# Supporting Information

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# 1 Experimental Section

## 1.1 General methods and Instrumentation

### Materials

All mentioned reactions were carried out in properly dried borosilicate glassware, filled with argon 4.6 (≥99.996%; *Westfalen* AG) or in *LABstar* gloveboxes from *MBraun Inertgas-Systeme* GmbH with $H_2O$ and $O_2$ levels not exceeding 5 ppm. In each reaction small overpressure of argon atmosphere was used to additionally prevent the intrusion of air. For sealing glass apparatuses *Triboflon III* PTFE/PEPE grease from *Freudenberg* & Co. KG was used. All heat-sensitive plastic materials such as syringes or cannulas were stored originally packed and flushed three times with argon.

### Chemicals

The Chemicals for this project were purchased from the commercial distributers: *Merck KGaA* (*Sigma-Adrich*), *ABCR* GmbH *and TCI* Co. Ldt. The used hexafluoropinacol ($H_2pin^F$) was purchased from *Sigma-Aldrich* and *ABCR* GmbH and dried with molecular sieves (4 Å) in diluted $Et_2O$ solution. After filtration and solvent removal in fine vacuo a mixture of 80 – 88 w% $H_2pin^F$ in $Et_2O$ was obtained. $Li_2pin^F$,[1] $[Mes_3PH][HB(C_6F_5)_3]$[2] and $B(C_6F_5)_3$[3] were synthesized according to literature procedures. Safety note: The use of directly dried, $Et_2O$-free $H_2pin^F$ in one lithiation experiment resulted in an explosion in the glovebox when the product was scraped from the glass wall with a spatula. Reactants for catalytic experiments were degassed and stored over molecular sieves. The used solvents for applications were distillated over elemental sodium/benzophenone (toluene, *n*-hexane, $Et_2O$), calcium hydride (acetonitrile, chloroform, acetonitrile-$d_3$, chloroform-*d* and dichloromethande-$d_2$), additionally degassed and stored over molecular sieves.

### NMR-spectroscopy

All NMR samples were prepared in an argon (4.6) atmosphere using *J-Young* PTFE valve NMR tubes. The recorded $^1H$,$^{13}C$, $^{19}F$ and $^{29}Si$ NMR spectra were obtained from a *Bruker Avance Neo* 400 MHz spectrometer and a *Bruker AV500C* spectrometer at ambient temperatures (300 K), unless otherwise stated. The VT-NMR experiments were carried out the *Bruker Avance Neo* 400 MHz spectrometer at the given temperature. The obtained $^1H$- and $^{13}C$-NMR spectra were calibrated on the residual proton and natural abundance carbon signals of deuterated NMR solvents acetonitrile-$d_3$ and dichloromethane-$d_2$. The obtained chemical shifts δ are reported in ppm values, calibrated on tetramethylsilane. The observed signals were abbreviated as following: s = singlet, br = broad signal and combinations, d = doublet, t = triplet, q = quartet, p = quintet, h = septet, m = multiplet and qm = quartet of multiplets. The spectra were processed and analyzed on the software *MestReNova* (version 12.0.1-20560).

### FT-ATR-IR spectra

The attenuated total reflection infrared ATR-IR spectra were recorded on a *Perkin Elmer* spectrometer (*diamond ATR, Spectrum Two*) in the range of 400 – 4000 $cm^{-1}$ at room temperature under an argon atmosphere.

### Elemental analysis

The analysis was carried out by the central analytics laboratory of the *TUM Catalysis Research Center*. For the procedure 0.5 − 1.0 mg of the investigated compounds were closely packed within two layers of tin foil under an argon atmosphere and subsequently handed to the elemental analysis team. The Analysis was performed on a *EURO EA* (*HEKAtech*) instrument equipped with a CHNS combustion analyzer.

**LIFDI**

Liquid Injection Field Desorption Ionization Mass Spectrometry (LIFDI-MS) was measured directly from an argon-filled glovebox with a *Thermo Fisher Scientific Exactive Plus Orbitrap* equipped with a *Linden CMS* ion source.[4]

**Melting Point**

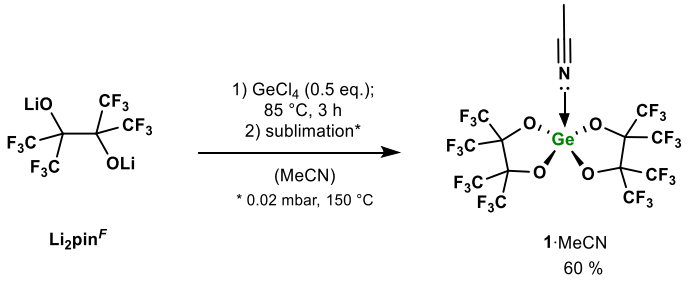
The Melting Points (m.p.) were determined in sealed glass capillaries under argon atmosphere using a *Büchi B-540* melting point apparatus.

**Single crystal X-ray diffraction analysis**

The X-ray intensity data were collected on an X-ray single crystal diffractometer equipped with a CMOS detector (Bruker Photon-100), a rotating anode (Bruker TXS) with MoKα radiation (λ = 0.71073 Å) and a Helios mirror optic by using the APEX4 software package[5] or an X-ray single crystal diffractometer equipped with a CMOS detector (Bruker Photon-100), an IMS microsource with MoKα radiation (λ = 0.71073 Å) and a Helios mirror optic by using the APEX III software package.[5] The measurement was performed on single crystals coated with perfluorinated ether. The crystal was fixed on the top of a microsampler, transferred to the diffractometer and measured under a stream of cold nitrogen. A matrix scan was used to determine the initial lattice parameters. Reflections were merged and corrected for Lorenz and polarization effects, scan speed, and background using SAINT.[6] Absorption corrections, including odd and even ordered spherical harmonics were performed using SADABS.[7] Space group assignments were based upon systematic absences, E statistics, and successful refinement of the structures. Structures were solved by direct methods with the aid of successive difference Fourier maps, and were refined against all data using the APEX4[5] and OLEX2[8] in conjunction with SHELXL-2014[9] and SHELXLE.[10] Methyl hydrogen atoms were refined as part of rigid rotating groups, with a C–H distance of 0.98 Å and Uiso(H) = 1.5·Ueq(C). Other H atoms were placed in calculated positions and refined using a riding model, with methylene and aromatic C–H distances of 0.99 and 0.95 Å, respectively, and Uiso(H) = 1.2·Ueq(C). If not mentioned otherwise, non-hydrogen atoms were refined with anisotropic displacement parameters. Full-matrix least-squares refinements were carried out by minimizing $\Delta w(Fo^2\text{-}Fc^2)^2$ with SHELXL-97[11] weighting scheme. Neutral atom scattering factors for all atoms and anomalous dispersion corrections for the non-hydrogen atoms were taken from International Tables for Crystallography.[12] Images of the crystal structures were generated by PLATON and MERCURY.[13] The CCDC numbers CCDC- (2286080-2286083, 2286830) contain the supplementary crystallographic data for the structures **1**MeCN, [K(18c6)][1-F], **2**, **3** and **1**. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/.

## 1.2 Synthesis and Characterization

### 1.2.1 Synthesis and characterization of 1·MeCN




To a solution of 3.0 g (8.67 mmol, 2.0 equiv.) $Li_2pin^F$ in 40 ml MeCN were added 0.49 ml (4.30 mmol, 1.0 equiv.) $GeCl_4$ at room temperature. The obtained solution slowly turned cloudy, and the reaction mixture was heated to 85 °C and stirred for 3 h. Afterwards, all volatiles were stripped off in vacuum and the obtained off-white solid was slowly heated to 150 °C and sublimated at a pressure of 0.02 mbar to give a colorless solid in 60 % yield.

Crystals suitable for SC-XRD analysis were obtained from a DCM solution at room temperature. For crystal structure please see Figure S 38.

**m.p.:** 142 -179 °C (sublimation and molten parts).
**$^1$H-NMR** (400 MHz, acetonitrile-$d_3$) δ (ppm) = 1.96 (s, 3H, NCC$H_3$).
**$^{13}$C NMR** (126 MHz, acetonitrile-$d_3$) δ (ppm) = 122.2 (q, $^1J_{C\text{-}F}$ = 293 Hz, $CF_3$), 81.5 (br, O$C$($CF_3$)$_2$).
**$^{19}$F NMR** (377 MHz, acetonitrile-$d_3$) δ (ppm) = -69.04 – -70.93 (m, 24F, C$F_3$).
**Elemental Analysis calcd. [%] for $C_{14}H_3F_{24}NO_4Ge$:** C (21.62), H (0.39), N (1.80), S (-); found (%): C (21,15), H (0.30), N (1.17), S (-).

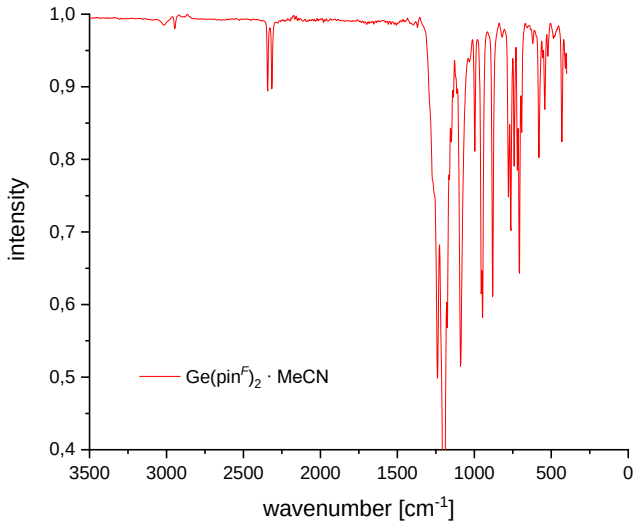
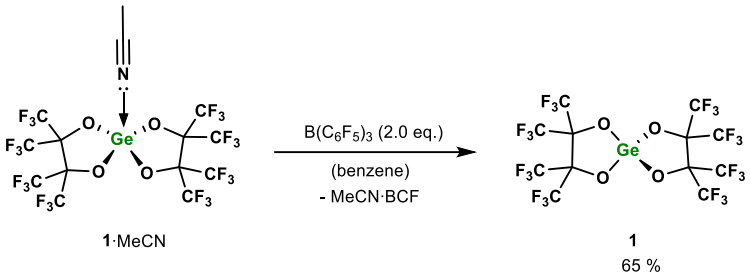



**Figure S 1:** FT-IR-spectrum of **1**·$CH_3CN$ showing two superimposed frequencies of blue-shifted C≡N and C–H vibrations originating from the coordinated acetonitrile.

### 1.2.2 Synthesis and characterization of acetonitrile-free germane 1




A mixture of 800 mg (1.03 mmol, 1.0 equiv.) **1**·MeCN and 1.05 g (2.06 mmol, 2.0 equiv.) $B(C_6F_5)_3$ were dissolved in 4 mL of benzene and heated to 80 °C. For ensuring a complete dissolution and thus mixture of the reactants, the walls of the glass vessel were additionally gently heated with a heat gun. Afterwards, the obtained clear solution was slowly cooled to 0 °C. The formed precipitation was collected by filtration dried under reduced pressure. For a complete product separation, the crude-product was sublimated at 60 °C and a pressure of 0.02 mbar. Compound **1** was then collected as a crystalline, colorless solid in 65 % yield.

In comparison to compound **1**·MeCN, donor-free **1** shows slightly enhanced solubility in non-coordinating solvents like DCM or benzene.

Crystals suitable for SC-XRD analysis were obtained from a slow sublimation at 40 °C temperature and 1 bar of argon atmosphere. For crystal structure please see S 42.

**m.p.:** 67.1 – 71.9 °C (partially sublimated).
**$^{13}$C NMR** (126 MHz, acetonitrile-$d_3$) δ (ppm) = 122.2 (q, $^1J_{C\text{-}F}$ = 293 Hz, $CF_3$), 81.5 (br, $OC(CF_3)_2$).
**$^{19}$F NMR** (377 MHz, acetonitrile-$d_3$) δ (ppm) = -68.93 – -71.19 (m, 24F, $CF_3$).
**Elemental Analysis calcd. [%] for $C_{12}F_{24}O_4Ge$:** C (19.56), H (-), N (-), S (-); found (%): C (20.02), H (0.06), N (-), S (-).

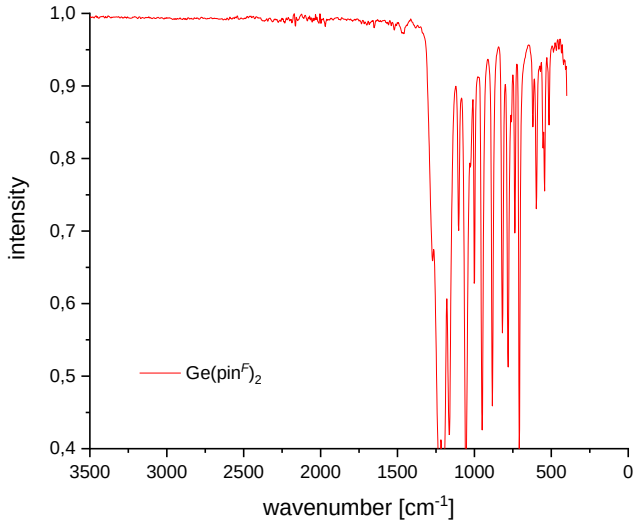
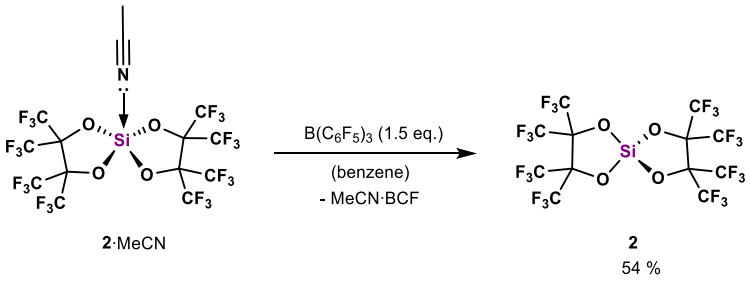



**Figure S 2:** FT-IR-spectrum of **1** showing the absence of the characteristic acetonitrile vibrations in the region of 2000 – 2500 $cm^{-1}$.

### 1.2.3 Synthesis and characterization of acetonitrile-free silane 2




A mixture of 500 mg (682 µmol, 1.0 equiv.) **2**·MeCN and 524 mg (614 µmol, 1.5 equiv.) $B(C_6F_5)_3$ were dissolved in 6 mL of benzene and heated to 80 °C. Complete dissolution was obtained by gently heating the glass walls with a heat gun. The obtained clear solution was slowly cooled to 0 °C and the formed precipitation was filtered off and washed with 1 ml benzene in the cold. After drying under reduced pressure, the solvent-free product **2** was obtained as a colorless solid in 54 % yield. Alternatively, the crude product can be purified by sublimation (60 °C, 0.04 mbar).

Crystals suitable for SC-XRD analysis were obtained from a slow sublimation at 40 °C temperature under 1 bar of argon atmosphere in a screw-cap glass vessel. For crystal structure please see Figure S 40.

**m.p.:** 66 – 68 °C.
**$^{13}$C NMR** (126 MHz, acetonitrile-$d_3$) δ (ppm) = 122.0 (qm, $^1J_{C\text{-}F}$ = 293 Hz, $CF_3$), 83.5 (br, $OC(CF_3)_2$).
**$^{19}$F NMR** (377 MHz, acetonitrile-$d_3$) δ (ppm) = -69.48 – -70.05 (m, 12F, $CF_3$), -70.05 – -70.55 (m, 12F, $CF_3$).
**$^{29}$Si NMR** (99 MHz, acetonitrile-$d_3$) δ (ppm) = -110.33 (*Si*).
**Elemental Analysis calcd. [%] for $C_{12}F_{24}O_4Si$:** C (20.82), H (-), N (-), S (-); found (%): C (21.19), H (0.09), N (-), S (-).

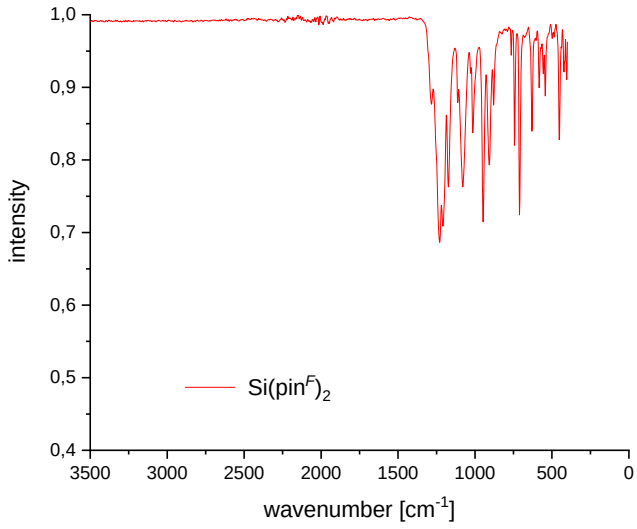
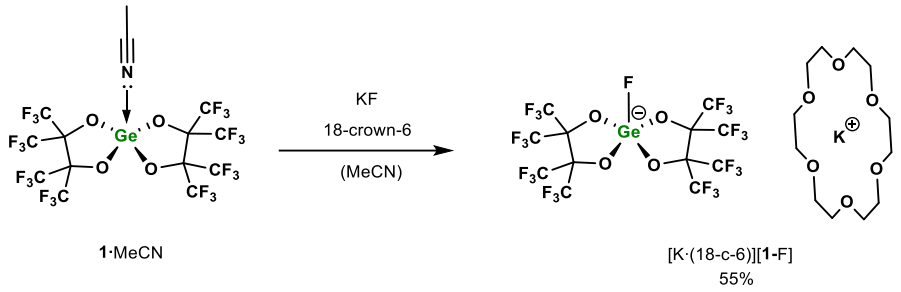



**Figure S 3:** FT-IR-spectrum of **2** showing the absence of the characteristic acetonitrile vibrations in the region of 2000 – 2500 $cm^{-1}$.

### 1.2.4 Synthesis of and characterization of [K·(18-c-6)][1-F]




**1**·MeCN

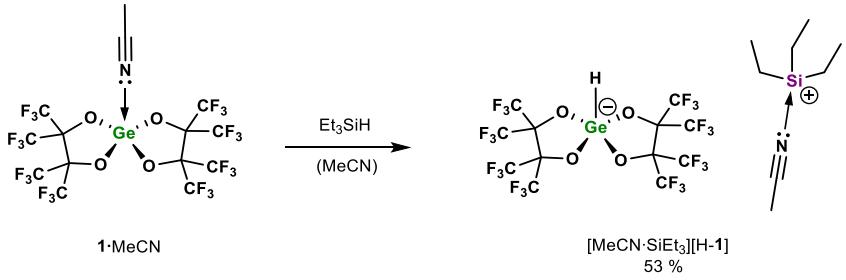
[K·(18-c-6)][**1**-F]
55%

To synthesize the pentavalent fluorogermanate species [**1**-F]$^-$, 100 mg **1**·MeCN (129 µmol, 1.0 equiv.), 7.50 mg KF (129 µmol, 1.0 equiv.) were dissolved in 1.0 ml acetonitrile. To this solution and 34.0 mg (129 µmol, 1.0 equiv.) 18-crown-6 dissolved in another 2.0 ml acetonitrile were added and the obtained solution was stirred for 230 minutes at room temperature. Afterwards, all volatile components were removed under reduced pressure. The obtained crude product was dissolved in 2.0 ml dichloromethane and precipitated by the addition of 10 ml hexane. The supernatant liquid phase was filtered off and the step was repeated once again. The obtained precipitation was then dried under reduced pressure to give a off-white solid in 55 % yield.

Crystals suitable for SC-XRD analysis were obtained from a saturated dichloromethane solution at -30 °C. For crystal structure please see Figure S 39.

**m.p.:** 204 -225 °C (decomposition).
**$^1$H NMR** (400 MHz, acetonitrile-$d_3$) δ (ppm) = 3.57 (s, 24H, O-C$H_2$-C$H_2$-O).
**$^{13}$C NMR** (126 MHz, acetonitrile-$d_3$) δ (ppm) = 122.8 (qm, $^1J_{C\text{-}F}$ = 293 Hz, $CF_3$), 81.6 (br, O$C$($CF_3$)$_2$), 70.8 (s, O$CH_2$).
**$^{19}$F NMR** (377 MHz, acetonitrile-$d_3$) δ (ppm) = -69.79 – -70.14(m, 12F, C$F_3$), -70.76 – -70.97 (m, 12F, C$F_3$), -145.04 – -145.25 (h, $J$ = 8.3 Hz, 1F, Si-$F$).
**Elemental Analysis calcd. [%] for $C_{24}H_{24}F_{25}GeKO_{10}$:** C (27.22), H (2.28), N (-), S (-); found (%): C (27.36), H (1.95), N (-), S (-).

### 1.2.5 Synthesis of and characterization of [MeCN·SiEt$_3$][H-1]




**1**·MeCN

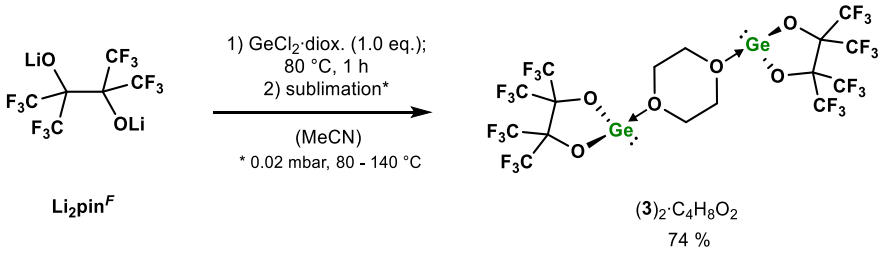
[MeCN·SiEt$_3$][H-**1**]
53 %

To a solution of 100 mg (129 µmol, 1.0 equiv.) **1**·MeCN diluted in 2.0 ml acetonitrile were added 15 mg (129 µmol, 5.0 equiv.) $Et_3SiH$ at room temperature. The obtained solution was heated to 80 °C for 30 minutes. Afterwards all volatiles were removed under reduced pressure to give the product as a colorless solid in 53 % yield.

**m.p.:** 81-86 °C.

**$^{1}$H NMR** (400 MHz, acetonitrile-$d_3$) δ (ppm) = 6.44 – 6.38 (m, 1H, Ge*H*), 1.96 (s, 3H, NCC*H*$_3$), 1.10 – 0.99 (m, 15H, C*H*$_2$C*H*$_3$).
**$^{13}$C NMR** (126 MHz, acetonitrile-$d_3$) δ (ppm) = 123.5 (q, $^{1}J_{C\text{-}F}$ = 293 Hz, *C*F$_3$), 123.1 (q, $^{1}J_{C\text{-}F}$ = 293 Hz, *C*F$_3$), 82.2 (br, O*C*(CF$_3$)$_2$), 6.13 (s, *C*H$_2$), 4.11 (s, *C*H$_3$).
**$^{19}$F-NMR** (377 MHz, acetonitrile-$d_3$) δ (ppm) = -70.18 – -70.35 (m, 12F, C*F*$_3$), -70.63 – -70.82 (m, 12F, C*F*$_3$).
**$^{29}$Si NMR** (99 MHz, acetonitrile-$d_3$) δ (ppm) = 36.38 (s, Et$_3$*Si*$^+$).
**Elemental Analysis calcd. [%] for $C_{20}H_{19}F_{24}GeNO_4Si$:** C (26.87), H (2.44), N (1.57), S (-); found (%): C (26.58), H (1.63), N (1.67), S (-).

### 1.2.6 Synthesis of and characterization of dioxane-bridged germylene 3




**Li$_2$pin$^F$** (**3**)$_2$·C$_4$H$_8$O$_2$
74 %

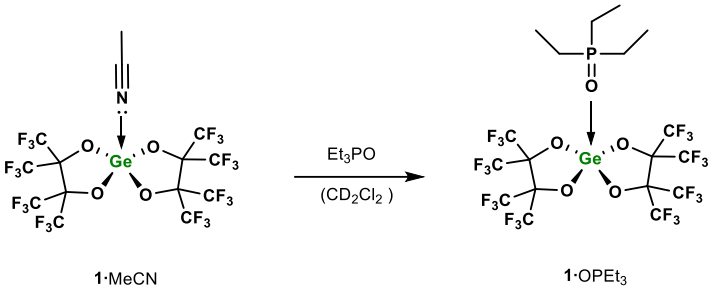
A mixture of 600 mg (1.73 mmol, 1.0 equiv.) Li$_2$pin$^F$ and 402 mg (1.73 mmol, 1.0 equiv.) GeCl$_2$·1,4-dioxane was dissolved in 5 ml acetonitrile. The solution immediately turned opaque because of LiCl precipitation and was further heated to 80 °C for 1 hour to ensure complete conversion. Afterwards all volatiles were removed under reduced pressure at 0 °C to give the crude product. The title compound was isolated by twofold sublimation at 0.02 mbar while slowly heating from 80 °C to 140 °C over a 2-hour period.

Dioxane could not be removed under reduced pressure. The product additionally contains impurities of acetonitrile, which could not be removed. Single crystals suitable for XRD analysis were obtained from saturated DCM solution at -30 °C (Figure S 41).

**m.p.:** 72 – 75 °C.
**$^{1}$H NMR** (500 MHz, dichloromethane-$d_2$) δ (ppm) = 3.89 (s, C*H*$_2$).
**$^{13}$C NMR** (126 MHz, dichloromethane-$d_2$) δ (ppm) = 122.2 (q, $^{1}J_{C\text{-}F}$ = 294 Hz), 88.4 (br, O*C*(CF$_3$)$_2$), 67.1 (s, *C*H$_2$).
**$^{19}$F-NMR** (377 MHz, dichloromethane-$d_2$) δ (ppm) = -70.6 (s, 12F, C*F*$_3$).

# 2 NMR experiments with 1·MeCN

## 2.1 Lewis acidity determination by *Gutmann-Beckett* method




**1**·MeCN **1**·OPEt$_3$

For the Lewis acidity assessment of the obtained compounds the by Gutmann-Beckett was applied. In case of **1**·MeCN, 6.00 mg (7.71 µmol, 1.0 equiv.) of the Lewis acid were dissolved in 0.4 ml dichloromethane-$d_2$ and reacted with 1.03 mg Et$_3$PO (7.71 µmol, 1.0 equiv.) in a gas-tight J-Young NMR tube. The obtained clear solution was analyzed by $^1$H, $^{19}$F and $^{31}$P NMR spectroscopy. The exact same spectra were also obtained for solvent free **1**. In this case, however, the broad signal overlapping signal at 2.03 ppm was absent.

**$^1$H NMR** (400 MHz, $CD_2Cl_2$) δ (ppm) = 2.03 (br, 3H, $NCCH_3$) 2.11 (dq, $^2J_{P\text{-}H}$ = 12.4 Hz, $^3J_{H\text{-}H}$ = 7.7 Hz, 6H, $PCH_2$), 1.26 (dt, $^2J_{P\text{-}H}$ = 12.4 Hz, $^3J_{H\text{-}H}$ = 7.7 Hz, 9H, $PCH_2CH_3$).
**$^{19}$F-NMR** (149 MHz, $CD_2Cl_2$) δ (ppm) = -69.19 – -69.99 (m, 24F, $CF_3$).
**$^{31}$P NMR** (162 MHz, CD2Cl2) δ (ppm) = 89.13 (s).

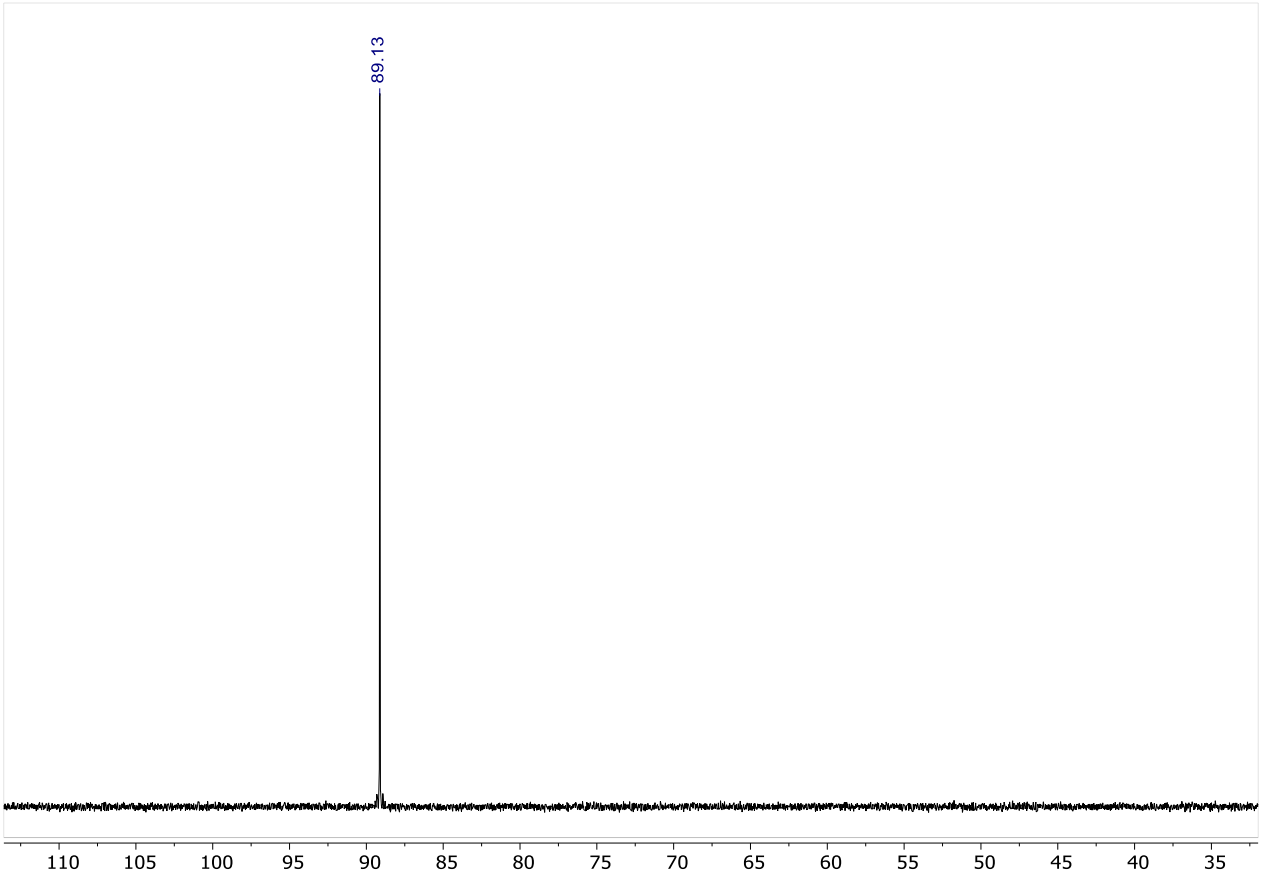



**Figure S 4:** $^{31}$P NMR spectrum of **1**·OPEt$_3$ obtained by the reaction of **1**·MeCN with Et$_3$PO in dichloromethande-$d_2$.

The same sample was additionally treated with another equivalent of $Et_3PO$ (total of 2.0 equiv.) and again analyzed by $^{31}P$ NMR spectroscopy. Figure S 5 shows a stack of free $Et_3PO$ and the obtained coordination products.

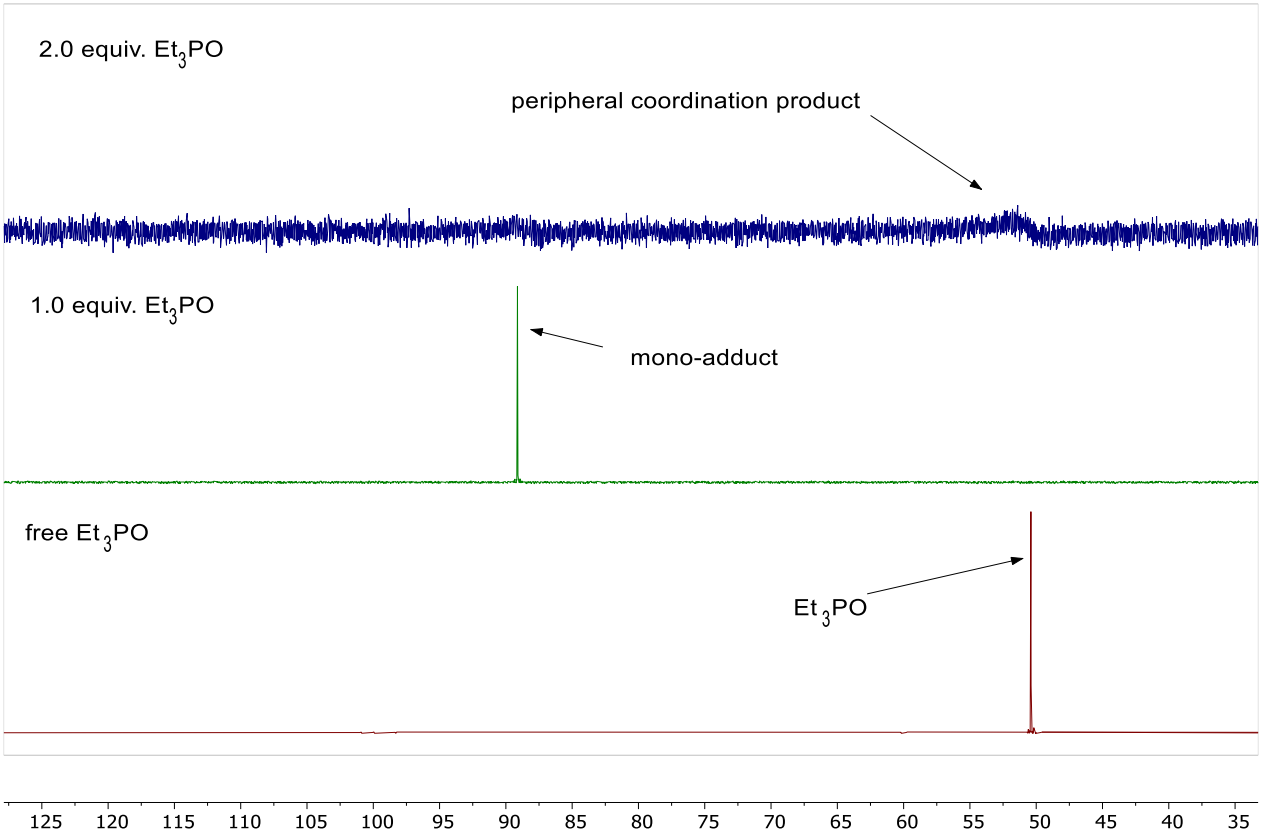
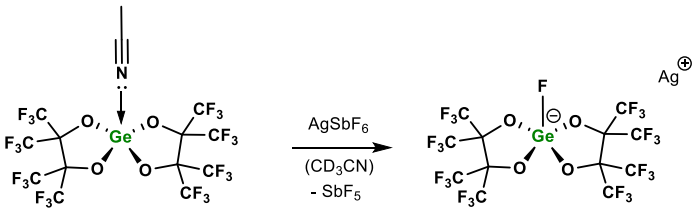



**Figure S 5:** Stacked $^{31}P$ NMR spectra of the reaction of **1**·MeCN with 1.0 and 2.0 equiv. of $Et_3PO$ in dichloromethane-$d_2$ at 300 K.

## 2.2 NMR-Scale Abstraction Experiments

### 2.2.1 Reaction of 1·MeCN with $AgSbF_6$




**1**·MeCN Ag[**1**-F]

A mixture of 16.0 mg (20.6 µmol, 1.0 equiv.) **1**·MeCN and 7.10 (20.7 µmol, 1.0 equiv.) $AgSbF_6$ was placed in a PTFE-valved J-Young NMR tube and dissolved in 0.4 ml of acetonitrile-$d_3$. The obtained solution was heated to 60 °C for one hour and afterwards analyzed by multinuclear NMR spectroscopy.

**$^{13}$C NMR** (126 MHz, acetonitrile-$d_3$) δ (ppm) = 122.7 (qm, $^1J_{C\text{-}F}$ = 295 Hz, *C*$F_3$), 81.6 (br, O*C*$(CF_3)_2$).
**$^{19}$F-NMR** (149 MHz, acetonitrile-$d_3$) δ (ppm) = -69.83 – -70.12 (m, 12F, C*F*$_3$), -70.67 – -71.02 (m, 12F, C*F*$_3$), -145.00 – -145.24(m, 1F, Ge-*F*).

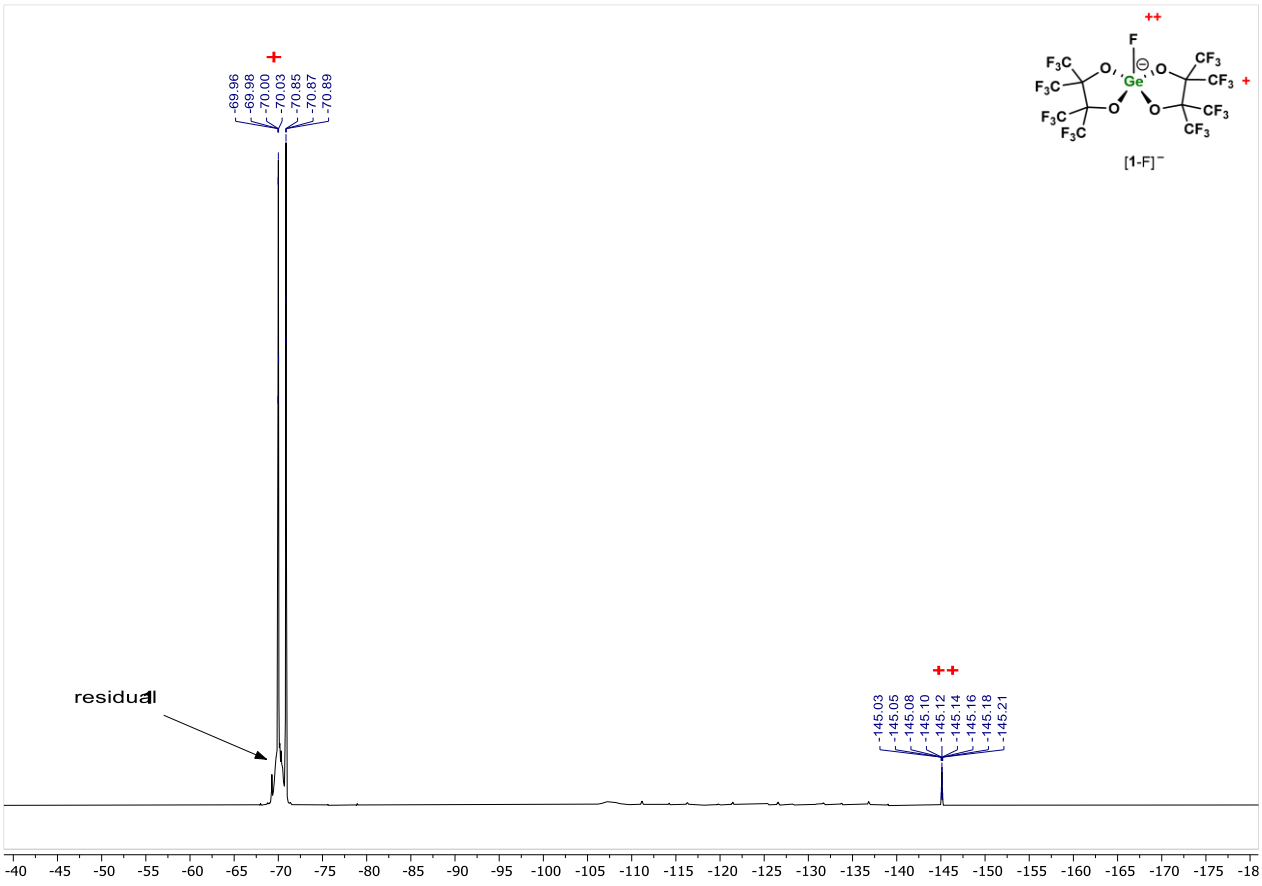
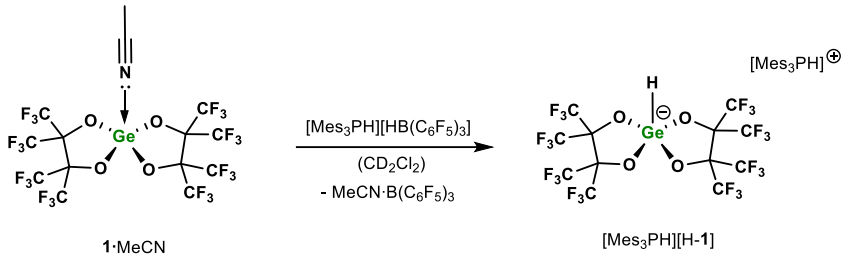



**Figure S 6:** $^{19}$F NMR of the reaction mixture after 1h at 60 °C showing the formation of the fluorogermanate anion [**1**-F]$^-$, thus confirming a successful fluoride abstraction.

### 2.2.2 Reaction of 1·MeCN with [Mes$_3$PH][HB(C$_6$F$_5$)$_3$]




To a solution of [Mes$_3$PH][HB(C$_6$F$_5$)$_3$] in 0.4 ml CD2Cl2 was added **1**·MeCN. The reaction mixture was transferred into a J-Young NMR tube and shaken until a clear solution was obtained. Reaction progress was traced by $^{1}$H, $^{11}$B and $^{19}$F NMR spectroscopy.

For further verifying the hydride abstraction from [HB(C$_6$F$_5$)$_3$]$^-$ the obtained reaction mixture was compared to separately synthesized MeCN·B(C$_6$F$_5$)$_3$.

**$^{1}$H NMR** (400 MHz, $CD_2Cl_2$) δ (ppm) = δ 8.25 (d, $^{1}J_{P\text{-}H}$ = 478.1 Hz, 1H, P*H*), 7.13 (d, $^{4}J_{P\text{-}H}$ = 36.1 Hz, 6H, *m*-Ar*H*), 6.47 – 6.41 (m, 1H, Ge*H*), 2.39 (s, 9H, *p*-Ar-C*H*$_3$), 2.30 (s, 9H, *o*-Ar-C*H*$_3$), 2.02 (s, 9H. *o*-Ar-C*H*$_3$).
**$^{11}$B NMR** (128 MHz, $CD_2Cl_2$) δ (ppm) = -10.68 (s, *B*(C$_6$F$_5$)$_3$).
**$^{19}$F-NMR** (377 MHz, $CD_2Cl_2$) δ (ppm) = -69.80 – -69.98 (m, 12F, C*F*$_3$), -70.36 – -70.53 (m, 12F, C*F*$_3$).

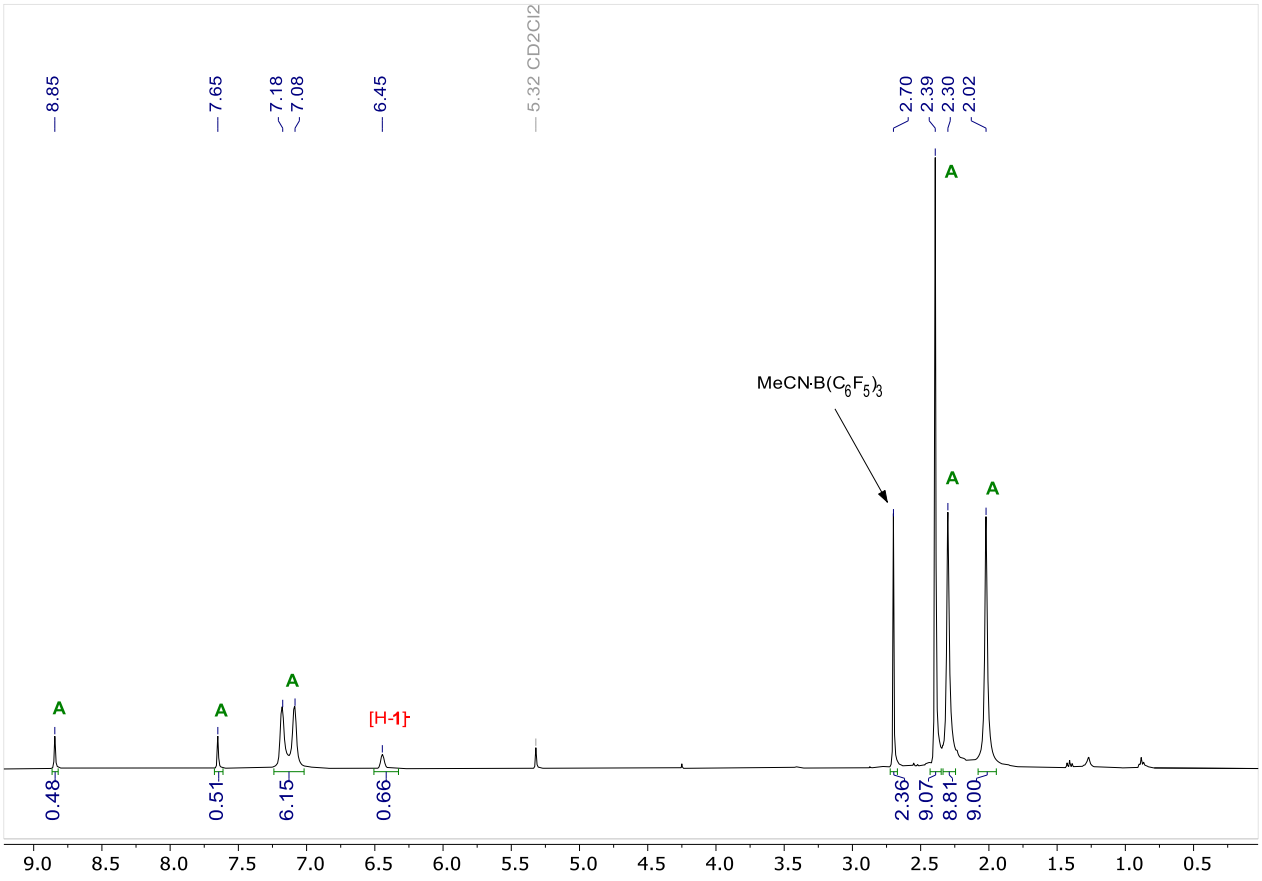



**Figure S 7:** $^{1}$H NMR of the reaction mixture after complete dissolution of the reactants in $CD_2Cl_2$ showing the formation of the hydrido germanate anion [H-**1**]$^-$ with the [Mes3PH] (**A**) counter cation . No [HB(C$_6$F$_5$)$_3$] signal could be observed.

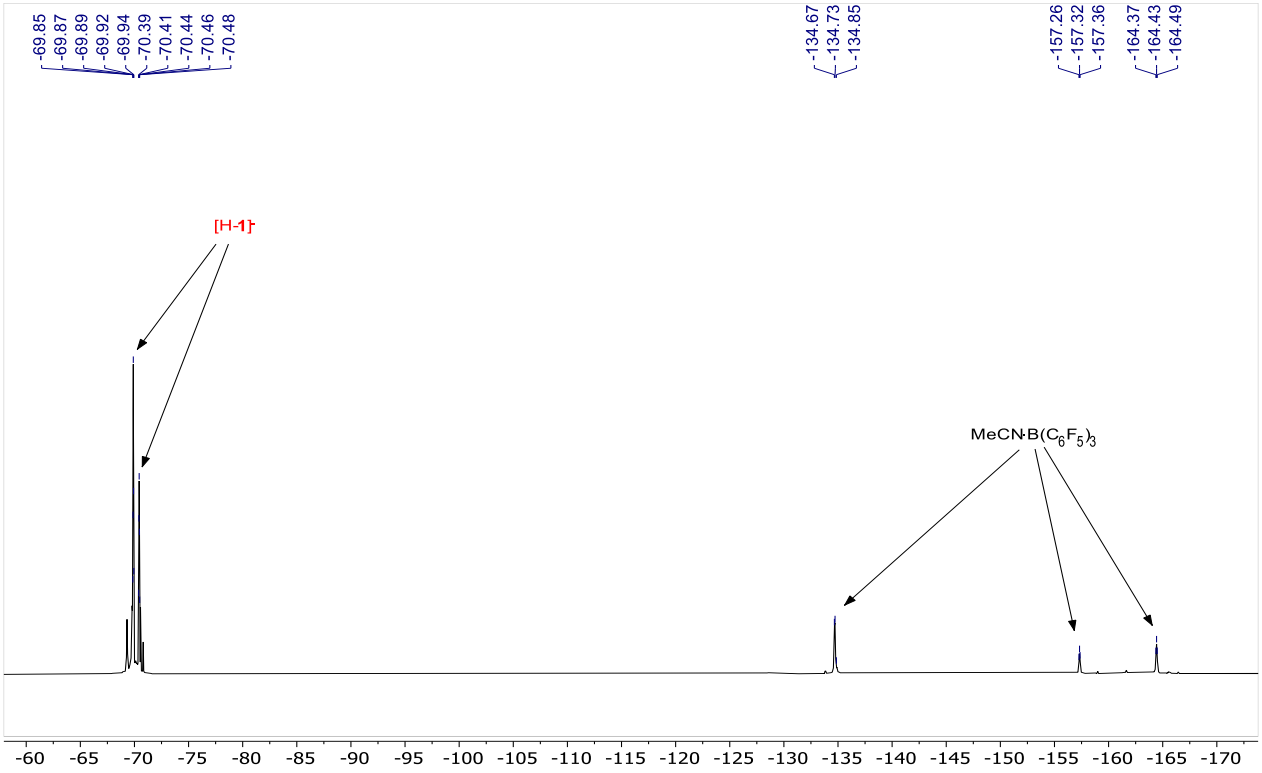



**Figure S 8:** $^{19}F$ NMR of the reaction mixture showing the presence of hydrido germanate anion [H-**1**]$^-$ and MeCN-coordinated BCF. No [$HB(C_6F_5)_3$] signals are present.

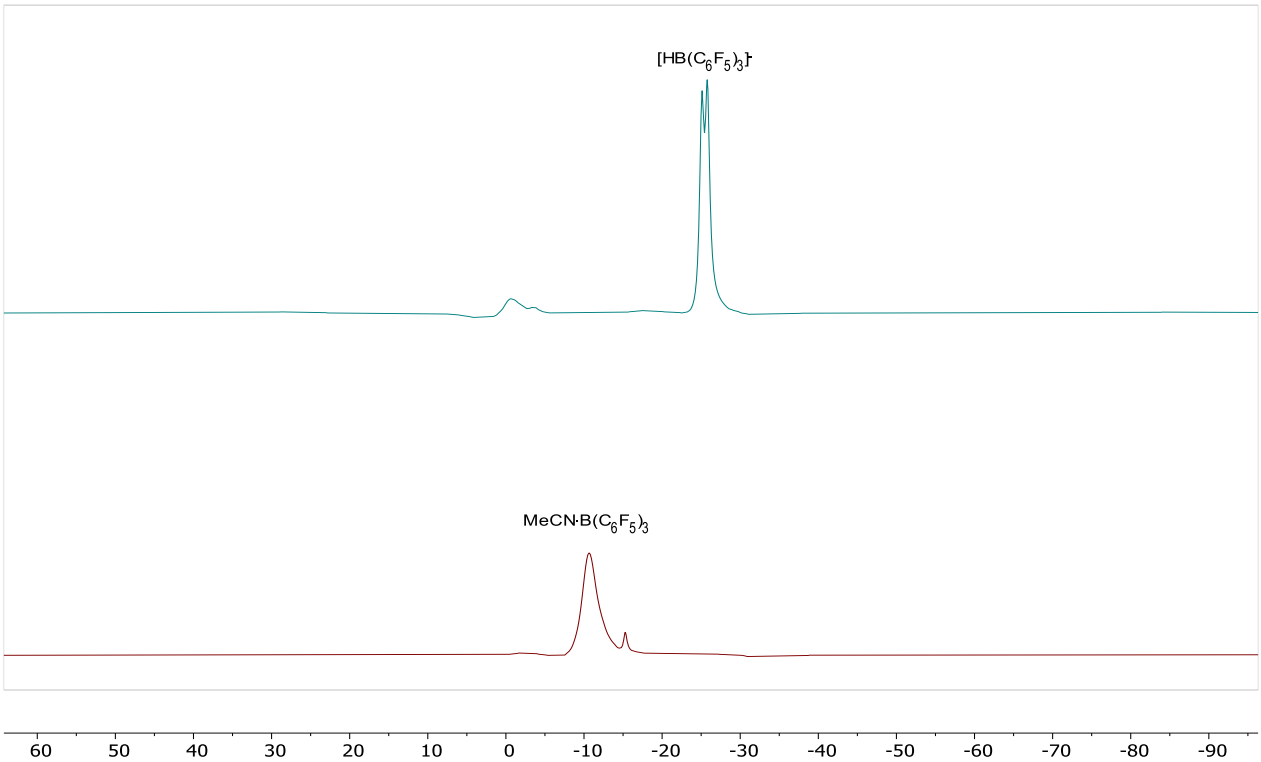
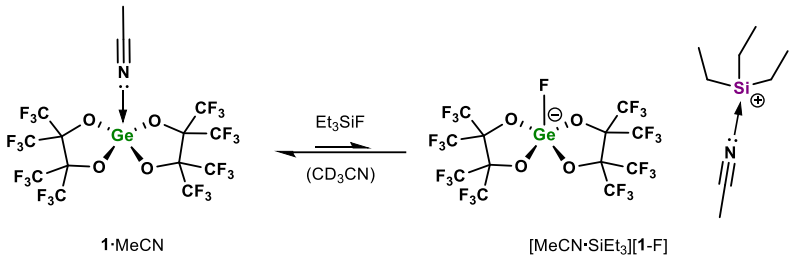



**Figure S 9:** Stacked $^{11}B$ NMR showing the characteristic doublet of [$HB(C_6F_5)_3$] before **1**·MeCN was added to the reaction mixture (top) and the signal of MeCN-coordinated BCF after addition of **1**·MeCN (bottom).

### 2.2.3 Reaction of 1·MeCN with $Et_3SiF$




**1**·MeCN [MeCN·$SiEt_3$][**1**-F]

To 10 mg (12.9 µmol, 1.0 equiv.) of **1**·MeCN in 0.4 ml acetonitrile-$d_3$ were added 17.3 mg (129 µmol, 10.0 equiv.) $Et_3SiF$ in a PTFE-valved J-Young NMR tube. The obtained solution was analyzed by multinuclear NMR spectroscopy. No difference in reaction conversion was observed at longer periods at room temperature or upon heating to 80 °C for several hours. The conversion progress correlated with the amount of added Et3SiF. When fewer equivalents $Et_3SiF$ were used, significantly lower conversion was observed.

**$^{1}$H-NMR** (500 MHz, acetonitrile-$d_3$) δ (ppm) = 1.96 (s, 3H, NCC$H_3$), 1.11 – 1.02 (m, 15H, C$H_3$).
**$^{13}$C NMR** (126 MHz, acetonitrile-$d_3$) δ (ppm) = 122.8 (qm, $^{1}J_{C\text{-}F}$ = 295 Hz, $CF_3$), 81.5 (br, O$C$($CF_3$)$_2$), 6.18 (s, $CH_2$), 4.16 (s, $CH_3$).
**$^{19}$F-NMR** (377 MHz, acetonitrile-$d_3$) δ (ppm) = -69.88 – -70.11 (m, 12F, $CF_3$), -70.76 – -70.99 (m, 12F, $CF_3$), -145.05 – -145.31 (m, 1F, Ge-$F$).
**$^{29}$Si NMR** (99 MHz, acetonitrile-$d_3$) δ (ppm) = 36.60 (s, $Et_3Si^+$).

