

Supporting Information

Electronic Nature of Zwitterionic Group 14 Anions of the Alkali Metals - A Combined Experimental and Computational Approach

Hui Li, Adelia J. A. Aquino, David B. Cordes, William L. Hase, Clemens Krempner*.

Texas Tech University, Department of Chemistry & Biochemistry, Box 41061, Lubbock, Texas,
79409-1061.

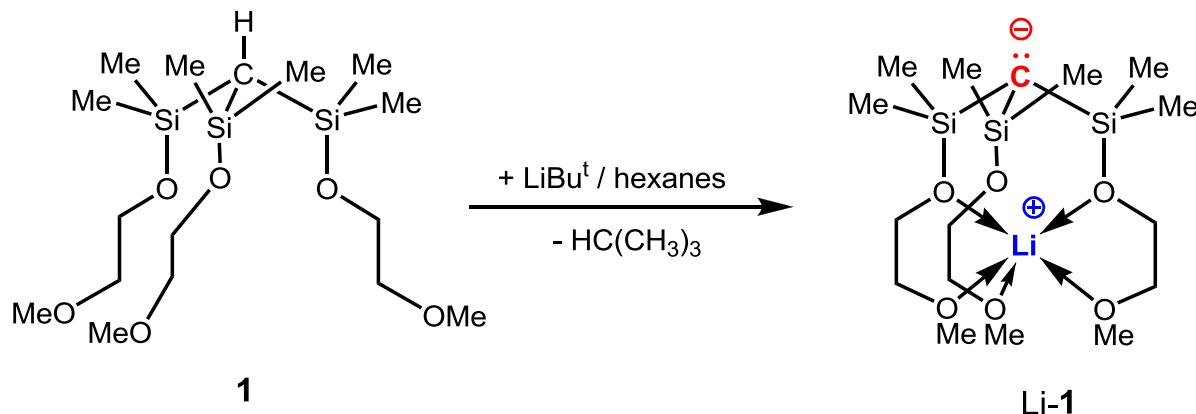
| | |
|---|------|
| 1. General Remarks..... | S3 |
| 2. Synthetic Procedures..... | S4 |
| 2.1. Synthesis of [C(SiMe₂OCH₂CH₂OMe)₃Li] (Li-1)..... | S4 |
| 2.2. Synthesis of [C(SiMe₂OCH₂CH₂OMe)₃K] (K-1)..... | S5 |
| 2.3. Synthesis of Ge(SiMe₂Cl)₄..... | S5 |
| 2.4. Synthesis of Ge(SiMe₂OCH₂CH₂OMe)₄ (3)..... | S6 |
| 2.5. Synthesis of [Ge(SiMe₂OCH₂CH₂OMe)₃Li] (Li-3)..... | S7 |
| 2.6. Synthesis of [Ge(SiMe₂OCH₂CH₂OMe)₃Na] (Na-3)..... | S8 |
| 2.7. Synthesis of [Ge(SiMe₂OCH₂CH₂OMe)₃K] (K-3)..... | S9 |
| 2.8. Synthesis of [HC(SiMe₂OCH₂CH₂OMe)₃Na][9-SiMe₂Ph-C₁₃H₈] (Na-4)..... | S10 |
| 2.9. Synthesis of [HC(SiMe₂OCH₂CH₂OMe)₃Li][BH₄] (Li-5)..... | S11 |
| 2.10. Synthesis of [HC(SiMe₂OCH₂CH₂OMe)₃Na][BPh₄] (Na-6)..... | S12 |
| 3. Estimation of the Basicities of M-1 – M-3..... | S13 |
| 4. X-ray crystallography..... | S16 |
| 5. DFT Calculations..... | S24 |
| 5.1. Results of calculations for M-1 and [M-1-H]⁺ (M = Li, Na, K)..... | S25 |
| 5.2. Results of calculations for M-2 and [M-2-H]⁺ (M = Li, Na, K)..... | S29 |
| 5.3. Results of calculations for M-3 and [M-3-H]⁺ (M = Li, Na, K)..... | S32 |
| 5.4. Results of calculations for the metal free anions 1⁻, 2⁻, 3⁻, 1, 2-H and 3-H..... | S35 |
| 5.5. Results of calculations for the metal free anions 7⁻, 8⁻, 9⁻, 7-H, 8-H and 9-H..... | S44 |
| 5.6. B3-LYP/TZVP Cartesian coordinates [Å]..... | S46 |
| 6. References..... | S128 |

1. General Remarks

All air- and moisture-sensitive manipulations were carried out using standard vacuum line, Schlenk or cannula techniques or in a Vacuum Atmospheres OMNI inert atmosphere drybox containing an atmosphere of purified nitrogen. THF, THF-D₈, toluene, diethyl ether and hexanes were distilled under nitrogen from alkali metals and stored over 4 Å molecular sieves prior to use. C₆D₆, THF-D₈, toluene-D₈, CD₂Cl₂ and MeOCH₂CH₂OH were dried and stored over 4 Å molecular sieves prior to use. NEt₃ and CH₂Cl₂ were dried over CaH₂, distilled under nitrogen and stored over 4 Å molecular sieves. All deuterated solvents were purchased from Cambridge Isotope Labs. Ph₂PCH₂PPh₂ (Alfa Aesar), Bu^tLi (Acros), Bu^tOK (Alfa Aesar), Bu^tONa (TCI), Bu^tOLi (Aldrich), fluorene (Aldrich), LiBH₄ (Alfa Aesar), NaBPh₄ (Alfa Aesar) and 4,7,13,16,21,24-Hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane [denoted as 2.2.2-cryptand] (Aldrich) were purchased from commercial sources and used without further purification. The compounds Ge(SiMe₃)₄ [1], Si(SiMe₂Cl)₄ [2], Si(SiMe₂OCH₂CH₂OMe)₄ (**2**) [3], Si(SiMe₂OCH₂CH₂OMe)₃Li (Li-**2**) [3], Si(SiMe₂OCH₂CH₂OMe)₃Li (Na-**2**) [3], Si(SiMe₂OCH₂CH₂OMe)₃Li (K-**2**), [3], HC(SiMe₃)₃ [4], HC(SiMe₂Cl)₃ [4], HC(SiMe₂OCH₂CH₂OMe)₃ (**1**) [4], C(SiMe₂OCH₂CH₂OMe)₃Na (Na-**1**) [4], Na-benzyl [4], K-benzyl [5], 9-Bu^t-fluorene [4], 9-Prⁱ-fluorene [4], 9-Buⁿ-fluorene [4], 9-Ph-fluorene [6], 9-Me₃Si-fluorene [7], 9-PhMe₂Si-fluorene [8] and 9-Ph₃Si-fluorene [8] were synthesized according to the literature procedures. The ¹H, ²³Na, ⁷Li, ¹³C, ³¹P and ²⁹Si NMR spectra were obtained from a Varian Unity Inova 500 and JOEL ECS 400. All measurements, unless noted otherwise, were carried out at 298 K and NMR chemical shifts were given in ppm. The ²³Na NMR spectra were referenced to a 0.1 M solution of NaCl in D₂O ($\delta = 0$), ⁷Li NMR spectra were referenced to a 0.1 M solution of LiCl in D₂O ($\delta = 0$) and the ²⁹Si NMR spectra to TMS ($\delta = 0$ ppm). ²⁹Si NMR spectra were obtained by using the INEPT pulse sequence. The ¹H-NMR spectra were referenced to the residual protonated solvent for ¹H and the ¹³C NMR spectra were referenced to the deuterated solvent peaks. The following abbreviations were used to describe peak multiplicities in the reported NMR spectroscopic data: ‘s’ for singlet, “d” for doublet, “t” for triplet, “quart.” for quartet, “sept” for septet, “m” for multiplet and “br” for broadened resonances. Elemental analyses were performed using a Perkin Elmer 2400 Series II CHNS/O Analyzer.

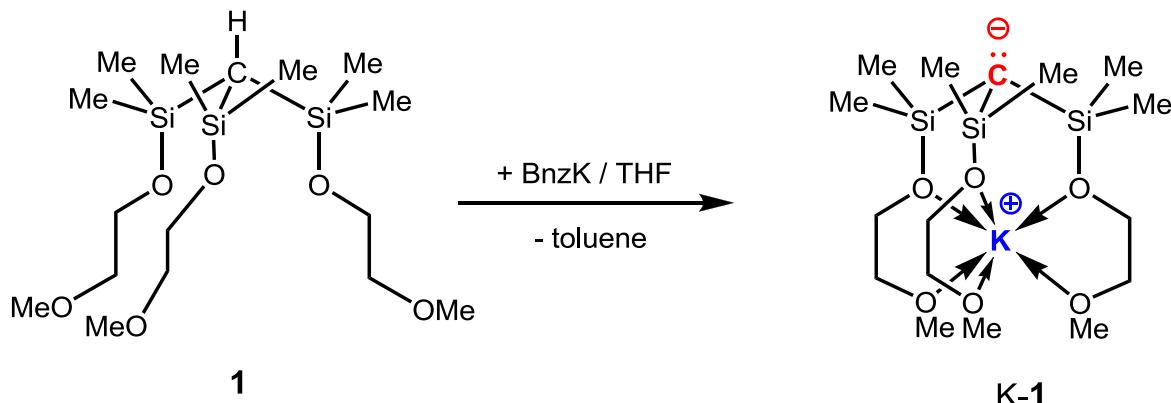
2. Synthetic Procedures

2.1. Synthesis of $\text{C}(\text{Si}(\text{CH}_3)_2\text{OCH}_2\text{CH}_2\text{OCH}_3)_3\text{Li}$ (Li-1)



In a Glove box a 25 mL Schlenk flask equipped with a magnetic stir bar was charged with $\text{HC}(\text{SiMe}_2\text{OCH}_2\text{CH}_2\text{OCH}_3)_3$ (**1**) (120 mg, 0.29 mmol) and 1 mL of hexane. The resulting solution was pre-cooled in a freezer and then a hexane solution of LiBu^t (0.2 mL, 1.5 M, 0.30 mmol) was added with stirring. After stirring the resulting solution for 2 hours at room temperature, the solvent was removed under vacuum to give raw **Li-1** as a colorless crystalline material. Recrystallization from hexanes gave an analytically pure sample of **Li-1** (92 mg, 76%). ^1H NMR (C_6D_6 , 400 MHz): δ 0.53 (s, $\text{Si}(\text{CH}_3)_2$, 18 H), 2.95 (s, OCH_3 , 9 H), 3.10 (t, $^3J_{\text{H-H}} = 4.8$ Hz, CH_2O , 6 H), 3.51 (t, $^3J_{\text{H-H}} = 4.8$ Hz, SiOCH_2 , 6 H) ppm. $^{13}\text{C}\{\text{H}\}$ NMR (C_6D_6 , 125.7 MHz): δ 4.3 ($\text{Si}(\text{CH}_3)_2$), 60.2 (OCH_3), 61.9 (OCH_2), 74.4 (CH_2OCH_3) ppm, signal from CSi_3 was not observed. $^{29}\text{Si}\{\text{H}\}$ NMR (C_6D_6 , 99.3 MHz): δ 12.2 ($\text{Si}(\text{CH}_3)_2\text{O}$) ppm. $^7\text{Li}\{\text{H}\}$ NMR (C_6D_6 , 194.2 MHz): δ -0.58 ppm. Anal. calc. for $\text{C}_{16}\text{H}_{39}\text{O}_6\text{Si}_3\text{Li}$ (418.67): C, 45.90; H, 9.39. Found: C, 46.20; H, 9.35%.

2.2. Synthesis of $[C(SiMe_2OCH_2CH_2OMe)_3K]$ (K-1)



In a Glove box a 25 mL Schlenk flask equipped with a magnetic stir bar was charged with benzyl potassium (30mg, 0.26 mmol), HC(Si(CH₃)₂OCH₂CH₂OCH₃)₄ (**1**) (100 mg, 0.24 mmol) and 1 mL of THF. After stirring the resulting solution for 3 hours, the solvent was removed under vacuum. The solid residue recrystallized from hexanes to give K-**1** (46 mg, 42%). ¹H NMR (C₆D₆, 300 MHz): δ 0.54 (s, Si(CH₃)₂, 18 H), 2.87 (s, OCH₃, 9 H), 3.04 (t, ³J_{H-H} = 4.5 Hz, CH₂O, 6 H), 3.47 (t, ³J_{H-H} = 4.5 Hz, SiOCH₂, 6 H) ppm. ¹³C{H} NMR (C₆D₆, 125.7 MHz): δ 3.6 (Si(CH₃)₂), 57.3(OCH₃), 60.1 (OCH₂), 75.0 (CH₂OCH₃) ppm, signal from CSi₃ was not observed. ²⁹Si{H} NMR (C₆D₆, 99.3 MHz): δ 8.7 (Si(CH₃)₂O) ppm. Anal. calc. for C₁₆H₃₉O₆Si₃K (450.83): C, 42.63; H, 8.72. Found: C, 42.79; H, 8.84%.

2.3. Synthesis of Ge(SiMe₂Cl)₄

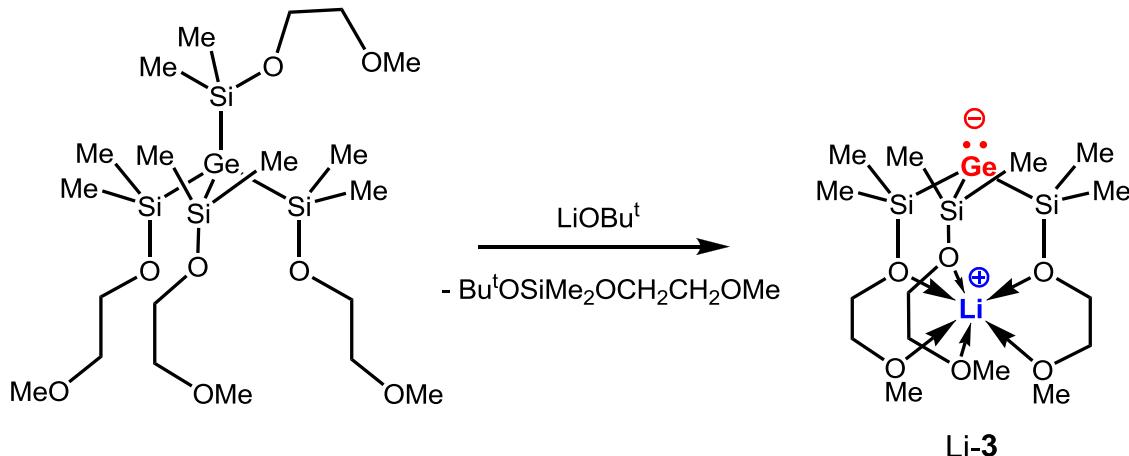
A 100 mL three-neck round bottom flask equipped with a reflux condenser, addition funnel and large magnetic stir bar was charged with $\text{Ge}(\text{SiMe}_3)_4$ (3 g, 8.2 mmol), AlCl_3 (6 g, 45 mmol) and 20 mL of dry hexanes. After the vigorously stirred suspension was heated (ca. 55-60°C), acetyl chloride (3 mL) dissolved in 10 mL of dry hexanes was slowly added via addition funnel within an hour. After the resulting emulsion (two liquid phases) was vigorously stirred with heating (ca. 55-60°C) overnight, 100 mL hexanes were added and the mixture was cooled to room temperature.

Then the upper phase was carefully separated from the viscous lower phase by decantation via cannula and the lower phase was extracted twice with hexanes. The solvent and other volatiles of the combined extracts were removed under vacuum to leave a solid. Vacuum distillation of the semi-solid using a Kugelrohrofen gave 2.6 g (71 %) of the title compound as a crystalline material. ^1H NMR (C_6D_6 , 400 MHz): δ 0.63 (s, $\text{Si}(\text{CH}_3)_2$, 24 H) ppm. $^{13}\text{C}\{\text{H}\}$ NMR (C_6D_6 , 125.7 MHz): δ 7.1 ($\text{Si}(\text{CH}_3)_2$) ppm. $^{29}\text{Si}\{\text{H}\}$ NMR (C_6D_6 , 99.3 MHz): δ 30.1 ($\text{Si}(\text{CH}_3)_2$) ppm. Anal. calc. for $\text{C}_{12}\text{H}_{36}\text{Si}_4\text{Ge}$ (366.11): C, 39.44; H, 9.93. Found: C, 39.28; H, 9.89%.

2.4. Synthesis of $\text{Ge}(\text{SiMe}_2\text{OCH}_2\text{CH}_2\text{OMe})_4$ (3)

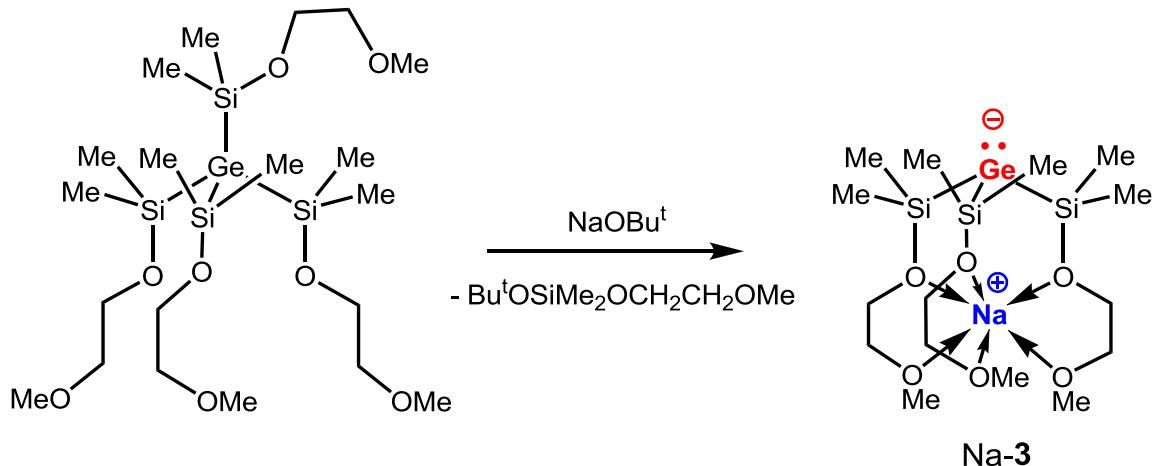
A 50 mL Schlenk flask equipped with a magnetic stir bar was charged with NEt_3 (10.8 ml, 5.72 mmol) $\text{Ge}(\text{Si}(\text{CH}_3)_2\text{Cl})_4$ (600 mg, 1.34 mmol) and hexanes (30 mL) and cooled to 0-5°C. Upon adding dropwise $\text{HOCH}_2\text{CH}_2\text{SCH}_3$ (2 ml, 25.4 mmol) via syringe a white suspension immediately formed, which was allowed to stir overnight at room temperature (the progress of the reaction was monitored by ^1H -NMR spectroscopy). Then the suspension was centrifuged, the liquid phase decanted and the solid phase washed two times with ca. 5 mL of hexanes. The organic phases were combined and solvent and excess $\text{HOCH}_2\text{CH}_2\text{OCH}_3$ were removed under high vacuum (ca. 10^{-1} mbar). Then 5 mL of hexanes were added to the residue, the mixture was centrifuged, the liquid phase decanted and the solvent evaporated under vacuum. Distillation of the liquid residue using a Kugelrohrofen afforded 470 mg (58%) of **3** as a colorless liquid. ^1H NMR (C_6D_6 , 400 MHz): δ 0.60 (s, $\text{Si}(\text{CH}_3)_2$, 24 H), 3.15 (s, OCH_3 , 12 H), 3.39 (t, $^3J_{\text{H-H}} = 5.5$ Hz, CH_2O , 8 H) 3.80 (t, $^3J_{\text{H-H}} = 5.5$ Hz, SiOCH_2 , 8 H) ppm. $^{13}\text{C}\{\text{H}\}$ NMR (C_6D_6 , 125.7 MHz): δ 4.6 ($\text{Si}(\text{CH}_3)_2$), 58.6 (OCH_3), 63.0 (OCH_2), 74.3 (CH_2OCH_3) ppm. $^{29}\text{Si}\{\text{H}\}$ NMR (C_6D_6 , 99.3 MHz): δ 25.1 ($\text{Si}(\text{CH}_3)_2\text{O}$) ppm. Anal. calc. for $\text{C}_{20}\text{H}_{52}\text{O}_8\text{Si}_4\text{Ge}$ (605.56): C, 39.67; H, 8.65. Found: C, 39.26; H, 8.77%.

2.5. Synthesis of $[\text{Ge}(\text{SiMe}_2\text{OCH}_2\text{CH}_2\text{OMe})_3\text{Li}]$ (Li-3)



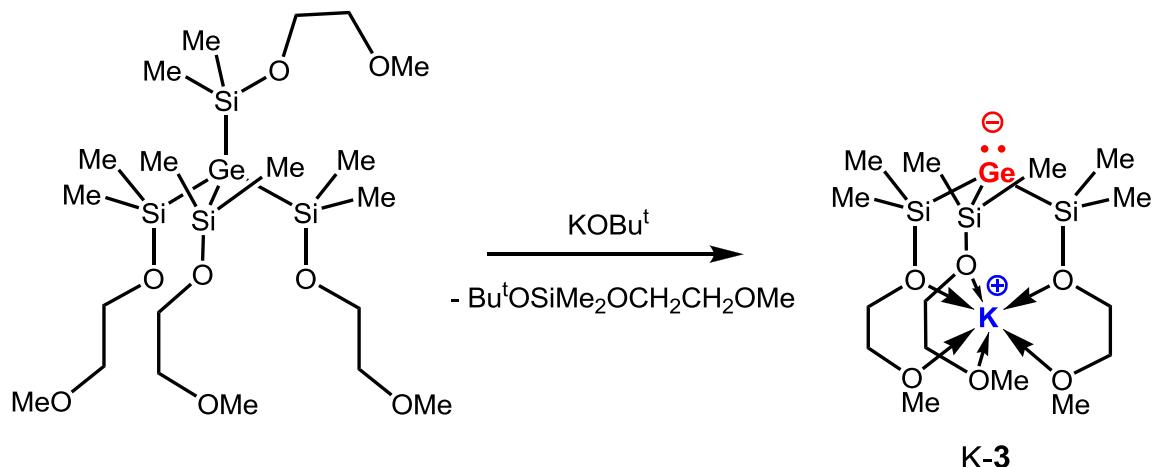
In a Glove box a 25 mL Schlenk flask equipped with a magnetic stir bar was charged with Bu^tOLi (14 mg, 0.17 mmol), $\text{Ge}(\text{Si}(\text{CH}_3)_2\text{OCH}_2\text{CH}_2\text{OCH}_3)_4$ (**3**) (100 mg, 0.17 mmol) and 1 mL of THF. After stirring the resulting solution for 1.5 hours, the solvent was removed under vacuum to give **Li-3** a yellow crystalline material nearly quantitatively (by ^1H and ^{13}C NMR). Recrystallization from toluene gave an analytically pure sample of **Li-3** (64 mg, 81%). ^1H NMR (C_6D_6 , 400 MHz): δ 0.66 (s, $\text{Si}(\text{CH}_3)_2$, 18 H), 2.94 (s, OCH_3 , 9 H), 2.99 (t, $^3J_{\text{H-H}} = 4.8$ Hz, CH_2O , 6 H), 3.39 (t, $^3J_{\text{H-H}} = 4.8$ Hz, SiOCH_2 , 6 H) ppm. $^{13}\text{C}\{\text{H}\}$ NMR (C_6D_6 , 125.7 MHz): δ 5.8 ($\text{Si}(\text{CH}_3)_2$), 58.5 (OCH_3), 61.1 (OCH_2), 73.6 (CH_2OCH_3) ppm. $^{29}\text{Si}\{\text{H}\}$ NMR (C_6D_6 , 99.3 MHz): δ 47.9 ($\text{Si}(\text{CH}_3)_2(\text{CH}_3)_2\text{O}$) ppm. $^7\text{Li}\{\text{H}\}$ NMR (C_6D_6 , 194.2 MHz): δ -1.1 ppm. Anal. calc. for $\text{C}_{15}\text{H}_{39}\text{O}_6\text{Si}_3\text{GeLi}$ (479.30): C, 37.59; H, 8.20. Found: C, 38.11; H, 8.09 %.

2.6. Synthesis of $[\text{Ge}(\text{SiMe}_2\text{OCH}_2\text{CH}_2\text{OMe})_3\text{Na}]$ (Na-3)



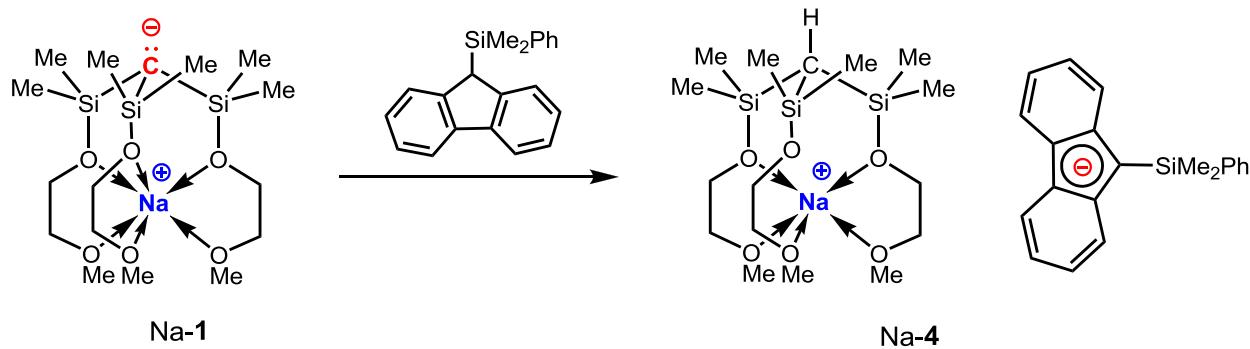
In a Glove box a 25 mL Schlenk flask equipped with a magnetic stir bar was charged with Bu^tONa (17 mg, 0.18 mmol), $\text{Ge}(\text{Si}(\text{CH}_3)_2\text{OCH}_2\text{CH}_2\text{OCH}_3)_4$ (**3**) (100 mg, 0.17 mmol) and 1 mL of THF. After stirring the resulting solution for 1.5 hours, the solvent was removed under vacuum to give raw **Na-3** as a red crystalline material nearly quantitatively (by ^1H and ^{13}C NMR). Recrystallization from hexanes gave an analytically pure sample of **Na-3** (68 mg, 83%). ^1H NMR (C_6D_6 , 400 MHz): δ 0.70 (s, $\text{Si}(\text{CH}_3)_2$, 18 H), 2.88 (s, OCH_3 , 9 H), 2.93 (t, $^3J_{\text{H-H}} = 4.4$ Hz, CH_2O , 6 H), 3.38 (t, $^3J_{\text{H-H}} = 4.4$ Hz, SiOCH_2 , 6 H) ppm. $^{13}\text{C}\{\text{H}\}$ NMR (C_6D_6 , 125.7 MHz): δ 5.7 ($\text{Si}(\text{CH}_3)_2$), 58.1 (OCH_3), 60.8(OCH_2), 74.4 (CH_2OCH_3) ppm. $^{29}\text{Si}\{\text{H}\}$ NMR (C_6D_6 , 99.3 MHz): δ 45.4 ($\text{Si}(\text{CH}_3)_2\text{O}$) ppm. $^{23}\text{Na}\{\text{H}\}$ NMR (C_6D_6 , 132.2 MHz): δ 0.4 ppm. Anal. calc. for $\text{C}_{15}\text{H}_{39}\text{O}_6\text{Si}_3\text{GeNa}$ (495.39): C, 36.37; H, 7.94. Found: C, 36.59; H, 7.99%.

2.7. Synthesis of $[\text{Ge}(\text{SiMe}_2\text{OCH}_2\text{CH}_2\text{OMe})_3\text{K}]$ (K-3)



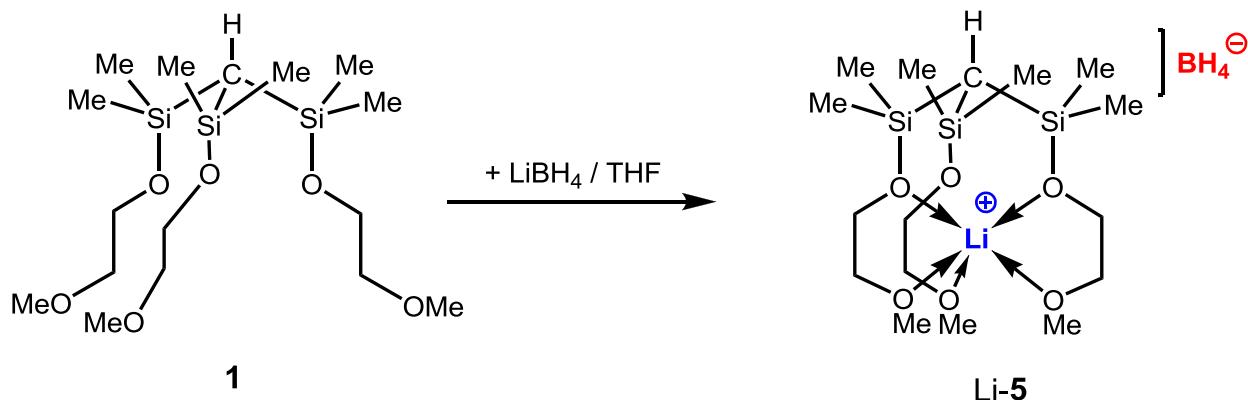
In a Glove box a 25 mL Schlenk flask equipped with a magnetic stir bar was charged with Bu^tOK (20 mg, 0.18 mmol), $\text{Ge}(\text{Si}(\text{CH}_3)_2\text{OCH}_2\text{CH}_2\text{OCH}_3)_4$ (**3**) (100 mg, 0.17 mmol) and 1 mL of THF. After stirring the resulting solution for 1.5 hours, the solvent was removed under vacuum to give **K-3** as a brown crystalline material nearly quantitatively (by ^1H and ^{13}C NMR). Recrystallization from hexanes gave an analytically pure sample of **K-3** (67 mg, 79%). ^1H NMR (C_6D_6 , 400 MHz): δ 0.73 (s, $\text{Si}(\text{CH}_3)_2$, 18 H), 2.86 (s, OCH_3 , 9 H), 2.97 (t, ${}^3J_{\text{H-H}} = 4.4$ Hz, CH_2O , 6 H), 3.44 (t, ${}^3J_{\text{H-H}} = 4.4$ Hz, SiOCH_2 , 6 H) ppm. $^{13}\text{C}\{\text{H}\}$ NMR (C_6D_6 , 125.7 MHz): δ 5.7 ($\text{Si}(\text{CH}_3)_2$), 57.6 (OCH_3), 60.9 (OCH_2), 74.9 (CH_2OCH_3) ppm. $^{29}\text{Si}\{\text{H}\}$ NMR (C_6D_6 , 99.3 MHz): δ 41.1 ($\text{Si}(\text{CH}_3)_2$) ppm. Anal. calc. for $\text{C}_{15}\text{H}_{39}\text{O}_6\text{Si}_3\text{GeK}$ (511.46): C, 35.22; H, 7.69. Found: C, 35.67; H, 8.08 %.

