.358954000	-1.432920000	2.530613000
1	-3.806025000	-2.943462000	1.767932000	1	3.445812000	-2.032887000	2.644919000
1	-5.418931000	-3.538284000	1.322603000	1	4.902438000	-1.460527000	3.482993000
35	3.326288000	-0.033912000	-0.810965000	35	-3.274516000	1.067120000	-0.380942000
13	1.536705000	0.168091000	0.793831000	13	-1.682117000	-0.758092000	-0.157166000
6	2.738328000	-0.863952000	2.333869000	6	-3.047489000	-2.053697000	0.948382000
6	2.727772000	0.535499000	2.599074000	6	-3.056241000	-2.407104000	-0.441331000
6	1.389499000	0.909291000	2.970720000	6	-1.810938000	-3.056506000	-0.734839000
6	1.394794000	-1.331889000	2.447875000	6	-1.779929000	-2.444151000	1.472286000
6	0.576375000	-0.241483000	2.881863000	6	-1.038603000	-3.083822000	0.444692000
6	3.938213000	-1.700668000	2.043334000	6	-4.207166000	-1.522809000	1.725739000
1	4.321079000	-2.144852000	2.973087000	1	-4.816788000	-2.351531000	2.112736000
1	3.699438000	-2.513595000	1.349551000	1	-3.876127000	-0.920516000	2.579534000
1	4.733236000	-1.100386000	1.592042000	1	-4.840128000	-0.890006000	1.096519000
6	0.998378000	2.280760000	3.417366000	6	-1.477842000	-3.643950000	-2.068247000
1	-0.027257000	2.287014000	3.793761000	1	-0.508014000	-4.146392000	-2.043658000
1	1.671805000	2.621983000	4.214346000	1	-2.245764000	-4.371985000	-2.362654000
1	1.039902000	3.013895000	2.602250000	1	-1.421481000	-2.879947000	-2.852907000
6	3.921886000	1.436105000	2.585687000	6	-4.225131000	-2.290918000	-1.367514000
1	4.574081000	1.204525000	1.735026000	1	-4.763315000	-1.350925000	-1.203069000
1	3.616115000	2.484972000	2.504958000	1	-3.897140000	-2.315341000	-2.412631000
1	4.510377000	1.327008000	3.506961000	1	-4.927697000	-3.122548000	-1.215736000
6	-0.865934000	-0.425467000	3.211872000	6	0.331676000	-3.637672000	0.655860000
1	-1.422121000	-0.774319000	2.332596000	1	1.042817000	-2.847224000	0.935221000
1	-0.969676000	-1.190689000	3.994536000	1	0.321491000	-4.375717000	1.470544000

1	-1.327763000	0.501123000	3.557883000	1	0.715246000	-4.117019000	-0.247867000
6	0.924958000	-2.748361000	2.414178000	6	-1.340698000	-2.372313000	2.895289000
1	0.000392000	-2.843879000	1.830799000	1	-0.286096000	-2.077362000	2.955339000
1	1.684695000	-3.408677000	1.986091000	1	-1.946027000	-1.660365000	3.466134000
1	0.715995000	-3.092656000	3.437118000	1	-1.442287000	-3.355847000	3.376062000