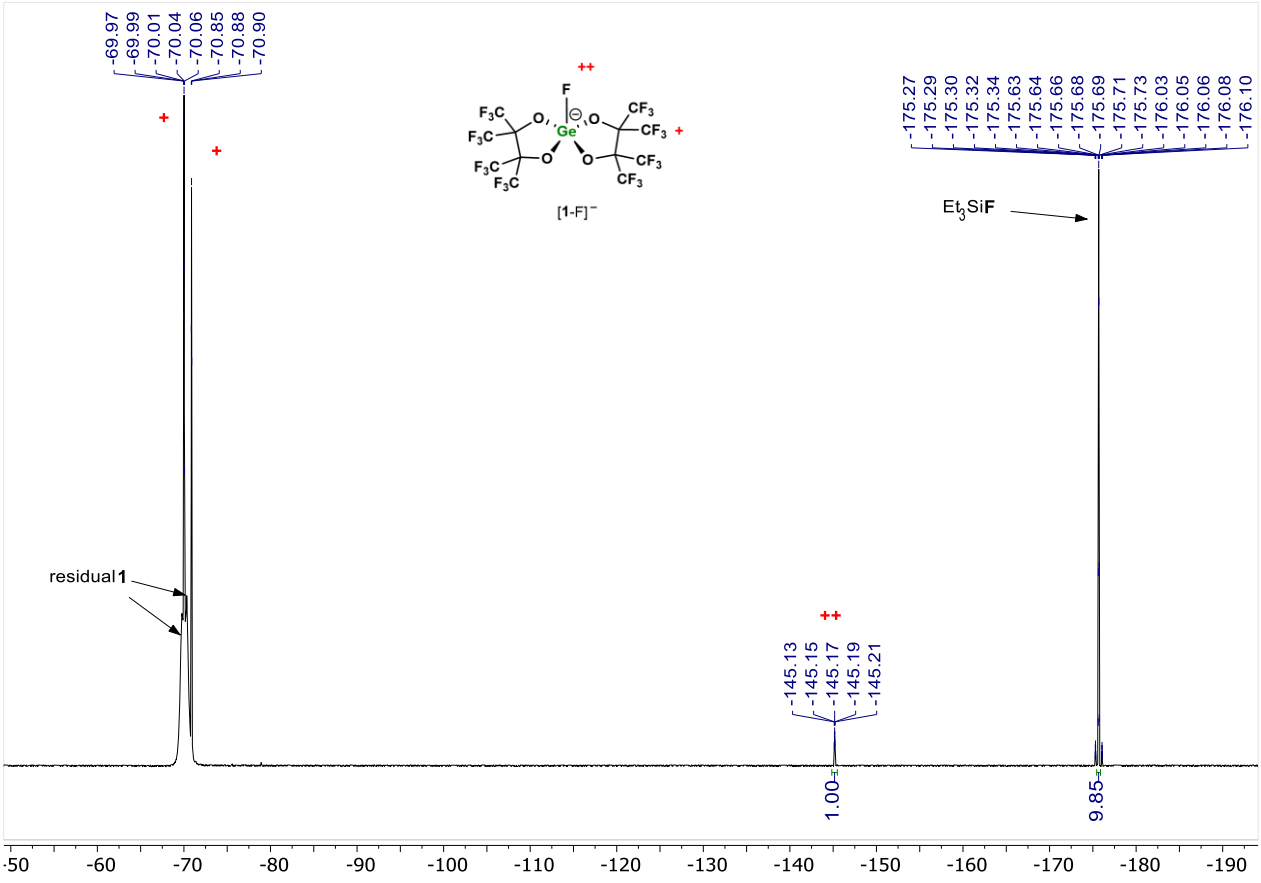


**Figure S 10:** $^{19}$F NMR of the reaction mixture showing the partial formation of the fluorogermanate anion [**1**-F]$^-$in an reaction equilibrium, thus confirming a successful fluoride abstraction when a surplus of $Et_3SiF$ is present. No further reaction progress was observed after various periods or upon heating.

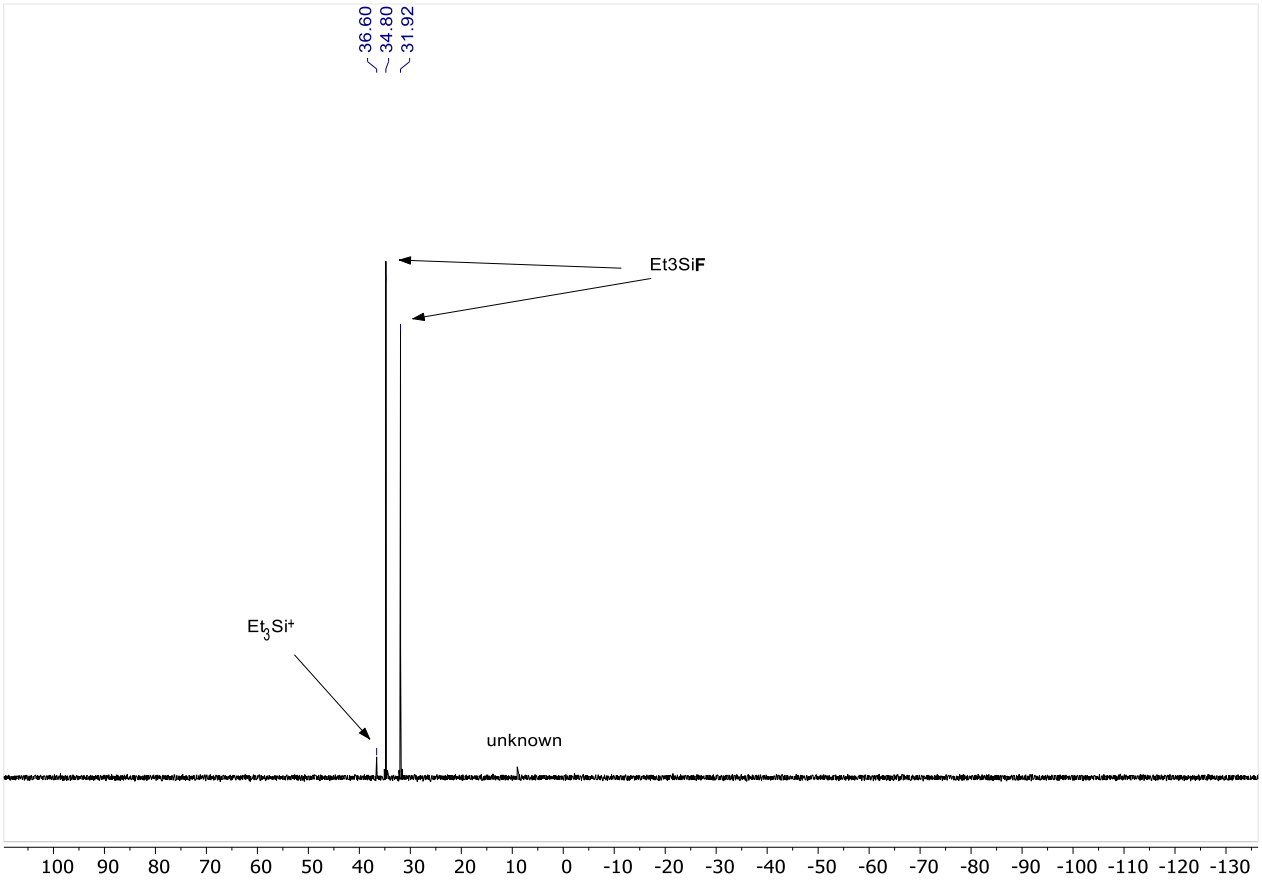
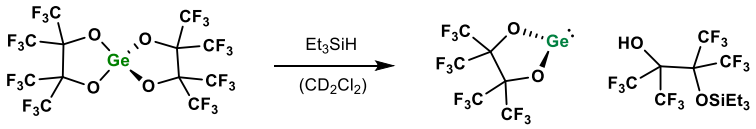



**Figure S 11:** $^{29}$Si{$^1$H} NMR of the reaction mixture showing the partial formation of the MeCN-coordinated silyl cation ($Et_3Si^+$) next to the characteristic doublet ($^1J_{Si\text{-}F}$ = 286 Hz) of $Et_3SiF$.

### 2.2.4 Reaction of acetonitrile-free 1 with $Et_3SiH$




To a suspension of 30 mg (40.7 mmol, 1.0 equiv.) of **1** in 0.4 ml of dichloromethande-$d_2$ were added 6.50 µl (40.7 mmol, 1.0 equiv.). $Et_3SiH$ in a PTFE-sealed J-Young NMR tube. The obtained solution was analyzed by multi nuclear NMR spectroscopy. Product separation and isolation failed in multiple attempts.

**$^1$H-NMR** (400 MHz, dichloromethane-$d_2$) δ (ppm) = 3.94(s, 1H, O*H*), 0.98 (t, $^3J_{H\text{-}H}$ = 7.9 Hz, 9H, C$H_3$), 0.80 (q, $^3J_{H\text{-}H}$ = 8.0 Hz, 6H, C$H_2$).
**$^{13}$C NMR** (126 MHz, dichloromethane-$d_2$) δ (ppm) = 121.5 (qm, $^1J_{C\text{-}F}$ = 293 Hz, *C*$F_3$), 121.9 (q, $^1J_{C\text{-}F}$ = 293 Hz, *C*$F_3$), 88.8 (br, GeO*C*$(CF_3)_2$), 82.9 (p, $^2J_{C\text{-}F}$ = 31.2 Hz, HO(*C*$(CF_3)$)$_2$OSi), 81.4(p, $^2J_{C\text{-}F}$ = 30.4 Hz, HO(*C*$(CF_3)$)$_2$OSi), 6.41 (s, *C*$H_2$), 5.76 (s, *C*$H_3$).

**$^{19}$F-NMR** (377 MHz, dichloromethane-$d_2$) δ (ppm) = -68.97 – -69.26 (m, 6F, HO-CC$F_3$), -69.90 – -70.14(m, 6F, SiO-CC$F_3$), -70.91 (s, 12F, Ge(OC(C$F_3$)$_2$)$_2$).
**$^{29}$Si NMR** (99 MHz, dichloromethane-$d_2$) δ (ppm) = 31.69 (s, *Si*Et$_3$).

## LIFDI-MS

For further investigation a high resolution LIFDI-MS analysis of the reaction mixture was performed, revealing the cleavage of the Si-O bond and consecutive hydride abstraction, by selectively giving the mass pattern for the hydrido germanate anion [H-**1**]$^-$ in negative mode:

| | |
|---|---|
| calculated for [$C_{12}HF_{24}GeO_4$]$^-$: | 738.87056 |
| observed: | 738.87157 |

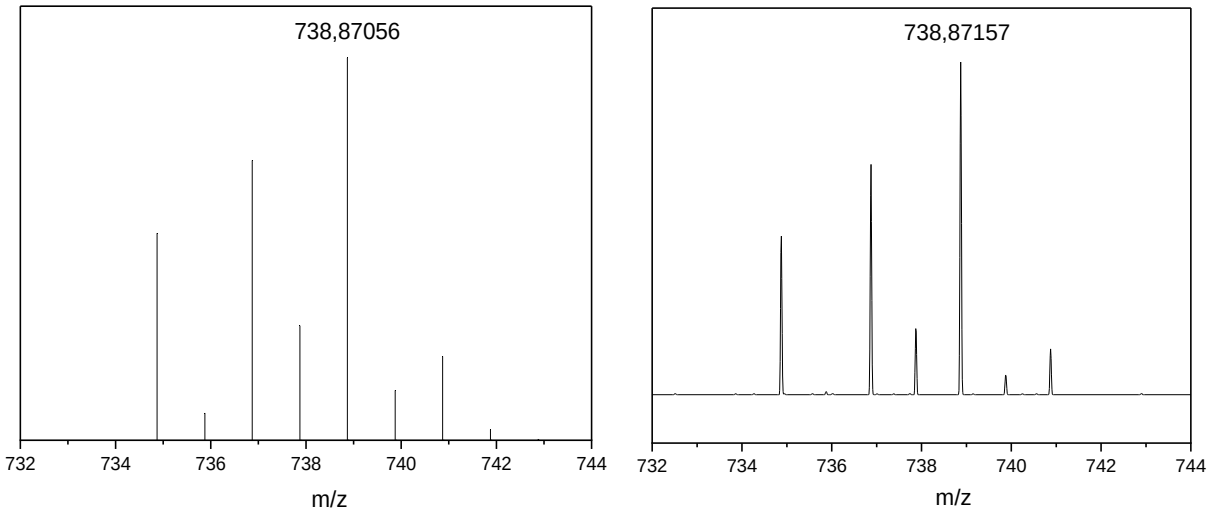
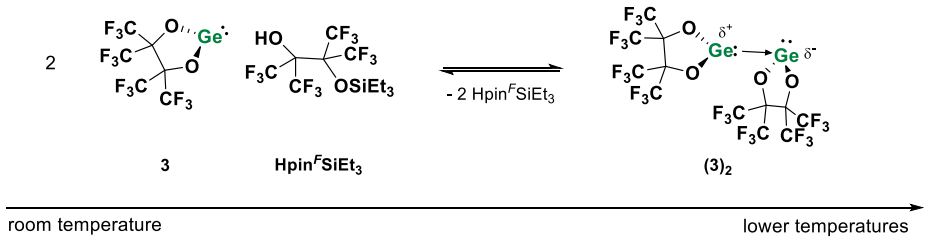



**Figure S12: :** LIDFI-MS spectrometry (detail view with isotope pattern) of **3** obtained in negative mode. Measured (right; *m*/*z* = 738.87157) and simulated (left; *m*/*z* = 738.87056) mass spectrum.

## Low Temperature NMR

At lower temperatures the thermodynamically favored dimerization of the perfluoropinacolato germylene is observed, leading to the formation of complex **4**. As a result of decreasing symmetry upon dimerization the sharp singlet at δ = -70.91 ppm completely disappears at -80 °C due to heavy broadening. A related trend is also seen in the $^{29}$Si NMR spectra were the silicon signal of the silylated alcohol shifts from δ = -31.69 ppm (25 °C) to δ = -33.65 ppm (-80 °C). This could be an effect of weak coordination at room temperature that decreases in favor of the germylene dimerization at low temperatures.



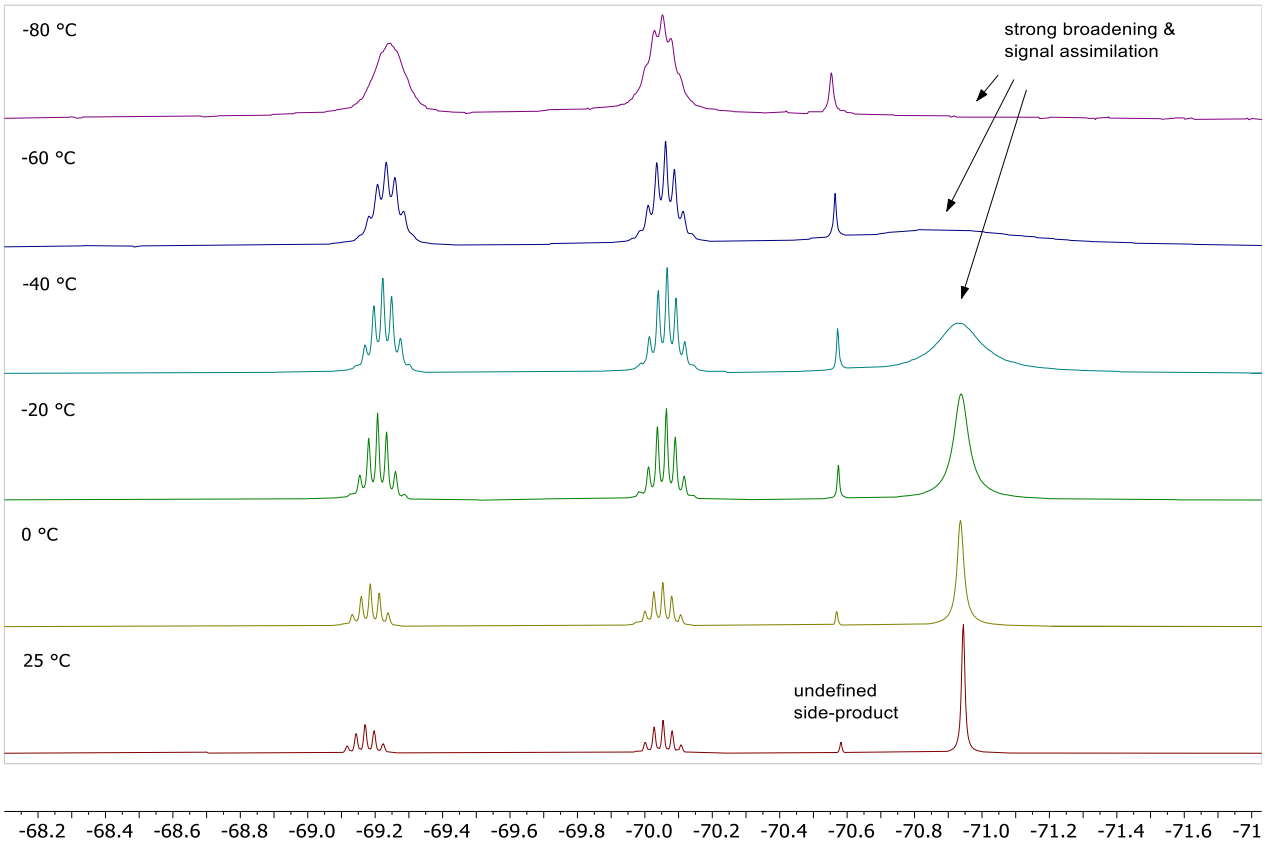



**Figure S 13:** Stacked $^{19}F$ NMR spectra in $CD_2Cl_2$ of a freshly prepared mixture of **3** and **4** at a temperature range from -80 °C to 25 °C.

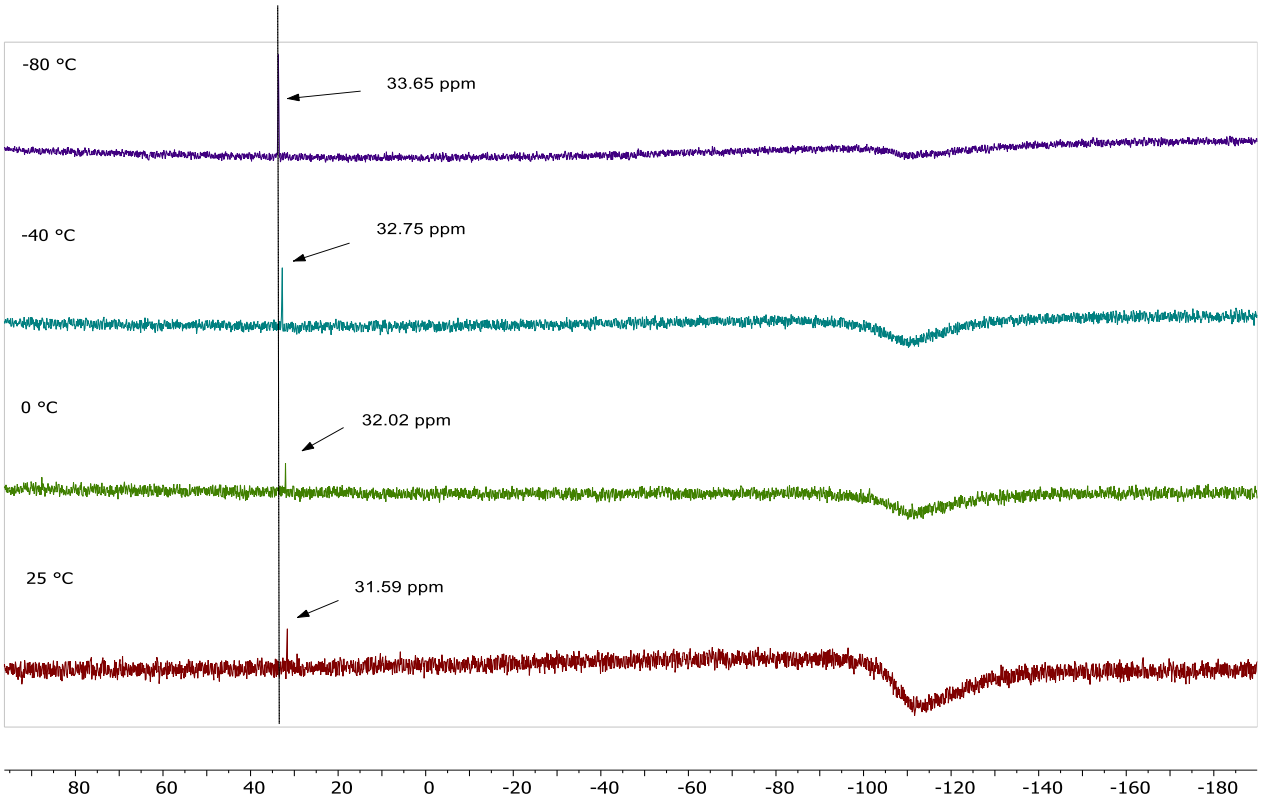
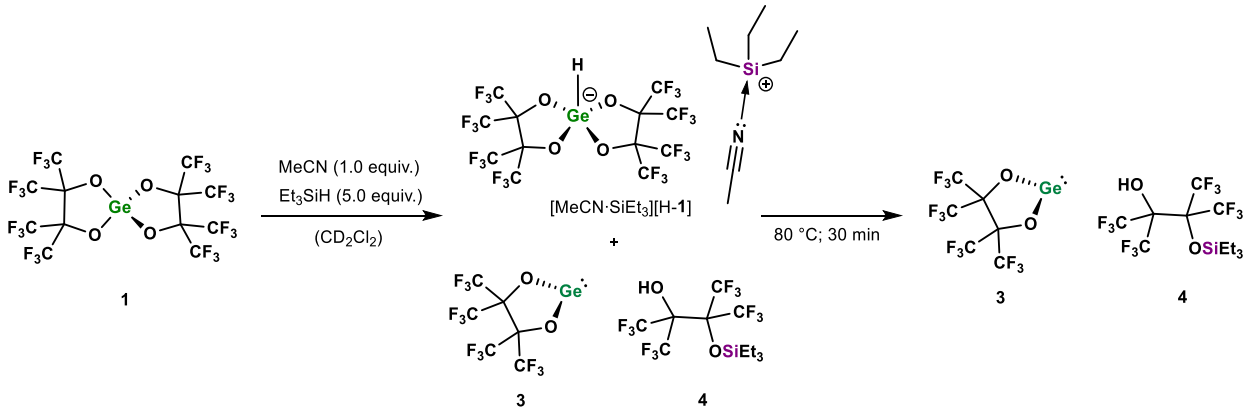


**Figure S 14:** Stacked $^{29}Si\{^{1}H\}$ NMR spectra in $CD_2Cl_2$ of freshly prepared **3** and **4** at a temperature range from -80 °C to 25 °C.

### 2.2.5 Reaction of 1 with $Et_3SiH$ in presence of acetonitrile




In a PTFE-sealed J-Young NMR tube was dissolved 15 mg (20.4 µmol, 1.0 equiv.) **1** in 0.4 ml $CD_2Cl_2$. To the mixture were subsequently added 1.2 µl (22.4 µmol, 1.0 equiv.) MeCN and 3.6 µl $Et_3SiH$. The NMR tube was shaken vigorously and analyzed by multinuclear NMR spectroscopy. Afterwards, the product mixture was heated to 80 °C for 30 min and again analyzed.

The first NMR outlined the presence of the two main reaction products **3** (with by-product **4**) and [MeCN·$SiEt_3$][H-**1**] in a molar ratio of 0.58/1.00 (referenced by integration of the Ge-H and OH signals). The second NMR (after heating) showed the selective formation of reaction product mixture **3** and **4**. No residual traces of ionic [MeCN·$SiEt_3$][H-**1**] could be observed.

Note: The same results were obtained when **1**·MeCN was used instead of **1** and additional MeCN.

Observed product signals for **3** and **4**:

**$^{1}$H-NMR** (400 MHz, dichloromethane-$d_2$) δ (ppm) = 4.04/4.07 (s, 1H, O*H*), 0.97 (t, $^{3}J_{H\text{-}H}$ = 7.9 Hz, 9H, C$H_3$), 0.80 (q, $^{3}J_{H\text{-}H}$ = 8.0 Hz, 6H, C$H_2$).
**$^{19}$F-NMR** (377 MHz, dichloromethane-$d_2$) δ (ppm) = -69.06 – -69.20/-69.03 – -69.25 (m, 6F, HO-CC$F_3$), -69.92 – -70.07/-69.90 – -70.11 (m, 6F, SiO-CC$F_3$), -70.61/-70.55 (s, 12F, Ge(OC(C$F_3$)$_2$)$_2$).
**$^{29}$Si NMR** (99 MHz, dichloromethane-$d_2$) δ (ppm) = 31.61/31.53 (s, *Si* $Et_3$).

Observed product signals of [MeCN·$SiEt_3$][H-**1**]:

**$^{1}$H-NMR** (400 MHz, dichloromethane-$d_2$) δ (ppm) = 6.50 (s, 1H, Ge*H*), 2.28 (s, 3H, C$H_3$CN), 1.14 – 1.02 (m, 15H, C$H_2$C$H_3$).
**$^{19}$F-NMR** (377 MHz, dichloromethane-$d_2$) δ (ppm) = -69.66 – -69.88 (m, 12F, C$F_3$), -70.25 – -70.43 (m, 12F, C$F_3$).
**$^{29}$Si NMR** (99 MHz, dichloromethane-$d_2$) δ (ppm) = 40.38 (s, *Si* $Et_3$).

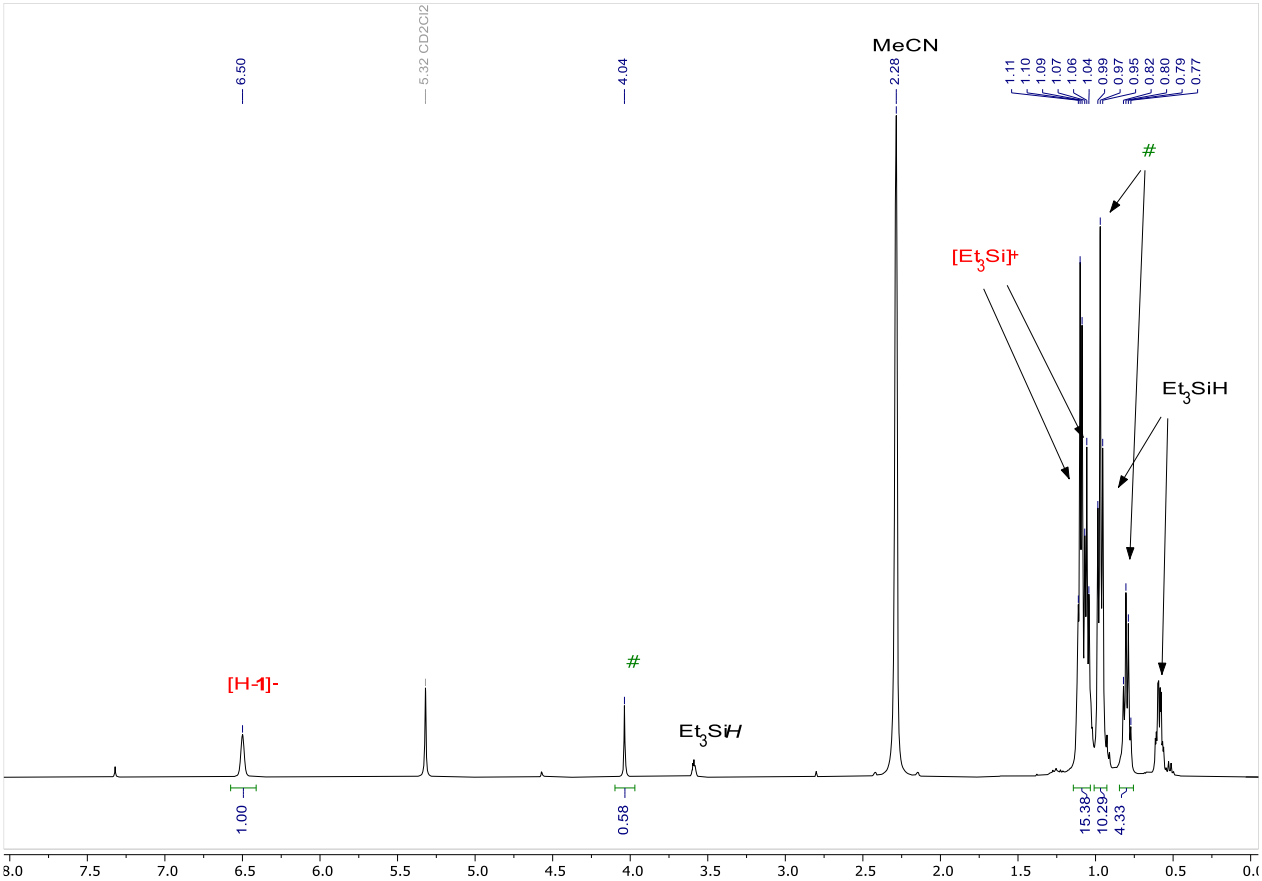



**Figure S 15:** $^{1}$H NMR spectrum of the reaction mixture after 10 minutes at room temperature in $CD_2Cl_2$, showing the formation of two main reaction products **4** (#) and [MeCN·SiEt$_3$][H-**1**] with an integral ratio of 0.58/1.00 and residual/unreacted $Et_3SiH$.

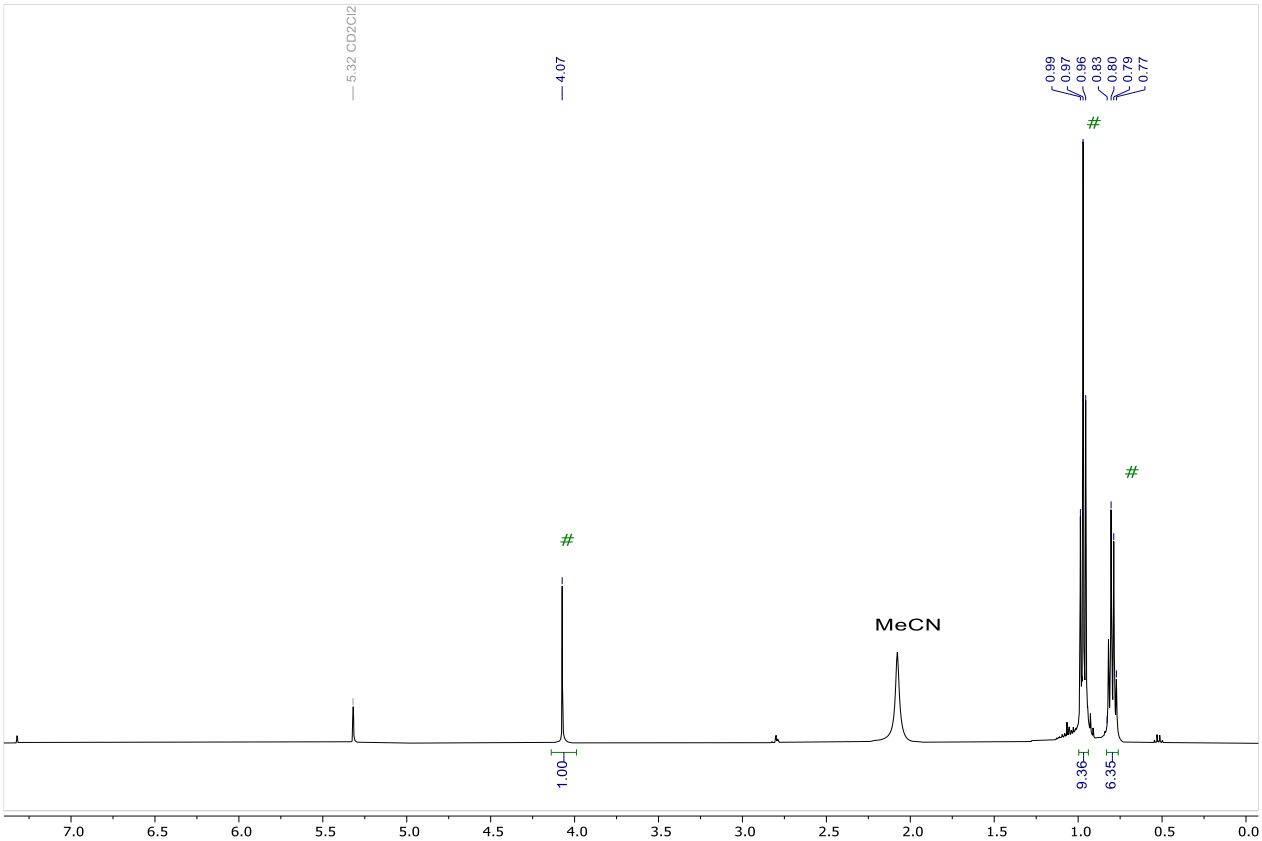


**Figure S 16:** $^{1}$H NMR spectrum of the reaction mixture after 30 minutes at 80 °C in $CD_2Cl_2$, showing the selective formation of **4** (#) as the main reaction product. No more [MeCN·SiEt$_3$][H-**1**] can be observed.

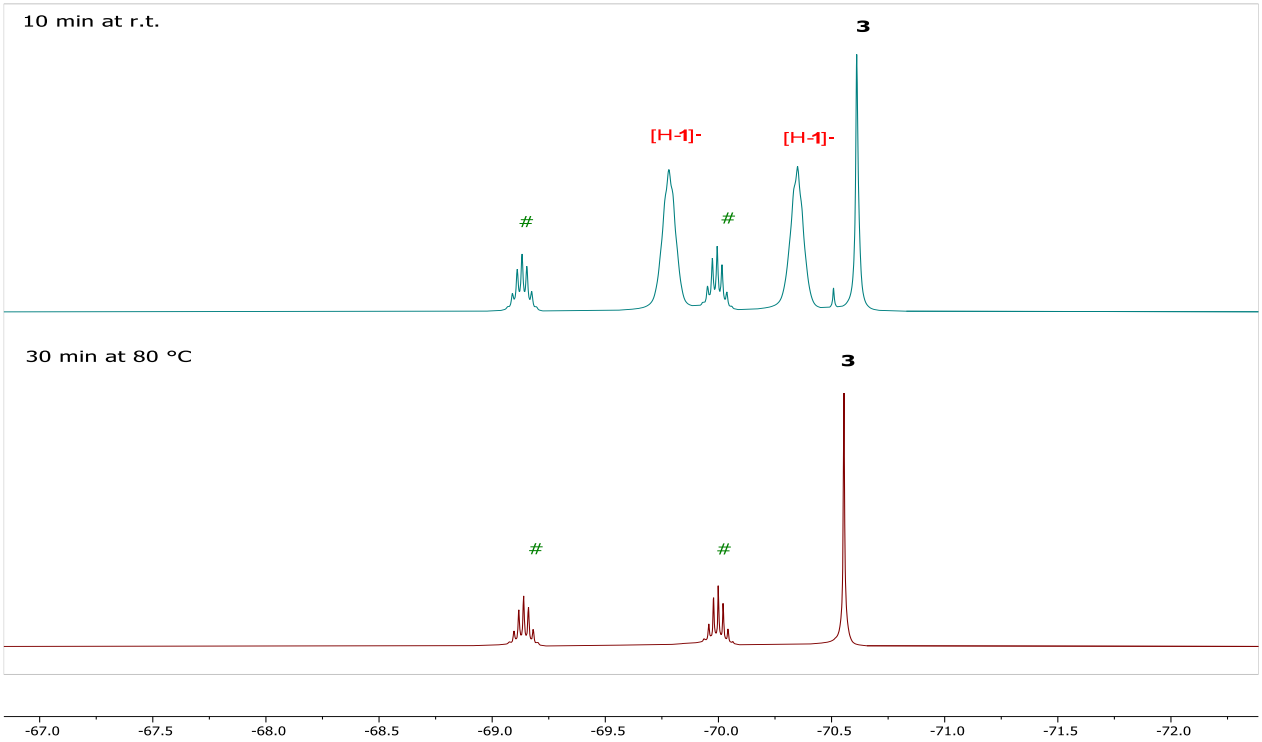



**Figure S 17:** Stacked $^{19}$F NMR spectra of the reaction mixture after 10 minutes at room temperature in $CD_2Cl_2$, showing the formation of two main reaction products **3**, **4**(#) and [MeCN·SiEt$_3$][H-**1**] (top) and the selective conversion to towards **3** and **4** (#) after 30 min at 80 °C (bottom).

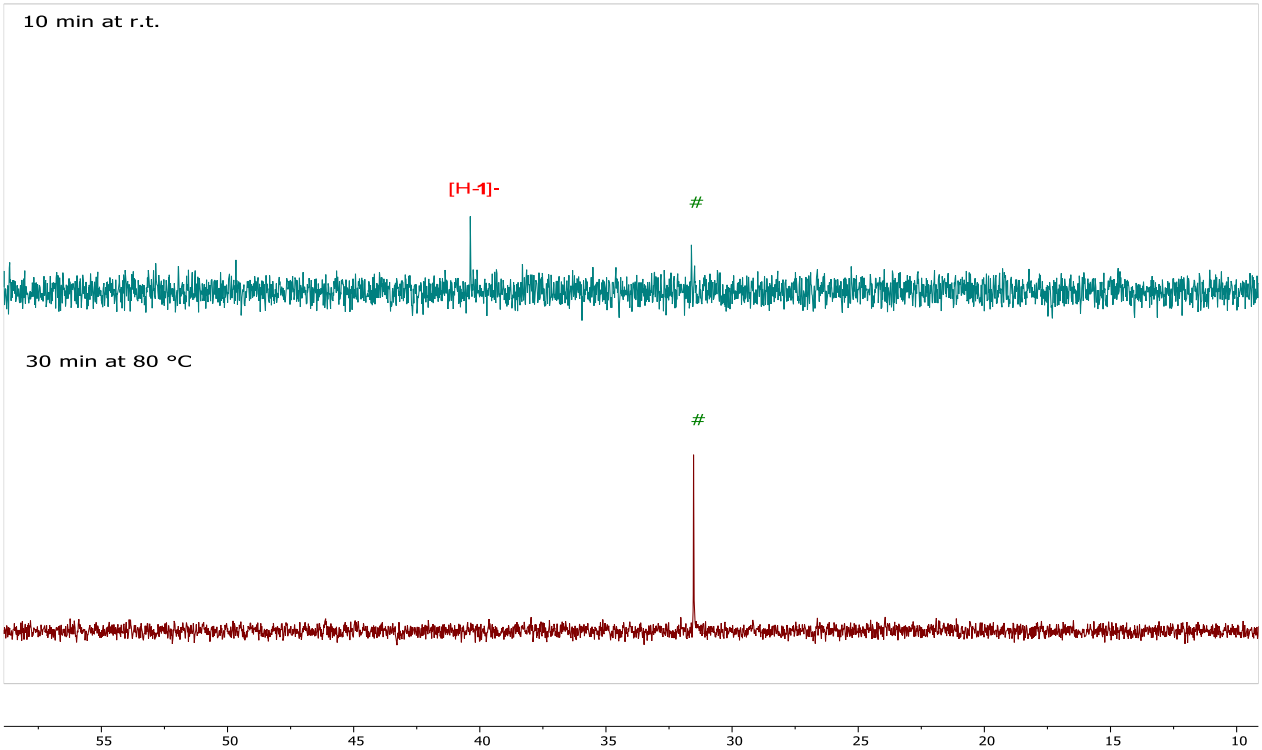
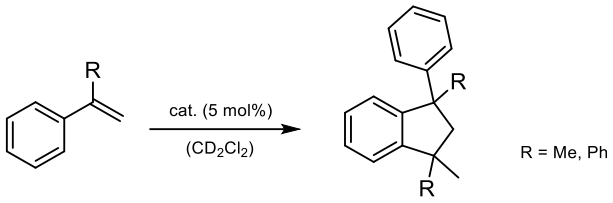



**Figure S 18:** Stacked $^{29}$Si{$^{1}$H} NMR spectra of the reaction mixture after 10 minutes at room temperature in $CD_2Cl_2$,

showing the formation of two main reaction products **4** (#) and [MeCN·$SiEt_3$][H-**1**] (top) and the selective conversion to **3** and **4** (#) after 30 min at 80 °C (bottom).

### 2.3.1 Dimerization of α-methylstyrene and 1,1-diphenylethylene




In a PTFE-sealed J-Young NMR tube was dissolved 15 µl a-methyl styrene or 15 µl 1,1-diphenylethylene as well as 3 µL of the internal standard mesitylene in 0.4 mL $CD_2Cl_2$. After zero-point measurements, 0.05 mol% of the respective catalyst were added and the NMR tube was vigorously shaken. The mixture was then analyzed by $^1$H NMR spectroscopy after 10 minutes at r.t. and several more intervals if necessary.

**1,1,3-Trimethyl-3-phenyl-2,3-dihydro-1H-indene (R = Me)**

**$^1$H NMR** (400 MHz, $CD_2Cl_2$) δ (ppm) = 7.34 – 7.07 (m, 9H, Ar*H*), 2.44(d, $^2J_{H\text{-}H}$ = 13.1 Hz, 1H, CH*H*), 2.22 (d, $^1J_{H\text{-}H}$ = 13.1 Hz, 1H, C*H*H), 1.69 (s, 3H, C$H_3$), 1.36 (s, 3H, C$H_3$), 1.05 (s, 3H, C$H_3$).

**$^{13}$C NMR** (101 MHz, $CD_2Cl_2$) δ (ppm) = 152.69, 151.53, 149.24(Ar*C*), 128.35, 127.09, 125.35, 122.96 (Ph*C*), 59.54(*C*$H_2$), 51.19 (*C*MePh), 43.21 (*C*$Me_2$), 31.17 (*C*$H_3$), 30.89 (*C*$H_3$), 30.50 (*C*$H_3$).

**1-Methyl-1,3,3-triphenyl-2,3-dihydro-1H-indene (R = Ph)**

**$^1$H NMR** (400 MHz, $CD_2Cl_2$) δ (ppm) = 7.36 – 7.01 (m, 19H, Ar*H*), 3.41 (d, $^2J_{H\text{-}H}$ = 13.5 Hz, 1H, CH*H*), 3.14(d, $^2J_{H\text{-}H}$ = 13.5 Hz, 1H, C*H*H), 1.57 (s, 3H, C$H_3$).

**$^{13}$C NMR** (101 MHz, $CD_2Cl_2$) δ (ppm) = 150.97, 149.81, 149.21, 149.08, 148.07 (Ar*C*), 129.11, 129.07, 128.36, 128.23, 127.98, 127.86, 127.22, 126.40, 126.06, 125.95, 125.49 (Ph*C*), 61.49 (*C*$H_2$), 61.33 (*C*$Ph_2$), 51.57 (*C*MePh), 29.28 (*C*$H_3$).

Product signals correspond with pattern given in the literature.[14]

**Table S 1:** Reaction conditions and conversion and yield of dimerization experiments after several hours at room temperature. Product yield and conversion of reactants were calculated by integration with respect to the internal standard.

| Sample | Reagent | Catalyst | Temp. [°C] | Time | Conversion [%] | Yield [%] |
|---|---|---|---|---|---|---|
| **I** | α-methyl styrene | **1** | 25 | 10 min | 99 | 65 |
| **II** | α-methyl styrene | **1**·MeCN | 25 | 10 min | 99 | 83 |
| **III** | 1,1-diphenylethylene | **1** | 25 | 1 h | 99 | 99 |
| **IV** | 1,1-diphenylethylene | **1**·MeCN | 25 | 10 min | 75 | 70 |
| **IV** | 1,1-diphenylethylene | **1**·MeCN | 25 | 5 h | 94 | 88 |
| **IV** | 1,1-diphenylethylene | **1**·MeCN | 25 | 48 h | 99 | 98 |

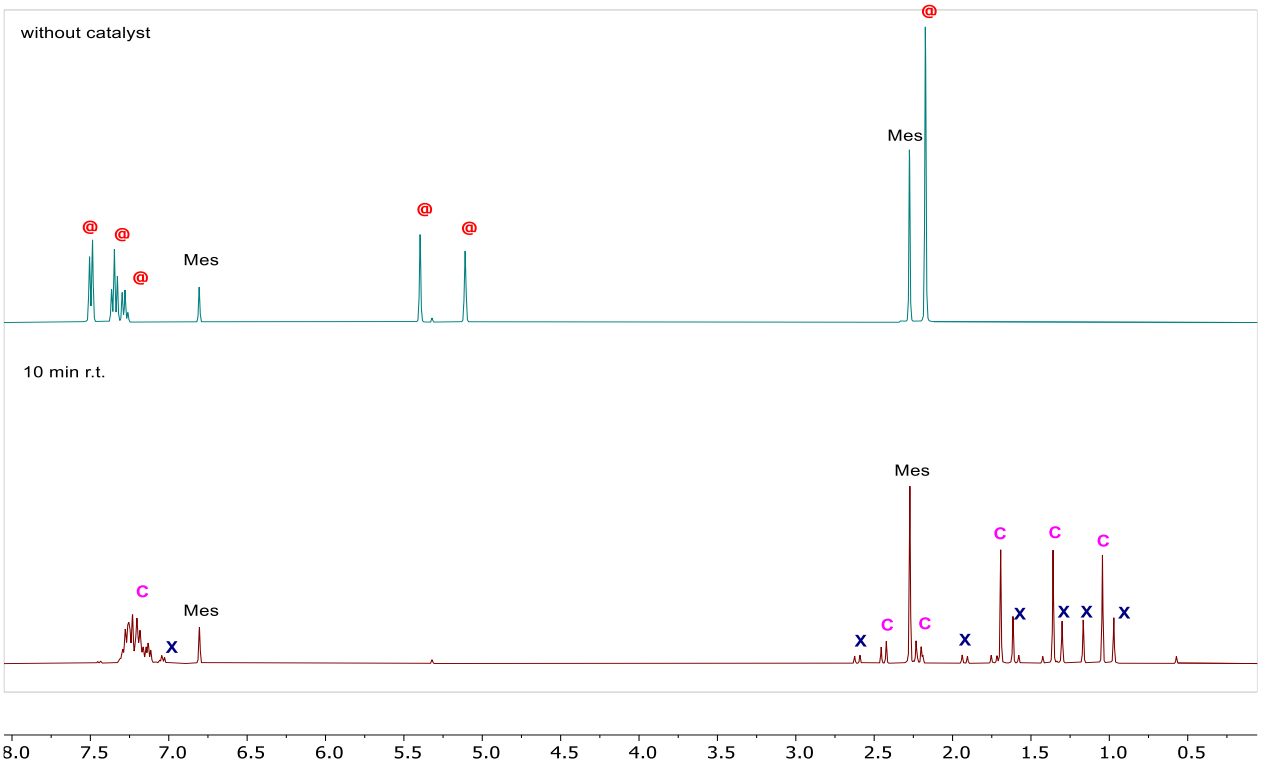



**Figure S 19:** Stacked $^{1}$H NMR spectra in $CD_2Cl_2$ of the dimerization experiment of α-methyl styrene (**@**) using **1** as catalyst. After 10 min full conversion was obtained showing giving the dimer (**C**) as the main reaction product as well as minor amounts of trimeric side product (**X**).[15]

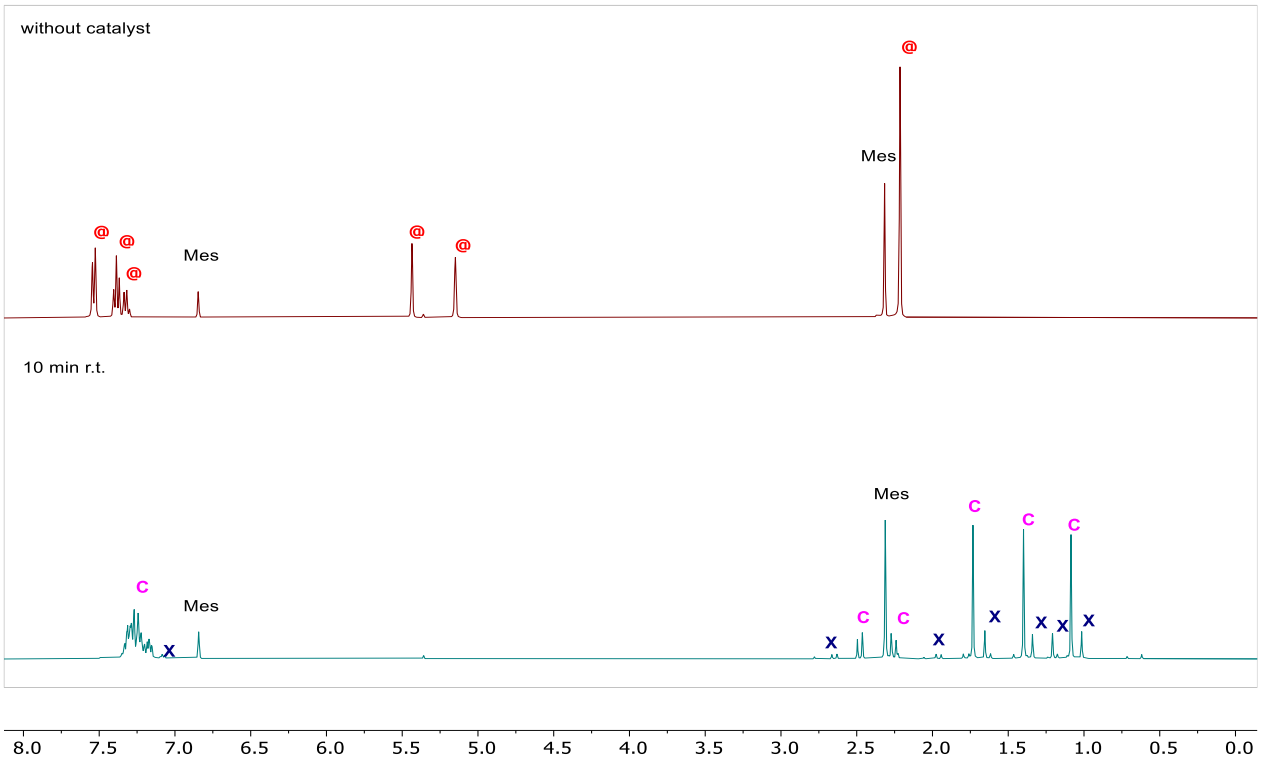



**Figure S 20:** Stacked $^{1}$H NMR spectra in $CD_2Cl_2$ of the dimerization experiment of α-methyl styrene (**@**) using **1**·MeCN as catalyst. After 10 min full conversion was obtained showing giving the dimer (**C**) as the main reaction product as well as minor amounts of trimeric side product (**X**).[15]

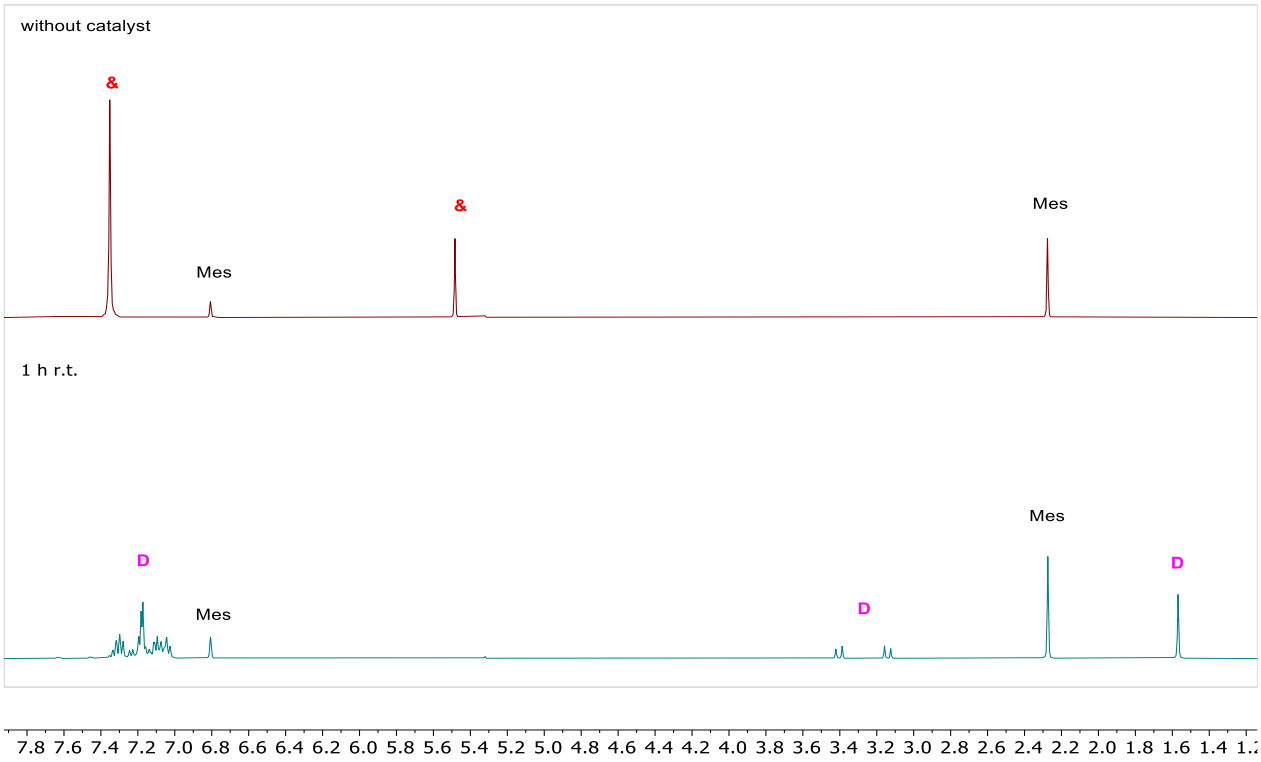



**Figure S 21:** Stacked $^{1}$H NMR spectra in $CD_2Cl_2$ of the dimerization experiment of 1,1-diphenylethylene (**&**) using **1** as catalyst. After 10 min full conversion was obtained selectively yielding the dimerization product (**D**).