2.8. Synthesis of $[\text{HC}(\text{SiMe}_2\text{OCH}_2\text{CH}_2\text{OMe})_3\text{Na}][9\text{-SiMe}_2\text{Ph-C}_{13}\text{H}_8]$ (Na-4)



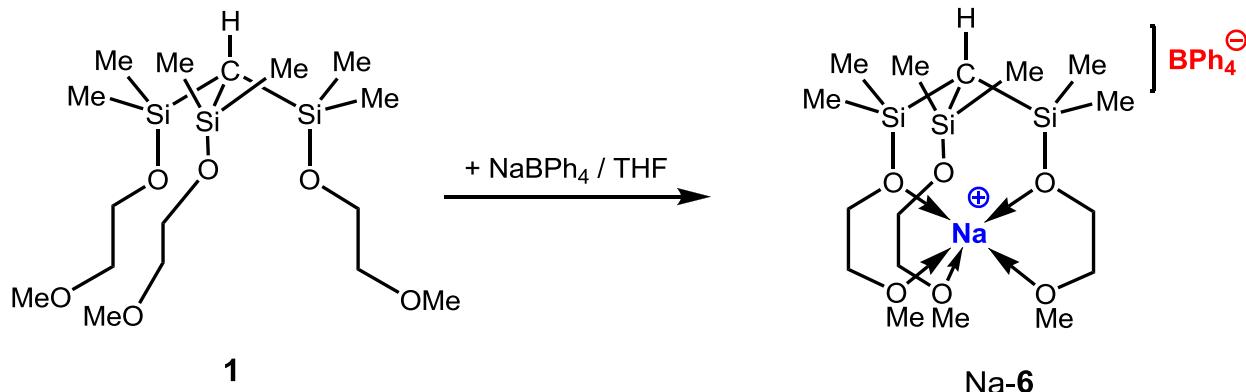
In a Glove box a 25 mL Schlenk flask equipped with a magnetic stir bar was charged with 9-
SiMe₂Ph-fluorene (55 mg, 0.18 mmol), Na-**1** (80 mg, 0.18 mmol) and 1 mL of THF. After stirring
the resulting solution for 3 hours, the solvent was removed under vacuum and the solid residue
was washed twice with hexanes to give 123 mg of Na-**4** as a pale yellow powder (91%). The
compound is thermally labile and slowly decomposes upon storage in the box. ¹H NMR (THF-D₈,
400 MHz): δ -0.25 (b, HCSi₃, 1 H) 0.26 (s, Si(CH₃)₂O, 18 H), 0.90 (s, Si(CH₃)₂Ph, 6 H) 3.15 (m, CH₂O
and OCH₃, 15 H), 3.43 (t, ³J_{H-H} = 4.6 Hz, SiOCH₂, 6 H), 6.85, 7.11, 7.29, 7.38, 7.81, 7.82, 8.22 (arom.
H, 13 H) ppm. ¹³C{H} NMR (THF-D₈, 125.7 MHz): δ 1.6 (Si(CH₃)₂O), 2.2 (Si(CH₃)₂Ph), 10.1 (CSi₃),
58.9 (OCH₃), 62.1 (OCH₂), 74.2 (CH₂OCH₃), 81.1 (C from CSi(CH₃)₂Ph) 111.1, 119.2, 119.4, 120.8,
126.8, 127.8, 127.9, 135.3, 144.8, 146.2 (arom. C) ppm. ²⁹Si{H} NMR (THF-D₈, 99.3 MHz): δ 17.5
(Si(CH₃)₂O), -16.4 (Si(CH₃)₂Ph) ppm. ²³Na{H} NMR (THF-D₈, 132.2 MHz): δ -9.0 ppm.

2.9. Synthesis of $[\text{HC}(\text{SiMe}_2\text{OCH}_2\text{CH}_2\text{OMe})_3\text{Li}][\text{BH}_4]$ (Li-5)



In a Glove box a 25 mL Schlenk flask equipped with a magnetic stir bar was charged with LiBH_4 (5 mg, 0.23 mmol), $\text{HC}(\text{Si}(\text{CH}_3)_2\text{OCH}_2\text{CH}_2\text{OCH}_3)_3$ (**1**) (100 mg, 0.24 mmol) and 1 mL of THF. The resulting suspension was stirred until it became a clear solution (approximately after a week). Then, the solvent was removed under vacuum to leave a crystalline residue, which was washed twice with hexanes and dried under vacuum. Yield (90 mg, 86%). ^1H NMR (C_6D_6 , 400 MHz): δ 0.31 (b, HCSi_3 , 1 H) 0.56 (quart., $^1J_{\text{H-B}} = 81.2$ Hz, BH_4 , 4 H), 1.16 (s, SiMe_2O , 18 H), 3.10 (t, $^3J_{\text{H-H}} = 4.6$ Hz, CH_2O , 6 H), 3.19 (s, OCH_3 , 9 H), 3.35 (t, $^3J_{\text{H-H}} = 4.6$ Hz, SiOCH_2 , 6 H), ppm. $^{13}\text{C}\{\text{H}\}$ NMR (C_6D_6 , 100.6 MHz): δ 0.6 (SiMe_2O), 9.4 (CSi_3), 58.6 (OMe), 60.9 (OCH_2), 72.5 (CH_2OMe) ppm. $^{29}\text{Si}\{\text{H}\}$ NMR (C_6D_6 , 79.5 MHz): δ 18.6 ppm. $^7\text{Li}\{\text{H}\}$ NMR (C_6D_6 , 155.5 MHz): δ 2.5 ppm. $^{11}\text{B}\{\text{H}\}$ NMR (C_6D_6 , 128.3 MHz): -40.2 (quintet, $^1J_{\text{H-B}} = 81.2$ Hz) ppm. Anal. calc. for $\text{C}_{16}\text{H}_{44}\text{O}_6\text{Si}_3\text{BLi}$ (434.525): C, 44.23; H, 10.21. Found: C, 43.97; H, 10.08 %.

2.10. Synthesis of $[\text{HC}(\text{SiMe}_2\text{OCH}_2\text{CH}_2\text{OMe})_3\text{Na}][\text{BPh}_4]$ (Na-6)



In a Glove box a 25 mL Schlenk flask equipped with a magnetic stir bar was charged with NaBPh₄ (50 mg, 0.15 mmol), HC(Si(CH₃)₂OCH₂CH₂OCH₃)₃ (**1**) (60 mg, 0.15 mmol) and 2 mL of CH₂Cl₂. The resulting suspension was stirred overnight until it became a clear solution. Then, the solvent was removed under vacuum to leave crystalline residue, which was washed twice with small amounts of benzene and dried under vacuum. Yield (98 mg, 89%). ¹H NMR (C₆D₆, 400 MHz): δ -1.38 (b, HCSi₃, 1 H) -0.11 (s, SiMe₂O, 18 H), 2.69 (t, ³J_{H-H} = 4.6 Hz, CH₂O, 6 H), 2.78 (s, OCH₃, 9 H), 2.89 (t, ³J_{H-H} = 4.6 Hz, SiOCH₂, 6 H), 7.27 (t, p-H 4 H), 7.44 (t, m-H, 8 H), 8.16 (b, o-H, 8 H) ppm. ¹H NMR (CDCl₃, 400 MHz): δ -0.72 (b, HCSi₃, 1 H) 0.22 (s, SiMe₂O, 18 H), 3.29 (s, OCH₃, 9 H), 3.33 (t, ³J_{H-H} = 4.6 Hz, CH₂O, 6 H), 3.55 (t, ³J_{H-H} = 4.6 Hz, SiOCH₂, 6 H), 6.89 (m, p-H, 4 H), 7.04 (m, m-H, 8 H), 7.40 (b, o-H, 8 H) ppm. ¹³C{H} NMR (CDCl₃, 100.6 MHz): δ 1.8 (SiMe₂O), 7.9 (CSi₃), 51.2 (OMe), 61.4 (OCH₂), 73.1 (CH₂OMe), 121.6, 125.5, 136.4, 163.6, 164.1, 164.6, 165.1 (aromatic C) ppm. ²⁹Si{H} NMR (CDCl₃, 79.5 MHz): δ 21.2 (SiMe₂O), ppm. ²³Na{H} NMR (CDCl₃, 105.8 MHz): δ 0.1 ppm. ¹¹B{H} NMR (CDCl₃, 128.3 MHz): δ -7.5 ppm. Anal. calc. for C₄₀H₆₀O₆Si₃BNa (754.958): C, 63.64; H, 8.01. Found: C, 63.61; H, 7.96 %.

3. Estimation of the Basicities of M-1 – M-3

General procedure: In the glove box, a J-Young NMR tube was charged with one equiv. (ca. 0.02 mmol) of the respective zwitterion **M-1**, **M-2** or **M-3**, one equivalent (ca. 0.02 mmol) of the hydrocarbon acid (Ind-H) and ca. 0.4 mL of solvent (THF-D₈ or C₆D₆). For some experiments (see Tables S1 and S2) one equivalent of 2.2.2-cryptand was added as well. ¹H NMR spectra of the resulting solutions were taken immediately and after ca. 3 hours if not mentioned otherwise. The ratios product to starting material were estimated from integrating the respective signals in ¹H-NMR spectrum. The relative pK_a-values were calculated according to the following equation:

$$pK_a(\text{acid}) = pK_a(\text{IndH}) + \lg \frac{[\text{acid}][\text{Ind}^-]}{[\text{base}][\text{IndH}]}$$

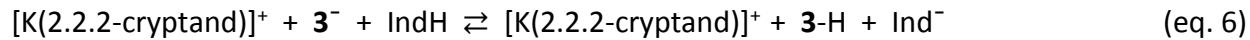
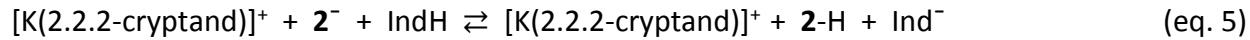
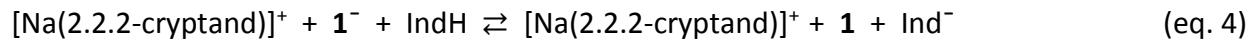


Table S1. Estimated pK_a values of M-**1** - M-**3** (M = Li, Na, K) derived from acid-base measurements by ^1H -NMR spectroscopy in THF-D₈.

| Acid [IndH] | pK_a [DMSO] ^a | Base [M- 1 – M- 3] | conv. [%] | pK_a [calc.] ^a |
|---|-------------------------------|--------------------------------------|--------------|--------------------------------|
| Ph ₃ PCH ₂ PPh ₃ | 29.9 | Na- 1 /(2.2.2-cryptand) | 30 | 29.2 |
| 9-Bu ^t -fluorene | 24.4 | K- 1 | 10 | - |
| 9-Pr ⁱ -fluorene | 23.2 | K- 1 | 82 | 24.5 |
| 9-Bu ^t -fluorene | 24.4 | Na- 1 | 0 | - |
| 9-Pr ⁱ -fluorene | 23.2 | Na- 1 | 62 | 23.6 |
| 9-Bu ⁿ -fluorene | 22.2 | Na- 1 | 86 | 23.8 |
| 9-Bu ^t -fluorene | 24.4 | Li- 1 | 0 | - |
| 9-Pr ⁱ -fluorene | 23.2 | Li- 1 | 62 | 23.6 |
| 9-Bu ⁿ -fluorene | 22.2 | K- 2 | 53 | 22.3 |
| 9-Me ₃ Si-fluorene | 21.5 | K- 2 | 70 | 22.2 |
| 9-Ph ₃ Si-fluorene | 18.6 | Li- 2 | 80 | 19.8 |
| 9-Ph-fluorene | 17.9 | Li- 2 | 100 | - |
| 9-Ph ₃ Si-fluorene | 18.6 | Na- 2 | 56 | 18.8 |
| 9-Ph ₃ Si-fluorene | 18.6 | K- 3 | 33 | 18.0 |
| 9-Ph-fluorene | 17.9 | Li- 3 | 9 | "15.9" |
| 9-Ph-fluorene | 17.9 | Na- 3 | 0 | - |

^a It is customary among chemists to use the term " pK_a of base" with the actual meaning of the pK_a of the conjugate acid of the respective base.

Table S2. Estimated pK_a values of M-**1** - M-**3** (M = Li, Na, K) derived from acid-base measurements by ^1H -NMR spectroscopy in C_6D_6 .

| Acid [Ind-H] | pK_a [DMSO] | Base [M- 1 - M- 3] | Conv. [%] | pK_a [calc.] ^a |
|---------------------------------------|------------------|--------------------------------------|--------------|--------------------------------|
| $\text{Ph}_3\text{PCH}_2\text{PPh}_3$ | 29.9 | K- 2 /(2.2.2-cryptand) | 0 | - |
| 9-Bu ^t -fluorene | 24.2 | K- 2 /(2.2.2-cryptand) | 100 | - |
| 9-Pr ⁱ -fluorene | 23.2 | K- 3 /(2.2.2-cryptand) | 42 | 22.9 |
| 9-Pr ⁱ -fluorene | 23.2 | Li- 1 | 45 | 23.0 |
| 9-Bu ⁿ -fluorene | 22.2 | Li- 1 | 69 | 22.9 |
| 9-Bu ^t -fluorene | 24.2 | Na- 1 | 0 | - |
| 9-Pr ⁱ -fluorene | 23.2 | Na- 1 | 0 | - |
| 9-Bu ⁿ -fluorene | 22.2 | Na- 1 | 59 | 22.5 |
| 9-Bu ⁿ -fluorene | 22.2 | K- 1 | 50 | 22.2 |
| 9-Ph ₃ Si-fluorene | 18.6 | K- 2 | 53 | 18.7 |
| 9-Ph ₃ Si-fluorene | 18.6 | Li- 2 | 33 | 18.0 |
| 9-Ph ₃ Si-fluorene | 18.6 | Na- 2 | 0 | - |
| 9-Ph-fluorene | 17.9 | Na- 2 | 10 | "16.0" |
| 9-Ph-fluorene | 17.9 | Li- 3 | 0 | - |
| 9-Ph-fluorene | 17.9 | Na- 3 | 0 | - |
| 9-Ph-fluorene | 17.9 | K- 3 | 0 | - |

^a It is customary among chemists to use the term " pK_a of base" with the actual meaning of the pK_a of the conjugate acid of the respective base.

4. X-ray crystallography

X-ray diffraction data for all compounds were obtained on a Bruker Smart Apex II CCD diffractometer, using graphite-monochromated Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$) at low temperature (150 K for Li-**1**, Na-**3**, and Na-**4**; 100 K for K-**1** and K-**3**). Intensity data were collected using ω -steps accumulating area detector images spanning at least a hemisphere of reciprocal space. All the data were corrected for Lorentz polarization effects. A multi-scan absorption correction was applied using SADABS [9]. Structures were solved by direct methods and refined by full-matrix least-squares against F^2 (SHELXTL) [10]. All hydrogen atoms were assigned riding isotropic displacement parameters and constrained to idealized geometries.

The flack parameter in Li-**1** was found to be meaningless, due to weak anomalous scattering by the crystals. In K-**1**, as refined as a pseudo-merohedral twin with a twin law of -1 0 0 0 -1 0 0 0 1 and a refined twin fraction of 0.44. The RIGU command was also used as a general constraint to the ellipsoids of the structure.

Crystallographic data for the five structures are listed in Tables S3 and S4. CCDC-1000501 (Li-**1**), CCDC-1013011 (K-**1**), CCDC-1000506 (Na-**3**), 1000507 (K-**3**) and CCDC-926164 (Na-**4**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/data_request/cif, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk.

Table S3. Crystallographic data for complexes Li-**1** and K-**1**.

| | Li- 1 | K- 1 |
|--|--|---|
| Formula | C ₁₆ H ₃₉ LiO ₆ Si ₃ | C ₁₆ H ₃₉ KO ₆ Si ₃ |
| Molecular weight | 418.68 | 450.84 |
| Crystal size (mm ³) | 0.27 × 0.20 × 0.08 | 0.48 × 0.39 × 0.15 |
| Crystal appearance | Colorless chunk | Colorless block |
| Crystal system | Monoclinic | Monoclinic |
| Space group | <i>Cc</i> (No. 9) | <i>P2₁/n</i> (No. 14) |
| a (Å) | 9.531(5) | 8.698(6) |
| b (Å) | 17.403(8) | 18.417(12) |
| c (Å) | 15.039(7) | 16.289(11) |
| α | | |
| β (°) | 90.873(6) | 90.200(10) |
| γ | | |
| Volume (Å ³) | 2494(2) | 2609(3) |
| Z | 4 | 4 |
| Temperature (K) | 150(2) | 100(2) |
| μ (mm ⁻¹) | 0.214 | 0.365 |
| θ range (°) | 2.34 to 27.78 | 1.106 to 25.816 |
| Reflections collected | 14494 | 26816 |
| Unique reflections (<i>R</i> _{int}) | 5737 (0.1480) | 4942 (0.1401) |
| R1 [<i>I</i> >2σ(<i>I</i>)] | 0.0762 | 0.0699 |
| wR2 indices (all data) | 0.1585 | 0.1863 |
| GOF | 0.949 | 0.936 |
| Data/restraints/parameters | 5737 / 2 / 244 | 4942 / 369 / 237 |

Table S4. Crystallographic data for complexes **Na-3** and **K-3** and **Na-4**

| | Na-3 | K-3 | Na-4 |
|--|--|---|--|
| Formula | C ₁₅ H ₃₉ GeNaO ₆ Si ₃ | C ₁₅ H ₃₉ GeKO ₆ Si ₃ | C ₃₇ H ₅₉ NaO ₆ Si ₄ |
| Molecular weight | 495.31 | 511.42 | 735.19 |
| Crystal size (mm ³) | 0.36 × 0.21 × 0.15 | 0.34 × 0.28 × 0.25 | 0.37 × 0.21 × 0.07 |
| Crystal appearance | Yellow prism | Yellow chunk | Orange prism |
| Crystal system | Monoclinic | Monoclinic | Monoclinic |
| Space group | P2 ₁ /c (No. 14) | P2 ₁ /n (No. 14) | C2/c (No. 15) |
| a (Å) | 15.729(2) | 8.141(2) | 23.272(4) |
| b (Å) | 9.9209(13) | 19.245(6) | 9.7485(17) |
| c (Å) | 17.212(2) | 16.727(5) | 37.173(6) |
| A | | | |
| β (°) | 90.3515(14) | 90.528(4) | 94.149(2) |
| Γ | | | |
| Volume (Å ³) | 2685.8(6) | 2620.5(13) | 8411(3) |
| Z | 4 | 4 | 8 |
| Temperature (K) | 150(2) | 100(2) | 150(2) |
| μ (mm ⁻¹) | 1.313 | 1.489 | 0.191 |
| θ range (°) | 2.37 to 27.88 | 1.06 to 27.91 | 1.10 to 27.92 |
| Reflections collected | 31353 | 27981 | 49332 |
| Unique reflections (<i>R</i> _{int}) | 6374 (0.0292) | 6104 (0.0539) | 9999 (0.0613) |
| R1 [<i>I</i> >2σ(<i>I</i>)] | 0.0266 | 0.0960 | 0.0779 |
| wR2 indices (all data) | 0.0682 | 0.2175 | 0.1178 |
| GOF | 1.035 | 1.279 | 1.035 |
| Data/restraints/parameters | 6374 / 0 / 244 | 6104 / 0 / 245 | 9999 / 0 / 444 |

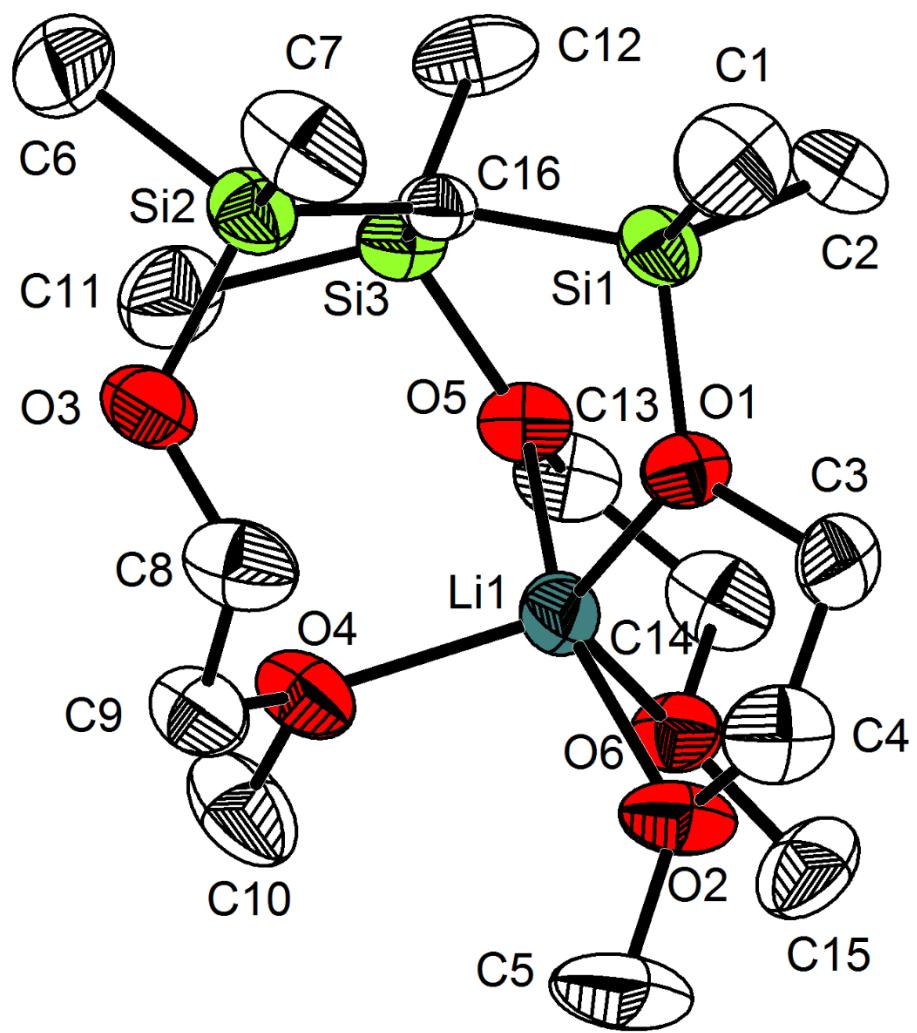


Figure S1. Solid-state structure of Li-1.

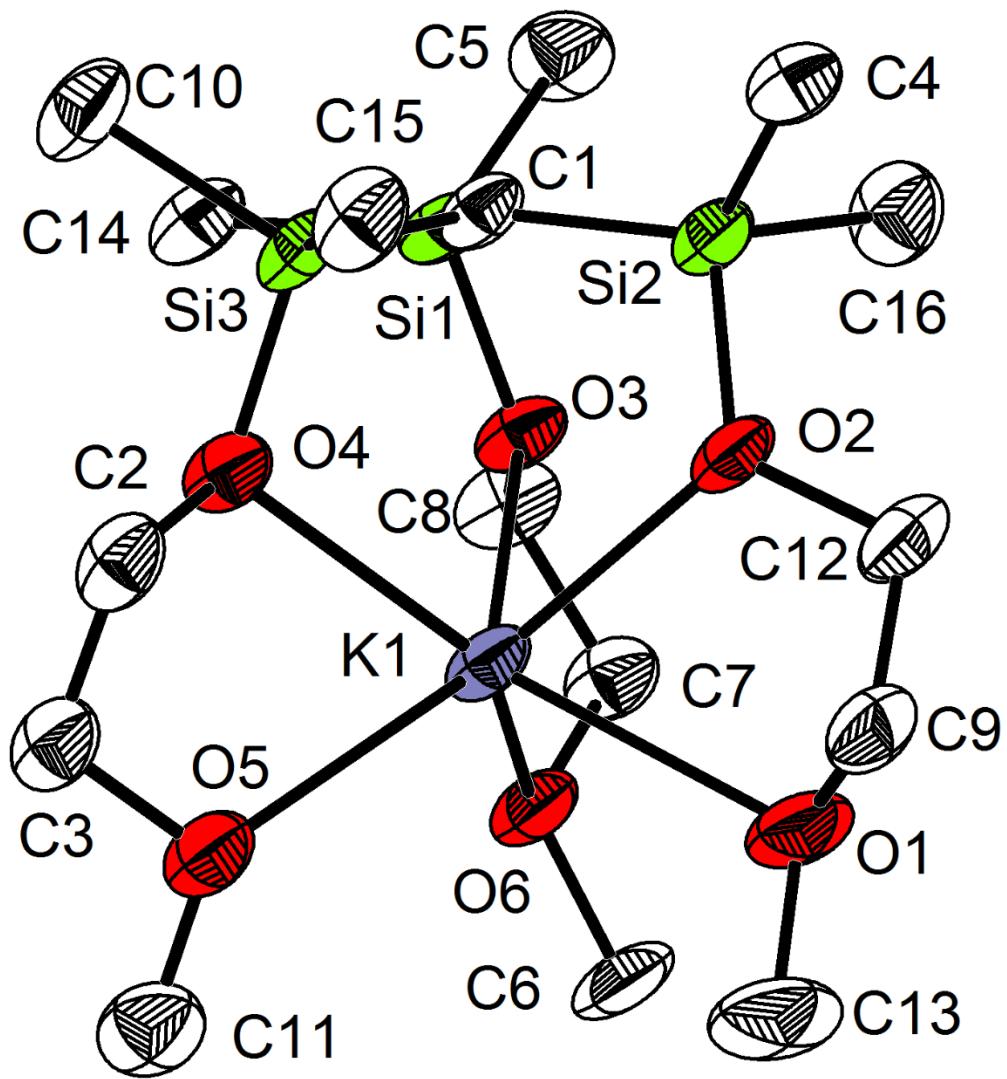


Figure S2. Solid-state structure of K-1.

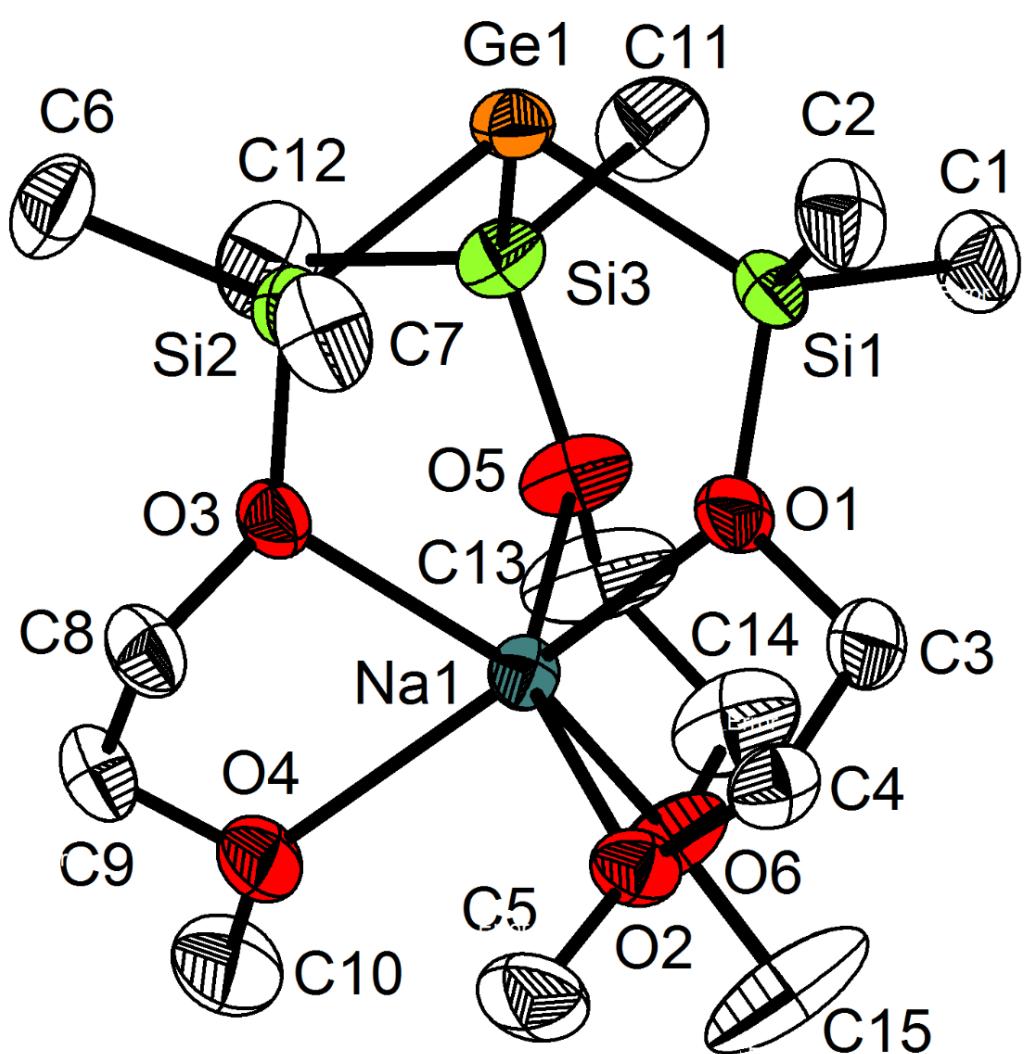


Figure S3. Solid-state structure of Na-3.

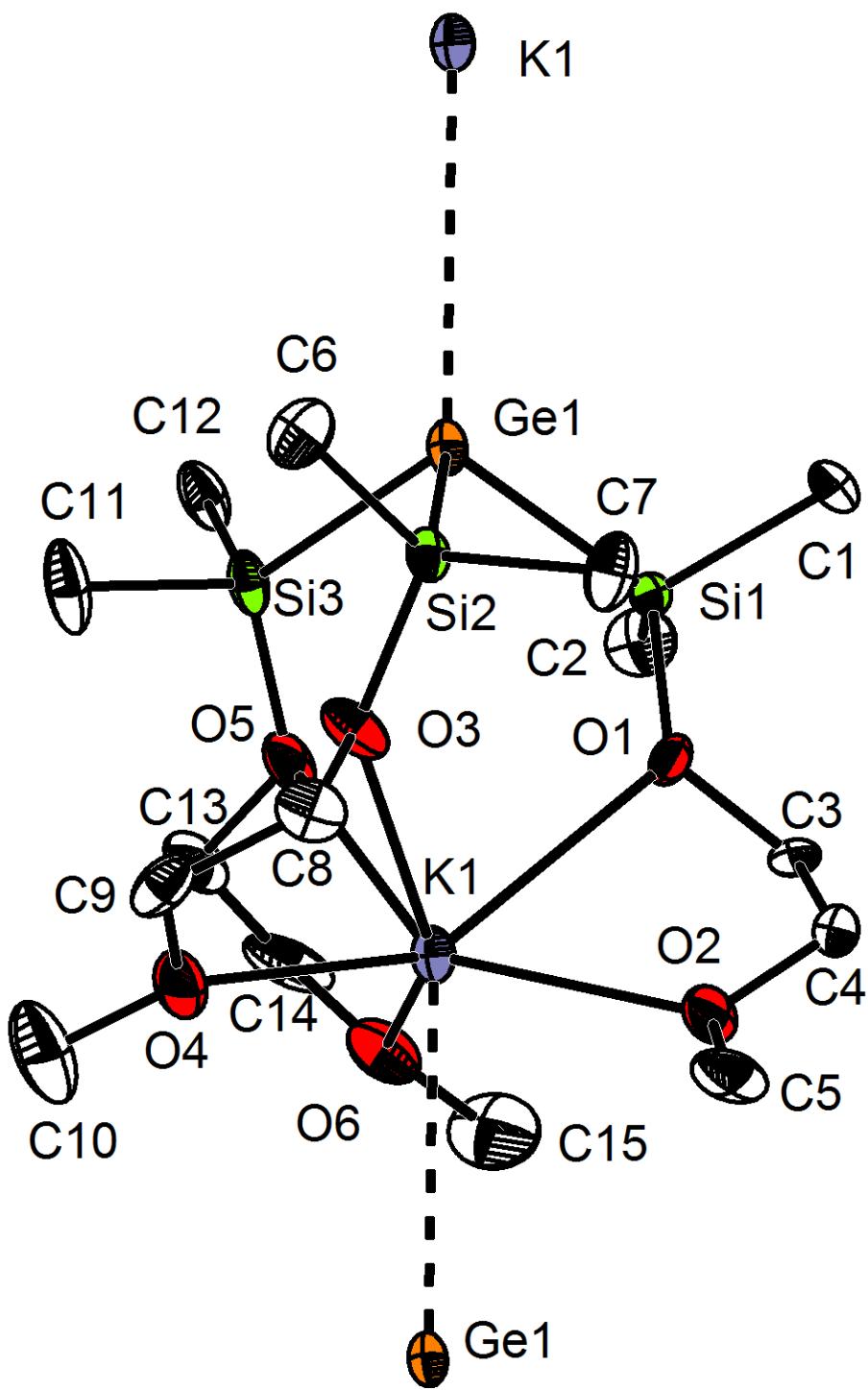


Figure S4. Solid-state structure of K-3.

