Electronic supporting information

Synthesis of tricyclic 1,4-dihydro-1,4-phosphagermines - trying to establish molecular fencing of reactive centers

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Contents

1. Experimental Section

General considerations

All manipulations and reactions of air and moisture sensitive compounds were performed under inert gas atmosphere (argon) using standard Schlenk line apparatus or working in a glove box. Removal of oxygen traces from Argon gas was done by a copper catalyst (BTS) while silica gel and phosphorus pentoxide was used for drying. Purification of solvents was ensured by boiling them over Na wire and benzophenone (in the case of dichloromethane over calcium hydride) under argon atmosphere prior to use. A MAT 90 or MAT 95 XL spectrometer (70 eV) was used to record mass spectra. The progress of the reactions was monitored via ^{1}H, ^{13}C and $^{31}P\{^{1}H\}$ NMR spectroscopy. NMR measurements were performed on a Bruker AVI (300, 400 and 500 MHz for ^{1}H). 85% H_3PO_4 was used as external standard for ^{31}P NMR spectra while ^{1}H and ^{13}C NMR spectra were referenced to the residual protons of the deuterated solvents. Infrared spectra were recorded on a Nicolet 380 (FT-IR) instrument. For single crystal X-ray diffraction studies, Bruker D8-Venture, STOE IPDS-2T and Bruker X8-Kappa Apex II diffractometers were used.

General synthetic method for 2a,b:

In 50 mL Schlenk flasks imidazole-2-thiones **1a** (100 mg, 0. 78 mmol) and **1b** (100 mg, 0. 47 mmol) were dissolved in 2 mL THF, cooled to –80 °C and then *n*-BuLi (0.532 mL, 0.86 mmol for **1a** & 0.324 mL, 0.518 mmol for **1b**) added while stirring. The reaction mixtures were slowly warmed to –15 °C and kept stirring for 3 h at this temperature. The reaction mixtures were again cooled to –50 °C and bis(diethylamino)dichlorogermane (0.11 mL, 0.39 mmol for **1a** & 0.065 mL, 0.235 mmol for **1b**) was added dropwise and the reaction mixtures then stirred for 12 hours while warming to ambient temperature. The solvent was then removed under reduced pressure (2.5 x 10^{-2} mbar), the residues re-dissolved in toluene and then filtered using a filter cannula to remove the lithium chloride salt. The filtrates were collected and the solvent removed under reduced pressure (3.8 × 10^{-2} mbar). The raw products **2a,b** were washed with *n*-pentane (3 x 5 mL) to remove other impurities and then dried under reduced pressure for an hour (1.2 x 10^{-2} mbar) to obtain white powders.

2a

Yield : 150.5 mg (0.32 mmol, 82 %), white powder, M.p. : 124 °C. ^{1}H NMR(500 MHz, $CDCl_3$): δ = 1.0 (t, 12H, $^{3}J_{H,H}$ = 7.0 Hz, Ge-(N-CH_2-CH_3)$_2$), 2.9 (q, 8H, $^{3}J_{H,H}$ = 7.0 Hz, Ge-(N-CH_2-CH_3)$_2$), 3.6 (d, 12H, $^{3}J_{H,H}$ = 7.0 Hz, N-CH_3), 6.7 (s, 2H, C^5-*H*). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ = 15.1 (s, Ge-(N-CH_2-*C*H_3)$_2$), 35.4 (s, Ge-(N-*C*H_2-CH_3)$_2$), 35.9 (s, Ge-(N-*C*H_2-CH_3)$_2$), 41.1 (s, N-*C*H_3), 117.5 (s, *C*^{5}), 123.8, 126.8 (s, *C*^{4}), 166.1 (s, *C*=S). IR: ṽ (cm^{-1}) = 2965 (*w*), 1442 (*m*), 1383 (*s*), 1182 (*s*), 1155 (*s*), 898 (*m*), 779 (*s*), 622 (*s*). EI-MS (70 eV): m/z (%) = 472.1 (90), $[M]^+$, 400.1 (90), $[C_{14}H_{24}N_5S_2Ge]^+$, 328.0 (100), $[C_{10}H_{14}N_4S_2Ge]^+$. HRMS: for $C_{18}H_{34}GeN_6S_2$ theor./exp. 468.1529/468.1524. EA (%): exp. C 45.13, H 6.66, N 17.55, S 14.04. Calc. C 45.88, H 7.27, N 17.83, S 13.61.

2b

Yield : 80 mg (0.124 mmol, 53 %), white powder, M.p. : 148 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.8 (t, 6H, $^{3}J_{H,H}$ = 7.5 Hz, $NCH_2CH_2CH_2CH_3$), 0.9 (t, 6H, $^{3}J_{H,H}$ = 7.3 Hz, $NCH_2CH_2CH_2CH_3$), 1.0 (t, 12H, $^{3}J_{H,H}$ = 7.0 Hz, Ge-(N-CH_2-CH_3)$_2$), 1.1–1.2 (m, 4H, $NCH_2CH_2CH_2$Me), 1.3–1.4 (m, 4H, $NCH_2CH_2CH_2$Me), 1.4–1.5 (m, 4H, $NCH_2CH_2CH_2$Me), 1.7–1.8 (m, 4H, $NCH_2CH_2CH_2$Me), 2.9 (q, 8H, $^{3}J_{H,H}$ = 7.0 Hz, Ge-(N-CH_2-CH_3)$_2$), 3.9 (t, 4H, $^{3}J_{H,H}$ = 8.1 Hz , N*C*$H_2$$CH_2CH_2$Me), 4.0 (t, 4H, $^{3}J_{H,H}$ = 7.5 Hz , N*C*$H_2$$CH_2CH_2$Me), 6.8 (s, 2H, C^5-*H*). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ = 13.8 (s, Ge-*(*N-CH_2-*C*H_3)$_2$), 15.2 (s, $NCH_2CH_2CH_2CH_3$), 20.0 (s, $NCH_2CH_2CH_2$Me), 20.2 (s, $NCH_2CH_2CH_2$Me), 30.2 (s, $NCH_2CH_2CH_2$Me), 31.0 (s, $NCH_2CH_2CH_2$Me), 41.4 (s, Ge-(N-*C*H_2-CH_3)$_2$), 47.9 (s, N*C*$H_2CH_2CH_2$Me), 48.6 (s, N*C*$H_2CH_2CH_2$Me), 123.1 (s, *C*^{5}), 125.5 (s, *C*^{4}), 165.2 (s, *C*=S). IR : ṽ (cm-1) = 2961 (*w*), 1417 (*w*), 1262 (*s*), 1091 (*s*), 1016 (*s*), 799 (*s*). EI-MS (70 eV): m/z (%) = 640.1 (20), $[M]^+$, 568.1 (30), $[C_{26}H_{48}GeN_5S_2]^+$, 496.2 (30), $[C_{22}H_{38}GeN_4S_2]^+$. HRMS: for $C_{30}H_{58}GeN_6S_2$ theor./exp. 636.3407/636.3402.

Synthetic method for 2c:

To a cooled suspension of IMes(S) (1.00 g, 2.97 mmol) in THF (30 mL) at −80 °C was added *n*-BuLi (1.86 mL, 2.97 mmol, 1.6 M in hexane, 2 eq.) with stirring. The reaction mixture was brought to room temperature over a period of 1 h and further stirred for 2 h. A colour change from pale yellow to maroon was observed. The solution was again cooled to −80 °C and a solution of Et_2NGeCl_3 (373 mg, 1.48 mmol) in THF (5 mL) was added dropwise with stirring. The reaction mixture was brought to −40 °C over a period of 1 h and stirred at this temperature for 16 h before warming it up to room temperature. The volatiles were removed in *vacuo* to give off white solid residue and the desired product was extracted in toluene (25 mL). Toluene was removed in *vacuo* and the residue was re-dissolved in THF (15 mL). The THF solution was concentrated (approx. 5 mL) until incipient crystallization was

observed and left undisturbed for a few hours. White crystals of **2c** were obtained and filtered. Thereafter, the supernatant was concentrated further (approx. 2 mL) and left undisturbed for a few hours to give another crop of crystals. The crystals were washed with cold (−80 °C) THF (2 mL) and dried under vacuum for 6 h. Even after drying under high vacuum (5×10^{-4} mbar), compound **2c** retained THF in it in 1:1 molar ratio. The crystals suitable for single crystal X-ray diffraction studies were grown from saturated solution of **2c** in toluene by keeping it at room temperature for 24 h.

