Electronic Supporting Information
to

Investigations on Non-Classical Siylium Ions and Cyclobutenyl Cations

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Contents:

General Considerations **3**

Experimental Details **4**

Reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with $Me_2C{=}CMe_2$ 4

Reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with $Ph_2C{=}CPh_2$ 6

Reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with $PhC{\equiv}CPh$ 8

Reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with $MeC{\equiv}CMe$ 9

Selective Synthesis of $[Me_4C_4{-}SiMe_3]^+[al{-}f{-}al]^-$ 10

Reactions of $[Ph_3C][al{-}f{-}al]$ with alkenes and alkynes in Me_3SiH 12

Reactions of $Ag[al{-}f{-}al]$ with bromoethyl/bromovinyl trimethyl silane 16

Reaction of $[Me_4C_4{-}SiMe_3][al{-}f{-}al]$ with $[NMe_4]F$ 21

Reaction of $[Me_4C_4{-}SiMe_3][al{-}f{-}al]$ with DMAP 25

Reactions of $[Me_4C_4{-}SiMe_3][al{-}f{-}al]$ with Et_2O and 2-butyne 28

Crystal Structure Data **33**

Crystal Structure of $[Me_4C_4{-}SiMe_3][al{-}f{-}al]$ 33

Crystal Structure of $DMAP{-}Al(OR^F)_3$ 35

Crystal Structure of $[Me_4C_4(SiMe_3)(DMAP)][f{-}al]$ (4) 37

Quantum Chemical Calculations **39**

Optimized coordinates and energies of the calculated compounds: 40

BP86−D3(BJ)/def-TZVP 40

COSMO(ε = 13.4)/BP86−D3(BJ)/def-TZVP 43

MP2/def2-TZVPP 46

Reaction path of $[Me_4C_4{-}SiMe_3]^+$ (BP86−D3(BJ)/def-TZVP) 50

General Considerations

All reactions were carried out in an inert gas atmosphere of argon, using standard vacuum and Schlenk techniques or a glove box to exclude air and moisture. All solvents and reagents were dried using standard drying agents (CaH_2, P_4O_{10}) and were subsequently distilled into airtight vessels. Solution NMR spectra were recorded on a Bruker Avance II WB 400 MHz, Bruker Avance III HD 300 MHz and a Bruker Avance DPX 200 MHz NMR spectrometer using the software package Bruker Topspin 3.2 for analysis. Samples were prepared in 5 mm NMR tubes and then flame-sealed in vacuo. Resonances are given in ppm and referenced to $SiMe_4$ for the ^{1}H, ^{13}C and ^{29}Si NMR spectra, to $CFCl_3$ for the ^{19}F NMR spectra and to a 1.1 M solution of $Al(NO_3)_3$ in D_2O for the ^{27}Al NMR spectra. Raman spectra were measured on a Bruker Vertex 70 with a Bruker RAM II module in a range of 50 – 4000 cm^{-1} and analyzed with the OPUS software package. IR spectra were measured on a Bruker Alpha Fourier transform IR spectrometer in a range of 400 – 4000 cm^{-1} using a diamond ATR unit and analyzed with the OPUS software package.

Single Crystal Diffraction: Obtained single crystals were coated with perfluoroether oil and mounted on 0.1 mm micromounts at the respective crystallization temperature. The crystal structure data were collected from the shock-cooled crystals at 100 K, on a Bruker SMART APEXII QUAZAR CCD area detector diffractometer using Mo-K_α radiation. Data reduction was done with SAINT[1] and scaling of the data and absorption correction was performed by SADABS[2]. The structures were solved by intrinsic phasing using SHELXT[3] and were refined by full matrix least squares minimization on F^2 using all reflections with SHELXL[4] in the ShelXle[5] GUI. In addition, a riding model was used to attribute idealized positions to all hydrogen atoms. The disorder of the OR^F groups in the compounds was treated using DSR.[6] The graphical representations were prepared using the software Mercury 3.6.[7] CCDC 1868136 (**1**), CCDC 1868137 (**4**) and CCDC 1868138 contain the supplementary crystallographic data for this paper.

[1] *SAINT*, BRUKER-AXS, Madison, Wisconsin, USA, **2013**.
[2] L. Krause, R. Herbst-Irmer, G. M. Sheldrick, D. Stalke, *J. Appl. Cryst.* **2015**, *48*, 3–10.
[3] G. M. Sheldrick, *Acta Cryst. A* **2015**, *71*, 3–8.
[4] G. M. Sheldrick, *Acta Cryst. C* **2015**, *71*, 3–8.
[5] C. B. Hubschle, G. M. Sheldrick and B. Dittrich, *J. Appl. Cryst.* **2011**, *44*, 1281-1284.
[6] D. Kratzert, J. J. Holstein, I. Krossing, *J. Appl. Cryst.* **2015**, *48*, 933–938. *www.xs3.uni-freiburg.de/research/dsr*
[7] C. F. Macrae, P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor, M. Towler, J. van de Streek, *J. Appl. Cryst.* **2006**, *39*, 453–457.

Experimental Details

$Me_3Si{-}F{-}Al(OR^F)_3$, Ag[*al*–*f*–*al*], and [Ph_3C][*al*–*f*–*al*] were synthesized according to the literature.[1] If not stated otherwise, the other starting materials were commercially available and were used as received.

Due to the high sensitivity of the presented compounds towards water, some of the NMR spectra show signals of these hydrolysis products, like $Me_3Si{-}O(H){-}Al(OR^F)_3$ or $(Me_3Si)_2O$.

[1] A. Martens, P. Weis, M. C. Krummer, M. Kreuzer, A. Meierhöfer, S. C. Meier, J. Bohnenberger, H. Scherer, I. Riddlestone and I. Krossing, *Chem. Sci.*, 2018 , **9**, 7058.

Reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with $Me_2C{=}CMe_2$

$Me_2C{=}CMe_2$ (0.06 mL, 42 mg, 0.51 mmol) was added to a solution of $Me_3Si{-}F{-}Al(OR^F)_3$ (0.42 g, 0.51 mmol, 1.0 eq.) in CH_2Cl_2 (2 mL) at rt. The solution was stirred for 1 h. After several minutes the solution changed color to yellow. This solution was analyzed NMR-spectroscopically. All relevant spectra are shown following this section.
The ^{29}Si NMR spectrum only showed signals of impurities and therefore is not shown.

^{1}H-NMR (300.18 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 0.57 (s, br, **Me**$_3$Si–F–Al(OR^F)$_3$), 0.7 - 1.8 (several overlapping signals, oligomerization products of $Me_2C{=}CMe_2$) ppm.
^{13}C-NMR (75.48 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 10 - 65 (several signals, oligomerization products of $Me_2C{=}CMe_2$) ppm.
^{19}F-NMR (282.45 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = –75.8 (s, [*al*–*f*–*al*]$^-$), –75.9 (s, $Me_3Si{-}F{-}Al(O\mathbf{R^F})_3$), −165.9 (s, br, $Me_3Si{-}\mathbf{F}{-}Al(OR^F)_3$/$Me_3Si\mathbf{F}$), −184.9 (s, [*al*–***f***–*al*]$^-$) ppm.
^{27}Al-NMR (78.22 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 36.5 (s, br, $Me_3Si{-}F{-}\mathbf{Al}(OR^F)_3$ / [***al***–*f*–***al***]$^-$) ppm.

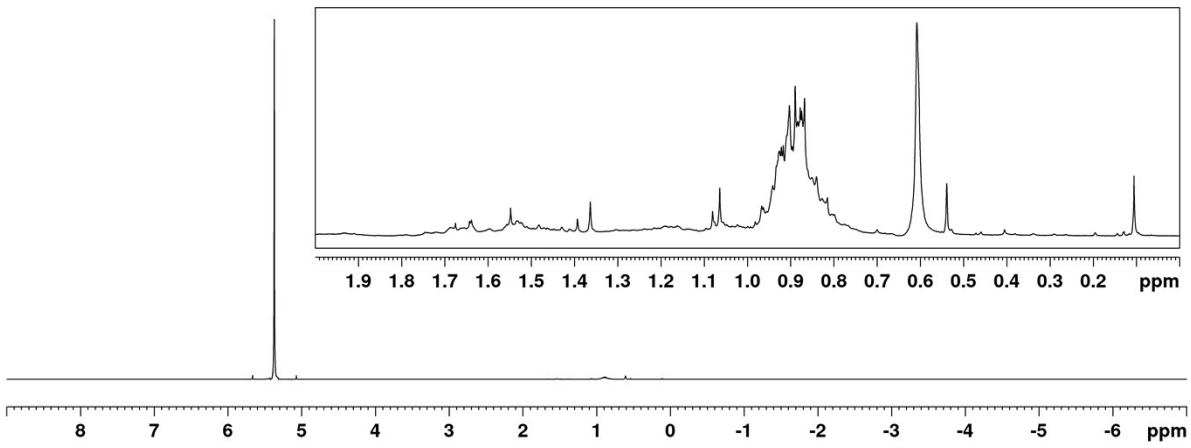

Figure S- 1: ^{1}H-NMR (300.18 MHz, 298 K, CH_2Cl_2/CD_2Cl_2) of the reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with $Me_2C{=}CMe_2$ in CH_2Cl_2.

The signals at 0.07 and 0.50 ppm result from impurities of $Me_3Si{-}O{-}SiMe_3$ and $Me_3Si{-}O(H){-}Al(OR^F)_3$, respectively. The $^3J_{H-F}$ coupling constant of $Me_3Si{-}F{-}Al(OR^F)_3$ is not visible, due to exchange reactions involving the Me_3Si moiety.

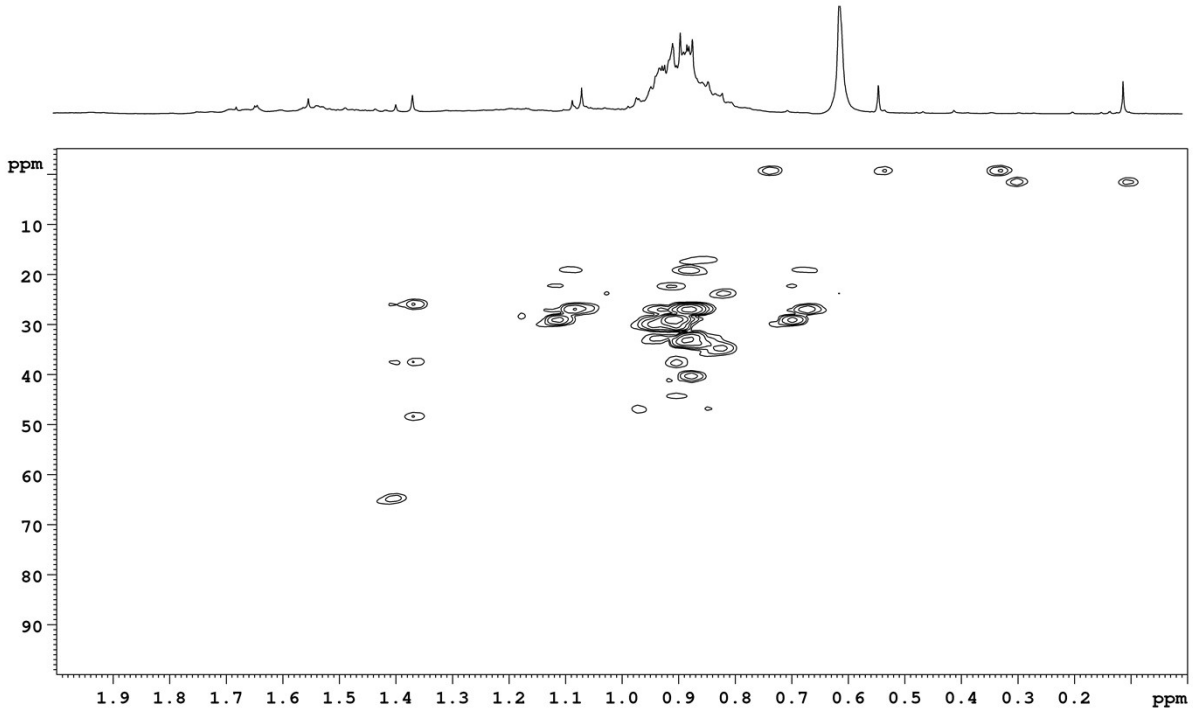

Figure S- 2: $^{1}H,^{13}C$-HMBC NMR spectrum (300.18 MHz, 298 K, optimized to 8 Hz) of the reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with $Me_2C{=}CMe_2$ in CH_2Cl_2.

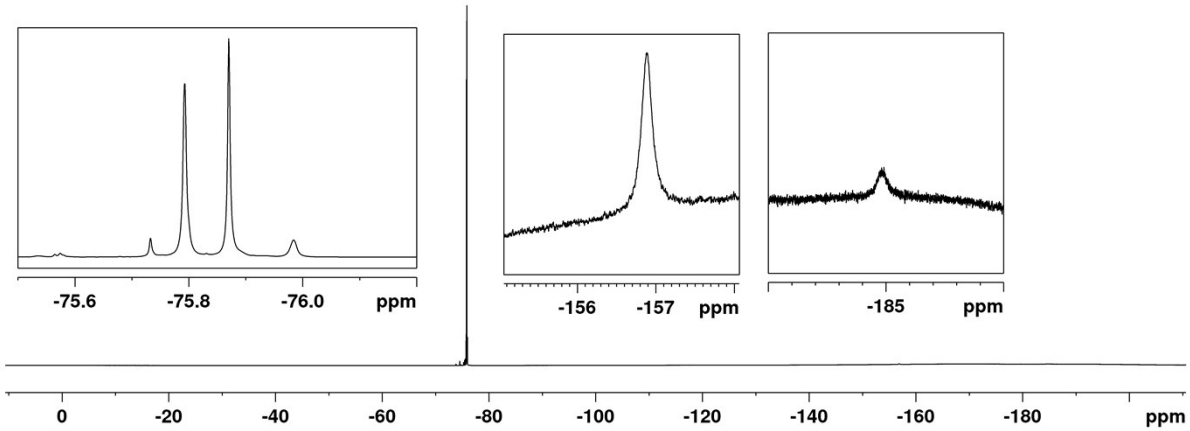

Figure S- 3: ^{19}F-NMR spectrum (282.45 MHz, 298 K, CH_2Cl_2/CD_2Cl_2) of the reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with $Me_2C{=}CMe_2$ in CH_2Cl_2.

The signal at −76.0 ppm results from an unidentified impurity.

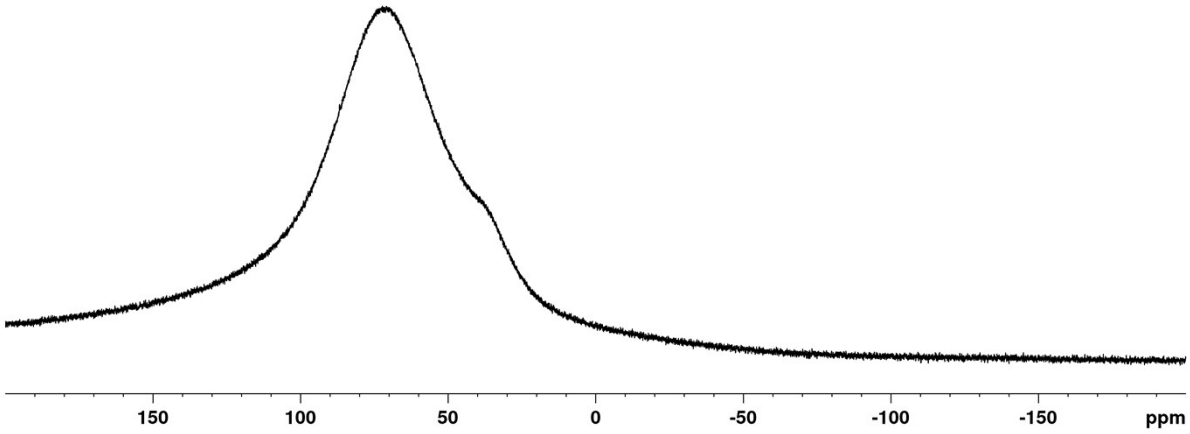

Figure S- 4: ^{27}Al NMR spectrum (78.22 MHz, 298 K, CH_2Cl_2/CD_2Cl_2) of the reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with $Me_2C{=}CMe_2$ in CH_2Cl_2. Note that the broad hump in the center (max. at 60 ppm) belongs to the ^{27}Al-nuclei in the probe head.

Reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with $Ph_2C{=}CPh_2$

$Me_3Si{-}F{-}Al(OR^F)_3$ (170 mg, 0.21 mmol) and $Ph_2C{=}CPh_2$ (70 mg, 0.21 mmol, 1.0 eq.) were dissolved in CH_2Cl_2 (2 mL) at rt. The solution was stirred for 1 h. After several minutes, the solution turned green. This solution was analyzed NMR-spectroscopically. All relevant spectra are shown following this section.

^{1}H-NMR (400.18 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 0.56 (d, $^3J_{H-F}$ = 11.8 Hz, **Me_3**Si−F−Al(OR^F)$_3$), 7.12 (s, br, $\nu_{1/2}$ = 160 Hz, oligomerization products of $Ph_2C{=}CPh_2$) ppm.
^{13}C{^{1}H}-NMR (100.62 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = –127.6 (s, br, $\nu_{1/2}$ = 240 Hz, oligomerization products of $Ph_2C{=}CPh_2$) ppm.
^{19}F-NMR (376.54 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = –75.9 (s, $Me_3Si{-}F{-}Al(O\mathbf{R^F})_3$), –156.7 (s, br $Me_3Si{-}\mathbf{F}{-}Al(OR^F)_3$) ppm.
^{27}Al-NMR (104.27 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 37 (s, br, $Me_3Si{-}F{-}\mathbf{Al}(OR^F)_3$) ppm.

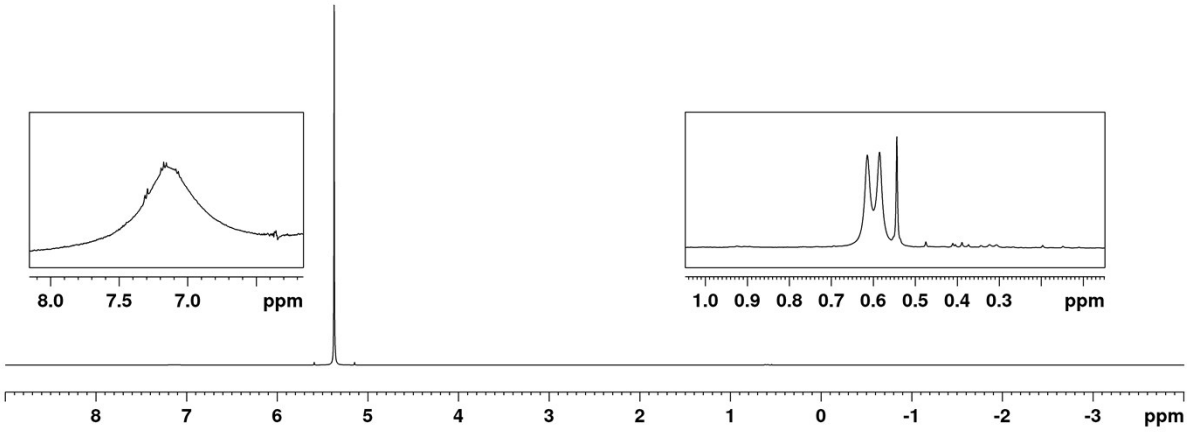

Figure S- 5: ^{1}H-NMR spectrum (400.17 MHz, 298 K, CH_2Cl_2/CD_2Cl_2) of the reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with $Ph_2C{=}CPh_2$ in CH_2Cl_2.

The signal at 0.52 ppm results from impurities of $Me_3Si{-}O(H){-}Al(OR^F)_3$. The signal of $Me_3Si{-}F{-}Al(OR^F)_3$ is broadened due to exchange reactions involving the Me_3Si moiety.

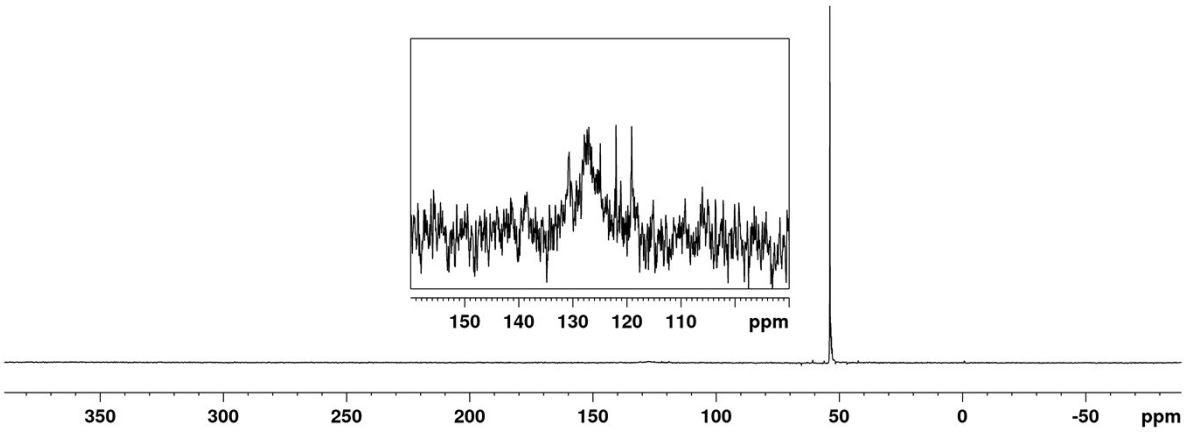

Figure S- 6: $^{13}C\{^{1}H\}$-NMR spectrum (100.62 MHz, 298 K, CH_2Cl_2/CD_2Cl_2) of the reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with $Ph_2C{=}CPh_2$ in CH_2Cl_2.

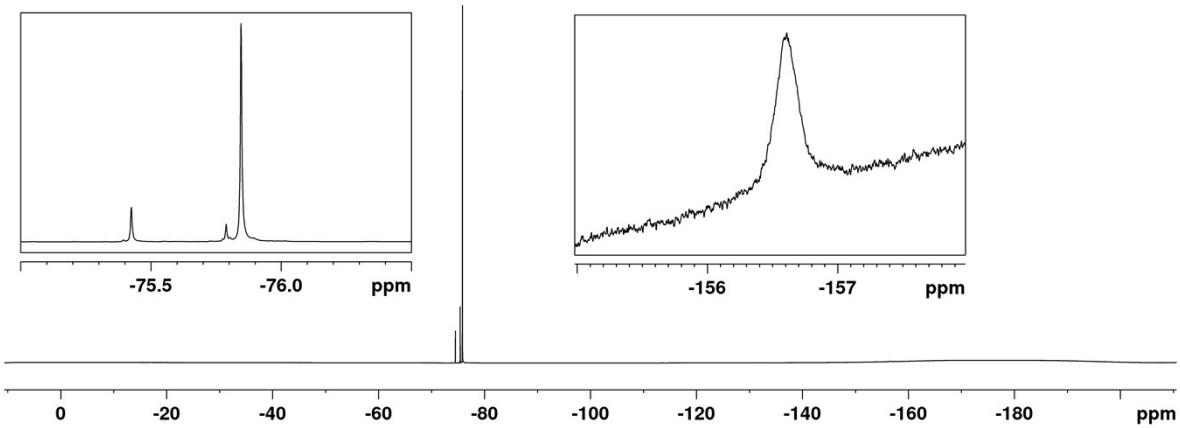

Figure S- 7: ^{19}F-NMR spectrum (376..54 MHz, 298 K, CH_2Cl_2/CD_2Cl_2) of the reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with $Ph_2C{=}CPh_2$ in CH_2Cl_2.

The signal at −75.4 ppm results from impurities of $Me_3Si{-}O(H){-}Al(OR^F)_3$. The signal at −75.8 ppm probably results from small amounts of [*f*–*al*]$^-$ or [*al*–*f*–*al*]$^-$.

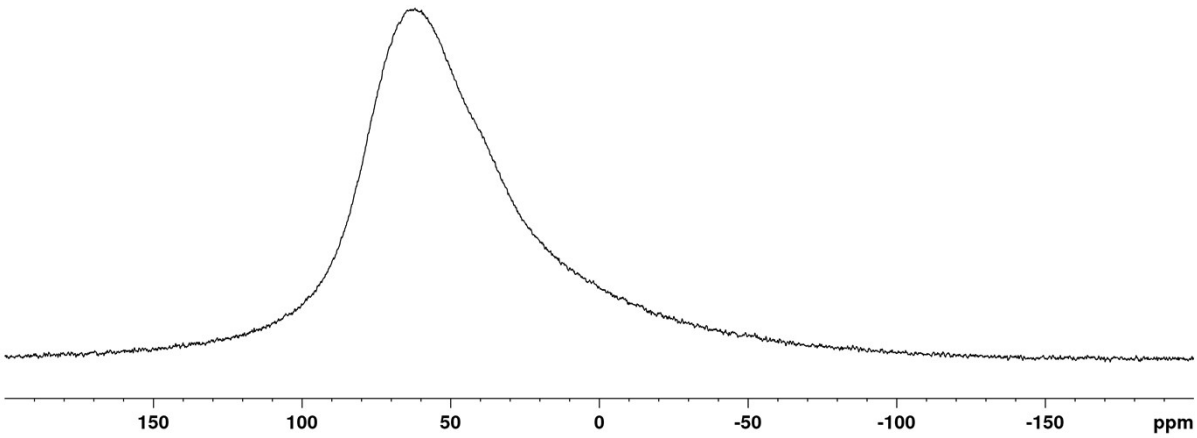

Figure S- 8: ^{27}Al-NMR spectrum (104.27 MHz, 298 K, CH_2Cl_2/CD_2Cl_2) of the reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with $Ph_2C{=}CPh_2$ in CH_2Cl_2. Note that the broad hump in the center (max. at 60 ppm) belongs to the ^{27}Al-nuclei in the probe head.

Reaction of $Me_3Si–F–Al(OR^F)_3$ with PhC≡CPh

$Me_3Si–F–Al(OR^F)_3$ (400 mg, 0.49 mmol) and PhC≡CPh (87 mg, 0.49 mmol, 1.0 eq.) were dissolved in CH_2Cl_2 (3 mL) at rt. The solution was stirred for 1 h. After several minutes the solution turned dark green. This solution was analyzed NMR-spectroscopically. All relevant spectra are shown following this section.

^{1}H-NMR after 1 h (300.18 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 0.56 (s, br, **Me_3**Si–F–Al$(OR^F)_3$ / **Me_3**SiF), 7.34 – 7.40 (m, H_{ortho}, PhC≡CPh), 7.50 – 7.57 (m, $H_{meta/para}$, PhC≡CPh) ppm.
^{1}H-NMR after 7 d (300.18 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 0.48 (d, $^3J_{H–F}$ = 8.7 Hz, **Me_3**SiF), 6.5 – 8.0 (several overlapping signals, oligomerization products of PhC≡CPh) ppm.
^{19}F-NMR (282.45 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = –75.8 (s, [*al*–*f*–*al*]$^-$), –75.9 (s, $Me_3Si–F–Al(OR^F)_3$), –156.6 (s, br, $Me_3Si–F–Al(OR^F)_3$ / Me_3SiF), –84.9 (s, [*al*–***f***–*al*]$^-$) ppm.
^{27}Al-NMR (78.22 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 37 (s, br, $Me_3Si–F–$**Al**$(OR^F)_3$ / [***al***–*f*–***al***]$^-$) ppm.

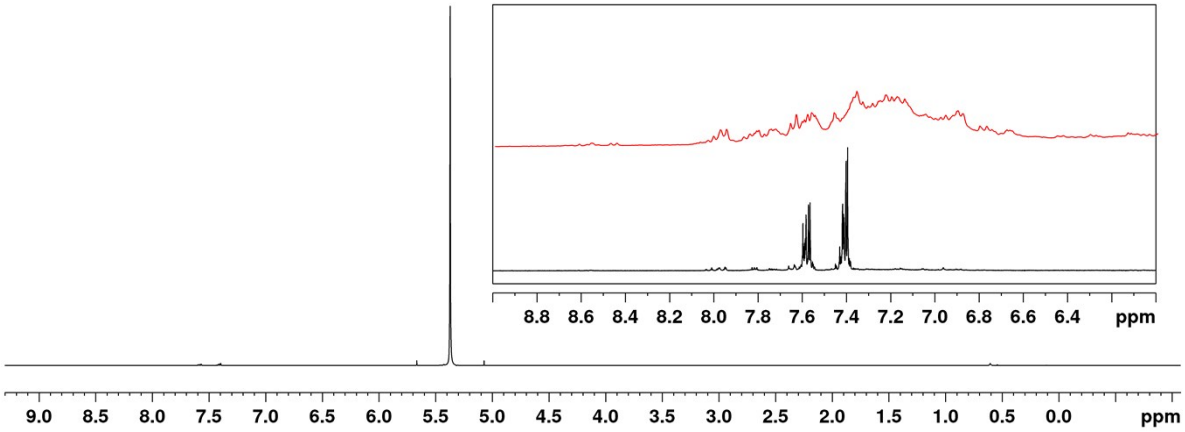

Figure S- 9: ^{1}H-NMR spectrum (300.18 MHz, 298 K, CH_2Cl_2/CD_2Cl_2) of the reaction of $Me_3Si–F–Al(OR^F)_3$ with PhC≡CPh in CH_2Cl_2. Black: NMR spectrum directly after reaction; red: NMR spectrum after 7 days.