Table S5. Selected average distances [Å] and angles [°] of M-**1**–M-**3**.

| M- 1 ^b | Li- 1 | Na- 1 | K- 1 | M- 2 ^b | Li- 2 | Na- 2 | K- 2 | M- 3 ^b | Na- 3 | K- 3 |
|--------------------------|--------------|--------------|-------------|--------------------------|--------------|--------------|-------------|--------------------------|--------------|-------------|
| CN ^a | 5 | 6 | 6 | CN | 6 | 6 | 7 | CN | 6 | 7 |
| C-Si | 1.78 | 1.79 | 1.80 | Si-Si | 2.32 | 2.32 | 2.32 | Ge-Si | 2.37 | 2.37 |
| Si-O | 1.71 | 1.70 | 1.70 | Si-O | 1.69 | 1.68 | 1.68 | Si-O | 1.68 | 1.67 |
| O-M | 2.01 | 2.37 | 2.69 | O-M | 2.08 | 2.32 | 2.74 | O-M | 2.32 | 2.75 |
| C···M | 3.30 | 3.23 | 3.32 | Si···M | 3.92 | 4.00 | 4.50 | Ge···M | 4.05 | 4.53 |
| Si-C-Si | 119 | 116 | 119 | Si-Si-Si | 96 | 99 | 100 | Si-Ge-Si | 97 | 98 |
| C-Si-O | 106 | 107 | 108 | Si-Si-O | 113 | 113 | 113 | Ge-Si-O | 113 | 114 |
| Si-O-M | 118 | 110 | 107 | Si-O-M | 126 | 122 | 125 | Si-O-M | 123 | 125 |

^a CN = coordination number; ^b M = metal.

5. DFT Calculations

The calculations were performed at density functional theory level through the functional B3-LYP [11] and the TZVP [12, 13] basis set. Geometry optimizations were performed for all systems studied in this work. Gas-phase basicity (GB) and proton affinity (PA) computations were carried out at the same level of theory by means of harmonic vibrational frequency calculations to get corresponding enthalpies and Gibbs free energies. The atomic charges were calculated using natural population analysis [14]. All calculations were performed using the Turbomole [15] suite program. The natural bond orbital (NBO) analysis [16] was performed with the optimized structures of the zwitterions Na-**1**, Na-**2** and Na-**3** (Table 3) at the B3-LYP/def2-TZVP [17, 18] level of theory using Gaussian 9 code [19].

5.1. Results of calculations for M-1 and $[M-1-H]^+$ ($M = Li, Na, K$)

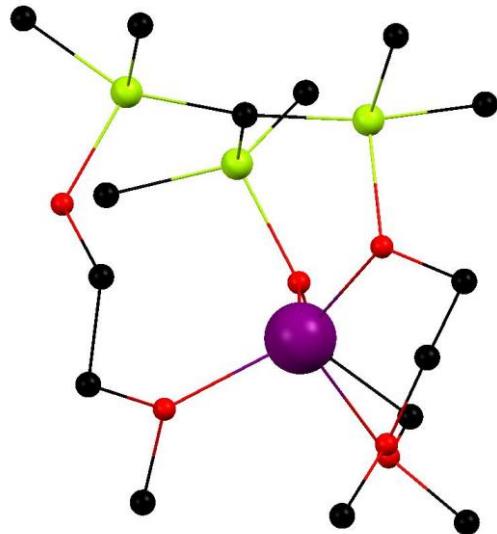


Figure S5. Calculated gas-phase structure of Li-1-A (purple = lithium; green = silicon; black = carbon; red = oxygen).

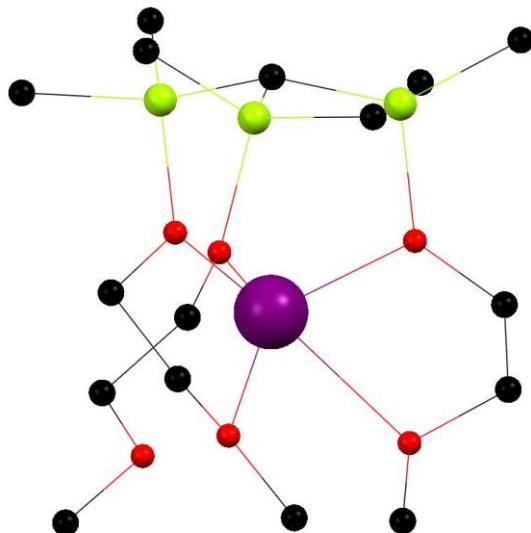


Figure S6. Calculated gas-phase structure of Li-1-B (purple = lithium; green = silicon; black = carbon; red = oxygen).

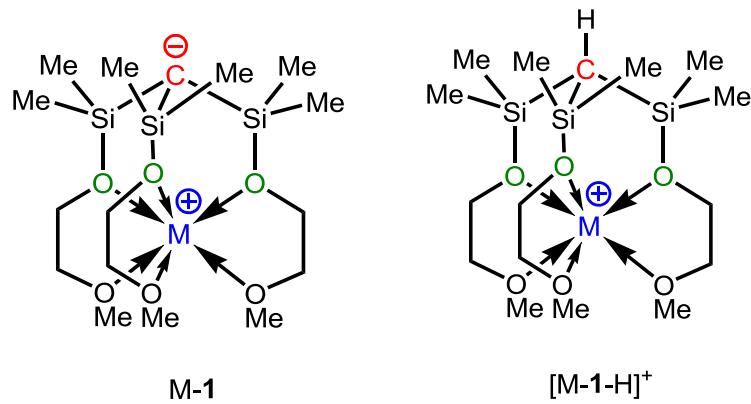


Table S6. Calculated average distances [\AA] and angles [$^\circ$] of M-1 and $[\text{M-1-H}]^+$ ($\text{M} = \text{Li}, \text{Na}, \text{K}$).

| | Li-1-A | Li-1-B | Na-1 | K-1 | $[\text{Li-1-H}]^+$ | $[\text{Na-1-H}]^+$ | $[\text{K-1-H}]^+$ |
|----------|--------|--------|-------|-------|---------------------|---------------------|--------------------|
| CN | 4 | 5 | 6 | 6 | 6 | 6 | 6 |
| C-Si | 1.81 | 1.81 | 1.81 | 1.81 | 1.90 | 1.91 | 1.91 |
| Si-O | 1.76 | 1.76 | 1.75 | 1.75 | 1.71 | 1.71 | 1.71 |
| O-M | 1.98 | 2.07 | 2.38 | 2.75 | 2.19 | 2.42 | 2.81 |
| C···M | 3.03 | 2.99 | 3.18 | 3.34 | 3.43 | 3.56 | 3.88 |
| Si-C-Si | 119.5 | 115.6 | 117.4 | 119.2 | 112.5 | 114.1 | 115.5 |
| C-Si-O | - | 103.9 | 105.1 | 106.6 | 101.6 | 103.1 | 105.1 |
| Si-O-M | - | 110.2 | 109.7 | 106.8 | 122.1 | 120.0 | 119.6 |
| C-Si-O-M | - | 20.8 | 24.7 | 27.1 | 33.5 | 34.3 | 37.2 |
| C-H | - | - | - | - | 1.10 | 1.10 | 1.10 |

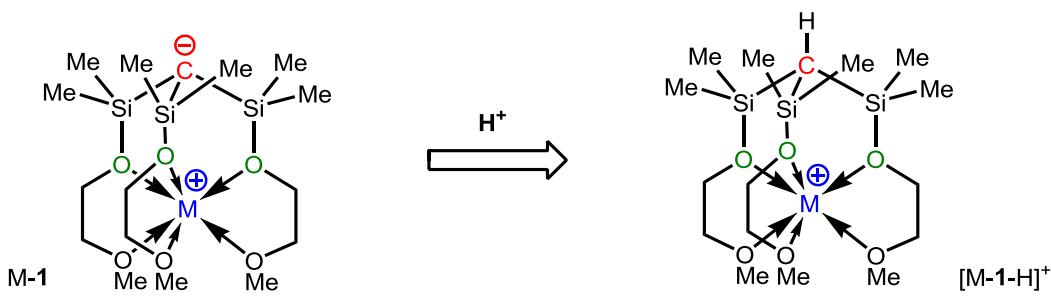


Table S7. Calculated absolute energies [au], HOMO energies [eV], gas-phase basicities [GPB in kcal/mol] and proton affinities [PA in kcal/mol] of **M-1** and $[\text{M-1-H}]^+$ ($\text{M} = \text{Li}, \text{Na}, \text{K}$).

| Comp. | Li-1-A | Li-1-B | Na-1 | K-1 |
|-------------------|---------------------|--------------|---------------------|--------------------|
| E | -1960.381346 | -1960.381167 | -2115.12458 | -2552.719709 |
| E_{HOMO} | -4.402 | -4.469 | -4.335 | -4.256 |
| G | -1229864.646 | -1229865.514 | -1326969.934 | -1601567.854 |
| H | -1229795.277 | -1229795.459 | -1326898.947 | -1601494.632 |
| GPB | -282.9 | -282.0 | -282.3 | -280.6 |
| PA | -291.9 | -291.8 | -290.7 | -289.2 |
| Comp. | $[\text{Li-1-H}]^+$ | - | $[\text{Na-1-H}]^+$ | $[\text{K-1-H}]^+$ |
| E | -1960.857087 | - | -2115.598906 | -2553.191823 |
| G | -1230153.848 | - | -1327258.551 | -1601854.708 |
| H | -1230085.719 | - | -1327188.14 | -1601782.359 |

Table S8. Calculated NPA charges [e] of M-**1** and [M-**1**-H]⁺ (M = Li, Na, K).

| Comp. | Li- 1 -A | Li- 1 -B | Na- 1 | K- 1 |
|---------------------|-----------------|-----------------|--------------|-------------|
| e (M) | +0.900 | +0.894 | +0.917 | +0.949 |
| e (C ⁻) | -2.195 | -2.155 | -2.168 | -2.189 |
| e (Si) | +2.087 | +2.081 | +2.082 | +2.089 |
| e (C) | -1.085 | -1.084 | -1.086 | -1.088 |
| e (O) | -0.977 | -0.991 | -0.974 | -0.966 |

| Comp. | [Li- 1 -H] ⁺ | [Na- 1 -H] ⁺ | [K- 1 -H] ⁺ |
|---------------------|--------------------------------|--------------------------------|-------------------------------|
| e (M) | +0.896 | +0.918 | +0.953 |
| e (C ⁻) | -1.774 | -1.769 | -1.769 |
| e (H) | +0.265 | +0.263 | +0.261 |
| e (Si) | +2.085 | +2.080 | +2.082 |
| e (C) | -1.103 | -1.103 | -1.103 |
| e (O) | -0.980 | -0.975 | -0.968 |

5.2. Results of calculations for M-2 and $[M\text{-}2\text{-H}]^+$ ($M = \text{Li}, \text{Na}, \text{K}$)

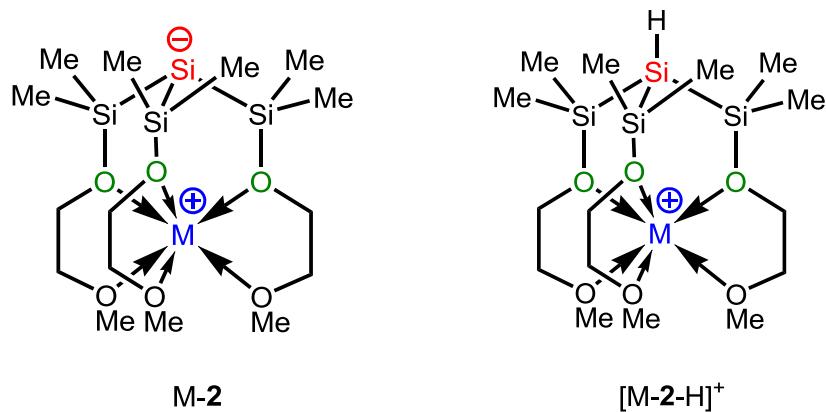


Table S9. Calculated average distances [\AA] and angles [$^\circ$] of M-2 and $[\text{M-2-H}]^+$ ($M = \text{Li}, \text{Na}, \text{K}$).

| Comp. | Li-2 | Na-2 | K-2 | $[\text{Li-2-H}]^+$ | $[\text{Na-2-H}]^+$ | $[\text{K-2-H}]^+$ |
|-----------|-------|-------|-------|---------------------|---------------------|--------------------|
| CN (M) | 6 | 6 | 6 | 6 | 6 | 6 |
| Si-Si | 2.35 | 2.35 | 2.35 | 2.36 | 2.37 | 2.38 |
| Si-O | 1.76 | 1.75 | 1.75 | 1.72 | 1.72 | 1.71 |
| O-M | 2.07 | 2.35 | 2.71 | 2.27 | 2.45 | 2.82 |
| Si···M | 3.79 | 3.94 | 4.07 | 3.72 | 3.74 | 3.94 |
| Si-Si-Si | 97.5 | 101.2 | 105.8 | 107.4 | 110.0 | 112.9 |
| Si-Si-O | 112.3 | 113.6 | 115.7 | 99.9 | 101.5 | 104.1 |
| Si-O-M | 120.5 | 119.9 | 114.4 | 128.3 | 125.6 | 122.6 |
| Si-Si-O-M | 21.9 | 21.0 | 21.0 | 29.2 | 23.7 | 24.7 |
| Si-H | - | - | - | 1.49 | 1.50 | 1.50 |

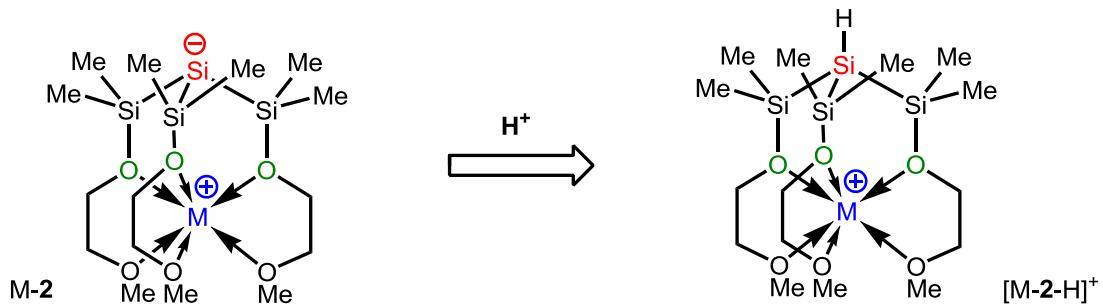


Table S10. Calculated absolute energies [au], HOMO energies [eV], gas-phase basicities [GPB in kcal/mol] and proton affinities [PA in kcal/mol] of M-2, and [M-2-H]⁺ (M = Li, Na, K).

| Comp. | Li-2 | Na-2 | K-2 |
|-------------------|-----------------------|-----------------------|----------------------|
| E | -2211.745006 | -2366.486518 | -2804.077403 |
| E _{HOMO} | -4.200 | -4.013 | -3.837 |
| G | -1387602.653 | -1484706.84 | -1759302.046 |
| H | -1387530.78 | -1484633.075 | -1759225.98 |
| GPB | -274.0 | -276.3 | -278.9 |
| PA | -281.4 | -283.8 | -286.3 |
| Comp. | [Li-2-H] ⁺ | [Na-2-H] ⁺ | [K-2-H] ⁺ |
| E | -2212.201368 | -2366.946799 | -2804.541748 |
| G | -1387882.999 | -1484989.394 | -1759587.22 |
| H | -1387810.643 | -1484915.362 | -1759510.76 |

Table S11. Calculated NPA charges [e] of **M-2**, and $[M\text{-}2\text{-H}]^+$ ($M = \text{Li}, \text{Na}, \text{K}$).

| Comp. | Li-2 | Na-2 | K-2 |
|--------|--------|--------|--------|
| e (M) | +0.891 | +0.913 | +0.945 |
| e (E) | -0.683 | -0.709 | -0.738 |
| e (Si) | +1.584 | +1.581 | +1.581 |
| e (C) | -1.084 | -1.081 | -1.080 |
| e (O) | -0.992 | -0.978 | -0.970 |

| Comp. | $[\text{Li-2-H}]^+$ | $[\text{Na-2-H}]^+$ | $[\text{K-2-H}]^+$ |
|--------|---------------------|---------------------|--------------------|
| e (M) | +0.898 | +0.917 | +0.950 |
| e (E) | -0.139 | -0.153 | -0.171 |
| e (H) | -0.131 | -0.136 | -0.139 |
| e (Si) | +1.643 | +1.640 | +1.643 |
| e (C) | -1.085 | -1.084 | -1.085 |
| e (O) | -0.976 | -0.974 | -0.968 |

5.3. Results of calculations for M-3 and $[M\text{-}3\text{-H}]^+$ ($M = \text{Li}, \text{Na}, \text{K}$)

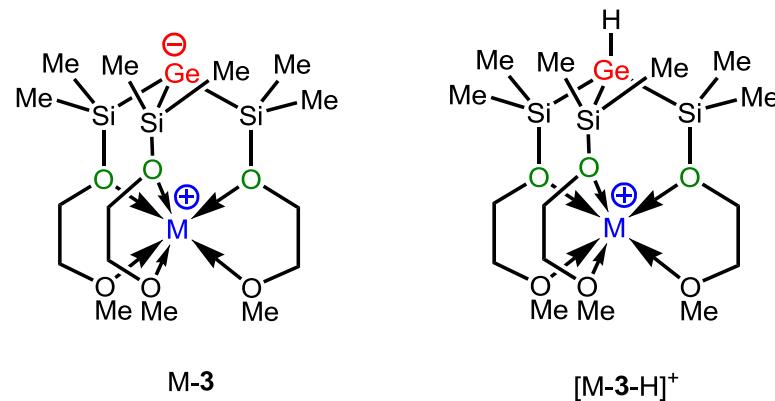


Table S12. Calculated average distances [\AA] and angles [$^\circ$] of M-3 and $[\text{M-3-H}]^+$ ($M = \text{Li}, \text{Na}, \text{K}$).

| Comp. | Li-3 | Na-3 | K-3 | $[\text{Li-3-H}]^+$ | $[\text{Na-3-H}]^+$ | $[\text{K-3-H}]^+$ |
|-----------|-------|-------|-------|---------------------|---------------------|--------------------|
| CN (M) | 6 | 6 | 6 | 6 | 6 | 6 |
| Ge-Si | 2.42 | 2.42 | 2.42 | 2.41 | 2.41 | 2.42 |
| Si-O | 1.76 | 1.75 | 1.75 | 1.72 | 1.72 | 1.71 |
| O-M | 2.08 | 2.35 | 2.71 | 2.28 | 2.46 | 2.82 |
| Ge···M | 3.88 | 4.01 | 4.14 | 3.74 | 3.74 | 3.93 |
| Si-Ge-Si | 95.3 | 99.1 | 103.9 | 107.1 | 109.7 | 112.8 |
| Ge-Si-O | 112.5 | 114.0 | 116.7 | 99.7 | 101.1 | 103.6 |
| Si-O-M | 120.5 | 119.7 | 115.5 | 129.0 | 125.4 | 122.2 |
| Ge-Si-O-M | 27.5 | 24.8 | 20.9 | 27.4 | 24.8 | 25.0 |
| Ge-H | - | - | - | 1.54 | 1.55 | 1.55 |

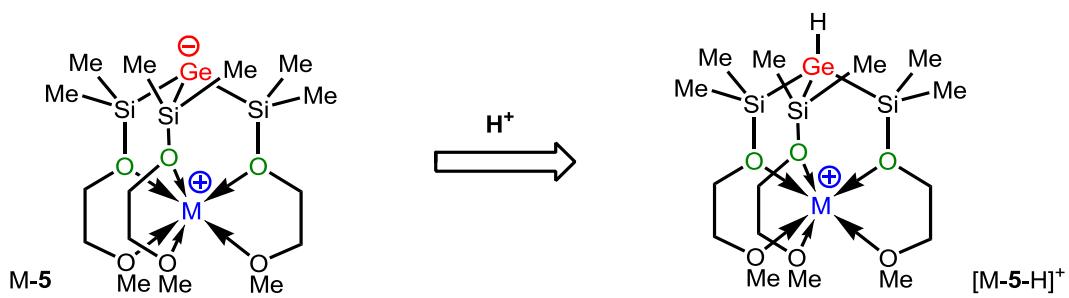


Table S13. Calculated absolute energies [au], HOMO energies [eV], gas-phase basicities [GPB in kcal/mol] and proton affinities [PA in kcal/mol] of M-3 and [M-3-H]⁺ (M = Li, Na, K).

| Comp. | Li-3 | Na-3 | K-3 |
|---------------------|-----------------------|-----------------------|----------------------|
| E | -3999.227947 | -4153.969879 | -4591.560881 |
| E _{HOMO} | -4.260 | -4.082 | -3.914 |
| E _{HOMO-1} | -5.523 | -5.506 | -5.504 |
| G | -2509267.985 | -2606372.612 | -2880967.572 |
| H | -2509194.52 | -2606297.148 | -2880890.103 |
| GPB | -267.5 | -269.1 | -272.7 |
| PA | -276.4 | -277.8 | -280.5 |
| Comp. | [Li-3-H] ⁺ | [Na-3-H] ⁺ | [K-3-H] ⁺ |
| E | -3999.674531 | -4154.420523 | -4592.015832 |
| G | -2509541.831 | -2606648.037 | -2881246.567 |
| H | -2509468.379 | -2606573.441 | -2881169.138 |

Table S14. Calculated NPA charges [e] of M-**3**, and [M-**3**-H]⁺ (M = Li, Na, K).

| Comp. | Li- 3 | Na- 3 | K- 3 |
|--------|--------------|--------------|-------------|
| e (M) | +0.890 | +0.912 | +0.945 |
| e (E) | -0.634 | -0.665 | -0.698 |
| e (Si) | +1.578 | +1.574 | +1.574 |
| e (C) | -1.088 | -1.085 | -1.083 |
| e (O) | -0.993 | -0.979 | -0.971 |

| Comp. | [Li- 3 -H] ⁺ | [Na- 3 -H] ⁺ | [K- 3 -H] ⁺ |
|--------|--------------------------------|--------------------------------|-------------------------------|
| e (M) | +0.899 | +0.917 | +0.949 |
| e (E) | -0.141 | -0.158 | -0.179 |
| e (H) | -0.125 | -0.127 | -0.130 |
| e (Si) | +1.647 | +1.647 | +1.651 |
| e (C) | -1.088 | -1.089 | -1.088 |
| e (O) | -0.978 | -0.977 | -0.971 |

5.4. Results of calculations for the metal free anions 1^- , 2^- , 3^- , 1 , 2-H and 3-H

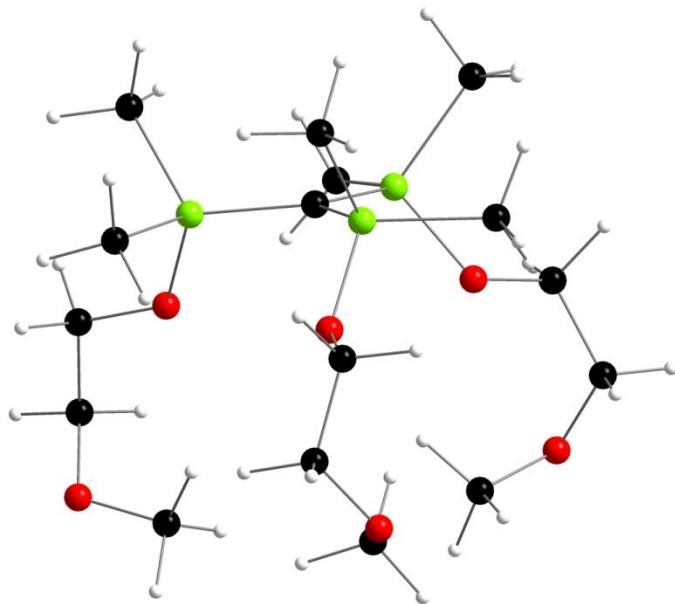


Figure S7. Calculated gas-phase structures of 1^- -A (white = hydrogen; green = silicon; black = carbon; red = oxygen).

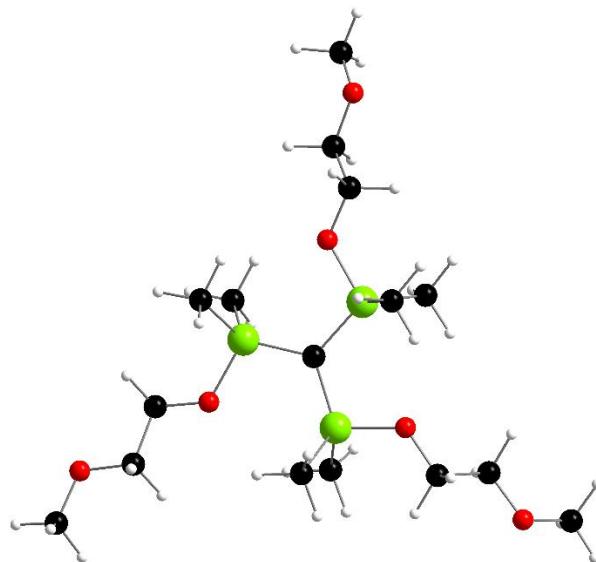


Figure S8. Calculated gas-phase structures of 1^- -B (white = hydrogen; green = silicon; black = carbon; red = oxygen).

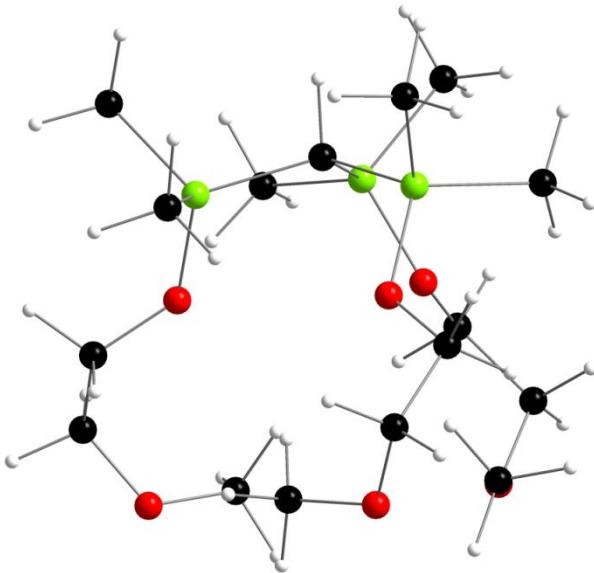


Figure S9. Calculated gas-phase structures of **1-A** (white = hydrogen; green = silicon; black = carbon; red = oxygen).

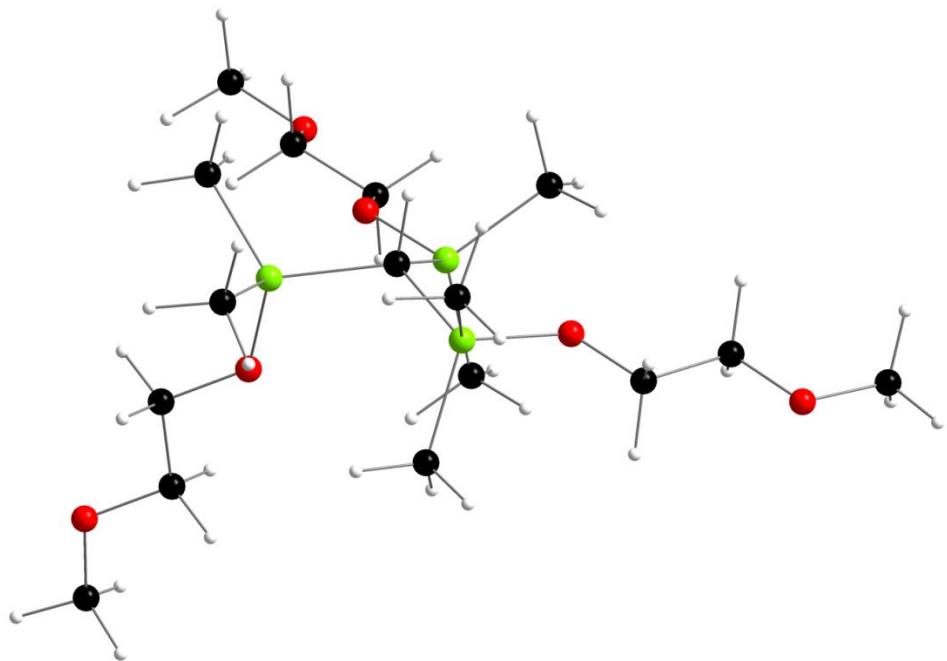


Figure S10. Calculated gas-phase structures of **1-B** (white = hydrogen; green = silicon; black = carbon; red = oxygen).

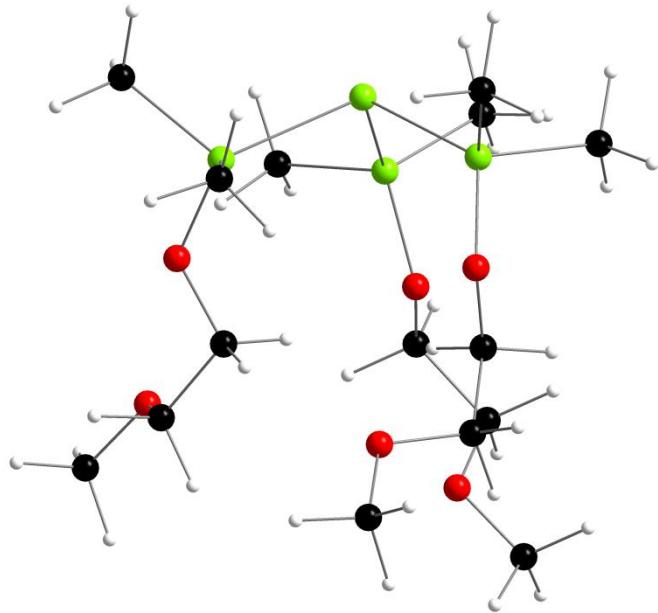


Figure S11. Calculated gas-phase structures of **2⁻**-A (white = hydrogen; green = silicon; black = carbon; red = oxygen).

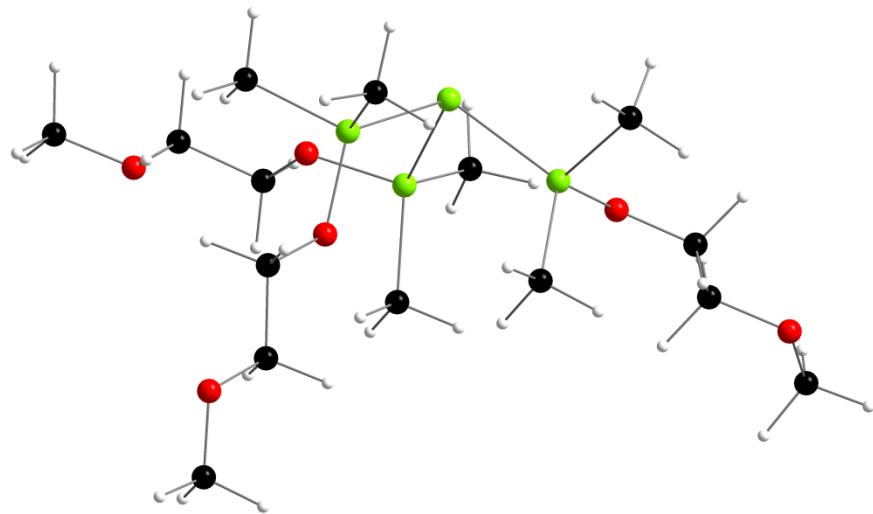


Figure S12. Calculated gas-phase structures of **2⁻**-B (white = hydrogen; green = silicon; black = carbon; red = oxygen).

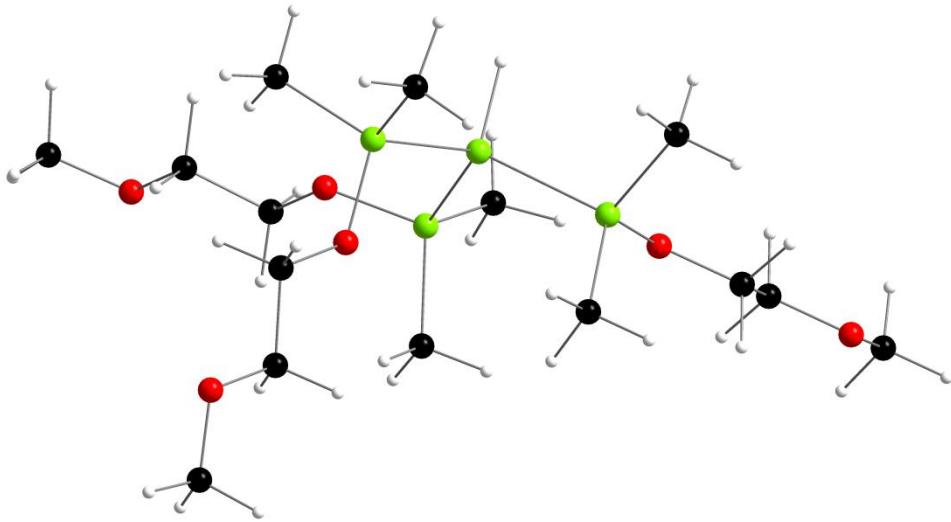


Figure S13. Calculated gas-phase structures of **2-H-B** (white = hydrogen; green = silicon; black = carbon; red = oxygen).