Yield: 900 mg (0.97 mmol, 66%), white powder, M.p. 252 °C. ^{1}H NMR (300 MHz, C_6D_6): δ = 0.87 (6H, t, $^3J_{HH}$ = 6.9 Hz, N(CH_2CH_3)$_2$), 1.42 (4H, m, (CH_2CH_2)$_2$O), 1.84 (6H, s), 2.05 (6H, s), 2.11 (6H, s), 2.18 (6H, s), 2.20 (6H, s), 2.26 (6H, s), 2.89 (4H, t, $^3J_{HH}$ = 6.8 Hz, N(CH_2CH_3)$_2$), 3.57 4H, m, (CH_2CH_2)$_2$O), 6.02 (2H, 2×(SCN_2C_2H)), 6.70-6.76 (8 H, m, 4×(2,4,6-$(CH_3)_3C_6H_2$). ^{1}H NMR (500 MHz, THF-d_8): δ = 1.00 (6H, t, $^3J_{HH}$ = 7.0 Hz, N(CH_2CH_3)$_2$), 2.01 (12H, b), 2.03 (6H, s), 2.04 (6H, s), 2.15 (6H, s), 2.32(6H, s), 3.00 (4H, t, $^3J_{HH}$ = 6.9 Hz, N(CH_2CH_3)$_2$), 6.35 (2H, 2×(SCN_2C_2H)), 6.82 (2H, s, 2,4,6-$(CH_3)_3C_6H_2$), 6.87 (2H, s, 2,4,6-$(CH_3)_3C_6H_2$), 6.98 (2H, s, 2,4,6-$(CH_3)_3C_6H_2$), 7.02 (2H, s, 2,4,6-$(CH_3)_3C_6H_2$). ^{13}C{^{1}H} NMR (125 MHz, THF-d_8): δ = 14.62 (N(CH_2CH_3)$_2$), 17.86, 18.31, 18.45, 18.52, 20.63, 20.94, 41.01 (N(CH_2CH_3)$_2$), 120.42, 129.40, 129.45, 129.57, 129.62, 129.79, 134.56, 134.82, 135.81, 136.63, 137.36, 137.74, 139.46, 139.75, 168.78 (>*C*=S). EA (%): exp. C 65.01, H 6.79, N 7.57, S 7.04. Calc. C 65.04, H 6.99, N 7.59, S 7.53.

General synthetic method for 3a and **4a:**

Ge-bridged derivative **2a** (100 mg, 0. 212 mmol) were taken in 50 mL Schlenk flasks, each dissolved in THF, and *n*-BuLi (0.29 mL, 0.466 mmol) was added on stirring at room temperature. The reaction mixtures were stirred for 4 h at this temperature. The reaction mixtures were cooled down to –80 °C and phosphanes (diisopropyl(dichloro)phosphane : 0.038 mL, 0.212 mmol, dichloro(phenyl)phosphane : 0.028 mL, 0.212 mmol) were added dropwise into the reaction mixture. The reaction mixture was then stirred for 12 hours while warming to ambient temperatures. The solvent was then removed under reduced pressure (1.7 x 10^{-2} mbar) , residue were re-dissolved in toluene and filtered using a filter cannula to remove the lithium chloride salt. The filtrates were collected and the solvent removed under reduced pressure (1.4 x 10^{-2} mbar). The raw products **3a** and **4a** were washed with *n*-pentane (3 x 5 mL) to remove other impurities and then dried under reduced pressure for an hour (1.5 x 10^{-2} mbar) to obtain white powders.

3a

Yield : 60 mg (0.1 mmol, 48 %), white powder, M.p. : 143 °C. ^{1}H NMR (300 MHz, $CDCl_3$) : δ = 0.9 (t, 6H, $^3J_{H,H}$ = 7.1 Hz, *Ge-(*N-CH_2-CH_3)$_2$), 1.1 (t, 6H, $^3J_{H,H}$ = 7.0 Hz, Ge-*(*N-CH_2-CH_3)$_2$), 1.1-1.2 (m, 12H, N-^{i}*Pr,* N-CH-((CH_3)$_2$), 2.8 (q, 4H, $^3J_{H,H}$ = 7.1 Hz, Ge-*(*N-CH_2-CH_3)$_2$), 3.0 (q, 4H, $^3J_{H,H}$ = 7.1 Hz, Ge-*(*N-CH_2-CH_3)$_2$), 3.3-3.5 (m, 2H, N-^{i}*Pr,* N-*C*H-Me_2), 3.7 (s, 6H, *N*-CH_3), 3.8 (s, 6H, *N*-CH_3). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) : δ = 14.6 (s, Ge-*(*N-CH_2-CH_3)$_2$), 14.7 (s, Ge-*(*N-CH_2-CH_3)$_2$), 34.7 (s, N-^{i}*Pr,* N-CH-((CH_3)$_2$), 34.8 (s, N-^{i}*Pr,* N-CH-((CH_3)$_2$), 35.7 (s, Ge-*(*N-CH_2-CH_3)$_2$), 35.8 (s, N-^{i}*Pr,* N-CH_2-Me_2), 39.6 (s, *N*-CH_3), 40.8 (s, *N*-CH_3), 130.6 (s, C^5), 133.3 (s, C^4), 167.3 (s, *C*=S). ^{31}P{^{1}H} NMR (121.5 Hz, $CDCl_3$) : δ = –17.5. IR : $\tilde{\nu}$ (cm^{-1}) = 2965 (*w*), 1430 (*w*), 1376 (*s*), 1160 (*s*), 1018 (*s*), 968 (*s*), 830 (*s*). EI-MS (70 eV): m/z (%) = 601.2 (100) $[M]^+$, 430.1 (90) $[C_{15}H_{28}GeN_6S_2]^+$. HRMS: for $C_{24}H_{46}GeN_7PS_2$ theor./exp. 601.2205/601.2213. EA(%) : exp. C 45.98, H 7.21, N 14.65, S 9.43. Calc. C 48.01, H 7.72, N 16.33, S 10.68.

4a

Yield : 82 mg (0.142 mmol, 67 %), white powder, M.p. : 145 °C. ^{1}H NMR (500 MHz, $CDCl_3$) : δ = 0.9 (*br*. t, 6H, Ge-*(*N-CH_2-CH_3)$_2$), 1.0 (*br*. t, 6H, Ge-*(*N-CH_2-CH_3)$_2$), 2.8 (*br*. q, 4H, Ge-*(*N-CH_2-CH_3)$_2$), 3.0 (*br*. q, 4H, Ge-*(*N-CH_2-CH_3)$_2$), 3.4 (s, 6H, *N*-CH_3), 3.7 (s, 6H, *N*-CH_3), 7.3 (*br*. m, 2H, P-*Ph* protons), 7.4 (*br*. m, 3H, P-*Ph* protons).^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) : δ = 14.4 (s, Ge-(N-CH_2-CH_3)$_2$), 14.6 (s, Ge-*(*N-CH_2-CH_3)$_2$), 33.7 (s, Ge-*(*N-CH_2-CH_3)$_2$), 33.8 (s, Ge-*(*N-CH_2-CH_3)$_2$), 39.8 (s, *N*-CH_3), 40.0 (s, *N*-CH_3), 130.1 (d, P-*Ph*), 130.3 1(d, P-*Ph*), 130.4 (d, P-*Ph*), 131.4 (s, C^5), 134.0 (s, C^4), 134.2 (s, C^4), 167.7 (s, *C*=S). ^{31}P{^{1}H} NMR (200 Hz, $CDCl_3$) : δ = –55.6. IR : $\tilde{\nu}$ (cm^{-1}) = 2970 (*w*), 1437 (*m*), 1378 (*s*), 1337 (*w*) 1161 (*s*), 1061 (*s*), 1016 (*w*), 834 (*s*), 695 (*s*). EI-MS (70 eV): m/z (%) = 578.1 (40) $[M]^+$, 434.0 (60) $[C_{16}H_{17}GeN_4PS_2]^{+\bullet}$. HRMS: for $C_{24}H_{37}GeN_6PS_2$ theor./exp. 578.1470/578.1467. EA(%) : exp. C 50.45, H 6.12, N 12.52, S 10.19. Calc. C 49.93, H 6.46, N 14.56, S 11.11.

Synthetic method for 5:

Compound **1** (70 mg, 0.08 mmol) was dissolved in THF (5 mL) and cooled down to −80 °C. To this was added MeLi (0.15 mL, 0.23 mmol, 1.6 M in diethylether) with stirring. The reaction mixture was brought to −40 °C and stirred at this temperature for 2 h upon which reaction solution turned yellow. Then −40 °C bath was replaced with ice-bath for 10 min. The reaction mixture was cooled down to −60 °C and diluted PCl_3 (7 µL, 0.08 mmol in 1 mL THF) was added to it dropwise with vigorous stirring. After

complete addition, the reaction mixture was allowed to warm up to room temperature and stirred for additional 3 h. All the volatiles were removed under reduced pressure and the product was extracted in diethylether (10 mL). The extract solution was concentrated to 2 mL and allowed to stand overnight upon which yellow precipitate was obtained. Single crystal suitable for X-ray diffraction analysis was obtained from slow evaporation of THF solution of the product. ^{31}P NMR (200 MHz, THF-d_8): δ = 17.07, 17.05.