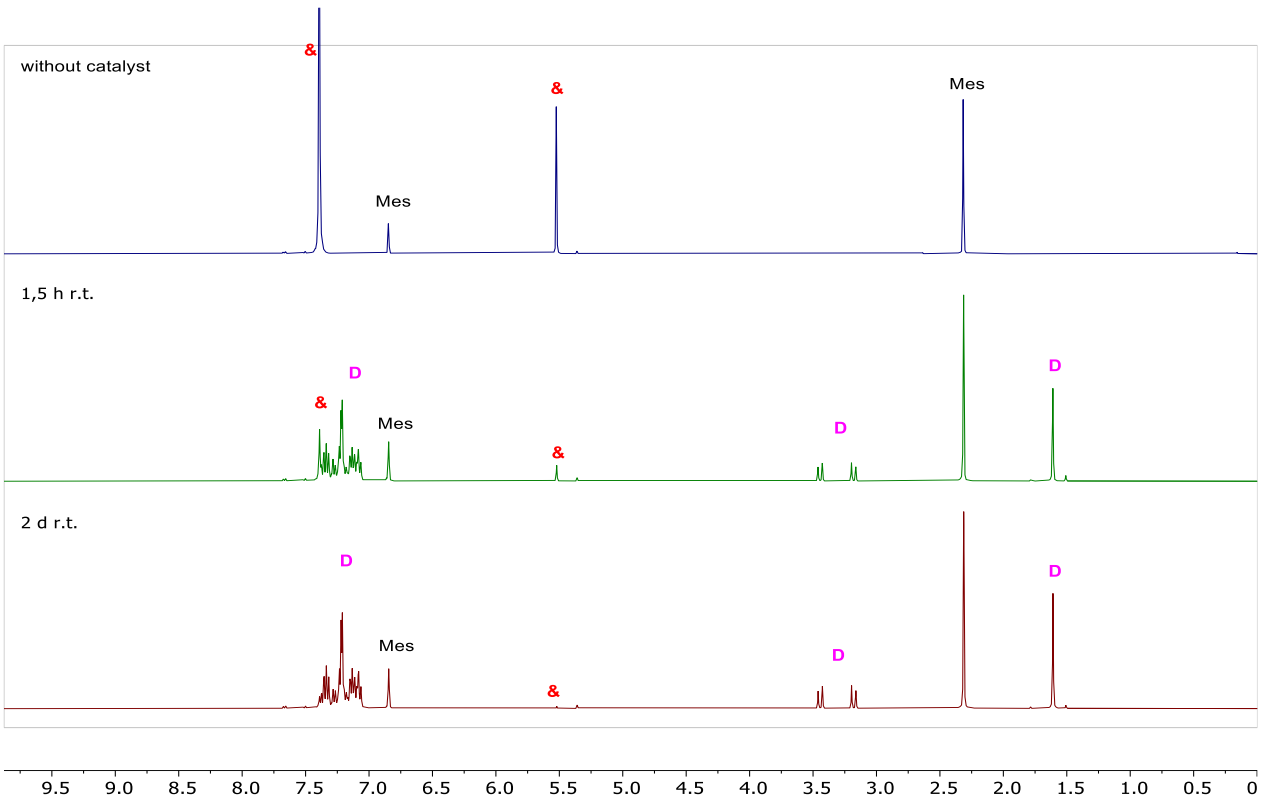



**Figure S 22:** Stacked $^{1}$H NMR spectra in $CD_2Cl_2$ of the dimerization experiment of 1,1-diphenylethylene (**&**) using **1**·MeCN as catalyst. After 2 days at room temperature nearly quantitative conversion was obtained selectively yielding the dimerization product (**D**).

### 2.3.2 Hydrosilylation of α-methylstyrene


To a solution 3.70 mg (500 µmol, 0.05 equiv.) **1** in 0.4 ml $CD_2Cl_2$ were added 16 µl (100 mmol, 1.00 equiv.) $Et_3SiH$ in a PTFE-sealed J-Young NMR tube. After complete dissolution 13.0 µl (100 mmol, 1.00 equiv.) α-methylstyrene and the internal standard mesitylene (3.00 µl) was added. The reaction mixture was analyzed by $^1$H NMR spectroscopy after several periods at defined temperatures.

Triethyl(2-phenylpropyl)silane:

**$^1$H NMR** (400 MHz, $CD_2Cl_2$) δ (ppm) = 7.32 – 7.21 (m, 4H, *o,m*-C*H*), 7.20 – 7.10 (m, 1H, *p*-C*H*), 2.96 – 2.83 (m, 1H, PhC*H*$CH_3$), 1.29 (d, $^3J_{H\text{-}H}$ = 6.9 Hz, 3H, PhCHC*H*$_3$), 0.97 (dd, $^1J_{H\text{-}H}$ = 17.2, $^3J_{H\text{-}H}$ = 7.5 Hz, 2H, CH($CH_3$)C*H*$_2$), 0.90 (t, $^3J_{H\text{-}H}$ = 7.9 Hz, 9H, $SiCH_2CH_3$), 0.54 – 0.35 (m, 6H, $SiCH_2CH_3$).

**$^{13}$C NMR** (101 MHz, $CD_2Cl_2$) δ (ppm) = 150.75 (*C*), 128.64(*o,m*-*C*H), 127.04(*o,m*-*C*H), 126.09 (*p*-*C*H), 36.60 (*C*H), 26.82 (*C*$H_3$), 21.92 (*C*$H_2$), 7.62 ($SiCH_2CH_3$), 4.09 ($SiCH_2CH_3$).

Product signals corresponds to separately synthesized triethyl(2-phenylpropyl)silane and NMR signals given in the literature.[16]

**Table S 2:** Reaction conditions and yield hydrosilylation experiments several hours at various temperatures. Product yield was calculated by integration of the PhC*H*$CH_3$-Signal with respect to the internal standard.

| Sample | Temp. [°C] | Time [h] | Conversion [%] | Yield [%] |
|---|---|---|---|---|
| **I** | 25 | 24 | 28 | 26 |
| **I** | 25 | 72 | 33 | 31 |
| **I** | 25 | 216 | 69 | 65 |
| **I** | 25 | 336 | 95 | 89 |
| **II** | -35 | 18 | 98 | 96 |

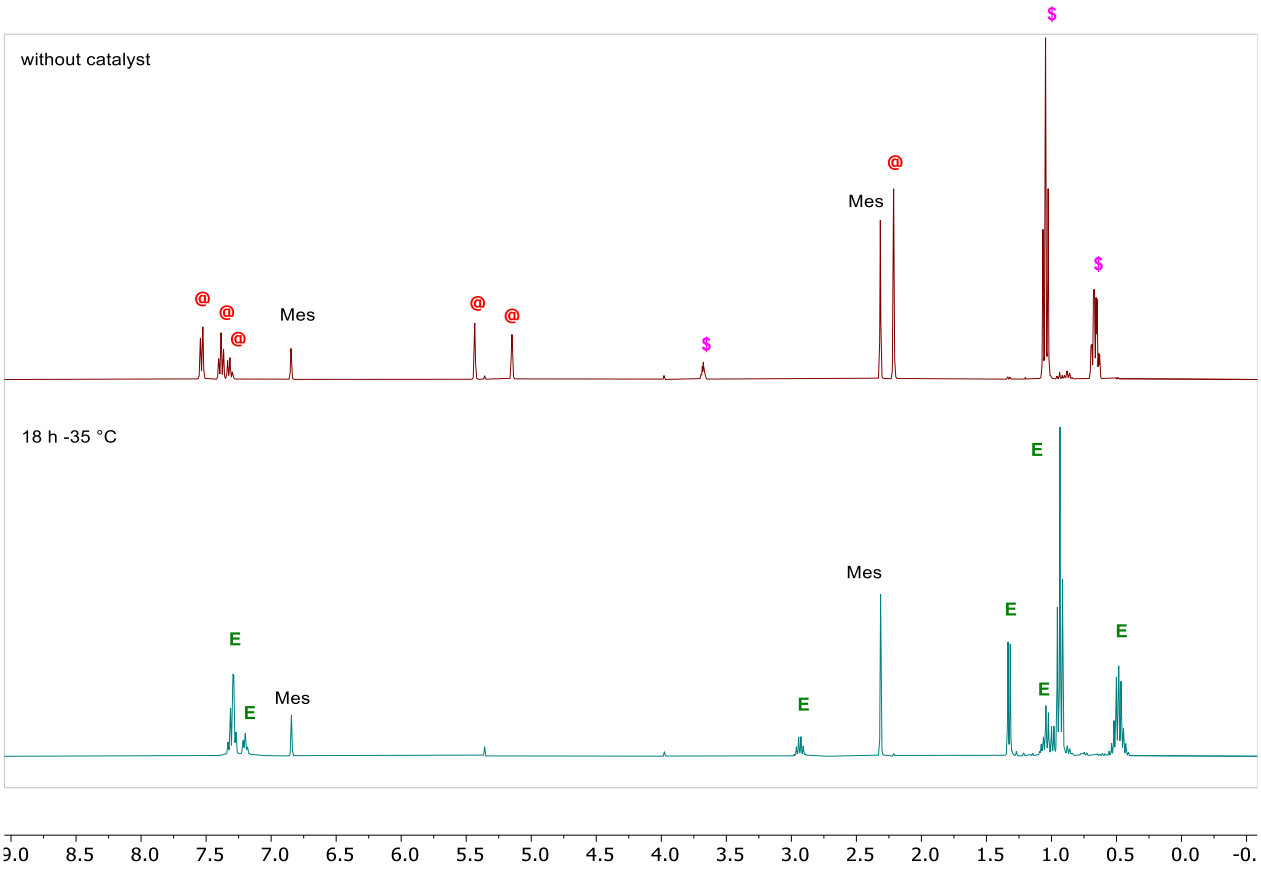



**Figure S 23:** Stacked $^{1}$H NMR spectra in $CD_2Cl_2$ of sample **II** after 18 hours at -35 °C, showing complete conversion, selectively forming the hydrosilylation product (**E**) from α-methylstyrene (**@**) and $Et_3SiH$ (**$**).

## Tracing the reaction progress

To additionally monitor the reaction progress, an equal NMR sample as described above was placed in a cooled NMR probe head at -44.3 °C (displayed value: -50 °C) and measured over the course of 12 hours. The obtained reaction progress is displayed in Table S 3.

**Table S 3:** Reaction progress of a freshly prepared sample at -44.3 °C. Conversion and product yield was calculated by integration of the $Et_3Si\mathit{H}$- and $PhC\mathit{H}CH_3$ signals with respect to the internal standard.

| Time [min] | Conversion [%] | Yield [%] |
|---|---|---|
| **1** | 19 | 17 |
| **2** | 30 | 29 |
| **3** | 41 | 39 |
| **4** | 49 | 47 |
| **6** | 59 | 59 |
| **9** | 72 | 71 |
| **12** | 78 | 77 |

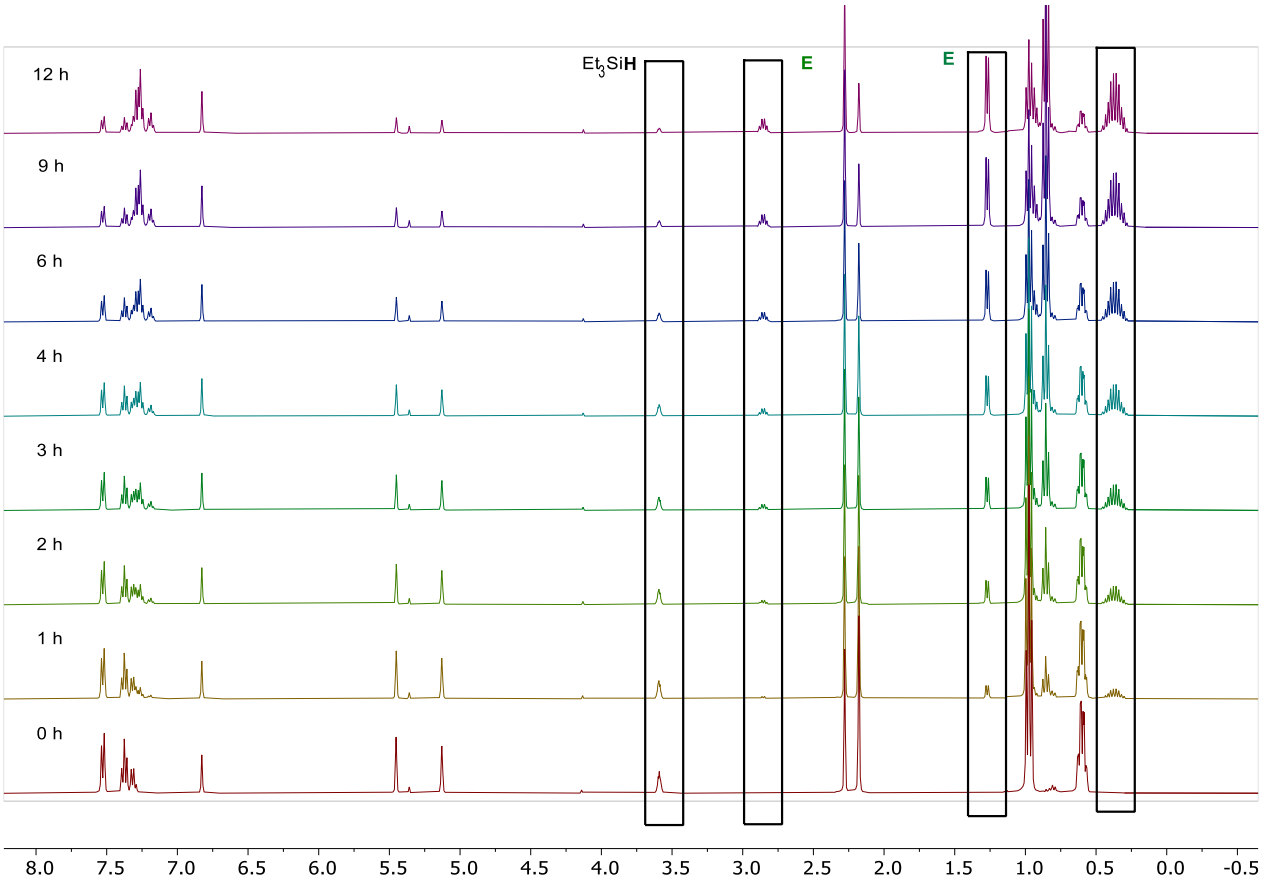
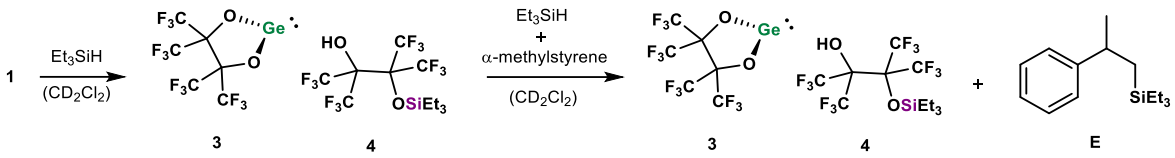



**Figure S 24:** Stacked $^{1}$H NMR spectra in $CD_2Cl_2$ of a freshly prepared hydrosilylation experiment after several hours at -44.3 °C. Selected reactant ($Et_3SiH$) and product (**E**) signals are highlighted by dashed frames.

### 2.3.3 Stoichiometric hydrosilylation of methylstyrene with $Et_3SiH$




In this stoichimetric experiment compound **1** (6.00 mg, 8.14 µmol, 1.00 equiv.) was reacted with $Et_3SiH$ (1.30 µl, 8.14 µmol, 1.00 equiv.) in 0.4 ml $CD_2Cl_2$ to selectively form hydrosilane activation products **3** and **4**. Afterwards another equivalent of $Et_3SiH$ (1.30 µl, 8.14 µmol, 1.00 equiv.) and one equivalent of α-methylstyrene (1.06 ml, 8.14 µmol, 1.00 equiv.) were added. The mixture was analysed after 15 min at room temoerature and then stored for 18 h at -36 °C. Multinuclear NMR analysis revealed the quantitative formation of hydrosilylation product **E**. The initially formed germylene species **3** as well as the silyated alcohol **4** stayed intact during this experiment, which could be observed by $^{19}$F NMR spectroscopy.

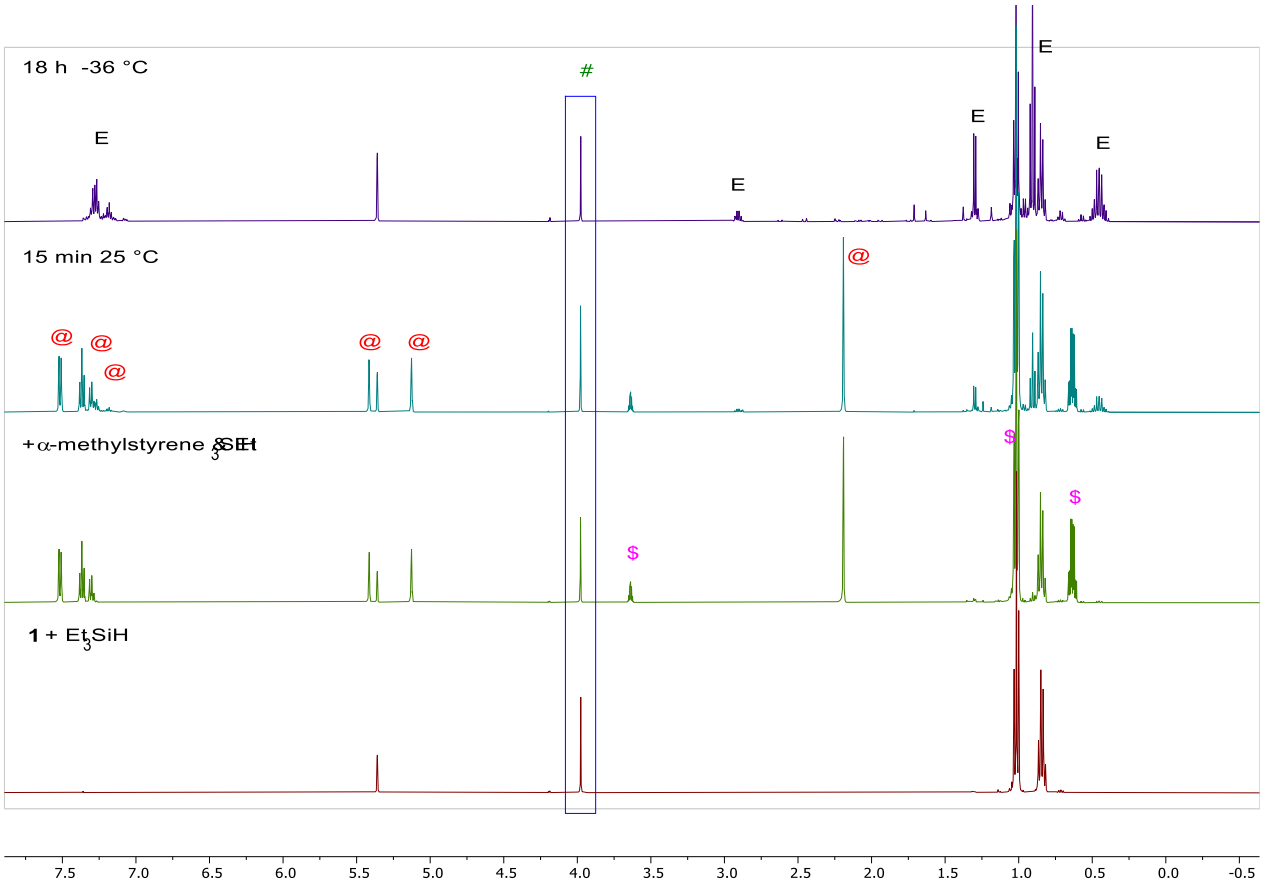



**Figure S 25:** Stacked $^{1}$H NMR spectra of stepwise hydrosilylation experiment in $CD_2Cl_2$. The experiments showed the selective formation of the product mixture containing **4** (#), which stayed intact over the course the catalytic reaction. $Et_3SiH$ ($) and α-methylstyrene (@) were fully converted to hydrosilylation product **E**.

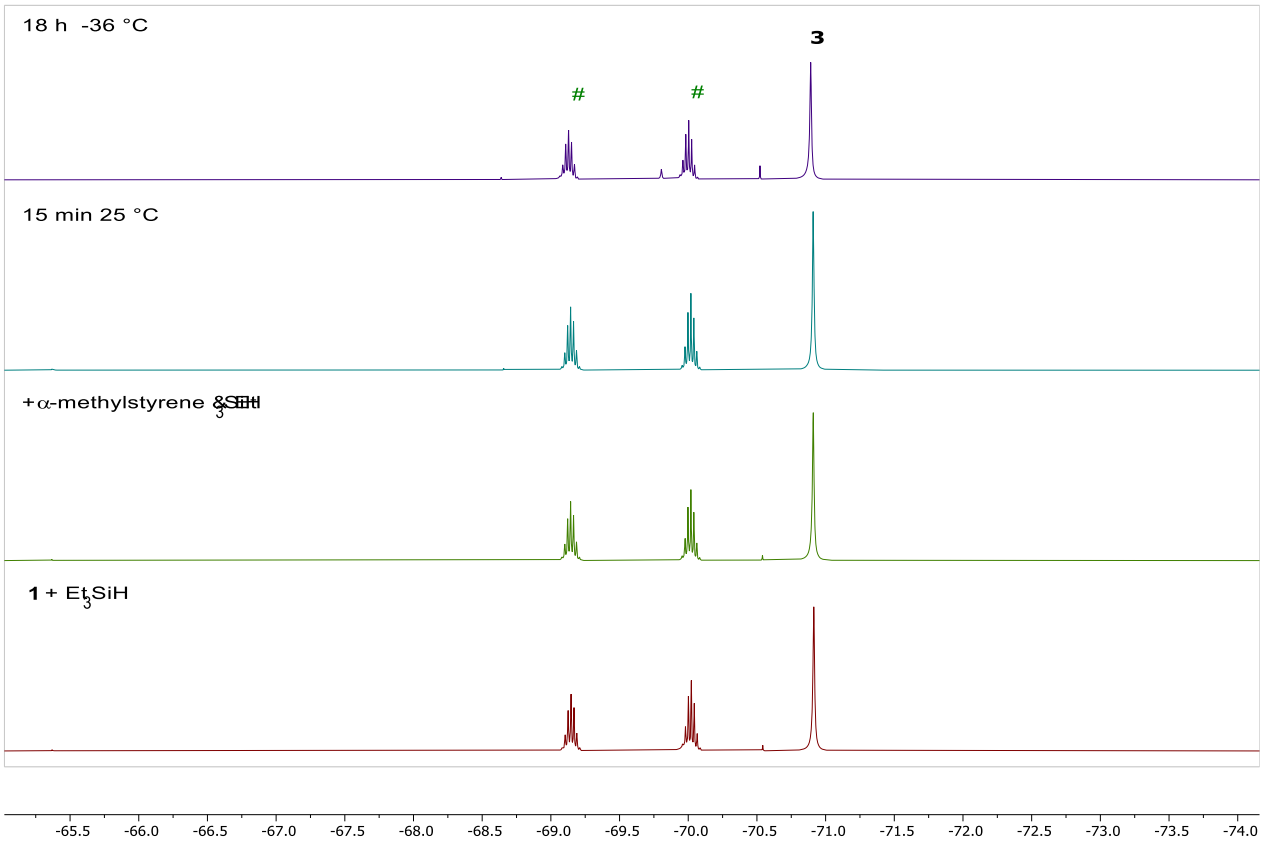
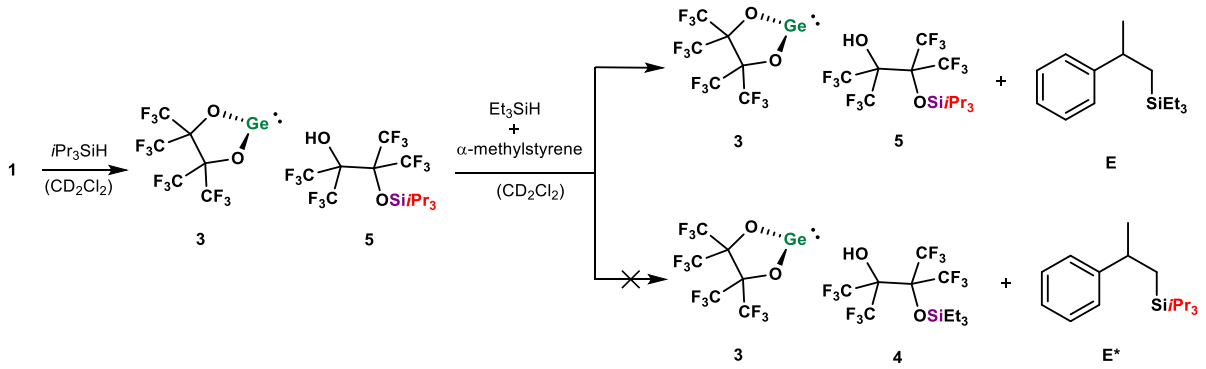



**Figure S 26:** Stacked $^{19}F$ NMR spectra of stepwise hydrosilylation experiment in $CD_2Cl_2$. No change of the germylene species **3** and triethylsilyl perfluoropinacol **4** (#) is observed over the course of the reaction.

### 2.3.4 Hydrosilylation of α-methylstyrene with mixed silanes ($iPr_3SiH$ vs $Et_3SiH$)

**Initiation with *i*$Pr_3SiH$**




In a first experiment **1** (6.00 mg, 8.14 µmol, 1.00 equiv.) was reacted with *i*$Pr_3SiH$ (1.67 µl, 8.14 µmol, 1.00 equiv.) in 0.4 ml $CD_2Cl_2$ to generate the hydrosilane activation products **3** and $Hpin^FSiiPr_3$. Full conversion but less selective product formation, when compared to $Et_3SiH$, was confirmed by NMR analysis. Afterwards $Et_3SiH$ (1.30 µl, 8.14 µmol, 1.00 equiv.) and α-methylstyrene (1.06 ml, 8.14 µmol, 1.00 equiv.) were added and the mixture was stored for 18 h at -36 °C. Subsquent multinuclear NMR analysis revealed the quantitative formation of hydrosilylationproduct **E**. The formation of **E*** was not observed. The catalyst mixutre stayed intact as no change could be observed within the $^{19}F$ NMR spectrum.

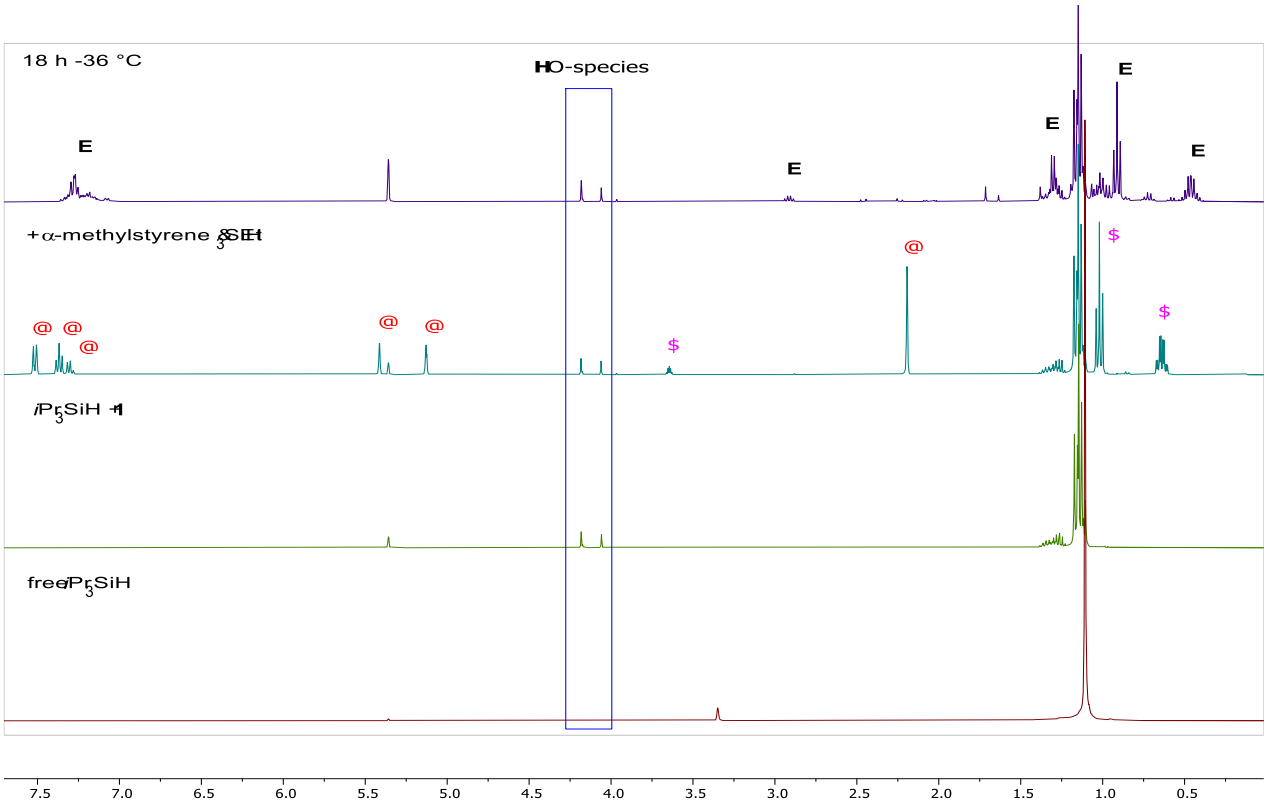



**Figure S 27:** Stacked $^{1}$H NMR spectra of stepwise hydrosilylation experiment in $CD_2Cl_2$ selectively forming product **E**. The experiments initiated with the addition of *i*Pr$_3$SiH, followed by Et$_3$SiH ($) and α-methylstyrene (@). The formation of two alcohol species is observed after *i*Pr$_3$SiH addition.

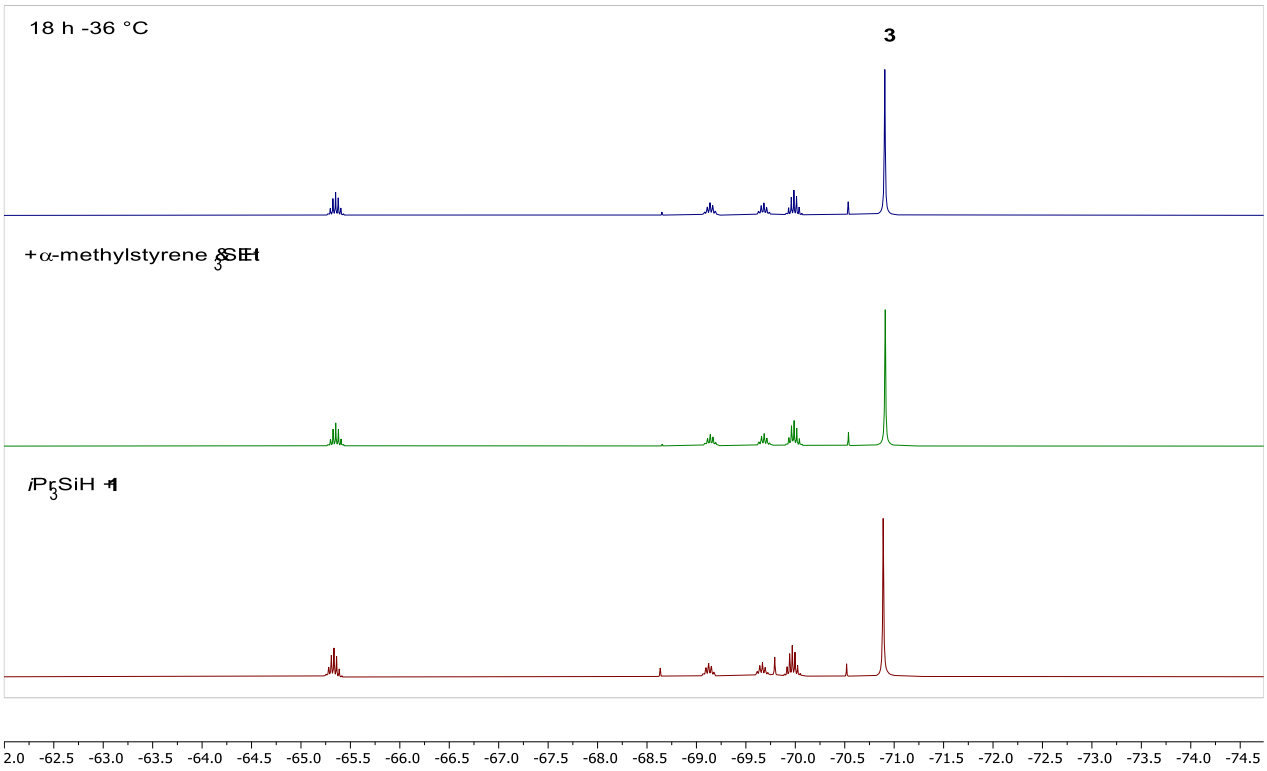
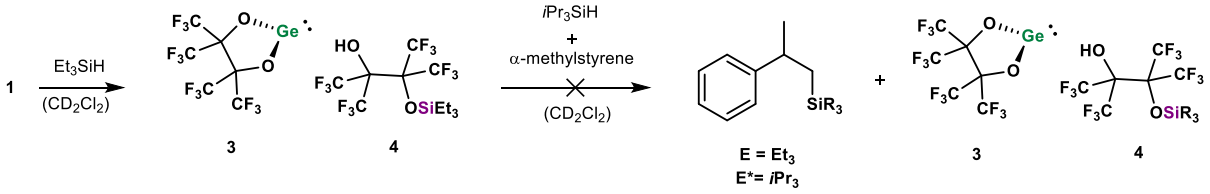



**Figure S 28:** Stacked $^{19}$F NMR spectra of stepwise hydrosilylation experiment in $CD_2Cl_2$. No change of the germylene species **3** is observed after reactant addition and after full conversion.

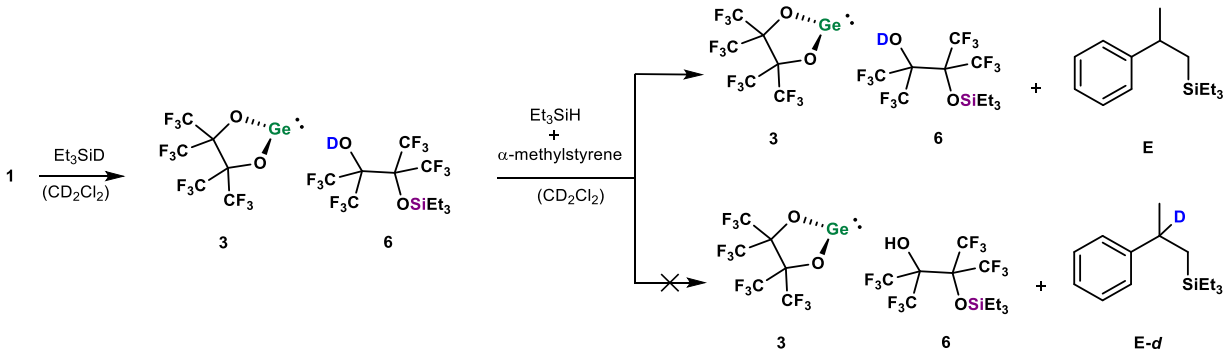
**Initiation with $Et_3SiH$**




In this experiment **1** (6.00 mg, 8.14 µmol, 1.00 equiv.) was reacted with $Et_3SiH$ (1.30 µl, 8.14 µmol, 1.00 equiv.) in 0.4 ml $CD_2Cl_2$ to generate the hydrosilane activation product **3** and **4**. Afterwards $iPr_3SiH$ (1.67 µl, 8.14 µmol, 1.00 equiv.) and α-methylstyrene (1.06 ml, 8.14 µmol, 1.00 equiv.) were added and the mixture was stored for 18 h at -36 °C. Subsquent multinuclear NMR analysis revealed the quantitative conversion of α-methylstyrene but no hydrosilylation product could be identified. An ill-defined product mixutre containing various dimerization products was obtained.

### 2.3.5 Hydrosilylation of α-methylstyrene with isotopically marked $Et_3SiD$

**Initiation with $Et_3SiD$**




Here **1** (6.00 mg, 8.14 µmol, 1.00 equiv.) was reacted with $Et_3SiD$ (1.67 µl, 8.14 µmol, 1.00 equiv.) in 0.4 ml $CD_2Cl_2$ to generate **3** and deuterated $Dpin^FSiEt_3$. Full conversion was confirmed by NMR analysis. Afterwards $Et_3SiH$ (1.30 µl, 8.14 µmol, 1.00 equiv.) and α-methylstyrene (1.06 ml, 8.14 µmol, 1.00 equiv.) were added and the mixture was stored for 18 h at -36 °C. NMR analysis revealed the quantitative formation of hydrosilylationproduct **E** while both **3** and **6** stayed intact. The formation of deuterated **E-*d*** was not observed.

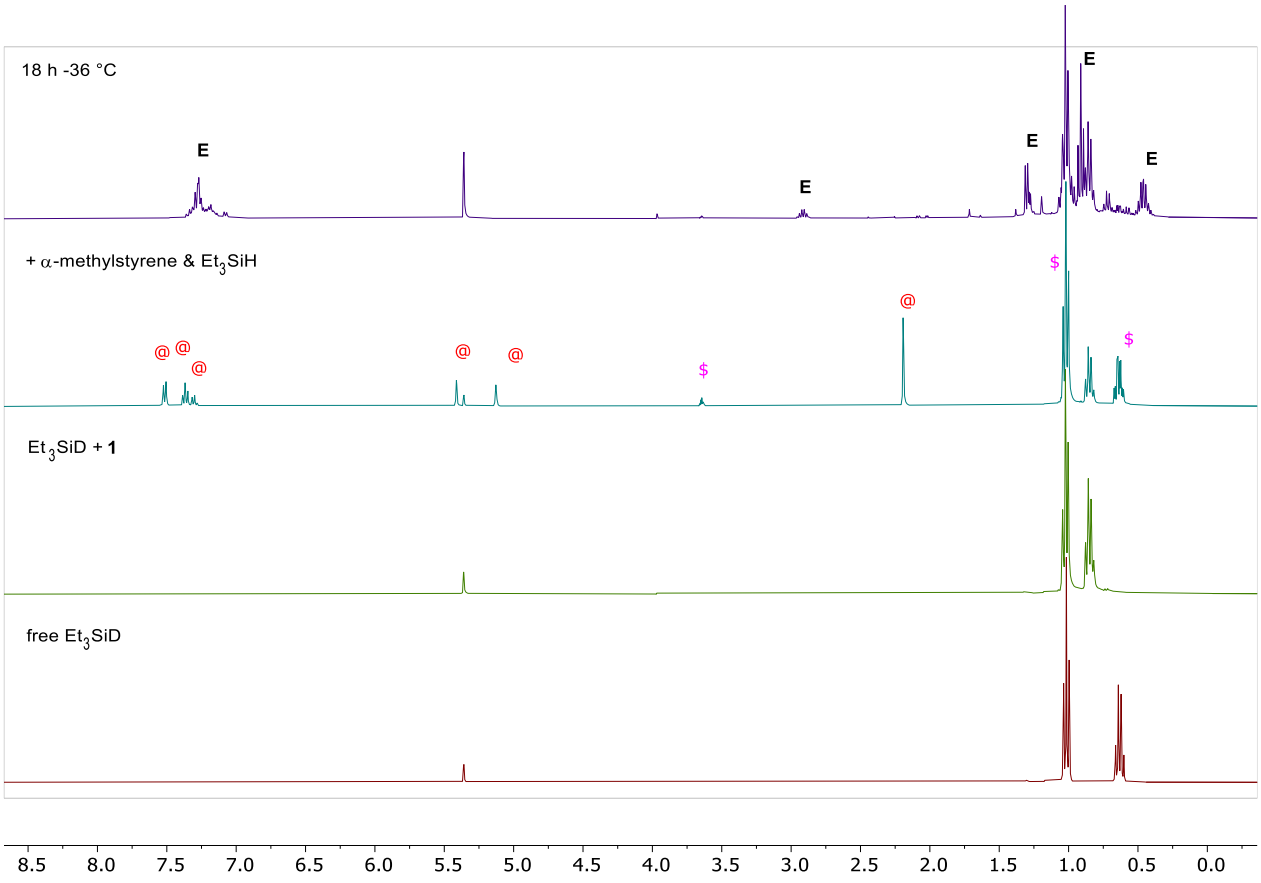



**Figure S 29:** Stacked $^{1}$H NMR spectra of stoichiometric hydrosilylation experiment with isotopically marked $Et_3SiD$ in $CD_2Cl_2$ selectively forming product **E**. The spectra show additionally show reactants $Et_3SiH$ ($) and α-methylstyrene (@) directly after the addition. No formation of the Ge-H species or potential reaction product **E-*d*** was observed.

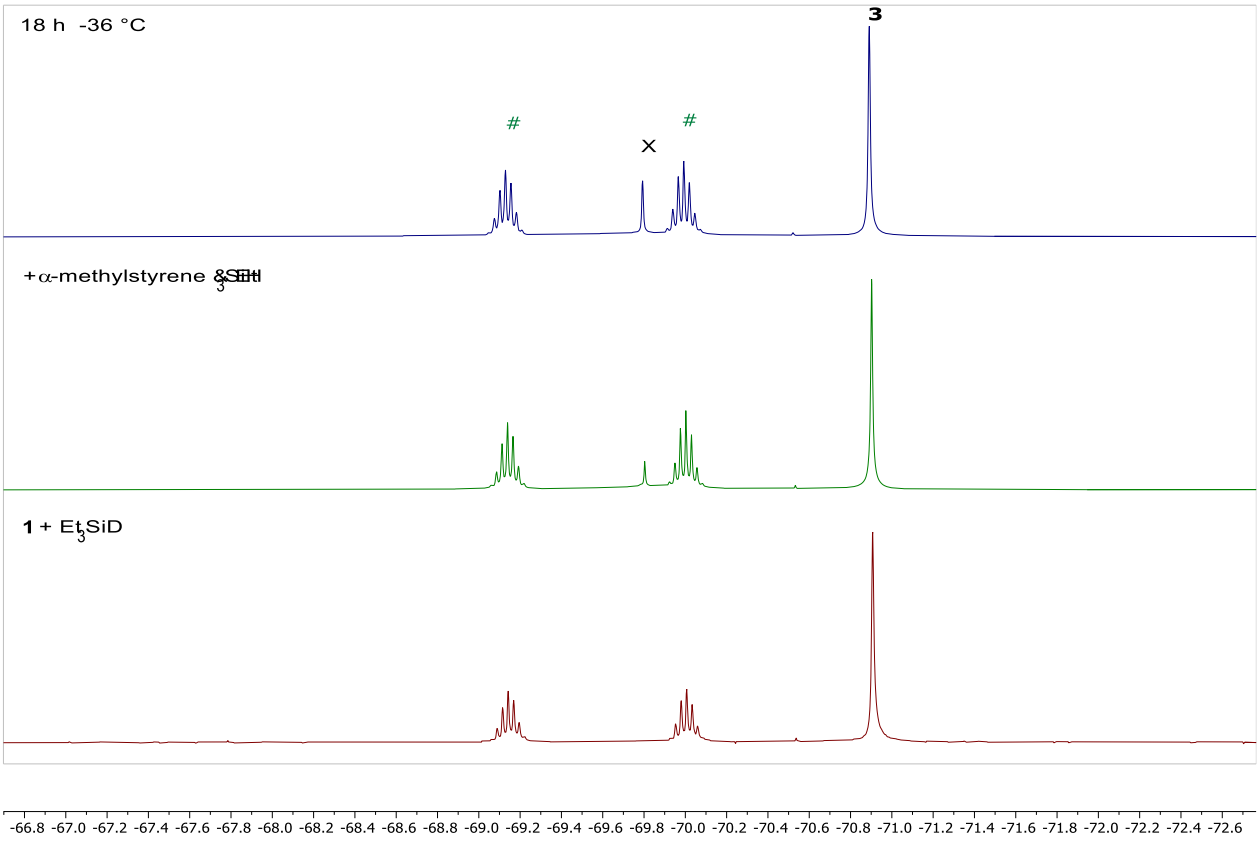
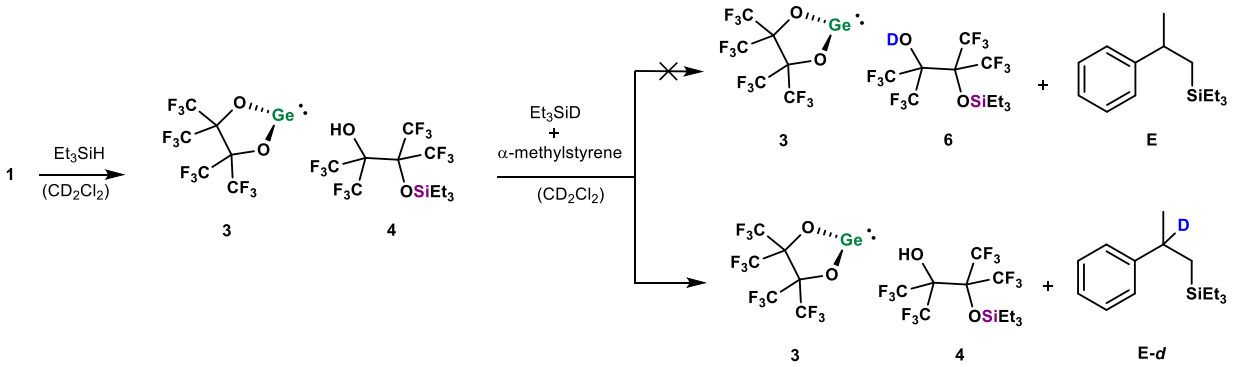



**Figure S 30:** Stacked $^{19}F$ NMR spectra of stoichiometric hydrosilylation experiment with $Et_3SiD$ in $CD_2Cl_2$. The formation of an undefined side product **X** is observed while the germylene species **3** and **6** (#) stayed intact.

### Initiation with $Et_3SiH$




To double check the obtained results **1** (6.00 mg, 8.14 µmol, 1.00 equiv.) was reacted with non-deuterated $Et_3SiH$ (1.67 µl, 8.14 µmol, 1.00 equiv.) in 0.4 ml $CD_2Cl_2$ to generate perfluoropinacolatogermylene **3** and triethylsilyl perfluoropinacol **4**. Full conversion was confirmed by NMR analysis. Afterwards deuterated $Et_3SiD$ (1.30 µl, 8.14 µmol, 1.00 equiv.) and α-methylstyrene (1.06 ml, 8.14 µmol, 1.00 equiv.) were added and the mixture was stored for 18 h at -36 °C. NMR analysis revealed the quantitative formation of hydrosilylationproduct **E-*d*** while catalyst **3** and **4** stayed intact. This time, no formation of non-deuterated **E** was observed.

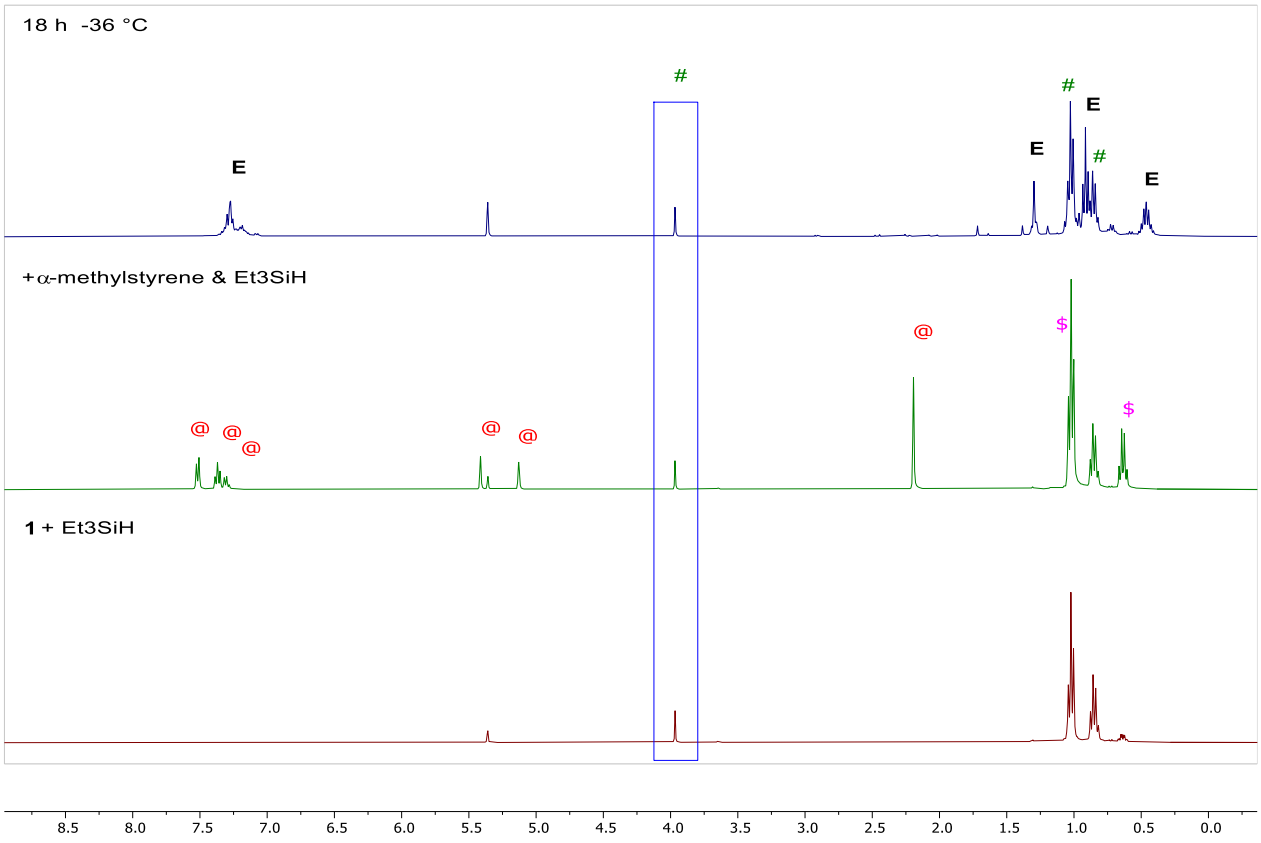



**Figure S 31:** Stacked $^{1}$H NMR spectra of stoichiometric hydrosilylation experiment with $Et_3SiD$ (initiating with $Et_3SiH$ addition) in $CD_2Cl_2$ selectively forming hydrosilylation product **E-*d***. The spectra additionally contain reactants isotopically marked $Et_3SiD$ ($) and α-methylstyrene (@) directly after the addition. No conversion of **4** (#) species or formation of reaction product **E** was observed in this case.

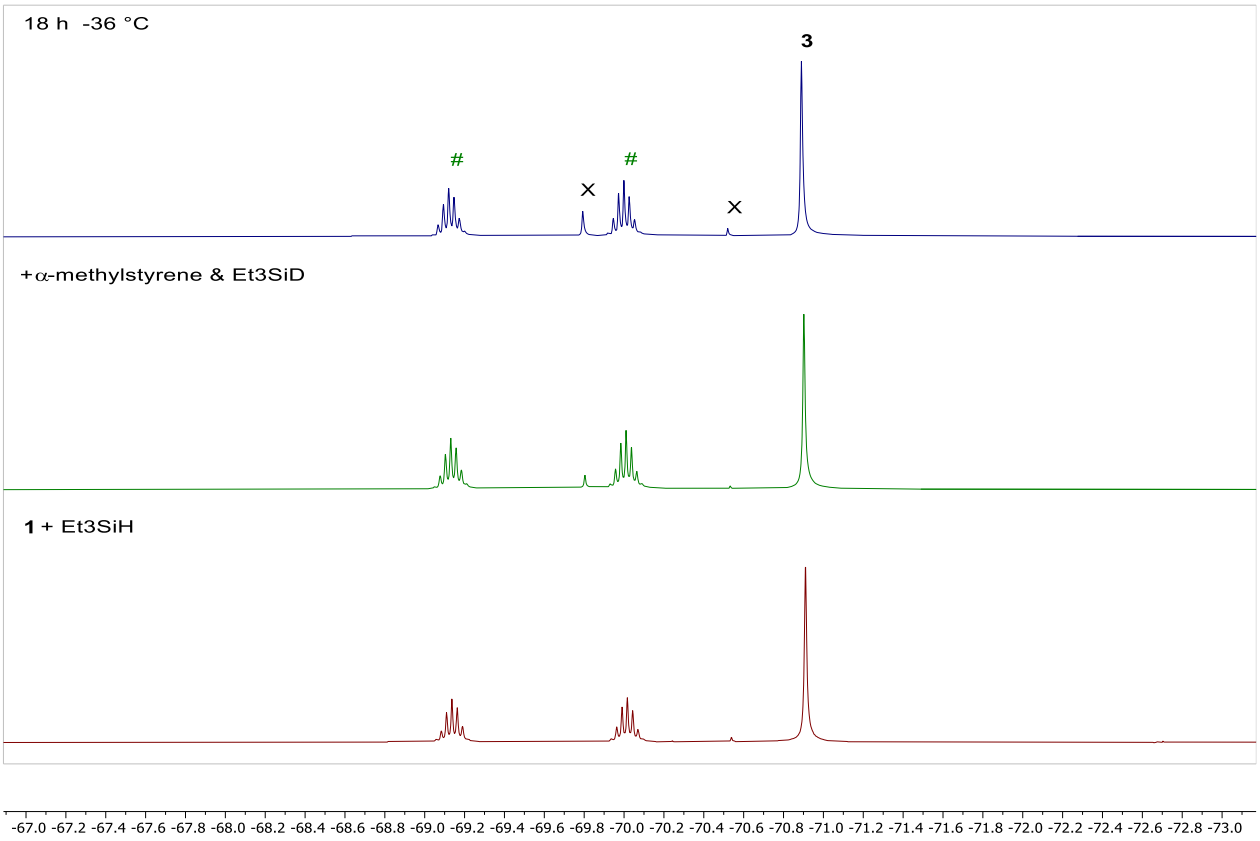



**Figure S 32:** Stacked $^{19}F$ NMR spectra of stoichiometric hydrosilylation experiment with $Et_3SiD$ (initiating with $Et_3SiH$ addition) in $CD_2Cl_2$. The formation of an undefined side product **X** was observed while the germylene species **3** and **4** (#) stayed untouched.

# 3 Computational Section

Calculations were carried out using ORCA 5.0.4.[17]

Geometry optimizations for the mechanistic investigations were carried out at the PBE0[18] level of theory. The calculations utilized the atom-pairwise dispersion correction based on tight binding partial charges (D4),[19] the def2-TZVP basis set,[20] CPCM solvation model with the corresponding parameters for dichloromethane, benzene, and acetonitrile. The method is denoted as PBE0-D4(CPCM)/def2-TZVP. The calculations were accelerated by resolution-of-identity (RI) approximation with def2/J auxiliary basis set.[21] The optimized geometries were verified as minima or transition states by analytical frequency calculations. The transition states were verified by IRC calculations. Cartesian coordinates of the optimized geometries are given in Appendix A.

For details regarding the ion affinities calculations see section 3.6 Calculation of ion affinities.

### 3.2 Hydrosilane activation mechanism

The activation of $HSiEt_3$ with donor-free germane **1** and silane **2** was calculated on the BPE0-D4(CPCM=DCM)/BPE0-D4(CPCM=DCM) level of theory (Figure S 33). The reactions are predicted to proceed in two step. First, the silane coordinates to the Lewis acidic center to form the intermediate **INT_A**. The second step involves the formal metathesis reaction of Si-H E-O bond to form the ring-opening product **3***. With a barrier of 12.8 kcal $mol^{-1}$ (TS(1_INT_A_Ge)) the hydride abstraction and the ring opening are easily accessible in the case of germane **1**. In the silicon case, the barrier (TS(INT_A_Si_3*)) is significantly higher in energy (28.8 kcal $mol^{-1}$). Furthermore, the overall process is endergonic by 5.9 kcal $mol^{-1}$. In contrast, for germane **1** the reaction is exergonic by 13.0 kcal $mol^{-1}$. The calculations align well with the experimentally observed reactivity, as no interaction between silane **2** and hydrosilanes was monitored. Germylene **1** on the other hand readily activates $Et_3SiH$ forming compound **3*** that decomposes to release the germylene **3** and mono-silylated perfluoropinacol **4**.