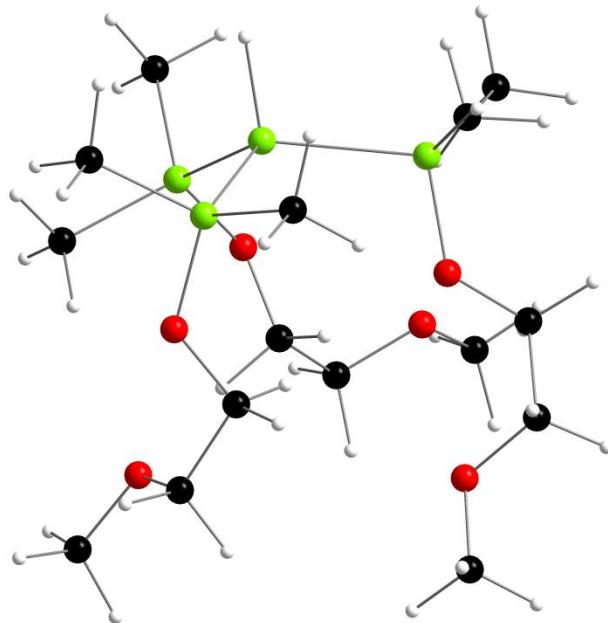


Figure S14. Calculated gas-phase structures of **2-H-A** (white = hydrogen; green = silicon; black = carbon; red = oxygen).

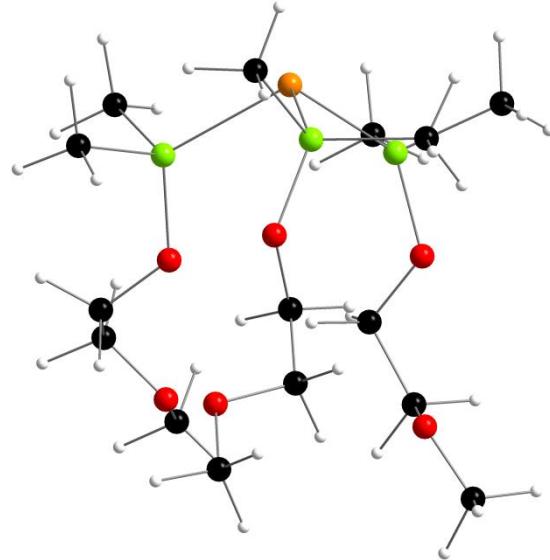


Figure S15. Calculated gas-phase structures of **3⁻**-A (white = hydrogen; green = silicon; black = carbon; red = oxygen; orange = germanium).

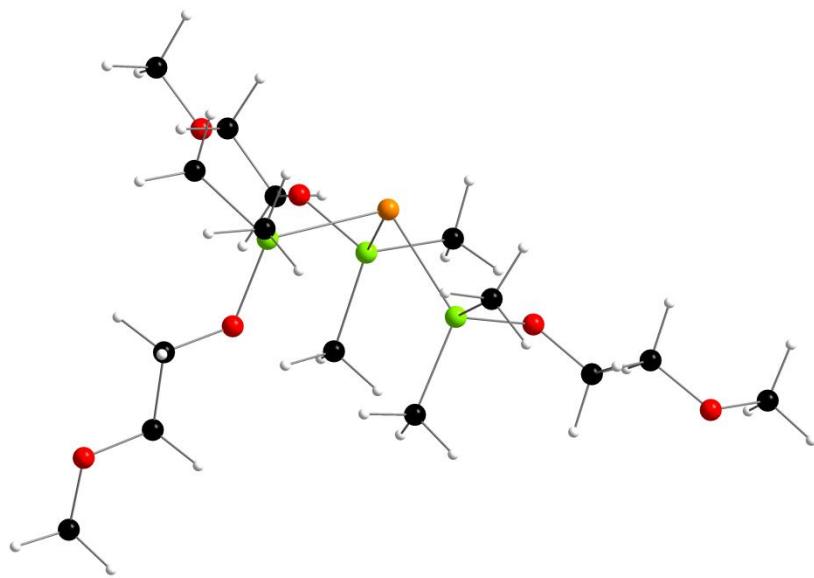


Figure S16. Calculated gas-phase structures of **3⁻**-B (white = hydrogen; green = silicon; black = carbon; red = oxygen; orange = germanium).

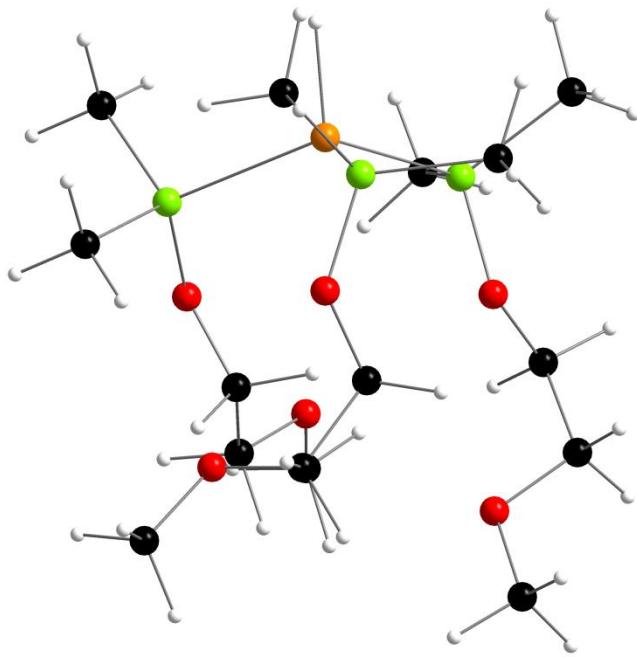


Figure S17. Calculated gas-phase structures of **3-H-A** (white = hydrogen; green = silicon; black = carbon; red = oxygen; orange = germanium).

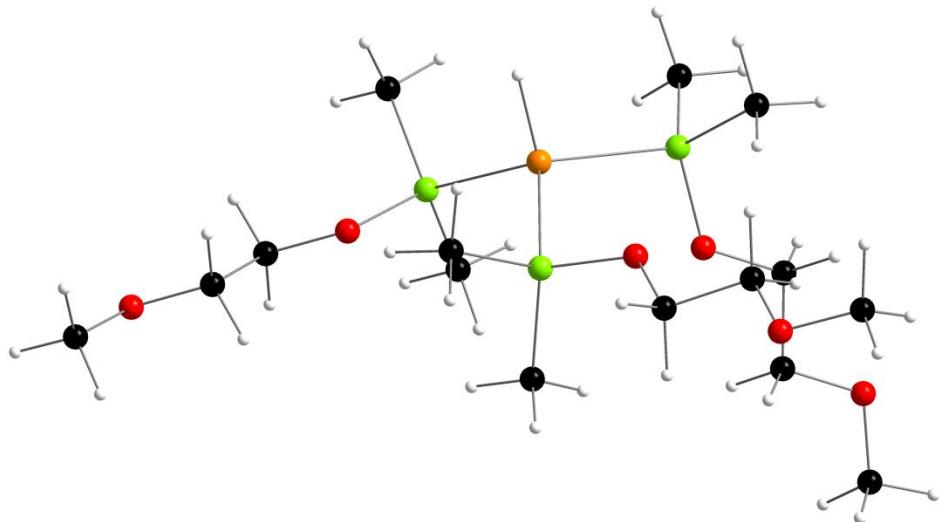


Figure S18. Calculated gas-phase structures of **3-H-B** (white = hydrogen; green = silicon; black = carbon; red = oxygen; orange = germanium).

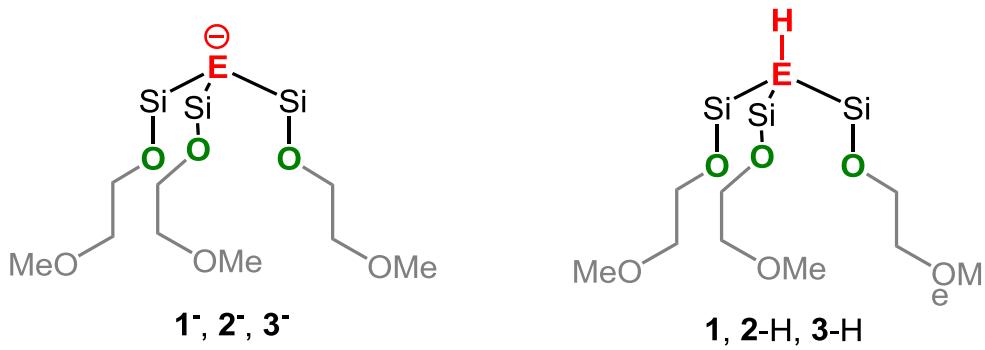


Table S15. Calculated average distances [Å] and angles [°] of the metal-free anions, **1⁻**, **2⁻** and **3⁻**, and their conjugated acids **1**, **2-H** and **3-H**.

| Comp. | 1⁻-A | 1⁻-B | 2⁻-A | 2⁻-B | 3⁻-A | 3⁻-B |
|---------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| E-Si | 1.81 | 1.80 | 2.36 | 2.36 | 2.43 | 2.43 |
| Si-O | 1.73 | 1.73 | 1.72 | 1.73 | 1.72 | 1.73 |
| Si-E-Si | 119.8 | 120.0 | 104.9 | 99.3 | 103.1 | 98.2 |
| E-Si-O | 110.6 | 106.9 | 120.2 | 110.0 | 121.6 | 109.7 |
| Comp. | 1-A | 1-B | 2-H-A | 2-H-B | 3-H-A | 3-H-B |
| E-H | 1.10 | 1.10 | 1.51 | 1.50 | 1.56 | 1.55 |
| E-Si | 1.91 | 1.90 | 2.38 | 2.37 | 2.43 | 2.41 |
| Si-O | 1.69 | 1.69 | 1.69 | 1.70 | 1.69 | 1.69 |
| Si-E-Si | 115.4 | 114.1 | 113.3 | 111.7 | 114.4 | 112.1 |
| E-Si-O | 106.9 | 105.3 | 108.9 | 104.3 | 108.5 | 104.1 |

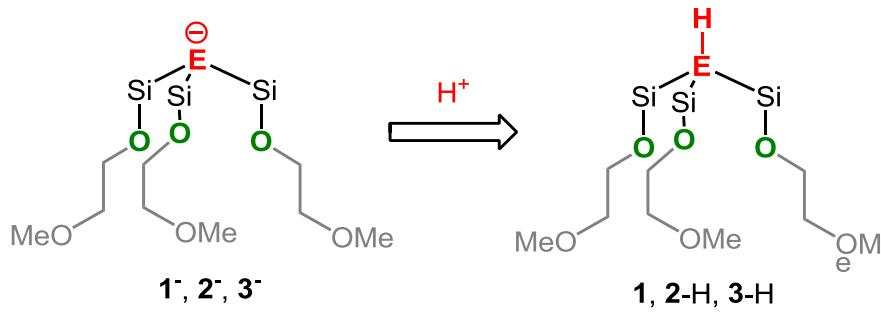


Table S16. Calculated absolute energies [au], HOMO energies [eV], gas-phase basicities [GPB in kcal/mol] and proton affinities [PA in kcal/mol] of **1⁻**, **2⁻**, **3⁻**, **1**, **2-H** and **3-H**.

| Comp. | 1⁻-B | 1⁻-A | 2⁻-A | 2⁻-B | 3⁻-A | 3⁻-B |
|-------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| E | -1952.81871 | -1952.81745 | -2204.17386 | -2204.17820 | -3991.65716 | -3991.66274 |
| E _{HOMO} | -0.9176 | -1.439 | -0.861 | -1.111 | -0.993 | -1.202 |
| G | -1225128.66 | -1225125.09 | -1382859.48 | -1382864.55 | -2504523.30 | -2504530.00 |
| H | -1225055.01 | -1225052.56 | -1382783.23 | -1382785.84 | -2504447.88 | -2504450.58 |
| GPB | -348.8 | - | - | -339.7 | - | -334.9 |
| PA | -352.3 | - | - | -351.6 | - | -344.3 |
| Comp. | 1-B | 1-A | 2-H-B | 2-H-A | 3-H-B | 3-H-A |
| E | -1953.39895 | -1953.38706 | -2204.74599 | -2204.74685 | -3992.21956 | -3992.22140 |
| G | -1225483.69 | -1225472.96 | -1383214.47 | -1383210.52 | -2504874.93 | -2504871.25 |
| H | -1225408.76 | -1225401.41 | -1383135.30 | -1383135.96 | -2504793.36 | -2504793.36 |

Table S17. Calculated NPA charges [e] of **1⁻**, **2⁻**, **3⁻**, **1**, **2-H** and **3-H**.

| Comp. | 1⁻-A | 1⁻-B | 2⁻-A | 2⁻-B | 3⁻-A | 3⁻-B |
|--------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| e (E) | -2.188 | -2.061 | -0.807 | -0.709 | -0.770 | -0.660 |
| e (Si) | +2.106 | +1.984 | +1.610 | +1.596 | +1.603 | +1.583 |
| e (C) | -1.086 | -1.130 | -1.084 | -1.085 | -1.079 | -1.084 |
| e (O) | -0.943 | -0.871 | -0.948 | -0.944 | -0.949 | -0.945 |
| Comp. | 1-A | 1-B | 2-H-A | 2-H-B | 3-H-A | 3-H-B |
| e (E) | -1.766 | -1.762 | -0.206 | -0.141 | -0.220 | -0.146 |
| e (H) | +0.249 | +0.256 | -0.161 | -0.156 | -0.153 | -0.149 |
| e (Si) | +2.096 | +2.089 | +1.664 | +1.650 | +1.672 | +1.657 |
| e (C) | -1.101 | -1.099 | -1.082 | -1.081 | -1.088 | -1.085 |
| e (O) | -0.953 | -0.950 | -0.945 | -0.946 | -0.946 | -0.949 |

5.5. Results of calculations for the metal free anions **7⁻**, **8⁻**, **9⁻**, **7-H**, **8-H** and **9-H**

Table S18. Calculated av. distances [Å] and angles [°] of ⁻E(SiMe₃)₃ and HE(SiMe₃)₃ (E = C, Si, Ge).

| Compound | ⁻ C(SiMe ₃) ₃ (7⁻) | ⁻ Si(SiMe ₃) ₃ (8⁻) | ⁻ Ge(SiMe ₃) ₃ (9⁻) |
|--------------------|--|---|---|
| E-Si | 1.83 | 2.38 | 2.45 |
| Si-CH ₃ | 1.93 | 1.93 | 1.93 |
| Si-E-Si | 119.7 | 102.0 | 100.3 |
| Comp. | HC(SiMe ₃) ₃ (7-H) | HSi(SiMe ₃) ₃ (8-H) | HGe(SiMe ₃) ₃ (9-H) |
| E-Si | 1.92 | 2.38 | 2.43 |
| Si-CH ₃ | 1.90 | 1.90 | 1.90 |
| Si-E-Si | 114.8 | 113.0 | 113.5 |

Table S19. Calculated NPA charges [e] of ⁻E(SiMe₃)₃ and HE(SiMe₃)₃ (E = C, Si, Ge).

| Compound | ⁻ C(SiMe ₃) ₃ (6⁻) | ⁻ Si(SiMe ₃) ₃ (7⁻) | ⁻ Ge(SiMe ₃) ₃ (8⁻) |
|----------|--|---|---|
| e (E) | -2.124 | -0.678 | -0.654 |
| e (Si) | +1.867 | +1.325 | +1.322 |
| e (C) | -1.052 | -1.042 | -1.044 |
| Comp. | HC(SiMe ₃) ₃ (6-H) | HSi(SiMe ₃) ₃ (7-H) | HGe(SiMe ₃) ₃ (8-H) |
| e (E) | -1.691 | -0.105 | -0.128 |
| e (H) | +0.248 | -0.160 | -0.152 |
| e (Si) | +1.813 | +1.359 | +1.373 |
| e (C) | -1.061 | -1.041 | -1.044 |

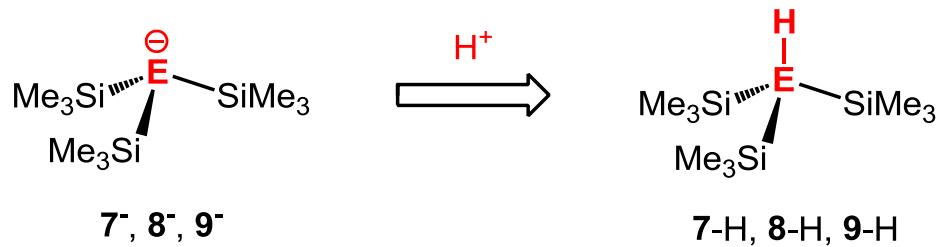


Table S20. Calculated absolute energies [au], HOMO energies [eV], gas-phase basicities [ΔG_B in kcal/mol] and proton affinities [ΔH_{PA} in kcal/mol] of ${}^{\text{-}}\text{E}(\text{SiMe}_3)_3$ and $\text{H}\text{E}(\text{SiMe}_3)_3$ ($\text{E} = \text{C}, \text{Si}, \text{Ge}$).

| Comp. | ${}^{\text{-}}\text{C}(\text{SiMe}_3)_3$ (7-) | ${}^{\text{-}}\text{Si}(\text{SiMe}_3)_3$ (8-) | ${}^{\text{-}}\text{Ge}(\text{SiMe}_3)_3$ (9-) |
|-------------------|--|---|---|
| E | -1265.672843 | -1517.049041 | -3304.533534 |
| E_{HOMO} | -0.590 | -0.682 | -0.778 |
| G | -794044.9347 | -951790.7426 | -2073457.08 |
| H | -793996.7535 | -951739.3945 | -2073404.219 |
| GPB | -355.1 | -349.3 | -342.8 |
| PA | -364.1 | -356.7 | -350.4 |
| Comp. | $\text{HC}(\text{SiMe}_3)_3$ (7-H) | $\text{HSi}(\text{SiMe}_3)_3$ (8-H) | $\text{HGe}(\text{SiMe}_3)_3$ (9-H) |
| E | -1266.265089 | -1517.625792 | -3305.100080 |
| G | -794406.2862 | -952146.3907 | -2073806.2220 |
| H | -794359.3980 | -952094.5646 | -2073753.1050 |

5.6. B3-LYP/TZVP Cartesian coordinates [Å]

[Li(MeOCH₂CH₂OSiMe₂)₃C] (Li-1-B)

| | | | |
|----|------------|------------|------------|
| C | 2.8044057 | -2.9873036 | -0.7144778 |
| Si | 1.5040104 | -2.0489628 | 0.3100591 |
| C | 1.9498073 | -2.4685070 | 2.1123918 |
| C | -0.2290699 | -2.1462751 | -0.2051599 |
| Si | -0.5962621 | -1.4952465 | -1.8539048 |
| C | 0.7413739 | -1.6200041 | -3.2043720 |
| O | 1.8835582 | -0.3412097 | 0.1563348 |
| C | 3.1307590 | 0.3073851 | 0.2636071 |
| C | 3.1848193 | 1.4325389 | -0.7524372 |
| O | 2.0393972 | 2.2578648 | -0.5686030 |
| C | 1.9561665 | 3.3101221 | -1.5169777 |
| O | -0.7974054 | 0.2370680 | -1.6104520 |
| C | -1.2228323 | 1.1688204 | -2.5843193 |
| C | -2.1063653 | 2.2201460 | -1.9446328 |
| O | -1.3690893 | 2.8836072 | -0.9272248 |
| C | -2.1495381 | 3.8045418 | -0.1878972 |
| C | -2.1781274 | -2.1059342 | -2.7193539 |
| Si | -1.4500194 | -1.7527944 | 1.0725542 |
| C | -1.5044644 | -2.8336606 | 2.6365332 |
| O | -0.9900669 | -0.1417067 | 1.5974935 |
| C | -1.5857254 | 0.6560065 | 2.5948484 |
| C | -0.5364795 | 1.5971406 | 3.1512199 |
| O | 0.0594667 | 2.2972898 | 2.0638474 |
| C | 1.0740926 | 3.1967605 | 2.4800905 |
| C | -3.2796994 | -1.5830867 | 0.5708823 |
| Li | 0.1686381 | 0.7924400 | 0.1525829 |

H -2.5156563 4.6211925 -0.8245945
H -1.5125681 4.2108718 0.5951933
H -3.0125962 3.3121729 0.2781088
H 1.8561065 2.6770540 3.0480323
H 0.6597738 3.9968350 3.1070415
H 1.5154855 3.6205257 1.5815604
H 2.7837782 4.0205555 -1.3935809
H 1.0050261 3.8123502 -1.3544239
H 1.9803533 2.9201905 -2.5421826
H -1.9841297 0.0551348 3.4223250
H -2.4178199 1.2366359 2.1747318
H -0.9965253 2.3046462 3.8563496
H 0.2339054 1.0257341 3.6861260
H 2.7679031 -2.7629186 -1.7796538
H 2.6272037 -4.0602117 -0.5971306
H 3.8196438 -2.7884072 -0.3572513
H 3.0234960 -2.3217367 2.2651116
H 1.7258331 -3.5112240 2.3488522
H 1.4221509 -1.8342856 2.8263229
H -3.0818937 -1.9627216 -2.1282218
H -2.0741594 -3.1784386 -2.9064514
H -2.3246204 -1.6226753 -3.6902384
H -3.8774453 -1.3154412 1.4478824
H -3.6732295 -2.5260312 0.1847066
H -3.4358077 -0.8128787 -0.1860273
H -1.7985421 0.6861230 -3.3832239
H -0.3555900 1.6540900 -3.0497866
H 3.9692854 -0.3726462 0.0707883
H 3.2598782 0.7152071 1.2748262

H -2.4422426 2.9395464 -2.7070918
 H -2.9936298 1.7410305 -1.5090455
 H -0.5315665 -2.9658453 3.1073469
 H -1.8768936 -3.8249484 2.3630009
 H -2.1931337 -2.4251564 3.3829016
 H 4.1061471 2.0189195 -0.6225386
 H 3.1787349 1.0181167 -1.7694576
 H 0.3784439 -1.1493102 -4.1232477
 H 0.9737864 -2.6608451 -3.4411306
 H 1.6682625 -1.1202211 -2.9183602

[Li(MeOCH₂CH₂OSiMe₂)₃C] (Li-1-A)

Si 5.0819167 2.4672337 0.4727102
 Si 4.5038025 2.0419805 -2.6379024
 Si 2.3654294 3.2673071 -0.7177749
 O 5.8743148 4.0589987 0.4585579
 O 7.2751430 6.5166738 0.1817138
 O 4.8271404 3.4520900 -3.5908931
 O 4.7790507 6.2081760 -2.2544933
 O 2.7854033 4.8167354 -0.0018584
 O 3.9155643 7.0362011 0.9226983
 C 6.5215031 1.2222707 0.5507478
 H 6.1368076 0.2091841 0.4113266
 H 7.0091267 1.2487756 1.5292930
 H 7.2826141 1.3909077 -0.2113676
 C 4.2961936 2.3995938 2.2071859
 H 3.8181932 1.4318776 2.3785745
 H 3.5446841 3.1775325 2.3498670

| | | | |
|---|-----------|-----------|------------|
| H | 5.0621315 | 2.5285648 | 2.9782798 |
| C | 6.9226019 | 4.4429932 | 1.3302160 |
| H | 7.4634555 | 3.5698925 | 1.7122998 |
| H | 6.5204624 | 4.9855707 | 2.1955333 |
| C | 7.9210056 | 5.3220981 | 0.6060360 |
| H | 8.7580824 | 5.5623699 | 1.2785707 |
| H | 8.3214337 | 4.7845983 | -0.2641969 |
| C | 8.1105013 | 7.3451245 | -0.6053667 |
| H | 8.9984196 | 7.6685650 | -0.0463965 |
| H | 7.5297034 | 8.2238470 | -0.8849203 |
| H | 8.4406529 | 6.8314360 | -1.5171963 |
| C | 3.2339917 | 1.1574813 | -3.7337408 |
| H | 2.3314890 | 1.7461229 | -3.8963764 |
| H | 2.9395606 | 0.2069228 | -3.2809731 |
| H | 3.6723112 | 0.9467235 | -4.7128399 |
| C | 6.0958814 | 1.0020447 | -2.7789875 |
| H | 6.9847917 | 1.5200050 | -2.4133959 |
| H | 6.2632351 | 0.7691399 | -3.8345058 |
| H | 6.0171855 | 0.0580949 | -2.2358920 |
| C | 5.8973619 | 4.3149151 | -3.3103970 |
| H | 6.7105000 | 4.1523729 | -4.0333882 |
| H | 6.3205407 | 4.1509155 | -2.3086239 |
| C | 5.4926414 | 5.7711421 | -3.4208085 |
| H | 6.3862025 | 6.4004914 | -3.5398139 |
| H | 4.8552048 | 5.9005055 | -4.3026782 |
| C | 4.1891786 | 7.4899623 | -2.4378169 |
| H | 3.4224328 | 7.4562284 | -3.2198147 |
| H | 4.9462726 | 8.2331519 | -2.7172626 |
| H | 3.7376700 | 7.7797247 | -1.4914150 |

| | | | |
|----|-----------|-----------|------------|
| C | 1.3512940 | 3.7225264 | -2.2599282 |
| H | 1.9778095 | 4.1225200 | -3.0588257 |
| H | 0.6069636 | 4.4805199 | -1.9959691 |
| H | 0.8049884 | 2.8619015 | -2.6515652 |
| C | 1.1087265 | 2.4968452 | 0.4880474 |
| H | 1.5279495 | 2.3168396 | 1.4788794 |
| H | 0.7908000 | 1.5300048 | 0.0880195 |
| H | 0.2096329 | 3.1111565 | 0.6006801 |
| C | 1.9153995 | 5.8242073 | 0.4619173 |
| H | 1.0154108 | 5.4097724 | 0.9318180 |
| H | 1.5915460 | 6.4643608 | -0.3691848 |
| C | 2.6615732 | 6.6514441 | 1.4898715 |
| H | 2.0790666 | 7.5414812 | 1.7640292 |
| H | 2.8414913 | 6.0593433 | 2.3962686 |
| C | 4.6848334 | 7.8577509 | 1.7934400 |
| H | 4.1940241 | 8.8253751 | 1.9510927 |
| H | 5.6563876 | 7.9979543 | 1.3270762 |
| H | 4.8258306 | 7.3708347 | 2.7659600 |
| C | 3.9686704 | 2.4574034 | -0.9439292 |
| Li | 4.6501675 | 5.3529370 | -0.3914053 |

[Li(MeOCH₂CH₂OSiMe₂)₃CH]⁺ [Li-1-H]⁺

| | | | |
|----|------------|-----------|------------|
| C | -0.2624048 | 2.7352742 | -3.1100635 |
| Si | -0.8472632 | 1.7225967 | -1.6289982 |
| C | -2.7338026 | 1.7421197 | -1.6785278 |
| C | -0.0164466 | 2.2707721 | -0.0067111 |
| Si | 1.8122772 | 1.7494118 | 0.0863716 |
| C | 2.7950545 | 1.7796066 | -1.5240891 |

| | | | |
|----|------------|------------|------------|
| O | -0.3176996 | 0.1014013 | -1.7544471 |
| C | -0.5254708 | -0.7379649 | -2.8869115 |
| C | 0.6018431 | -1.7446409 | -2.9582959 |
| O | 0.6953715 | -2.4029239 | -1.6971590 |
| C | 1.6767941 | -3.4382485 | -1.6884902 |
| O | 1.6812258 | 0.1274845 | 0.6124201 |
| C | 2.7760765 | -0.6947870 | 1.0059333 |
| C | 2.2807053 | -1.7149841 | 2.0076189 |
| O | 1.1592172 | -2.3901726 | 1.4430258 |
| C | 0.6777048 | -3.4467564 | 2.2721245 |
| C | 2.7854233 | 2.7806223 | 1.3313709 |
| Si | -1.0042653 | 1.7401334 | 1.5314437 |
| C | -2.5891405 | 2.7419154 | 1.7442662 |
| O | -1.3647196 | 0.1105675 | 1.1593403 |
| C | -2.2434283 | -0.7261828 | 1.9055714 |
| C | -2.8529266 | -1.7469823 | 0.9696672 |
| O | -1.7969121 | -2.4054683 | 0.2735347 |
| C | -2.2651389 | -3.4626904 | -0.5624235 |
| C | -0.1036097 | 1.7936870 | 3.1883266 |
| Li | 0.0102470 | -1.1589131 | 0.0073910 |
| H | 1.4389875 | -4.2248553 | 2.3911627 |
| H | -0.2003535 | -3.8611497 | 1.7843777 |
| H | 0.3978286 | -3.0716072 | 3.2628307 |
| H | -2.9907788 | -3.0921688 | -1.2953082 |
| H | -2.7373811 | -4.2499420 | 0.0344414 |
| H | -1.4005981 | -3.8641408 | -1.0843439 |
| H | 1.4119702 | -4.2308880 | -2.3959536 |
| H | 1.7083110 | -3.8401677 | -0.6794749 |
| H | 2.6648807 | -3.0448364 | -1.9525510 |

H -3.0526536 -0.1544914 2.3720595
H -1.6836262 -1.2303559 2.7002561
H -3.4411879 -2.4705589 1.5479178
H -3.5202275 -1.2582683 0.2485207
H 0.8150463 2.7043076 -3.2666598
H -0.5481722 3.7813557 -2.9654914
H -0.7493888 2.4034400 -4.0307660
H -3.0693280 1.3841857 -2.6562240
H -3.1254553 2.7554643 -1.5615693
H -3.1856736 1.1079426 -0.9162576
H 2.3829287 2.7429381 2.3427082
H 2.7839558 3.8265546 1.0110046
H 3.8317678 2.4670642 1.3693002
H -0.7800829 1.4461164 3.9745611
H 0.1876503 2.8135576 3.4506475
H 0.7855485 1.1648051 3.2071915
H 3.5772071 -0.1107029 1.4712819
H 3.1909376 -1.2000536 0.1276820
H -0.5408224 -0.1655136 -3.8204153
H -1.4862353 -1.2540576 -2.7902306
H 3.0835064 -2.4275060 2.2341496
H 1.9820657 -1.2232185 2.9418764
H -3.2619286 2.6825184 0.8898014
H -2.3339964 3.7950200 1.8946205
H -3.1400930 2.4246005 2.6334633
H 0.3977717 -2.4695230 -3.7562110
H 1.5515785 -1.2431230 -3.1831890
H 3.8152931 1.4374603 -1.3277615
H 2.8726770 2.7932837 -1.9244803

H 2.3674073 1.1365556 -2.2927176
H -0.0220404 3.3694421 -0.0134378

[Na(MeOCH₂CH₂OSiMe₂)₃C] (Na-1)