2. Spectra for compound **2a**

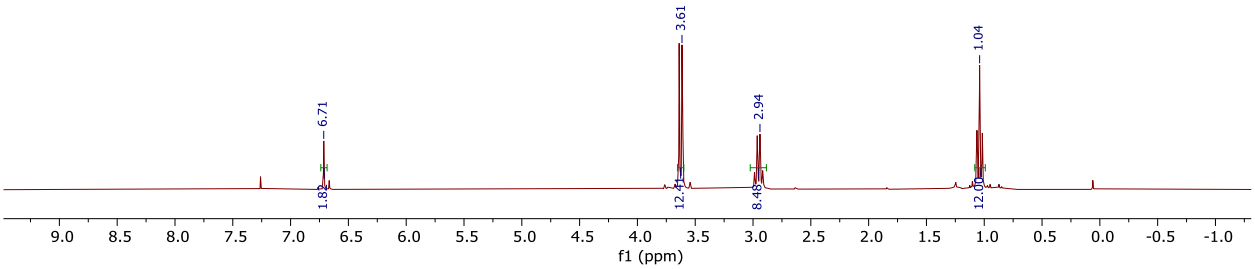

Figure S1. ^{1}H NMR spectrum in $CDCl_3$ (300 MHz, 25 °C).

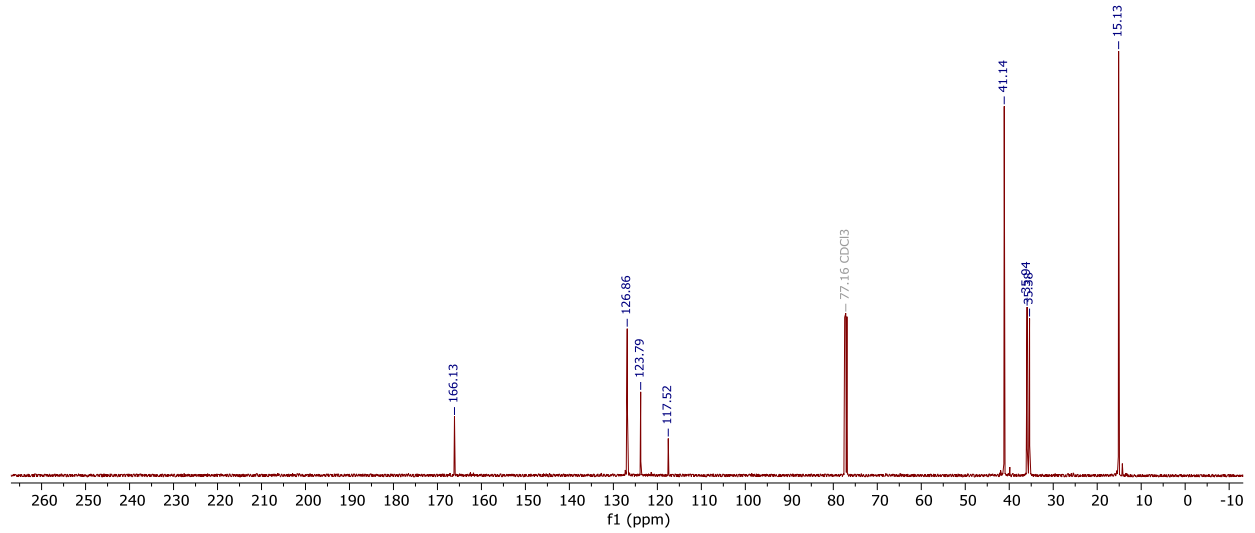

Figure S2.^{13}C NMR spectrum in $CDCl_3$ (75 MHz, 25 °C).

3. Spectra for compound **2b**

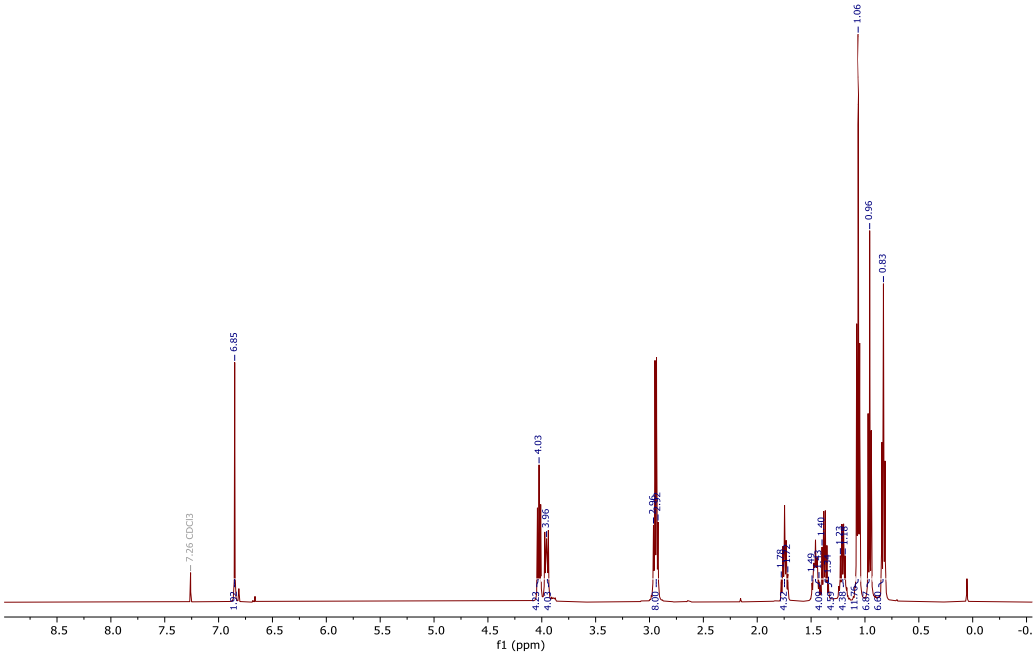

Figure S3.^{1}H NMR spectrum in $CDCl_3$ (300 MHz, 25 °C).

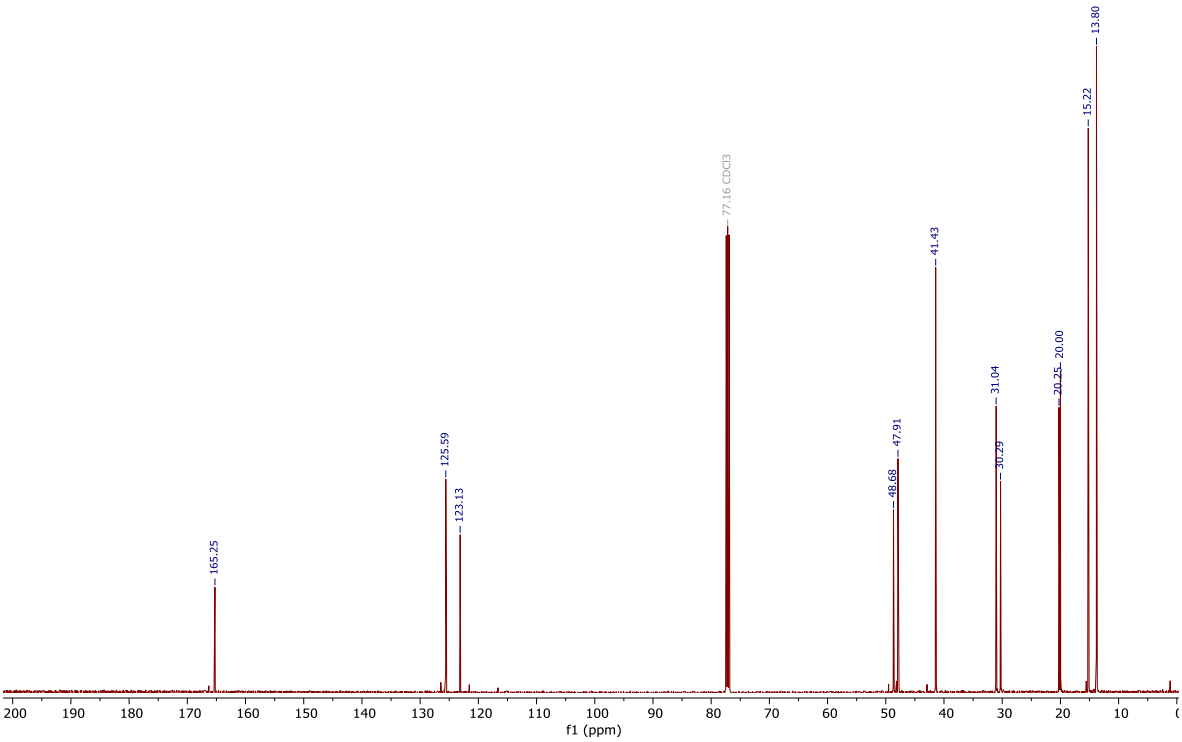

Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum in $CDCl_3$ (75 MHz, 25 °C).