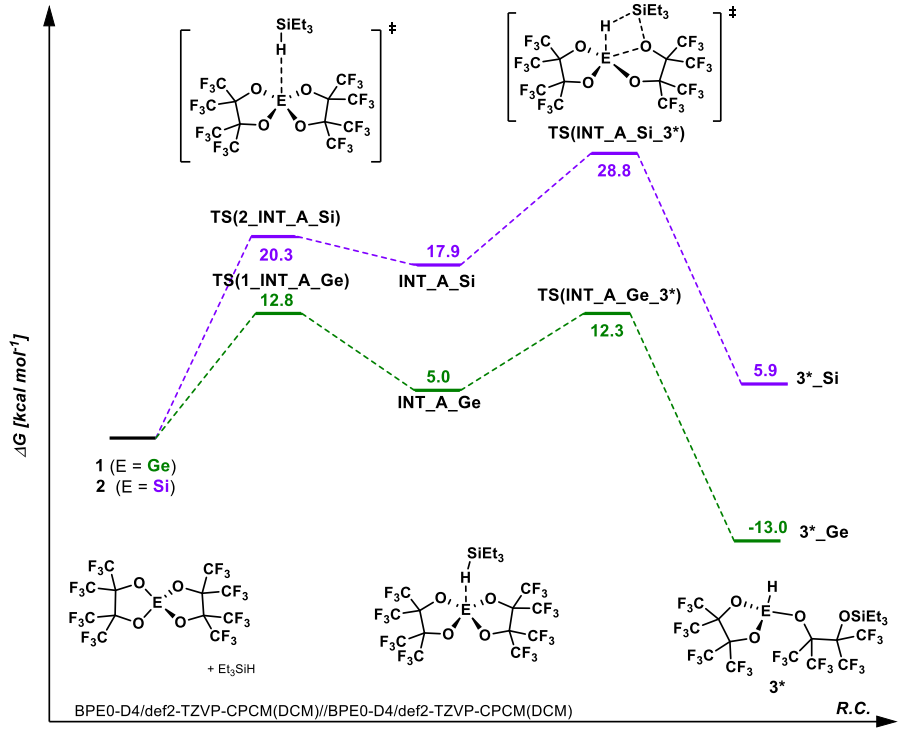



**Figure S 33:** Reaction mechanism for the activation $Et_3SiH$ with **1** and **2**.

**Table S 4:** PBE0-D4(CPCM=DCM)/def2-TZVP//PBE0-D4(CPCM=DCM)//def2-TZVP calculated energies ($E_h$) (E – electronic energy; H – total enthalpy; G – Gibbs energy; $G_S = G + G_{conc}$) of the compounds in Figure **S33**. Thermochemistry at 298.15 K.

| Compound | E | H | G | $G_S$ |
|---|---|---|---|---|
| $HSiEt_3$ | -527.47794089 | -527.26095375 | -527.30955265 | -527.3065325 |
| **1** | -5229.60383427 | -5229.40102877 | -5229.50026724 | -5229.497247 |
| **TS(1_INT_A_Ge)** | -5757.08372525 | -5756.66273811 | -5756.78633436 | -5756.783314 |
| **INT_A_Ge** | -5757.09570753 | -5756.67461003 | -5756.79886433 | -5756.795844 |
| **TS(INT_A_3*_Ge)** | -5757.08459280 | -5756.66407390 | -5756.78714612 | -5756.784126 |
| **3*_Ge** | -5757.12723823 | -5756.70436594 | -5756.82749411 | -5756.784126 |
| **2** | -3442.33762144 | -3442.13280403 | -3442.23043761 | -3442.227417 |
| **TS(1_INT_A_Si)** | -3969.80591658 | -3969.38299325 | -3969.50463621 | -3969.501616 |
| **INT_A_Si** | -3969.80988667 | -3969.38569342 | -3969.50849320 | -3969.505473 |
| **TS(INT_A_3*_Si)** | -3969.79415802 | -3969.37080317 | -3969.49109157 | -3969.488071 |
| **3*_Si** | -3969.83058328 | -3969.40556420 | -3969.52758424 | -3969.524564 |

### 3.3 Thermochemistry analysis of the hydrosilylation catalytic cycle

The reported energy differences for reaction components are at the PBE0-D4(CPCM)/def2-TZVP//PBE0-D4(CPCM)/def2-TZVP level of theory with the gas to liquid phase correction term, i.e. concentration-induced free-energy shift $G_{conc}$ = RTln(24.5) (1.51, 1.90 and 2.24 kcal mol$^{-1}$ at 238.15, 298.15 and 298.15K, respectively) is included in the free energy $G_S$ of each compound.

**Table S 5**: Thermochemistry analysis at 238.15, 298.15 and 353.15 K for the components of the reaction mechanism in Figure 4, calculated at the PBE0-D4(CPCM=DCM)/def2-TZVP level of theory. E – Electronic energy ($E_h$) ; $(G-E)_T$ - Gibbs energy minus the electronic energy at the different temperatures ($E_h$); $G_T$ – Gibbs energy at the different temperatures ($E_h$) , $G_T = E + (G-E)_T + G_{conc\,T}$.

| Compound | E | $(G-E)_{238.15K}$ | $(G-E)_{298.15K}$ | $(G-E)_{353.15K}$ | $G_{S,238.15K}$ | $G_{S,298.15K}$ | $G_{S,353.15K}$ |
|---|---|---|---|---|---|---|---|
| $HSiEt_3$ | -527.47794 | 0.17746 | 0.16839 | 0.15941 | -527.29806 | -527.30653 | -527.31495 |
| $C_6H_5C(CH_3)=CH_2$ | -348.67931 | 0.13738 | 0.12950 | 0.12174 | -348.53952 | -348.54679 | -348.55399 |
| $PhC(H)(CH_3)\text{-}CH_2SiEt_3$ | -876.20164 | 0.33974 | 0.32769 | 0.31545 | -875.85948 | -875.87093 | -875.88261 |
| $(pin^F)Ge$: (**3**) | -3653.18557 | 0.04907 | 0.03726 | 0.02535 | -3653.13409 | -3653.14529 | -3653.15664 |
| **INT1** | -7655.09020 | 0.27477 | 0.25312 | 0.23058 | -7654.81303 | -7654.83406 | -7654.85605 |
| **TS1** | -7655.08522 | 0.27506 | 0.25363 | 0.23130 | -7654.80775 | -7654.82857 | -7654.85034 |
| **INT2** | -8182.57273 | 0.47418 | 0.44852 | 0.42165 | -8182.09614 | -8182.12119 | -8182.14750 |
| **TS2** | -8182.56381 | 0.47632 | 0.45096 | 0.42439 | -8182.08508 | -8182.10984 | -8182.13585 |

### 3.4 Alternative mechanisms for the catalytic hydrosilylation

Initially we considered a few proposed mechanisms for catalytic hydrosilylation of the α-methylstyrene mediated by the germylene **3**, which involved one molecule of the germylene.

In the mechanism shown in Figure S34, α-methylstyrene coordinates to the germylene to form the coordination intermediate **INT1'**. The concerted addition of the silane across the C-C bond is exergonic by 12.3 kcal mol$^{-1}$, however it need to overcome a very high lying transition state **TS3** at 37.0 kcal mol$^{-1}$, making this reaction pathway infeasible under the experimental conditions.

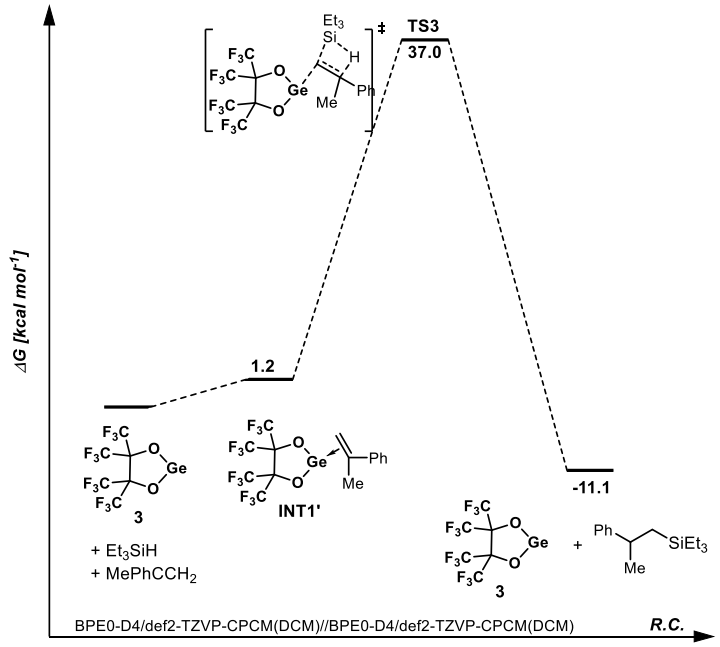



**Figure S 34:** Alternative mechanism for hydrosilylation by **3**, via olefin activation.

In an additional mechanism that was considered by us, the silane an the olefin are activated in a concerted fashion via a 5-membered transition state **TS4** at 23.8 kcal mol$^{-1}$ to form the Ge(IV) intermediate **INT3**. However, **TS4** is by 2.0 kcal mol$^{-1}$ higher in energy that the rate determining transition state **TS2**. Additionally, the intermediate **INT3** is a very deep minimum. The reductive elimination of the silylated product from **INT3** is endergonic by 8.8 kcal mol$^{-1}$ and would need to overcome a barrier of 54.6 kcal mol$^{-1}$, which is unfeasible. Since **INT3** is not observed in the catalytic reaction mixtures we also rule out this scenario.

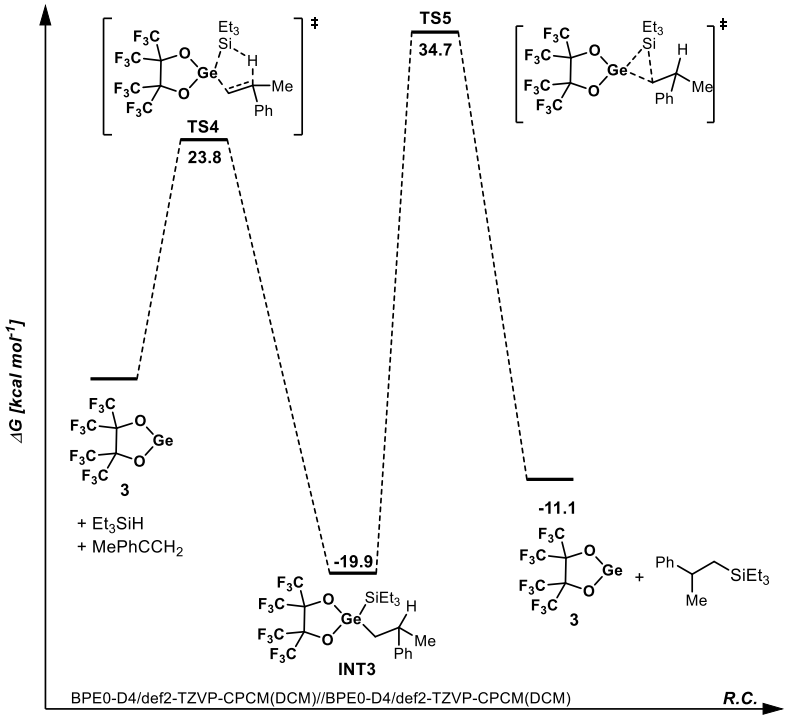



**Figure S 35:** Alternative mechanism for hydrosilylation by **3**, via concerted activation of the silane and the olefin.

We also considered a possibility in which the germylene activates the silane at the first step of the catalytic cycle. Thus, we calculated the transition states and the products of the oxidation addition of the germanium center across the Si-H bond to form the corresponding germane **5** (Figure 36, purple), as well the addition across the Ge-O bond to form the silyl ether **6** (Figure 36, orange). In the former case, the reaction is exergonic by 2.5 kcal mol$^{-1}$, however the barrier, **TS6** at 34.5 kcal mol$^{-1}$ is too high to overcome at rt. The formation of **6**, is both endergonic and requires a very high barrier, **TS7** at 36.0 kcal mol$^{-1}$. Thus, we had to rule out the mechanism of the catalytic hydrosilylation that involve initial activation of the silane by **3**.

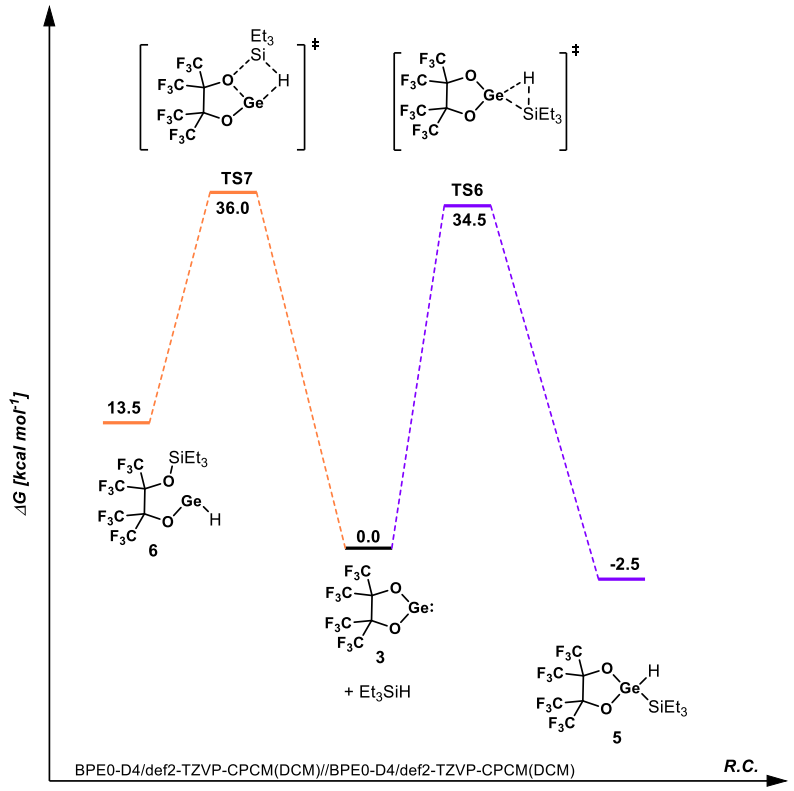



**Figure S 36.** Activation of $Et_3SiH$ by **3**. .

**Table S 6:** PBE0-D4(CPCM=**DCM**)/def2-TZVP//PBE0-D4(CPCM=**DCM**)//def2-TZVP calculated energies ($E_h$) (E – electronic energy; H – total enthalpy; G – Gibbs energy; $G_S = G + G_{conc}$) of the compounds in Figures S34, S35, S36.Thermochemistry at 298.15 K.

| Compound | E | H | G | $G_S$ |
|---|---|---|---|---|
| $Et_3SiH$ | -527.47794089 | -527.26095375 | -527.30955265 | -527.3065325 |
| $C_6H_5C(CH_3)=CH_2$ | -348.67930941 | -348.50860159 | -348.54980691 | -348.5467868 |
| $PhC(H)(CH_3)-CH_2SiEt_3$ | -876.20163736 | -875.80789303 | -875.87394682 | -875.8709267 |
| $(pin^F)Ge$: (**3**) | -3653.18556968 | -3653.08432860 | -3653.14830528 | -3653.145285 |
| **INT1'** | -4001.88343534 | -4001.60950462 | -4001.69322602 | -4001.690206 |
| **INT3** | -4529.42479979 | -4528.92716084 | -4529.03327144 | -4529.030251 |
| **5** | -4180.68961685 | -4180.36895133 | -4180.45874709 | -4180.455727 |
| **6** | 4180.66063500 | -4180.34073622 | -4180.43037547 | -4180.427355 |
| **TS3** | -4529.33050459 | -4528.83632640 | -4528.94268493 | -4528.939665 |
| **TS4** | -4529.34815297 | -4528.85730789 | -4528.96362146 | -4528.960601 |
| **TS5** | -4529.33432713 | -4528.83959212 | -4528.94643774 | -4528.943418 |
| **TS6** | -4180.62860727 | -4180.31071973 | -4180.39985862 | -4180.396838 |
| **TS7** | -4180.62859703 | -4180.31011627 | -4180.39745030 | -4180.394430 |

## 3.5 **Calculated energies for compounds in Figure 3 and Scheme 2B**.

**Table S 7:** PBE0-D4(CPCM=**Benzene**)/def2-TZVP//PBE0-D4(CPCM=**Benzene**)//def2-TZVP calculated energies ($E_h$) (E – electronic energy; H – total enthalpy; G – Gibbs energy; $G_S = G + G_{conc}$) of the compounds in Figure 3. Thermochemistry at 298.15 K.

| Compound | E | H | G | $G_S$ |
|---|---|---|---|---|
| **1**·MeCN | -5362.27989486 | -5362.02487581 | -5362.13407019 | -5362.13105 |
| **2**·MeCN | -3575.00611941 | -3574.74907229 | -3574.85531876 | -3574.852299 |
| $B(C_6F_5)_3$ | -2207.04435998 | -2206.85835763 | -2206.94390926 | -2206.940889 |
| $MeCN{\cdot}B(C_6F_5)_3$ | -2339.72502805 | -2339.48685703 | -2339.58041533 | -2339.577602 |
| **1** | -5229.60274820 | -5229.39943902 | -5229.49860457 | -5229.495584 |
| **2** | -3442.33672263 | -3442.13138544 | -3442.22895812 | -3442.225938 |

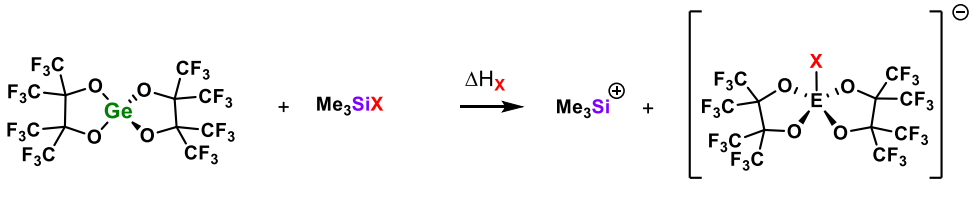
**Table S 8:** PBE0-D4(CPCM=**DCM**)/def2-TZVP//PBE0-D4(CPCM=**DCM**)//def2-TZVP calculated energies ($E_h$) (E – electronic energy; H – total enthalpy; G – Gibbs energy; $G_S = G + G_{conc}$) of the compounds in Scheme 2B. Thermochemistry at 298.15 K.

| Compound | E | H | G | $G_S$ |
|---|---|---|---|---|
| $Et_3SiH$ | -527.47794089 | -527.26095375 | -527.30955265 | -527.3065325 |
| **1** | -5229.60383427 | -5229.40102877 | -5229.50026724 | -5229.497247 |
| **1**·MeCN | -5362.28957277 | -5362.03518325 | -5362.14349099 | -5362.140471 |
| B[H-**1**] | -5230.38307456 | -5230.17303971 | -5230.27259092 | -5230.269571 |
| $[MeCN{\rightarrow}Et_3Si]^+$ | -659.40109109 | -659.13947027 | -659.19731608 | -659.1942959 |
| **3** | -3653.18556968 | -3653.08432860 | -3653.14830528 | -3653.145285 |
| **3**·MeCN | -3785.85639647 | -3785.70362806 | -3785.77885706 | -3785.775837 |
| **3*_Ge** | -5757.12723823 | -5756.70436594 | -5756.82749411 | -5756.784126 |
| **4** | -2103.92509554 | -2103.60313079 | -2103.68923676 | -2103.686217 |

**Table S 9:** PBE0-D4(CPCM=**acetonitrile**)/def2-TZVP//PBE0-D4(CPCM=**acetonitrile**)//def2-TZVP calculated energies ($E_h$) (E – electronic energy; H – total enthalpy; G – Gibbs energy; $G_S = G + G_{conc}$) of the compounds in Scheme 2B. Thermochemistry at 298.15 K.

| Compound | E | H | G | $G_S$ |
|---|---|---|---|---|
| $Et_3SiH$ | -527.47814599 | -527.26125033 | -527.30985532 | -527.3068352 |
| **1** | -5229.60411347 | -5229.40144558 | -5229.50070480 | -5229.497685 |
| **1**·MeCN | -5362.29230028 | -5362.03809409 | -5362.14640094 | -5362.143381 |
| B[H-**1**] | -5230.38799575 | -5230.17806933 | -5230.27760702 | -5230.274587 |
| $[MeCN{\rightarrow}Et_3Si]^+$ | -659.40790905 | -659.14636791 | -659.20410583 | -659.2010857 |
| **3**·MeCN | -3785.85836779 | -3785.70572528 | -3785.78067625 | -3785.777656 |
| **4** | -2103.92589053 | -2103.60407120 | -2103.69020638 | -2103.687186 |

For comparison with the previously published results,[1] the gas phase ion affinities of **1** were calculated at the same level of theory, i.e. PBE0-D3BJ[22]/def2-TZVPP//DLPNO-CCSD(T)/aug-cc-pVQZ.[23] The ion affinity values of the reference compound $Me_3Si^+$ (FIA = 953 kJ, HIA = 924 kJ) calculated at the CCSD(T)/CBS level of theory are taken from literature (Figure S 37).[24] The calculated energies are given in Table 1.




| | $\Delta H_H$ | $\Delta H_F$ | HIA | FIA |
|---|---|---|---|---|
| PBE0 | 388.1 | 460.9 | 535.9 | 492.1 |
| DLPNO-CCSD(T) | 399.9 | 467.9 | 524.1 | 485.1 |

**Figure S 37.** . Hydride and fluoride ion affinities of **1**, relative to the reference compound $Me_3Si^+$.

Table 1. Calculated $E_{PBE0\text{-}D3}$ (electronic energy, ($E_h$)) and $H_{PBE0\text{-}D3}$ (enthalpy, ($E_h$)) at the PBE0-D3/def2-TZVPP//PBE0-D3/def2-TZVPP level of theory. $E_{(DLPNO\text{-}CCSD(T))}$ – electronic energy at the DLPNO-CCSD(T)/aug-cc-pVQZ//PBE0-D3/def2-TZVPP level of theory.

| Compound | $E_{PBE0\text{-}D3}$ | $H_{PBE0\text{-}D3}$ | $E_{(DLPNO\text{-}CCSD(T))}$ |
|---|---|---|---|
| $(pin^F)_2Ge$ | -5229.589261 | -5229.385278 | -5227.503704 |
| $[(pin^F)_2GeH]^-$ (**B[H-1]**) | -5230.319351 | -5230.108305 | -5228.237155 |
| $[(pin^F)_2GeF]^-$ (**B[F-1]**) | -5329.565126 | -5329.358558 | -5327.464448 |
| $Me_3SiH$ | -409.6509397 | -409.5238372 | -409.254734 |
| $Me_3SiF$ | -508.9243983 | -508.8018046 | -508.5078966 |
| $Me_3Si^+$ | -408.7706389 | -408.6529826 | -408.3665695 |

# 4 Single-Crystal X-ray Diffraction Analysis

## 4.1 Crystal Structure of 1·MeCN

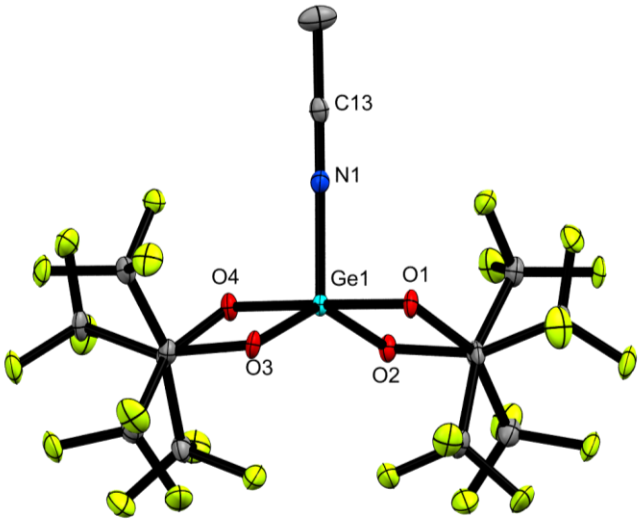



**Figure S 38:** Molecular structure of **1**·MeCN with translational ellipsoids plotted at 50% probability level. Hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles [deg]: Ge1−N1 1.933(4), Ge1−O1 1.827(3), Ge1−O2 1.794(3), Ge1−O3 1.782(3), Ge1−O4 1.833(3); O1−Ge1−O2 88.39(12), O1−Ge1−O4 179.20(13), O3−Ge1−O4 88.12(12), O2−Ge1−O3 136.47(13).

## 4.2 Crystal Structure of [K·(18-c-6)][F-1]

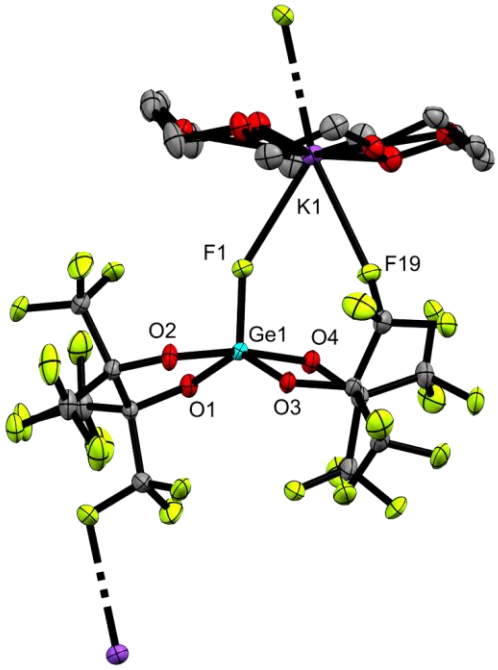



**Figure S 39:** Molecular structure of [K·(18-c-6)][F-**1**] with translational ellipsoids plotted at 50% probability level. Hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles [deg]: Ge1−F1 1.7274(16), Ge1−O1 1.8122(19), Ge1−O2 1.841(2), Ge1−O3 1.8100(19), Ge1−O4 1.8467(19), F1−K1 2.8189(18); O1−Ge1−O4 90.60(9), O2−Ge1−O3 87.58(8), O1−Ge1−O2 86.70(9), O3−Ge1−O4 86.88(8).

## 4.3 Crystal Structure of donor-free silane 2

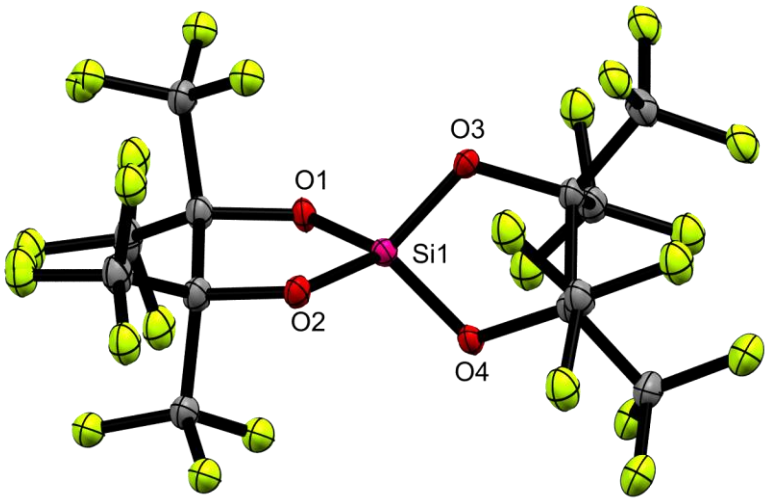



**Figure S 40:** Molecular structure of MeCN-free **2** with translational ellipsoids plotted at 50% probability level. Hydrogen atoms are omitted for clarity. The structure contains a second, twisted overlaying disordered, that is also omitted for clarity reasons. Selected bond lengths [Å] and angles [°]: Si1–O1 1.744(18), Si1–O2 1.754(17), Si1–O3 1.779(18), Si1–O4 1.684(18); O1–Si1–O4 131.7(8), O2–Si1–O3 166.0(8).

## 4.4 Crystal Structure of dioxane-coordinated germylene 3

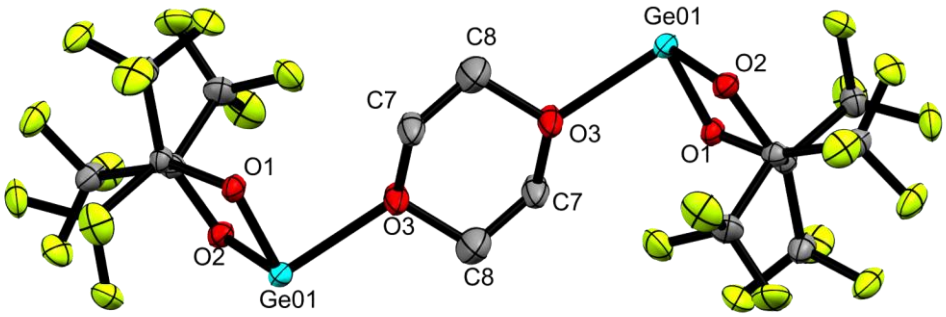



**Figure S 41:** Molecular structure of 1,4-dioxane-coordinted germylene **3** with translational ellipsoids plotted at 50% probability. Hydrogen atoms are omitted for clarity. The figure contains two symmetry-generated unit cells. Selected bond lengths [Å] and angles [°]: Ge011–O1 1.853(2), Ge01–O2 1.853(2), Ge01–O3 2.241(3); O1–Ge01–O2 85.60(10), O1–Ge01–O3 84.71(10), O2–Ge01–O3 106.29(11).

## 4.5 Preliminary crystal structure of donor-free 1

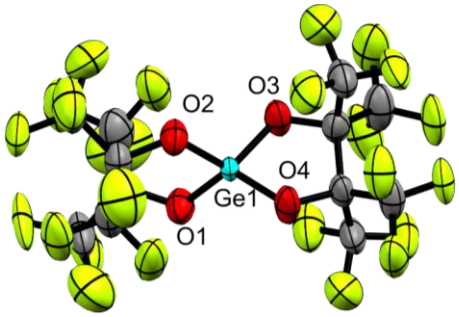



**Figure S 42:** Preliminary molecular structure of **1** with translational ellipsoids plotted at 50% probability. Because of heavy disorder only insufficient data refinement was possible. The depicted structure demonstrates a similar connectivity as for compound **2**. However, no bond lengths and angles can be discussed. This depiction is no structure evidence due to lacking data quality.

**Table S 10:** Crystallographic Details.

| | **1·MeCN** | **[K·(18-c-6)][F-1]** | **2** |
|---|---|---|---|
| CCDC-Number | 2286080 | 2286083 | 2286081 |
| | | **Crystal Data** | |
| Chemical formula | $C_{14}H_3F_{24}GeNO_4$ | $C_{48}H_{47}F_{50}Ge_2K_2O_{20}$ | $C_{12}F_{24}O_4Si$ |
| $M_r$ | 777.78 | 2116.91 | 692.21 |
| Crystal system, space group | Orthorhombic, *Pbcn* | Triclinic, -*P*1 | Orthorhombic, $P2_12_12$ |
| Temperature (K) | 100 | 100 | 100 |
| *a*, *b*, *c* (Å) | 23.5238(15), 8.6067(5), 21.8982(13) | 11.2001(10), 15.7831(14), 22.3057(19) | 8.3174(7), 10.3383(8), 11.4253(8) |
| α, β, γ (°) | 90, 90, 90 | 107.062(3), 102.834(3), 95.235(3) | 90, 90, 90 |
| *V* (Å$^3$) | 4433.6(5) | 3623.2(6) | 982.44(13) |
| *Z* | 8 | 2 | 2 |
| Radiation type | Mo *K*a | Mo *K*a | Mo *K*a |
| μ (mm$^{-1}$) | 1.611 | 1.141 | 0.369 |
| Crystal size (mm) | 0.174 × 0.112 × 0.068 | 0.58 × 0.318 × 0.279 | 0.255 × 0.207 × 0.160 |
| Crystal shape | Fragment | Block | Fragment |
| Color | Clear colorless | Clear colorless | Clear colorless |
| | | **Data Collection** | |
| Diffractometer | Bruker Photon CMOS | Bruker Photon CMOS | Bruker Photon CMOS |
| Absorption correction | Multi-scan | Multi-scan | Multi-scan |
| $T_{min}$, $T_{max}$ | 0.7453, 0.6764 | 0.7453, 0.6350 | 0.7452, 0.5419 |
| No. of measured, independent, and observed [$I > 2\sigma(I)$] reflections | 117042, 4064, 3029 | 133009, 13270, 11373 | 6489, 1797, 1437 |
| $R_{int}$ | 0.0960 | 0.0472 | 0.0820 |
| θ range (°) for cell measurement | 2.52- 25.35 | 2.33-25.72 | 2.66-25.34 |
| Data completeness | 0.999 | 1.000 | 0.998 |
| | | **Refinement** | |
| $R[F^2 > 2\sigma(F^2)]$, $R(F^2)$, *S* | 0.0458, 0.1171, 1.017 | 0.0348, 0.0717, 1.087 | 0.0619, 0.1409, 1.047 |
| No. of reflections | 4046 | 13270 | 1797 |
| No. of parameters | 270 | 1277 | 177 |
| No. of restraints | 398 | 56 | 523 |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 2.38, –2.38 | 0.55, –0.48 | 0.47, -0.49 |

| | **1** | **$(3)_2 \cdot C_4H_8O_2$** |
|---|---|---|
| CCDC-Number | 2286830 | 2286082 |
| | **Crystal Data** | |
| Chemical formula | $C_{12}F24GeO4_7$ | $C_{16}H_8F_{24}Ge_2O_6$ |
| $M_r$ | 736.73 | 897.40 |
| Crystal system, space group | Orthorhombic, $P2_12_12$ | Monoclinic, $P2_1/n$ |
| Temperature (K) | 100 | 100 |
| *a*, *b*, *c* (Å) | 18.5204(10), 18.7351(9), 11.6382(6) | 11.8448(8), 7.7953(5), 14.4848(9) |
| α, β, γ (°) | 90, 90, 90 | 90, 93.398(2), 90 |
| *V* (Å$^3$) | 4038.2(4) | 1335.08(15) |
| *Z* | 8 | 2 |
| Radiation type | Mo *K*a | Mo *K*a |
| μ (mm$^{-1}$) | 1.760 | 2.454 |
| Crystal size (mm) | 0.258 × 0.245 × 0.201 | 0.298 × 0.25 × 0.154 |
| Crystal shape | Fragment | Block |
| Color | Clear colorless | Clear colorless |
| | **Data Collection** | |
| Diffractometer | Bruker Photon CMOS | Bruker Photon CMOS |
| Absorption correction | Multi-scan | Multi-scan |
| $T_{min}$, $T_{max}$ | 0.7453, 0.5705 | 0.7453, 0.5707 |
| No. of measured, independent, and observed [$I > 2\sigma(I)$] reflections | 154374, 8248, 7776 | 54591, 2443, 2328 |
| $R_{int}$ | 0.0486 | 0.0412 |
| θ range (°) for cell measurement | 2.20-26.67 | 2.16-25.35 |
| Data completeness | 0.999 | 1.000 |
| | **Refinement** | |
| $R[F^2 > 2\sigma(F^2)]$, $R(F^2)$, *S* | 0.1054, 0.3131, 1.618 | 0.0374, 0.0891, 1.157 |
| No. of reflections | 8248 | 2443 |
| No. of parameters | 720 | 217 |
| No. of restraints | 2945 | 0 |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 1.93, -1.34 | 1.59, -0.62 |

The data have been assigned the following deposition numbers which can either be quoted as CCDC Numbers or CSD Numbers. A CCDC Number is usually quoted for an organic or metal-organic structure, whereas a CSD Number is usually quoted for an inorganic structure.

CCDC XXXXXXX-YYYYYYY (generally used for organic and metal-organic structures)

CSD XXXXXXX-YYYYYYY (generally used for inorganic structures)

Deposition Number 2286080-2286083, 2286830

---
Summary of Data - Deposition Number 2286080
---
Compound Name:
Data Block Name: data_GraAn1_fine
Unit Cell Parameters: a 23.5238(15) b 8.6067(5) c 21.8982(13) Pbcn
---
---
Summary of Data - Deposition Number 2286081
---
Compound Name:
Data Block Name: data_TscFl23_fine
Unit Cell Parameters: a 8.3174(7) b 10.3383(8) c 11.4253(8) P21212
---
---
Summary of Data - Deposition Number 2286082
---
Compound Name:
Data Block Name: data_mo_tscfl32_0ma_a
Unit Cell Parameters: a 11.8448(8) b 7.7953(5) c 14.4848(9) P21/n
---
---
Summary of Data - Deposition Number 2286083
---
Compound Name:
Data Block Name: data_mo_tscfl29_0m
Unit Cell Parameters: a 11.2001(10) b 15.7831(14) c 22.3057(19) P-1
---

---
Summary of Data - Deposition Number 2286830
---
Compound Name:
Data Block Name: data_TscFl26_fine2
Unit Cell Parameters: a 18.5204(10) b 18.7351(9) c 11.6382(6) P21212