C 2.7202967 -2.8437979 -1.5066044
Si 1.7799162 -1.8251656 -0.2020030
C 2.8908534 -1.9005479 1.3441689
C 0.0084393 -2.1345868 0.0126983
Si -1.0659571 -1.8549662 -1.4182682
C -0.2819299 -1.9562483 -3.1521224
O 1.8929297 -0.1585814 -0.7344601
C 3.0535719 0.5926642 -0.9949760
C 2.6993035 1.7625645 -1.8912078
O 1.6760402 2.5443118 -1.2733080
C 1.2815097 3.6469868 -2.0738111
O -1.5927230 -0.1889447 -1.2777327
C -2.3711331 0.5547435 -2.1831728
C -2.9850395 1.7357902 -1.4573366
O -1.9493328 2.5193417 -0.8613058
C -2.4588930 3.6330792 -0.1449575
C -2.6595338 -2.8859180 -1.5602031
Si -0.6950180 -1.8459198 1.6564766
C -0.0184468 -2.8644308 3.1151682
O -0.3144786 -0.1761850 2.0258220
C -0.6777516 0.5684543 3.1622468
C 0.2658204 1.7459378 3.3070822
O 0.2323297 2.5316150 2.1142019
C 1.1168688 3.6393985 2.1712266

| | | | |
|----|------------|------------|------------|
| C | -2.5880432 | -1.9498752 | 1.8474981 |
| Na | -0.0157671 | 1.0457949 | 0.0055890 |
| H | -2.9781069 | 4.3312690 | -0.8137418 |
| H | -1.6141902 | 4.1387919 | 0.3197739 |
| H | -3.1536655 | 3.3159008 | 0.6419146 |
| H | 2.1497802 | 3.3153951 | 2.3479028 |
| H | 0.8256111 | 4.3388295 | 2.9649116 |
| H | 1.0715182 | 4.1456647 | 1.2085306 |
| H | 2.1128569 | 4.3481612 | -2.2206383 |
| H | 0.4687627 | 4.1537854 | -1.5566017 |
| H | 0.9201970 | 3.3174192 | -3.0555937 |
| H | -0.6164856 | -0.0237635 | 4.0857289 |
| H | -1.7099087 | 0.9356828 | 3.0749959 |
| H | -0.0310174 | 2.3610861 | 4.1685070 |
| H | 1.2884561 | 1.3831214 | 3.4741586 |
| H | 2.2651691 | -2.7963080 | -2.4955889 |
| H | 2.7323554 | -3.8927522 | -1.1981260 |
| H | 3.7619791 | -2.5192264 | -1.5956336 |
| H | 3.9075853 | -1.5906453 | 1.0834309 |
| H | 2.9541762 | -2.9174349 | 1.7385053 |
| H | 2.5350259 | -1.2464564 | 2.1424348 |
| H | -3.2798829 | -2.8357666 | -0.6658863 |
| H | -2.3932538 | -3.9344011 | -1.7203255 |
| H | -3.2674578 | -2.5705316 | -2.4142898 |
| H | -2.8744440 | -1.6606747 | 2.8634539 |
| H | -2.9462205 | -2.9696575 | 1.6890259 |
| H | -3.1109573 | -1.2923039 | 1.1508730 |
| H | -3.1927001 | -0.0369515 | -2.6102139 |
| H | -1.7580212 | 0.9178826 | -3.0198384 |

H 3.8252253 0.0022764 -1.5079366
 H 3.4933458 0.9681850 -0.0605284
 H -3.5602736 2.3516854 -2.1631181
 H -3.6651641 1.3772490 -0.6738158
 H 1.0662937 -2.8128432 3.2054194
 H -0.2887117 -3.9141945 2.9707527
 H -0.4542710 -2.5446280 4.0671630
 H 3.5895668 2.3836052 -2.0661645
 H 2.3383768 1.3917077 -2.8593891
 H -1.0207223 -1.6797954 -3.9109301
 H 0.0473074 -2.9731181 -3.3782134
 H 0.5750772 -1.2887821 -3.2578948

[Na(MeOCH₂CH₂OSiMe₂)₃CH]⁺ [Na-1-H]⁺

C -3.0234777 2.8958868 0.5904690
 Si -1.5439070 1.8032548 1.0137335
 C -1.3498292 1.8416603 2.8905732
 C 0.0010428 2.2755984 0.0006349
 Si -0.1017151 1.8039823 -1.8436091
 C -1.8226425 1.8366401 -2.6174635
 O -1.8442958 0.1905162 0.5336810
 C -2.9282890 -0.6026557 1.0129435
 C -3.2362323 -1.7029200 0.0209224
 O -2.0696937 -2.5004785 -0.1758056
 C -2.3017960 -3.6145770 -1.0357151
 O 0.4669553 0.1915668 -1.8650896
 C 0.5919103 -0.5971521 -3.0468729
 C 1.6032854 -1.7001632 -2.8246910

| | | | |
|----|------------|------------|------------|
| O | 1.1900039 | -2.5041419 | -1.7204583 |
| C | 2.0479860 | -3.6226492 | -1.5021372 |
| C | 1.0028754 | 2.9001396 | -2.9108349 |
| Si | 1.6498220 | 1.8021287 | 0.8329347 |
| C | 2.0308282 | 2.9050569 | 2.3161362 |
| O | 1.3778992 | 0.1935361 | 1.3436430 |
| C | 2.3326086 | -0.5934026 | 2.0539570 |
| C | 1.6250966 | -1.6964414 | 2.8099731 |
| O | 0.8863275 | -2.4991366 | 1.8898183 |
| C | 0.2419880 | -3.6063140 | 2.5182908 |
| C | 3.1802596 | 1.8229763 | -0.2713084 |
| Na | 0.0065124 | -1.2832115 | -0.0009362 |
| H | 2.0311599 | -4.3005214 | -2.3617472 |
| H | 1.6825109 | -4.1448538 | -0.6201677 |
| H | 3.0794111 | -3.2994460 | -1.3236836 |
| H | -0.4382821 | -3.2698914 | 3.3082455 |
| H | 0.9784823 | -4.2920580 | 2.9496538 |
| H | -0.3324889 | -4.1247551 | 1.7529982 |
| H | -3.0328315 | -4.3009291 | -0.5958779 |
| H | -1.3515949 | -4.1290081 | -1.1641958 |
| H | -2.6655329 | -3.2866791 | -2.0155501 |
| H | 2.8911672 | 0.0095405 | 2.7783803 |
| H | 3.0520819 | -1.0284166 | 1.3513251 |
| H | 2.3707442 | -2.3083328 | 3.3335919 |
| H | 0.9437606 | -1.2699923 | 3.5573519 |
| H | -3.3187645 | 2.8384787 | -0.4566064 |
| H | -2.7870242 | 3.9402107 | 0.8146693 |
| H | -3.8910837 | 2.6330761 | 1.2014410 |
| H | -2.2828348 | 1.5165610 | 3.3596799 |

H -1.1543000 2.8558435 3.2470769
 H -0.5492633 1.1919119 3.2440347
 H 2.0540448 2.8617738 -2.6277959
 H 0.6730315 3.9401824 -2.8345044
 H 0.9261702 2.6233411 -3.9655740
 H 4.0486618 1.4958649 0.3078292
 H 3.4000040 2.8330720 -0.6247738
 H 3.0857698 1.1675840 -1.1370484
 H 0.9298877 0.0050272 -3.8976281
 H -0.3789423 -1.0327367 -3.3071897
 H -3.8360163 -0.0036417 1.1468370
 H -2.6678088 -1.0410534 1.9826341
 H 1.6707782 -2.3118752 -3.7335847
 H 2.5939615 -1.2742069 -2.6213825
 H 1.2651364 2.8731308 3.0905828
 H 2.1287465 3.9430951 1.9854221
 H 2.9851231 2.6301608 2.7732873
 H -4.0552192 -2.3198573 0.4129106
 H -3.5560529 -1.2737398 -0.9368577
 H -1.7564814 1.5183764 -3.6616754
 H -2.2371082 2.8474716 -2.6210543
 H -2.5258233 1.1779051 -2.1075329
 H 0.0009125 3.3760679 0.0009126

[K(MeOCH₂CH₂OSiMe₂)₃C] (K-1)

C 2.5896182 2.9978862 1.5716224
 Si 1.7850869 1.8127430 0.3155921
 C 2.9423037 1.8658518 -1.1989014

| | | | |
|----|------------|------------|------------|
| C | 0.0092275 | 1.9802557 | -0.0063843 |
| Si | -1.1568494 | 1.8326282 | 1.3735737 |
| C | -0.4210551 | 1.9117153 | 3.1307890 |
| O | 2.0229041 | 0.2135849 | 0.9870155 |
| C | 3.2566651 | -0.3882256 | 1.2912597 |
| C | 3.0416203 | -1.6200665 | 2.1468541 |
| O | 2.2622706 | -2.5858517 | 1.4355450 |
| C | 2.0989681 | -3.7896042 | 2.1653958 |
| O | -1.8571229 | 0.2319936 | 1.2674707 |
| C | -2.7314632 | -0.3581985 | 2.1965785 |
| C | -3.3817990 | -1.5873320 | 1.5943197 |
| O | -2.3880581 | -2.5625182 | 1.2665767 |
| C | -2.9554445 | -3.7585403 | 0.7598785 |
| C | -2.6466988 | 3.0186987 | 1.4252897 |
| Si | -0.6029774 | 1.8176414 | -1.7046460 |
| C | 0.1037976 | 2.9870551 | -3.0321649 |
| O | -0.1700145 | 0.2082382 | -2.2401281 |
| C | -0.5279828 | -0.3897369 | -3.4610337 |
| C | 0.3176234 | -1.6226479 | -3.7069115 |
| O | 0.0916097 | -2.5923264 | -2.6802947 |
| C | 0.7943667 | -3.7999057 | -2.9175833 |
| C | -2.4919892 | 1.9064573 | -1.9519253 |
| K | -0.0071551 | -1.3617746 | 0.0057529 |
| H | -3.6302195 | -4.2208993 | 1.4913642 |
| H | -2.1380198 | -4.4494991 | 0.5527924 |
| H | -3.5139219 | -3.5783637 | -0.1674699 |
| H | 1.8792981 | -3.6367172 | -2.9434637 |
| H | 0.4867030 | -4.2611906 | -3.8647120 |
| H | 0.5585931 | -4.4843057 | -2.1024200 |

| | | | |
|---|------------|------------|------------|
| H | 3.0667801 | -4.2580349 | 2.3846478 |
| H | 1.5119755 | -4.4717670 | 1.5498934 |
| H | 1.5699868 | -3.6183788 | 3.1116356 |
| H | -0.3710640 | 0.2864513 | -4.3135205 |
| H | -1.5887949 | -0.6785783 | -3.4644210 |
| H | 0.0547535 | -2.0548874 | -4.6831267 |
| H | 1.3807458 | -1.3483074 | -3.7238662 |
| H | 2.1128793 | 2.9598182 | 2.5513636 |
| H | 2.5094120 | 4.0238205 | 1.2023940 |
| H | 3.6544744 | 2.7815425 | 1.7052171 |
| H | 3.9589461 | 1.5902568 | -0.9024000 |
| H | 2.9929973 | 2.8721842 | -1.6209878 |
| H | 2.6233651 | 1.1816454 | -1.9878155 |
| H | -3.2488805 | 2.9774179 | 0.5175982 |
| H | -2.2864132 | 4.0448270 | 1.5384738 |
| H | -3.3012007 | 2.8068238 | 2.2767619 |
| H | -2.7482485 | 1.6419929 | -2.9825837 |
| H | -2.8631625 | 2.9193319 | -1.7794383 |
| H | -3.0299400 | 1.2294825 | -1.2855473 |
| H | -3.5407153 | 0.3244015 | 2.4937964 |
| H | -2.1977959 | -0.6501198 | 3.1123211 |
| H | 3.9172950 | 0.2869144 | 1.8543029 |
| H | 3.7913586 | -0.6800155 | 0.3760453 |
| H | -4.0917062 | -2.0152882 | 2.3168460 |
| H | -3.9351504 | -1.3094991 | 0.6873662 |
| H | 1.1910370 | 2.9426301 | -3.0986705 |
| H | -0.1724114 | 4.0164003 | -2.7876425 |
| H | -0.3048438 | 2.7666581 | -4.0236817 |
| H | 4.0165330 | -2.0558748 | 2.4085478 |

| | | | |
|---|------------|------------|-----------|
| H | 2.5245509 | -1.3438495 | 3.0754247 |
| H | -1.1864224 | 1.6597298 | 3.8712637 |
| H | -0.0686128 | 2.9187507 | 3.3650282 |
| H | 0.4145462 | 1.2209086 | 3.2593326 |

[K(MeOCH₂CH₂OSiMe₂)₃CH]⁺ [K-1-H]⁺

| | | | |
|----|------------|------------|------------|
| C | -2.1917959 | -3.0336190 | -2.0758269 |
| Si | -0.8086450 | -1.8102760 | -1.6795210 |
| C | 0.3568422 | -1.7885463 | -3.1646464 |
| C | 0.0019766 | -2.2191558 | -0.0019419 |
| Si | -1.0509207 | -1.8067955 | 1.5345378 |
| C | -2.9196154 | -1.8281496 | 1.2656321 |
| O | -1.4546861 | -0.2393792 | -1.4903045 |
| C | -2.1854050 | 0.4137489 | -2.5289163 |
| C | -3.0790337 | 1.4990384 | -1.9705546 |
| O | -2.2948444 | 2.5354239 | -1.3815418 |
| C | -3.0753789 | 3.6780948 | -1.0362393 |
| O | -0.5924935 | -0.2214510 | 1.9754183 |
| C | -1.1598903 | 0.4564285 | 3.0952197 |
| C | -0.2248830 | 1.5236133 | 3.6215690 |
| O | -0.0305913 | 2.5409940 | 2.6398798 |
| C | 0.7024846 | 3.6542616 | 3.1471984 |
| C | -0.6796230 | -3.0001386 | 2.9506870 |
| Si | 1.8593405 | -1.8086884 | 0.1381426 |
| C | 2.8972504 | -3.0068361 | -0.8887818 |
| O | 2.0164120 | -0.2256130 | -0.4846447 |
| C | 3.2727539 | 0.4503150 | -0.5376500 |
| C | 3.2736535 | 1.5246688 | -1.6026648 |

O 2.3276240 2.5427603 -1.2812703
C 2.4297394 3.6733983 -2.1444922
C 2.5642979 -1.8231764 1.8898538
K -0.0077054 1.6648572 -0.0189207
H 0.1718870 4.1259602 3.9808880
H 0.8026393 4.3762732 2.3377227
H 1.7003196 3.3526245 3.4846978
H 2.2407801 3.3958272 -3.1874840
H 3.4209320 4.1335252 -2.0718747
H 1.6802713 4.3968436 -1.8262801
H -3.5472030 4.1134574 -1.9233728
H -2.4023247 4.4135231 -0.5974318
H -3.8528187 3.4228999 -0.3076091
H 4.0868883 -0.2439595 -0.7744021
H 3.4944153 0.9040339 0.4352219
H 4.2815802 1.9572464 -1.6530624
H 3.0375209 1.0906743 -2.5828222
H -2.9885965 -3.0393651 -1.3322652
H -1.7809489 -4.0454695 -2.1350572
H -2.6409326 -2.8196866 -3.0491428
H -0.1948671 -1.4851870 -4.0589971
H 0.7602817 -2.7835245 -3.3657767
H 1.1912015 -1.0994105 -3.0303906
H 0.3589970 -2.9662939 3.2785988
H -0.8999998 -4.0253729 2.6392247
H -1.3134767 -2.7933934 3.8169238
H 3.6181153 -1.5317981 1.8630214
H 2.5254769 -2.8243066 2.3251081
H 2.0400415 -1.1374182 2.5562211

H -1.3591475 -0.2371548 3.9199935
 H -2.1127742 0.9174784 2.8103770
 H -2.8274776 -0.2938333 -3.0658464
 H -1.4923820 0.8532856 -3.2556534
 H -0.6732565 1.9588996 4.5242058
 H 0.7412136 1.0817724 3.8973970
 H 2.6441633 -2.9939323 -1.9485564
 H 2.7568268 -4.0277393 -0.5221759
 H 3.9633127 -2.7841499 -0.7945416
 H -3.6759681 1.9097210 -2.7953659
 H -3.7677679 1.0811710 -1.2249395
 H -3.4264156 -1.5281160 2.1871961
 H -3.2730328 -2.8333302 1.0248567
 H -3.2337071 -1.1528074 0.4695668
 H 0.0025411 -3.3211980 -0.0009462

[Li(MeOCH₂CH₂OSiMe₂)₃Si] (Li-**2**)

C -0.2337487 1.6121749 3.5250142
 H -1.0814468 0.9260450 3.4701790
 H -0.6092729 2.5792193 3.8690372
 H 0.4579742 1.2361453 4.2855749
 C 2.2188527 2.7978524 2.1831183
 H 2.8130489 2.3900456 3.0065677
 H 1.9336970 3.8156780 2.4624474
 H 2.8592157 2.8721653 1.3017168
 C 2.3972647 2.4031385 -1.7765197
 H 2.9543745 1.9796647 -0.9383976
 H 2.5134943 3.4893564 -1.7400319

| | | | |
|---|------------|------------|------------|
| H | 2.8606680 | 2.0518510 | -2.7038921 |
| C | -0.1870108 | 2.4956455 | -3.3687062 |
| H | 0.3793113 | 2.1429000 | -4.2360476 |
| H | -0.1753023 | 3.5885488 | -3.3956588 |
| H | -1.2256091 | 2.1798430 | -3.4858861 |
| C | -3.4225067 | 1.1073520 | -1.5060022 |
| H | -2.8142431 | 0.7664559 | -2.3462704 |
| H | -3.8208531 | 2.0927223 | -1.7605734 |
| H | -4.2716232 | 0.4240554 | -1.4029386 |
| C | -3.6695836 | 1.5131969 | 1.4952772 |
| H | -4.5100372 | 0.8125047 | 1.4809734 |
| H | -4.0825271 | 2.5173551 | 1.3669324 |
| H | -3.2084129 | 1.4768875 | 2.4843864 |
| C | 2.1077286 | -0.5445331 | 2.1861190 |
| H | 1.5875491 | -1.2683178 | 2.8249028 |
| H | 2.6936643 | 0.1113590 | 2.8386883 |
| C | 3.0664245 | -1.2724058 | 1.2679129 |
| H | 3.6470384 | -0.5502355 | 0.6786084 |
| H | 3.7665953 | -1.8760659 | 1.8639767 |
| C | 1.0492763 | -0.5738960 | -2.8399122 |
| H | 2.0653454 | -0.9180865 | -2.6137796 |
| H | 1.0985636 | 0.0261499 | -3.7551276 |
| C | 0.1567695 | -1.7660047 | -3.1068710 |
| H | -0.8453073 | -1.4286553 | -3.4033959 |
| H | 0.5752800 | -2.3696986 | -3.9259928 |
| C | 3.1166826 | -2.8580754 | -0.4915521 |
| H | 3.7588897 | -2.2049341 | -1.0958180 |
| H | 2.4430158 | -3.4033272 | -1.1486910 |
| H | 3.7549493 | -3.5645037 | 0.0548540 |

C -0.7281978 -3.6978497 -2.0610496
 H -1.7443676 -3.4420825 -2.3870004
 H -0.7771296 -4.1760039 -1.0854231
 H -0.2921503 -4.3903520 -2.7927325
 C -0.0940308 -3.7148054 2.0622980
 H -0.0331013 -3.3011184 3.0767144
 H 0.9118480 -3.8670183 1.6781342
 H -0.6247165 -4.6744281 2.1087829
 C -2.6607197 -1.5460654 0.5658763
 H -2.7934137 -2.0945457 -0.3747427
 H -3.6536754 -1.2426419 0.9150566
 C -2.0525889 -2.4609444 1.6074776
 H -1.9995776 -1.9490551 2.5774646
 H -2.6747848 -3.3604644 1.7230207
 Li 0.1664040 -0.9179840 -0.0246362
 O 1.1649460 0.1817011 1.4153429
 O 0.5381216 0.1718682 -1.7474567
 O -1.8093602 -0.4324333 0.3587261
 O 2.3091308 -2.1055892 0.3984498
 O 0.0728497 -2.5377434 -1.9152074
 O -0.7431528 -2.8157528 1.1786638
 Si -0.6593039 2.7807586 0.1258670
 Si 0.6275572 1.8000254 1.8310631
 Si 0.5499371 1.9268426 -1.6999100
 Si -2.3988538 1.1999280 0.1033130

$[\text{Li}(\text{MeOCH}_2\text{CH}_2\text{OSiMe}_2)_3\text{SiH}]^+ [\text{Li-2-H}]^+$

C 1.8213095 2.4731613 3.0571727

| | | | |
|----|------------|------------|------------|
| Si | 1.7487364 | 1.6826084 | 1.3408020 |
| C | 3.4702028 | 1.7325650 | 0.5638485 |
| Si | 0.0015453 | 2.5513344 | 0.0056475 |
| Si | -2.0309752 | 1.6879576 | 0.8488169 |
| C | -2.2147624 | 1.7208916 | 2.7295775 |
| O | 1.2353077 | 0.0469475 | 1.4693261 |
| C | 1.8149973 | -0.8774771 | 2.3905796 |
| C | 0.7385631 | -1.7970488 | 2.9193043 |
| O | 0.0825991 | -2.4101744 | 1.8113415 |
| C | -0.8232989 | -3.4381293 | 2.2103582 |
| O | -1.8932254 | 0.0573915 | 0.3221686 |
| C | -2.9807891 | -0.8665778 | 0.3726522 |
| C | -2.9080528 | -1.7879016 | -0.8227796 |
| O | -1.6235114 | -2.4077546 | -0.8398996 |
| C | -1.5191702 | -3.4252578 | -1.8345883 |
| C | -3.5521129 | 2.4937313 | 0.0666012 |
| Si | 0.2831967 | 1.6833421 | -2.1756100 |
| C | 1.7202070 | 2.4903296 | -3.1025959 |
| O | 0.6711719 | 0.0510786 | -1.7995818 |
| C | 1.1871950 | -0.8626591 | -2.7680223 |
| C | 2.1755148 | -1.7915794 | -2.1018237 |
| O | 1.5303592 | -2.4232158 | -0.9976871 |
| C | 2.3258133 | -3.4534200 | -0.4127716 |
| C | -1.2564331 | 1.7192444 | -3.2704233 |
| Li | 0.0016053 | -1.1667624 | -0.0071144 |
| H | -2.2318960 | -4.2331445 | -1.6385347 |
| H | -0.5044344 | -3.8110436 | -1.7918577 |
| H | -1.7132607 | -3.0193177 | -2.8335127 |
| H | 3.2851969 | -3.0574623 | -0.0620610 |

H 2.5181432 -4.2522735 -1.1364168
H 1.7674087 -3.8479755 0.4315988
H -0.2911595 -4.2447008 2.7253224
H -1.2887102 -3.8220570 1.3068082
H -1.5958983 -3.0433620 2.8795960
H 1.6993275 -0.3425779 -3.5840865
H 0.3630770 -1.4378260 -3.2009679
H 2.5150605 -2.5430588 -2.8258554
H 3.0508800 -1.2328088 -1.7480716
H 0.8798834 2.3741345 3.6003855
H 2.0298296 3.5412334 2.9502422
H 2.6210213 2.0522110 3.6722314
H 4.2065632 1.2604922 1.2205543
H 3.7926769 2.7643220 0.4026433
H 3.4913200 1.2165252 -0.3970942
H -3.5488811 2.4166421 -1.0220876
H -3.5660424 3.5567809 0.3220498
H -4.4851550 2.0638248 0.4403520
H -1.0573656 1.2506320 -4.2386140
H -1.5665349 2.7489390 -3.4661636
H -2.0932191 1.1959420 -2.8053456
H -3.9491650 -0.3557506 0.3560168
H -2.9223835 -1.4462780 1.2989519
H 2.2808319 -0.3669626 3.2396908
H 2.5896917 -1.4592539 1.8818113
H -3.6970911 -2.5472182 -0.7475623
H -3.0589506 -1.2247186 -1.7521140
H 2.6656712 2.3982291 -2.5647894
H 1.5134566 3.5570371 -3.2248446

H 1.8513789 2.0739848 -4.1049351
 H 1.1945279 -2.5606111 3.5624741
 H 0.0094977 -1.2347420 3.5158122
 H -3.1556420 1.2555982 3.0376043
 H -2.2257626 2.7497834 3.0980552
 H -1.3973373 1.1935804 3.2240985
 H 0.0045238 4.0455693 0.0031252

[Na(MeOCH₂CH₂OSiMe₂)₃Si] (Na-2)

Na -0.0011619 -1.1119807 -0.0061828
 Si -0.0041744 2.8252784 0.0027447
 Si -2.0004568 1.7587392 0.6427387
 Si 1.5570954 1.7683392 1.4088576
 Si 0.4399141 1.7665872 -2.0504366
 O -2.0230739 0.0456935 0.2888345
 O 1.2858695 0.0494410 1.5856037
 O 0.7604353 0.0534666 -1.9010336
 O -1.9681139 -2.6064516 -0.5810191
 O 0.4812874 -2.5876915 1.9857317
 O 1.4695603 -2.5979781 -1.4162315
 C -2.4113142 1.8858114 2.5037844
 C -3.5145754 2.4809119 -0.2704669
 C 1.5094895 2.4697143 3.1853146
 C 3.3734869 1.9300484 0.8408647
 C -0.9706915 1.8984004 -3.3317188
 C 1.9856259 2.4943336 -2.9049775
 C -3.1216161 -0.8130827 0.5224891
 C -3.1895355 -1.8683683 -0.5624546

| | | | |
|---|------------|------------|------------|
| C | 2.0395276 | -0.8122384 | 2.4149201 |
| C | 1.1319101 | -1.8600432 | 3.0267036 |
| C | 1.1260130 | -0.7990487 | -2.9679249 |
| C | 2.0866787 | -1.8602384 | -2.4706983 |
| C | -1.9372020 | -3.5888127 | -1.6055749 |
| C | -0.4193257 | -3.5670020 | 2.4809114 |
| C | 2.3259332 | -3.5856109 | -0.8621493 |
| H | -3.3998061 | 1.4715944 | 2.7277778 |
| H | -2.4131620 | 2.9319417 | 2.8197924 |
| H | -1.6757878 | 1.3547569 | 3.1117159 |
| H | -3.4069743 | 2.4044003 | -1.3543845 |
| H | -3.6055980 | 3.5422856 | -0.0255184 |
| H | -4.4537008 | 1.9970478 | 0.0160353 |
| H | 0.5204038 | 2.3659211 | 3.6365845 |
| H | 1.7428230 | 3.5371367 | 3.1529130 |
| H | 2.2396091 | 1.9950105 | 3.8486011 |
| H | 4.0645320 | 1.5112772 | 1.5794293 |
| H | 3.6356164 | 2.9820184 | 0.7027060 |
| H | 3.5418439 | 1.4176340 | -0.1089425 |
| H | -0.6704670 | 1.4924901 | -4.3029265 |
| H | -1.2502779 | 2.9440636 | -3.4826693 |
| H | -1.8611700 | 1.3597496 | -3.0000195 |
| H | 2.8750400 | 2.4029343 | -2.2779038 |
| H | 1.8230089 | 3.5598220 | -3.0870098 |
| H | 2.1985756 | 2.0260146 | -3.8712853 |
| H | -4.0761045 | -0.2726132 | 0.5207451 |
| H | -3.0217666 | -1.3001922 | 1.5017502 |
| H | -4.0341043 | -2.5454220 | -0.3707048 |
| H | -3.3425267 | -1.3889256 | -1.5380424 |

H 2.5276330 -0.2744525 3.2368000
 H 2.8288687 -1.3052006 1.8315438
 H 1.7226741 -2.5455337 3.6511973
 H 0.3777385 -1.3748525 3.6598687
 H 1.6230232 -0.2549639 -3.7804361
 H 0.2347641 -1.2806179 -3.3916094
 H 2.3543687 -2.5362671 -3.2952708
 H 3.0036139 -1.3860099 -2.0974700
 H -2.6995721 -4.3596233 -1.4370901
 H -0.9477989 -4.0418010 -1.5905727
 H -2.1048932 -3.1380703 -2.5913255
 H 0.1122090 -4.3478905 3.0390489
 H -0.9223635 -4.0077154 1.6221918
 H -1.1717627 -3.1157912 3.1394876
 H 2.5730660 -4.3551412 -1.6040242
 H 1.7988730 -4.0389580 -0.0249231
 H 3.2579665 -3.1401671 -0.4936074

[Na(MeOCH2CH2OSiMe2)3SiH]+ [Na-2-H]+

C 1.5825339 2.5898558 3.1941192
 Si 1.6827020 1.7769396 1.4903151
 C 3.4429100 1.9445176 0.8223576
 Si 0.0003978 2.5473703 0.0042112
 Si -2.1301011 1.7770578 0.7113896
 C -2.4294388 1.9138714 2.5726613
 O 1.2851218 0.1125714 1.6198529
 C 2.0029448 -0.8070826 2.4452792
 C 1.0523465 -1.8185223 3.0468724

| | | | |
|----|------------|------------|------------|
| O | 0.3737220 | -2.5079908 | 1.9994142 |
| C | -0.4734966 | -3.5490136 | 2.4829471 |
| O | -2.0556658 | 0.1185887 | 0.2767680 |
| C | -3.1312775 | -0.7982462 | 0.4906377 |
| C | -3.1756846 | -1.8179623 | -0.6257919 |
| O | -1.9318815 | -2.5132219 | -0.6780875 |
| C | -1.9189678 | -3.5457097 | -1.6628664 |
| C | -3.5502620 | 2.6151381 | -0.2120370 |
| Si | 0.4509909 | 1.7775940 | -2.1954118 |
| C | 1.9552292 | 2.6222084 | -2.9682313 |
| O | 0.7993629 | 0.1206176 | -1.9140020 |
| C | 1.1752288 | -0.7877958 | -2.9518071 |
| C | 2.1442742 | -1.8186982 | -2.4164553 |
| O | 1.5346456 | -2.5231124 | -1.3373472 |
| C | 2.3505278 | -3.5817581 | -0.8386304 |
| C | -1.0178699 | 1.9085923 | -3.3779961 |
| Na | -0.0031938 | -1.1891709 | -0.0067992 |
| H | -2.6500504 | -4.3243273 | -1.4216374 |
| H | -0.9181730 | -3.9721040 | -1.6688897 |
| H | -2.1442718 | -3.1434969 | -2.6569563 |
| H | 3.3265431 | -3.2058383 | -0.5120449 |
| H | 2.5047677 | -4.3491978 | -1.6043823 |
| H | 1.8316477 | -4.0143883 | 0.0139408 |
| H | 0.1117163 | -4.3310861 | 2.9779424 |
| H | -0.9905456 | -3.9684614 | 1.6225125 |
| H | -1.2124900 | -3.1579767 | 3.1914773 |
| H | 1.6616247 | -0.2691717 | -3.7849933 |
| H | 0.2807796 | -1.2848135 | -3.3422009 |
| H | 2.4067504 | -2.5148455 | -3.2235133 |

H 3.0639211 -1.3313763 -2.0683576
H 0.6029251 2.4598005 3.6574825
H 1.7665013 3.6634414 3.1005499
H 2.3386609 2.1923532 3.8767160
H 4.1727651 1.5550842 1.5378263
H 3.6902540 2.9946650 0.6470273
H 3.5691251 1.4058347 -0.1183856
H -3.4587896 2.5062567 -1.2939399
H -3.5581668 3.6843051 0.0157280
H -4.5217471 2.2151143 0.0911728
H -0.7567503 1.5287905 -4.3697900
H -1.3224881 2.9511838 -3.4998470
H -1.8789429 1.3449246 -3.0143915
H -4.0989870 -0.2857708 0.5181907
H -2.9922256 -1.3041932 1.4521419
H 2.5173852 -0.2969935 3.2666885
H 2.7605526 -1.3199344 1.8429390
H -3.9961117 -2.5220764 -0.4357609
H -3.3630907 -1.3212778 -1.5863865
H 2.8508387 2.5074401 -2.3554326
H 1.7614694 3.6926642 -3.0766015
H 2.1717919 2.2324273 -3.9666550
H 1.6248193 -2.5276061 3.6590196
H 0.3216852 -1.3161185 3.6935872
H -3.4155982 1.5239788 2.8408450
H -2.3969150 2.9588846 2.8908791
H -1.6798892 1.3629407 3.1434839
H 0.0001146 4.0440244 0.0032249