4. Spectra for **2c**

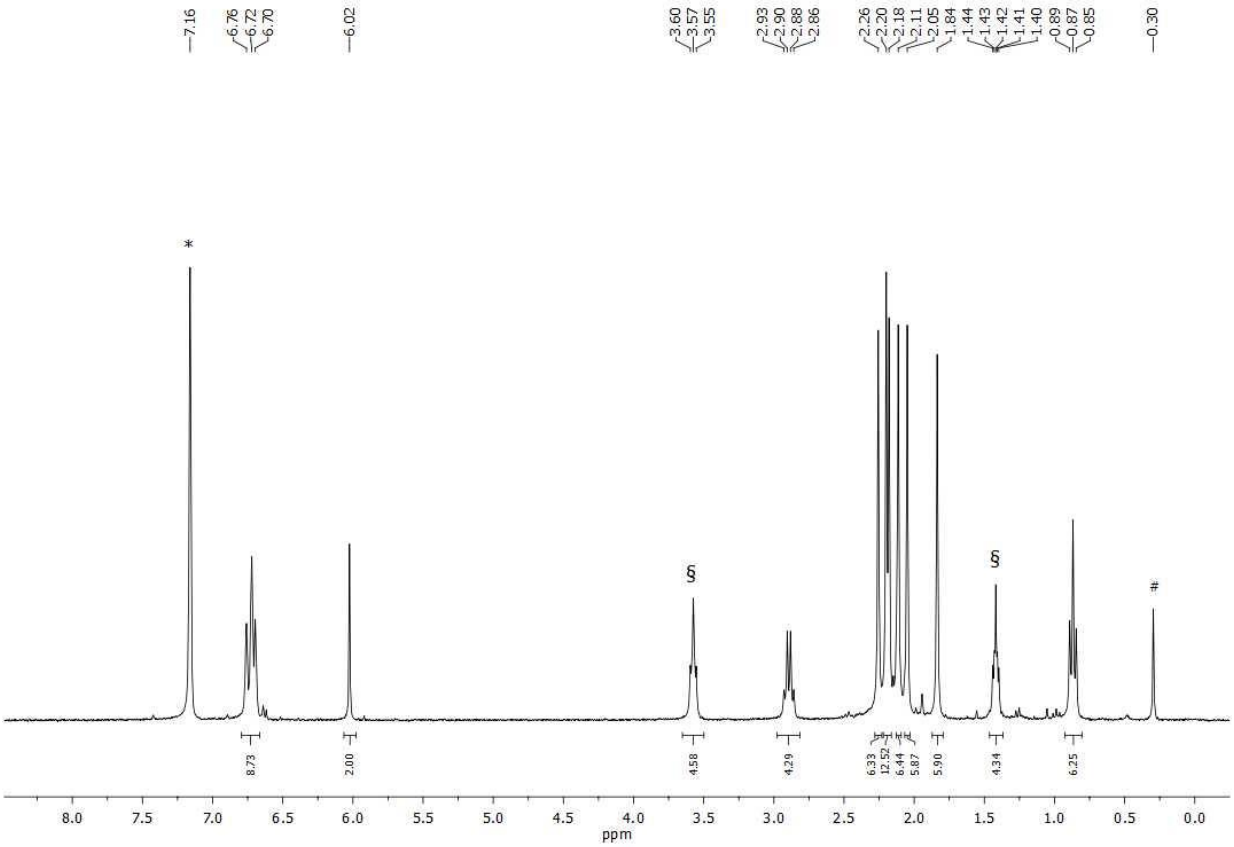

Figure S5. ^{1}H NMR spectrum in C_6D_6 (300 MHz, 25 °C). Residual solvent and grease signals are marked with * and #, respectively. Signals marked with § correspond to THF.

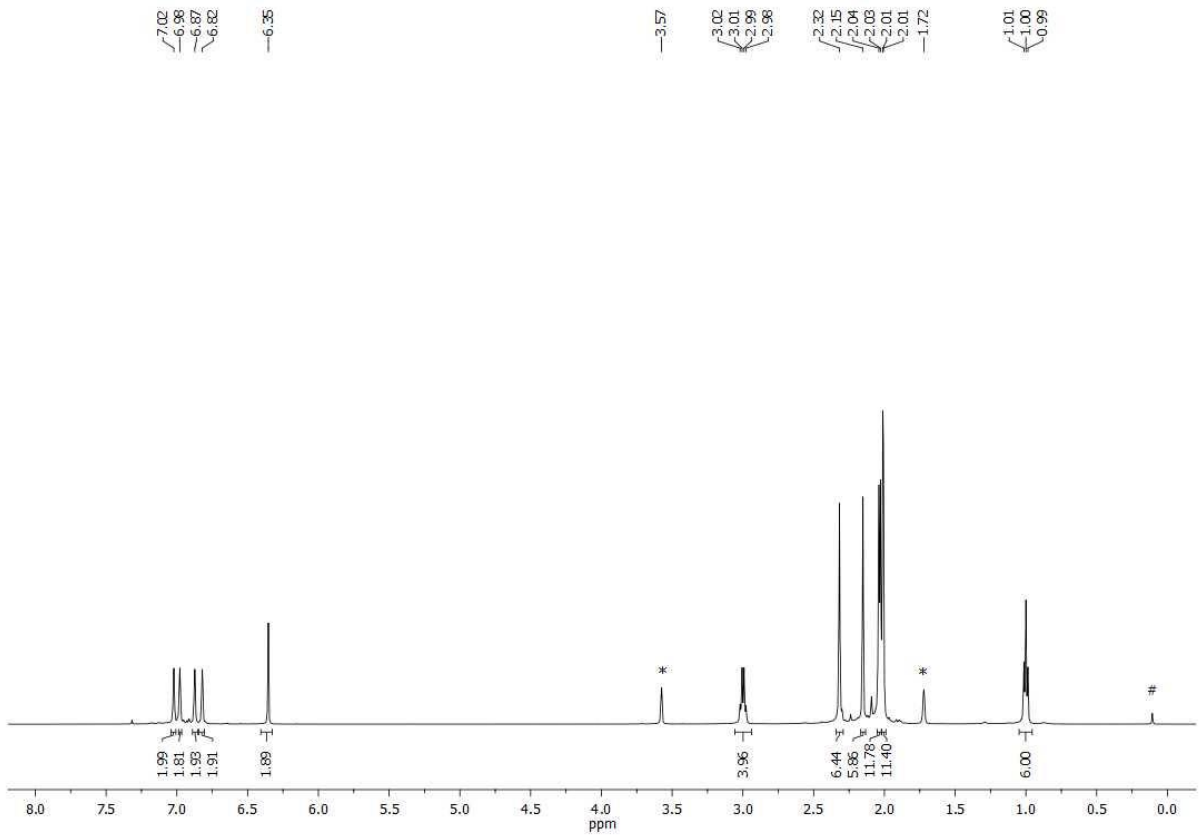

Figure S6. ^{1}H NMR spectrum in THF-d_8 (500 MHz, 25 °C). Residual solvent and grease signals are marked with * and #, respectively.

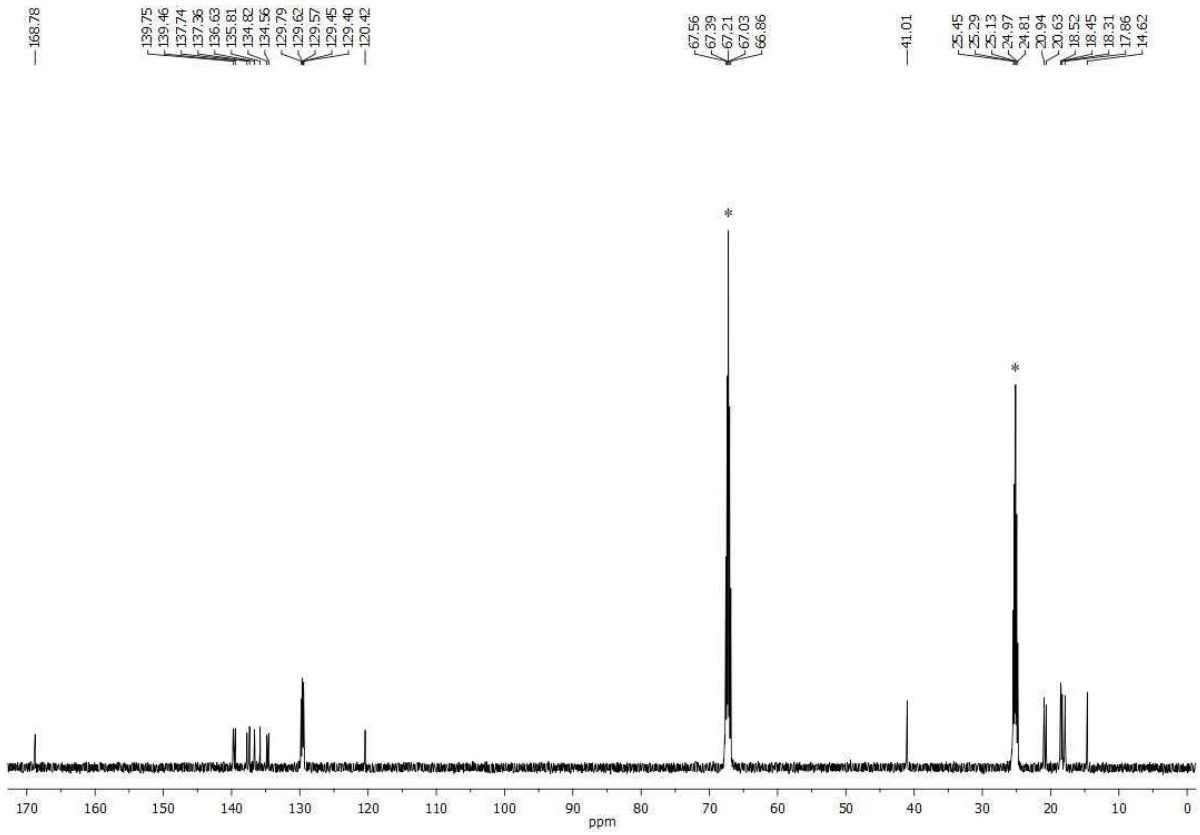

Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum in THF-d_8 (125 MHz, 25 °C). Residual solvent signals are marked with *.