III-IV

IV

35	2.504871000	-1.552607000	-1.895800000	35	-2.350574000	-1.114714000	-2.474223000
13	0.981953000	0.061747000	-1.055181000	13	-1.787937000	-0.710190000	-0.188560000
7	-0.613959000	0.928399000	2.055661000	7	-1.619002000	2.114177000	-0.051910000
6	0.211633000	0.120667000	1.438605000	6	-0.750608000	0.978326000	-0.078953000
6	-1.623821000	3.190409000	2.087794000	6	-2.414134000	4.126658000	1.121976000
1	-2.085456000	3.054282000	1.101698000	1	-1.769968000	4.787857000	0.525875000
1	-1.356051000	4.246714000	2.195783000	1	-2.519560000	4.570475000	2.119999000
6	-0.347535000	2.370590000	2.139696000	6	-1.739749000	2.767777000	1.247629000
1	0.320254000	2.613926000	1.309157000	1	-0.728679000	2.883337000	1.646089000
1	0.174647000	2.564448000	3.090778000	1	-2.314818000	2.140375000	1.944930000
6	-1.725650000	0.383169000	2.845537000	6	-2.851201000	1.996771000	-0.798172000
1	-1.337332000	0.182804000	3.855635000	1	-3.553829000	1.261385000	-0.340393000
1	-1.991646000	-0.571404000	2.388302000	1	-2.612364000	1.613421000	-1.794334000
6	-2.584469000	2.738256000	3.179703000	6	-3.768221000	3.987982000	0.435738000
1	-2.102478000	2.848711000	4.163479000	1	-4.424554000	3.355860000	1.053314000
1	-3.487626000	3.358773000	3.184922000	1	-4.260671000	4.962578000	0.329575000
6	-2.952295000	1.282978000	2.924814000	6	-3.568759000	3.334883000	-0.926321000
1	-3.498226000	1.217176000	1.979143000	1	-2.954738000	3.995693000	-1.553249000
1	-3.601355000	0.889261000	3.716521000	1	-4.524848000	3.178659000	-1.440726000
6	-0.157713000	1.893463000	-2.587744000	6	-2.527712000	-2.613180000	0.594035000
6	1.256759000	1.727279000	-2.199193000	6	-3.571468000	-1.651774000	0.703126000
6	1.505627000	2.799644000	-1.227050000	6	-3.174666000	-0.675928000	1.673147000
6	-0.694898000	2.934860000	-1.870862000	6	-1.456433000	-2.187966000	1.454139000
6	0.337693000	3.500355000	-1.040097000	6	-1.878857000	-1.007528000	2.135917000
6	-0.832919000	1.059561000	-3.629220000	6	-2.611759000	-3.870597000	-0.207910000
1	-0.783741000	1.530156000	-4.622566000	1	-3.390926000	-4.526318000	0.202663000
1	-1.888039000	0.896906000	-3.379095000	1	-1.666416000	-4.421564000	-0.190951000
1	-0.353517000	0.074193000	-3.716520000	1	-2.864101000	-3.655172000	-1.253193000
6	2.827091000	3.122633000	-0.610441000	6	-4.091266000	0.371366000	2.221077000
1	2.854929000	2.884171000	0.464033000	1	-3.623332000	0.901207000	3.056127000
1	3.059435000	4.191563000	-0.711745000	1	-5.008124000	-0.104889000	2.592608000
1	3.634419000	2.557608000	-1.090599000	1	-4.389783000	1.122258000	1.481347000
6	2.274623000	1.513856000	-3.309008000	6	-4.893025000	-1.712617000	0.010842000
1	3.269591000	1.289853000	-2.908021000	1	-5.370038000	-0.726287000	-0.000045000
1	2.341126000	2.416454000	-3.933409000	1	-5.571277000	-2.411671000	0.520174000
1	1.993520000	0.669256000	-3.947107000	1	-4.773618000	-2.042666000	-1.026960000
6	0.174791000	4.728595000	-0.200358000	6	-1.044553000	-0.233602000	3.100213000
1	0.515299000	5.622396000	-0.744097000	1	-0.412601000	0.494136000	2.574452000
1	0.761409000	4.678234000	0.726881000	1	-0.378503000	-0.898630000	3.660139000
1	-0.874702000	4.892679000	0.066362000	1	-1.673019000	0.312378000	3.813046000
6	-2.090166000	3.460204000	-1.947093000	6	-0.227955000	-2.975542000	1.780668000
1	-2.104514000	4.481145000	-2.356171000	1	0.665945000	-2.349336000	1.855990000
1	-2.569524000	3.496670000	-0.959383000	1	-0.043250000	-3.754252000	1.036363000
1	-2.714433000	2.825815000	-2.583438000	1	-0.350976000	-3.470763000	2.753490000