[K(MeOCH₂CH₂OSiMe₂)₃Si] (K-2)

| | | | |
|----|------------|------------|------------|
| C | 1.7457347 | 2.7964673 | 3.1125845 |
| Si | 1.7026038 | 1.9806623 | 1.3868349 |
| C | 3.4546096 | 2.1913244 | 0.6541531 |
| Si | 0.0289839 | 2.9265519 | 0.0356035 |
| Si | -2.0024788 | 2.0216524 | 0.7935656 |
| C | -2.2481659 | 2.2102600 | 2.6790895 |
| O | 1.5435046 | 0.2701307 | 1.7069144 |
| C | 2.4898740 | -0.4951517 | 2.4242160 |
| C | 1.8147466 | -1.6386865 | 3.1534473 |
| O | 1.2048809 | -2.5301515 | 2.2182152 |
| C | 0.5821076 | -3.6357551 | 2.8518078 |
| O | -2.2433674 | 0.3215799 | 0.4680311 |
| C | -3.3699371 | -0.4143352 | 0.8986195 |
| C | -3.6644370 | -1.5522504 | -0.0563807 |
| O | -2.5716112 | -2.4720730 | -0.0821763 |
| C | -2.8211849 | -3.5852200 | -0.9241224 |
| C | -3.4925428 | 2.8899076 | -0.0263433 |
| Si | 0.3640345 | 2.0287401 | -2.1096455 |
| C | 1.8311528 | 2.8760684 | -2.9904342 |
| O | 0.7340118 | 0.3215780 | -2.1681349 |
| C | 0.8957252 | -0.4091620 | -3.3663273 |
| C | 1.8300171 | -1.5832512 | -3.1584715 |
| O | 1.2767792 | -2.4935665 | -2.2055277 |
| C | 2.0888587 | -3.6407919 | -2.0174937 |
| C | -1.1451092 | 2.2512265 | -3.2601794 |
| K | -0.0106977 | -1.1444369 | -0.0062832 |
| H | -3.6885712 | -4.1603050 | -0.5761034 |

H -1.9391120 -4.2244477 -0.8952874
H -2.9997272 -3.2729923 -1.9606552
H 3.0890198 -3.3698966 -1.6570568
H 2.1933106 -4.2110824 -2.9489869
H 1.6033291 -4.2698203 -1.2714529
H 1.3112980 -4.2371456 3.4091987
H 0.1368567 -4.2541412 2.0724968
H -0.2063799 -3.3109802 3.5418023
H 1.3261334 0.2065195 -4.1675762
H -0.0736824 -0.7802403 -3.7253318
H 1.9778699 -2.1000754 -4.1178397
H 2.8049918 -1.2257610 -2.8026164
H 0.7889288 2.6911981 3.6284325
H 1.9459161 3.8654520 3.0051223
H 2.5269416 2.3764183 3.7541523
H 4.2298709 1.8642686 1.3542638
H 3.6424746 3.2424548 0.4218701
H 3.5698043 1.6207209 -0.2703312
H -3.4576669 2.8007461 -1.1142898
H -3.4718511 3.9551108 0.2165874
H -4.4523899 2.4915915 0.3178715
H -0.9179764 1.9487617 -4.2872822
H -1.4495962 3.3002488 -3.2844651
H -1.9999146 1.6646989 -2.9149874
H -4.2733368 0.2080064 0.9469863
H -3.2015425 -0.8231486 1.9043859
H 3.0143591 0.1038983 3.1800508
H 3.2516457 -0.9009145 1.7443226
H -4.5755472 -2.0734181 0.2718639

H -3.8361280 -1.1560290 -1.0657670
 H 2.7575647 2.7634715 -2.4230068
 H 1.6302461 3.9463568 -3.0815144
 H 1.9992983 2.4844408 -3.9989749
 H 2.5644424 -2.1828838 3.7460409
 H 1.0513871 -1.2445517 3.8372019
 H -3.2511892 1.9022120 2.9903168
 H -2.1172295 3.2549039 2.9714406
 H -1.5219408 1.6150362 3.2375560

[K(MeOCH₂CH₂OSiMe₂)₃SiH]⁺ [K-2-H]⁺

C 3.0493185 2.7460328 1.7913396
 Si 2.2699892 1.7809809 0.3645641
 C 3.3441419 1.9644440 -1.1812061
 Si 0.0099417 2.4264661 -0.0008078
 Si -1.4376496 1.7872518 1.7755081
 C -0.6250616 1.9406566 3.4764030
 O 2.1680874 0.1228746 0.7824006
 C 3.3238415 -0.6844002 1.0176147
 C 3.0450685 -1.7504567 2.0540446
 O 2.0367993 -2.6429528 1.5830995
 C 1.8567196 -3.7648809 2.4441126
 O -1.7769169 0.1372127 1.4639251
 C -2.5899718 -0.6567808 2.3315176
 C -3.3150003 -1.7386089 1.5621981
 O -2.3774080 -2.6419364 0.9805175
 C -3.0080685 -3.7656714 0.3709418
 C -3.0467543 2.7792044 1.7547422

| | | | |
|----|------------|------------|------------|
| Si | -0.8104229 | 1.7740497 | -2.1354540 |
| C | 0.0373039 | 2.7252805 | -3.5321577 |
| O | -0.4084906 | 0.1126815 | -2.2483643 |
| C | -0.7914005 | -0.6949536 | -3.3639339 |
| C | 0.2350398 | -1.7717163 | -3.6369860 |
| O | 0.3194975 | -2.6653241 | -2.5288221 |
| C | 1.1427557 | -3.7958634 | -2.8039863 |
| C | -2.6857207 | 1.9679974 | -2.2881484 |
| K | 0.0026504 | -1.5148434 | 0.0160228 |
| H | -3.5694628 | -4.3484495 | 1.1090328 |
| H | -2.2235359 | -4.3918509 | -0.0521939 |
| H | -3.6889693 | -3.4542172 | -0.4291143 |
| H | 2.1665950 | -3.4916072 | -3.0492226 |
| H | 0.7380676 | -4.3832002 | -3.6352457 |
| H | 1.1599183 | -4.4143018 | -1.9077467 |
| H | 2.7737289 | -4.3599183 | 2.5104059 |
| H | 1.0644318 | -4.3799727 | 2.0192271 |
| H | 1.5633934 | -3.4490476 | 3.4514576 |
| H | -0.8883195 | -0.0954568 | -4.2763886 |
| H | -1.7642236 | -1.1585509 | -3.1655678 |
| H | -0.0710611 | -2.3216129 | -4.5371937 |
| H | 1.2170987 | -1.3203837 | -3.8283829 |
| H | 2.4962460 | 2.6154049 | 2.7230648 |
| H | 3.0622046 | 3.8135315 | 1.5567120 |
| H | 4.0850713 | 2.4408488 | 1.9644149 |
| H | 4.3784549 | 1.6729984 | -0.9788250 |
| H | 3.3597223 | 3.0047918 | -1.5157902 |
| H | 2.9730773 | 1.3509499 | -2.0045520 |
| H | -3.5841450 | 2.6667789 | 0.8116312 |

H -2.8303268 3.8417086 1.8923143
 H -3.7148078 2.4777128 2.5660682
 H -3.0341468 1.6673263 -3.2800994
 H -2.9751976 3.0121674 -2.1451879
 H -3.2144643 1.3669390 -1.5456563
 H -3.3495217 -0.0471343 2.8341036
 H -1.9642972 -1.1150796 3.1053659
 H 4.1635520 -0.0826109 1.3844248
 H 3.6378458 -1.1577132 0.0808514
 H -3.9707733 -2.2787034 2.2582910
 H -3.9406433 -1.2929321 0.7780771
 H 1.1205492 2.5929759 -3.5171668
 H -0.1708976 3.7940299 -3.4358138
 H -0.3302951 2.4119802 -4.5132580
 H 3.9756083 -2.3034620 2.2405103
 H 2.7247311 -1.2890324 2.9970017
 H -1.3160412 1.6458552 4.2712293
 H -0.3317073 2.9755698 3.6703236
 H 0.2674199 1.3166607 3.5529166
 H 0.0116765 3.9261285 -0.0043645

[Li(MeOCH₂CH₂OSiMe₂)₃Ge] (Li-3)

C 3.2586258 2.1932548 1.3962541
 Si 2.0638961 1.5253312 0.0619158
 C 3.0847571 1.5039083 -1.5523606
 Ge 0.0067531 2.7991324 -0.0022651
 Si -1.0871197 1.5426905 1.7534421
 C -0.2022147 1.5248268 3.4462457

| | | | |
|----|------------|------------|------------|
| O | 1.7977817 | -0.1627963 | 0.4614097 |
| C | 2.8424580 | -1.0525628 | 0.8190755 |
| C | 2.3598605 | -1.9966095 | 1.8991818 |
| O | 1.1996719 | -2.6686369 | 1.4227988 |
| C | 0.6852439 | -3.6108145 | 2.3487288 |
| O | -1.3089406 | -0.1459837 | 1.3293365 |
| C | -2.1396906 | -1.0325907 | 2.0600014 |
| C | -2.8234887 | -1.9886105 | 1.1070396 |
| O | -1.8240252 | -2.6563204 | 0.3452571 |
| C | -2.3600002 | -3.6133900 | -0.5526826 |
| C | -2.8367187 | 2.2226236 | 2.1155484 |
| Si | -0.9757876 | 1.5402965 | -1.8211167 |
| C | -0.4069957 | 2.2070491 | -3.5198917 |
| O | -0.5098713 | -0.1513146 | -1.7931436 |
| C | -0.7182906 | -1.0380947 | -2.8797417 |
| C | 0.4577643 | -1.9836508 | -2.9985066 |
| O | 0.6170888 | -2.6602247 | -1.7571085 |
| C | 1.6664968 | -3.6131586 | -1.7743754 |
| C | -2.8842032 | 1.5368928 | -1.9044842 |
| Li | -0.0099401 | -1.0796409 | -0.0003387 |
| H | -2.8654342 | -4.4228474 | -0.0104928 |
| H | -1.5264679 | -4.0162890 | -1.1233576 |
| H | -3.0800702 | -3.1540990 | -1.2418625 |
| H | 2.6232585 | -3.1485174 | -2.0438151 |
| H | 1.4565587 | -4.4177378 | -2.4908246 |
| H | 1.7392993 | -4.0242631 | -0.7701031 |
| H | 1.4055884 | -4.4187620 | 2.5304427 |
| H | -0.2244912 | -4.0192024 | 1.9148040 |
| H | 0.4449062 | -3.1366587 | 3.3087094 |

H -0.8200564 -0.5019041 -3.8293320
H -1.6385822 -1.6130991 -2.7225245
H 0.2734480 -2.7062048 -3.8067418
H 1.3720533 -1.4239709 -3.2366208
H 2.8362964 2.1198265 2.4008187
H 3.4328694 3.2539426 1.1957999
H 4.2348008 1.6986298 1.3939501
H 4.0359538 0.9781988 -1.4209968
H 3.3124482 2.5255300 -1.8680013
H 2.5376161 1.0188767 -2.3631063
H -3.4903221 2.1589861 1.2429513
H -2.7431522 3.2809233 2.3737192
H -3.3320826 1.7265666 2.9559492
H -3.2462373 1.0159195 -2.7968473
H -3.2612071 2.5623089 -1.9453214
H -3.3226624 1.0560736 -1.0279731
H -2.9149240 -0.4972134 2.6186355
H -1.5402192 -1.5982114 2.7831473
H 3.7191534 -0.5186962 1.2015025
H 3.1611328 -1.6283244 -0.0579795
H -3.4208226 -2.7166925 1.6751997
H -3.4958147 -1.4383248 0.4357348
H 0.6744292 2.1285693 -3.6511980
H -0.6632321 3.2687225 -3.5711815
H -0.8950083 1.7154850 -4.3673192
H 3.1504370 -2.7222640 2.1392589
H 2.1158846 -1.4361382 2.8114636
H -0.7983400 1.0087006 4.2056134
H -0.0362083 2.5474774 3.7950198

H 0.7699105 1.0320321 3.3838352

[Li(MeOCH₂CH₂OSiMe₂)₃GeH]⁺ [Li-3-H]⁺

C -2.6678060 -2.1926094 -2.4001666
Si -0.9897077 -1.4205118 -1.9985104
C 0.1052478 -1.4727870 -3.5371181
Ge 0.0012097 -2.3203618 -0.0006957
Si -1.2344398 -1.4318925 1.8612221
C -3.1139127 -1.5064566 1.6859282
O -1.2032303 0.2143339 -1.5088783
C -1.9703379 1.1470209 -2.2719754
C -2.7124874 2.0736740 -1.3366338
O -1.7684567 2.6863785 -0.4606346
C -2.3495492 3.7136935 0.3400290
O -0.7196638 0.2066968 1.7950583
C -0.9900154 1.1403581 2.8413572
C 0.1930380 2.0664804 3.0071315
O 0.4757312 2.6725019 1.7470803
C 1.4510874 3.7093733 1.8434209
C -0.7298315 -2.1948424 3.5153449
Si 2.2329467 -1.4384008 0.1435542
C 3.4168968 -2.2010153 -1.1174861
O 1.9152609 0.1989181 -0.2714812
C 2.9545398 1.1355215 -0.5589718
C 2.5095524 2.0556597 -1.6728918
O 1.2737653 2.6609135 -1.2971313
C 0.8727396 3.6923965 -2.1975563
C 3.0205741 -1.5093516 1.8591828

| | | | |
|----|------------|------------|------------|
| Li | -0.0056245 | 1.4157165 | 0.0016479 |
| H | 1.0893228 | 4.5232163 | 2.4804886 |
| H | 1.6239476 | 4.0792412 | 0.8365689 |
| H | 2.3905809 | 3.3281463 | 2.2584077 |
| H | 0.7679656 | 3.3056030 | -3.2173269 |
| H | 1.6048017 | 4.5069513 | -2.2043247 |
| H | -0.0874395 | 4.0635277 | -1.8504515 |
| H | -2.7280713 | 4.5271165 | -0.2879514 |
| H | -1.5678273 | 4.0885353 | 0.9952753 |
| H | -3.1752952 | 3.3222612 | 0.9448142 |
| H | 3.8761889 | 0.6356743 | -0.8747545 |
| H | 3.1781447 | 1.7161677 | 0.3411835 |
| H | 3.2756422 | 2.8240960 | -1.8364534 |
| H | 2.3780459 | 1.4959108 | -2.6074392 |
| H | -3.3733926 | -2.0984419 | -1.5729335 |
| H | -2.5352165 | -3.2589975 | -2.6014698 |
| H | -3.1220112 | -1.7530237 | -3.2921012 |
| H | -0.3924581 | -0.9980091 | -4.3875204 |
| H | 0.3193579 | -2.5065285 | -3.8203434 |
| H | 1.0564108 | -0.9637825 | -3.3729476 |
| H | 0.3370567 | -2.0801575 | 3.7148153 |
| H | -0.9491869 | -3.2658157 | 3.5003977 |
| H | -1.2854597 | -1.7669804 | 4.3540156 |
| H | 4.0080771 | -1.0391183 | 1.8549253 |
| H | 3.1544895 | -2.5463527 | 2.1776963 |
| H | 2.4068376 | -1.0030699 | 2.6059540 |
| H | -1.1697310 | 0.6382608 | 3.7975987 |
| H | -1.8854664 | 1.7165855 | 2.5899336 |
| H | -2.7044830 | 0.6428862 | -2.9089779 |

H -1.3020104 1.7226527 -2.9190565
 H -0.0482600 2.8340854 3.7531269
 H 1.0727952 1.5111618 3.3557104
 H 3.0607966 -2.0846252 -2.1425417
 H 3.5114338 -3.2723747 -0.9210334
 H 4.4211342 -1.7741771 -1.0509865
 H -3.2393159 2.8368331 -1.9237464
 H -3.4543152 1.5169987 -0.7505254
 H -3.6061424 -1.0370967 2.5426444
 H -3.4534383 -2.5445835 1.6438487
 H -3.4546614 -1.0027841 0.7800667
 H -0.0073474 -3.8641339 -0.0063682

[Na(MeOCH₂CH₂OSiMe₂)₃Ge] (Na-3)

C 3.1961143 2.3302007 1.5778812
 Si 2.1187202 1.5939872 0.1816708
 C 3.2024716 1.6593554 -1.3904110
 Ge 0.0040869 2.7583262 -0.0038525
 Si -1.2187419 1.6079409 1.7397049
 C -0.3978993 1.6865183 3.4630912
 O 1.9652753 -0.1064152 0.5621003
 C 3.0439748 -0.9742229 0.8511672
 C 2.6126306 -2.0080156 1.8713522
 O 1.4998912 -2.7416798 1.3611447
 C 1.0198420 -3.7153838 2.2759418
 O -1.4725091 -0.0947778 1.4302674
 C -2.2532603 -0.9594390 2.2316434
 C -2.9312827 -1.9968350 1.3599171

| | | | |
|----|------------|------------|------------|
| O | -1.9417988 | -2.7288038 | 0.6373132 |
| C | -2.5034041 | -3.7133883 | -0.2175015 |
| C | -2.9673495 | 2.3447720 | 1.9665618 |
| Si | -0.8976516 | 1.6072677 | -1.9329008 |
| C | -0.2208350 | 2.3459035 | -3.5601714 |
| O | -0.4959092 | -0.0935787 | -1.9937916 |
| C | -0.7780839 | -0.9552709 | -3.0789162 |
| C | 0.3206100 | -1.9900410 | -3.2122235 |
| O | 0.4215191 | -2.7330454 | -1.9974665 |
| C | 1.4479901 | -3.7132452 | -2.0394025 |
| C | -2.8008114 | 1.6802064 | -2.0891181 |
| Na | -0.0088847 | -1.2514085 | -0.0040577 |
| H | -3.0183000 | -4.4908692 | 0.3604986 |
| H | -1.6851609 | -4.1568194 | -0.7820567 |
| H | -3.2179422 | -3.2671389 | -0.9203547 |
| H | 2.4198708 | -3.2594078 | -2.2688926 |
| H | 1.2310720 | -4.4793846 | -2.7940174 |
| H | 1.4987584 | -4.1722880 | -1.0539923 |
| H | 1.7780173 | -4.4850214 | 2.4668406 |
| H | 0.1377034 | -4.1714198 | 1.8311182 |
| H | 0.7370274 | -3.2562571 | 3.2311659 |
| H | -0.8408866 | -0.4129809 | -4.0302173 |
| H | -1.7404714 | -1.4608442 | -2.9235855 |
| H | 0.0943200 | -2.6674913 | -4.0478048 |
| H | 1.2774048 | -1.4921675 | -3.4165221 |
| H | 2.7077386 | 2.2466910 | 2.5514651 |
| H | 3.3511910 | 3.3944030 | 1.3810822 |
| H | 4.1837991 | 1.8631580 | 1.6470206 |
| H | 4.1894572 | 1.2170672 | -1.2207867 |

H 3.3537115 2.6964252 -1.7012238
 H 2.7300102 1.1291539 -2.2201691
 H -3.5621117 2.2563195 1.0547768
 H -2.8770292 3.4096067 2.1965911
 H -3.5238532 1.8792122 2.7863328
 H -3.1469069 1.2408674 -3.0304526
 H -3.1412202 2.7186798 -2.0646616
 H -3.2880553 1.1511846 -1.2671711
 H -3.0371829 -0.4198440 2.7766701
 H -1.6215973 -1.4621232 2.9760052
 H 3.9056103 -0.4369688 1.2662362
 H 3.3811656 -1.4801153 -0.0630632
 H -3.5205857 -2.6811091 1.9870940
 H -3.6091248 -1.5025675 0.6520332
 H 0.8668347 2.2625434 -3.6179300
 H -0.4688500 3.4100301 -3.5954555
 H -0.6497785 1.8811085 -4.4536814
 H 3.4469468 -2.6917052 2.0842014
 H 2.3238577 -1.5095627 2.8056313
 H -1.0372062 1.2501248 4.2374728
 H -0.2036607 2.7253921 3.7419106
 H 0.5563874 1.1554693 3.4703583



C 3.1618686 -2.3508250 1.7072016
 Si 1.4609774 -1.5289633 1.7463720
 C 0.7299321 -1.6676220 3.4830815
 Ge -0.0003658 -2.3194310 -0.0033348

| | | | |
|----|------------|------------|------------|
| Si | 0.7777916 | -1.5267895 | -2.1455840 |
| C | 2.6497290 | -1.6377032 | -2.3798839 |
| O | 1.6076262 | 0.1289759 | 1.3281894 |
| C | 2.4142071 | 1.0555929 | 2.0589259 |
| C | 3.0274562 | 2.0681405 | 1.1171381 |
| O | 1.9896173 | 2.7496815 | 0.4162807 |
| C | 2.4843177 | 3.7941818 | -0.4200780 |
| O | 0.3195468 | 0.1254542 | -2.0705775 |
| C | 0.5436503 | 1.0500247 | -3.1377249 |
| C | -0.5692727 | 2.0734952 | -3.1826111 |
| O | -0.6284468 | 2.7618392 | -1.9353175 |
| C | -1.5996176 | 3.8073001 | -1.9289489 |
| C | -0.0951729 | -2.3683799 | -3.5944614 |
| Si | -2.2430544 | -1.5208818 | 0.3925829 |
| C | -3.0701131 | -2.3690173 | 1.8643927 |
| O | -1.9460086 | 0.1283797 | 0.7633590 |
| C | -2.9810847 | 1.0465685 | 1.1239200 |
| C | -2.4498798 | 2.0736747 | 2.0991918 |
| O | -1.3559847 | 2.7670214 | 1.5035608 |
| C | -0.8628538 | 3.8268647 | 2.3210816 |
| C | -3.3764721 | -1.6216040 | -1.1158603 |
| Na | -0.0026302 | 1.4188363 | -0.0045066 |
| H | -1.3381785 | 4.5869583 | -2.6519779 |
| H | -1.6133408 | 4.2273519 | -0.9255995 |
| H | -2.5958669 | 3.4198223 | -2.1699012 |
| H | -0.5548985 | 3.4548497 | 3.3046046 |
| H | -1.6253010 | 4.6008899 | 2.4580461 |
| H | 0.0014026 | 4.2494770 | 1.8134813 |
| H | 2.9618157 | 4.5788210 | 0.1762416 |

| | | | |
|---|------------|------------|------------|
| H | 1.6324183 | 4.2081778 | -0.9553142 |
| H | 3.2108958 | 3.4078163 | -1.1437704 |
| H | -3.8249579 | 0.5351693 | 1.5993940 |
| H | -3.3548683 | 1.5463306 | 0.2239388 |
| H | -3.2541078 | 2.7776654 | 2.3492036 |
| H | -2.1194321 | 1.5845898 | 3.0244803 |
| H | 3.6549596 | -2.2297729 | 0.7411322 |
| H | 3.0554462 | -3.4225634 | 1.8947426 |
| H | 3.8230593 | -1.9524792 | 2.4817032 |
| H | 1.4162082 | -1.2612853 | 4.2316399 |
| H | 0.5490895 | -2.7137543 | 3.7426907 |
| H | -0.2167376 | -1.1305949 | 3.5631479 |
| H | -1.1801564 | -2.2674813 | -3.5337557 |
| H | 0.1402342 | -3.4359297 | -3.5951636 |
| H | 0.2333233 | -1.9658526 | -4.5566768 |
| H | -4.3678797 | -1.2186321 | -0.8898582 |
| H | -3.5112160 | -2.6611065 | -1.4253585 |
| H | -2.9687939 | -1.0665044 | -1.9625796 |
| H | 0.5755030 | 0.5443895 | -4.1089674 |
| H | 1.5056754 | 1.5520619 | -2.9887302 |
| H | 3.2293783 | 0.5513754 | 2.5889523 |
| H | 1.7955737 | 1.5666487 | 2.8044712 |
| H | -0.3708481 | 2.7817618 | -3.9973814 |
| H | -1.5302399 | 1.5814876 | -3.3800995 |
| H | -2.4871084 | -2.2622037 | 2.7808308 |
| H | -3.1744862 | -3.4377580 | 1.6596341 |
| H | -4.0742088 | -1.9772915 | 2.0491427 |
| H | 3.6241016 | 2.7823874 | 1.6995566 |
| H | 3.6913912 | 1.5680111 | 0.4005547 |

H 2.9496540 -1.2312371 -3.3501935
 H 2.9795317 -2.6790977 -2.3480070
 H 3.1849406 -1.0897048 -1.6022563
 H -0.0051048 -3.8662526 -0.0026728

[K(MeOCH₂CH₂OSiMe₂)₃Ge] (K-3)

C 3.0230111 2.5127848 1.8790692
 Si 2.1598780 1.6564346 0.4056268
 C 3.3526401 1.8281223 -1.0781993
 Ge 0.0007773 2.6643154 -0.0020034
 Si -1.4309029 1.6606811 1.6673514
 C -0.7488452 1.8721259 3.4400824
 O 2.1721257 -0.0443224 0.8059491
 C 3.3531736 -0.7923831 1.0149346
 C 3.0948510 -1.9559852 1.9493830
 O 2.1476353 -2.8554136 1.3699610
 C 1.9211673 -3.9979297 2.1788838
 O -1.7536711 -0.0476668 1.4995286
 C -2.5084640 -0.8062560 2.4228158
 C -3.2124474 -1.9532743 1.7269833
 O -2.2553751 -2.8506926 1.1617486
 C -2.8645104 -3.9592660 0.5201249
 C -3.1519678 2.4892760 1.6585651
 Si -0.7304937 1.6569506 -2.0729826
 C 0.1555328 2.4625789 -3.5612636
 O -0.4418135 -0.0557984 -2.2567469
 C -0.8731361 -0.8161214 -3.3671267
 C 0.0808608 -1.9609062 -3.6375829

O 0.1123096 -2.8520946 -2.5216340
C 0.9576079 -3.9683371 -2.7449288
C -2.6027428 1.8886634 -2.3798806
K 0.0063116 -1.4744836 0.0099064
H -3.4504279 -4.5570182 1.2296387
H -2.0684590 -4.5799456 0.1091466
H -3.5227459 -3.6382961 -0.2965799
H 1.9918141 -3.6565091 -2.9371480
H 0.6075839 -4.5677139 -3.5948327
H 0.9360131 -4.5838328 -1.8459709
H 2.8428467 -4.5772207 2.3161624
H 1.1850918 -4.6205341 1.6706476
H 1.5305208 -3.7202030 3.1657832
H -0.9229372 -0.2140130 -4.2839607
H -1.8788246 -1.2200055 -3.1874772
H -0.2520857 -2.5052183 -4.5334005
H 1.0893047 -1.5692057 -3.8245977
H 2.4404476 2.4075230 2.7971910
H 3.1185090 3.5816909 1.6722937
H 4.0285421 2.1217800 2.0658139
H 4.3692460 1.5131336 -0.8222436
H 3.4011793 2.8705414 -1.4024960
H 3.0162868 1.2315489 -1.9297851
H -3.6491107 2.3655199 0.6938973
H -3.0391317 3.5621337 1.8341520
H -3.8132911 2.0946447 2.4365997
H -2.8974713 1.5656049 -3.3832817
H -2.8680789 2.9440643 -2.2804286
H -3.1961977 1.3278804 -1.6539308

| | | | |
|---|------------|------------|------------|
| H | -3.2833324 | -0.2025254 | 2.9130010 |
| H | -1.8594718 | -1.2073693 | 3.2132503 |
| H | 4.1474168 | -0.1852600 | 1.4695307 |
| H | 3.7400719 | -1.1762387 | 0.0614221 |
| H | -3.8363996 | -2.4905754 | 2.4560065 |
| H | -3.8636464 | -1.5629835 | 0.9338769 |
| H | 1.2383377 | 2.3357875 | -3.4944373 |
| H | -0.0492026 | 3.5360551 | -3.5722759 |
| H | -0.1773326 | 2.0532826 | -4.5206043 |
| H | 4.0406744 | -2.4864007 | 2.1330241 |
| H | 2.7121373 | -1.5865175 | 2.9095497 |
| H | -1.4685195 | 1.5474205 | 4.1984761 |
| H | -0.5203777 | 2.9238312 | 3.6305569 |
| H | 0.1730797 | 1.3025567 | 3.5799329 |

[K(MeOCH₂CH₂OSiMe₂)₃GeH]⁺ [K-3-H]⁺

| | | | |
|----|------------|------------|------------|
| C | 1.9790045 | 2.5752216 | 2.9624143 |
| Si | 1.8976409 | 1.5951007 | 1.3488119 |
| C | 3.5411138 | 1.7441591 | 0.4260746 |
| Ge | 0.0000934 | 2.2458153 | -0.0029012 |
| Si | -2.1062056 | 1.5760544 | 0.9806749 |
| C | -2.1110670 | 1.7383782 | 2.8645987 |
| O | 1.5941859 | -0.0548013 | 1.6931981 |
| C | 2.4993667 | -0.8638974 | 2.4483240 |
| C | 1.7595607 | -1.9387793 | 3.2128002 |
| O | 1.1148034 | -2.8322198 | 2.3072602 |
| C | 0.5237544 | -3.9471883 | 2.9705190 |
| O | -2.2367442 | -0.0781603 | 0.5586255 |

| | | | |
|----|------------|------------|------------|
| C | -3.3182331 | -0.9063360 | 0.9916774 |
| C | -3.6478799 | -1.9578452 | -0.0445044 |
| O | -2.5393828 | -2.8367597 | -0.2245322 |
| C | -2.8488451 | -3.9333621 | -1.0809039 |
| C | -3.5637881 | 2.5350545 | 0.2546813 |
| Si | 0.2232574 | 1.5815819 | -2.3188335 |
| C | 1.5897890 | 2.5485789 | -3.1952817 |
| O | 0.6590528 | -0.0724453 | -2.2305263 |
| C | 0.8398549 | -0.8852747 | -3.3926976 |
| C | 1.8742037 | -1.9625173 | -3.1517110 |
| O | 1.4315563 | -2.8484120 | -2.1251669 |
| C | 2.2833043 | -3.9816299 | -1.9760983 |
| C | -1.3951832 | 1.7485802 | -3.2810818 |
| K | 0.0152551 | -1.6796712 | -0.0042820 |
| H | -3.6561025 | -4.5435360 | -0.6616288 |
| H | -1.9513866 | -4.5440132 | -1.1689219 |
| H | -3.1459416 | -3.5870992 | -2.0771912 |
| H | 3.3027594 | -3.6808079 | -1.7095288 |
| H | 2.3160421 | -4.5720850 | -2.8978332 |
| H | 1.8726622 | -4.5960550 | -1.1758577 |
| H | 1.2823929 | -4.5403128 | 3.4922160 |
| H | 0.0507045 | -4.5676540 | 2.2103769 |
| H | -0.2343784 | -3.6242801 | 3.6928856 |
| H | 1.1806234 | -0.2890170 | -4.2471020 |
| H | -0.1134426 | -1.3491609 | -3.6685367 |
| H | 2.0187473 | -2.5188802 | -4.0876110 |
| H | 2.8342397 | -1.5118689 | -2.8687156 |
| H | 1.0710856 | 2.4556088 | 3.5556654 |
| H | 2.0997781 | 3.6396267 | 2.7455306 |

H 2.8312504 2.2715509 3.5766169
H 4.3785264 1.4366394 1.0589927
H 3.7214220 2.7808140 0.1306107
H 3.5519268 1.1288824 -0.4757154
H -3.6340862 2.4124686 -0.8275733
H -3.4485875 3.6016824 0.4639415
H -4.5133491 2.2195412 0.6961642
H -1.2682297 1.4433996 -4.3234765
H -1.7311536 2.7885914 -3.2855601
H -2.1882912 1.1401589 -2.8419762
H -4.2271262 -0.3189007 1.1651208
H -3.0521070 -1.3941927 1.9360851
H 3.0546791 -0.2647203 3.1787754
H 3.2281264 -1.3287310 1.7748858
H -4.5218302 -2.5254159 0.3029954
H -3.9056683 -1.4815892 -0.9992795
H 2.5578563 2.4164876 -2.7085698
H 1.3548442 3.6159418 -3.1886633
H 1.6894294 2.2450925 -4.2411464
H 2.4841807 -2.4895985 3.8272294
H 1.0172089 -1.4847535 3.8822304
H -3.0713292 1.4278664 3.2859098
H -1.9478250 2.7782492 3.1588201
H -1.3266306 1.1317103 3.3215643
H -0.0067436 3.7970777 -0.0077105