5. Spectra for compound **3a**

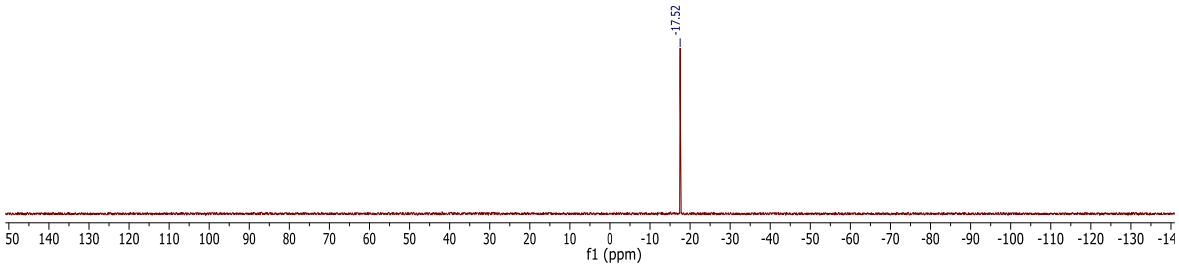

Figure S8. $^{31}P\{^{1}H\}$ NMR spectrum in $CDCl_3$ (121.5 MHz, 25 °C).

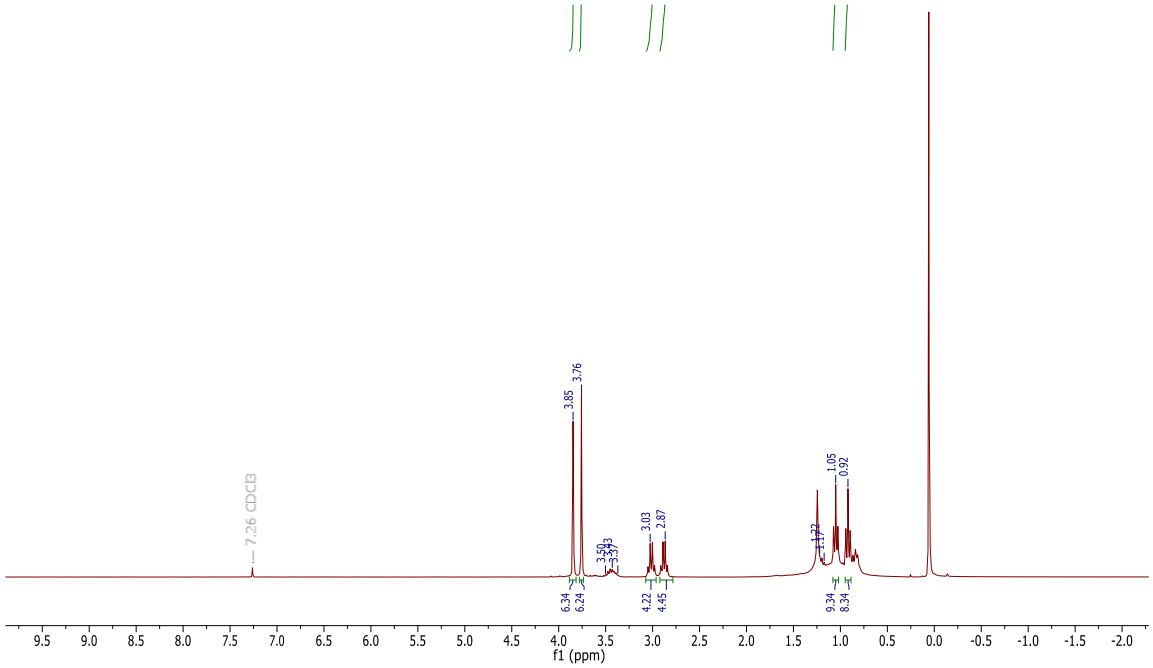

Figure S9.^{1}H NMR spectrum in $CDCl_3$ (300 MHz, 25 °C). *Here, the significant signal at δ = 0.07 ppm corresponds to the silicone grease present in the deuterated solvent.*

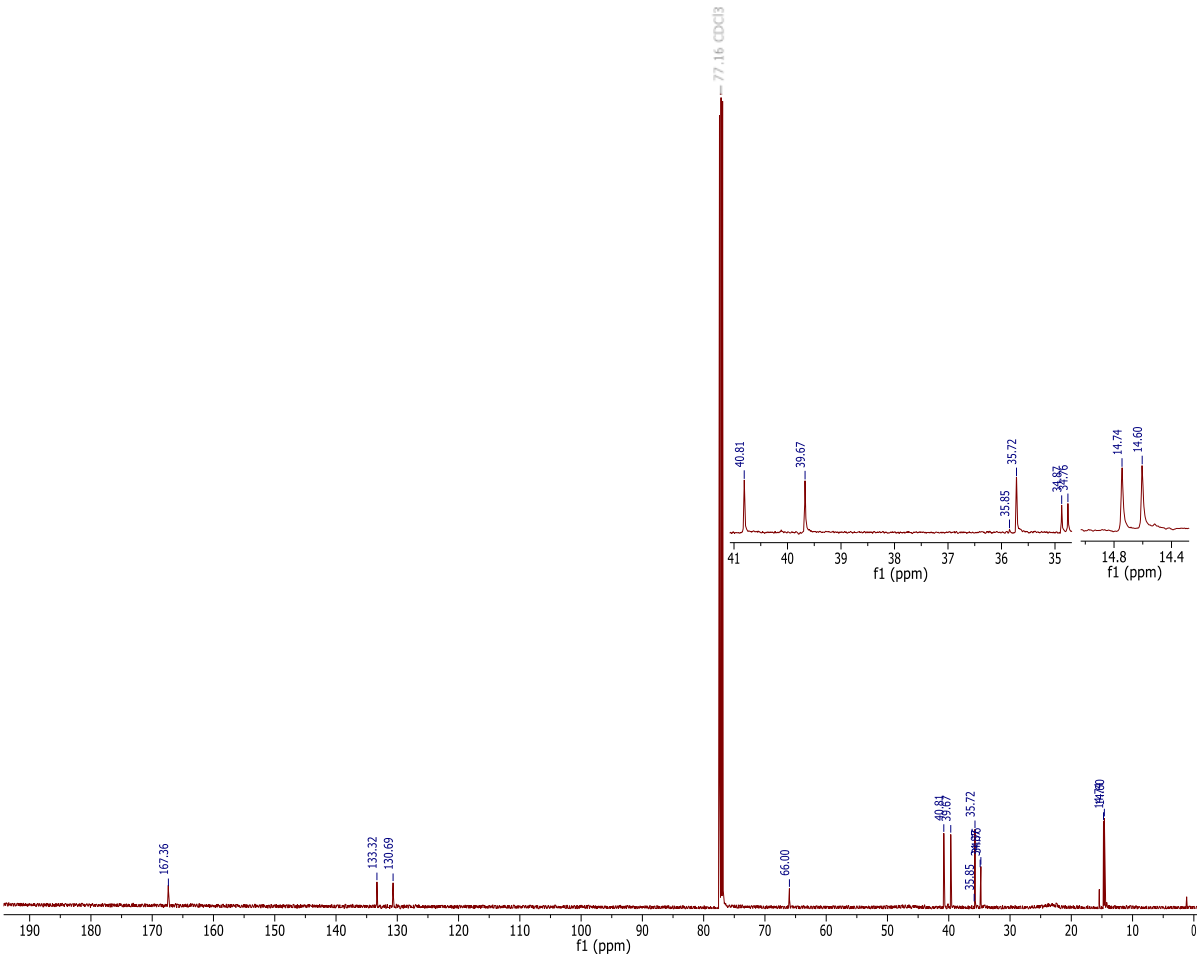

Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum in $CDCl_3$ (75 MHz, 25 °C).

6. Spectra for **4a**

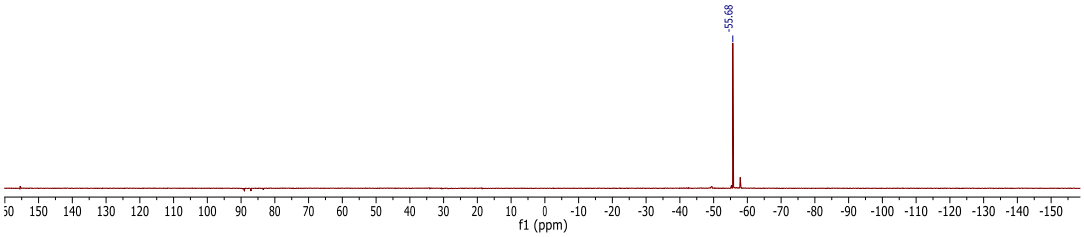

Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum in $CDCl_3$ (121.5 MHz, 25 °C).