# 5 NMR Spectra

## 5.1 NMR spectra of 1·MeCN

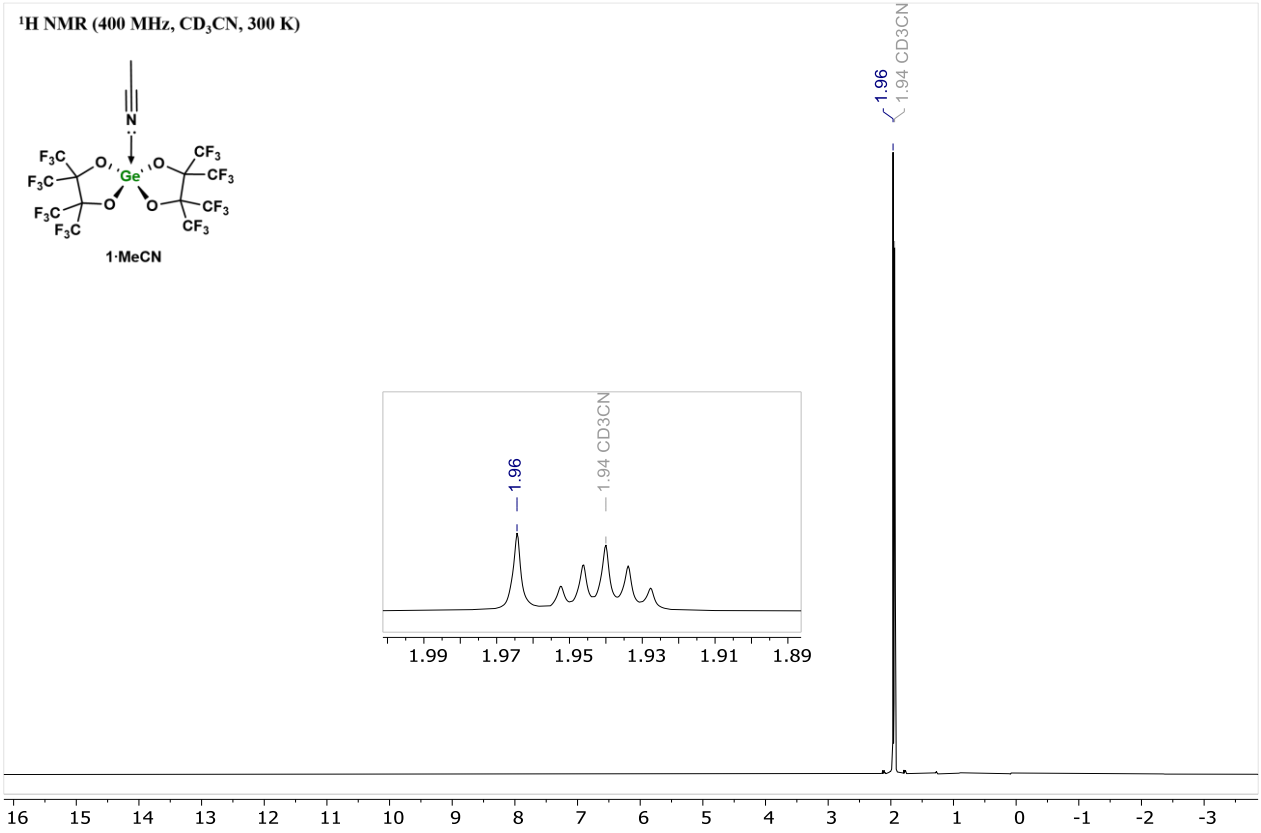



**Figure S 43:** $^{1}$H NMR spectrum of **1**·MeCN in $CD_3CN$ at 300 K.

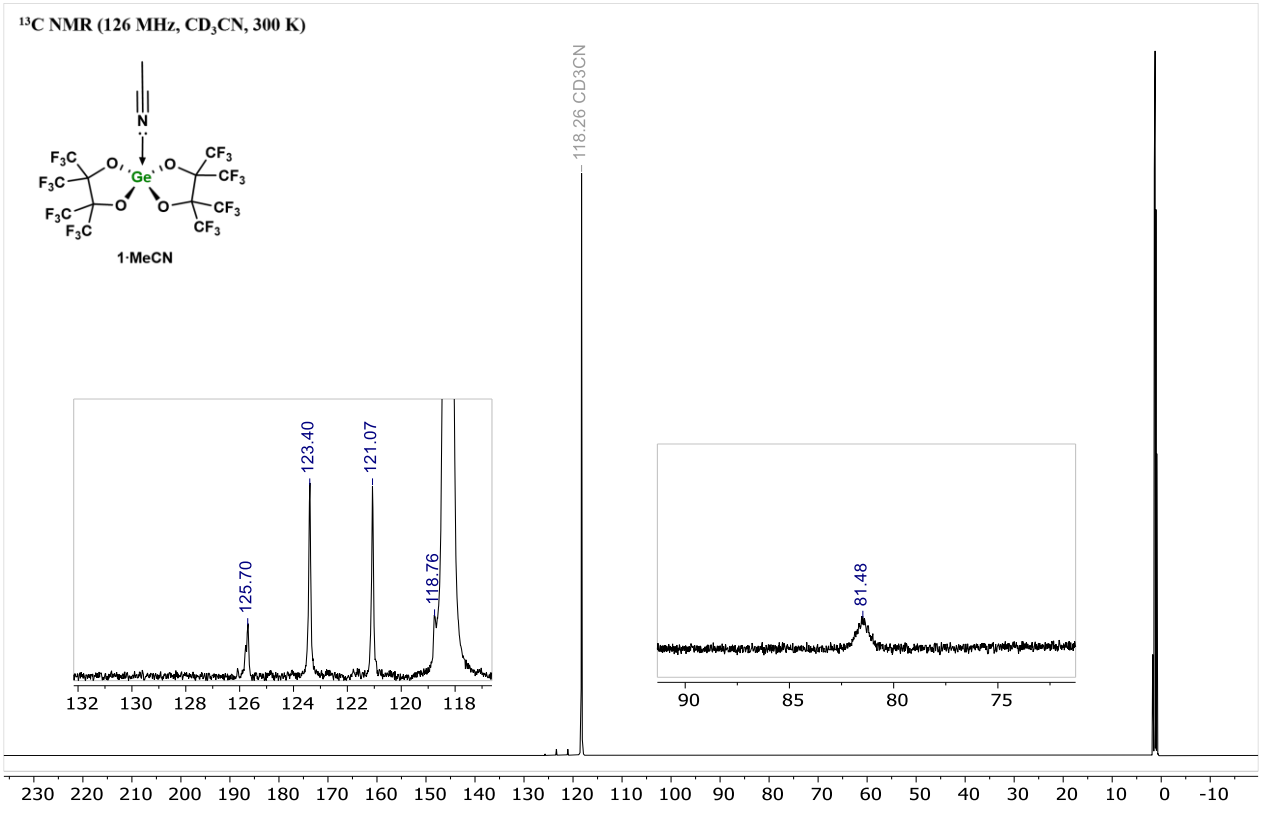



**Figure S 44:** $^{13}$C NMR spectrum of **1**·MeCN in $CD_3CN$ at 300 K.

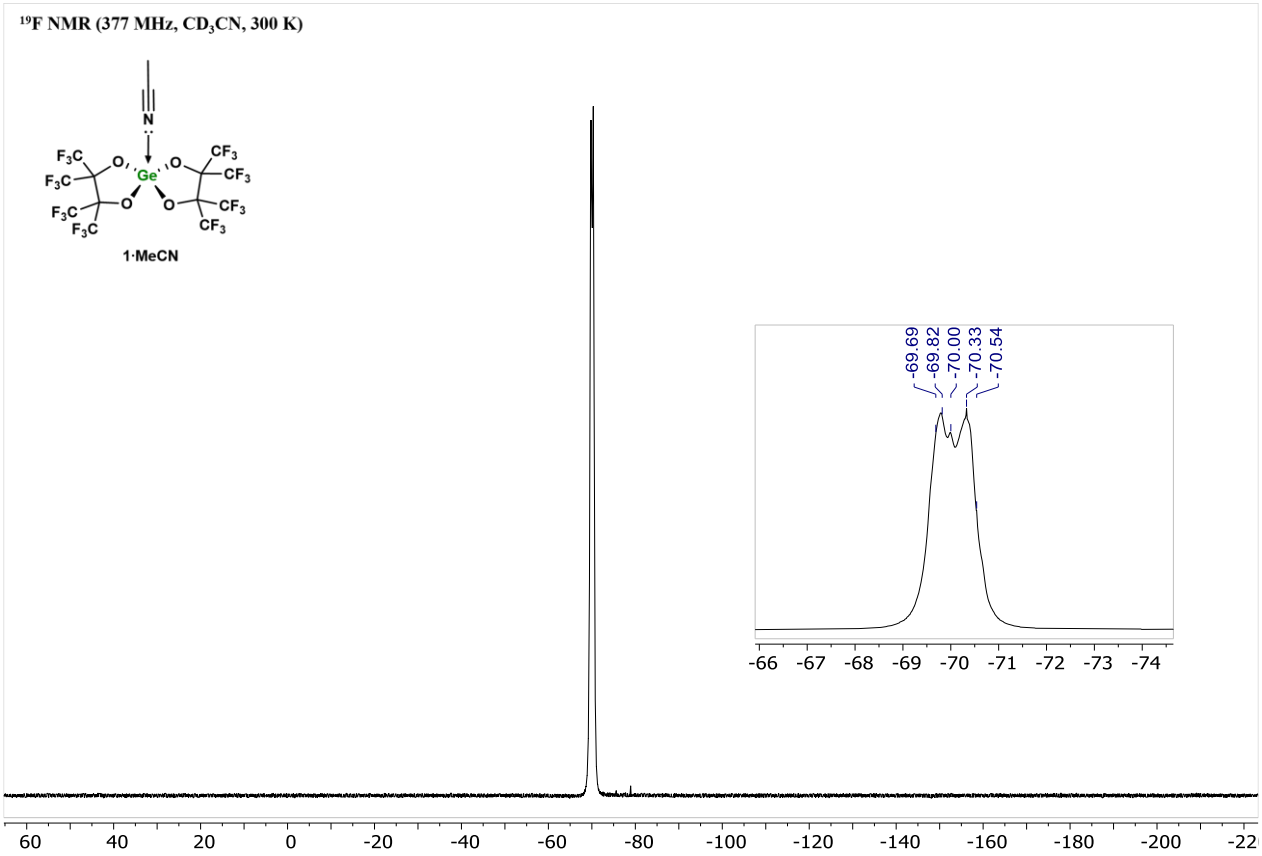



**Figure S 45:** $^{19}$F NMR spectrum of **1**·MeCN in $CD_3CN$ at 300 K.

## 5.2 NMR spectra of 1

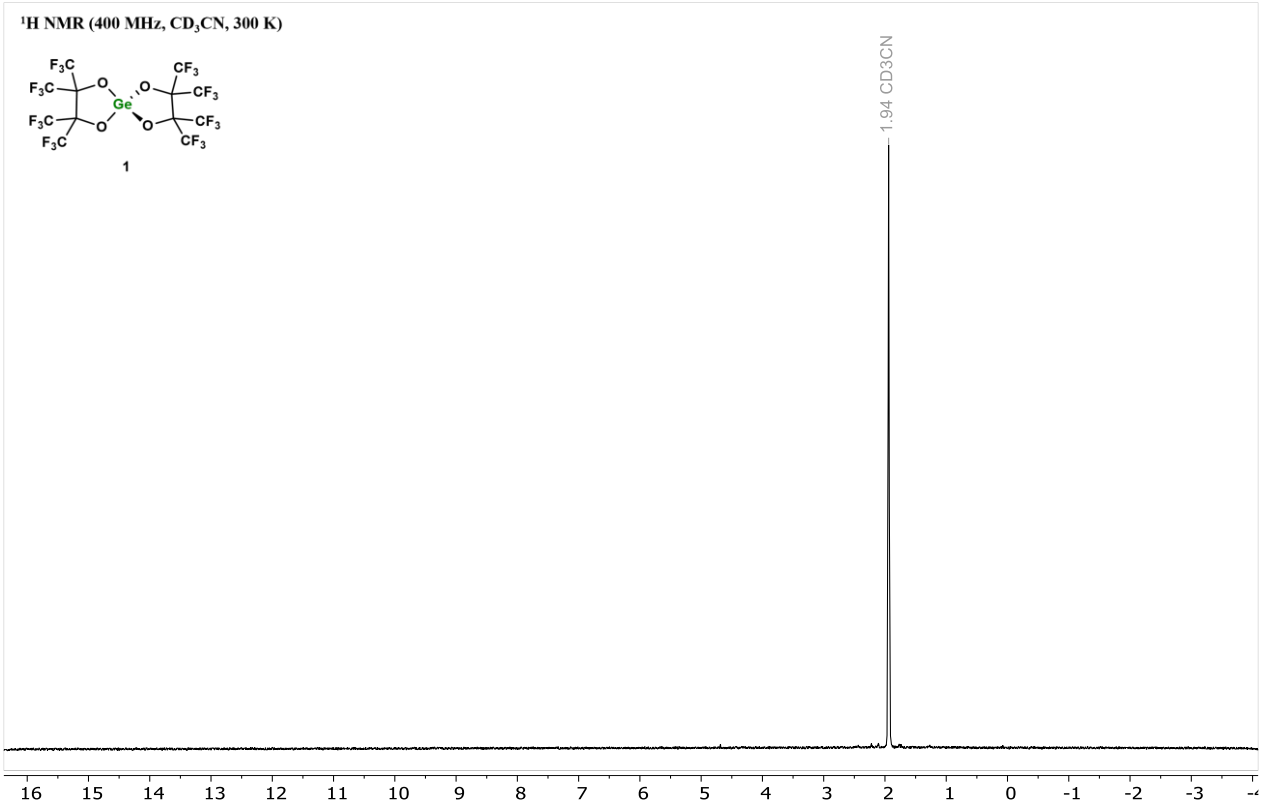



**Figure S 46:** $^1$H NMR spectrum of **1** in $CD_3CN$ at 300 K.

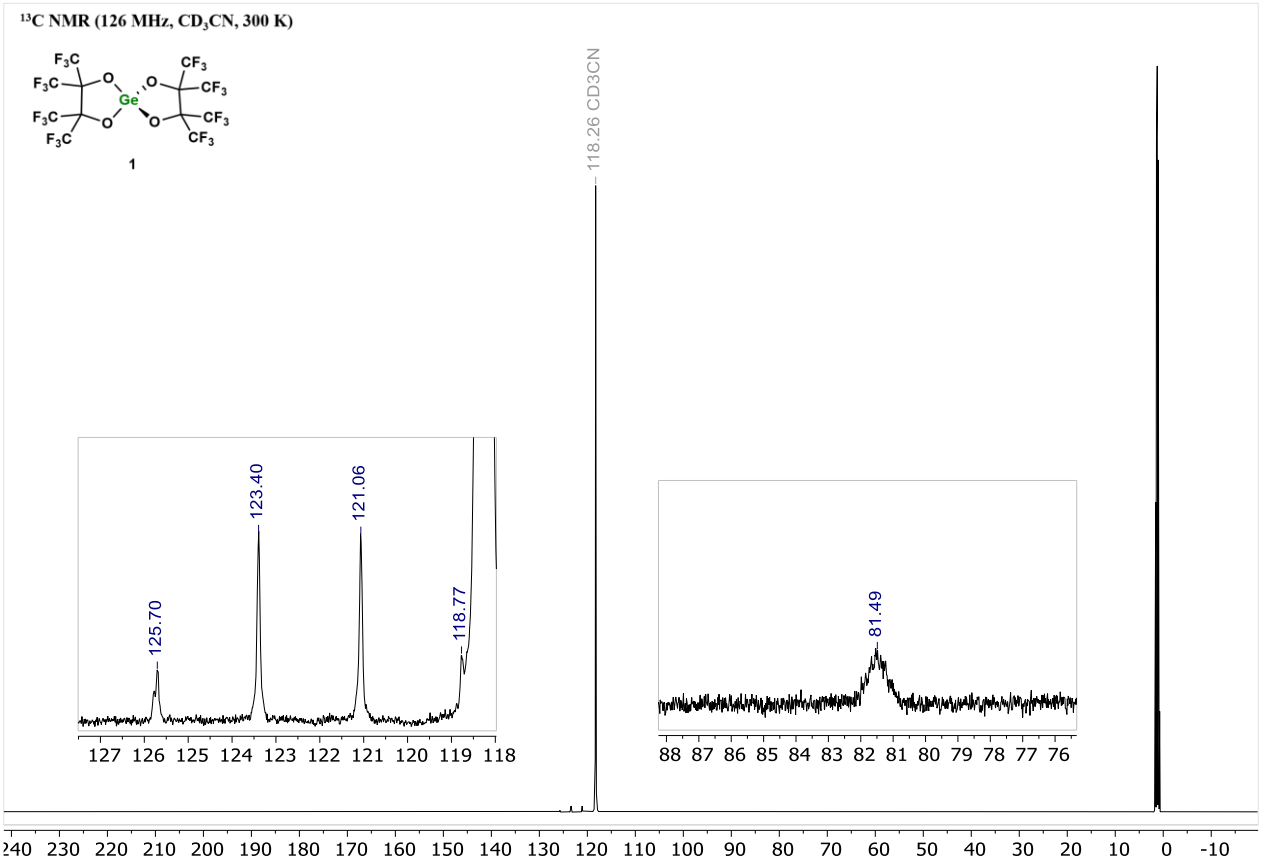



**Figure S 47:** $^{13}$C NMR spectrum of **1** in $CD_3CN$ at 300 K.

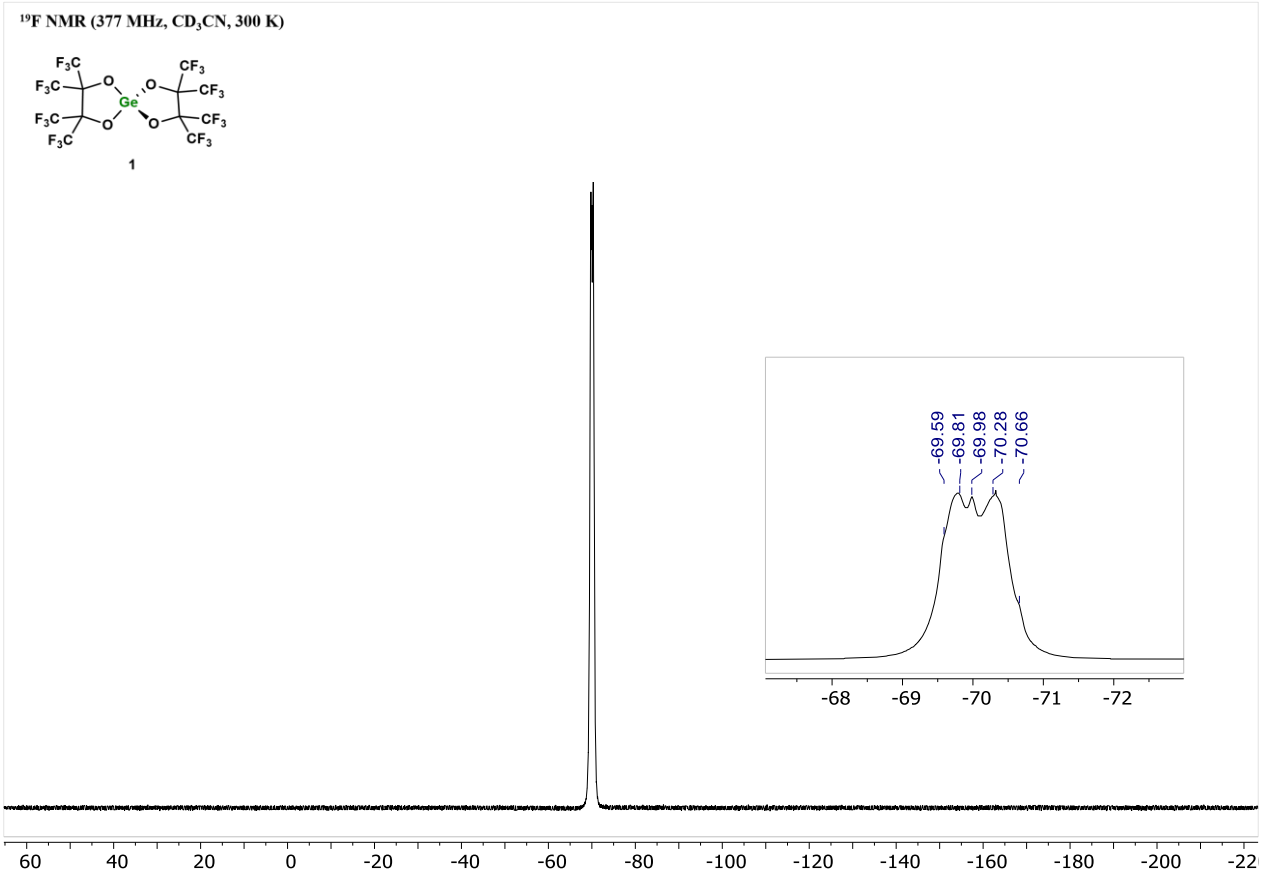



**Figure S 48:** $^{19}F$ NMR spectrum of **1** in $CD_3CN$ at 300 K.

## 5.3 NMR spectra of 2

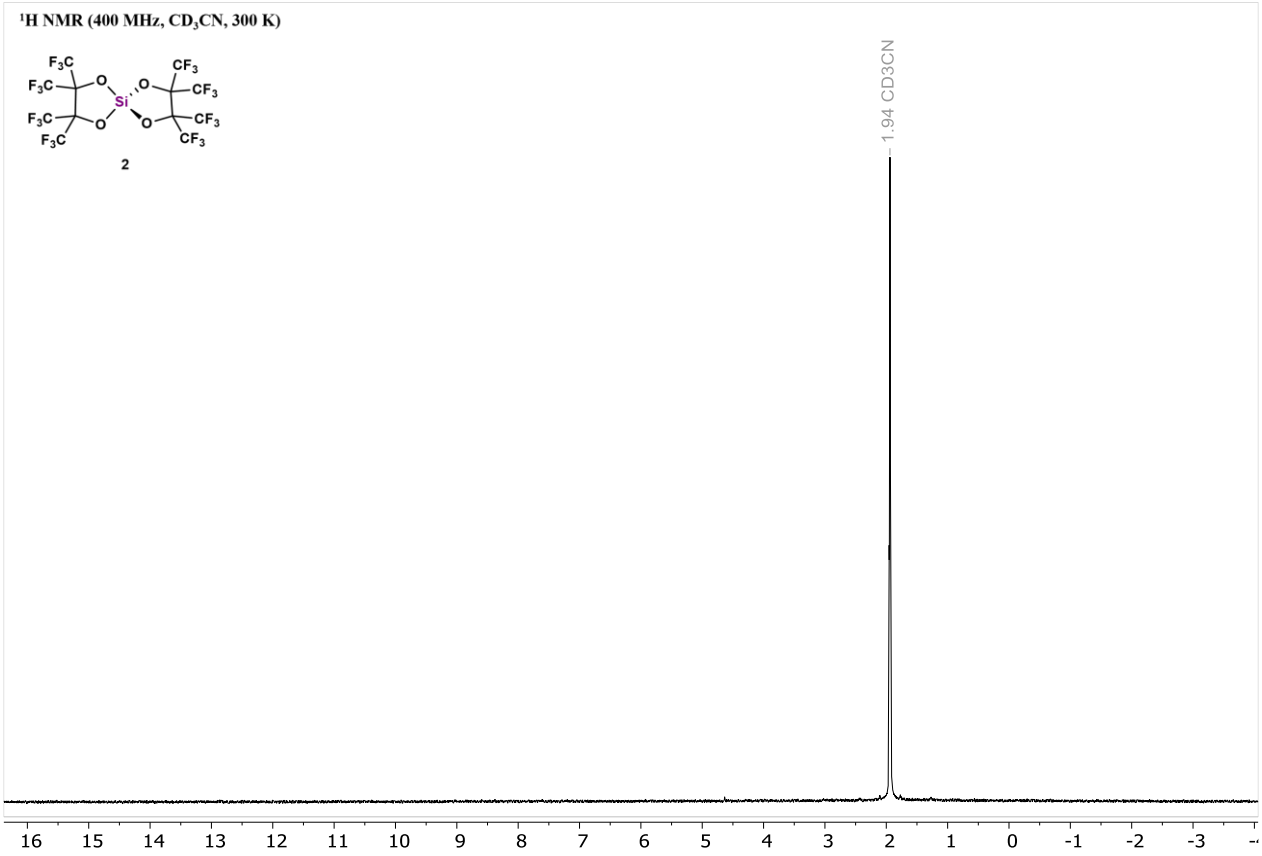



**Figure S 49:** $^{1}$H NMR spectrum of **2** in $CD_3CN$ at 300 K.

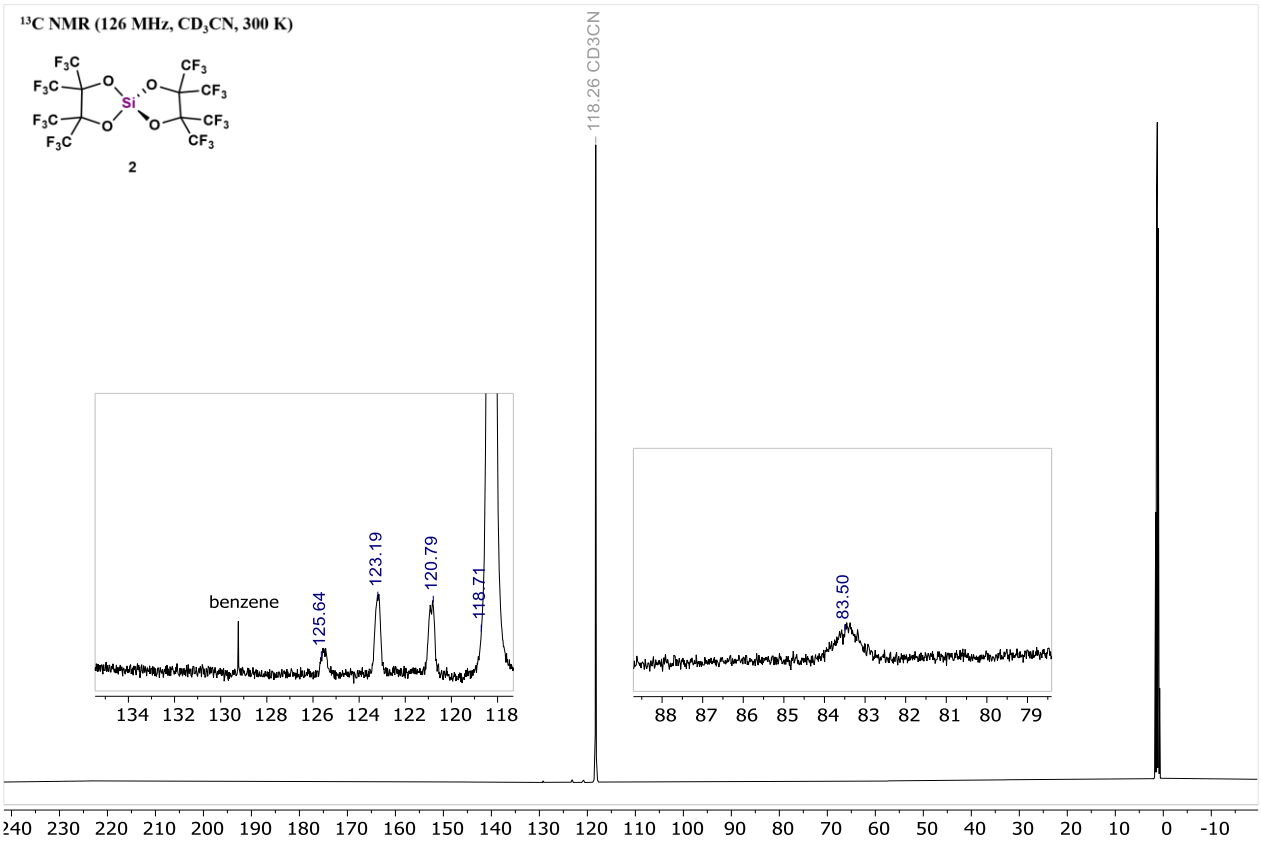



**Figure S 50:** $^{13}$C NMR spectrum of **2** in $CD_3CN$ at 300 K.

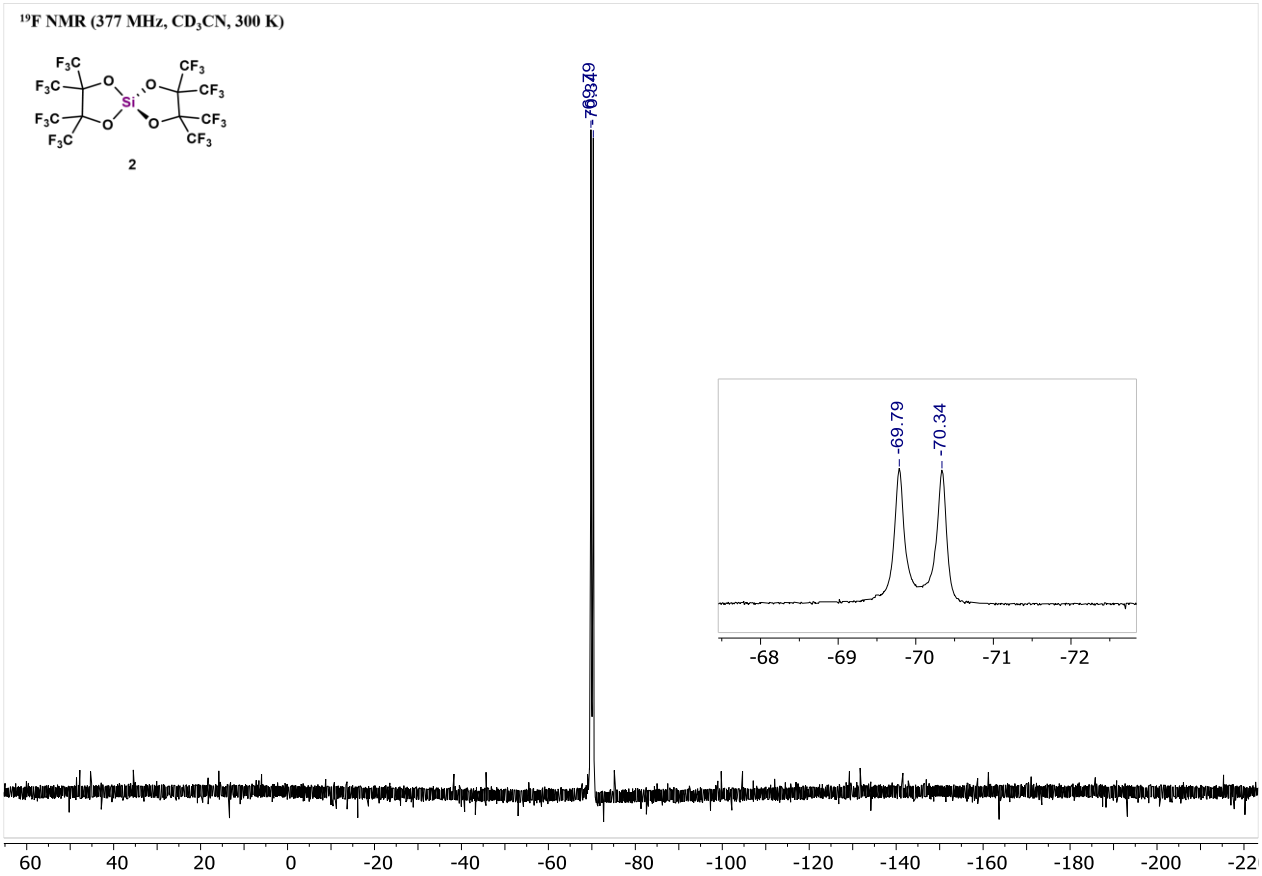



**Figure S 51:** $^{19}F$ NMR spectrum of **2** in $CD_3CN$ at 300 K.

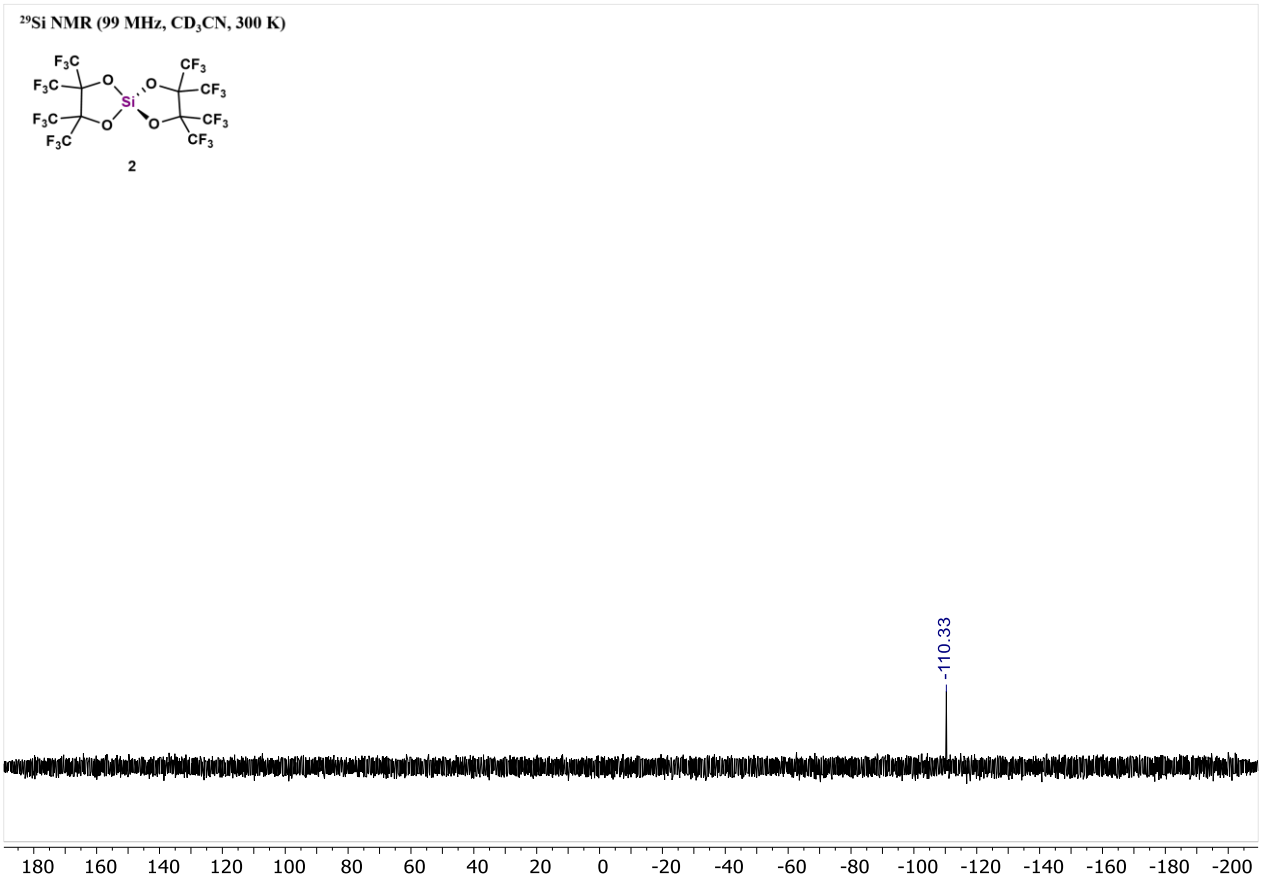



**Figure S 52:** $^{29}Si\{^1H\}$ NMR spectrum of **2** in $CD_3CN$ at 300 K.

## 5.4 NMR spectra of [K·18-c-6][1-F]

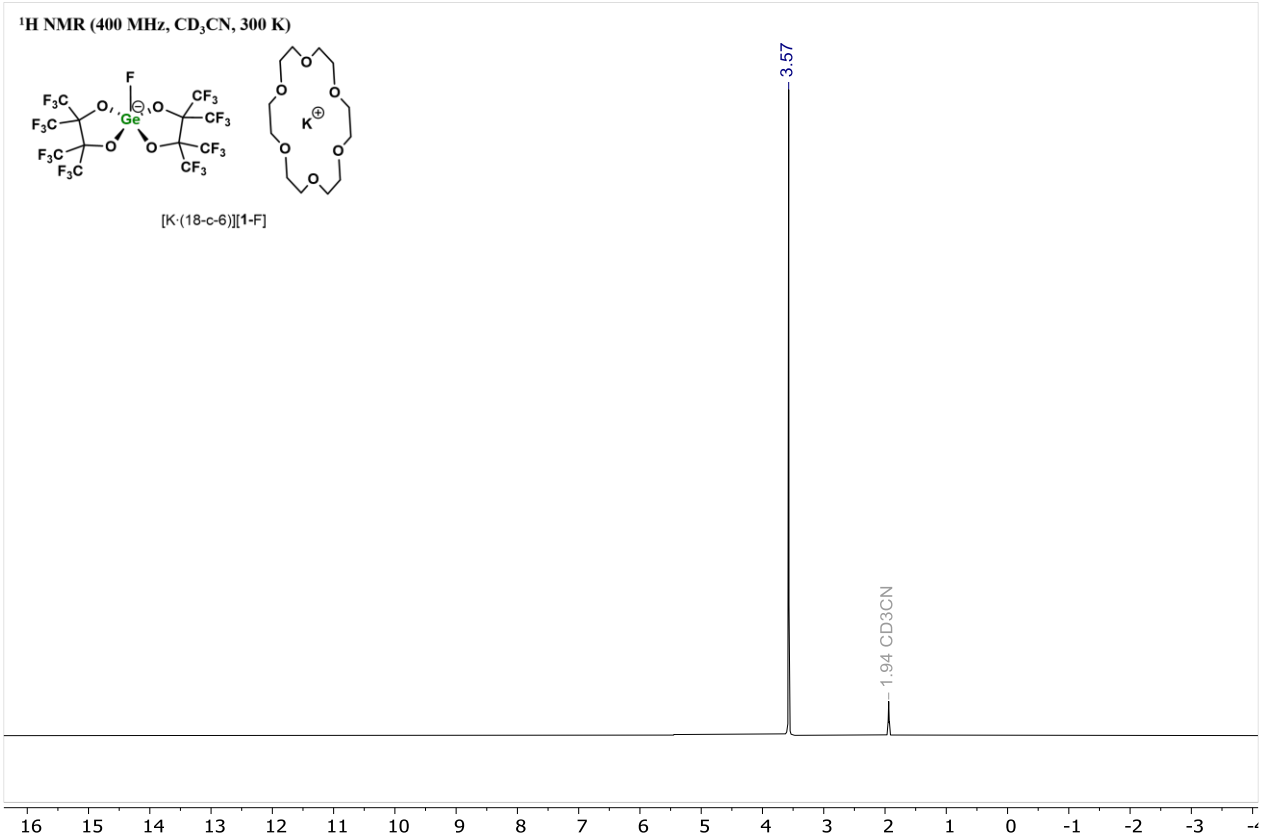



**Figure S 53:** $^{1}$H NMR spectrum of [K·(18-c-6)][**1**-F] in $CD_3CN$ at 300 K.

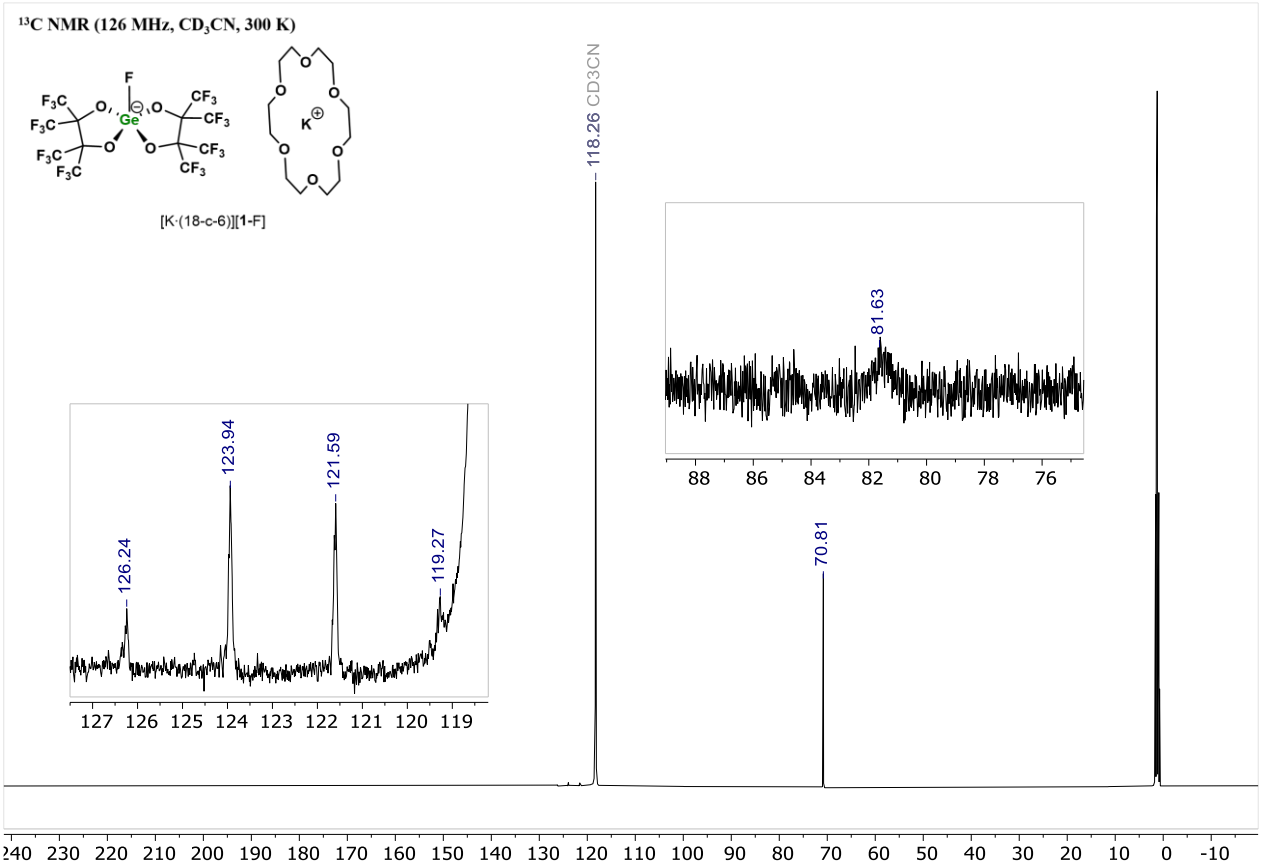



**Figure S 54:** $^{13}$C NMR spectrum of [K·(18-c-6)][**1**-F] in $CD_3CN$ at 300 K.

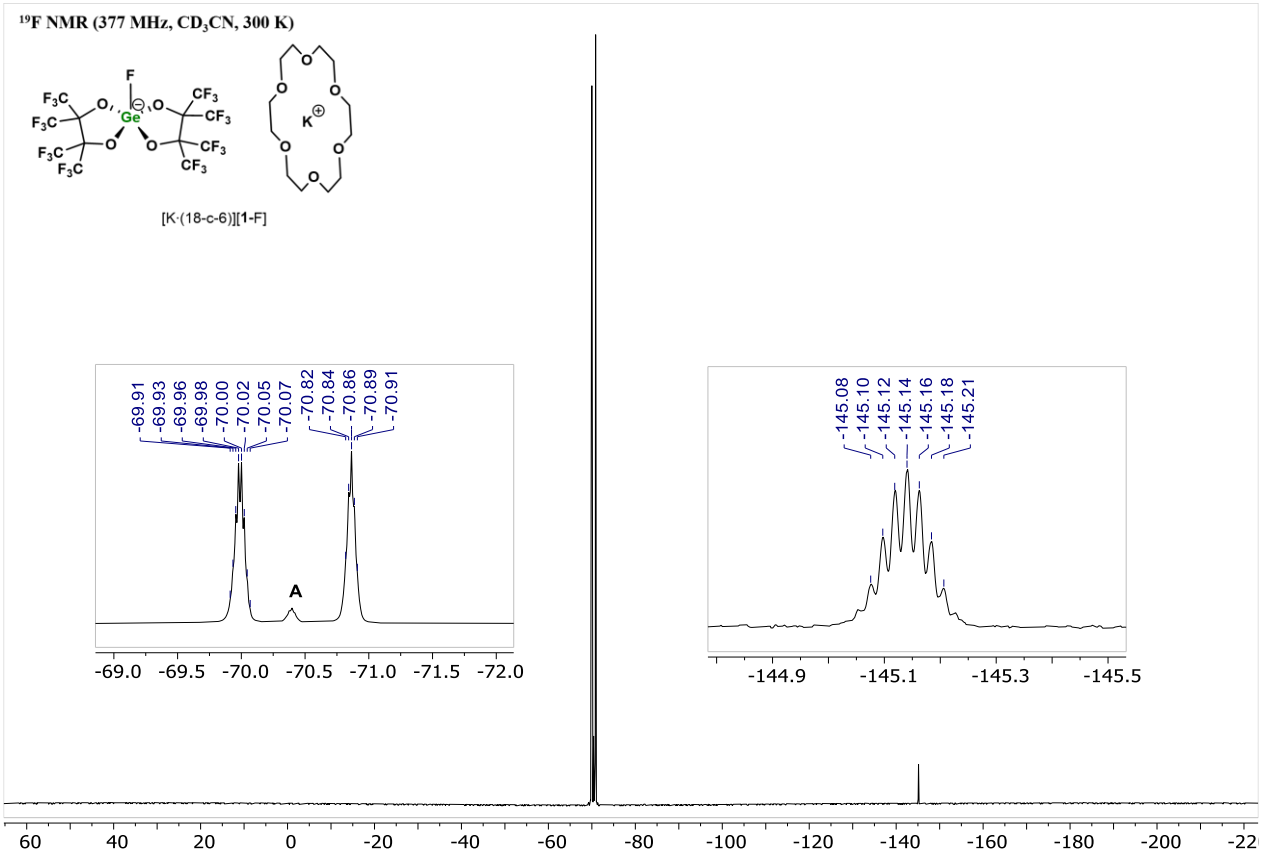



**Figure S 55:** $^{19}$F NMR spectrum of [K·(18-c-6)][**1**-F] in $CD_3CN$ at 300 K. The spectrum additionally contains little amounts of an impurity (**A**) which could be identified as unreacted **1**·MeCN.