[(MeOCH2CH2OSiMe2)3CH] (1-A)

| | | | |
|----|------------|------------|------------|
| C | 0.2122341 | 3.3292480 | 2.3880367 |
| Si | -0.3940611 | 2.1060616 | 1.0695136 |
| O | 0.7397753 | 2.0281479 | -0.1792761 |
| C | 1.0141696 | 3.1153568 | -1.0561565 |
| C | 2.3277641 | 2.9212911 | -1.7974775 |
| O | 2.3039200 | 1.8990581 | -2.7756805 |
| C | 2.6659733 | 0.6054824 | -2.3024448 |
| C | -2.0173434 | 2.8065544 | 0.3973275 |
| C | -0.5104324 | 0.3601046 | 1.8226213 |
| Si | -1.9559233 | -0.7067701 | 1.1895349 |
| C | -1.7962766 | -2.5617578 | 1.5224355 |
| Si | 1.1488632 | -0.5528601 | 2.0277336 |
| C | 1.1130738 | -1.5860663 | 3.6193145 |
| C | 2.6742552 | 0.5591858 | 2.1475716 |
| O | 1.3114048 | -1.5828337 | 0.7000407 |
| C | 2.4864529 | -2.3413676 | 0.4368210 |
| C | 2.2231977 | -3.4567144 | -0.5630776 |
| O | 1.9965670 | -3.0167070 | -1.8886329 |
| C | 0.6360970 | -2.7374276 | -2.2054453 |
| C | -3.5690635 | -0.1481240 | 2.0184228 |
| O | -2.0673486 | -0.4451878 | -0.4748156 |
| C | -2.9564543 | -1.1625607 | -1.3235290 |
| C | -3.1480766 | -0.4607362 | -2.6591811 |
| O | -2.0202567 | -0.5023107 | -3.5127679 |
| C | -1.1036101 | 0.5760828 | -3.3527225 |
| H | 0.0105179 | -3.6263397 | -2.0481977 |
| H | 0.6056245 | -2.4744843 | -3.2615433 |

H 0.2383531 -1.9110207 -1.6144217
H -0.6441464 0.5812533 -2.3630570
H -1.6036852 1.5392157 -3.5221078
H -0.3311771 0.4485453 -4.1094835
H 3.6772013 0.6178595 -1.8735096
H 2.6637825 -0.0586730 -3.1651938
H 1.9647618 0.2310305 -1.5549021
H -3.9484487 -1.2639268 -0.8594961
H -2.5680475 -2.1708536 -1.5087948
H -3.9529967 -0.9810497 -3.1885960
H -3.4700735 0.5757273 -2.4893418
H 1.1844278 3.0526217 2.7983367
H -0.5004562 3.3844970 3.2161896
H 0.2996765 4.3369567 1.9727488
H -1.8387987 3.7898107 -0.0474366
H -2.7489815 2.9457538 1.1969510
H -2.4526195 2.1582301 -0.3626388
H 0.3040876 -2.3180614 3.6246607
H 0.9883492 -0.9388003 4.4923547
H 2.0534072 -2.1278549 3.7536678
H -2.6506954 -3.0896292 1.0896353
H -1.7984598 -2.7719745 2.5946830
H -0.8829564 -2.9703716 1.0910811
H 2.8693052 -2.8068304 1.3568346
H 3.2732536 -1.6904110 0.0383003
H 1.0856399 4.0617534 -0.5001042
H 0.2077794 3.2185015 -1.7912321
H 3.1205662 -4.0834248 -0.5965320
H 1.3892310 -4.0794549 -0.2114396

| | | | |
|---|------------|------------|------------|
| H | -3.7953913 | 0.9014428 | 1.8259764 |
| H | -3.5107975 | -0.2885689 | 3.1018212 |
| H | -4.4152099 | -0.7429566 | 1.6637550 |
| H | 2.5423651 | 3.8531299 | -2.3311698 |
| H | 3.1381844 | 2.7511519 | -1.0759008 |
| H | 3.5755661 | -0.0558806 | 2.2213954 |
| H | 2.6380226 | 1.1817102 | 3.0451212 |
| H | 2.7698184 | 1.2097384 | 1.2787086 |
| H | -0.8018814 | 0.5664879 | 2.8647113 |

[(MeOCH₂CH₂OSiMe₂)₃CH] (1-B)

| | | | |
|----|------------|------------|------------|
| C | -0.6160180 | 0.7761917 | -0.8162385 |
| Si | -2.2484204 | -0.1678922 | -1.0234892 |
| Si | -0.0854548 | 0.9850491 | 1.0042499 |
| Si | 0.7836767 | 0.2155769 | -1.9722035 |
| C | -0.1781249 | -0.6163845 | 1.9992094 |
| C | -1.0865230 | 2.3542495 | 1.8380791 |
| C | -3.2038527 | 0.4217624 | -2.5477878 |
| C | -2.0456113 | -2.0465314 | -1.0720904 |
| C | 2.0806125 | 1.5639792 | -2.2267822 |
| C | 0.1982171 | -0.2777193 | -3.7109928 |
| O | -3.1705825 | 0.2290338 | 0.3424336 |
| C | -4.4781735 | -0.2652295 | 0.5916087 |
| O | 1.4377106 | -1.1477202 | -1.2226984 |
| C | 2.5734394 | -1.8585854 | -1.6870674 |
| O | 1.5309909 | 1.4946207 | 0.9585047 |
| C | 2.3072190 | 1.7550782 | 2.1161513 |
| C | -5.0011355 | 0.3735332 | 1.8672598 |

| | | | |
|---|------------|------------|------------|
| O | -6.3026162 | -0.1327959 | 2.1014566 |
| C | -6.8963890 | 0.3856748 | 3.2750388 |
| C | 2.7989862 | -3.0471345 | -0.7685394 |
| O | 3.9318958 | -3.7543455 | -1.2398524 |
| C | 4.2405388 | -4.8895089 | -0.4566521 |
| C | 3.6623694 | 2.2839533 | 1.6772827 |
| O | 4.4279690 | 2.5410596 | 2.8405306 |
| C | 5.7195895 | 3.0379666 | 2.5534569 |
| H | 0.2262356 | -0.4709248 | 3.0043526 |
| H | 0.3983967 | -1.4029599 | 1.5088789 |
| H | -1.2116080 | -0.9516055 | 2.1030817 |
| H | -0.7937557 | 2.4812940 | 2.8838979 |
| H | -0.9339045 | 3.3103608 | 1.3299170 |
| H | -2.1493094 | 2.1137037 | 1.8060660 |
| H | -4.1774125 | -0.0716569 | -2.6114222 |
| H | -3.3796826 | 1.4997333 | -2.5026804 |
| H | -2.6676943 | 0.2057138 | -3.4734182 |
| H | -3.0205639 | -2.5363338 | -1.1427628 |
| H | -1.5467555 | -2.4109753 | -0.1724695 |
| H | -1.4519185 | -2.3677260 | -1.9294392 |
| H | 2.8930956 | 1.2096791 | -2.8671721 |
| H | 2.4920007 | 1.8908644 | -1.2734141 |
| H | 1.6304072 | 2.4291561 | -2.7224124 |
| H | 1.0609263 | -0.5645933 | -4.3191220 |
| H | -0.4995454 | -1.1165735 | -3.7150402 |
| H | -0.2814948 | 0.5653344 | -4.2151171 |
| H | -4.4730696 | -1.3543905 | 0.7142192 |
| H | -5.1595861 | -0.0229942 | -0.2320056 |
| H | 2.4276809 | -2.2223250 | -2.7112603 |

H 3.4673260 -1.2245397 -1.6792701
 H 2.4549053 0.8442210 2.7079140
 H 1.8274644 2.5005434 2.7616643
 H -5.0207671 1.4666485 1.7535673
 H -4.3309129 0.1333584 2.7044075
 H -7.8856750 -0.0624620 3.3622170
 H -7.0025651 1.4776278 3.2248944
 H -6.3101135 0.1330907 4.1687519
 H 2.9578592 -2.6934940 0.2597586
 H 1.9073804 -3.6897765 -0.7707923
 H 5.1189297 -5.3589630 -0.8982335
 H 4.4676246 -4.6136097 0.5819705
 H 3.4140147 -5.6131314 -0.4518411
 H 3.5281330 3.2016594 1.0870660
 H 4.1602575 1.5411188 1.0380874
 H 6.2221775 3.2040761 3.5058097
 H 6.3051268 2.3215217 1.9615109
 H 5.6734786 3.9881052 2.0040938
 H -0.8499991 1.7988428 -1.1471244

[(MeOCH₂CH₂OSiMe₂)₃C]⁻ (1**⁻-A)**

C 2.4747882 2.8445139 1.3552195
 Si 1.9416991 1.7493069 -0.1302123
 O 3.1796276 2.0068667 -1.3116193
 C 3.7130373 3.2622886 -1.6493475
 C 4.6999268 3.1500010 -2.8040285
 O 4.1162458 2.9356843 -4.0827077
 C 3.7115452 1.5940926 -4.3326835

| | | | |
|----|------------|------------|------------|
| C | 0.3990044 | 2.6359425 | -0.8296545 |
| C | 1.7449529 | -0.0153263 | 0.2083492 |
| Si | 0.1617225 | -0.8230479 | -0.1201599 |
| C | 0.1227730 | -2.7115812 | 0.1717993 |
| Si | 3.1659651 | -0.9945265 | 0.7466855 |
| C | 2.9780466 | -1.9109571 | 2.4245822 |
| C | 4.8095399 | -0.0348306 | 0.9251914 |
| O | 3.5024236 | -2.2544464 | -0.3909632 |
| C | 4.4083230 | -3.3062986 | -0.1746664 |
| C | 4.5633616 | -4.1657174 | -1.4224644 |
| O | 5.3274615 | -3.5819931 | -2.4701548 |
| C | 4.6258564 | -2.6199505 | -3.2500052 |
| C | -1.3488868 | -0.1670949 | 0.8692053 |
| O | -0.2961623 | -0.6152127 | -1.7765417 |
| C | -1.5633670 | -0.9231409 | -2.2998392 |
| C | -1.5988579 | -0.7245756 | -3.8094243 |
| O | -0.9272106 | -1.7219246 | -4.5682462 |
| C | 0.4892398 | -1.5844866 | -4.6057220 |
| H | 3.7278363 | -3.0632867 | -3.7023206 |
| H | 5.3059930 | -2.3106837 | -4.0456539 |
| H | 4.3210331 | -1.7551851 | -2.6589167 |
| H | 0.9386170 | -1.6899880 | -3.6173523 |
| H | 0.7764885 | -0.6050801 | -5.0128280 |
| H | 0.8581062 | -2.3659691 | -5.2723912 |
| H | 4.5610699 | 0.9044578 | -4.2311503 |
| H | 3.3547981 | 1.5655467 | -5.3637092 |
| H | 2.9226417 | 1.2694857 | -3.6526759 |
| H | -2.3421966 | -0.2727189 | -1.8679173 |
| H | -1.8547884 | -1.9628455 | -2.0853563 |

| | | | |
|---|------------|------------|------------|
| H | -2.6425212 | -0.7651993 | -4.1384692 |
| H | -1.1984545 | 0.2708130 | -4.0496058 |
| H | 3.4300520 | 2.5225872 | 1.7767921 |
| H | 1.7231669 | 2.7635257 | 2.1458861 |
| H | 2.5636821 | 3.9034682 | 1.0883539 |
| H | 0.6664173 | 3.6317742 | -1.1971908 |
| H | -0.3690688 | 2.7692915 | -0.0631930 |
| H | -0.0349622 | 2.0688970 | -1.6549470 |
| H | 2.1335449 | -2.6042337 | 2.4191176 |
| H | 2.7929152 | -1.1747628 | 3.2119059 |
| H | 3.8757792 | -2.4753994 | 2.7002939 |
| H | -0.7921408 | -3.1426082 | -0.2468835 |
| H | 0.1383208 | -2.9517863 | 1.2381098 |
| H | 0.9792014 | -3.1958138 | -0.3006066 |
| H | 4.0632871 | -3.9696297 | 0.6361375 |
| H | 5.4051824 | -2.9375317 | 0.1119392 |
| H | 4.2571353 | 3.7066770 | -0.7991124 |
| H | 2.9281852 | 3.9773681 | -1.9393617 |
| H | 5.1005012 | -5.0795121 | -1.1472718 |
| H | 3.5663008 | -4.4479103 | -1.7899482 |
| H | -1.5316294 | 0.8935977 | 0.6813743 |
| H | -1.1512552 | -0.2823986 | 1.9387471 |
| H | -2.2706824 | -0.7136570 | 0.6410476 |
| H | 5.2400581 | 4.0988947 | -2.8888928 |
| H | 5.4264350 | 2.3562601 | -2.5792524 |
| H | 5.6448160 | -0.7290135 | 1.0614124 |
| H | 4.7928243 | 0.6266701 | 1.7955112 |
| H | 5.0046275 | 0.5720262 | 0.0395003 |

$[(\text{MeOCH}_2\text{CH}_2\text{OSiMe}_2)_3\text{C}]^- (\mathbf{1}^-\text{-B})$

C -0.6072186 0.3128240 -0.7557144
Si -2.3655746 0.3142979 -1.1373876
Si -0.1215652 0.9672475 0.8676368
Si 0.6951692 -0.3830185 -1.7904281
C -0.1783532 -0.2939774 2.3027660
C -1.0903867 2.4996532 1.4830153
C -3.0810529 1.9458345 -1.8550380
C -3.0461953 -1.0452302 -2.2998674
C 1.9934810 0.8655153 -2.4394498
C 0.1535102 -1.3296891 -3.3667056
O -3.2394072 0.0904542 0.3413059
C -4.6194434 0.2941986 0.4922198
O 1.6034136 -1.5494224 -0.8911533
C 2.8600142 -2.0455464 -1.2666619
O 1.5202393 1.4964817 0.7956233
C 2.2962664 1.7954020 1.9251111
C -5.0341048 -0.2940327 1.8319456
O -6.4326068 -0.0911172 2.0197067
C -6.8955527 -0.6022069 3.2464193
C 3.1946762 -3.2072417 -0.3444190
O 4.4762566 -3.7298765 -0.6896165
C 4.8589226 -4.8095059 0.1269215
C 3.6116725 2.3882625 1.4447312
O 4.4222488 2.7056357 2.5738905
C 5.6700356 3.2449723 2.2108385
H 0.1265305 0.1206697 3.2701711
H 0.4632581 -1.1466874 2.0662383

H -1.2028185 -0.6635420 2.3946531
H -0.7177485 2.8445675 2.4533758
H -0.9970531 3.3236911 0.7705933
H -2.1505951 2.2629472 1.5958608
H -4.1647568 1.9134619 -2.0151830
H -2.8563123 2.7880729 -1.1952891
H -2.6077074 2.1547556 -2.8195048
H -4.1410718 -1.0185353 -2.3060660
H -2.7330901 -2.0369222 -1.9664124
H -2.7110111 -0.9135293 -3.3307508
H 2.8145389 0.3892631 -2.9871834
H 2.4047754 1.4375094 -1.6063909
H 1.5038902 1.5703199 -3.1187357
H 1.0391502 -1.7140926 -3.8838036
H -0.4948511 -2.1762978 -3.1352664
H -0.3748795 -0.6792615 -4.0693152
H -5.2044958 -0.1936045 -0.3007432
H -4.8794804 1.3618776 0.4765471
H 2.8773847 -2.4074163 -2.3057721
H 3.6457026 -1.2824742 -1.1756690
H 2.5083921 0.9001685 2.5253824
H 1.8052519 2.5229118 2.5883119
H -4.4656725 0.1911788 2.6369720
H -4.7969834 -1.3665839 1.8507375
H -7.9666026 -0.4013037 3.3044094
H -6.3986086 -0.1220776 4.1022629
H -6.7345023 -1.6878557 3.3234086
H 3.1919349 -2.8587910 0.6970247
H 2.4259327 -3.9864991 -0.4420337

| | | | |
|---|-----------|------------|------------|
| H | 5.8452325 | -5.1402171 | -0.2029629 |
| H | 4.9191572 | -4.5193046 | 1.1862978 |
| H | 4.1575163 | -5.6533837 | 0.0443230 |
| H | 3.4127991 | 3.2913367 | 0.8512034 |
| H | 4.1250764 | 1.6649283 | 0.7970209 |
| H | 6.2192129 | 3.4546043 | 3.1302940 |
| H | 6.2564994 | 2.5425566 | 1.6005469 |
| H | 5.5610599 | 4.1811444 | 1.6430543 |

[(MeOCH₂CH₂OSiMe₂)₃Si]⁻ (2**⁻-A)**

| | | | |
|----|-----------|------------|------------|
| C | 2.2970855 | 2.4651264 | 2.9358272 |
| Si | 2.0084997 | 1.6066614 | 1.2405265 |
| O | 3.5956968 | 1.5143800 | 0.5446404 |
| C | 4.3259156 | 2.6434208 | 0.1315843 |
| C | 5.8199390 | 2.4028313 | 0.2316666 |
| O | 6.2567020 | 1.5191041 | -0.7912361 |
| C | 7.6186739 | 1.1880834 | -0.6775575 |
| C | 1.0432147 | 2.8803623 | 0.1845952 |
| Si | 0.8351317 | -0.4098328 | 1.4780043 |
| Si | 0.2291686 | -0.9544876 | -0.7498827 |
| C | 0.3032838 | -2.8366779 | -1.1022652 |
| Si | 2.4508870 | -2.0034314 | 2.1223084 |
| C | 1.6179610 | -3.6475995 | 2.6224057 |
| C | 3.4276357 | -1.4204671 | 3.6708012 |
| O | 3.6490570 | -2.6224571 | 1.0485509 |
| C | 4.6743792 | -1.8450431 | 0.4784391 |
| C | 5.4935908 | -2.6802933 | -0.4833273 |
| O | 4.7629236 | -2.9544904 | -1.6712250 |

C 5.4329289 -3.8409233 -2.5307505
C -1.5697870 -0.4211542 -1.1036880
O 1.0034903 -0.1877831 -2.0772118
C 2.3959505 -0.2064826 -2.3135015
C 2.7142666 0.4626297 -3.6324725
O 2.5307417 1.8718728 -3.5458224
C 2.7374246 2.5203672 -4.7736252
H 6.4030086 -3.4386063 -2.8636750
H 4.7990849 -3.9922746 -3.4054503
H 5.6131605 -4.8155486 -2.0527206
H 2.0327588 2.1727107 -5.5447627
H 3.7605526 2.3682832 -5.1533036
H 2.5802145 3.5881186 -4.6130635
H 8.2641871 2.0778502 -0.7495059
H 7.8614659 0.5120012 -1.4980293
H 7.8386200 0.6824878 0.2739925
H 2.7812256 -1.2333406 -2.3671982
H 2.9408603 0.3032737 -1.5117247
H 3.7607039 0.2448059 -3.8992105
H 2.0631941 0.0521724 -4.4188798
H 2.8531082 1.8132121 3.6141387
H 1.3351148 2.6879610 3.4053879
H 2.8498621 3.4064886 2.8382867
H 1.5210150 3.8660869 0.1886510
H 0.0314573 2.9981287 0.5828024
H 0.9629298 2.5420172 -0.8508896
H 1.0763288 -4.0826079 1.7794679
H 0.9023134 -3.4810744 3.4314976
H 2.3673645 -4.3725962 2.9551420

H -0.0801928 -3.0527247 -2.1053633
 H -0.3051926 -3.3868739 -0.3785141
 H 1.3255427 -3.2155989 -1.0317138
 H 5.3696769 -1.4822770 1.2530424
 H 4.2849940 -0.9586015 -0.0317046
 H 4.1069769 3.5237850 0.7558805
 H 4.0789847 2.9071403 -0.9056068
 H 6.4178289 -2.1353566 -0.7375153
 H 5.7739097 -3.6245034 0.0072083
 H -1.6898280 0.6547928 -0.9545907
 H -2.2599561 -0.9306626 -0.4259069
 H -1.8475572 -0.6570831 -2.1359046
 H 6.3493024 3.3661504 0.1338912
 H 6.0532652 1.9826786 1.2203740
 H 4.0838420 -2.2193466 4.0328374
 H 2.7397923 -1.1484923 4.4758434
 H 4.0440264 -0.5444779 3.4540154

[$(\text{MeOCH}_2\text{CH}_2\text{OSiMe}_2)_3\text{Si}]^-$ (2⁻**-B)**

Si -0.6116660 1.6187414 -1.4519933
 Si -2.4332814 0.1085805 -1.3356280
 Si 0.0957634 1.5124945 0.8021488
 Si 1.0109043 0.2131923 -2.4245616
 C 0.1689383 -0.1438259 1.7625535
 C -0.9546980 2.6771200 1.9019305
 C -3.5878474 0.3048234 -2.8565504
 C -2.1877389 -1.7873805 -1.1698619
 C 2.6994950 1.1044618 -2.5699440

| | | | |
|---|------------|------------|------------|
| C | 0.5609453 | -0.2996118 | -4.2225905 |
| O | -3.3803305 | 0.5591704 | 0.0370318 |
| C | -4.6791430 | 0.0826185 | 0.2935387 |
| O | 1.3400054 | -1.2689445 | -1.5968209 |
| C | 2.2527857 | -2.2422826 | -2.0418535 |
| O | 1.7083917 | 2.1326047 | 0.8376243 |
| C | 2.4127432 | 2.4229578 | 2.0177937 |
| C | -4.9124933 | 0.1283646 | 1.7951105 |
| O | -6.2363431 | -0.3186231 | 2.0750792 |
| C | -6.5187504 | -0.3462557 | 3.4540757 |
| C | 2.2483606 | -3.3834011 | -1.0368795 |
| O | 3.1546087 | -4.3917925 | -1.4766951 |
| C | 3.2098231 | -5.4918691 | -0.6000085 |
| C | 3.8068374 | 2.8878905 | 1.6286084 |
| O | 4.5370875 | 3.2053915 | 2.8107720 |
| C | 5.8484984 | 3.6389439 | 2.5397028 |
| H | 0.6020683 | -0.0240001 | 2.7622195 |
| H | 0.7563878 | -0.8768209 | 1.2064420 |
| H | -0.8425999 | -0.5415306 | 1.8825999 |
| H | -0.6575657 | 2.6491870 | 2.9558916 |
| H | -0.8882017 | 3.7090009 | 1.5470091 |
| H | -2.0013587 | 2.3693095 | 1.8316894 |
| H | -4.4819579 | -0.3240792 | -2.7913415 |
| H | -3.9011052 | 1.3464365 | -2.9629837 |
| H | -3.0518295 | 0.0282718 | -3.7699605 |
| H | -3.1421226 | -2.3213754 | -1.0915654 |
| H | -1.5795095 | -2.0251908 | -0.2956700 |
| H | -1.6573607 | -2.1743478 | -2.0440934 |
| H | 3.4741242 | 0.4644887 | -3.0061814 |

H 3.0278010 1.4362841 -1.5828796
H 2.5988633 1.9914101 -3.2021509
H 1.3751215 -0.8422682 -4.7142718
H -0.3305676 -0.9321048 -4.2498698
H 0.3502689 0.5947749 -4.8153888
H -4.8257242 -0.9505091 -0.0511723
H -5.4348572 0.7039411 -0.2064560
H 1.9792471 -2.6419265 -3.0284118
H 3.2738635 -1.8436416 -2.1215942
H 2.5027175 1.5451169 2.6735558
H 1.9252541 3.2175469 2.5997243
H -4.7698045 1.1550889 2.1588001
H -4.1768415 -0.5133759 2.2985316
H -7.5454389 -0.6963497 3.5730003
H -6.4299346 0.6511473 3.9086934
H -5.8457619 -1.0283674 3.9941136
H 2.5454400 -3.0059289 -0.0491767
H 1.2325786 -3.7922974 -0.9507568
H 3.9158797 -6.2108622 -1.0184631
H 3.5546699 -5.1988222 0.4025627
H 2.2292179 -5.9787340 -0.4946234
H 3.7304993 3.7690562 0.9769479
H 4.3160203 2.0939619 1.0653543
H 6.3266940 3.8607713 3.4953580
H 6.4351107 2.8658465 2.0224063
H 5.8578183 4.5475234 1.9195287

[(MeOCH2CH2OSiMe2)3SiH] (**2**-H-A)

| | | | |
|----|------------|------------|------------|
| C | 2.0068629 | 2.5408007 | 2.9242255 |
| Si | 2.0021877 | 1.7690655 | 1.1881720 |
| O | 3.6077939 | 1.5931002 | 0.6635035 |
| C | 4.3868554 | 2.6386239 | 0.0998598 |
| C | 5.8489690 | 2.2521142 | 0.0587888 |
| O | 6.0598847 | 1.2328971 | -0.9034849 |
| C | 7.4137877 | 0.8405620 | -0.9936501 |
| C | 1.0477258 | 2.9148796 | 0.0218237 |
| Si | 1.1526111 | -0.4432635 | 1.1909110 |
| Si | 0.4383245 | -1.1267286 | -0.9926972 |
| C | 0.7967764 | -2.9606234 | -1.2945264 |
| Si | 2.5631585 | -2.0116158 | 2.3064548 |
| C | 1.5548384 | -3.4932854 | 2.9048162 |
| C | 3.4669573 | -1.2141301 | 3.7727666 |
| O | 3.6891268 | -2.6974835 | 1.2541305 |
| C | 4.7673765 | -2.0343706 | 0.6152157 |
| C | 5.3800097 | -2.9428756 | -0.4280090 |
| O | 4.5013545 | -3.0856759 | -1.5323453 |
| C | 4.9642653 | -4.0221642 | -2.4839975 |
| C | -1.4039687 | -0.7697769 | -1.2111257 |
| O | 1.1732152 | -0.1886654 | -2.1855899 |
| C | 2.5705900 | -0.0970423 | -2.4323839 |
| C | 2.8307040 | 0.8607777 | -3.5720376 |
| O | 2.5742249 | 2.1949289 | -3.1575811 |
| C | 2.6828628 | 3.1268986 | -4.2127646 |
| H | 5.9321051 | -3.7225023 | -2.9102438 |
| H | 4.2257729 | -4.0657935 | -3.2840961 |

H 5.0716940 -5.0230673 -2.0453030
H 1.9648917 2.9120077 -5.0156950
H 3.6940680 3.1367671 -4.6434625
H 2.4650262 4.1123189 -3.8009759
H 8.0602084 1.6796037 -1.2872052
H 7.4772931 0.0650283 -1.7565306
H 7.7836697 0.4361032 -0.0413193
H 2.9840578 -1.0761299 -2.7001498
H 3.1047460 0.2548997 -1.5431182
H 3.8800741 0.7616000 -3.8877758
H 2.1863038 0.5994717 -4.4232562
H 2.5758259 1.9358288 3.6326154
H 0.9858926 2.6349274 3.3041053
H 2.4463862 3.5426621 2.9040517
H 1.4248100 3.9403654 0.0812411
H -0.0089755 2.9371585 0.3022511
H 1.1242886 2.5788025 -1.0137390
H 1.0765596 -4.0049360 2.0675530
H 0.7758817 -3.1832871 3.6054779
H 2.2065504 -4.2112690 3.4099857
H 0.4687023 -3.2464214 -2.2984330
H 0.2538732 -3.5804271 -0.5753476
H 1.8609454 -3.1840144 -1.1956005
H 5.5498845 -1.7896516 1.3460032
H 4.4507357 -1.0956560 0.1484810
H 4.3084342 3.5575888 0.6976676
H 4.0421182 2.8597107 -0.9160165
H 6.3366975 -2.5112816 -0.7603285
H 5.5850894 -3.9241587 0.0228394

H -1.6182596 0.2911369 -1.0700779
 H -2.0009119 -1.3368023 -0.4927374
 H -1.7212338 -1.0491269 -2.2193379
 H 6.4399718 3.1445432 -0.2024186
 H 6.1701439 1.9115371 1.0535612
 H 4.0924623 -1.9526697 4.2827808
 H 2.7508782 -0.8203457 4.4989480
 H 4.1054575 -0.3875172 3.4532656
 H -0.0943122 -0.3894834 2.0329831

[(MeOCH₂CH₂OSiMe₂)₃SiH] (2-H-B)

Si -0.4691057 1.3470298 -0.1088820
 Si -2.3353928 0.5601406 -1.3414318
 Si -0.0358952 -0.0566258 1.7484379
 Si 1.4579823 1.6357675 -1.4535843
 C 0.0212445 -1.8822809 1.2445229
 C -1.3337307 0.1818351 3.1073490
 C -3.1826491 1.9613804 -2.2992939
 C -1.8881970 -0.8317697 -2.5476018
 C 2.8653002 2.4549980 -0.4883380
 C 1.1199712 2.6550633 -3.0203005
 O -3.3922818 -0.0374227 -0.1578739
 C -4.6839488 -0.5648352 -0.4312624
 O 1.8814911 0.0558122 -1.8905571
 C 3.0261669 -0.2872342 -2.6589089
 O 1.4868768 0.4263718 2.3148261
 C 2.1053464 -0.1084940 3.4768584
 C -5.3573485 -0.8850206 0.8919479

O -6.6400296 -1.4143967 0.6097698
 C -7.3730274 -1.7398313 1.7737955
 C 3.0610184 -1.7984835 -2.8114173
 O 4.2046978 -2.1314517 -3.5775278
 C 4.3450738 -3.5222794 -3.7880851
 C 3.4826830 0.5174043 3.6151241
 O 4.0885018 -0.0173939 4.7783229
 C 5.3856326 0.4935980 5.0115549
 H 0.2894672 -2.5215341 2.0904618
 H 0.7490856 -2.0452638 0.4470528
 H -0.9593253 -2.2037301 0.8845126
 H -1.1690898 -0.4992731 3.9471097
 H -1.3223782 1.2051180 3.4890290
 H -2.3280792 -0.0157309 2.6999054
 H -4.0464665 1.5981562 -2.8633669
 H -3.5222117 2.7485796 -1.6228328
 H -2.4891784 2.4114755 -3.0145709
 H -2.7711553 -1.1824280 -3.0893321
 H -1.4469177 -1.6827997 -2.0250483
 H -1.1592445 -0.4841092 -3.2835468
 H 3.7758518 2.5295450 -1.0897049
 H 3.0862563 1.8908827 0.4193148
 H 2.5792576 3.4678893 -0.1924951
 H 2.0310758 2.7857656 -3.6115560
 H 0.3712127 2.1797101 -3.6579987
 H 0.7540143 3.6512017 -2.7572954
 H -4.6181368 -1.4795299 -1.0317674
 H -5.3006480 0.1559387 -0.9802555
 H 2.9899766 0.1726923 -3.6533521

H 3.9480670 0.0443152 -2.1675051
 H 2.2137829 -1.1971967 3.4064231
 H 1.5183715 0.1141729 4.3751996
 H -5.4340804 0.0291870 1.4971666
 H -4.7491349 -1.6099745 1.4510216
 H -8.3368012 -2.1318627 1.4506368
 H -7.5409768 -0.8565157 2.4047701
 H -6.8599203 -2.5039885 2.3731625
 H 3.1035567 -2.2684972 -1.8190390
 H 2.1426268 -2.1413879 -3.3081813
 H 5.2462749 -3.6704517 -4.3821942
 H 4.4497437 -4.0652666 -2.8391596
 H 3.4862843 -3.9363016 -4.3334407
 H 3.3859673 1.6095555 3.6896100
 H 4.0830334 0.2914645 2.7225953
 H 5.7610797 0.0226794 5.9194815
 H 6.0661394 0.2606798 4.1812993
 H 5.3706859 1.5825600 5.1548297
 H -0.8404886 2.7038217 0.4170616

[(MeOCH₂CH₂OSiMe₂)₃Ge]⁻ (3⁻**-A)**

C 1.4428250 1.6836405 3.8287809
 Si 0.3014431 1.4786265 2.3120572
 O 1.3021590 2.1577074 1.0947906
 C 0.9803141 2.1330018 -0.2825560
 C 1.5152615 3.3596170 -0.9874598
 O 2.9359336 3.3108182 -1.0969728
 C 3.4695975 4.4720797 -1.6771613

| | | | |
|----|------------|------------|------------|
| C | -1.1267826 | 2.7362131 | 2.5607670 |
| Ge | -0.5093274 | -0.8134648 | 2.1962064 |
| Si | -2.3966514 | -0.7224141 | 0.6736628 |
| C | -2.9244772 | -2.5028622 | 0.1748216 |
| Si | 1.2265033 | -1.8510448 | 0.8789164 |
| C | 1.1012023 | -3.7693111 | 0.9706977 |
| C | 2.9791557 | -1.4478237 | 1.5465218 |
| O | 1.2769484 | -1.4900256 | -0.8141256 |
| C | 2.2356850 | -1.9975887 | -1.7091288 |
| C | 1.6528507 | -2.9848551 | -2.7064346 |
| O | 0.8633107 | -2.3070028 | -3.6744192 |
| C | 0.1960623 | -3.1876819 | -4.5458877 |
| C | -3.9139349 | 0.0381551 | 1.5499967 |
| O | -2.4328613 | 0.1815516 | -0.7912742 |
| C | -1.6575923 | -0.1325949 | -1.9263538 |
| C | -2.0025886 | 0.7936555 | -3.0725956 |
| O | -1.5087650 | 2.1077458 | -2.8391845 |
| C | -1.9207352 | 3.0233683 | -3.8218272 |
| H | 0.9013119 | -3.8156465 | -5.1127702 |
| H | -0.3758441 | -2.5815998 | -5.2494362 |
| H | -0.4955211 | -3.8503890 | -4.0064543 |
| H | -3.0165424 | 3.1169766 | -3.8590921 |
| H | -1.5675735 | 2.7377025 | -4.8254596 |
| H | -1.4959518 | 3.9951293 | -3.5656518 |
| H | 3.0887650 | 4.6367091 | -2.6982779 |
| H | 4.5531631 | 4.3501249 | -1.7248094 |
| H | 3.2424488 | 5.3702744 | -1.0822154 |
| H | -1.8654736 | -1.1553325 | -2.2763439 |
| H | -0.5854339 | -0.0916858 | -1.7132396 |