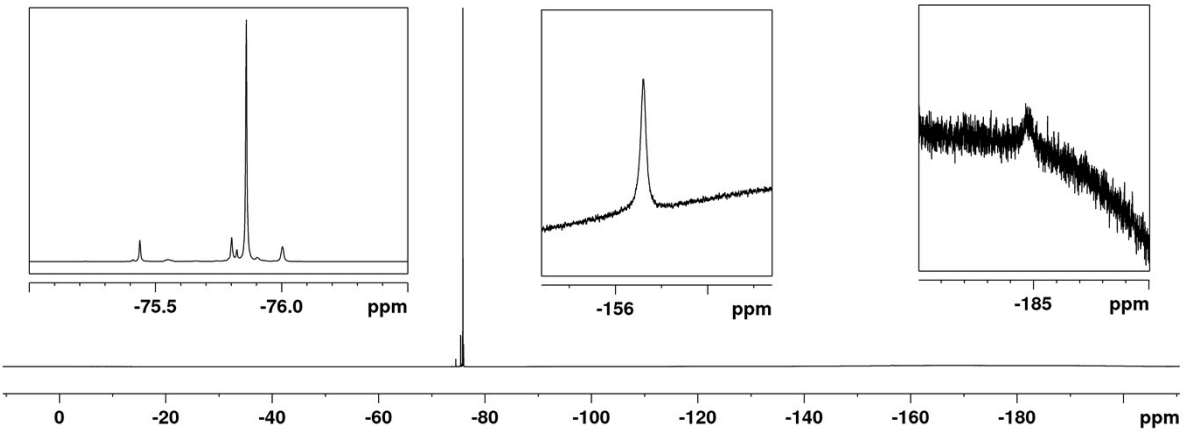

Figure S- 10: ^{19}F-NMR spectrum (282.45 MHz, 298 K, CH_2Cl_2/CD_2Cl_2) of the reaction of $Me_3Si–F–Al(OR^F)_3$ with PhC≡CPh in CH_2Cl_2.

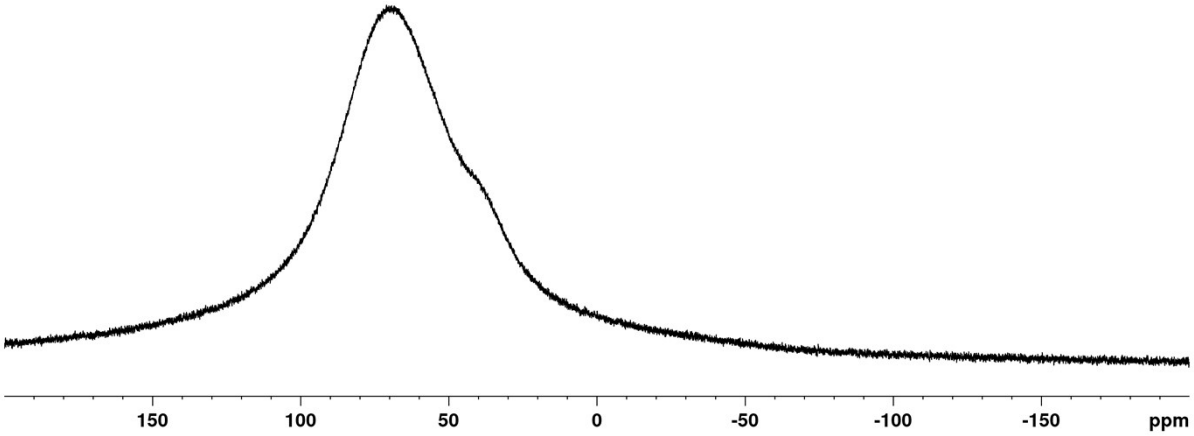

Figure S- 11: ^{27}Al-NMR spectrum (78.22 MHz, 298 K, CH_2Cl_2/CD_2Cl_2) of the reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with PhC≡CPh in CH_2Cl_2.

Reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with MeC≡CMe

2-butyne (0.04 mL, 28 mg, 0.51 mmol) was added to a solution of $Me_3Si{-}F{-}Al(OR^F)_3$ (420 mg, 0.51 mmol, 1.0 eq.) in CH_2Cl_2 (3 mL) at rt. The solution was stirred for 1 h. After several minutes the solution turned orange. This solution was analyzed NMR-spectroscopically. All relevant spectra are shown following this section.

^{1}H–NMR (400.17 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 0.18 (s, 9 H, $[Me_4C_4{-}Si\mathbf{Me_3}]^+$), 0.55 (s, br, $\mathbf{Me_3}Si{-}F{-}Al(OR^F)_3$), 1.35 (s, 3 H, C1–**Me**, $[Me_4C_4{-}SiMe_3]^+$), 1.72 (s, MeC≡CMe), 2.20 (s, $C_6\mathbf{Me_6}$), 2.35 (sept, $^5J_{H-H}$ = 0.48 Hz, 3 H, C3–**Me**, $[Me_4C_4{-}SiMe_3]^+$), 2.45 (q, $^5J_{H-H}$ = 0.48 Hz, 6 H, C2–**Me**, $[Me_4C_4{-}SiMe_3]^+$) ppm.
^{13}C–NMR (^{1}H,^{13}C HMBC and HSQC) (100.62 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = −3.3 ($[Me_4C_4{-}Si\mathbf{Me_3}]^+$), 10.3 (C3–**Me**, $[Me_4C_4{-}SiMe_3]^+$), 13.3 (C1–**Me**, $[Me_4C_4{-}SiMe_3]^+$), 13.6 (C2–**Me**, $[Me_4C_4{-}SiMe_3]^+$), 16.5 ($C_6\mathbf{Me_6}$), 66.8 (**C1**, $[Me_4C_4{-}SiMe_3]^+$), 131.2 ($\mathbf{C_6}Me_6$), 166.0 (**C2**, $[Me_4C_4{-}SiMe_3]^+$), 170.4 (**C3**, $[Me_4C_4{-}SiMe_3]^+$) ppm.
^{19}F–NMR (376.54 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = –75.8 (s, $[al{-}f{-}al]^-$), –75.9 (s, $Me_3Si{-}F{-}Al(O\mathbf{R^F})_3$), −156.6 (s, br, $Me_3Si{-}\mathbf{F}{-}Al(OR^F)_3$ / $Me_3Si\mathbf{F}$), −184.8 (s, br, $[al{-}\boldsymbol{f}{-}al]^-$) ppm.
^{27}Al–NMR (78.22 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 37 (s, br, $[\boldsymbol{al}{-}f{-}\boldsymbol{al}]^-$ / $Me_3Si{-}F{-}\mathbf{Al}(OR^F)_3$) ppm.
^{29}Si–NMR (59.64 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 17.5 ($[Me_4C_4{-}\mathbf{Si}Me_3]^+$) ppm.

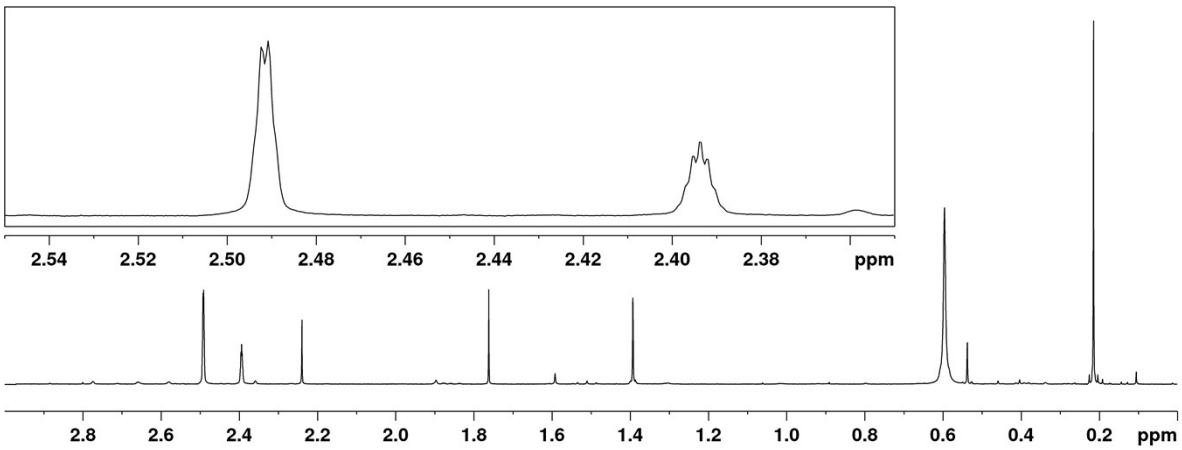

Figure S- 12: ^{1}H- NMR spectrum (300.18 MHz, 298 K, CH_2Cl_2/CD_2Cl_2) of the reaction of $Me_3Si{-}F{-}Al(OR^F)_3$ with MeC≡CMe in CH_2Cl_2.

Selective Synthesis of $[Me_4C_4{-}SiMe_3]^+[\mathit{al}{-}\mathit{f}{-}\mathit{al}]^-$

2-butyne (0.50 mL, 345 mg, 6.4 mmol, 1.05 eq.) was added to a solution of $Me_3Si{-}F{-}Al(OR^F)_3$ (4.99 g, 6.1 mmol) in *o*−DFB (10 mL) at rt within 2 min. The solution was stirred for 30 min. Parts of the solvent (~ 3 mL) were removed in vacuo, then CH_2Cl_2 (10 mL) was added. The solution was stored at −30°C overnight. The solution was filtered and concentrated to a volume of 5 mL in vacuo. Then hexane (10 mL) was added, which led to precipitation of an orange solid. After 2 h the solvent was filtered off and the precipitate was washed with hexane (10 mL), then with CH_2Cl_2 (5 mL). The orange solid (2.35 g raw yield) was dissolved in *o*−DFB (5 g) and layered with pentane (10 mL). After 2 days the precipitated crystals were isolated by filtering off the solvent. The product was obtained as orange crystals (1.42 g, 0.85 mmol, 28%).

^{1}H–NMR (300.18 MHz, 298 K, *o*–DFB/CD_2Cl_2): δ = 0.35 (s, 9 H, $[Me_4C_4{-}Si\mathbf{Me_3}]^+$), 1.56 (s, 3 H, C1−**Me**, $[Me_4C_4{-}SiMe_3]^+$), 2.55 (sept, $^{5}J_{H-H}$ = 0.48 Hz, 3 H, C3−**Me**, $[Me_4C_4{-}SiMe_3]^+$), 2.64 (q, $^{5}J_{H-H}$ = 0.48 Hz, 6 H, C2−**Me**, $[Me_4C_4{-}SiMe_3]^+$) ppm.
^{19}F–NMR (282.45 MHz, 298 K, *o*–DFB/CD_2Cl_2): δ = –75.5 (s, $[\mathit{al}{-}\mathit{f}{-}\mathit{al}]^-$), −184.5 (s, br, $[\mathit{al}{-}\mathbf{\mathit{f}}{-}\mathit{al}]^-$) ppm.
^{27}Al–NMR (78.22 MHz, 298 K, *o*–DFB/CD_2Cl_2): δ = 37 (s, br, $[\mathbf{\mathit{al}}{-}\mathit{f}{-}\mathbf{\mathit{al}}]^-$) ppm.
^{29}Si–NMR (59.64 MHz, 298 K, *o*–DFB/CD_2Cl_2): δ = 17.6 ($[Me_4C_4{-}\mathbf{Si}Me_3]^+$) ppm.

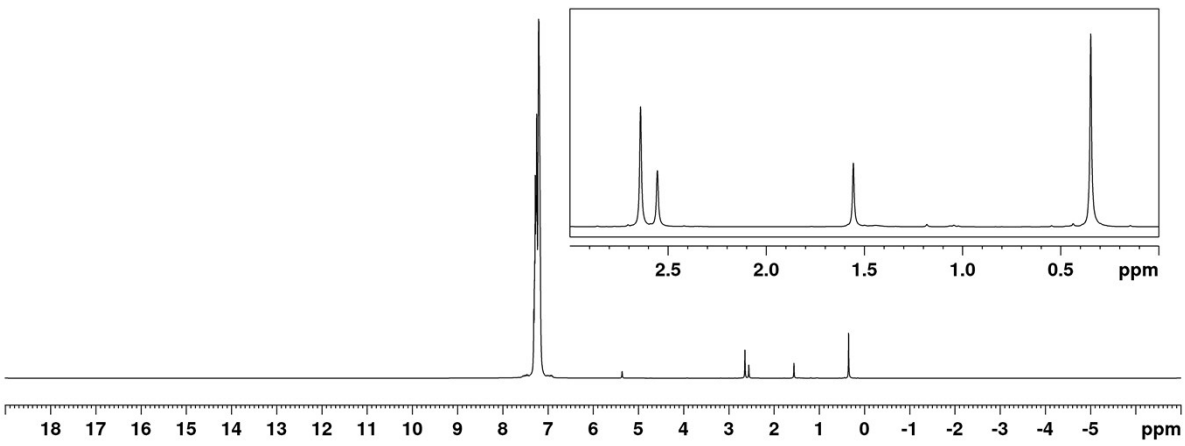

Figure S- 13: ^{1}H- NMR spectrum (300.18 MHz, 298 K, *o*−DFB/CD_2Cl_2) of $[Me_4C_4–SiMe_3]^+[al–f–al]^–$.

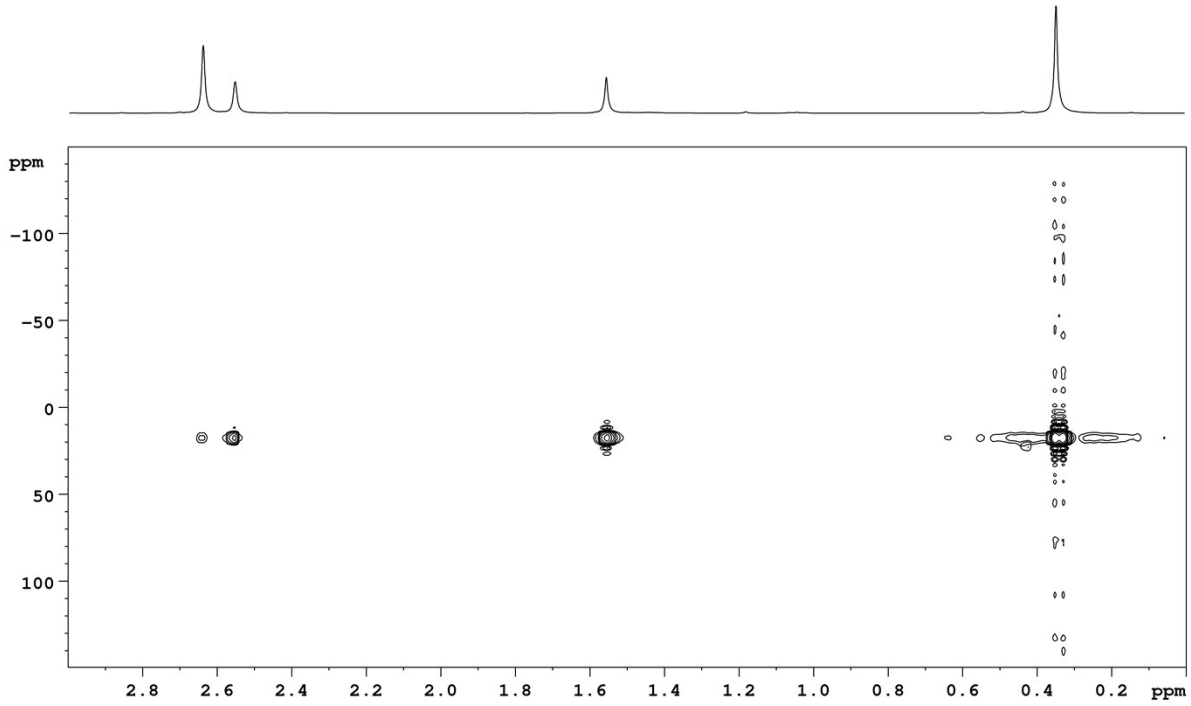

Figure S- 14: ^{1}H,^{29}Si HMBC NMR spectrum (300.18 MHz, 298 K, *o*−DFB/CD_2Cl_2, optimized to 8 Hz) of $[Me_4C_4–SiMe_3]^+[al–f–al]^–$.

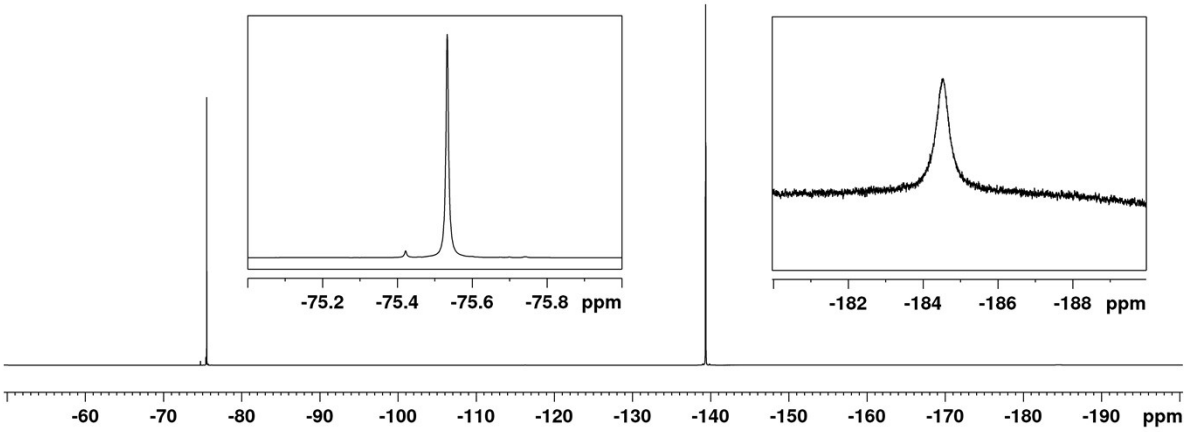

Figure S- 15: ^{19}F-NMR spectrum (282.45 MHz, 298 K, *o*−DFB/CD_2Cl_2) of $[Me_4C_4–SiMe_3]^+[al–f–al]^–$.

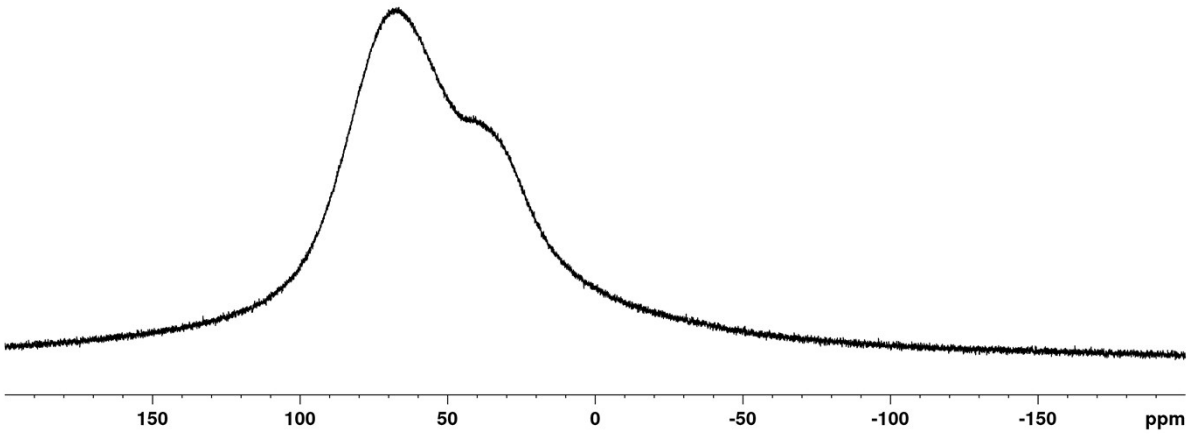

Figure S- 16: ^{27}Al-NMR spectrum (78.22 MHz, 298 K, *o*−DFB/CD_2Cl_2) of $[Me_4C_4–SiMe_3]^+[al–f–al]^-$.

Reactions of $[Ph_3C][al–f–al]$ with alkenes and alkynes in Me_3SiH

In a general procedure a catalytic amount of $[Ph_3C][al–f–al]$ (tip of a small spatula) and alkene/alkyne (see below for weights) were filled into a Schlenk vessel and cooled to −78°C. Then an excess of Me_3SiH (~ 2 mL) was condensed onto this mixture. The suspension was allowed to reach rt and the brown solution was stirred for 1 h.

a) $Me_2C=CMe_2$ (0.2 mL, 141 mg, 1.7 mmol)

The main product of this reaction is shown in Figure S- 17.

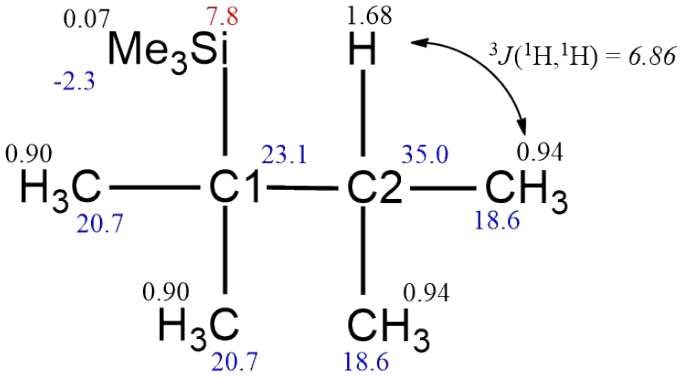

Figure S- 17: Main product of the reaction of $[Ph_3C][al–f–al]$ with $Me_2C=CMe_2$ in Me_3SiH and ^{1}H (black), ^{13}C (blue) and ^{29}Si (red) NMR chemical shifts in ppm.

^{1}H-NMR (300.18 MHz, 298 K, CD_2Cl_2): δ = 0.07 (s, 9H, **Me**$_3$Si−C1), 0.07(4) (s, 12H, **Me$_4$**Si) 0.15 (d, $^3J_{H–H}$ = 3.63 Hz, 9H, **Me**$_3$SiH), 0.50 (s, 9H, **Me**$_3$SiCl), 0.90 (s, 6H, C1−**Me**$_2$), 0.94 (d, $^3J_{H–H}$ = 6.86 Hz, 6H, C2−**Me**$_2$), 1.68 (sep, $^3J_{H–H}$ = 6.86 Hz, 1H, C2−**H**), 4.00 (dec, $^3J_{H–H}$ = 3.60 Hz, Me$_3$Si**H**) ppm.
^{13}C-NMR (75.48 MHz, 298 K, CD_2Cl_2): δ = −2.3 (**Me**$_3$Si−C1), −0.4 (**Me$_4$**Si), 2.9 (**Me**$_3$SiCl), 18.6 (C1−**Me$_2$**) 20.7 (C2−**Me**$_2$), 23.1 (**C1**), 35.0 (**C2**) ppm.
^{29}Si-NMR (59.64 MHz, 298 K, CD_2Cl_2): δ = −16.1 (Me$_3$**Si**H), 0.0 (Me$_4$**Si**), 7.8 (**Me**$_3$Si−C1), 31.7 (Me$_3$**Si**Cl) ppm.

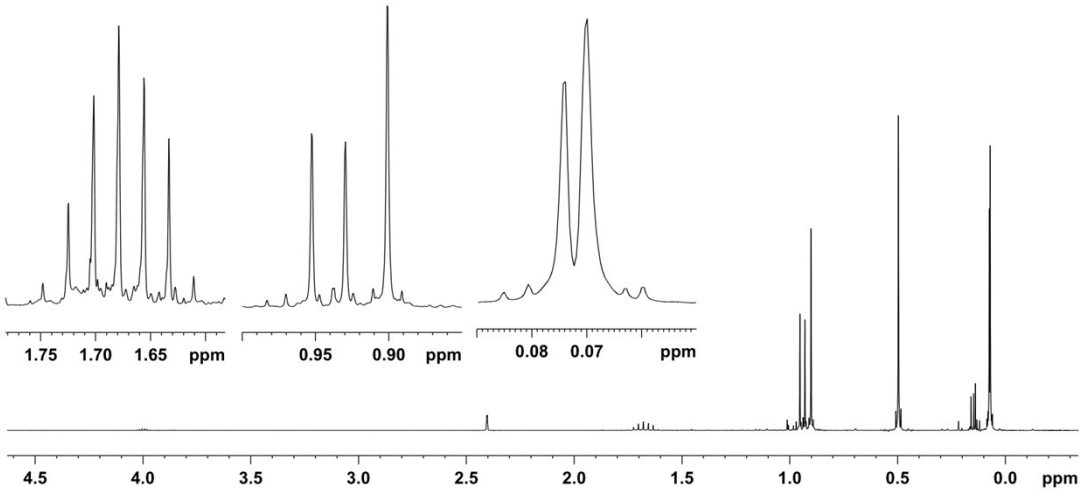

Figure S- 18: ^{1}H- NMR spectrum (300.18 MHz, 298 K, CD_2Cl_2) of the reaction of $[Ph_3C][al{-}f{-}al]$ with 2-butyne in Me_3SiH.

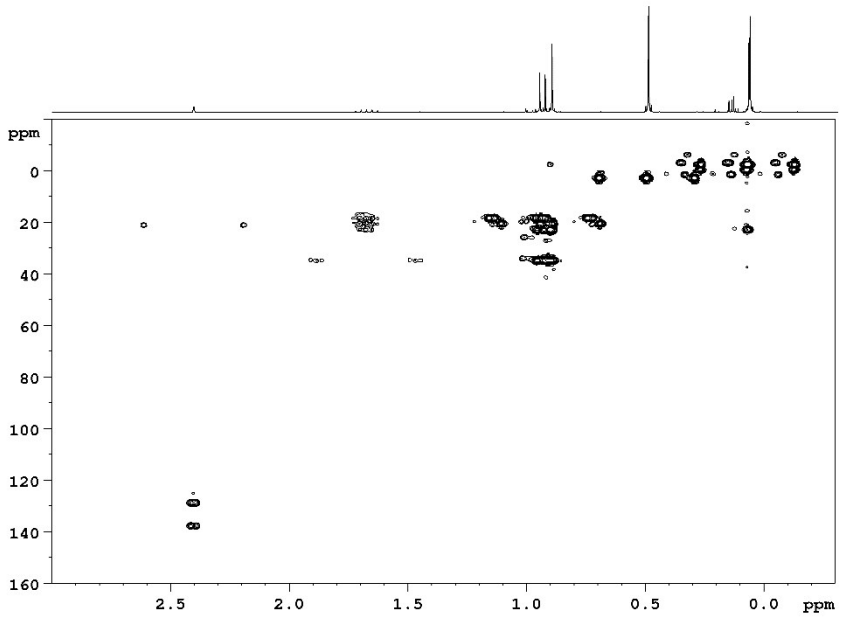

Figure S- 19: ^{1}H,^{13}C HMBC NMR spectrum (300.18 MHz, 298 K, CD_2Cl_2, optimized to 8 Hz) of the reaction of $[Ph_3C][al{-}f{-}al]$ with $Me_2C{=}CMe_2$ in Me_3SiH.

b) $Ph_2C{=}CPh_2$ (830 mg, 2.5 mmol)

No reaction with the alkene could be observed.

c) MeC≡CMe (0.2 mL, 138 mg, 2.6 mmol)

The main product of this reaction is shown in Figure S- 20.

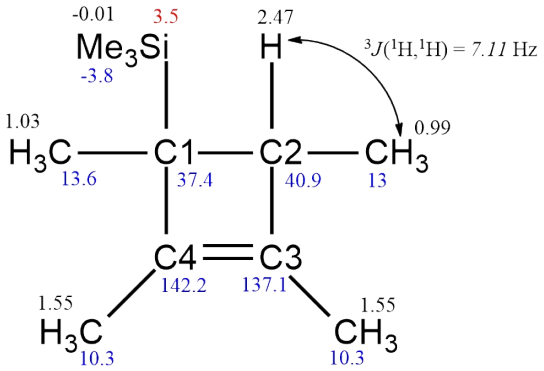

Figure S- 20: Main product of the reaction of [Ph_3C][*al–f–al*] with 2-butyne in Me_3SiH and ^{1}H (black), ^{13}C (blue) and ^{29}Si (red) NMR chemical shifts in ppm.

^{1}H-NMR (300.18 MHz, 298 K, CD_2Cl_2): δ = −0.01 (s, 9H, **Me**$_3$Si−C1), 0.05 (s, 12H, **Me**$_4$Si), 0.13 (d, $^{3}J_{HH}$ = 3.62 Hz, 9H, **Me**$_3$SiH), 0.20 (t, $^{3}J_{HH}$ = 4.13 Hz, **Me**$_2$SiH$_2$), 0.48 (s, 9H, **Me**$_3$SiCl), 0.99 (d, $^{3}J_{HH}$ = 7.11 Hz, 3H, C2−**Me**), 1.03 (s, 3H, C1−**Me**), 1.53-1.57 (m, 6H, **Me**C3=C4**Me**), 1.77 (s, 6H, **Me**C≡C**Me**), 2.42-2.52 (m, 1H, C2−**H**), 3.80 (sep, $^{3}J_{HH}$ = 4.14 Hz, Me$_2$Si**H**$_2$), 3.97 (dec, $^{3}J_{HH}$ = 3.62 Hz, **Me**$_3$SiH) ppm.