## 5.5 NMR spectra of [Et$_3$Si·MeCN][H-1]

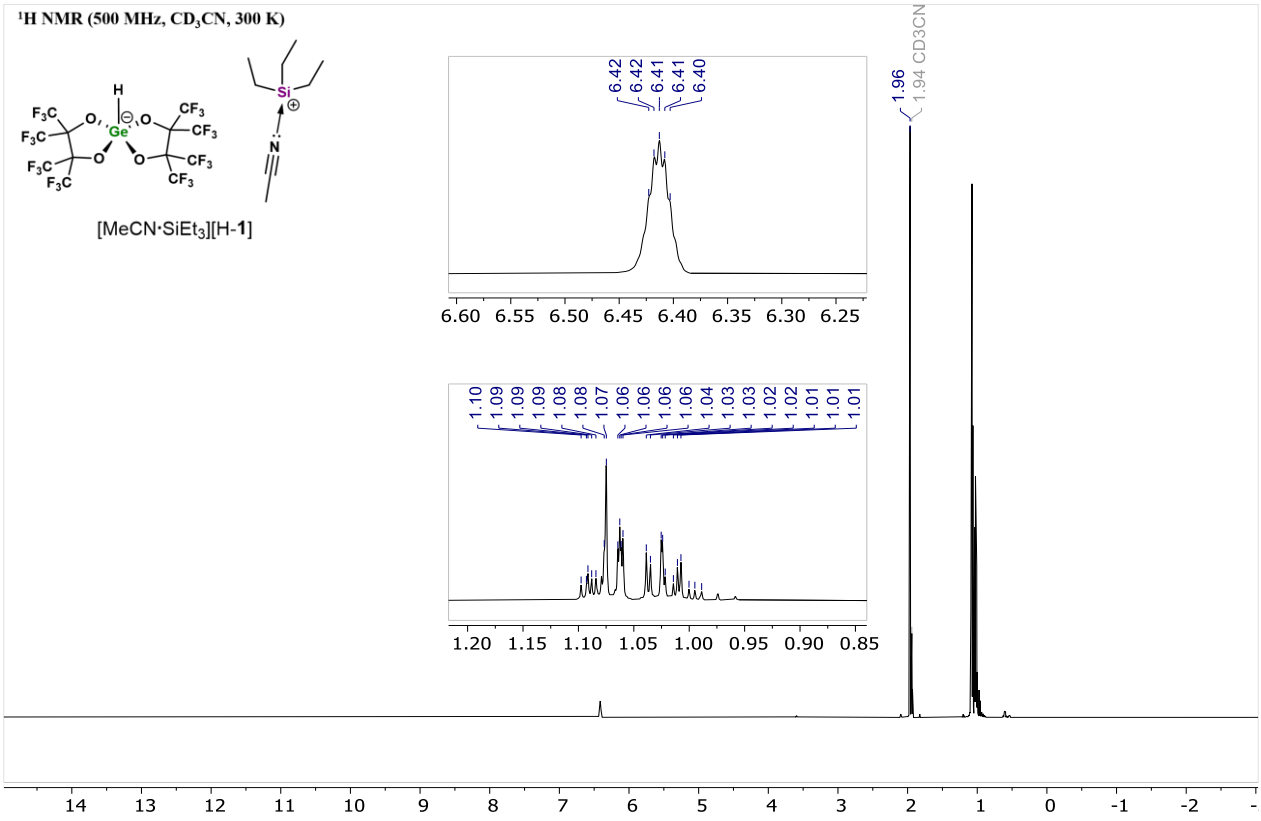



**Figure S 56:** $^1$H NMR spectrum of [Et$_3$Si·MeCN][H-**1**] in CD$_3$CN at 300 K.

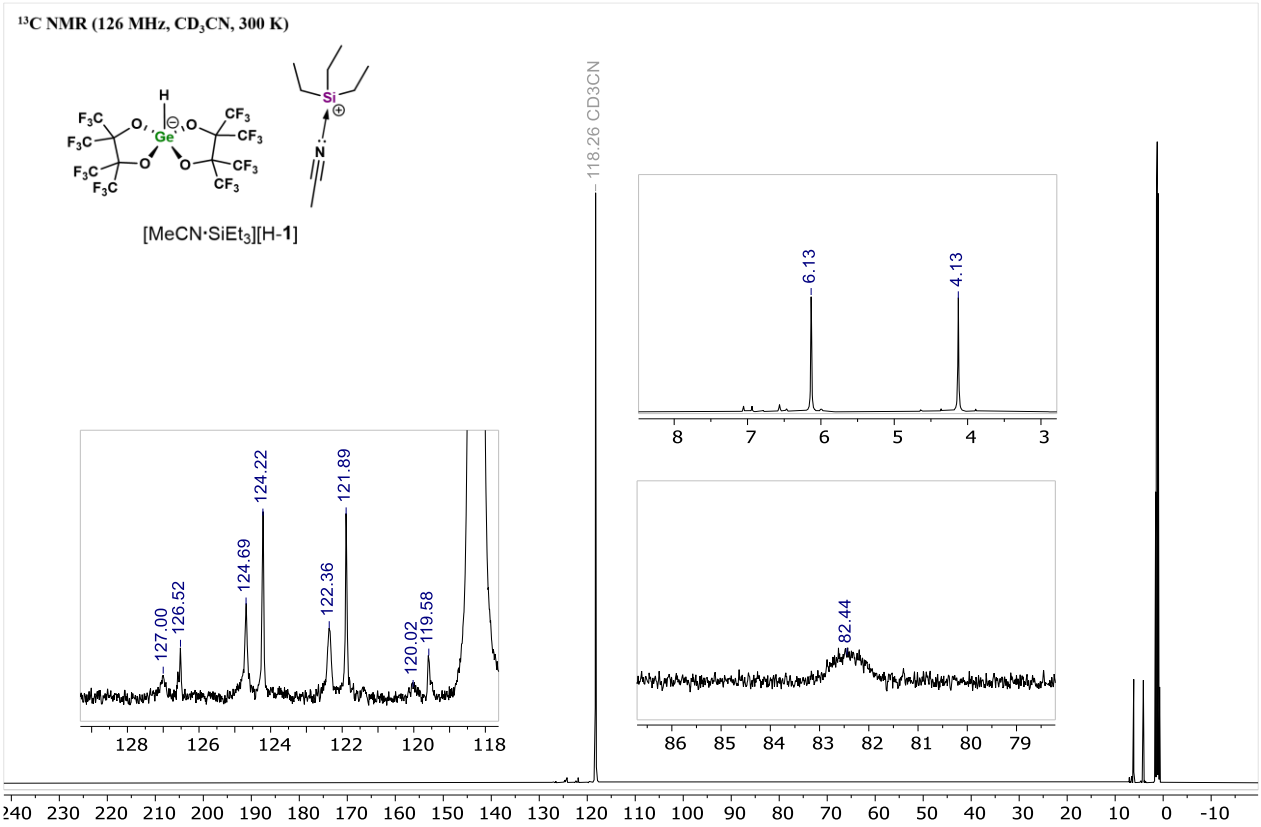



**Figure S 57**: $^{13}$C NMR spectrum of [Et$_3$Si·MeCN][**1**-F] in CD$_3$CN at 300 K.

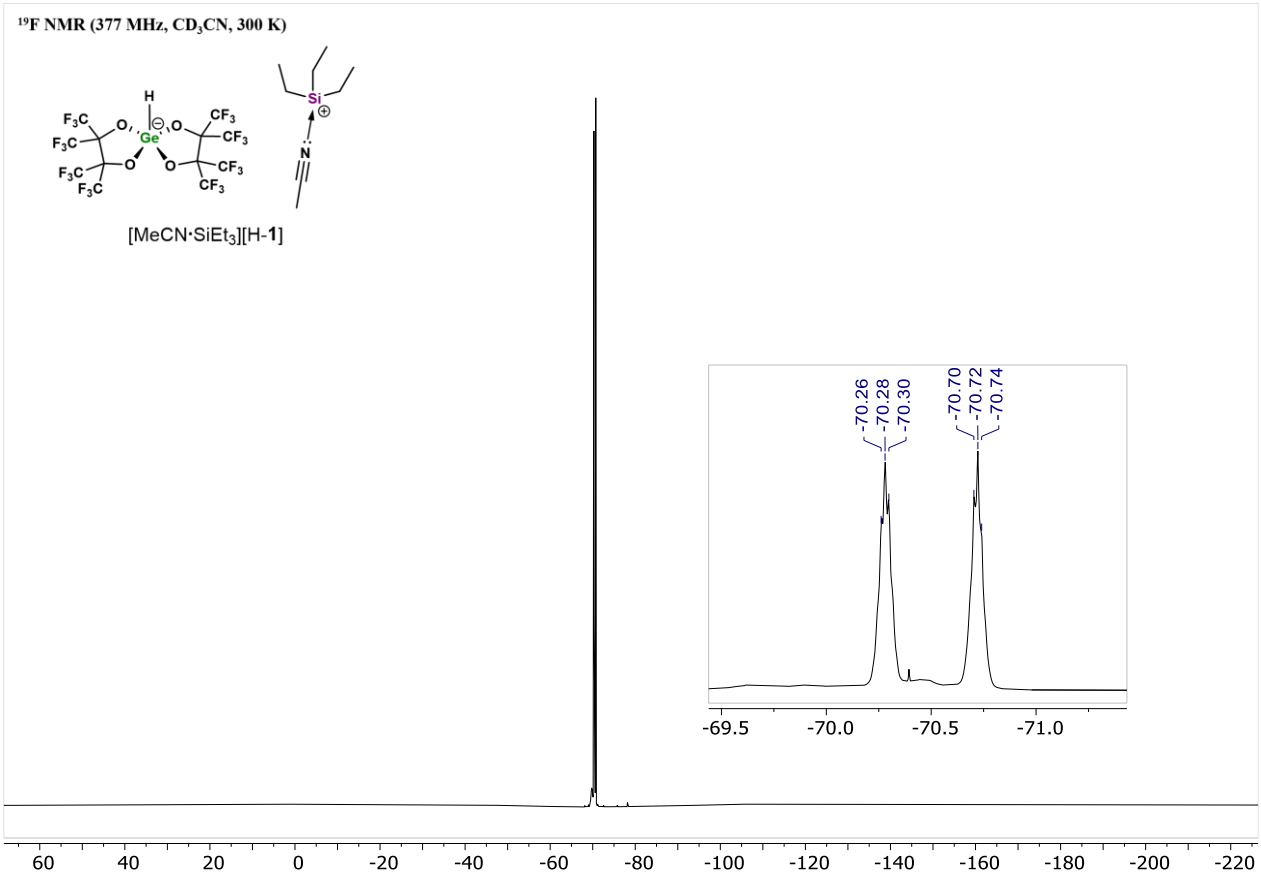



**Figure S 58**: $^{19}F$ NMR spectrum of [$Et_3Si$·MeCN][**1**-F] in $CD_3CN$ at 300 K.

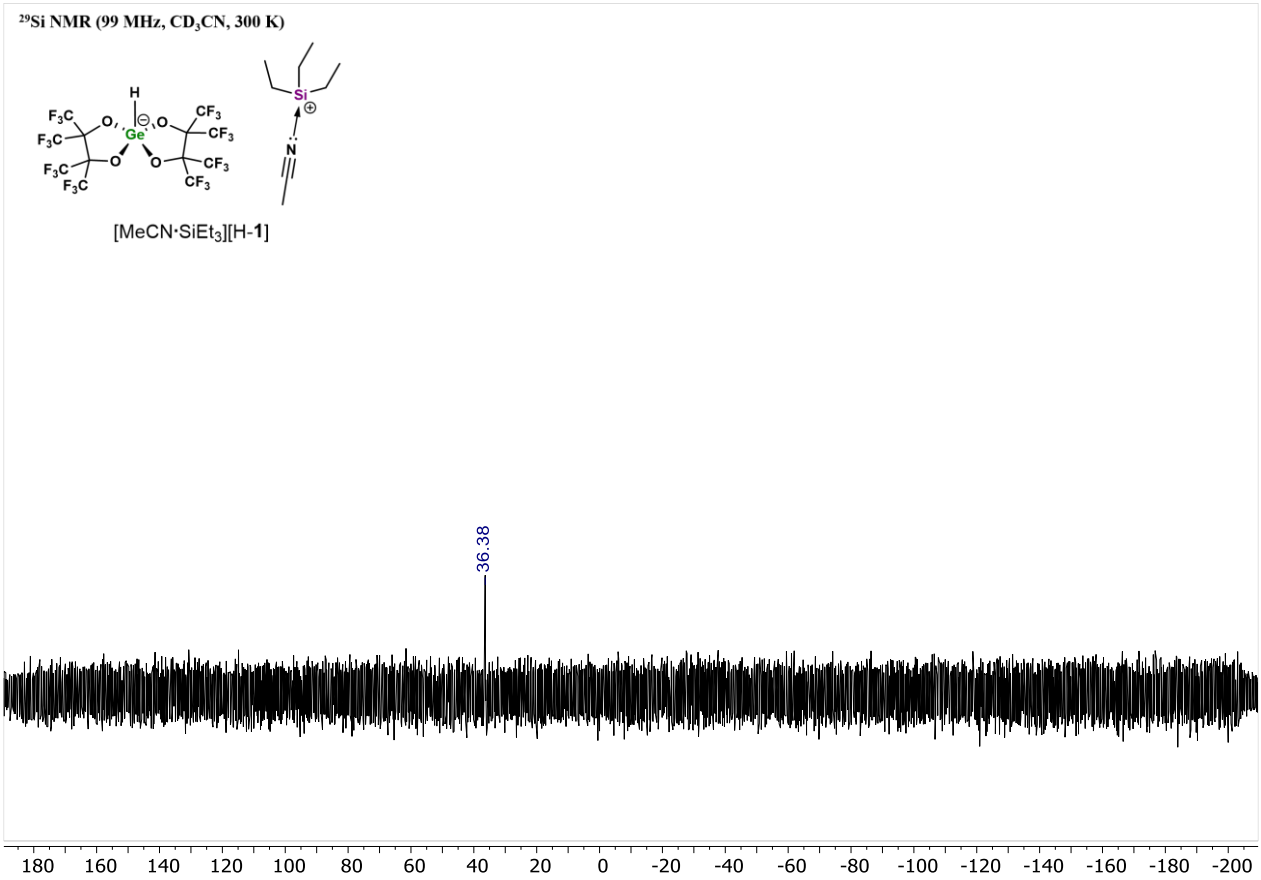



**Figure S 59**: $^{29}Si\{^1H\}$ NMR spectrum of [$Et_3Si$·MeCN][**1**-F] in $CD_3CN$ at 300 K.

## 5.6 NMR spectra of compound mixture 3 and 4

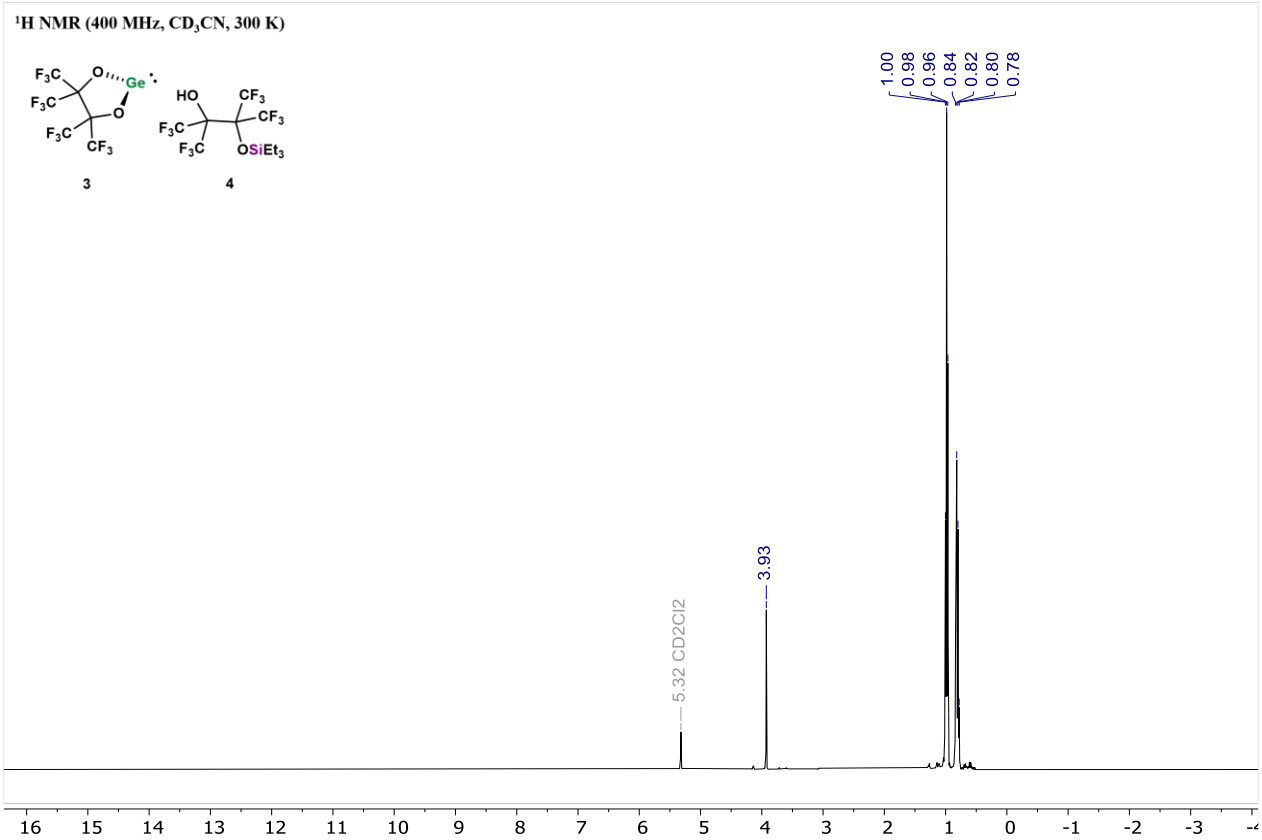



**Figure S 60:** $^{1}$H NMR spectrum of **3** and **4** in $CD_2Cl_2$ at 300 K.

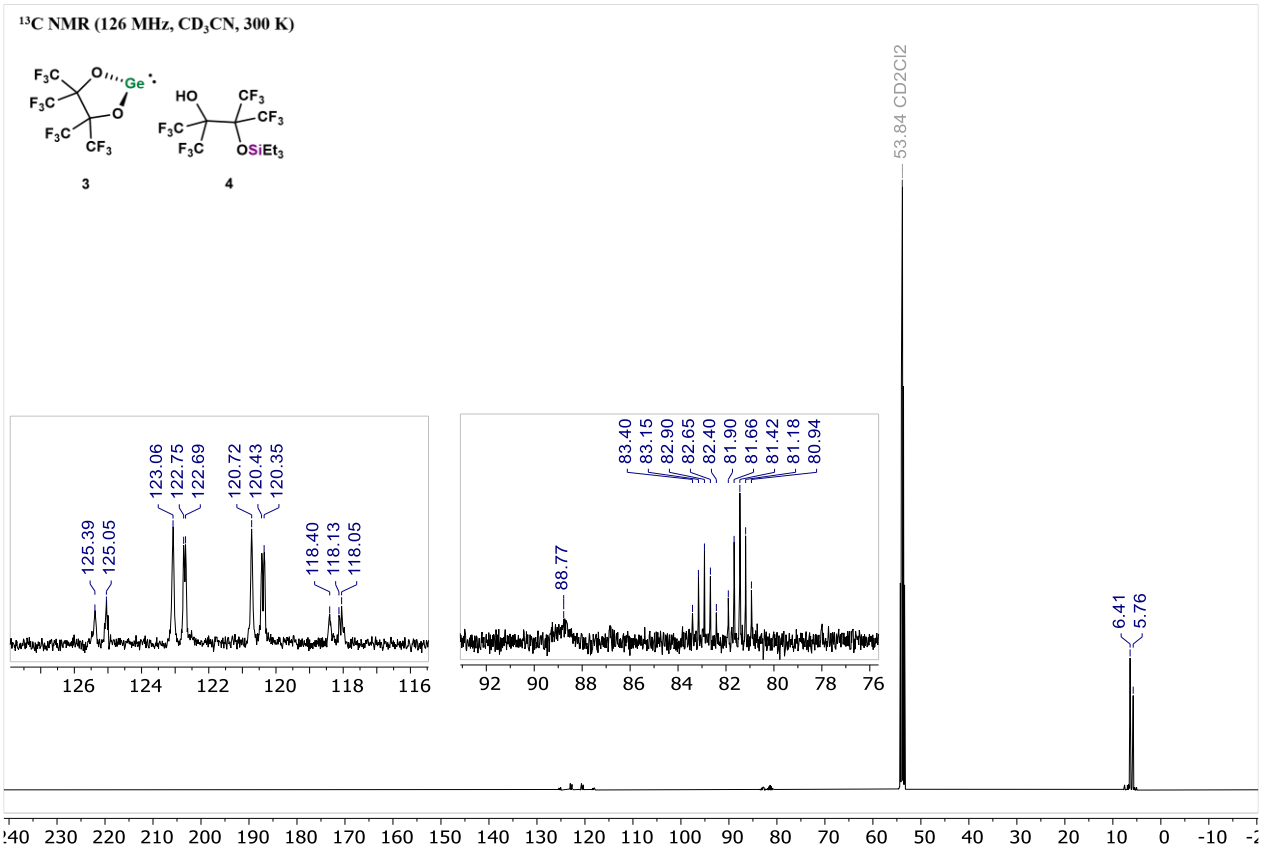



**Figure S 61:** $^{13}$C NMR spectrum of **3** and **4** in $CD_2Cl_2$ at 300 K.

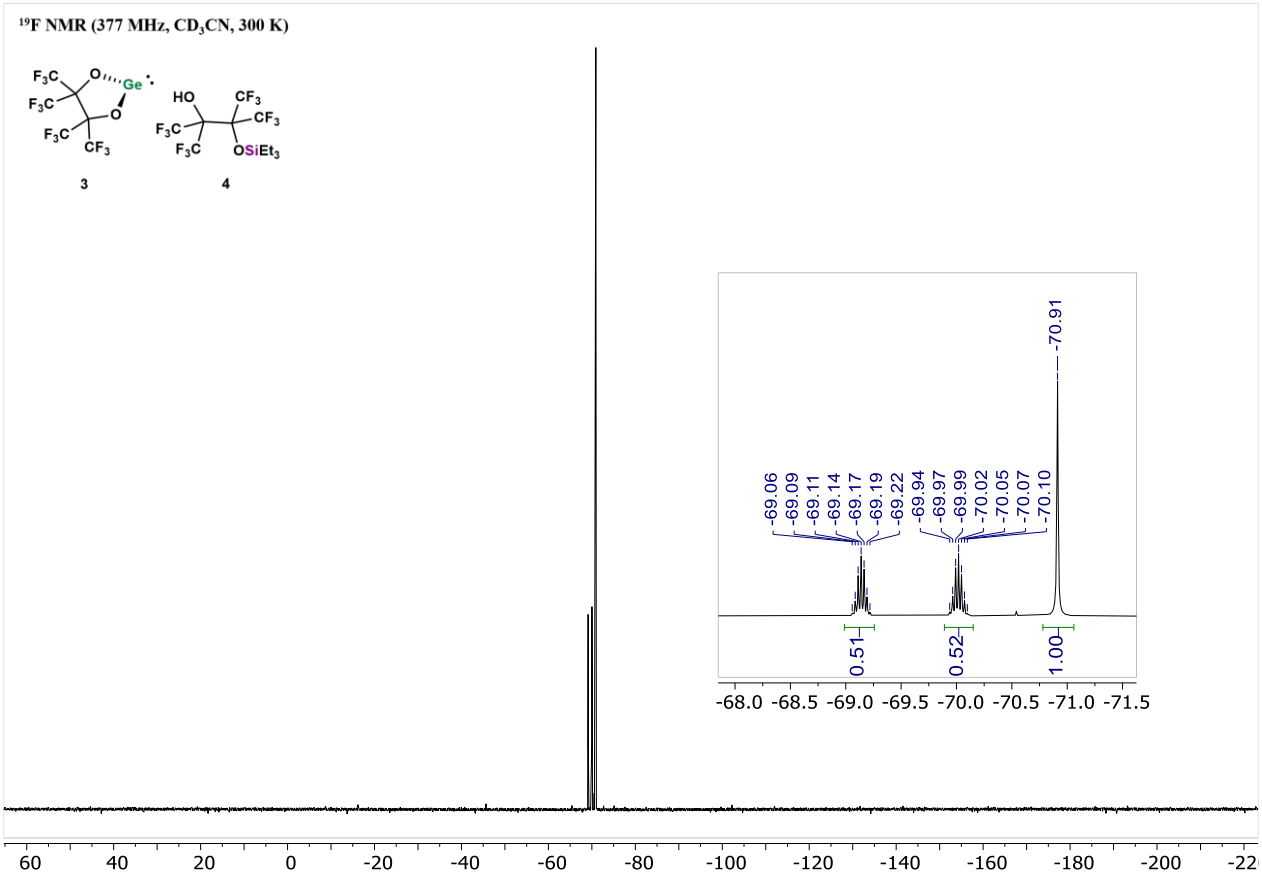



**Figure S 62:** $^{19}F$ NMR spectrum of **3** and **4** in $CD_2Cl_2$ at 300 K.

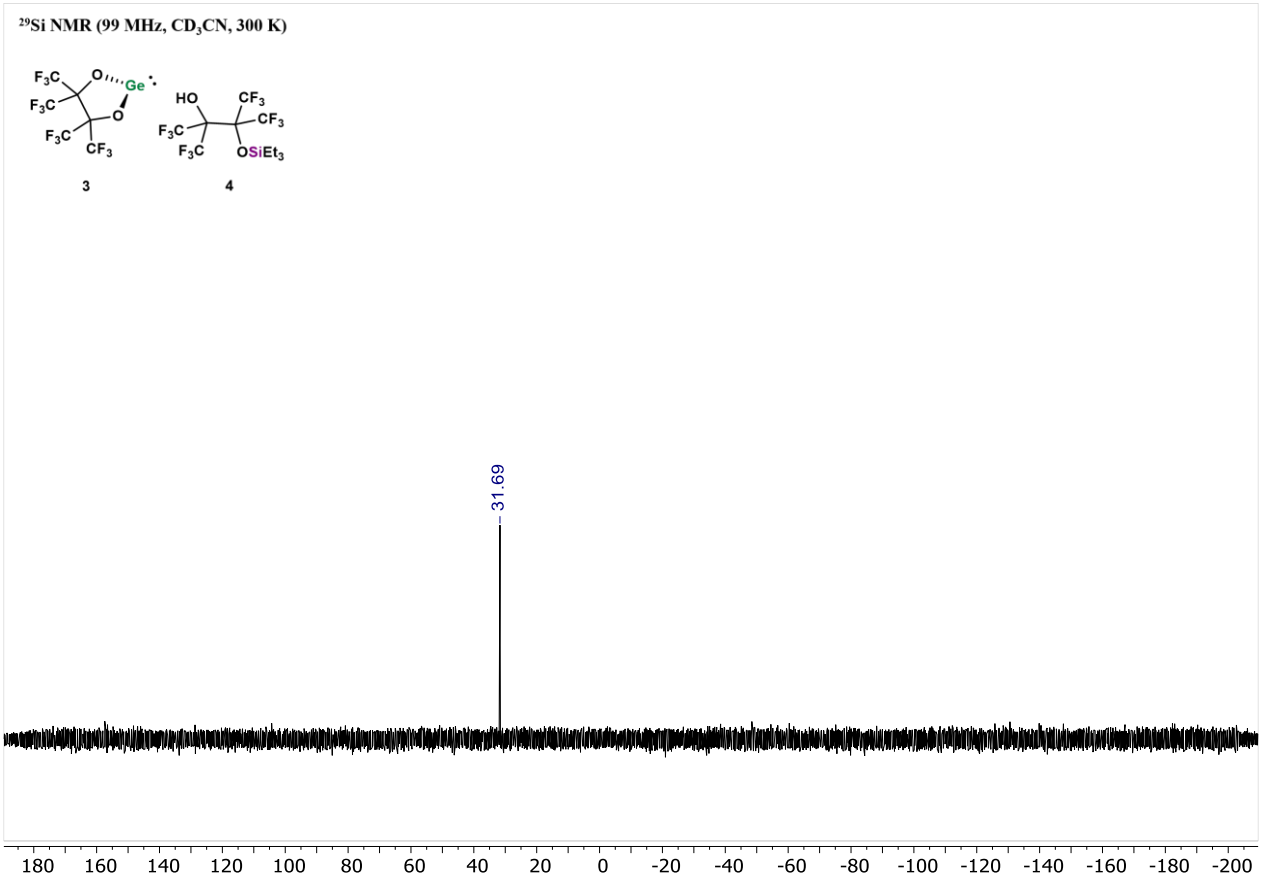



**Figure S 63:** $^{29}Si\{^1H\}$ NMR spectrum of **3** and **4** in $CD_2Cl_2$ at 300 K.

## 5.7 NMR spectra of 1,4-dioxane-coordinated germylene 3

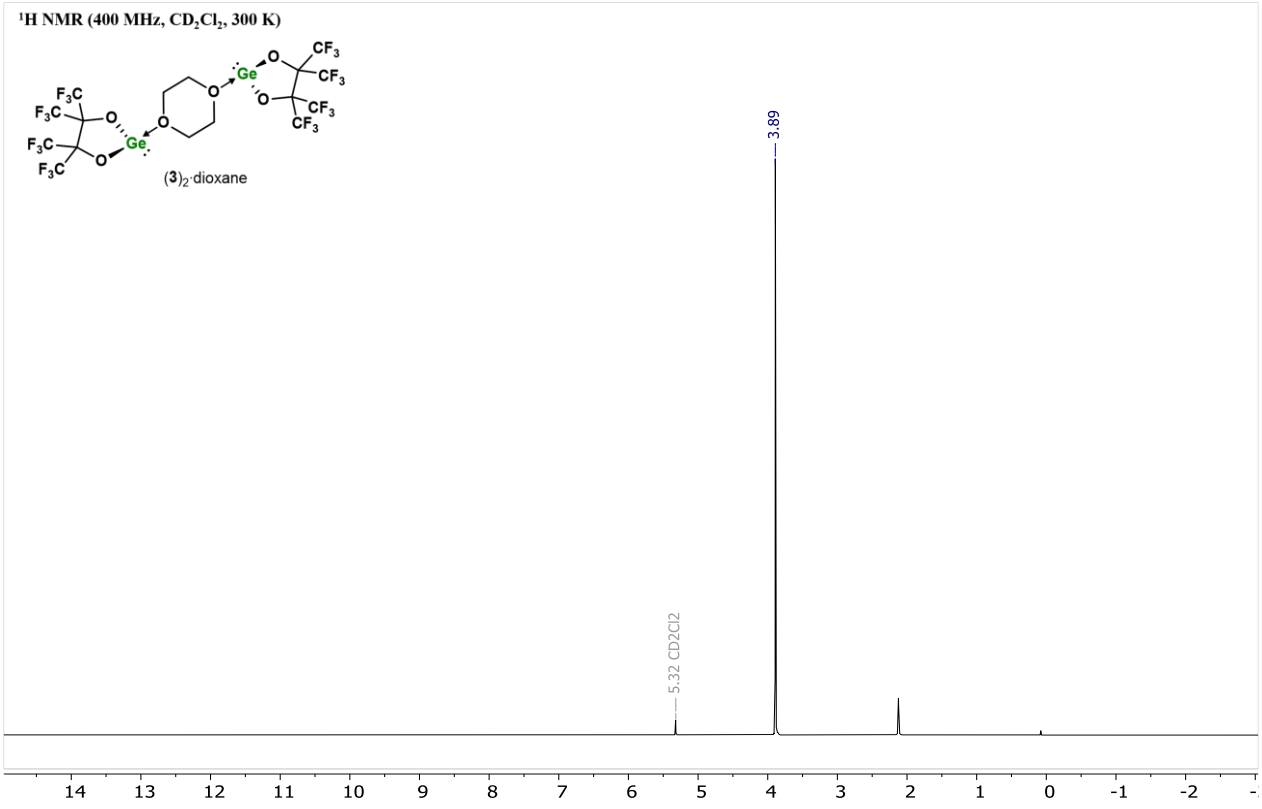



**Figure S 64:** $^1$H NMR spectrum of (**3**)$_2$·dioxane in $CD_2Cl_2$ at 300 K.

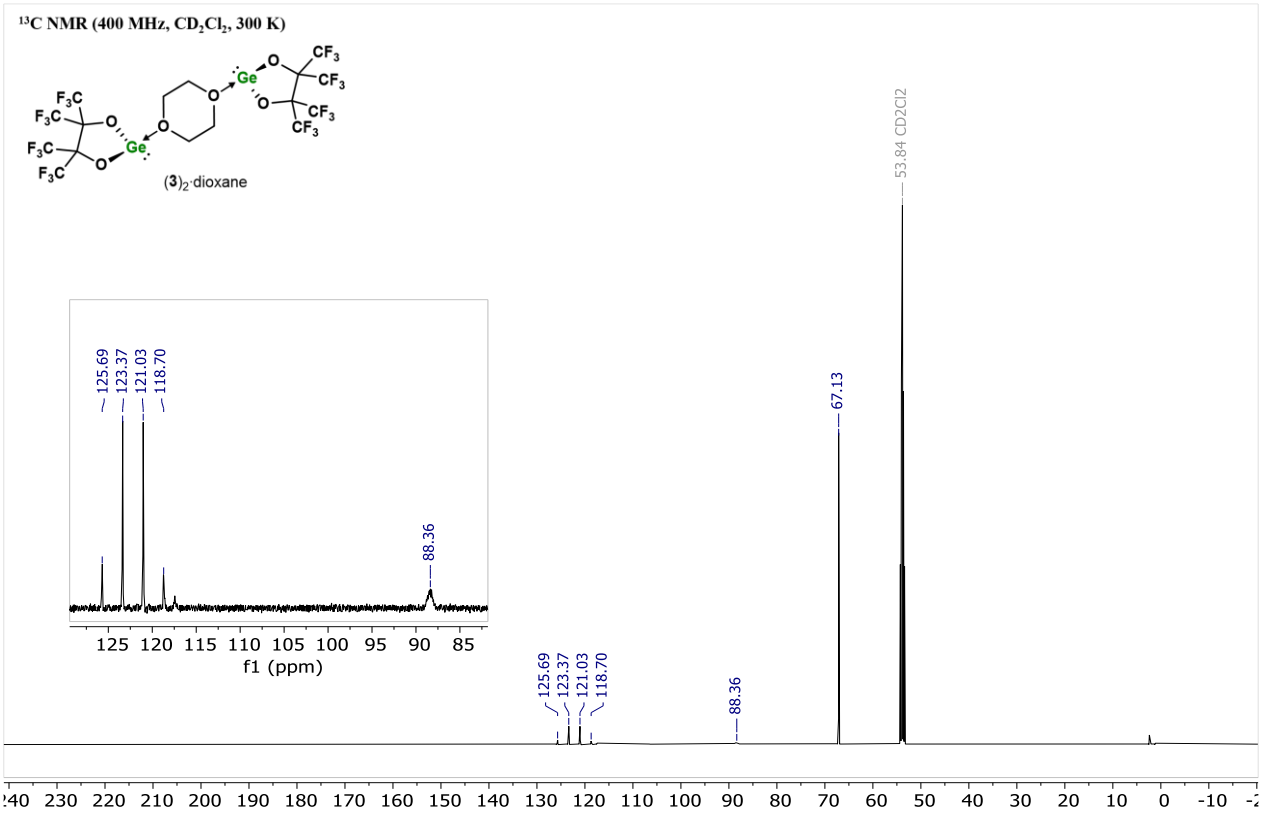



**Figure S 65:** $^{13}$C NMR spectrum of (**3**)$_2$·dioxane in $CD_2Cl_2$ at 300 K.

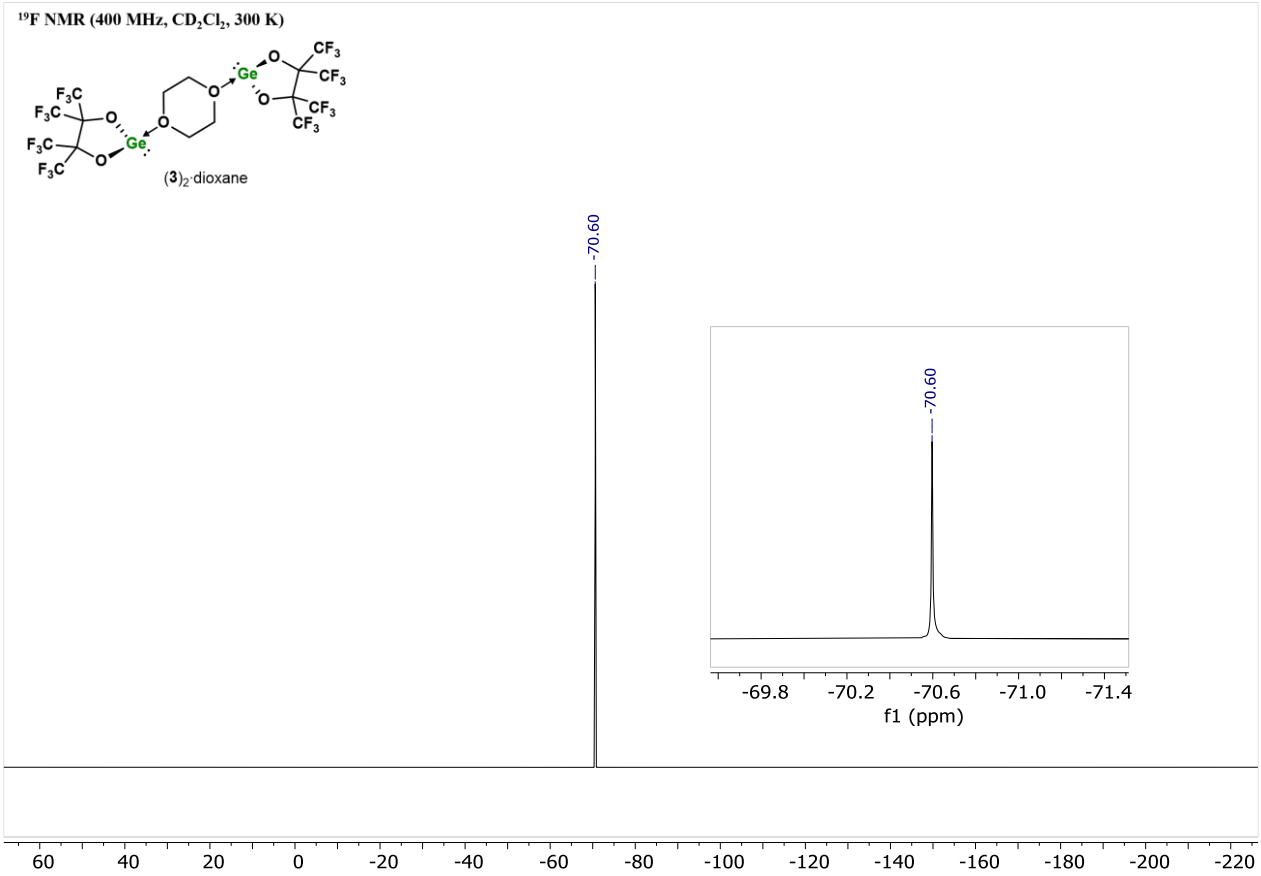



**Figure S 66:** $^{19}F$ NMR spectrum of (**3**)$_2$·dioxane in $CD_2Cl_2$ at 300 K.

# 6 References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# 7 Appendix A

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Calculated energies and coordinates of **1** at PBE0-D4(CPCM=DCM)/def2-TZVP

Electronic energy ... -5229.60383427 Eh
Total Enthalpy ... -5229.40102877 Eh
Final Gibbs free energy ... -5229.50026724 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 4.685199 | 14.396301 | 8.765874 |
| O | 3.400303 | 14.407805 | 7.561079 |
| O | 5.968291 | 14.387158 | 7.558922 |
| O | 4.503637 | 13.123260 | 9.970294 |
| O | 4.867964 | 15.666865 | 9.972762 |
| C | 3.918783 | 14.673253 | 6.291482 |
| C | 5.447681 | 14.122588 | 6.289949 |
| C | 2.933721 | 14.010537 | 5.270178 |
| F | 2.726050 | 12.736069 | 5.563454 |
| F | 3.400052 | 14.098629 | 4.031885 |
| F | 1.750827 | 14.612131 | 5.307761 |
| C | 3.834705 | 16.236199 | 6.149355 |
| F | 4.150103 | 16.662887 | 4.937730 |
| F | 4.654749 | 16.797439 | 7.045402 |
| F | 2.617044 | 16.666525 | 6.437658 |
| C | 5.531834 | 12.559691 | 6.146527 |
| F | 6.750730 | 12.129629 | 6.429950 |
| F | 5.211964 | 12.133313 | 4.936010 |
| F | 4.715328 | 11.997694 | 7.045382 |
| C | 6.430489 | 14.786252 | 5.267081 |
| F | 7.614271 | 14.186346 | 5.303116 |
| F | 6.636861 | 16.061142 | 5.559341 |
| F | 5.962245 | 14.696999 | 4.029548 |
| C | 4.844835 | 13.598852 | 11.239649 |
| C | 4.527968 | 15.188572 | 11.241476 |
| C | 4.045778 | 12.726153 | 12.265204 |
| F | 2.756748 | 12.695973 | 11.965633 |
| F | 4.188409 | 13.182577 | 13.502119 |
| F | 4.481358 | 11.473039 | 12.238279 |
| C | 6.377693 | 13.284298 | 11.385876 |
| F | 6.832931 | 13.511492 | 12.607785 |
| F | 7.064497 | 14.028300 | 10.512440 |
| F | 6.625161 | 12.022199 | 11.075366 |
| C | 2.995291 | 15.502877 | 11.390005 |
| F | 2.307268 | 14.760211 | 10.516445 |
| F | 2.747454 | 16.765457 | 11.081687 |
| F | 2.541760 | 15.273873 | 12.612236 |
| C | 5.327789 | 16.058812 | 12.268524 |
| F | 4.890622 | 17.311460 | 12.247018 |
| F | 6.616231 | 16.091654 | 11.966783 |
| F | 5.187776 | 15.597790 | 13.504033 |

---

Calculated energies and coordinates of **1** at PBE0-D4(CPCM=acetonitrile)/def2-TZVP level of theory

Electronic energy ... -5229.60411347 Eh
Total Enthalpy ... -5229.40144558 Eh
Final Gibbs free energy ... -5229.50070480 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 4.685208 | 14.396305 | 8.765831 |
| O | 3.400375 | 14.407608 | 7.560853 |
| O | 5.968231 | 14.387365 | 7.558691 |
| O | 4.503546 | 13.123351 | 9.970455 |
| O | 4.868078 | 15.666779 | 9.972926 |
| C | 3.918751 | 14.673209 | 6.291305 |
| C | 5.447717 | 14.122640 | 6.289769 |
| C | 2.933685 | 14.010358 | 5.270076 |
| F | 2.726365 | 12.735773 | 5.563236 |
| F | 3.399694 | 14.098727 | 4.031695 |
| F | 1.750524 | 14.611511 | 5.308049 |
| C | 3.834579 | 16.236193 | 6.149051 |
| F | 4.150346 | 16.662657 | 4.937426 |
| F | 4.654262 | 16.797565 | 7.045179 |
| F | 2.616702 | 16.666361 | 6.436814 |
| C | 5.531953 | 12.559704 | 6.146226 |
| F | 6.751059 | 12.129792 | 6.429107 |
| F | 5.211703 | 12.133548 | 4.935714 |
| F | 4.715805 | 11.997585 | 7.045166 |
| C | 6.430526 | 14.786426 | 5.266964 |
| F | 7.614566 | 14.186940 | 5.303368 |
| F | 6.636575 | 16.061428 | 5.559107 |
| F | 5.962584 | 14.696905 | 4.029350 |
| C | 4.844797 | 13.598832 | 11.239770 |
| C | 4.528018 | 15.188596 | 11.241595 |
| C | 4.045565 | 12.726174 | 12.265220 |
| F | 2.756451 | 12.696478 | 11.965869 |
| F | 4.188539 | 13.182175 | 13.502250 |
| F | 4.480579 | 11.472822 | 12.237822 |
| C | 6.377681 | 13.284214 | 11.386250 |
| F | 6.832579 | 13.511656 | 12.608282 |
| F | 7.064600 | 14.027991 | 10.512912 |
| F | 6.625052 | 12.021961 | 11.076178 |
| C | 2.995313 | 15.502957 | 11.390361 |
| F | 2.307189 | 14.760504 | 10.516897 |
| F | 2.747567 | 16.765685 | 11.082467 |
| F | 2.542109 | 15.273711 | 12.612708 |
| C | 5.327996 | 16.058793 | 12.268554 |
| F | 4.891368 | 17.311672 | 12.246598 |
| F | 6.616521 | 16.091182 | 11.967037 |
| F | 5.187644 | 15.598168 | 13.504173 |

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Calculated energies and coordinates of **1** at PBE0-D4(CPCM=benzene)/def2-TZVP level of theory

Electronic energy ... -5229.60274820 Eh
Total Enthalpy ... -5229.39943902 Eh
Final Gibbs free energy ... -5229.49860457 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 4.685159 | 14.396278 | 8.766037 |
| O | 3.400027 | 14.408503 | 7.561928 |
| O | 5.968514 | 14.386406 | 7.559797 |
| O | 4.503965 | 13.122915 | 9.969689 |
| O | 4.867537 | 15.667182 | 9.972142 |
| C | 3.918895 | 14.673396 | 6.292163 |
| C | 5.447549 | 14.122414 | 6.290641 |
| C | 2.933897 | 14.011170 | 5.270558 |
| F | 2.724846 | 12.737162 | 5.564280 |
| F | 3.401474 | 14.098159 | 4.032600 |
| F | 1.752007 | 14.614445 | 5.306566 |
| C | 3.835142 | 16.236194 | 6.150513 |
| F | 4.149021 | 16.663698 | 4.938822 |
| F | 4.656629 | 16.796962 | 7.046130 |
| F | 2.618322 | 16.667110 | 6.440935 |
| C | 5.531425 | 12.559665 | 6.147664 |
| F | 6.749502 | 12.129044 | 6.433206 |
| F | 5.213111 | 12.132489 | 4.937059 |
| F | 4.713488 | 11.998092 | 7.046072 |
| C | 6.430309 | 14.785644 | 5.267529 |
| F | 7.613125 | 14.184130 | 5.302067 |
| F | 6.637957 | 16.060091 | 5.560250 |
| F | 5.960903 | 14.697465 | 4.030303 |
| C | 4.844963 | 13.598921 | 11.239188 |
| C | 4.527789 | 15.188490 | 11.241016 |
| C | 4.046565 | 12.726069 | 12.265129 |
| F | 2.757850 | 12.694010 | 11.964770 |
| F | 4.187900 | 13.184070 | 13.501630 |
| F | 4.484300 | 11.473848 | 12.240018 |
| C | 6.377710 | 13.284568 | 11.384469 |
| F | 6.834191 | 13.510772 | 12.605975 |
| F | 7.064131 | 14.029418 | 10.510749 |
| F | 6.625511 | 12.023050 | 11.072317 |
| C | 2.995232 | 15.502637 | 11.388668 |
| F | 2.307528 | 14.759179 | 10.514830 |
| F | 2.747098 | 16.764657 | 11.078757 |
| F | 2.540502 | 15.274615 | 12.610514 |
| C | 5.327033 | 16.058878 | 12.268384 |
| F | 4.887846 | 17.310671 | 12.248584 |

| | | | |
|---|---|---|---|
| F | 6.615158 | 16.093442 | 11.965846 |
| F | 5.188286 | 15.596394 | 13.503507 |

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Calculated energies and coordinates of **1** at PBE0-D3/def2-TZVPP

Electronic energy ... -5229.58926089 Eh
Total Enthalpy ... -5229.38527772 Eh
Final Gibbs free energy ... -5229.48435440 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 4.684919 | 14.396541 | 8.766367 |
| O | 3.399086 | 14.412018 | 7.562320 |
| O | 5.969183 | 14.382601 | 7.560445 |
| O | 4.506453 | 13.121920 | 9.969751 |
| O | 4.864792 | 15.668539 | 9.972346 |
| C | 3.918862 | 14.674686 | 6.291791 |
| C | 5.447532 | 14.121081 | 6.290399 |
| C | 2.933239 | 14.012655 | 5.269991 |
| F | 2.722095 | 12.739530 | 5.565186 |
| F | 3.402303 | 14.097044 | 4.032190 |
| F | 1.752695 | 14.618443 | 5.303234 |
| C | 3.836937 | 16.237708 | 6.149144 |
| F | 4.149339 | 16.664890 | 4.936867 |
| F | 4.661179 | 16.798339 | 7.043268 |
| F | 2.621726 | 16.671221 | 6.441714 |
| C | 5.528933 | 12.558146 | 6.146174 |
| F | 6.745049 | 12.124259 | 6.434428 |
| F | 5.212506 | 12.131806 | 4.934668 |
| F | 4.707386 | 11.996959 | 7.042419 |
| C | 6.431544 | 14.783798 | 5.267429 |
| F | 7.612518 | 14.178800 | 5.299191 |
| F | 6.642368 | 16.057085 | 5.562082 |
| F | 5.960840 | 14.699001 | 4.030238 |
| C | 4.846105 | 13.598709 | 11.240026 |
| C | 4.526538 | 15.188882 | 11.241986 |
| C | 4.048964 | 12.723829 | 12.266021 |
| F | 2.760739 | 12.687565 | 11.964553 |
| F | 4.187659 | 13.183269 | 13.502525 |
| F | 4.491165 | 11.473290 | 12.242906 |
| C | 6.379292 | 13.285847 | 11.385148 |
| F | 6.836488 | 13.510751 | 12.606599 |
| F | 7.065632 | 14.032787 | 10.512081 |
| F | 6.629081 | 12.025397 | 11.070870 |
| C | 2.993620 | 15.501896 | 11.389709 |
| F | 2.305667 | 14.756853 | 10.516345 |
| F | 2.743842 | 16.763008 | 11.078032 |
| F | 2.538224 | 15.275022 | 12.611489 |
| C | 5.324900 | 16.060913 | 12.269420 |
| F | 4.881691 | 17.311181 | 12.251892 |
| F | 6.612498 | 16.099226 | 11.965588 |
| F | 5.188811 | 15.596806 | 13.504466 |

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Calculated energies and coordinates of **1**·MeCN at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -5362.28957277 Eh
Total Enthalpy ... -5362.03518325 Eh
Final Gibbs free energy ... -5362.14349099 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 7.941027 | 6.425840 | 12.129435 |
| F | 10.650589 | 5.585874 | 13.222187 |
| F | 10.003093 | 3.775457 | 14.131377 |
| F | 10.993176 | 5.254610 | 15.333120 |
| F | 8.275080 | 3.786967 | 15.924550 |
| F | 8.797273 | 5.563325 | 17.009722 |
| F | 6.861235 | 5.370436 | 16.083213 |
| F | 11.097633 | 7.784765 | 14.388082 |
| F | 10.253484 | 7.702834 | 16.369903 |
| F | 9.880015 | 9.383743 | 15.089405 |
| F | 7.501127 | 7.967676 | 16.520499 |
| F | 7.406383 | 9.306875 | 14.843194 |
| F | 6.366733 | 7.456059 | 14.750052 |
| F | 9.838419 | 3.420537 | 9.189356 |
| F | 11.086210 | 4.991779 | 9.900026 |
| F | 10.261287 | 5.091347 | 7.910933 |
| F | 6.366974 | 5.426940 | 9.495620 |
| F | 7.505170 | 4.888682 | 7.735565 |
| F | 7.366022 | 3.553359 | 9.412842 |
| F | 11.046699 | 7.522922 | 8.947431 |
| F | 10.681527 | 7.203471 | 11.056494 |
| F | 10.081800 | 9.026340 | 10.139616 |
| F | 8.858120 | 7.263922 | 7.255576 |
| F | 6.919424 | 7.499549 | 8.166545 |
| F | 8.365936 | 9.052019 | 8.335627 |
| O | 7.912244 | 5.318295 | 13.587399 |
| O | 8.672917 | 7.679395 | 13.196825 |
| O | 8.652723 | 5.154543 | 11.069285 |
| O | 7.952680 | 7.532476 | 10.670618 |
| N | 6.014015 | 6.451158 | 12.121214 |
| C | 8.720782 | 5.731518 | 14.614932 |
| C | 8.746126 | 7.355197 | 14.536179 |
| C | 8.746106 | 5.475172 | 9.730490 |
| C | 8.758984 | 7.099198 | 9.649744 |
| C | 10.127604 | 5.081240 | 14.339260 |
| C | 8.154227 | 5.112732 | 15.936520 |
| C | 10.021270 | 8.059976 | 15.110325 |
| C | 7.486580 | 8.027801 | 15.192919 |
| C | 10.010057 | 4.740717 | 9.168702 |
| C | 7.477774 | 4.830068 | 9.062944 |
| C | 10.178203 | 7.717680 | 9.934794 |
| C | 8.216496 | 7.729188 | 8.323374 |
| C | 4.871807 | 6.456613 | 12.108538 |
| C | 3.444045 | 6.465372 | 12.092814 |
| H | 3.099708 | 6.220020 | 11.085471 |
| H | 3.095965 | 7.462334 | 12.373813 |
| H | 3.076746 | 5.725778 | 12.807771 |

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Calculated energies and coordinates of **1**·MeCN at PBE0-D4(CPCM=acetonitrile)/def2-TZVP level of theory

Electronic energy ... -5362.29230028 Eh
Total Enthalpy ... -5362.03809409 Eh
Final Gibbs free energy ... -5362.14640094 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 7.930206 | 6.422622 | 12.129657 |
| F | 10.652518 | 5.589092 | 13.218577 |
| F | 10.010828 | 3.777110 | 14.128164 |
| F | 10.998191 | 5.259113 | 15.328957 |
| F | 8.286886 | 3.783436 | 15.924501 |
| F | 8.806611 | 5.561343 | 17.008514 |
| F | 6.868719 | 5.362555 | 16.087213 |
| F | 11.093057 | 7.789951 | 14.381337 |
| F | 10.253640 | 7.706748 | 16.364935 |
| F | 9.871969 | 9.385565 | 15.084002 |
| F | 7.502475 | 7.961833 | 16.522945 |
| F | 7.398174 | 9.300596 | 14.845654 |
| F | 6.364201 | 7.446211 | 14.756276 |
| F | 9.839248 | 3.419613 | 9.194039 |
| F | 11.085562 | 4.991525 | 9.905478 |
| F | 10.263986 | 5.089612 | 7.915064 |
| F | 6.367163 | 5.425837 | 9.491312 |
| F | 7.509609 | 4.888113 | 7.733932 |
| F | 7.366787 | 3.552282 | 9.410692 |
| F | 11.046778 | 7.523820 | 8.951148 |
| F | 10.680849 | 7.202661 | 11.059558 |
| F | 10.080360 | 9.025752 | 10.144221 |
| F | 8.863042 | 7.264189 | 7.257320 |
| F | 6.922181 | 7.498763 | 8.163889 |
| F | 8.367666 | 9.051632 | 8.337146 |
| O | 7.914313 | 5.313411 | 13.588064 |
| O | 8.665882 | 7.676754 | 13.195626 |
| O | 8.649985 | 5.153681 | 11.070542 |
| O | 7.950898 | 7.531590 | 10.670971 |
| N | 6.010001 | 6.444837 | 12.120900 |
| C | 8.723110 | 5.729491 | 14.613649 |
| C | 8.742881 | 7.353154 | 14.534762 |

| | | | |
|---|---|---|---|
| C | 8.745315 | 5.474331 | 9.731986 |
| C | 8.758339 | 7.098337 | 9.651577 |
| C | 10.131579 | 5.083612 | 14.336110 |
| C | 8.161588 | 5.109088 | 15.936818 |
| C | 10.016858 | 8.062091 | 15.105704 |
| C | 7.482637 | 8.021439 | 15.195072 |
| C | 10.010099 | 4.739996 | 9.172598 |
| C | 7.478119 | 4.829513 | 9.061562 |
| C | 10.177202 | 7.716942 | 9.938149 |
| C | 8.218308 | 7.728491 | 8.324043 |
| C | 4.867424 | 6.457451 | 12.108450 |
| C | 3.440968 | 6.476778 | 12.091577 |
| H | 3.096587 | 6.228996 | 11.084651 |
| H | 3.101154 | 7.478342 | 12.366940 |
| H | 3.067547 | 5.743499 | 12.810017 |

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Calculated energies and coordinates of **1**·MeCN at PBE0-D4(CPCM=benzene)/def2-TZVP level of theory

Electronic energy ... -5362.27989486 Eh
Total Enthalpy ... -5362.02487581 Eh
Final Gibbs free energy ... -5362.13407019 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 7.979426 | 6.424732 | 12.128480 |
| F | 10.649927 | 5.576141 | 13.235244 |
| F | 9.991239 | 3.767957 | 14.142598 |
| F | 10.981727 | 5.242783 | 15.348469 |
| F | 8.251139 | 3.788144 | 15.925208 |
| F | 8.767469 | 5.563868 | 17.013445 |
| F | 6.840568 | 5.376560 | 16.066835 |
| F | 11.105869 | 7.771797 | 14.411163 |
| F | 10.247176 | 7.687402 | 16.387079 |
| F | 9.890646 | 9.374289 | 15.110198 |
| F | 7.490642 | 7.974244 | 16.512473 |
| F | 7.419747 | 9.312157 | 14.833506 |
| F | 6.370072 | 7.468114 | 14.731497 |
| F | 9.851700 | 3.429953 | 9.165345 |
| F | 11.096649 | 5.004028 | 9.876352 |
| F | 10.258730 | 5.108506 | 7.892552 |
| F | 6.371651 | 5.413639 | 9.512165 |
| F | 7.496644 | 4.884165 | 7.740782 |
| F | 7.381825 | 3.547172 | 9.418031 |
| F | 11.037518 | 7.536977 | 8.933571 |
| F | 10.681411 | 7.211462 | 11.044070 |
| F | 10.070029 | 9.033519 | 10.131563 |
| F | 8.832608 | 7.264837 | 7.250374 |
| F | 6.901702 | 7.493844 | 8.179523 |
| F | 8.344869 | 9.051491 | 8.333943 |
| O | 7.912341 | 5.321924 | 13.583823 |
| O | 8.691794 | 7.679396 | 13.201197 |
| O | 8.672826 | 5.153258 | 11.063041 |
| O | 7.952376 | 7.527563 | 10.671940 |
| N | 6.027545 | 6.449310 | 12.120395 |
| C | 8.716637 | 5.729745 | 14.618866 |
| C | 8.752658 | 7.353077 | 14.541323 |
| C | 8.754503 | 5.476781 | 9.723523 |
| C | 8.756331 | 7.100588 | 9.644481 |
| C | 10.121394 | 5.071844 | 14.350489 |
| C | 8.135509 | 5.113381 | 15.934614 |
| C | 10.027490 | 8.050406 | 15.126988 |
| C | 7.492160 | 8.034322 | 15.186062 |
| C | 10.018890 | 4.750354 | 9.150381 |
| C | 7.485297 | 4.823314 | 9.067058 |
| C | 10.173144 | 7.727043 | 9.924616 |
| C | 8.200778 | 7.729037 | 8.323417 |
| C | 4.886662 | 6.455184 | 12.111010 |
| C | 3.455042 | 6.465799 | 12.099322 |
| H | 3.104217 | 6.112203 | 11.127500 |
| H | 3.107792 | 7.487450 | 12.268202 |
| H | 3.085131 | 5.812042 | 12.891586 |

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Calculated energies and coordinates of **B[H-1]** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -5230.38307456 Eh
Total Enthalpy ... -5230.17303971 Eh
Final Gibbs free energy ... -5230.27259092 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 1.084469 | -2.222684 | -0.633854 |
| O | -0.173615 | -1.450155 | -1.721323 |
| O | 1.787132 | -2.932278 | -2.238259 |
| O | 0.881109 | -3.926621 | 0.017242 |
| O | 0.054349 | -1.710609 | 0.866204 |
| C | 0.116479 | -1.430656 | -3.059612 |
| C | 1.030650 | -2.750814 | -3.350123 |
| C | -1.245689 | -1.337826 | -3.822472 |
| F | -2.090048 | -2.290435 | -3.448007 |
| F | -1.087875 | -1.416225 | -5.143006 |
| F | -1.858938 | -0.180207 | -3.568047 |
| C | 0.895750 | -0.088022 | -3.308534 |
| F | 1.095826 | 0.178226 | -4.599145 |
| F | 2.077912 | -0.107666 | -2.691840 |
| F | 0.232100 | 0.943606 | -2.789161 |
| C | 0.175547 | -4.058817 | -3.522639 |
| F | 0.959134 | -5.135558 | -3.471789 |
| F | -0.490835 | -4.110013 | -4.680300 |
| F | -0.694780 | -4.190781 | -2.527487 |
| C | 1.990192 | -2.652943 | -4.584818 |
| F | 2.606404 | -3.815908 | -4.805081 |
| F | 2.953642 | -1.758528 | -4.394460 |
| F | 1.346042 | -2.334244 | -5.708154 |
| C | 0.455542 | -4.023072 | 1.315870 |
| C | -0.492793 | -2.722688 | 1.584419 |
| C | -0.217838 | -5.423845 | 1.484724 |
| F | -1.161974 | -5.633840 | 0.576828 |
| F | -0.763520 | -5.572849 | 2.691166 |
| F | 0.672265 | -6.406868 | 1.331716 |
| C | 1.760823 | -4.013033 | 2.189944 |
| F | 1.540355 | -4.286306 | 3.475633 |
| F | 2.374135 | -2.832454 | 2.106037 |
| F | 2.635344 | -4.909845 | 1.735505 |
| C | -1.957385 | -2.913115 | 1.043074 |
| F | -1.949962 | -3.375131 | -0.202061 |
| F | -2.587737 | -1.739599 | 0.996561 |
| F | -2.700314 | -3.732095 | 1.795037 |
| C | -0.603390 | -2.246875 | 3.072607 |
| F | -1.478442 | -1.244406 | 3.184550 |
| F | 0.553938 | -1.779391 | 3.527289 |
| F | -1.010197 | -3.211488 | 3.897797 |
| H | 2.327244 | -1.427602 | -0.254208 |

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Calculated energies and coordinates of **B[H-1]** at PBE0-D4(CPCM=acetonitrile)/def2-TZVP level of theory

Electronic energy ... -5230.38799575 Eh
Total Enthalpy ... -5230.17806933 Eh
Final Gibbs free energy ... -5230.27760702 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 1.081630 | -2.224234 | -0.634726 |
| O | -0.176247 | -1.451850 | -1.723010 |
| O | 1.783342 | -2.936136 | -2.238893 |
| O | 0.878953 | -3.928015 | 0.017599 |
| O | 0.049629 | -1.711907 | 0.864466 |
| C | 0.116819 | -1.430205 | -3.061097 |
| C | 1.028507 | -2.751378 | -3.351873 |
| C | -1.243440 | -1.333125 | -3.826880 |
| F | -2.090118 | -2.285684 | -3.456565 |
| F | -1.082697 | -1.408385 | -5.146803 |
| F | -1.855248 | -0.175448 | -3.569830 |
| C | 0.899155 | -0.088518 | -3.306124 |
| F | 1.101498 | 0.179438 | -4.595562 |
| F | 2.080173 | -0.111816 | -2.687351 |
| F | 0.236329 | 0.942878 | -2.785202 |
| C | 0.171015 | -4.057419 | -3.526999 |
| F | 0.952410 | -5.135950 | -3.474755 |
| F | -0.493209 | -4.106629 | -4.685322 |

| | | | |
|---|---|---|---|
| F | -0.701244 | -4.188521 | -2.532843 |
| C | 1.990159 | -2.654207 | -4.585057 |
| F | 2.604727 | -3.818283 | -4.803933 |
| F | 2.954644 | -1.761547 | -4.392174 |
| F | 1.348395 | -2.334103 | -5.708909 |
| C | 0.455820 | -4.023063 | 1.317600 |
| C | -0.494430 | -2.724464 | 1.585181 |
| C | -0.214676 | -5.424853 | 1.490008 |
| F | -1.160572 | -5.637335 | 0.584115 |
| F | -0.757241 | -5.573100 | 2.697467 |
| F | 0.676940 | -6.406056 | 1.335344 |
| C | 1.762569 | -4.009209 | 2.189629 |
| F | 1.544318 | -4.280642 | 3.475617 |
| F | 2.373521 | -2.827632 | 2.102371 |
| F | 2.637701 | -4.905167 | 1.734678 |
| C | -1.959085 | -2.918459 | 1.045610 |
| F | -1.951595 | -3.381205 | -0.199685 |
| F | -2.591615 | -1.745912 | 0.997884 |
| F | -2.699635 | -3.737775 | 1.798477 |
| C | -0.604172 | -2.246635 | 3.072846 |
| F | -1.480459 | -1.245092 | 3.183494 |
| F | 0.553118 | -1.776736 | 3.524977 |
| F | -1.008655 | -3.210459 | 3.899487 |
| H | 2.324015 | -1.428819 | -0.255437 |

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Calculated energies and coordinates of **B[H-1]** at PBE0-D3/def2-TZVPP

Electronic energy ... -5230.31935171 Eh
Total Enthalpy ... -5230.10830518 Eh
Final Gibbs free energy ... -5230.20821438 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 7.823400 | 6.436069 | 12.130075 |
| F | 10.826701 | 5.806517 | 13.319296 |
| F | 10.290230 | 3.915316 | 14.127873 |
| F | 11.080994 | 5.430654 | 15.432488 |
| F | 8.570607 | 3.749251 | 15.935007 |
| F | 8.864150 | 5.572819 | 17.023877 |
| F | 6.982468 | 5.161948 | 16.063516 |
| F | 10.991087 | 8.042926 | 14.474086 |
| F | 10.119053 | 7.832470 | 16.431051 |
| F | 9.595996 | 9.490088 | 15.177262 |
| F | 7.356366 | 7.846098 | 16.522433 |
| F | 7.145428 | 9.166852 | 14.842430 |
| F | 6.302419 | 7.219073 | 14.741018 |
| F | 9.518145 | 3.325227 | 9.090864 |
| F | 10.957480 | 4.719034 | 9.812361 |
| F | 10.109938 | 4.968063 | 7.849403 |
| F | 6.301136 | 5.702229 | 9.511787 |
| F | 7.344502 | 5.029538 | 7.740761 |
| F | 7.078729 | 3.727439 | 9.427965 |
| F | 11.140745 | 7.323893 | 8.856201 |
| F | 10.849100 | 6.969724 | 10.967928 |
| F | 10.386418 | 8.873311 | 10.141873 |
| F | 8.930690 | 7.255678 | 7.243526 |
| F | 7.052976 | 7.724820 | 8.185031 |
| F | 8.680792 | 9.089686 | 8.325762 |
| O | 8.064273 | 5.265838 | 13.584850 |
| O | 8.629398 | 7.681948 | 13.219083 |
| O | 8.602713 | 5.164900 | 11.050579 |
| O | 8.114790 | 7.596831 | 10.676345 |
| C | 8.810766 | 5.732181 | 14.612606 |
| C | 8.691221 | 7.362077 | 14.545357 |
| C | 8.682052 | 5.480072 | 9.724039 |
| C | 8.852156 | 7.104006 | 9.653999 |
| C | 10.280274 | 5.222723 | 14.376880 |
| C | 8.299589 | 5.057779 | 15.928970 |
| C | 9.870234 | 8.181552 | 15.166615 |
| C | 7.359218 | 7.897626 | 15.186627 |
| C | 9.838067 | 4.623027 | 9.109863 |
| C | 7.337195 | 4.985952 | 9.076960 |
| C | 10.335261 | 7.565462 | 9.900659 |
| C | 8.371561 | 7.790021 | 8.332018 |
| H | 6.299502 | 6.460467 | 12.122742 |

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Calculated energies and coordinates of **B[F-1]** at PBE0-D3/def2-TZVPP

Electronic energy ... -5329.56512578 Eh
Total Enthalpy ... -5329.35855798 Eh
Final Gibbs free energy ... -5329.46017603 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 7.892306 | 6.433745 | 12.130303 |
| F | 10.806868 | 5.808770 | 13.312452 |
| F | 10.271362 | 3.921531 | 14.128929 |
| F | 11.071891 | 5.436697 | 15.425557 |
| F | 8.538057 | 3.752433 | 15.911734 |
| F | 8.853375 | 5.564069 | 17.014963 |
| F | 6.964327 | 5.177865 | 16.058274 |
| F | 10.989581 | 8.042717 | 14.459325 |
| F | 10.139066 | 7.819969 | 16.424582 |
| F | 9.612114 | 9.491760 | 15.190988 |
| F | 7.392955 | 7.874086 | 16.550071 |
| F | 7.159013 | 9.191349 | 14.868156 |
| F | 6.299891 | 7.249317 | 14.794033 |
| F | 9.533155 | 3.323402 | 9.071044 |
| F | 10.952511 | 4.717835 | 9.828689 |
| F | 10.132359 | 4.983608 | 7.856164 |
| F | 6.296275 | 5.672579 | 9.454613 |
| F | 7.380235 | 4.999294 | 7.710573 |
| F | 7.088924 | 3.702470 | 9.400021 |
| F | 11.130596 | 7.319276 | 8.868315 |
| F | 10.824107 | 6.966195 | 10.978722 |
| F | 10.363051 | 8.866748 | 10.146229 |
| F | 8.921817 | 7.268011 | 7.252852 |
| F | 7.034854 | 7.712349 | 8.188162 |
| F | 8.649258 | 9.088899 | 8.352408 |
| O | 8.060187 | 5.283612 | 13.570686 |
| O | 8.613160 | 7.704294 | 13.227711 |
| O | 8.583671 | 5.141420 | 11.039614 |
| O | 8.105064 | 7.576733 | 10.689274 |
| C | 8.799087 | 5.746172 | 14.611933 |
| C | 8.684757 | 7.375781 | 14.554962 |
| C | 8.673116 | 5.465890 | 9.712455 |
| C | 8.837602 | 7.089598 | 9.654567 |
| C | 10.266462 | 5.228164 | 14.376978 |
| C | 8.277442 | 5.062546 | 15.919803 |
| C | 9.877870 | 8.182836 | 15.167417 |
| C | 7.362939 | 7.920823 | 15.212569 |
| C | 9.844361 | 4.621837 | 9.107409 |
| C | 7.338616 | 4.962350 | 9.048342 |
| C | 10.318198 | 7.559807 | 9.904276 |
| C | 8.349491 | 7.787533 | 8.341436 |
| F | 6.167886 | 6.460910 | 12.124341 |

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Calculated energies and coordinates of **2** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -3442.33762144 Eh
Total Enthalpy ... -3442.13280403 Eh
Final Gibbs free energy ... -3442.23043761 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Si | 6.241492 | 7.760971 | 4.237656 |
| O | 6.213586 | 6.537301 | 5.325411 |
| O | 6.278562 | 8.983590 | 5.326575 |
| O | 5.012339 | 7.710685 | 3.156829 |
| O | 7.457513 | 7.812316 | 3.141670 |
| C | 6.492106 | 6.989285 | 6.619950 |
| C | 6.003057 | 8.530428 | 6.621419 |
| C | 5.452926 | 7.997748 | 1.860262 |
| C | 6.999952 | 7.530484 | 1.849380 |
| C | 5.789244 | 6.017728 | 7.624251 |
| C | 6.707763 | 9.501203 | 7.625183 |
| C | 4.484088 | 7.283945 | 0.861241 |
| C | 7.953533 | 8.248474 | 0.838467 |
| C | 5.280406 | 9.553708 | 1.716583 |

| | | | |
|---|---|---|---|
| C | 7.170630 | 5.975172 | 1.696457 |
| C | 4.445381 | 8.680576 | 6.772567 |
| C | 8.049986 | 6.838437 | 6.766452 |
| F | 6.344312 | 4.813274 | 7.574040 |
| F | 4.507221 | 5.864056 | 7.333336 |
| F | 5.898196 | 6.472486 | 8.865994 |
| F | 6.601174 | 9.045054 | 8.866632 |
| F | 6.152235 | 10.705548 | 7.577313 |
| F | 7.989169 | 9.655713 | 7.332150 |
| F | 4.025210 | 8.407999 | 7.997428 |
| F | 4.064525 | 9.908784 | 6.461843 |
| F | 3.839062 | 7.867741 | 5.904342 |
| F | 8.473701 | 7.109437 | 7.990489 |
| F | 8.429381 | 5.610388 | 6.453344 |
| F | 8.654122 | 7.651716 | 5.897118 |
| F | 9.165063 | 7.707985 | 0.875357 |
| F | 8.094115 | 9.531455 | 1.131345 |
| F | 7.488181 | 8.137500 | -0.399250 |
| F | 4.928434 | 7.398783 | -0.383651 |
| F | 3.273814 | 7.825358 | 0.920563 |
| F | 4.347798 | 6.000023 | 1.152363 |
| F | 5.532276 | 9.980930 | 0.489516 |
| F | 4.051309 | 9.916814 | 2.043992 |
| F | 6.095137 | 10.168572 | 2.576960 |
| F | 6.897793 | 5.552831 | 0.472274 |
| F | 8.405519 | 5.611406 | 2.000780 |
| F | 6.370692 | 5.356095 | 2.567471 |

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Calculated energies and coordinates of **2** at PBE0-D4(CPCM=benzene)/def2-TZVP level of theory

Electronic energy ... -3442.33672263 Eh
Total Enthalpy ... -3442.13138544 Eh
Final Gibbs free energy ... -3442.22895812 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Si | 6.241477 | 7.760966 | 4.237644 |
| O | 6.213627 | 6.537278 | 5.325321 |
| O | 6.278502 | 8.983605 | 5.326480 |
| O | 5.012309 | 7.710710 | 3.156898 |
| O | 7.457520 | 7.812266 | 3.141744 |
| C | 6.492019 | 6.989255 | 6.619875 |
| C | 6.003131 | 8.530460 | 6.621340 |
| C | 5.452882 | 7.997668 | 1.860322 |
| C | 6.999971 | 7.530564 | 1.849439 |
| C | 5.789252 | 6.017675 | 7.624073 |
| C | 6.707750 | 9.501273 | 7.624982 |
| C | 4.484025 | 7.283959 | 0.861382 |
| C | 7.953604 | 8.248448 | 0.838635 |
| C | 5.279901 | 9.553507 | 1.716809 |
| C | 7.171131 | 5.975382 | 1.696645 |
| C | 4.445577 | 8.681086 | 6.772399 |
| C | 8.049776 | 6.837924 | 6.766269 |
| F | 6.344982 | 4.813595 | 7.574377 |
| F | 4.507378 | 5.863349 | 7.333005 |
| F | 5.897808 | 6.472635 | 8.865798 |
| F | 6.601577 | 9.044940 | 8.866420 |
| F | 6.151562 | 10.705243 | 7.577617 |
| F | 7.989005 | 9.656436 | 7.331780 |
| F | 4.025086 | 8.410615 | 7.997683 |
| F | 4.064829 | 9.908811 | 6.459952 |
| F | 3.838814 | 7.867298 | 5.905322 |
| F | 8.473843 | 7.106867 | 7.990702 |
| F | 8.429052 | 5.610347 | 6.451478 |
| F | 8.654351 | 7.652112 | 5.898027 |
| F | 9.164764 | 7.707297 | 0.875060 |
| F | 8.094845 | 9.531295 | 1.131642 |
| F | 7.488088 | 8.137856 | -0.399073 |
| F | 4.928528 | 7.398510 | -0.383503 |
| F | 3.274066 | 7.825926 | 0.920261 |
| F | 4.347188 | 6.000145 | 1.152578 |
| F | 5.529694 | 9.981097 | 0.489382 |
| F | 4.051323 | 9.916514 | 2.045960 |
| F | 6.095558 | 10.168783 | 2.576074 |
| F | 6.900359 | 5.552705 | 0.472058 |
| F | 8.405560 | 5.611742 | 2.002674 |
| F | 6.370288 | 5.355857 | 2.566567 |

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Calculated energies and coordinates of **2**·MeCN at PBE0-D4(CPCM=benzene)/def2-TZVP level of theory

Electronic energy ... -3575.00611941 Eh
Total Enthalpy ... -3574.74907229 Eh
Final Gibbs free energy ... -3574.85531876 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Si | 7.968816 | 6.417901 | 12.130199 |
| F | 10.651801 | 5.509481 | 13.194334 |
| F | 9.930128 | 3.725002 | 14.096314 |
| F | 10.935683 | 5.182846 | 15.313637 |
| F | 8.172199 | 3.781415 | 15.847277 |
| F | 8.716822 | 5.551328 | 16.934100 |
| F | 6.794146 | 5.397694 | 15.971660 |
| F | 11.107344 | 7.711511 | 14.284951 |
| F | 10.267011 | 7.679465 | 16.270438 |
| F | 9.929488 | 9.348265 | 14.962164 |
| F | 7.532046 | 8.000424 | 16.442965 |
| F | 7.464743 | 9.321677 | 14.749159 |
| F | 6.369517 | 7.504567 | 14.688391 |
| F | 9.905416 | 3.457569 | 9.311339 |
| F | 11.103727 | 5.074148 | 10.001026 |
| F | 10.281031 | 5.122613 | 8.008659 |
| F | 6.372956 | 5.356143 | 9.557116 |
| F | 7.543105 | 4.842289 | 7.812956 |
| F | 7.440428 | 3.522333 | 9.506160 |
| F | 10.979314 | 7.608347 | 8.970343 |
| F | 10.674777 | 7.283601 | 11.086887 |
| F | 9.986732 | 9.079889 | 10.182044 |
| F | 8.767833 | 7.273399 | 7.332301 |
| F | 6.840574 | 7.457850 | 8.280064 |
| F | 8.243666 | 9.051591 | 8.415520 |
| O | 7.907768 | 5.357852 | 13.483132 |
| O | 8.642800 | 7.601097 | 13.110591 |
| O | 8.631488 | 5.224299 | 11.154689 |
| O | 7.934709 | 7.478595 | 10.776713 |
| N | 6.129225 | 6.433397 | 12.122930 |
| C | 8.695209 | 5.716926 | 14.546516 |
| C | 8.748114 | 7.329780 | 14.460986 |
| C | 8.752207 | 5.494120 | 9.805300 |
| C | 8.725190 | 7.107614 | 9.719744 |
| C | 10.090159 | 5.027144 | 14.299203 |
| C | 8.084708 | 5.108386 | 15.851161 |
| C | 10.041795 | 8.023259 | 15.005027 |
| C | 7.512160 | 8.046756 | 15.116437 |
| C | 10.039412 | 4.780672 | 9.271518 |
| C | 7.510834 | 4.796315 | 9.139275 |
| C | 10.128636 | 7.775732 | 9.978597 |
| C | 8.134761 | 7.726203 | 8.410535 |
| C | 4.988988 | 6.442476 | 12.110941 |
| C | 3.558060 | 6.456184 | 12.097399 |
| H | 3.210047 | 6.721974 | 11.097333 |
| H | 3.206781 | 7.194111 | 12.822347 |
| H | 3.189331 | 5.465863 | 12.372601 |

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Calculated energies and coordinates of Compound **3** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -3653.18556968 Eh
Total Enthalpy ... -3653.08432860 Eh
Final Gibbs free energy ... -3653.14830528 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | -0.000129 | 2.529572 | 0.000093 |
| O | -0.971458 | 1.204605 | 0.792892 |
| O | 0.971511 | 1.204906 | -0.792825 |
| C | -0.757176 | -0.063161 | 0.285918 |
| C | 0.757212 | -0.063020 | -0.286240 |
| C | -1.069636 | -1.081325 | 1.430953 |
| F | -0.412555 | -0.770233 | 2.540674 |

| | | | |
|---|---|---|---|
| F | -0.753468 | -2.324591 | 1.085207 |
| F | -2.363709 | -1.067533 | 1.739124 |
| C | -1.838791 | -0.236670 | -0.843042 |
| F | -1.867504 | -1.463007 | -1.350781 |
| F | -1.613590 | 0.635383 | -1.830044 |
| F | -3.050957 | 0.040123 | -0.378364 |
| C | 1.838341 | -0.236669 | 0.843143 |
| F | 3.050625 | 0.041169 | 0.379393 |
| F | 1.867438 | -1.463323 | 1.350087 |
| F | 1.611950 | 0.634530 | 1.830632 |
| C | 1.070264 | -1.081046 | -1.431311 |
| F | 0.413712 | -0.769984 | -2.541345 |
| F | 0.754119 | -2.324391 | -1.085823 |
| F | 2.364466 | -1.067105 | -1.738918 |

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Calculated energies and coordinates of **3**·MeCN at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -3785.85639647 Eh
Total Enthalpy ... -3785.70362806 Eh
Final Gibbs free energy ... -3785.77885706 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 1.510846 | 1.421875 | -0.648441 |
| O | 0.478545 | 0.012467 | -1.307624 |
| O | 0.520514 | 1.179007 | 0.926000 |
| C | -0.442759 | -0.535898 | -0.451338 |
| C | -0.687297 | 0.566834 | 0.721116 |
| C | -1.702441 | -0.922584 | -1.298596 |
| F | -1.435224 | -1.943718 | -2.114505 |
| F | -2.095111 | 0.081299 | -2.073364 |
| F | -2.731468 | -1.289764 | -0.537877 |
| C | 0.183620 | -1.874802 | 0.076704 |
| F | 1.208051 | -1.652488 | 0.892324 |
| F | 0.671504 | -2.586203 | -0.938314 |
| F | -0.703372 | -2.640972 | 0.715944 |
| C | -1.668517 | 1.712061 | 0.269555 |
| F | -1.635657 | 2.722809 | 1.132068 |
| F | -2.936071 | 1.330381 | 0.149352 |
| F | -1.264838 | 2.218480 | -0.903346 |
| C | -1.186457 | 0.030776 | 2.102693 |
| F | -1.407109 | 1.039344 | 2.946428 |
| F | -0.285211 | -0.750367 | 2.684015 |
| F | -2.322919 | -0.655780 | 1.999215 |
| N | 3.105356 | 0.172225 | 0.150571 |
| C | 4.032149 | -0.388554 | 0.523460 |
| C | 5.171490 | -1.120706 | 1.004298 |
| H | 5.452141 | -1.871363 | 0.263121 |
| H | 4.908191 | -1.613489 | 1.942202 |
| H | 6.005035 | -0.436090 | 1.168715 |