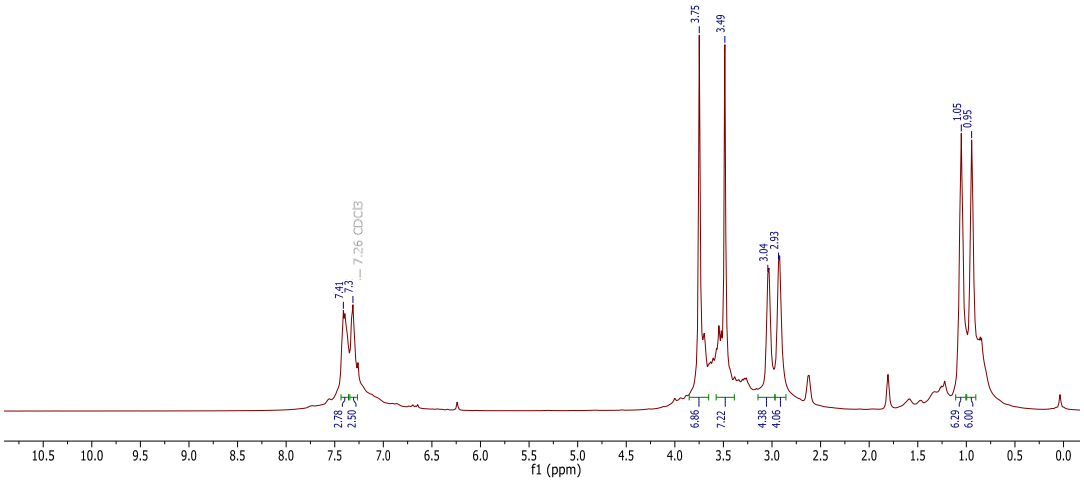

Figure S12.^{1}H NMR spectrum in $CDCl_3$ (300 MHz, 25 °C).

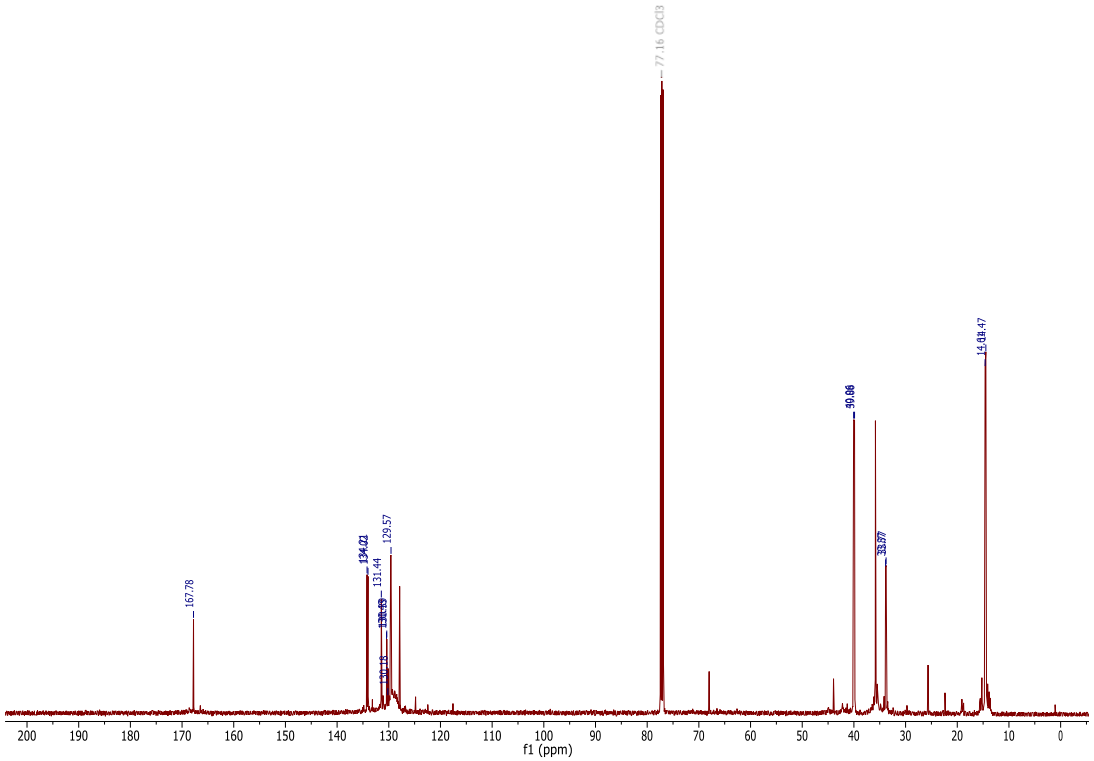

Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum in $CDCl_3$ (75 MHz, 25 °C).

7. Spectrum for **5**

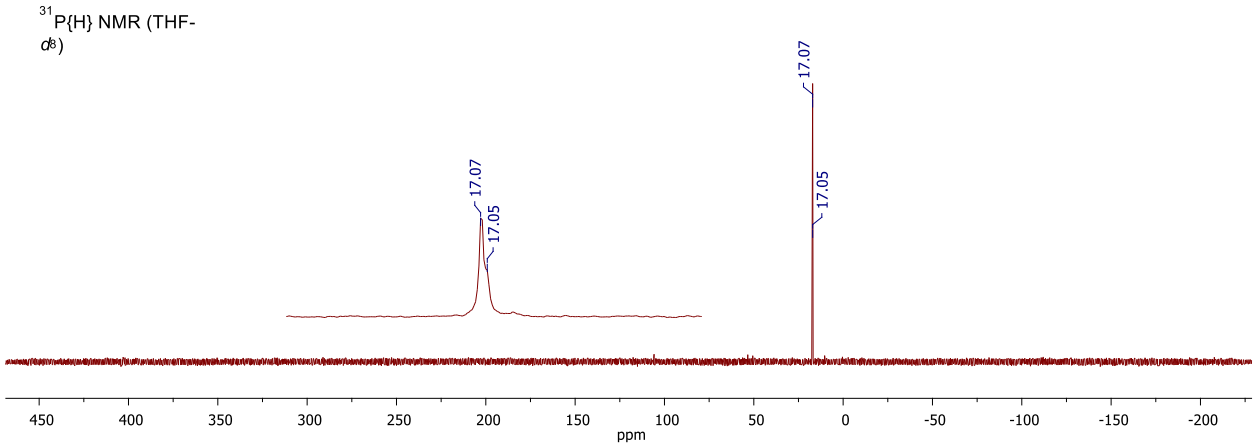

Figure S14. $^{31}P\{^{1}H\}$ NMR spectrum in THF-d_8 (121.5 MHz, 25 °C).

8. X-ray diffraction studies

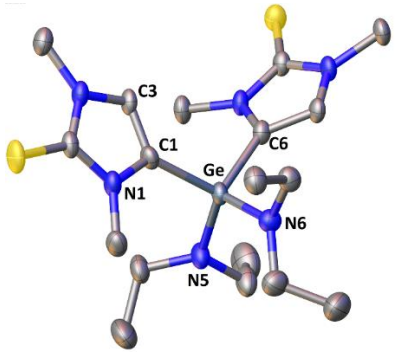

Figure S15. Molecular structure of compound **2a** (50 % probability level)**:** hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Ge-C1 1.936(4) , Ge-N6 1.823(3), C1-N1 1.404(5), C1-C3 1.352(6) ; C1-Ge-C6 107.38(16), N5-Ge-C6 111.58(16), N5-Ge-N6 107.68(16), N6-Ge-C1 110.96(15).