^{13}C-NMR (75.48 MHz, 298 K, CD_2Cl_2): δ = −3.9 (**Me**$_3$Si−C1), −3.0 (**Me**$_3$SiH), −0.3 (**Me**$_4$Si), 2.9 (**Me**$_3$SiCl), 3.0 (**Me**C≡C**Me**), 10.3 (**Me**-C3/**Me**-C4), 13.0 (**Me**−C2), 13.6 (**Me**-C1), 37.4 (**C1**), 40.9 (s, 1C, **C**2), 74.3 (Me**C**≡**C**Me), 137.1 (**C**3), 142.2 (**C**4) ppm.

^{29}Si-NMR (59.64 MHz, 298 K, CD_2Cl_2): δ = −38.0 (Me$_2$**Si**H$_2$), −16.0 (Me$_3$**Si**H), −6.9 (**Me**$_2$SiH$_2$), 0.0 (Me$_4$**Si**), 3.5 (Me$_3$**Si**−C1), 31.5 (Me$_3$**Si**Cl) ppm.

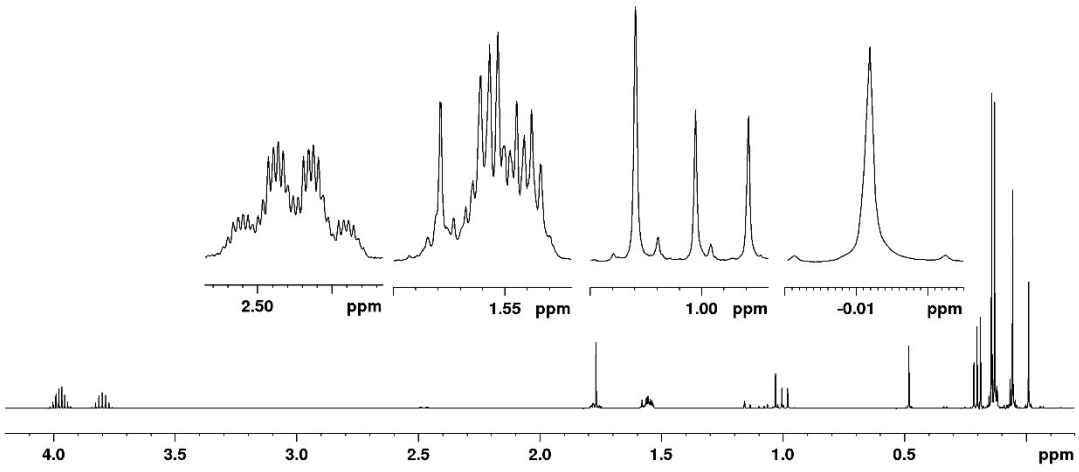

Figure S- 21: ^{1}H- NMR spectrum (300.18 MHz, 298 K, CD_2Cl_2) of the reaction of [Ph_3C][*al–f–al*] with 2-butyne in Me_3SiH.

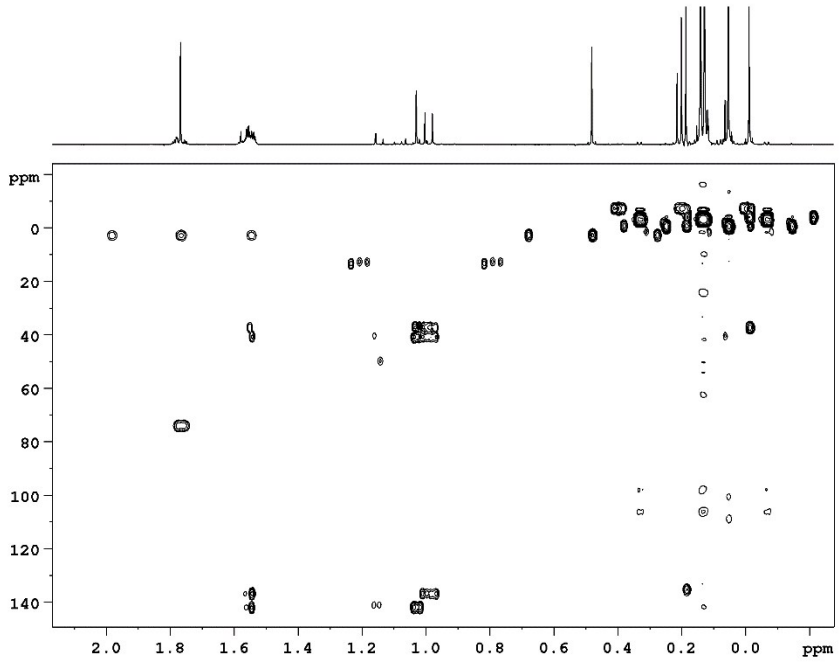

Figure S- 22: $^{1}H,^{13}C$ HMBC NMR spectrum (300.18 MHz, 298 K, CD_2Cl_2, optimized to 8 Hz) of the reaction of $[Ph_3C][al–f–al]$ with 2-butyne in Me_3SiH.

d) PhC≡CPh (0.5 mL, 495 mg, 2.78 mmol)

The main product of this reaction is shown in Figure S- 23.

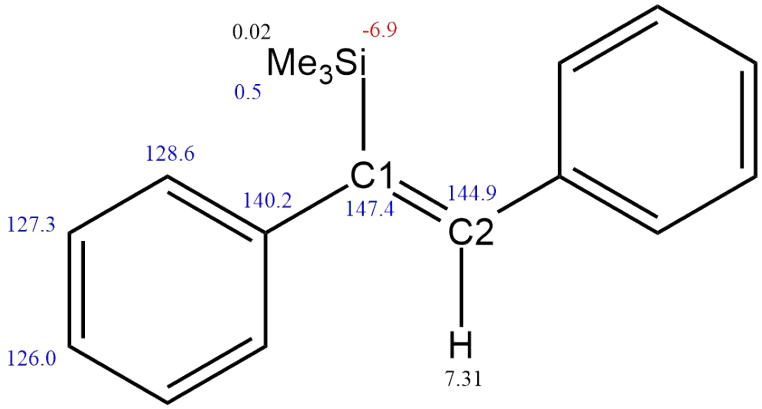

Figure S- 23: Main product of the reaction of $[Ph_3C][al–f–al]$ with PhC≡CPh in Me_3SiH and ^{1}H (black), ^{13}C (blue) and ^{29}Si (red) NMR chemical shifts in ppm.

^{1}H-NMR (300.18 MHz, 298 K, CD_2Cl_2): δ = 0.02 (s, 9H, **Me**$_3$Si–C1), 0.13 (d, $^{3}J_{H–H}$ = 3.56 Hz, **Me**$_3$SiH), 0.47 (s, **Me**$_3$SiCl), 4.0 (dec, $^{3}J_{H–H}$ = 3.64 Hz, Me$_3$Si**H**), 7.22-7.44 (m, 10H, **Ph**C1=C2**Ph**), 7.54-7.61 (m, 1H, C2–**H**) ppm.

^{13}C-NMR (75.48 MHz, 298 K, CD_2Cl_2): δ = −3.0 (**Me**$_3$SiH), 0.5 (**Me**$_3$Si–C1), 3.0 (**Me**$_3$SiCl), 126.0 (*p*-C, C1–**Ph**, C2-**Ph**), 127.3 (*m*-C, C1–**Ph**, C2-**Ph**), 128.6 (*o*-C, C1–**Ph**, C2-**Ph**), 147.4 (**C1**), 144.9 (**C2**) ppm.

^{29}Si-NMR (59.64 MHz, 298 K, CD_2Cl_2): δ = −6.6 (Me$_3$**Si**–C1), −16.0 (Me$_3$**Si**H), 31.5 (Me$_3$**Si**Cl) ppm.

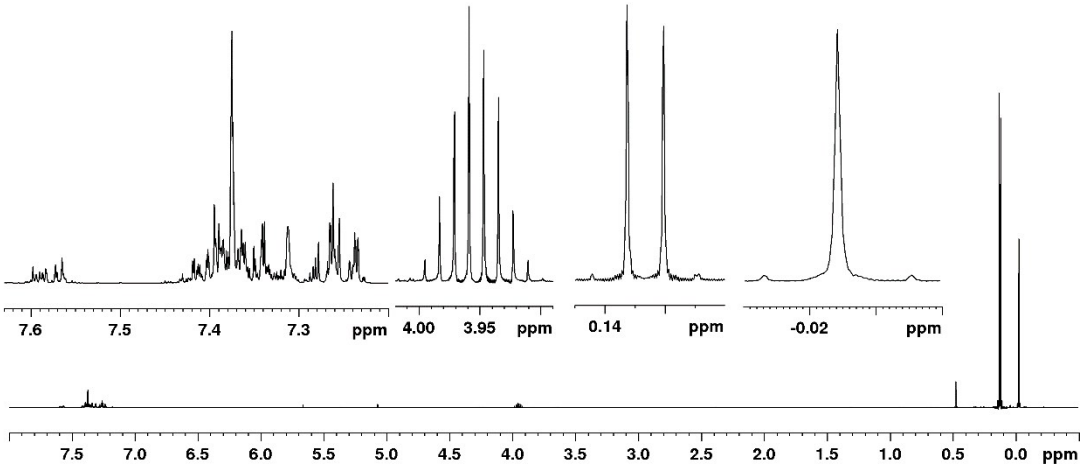

Figure S- 24: ^{1}H- NMR spectrum (300.18 MHz, 298 K, CD_2Cl_2) of the reaction of $[Ph_3C][al–f–al]$ with PhC≡CPh in Me_3SiH.

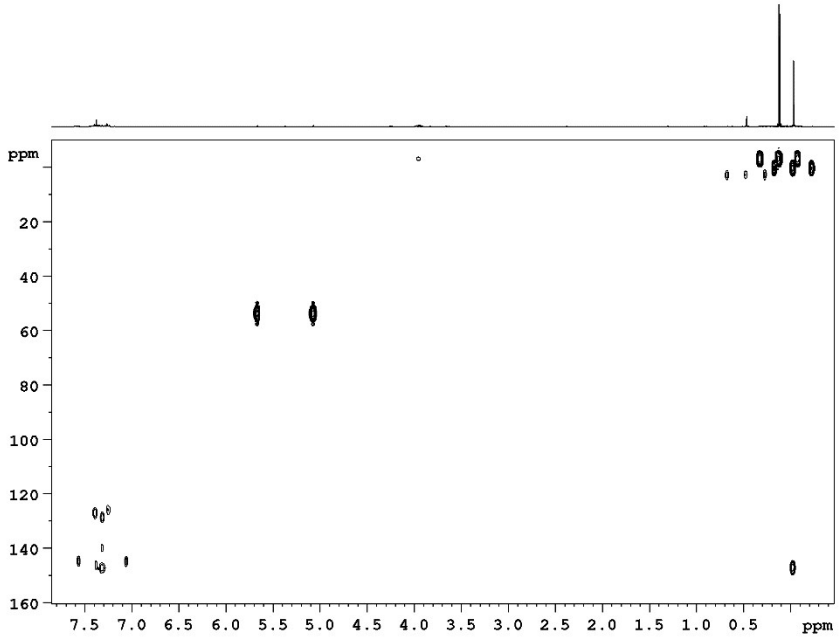

Figure S- 25: ^{1}H,^{13}C HMBC NMR spectrum (300.18 MHz, 298 K, CD_2Cl_2, optimized to 8 Hz) of the reaction of $[Ph_3C][al–f–al]$ with PhC≡CPh in Me_3SiH.

Reactions of Ag[*al–f–al*] with bromoethyl/bromovinyl trimethyl silane

a) Synthesis of bromoethyl trimethyl silane

Benzoyl peroxide (21 mg, 0.1 mmol, 0.3 mol-%) and trimethylvinylsilane (4.4 mL, 3.0 g, 30 mmol) were weighed into a Schlenk vessel and cooled to 0°C. In a round bottom flask conc. H_2SO_4 (30 mL) was added dropwise onto KBr (30 g). The evolving HBr was bubbled through the trimethylvinylsilane for 1 h under vigorous stirring. Condensation of the volatiles yielded the product as colorless liquid.

^{1}H-NMR (400.17 MHz, 298 K, CD_2Cl_2): δ = 0.06 (s, 9H, **Me**$_3$Si–CH_2–CH_2Br), 1.40 (m, 2H, Me_3Si–C**H**$_2$–CH_2Br), 3.59 (m, 2H, Me_3Si–CH_2–C**H**$_2$Br) ppm.

^{13}C-NMR (100.62 MHz, 298 K, CD_2Cl_2): δ = −1.7 (**Me**$_3$Si−CH_2−CH_2Br), 24.0 (Me_3Si−**C**H_2−CH_2Br), 32.0 (Me_3Si−CH_2−**C**H_2Br) ppm.
^{29}Si-NMR (79.50 MHz, 298 K, CD_2Cl_2): δ = 1.3 (Me_3**Si**−CH_2−CH_2Br) ppm.

b) Synthesis of bromovinyl trimethyl silane

Benzoyl peroxide (26 mg, 0.1 mmol, 0.3 mol-%) and trimethylsilylacetylene (5.0 mL, 3.45 g, 36 mmol) were weighed into a Schlenk vessel and cooled to 0°C. In a round bottom flask conc. H_2SO_4 (30 mL) was added dropwise onto KBr (30 g). The evolving HBr was bubbled through the trimethylvinylsilane for 45 min under vigorous stirring. Condensation of the volatiles yielded the product as colorless liquid.
The product contained small amounts of impurities, which were identified as Me_3Si−C≡CH (14%) and Me_3Si−CHBr−CH_2Br (9%).

^{1}H-NMR (400.17 MHz, 298 K, CD_2Cl_2): δ = 0.13 (s, 9H, **Me**$_3$Si−CH=CHBr), 0.15 (s, **Me**$_3$Si−CHBr−CH_2Br), 0.22 (s, **Me**$_3$Si−C≡CH), 2.31 (d, $^3J_{HH}$ = 7.39 Hz **,**Me_3Si−CHBr−C**H**$_2$Br), 2.39 (s, Me_3Si−C≡C**H**), 5.95 (t, $^3J_{HH}$ = 7.39 Hz, Me_3Si−C**H**Br−CH_2Br), 6.49 (t, 1H, Me_3Si−CH=C**H**Br), 6.59 (d, 1H, Me_3Si−C**H**=CHBr) ppm.
^{13}C-NMR (100.62 MHz, 298 K, CD_2Cl_2): δ = −1.4 (**Me**$_3$Si−CH=CHBr), 116.7 (Me_3Si−**C**H=CHBr), 139.1 (Me_3Si−CH=**C**HBr) ppm.
^{29}Si-NMR (79.5 MHz, 298 K, CD_2Cl_2): δ = −17.2 (Me_3**Si**−C≡CH), −4.8 (Me_3**Si**−CH=CHBr), 2.0 (Me_3**Si**−CHBr−CH_2Br) ppm.

c) Reaction of bromoethyl trimethyl silane with Ag[*al–f–al*]

Ag[*al–f–al*] (196 mg, 0.13 mmol) was dissolved in CH_2Cl_2 (5 mL) and cooled to −40°C. To this solution bromoethyl trimethyl silane (0.02 mL, 23 mg, 0.13 mmol, 1 eq.) was added. After few seconds the solution turned brown, which usually indicates decomposition of the anion. The formation of a precipitate was not observed. The solution was stirred for 1 h at −40°C, then analyzed by NMR spectroscopy at rt.

^{1}H-NMR (300.18 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 0.04 (s, **Me$_4$**Si), 0.47 (s, **Me$_3$**SiCl), 0.62 (s, **Me$_3$**SiBr) ppm.
^{13}C-NMR (75.48 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 0.0 (Si**Me$_4$**), 3.0 (**Me$_3$**SiCl), 3.9 (**Me$_3$**SiBr) ppm.
^{19}F-NMR (282.45 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = −74.5 (s, HO**R^F**, 43%), −75.4 (s, O**R^F**), −75.6 (s, O**R^F**), −75.8 (s, [*al–f–al*]$^-$, 57%), −75.9 (s, O**R^F**), −157.1 (Me_3Si**F**), −184.8 (s, [*al–**f**–al*]$^-$) ppm.
^{29}Si-NMR (59.64 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 0.0 (**Si**Me_4), 28.1 (Me_3**Si**Br), 31.3 (Me_3**Si**Cl) ppm.

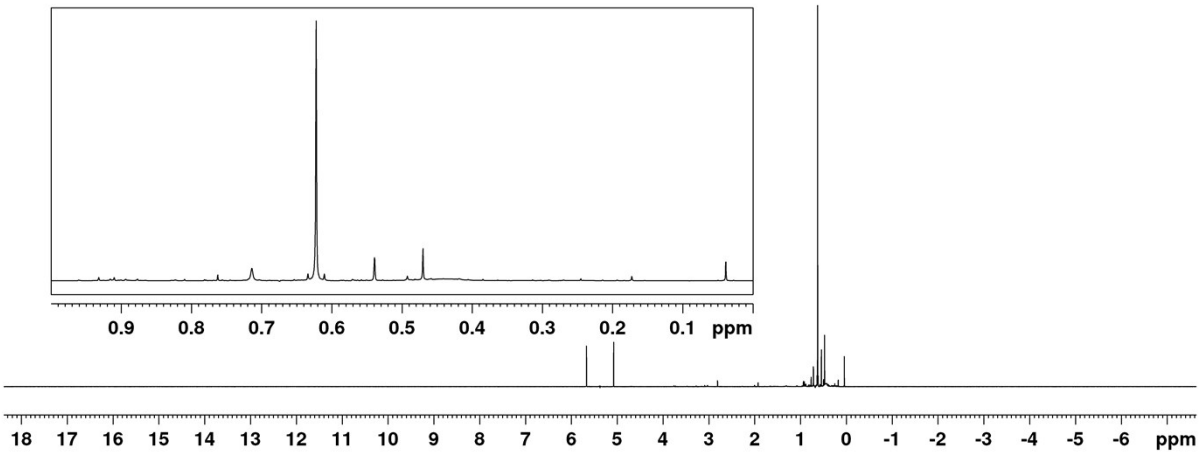

Figure S- 26: ^{1}H- NMR spectrum (300.18 MHz, 298 K, CH_2Cl_2/CD_2Cl_2) of the reaction of Ag[*al–f–al*] with bromoethyl trimethyl silane in CH_2Cl_2.

The signal at 0.54 ppm results from impurities of $Me_3Si–O(H)–Al(OR^F)_3$, that were already present in the used Ag[*al–f–al*].

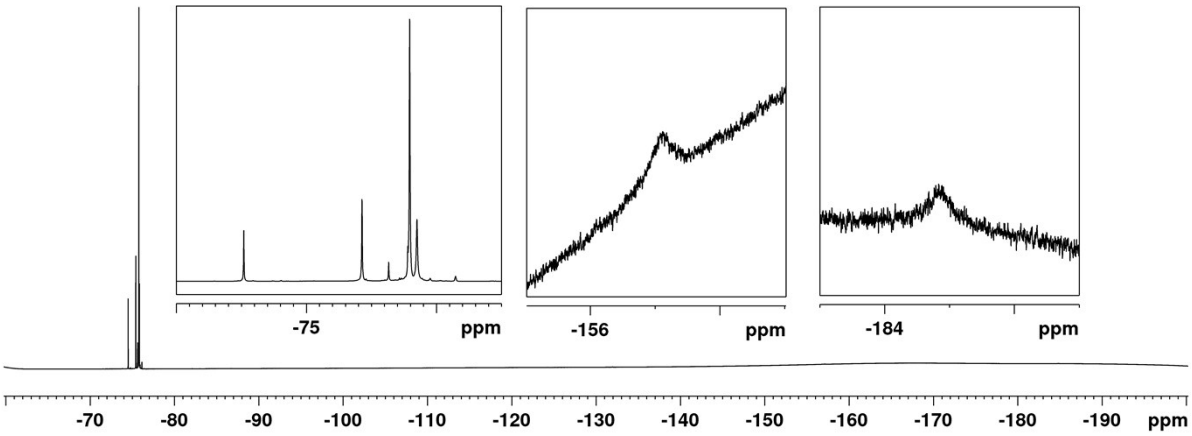

Figure S- 27: ^{19}F- NMR spectrum (282.54 MHz, 298 K, CH_2Cl_2/CD_2Cl_2) of the reaction of Ag[*al–f–al*] with bromoethyl trimethyl silane in CH_2Cl_2.

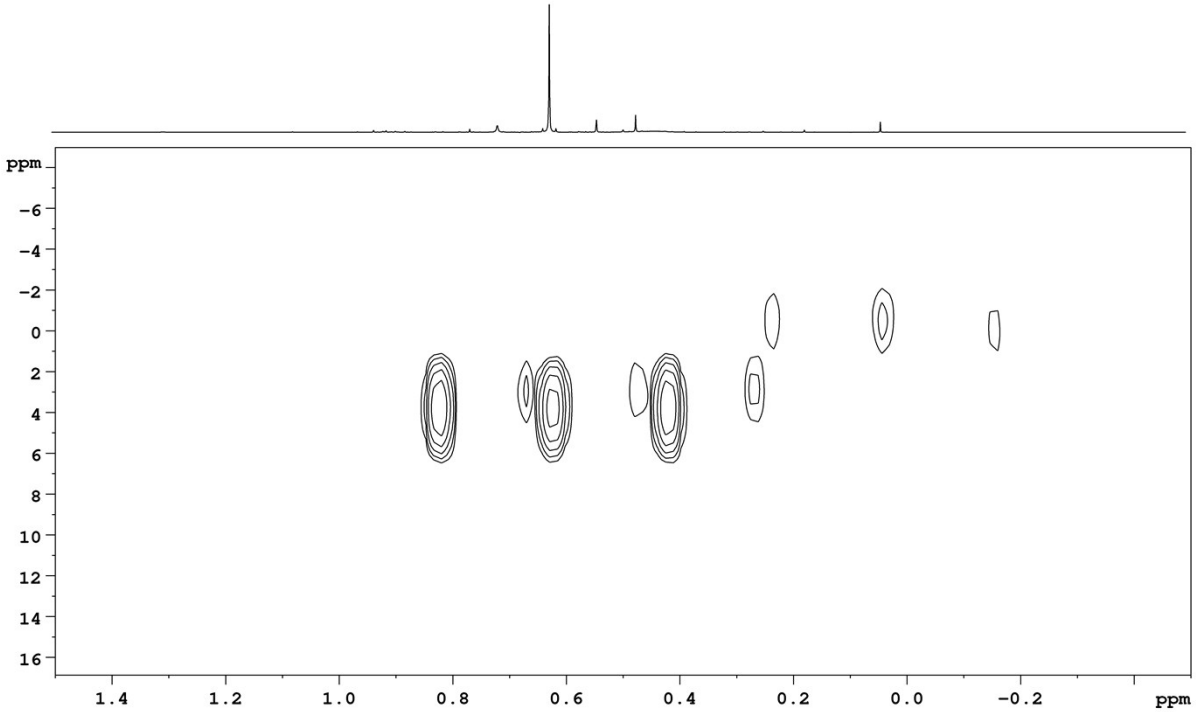

Figure S- 28: $^{1}H,^{13}C$-HMBC NMR spectrum (300.18 MHz, 298 K, CH_2Cl_2/CD_2Cl_2, optimized to 8 Hz) of the reaction of Ag[*al*–*f*–*al*] with bromoethyl trimethyl silane in CH_2Cl_2.

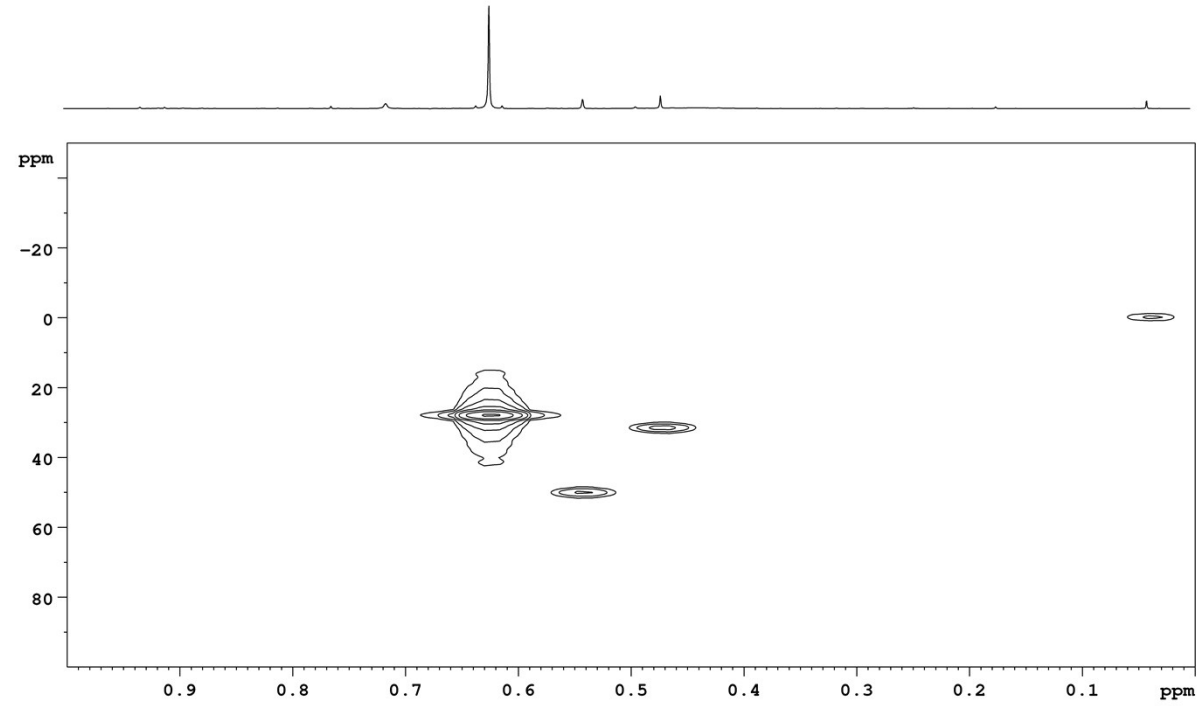

Figure S- 29: $^{1}H,^{29}Si$-HMBC NMR spectrum (300.18 MHz, 298 K, CH_2Cl_2/CD_2Cl_2, optimized to 8 Hz) of the reaction of Ag[*al*–*f*–*al*] with bromoethyl trimethyl silane in CH_2Cl_2.

The signal at $\delta(^{29}Si)$ = 50 ppm results from impurities of $Me_3Si{-}O(H){-}Al(OR^F)_3$, that were already present in the used Ag[*al*–*f*–*al*].

d) Reaction of bromovinyl trimethyl silane with Ag[*al–f–al*]

Ag[*al–f–al*] (199 mg, 0.13 mmol) was dissolved in CH_2Cl_2 (3 mL). To this solution bromovinyl trimethyl silane (0.02 mL, 23 mg, 0.13 mmol, 1 eq.) was added at rt. The reaction mixture turned immediately turbid and after few minutes it turned red. The solution was stirred for 1 h at rt, then analyzed by NMR spectroscopy.

^{1}H-NMR (400.17 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 0.04 (s, **Me_4**Si), 0.62 (s, **Me_3**SiBr) ppm.
^{13}C-NMR (100.62 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 0.0 (Si**Me_4**), 3.8 (**Me_3**SiBr) ppm.
^{19}F-NMR (376.54 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = −75.7 (s, O**R^F**), −75.8 (s, [*al–f–al*]$^-$), −75.9 (s, O**R^F**), −157.6 (Me_3Si**F**), −184.9 (s, [*al–**f**–al*]$^-$) ppm.
^{29}Si-NMR (79.50 MHz, 298 K, CH_2Cl_2/CD_2Cl_2): δ = 0.0 (**Si**Me_4), 28.1 (Me_3**Si**Br) ppm.

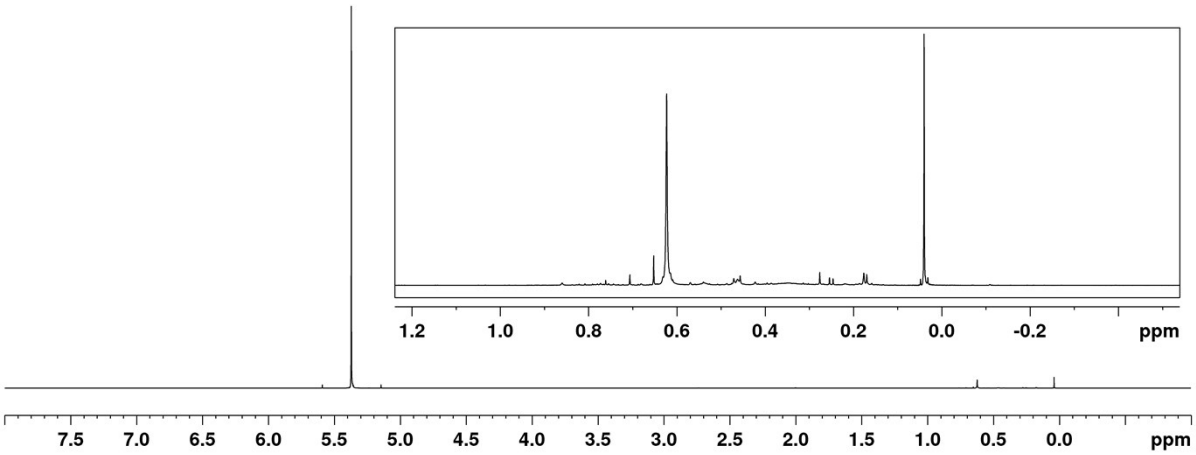

Figure S- 30: ^{1}H- NMR spectrum (400.17 MHz, 298 K, CH_2Cl_2/CD_2Cl_2) of the reaction of Ag[*al–f–al*] with bromovinyl trimethyl silane in CH_2Cl_2.