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Calculated energies and coordinates of **3**·MeCN at PBE0-D4(CPCM=acetonitrile)/def2-TZVP level of theory

Electronic energy ... -3785.85836779 Eh
Total Enthalpy ... -3785.70572528 Eh
Final Gibbs free energy ... -3785.78067625 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 1.558017 | 1.267225 | -0.631483 |
| O | 0.423254 | -0.014588 | -1.376760 |
| O | 0.585183 | 0.959432 | 0.941971 |
| C | -0.517117 | -0.570638 | -0.547590 |
| C | -0.661737 | 0.440346 | 0.724630 |
| C | -1.816198 | -0.792939 | -1.394325 |
| F | -1.632816 | -1.739015 | -2.317254 |
| F | -2.161261 | 0.307121 | -2.053850 |
| F | -2.850526 | -1.171611 | -0.645980 |
| C | 0.028944 | -1.987052 | -0.149900 |
| F | 1.099920 | -1.895652 | 0.629975 |
| F | 0.418763 | -2.654813 | -1.234911 |
| F | -0.883761 | -2.735834 | 0.473839 |
| C | -1.583222 | 1.677205 | 0.409260 |
| F | -1.451895 | 2.611622 | 1.346661 |
| F | -2.876630 | 1.381695 | 0.316982 |
| F | -1.195893 | 2.253959 | -0.735044 |
| C | -1.152269 | -0.192194 | 2.068615 |
| F | -1.322913 | 0.747144 | 3.000442 |
| F | -0.267110 | -1.049194 | 2.562493 |
| F | -2.313599 | -0.828959 | 1.932223 |
| N | 3.096472 | -0.058874 | 0.092034 |
| C | 4.078768 | -0.369973 | 0.596241 |
| C | 5.304427 | -0.771137 | 1.227595 |
| H | 5.105099 | -1.596483 | 1.913445 |
| H | 5.714282 | 0.076146 | 1.781147 |
| H | 6.016809 | -1.088160 | 0.463920 |

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Calculated energies and coordinates of Compound **3*_Ge** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -5757.12723823 Eh
Total Enthalpy ... -5756.70436594 Eh
Final Gibbs free energy ... -5756.82749411 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 0.682796 | -1.060073 | -0.827283 |
| O | -0.855276 | -0.498433 | -1.554416 |
| O | 0.930780 | -2.184535 | -2.210720 |
| O | 0.315017 | -2.159560 | 0.498172 |
| O | 0.174515 | 0.305897 | 1.399935 |
| C | -0.961172 | -0.857607 | -2.890068 |
| C | -0.157555 | -2.261202 | -3.056956 |
| C | -2.488959 | -0.876560 | -3.230158 |
| F | -3.166101 | -1.668659 | -2.412868 |
| F | -2.699455 | -1.277609 | -4.479919 |
| F | -3.013082 | 0.338883 | -3.100138 |
| C | -0.291383 | 0.315358 | -3.699085 |
| F | -0.415598 | 0.188315 | -5.011959 |
| F | 1.009135 | 0.383384 | -3.390516 |
| F | -0.812899 | 1.485802 | -3.356487 |
| C | -0.990372 | -3.507727 | -2.585160 |
| F | -0.201612 | -4.566956 | -2.443376 |
| F | -1.951154 | -3.826962 | -3.448785 |
| F | -1.534009 | -3.286389 | -1.392591 |
| C | 0.403297 | -2.568317 | -4.488303 |
| F | 0.917303 | -3.794518 | -4.540497 |
| F | 1.382400 | -1.733191 | -4.807199 |
| F | -0.540953 | -2.490776 | -5.420166 |
| C | 0.474763 | -2.025990 | 1.855641 |
| C | -0.201864 | -0.632442 | 2.338060 |
| C | -0.162634 | -3.367129 | 2.399487 |
| F | -1.379888 | -3.539778 | 1.903824 |
| F | -0.238397 | -3.432971 | 3.719375 |
| F | 0.572462 | -4.399049 | 1.991194 |
| C | 2.021687 | -2.066446 | 2.146881 |
| F | 2.300671 | -2.298497 | 3.422585 |
| F | 2.593586 | -0.916071 | 1.790851 |
| F | 2.603975 | -3.013061 | 1.420971 |
| C | -1.768810 | -0.703561 | 2.280750 |
| F | -2.190580 | -1.206289 | 1.128916 |
| F | -2.287592 | 0.517154 | 2.372960 |
| F | -2.261714 | -1.431745 | 3.281024 |
| C | 0.206893 | -0.195274 | 3.798451 |
| F | -0.651752 | 0.689765 | 4.295303 |
| F | 1.408054 | 0.378645 | 3.776280 |
| F | 0.247071 | -1.201380 | 4.655820 |
| Si | 0.491637 | 2.022801 | 1.309402 |
| C | -0.236790 | 3.021070 | 2.712629 |
| C | -0.307242 | 2.521215 | -0.294966 |
| C | 2.349384 | 2.285251 | 1.272556 |
| H | -1.266675 | 2.728384 | 2.921317 |
| C | -0.183517 | 4.511683 | 2.359917 |
| H | 0.335869 | 2.845551 | 3.626035 |
| H | -0.832120 | 4.750568 | 1.514604 |
| H | 0.827876 | 4.838249 | 2.101974 |
| H | -0.512423 | 5.116572 | 3.208109 |
| C | -1.828056 | 2.415984 | -0.335222 |
| H | 0.141650 | 1.971622 | -1.125038 |
| H | 0.005443 | 3.561449 | -0.451541 |

| | | | |
|---|---|---|---|
| H | -2.157149 | 1.381095 | -0.238938 |
| H | -2.223464 | 2.798263 | -1.278956 |
| H | -2.290041 | 2.988081 | 0.473073 |
| H | 2.843736 | 1.449174 | 1.771607 |
| H | 2.524761 | 3.151226 | 1.921914 |
| C | 2.985115 | 2.546712 | -0.091054 |
| H | 2.872732 | 1.701166 | -0.773925 |
| H | 4.056531 | 2.737592 | 0.008543 |
| H | 2.540097 | 3.415379 | -0.581315 |
| H | 1.867915 | -0.138768 | -0.685677 |

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Calculated energies and coordinates of Compound **3*_Si** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -3969.83058328 Eh
Total Enthalpy ... -3969.40556420 Eh
Final Gibbs free energy ... -3969.52758424 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Si | 0.590319 | -1.126301 | -0.923720 |
| O | -0.804881 | -0.508939 | -1.578391 |
| O | 0.871172 | -2.176068 | -2.186058 |
| O | 0.260584 | -2.006267 | 0.396751 |
| O | 0.179193 | 0.386232 | 1.431928 |
| C | -0.970318 | -0.852257 | -2.915380 |
| C | -0.188266 | -2.264650 | -3.077317 |
| C | -2.502869 | -0.856565 | -3.224495 |
| F | -3.170183 | -1.639658 | -2.391507 |
| F | -2.729300 | -1.266053 | -4.468606 |
| F | -3.015384 | 0.362062 | -3.093862 |
| C | -0.300809 | 0.319703 | -3.725769 |
| F | -0.446488 | 0.194094 | -5.036358 |
| F | 1.000649 | 0.377520 | -3.433734 |
| F | -0.813619 | 1.489139 | -3.368748 |
| C | -1.028196 | -3.508809 | -2.610539 |
| F | -0.244945 | -4.572559 | -2.482658 |
| F | -1.997331 | -3.810205 | -3.467503 |
| F | -1.557160 | -3.289276 | -1.410935 |
| C | 0.399660 | -2.573833 | -4.494648 |
| F | 0.915556 | -3.797556 | -4.540907 |
| F | 1.379098 | -1.736516 | -4.801708 |
| F | -0.540207 | -2.494761 | -5.430616 |
| C | 0.492135 | -1.956418 | 1.749633 |
| C | -0.168231 | -0.592223 | 2.324099 |
| C | -0.101702 | -3.334968 | 2.248464 |
| F | -1.341083 | -3.495203 | 1.806174 |
| F | -0.107920 | -3.478531 | 3.563065 |
| F | 0.622549 | -4.330092 | 1.739251 |
| C | 2.052341 | -1.996863 | 1.955082 |
| F | 2.381509 | -2.371594 | 3.184442 |
| F | 2.607347 | -0.815219 | 1.711607 |
| F | 2.598213 | -2.854453 | 1.098403 |
| C | -1.737207 | -0.677894 | 2.309413 |
| F | -2.189200 | -1.135849 | 1.149598 |
| F | -2.266243 | 0.530233 | 2.469778 |
| F | -2.193651 | -1.457344 | 3.288697 |
| C | 0.280791 | -0.229422 | 3.791637 |
| F | -0.556481 | 0.646044 | 4.340353 |
| F | 1.486562 | 0.331864 | 3.775563 |
| F | 0.326506 | -1.276103 | 4.600102 |
| Si | 0.492679 | 2.084644 | 1.346970 |
| C | -0.265300 | 3.060438 | 2.753285 |
| C | -0.291861 | 2.572295 | -0.268812 |
| C | 2.333319 | 2.412291 | 1.341549 |
| H | -1.275894 | 2.710276 | 2.969403 |
| C | -0.301715 | 4.554537 | 2.417645 |
| H | 0.321361 | 2.904655 | 3.662538 |
| H | -0.949209 | 4.760692 | 1.562582 |
| H | 0.689976 | 4.947886 | 2.179878 |
| H | -0.684320 | 5.130339 | 3.263943 |
| C | -1.811126 | 2.444736 | -0.314763 |
| H | 0.166697 | 2.005207 | -1.082045 |
| H | 0.009456 | 3.613191 | -0.441285 |
| H | -2.126797 | 1.407936 | -0.191140 |
| H | -2.209444 | 2.794819 | -1.269903 |
| H | -2.287202 | 3.030426 | 0.475571 |
| H | 2.787750 | 1.923557 | 2.208259 |
| H | 2.389094 | 3.487739 | 1.558281 |
| C | 3.132831 | 2.119678 | 0.075895 |
| H | 3.251709 | 1.048350 | -0.092168 |
| H | 4.136747 | 2.547087 | 0.141356 |
| H | 2.655590 | 2.541335 | -0.812118 |
| H | 1.711674 | -0.214318 | -0.774573 |

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Calculated energies and coordinates of **4** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -2103.92509554 Eh
Total Enthalpy ... -2103.60313079 Eh
Final Gibbs free energy ... -2103.68923676 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| O | -2.560390 | -0.458770 | 1.112834 |
| O | 0.647962 | 0.190914 | -0.165216 |
| C | -1.672346 | 0.212335 | 0.295832 |
| C | -0.337001 | -0.634404 | 0.267369 |
| C | -2.350036 | 0.413034 | -1.110235 |
| F | -3.356866 | 1.287768 | -0.978701 |
| F | -2.890610 | -0.715778 | -1.549394 |
| F | -1.530505 | 0.874562 | -2.043661 |
| C | -1.404458 | 1.682165 | 0.841922 |
| F | -2.539242 | 2.121024 | 1.400099 |
| F | -1.081662 | 2.529044 | -0.131753 |
| F | -0.462927 | 1.779139 | 1.765708 |
| C | -0.042929 | -1.252232 | 1.703124 |
| F | 1.262161 | -1.522015 | 1.785476 |
| F | -0.703774 | -2.391102 | 1.894740 |
| F | -0.335661 | -0.457347 | 2.720409 |
| C | -0.395732 | -1.879078 | -0.701662 |
| F | -1.483756 | -2.625004 | -0.555823 |
| F | 0.661085 | -2.664522 | -0.481657 |
| F | -0.323749 | -1.486187 | -1.968396 |
| Si | 2.319227 | 0.468045 | -0.250706 |
| C | 2.939990 | 1.034089 | 1.426504 |
| C | 2.393450 | 1.843176 | -1.511840 |
| C | 3.223068 | -1.047817 | -0.867634 |
| H | 2.088033 | 1.434617 | 1.984655 |
| C | 4.054746 | 2.079146 | 1.371523 |
| H | 3.278207 | 0.154180 | 1.983000 |
| H | 3.720607 | 2.994428 | 0.877770 |
| H | 4.928799 | 1.714913 | 0.825909 |
| H | 4.387974 | 2.350585 | 2.376657 |
| C | 1.942111 | 1.439713 | -2.913162 |
| H | 3.424390 | 2.213851 | -1.539777 |
| H | 1.787112 | 2.675159 | -1.135591 |
| H | 1.975556 | 2.286457 | -3.603796 |
| H | 0.919282 | 1.057499 | -2.909239 |
| H | 2.581950 | 0.655487 | -3.326263 |
| H | 2.720180 | -1.416442 | -1.767611 |
| H | 3.143388 | -1.844121 | -0.122361 |
| C | 4.694648 | -0.761978 | -1.172921 |
| H | 4.805104 | 0.012605 | -1.936453 |
| H | 5.202291 | -1.657549 | -1.540181 |
| H | 5.233727 | -0.424326 | -0.284126 |
| H | -3.371183 | 0.049921 | 1.243635 |

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Calculated energies and coordinates of **4** at PBE0-D4(CPCM=acetonitrile)/def2-TZVP level of theory

Electronic energy ... -2103.92589053 Eh
Total Enthalpy ... -2103.60407120 Eh
Final Gibbs free energy ... -2103.69020638 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| O | -2.560156 | -0.463934 | 1.111694 |
| O | 0.647741 | 0.193354 | -0.162901 |
| C | -1.673303 | 0.212735 | 0.298573 |
| C | -0.337182 | -0.633169 | 0.266436 |
| C | -2.349040 | 0.420726 | -1.107500 |

| | | | |
|---|---|---|---|
| F | -3.353448 | 1.297625 | -0.975730 |
| F | -2.891512 | -0.705491 | -1.551655 |
| F | -1.526410 | 0.883135 | -2.038224 |
| C | -1.406093 | 1.680069 | 0.851680 |
| F | -2.540899 | 2.116876 | 1.410343 |
| F | -1.081824 | 2.531157 | -0.118335 |
| F | -0.465050 | 1.772839 | 1.776476 |
| C | -0.043064 | -1.256557 | 1.700008 |
| F | 1.262245 | -1.523998 | 1.782753 |
| F | -0.701690 | -2.398222 | 1.885905 |
| F | -0.339028 | -0.467477 | 2.720882 |
| C | -0.396065 | -1.874658 | -0.706890 |
| F | -1.485031 | -2.620620 | -0.564994 |
| F | 0.659651 | -2.662029 | -0.488615 |
| F | -0.322828 | -1.477971 | -1.972337 |
| Si | 2.319994 | 0.469097 | -0.250574 |
| C | 2.939561 | 1.039163 | 1.425514 |
| C | 2.394175 | 1.840134 | -1.515999 |
| C | 3.223390 | -1.048685 | -0.863370 |
| H | 2.086954 | 1.440046 | 1.982450 |
| C | 4.053298 | 2.085269 | 1.368382 |
| H | 3.278757 | 0.160581 | 1.983582 |
| H | 3.718232 | 2.998819 | 0.872005 |
| H | 4.927806 | 1.720299 | 0.824020 |
| H | 4.385665 | 2.359525 | 2.373077 |
| C | 1.944120 | 1.431514 | -2.916292 |
| H | 3.425332 | 2.210127 | -1.544519 |
| H | 1.787940 | 2.673583 | -1.142843 |
| H | 1.977804 | 2.275858 | -3.609911 |
| H | 0.921435 | 1.048736 | -2.912041 |
| H | 2.584799 | 0.646092 | -3.325812 |
| H | 2.720735 | -1.419815 | -1.762443 |
| H | 3.144399 | -1.842721 | -0.115585 |
| C | 4.694874 | -0.762957 | -1.169692 |
| H | 4.804553 | 0.009278 | -1.935700 |
| H | 5.202695 | -1.659623 | -1.534145 |
| H | 5.233723 | -0.422120 | -0.281983 |
| H | -3.375034 | 0.038594 | 1.243322 |

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Calculated Energies and Coordinates of **5** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -4180.68961685 Eh
Total Enthalpy ... -4180.36895133 Eh
Final Gibbs free energy ... -4180.45874709 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 1.250435 | -0.269376 | 0.955904 |
| O | -0.004367 | 1.072603 | 0.962854 |
| O | 0.052254 | -1.304277 | 0.031089 |
| C | -1.050391 | 0.836954 | 0.104142 |
| C | -1.219019 | -0.779462 | 0.014031 |
| C | -2.278435 | 1.635384 | 0.655360 |
| C | -0.638624 | 1.476997 | -1.272337 |
| C | -1.960365 | -1.379304 | 1.263426 |
| C | -1.916866 | -1.335062 | -1.272224 |
| F | -2.511637 | 1.356248 | 1.930709 |
| F | -3.387347 | 1.387120 | -0.036165 |
| F | -2.052259 | 2.947503 | 0.591777 |
| F | -1.628786 | 1.510956 | -2.159396 |
| F | 0.386896 | 0.810203 | -1.808271 |
| F | -0.213016 | 2.724662 | -1.096536 |
| F | -1.801695 | -2.699199 | 1.305430 |
| F | -3.268710 | -1.129579 | 1.264553 |
| F | -1.435812 | -0.908240 | 2.393506 |
| F | -2.084711 | -2.654074 | -1.185708 |
| F | -1.182303 | -1.120016 | -2.356518 |
| F | -3.115924 | -0.794002 | -1.466835 |
| Si | 3.306104 | 0.156925 | -0.249563 |
| C | 3.345839 | 1.989893 | -0.644177 |
| C | 3.294853 | -0.879333 | -1.814596 |
| C | 4.649436 | -0.281254 | 0.985527 |
| H | 2.561261 | 2.205110 | -1.374600 |
| H | 4.296803 | 2.157562 | -1.166202 |
| C | 3.232519 | 2.924664 | 0.556229 |
| H | 4.499483 | 0.354018 | 1.865919 |
| H | 5.596109 | 0.049513 | 0.539980 |
| C | 4.746891 | -1.745757 | 1.401877 |
| H | 4.313599 | -0.812461 | -2.217974 |
| H | 2.655783 | -0.357784 | -2.534575 |
| C | 2.867884 | -2.340704 | -1.698576 |
| H | 3.311775 | 3.970379 | 0.248785 |
| H | 4.019527 | 2.737619 | 1.290421 |
| H | 2.271819 | 2.810168 | 1.065931 |
| H | 5.502335 | -1.883117 | 2.179544 |
| H | 5.023201 | -2.382855 | 0.559914 |
| H | 3.799967 | -2.122828 | 1.799993 |
| H | 1.839653 | -2.430272 | -1.342101 |
| H | 3.505765 | -2.899342 | -1.011620 |
| H | 2.919797 | -2.837959 | -2.670539 |
| H | 1.256443 | -0.755094 | 2.419695 |

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Calculated energies and coordinates of **6** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -4180.66063500 Eh
Total Enthalpy ... -4180.34073622 Eh
Final Gibbs free energy ... -4180.43037547 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 0.093836 | 2.665039 | 0.723946 |
| O | -1.149136 | 1.310592 | 0.845998 |
| O | 0.914745 | -0.110126 | 0.058480 |
| C | -1.423598 | 0.284039 | -0.010243 |
| C | -0.241077 | -0.824563 | 0.134235 |
| C | -2.873382 | -0.154941 | 0.425558 |
| C | -1.511500 | 0.826943 | -1.486672 |
| C | -0.278441 | -1.533846 | 1.534979 |
| C | -0.244358 | -1.949578 | -0.968190 |
| F | -3.347972 | -1.225439 | -0.197875 |
| F | -3.720903 | 0.848128 | 0.189611 |
| F | -2.916888 | -0.394866 | 1.731354 |
| F | -2.185151 | 1.976958 | -1.511809 |
| F | -2.132455 | -0.024253 | -2.301112 |
| F | -0.312835 | 1.085873 | -2.000295 |
| F | 0.884355 | -2.145547 | 1.764290 |
| F | -1.238475 | -2.457013 | 1.595347 |
| F | -0.447127 | -0.676927 | 2.531926 |
| F | 0.235942 | -1.473029 | -2.112566 |
| F | -1.444659 | -2.459217 | -1.203160 |
| F | 0.541007 | -2.965234 | -0.609687 |
| Si | 2.610240 | -0.166514 | -0.068592 |
| C | 3.280370 | -1.840617 | -0.555227 |
| C | 3.235508 | 0.321003 | 1.624746 |
| C | 2.968609 | 1.137090 | -1.364621 |
| H | 2.827818 | -2.156610 | -1.499209 |
| H | 2.984571 | -2.577966 | 0.195862 |
| C | 4.804958 | -1.826173 | -0.698205 |
| H | 2.171355 | 1.884940 | -1.313188 |
| H | 2.864410 | 0.659604 | -2.346164 |
| C | 4.326013 | 1.828035 | -1.246078 |
| H | 4.309340 | 0.519246 | 1.534004 |
| H | 3.141920 | -0.547219 | 2.285436 |
| C | 2.535340 | 1.523336 | 2.243375 |
| H | 5.182638 | -2.827936 | -0.917189 |
| H | 5.297853 | -1.483378 | 0.215101 |
| H | 5.127564 | -1.172679 | -1.511744 |
| H | 5.156220 | 1.120300 | -1.296408 |
| H | 4.415163 | 2.366502 | -0.299308 |
| H | 4.467478 | 2.554728 | -2.050265 |
| H | 2.946330 | 1.789184 | 3.220687 |
| H | 1.472804 | 1.309877 | 2.419467 |
| H | 2.633718 | 2.414851 | 1.611989 |
| H | -0.262165 | 3.065610 | 2.231063 |

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Calculated energies and coordinates of **INT1** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -7655.09020443 Eh

Total Enthalpy ... -7654.71296486 Eh
Final Gibbs free energy ... -7654.83708072 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| O | 1.587694 | -0.731176 | -1.302240 |
| O | 2.553278 | 1.257381 | -0.104446 |
| C | 2.711852 | -1.082982 | -0.594523 |
| C | 3.515059 | 0.299550 | -0.309282 |
| C | 2.204068 | -1.773814 | 0.720084 |
| F | 1.619421 | -0.888265 | 1.531094 |
| F | 3.181626 | -2.378242 | 1.393612 |
| F | 1.276511 | -2.683884 | 0.445220 |
| C | 3.478644 | -2.164590 | -1.428778 |
| F | 2.803796 | -3.314272 | -1.452167 |
| F | 4.684769 | -2.425901 | -0.930631 |
| F | 3.623499 | -1.784549 | -2.692347 |
| C | 4.476138 | 0.324416 | 0.923943 |
| F | 5.112513 | 1.493367 | 1.000486 |
| F | 5.401611 | -0.629406 | 0.858091 |
| F | 3.815510 | 0.185128 | 2.065780 |
| C | 4.327301 | 0.790068 | -1.565049 |
| F | 4.729032 | 2.046999 | -1.402508 |
| F | 3.533172 | 0.798018 | -2.643210 |
| F | 5.399356 | 0.054726 | -1.836401 |
| Ge | 1.045510 | 1.047539 | -1.183120 |
| Ge | -0.908522 | 0.666631 | 0.920318 |
| O | -2.630242 | 0.985017 | 0.323847 |
| O | -1.551639 | -0.918575 | 1.593355 |
| C | -3.371649 | -0.165625 | 0.196187 |
| C | -2.895842 | -1.147959 | 1.407803 |
| C | -4.881201 | 0.252583 | 0.179812 |
| C | -3.013318 | -0.737810 | -1.225206 |
| C | -3.574404 | -0.801165 | 2.778877 |
| C | -3.063516 | -2.685418 | 1.158592 |
| F | -5.689114 | -0.803094 | 0.159395 |
| F | -5.156263 | 0.987977 | -0.896758 |
| F | -5.196158 | 0.998390 | 1.230992 |
| F | -3.745875 | -1.785986 | -1.577921 |
| F | -1.720128 | -1.086488 | -1.260829 |
| F | -3.161673 | 0.195515 | -2.158197 |
| F | -2.943813 | -1.408287 | 3.779398 |
| F | -4.854797 | -1.160542 | 2.827995 |
| F | -3.489000 | 0.505306 | 3.027863 |
| F | -4.305351 | -3.002732 | 0.804273 |
| F | -2.772798 | -3.379347 | 2.258092 |
| F | -2.235073 | -3.113831 | 0.215025 |
| C | -0.769169 | 2.113534 | 2.707297 |
| C | -1.320508 | 3.164392 | 2.005018 |
| H | 0.307949 | 1.973603 | 2.733814 |
| H | -1.327462 | 1.667275 | 3.522485 |
| C | -0.560414 | 3.803912 | 0.936895 |
| C | -2.741257 | 3.541152 | 2.213830 |
| H | -3.119421 | 3.146369 | 3.154296 |
| H | -3.359728 | 3.138786 | 1.404312 |
| H | -2.853319 | 4.626840 | 2.199929 |
| C | -1.232744 | 4.364231 | -0.158013 |
| C | -0.526392 | 4.844088 | -1.245259 |
| C | 0.861883 | 4.801077 | -1.248300 |
| C | 1.544229 | 4.282295 | -0.153963 |
| C | 0.841749 | 3.779652 | 0.924626 |
| H | -2.314771 | 4.390469 | -0.173817 |
| H | -1.059833 | 5.250495 | -2.096071 |
| H | 1.414626 | 5.181655 | -2.099343 |
| H | 2.626904 | 4.262350 | -0.145270 |
| H | 1.389166 | 3.388710 | 1.772748 |

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Calculated energies and coordinates of **INT1'** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -4001.88343534 Eh
Total Enthalpy ... -4001.60950462 Eh
Final Gibbs free energy ... -4001.69322602 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | -0.353138 | -2.112188 | 0.243427 |
| O | 1.068321 | -1.536388 | -0.804147 |
| O | -0.433026 | -0.345211 | 0.818608 |
| C | 1.418539 | -0.210968 | -0.705165 |
| C | 0.749520 | 0.334717 | 0.675295 |
| C | 2.979487 | -0.132427 | -0.791674 |
| F | 3.554571 | -0.941019 | 0.089995 |
| F | 3.436348 | 1.101752 | -0.588921 |
| F | 3.408971 | -0.521582 | -1.992115 |
| C | 0.837042 | 0.481552 | -1.987072 |
| F | 1.266197 | 1.733677 | -2.144014 |
| F | -0.493214 | 0.491146 | -1.957818 |
| F | 1.176046 | -0.199532 | -3.079158 |
| C | 1.594781 | -0.033910 | 1.950323 |
| F | 0.892044 | 0.187297 | 3.056519 |
| F | 2.733319 | 0.642018 | 2.054771 |
| F | 1.871925 | -1.344688 | 1.951177 |
| C | 0.440010 | 1.867372 | 0.742516 |
| F | 1.533125 | 2.600923 | 0.536209 |
| F | -0.043577 | 2.199852 | 1.939653 |
| F | -0.475477 | 2.230812 | -0.143836 |
| C | -2.376485 | -1.987688 | -1.374523 |
| C | -3.181155 | -1.574517 | -0.364674 |
| H | -1.977906 | -1.298875 | -2.108151 |
| H | -2.267111 | -3.047606 | -1.578788 |
| C | -3.704699 | -2.569019 | 0.616297 |
| C | -3.493630 | -0.156817 | -0.150257 |
| H | -3.196776 | -2.457927 | 1.582885 |
| H | -3.541143 | -3.588000 | 0.267948 |
| H | -4.769127 | -2.413480 | 0.803669 |
| C | -3.754323 | 0.323793 | 1.135818 |
| C | -4.012808 | 1.667163 | 1.349797 |
| C | -4.038923 | 2.550978 | 0.280148 |
| C | -3.805158 | 2.082022 | -1.006076 |
| C | -3.532923 | 0.742281 | -1.218765 |
| H | -3.369720 | 0.384383 | -2.228222 |
| H | -3.730345 | -0.351843 | 1.981762 |
| H | -4.195220 | 2.025280 | 2.356525 |
| H | -4.247175 | 3.601643 | 0.447311 |
| H | -3.838006 | 2.764142 | -1.847820 |

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Calculated energies and coordinates of **TS1** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -8182.56427396 Eh
Total Enthalpy ... -8181.96958506 Eh
Final Gibbs free energy ... -8182.11783335 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| O | 1.820067 | -2.804771 | -2.743941 |
| O | 2.325025 | -0.580658 | -1.662804 |
| C | 2.830037 | -2.917169 | -1.828886 |
| C | 3.405945 | -1.411367 | -1.593728 |
| C | 2.194913 | -3.536662 | -0.534566 |
| F | 1.378481 | -2.662310 | 0.067959 |
| F | 3.099601 | -3.932054 | 0.360912 |
| F | 1.442545 | -4.586847 | -0.839467 |
| C | 3.855017 | -3.966508 | -2.378276 |
| F | 3.323201 | -5.190509 | -2.390490 |
| F | 4.964157 | -4.027799 | -1.642618 |
| F | 4.204067 | -3.696842 | -3.629696 |
| C | 4.129966 | -1.132235 | -0.232391 |
| F | 4.602145 | 0.115413 | -0.195915 |
| F | 5.160668 | -1.948328 | -0.024550 |
| F | 3.303748 | -1.242434 | 0.802614 |
| C | 4.381366 | -0.956076 | -2.742996 |
| F | 4.593726 | 0.357148 | -2.683473 |
| F | 3.827197 | -1.180230 | -3.937645 |
| F | 5.570769 | -1.552963 | -2.709993 |
| Ge | 1.039969 | -1.100548 | -2.964978 |
| Ge | -0.818254 | -1.330274 | -1.039221 |
| O | -2.609415 | -0.971271 | -1.369285 |
| O | -1.364314 | -3.031409 | -0.577138 |
| C | -3.353274 | -2.105164 | -1.575574 |

| | | | |
|---|---|---|---|
| C | -2.717243 | -3.250259 | -0.603781 |
| C | -4.852714 | -1.731894 | -1.321221 |
| C | -3.204390 | -2.446814 | -3.102832 |
| C | -3.198213 | -3.125724 | 0.886003 |
| C | -2.933625 | -4.737308 | -1.048586 |
| F | -5.649696 | -2.795309 | -1.363123 |
| F | -5.292485 | -0.868808 | -2.237190 |
| F | -5.014352 | -1.138876 | -0.144440 |
| F | -4.019239 | -3.414344 | -3.511182 |
| F | -1.946266 | -2.802073 | -3.380317 |
| F | -3.452053 | -1.371566 | -3.844855 |
| F | -2.436223 | -3.868296 | 1.684884 |
| F | -4.462422 | -3.506380 | 1.064236 |
| F | -3.069871 | -1.872184 | 1.319676 |
| F | -4.220161 | -5.025589 | -1.233939 |
| F | -2.466076 | -5.580888 | -0.128419 |
| F | -2.279607 | -5.009877 | -2.170156 |
| C | -0.448886 | -0.255207 | 0.699135 |
| C | -1.147052 | 0.983686 | 0.506776 |
| H | 0.633717 | -0.196418 | 0.591548 |
| H | -0.743820 | -0.827367 | 1.574617 |
| C | -0.800211 | 1.763813 | -0.690598 |
| C | -2.511491 | 1.127086 | 1.087285 |
| H | -2.559930 | 0.669011 | 2.073381 |
| H | -3.214625 | 0.600708 | 0.434394 |
| H | -2.817685 | 2.169859 | 1.148690 |
| C | -1.803081 | 2.385551 | -1.437304 |
| C | -1.498473 | 2.992406 | -2.644280 |
| C | -0.191612 | 3.005926 | -3.109321 |
| C | 0.818604 | 2.413241 | -2.360593 |
| C | 0.516366 | 1.796450 | -1.161836 |
| H | -2.830068 | 2.363197 | -1.097694 |
| H | -2.288370 | 3.450882 | -3.227044 |
| H | 0.042894 | 3.482117 | -4.054229 |
| H | 1.844026 | 2.433679 | -2.710014 |
| H | 1.315703 | 1.354665 | -0.582122 |
| Si | 0.338052 | 2.718900 | 2.713214 |
| C | 1.078793 | 1.335633 | 3.731889 |
| C | -0.981960 | 3.738974 | 3.562237 |
| C | 1.613427 | 3.745009 | 1.810726 |
| C | 1.030098 | 4.831243 | 0.910853 |
| C | 2.034646 | 1.793903 | 4.834125 |
| C | -0.444806 | 4.785494 | 4.539718 |
| H | 2.440160 | 0.939179 | 5.381307 |
| H | 1.535525 | 2.440117 | 5.559168 |
| H | 2.879396 | 2.352021 | 4.423845 |
| H | 1.599286 | 0.662337 | 3.041411 |
| H | 0.253369 | 0.755080 | 4.158134 |
| H | -1.259411 | 5.376505 | 4.966009 |
| H | 0.240684 | 5.479526 | 4.046890 |
| H | 0.095720 | 4.325050 | 5.369597 |
| H | -1.667000 | 3.051481 | 4.070153 |
| H | -1.569961 | 4.227906 | 2.777296 |
| H | 2.243034 | 3.058744 | 1.233406 |
| H | 2.272776 | 4.189180 | 2.566587 |
| H | 0.382693 | 4.408092 | 0.139187 |
| H | 1.819656 | 5.392873 | 0.405230 |
| H | 0.432883 | 5.545945 | 1.482272 |
| H | -0.428088 | 1.964330 | 1.597335 |

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Calculated energies and coordinates of **INT2** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -8182.57273282 Eh
Total Enthalpy ... -8181.97493985 Eh
Final Gibbs free energy ... -8182.12421382 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| O | 1.840294 | -2.913531 | -2.533007 |
| O | 2.375046 | -0.702835 | -1.416829 |
| C | 2.824361 | -3.049373 | -1.598424 |
| C | 3.433789 | -1.555722 | -1.346544 |
| C | 2.148247 | -3.649482 | -0.316725 |
| F | 1.346502 | -2.757510 | 0.276009 |
| F | 3.028170 | -4.078318 | 0.591553 |
| F | 1.370239 | -4.678557 | -0.636901 |
| C | 3.835349 | -4.120859 | -2.128169 |
| F | 3.280646 | -5.335950 | -2.146033 |
| F | 4.934507 | -4.205027 | -1.378290 |
| F | 4.208739 | -3.862079 | -3.375831 |
| C | 4.151219 | -1.300945 | 0.022560 |
| F | 4.632210 | -0.055356 | 0.079461 |
| F | 5.176737 | -2.124896 | 0.230834 |
| F | 3.319302 | -1.417657 | 1.052662 |
| C | 4.434076 | -1.118676 | -2.483194 |
| F | 4.672344 | 0.191607 | -2.415315 |
| F | 3.900362 | -1.327813 | -3.688262 |
| F | 5.614353 | -1.736602 | -2.434880 |
| Ge | 1.080323 | -1.182479 | -2.749550 |
| Ge | -0.820219 | -1.286533 | -0.907366 |
| O | -2.537328 | -0.850733 | -1.497801 |
| O | -1.540981 | -2.940286 | -0.437808 |
| C | -3.322905 | -1.949152 | -1.722282 |
| C | -2.896718 | -3.049865 | -0.598465 |
| C | -4.812165 | -1.461622 | -1.702145 |
| C | -3.009681 | -2.439442 | -3.185762 |
| C | -3.538042 | -2.752742 | 0.803837 |
| C | -3.199315 | -4.548111 | -0.939136 |
| F | -5.682169 | -2.466683 | -1.760837 |
| F | -5.061523 | -0.665514 | -2.743941 |
| F | -5.082590 | -0.748215 | -0.614492 |
| F | -3.858500 | -3.369316 | -3.621263 |
| F | -1.768922 | -2.926102 | -3.271402 |
| F | -3.058638 | -1.422003 | -4.041025 |
| F | -2.919061 | -3.446474 | 1.756712 |
| F | -4.835563 | -3.058455 | 0.860926 |
| F | -3.397452 | -1.471507 | 1.136833 |
| F | -4.477642 | -4.754373 | -1.251798 |
| F | -2.917017 | -5.333185 | 0.102515 |
| F | -2.453307 | -4.981220 | -1.946729 |
| C | -0.565117 | -0.240933 | 0.779552 |
| C | -1.036309 | 1.189379 | 0.652668 |
| H | 0.520344 | -0.284190 | 0.896344 |
| H | -1.021110 | -0.744376 | 1.631966 |
| C | -0.662422 | 1.818744 | -0.664267 |
| C | -2.461439 | 1.415770 | 1.096461 |
| H | -2.615478 | 1.006769 | 2.095071 |
| H | -3.139407 | 0.901878 | 0.413907 |
| H | -2.713818 | 2.476991 | 1.104394 |
| C | -1.623968 | 2.366796 | -1.507050 |
| C | -1.262837 | 2.880198 | -2.744962 |
| C | 0.061569 | 2.860546 | -3.152694 |
| C | 1.029237 | 2.319158 | -2.316467 |
| C | 0.667918 | 1.803516 | -1.082594 |
| H | -2.665083 | 2.381183 | -1.213027 |
| H | -2.026185 | 3.294662 | -3.393344 |
| H | 0.340409 | 3.261207 | -4.120333 |
| H | 2.068047 | 2.293158 | -2.624320 |
| H | 1.432751 | 1.372801 | -0.447315 |
| Si | 0.548698 | 2.784006 | 2.618696 |
| C | 1.894873 | 1.539617 | 2.873491 |
| C | -0.760952 | 2.973870 | 3.911808 |
| C | 0.906797 | 4.245598 | 1.548459 |
| C | -0.302141 | 5.094792 | 1.165118 |
| C | 2.900047 | 1.986725 | 3.946111 |
| C | -0.353913 | 4.005798 | 4.975659 |
| H | 3.694080 | 1.242990 | 4.036620 |
| H | 2.427185 | 2.089302 | 4.924675 |
| H | 3.366239 | 2.941363 | 3.693488 |
| H | 2.402790 | 1.380158 | 1.917739 |
| H | 1.434565 | 0.588069 | 3.157621 |
| H | -1.155425 | 4.115294 | 5.708690 |
| H | -0.170210 | 4.987964 | 4.534573 |
| H | 0.547753 | 3.704237 | 5.512082 |
| H | -0.952564 | 1.997410 | 4.365309 |
| H | -1.685910 | 3.288748 | 3.418774 |
| H | 1.452399 | 3.895611 | 0.666759 |
| H | 1.632797 | 4.836267 | 2.127664 |
| H | -1.011165 | 4.525793 | 0.560568 |
| H | 0.012373 | 5.961508 | 0.581006 |

| | | | |
|---|---|---|---|
| H | -0.832100 | 5.461584 | 2.046465 |
| H | -0.392692 | 1.776375 | 1.440934 |

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Calculated energies and coordinates of Compound **INT3** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -4529.42479979 Eh
Total Enthalpy ... -4528.92716084 Eh
Final Gibbs free energy ... -4529.03327144 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| H | 3.280049 | -0.788382 | -2.281279 |
| Ge | 0.709949 | -0.016175 | -0.544009 |
| O | -0.276614 | -0.835179 | 0.788039 |
| O | -0.897130 | 0.599280 | -1.217935 |
| C | -1.594550 | -0.458777 | 0.840390 |
| C | -2.011060 | 0.020723 | -0.668707 |
| C | -2.400743 | -1.670189 | 1.420129 |
| C | -1.674968 | 0.703546 | 1.893088 |
| C | -2.391896 | -1.179233 | -1.610273 |
| C | -3.164326 | 1.077357 | -0.769488 |
| F | -3.712246 | -1.436959 | 1.421318 |
| F | -2.041122 | -1.925038 | 2.677962 |
| F | -2.175606 | -2.785891 | 0.739568 |
| F | -2.919799 | 1.089577 | 2.164428 |
| F | -0.986931 | 1.759930 | 1.463844 |
| F | -1.112712 | 0.341128 | 3.043265 |
| F | -2.426934 | -0.780922 | -2.879084 |
| F | -3.578298 | -1.715112 | -1.326102 |
| F | -1.468847 | -2.136692 | -1.554807 |
| F | -3.475545 | 1.314254 | -2.044347 |
| F | -2.803451 | 2.246129 | -0.253282 |
| F | -4.277803 | 0.675372 | -0.160822 |
| C | 1.378172 | -1.511412 | -1.620992 |
| C | 2.895811 | -1.629544 | -1.695122 |
| H | 0.962115 | -1.394921 | -2.625438 |
| H | 0.935651 | -2.416738 | -1.199578 |
| C | 3.574506 | -1.573222 | -0.347679 |
| C | 3.289106 | -2.910173 | -2.434026 |
| H | 2.846021 | -2.928098 | -3.432659 |
| H | 2.936916 | -3.788403 | -1.886029 |
| H | 4.374017 | -2.984198 | -2.537021 |
| C | 2.932476 | -1.955815 | 0.827269 |
| C | 3.593632 | -1.911066 | 2.049373 |
| C | 4.911348 | -1.488948 | 2.115225 |
| C | 5.566218 | -1.111230 | 0.948358 |
| C | 4.901911 | -1.152460 | -0.266127 |
| H | 1.908517 | -2.312773 | 0.802664 |
| H | 3.071017 | -2.208655 | 2.951483 |
| H | 5.426609 | -1.448688 | 3.068046 |
| H | 6.596022 | -0.773696 | 0.988080 |
| H | 5.416919 | -0.847409 | -1.172092 |
| Si | 2.080603 | 1.947441 | -0.126084 |
| C | 0.970760 | 3.465866 | -0.116936 |
| C | 3.224556 | 2.011490 | -1.615287 |
| C | 3.036466 | 1.746984 | 1.470923 |
| H | 0.445258 | 3.504703 | 0.839626 |
| H | 0.199322 | 3.360759 | -0.885584 |
| C | 1.760247 | 4.757666 | -0.327787 |
| H | 3.614577 | 2.672168 | 1.592683 |
| H | 3.770837 | 0.948553 | 1.330729 |
| C | 2.193610 | 1.482116 | 2.713111 |
| H | 3.922226 | 1.171256 | -1.567402 |
| H | 3.837163 | 2.912526 | -1.489209 |
| C | 2.505967 | 2.053148 | -2.960997 |
| H | 2.230326 | 4.788615 | -1.313391 |
| H | 2.552424 | 4.874206 | 0.417143 |
| H | 1.107295 | 5.630920 | -0.248931 |
| H | 2.820658 | 1.404230 | 3.605162 |
| H | 1.636954 | 0.546595 | 2.622747 |
| H | 1.467796 | 2.279821 | 2.888491 |
| H | 3.213113 | 2.131945 | -3.790557 |
| H | 1.825072 | 2.905638 | -3.026001 |
| H | 1.909725 | 1.151760 | -3.135072 |

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Calculated Energies and Coordinates **TS2** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -8182.56381263 Eh
Total Enthalpy ... -8181.96541925 Eh
Final Gibbs free energy ... -8182.11285675 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| O | -3.304682 | -1.936539 | 1.401643 |
| O | -2.952351 | -1.726895 | -1.101508 |
| C | -3.524921 | -3.125126 | 0.774640 |
| C | -2.793978 | -3.016224 | -0.683013 |
| C | -3.017225 | -4.259238 | 1.727124 |
| F | -1.770991 | -4.041196 | 2.131152 |
| F | -3.061317 | -5.464686 | 1.159130 |
| F | -3.762012 | -4.320188 | 2.832883 |
| C | -5.085538 | -3.282689 | 0.647798 |
| F | -5.469186 | -4.487266 | 0.223376 |
| F | -5.589413 | -2.365298 | -0.181899 |
| F | -5.673873 | -3.068950 | 1.822717 |
| C | -1.249694 | -3.283344 | -0.596151 |
| F | -0.638396 | -2.894670 | -1.714722 |
| F | -0.941314 | -4.566360 | -0.403619 |
| F | -0.690013 | -2.572454 | 0.386497 |
| C | -3.356613 | -3.943673 | -1.812925 |
| F | -2.608066 | -3.854575 | -2.916896 |
| F | -4.585388 | -3.590493 | -2.170565 |
| F | -3.382159 | -5.229132 | -1.463019 |
| Ge | -3.368196 | -0.431312 | 0.237727 |
| Ge | -0.890351 | 0.275306 | 0.819401 |
| O | -0.750419 | 1.851698 | 1.809490 |
| O | -0.205951 | -0.570226 | 2.336035 |
| C | -0.715891 | 1.640737 | 3.158991 |
| C | 0.114012 | 0.252291 | 3.380868 |
| C | -0.112041 | 2.928491 | 3.813221 |
| C | -2.211461 | 1.533708 | 3.636647 |
| C | 1.670114 | 0.460374 | 3.318290 |
| C | -0.194264 | -0.532728 | 4.701844 |
| F | 1.040027 | 3.274909 | 3.251317 |
| F | 0.093030 | 2.785978 | 5.121204 |
| F | -0.932520 | 3.968667 | 3.653262 |
| F | -2.348670 | 1.530042 | 4.960945 |
| F | -2.783733 | 0.427220 | 3.153632 |
| F | -2.926969 | 2.549402 | 3.160821 |
| F | 2.290620 | -0.709741 | 3.177564 |
| F | 2.165389 | 1.047710 | 4.408667 |
| F | 2.022953 | 1.187856 | 2.258741 |
| F | 0.631127 | -1.573007 | 4.837885 |
| F | -1.424301 | -1.029917 | 4.700422 |
| F | -0.053976 | 0.223126 | 5.790223 |
| C | 0.637525 | 0.424256 | -0.453471 |
| C | 0.238693 | 1.132266 | -1.756622 |
| H | 0.969282 | -0.600673 | -0.631205 |
| H | 1.405871 | 0.972648 | 0.090537 |
| C | -0.547632 | 2.384743 | -1.431642 |
| C | -0.450398 | 0.193493 | -2.729060 |
| H | 0.209297 | -0.633627 | -2.998816 |
| H | -0.743300 | 0.715833 | -3.641413 |
| H | -1.340609 | -0.258823 | -2.288051 |
| C | 0.105935 | 3.500291 | -0.913409 |
| C | -0.605628 | 4.617222 | -0.510574 |
| C | -1.991282 | 4.635159 | -0.611400 |
| C | -2.651870 | 3.535100 | -1.133233 |
| C | -1.934148 | 2.420524 | -1.549871 |
| H | 1.185932 | 3.489900 | -0.811428 |
| H | -0.078333 | 5.475120 | -0.108942 |
| H | -2.550648 | 5.505511 | -0.288247 |
| H | -3.732153 | 3.538184 | -1.224486 |
| H | -2.471268 | 1.582753 | -1.979269 |
| H | 1.151301 | 1.519632 | -2.269712 |
| Si | 3.093793 | 0.477255 | -2.155347 |
| C | 2.889180 | 0.799925 | -3.964291 |
| C | 3.274414 | -1.287035 | -1.659956 |
| C | 3.849173 | 1.786463 | -1.107747 |

| | | | |
|---|---|---|---|
| C | 4.022102 | 0.169909 | -4.788754 |
| C | 3.576262 | -1.585071 | -0.196946 |
| C | 5.352380 | 1.803576 | -1.450562 |
| H | 3.883324 | 0.419345 | -5.842326 |
| H | 4.023677 | -0.917728 | -4.701229 |
| H | 5.005565 | 0.536628 | -4.488553 |
| H | 2.847315 | 1.883228 | -4.111850 |
| H | 1.927234 | 0.392963 | -4.289397 |
| H | 4.110856 | -1.613774 | -2.299968 |
| H | 2.409238 | -1.846371 | -2.033450 |
| H | 4.455844 | -1.039591 | 0.150022 |
| H | 3.772022 | -2.650680 | -0.066162 |
| H | 2.741553 | -1.319877 | 0.452589 |
| H | 5.856073 | 2.535441 | -0.816458 |
| H | 5.529929 | 2.087458 | -2.489769 |
| H | 5.826086 | 0.834574 | -1.273466 |
| H | 3.699981 | 1.566787 | -0.049140 |
| H | 3.396034 | 2.755474 | -1.326766 |

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Calculated energies and coordinates of **TS3** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -4529.33050459 Eh
Total Enthalpy ... -4528.83632640 Eh
Final Gibbs free energy ... -4528.94268493 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 1.387864 | -1.270136 | 1.313157 |
| O | 2.715831 | -1.552813 | -0.063594 |
| O | 2.107709 | 0.517446 | 1.272523 |
| C | 3.536154 | -0.511461 | -0.360869 |
| C | 3.399626 | 0.568875 | 0.868225 |
| C | 4.971447 | -1.090070 | -0.610439 |
| F | 5.373129 | -1.866823 | 0.390047 |
| F | 5.895793 | -0.143260 | -0.786666 |
| F | 4.994539 | -1.859267 | -1.705098 |
| C | 3.048274 | 0.082250 | -1.731142 |
| F | 3.900796 | 0.965506 | -2.264015 |
| F | 1.862392 | 0.678151 | -1.620056 |
| F | 2.882085 | -0.888901 | -2.631226 |
| C | 4.294956 | 0.184710 | 2.107345 |
| F | 3.928325 | 0.887405 | 3.180643 |
| F | 5.599191 | 0.407834 | 1.917433 |
| F | 4.141071 | -1.095490 | 2.446237 |
| C | 3.725837 | 2.061793 | 0.523624 |
| F | 4.934966 | 2.220780 | -0.016887 |
| F | 3.688719 | 2.824497 | 1.621537 |
| F | 2.835910 | 2.586130 | -0.313542 |
| C | -0.249056 | -0.856667 | 0.109761 |
| C | -1.444225 | -0.447167 | 0.972056 |
| H | 0.058440 | -0.065001 | -0.566267 |
| H | -0.435816 | -1.781063 | -0.448489 |
| C | -1.970857 | -1.591269 | 1.819585 |
| C | -1.124876 | 0.819839 | 1.734713 |
| H | -1.195183 | -1.948101 | 2.499819 |
| H | -2.255056 | -2.433199 | 1.188124 |
| H | -2.838305 | -1.287641 | 2.407761 |
| C | -0.966838 | 0.823076 | 3.116087 |
| C | -0.590872 | 1.984070 | 3.780684 |
| C | -0.382993 | 3.158485 | 3.075710 |
| C | -0.554269 | 3.168024 | 1.696877 |
| C | -0.918478 | 2.007796 | 1.036744 |
| H | -1.025366 | 2.027669 | -0.043115 |
| H | -1.125173 | -0.083288 | 3.686770 |
| H | -0.461672 | 1.964958 | 4.856997 |
| H | -0.089859 | 4.063464 | 3.595456 |
| H | -0.395698 | 4.080961 | 1.134134 |
| H | -2.350891 | -0.124894 | 0.369224 |
| Si | -2.550530 | -0.402103 | -1.530964 |
| C | -1.327955 | 0.092787 | -2.826783 |
| C | -3.782762 | 0.955186 | -1.234430 |
| C | -3.267076 | -2.101921 | -1.439382 |
| C | -0.419021 | -0.956896 | -3.448626 |
| C | -4.750171 | 0.802044 | -0.068506 |
| C | -2.419999 | -3.352302 | -1.634362 |
| H | 0.242685 | -0.491638 | -4.181454 |
| H | -0.996780 | -1.725325 | -3.964185 |
| H | 0.207898 | -1.445468 | -2.702960 |
| H | -0.762457 | 0.946394 | -2.439386 |
| H | -1.995622 | 0.524752 | -3.590298 |
| H | -4.330366 | 0.984791 | -2.189670 |
| H | -3.240019 | 1.904372 | -1.183179 |
| H | -5.307625 | -0.134893 | -0.124570 |
| H | -5.473508 | 1.619682 | -0.063954 |
| H | -4.228236 | 0.824312 | 0.891414 |
| H | -4.009224 | -2.022267 | -2.253792 |
| H | -3.867563 | -2.161272 | -0.526464 |
| H | -1.842057 | -3.313816 | -2.557344 |
| H | -3.065222 | -4.231816 | -1.680993 |
| H | -1.721959 | -3.501808 | -0.809979 |

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Calculated energies and coordinates of **TS4** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -4529.34815297 Eh
Total Enthalpy ... -4528.85730789 Eh
Final Gibbs free energy ... -4528.96362146 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| H | 2.511085 | 0.285203 | -0.728478 |
| Ge | 0.208824 | 0.210682 | -1.189824 |
| O | -0.485539 | -0.257040 | 0.495169 |
| O | -1.540584 | -0.108511 | -1.802187 |
| C | -1.848238 | -0.185632 | 0.583362 |
| C | -2.429267 | -0.597468 | -0.883739 |
| C | -2.283752 | -1.087524 | 1.785082 |
| C | -2.182236 | 1.303999 | 0.963703 |
| C | -2.475720 | -2.151797 | -1.108087 |
| C | -3.844210 | -0.031462 | -1.247562 |
| F | -3.607316 | -1.170226 | 1.904089 |
| F | -1.812069 | -0.603642 | 2.935551 |
| F | -1.801168 | -2.319826 | 1.676710 |
| F | -3.465174 | 1.507382 | 1.257655 |
| F | -1.842355 | 2.128335 | -0.029720 |
| F | -1.466379 | 1.688157 | 2.017953 |
| F | -2.638958 | -2.432617 | -2.399427 |
| F | -3.463474 | -2.751402 | -0.440386 |
| F | -1.324638 | -2.721656 | -0.755418 |
| F | -4.282687 | -0.548702 | -2.397133 |
| F | -3.812305 | 1.285035 | -1.420586 |
| F | -4.761311 | -0.305012 | -0.321028 |
| C | 1.392231 | -1.500908 | -1.559417 |
| C | 2.721957 | -1.174395 | -1.137178 |
| H | 1.277425 | -1.641464 | -2.632436 |
| H | 0.882962 | -2.258874 | -0.975347 |
| C | 3.205701 | -1.663611 | 0.173384 |
| C | 3.723632 | -0.934498 | -2.229174 |
| H | 3.247830 | -0.429518 | -3.070370 |
| H | 4.091647 | -1.901582 | -2.588650 |
| H | 4.581701 | -0.346874 | -1.904681 |
| C | 2.314938 | -1.896656 | 1.226317 |
| C | 2.772525 | -2.331385 | 2.456916 |
| C | 4.128714 | -2.556180 | 2.662463 |
| C | 5.020604 | -2.337859 | 1.623726 |
| C | 4.565142 | -1.889950 | 0.392878 |
| H | 1.255072 | -1.716196 | 1.094809 |
| H | 2.065608 | -2.493790 | 3.262707 |
| H | 4.485721 | -2.898489 | 3.627020 |
| H | 6.080468 | -2.512265 | 1.770254 |
| H | 5.280246 | -1.722283 | -0.401983 |
| Si | 2.701698 | 1.909124 | -0.602182 |
| C | 1.461756 | 2.957289 | 0.341642 |
| C | 3.050590 | 2.568028 | -2.322192 |
| C | 4.303674 | 1.829404 | 0.383844 |
| H | 1.112951 | 2.401315 | 1.217539 |
| H | 0.585246 | 3.096518 | -0.297185 |
| C | 2.031339 | 4.313143 | 0.757427 |
| H | 4.762175 | 2.822837 | 0.293264 |
| H | 4.994693 | 1.137371 | -0.107708 |
| C | 4.136453 | 1.456913 | 1.854228 |

| | | | |
|---|---|---|---|
| H | 3.909796 | 2.024478 | -2.727538 |
| H | 3.409438 | 3.591242 | -2.144010 |
| C | 1.905551 | 2.590006 | -3.325977 |
| H | 2.369083 | 4.888338 | -0.108830 |
| H | 2.882603 | 4.208599 | 1.433734 |
| H | 1.274657 | 4.911142 | 1.272221 |
| H | 5.096149 | 1.469359 | 2.377840 |
| H | 3.713538 | 0.456957 | 1.968823 |
| H | 3.472808 | 2.153408 | 2.372460 |
| H | 2.191906 | 3.119436 | -4.238982 |
| H | 1.020909 | 3.086799 | -2.919344 |
| H | 1.607689 | 1.578498 | -3.613006 |