Crystal Data for **2a**: Suitable single-crystals of **2a** were obtained from a concentrated diethyl ether solution at −20 °C. Data were collected with a with a STOE STADIVARI diffractometer equipped with a low-temperature device at 100 K by using graphite monochromated Cu Kα radiation (λ = 1.54186 Å). $C_{40}H_{78}Ge_2N_{12}OS_4$, M = 1016.56, crystal dimensions 0.4 × 0.1 × 0.05 mm^3, triclinic, space group *P*-1, Z = 2, a = 10.4910(7) Å, b = 15.5099(8) Å, c = 17.3593(10) Å, α = 75.118(4)°, β = 72.831(5)°, γ = 81.836(5)°, V = 2601.5(3) $Å^3$, ρ_{calc} = 1.298 gcm^{-3}, μ = 3.251 mm^{-1}, T = 100 K, transmission factors (min./max.) 0.2573/ 0.4835, empirical absorption correction, $2\theta_{max}$= 135.468°, no. of unique data 9314 [R_{int} = 0.0777, R_{sigma} = 0.0480], R_1 (for I > 2σ(I)) = 0.0545, wR_2 (for all data) = 0.1582, final R = 0.0769, goodness of fit 1.020, ΔF(max./min.) 0.62/-0.87e $Å^{-3}$. CCDC number **2330268.**

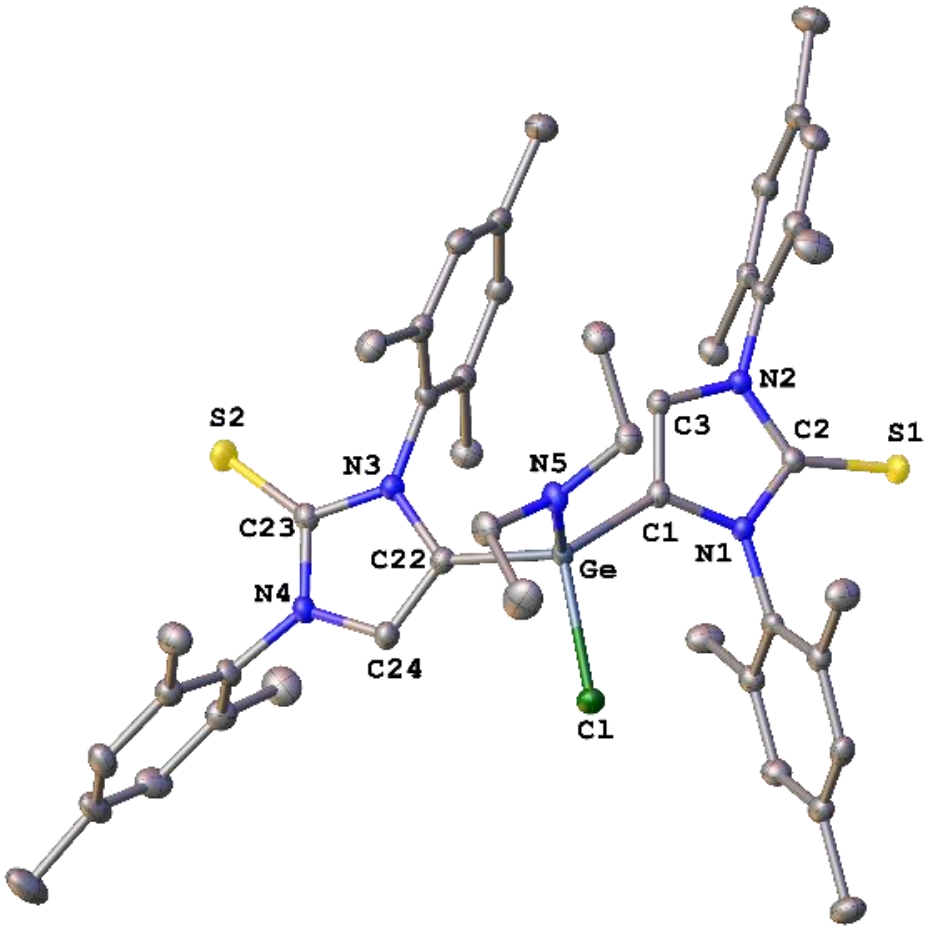

Figure S16. Molecular structure of **2c**. Hydrogen atoms and solvent molecule are omitted for clarity (50 % probability level). Selected bond lengths [Å] and angles [°]: Ge-Cl 2.180(3), Ge-N5 1.794(2), Ge-C1 1.928(2), Ge-C22 1.933(3); Cl-Ge-N5 110.86(9), Cl-Ge-C1 111.06(12), Cl-Ge-C22 99.72(10), C1-Ge-C22 115.81(8), N5-Ge-C1 108.08(12), N5-Ge-C22 111.15(13).

Crystal Data for **2c**: Suitable single were grown from saturated solution of **2c** in toluene by keeping it at room temperature for 24 h Data were collected with a with a STOE STADIVARI diffractometer equipped with a low-temperature device at 100 K by using graphite monochromated Cu Kα radiation (λ = 1.54186 Å). $C_{46}H_{56}ClGeN_5S_2$, M = 943.25, crystal dimensions 0.19 × 0.14 × 0.09 mm^3, monoclinic, space group $P2_1/n$, Z = 4, a = 10.74459(15) Å, b = 26.5970(5) Å, c = 17.9341(3) Å, α = 90.00°, β = 104.142(1) °, γ = 90.00°, V = 4969.8(1) $Å^3$, ρ_{calc} = 1.261 gcm^{-3}, μ = 2.418 mm^{-1}, T = 100 K, transmission factors (min./max.) 0.5369/0.6023, empirical absorption correction, $2\theta_{max}$= 140.938 °, no. of unique data 9383 [R_{int} = 0.0286, R_{sigma} = 0.0190], R_1 (for I > 2σ(I)) = 0.0276, wR_2 (for all data) = 0.0706, final R = 0.0335, goodness of fit 1.017, ΔF(max./min.) 0.32/-0.54e $Å^{-3}$. CCDC number: **2330269**.

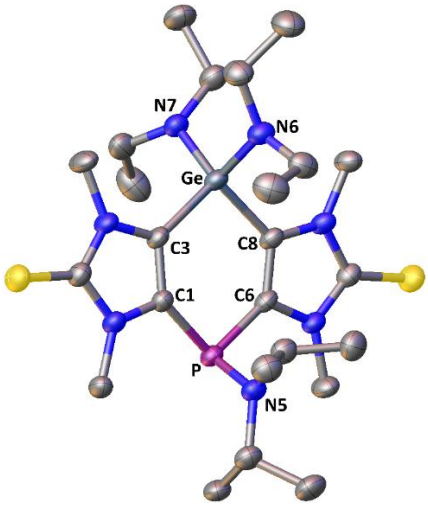

Figure S17. Molecular structure of **3a;** hydrogen atoms are omitted for clarity (50 % probability level). Selected bond lengths [Å] and angles [°]: Ge-N6 1.810(3), P-N5 1.689(3), P-C1 1.835(4), Ge-C3 1.936(4), C1-C3 1.376(5); Σ<°P 306.83, C3-Ge-C8 98.39(15), N6-Ge-C3 118.23(16), N6-Ge-N7 105.19(15), N6-Ge-C8 107.45(15).

Crystal Data for **3a**: Suitable single-crystals of **3a** were obtained from a concentrated diethyl ether solution at −20 °C. Data were collected with a with a STOE STADIVARI diffractometer equipped with a low-temperature device at 100 K by using graphite monochromated Cu Kα radiation (λ = 1.54186 Å). $C_{24}H_{46}GeN_7PS_2$, M = 600.36, crystal dimensions 0.21 × 0.15 × 0.05 mm^3, triclinic, space group *P*-1, Z = 2, a = 8.9922(3) Å, b = 10.9651(3) Å, c = 15.4675(5) Å, α = 87.642(3)°, β = 81.540(3)°, γ = 79.789(3)°, V = 1484.44(8) Å^3, ρ_{calc} = 1.343 g cm^{-3}, μ = 3.423 mm^{-1}, T = 100 K, transmission factors (min./max.) 0.3874/0.5059, empirical absorption correction, $2\theta_{max}$= 140.974°, no. of unique data 5589 [R_{int} = 0.0516, R_{sigma} = 0.0321], R_1 (for I > 2σ(I)) = 0.0547, wR_2 (for all data) = 0.1599, final R = 0.0697, goodness of fit 1.071, ΔF(max./min.) 1.57/-0.45e Å^{-3}. CCDC number: **2330270**

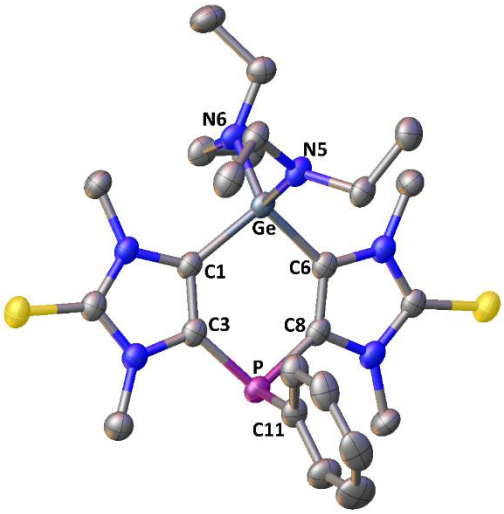

Figure S18. Molecular structure of **4a;** hydrogen atoms are omitted for clarity (50 % probability level). Selected bond lengths [Å] and angles [°]: Ge-N5 1.8092(18), P-C11 1.847(2), P-C8 1.818(2), Ge-C1 1.939(2), C6-C8 1.361(3); Σ<°P 302.1, C1-Ge-C6 98.42(10), N5-Ge-C6 109(9), N5-Ge-N6 107.6(9), N6-Si-C1 108.6(9).