The signal at 0.65 ppm results from impurities of $Me_3Si–O(H)–Al(OR^F)_3$, that were already present in the used Ag[*al–f–al*].

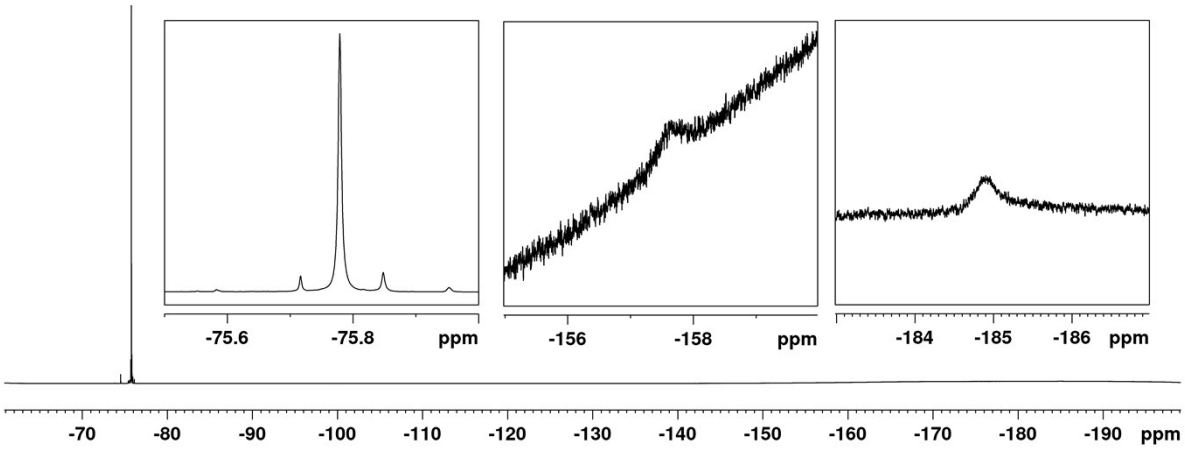

Figure S- 31: ^{19}F- NMR spectrum (376.54 MHz, 298 K, CH_2Cl_2/CD_2Cl_2) of the reaction of Ag[*al–f–al*] with bromovinyl trimethyl silane in CH_2Cl_2.

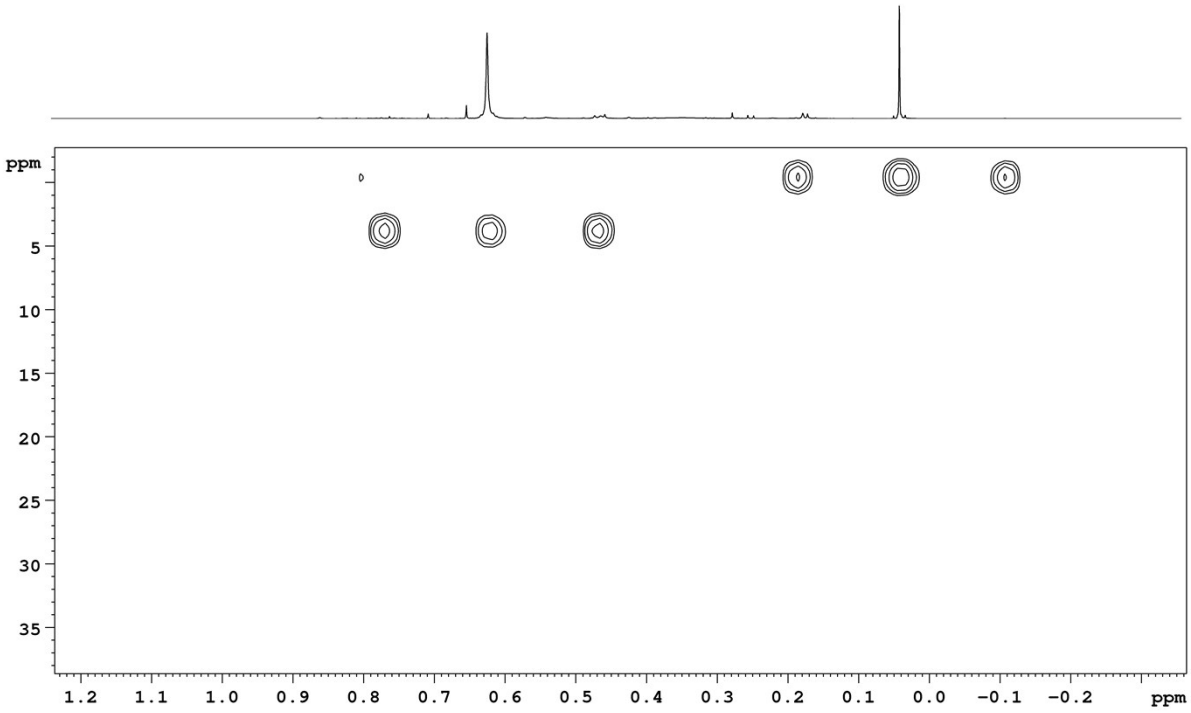

Figure S- 32: $^{1}H,^{13}C$-HMBC NMR spectrum (400.17 MHz, 298 K, CH_2Cl_2/CD_2Cl_2, optimized to 8 Hz) of the reaction of Ag[*al*−*f*−*al*] with bromovinyl trimethyl silane in CH_2Cl_2.

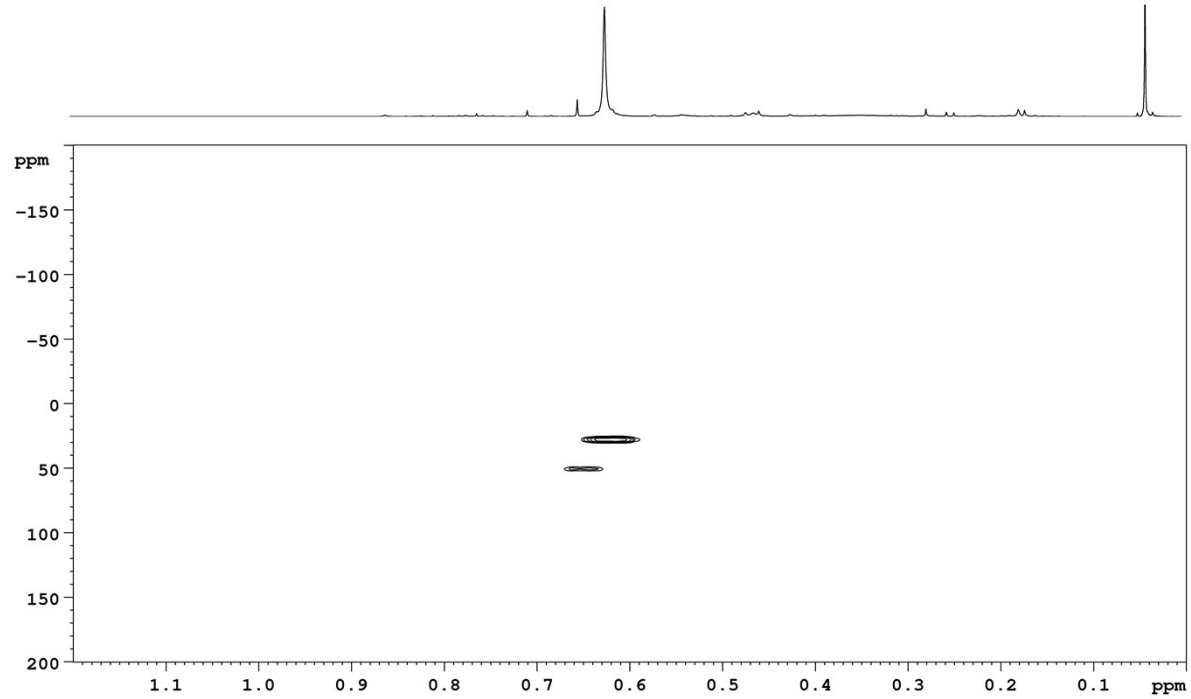

Figure S- 33: $^{1}H,^{29}Si$-HMBC NMR spectrum (400.17 MHz, 298 K, CH_2Cl_2/CD_2Cl_2, optimized to 8 Hz) of the reaction of Ag[*al*−*f*−*al*] with bromovinyl trimethyl silane in CH_2Cl_2.

The signal at $\delta(^{29}Si)$ = 50 ppm results from impurities of $Me_3Si{-}O(H){-}Al(OR^F)_3$, that were already present in the used Ag[*al*−*f*−*al*].

Reaction of [Me_4C_4–$SiMe_3$][*al*–*f*–*al*] with [NMe_4]F

[Me_4C_4–$SiMe_3$][*al*–*f*–*al*] was filled into a NMR tube with J. Young valve and dissolved in a 1:1 mixture of *o*–DFB and CD_2Cl_2. Then an excess of dry [NMe_4]F was added to this solution and the NMR tube was immediately closed. The solution was analyzed by NMR spectroscopy. The main product of this reaction is shown in Figure S- 34.

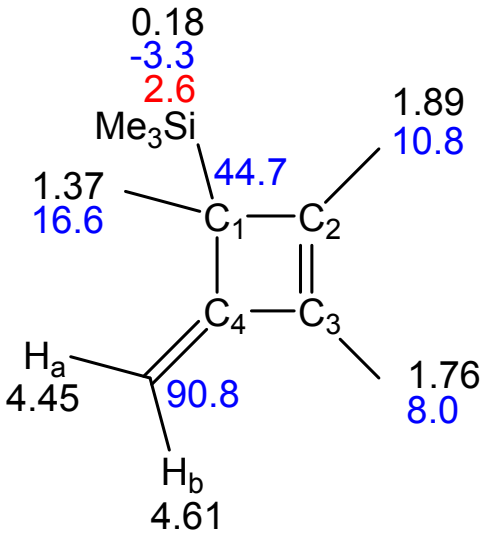

Figure S- 34: Main product of the reaction of [Me_4C_4–$SiMe_3$][*al*–*f*–*al*] with [NMe_4]F in *o*–DFB/CD_2Cl_2 and ^{1}H (black), ^{13}C (blue) and ^{29}Si (red) NMR chemical shifts in ppm.

^{1}H-NMR (400.17 MHz, 298 K, *o*–DFB/CD_2Cl_2): δ = 0.18 (s, **Me_3Si**), 1.37 (s, C_1–**Me**), 1.76 (q, $^{5}J_{H-H}$ = 1.21 Hz, C_3–**Me**), 1.89 (m, $^{5}J_{H-H}$ = 1.21 Hz, $^{6}J_{H-H}$ = 0.60/0.58 Hz, C_2–**Me**), 2.24 (s C_6**Me_6**), 3.32 (t, $^{2}J_{H-N}$ = 0.40 Hz, [N**Me_4**]$^{+}$), 4.45 (q, $^{6}J_{H-H}$ = 0.60 Hz, **H_a**), 4.61 (q, $^{6}J_{H-H}$ = 0.58 Hz, **H_b**) ppm.
^{13}C-NMR (100.62 MHz, 298 K, *o*–DFB/CD_2Cl_2): δ = −3.3 (**Me_3Si**), 8.0 (C_3–**Me**), 10.8 (C_2–**Me**), 16.6 (C_1–**Me**), 44.7 (**C_1**), 90.8 (C_4=**C**H_2), 133.8 (**C_3**), 152.6 (**C_2**), 157.1 (**C_4**) ppm.
^{19}F-NMR (376.54 MHz, 298 K, *o*–DFB/CD_2Cl_2): δ = −74.6 (s, HO**R^{F}**), −75.6 (d, $^{5}J_{F-F}$ = 1.4 Hz, [*f*–*al*]$^{-}$), −75.7 (s, br, [F_2Al(O**R^{F}**)$_2$]$^{-}$), −180.4 (m, br, [***f***–*al*]$^{-}$), −185.3 (m, br, [**F_2**Al(OR^{F})$_2$]$^{-}$) ppm.
^{27}Al-NMR (78.22 MHz, 298 K, *o*–DFB/CD_2Cl_2): δ = 41 (d, $^{1}J_{Al-F}$ = 24 Hz, [*f*–***al***]$^{-}$), 45 (s, [F_2**Al**(OR^{F})$_2$]$^{-}$) ppm.
^{29}Si-NMR (79.50 MHz, 298 K, *o*–DFB/CD_2Cl_2): δ = 2.6 (Me_3**Si**) ppm.

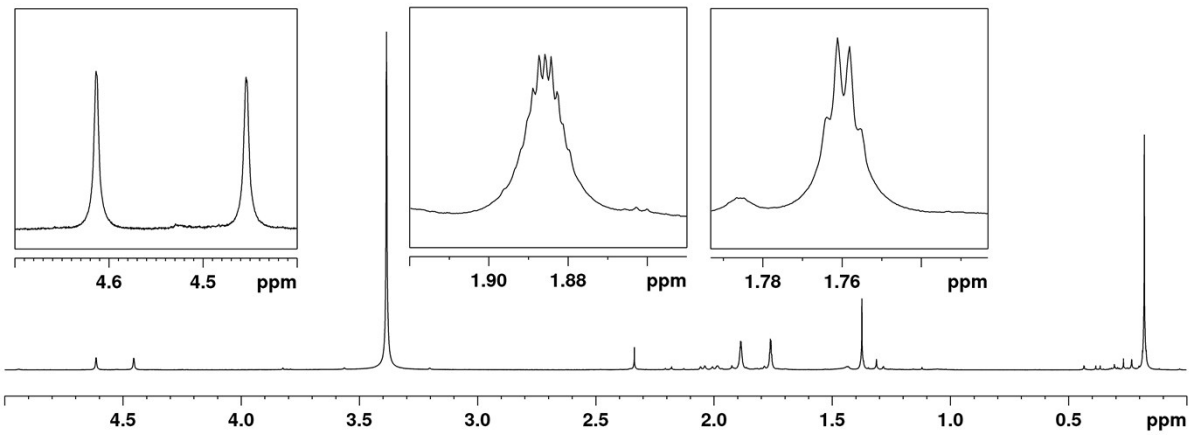

Figure S- 35: ^{1}H- NMR spectrum (400.17 MHz, 298 K, *o*–DFB/CD_2Cl_2) of the reaction of [Me_4C_4–$SiMe_3$][*al*–*f*–*al*] with [NMe_4]F in *o*–DFB/CD_2Cl_2.

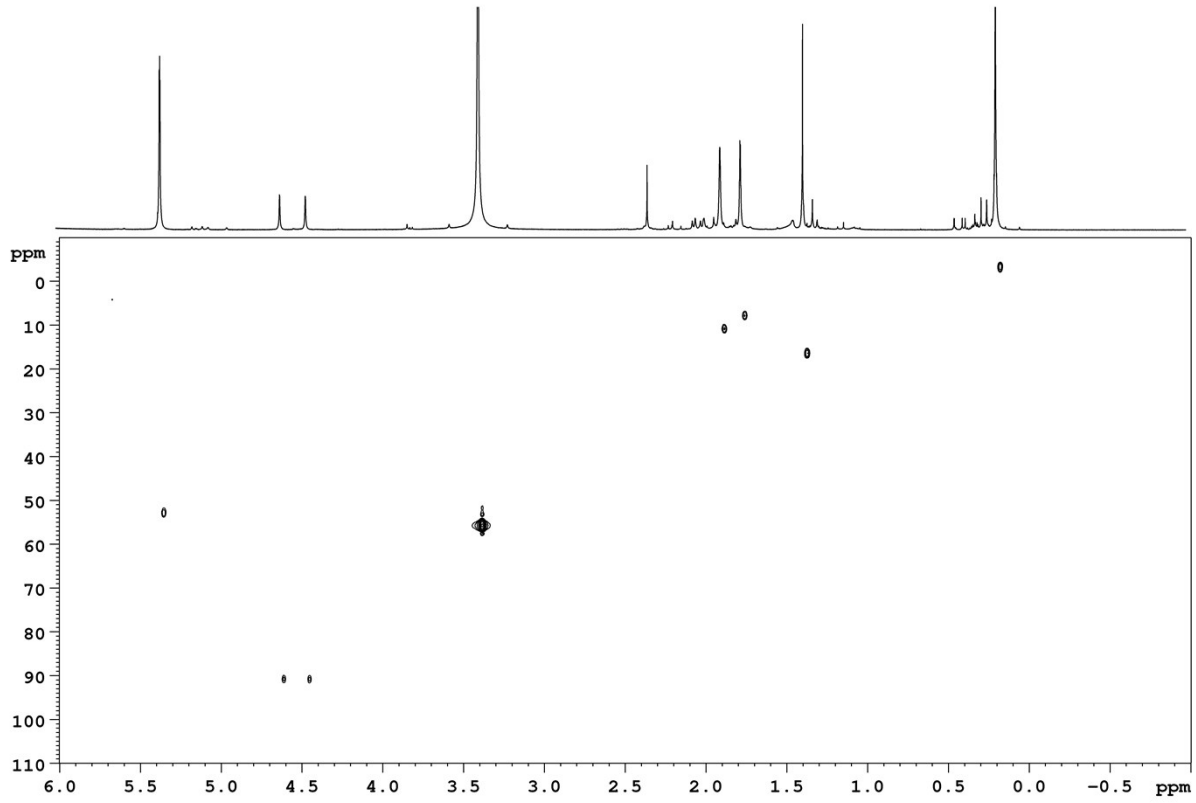

Figure S- 36: $^{1}H,^{13}C$-HSQC NMR spectrum (400.17 MHz, 298 K, *o*−DFB/CD_2Cl_2, optimized to 145 Hz) of the reaction of [Me_4C_4−$SiMe_3$][*al*−*f*−*al*] with [NMe_4]F in *o*−DFB/CD_2Cl_2.

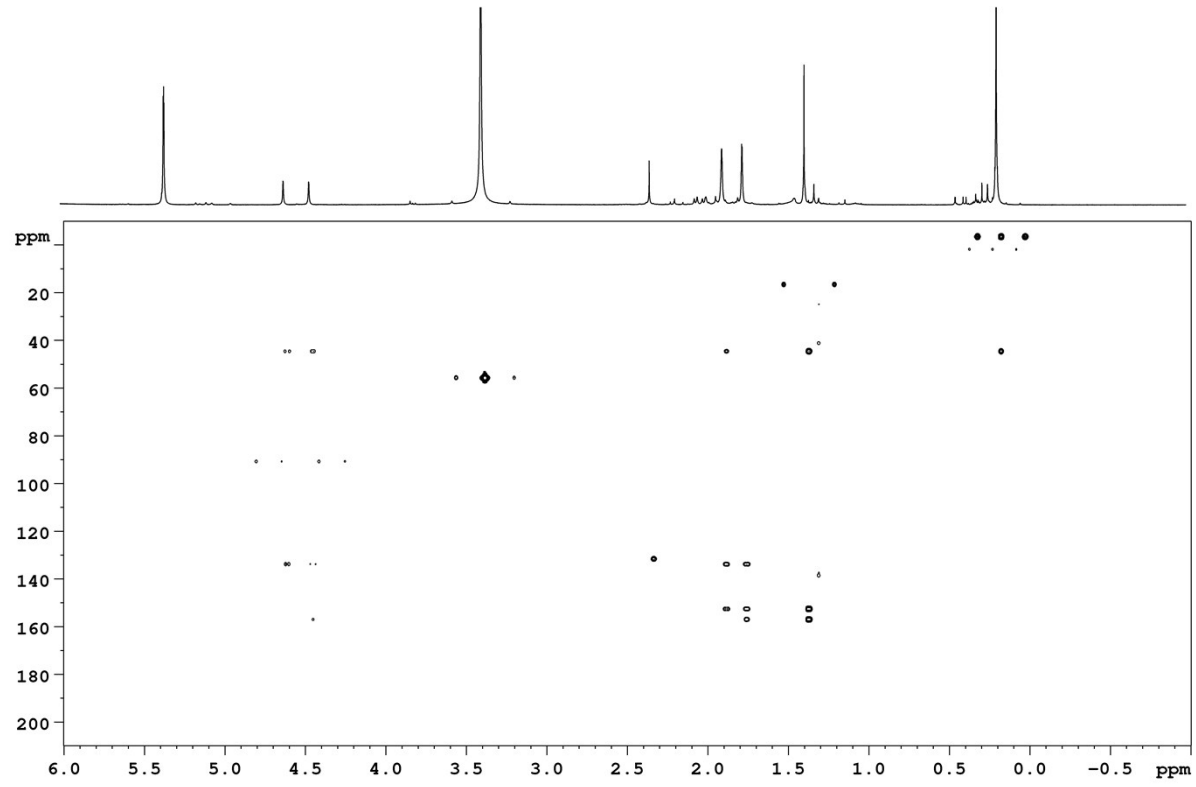

Figure S- 37: $^{1}H,^{13}C$-HMBC NMR spectrum (400.17 MHz, 298 K, *o*−DFB/CD_2Cl_2, optimized to 8 Hz) of the reaction of [Me_4C_4−$SiMe_3$][*al*−*f*−*al*] with [NMe_4]F in *o*−DFB/CD_2Cl_2.

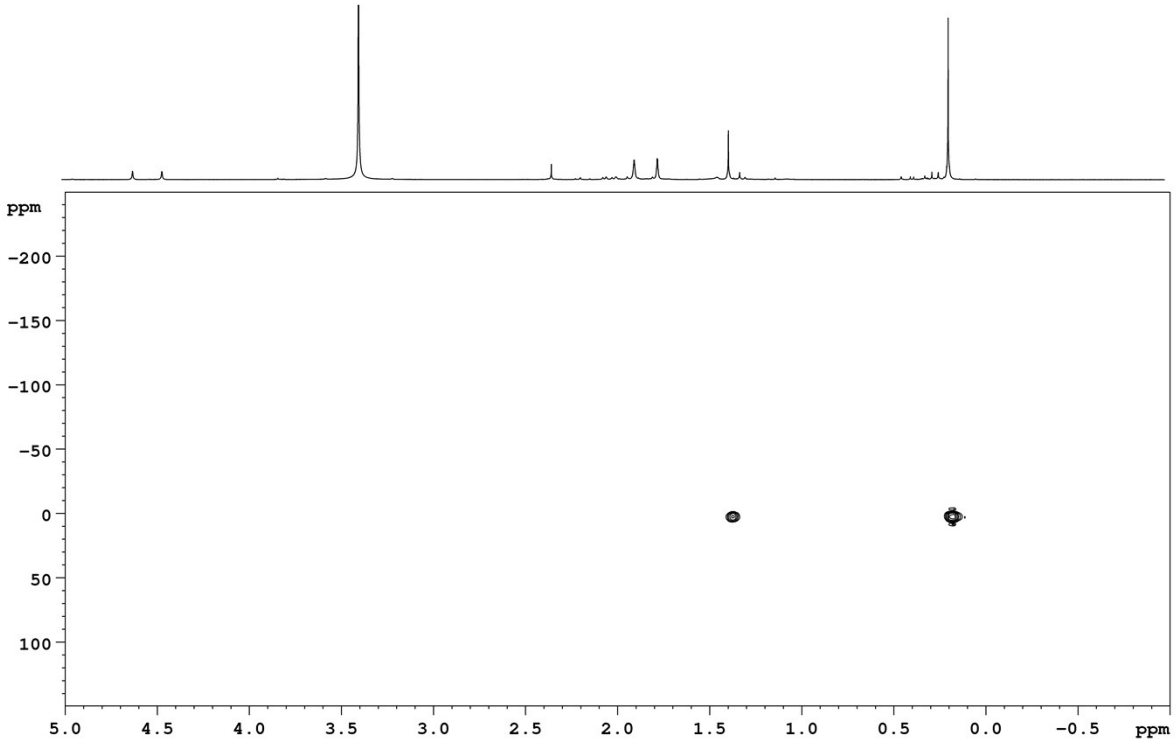

Figure S- 38: $^{1}H,^{29}Si$-HMBC NMR spectrum (400.17 MHz, 298 K, *o*−DFB/CD_2Cl_2, optimized to 8 Hz) of the reaction of [Me_4C_4−$SiMe_3$][*al*−*f*−*al*] with [NMe_4]F in *o*−DFB/CD_2Cl_2.

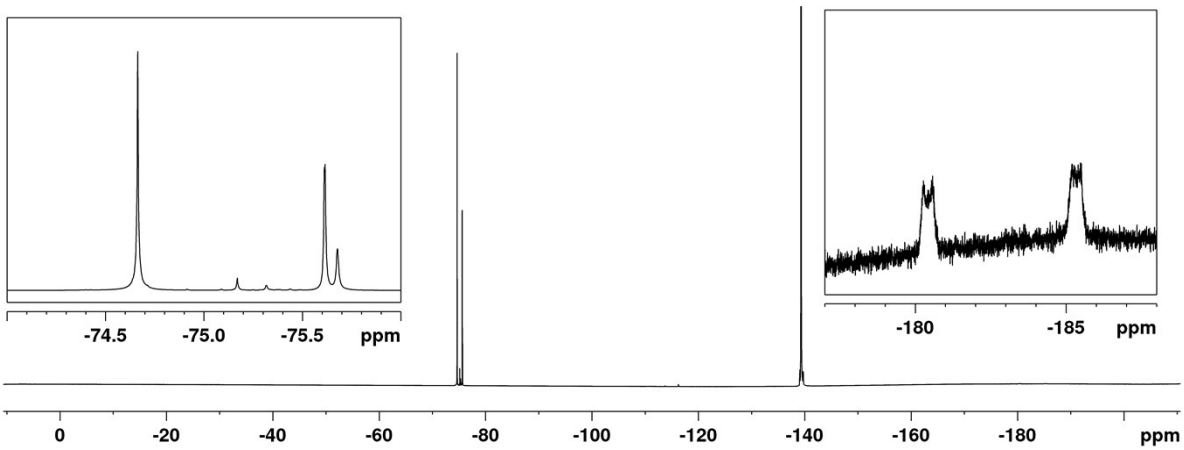

Figure S- 39: ^{19}F NMR spectrum (376.54 MHz, 298 K, *o*−DFB/CD_2Cl_2) of the reaction of [Me_4C_4−$SiMe_3$][*al*−*f*−*al*] with [NMe_4]F in *o*−DFB/CD_2Cl_2.

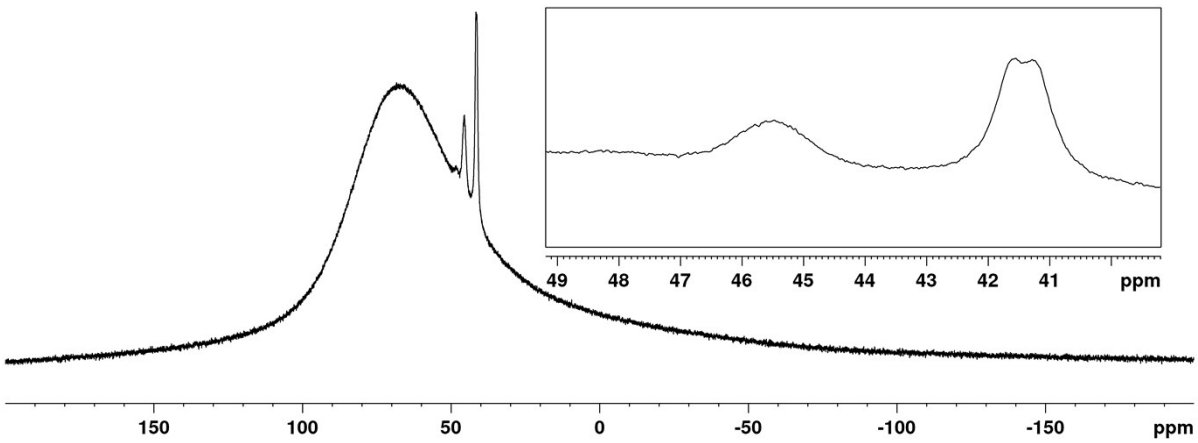

Figure S- 40: ^{27}Al NMR spectrum (78.22 MHz, 298 K, *o*–DFB/CD_2Cl_2) of the reaction of [Me_4C_4–$SiMe_3$][*al*–*f*–*al*] with [NMe_4]F in *o*–DFB/CD_2Cl_2.

Reaction of [Me_4C_4–$SiMe_3$][*al*–*f*–*al*] with DMAP

[Me_4C_4–$SiMe_3$][*al*–*f*–*al*] (400 mg, 0.24 mmol) and DMAP (58 mg, 0.48 mmol, 2 eq.) were dissolved in *o*–DFB (0.5 mL) and CH_2Cl_2 (0.3 mL) at rt. The orange solution was stored at −40°C overnight, which led to formation of crystals (DMAP-Al(OR^F)$_3$). The supernatant solution was filtered and then narrow down to a volume of ~0.4 mL. The concentrated solution was again stored at −40°C overnight, which led to formation of crystals of [Me_4C_4($SiMe_3$)(DMAP)][*f*–*al*].