H -1.5603090 0.3956761 -3.9999380
H -3.0956409 0.8256775 -3.1945280
H 2.3019781 1.0120051 3.7652174
H 0.9003705 1.4482775 4.7486408
H 1.8167080 2.7104585 3.8922074
H -0.7245859 3.7256457 2.8037026
H -1.7870624 2.4224860 3.3742910
H -1.7354543 2.8277151 1.6577786
H 0.1449964 -4.1227164 0.5755223
H 1.1613161 -4.0880167 2.0149442
H 1.9061391 -4.2695359 0.4199177
H -3.8446199 -2.4855270 -0.4195708
H -3.1050534 -3.1025375 1.0710648
H -2.1509997 -3.0101656 -0.4072412
H 3.0571106 -2.5123406 -1.1898978
H 2.6821372 -1.1660339 -2.2692637
H -0.1023943 2.1144161 -0.4520184
H 1.3927931 1.2340184 -0.7537770
H 2.4769625 -3.5163580 -3.2130226
H 1.0445252 -3.7280285 -2.1736244
H -3.7327757 1.0834933 1.8090347
H -4.1338803 -0.5028486 2.4741291
H -4.7936835 -0.0039728 0.8998688
H 1.0703820 3.4085318 -1.9931590
H 1.2176154 4.2604888 -0.4305260
H 3.7641899 -2.0282595 1.0495456
H 3.0282012 -1.6727552 2.6157220
H 3.2023375 -0.3863803 1.4163518

$[(\text{MeOCH}_2\text{CH}_2\text{OSiMe}_2)_3\text{Ge}]^-$ (**3⁻-B**)

| | | | |
|----|------------|------------|------------|
| Ge | -0.4716294 | 0.2694362 | -1.5708237 |
| Si | -2.1773915 | -1.0883987 | -0.4918719 |
| Si | 0.1926162 | 1.5788787 | 0.3640046 |
| Si | 1.3498469 | -1.3332728 | -1.5282207 |
| C | 0.4879420 | 0.7991562 | 2.0904909 |
| C | -1.0580574 | 2.9985490 | 0.6729193 |
| C | -3.0789851 | -2.1784381 | -1.7914806 |
| C | -1.8237271 | -2.2863390 | 0.9641413 |
| C | 2.9810362 | -0.5132815 | -2.1118547 |
| C | 1.0706146 | -2.7925522 | -2.7493415 |
| O | -3.3629631 | 0.0179207 | 0.1042759 |
| C | -4.5981696 | -0.3612076 | 0.6594469 |
| O | 1.7132003 | -2.0765948 | -0.0095088 |
| C | 2.7291484 | -3.0307514 | 0.1867140 |
| O | 1.6861592 | 2.3340692 | -0.0640176 |
| C | 2.3519133 | 3.2836527 | 0.7300702 |
| C | -5.3675836 | 0.9075173 | 0.9894529 |
| O | -6.6279930 | 0.5554619 | 1.5534090 |
| C | -7.4054272 | 1.6804762 | 1.8870561 |
| C | 2.7585052 | -3.3823465 | 1.6654757 |
| O | 3.7736662 | -4.3571551 | 1.8914264 |
| C | 3.8729562 | -4.7328906 | 3.2445993 |
| C | 3.4678456 | 3.8888764 | -0.1072278 |
| O | 4.1782578 | 4.8413072 | 0.6800166 |
| C | 5.2325167 | 5.4512381 | -0.0253189 |
| H | 0.8949622 | 1.5229580 | 2.8063623 |
| H | 1.1706100 | -0.0493818 | 2.0151262 |

H -0.4588965 0.4303126 2.4944594
H -0.7944602 3.6241592 1.5325944
H -1.1401047 3.6372410 -0.2105388
H -2.0434698 2.5615446 0.8560074
H -3.9132433 -2.7450380 -1.3635832
H -3.4601803 -1.5629180 -2.6103845
H -2.3771887 -2.8985198 -2.2230111
H -2.7157957 -2.8504511 1.2599385
H -1.4512586 -1.7440526 1.8358104
H -1.0463756 -2.9968072 0.6739324
H 3.8235824 -1.2132438 -2.1312684
H 3.2331927 0.3265691 -1.4607199
H 2.8498892 -0.1176222 -3.1231214
H 1.9573086 -3.4281352 -2.8476021
H 0.2351773 -3.4239543 -2.4347971
H 0.8303120 -2.3985375 -3.7407526
H -4.4718955 -0.9503104 1.5786835
H -5.1946997 -0.9656688 -0.0378972
H 2.5479857 -3.9472472 -0.3922067
H 3.7163245 -2.6483162 -0.1067728
H 2.7890425 2.8292251 1.6300821
H 1.6824242 4.0894377 1.0622768
H -5.5084738 1.4987762 0.0742806
H -4.7876392 1.5152125 1.6970766
H -8.3469383 1.3189163 2.3034443
H -7.6230812 2.3014906 1.0056041
H -6.9069487 2.3136310 2.6357206
H 2.9589415 -2.4769583 2.2542932
H 1.7781152 -3.7719509 1.9703635

| | | | |
|---|-----------|------------|------------|
| H | 4.6668474 | -5.4774022 | 3.3225539 |
| H | 4.1256404 | -3.8773935 | 3.8880392 |
| H | 2.9360580 | -5.1738857 | 3.6152005 |
| H | 3.0391211 | 4.3697194 | -0.9968966 |
| H | 4.1437109 | 3.0925689 | -0.4470084 |
| H | 5.7184343 | 6.1554046 | 0.6519924 |
| H | 5.9764288 | 4.7153085 | -0.3639625 |
| H | 4.8698710 | 6.0008376 | -0.9065895 |

[(MeOCH₂CH₂OSiMe₂)₃GeH] (3-H-A)

| | | | |
|----|------------|------------|------------|
| C | 2.8153223 | 2.8062408 | 1.5650198 |
| Si | 2.2691412 | 1.9067028 | -0.0026074 |
| O | 3.6411064 | 1.9258659 | -0.9799700 |
| C | 3.7525245 | 1.3407611 | -2.2712782 |
| C | 5.1398262 | 1.5676720 | -2.8255433 |
| O | 6.0854929 | 0.7760493 | -2.1207911 |
| C | 7.4147269 | 1.0201060 | -2.5303499 |
| C | 0.8524577 | 2.8342759 | -0.8469467 |
| Ge | 1.6319419 | -0.3875326 | 0.5154923 |
| Si | -0.3982803 | -1.1546738 | -0.5747009 |
| C | -0.5085593 | -3.0486886 | -0.5611473 |
| Si | 3.4877084 | -1.9098788 | 0.2755129 |
| C | 3.2207722 | -3.5278901 | 1.2323592 |
| C | 5.1311106 | -1.1434761 | 0.8182739 |
| O | 3.5167261 | -2.2558484 | -1.3860500 |
| C | 4.6612165 | -2.7068409 | -2.0959070 |
| C | 4.2794893 | -3.1589306 | -3.4879773 |
| O | 3.9155700 | -2.0435234 | -4.2836347 |

C 3.5594555 -2.4079324 -5.6008909
C -1.9184957 -0.4073842 0.2594300
O -0.4953248 -0.5952673 -2.1629135
C 0.3560136 -0.9584567 -3.2370908
C 0.0965232 -0.0566243 -4.4236088
O 0.5973110 1.2458685 -4.1687409
C 0.2618401 2.1713157 -5.1826238
H 4.3904235 -2.9029282 -6.1226894
H 3.3052267 -1.4925298 -6.1345222
H 2.6917746 -3.0819304 -5.6153567
H -0.8260608 2.2769594 -5.2876442
H 0.6786215 1.8756340 -6.1556965
H 0.6834193 3.1344987 -4.8964801
H 7.5610980 0.7865632 -3.5944693
H 8.0628426 0.3766552 -1.9355916
H 7.7029637 2.0664430 -2.3614582
H 0.1532620 -1.9914880 -3.5504375
H 1.4131719 -0.9037673 -2.9562126
H 0.5886178 -0.4822614 -5.3118071
H -0.9845291 -0.0165800 -4.6168716
H 3.6534073 2.2922836 2.0390694
H 1.9983306 2.8665040 2.2880799
H 3.1350539 3.8231462 1.3214370
H 1.1650965 3.8547154 -1.0889374
H -0.0136065 2.8970430 -0.1820978
H 0.5361379 2.3372858 -1.7664087
H 2.3032142 -4.0311454 0.9212989
H 3.1510720 -3.3315856 2.3056193
H 4.0558964 -4.2170689 1.0739733

H -1.4274999 -3.3829114 -1.0519516
 H -0.5176196 -3.4261044 0.4648003
 H 0.3406014 -3.5041316 -1.0753518
 H 5.1279994 -3.5632928 -1.5893310
 H 5.4029979 -1.9040455 -2.1689619
 H 3.0270177 1.7830343 -2.9635393
 H 3.5574482 0.2639866 -2.2323437
 H 5.1421794 -3.6759155 -3.9375136
 H 3.4469639 -3.8750391 -3.4290095
 H -1.8954686 0.6826591 0.2071869
 H -1.9694969 -0.6972645 1.3115605
 H -2.8297948 -0.7507871 -0.2376985
 H 5.1435767 1.2949623 -3.8914595
 H 5.3998272 2.6322063 -2.7391992
 H 5.9498846 -1.8648587 0.7349752
 H 5.0706391 -0.8344299 1.8654106
 H 5.3800384 -0.2689503 0.2138935
 H 1.2838393 -0.3987594 2.0355944

[(MeOCH₂CH₂OSiMe₂)₃GeH] (3-H-B)

Ge -0.6877535 0.9937979 -0.9909959
 Si -2.7226528 -0.2934269 -1.1319452
 Si 0.0251379 1.2092012 1.3015209
 Si 1.1105422 0.1785517 -2.3685274
 C -0.0286681 -0.4598201 2.1950733
 C -1.0369479 2.4642197 2.2408896
 C -3.7489978 0.1721362 -2.6570460
 C -2.4039313 -2.1616977 -1.1451777

| | | | |
|---|------------|------------|------------|
| C | 2.5231672 | 1.4368134 | -2.4348461 |
| C | 0.5741606 | -0.2429492 | -4.1400035 |
| O | -3.5648023 | 0.1284648 | 0.2769323 |
| C | -4.8682181 | -0.3366520 | 0.6037476 |
| O | 1.6070665 | -1.2327131 | -1.5790215 |
| C | 2.7465511 | -1.9996761 | -1.9414645 |
| O | 1.6256779 | 1.7564298 | 1.2108904 |
| C | 2.4493914 | 1.9820087 | 2.3465943 |
| C | -5.2936918 | 0.3146037 | 1.9090696 |
| O | -6.5889129 | -0.1610776 | 2.2277756 |
| C | -7.0997553 | 0.3798549 | 3.4299042 |
| C | 2.8964927 | -3.1279694 | -0.9360079 |
| O | 4.0387292 | -3.8838966 | -1.2962601 |
| C | 4.2848475 | -4.9655469 | -0.4204465 |
| C | 3.8122313 | 2.4462252 | 1.8630022 |
| O | 4.6272163 | 2.6609046 | 3.0011893 |
| C | 5.9308246 | 3.0979744 | 2.6733166 |
| H | 0.3356507 | -0.3748078 | 3.2226443 |
| H | 0.5808609 | -1.2008443 | 1.6737656 |
| H | -1.0563893 | -0.8288848 | 2.2352975 |
| H | -0.7408866 | 2.5373606 | 3.2913527 |
| H | -0.9634707 | 3.4577377 | 1.7935359 |
| H | -2.0838752 | 2.1539385 | 2.2047062 |
| H | -4.6760875 | -0.4057649 | -2.7094949 |
| H | -4.0068291 | 1.2333213 | -2.6502221 |
| H | -3.1829503 | -0.0284846 | -3.5705565 |
| H | -3.3418080 | -2.7242646 | -1.1654733 |
| H | -1.8370962 | -2.4730392 | -0.2655199 |
| H | -1.8266452 | -2.4453475 | -2.0287646 |

H 3.3764076 1.0610307 -3.0066451
H 2.8564969 1.6880070 -1.4264562
H 2.1814857 2.3578299 -2.9145428
H 1.4212514 -0.5953753 -4.7358217
H -0.1927516 -1.0207331 -4.1537045
H 0.1667234 0.6410530 -4.6375653
H -4.8812785 -1.4258904 0.7263424
H -5.5913728 -0.0762322 -0.1775883
H 2.6365415 -2.4254211 -2.9458909
H 3.6565892 -1.3890830 -1.9313025
H 2.5735529 1.0658877 2.9356549
H 2.0216225 2.7492798 3.0026549
H -5.2939850 1.4075042 1.7934560
H -4.5760582 0.0589558 2.7014612
H -8.0925050 -0.0437820 3.5788303
H -7.1834958 1.4736084 3.3768391
H -6.4682586 0.1198920 4.2900863
H 3.0063481 -2.7078177 0.0734693
H 1.9931858 -3.7537935 -0.9447634
H 5.1761240 -5.4780894 -0.7811653
H 4.4630512 -4.6201244 0.6068503
H 3.4455560 -5.6741043 -0.4088585
H 3.7027845 3.3705600 1.2787420
H 4.2506248 1.6814577 1.2061401
H 6.4708564 3.2372317 3.6093360
H 6.4629007 2.3569733 2.0614604
H 5.9112364 4.0509076 2.1274975
H -1.0344112 2.4150872 -1.5159568

$[(\text{SiMe}_3)_3\text{C}]^-$ (**7⁻**)

| | | | |
|----|------------|------------|------------|
| C | 2.2562551 | 2.7725955 | 1.4373531 |
| Si | 1.9693161 | 1.7580082 | -0.1818432 |
| C | 3.3997730 | 2.3264087 | -1.3439781 |
| C | 0.4491840 | 2.6442820 | -0.9662173 |
| C | 1.7914155 | -0.0455709 | 0.0457084 |
| Si | 0.1564246 | -0.8293924 | -0.1744601 |
| C | 0.1215141 | -2.7435154 | 0.0432032 |
| Si | 3.1756377 | -1.0170325 | 0.7358430 |
| C | 2.9082873 | -1.6865568 | 2.5287145 |
| C | 4.8499993 | -0.0766078 | 0.8878525 |
| C | 3.6939836 | -2.5779427 | -0.2715998 |
| C | -1.2122378 | -0.2405174 | 1.0558232 |
| C | -0.6534423 | -0.6191800 | -1.9121505 |
| H | 3.1404073 | 2.4255225 | 1.9791792 |
| H | 1.3989623 | 2.6542511 | 2.1071394 |
| H | 2.3855809 | 3.8425976 | 1.2345214 |
| H | 0.6237235 | 3.7255067 | -0.9517595 |
| H | -0.4831789 | 2.4535058 | -0.4292600 |
| H | 0.3027759 | 2.3466452 | -2.0075506 |
| H | 2.0063737 | -2.3000089 | 2.6025011 |
| H | 2.7888188 | -0.8501162 | 3.2243290 |
| H | 3.7556283 | -2.2940834 | 2.8689047 |
| H | -0.9178837 | -3.0858849 | -0.0069774 |
| H | 0.5325023 | -3.0756294 | 0.9994359 |
| H | 0.6745183 | -3.2491256 | -0.7524370 |
| H | -1.3508806 | 0.8433606 | 1.0157660 |
| H | -0.9224005 | -0.4918639 | 2.0808930 |

H -2.1814814 -0.7109865 0.8508641
 H 5.5706474 -0.7196217 1.4045751
 H 4.7710276 0.8533618 1.4559509
 H 5.2660231 0.1649431 -0.0934192
 H 3.3771251 3.4132017 -1.4870061
 H 3.2977951 1.8520773 -2.3246357
 H 4.3829474 2.0626445 -0.9496956
 H 2.8995127 -3.3255402 -0.3194871
 H 4.5756318 -3.0546688 0.1728535
 H 3.9423875 -2.2939096 -1.2986475
 H -0.8785514 0.4238966 -2.1429131
 H -1.5894716 -1.1862195 -1.9771408
 H 0.0239002 -0.9904730 -2.6871372

[(SiMe₃)₃CH] (7-H)

C 0.4229467 3.3225047 2.3772272
 Si -0.3716271 2.1274520 1.1284152
 C 0.6522427 2.1092534 -0.4732961
 C -2.0444299 2.9319881 0.7008160
 C -0.5321154 0.3734616 1.8981868
 Si -1.9938237 -0.6722233 1.2179991
 C -1.9627848 -2.4921404 1.7784564
 Si 1.1263236 -0.5800449 2.0817234
 C 1.0256312 -1.7894026 3.5467314
 C 2.6119474 0.5400824 2.4886992
 C 1.5787589 -1.5354367 0.5007507
 C -3.6440666 0.0008005 1.8828052
 C -2.0316326 -0.6894522 -0.6829555

| | | | |
|---|------------|------------|------------|
| H | 1.4536150 | 3.0677673 | 2.6229226 |
| H | -0.1484238 | 3.3428491 | 3.3096104 |
| H | 0.4185406 | 4.3374656 | 1.9692048 |
| H | -1.8534301 | 3.9323080 | 0.3005417 |
| H | -2.6739148 | 3.0509988 | 1.5857628 |
| H | -2.6163571 | 2.3843260 | -0.0497138 |
| H | 0.2934545 | -2.5831241 | 3.4002769 |
| H | 0.7660755 | -1.2598175 | 4.4679461 |
| H | 2.0000966 | -2.2605303 | 3.7045113 |
| H | -2.8473944 | -2.9916635 | 1.3721581 |
| H | -2.0081682 | -2.5839611 | 2.8661720 |
| H | -1.0879793 | -3.0430638 | 1.4296116 |
| H | -3.8670262 | 1.0114419 | 1.5426605 |
| H | -3.6447263 | 0.0072650 | 2.9765559 |
| H | -4.4634012 | -0.6482620 | 1.5601683 |
| H | 3.4962927 | -0.0923801 | 2.6112861 |
| H | 2.4665982 | 1.0811140 | 3.4267289 |
| H | 2.8372020 | 1.2688803 | 1.7089010 |
| H | -0.8259388 | 0.5768538 | 2.9400060 |
| H | 0.1997651 | 1.4652183 | -1.2307103 |
| H | 1.6767448 | 1.7680299 | -0.3142246 |
| H | 0.7035258 | 3.1196914 | -0.8883272 |
| H | 0.8470695 | -2.3058624 | 0.2504832 |
| H | 2.5443788 | -2.0309885 | 0.6350884 |
| H | 1.6683976 | -0.8691445 | -0.3603251 |
| H | -2.1732939 | 0.3045684 | -1.1112979 |
| H | -2.8591884 | -1.3157540 | -1.0279060 |
| H | -1.1101625 | -1.1032721 | -1.0985961 |

$[(\text{SiMe}_3)_3\text{Si}]^-$ (**8⁻**)

| | | | |
|----|------------|------------|------------|
| C | 2.1538672 | 2.3852095 | 3.0547372 |
| Si | 1.8588808 | 1.5903468 | 1.3252717 |
| C | 3.5850108 | 1.6797568 | 0.4672308 |
| C | 0.7957999 | 2.8900549 | 0.3810017 |
| Si | 0.6977692 | -0.4711762 | 1.5754598 |
| Si | 0.1980861 | -1.0360650 | -0.6805408 |
| C | -0.2762724 | -2.8955167 | -0.8514670 |
| Si | 2.4674379 | -1.9774828 | 2.0852169 |
| C | 1.7439921 | -3.6926993 | 2.5801107 |
| C | 3.4482290 | -1.4109814 | 3.6436593 |
| C | 3.8381763 | -2.4011647 | 0.7949537 |
| C | -1.3774538 | -0.0915295 | -1.2596774 |
| C | 1.4690231 | -0.7401654 | -2.1021182 |
| H | 2.7916255 | 1.7525630 | 3.6778550 |
| H | 1.2041166 | 2.5108249 | 3.5816514 |
| H | 2.6322929 | 3.3678136 | 2.9678142 |
| H | 1.2542280 | 3.8841279 | 0.4358446 |
| H | -0.2090528 | 2.9542811 | 0.8070060 |
| H | 0.6901086 | 2.6284955 | -0.6753464 |
| H | 1.1966417 | -4.1473610 | 1.7499212 |
| H | 1.0427089 | -3.5824541 | 3.4115589 |
| H | 2.5347698 | -4.3877816 | 2.8854778 |
| H | -0.6748475 | -3.1067631 | -1.8504241 |
| H | -1.0360379 | -3.1725283 | -0.1157390 |
| H | 0.5886310 | -3.5453930 | -0.6927956 |
| H | -1.2156995 | 0.9897811 | -1.2589819 |
| H | -2.2133436 | -0.2967141 | -0.5856082 |

H -1.6705770 -0.3896487 -2.2730753
 H 4.1373287 -2.1958244 3.9759948
 H 2.7692929 -1.1815113 4.4693009
 H 4.0374695 -0.5124646 3.4413857
 H 3.5357408 1.3010773 -0.5567066
 H 4.3225695 1.0766518 1.0039530
 H 3.9564448 2.7113237 0.4328214
 H 3.4084076 -2.8657353 -0.0965607
 H 4.5741719 -3.0978649 1.2150189
 H 4.3668186 -1.5008349 0.4725884
 H 1.7179858 0.3207693 -2.1911326
 H 1.0674328 -1.0732974 -3.0670827
 H 2.4007680 -1.2802826 -1.9172399

[(SiMe₃)₃SiH] (8-H)

C 1.8794022 2.4418123 3.0364090
 Si 1.8884548 1.7722272 1.2539407
 C 3.6615246 1.8822229 0.5655535
 C 0.7665661 2.8929170 0.1980925
 Si 1.1084808 -0.4799907 1.2340187
 Si 0.3678273 -1.1896790 -0.9175527
 C 0.0119035 -3.0612604 -0.9350679
 Si 2.6387708 -2.0049906 2.2402126
 C 1.7331435 -3.6130538 2.7088266
 C 3.3897038 -1.2704850 3.8297805
 C 4.0601985 -2.4255044 1.0433997
 C -1.2416806 -0.2813431 -1.3759695
 C 1.6824240 -0.8186645 -2.2456129

| | | | |
|---|------------|------------|------------|
| H | 2.5295244 | 1.8585737 | 3.6917794 |
| H | 0.8727980 | 2.4203243 | 3.4608572 |
| H | 2.2282608 | 3.4788254 | 3.0535372 |
| H | 1.1013527 | 3.9324074 | 0.2661773 |
| H | -0.2709203 | 2.8535809 | 0.5378054 |
| H | 0.7852967 | 2.6066704 | -0.8558095 |
| H | 1.3038724 | -4.1073470 | 1.8349240 |
| H | 0.9211320 | -3.4153957 | 3.4124081 |
| H | 2.4259261 | -4.3140475 | 3.1844828 |
| H | -0.3858960 | -3.3599740 | -1.9096880 |
| H | -0.7243833 | -3.3353539 | -0.1759608 |
| H | 0.9157420 | -3.6468801 | -0.7525940 |
| H | -1.1000926 | 0.8006545 | -1.4164518 |
| H | -2.0304230 | -0.4874477 | -0.6487039 |
| H | -1.5959471 | -0.6103308 | -2.3575843 |
| H | 4.0441714 | -2.0039476 | 4.3105326 |
| H | 2.6140365 | -0.9944232 | 4.5477229 |
| H | 3.9867903 | -0.3797070 | 3.6217423 |
| H | -0.1157357 | -0.4938683 | 2.1098075 |
| H | 3.7189881 | 1.5120567 | -0.4608838 |
| H | 4.3642373 | 1.3024645 | 1.1687946 |
| H | 4.0050197 | 2.9210250 | 0.5635613 |
| H | 3.6906672 | -2.9024939 | 0.1326661 |
| H | 4.7642342 | -3.1159002 | 1.5174117 |
| H | 4.6172097 | -1.5328026 | 0.7496379 |
| H | 1.8853124 | 0.2521245 | -2.3222863 |
| H | 1.3388611 | -1.1624915 | -3.2257773 |
| H | 2.6277268 | -1.3220432 | -2.0294493 |

$[(\text{SiMe}_3)_3\text{Ge}]^-$ (**9⁻**)

| | | | |
|----|------------|------------|------------|
| C | 1.5448675 | 1.7763516 | 3.6830504 |
| Si | 0.2171742 | 1.5014432 | 2.3141402 |
| C | 0.9977950 | 2.2931348 | 0.7377871 |
| C | -1.2073779 | 2.7077222 | 2.7936762 |
| Ge | -0.5325371 | -0.8267124 | 2.3713038 |
| Si | -2.3577915 | -0.7402620 | 0.7442203 |
| C | -2.8149872 | -2.5033082 | 0.1149348 |
| Si | 1.2155647 | -1.8825864 | 1.0236306 |
| C | 0.9795402 | -3.7944685 | 1.0581427 |
| C | 2.9551466 | -1.6087143 | 1.8061550 |
| C | 1.4659249 | -1.4741162 | -0.8450370 |
| C | -3.9597135 | -0.1213632 | 1.6181544 |
| C | -2.2586263 | 0.3255401 | -0.8603580 |
| H | 2.4381735 | 1.1746227 | 3.4946451 |
| H | 1.1530946 | 1.4799418 | 4.6599980 |
| H | 1.8502396 | 2.8278384 | 3.7398024 |
| H | -0.8260753 | 3.7224920 | 2.9575012 |
| H | -1.7021898 | 2.3780339 | 3.7113930 |
| H | -1.9687329 | 2.7594642 | 2.0102303 |
| H | 0.0414268 | -4.0862870 | 0.5779186 |
| H | 0.9438182 | -4.1562945 | 2.0894060 |
| H | 1.7986222 | -4.3090610 | 0.5419755 |
| H | -3.7468374 | -2.4867673 | -0.4623274 |
| H | -2.9463809 | -3.1934958 | 0.9527920 |
| H | -2.0304232 | -2.9122849 | -0.5276912 |
| H | -3.8466512 | 0.9082495 | 1.9686764 |
| H | -4.1814025 | -0.7405810 | 2.4917993 |

H -4.8240627 -0.1571664 0.9442914
 H 3.7103508 -2.2360076 1.3181790
 H 2.9449141 -1.8553782 2.8713760
 H 3.2746497 -0.5670042 1.7136770
 H 1.2594289 3.3443283 0.9119263
 H 0.3068887 2.2501241 -0.1077705
 H 1.9089379 1.7657632 0.4428439
 H 1.6706442 -0.4107828 -0.9918446
 H 0.5706357 -1.7175616 -1.4238697
 H 2.3034463 -2.0443871 -1.2657693
 H -2.1319091 1.3845421 -0.6197045
 H -3.1722409 0.2233728 -1.4588274
 H -1.4098202 0.0278006 -1.4809352

[(SiMe₃)₃GeH] (9-H)

C 3.2869253 2.6019331 1.4584457
 Si 2.1627996 1.9254114 0.0801125
 C 3.0728415 2.0710510 -1.5862193
 C 0.5930129 3.0007292 0.0086838
 Ge 1.5952469 -0.3875100 0.5454796
 Si -0.3546848 -1.1634198 -0.6737201
 C -0.5935241 -3.0377472 -0.4371014
 Si 3.4861150 -1.9004428 0.3883045
 C 3.1056280 -3.5010297 1.3445872
 C 5.0482349 -1.1137513 1.1407086
 C 3.8459350 -2.3359314 -1.4301706
 C -1.9117903 -0.2779638 -0.0315433
 C -0.1642400 -0.8085657 -2.5349288

H 4.2214865 2.0414466 1.5277445
H 2.7925936 2.5481748 2.4312901
H 3.5374711 3.6499000 1.2665914
H 0.8602739 4.0502955 -0.1482539
H 0.0239427 2.9363592 0.9388690
H -0.0656397 2.6999686 -0.8092114
H 2.2320473 -4.0158327 0.9389838
H 2.9095753 -3.2929089 2.3990877
H 3.9555368 -4.1883163 1.2902955
H -1.5011938 -3.3720195 -0.9491846
H -0.6920405 -3.2961856 0.6197230
H 0.2457247 -3.6058957 -0.8446811
H -1.8457104 0.8035799 -0.1669752
H -2.0636642 -0.4718493 1.0328125
H -2.7986165 -0.6301928 -0.5673473
H 5.8793640 -1.8251581 1.1138718
H 4.8875384 -0.8268122 2.1823855
H 5.3569155 -0.2216965 0.5910911
H 1.1766242 -0.4114060 2.0479961
H 2.4652722 1.6917165 -2.4112338
H 4.0121897 1.5132681 -1.5801603
H 3.3086725 3.1178603 -1.8002744
H 4.0699035 -1.4437663 -2.0198099
H 2.9969913 -2.8398820 -1.8981121
H 4.7086125 -3.0054686 -1.4985698
H -0.0739950 0.2621698 -2.7324381
H -1.0374499 -1.1751663 -3.0829849
H 0.7193385 -1.2994518 -2.9494806

6. References

- 1) A. G. Brook, F. Abdesaken and H. Söllradl, *J. Organomet. Chem.* **1986**, 299, 9-13.
- 2) U. Herzog, N. Schulze, K. Trommer and G. Roewer, *J. Organomet. Chem.* **1997**, 547, 133.
- 3) H. Li, L. J. Hope-Weeks and C. Krempner, *Chem. Comm.* **2011**, 47, 4117-4119.
- 4) H. Li, A. J. A. Aquino, D. B. Cordes, F. Hung-Low, W. L. Hase and C. Krempner, *J. Am. Chem. Soc.* **2013**, 135, 16066-16069.
- 5) M. Schlosser and J. Hartmann, *Angew. Chem.* **1973**, 85, 544-5.
- 6) G. C. Vougioukalakis, M. M. Roubelakis and M. Orfanopoulos, *J. Org. Chem.* **2010**, 75, 4124-4130.
- 7) H. Nakamura, Y. Nakayama, H. Yasuda, T. Maruo, N. Kanehisa and Y. Kai, *Organometallics* **2000**, 19, 5392–5399.
- 8) L. A. Carpino and A. C. Wu, PCT Int. Appl. **1991**, WO 9108190 A1 19910613.
- 9) G. M. Sheldrick, *SADABS v2008/1*, 2008.
- 10) G. M. Sheldrick, *Acta Crystallogr.*, **2008**, A64, 112-122.
- 11) A. D. Becke, *J. Chem. Phys.* **1993**, 98, 5648.
- 12) A. Schäfer, H. Horne and R. Ahlrichs, *J. Chem. Phys.* **1992**, 97, 2571-2577.
- 13) A. Schäfer, C. Huber and R. Ahlrichs, *J. Chem. Phys.* **1994**, 100, 5829-5835.
- 14) A. E. Reed, R. B. Weinstock and F. Weinhold, *J. Chem. Phys.* **1985**, 83, 735-46.
- 15) R. Ahlrichs, M. Bär, M.; Häser, H. Horn and C. Kölmel, *Chem. Phys. Lett.* **1989**, 162, 165.
- 16) NBO, version 3.1 E. D. Glendening, A. E. Reed, J. E Carpenter and F. Weinhold
Theoretical Chemistry Institute WISC-TCI, University of Wisconsin-Madison
- 17) F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, **2005**, 7, 3297-305.
- 18) F. Weigend, *Phys. Chem. Chem. Phys.* **2006**, 8, 1057-65.
- 19) Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O.

Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2009**.