7	2.553043000	0.643858000	1.563029000	7	1.042164000	2.500862000	0.373558000
6	1.450474000	0.342187000	0.878862000	6	0.588111000	1.167307000	0.164115000
6	4.345975000	-1.005077000	1.393785000	6	2.022569000	3.296651000	-1.724858000
1	3.675360000	-1.745368000	0.939388000	1	1.959704000	2.280770000	-2.134198000
1	5.349645000	-1.180409000	0.988684000	1	1.902837000	4.000041000	-2.559707000
6	3.859654000	0.376661000	0.967892000	6	0.878285000	3.442468000	-0.726565000
1	3.762947000	0.442746000	-0.117686000	1	-0.098086000	3.279738000	-1.186604000
1	4.549386000	1.159353000	1.312174000	1	0.884388000	4.459116000	-0.300470000
6	2.578568000	0.635443000	3.022533000	6	2.272960000	2.759177000	1.092451000
1	3.315537000	1.378865000	3.354989000	1	2.213441000	3.793868000	1.464779000
1	1.597161000	0.929555000	3.402145000	1	2.333774000	2.100958000	1.961395000
6	4.342573000	-1.138246000	2.917467000	6	3.368086000	3.518240000	-1.030370000
1	5.106109000	-0.468273000	3.340986000	1	3.420229000	4.570134000	-0.710153000
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6	2.979486000	-0.759757000	3.500411000	6	3.512461000	2.633478000	0.209316000
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6	-2.457343000	-2.697125000	0.608362000	6	3.743148000	-1.289262000	-0.642536000
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1	1.257138000	-4.265018000	1.420392000	1	0.536753000	-0.919777000	-3.658689000
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6	-0.897610000	-2.783869000	2.713214000	6	4.135515000	0.582166000	-2.375707000
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1	-1.795060000	-2.572223000	3.304158000	1	4.851193000	1.056158000	-1.696944000
1	-0.475505000	-3.733592000	3.068062000	1	4.717651000	0.060255000	-3.147717000
V				VI			
35	-2.623699000	-0.138883000	2.532663000	35	-2.508167000	1.315187000	2.319054000
13	-2.302904000	-0.278697000	0.174215000	13	-2.105394000	0.098631000	0.313906000
7	0.452519000	-1.426848000	0.001652000	7	0.734553000	-1.541122000	0.628352000
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1	-3.616513000	-3.488515000	0.052837000	1	-2.355864000	-3.251842000	1.713512000
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6	-2.090914000	-1.305006000	-3.192073000	6	-1.966472000	-3.037097000	-2.218864000
1	-1.166637000	-0.718820000	-3.258135000	1	-1.080271000	-2.542574000	-2.650054000
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1	-2.269352000	4.366354000	0.774104000	1	-1.874420000	2.873167000	-3.518295000
35	2.845975000	-0.742368000	-2.368931000	35	2.516166000	-1.442698000	-2.278527000
13	2.160132000	-0.147054000	-0.140900000	13	2.083975000	-0.162657000	-0.332264000
6	4.034101000	-0.498970000	0.888509000	6	3.875267000	0.257306000	0.673422000
6	4.086507000	0.858781000	0.423964000	6	3.856915000	1.171522000	-0.456433000
6	3.170423000	1.615671000	1.197113000	6	3.154805000	2.332606000	-0.063220000
6	3.080730000	-0.544630000	1.960508000	6	3.205311000	0.935753000	1.748364000
6	2.534770000	0.754953000	2.118598000	6	2.764635000	2.185442000	1.289321000
6	4.950254000	-1.602645000	0.465888000	6	4.858655000	-0.873848000	0.807063000
1	5.899998000	-1.565412000	1.018207000	1	5.887853000	-0.489079000	0.871309000
1	4.496608000	-2.585133000	0.644060000	1	4.672223000	-1.457200000	1.713927000
1	5.171894000	-1.530489000	-0.604381000	1	4.816446000	-1.555851000	-0.053231000
6	2.914416000	3.080032000	1.081864000	6	2.921791000	3.501378000	-0.958576000
1	1.852698000	3.295708000	1.231694000	1	2.463696000	4.340325000	-0.416055000
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6	1.407007000	1.124561000	3.026140000	6	2.031746000	3.177730000	2.135060000
1	0.438967000	1.053672000	2.506830000	1	1.198365000	2.707163000	2.683269000
1	1.362832000	0.459017000	3.896721000	1	2.695968000	3.624541000	2.884764000
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VII