NMR spectra of the reaction solution showed a mixture of several reaction products and will therefore not be discussed. NMR spectra after crystallization of DMAP-Al(OR^F)$_3$ allowed for assignment of the signals of [Me_4C_4($SiMe_3$)(DMAP)][*f*–*al*] (Figure S- 41).

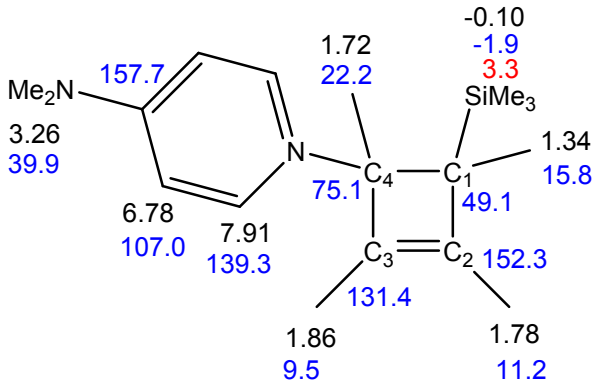

Figure S- 41: Main product of the reaction of [Me_4C_4–$SiMe_3$][*al*–*f*–*al*] with DMAP in *o*–DFB/CH_2Cl_2/CD_2Cl_2 after crystallization of DMAP-Al(OR^F)$_3$ and ^{1}H (black), ^{13}C (blue) and ^{29}Si (red) NMR chemical shifts in ppm.

^{1}H-NMR (300.18 MHz, 298 K, *o*–DFB/CH_2Cl_2/CD_2Cl_2): δ = −0.10 (s, **Me_3**Si), 1.34 (s, C_1–**Me**), 1.72 (s, C_4–**Me**), 1.78 (q, $^5J_{H-H}$ = 1.2 Hz, C_2–**Me**), 1.86 (q, $^5J_{H-H}$ = 1.2 Hz, C_3–**Me**), 3.26 (s, N**Me_2**), 6.78 (m, DMAP), 7.91 (m, DMAP) ppm.
^{13}C-NMR (75.48 MHz, 298 K, *o*–DFB/CH_2Cl_2/CD_2Cl_2): δ = −1.9 (**Me_3**Si), 9.5 (C_3-**Me**), 11.2 (C_2-**Me**), 15.8 (C_1-**Me**), 22.2 (C_4-**Me**), 39.9 (N**Me_2**), 49.1 (**C_1**), 75.1 (**C_4**), 107.0 (DMAP, *o*-**C**), 131.4 (**C_3**), 139.3 (DMAP, *m*-**C**) 152.3 (**C_2**), 157.7 (**C**-NMe_2) ppm.

^{19}F-NMR (282.45 MHz, 298 K, *o*–DFB/CH_2Cl_2/CD_2Cl_2): δ = −75.8 (d, $^5J_{F-F}$ = 1.8 Hz, [*f*–*al*]$^-$), −182.2 (m, br, [***f***–*al*]$^-$) ppm.

^{27}Al-NMR (78.22 MHz, 298 K, *o*–DFB/CH_2Cl_2/CD_2Cl_2): δ = 41 (d, $^1J_{Al-F}$ = 37 Hz, [*f*–***al***]$^-$), 44 (s, br, DMAP-Al(OR^F)$_3$) ppm.

^{29}Si-NMR (59.64 MHz, 298 K, *o*–DFB/CH_2Cl_2/CD_2Cl_2): δ = 3.3 (Me_3**Si**) ppm.

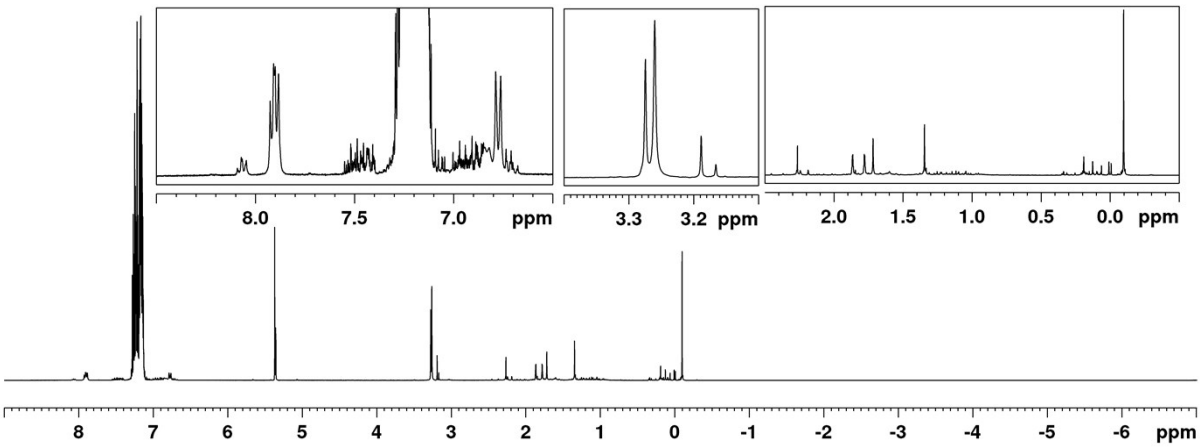

Figure S- 42: ^{1}H- NMR spectrum (300.18 MHz, 298 K, *o*–DFB/CH_2Cl_2/CD_2Cl_2) of the reaction of [Me_4C_4–$SiMe_3$][*al*–*f*–*al*] with DMAP in *o*–DFB/CH_2Cl_2 after crystallization of DMAP-Al(OR^F)$_3$.

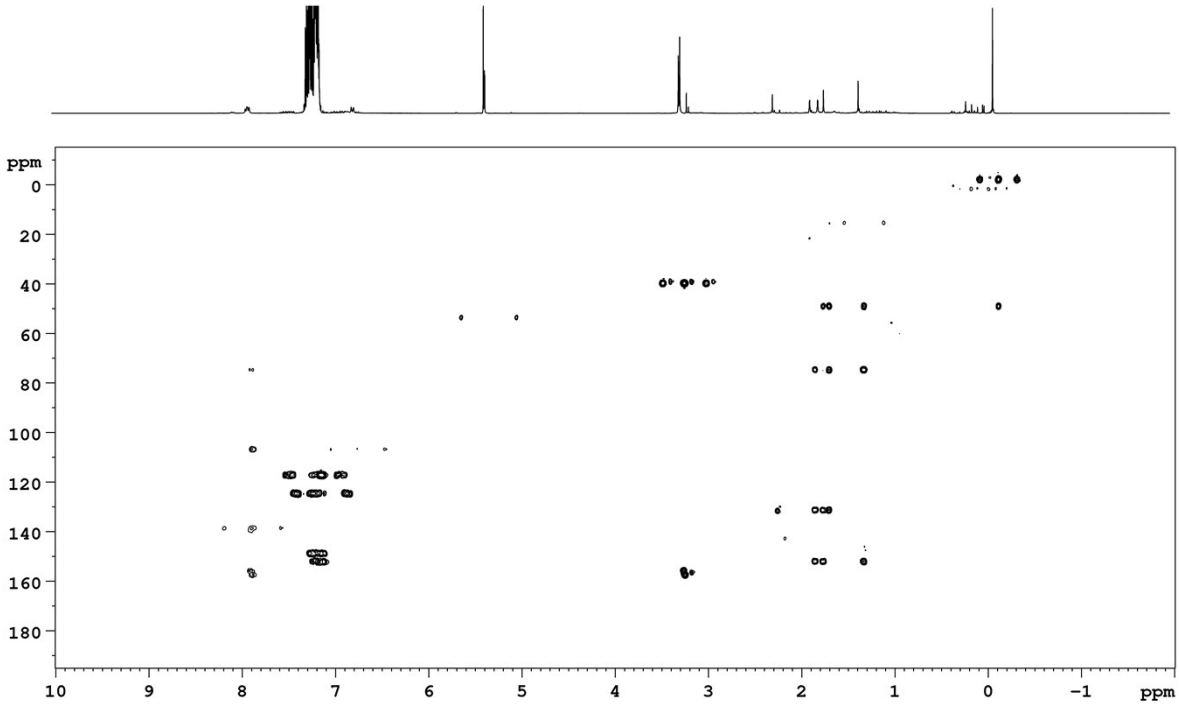

Figure S- 43: ^{1}H,^{13}C-HMBC NMR spectrum (300.18 MHz, 298 K, *o*–DFB/CH_2Cl_2/CD_2Cl_2) of the reaction of [Me_4C_4–$SiMe_3$][*al*–*f*–*al*] with DMAP in *o*–DFB/CH_2Cl_2 after crystallization of DMAP-Al(OR^F)$_3$.

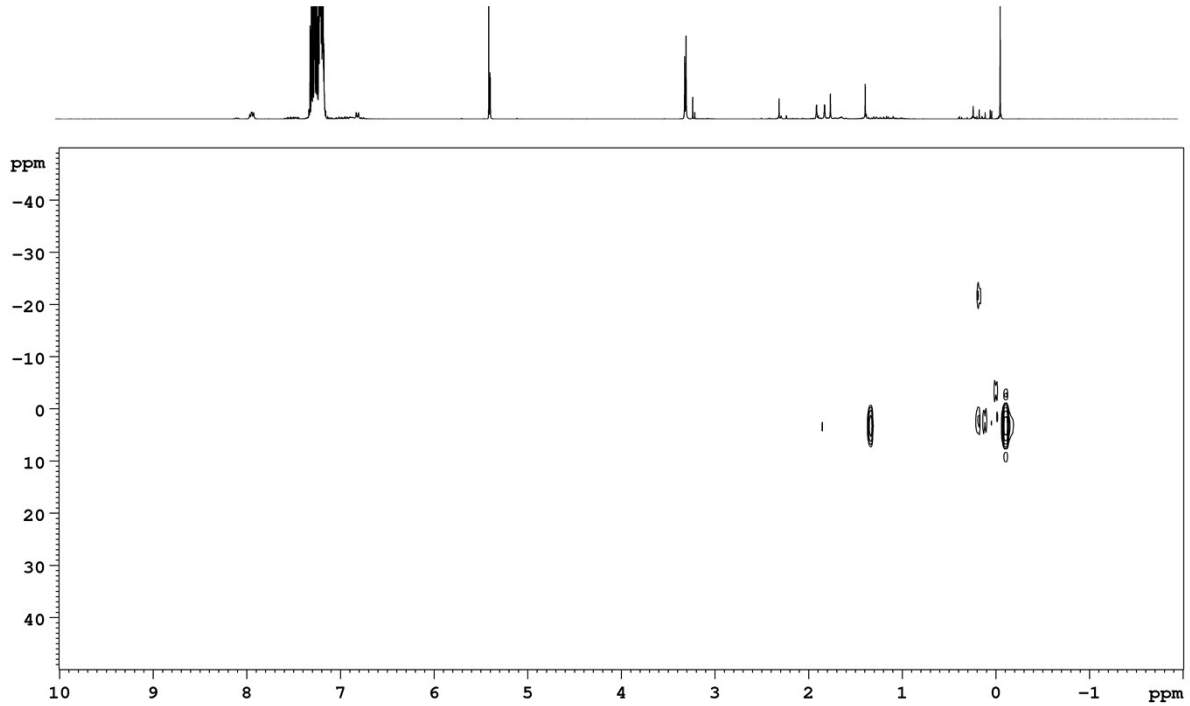

Figure S- 44: $^{1}H,^{29}Si$-HMBC NMR spectrum (300.18 MHz, 298 K, *o*–DFB/CH_2Cl_2/CD_2Cl_2 optimized to 8 Hz) of the reaction of [Me_4C_4–$SiMe_3$][*al*–*f*–*al*] with DMAP in *o*–DFB/CH_2Cl_2 after crystallization of DMAP-Al(OR^F)$_3$.

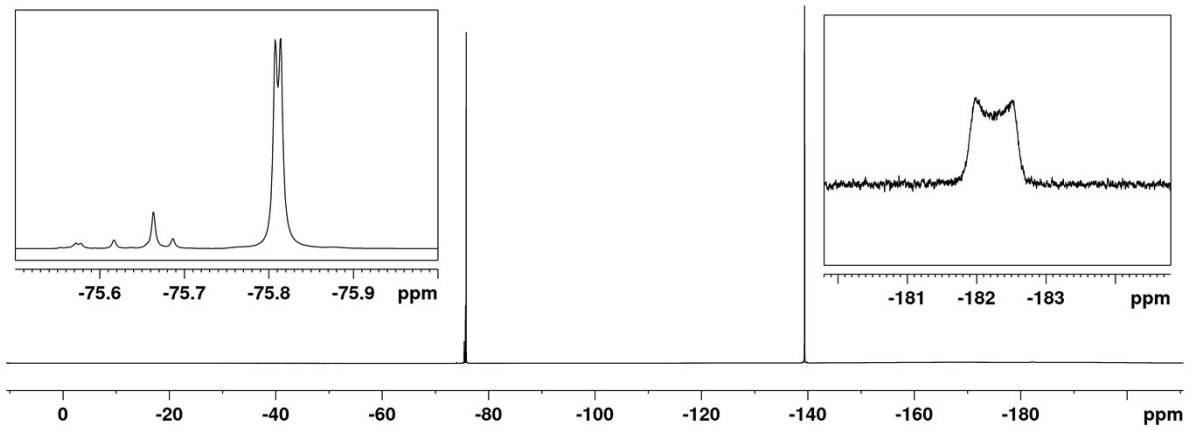

Figure S- 45: ^{19}F- NMR spectrum (282.45 MHz, 298 K, *o*–DFB/CH_2Cl_2/CD_2Cl_2) of the reaction of [Me_4C_4–$SiMe_3$][*al*–*f*–*al*] with DMAP in *o*–DFB/CH_2Cl_2 after crystallization of DMAP-Al(OR^F)$_3$.

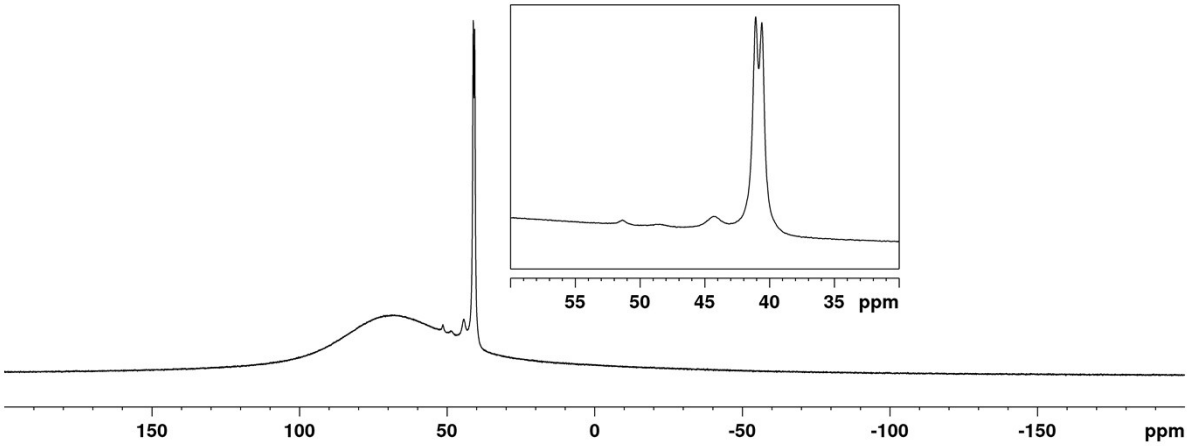

Figure S- 46: ^{27}Al- NMR spectrum (300.18 MHz, 298 K, *o*–DFB/CH_2Cl_2/CD_2Cl_2) of the reaction of [Me_4C_4–$SiMe_3$][*al*–*f*–*al*] with DMAP in *o*–DFB/CH_2Cl_2 after crystallization of DMAP-Al(OR^F)$_3$.

Reactions of [Me_4C_4–$SiMe_3$][*al*–*f*–*al*] with Et_2O and 2-butyne

a) Reaction with Et_2O

[Me_4C_4–$SiMe_3$][*al*–*f*–*al*] was dissolved in CD_2Cl_2 (0.4 mL) and Et_2O (0.4 mL) in a NMR tube. The tube was immediately closed and analyzed by NMR spectroscopy. NMR spectra revealed formation of Me_3SiF, Me_3SiOEt (decomposition of Et_2O), Et_2O–$Al(OR^F)_3$ and [*f*–*al*]$^-$. The according cation could not be identified.

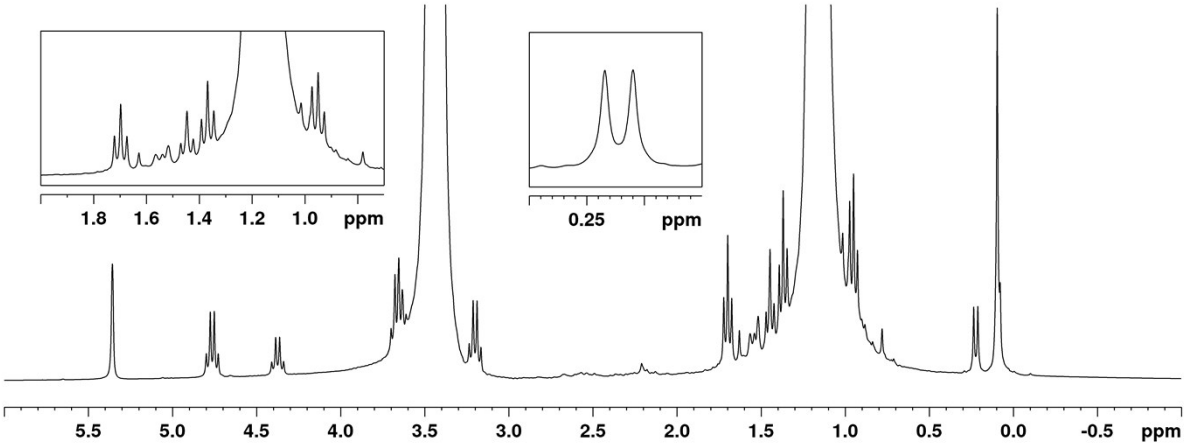

Figure S- 47: ^1H- NMR spectrum (300.18 MHz, 298 K, Et_2O/CD_2Cl_2) of the reaction of [Me_4C_4–$SiMe_3$][*al*–*f*–*al*] with Et_2O in Et_2O/CD_2Cl_2.

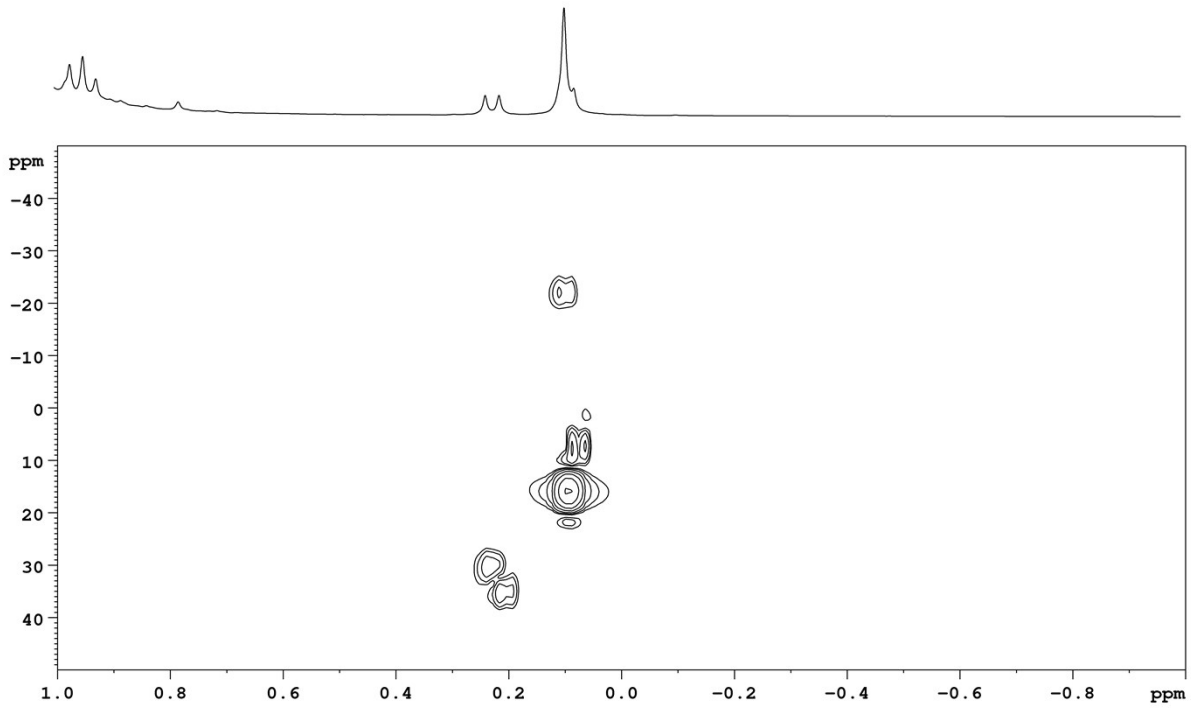

Figure S- 48: ^1H,^{29}Si-HMBC NMR spectrum (300.18 MHz, 298 K, Et_2O/CD_2Cl_2, optimized to 8 Hz) of the reaction of [Me_4C_4–$SiMe_3$][*al*–*f*–*al*] with Et_2O in Et_2O/CD_2Cl_2.

The signal at $\delta(^{29}Si)$ = 16 ppm results from Me_3SiOEt due to decomposition of Et_2O.

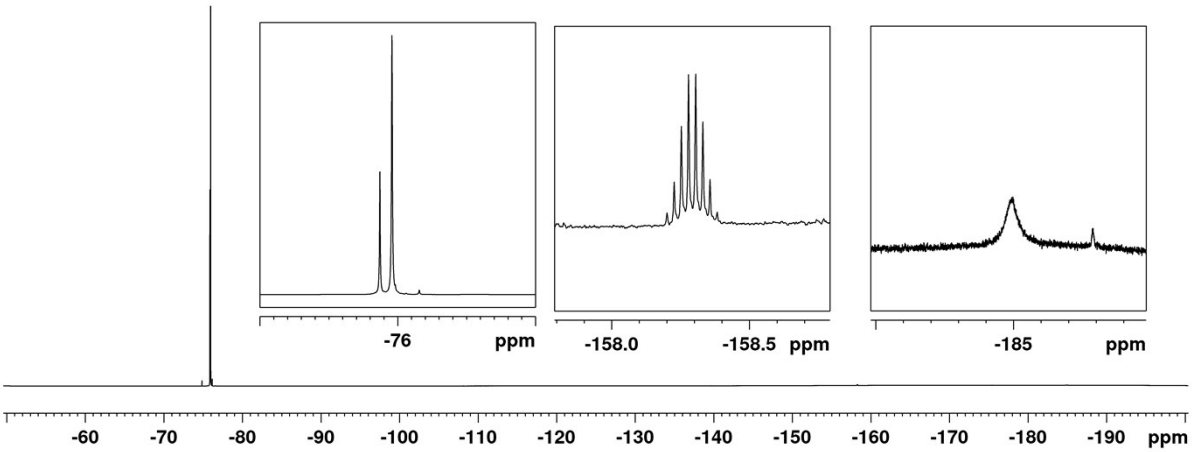

Figure S- 49: ^{19}F- NMR spectrum (282.45 MHz, 298 K, Et_2O/CD_2Cl_2) of the reaction of $[Me_4C_4–SiMe_3][al–f–al]$ with Et_2O in Et_2O/CD_2Cl_2.

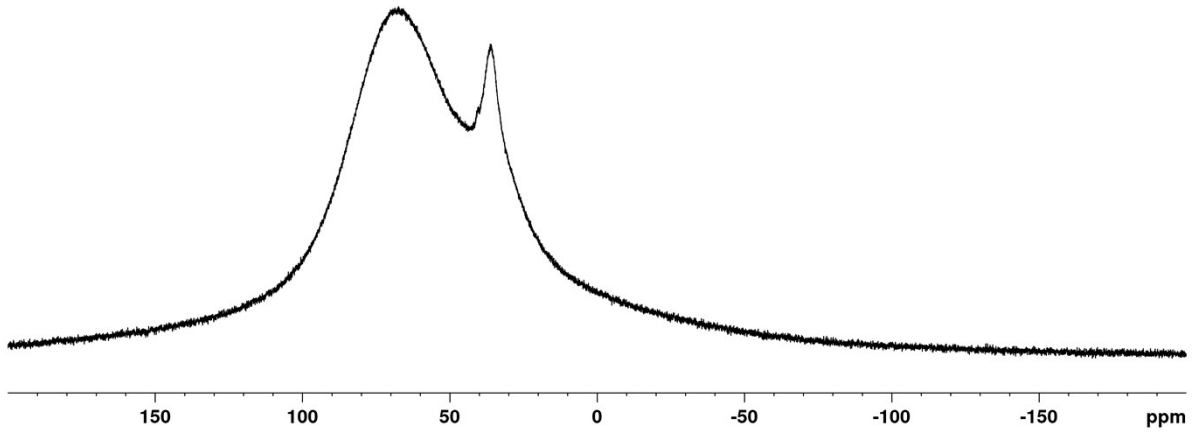

Figure S- 50: ^{27}Al- NMR spectrum (78.22 MHz, 298 K, Et_2O/CD_2Cl_2) of the reaction of $[Me_4C_4–SiMe_3][al–f–al]$ with Et_2O in Et_2O/CD_2Cl_2.

b) Reaction with Et_2O and 2-butyne

$[Me_4C_4–SiMe_3][al–f–al]$ (327 mg, 0.20 mmol) and 2-butyne (0.03 mL, 21 mg, 0.39 mmol, 1.95 eq.) were dissolved in *o*–DFB (1.0 mL). Parts of this solution was transferred into a NMR tube, then CD_2Cl_2 and Et_2O were added. The tube was immediately closed and analyzed by NMR spectroscopy. NMR spectra revealed formation of Me_3SiF, $(Me_3Si)_2O$ (residual water in the Et_2O), $Et_2O–Al(OR^F)_3$, C_6Me_6 and decomposition of $[Me_4C_4–SiMe_3]^+$. Parts of $[al–f–al]^-$ did not decompose, but the according cation could not be identified.

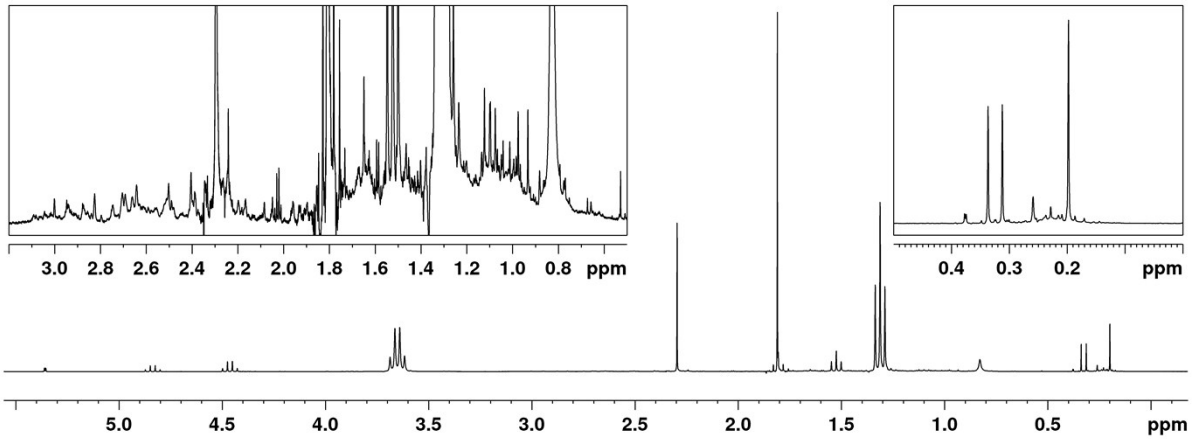

Figure S- 51: ^{1}H- NMR spectrum (300.18 MHz, 298 K, *o*−DFB/Et_2O/CD_2Cl_2) of the reaction of [Me_4C_4−$SiMe_3$][*al*−*f*−*al*] with 2-butyne and Et_2O in *o*−DFB/Et_2O/CD_2Cl_2.

The signals at δ(^{1}H) = 2.30 and 1.81 ppm result from C_6Me_6 and 2-butyne, respectively (molar ratio 1:7).