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Calculated energies and coordinates of **TS5** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -4529.33432713 Eh
Total Enthalpy ... -4528.83959212 Eh
Final Gibbs free energy ... -4528.94643774 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| H | 3.885854 | -0.297343 | -0.828542 |
| Ge | 0.874910 | 0.641874 | 0.422674 |
| O | 0.077399 | -0.890503 | 1.151901 |
| O | -0.840094 | 0.968708 | -0.300883 |
| C | -1.265046 | -0.725725 | 1.357280 |
| C | -1.823360 | 0.092791 | 0.056931 |
| C | -1.870435 | -2.149170 | 1.608194 |
| C | -1.429907 | 0.090456 | 2.696315 |
| C | -2.072266 | -0.835980 | -1.186090 |
| C | -3.134726 | 0.927035 | 0.272675 |
| F | -3.201148 | -2.126946 | 1.665148 |
| F | -1.433216 | -2.652978 | 2.764057 |
| F | -1.514390 | -3.016233 | 0.669392 |
| F | -2.689411 | 0.156722 | 3.124468 |
| F | -0.971791 | 1.337082 | 2.557420 |
| F | -0.704959 | -0.455610 | 3.669881 |
| F | -2.169962 | -0.106163 | -2.296268 |
| F | -3.188483 | -1.561302 | -1.081007 |
| F | -1.057514 | -1.673170 | -1.391386 |
| F | -3.586256 | 1.408266 | -0.888874 |
| F | -2.917248 | 1.980558 | 1.051506 |
| F | -4.125294 | 0.214968 | 0.807812 |
| C | 1.768047 | -0.300568 | -1.293365 |
| C | 3.093703 | -1.025996 | -1.034767 |
| H | 1.727900 | 0.168562 | -2.279034 |
| H | 0.960736 | -1.036807 | -1.326221 |
| C | 2.971838 | -1.871302 | 0.212924 |
| C | 3.525558 | -1.821482 | -2.262011 |
| H | 3.682340 | -1.149788 | -3.109422 |
| H | 2.760787 | -2.544344 | -2.554654 |
| H | 4.456599 | -2.362674 | -2.074274 |
| C | 2.355212 | -3.120057 | 0.188447 |
| C | 2.197355 | -3.857249 | 1.350937 |
| C | 2.647777 | -3.356011 | 2.565819 |
| C | 3.263945 | -2.114942 | 2.604609 |
| C | 3.426975 | -1.383393 | 1.434855 |
| H | 1.985530 | -3.521918 | -0.748277 |
| H | 1.715802 | -4.828142 | 1.310151 |
| H | 2.520858 | -3.932666 | 3.475018 |
| H | 3.626234 | -1.714374 | 3.544874 |
| H | 3.927015 | -0.420940 | 1.473589 |
| Si | 2.506809 | 2.127985 | -0.897191 |
| C | 1.111886 | 3.365918 | -1.078539 |
| C | 3.446015 | 1.991526 | -2.511912 |
| C | 3.774284 | 2.435001 | 0.437571 |
| H | 0.588907 | 3.485068 | -0.128361 |
| H | 0.381310 | 2.986985 | -1.798549 |
| C | 1.684859 | 4.711136 | -1.541141 |
| H | 4.312793 | 3.296108 | 0.011957 |
| H | 4.499765 | 1.615391 | 0.422533 |
| C | 3.312913 | 2.750053 | 1.848894 |
| H | 4.170826 | 1.175074 | -2.462789 |
| H | 4.051047 | 2.909636 | -2.464645 |
| C | 2.671458 | 1.963532 | -3.822673 |
| H | 2.168301 | 4.642261 | -2.517336 |
| H | 2.416718 | 5.103847 | -0.831063 |
| H | 0.879620 | 5.445088 | -1.623233 |
| H | 4.153487 | 3.088085 | 2.460207 |
| H | 2.876349 | 1.871712 | 2.327528 |
| H | 2.553831 | 3.535775 | 1.857508 |
| H | 3.347887 | 2.099164 | -4.669884 |
| H | 1.919545 | 2.753907 | -3.871335 |
| H | 2.155886 | 1.013206 | -3.976341 |

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Calculated energies and coordinates of **TS6** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -4180.62860727 Eh
Total Enthalpy ... -4180.31071973 Eh
Final Gibbs free energy ... -4180.39985862 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | -0.122363 | 0.655842 | -0.399763 |
| O | -1.451412 | 0.880317 | 0.871655 |
| O | -1.253337 | -0.511568 | -1.268521 |
| C | -2.678390 | 0.466954 | 0.412201 |
| C | -2.400758 | -0.802205 | -0.570017 |
| C | -3.575869 | 0.194918 | 1.667455 |
| C | -3.293082 | 1.696341 | -0.356160 |
| C | -2.125572 | -2.129781 | 0.226382 |
| C | -3.497326 | -1.107888 | -1.645813 |
| F | -3.009230 | -0.657118 | 2.510953 |
| F | -4.769499 | -0.287892 | 1.329884 |
| F | -3.780227 | 1.319333 | 2.352869 |
| F | -4.562265 | 1.517273 | -0.712734 |
| F | -2.576444 | 1.969115 | -1.450464 |
| F | -3.238737 | 2.790162 | 0.397898 |
| F | -1.578471 | -3.043389 | -0.572050 |
| F | -3.235878 | -2.661210 | 0.738935 |
| F | -1.257639 | -1.933829 | 1.214863 |
| F | -3.199312 | -2.224234 | -2.312094 |
| F | -3.572530 | -0.139871 | -2.550893 |
| F | -4.704660 | -1.273567 | -1.113406 |
| Si | 2.366104 | 0.456902 | -0.238710 |
| C | 2.965073 | 1.987297 | -1.132346 |
| C | 2.739180 | -1.056869 | -1.263117 |
| C | 2.865584 | 0.532424 | 1.555224 |
| H | 2.599345 | 1.937268 | -2.162545 |
| H | 4.057517 | 1.863120 | -1.182696 |
| C | 2.609809 | 3.318143 | -0.486850 |
| H | 2.273982 | 1.321957 | 2.032744 |
| H | 3.893096 | 0.921137 | 1.524258 |
| C | 2.799294 | -0.758492 | 2.358543 |
| H | 3.828680 | -1.153216 | -1.137821 |
| H | 2.592572 | -0.778780 | -2.311828 |
| C | 2.049338 | -2.375706 | -0.947488 |
| H | 2.996496 | 4.155869 | -1.071889 |
| H | 3.022019 | 3.400344 | 0.521490 |
| H | 1.524811 | 3.440307 | -0.413768 |
| H | 3.122290 | -0.590426 | 3.388624 |
| H | 3.442421 | -1.530555 | 1.930507 |
| H | 1.781425 | -1.154567 | 2.390184 |
| H | 0.979412 | -2.321315 | -1.156439 |
| H | 2.167068 | -2.656826 | 0.100192 |
| H | 2.464229 | -3.180727 | -1.559086 |
| H | 0.743254 | -0.494990 | 0.491639 |

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Calculated energies and coordinates of Compound **TS7** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -4180.62859703 Eh
Total Enthalpy ... -4180.31011627 Eh
Final Gibbs free energy ... -4180.39745030 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 0.564790 | 1.816858 | -0.702186 |
| O | -1.052986 | 1.443030 | 0.160461 |
| O | 0.693344 | -0.201719 | -0.718255 |

| | | | |
|---|---|---|---|
| C | -1.627616 | 0.265784 | -0.218156 |
| C | -0.424390 | -0.841220 | -0.211522 |
| C | -2.841215 | 0.023201 | 0.752423 |
| C | -2.225224 | 0.480117 | -1.660086 |
| C | -0.131448 | -1.292348 | 1.260820 |
| C | -0.661205 | -2.125355 | -1.079289 |
| F | -3.392994 | -1.177338 | 0.607041 |
| F | -3.798817 | 0.923925 | 0.526354 |
| F | -2.484659 | 0.171575 | 2.022066 |
| F | -2.933378 | 1.602803 | -1.711141 |
| F | -3.009381 | -0.515350 | -2.061170 |
| F | -1.240985 | 0.629071 | -2.555128 |
| F | 0.986955 | -2.014616 | 1.333110 |
| F | -1.107289 | -2.039622 | 1.767025 |
| F | 0.060662 | -0.237832 | 2.046975 |
| F | -0.631196 | -1.840688 | -2.374642 |
| F | -1.823395 | -2.712085 | -0.808683 |
| F | 0.294402 | -3.031061 | -0.868040 |
| Si | 2.769894 | 0.104701 | 0.022883 |
| C | 3.187087 | -1.577825 | -0.705700 |
| C | 3.384190 | 0.135249 | 1.798992 |
| C | 3.529807 | 1.325607 | -1.189219 |
| H | 2.949866 | -1.534103 | -1.773771 |
| H | 2.573301 | -2.369783 | -0.283519 |
| C | 4.666499 | -1.917765 | -0.504681 |
| H | 2.910867 | 1.386627 | -2.094250 |
| H | 4.435665 | 0.806450 | -1.525707 |
| C | 3.875896 | 2.712348 | -0.671301 |
| H | 4.472483 | 0.038963 | 1.677521 |
| H | 3.060874 | -0.799039 | 2.267645 |
| C | 3.055079 | 1.327396 | 2.682252 |
| H | 4.924901 | -2.835804 | -1.039013 |
| H | 4.900777 | -2.077931 | 0.549977 |
| H | 5.332425 | -1.132769 | -0.873597 |
| H | 4.592312 | 2.661777 | 0.151311 |
| H | 2.995212 | 3.246585 | -0.301181 |
| H | 4.316507 | 3.326276 | -1.460347 |
| H | 3.531872 | 1.228784 | 3.660983 |
| H | 1.978790 | 1.415249 | 2.844276 |
| H | 3.396155 | 2.265428 | 2.240318 |
| H | 1.645551 | 1.434656 | 0.567801 |

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Calculated Energies and Coordinates **TS(1_INT_A_Ge)** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -5757.08372525 Eh
Total Enthalpy ... -5756.66273811 Eh
Final Gibbs free energy ... -5756.78633436 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | -0.535373 | -1.190453 | -0.126389 |
| O | -1.822951 | -1.727008 | -1.232043 |
| O | 0.512519 | -0.756597 | -1.495006 |
| O | 0.180943 | -2.490850 | 0.847071 |
| O | -1.311169 | -0.466543 | 1.302332 |
| C | -1.596541 | -1.322465 | -2.537857 |
| C | 0.009079 | -1.238211 | -2.706577 |
| C | -2.350398 | -2.337885 | -3.461572 |
| F | -1.994644 | -3.586542 | -3.203714 |
| F | -2.123115 | -2.086277 | -4.744668 |
| F | -3.660419 | -2.262569 | -3.254875 |
| C | -2.301220 | 0.079494 | -2.646686 |
| F | -2.308151 | 0.572710 | -3.874807 |
| F | -1.683322 | 0.942933 | -1.831826 |
| F | -3.553032 | 0.003119 | -2.222344 |
| C | 0.682579 | -2.644780 | -2.896612 |
| F | 1.991534 | -2.557781 | -2.708829 |
| F | 0.469146 | -3.148992 | -4.104259 |
| F | 0.227252 | -3.495762 | -1.976011 |
| C | 0.536701 | -0.274842 | -3.822234 |
| F | 1.851588 | -0.390661 | -3.961470 |
| F | 0.287364 | 0.989445 | -3.516241 |
| F | -0.018462 | -0.547046 | -4.996035 |
| C | -0.024080 | -2.316203 | 2.211892 |
| C | -1.336794 | -1.368343 | 2.367264 |
| C | -0.125935 | -3.745254 | 2.849795 |
| F | -1.021559 | -4.495322 | 2.228909 |
| F | -0.445799 | -3.672212 | 4.136271 |
| F | 1.036597 | -4.380842 | 2.755690 |
| C | 1.294757 | -1.642721 | 2.738615 |
| F | 1.326444 | -1.551276 | 4.061114 |
| F | 1.416959 | -0.425161 | 2.212488 |
| F | 2.360282 | -2.325379 | 2.345478 |
| C | -2.686968 | -2.164123 | 2.206038 |
| F | -2.634064 | -2.920917 | 1.109659 |
| F | -3.702097 | -1.330245 | 2.033719 |
| F | -2.956468 | -2.931974 | 3.252465 |
| C | -1.431495 | -0.503302 | 3.670139 |
| F | -2.583674 | 0.158449 | 3.698454 |
| F | -0.467853 | 0.401840 | 3.726653 |
| F | -1.369677 | -1.261409 | 4.757475 |
| Si | 1.227036 | 2.219833 | 0.337895 |
| C | 1.009431 | 2.879192 | 2.080832 |
| C | 0.533085 | 3.414844 | -0.928685 |
| C | 3.025881 | 1.799177 | 0.018874 |
| H | -0.060668 | 2.936896 | 2.304568 |
| C | 1.668889 | 4.243458 | 2.283469 |
| H | 1.427666 | 2.151454 | 2.782293 |
| H | 1.250907 | 4.997710 | 1.611542 |
| H | 2.745093 | 4.201505 | 2.096455 |
| H | 1.529672 | 4.603659 | 3.306233 |
| C | -0.859254 | 3.942502 | -0.591386 |
| H | 0.533351 | 2.927764 | -1.907696 |
| H | 1.243097 | 4.247251 | -1.008964 |
| H | -1.579838 | 3.130474 | -0.467877 |
| H | -1.238959 | 4.600469 | -1.377600 |
| H | -0.853564 | 4.514172 | 0.339847 |
| H | 3.339558 | 1.071010 | 0.774943 |
| H | 3.589018 | 2.715141 | 0.238829 |
| C | 3.373469 | 1.299071 | -1.378800 |
| H | 2.886813 | 0.346501 | -1.591954 |
| H | 4.450952 | 1.150693 | -1.490793 |
| H | 3.059170 | 2.007232 | -2.149742 |
| H | 0.405589 | 0.942889 | 0.234055 |

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Calculated energies and coordinates of **INT_A_Ge** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -5757.09570753 Eh
Total Enthalpy ... -5756.67461003 Eh
Final Gibbs free energy ... -5756.79886433 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 0.015597 | -0.722304 | -0.120794 |
| O | -1.398932 | -0.591784 | -1.236586 |
| O | 0.992150 | -1.313797 | -1.572943 |
| O | 0.435506 | -2.208049 | 0.821362 |
| O | -0.881873 | -0.150836 | 1.388464 |
| C | -1.133817 | -0.850896 | -2.567280 |
| C | 0.201547 | -1.771123 | -2.597805 |
| C | -2.435656 | -1.462824 | -3.184545 |
| F | -2.861678 | -2.516250 | -2.504908 |
| F | -2.257832 | -1.825779 | -4.451639 |
| F | -3.421693 | -0.567307 | -3.157510 |
| C | -0.908000 | 0.551005 | -3.235284 |
| F | -0.836315 | 0.494030 | -4.560540 |
| F | 0.214843 | 1.102301 | -2.773441 |
| F | -1.888706 | 1.388851 | -2.917890 |
| C | -0.100244 | -3.290898 | -2.304331 |
| F | 1.021446 | -3.934174 | -1.999098 |
| F | -0.660089 | -3.911743 | -3.342168 |
| F | -0.902102 | -3.422906 | -1.253107 |
| C | 1.054579 | -1.719905 | -3.911958 |
| F | 2.034386 | -2.620955 | -3.863006 |
| F | 1.634999 | -0.539605 | -4.078967 |
| F | 0.325333 | -1.983707 | -4.992301 |
| C | 0.089007 | -2.209552 | 2.151924 |

| | | | |
|---|---|---|---|
| C | -1.123728 | -1.134966 | 2.312945 |
| C | -0.240514 | -3.686801 | 2.552149 |
| F | -1.159946 | -4.219955 | 1.761244 |
| F | -0.669812 | -3.763592 | 3.809355 |
| F | 0.838902 | -4.458989 | 2.450054 |
| C | 1.406515 | -1.787273 | 2.893455 |
| F | 1.321262 | -1.858735 | 4.216723 |
| F | 1.737390 | -0.542088 | 2.543364 |
| F | 2.422233 | -2.553919 | 2.514036 |
| C | -2.535497 | -1.727517 | 1.941977 |
| F | -2.483485 | -2.331113 | 0.757603 |
| F | -3.425688 | -0.747307 | 1.819988 |
| F | -3.003750 | -2.588491 | 2.841968 |
| C | -1.248282 | -0.449745 | 3.714915 |
| F | -2.280378 | 0.390332 | 3.733931 |
| F | -0.176230 | 0.272925 | 4.015229 |
| F | -1.431643 | -1.340197 | 4.685551 |
| Si | 1.204626 | 2.395770 | 0.280904 |
| C | 1.195665 | 2.505449 | 2.128245 |
| C | -0.211393 | 3.273932 | -0.525560 |
| C | 2.878649 | 2.508716 | -0.502110 |
| H | 0.273706 | 2.063394 | 2.505875 |
| C | 1.293524 | 3.975865 | 2.562824 |
| H | 2.026415 | 1.927345 | 2.537403 |
| H | 0.440275 | 4.559275 | 2.209991 |
| H | 2.203857 | 4.454342 | 2.194018 |
| H | 1.306619 | 4.037495 | 3.652989 |
| C | -1.600713 | 2.996212 | 0.041489 |
| H | -0.176679 | 3.144937 | -1.607248 |
| H | 0.060544 | 4.327476 | -0.349652 |
| H | -1.920453 | 1.972162 | -0.156193 |
| H | -2.335329 | 3.664153 | -0.412627 |
| H | -1.633972 | 3.150272 | 1.122025 |
| H | 3.524155 | 1.778853 | -0.002759 |
| H | 3.231660 | 3.493570 | -0.157717 |
| C | 2.982243 | 2.404950 | -2.018187 |
| H | 2.740156 | 1.399024 | -2.362657 |
| H | 3.998678 | 2.632915 | -2.345474 |
| H | 2.308078 | 3.102896 | -2.518728 |
| H | 0.909681 | 0.663844 | -0.048971 |

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Calculated energies and coordinates of **TS(INT_A_3*_Ge)** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -5757.08459280 Eh
Total Enthalpy ... -5756.66407390 Eh
Final Gibbs free energy ... -5756.78714612 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Ge | 0.265890 | -0.756781 | -0.339418 |
| O | -1.235576 | -0.560912 | -1.340652 |
| O | 1.018782 | -1.580589 | -1.826779 |
| O | 0.462542 | -2.263455 | 0.640955 |
| O | -0.487279 | -0.020863 | 1.256706 |
| C | -1.107212 | -0.881543 | -2.675411 |
| C | 0.121138 | -1.945845 | -2.787803 |
| C | -2.511172 | -1.364632 | -3.170540 |
| F | -2.976477 | -2.380548 | -2.459740 |
| F | -2.475054 | -1.733341 | -4.448898 |
| F | -3.411113 | -0.387605 | -3.057971 |
| C | -0.788653 | 0.471420 | -3.406030 |
| F | -0.779158 | 0.374684 | -4.730379 |
| F | 0.396169 | 0.939913 | -3.005079 |
| F | -1.680929 | 1.404272 | -3.080820 |
| C | -0.314889 | -3.423424 | -2.462981 |
| F | 0.755957 | -4.177252 | -2.227850 |
| F | -0.998824 | -3.991265 | -3.458712 |
| F | -1.052057 | -3.474272 | -1.359440 |
| C | 0.890470 | -1.979548 | -4.155193 |
| F | 1.787089 | -2.966183 | -4.159688 |
| F | 1.571808 | -0.859892 | -4.365894 |
| F | 0.080996 | -2.175825 | -5.193622 |
| C | 0.234202 | -2.177195 | 1.990200 |
| C | -0.816842 | -0.954973 | 2.206924 |
| C | -0.231846 | -3.596096 | 2.458366 |
| F | -1.277477 | -4.020838 | 1.763728 |
| F | -0.551047 | -3.617787 | 3.749495 |
| F | 0.737249 | -4.491334 | 2.272876 |
| C | 1.648904 | -1.899470 | 2.617680 |
| F | 1.669373 | -1.985273 | 3.943667 |
| F | 2.084999 | -0.687138 | 2.256421 |
| F | 2.542976 | -2.761034 | 2.144400 |
| C | -2.310913 | -1.360394 | 1.922291 |
| F | -2.417712 | -2.006373 | 0.768087 |
| F | -3.064061 | -0.267605 | 1.813385 |
| F | -2.839771 | -2.116304 | 2.883673 |
| C | -0.786982 | -0.297834 | 3.625986 |
| F | -1.716264 | 0.653894 | 3.727230 |
| F | 0.377875 | 0.283505 | 3.879098 |
| F | -1.015220 | -1.181926 | 4.591928 |
| Si | 0.959383 | 2.367195 | 0.761840 |
| C | 0.738699 | 2.832968 | 2.528199 |
| C | -0.362605 | 2.923604 | -0.387419 |
| C | 2.720677 | 2.377399 | 0.200139 |
| H | -0.245511 | 2.539716 | 2.889903 |
| C | 0.881907 | 4.367123 | 2.579788 |
| H | 1.493724 | 2.355697 | 3.153293 |
| H | 0.121537 | 4.870243 | 1.978166 |
| H | 1.863789 | 4.705288 | 2.241541 |
| H | 0.757504 | 4.700572 | 3.611981 |
| C | -1.801720 | 2.845643 | 0.106050 |
| H | -0.233491 | 2.469751 | -1.368326 |
| H | -0.060638 | 3.977467 | -0.526365 |
| H | -2.127096 | 1.811037 | 0.211352 |
| H | -2.467123 | 3.340955 | -0.603245 |
| H | -1.922045 | 3.335378 | 1.074447 |
| H | 3.265186 | 1.622120 | 0.777090 |
| H | 3.071950 | 3.344041 | 0.595759 |
| C | 3.007234 | 2.271595 | -1.290215 |
| H | 2.744564 | 1.286926 | -1.681255 |
| H | 4.071260 | 2.425097 | -1.479451 |
| H | 2.454416 | 3.018502 | -1.863086 |
| H | 1.268505 | 0.429344 | -0.310383 |

---

Calculated Energies and Coordinates **TS(1_INT_A_Si)** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -3969.80591658 Eh
Total Enthalpy ... -3969.38299325 Eh
Final Gibbs free energy ... -3969.50463621 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Si | -0.488255 | -1.038130 | -0.110509 |
| O | -1.777341 | -1.420063 | -1.084116 |
| O | 0.519356 | -0.757576 | -1.409744 |
| O | 0.249532 | -2.263897 | 0.722447 |
| O | -1.247174 | -0.433298 | 1.247001 |
| C | -1.574941 | -1.204818 | -2.437453 |
| C | 0.024802 | -1.263665 | -2.611367 |
| C | -2.418798 | -2.251351 | -3.238079 |
| F | -2.188729 | -3.488485 | -2.826741 |
| F | -2.153629 | -2.177139 | -4.537683 |
| F | -3.717640 | -2.028566 | -3.072535 |
| C | -2.176679 | 0.223644 | -2.693736 |
| F | -2.166915 | 0.566237 | -3.973412 |
| F | -1.485332 | 1.122506 | -1.993329 |
| F | -3.424228 | 0.293542 | -2.253241 |
| C | 0.590241 | -2.727516 | -2.708403 |
| F | 1.903484 | -2.726126 | -2.524113 |
| F | 0.332506 | -3.288694 | -3.882390 |
| F | 0.076678 | -3.483955 | -1.742486 |
| C | 0.636630 | -0.426995 | -3.783686 |
| F | 1.941355 | -0.648185 | -3.893127 |
| F | 0.480976 | 0.872519 | -3.584752 |
| F | 0.073067 | -0.751707 | -4.941645 |
| C | 0.040283 | -2.256574 | 2.094849 |
| C | -1.284437 | -1.345658 | 2.299107 |
| C | -0.044122 | -3.740534 | 2.592818 |
| F | -0.909931 | -4.450603 | 1.888612 |

| | | | |
|---|---|---|---|
| F | -0.394255 | -3.781478 | 3.873597 |
| F | 1.129875 | -4.349270 | 2.471967 |
| C | 1.348229 | -1.619569 | 2.692564 |
| F | 1.358311 | -1.630650 | 4.018667 |
| F | 1.476025 | -0.365784 | 2.265364 |
| F | 2.423427 | -2.265790 | 2.264326 |
| C | -2.634830 | -2.141588 | 2.118045 |
| F | -2.599318 | -2.870866 | 1.007732 |
| F | -3.648923 | -1.298605 | 1.978688 |
| F | -2.895050 | -2.937045 | 3.147771 |
| C | -1.386742 | -0.537126 | 3.635116 |
| F | -2.539572 | 0.120813 | 3.694955 |
| F | -0.426739 | 0.366702 | 3.743578 |
| F | -1.323402 | -1.351601 | 4.682316 |
| Si | 1.168159 | 2.185825 | 0.333294 |
| C | 0.908528 | 2.829437 | 2.073744 |
| C | 0.477162 | 3.376507 | -0.935878 |
| C | 2.970019 | 1.776083 | 0.034033 |
| H | -0.165748 | 2.869690 | 2.279604 |
| C | 1.542416 | 4.205433 | 2.284482 |
| H | 1.329313 | 2.111797 | 2.782282 |
| H | 1.126472 | 4.952605 | 1.603819 |
| H | 2.622708 | 4.179640 | 2.120213 |
| H | 1.375979 | 4.563229 | 3.303852 |
| C | -0.904988 | 3.929456 | -0.595970 |
| H | 0.471876 | 2.890836 | -1.915183 |
| H | 1.201384 | 4.197060 | -1.015447 |
| H | -1.639066 | 3.132099 | -0.460578 |
| H | -1.276235 | 4.585792 | -1.387346 |
| H | -0.884346 | 4.510678 | 0.328848 |
| H | 3.285228 | 1.052911 | 0.793439 |
| H | 3.514901 | 2.701271 | 0.262742 |
| C | 3.342562 | 1.284249 | -1.360086 |
| H | 2.889659 | 0.315155 | -1.570953 |
| H | 4.425086 | 1.172097 | -1.462814 |
| H | 3.010024 | 1.978609 | -2.135685 |
| H | 0.355980 | 0.887426 | 0.210418 |

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Calculated energies and coordinates of **INT_A_Si** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -3969.80988667 Eh
Total Enthalpy ... -3969.38569342 Eh
Final Gibbs free energy ... -3969.50849320 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Si | -0.049211 | -0.716556 | -0.107526 |
| O | -1.363990 | -0.588310 | -1.141505 |
| O | 0.947879 | -1.166112 | -1.437573 |
| O | 0.376994 | -2.107496 | 0.735100 |
| O | -0.856516 | -0.141775 | 1.297133 |
| C | -1.136561 | -0.855399 | -2.482093 |
| C | 0.241958 | -1.695020 | -2.495914 |
| C | -2.413801 | -1.544256 | -3.078750 |
| F | -2.880919 | -2.498511 | -2.291761 |
| F | -2.159561 | -2.068202 | -4.274177 |
| F | -3.400969 | -0.662594 | -3.232810 |
| C | -0.991580 | 0.542343 | -3.176315 |
| F | -0.980883 | 0.449260 | -4.502169 |
| F | 0.129229 | 1.143581 | -2.786464 |
| F | -1.986225 | 1.348207 | -2.825924 |
| C | 0.045013 | -3.237534 | -2.212367 |
| F | 1.185936 | -3.766846 | -1.787788 |
| F | -0.341930 | -3.903030 | -3.299598 |
| F | -0.851099 | -3.452899 | -1.257802 |
| C | 1.125370 | -1.605322 | -3.789641 |
| F | 2.119427 | -2.490324 | -3.730242 |
| F | 1.687076 | -0.415477 | -3.937182 |
| F | 0.418352 | -1.870487 | -4.883974 |
| C | 0.055311 | -2.180091 | 2.072753 |
| C | -1.127673 | -1.094417 | 2.254850 |
| C | -0.283053 | -3.664891 | 2.430289 |
| F | -1.270366 | -4.151424 | 1.694896 |
| F | -0.621661 | -3.770702 | 3.713529 |
| F | 0.766435 | -4.453265 | 2.217768 |
| C | 1.397928 | -1.808350 | 2.801129 |
| F | 1.328162 | -1.897631 | 4.122945 |
| F | 1.764150 | -0.571360 | 2.464684 |
| F | 2.379977 | -2.602725 | 2.392537 |
| C | -2.563543 | -1.647292 | 1.912099 |
| F | -2.560507 | -2.254555 | 0.730595 |
| F | -3.423822 | -0.639024 | 1.809488 |
| F | -3.032061 | -2.490614 | 2.827632 |
| C | -1.213297 | -0.402175 | 3.654750 |
| F | -2.213369 | 0.473712 | 3.690588 |
| F | -0.113127 | 0.275520 | 3.951134 |
| F | -1.417064 | -1.298808 | 4.616422 |
| Si | 1.132367 | 2.286525 | 0.268273 |
| C | 1.147768 | 2.473221 | 2.111764 |
| C | -0.248935 | 3.241036 | -0.520465 |
| C | 2.820349 | 2.405439 | -0.491148 |
| H | 0.195637 | 2.130311 | 2.515291 |
| C | 1.373304 | 3.944347 | 2.482577 |
| H | 1.928788 | 1.847813 | 2.547029 |
| H | 0.576872 | 4.586565 | 2.099888 |
| H | 2.323336 | 4.324808 | 2.099664 |
| H | 1.389173 | 4.056046 | 3.569010 |
| C | -1.640834 | 3.002515 | 0.058438 |
| H | -0.236112 | 3.119126 | -1.602846 |
| H | 0.057444 | 4.282536 | -0.340473 |
| H | -1.985244 | 1.984187 | -0.126032 |
| H | -2.364599 | 3.683283 | -0.394697 |
| H | -1.662034 | 3.167032 | 1.137869 |
| H | 3.451595 | 1.662489 | 0.008169 |
| H | 3.182637 | 3.381738 | -0.137678 |
| C | 2.943387 | 2.308003 | -2.005649 |
| H | 2.689178 | 1.308683 | -2.358506 |
| H | 3.966900 | 2.521593 | -2.321331 |
| H | 2.285739 | 3.018307 | -2.511169 |
| H | 0.801752 | 0.676186 | -0.038931 |

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Calculated energies and coordinates of **TS(INT_A_3*_Si)** at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -3969.79415802 Eh
Total Enthalpy ... -3969.37080317 Eh
Final Gibbs free energy ... -3969.49109157 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Si | 0.247401 | -0.734093 | -0.346059 |
| O | -1.158133 | -0.502826 | -1.251995 |
| O | 0.997394 | -1.464050 | -1.730886 |
| O | 0.485499 | -2.128988 | 0.561835 |
| O | -0.400078 | 0.017716 | 1.169952 |
| C | -1.101288 | -0.841283 | -2.592624 |
| C | 0.134108 | -1.882255 | -2.706634 |
| C | -2.511962 | -1.355414 | -3.040317 |
| F | -2.980367 | -2.305503 | -2.247408 |
| F | -2.465905 | -1.830059 | -4.283239 |
| F | -3.412996 | -0.374486 | -3.017395 |
| C | -0.825653 | 0.501645 | -3.356974 |
| F | -0.868688 | 0.363263 | -4.677437 |
| F | 0.366132 | 0.992782 | -3.019646 |
| F | -1.717300 | 1.428422 | -3.017859 |
| C | -0.267278 | -3.371218 | -2.371763 |
| F | 0.819251 | -4.090774 | -2.108004 |
| F | -0.917785 | -3.963550 | -3.374725 |
| F | -1.027444 | -3.436851 | -1.286561 |
| C | 0.915969 | -1.919942 | -4.067219 |
| F | 1.826696 | -2.892938 | -4.050462 |
| F | 1.580033 | -0.794903 | -4.294366 |
| F | 0.111461 | -2.144876 | -5.103112 |
| C | 0.254993 | -2.118174 | 1.914868 |
| C | -0.765783 | -0.890982 | 2.150469 |
| C | -0.237498 | -3.546049 | 2.328654 |
| F | -1.298757 | -3.922624 | 1.632003 |
| F | -0.544339 | -3.602925 | 3.621306 |
| F | 0.710373 | -4.451772 | 2.100318 |
| C | 1.678414 | -1.893511 | 2.547791 |
| F | 1.694242 | -2.026084 | 3.868839 |

| | | | |
|---|---|---|---|
| F | 2.140594 | -0.681280 | 2.226821 |
| F | 2.548527 | -2.760077 | 2.043272 |
| C | -2.277712 | -1.245720 | 1.877982 |
| F | -2.425954 | -1.892541 | 0.732005 |
| F | -2.987621 | -0.125178 | 1.776544 |
| F | -2.815998 | -1.979900 | 2.849433 |
| C | -0.712168 | -0.261323 | 3.580561 |
| F | -1.620525 | 0.703718 | 3.715466 |
| F | 0.467283 | 0.277754 | 3.848267 |
| F | -0.955571 | -1.175094 | 4.514107 |
| Si | 0.888703 | 2.179435 | 0.762564 |
| C | 0.673695 | 2.761607 | 2.505810 |
| C | -0.370678 | 2.869699 | -0.391880 |
| C | 2.676305 | 2.231725 | 0.263019 |
| H | -0.300699 | 2.488523 | 2.904486 |
| C | 0.807772 | 4.294495 | 2.485662 |
| H | 1.440608 | 2.327069 | 3.147115 |
| H | 0.009651 | 4.766069 | 1.909213 |
| H | 1.764108 | 4.628584 | 2.076710 |
| H | 0.742449 | 4.671624 | 3.508502 |
| C | -1.832886 | 2.764520 | 0.020649 |
| H | -0.200608 | 2.515932 | -1.405737 |
| H | -0.054498 | 3.926750 | -0.402928 |
| H | -2.180878 | 1.733902 | -0.031697 |
| H | -2.456318 | 3.367190 | -0.642659 |
| H | -1.991308 | 3.120610 | 1.040947 |
| H | 3.208733 | 1.459451 | 0.828013 |
| H | 3.014523 | 3.186872 | 0.690573 |
| C | 3.001206 | 2.164026 | -1.221293 |
| H | 2.724409 | 1.199051 | -1.650345 |
| H | 4.073032 | 2.298053 | -1.381053 |
| H | 2.480639 | 2.941714 | -1.783921 |
| H | 1.200470 | 0.425046 | -0.347560 |

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Calculated energies and coordinates of $Et_3SiH$ at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -527.47794089 Eh
Total Enthalpy ... -527.26095375 Eh
Final Gibbs free energy ... -527.30955265 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Si | -8.707706 | 2.248089 | 0.288698 |
| C | -7.234249 | 3.042892 | -0.567388 |
| C | -8.214948 | 1.534636 | 1.957132 |
| C | -9.481178 | 0.928363 | -0.804467 |
| H | -6.778513 | 3.754545 | 0.130201 |
| H | -6.481327 | 2.263204 | -0.735862 |
| C | -7.574093 | 3.742204 | -1.881307 |
| H | -6.691688 | 4.202032 | -2.335238 |
| H | -8.314517 | 4.533037 | -1.730941 |
| H | -7.990147 | 3.043610 | -2.611965 |
| C | -7.632872 | 2.554894 | 2.932329 |
| H | -7.495592 | 0.726216 | 1.777728 |
| H | -9.098530 | 1.056767 | 2.395249 |
| H | -6.718508 | 3.007973 | 2.540457 |
| H | -7.384981 | 2.099172 | 3.895122 |
| H | -8.339662 | 3.366803 | 3.125920 |
| H | -8.723534 | 0.156064 | -0.985384 |
| H | -9.689126 | 1.378868 | -1.781717 |
| C | -10.751932 | 0.300611 | -0.238168 |
| H | -11.523184 | 1.055987 | -0.062494 |
| H | -11.173081 | -0.445101 | -0.918449 |
| H | -10.563209 | -0.197908 | 0.716313 |
| H | -9.735931 | 3.317661 | 0.523044 |

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Calculated energies and coordinates of $Et_3SiH$ at PBE0-D4(CPCM=acetonitrile)/def2-TZVP level of theory

Electronic energy ... -527.47814599 Eh
Total Enthalpy ... -527.26125033 Eh
Final Gibbs free energy ... -527.30985532 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Si | -8.705984 | 2.246198 | 0.288291 |
| C | -7.233612 | 3.041709 | -0.568696 |
| C | -8.213177 | 1.534256 | 1.957173 |
| C | -9.480123 | 0.926167 | -0.803774 |
| H | -6.775647 | 3.751207 | 0.129647 |
| H | -6.482312 | 2.261104 | -0.740176 |
| C | -7.575179 | 3.744009 | -1.880642 |
| H | -6.692733 | 4.202391 | -2.336049 |
| H | -8.313209 | 4.536525 | -1.727056 |
| H | -7.994939 | 3.047543 | -2.611248 |
| C | -7.633971 | 2.555687 | 2.932901 |
| H | -7.491701 | 0.727750 | 1.777621 |
| H | -9.095948 | 1.054043 | 2.394402 |
| H | -6.720985 | 3.011617 | 2.541076 |
| H | -7.384746 | 2.099998 | 3.895411 |
| H | -8.343130 | 3.365451 | 3.127080 |
| H | -8.723292 | 0.152198 | -0.980955 |
| H | -9.684893 | 1.375018 | -1.782474 |
| C | -10.753206 | 0.301930 | -0.238694 |
| H | -11.523931 | 1.058924 | -0.067434 |
| H | -11.173571 | -0.445366 | -0.917789 |
| H | -10.567447 | -0.193723 | 0.717884 |
| H | -9.734776 | 3.315984 | 0.522312 |

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Calculated energies and coordinates of $[MeCN{\rightarrow}Et_3Si]^+$ at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -659.40109109 Eh
Total Enthalpy ... -659.13947027 Eh
Final Gibbs free energy ... -659.19731608 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Si | 0.460150 | -0.004765 | -0.256712 |
| N | -1.326818 | -0.011546 | 0.157921 |
| C | -2.442228 | -0.001290 | 0.413515 |
| C | -3.835502 | 0.009823 | 0.728861 |
| H | -4.307075 | -0.869231 | 0.283155 |
| H | -3.956399 | -0.012221 | 1.814355 |
| H | -4.283987 | 0.919272 | 0.321982 |
| C | 1.269931 | -0.002775 | 1.416255 |
| H | 0.920556 | 0.872123 | 1.973742 |
| H | 0.930178 | -0.882928 | 1.971409 |
| C | 2.795756 | 0.005743 | 1.300513 |
| H | 3.163003 | -0.873462 | 0.765121 |
| H | 3.153344 | 0.890448 | 0.767659 |
| H | 3.259872 | 0.006894 | 2.288959 |
| C | 0.680698 | -1.562988 | -1.243136 |
| H | 0.056185 | -1.484831 | -2.139636 |
| H | 1.717988 | -1.551279 | -1.600171 |
| C | 0.665964 | 1.558121 | -1.239213 |
| H | 1.703180 | 1.556309 | -1.596714 |
| H | 0.041710 | 1.476610 | -2.135582 |
| C | 0.366834 | 2.846119 | -0.476553 |
| H | 1.018872 | 2.956287 | 0.392896 |
| H | 0.516337 | 3.720020 | -1.114222 |
| H | -0.666258 | 2.872127 | -0.120854 |
| C | 0.392369 | -2.855440 | -0.483781 |
| H | 0.549110 | -3.726415 | -1.123720 |
| H | 1.045363 | -2.962482 | 0.385348 |
| H | -0.640438 | -2.890908 | -0.128084 |

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Calculated energies and coordinates of $[MeCN{\rightarrow}Et_3Si]^+$ at PBE0-D4(CPCM=acetonitrile)/def2-TZVP level of theory

Electronic energy ... -659.40790905 Eh
Total Enthalpy ... -659.14636791 Eh
Final Gibbs free energy ... -659.20410583 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Si | 0.458256 | -0.005492 | -0.255322 |
| N | -1.325307 | -0.013063 | 0.158303 |
| C | -2.441073 | -0.001210 | 0.412641 |
| C | -3.834217 | 0.011886 | 0.725905 |
| H | -4.305439 | -0.867059 | 0.279545 |

| | | | |
|---|---|---|---|
| H | -3.955827 | -0.009453 | 1.811347 |
| H | -4.279983 | 0.922037 | 0.317524 |
| C | 1.271738 | -0.003308 | 1.415868 |
| H | 0.922202 | 0.871373 | 1.973642 |
| H | 0.932977 | -0.883905 | 1.970969 |
| C | 2.797297 | 0.006246 | 1.297604 |
| H | 3.163720 | -0.872591 | 0.760862 |
| H | 3.152884 | 0.891277 | 0.763771 |
| H | 3.263658 | 0.007522 | 2.285177 |
| C | 0.681784 | -1.563190 | -1.241876 |
| H | 0.057099 | -1.484219 | -2.138238 |
| H | 1.719546 | -1.551847 | -1.597430 |
| C | 0.665545 | 1.557354 | -1.237539 |
| H | 1.703122 | 1.556661 | -1.593894 |
| H | 0.040889 | 1.474853 | -2.133585 |
| C | 0.363551 | 2.844446 | -0.474179 |
| H | 1.015118 | 2.954767 | 0.395708 |
| H | 0.511346 | 3.719301 | -1.111217 |
| H | -0.669702 | 2.867108 | -0.118679 |
| C | 0.391136 | -2.855151 | -0.482263 |
| H | 0.546776 | -3.726842 | -1.121775 |
| H | 1.043517 | -2.962253 | 0.387424 |
| H | -0.641918 | -2.887914 | -0.126980 |

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Calculated energies and coordinates of $Me_3SiH$ at PBE0-D3/def2-TZVPP

Electronic energy ... -409.65093967 Eh
Total Enthalpy ... -409.52383724 Eh
Final Gibbs free energy ... -409.56248516 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Si | 0.000000 | -0.000691 | -0.369206 |
| H | -0.000000 | 0.000800 | -1.863390 |
| C | 1.538522 | -0.887019 | 0.228598 |
| H | 1.559308 | -1.922108 | -0.118581 |
| H | 2.443485 | -0.394280 | -0.132867 |
| H | 1.577937 | -0.899397 | 1.320733 |
| C | -1.538521 | -0.887019 | 0.228598 |
| H | -1.577931 | -0.899408 | 1.320733 |
| H | -2.443485 | -0.394274 | -0.132857 |
| H | -1.559312 | -1.922105 | -0.118591 |
| C | -0.000001 | 1.773125 | 0.232764 |
| H | 0.882553 | 2.310460 | -0.120600 |
| H | -0.882548 | 2.310462 | -0.120610 |
| H | -0.000007 | 1.811454 | 1.324998 |

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Calculated energies and coordinates of $Me_3SiF$ at PBE0-D3/def2-TZVPP

Electronic energy -508.92439829 Eh
Total Enthalpy -508.80180456 Eh
Final Gibbs free energy -508.84275550 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Si | 0.000000 | -0.000696 | 0.011616 |
| C | -0.000000 | 1.773410 | 0.570554 |
| H | 0.883505 | 2.301611 | 0.205969 |
| H | -0.883510 | 2.301607 | 0.205976 |
| H | 0.000004 | 1.834268 | 1.661777 |
| C | 1.538663 | -0.887273 | 0.566638 |
| H | 1.597062 | -0.911164 | 1.657753 |
| H | 1.551666 | -1.918631 | 0.208160 |
| H | 2.436166 | -0.388781 | 0.194594 |
| C | -1.538663 | -0.887271 | 0.566638 |
| H | -2.436166 | -0.388785 | 0.194586 |
| H | -1.551663 | -1.918633 | 0.208170 |
| H | -1.597067 | -0.911152 | 1.657753 |
| F | 0.000002 | 0.001490 | -1.601685 |

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Calculated energies and coordinates of $Me_3Si^+$ at PBE0-D3/def2-TZVPP

Electronic energy ... -408.77063889 Eh
Total Enthalpy ... -408.65298264 Eh
Final Gibbs free energy ... -408.69323035 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| Si | 0.000200 | 0.000381 | 0.272820 |
| C | 1.574957 | -0.916094 | 0.281046 |
| H | 1.439742 | -1.996915 | 0.274653 |
| H | 2.175624 | -0.617559 | -0.585751 |
| H | 2.155888 | -0.627777 | 1.165098 |
| C | -1.580645 | -0.905301 | 0.273412 |
| H | -1.611589 | -1.585573 | 1.132088 |
| H | -2.449608 | -0.249031 | 0.296212 |
| H | -1.629843 | -1.542176 | -0.617923 |
| C | 0.005615 | 1.821875 | 0.265349 |
| H | 1.008367 | 2.246538 | 0.241903 |
| H | -0.566142 | 2.184442 | -0.596527 |
| H | -0.523065 | 2.187182 | 1.153771 |

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Calculated energies and coordinates of $C_6H_5C(CH_3)=CH_2$ at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -348.67930941 Eh
Total Enthalpy ... -348.50860159 Eh
Final Gibbs free energy ... -348.54980691 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| C | 6.998511 | 16.657443 | 6.464318 |
| C | 7.913759 | 16.576471 | 7.433194 |
| H | 6.216591 | 17.407760 | 6.471157 |
| H | 7.020327 | 15.974182 | 5.622694 |
| C | 7.890974 | 17.488014 | 8.598196 |
| C | 9.018971 | 15.566769 | 7.361350 |
| H | 8.867195 | 14.890013 | 6.520245 |
| H | 9.079810 | 14.978865 | 8.281646 |
| H | 9.991156 | 16.051540 | 7.230792 |
| C | 9.063480 | 17.794202 | 9.292346 |
| C | 9.050895 | 18.669607 | 10.368739 |
| C | 7.861547 | 19.247035 | 10.787087 |
| C | 6.682861 | 18.935937 | 10.120359 |
| C | 6.698257 | 18.065447 | 9.044164 |
| H | 10.004231 | 17.355815 | 8.981934 |
| H | 9.977320 | 18.898231 | 10.883924 |
| H | 7.849545 | 19.926428 | 11.631853 |
| H | 5.743009 | 19.365998 | 10.448538 |
| H | 5.766502 | 17.813432 | 8.551203 |

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Calculated energies and coordinates of $PhC(H)(CH_3)$-$CH_2SiEt_3$ at PBE0-D4(CPCM=DCM)/def2-TZVP level of theory

Electronic energy ... -876.20163736 Eh
Total Enthalpy ... -875.80789303 Eh
Final Gibbs free energy ... -875.87394682 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| C | 0.578366 | 0.739710 | 0.902179 |
| C | 1.001924 | 1.758990 | -0.169543 |
| C | 1.631291 | -0.317752 | 1.149736 |
| C | 0.084642 | 1.422733 | 2.166978 |
| Si | 2.588710 | 2.794035 | -0.072762 |
| H | 1.074609 | 1.248644 | -1.137927 |
| H | 0.179895 | 2.476196 | -0.291050 |
| C | 2.047904 | -1.128038 | 0.092161 |
| C | 2.192218 | -0.546150 | 2.402644 |
| H | -0.323508 | 0.699242 | 2.876967 |
| H | -0.707843 | 2.131387 | 1.917338 |
| H | 0.877713 | 1.977183 | 2.671943 |
| C | 2.367192 | 4.129177 | -1.389758 |
| C | 2.860697 | 3.642511 | 1.587905 |
| C | 4.143949 | 1.822839 | -0.536017 |
| C | 2.992522 | -2.123665 | 0.276013 |
| H | 1.619812 | -0.976626 | -0.893591 |
| C | 3.138005 | -1.547179 | 2.594987 |
| H | 1.893596 | 0.060799 | 3.248469 |

| | | | |
|---|---|---|---|
| H | 1.476301 | 4.718511 | -1.144162 |
| C | 2.264657 | 3.600646 | -2.818430 |
| H | 3.216923 | 4.818239 | -1.306303 |
| C | 1.823262 | 4.700807 | 1.952759 |
| H | 3.857931 | 4.098556 | 1.547548 |
| H | 2.920104 | 2.878336 | 2.370816 |
| H | 4.792079 | 2.536443 | -1.060999 |
| H | 3.869118 | 1.068464 | -1.281752 |
| C | 4.921673 | 1.172803 | 0.603067 |
| C | 3.544052 | -2.339486 | 1.533605 |
| H | 3.297796 | -2.738225 | -0.563938 |
| H | 3.559303 | -1.702928 | 3.582245 |
| H | 1.400500 | 2.942095 | -2.940853 |
| H | 3.151864 | 3.024885 | -3.096363 |
| H | 2.161272 | 4.410677 | -3.546513 |
| H | 1.815498 | 5.516065 | 1.224960 |
| H | 2.021054 | 5.141478 | 2.934314 |
| H | 0.813227 | 4.284180 | 1.980936 |
| H | 4.323776 | 0.419035 | 1.116737 |
| H | 5.227930 | 1.911892 | 1.348222 |
| H | 5.829632 | 0.681777 | 0.239894 |
| H | 4.282778 | -3.119183 | 1.681248 |
| H | -0.284051 | 0.201365 | 0.485229 |

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Calculated energies and coordinates of $B(C_6F_5)_3$ at PBE0-D4(CPCM=benzene)/def2-TZVP level of theory

Electronic energy ... -2207.04435998 Eh
Total Enthalpy ... -2206.85835763 Eh
Final Gibbs free energy ... -2206.94390926 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| B | 3.698587 | 5.581018 | 1.345145 |
| F | 3.303145 | 3.970409 | -1.021796 |
| F | 2.191593 | 1.549785 | -1.063226 |
| F | 1.285300 | 0.431290 | 1.222512 |
| F | 1.510706 | 1.754188 | 3.570224 |
| F | 2.658410 | 4.159766 | 3.645474 |
| F | 5.657996 | 7.191806 | -0.043334 |
| F | 5.116893 | 8.877199 | -2.044274 |
| F | 2.567081 | 9.234693 | -2.862683 |
| F | 0.547786 | 7.882349 | -1.673369 |
| F | 1.072886 | 6.156910 | 0.297870 |
| F | 5.648246 | 3.816855 | 2.566912 |
| F | 7.350463 | 4.517801 | 4.495754 |
| F | 7.329049 | 7.034709 | 5.472160 |
| F | 5.563490 | 8.851518 | 4.530614 |
| F | 3.865814 | 8.182259 | 2.583401 |
| C | 3.028394 | 4.174809 | 1.315184 |
| C | 2.865801 | 3.465051 | 0.127763 |
| C | 2.297726 | 2.206801 | 0.081214 |
| C | 1.838017 | 1.628065 | 1.252310 |
| C | 1.962361 | 2.305357 | 2.454489 |
| C | 2.562736 | 3.548824 | 2.468638 |
| C | 3.387186 | 6.601616 | 0.207206 |
| C | 4.388573 | 7.341088 | -0.414005 |
| C | 4.133640 | 8.215770 | -1.452420 |
| C | 2.827727 | 8.396295 | -1.878373 |
| C | 1.796559 | 7.696303 | -1.272832 |
| C | 2.092507 | 6.806126 | -0.259090 |
| C | 4.681458 | 5.969395 | 2.488143 |
| C | 5.589748 | 5.061559 | 3.028805 |
| C | 6.486927 | 5.402907 | 4.021534 |
| C | 6.478883 | 6.693451 | 4.524508 |
| C | 5.579739 | 7.625303 | 4.031677 |
| C | 4.713373 | 7.256325 | 3.021367 |

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Calculated energies and coordinates of $MeCN{\cdot}B(C_6F_5)_3$ at PBE0-D4(CPCM=benzene)/def2-TZVP level of theory

Electronic energy ... -2339.72502805 Eh
Total Enthalpy ... -2339.48685703 Eh
Final Gibbs free energy ... -2339.58041533 Eh

CARTESIAN COORDINATES (ANGSTROEM)

| | | | |
|---|---|---|---|
| B | 3.092101 | 5.834674 | 1.723721 |
| N | 1.882290 | 6.397605 | 2.558964 |
| F | 3.314507 | 4.210446 | -0.798340 |
| F | 2.731055 | 1.647022 | -1.030344 |
| F | 1.882808 | 0.217796 | 1.110638 |
| F | 1.629577 | 1.437419 | 3.523425 |
| F | 2.221437 | 4.014866 | 3.791249 |
| F | 5.423893 | 7.078766 | 0.300452 |
| F | 5.290098 | 8.522426 | -1.907097 |
| F | 2.914888 | 8.949322 | -3.141208 |
| F | 0.649986 | 7.870640 | -2.102996 |
| F | 0.754306 | 6.404690 | 0.109553 |
| F | 5.351083 | 3.949983 | 2.371676 |
| F | 7.411323 | 4.501093 | 3.927466 |
| F | 7.675830 | 6.945923 | 5.064561 |
| F | 5.796179 | 8.850334 | 4.605578 |
| F | 3.714403 | 8.329652 | 3.037772 |
| C | 1.010496 | 6.816180 | 3.160322 |
| C | -0.089674 | 7.344249 | 3.915723 |
| C | 2.749907 | 4.259785 | 1.503416 |
| C | 2.877092 | 3.587602 | 0.297464 |
| C | 2.590886 | 2.239797 | 0.148951 |
| C | 2.160721 | 1.506059 | 1.237653 |
| C | 2.029744 | 2.131587 | 2.464177 |
| C | 2.329851 | 3.476083 | 2.569064 |
| C | 3.084156 | 6.710628 | 0.351989 |
| C | 4.214226 | 7.264039 | -0.230538 |
| C | 4.176150 | 8.013486 | -1.395309 |
| C | 2.968651 | 8.230441 | -2.030843 |
| C | 1.816724 | 7.682711 | -1.496781 |
| C | 1.900483 | 6.937682 | -0.336040 |
| C | 4.395577 | 6.100085 | 2.662379 |
| C | 5.390103 | 5.167559 | 2.915838 |
| C | 6.489871 | 5.432855 | 3.716345 |
| C | 6.630733 | 6.678301 | 4.297219 |
| C | 5.669867 | 7.644818 | 4.062958 |
| C | 4.590989 | 7.339566 | 3.255669 |
| H | -0.369086 | 6.630090 | 4.692483 |
| H | -0.936271 | 7.512118 | 3.247261 |
| H | 0.209941 | 8.288722 | 4.373934 |

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