35	3.238506000	-0.290481000	2.318465000
13	2.459430000	-0.010230000	0.090074000
7	0.386404000	1.834868000	-0.061637000
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6	0.883006000	4.092870000	0.891758000
1	1.637517000	4.386854000	0.153662000
1	1.156050000	4.560311000	1.845404000
6	0.907546000	2.579704000	1.079034000
1	1.943585000	2.254980000	1.258937000
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1	-1.007380000	1.791510000	-1.565966000
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6	3.100779000	-0.854202000	-1.896660000
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6	3.108437000	2.863920000	-1.476708000
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1	3.620906000	3.323089000	-2.332751000
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6	5.427415000	1.321856000	0.092899000
1	5.097504000	2.275388000	0.519246000
1	6.323881000	1.515290000	-0.512243000
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6	1.343958000	0.694257000	-2.993521000
1	0.471763000	0.184321000	-2.560248000
1	1.467616000	0.345606000	-4.026800000
1	1.119580000	1.765135000	-3.018019000
6	2.631085000	-2.138405000	-2.494095000
1	1.554498000	-2.110348000	-2.689473000
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1	3.140311000	-2.329976000	-3.448580000
7	-0.386431000	-1.834703000	0.061214000
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6	-0.883093000	-4.092882000	-0.892003000
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6	0.482842000	-4.569813000	-0.415088000
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1	0.480738000	-5.654537000	-0.254629000
6	0.833108000	-3.827579000	0.867386000
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1	-3.144456000	2.332219000	3.446680000

References

- 1 Manipulation of Air Sensitive Compounds; 2 ed.; D. F. Shriver and M. A. Drezdson, Eds.; Wiley: New York, 1986
- 2 F. X. Kohl and P. Jutzi, *J. Organomet. Chem.*, 1983, **243**, 119.
- 3 Z. J. Tonzetich and R. Eisenberg, *Inorg. Chim. Acta*, 2003, **345**, 340.
- 4 M. Schormann, *J. Solid State Chem.*, 2001, **162**, 225.
- 5 Purification of Laboratory Chemicals; 6 ed., W. L. F. Armarego and C. L. L. Chai; Elsevier: Oxford, 2009.
- 6 G. Sheldrick, *Acta Cryst.*, 2015, **A71**, 3–8.
- 7 G. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112–122.
- 8 C. Adamo and V. Barone, *J. Chem. Phys.*, 1999, **110**, 6158-6169.
- 9 S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104-1541019.
- 10 (a) T. H. Dunning Jr. and P. J. Hay, in *Methods of Electronic Structure Theory*, Vol. 2, H. F. Schaefer III, ed., Plenum Press, 1977. (b) Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.
- 11 Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.
- 12 A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378-6396.
- 13 (a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652. (b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789. (c) S. H. Vosko, L. Wilk and M. Nusair, *Can. J. Phys.*, 1980, **58**, 1200-1211. (d) P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.*, 1994, **98**, 11623-11627.
- 14 Y. Zhao and D. G. Truhlar, *J. Chem. Phys.*, 2006, **125**, 194101.
- 15 (a) F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1057-1065. (b) F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.
- 16 J. Gauss, U. Scheiner, R. Ahlrichs, C. Dohmeierer and H. Schnöckel, *J. Am. Chem. Soc.*, 1993, **115**, 2402-2408.