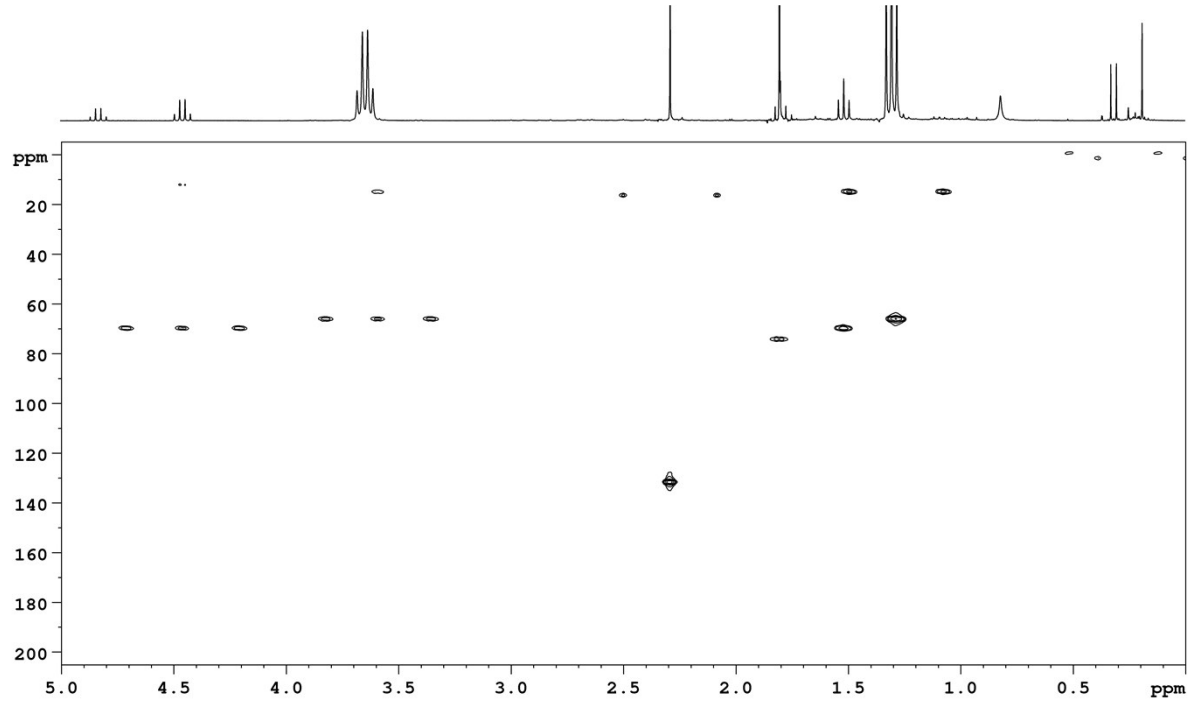

Figure S- 52: ^{1}H,^{13}C-HMBC NMR spectrum (300.18 MHz, 298 K, *o*−DFB/Et_2O/CD_2Cl_2) of the reaction of [Me_4C_4−$SiMe_3$][*al*−*f*−*al*] with 2-butyne and Et_2O in *o*−DFB/Et_2O/CD_2Cl_2.

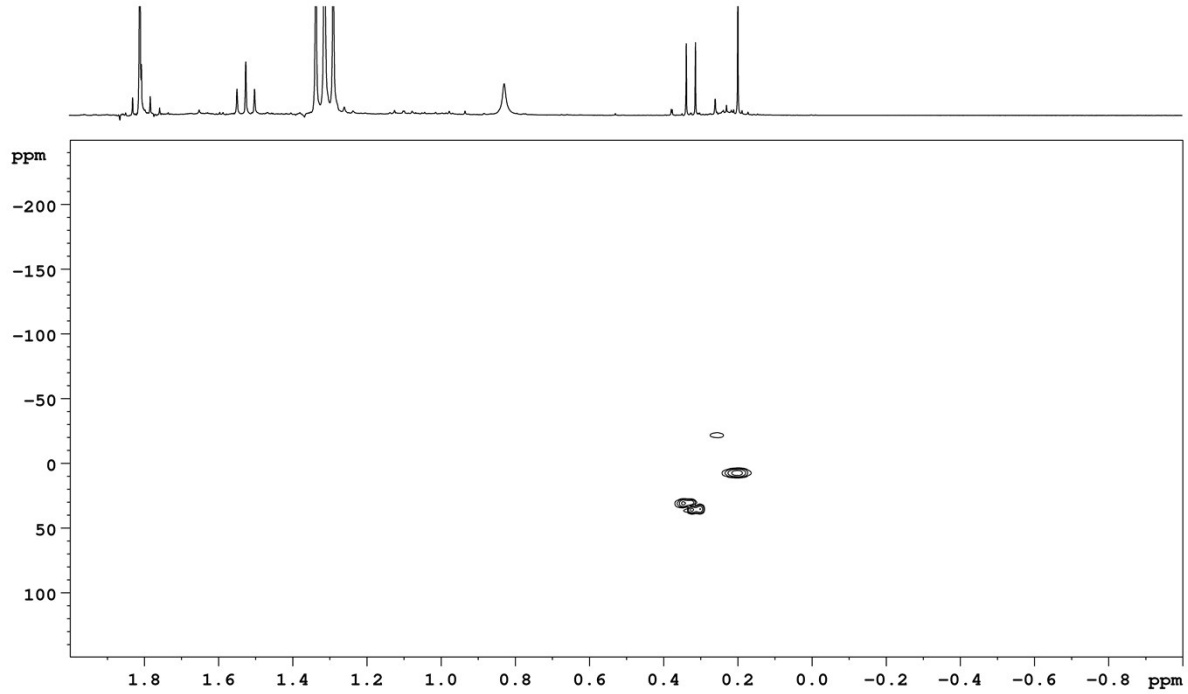

Figure S- 53: $^{1}H,^{29}Si$-HMBC NMR spectrum (300.18 MHz, 298 K, *o*−DFB/Et_2O/CD_2Cl_2) of the reaction of [Me_4C_4−$SiMe_3$][*al*−*f*−*al*] with 2-butyne and Et_2O in *o*−DFB/Et_2O/CD_2Cl_2.

The signals at δ(^{29}Si) = 33.6 and 7.8 ppm result from Me_3SiF and $(Me_3Si)_2O$, respectively.

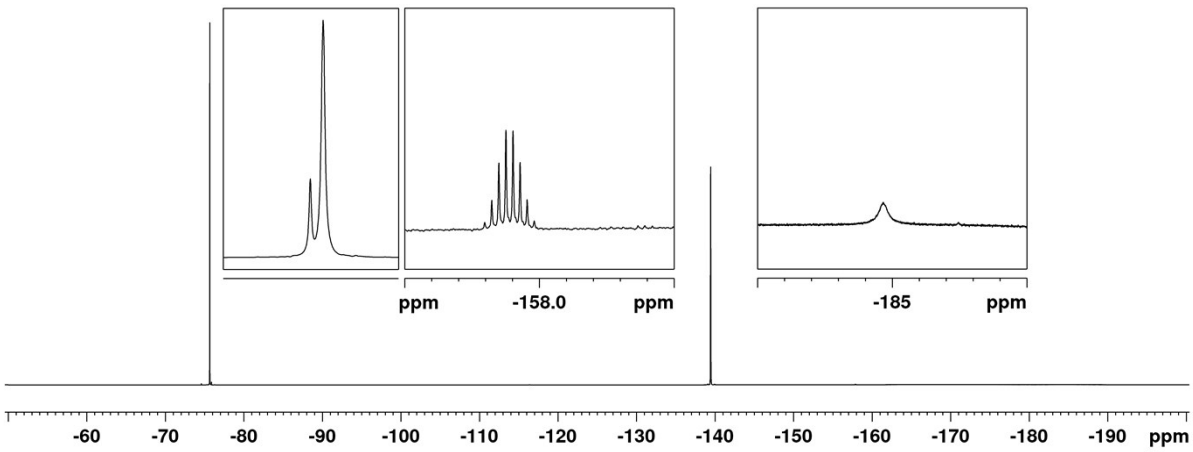

Figure S- 54: ^{19}F- NMR spectrum (282.45 MHz, 298 K, *o*−DFB/Et_2O/CD_2Cl_2) of the reaction of [Me_4C_4−$SiMe_3$][*al*−*f*−*al*] with 2-butyne and Et_2O in *o*−DFB/Et_2O/CD_2Cl_2.

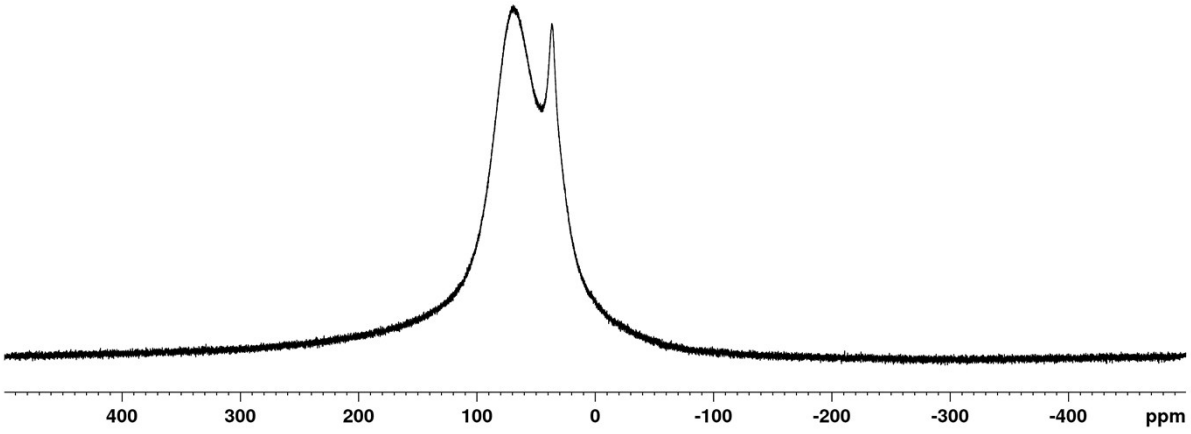

Figure S- 55: ^{27}Al- NMR spectrum (78.22 MHz, 298 K, *o*−DFB/Et_2O/CD_2Cl_2) of the reaction of [Me_4C_4–$SiMe_3$][*al*–*f*–*al*] with 2-butyne and Et_2O in *o*−DFB/Et_2O/CD_2Cl_2.

The signal at δ(^{27}Al) = 36.5 ppm results from Et_2O−Al(OR^F)$_3$ and [*al*–*f*–*al*]$^-$.

c) Reaction with Et_2O and MeO_2C−C≡C−CO_2Me

[Me_4C_4−$SiMe_3$][*al*–*f*–*al*] (263 mg, 0.16 mmol) and MeO_2C−C≡C−CO_2Me (0.02 mL, 16 mg, 0.16 mmol, 1.0 eq.) were dissolved in *o*−DFB (1.0 mL) and stirred for 15 min. Then Et_2O (0.1 mL) was added and the solution was stirred for another 30 min. NMR spectra of the reaction solution revealed decomposition of [Me_4C_4–$SiMe_3$]$^+$ and retention of MeO_2C−C≡C−CO_2Me.

d) Reaction with Et_2O and Me_3Si−C≡C−$SiMe_3$

[Me_4C_4−$SiMe_3$][*al*–*f*–*al*] (146 mg, 0.09 mmol) and Me_3Si−C≡C−$SiMe_3$ (0.02 mL, 23 mg, 0.09 mmol, 1.0 eq.) were dissolved in *o*−DFB (1.0 mL) and stirred for 15 min. Then Et_2O (0.06 mL) was added and the solution was stirred for another 30 min. NMR spectra of the reaction solution revealed decomposition of [Me_4C_4–$SiMe_3$]$^+$ and retention of Me_3Si−C≡C−$SiMe_3$.

Crystal Structure Data

Crystal Structure of [Me_4C_4–$SiMe_3$][*al–f–al*]

[Me_4C_4–$SiMe_3$][*al–f–al*] was synthesized as described above and crystals suited for SC-XRD could be obtained from the reaction solution in *o*–DFB by addition of CH_2Cl_2. Equivalent C–C and C–F bond distances in the anion and thermal ellipsoids were equalized by using SADI, SIMU and RIGU commands.

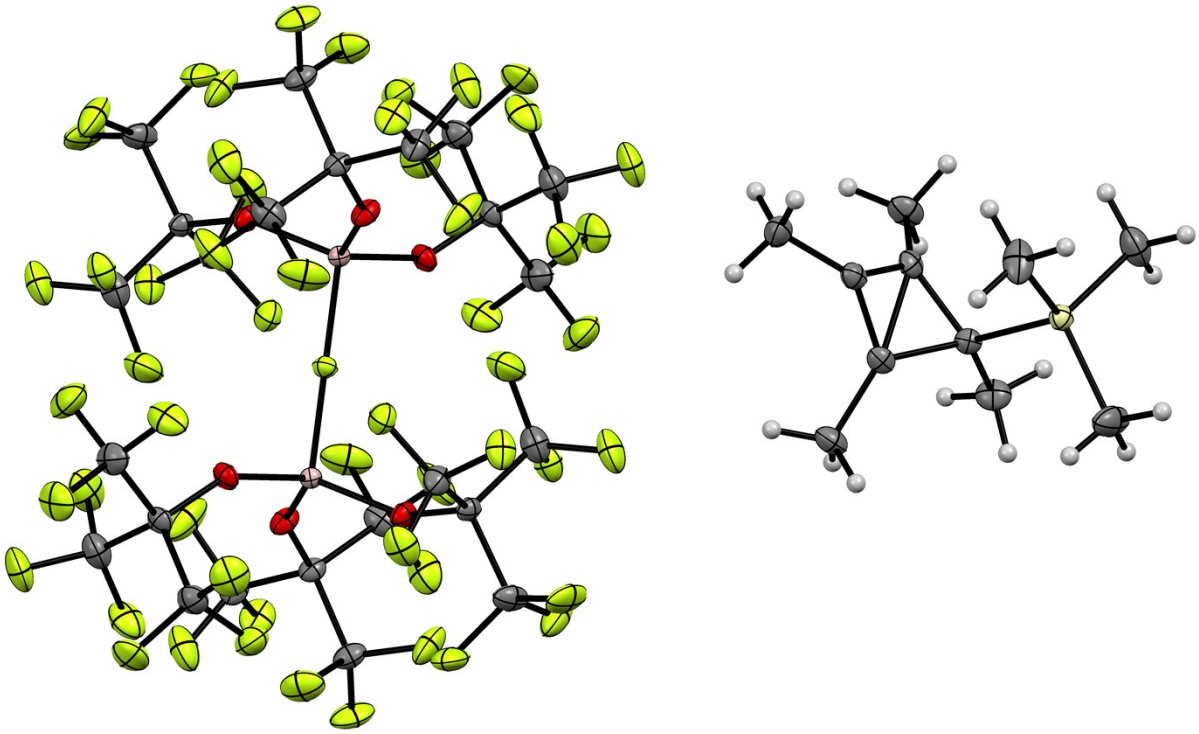

Figure S- 56: Molecular structure of [Me_4C_4–$SiMe_3$][*al–f–al*] with thermal ellipsoids set at 50% probability level. The cation and some of the OR^F moieties were disordered over two positions. For clarity, only the most occupied moieties are shown and H atoms are shown as spheres of arbitrary radius. Scheme: Al (pink), O (red), F (light green), Si (yellow), C (grey), H (white).

Table S-1. Crystal data and structure refinement for **1**.

Identification code	**1**	
Empirical formula	C35 H21 Al2 F55 O6 Si	
Formula weight	1664.47	
Temperature	100(2) K	
Wavelength	71.073 pm	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 1040.39(2) pm	a= 88.2350(10)°.
	b = 1268.20(3) pm	b= 80.1750(10)°.
	c = 2140.37(5) pm	g = 82.3730(10)°.
Volume	2.75792(11) nm^3	

Z	2
Density (calculated)	2.004 Mg/m^3
Absorption coefficient	0.305 mm^{-1}
F(000)	1628
Crystal size	0.280 x 0.220 x 0.060 mm^3
Theta range for data collection	0.966 to 31.583°.
Index ranges	-15<=h<=15, -18<=k<=18, -31<=l<=31
Reflections collected	82248
Independent reflections	17826 [R(int) = 0.0205]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7463 and 0.7201
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	17826 / 13040 / 1262
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0355, wR2 = 0.0853
R indices (all data)	R1 = 0.0479, wR2 = 0.0908
Extinction coefficient	n/a
Largest diff. peak and hole	0.580 and -0.326 $e.Å^{-3}$

Crystal Structure of DMAP−Al(OR^F)$_3$

DMAP−Al(OR^F)$_3$ was synthesized as described above by reaction of [Me$_4$C$_4$−SiMe$_3$][*al*−*f*−*al*] with an excess DMAP. Crystals suited for SC-XRD could be obtained from the reaction solution at −40°C. Equivalent C−C and C−F bond distances and thermal ellipsoids in the disordered OC(CF$_3$)$_3$ groups were equalized by using SADI, SIMU and RIGU commands.

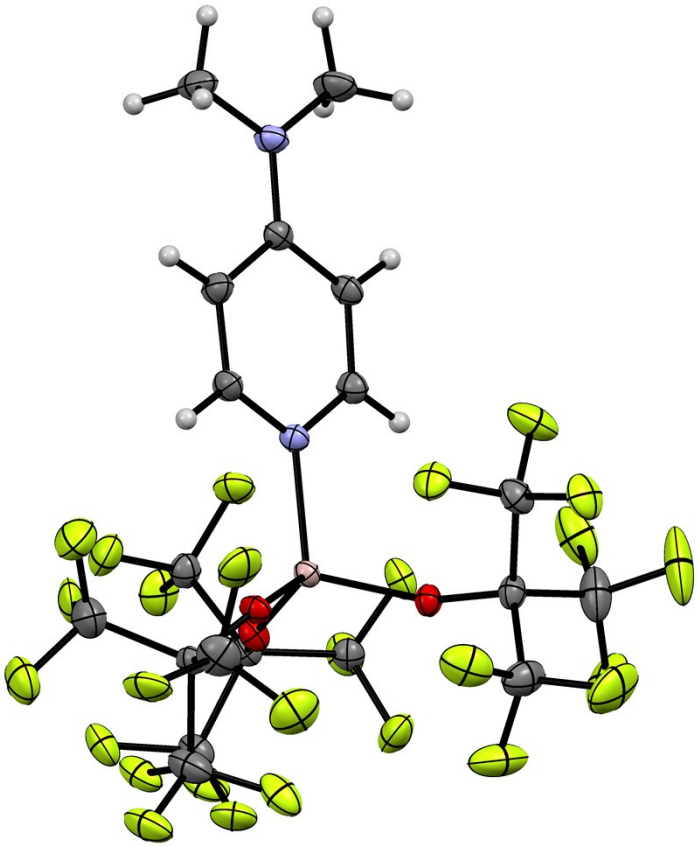

Figure S- 57: Molecular structure of DMAP−Al(OR^F)$_3$ with thermal ellipsoids set at 50% probability level. H atoms are shown as spheres of arbitrary radius. Some of the OR^F groups were disordered over two positions. Only the most occupied moiety is shown. Scheme: Al (pink), O (red), F (light green), N (blue), C (grey), H (white).

Table S-2. Crystal data and structure refinement for DMAP−Al(OR^F)$_3$.

Identification code	DMAP−Al(OR^F)$_3$	
Empirical formula	C19 H10 Al F27 N2 O3	
Formula weight	854.27	
Temperature	100(2) K	
Wavelength	71.073 pm	
Crystal system	Monoclinic	
Space group	P2$_1$/c	
Unit cell dimensions	a = 1221.82(8) pm	a= 90°.
	b = 1139.50(7) pm	b= 105.383(3)°.
	c = 2117.52(14) pm	g = 90°.
Volume	2.8425(3) nm^3	
Z	4	

Density (calculated)	1.996 Mg/m^3
Absorption coefficient	0.279 mm^{-1}
F(000)	1672
Crystal size	0.34 x 0.32 x 0.1 mm^3
Theta range for data collection	1.729 to 26.039°.
Index ranges	-15<=h<=15, -12<=k<=14, -26<=l<=26
Reflections collected	106462
Independent reflections	5604 [R(int) = 0.0287]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7453 and 0.7026
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5604 / 2973 / 568
Goodness-of-fit on F^2	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0277, wR2 = 0.0685
R indices (all data)	R1 = 0.0295, wR2 = 0.0697
Extinction coefficient	n/a
Largest diff. peak and hole	0.407 and -0.248 $e.Å^{-3}$

Crystal Structure of $[Me_4C_4(SiMe_3)(DMAP)][f\text{–}al]$ (4)

4 was synthesized as described above by reaction of $[Me_4C_4\text{–}SiMe_3][al\text{–}f\text{–}al]$ with an excess DMAP. Crystals suited for SC-XRD could be obtained from the concentrated reaction solution at −40°C after crystallization of DMAP–$Al(OR^F)_3$. Equivalent C–C and C–F bond distances and thermal ellipsoids in the disordered $OC(CF_3)_3$ groups were equalized by using SADI, SIMU and RIGU commands.

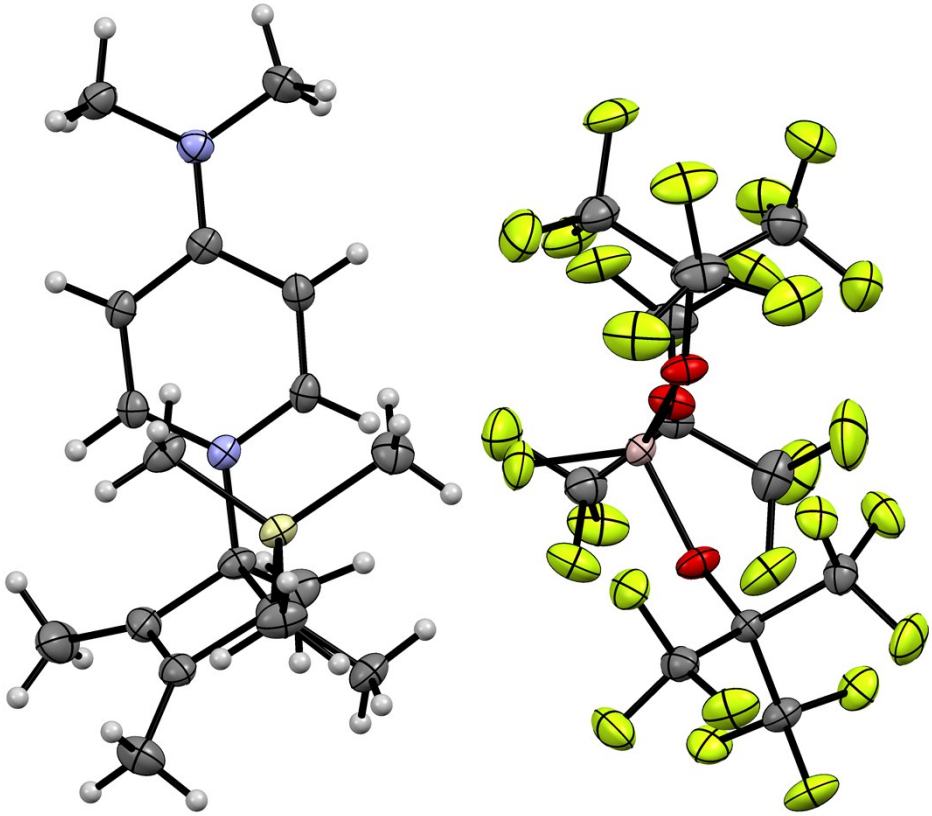

Figure S- 58: Molecular structure of $[Me_4C_4(SiMe_3)(DMAP)][f\text{–}al]$ (**4**) with thermal ellipsoids set at 50% probability level. H atoms are shown as spheres of arbitrary radius. Scheme: Al (pink), O (red), F (light green), N (blue), Si (yellow), C (grey), H (white).

Table S-3. Crystal data and structure refinement for $[Me_4C_4(SiMe_3)(DMAP)][f\text{–}al]$.

Identification code	**4**	
Empirical formula	C30 H31 Al F28 N2 O3 Si	
Formula weight	1054.64	
Temperature	100(2) K	
Wavelength	71.073 pm	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 942.36(2) pm	a= 78.2070(10)°.
	b = 1096.84(3) pm	b= 88.952(2)°.
	c = 2066.76(5) pm	g = 83.352(2)°.
Volume	2.07706(9) nm^3	

Z	2
Density (calculated)	1.686 Mg/m^3
Absorption coefficient	0.239 mm^{-1}
F(000)	1056
Crystal size	0.24 x 0.19 x 0.14 mm^3
Theta range for data collection	1.006 to 30.547°.
Index ranges	-13<=h<=12, -15<=k<=15, -28<=l<=29
Reflections collected	53293
Independent reflections	12146 [R(int) = 0.0259]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.6945
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12146 / 372 / 595
Goodness-of-fit on F^2	1.048
Final R indices [I>2sigma(I)]	R1 = 0.0475, wR2 = 0.1241
R indices (all data)	R1 = 0.0642, wR2 = 0.1330
Extinction coefficient	n/a
Largest diff. peak and hole	0.495 and -0.290 $e.Å^{-3}$

Quantum Chemical Calculations

DFT and MP2 optimizations were carried out with TURBOMOLE[QC 1,2] using the BP86[QC 3,4] density functional (RI approximation[5a]) in combination with the def-TZVP and def2-TZVPP basis sets[QC 5b,c] and D3 dispersion correction with Becke-Johnson damping.[QC 5d,e] Vibrational frequencies were calculated analytically with the AOFORCE[QC 6,7] module and all structures represented true minima without imaginary frequencies on the respective hypersurface. Thermodynamic terms were calculated with inclusion of zero-point energy and thermal contributions to the enthalpy/entropy (FREEH tool; unscaled BP86 vibrational frequencies).

[QC 1] O. Treutler, R. Ahlrichs, *J. Chem. Phys.* **1995**, *102*, 346.
[QC 2] R. Ahlrichs, M. Baer, M. Haeser, H. Horn, C. Koelmel, *Chem. Phys. Lett.* **1989**, *162*, 165.
[QC 3] J. P. Perdew, *Phys. Rev. B* **1986**, *34*.
[QC 4] A. D. Becke, *Phys. Rev. A: Gen. Phys.* **1988**, *38*, 3098.
[QC 5] a) K. Eichkorn, O. Treutler, H. Oehm, M. Haeser, R. Ahlrichs, *Chem. Phys. Lett.* **1995**, *242*, 652; b) A. Schäfer, C. Huber, R. Ahlrichs, *The Journal of Chemical Physics* **1994**, *100*, 5829; c) F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297; d) S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *The Journal of Chemical Physics* **2010**, *132*, 154104; e) S. Grimme, S. Ehrlich, L. Goerigk, *Journal of Computational chemistry* **2011**, *32*, 1456.
[QC 6] P. Deglmann, F. Furche, R. Ahlrichs, *Chem. Phys. Lett.* **2002**, *362*, 511.
[QC 7] P. Deglmann, F. Furche, *J. Chem. Phys.* **2002**, *117*, 9535.
[QC 8] A. Klamt, G. Schueuermann, *J. Chem. Soc., Perkin Trans. 2* **1993**, 799.
[QC 9] A. Schäfer, A. Klamt, D. Sattel, J. C. W. Lohrenz, F. Eckert, *Phys. Chem. Chem. Phys.* **2000**, *2*, 2187.

SCF energy of $[Me_3Si(MeCCMe)]^+$ in dependence of the C–C–Si angle (BP86–D3(BJ)/def-TZVP)

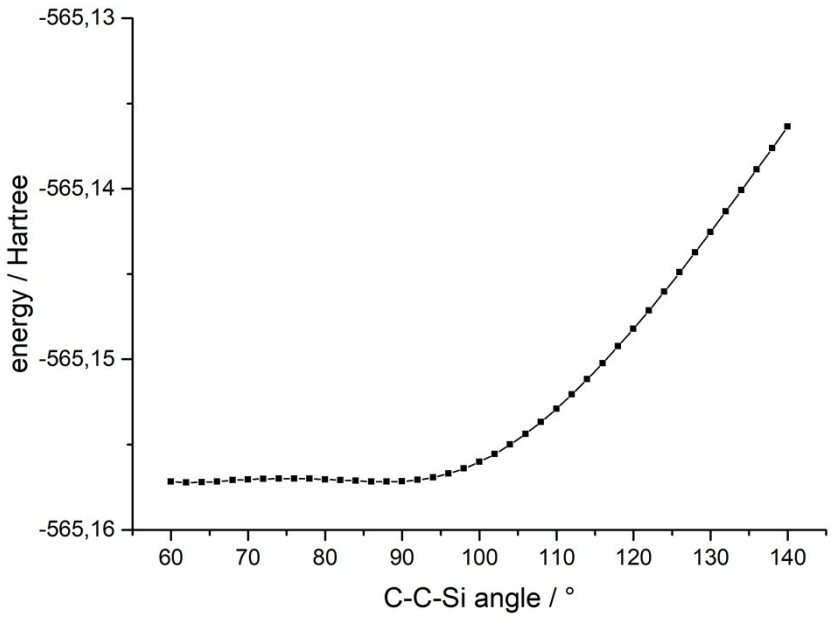

Figure S- 59: SCF energy of $[Me_3Si(MeCCMe)]^+$ in dependence of the C–C–Si angle. The minimum structure features inequivalent Si–C distances between the $[Me_3Si]^+$ moiety and the ligand. Therefore, both minima at 87.6° and 62.4°, respectively, represent the same *non-classical* structure. The *classical* structure with a C–C–Si angle of approximately 100 to 120° is not a minimum structure.

Images of the LUMO of 1

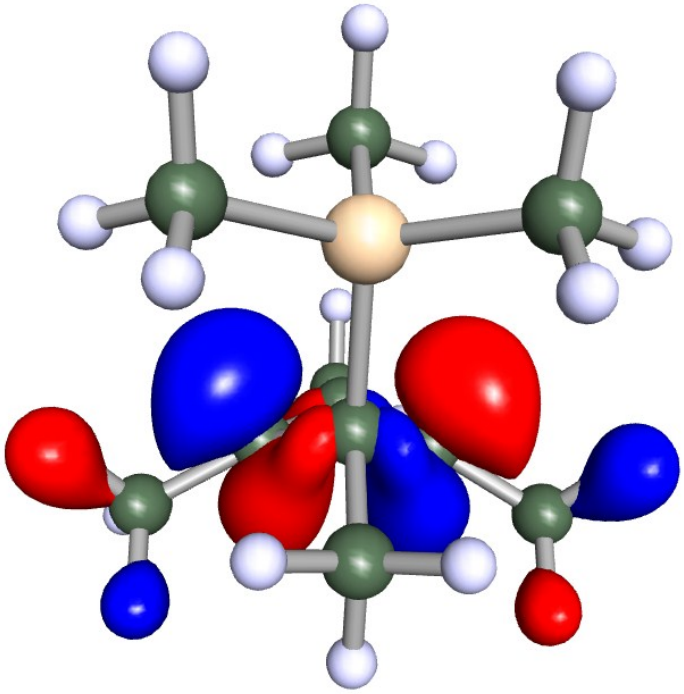

Figure S- 60: Calculated LUMO of $[Me_4C_4{-}SiMe_3]^+$ (−7.01 eV) at BP86−D3(BJ)/def-TZVP level. The LUMO is mainly located at C2 and C2'.

Optimized coordinates and energies of the calculated compounds:

Atomic coordinates are given in Å, SCF and MP2 energies are given in Hartree, the FREEH energy is given in kJ mol^{-1}, and the FREEH entropy is given in kJ mol^{-1} K^{-1}. Calculations at MP2 level were performed by using thermal contributions (FREEH energy and FREEH entropy) and solvation energies ($\Delta_{solv}G^0$) from BP86-D3(BJ)/def-TZVP calculations. $H^0_{(g)}$, $G^0_{(g)}$ and $G^0_{(solv)}$ are calculated by the following equations:

$H^0_{(g)}$ = SCF/MP2 energy + FREEH energy + R·T
$G^0_{(g)}$ = SCF/MP2 energy + FREEH energy + R·T – T·FREEH entropy
$G^0_{solv} = G^0_{(g)} + \Delta_{solv}G^0$ with $\Delta_{solv}G^0$ = COSMO energy - SCF energy + 7.96 kJ mol^{-1}

BP86–D3(BJ)/def-TZVP

$[Me_3Si]^+$

Si	-0.00000	0.00000	0.00112
C	0.52047	1.77035	-0.00060
C	-1.79340	-0.43444	-0.00060
C	1.27294	-1.33592	-0.00060
H	1.60980	1.89658	0.00703
H	0.09951	2.27532	-0.88737
H	0.08501	2.28366	0.87404
H	-2.44739	0.44584	0.00703
H	-2.02024	-1.05148	-0.88737
H	-2.02021	-1.06821	0.87404
H	1.92073	-1.22384	-0.88737
H	1.93520	-1.21545	0.87404
H	0.83759	-2.34242	0.00703

SCF energy = -409.0711201408
FREEH energy = 299.76
FREEH entropy = 0.36071

$H_2C=CH_2$

C	-0.66688	0.00000	0.00000
C	0.66688	0.00000	0.00000
H	-1.24150	-0.92854	0.00000
H	-1.24150	0.92854	0.00000
H	1.24150	0.92854	0.00000
H	1.24150	-0.92854	0.00000

SCF energy = -78.620109348
FREEH energy = 138.22
FREEH entropy = 0.21962

$[Me_3Si(H_2C=CH_2)]^+$

C	-1.09870	1.64881	0.37827
C	0.05218	1.99702	-0.25189
Si	0.12516	-0.42482	-0.00673
C	-1.51042	-1.32289	-0.15632
C	1.18128	-0.50706	-1.55060
C	1.02210	-0.59013	1.62124
H	-1.15318	1.57720	1.46736
H	-2.03367	1.52970	-0.17209
H	0.96401	2.21952	0.30796
H	0.07953	2.17040	-1.32916
H	-1.26792	-2.39700	-0.22681
H	-2.16112	-1.18495	0.71597
H	-2.05578	-1.04843	-1.06863
H	1.49909	-1.55913	-1.64942
H	2.08635	0.10973	-1.48949
H	0.61945	-0.24657	-2.45693
H	1.89395	0.07343	1.69183
H	0.36521	-0.41866	2.48399
H	1.39249	-1.62618	1.69146

SCF energy = -487.7335919317
FREEH energy = 450.82
FREEH entropy = 0.41480

$Me_2C=CMe_2$

C	0.00000	0.00000	-0.67642
C	0.00000	0.00000	0.67642
C	0.00193	1.25013	-1.52337
C	-0.00193	-1.25013	-1.52337
C	0.00193	-1.25013	1.52337
C	-0.00193	1.25013	1.52337
H	0.01735	2.18103	-0.94765
H	0.87720	1.25726	-2.19473
H	-0.88703	1.27408	-2.17625
H	-0.01735	-2.18103	-0.94765
H	-0.87720	-1.25726	-2.19473
H	0.88703	-1.27408	-2.17625
H	0.01735	-2.18103	0.94765
H	0.87720	-1.25726	2.19473
H	-0.88703	-1.27408	2.17625
H	0.88703	1.27408	2.17625
H	-0.01735	2.18103	0.94765
H	-0.87720	1.25726	2.19473

SCF energy = -235.9565983791
FREEH energy = 440.07
FREEH entropy = 0.36567

$[Me_3Si(Me_2C=CMe_2)]^+$

Si	-0.02188	0.93905	0.82938
C	-1.71822	1.72716	0.68347

C	1.37238	2.07758	0.31343
C	0.24511	0.14645	2.50856
C	-0.41963	-0.46926	-1.13697
C	-1.88636	-0.82191	-1.18145
C	0.01860	0.42212	-2.27094
C	0.47032	-1.17495	-0.32880
C	1.96673	-1.11721	-0.49500
C	0.00483	-2.31832	0.53815
H	-2.53086	1.04381	0.95752
H	-1.91637	2.14626	-0.31067
H	-1.72877	2.56261	1.40300
H	1.23053	2.50729	-0.68531
H	1.36908	2.91318	1.03289
H	2.35942	1.60348	0.36943
H	1.21133	-0.36509	2.59636
H	-0.55843	-0.54656	2.78553
H	0.23920	0.97156	3.23991
H	-2.01431	-1.63918	-1.91106
H	-2.29537	-1.17651	-0.22990
H	-2.48983	0.02231	-1.53417
H	-0.16642	-0.12340	-3.21112
H	1.07524	0.70024	-2.25283
H	-0.59264	1.33413	-2.32179
H	2.47611	-1.09358	0.47870
H	2.28196	-2.05472	-0.98246
H	2.32804	-0.28820	-1.10838
H	0.69570	-2.49689	1.37006
H	-1.00787	-2.20095	0.93669
H	0.00238	-3.23050	-0.08224

SCF energy = -645.0954455209
FREEH energy = 753.26
FREEH entropy = 0.52255

$Ph_2C{=}CPh_2$

C	0.00000	0.00000	-0.68526
C	0.00000	0.00000	0.68526
C	0.13393	1.24813	-1.47853
C	-0.13393	-1.24813	-1.47853
C	0.13393	-1.24813	1.47853
C	-0.13393	1.24813	1.47853
C	1.10798	2.21210	-1.16085
C	1.23094	3.37732	-1.91624
C	0.38217	3.60393	-3.00518
C	-0.57971	2.64614	-3.34168
C	-0.69479	1.47446	-2.59274
C	0.69479	-1.47446	-2.59274
C	0.57971	-2.64614	-3.34168
C	-0.38217	-3.60393	-3.00518
C	-1.23094	-3.37732	-1.91624
C	-1.10798	-2.21210	-1.16085
C	-0.69479	-1.47446	2.59274
C	-0.57971	-2.64614	3.34168
C	0.38217	-3.60393	3.00518
C	1.23094	-3.37732	1.91624
C	1.10798	-2.21210	1.16085
C	0.69479	1.47446	2.59274
C	0.57971	2.64614	3.34168
C	-0.38217	3.60393	3.00518
C	-1.23094	3.37732	1.91624
C	-1.10798	2.21210	1.16085
H	1.76808	2.03802	-0.31095
H	1.99504	4.11171	-1.65623
H	0.47653	4.51760	-3.59404
H	-1.24154	2.81167	-4.19351
H	-1.43927	0.72343	-2.86129
H	1.43927	-0.72343	-2.86129
H	1.24154	-2.81167	-4.19351
H	-0.47653	-4.51760	-3.59404
H	-1.99504	-4.11171	-1.65623
H	-1.76808	-2.03802	-0.31095
H	-1.43927	-0.72343	2.86129
H	-1.24154	-2.81167	4.19351
H	0.47653	-4.51760	3.59404
H	1.99504	-4.11171	1.65623
H	1.76808	-2.03802	0.31095
H	1.43927	0.72343	2.86129
H	1.24154	2.81167	4.19351
H	-0.47653	4.51760	3.59404
H	-1.99504	4.11171	1.65623
H	-1.76808	2.03802	0.31095

SCF energy = -1003.261793521
FREEH energy = 1014.65
FREEH entropy = 0.63855

$[Me_3Si(Ph_2C{=}CPh_2)]^+$

C	0.18720	0.38962	0.82472
C	-0.06825	0.01987	-0.56415
C	-0.94103	0.73584	1.70447
C	1.51846	0.49402	1.40947
C	-1.50846	0.08740	-1.07758
C	0.92522	0.56135	-1.58110
C	-1.80864	1.77606	1.30809
C	-2.83220	2.19358	2.15205
C	-3.04791	1.54123	3.37213
C	-2.20391	0.49857	3.76840
C	-1.13919	0.11645	2.95452
C	1.67836	1.12066	2.67793
C	2.93181	1.25318	3.26467
C	4.06879	0.77521	2.60718
C	3.94359	0.18345	1.34154
C	2.69805	0.05945	0.74712
C	-1.79147	0.75134	-2.28186
C	-3.09877	0.82098	-2.77370
C	-4.14821	0.21645	-2.08236
C	-3.87911	-0.45870	-0.88668
C	-2.57941	-0.52051	-0.39363
C	1.30547	-0.14722	-2.72915
C	2.15882	0.42718	-3.67444
C	2.63195	1.72888	-3.49444
C	2.22940	2.45947	-2.37185
C	1.38203	1.88167	-1.42771
Si	0.17714	-2.12753	-0.39766
C	-0.91265	-2.83738	-1.76823
C	-0.35010	-2.75768	1.29871

C	1.96820	-2.68448	-0.63419
H	-1.66195	2.26478	0.34572
H	-3.47644	3.01961	1.85060
H	-3.87227	1.84933	4.01611
H	-2.36844	-0.00897	4.71916
H	-0.47141	-0.68322	3.27143
H	0.81191	1.53819	3.18439
H	3.02415	1.74558	4.23274
H	5.05269	0.88207	3.06558
H	4.82976	-0.16818	0.81283
H	2.63456	-0.36278	-0.24830
H	-0.99046	1.23231	-2.83924
H	-3.29027	1.35260	-3.70646
H	-5.16625	0.26677	-2.46936
H	-4.68688	-0.93853	-0.33301
H	-2.40590	-1.03775	0.54758
H	0.92478	-1.15170	-2.90770
H	2.44666	-0.14368	-4.55786
H	3.29654	2.17834	-4.23266
H	2.56861	3.48705	-2.23602
H	1.06716	2.46293	-0.55983
H	-0.92364	-2.23157	-2.68165
H	-0.52152	-3.83641	-2.01592
H	-1.94985	-2.93872	-1.42862
H	0.35997	-2.44947	2.07736
H	-0.31712	-3.85763	1.24293
H	-1.36277	-2.47429	1.60547
H	1.89274	-3.76712	-0.83114
H	2.48576	-2.22928	-1.48616
H	2.57471	-2.55867	0.26979

SCF energy GEOOPT = -1412.395420558
FREEH energy = 1329.36
FREEH entropy = 0.77469

HC≡CH

C	0.00000	0.00000	-0.60416
C	0.00000	0.00000	0.60416
H	0.00000	0.00000	-1.67462
H	0.00000	0.00000	1.67462

SCF energy = -77.360512839
FREEH energy = 75.96
FREEH entropy = 0.20179

$[Me_3Si(HC{\equiv}CH)]^+$

C	-0.6614554	-2.1273591	-0.0767096
C	0.5536276	-2.0207460	-0.0612274
Si	0.0388224	0.2276544	0.0064874
C	-1.7907118	0.6237940	0.0421886
C	0.9418857	0.5453642	1.6083891
C	0.9063341	0.6498621	-1.5903147
H	-1.7311543	-2.2487667	-0.0913066
H	1.6257676	-2.1332545	-0.0552716
H	-1.8590522	1.7240337	0.0860107
H	-2.3194351	0.3015077	-0.8640875
H	-2.2987464	0.2312800	0.9325038
H	0.9018088	1.6309472	1.7989981
H	1.9992369	0.2538447	1.5673125
H	0.4595227	0.0402858	2.4557667
H	1.9608642	0.3454091	-1.5963206
H	0.3980557	0.2097154	-2.4585372
H	0.8746295	1.7464279	-1.7038817

SCF energy = -486.4700515204
FREEH energy = 385.76
FREEH entropy = 0.41154

MeC≡CMe

C	0.00000	0.00000	-2.06323
C	0.00000	0.00000	-0.60681
C	0.00000	0.00000	0.60681
C	0.00000	0.00000	2.06323
H	1.02576	0.00000	-2.46315
H	-0.51288	-0.88833	-2.46315
H	-0.51288	0.88833	-2.46315
H	1.02576	0.00000	2.46315
H	-0.51288	0.88833	2.46315
H	-0.51288	-0.88833	2.46315

SCF energy = -156.0424242801
FREEH energy = 229.59
FREEH entropy = 0.29468

$[Me_3Si(MeC{\equiv}CMe)]^+$

C	0.20693	-2.75829	-0.38542
C	0.80804	-1.46432	-0.15538
C	1.37617	-0.38042	0.01639
C	2.48233	0.57532	0.19409
Si	-0.60652	0.54898	0.04253
C	-2.08061	-0.59308	0.24213
C	-0.32757	1.59525	1.57355
C	-0.55954	1.43409	-1.60506
H	-0.32206	-2.80419	-1.34735
H	-0.46733	-3.05652	0.42829
H	1.03215	-3.49052	-0.42273
H	3.41814	0.07605	-0.09205
H	2.35769	1.46639	-0.43433
H	2.55592	0.89254	1.24258
H	-2.25057	-1.25149	-0.61818
H	-2.03392	-1.19031	1.16190
H	-2.96120	0.06457	0.32652
H	-1.26099	2.15045	1.76020
H	0.47865	2.32838	1.45080
H	-0.12534	0.97808	2.45920
H	0.32341	2.07543	-1.72082
H	-0.59357	0.72465	-2.44280
H	-1.45019	2.07895	-1.67407

SCF energy = -565.1751674480
FREEH energy = 540.62
FREEH entropy = 0.47542

PhC≡CPh

C	-2.74853	-1.21612	0.00000
C	-4.14170	-1.21021	0.00000

C	-4.84420	0.00000	0.00000
C	-4.14170	1.21021	0.00000
C	-2.74853	1.21612	0.00000
C	-2.02880	0.00000	0.00000
C	4.14170	-1.21021	0.00000
C	2.74853	-1.21612	0.00000
C	2.02880	0.00000	0.00000
C	2.74853	1.21612	0.00000
C	4.14170	1.21021	0.00000
C	4.84420	0.00000	0.00000
C	0.61068	0.00000	0.00000
C	-0.61068	0.00000	0.00000
H	-2.19734	-2.15669	0.00000
H	-4.68462	-2.15661	0.00000
H	-5.93498	0.00000	0.00000
H	-4.68462	2.15661	0.00000
H	-2.19734	2.15669	0.00000
H	4.68462	-2.15661	0.00000
H	2.19734	-2.15669	0.00000
H	2.19734	2.15669	0.00000
H	4.68462	2.15661	0.00000
H	5.93498	0.00000	0.00000

SCF energy = -539.6929888251
FREEH energy = 516.60
FREEH entropy = 0.44867

$[Me_3Si(PhC{\equiv}CPh)]^+$

C	-1.27209	-2.46155	1.70865
C	-2.06799	-3.58279	1.89485
C	-2.42274	-4.38033	0.79669
C	-1.98133	-4.06461	-0.49691
C	-1.18447	-2.94773	-0.70392
C	-0.82336	-2.13076	0.40140
C	3.70273	1.94083	0.98353
C	2.46173	1.31070	1.07286
C	1.89410	0.73606	-0.07686
C	2.55540	0.81729	-1.31397
C	3.79579	1.45055	-1.38829
C	4.36784	2.01620	-0.24435
C	0.59731	0.06563	0.01059
C	-0.02195	-1.00930	0.20462
Si	-0.99502	1.36273	-0.31391
C	-0.62179	1.99183	-2.04212
C	-2.65938	0.49902	-0.20659
C	-0.74682	2.61689	1.05987
H	-0.98135	-1.83161	2.54913
H	-2.41515	-3.84480	2.89416
H	-3.04846	-5.26020	0.95126
H	-2.26180	-4.69755	-1.33864
H	-0.82709	-2.68794	-1.70017
H	4.15189	2.37340	1.87780
H	1.94128	1.24568	2.02813
H	2.10720	0.37160	-2.20169
H	4.31756	1.50069	-2.34425
H	5.33541	2.51428	-0.30938
H	-1.39849	2.72349	-2.31526
H	0.35418	2.49037	-2.09045
H	-0.64793	1.18310	-2.78474
H	-3.43659	1.25717	-0.39021
H	-2.84713	0.06518	0.78415
H	-2.77760	-0.28688	-0.96382
H	-0.84186	2.15762	2.05298
H	0.22958	3.11142	0.98632
H	-1.53162	3.38432	0.96855

SCF energy = -948.8404400839
FREEH energy = 829.22
FREEH entropy = 0.62404

COSMO(ε = 13.4)/BP86−D3(BJ)/def-TZVP

$[Me_3Si]^+$

Si	0.00000	-0.00000	-0.02264
C	0.51853	1.76777	-0.00630
C	-1.79020	-0.43482	-0.00630
C	1.27167	-1.33295	-0.00630
H	1.60804	1.88408	-0.03038
H	0.06456	2.28468	-0.86654
H	0.11215	2.23833	0.90424
H	-2.43568	0.45056	-0.03038
H	-2.01087	-1.08643	-0.86654
H	-1.99452	-1.02204	0.90424
H	1.94631	-1.19825	-0.86654
H	1.88237	-1.21629	0.90424
H	0.82764	-2.33464	-0.03038

COSMO energy = -409.1528251959

$H_2C{=}CH_2$

C	0.00000	0.00000	-0.60522
C	0.00000	0.00000	0.60522
H	0.00000	0.00000	-1.67866
H	0.00000	0.00000	1.67866

COSMO energy = -77.3660170332

$[Me_3Si(H_2C{=}CH_2)]^+$

C	-0.65731	-2.09584	-0.07552
C	0.55895	-1.99341	-0.06125
Si	0.03608	0.21527	0.00634
C	-1.79094	0.61370	0.04178
C	0.93912	0.54141	1.60510
C	0.90393	0.64643	-1.58661
H	-1.72830	-2.21402	-0.08882
H	1.63316	-2.09531	-0.05652
H	-1.85210	1.71336	0.08452
H	-2.31077	0.27914	-0.86461
H	-2.28967	0.21051	0.93199
H	0.91753	1.63027	1.77246
H	1.98702	0.21899	1.56226
H	0.43748	0.05178	2.44993
H	1.95046	0.31662	-1.59047
H	0.37997	0.21702	-2.45051
H	0.88539	1.74409	-1.68006

COSMO energy = -486.5446438885

$Me_2C=CMe_2$

C	0.00000	0.00000	-0.67638
C	0.00000	0.00000	0.67638
C	-0.00009	1.25135	-1.52357
C	0.00009	-1.25135	-1.52357
C	-0.00009	-1.25135	1.52357
C	0.00009	1.25135	1.52357
H	-0.00114	2.18240	-0.94729
H	0.88230	1.26542	-2.18575
H	-0.88149	1.26422	-2.18705
H	0.00114	-2.18240	-0.94729
H	-0.88230	-1.26542	-2.18575
H	0.88149	-1.26422	-2.18705
H	-0.00114	-2.18240	0.94729
H	0.88230	-1.26542	2.18575
H	-0.88149	-1.26422	2.18705
H	0.88149	1.26422	2.18705
H	0.00114	2.18240	0.94729
H	-0.88230	1.26542	2.18575

COSMO energy = -235.9589522222

$[Me_3Si(Me_2C=CMe_2)]^+$

Si	-0.02101	0.92725	0.81936
C	-1.71681	1.71481	0.67899
C	1.36898	2.07078	0.30586
C	0.25076	0.14015	2.49921
C	-0.41907	-0.46320	-1.13329
C	-1.88408	-0.81650	-1.17799
C	0.02094	0.42947	-2.26361
C	0.46873	-1.16822	-0.32297
C	1.96419	-1.10998	-0.48563
C	-0.00126	-2.30899	0.54300
H	-2.52203	1.02322	0.95396
H	-1.91133	2.13015	-0.31748
H	-1.71918	2.54769	1.40102
H	1.22177	2.49586	-0.69398
H	1.35643	2.90192	1.02990
H	2.35422	1.59310	0.36213
H	1.21765	-0.37183	2.57689
H	-0.55536	-0.55165	2.77110
H	0.24648	0.97162	3.22277
H	-2.00396	-1.63557	-1.90663
H	-2.29092	-1.16931	-0.22496
H	-2.48502	0.02856	-1.53300
H	-0.16601	-0.11927	-3.20134
H	1.07837	0.70439	-2.24277
H	-0.59063	1.34141	-2.31058
H	2.46894	-1.08244	0.49028
H	2.27417	-2.05085	-0.96956
H	2.32421	-0.28293	-1.10247
H	0.69344	-2.49057	1.37105
H	-1.01174	-2.18280	0.94478
H	-0.01086	-3.21629	-0.08403

COSMO energy = -645.1583094192

$Ph_2C=CPh_2$

C	0.00000	0.00000	-0.68526
C	0.00000	0.00000	0.68526
C	0.13114	1.25320	-1.46976
C	-0.13114	-1.25320	-1.46976
C	0.13114	-1.25320	1.46976
C	-0.13114	1.25320	1.46976
C	1.11135	2.20946	-1.14529
C	1.21034	3.40164	-1.86208
C	0.33162	3.66025	-2.92149
C	-0.62925	2.70441	-3.27250
C	-0.71994	1.50590	-2.56108
C	0.71994	-1.50590	-2.56108
C	0.62925	-2.70441	-3.27250
C	-0.33162	-3.66025	-2.92149
C	-1.21034	-3.40164	-1.86208
C	-1.11135	-2.20946	-1.14529
C	-0.71994	-1.50590	2.56108
C	-0.62925	-2.70441	3.27250
C	0.33162	-3.66025	2.92149
C	1.21034	-3.40164	1.86208
C	1.11135	-2.20946	1.14529
C	0.71994	1.50590	2.56108
C	0.62925	2.70441	3.27250
C	-0.33162	3.66025	2.92149
C	-1.21034	3.40164	1.86208
C	-1.11135	2.20946	1.14529
H	1.79240	2.01169	-0.31715
H	1.97701	4.13168	-1.59661
H	0.40374	4.59564	-3.47897
H	-1.31107	2.89442	-4.10344
H	-1.47156	0.76346	-2.83494
H	1.47156	-0.76346	-2.83494
H	1.31107	-2.89442	-4.10344
H	-0.40374	-4.59564	-3.47897
H	-1.97701	-4.13168	-1.59661
H	-1.79240	-2.01169	-0.31715
H	-1.47156	-0.76346	2.83494
H	-1.31107	-2.89442	4.10344
H	0.40374	-4.59564	3.47897
H	1.97701	-4.13168	1.59661
H	1.79240	-2.01169	0.31715
H	1.47156	0.76346	2.83494
H	1.31107	2.89442	4.10344
H	-0.40374	4.59564	3.47897
H	-1.97701	4.13168	1.59661
H	-1.79240	2.01169	0.31715

COSMO energy = -1003.2725446186

$[Me_3Si(Ph_2C=CPh_2)]^+$

C	0.18850	0.39009	0.82073
C	-0.06753	0.01732	-0.56624
C	-0.94075	0.73899	1.69833
C	1.51849	0.49179	1.40503
C	-1.50873	0.08670	-1.07535
C	0.92178	0.56149	-1.58559

C	-1.79680	1.78847	1.30188
C	-2.82514	2.20650	2.14046
C	-3.05473	1.54599	3.35443
C	-2.21913	0.49601	3.75049
C	-1.15000	0.11235	2.94228
C	1.67699	1.10635	2.67941
C	2.93043	1.23172	3.26813
C	4.06768	0.75912	2.60592
C	3.94341	0.17849	1.33440
C	2.69765	0.06122	0.73903
C	-1.79725	0.75660	-2.27491
C	-3.10717	0.83021	-2.76090
C	-4.15466	0.22338	-2.06642
C	-3.87918	-0.45942	-0.87576
C	-2.57644	-0.52472	-0.38998
C	1.30842	-0.14905	-2.72999
C	2.16057	0.42812	-3.67546
C	2.62465	1.73445	-3.49895
C	2.21450	2.46661	-2.37897
C	1.36836	1.88589	-1.43473
Si	0.18679	-2.13321	-0.38932
C	-0.90235	-2.84325	-1.75899
C	-0.34284	-2.75165	1.30705
C	1.97794	-2.67834	-0.63020
H	-1.63601	2.28780	0.34721
H	-3.46118	3.03937	1.83963
H	-3.88299	1.85411	3.99376
H	-2.39268	-0.01755	4.69648
H	-0.49043	-0.69318	3.26070
H	0.81199	1.51908	3.19185
H	3.02206	1.71319	4.24175
H	5.05137	0.85961	3.06623
H	4.82923	-0.17159	0.80428
H	2.63432	-0.35741	-0.25782
H	-0.99920	1.24012	-2.83446
H	-3.30193	1.36710	-3.69047
H	-5.17536	0.27746	-2.44737
H	-4.68295	-0.94411	-0.32016
H	-2.39976	-1.05221	0.54472
H	0.94011	-1.15836	-2.90572
H	2.45631	-0.14657	-4.55403
H	3.29003	2.18531	-4.23630
H	2.54791	3.49643	-2.24342
H	1.04817	2.46858	-0.56983
H	-0.88018	-2.25952	-2.68660
H	-0.52142	-3.85430	-1.97145
H	-1.94478	-2.91726	-1.42856
H	0.35812	-2.42842	2.08769
H	-0.29182	-3.85097	1.25134
H	-1.36267	-2.48085	1.60146
H	1.89602	-3.76021	-0.82909
H	2.49199	-2.22080	-1.48297
H	2.58225	-2.55306	0.27532

COSMO energy = -1412.4478093524

HC≡CH

C	0.00000	0.00000	-0.60522
C	0.00000	0.00000	0.60522
H	0.00000	0.00000	-1.67866
H	0.00000	0.00000	1.67866

COSMO energy = -77.3660170332

$[Me_3Si(HC{\equiv}CH)]^+$

C	-0.65731	-2.09584	-0.07552
C	0.55895	-1.99341	-0.06125
Si	0.03608	0.21527	0.00634
C	-1.79094	0.61370	0.04178
C	0.93912	0.54141	1.60510
C	0.90393	0.64643	-1.58661
H	-1.72830	-2.21402	-0.08882
H	1.63316	-2.09531	-0.05652
H	-1.85210	1.71336	0.08452
H	-2.31077	0.27914	-0.86461
H	-2.28967	0.21051	0.93199
H	0.91753	1.63027	1.77246
H	1.98702	0.21899	1.56226
H	0.43748	0.05178	2.44993
H	1.95046	0.31662	-1.59047
H	0.37997	0.21702	-2.45051
H	0.88539	1.74409	-1.68006

COSMO energy = -486.5446438885

MeC≡CMe

C	-0.00000	0.00000	-2.06692
C	-0.00000	0.00000	-0.60798
C	-0.00000	0.00000	0.60798
C	-0.00000	0.00000	2.06692
H	1.02596	0.00000	-2.46547
H	-0.51298	-0.88851	-2.46547
H	-0.51298	0.88851	-2.46547
H	1.02596	0.00000	2.46547
H	-0.51298	0.88851	2.46547
H	-0.51298	-0.88851	2.46547

COSMO energy = -156.0473134584

$[Me_3Si(MeC{\equiv}CMe)]^+$

C	0.19516	-2.75444	-0.35722
C	0.80498	-1.46468	-0.14941
C	1.36511	-0.37417	0.01018
C	2.46772	0.58733	0.17347
Si	-0.59666	0.54204	0.04306
C	-2.07314	-0.59760	0.21959
C	-0.32942	1.58020	1.58045
C	-0.54281	1.44127	-1.59661
H	-0.36581	-2.79736	-1.30044
H	-0.44871	-3.04783	0.48209
H	1.02077	-3.48382	-0.42268
H	3.40148	0.09007	-0.12088
H	2.32931	1.47578	-0.45543
H	2.54664	0.90696	1.22058
H	-2.22918	-1.24233	-0.65351
H	-2.02246	-1.20840	1.12978

H	-2.94799	0.06627	0.30779
H	-1.26529	2.13298	1.75812
H	0.48316	2.30682	1.46132
H	-0.13144	0.94876	2.45671
H	0.34878	2.07265	-1.69987
H	-0.57933	0.72974	-2.43243
H	-1.43088	2.08974	-1.65465

COSMO energy = -565.2413754350

PhC≡CPh

C	-2.74969	-1.21828	0.00000
C	-4.14416	-1.21178	0.00000
C	-4.84637	0.00000	0.00000
C	-4.14416	1.21178	0.00000
C	-2.74969	1.21828	0.00000
C	-2.03146	0.00000	0.00000
C	4.14416	-1.21178	0.00000
C	2.74969	-1.21828	0.00000
C	2.03146	0.00000	0.00000
C	2.74969	1.21828	0.00000
C	4.14416	1.21178	0.00000
C	4.84637	0.00000	0.00000
C	0.61140	0.00000	0.00000
C	-0.61140	0.00000	0.00000
H	-2.20179	-2.16103	0.00000
H	-4.68707	-2.15824	0.00000
H	-5.93731	0.00000	0.00000
H	-4.68707	2.15824	0.00000
H	-2.20179	2.16103	0.00000
H	4.68707	-2.15824	0.00000
H	2.20179	-2.16103	0.00000
H	2.20179	2.16103	0.00000
H	4.68707	2.15824	0.00000
H	5.93731	0.00000	0.00000

COSMO energy = -539.7014627852

$[Me_3Si(PhC{\equiv}CPh)]^+$

C	-1.26497	-2.45231	1.70948
C	-2.07787	-3.56214	1.89170
C	-2.44021	-4.35386	0.79109
C	-1.99053	-4.04469	-0.50185
C	-1.17660	-2.93961	-0.70683
C	-0.80879	-2.13069	0.40237
C	3.70525	1.94675	0.98146
C	2.46525	1.31234	1.07197
C	1.89877	0.73558	-0.07688
C	2.55894	0.81647	-1.31426
C	3.79835	1.45390	-1.39055
C	4.37071	2.02256	-0.24720
C	0.59872	0.07014	0.01000
C	-0.00685	-1.01208	0.20615
Si	-0.99686	1.35408	-0.31168
C	-0.62357	1.97967	-2.04006
C	-2.64959	0.47361	-0.20312
C	-0.75135	2.60240	1.06654
H	-0.97258	-1.82344	2.54994
H	-2.43507	-3.81710	2.88920
H	-3.08129	-5.22303	0.94287
H	-2.28056	-4.67084	-1.34531
H	-0.81690	-2.68115	-1.70239
H	4.15091	2.38462	1.87531
H	1.94351	1.25043	2.02671
H	2.10931	0.37222	-2.20194
H	4.31673	1.50707	-2.34856
H	5.33657	2.52474	-0.31365
H	-1.41713	2.69205	-2.31469
H	0.34270	2.49748	-2.08286
H	-0.62902	1.16119	-2.77248
H	-3.42717	1.23109	-0.38711
H	-2.82859	0.04008	0.78941
H	-2.75648	-0.31153	-0.96288
H	-0.82707	2.12868	2.05460
H	0.21631	3.11249	0.98270
H	-1.55297	3.35280	0.98280

COSMO energy = -948.8969889648

MP2/def2-TZVPP

$[Me_3Si]^+$

Si	0.00001	-0.00000	0.00092
C	0.51571	1.74984	0.00033
C	-1.77326	-0.42828	0.00034
C	1.25755	-1.32156	0.00031
H	1.59483	1.87513	0.00310
H	0.09176	2.24696	-0.87633
H	0.08649	2.24998	0.87261
H	-2.42129	0.44364	0.00302
H	-1.99181	-1.04408	-0.87627
H	-1.99181	-1.04997	0.87267
H	1.90010	-1.20293	-0.87631
H	1.90525	-1.19998	0.87263
H	0.82646	-2.31873	0.00299

MP2 energy = -408.2380332879

$H_2C{=}CH_2$

C	-0.66615	0.00000	0.00000
C	0.66615	0.00000	0.00000
H	-1.22816	-0.92262	0.00000
H	-1.22816	0.92262	0.00000
H	1.22816	0.92262	0.00000
H	1.22816	-0.92262	0.00000

MP2 energy = -78.4006926122

$[Me_3Si(H_2C{=}CH_2)]^+$

C	-0.97938	-1.56492	-0.67708
C	-0.97938	-1.56492	0.67708
Si	0.22569	0.35699	0.00000
C	-0.32804	1.19431	-1.55357
C	-0.32804	1.19431	1.55357
C	1.94500	-0.31313	0.00000
H	-0.17183	-2.01996	-1.23672

H	-1.82570	-1.18699	-1.23339
H	-0.17183	-2.01996	1.23672
H	-1.82570	-1.18699	1.23339
H	0.20807	2.14599	-1.60198
H	-0.08418	0.63088	-2.45126
H	-1.39284	1.41889	-1.54299
H	0.20807	2.14599	1.60198
H	-0.08418	0.63088	2.45126
H	-1.39284	1.41889	1.54299
H	2.16299	-0.90368	0.88774
H	2.16299	-0.90368	-0.88774
H	2.62910	0.53890	0.00000

MP2 energy = -486.6842114601

$Me_2C=CMe_2$

C	0.00000	0.00000	-0.67422
C	0.00000	0.00000	0.67422
C	1.24354	0.00000	-1.52022
C	-1.24354	0.00000	-1.52022
C	-1.24354	0.00000	1.52022
C	1.24354	0.00000	1.52022
H	2.16703	0.00000	-0.95244
H	1.24961	-0.87506	-2.17344
H	1.24961	0.87506	-2.17344
H	-2.16703	0.00000	-0.95244
H	-1.24961	0.87506	-2.17344
H	-1.24961	-0.87506	-2.17344
H	-2.16703	0.00000	0.95244
H	-1.24961	-0.87506	2.17344
H	-1.24961	0.87506	2.17344
H	1.24961	-0.87506	2.17344
H	2.16703	0.00000	0.95244
H	1.24961	0.87506	2.17344

MP2 energy = -235.3044148381

$[Me_3Si(Me_2C=CMe_2)]^+$

Si	-0.01762	1.18842	0.00000
C	-0.92567	1.69647	-1.53666
C	1.75520	1.72517	0.00000
C	-0.92567	1.69647	1.53666
C	0.02787	-1.06349	-0.69154
C	-1.22361	-1.37016	-1.46947
C	1.27599	-1.12343	-1.52749
C	0.02787	-1.06349	0.69154
C	1.27599	-1.12343	1.52749
C	-1.22361	-1.37016	1.46947
H	-1.96483	1.37700	-1.54264
H	-0.44200	1.36889	-2.45392
H	-0.91694	2.78996	-1.53346
H	2.30164	1.41775	-0.88780
H	1.72723	2.81847	0.00000
H	2.30164	1.41775	0.88780
H	-0.44200	1.36889	2.45392
H	-1.96483	1.37700	1.54264
H	-0.91694	2.78996	1.53346
H	-1.30084	-2.45808	-1.53845
H	-2.13698	-1.00763	-1.00998
H	-1.15789	-0.98177	-2.48207
H	1.32105	-2.13057	-1.94834
H	2.19547	-0.94304	-0.98468
H	1.21433	-0.43792	-2.37212
H	1.21433	-0.43792	2.37212
H	1.32105	-2.13057	1.94834
H	2.19547	-0.94304	0.98468
H	-1.15789	-0.98177	2.48207
H	-2.13698	-1.00763	1.00998
H	-1.30084	-2.45808	1.53845

MP2 energy = -643.6127868675

$Ph_2C=CPh_2$

C	0.00000	0.00000	-0.68434
C	0.00000	0.00000	0.68434
C	0.12588	1.24428	-1.46759
C	-0.12588	-1.24428	-1.46759
C	0.12588	-1.24428	1.46759
C	-0.12588	1.24428	1.46759
C	1.09295	2.20702	-1.14530
C	1.20284	3.37717	-1.88958
C	0.34744	3.60602	-2.96777
C	-0.60636	2.64703	-3.30792
C	-0.70743	1.46943	-2.57222
C	0.70743	-1.46943	-2.57222
C	0.60636	-2.64703	-3.30792
C	-0.34744	-3.60602	-2.96777
C	-1.20284	-3.37717	-1.88958
C	-1.09295	-2.20702	-1.14530
C	-0.70743	-1.46943	2.57222
C	-0.60636	-2.64703	3.30792
C	0.34744	-3.60602	2.96777
C	1.20284	-3.37717	1.88958
C	1.09295	-2.20702	1.14530
C	0.70743	1.46943	2.57222
C	0.60636	2.64703	3.30792
C	-0.34744	3.60602	2.96777
C	-1.20284	3.37717	1.88958
C	-1.09295	2.20702	1.14530
H	1.75536	2.02806	-0.30788
H	1.95726	4.10829	-1.63138
H	0.43051	4.51782	-3.54340
H	-1.26720	2.81422	-4.14799
H	-1.44199	0.72007	-2.84040
H	1.44199	-0.72007	-2.84040
H	1.26720	-2.81422	-4.14799
H	-0.43051	-4.51782	-3.54340
H	-1.95726	-4.10829	-1.63138
H	-1.75536	-2.02806	-0.30788
H	-1.44199	-0.72007	2.84040
H	-1.26720	-2.81422	4.14799
H	0.43051	-4.51782	3.54340
H	1.95726	-4.10829	1.63138
H	1.75536	-2.02806	0.30788
H	1.44199	0.72007	2.84040
H	1.26720	2.81422	4.14799

H	-0.43051	4.51782	3.54340
H	-1.95726	4.10829	1.63138
H	-1.75536	2.02806	0.30788

MP2 energy = -1000.6575319576

$[Me_3Si(Ph_2C{=}CPh_2)]^+$

C	0.17988	0.35916	0.79770
C	-0.08645	0.08411	-0.57612
C	-0.94033	0.67185	1.69608
C	1.51736	0.48575	1.37394
C	-1.50718	0.11759	-1.08784
C	0.92011	0.56043	-1.58635
C	-1.78070	1.73768	1.32812
C	-2.79967	2.14691	2.17808
C	-3.02898	1.46820	3.37653
C	-2.19921	0.41059	3.74690
C	-1.13977	0.03126	2.92756
C	1.65347	1.09702	2.64293
C	2.90454	1.26935	3.22283
C	4.05254	0.83714	2.56494
C	3.93923	0.25196	1.30123
C	2.69872	0.09088	0.70611
C	-1.78345	0.77918	-2.29266
C	-3.08539	0.83979	-2.78923
C	-4.13124	0.22696	-2.10572
C	-3.86658	-0.44569	-0.91213
C	-2.57288	-0.49677	-0.40881
C	1.28082	-0.16530	-2.72599
C	2.15712	0.37969	-3.66300
C	2.66138	1.66678	-3.48714
C	2.27297	2.41484	-2.37544
C	1.40772	1.86682	-1.43460
Si	0.15950	-2.10563	-0.33840
C	-0.92175	-2.76639	-1.71151
C	-0.37300	-2.73990	1.32845
C	1.93219	-2.63517	-0.57376
H	-1.61965	2.24824	0.38723
H	-3.42396	2.98463	1.89992
H	-3.84168	1.76992	4.02245
H	-2.36464	-0.10707	4.68160
H	-0.47648	-0.76351	3.23629
H	0.78186	1.47444	3.15476
H	2.97978	1.75090	4.18767
H	5.02511	0.96969	3.01842
H	4.82608	-0.06758	0.77132
H	2.65098	-0.32546	-0.28451
H	-0.98729	1.26463	-2.83889
H	-3.27499	1.36633	-3.71440
H	-5.13849	0.26996	-2.49555
H	-4.66776	-0.92912	-0.36984
H	-2.40270	-1.00961	0.52716
H	0.87778	-1.15280	-2.90065
H	2.43428	-0.19769	-4.53420
H	3.33720	2.08921	-4.21728
H	2.63575	3.42521	-2.24565
H	1.10440	2.45326	-0.57548
H	-1.00459	-2.11120	-2.57481
H	-0.48448	-3.71564	-2.03147
H	-1.92848	-2.95460	-1.34362
H	0.34209	-2.46930	2.10358
H	-0.34934	-3.83007	1.23172
H	-1.37357	-2.45945	1.64370
H	1.84639	-3.71386	-0.74423
H	2.43680	-2.20510	-1.43460
H	2.53862	-2.49343	0.31668

MP2 energy GEOOPT= -1408.9550547501

HC≡CH

C	0.00000	0.00000	-0.60567
C	0.00000	0.00000	0.60567
H	0.00000	0.00000	-1.66747
H	0.00000	0.00000	1.66747

MP2 energy = -77.1605909390

$[Me_3Si(HC{\equiv}CH)]^+$

C	-0.51123	-2.09444	0.00000
C	0.70362	-1.97060	0.00000
Si	0.00838	0.23259	0.00000
C	-1.81917	0.51004	0.00000
C	0.86999	0.63514	1.57878
C	0.86999	0.63514	-1.57878
H	-1.56622	-2.26391	0.00000
H	1.77316	-1.98106	0.00000
H	-1.96193	1.59419	0.00000
H	-2.30459	0.11775	-0.89125
H	-2.30459	0.11775	0.89125
H	0.79731	1.71482	1.73135
H	1.92639	0.37542	1.55885
H	0.39652	0.14721	2.42893
H	1.92639	0.37542	-1.55885
H	0.39652	0.14721	-2.42893
H	0.79731	1.71482	-1.73135

MP2 energy = -485.4389988239

MeC≡CMe

C	-0.00000	0.00000	-2.06787
C	-0.00000	0.00000	-0.60807
C	-0.00000	0.00000	0.60807
C	-0.00000	0.00000	2.06787
H	1.01721	0.00000	-2.45557
H	-0.50860	-0.88093	-2.45557
H	-0.50860	0.88093	-2.45557
H	1.01721	0.00000	2.45557
H	-0.50860	0.88093	2.45557
H	-0.50860	-0.88093	2.45557

MP2 energy = -155.6223194210

$[Me_3Si(MeC{\equiv}CMe)]^+$

C	1.63970	-0.27816	-2.05691
C	1.38583	-0.28236	-0.61622

C	1.38583	-0.28236	0.61622
C	1.63970	-0.27816	2.05691
Si	-0.77153	0.14048	0.00000
C	-1.42326	-0.68050	-1.52735
C	-1.42326	-0.68050	1.52735
C	-0.78541	1.98690	0.00000
H	1.25818	0.62836	-2.52170
H	1.19951	-1.14763	-2.53698
H	2.72028	-0.30687	-2.19296
H	2.72028	-0.30687	2.19296
H	1.25818	0.62836	2.52170
H	1.19951	-1.14763	2.53698
H	-1.11662	-0.19645	-2.45024
H	-1.16602	-1.73778	-1.56579
H	-2.51229	-0.61170	-1.46444
H	-2.51229	-0.61170	1.46444
H	-1.11662	-0.19645	2.45024
H	-1.16602	-1.73778	1.56579
H	-0.29777	2.39412	0.88438
H	-0.29777	2.39412	-0.88438
H	-1.82029	2.33455	0.00000

MP2 energy = -563.9234579469

PhC≡CPh

C	-2.74524	-1.21098	0.00000
C	-4.13544	-1.20605	0.00000
C	-4.83531	0.00000	0.00000
C	-4.13544	1.20605	0.00000
C	-2.74524	1.21098	0.00000
C	-2.03415	0.00000	0.00000
C	4.13544	-1.20605	0.00000
C	2.74524	-1.21098	0.00000
C	2.03415	0.00000	0.00000
C	2.74524	1.21098	0.00000
C	4.13544	1.20605	0.00000
C	4.83531	0.00000	0.00000
C	0.61269	0.00000	0.00000
C	-0.61269	0.00000	0.00000
H	-2.19720	-2.14326	0.00000
H	-4.67343	-2.14420	0.00000
H	-5.91654	0.00000	0.00000
H	-4.67343	2.14420	0.00000
H	-2.19720	2.14326	0.00000
H	4.67343	-2.14420	0.00000
H	2.19720	-2.14326	0.00000
H	2.19720	2.14326	0.00000
H	4.67343	2.14420	0.00000
H	5.91654	0.00000	0.00000

MP2 energy = -538.2917773454

[Me_3Si(PhC≡CPh)]$^+$

C	-1.29010	-2.61675	1.30776
C	-2.16270	-3.69690	1.27738
C	-2.62433	-4.19348	0.05745
C	-2.20170	-3.62098	-1.14275
C	-1.32499	-2.54298	-1.13230
C	-0.87017	-2.04120	0.09803
C	3.85615	1.93253	1.17094
C	2.72080	1.13520	1.23691
C	2.09619	0.73288	0.04568
C	2.60442	1.13041	-1.20174
C	3.73829	1.93231	-1.24782
C	4.35987	2.33735	-0.06611
C	0.93797	-0.09169	0.09973
C	0.03080	-0.94020	0.11565
Si	-1.02252	1.09281	-0.03418
C	-1.20642	1.25512	-1.86677
C	-2.52103	0.46881	0.86051
C	-0.28340	2.56164	0.82116
H	-0.92170	-2.22641	2.24672
H	-2.48337	-4.15203	2.20368
H	-3.30550	-5.03260	0.04199
H	-2.55126	-4.01775	-2.08531
H	-0.97460	-2.10438	-2.05679
H	4.34875	2.23876	2.08286
H	2.32414	0.81108	2.18945
H	2.12634	0.79346	-2.11153
H	4.14007	2.23710	-2.20370
H	5.24226	2.96016	-0.10928
H	-1.94037	2.03622	-2.07651
H	-0.26921	1.54378	-2.33965
H	-1.56600	0.33136	-2.31694
H	-3.22572	1.30373	0.90228
H	-2.29190	0.17731	1.88423
H	-3.00116	-0.36349	0.35187
H	0.01114	2.33161	1.84381
H	0.56947	2.97586	0.28917
H	-1.06854	3.32134	0.86413

MP2 energy = -946.6052153959

Reaction path of $[Me_4C_4–SiMe_3]^+$ (BP86–D3(BJ)/def-TZVP)

Starting point S

Si	0.27368	-1.55245	0.03499
C	0.30878	-1.05266	1.82195
C	1.45455	-0.70885	-1.11880
C	-0.51967	-3.16333	-0.44880
H	-0.54985	-1.44176	2.38374
H	1.22705	-1.45892	2.28015
H	0.35279	0.04228	1.91428
H	2.48456	-0.85204	-0.75257
H	1.38468	-1.08805	-2.14555
H	1.25869	0.37686	-1.10717
H	-0.74901	-3.20588	-1.52162
H	0.20458	-3.96960	-0.23213
H	-1.42598	-3.36966	0.13567
C	0.65657	3.79292	0.10289
C	-0.17589	2.61390	-0.04754
C	-0.90373	1.64796	-0.17718
C	-1.79858	0.53550	-0.33282
H	0.02705	4.67688	0.28635
H	1.34753	3.69252	0.95249
H	1.24546	3.98413	-0.80591
H	-2.45873	0.62508	-1.20925
H	-1.24636	-0.44471	-0.57541
H	-2.39816	0.31988	0.56222

SCF energy = -565.1374887481
FREEH energy = 535.22
FREEH entropy = 0.51323

Transition state 1 (TS1)

Si	0.32759	-1.25515	0.26121
C	0.54102	-0.50898	1.94294
C	1.36231	-0.72860	-1.18283
C	-0.43937	-2.94848	0.17327
H	-0.34274	-0.66245	2.57627
H	1.38412	-1.03830	2.42430
H	0.78242	0.55837	1.88942
H	2.03643	-1.56191	-1.44499
H	0.73468	-0.52843	-2.06362
H	1.94900	0.16878	-0.95862
H	-0.74796	-3.22132	-0.84451
H	0.34227	-3.66667	0.48421
H	-1.28408	-3.06741	0.86435
C	0.69925	3.39266	-0.60895
C	-0.22761	2.28401	-0.45706
C	-1.01583	1.36849	-0.33272
C	-2.01510	0.32148	-0.20084
H	0.14642	4.33495	-0.73814
H	1.34511	3.50395	0.27447
H	1.34110	3.25971	-1.49230
H	-2.83058	0.43344	-0.93401
H	-1.63368	-0.71259	-0.43753
H	-2.45477	0.27444	0.80570

SCF energy = -565.1348922380
FREEH energy = 534.03
FREEH entropy = 0.49880

Intermediate 1 (I1)

C	0.20693	-2.75829	-0.38542
C	0.80804	-1.46432	-0.15538
C	1.37617	-0.38042	0.01639
C	2.48233	0.57532	0.19409
Si	-0.60652	0.54898	0.04253
C	-2.08061	-0.59308	0.24213
C	-0.32757	1.59525	1.57355
C	-0.55954	1.43409	-1.60506
H	-0.32206	-2.80419	-1.34735
H	-0.46733	-3.05652	0.42829
H	1.03215	-3.49052	-0.42273
H	3.41814	0.07605	-0.09205
H	2.35769	1.46639	-0.43433
H	2.55592	0.89254	1.24258
H	-2.25057	-1.25149	-0.61818
H	-2.03392	-1.19031	1.16190
H	-2.96120	0.06457	0.32652
H	-1.26099	2.15045	1.76020
H	0.47865	2.32838	1.45080
H	-0.12534	0.97808	2.45920
H	0.32341	2.07543	-1.72082
H	-0.59357	0.72465	-2.44280
H	-1.45019	2.07895	-1.67407

SCF energy = -565.1751674480
FREEH energy = 540.62
FREEH entropy = 0.47542

Intermediate 2 (I2)

C	-3.36659	0.21204	-0.82879
C	-2.05448	-0.04787	-1.42047
C	-1.11500	-0.26185	-2.23768
C	-0.36599	-0.45755	-3.48117
C	-0.64426	-0.50989	-0.67810
C	0.09483	0.50293	-0.08273
C	-0.59230	-1.96344	-0.26021
Si	1.27783	0.17422	1.43610
C	0.00252	1.92108	-0.51818
C	2.34272	1.71322	1.67114
C	0.10843	-0.05959	2.90850
C	2.38295	-1.32440	1.11596
H	-4.10175	0.36887	-1.63092
H	-3.69147	-0.64283	-0.21784
H	-3.34069	1.10327	-0.18590
H	-1.03786	-0.30218	-4.33691
H	0.47293	0.24933	-3.55111
H	0.03891	-1.47826	-3.53410
H	-1.47637	-2.50139	-0.62437
H	0.29353	-2.46700	-0.67211
H	-0.56072	-2.07095	0.83096
H	-0.70077	2.11055	-1.33646
H	-0.26720	2.55392	0.34486

H	1.00420	2.28056	-0.80921
H	2.99022	1.56134	2.54754
H	3.00171	1.89741	0.81066
H	1.75249	2.62054	1.85772
H	0.71463	-0.21116	3.81423
H	-0.55393	-0.92848	2.80143
H	-0.51280	0.83248	3.06886
H	2.86004	-1.27624	0.12697
H	3.18764	-1.31670	1.86649
H	1.85661	-2.28196	1.20482

SCF energy = -721.2601221156
FREEH energy = 778.72
FREEH entropy = 0.58851

Transition state 3-4 (TS3-4)

C	-2.39165	0.86163	-2.92294
C	-1.40708	0.88213	-1.82362
C	-0.66008	1.60341	-1.04789
C	-0.09318	2.78176	-0.39856
C	-1.05357	-0.02212	-0.66559
C	0.30566	-0.34909	-0.49670
C	-2.15359	-0.40089	0.29077
Si	1.02216	-0.91326	1.23354
C	1.27435	-0.34379	-1.63365
C	2.88904	-1.09827	1.04746
C	0.64320	0.44720	2.49498
C	0.22882	-2.57375	1.66406
H	-2.07084	0.15278	-3.70095
H	-3.36534	0.50958	-2.55020
H	-2.51418	1.85601	-3.36692
H	1.00559	2.76499	-0.39012
H	-0.42288	3.67538	-0.95125
H	-0.45211	2.86523	0.63734
H	-3.03265	0.24239	0.16017
H	-2.45937	-1.43921	0.09677
H	-1.83655	-0.33927	1.33874
H	0.83191	-0.08838	-2.60310
H	2.13549	0.31598	-1.44379
H	1.71019	-1.35710	-1.69098
H	3.31322	-1.38420	2.02152
H	3.16705	-1.88283	0.33039
H	3.37822	-0.16211	0.74382
H	1.01150	0.12096	3.47907
H	-0.42481	0.67498	2.60629
H	1.17381	1.37596	2.24293
H	0.35103	-3.30172	0.84978
H	0.73647	-2.98239	2.55072
H	-0.83983	-2.49198	1.89791

SCF energy = -721.2571991876
FREEH energy = 777.01
FREEH entropy = 0.55710

$[Me_4C_4–SiMe_3]^+$ (P-4)

C	-0.10953	-2.83322	-1.66117
C	-0.06787	-1.71640	-0.69910
C	0.86876	-1.13765	0.16816
C	2.12155	-1.66132	0.74421
C	-0.96160	-1.05948	0.15769
C	-0.00191	0.00778	0.68062
C	-2.26068	-1.47401	0.71979
Si	0.07074	1.63880	-0.40146
C	0.00135	0.27318	2.18391
C	1.63789	2.55791	0.10493
C	0.12634	1.11496	-2.21347
C	-1.49202	2.62038	-0.01121
H	0.75491	-3.49993	-1.54025
H	-1.03416	-3.41705	-1.55926
H	-0.08006	-2.44096	-2.68987
H	2.07439	-1.66885	1.84310
H	2.38095	-2.65863	0.37257
H	2.92965	-0.95537	0.48268
H	-2.60371	-2.44191	0.33834
H	-2.22240	-1.49458	1.81893
H	-3.00126	-0.69737	0.45946
H	-0.04924	-0.64923	2.78306
H	0.91055	0.81463	2.47762
H	-0.85217	0.90382	2.46673
H	1.74766	3.46779	-0.50316
H	1.61225	2.87066	1.15787
H	2.53968	1.94881	-0.05284
H	0.16345	2.01283	-2.84787
H	-0.76504	0.54463	-2.51203
H	1.01703	0.51471	-2.44873
H	-1.55119	2.90145	1.04935
H	-1.50186	3.55182	-0.59605
H	-2.40242	2.06179	-0.27258

SCF energy = -721.2994748191
FREEH energy = 781.05
FREEH entropy = 0.57707

Transition state 3-5 (TS3-5)

C	-3.38151	0.67803	-0.06657
C	-1.96588	1.02403	0.38829
C	-1.68535	2.17658	0.87799
C	-1.56850	3.40834	1.58780
C	-0.87979	-0.06234	0.27992
C	0.37913	0.22459	-0.11118
C	-1.41490	-1.41987	0.65098
Si	1.63145	-1.19784	-0.60171
C	0.91212	1.60705	-0.21424
C	3.07175	-0.37548	-1.50329
C	2.23741	-1.97518	1.01538
C	0.79986	-2.44068	-1.75576
H	-4.04578	1.54733	-0.02652
H	-3.33095	0.31232	-1.10126
H	-3.78862	-0.11236	0.57668
H	-2.56839	3.66288	1.99541
H	-0.93930	3.25876	2.48537
H	-1.17816	4.24459	0.99201
H	-1.93178	-1.38510	1.62201
H	-2.12846	-1.80366	-0.09211
H	-0.59600	-2.13855	0.74820
H	0.07986	2.34062	-0.10818

H	1.61265	1.81981	0.60942
H	1.44098	1.81084	-1.15473
H	3.80847	-1.14725	-1.77131
H	2.75370	0.10815	-2.43783
H	3.58893	0.36934	-0.88271
H	2.99144	-2.74137	0.77860
H	1.44109	-2.46082	1.59459
H	2.71528	-1.22178	1.65709
H	0.34667	-1.93197	-2.61848
H	1.56540	-3.12937	-2.14364
H	0.02719	-3.04966	-1.27023

SCF energy = -721.2443028259
FREEH energy = 773.38
FREEH entropy = 0.56053

5-membered ring (P-5)

C	-1.61533	2.65479	-1.51744
C	-0.64524	1.74943	-0.87576
C	0.69265	2.18992	-0.39624
C	0.63644	3.39459	0.57109
C	-0.86527	0.38183	-0.61558
C	0.27401	-0.15716	0.00415
C	-2.12610	-0.34354	-0.97556
Si	0.55812	-1.98327	0.55970
C	1.29489	0.90769	0.19663
C	2.32156	-2.10303	1.21138
C	-0.70764	-2.31654	1.92782
C	0.30651	-3.07933	-0.96040
H	-1.14230	3.54448	-1.94994
H	-2.22275	2.13898	-2.27399
H	-2.32717	3.00864	-0.74602
H	0.17325	4.26825	0.09592
H	0.06220	3.13970	1.47235
H	1.65343	3.67327	0.87304
H	-3.01292	0.20925	-0.63535
H	-2.21227	-0.46182	-2.06649
H	-2.16063	-1.34193	-0.52920
H	1.27167	2.50870	-1.28551
H	1.53594	1.01139	1.27031
H	2.25473	0.61832	-0.26696
H	2.51473	-3.12899	1.55727
H	3.06601	-1.87714	0.43473
H	2.49603	-1.43424	2.06607
H	-0.55456	-3.34019	2.30130
H	-1.74513	-2.23789	1.57835
H	-0.57258	-1.62762	2.77279
H	0.99747	-2.80514	-1.76933
H	0.51867	-4.12150	-0.67848
H	-0.71842	-3.03991	-1.35062

SCF energy = -721.3363315601
FREEH energy = 784.81
FREEH entropy = 0.56275