Crystal Data for **4a**: Suitable single-crystals of **4a** were obtained from a concentrated diethyl ether solution at −20 °C. Data were collected with a with a STOE STADIVARI diffractometer equipped with a low-temperature device at 100 K by using graphite monochromated Cu Kα radiation (λ = 1.54186 Å). $C_{52}H_{84}Ge_2N_{12}OP_2S_4$, M = 1228.71, crystal dimensions 0.3 × 0.3 × 0.1 mm^3, monoclinic, space group *C2/c*, Z = 4, a = 19.4838(7) Å, b = 11.2254(3) Å, c = 30.2357(11) Å, α = 90.00°, β = 112.700(3)°, γ = 90.00

°, V = 6100.7(4) Å^3, ρ_{calc} = 1.338 gcm^{-3}, μ = 3.352 mm^{-1}, T = 100 K, transmission factors (min./max.) 0.1971/0.3168, empirical absorption correction, $2\theta_{max}$= 140.984°, no. of unique data 5798 [R_{int} = 0.0562, R_{sigma} = 0.0281], R_1 (for I > 2σ(I)) = 0.0460, wR_2 (for all data) = 0.1271, final R = 0.0498, goodness of fit 1.042, ΔF(max./min.) 0.92/-0.83e Å^{-3}. CCDC number: **2330271**

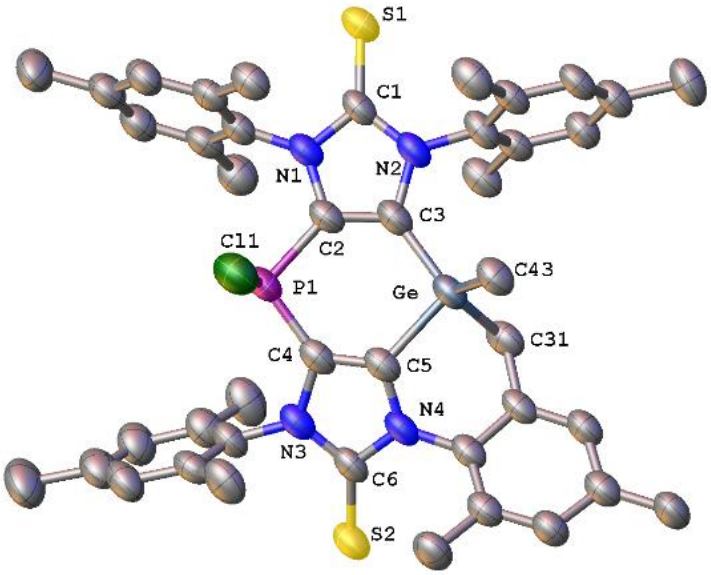

Figure S19. Molecular structure of **5**. Hydrogen atoms and solvent molecules are omitted for clarity (50 % probability level). Selected bond lengths [Å] and angles [°]: Ge-C3 1.891(18), Ge-C5 1.967(15), Ge-C31 1.991(17), Ge-C43 1.956(19), P1-C2 1.835 (15), P1-C4 1.777(18), P1-Cl1 2.065(8); Σ<°P1 302, C2-P1-C4 98.7(7), C3-Ge-C5 97.5 (7), C3-Ge-C31 119.3(8), C5-Ge-C31 92.6(7).

Crystal Data for **5**: Suitable single-crystals of **5** were obtained from slow eevaporation of a THF solution. Data were collected with a with a STOE STADIVARI diffractometer equipped with a low-temperature device at 100 K by using graphite monochromated Cu Kα radiation (λ = 1.54186 Å). $C_{43}H_{46}ClGeN_4PS_2$, M = 966.17, crystal dimensions 0.14 × 0.08 × 0.03 mm^3, triclinic, space group *P*-1, Z = 2, a = 13.9471(11) Å, b = 14.1197(13) Å, c = 14.5100(12) Å, α = 70.439(7)°, β = 78.468(6)°, γ = 66.212(7)°, V = 6100.7(4) Å^3, ρ_{calc} = 1.306 gcm^{-3}, μ = 2.782 mm^{-1}, T = 100 K, transmission factors (min./max.) 0.1228/0.6334, empirical absorption correction, $2\theta_{max}$= 135.496°, no. of unique data 113633 [R_{int} = --, R_{sigma} = 0.5668], R_1 (for I > 2σ(I)) = 0.1397, wR_2 (for all data) = 0.4121, final R = 0.3739, goodness of fit 0.924, ΔF(max./min.) 1.39/-0.80e Å^{-3}. CCDC number: **2330272**

9. Computational details

All DFT calculations are performed with the TURBOMOLE 7.4 suite of programs.[1] The structures are fully optimized at the TPSS-D3/def2-SVP + COSMO level in THF solution, which combines the TPSS meta-GGA density functional[2] with the BJ-damped DFT-D3 dispersion correction[3] and the def2-SVP basis set,[4] using the Conductor-like Screening Model (COSMO)[5] for THF solvent (dielectric constant ε = 7.58 and radius R_{solv} = 3.18 Å). The density-fitting RI-J approach[6] is used to accelerate the calculations. The optimized structures are characterized by frequency analysis (no imaginary frequency for true minima and only one imaginary frequency for transition states) to provide thermal free-energy corrections (at 298.15 K and 1 atm) according to the modified ideal gas–rigid rotor–harmonic oscillator model.[7] The connection between TSs and minima is established by visually examining the imaginary vibrational mode of each TS structure.

More accurate solvation free energies in THF solution are computed with the COSMO-RS model[8] (parameter file: BP_TZVP_C30_1601.ctd) using the COSMOtherm package[9] based on the TPSS-D3 optimized structures, corrected by +1.89 kcal/mol to account for the 1 mol/L reference concentration in solution. To check the effects of the chosen DFT functional on the reaction energies and barriers, single-point calculations at both TPSS-D3[2] and hybrid-meta-GGA PW6B95-D3[10] levels are performed using the larger def2-TZVP[4] basis set. Final reaction free energies (ΔG) are determined from the electronic single-point energies plus TPSS-D3 thermal corrections and COSMO-RS solvation free energies. In our discussion, the more reliable PW6B95-D3 + COSMO-RS free energies (in kcal/mol, at 298.15 K and 1 mol/L concentration) are used unless specified otherwise. The applied DFT methods in combination with the large AO basis set provide usually accurate electronic energies leading to errors for chemical energies (including barriers) on the order of typically 1-2 kcal/mol. This has been tested thoroughly for the huge data base GMTKN55[11] which is the common standard in the field of DFT benchmarking.

[1] TURBOMOLE V7.4, **2019**, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com. .

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Table S1. DFT-computed energies for the reaction of FLP with ester in toluene solution. See main-text **Scheme 5** for structural labelling.
TPSS-D3/def2-SVP + COSMO computed imaginary frequency (ImF), zero-point energies (ZPE), enthalpic (Hc) and Gibbs free-energy (Gc) corrections; the COSMO-RS computed solvation enthalpic (Hsol) and Gibbs free-energy (Gsol) corrections; TPSS-D3 and PW6B95-D3 single-point energies using def2-TZVP basis set (TPSS-D3 and PW6B95-D3 (E_P)); total PW6B95-D3 Gibbs free energies ($G_P = E_P + Gc + Gsol$), relative electronic energies (ΔE_T and ΔE_P) and final Gibbs free-energies (ΔG_T and ΔG_P) at the TPSS-D3 and PW6B95-D3 levels at 298 K. Each structure is labeled either by its molecular formula or a specific name in bold. Transition structures (with only one imaginary frequency) are indicated by the "**TS**" prefixes.

Reactions in THF (1M)	ImF cm^{-1}	ZPE kcal /mol	Hc kcal /mol	Gc kcal /mol	Hsol kcal /mol	Gsol kcal /mol	TPSS-D3 E_h	PW6B95-D3 E_h	G_P E_h	ΔE_T kcal /mol	ΔE_P kcal /mol	ΔG_p kcal /mol	ΔG_T kcal /mol
MeLi exists as tetramer Me_4Li_4 in THF solution; Et_2NLi exists as dimer Et_2NLi_2.													
Et_2NLi_2	0	170.54	182.03	143.84	-23.15	-15.02	-441.77155	-442.23430	-442.02600				
Et_2NLim (monomer)	0	85.27	91.01	71.92	-11.57	-7.51	-220.88578	-221.11715	-221.01300				
Me_4Li_4 (tetramer)	0	88.16	97.90	67.04	-23.84	-15.59	-189.93151	-190.15238	-190.06737				
MeLim (monomer)	0	22.04	24.47	16.76	-5.96	-3.90	-47.48288	-47.53810	-47.51684				
MeLim + THF	0	94.17	100.32	71.79	-12.55	-8.11	-280.07046	-280.36226	-280.25701	0.00	0.00	*0.00*	0.00
MeLi.THF	0	93.62	100.45	72.07	-21.88	-16.65	-280.04494	-280.33586	-280.24453	16.01	16.57	*7.83*	7.28
THF + LiCl	0	72.89	78.80	42.73	-40.19	-29.05	-700.41809	-701.00577	-700.97794	0.00	0.00	*0.00*	0.00
LiClThf	0	74.43	80.26	53.26	-27.81	-21.51	-700.45667	-701.04413	-700.99052	-24.21	-24.08	*-7.89*	-8.03
Transmetalation of Ge-Cl bond is highly exergonic													
MeLi.THF + **2c**	0	662.67	709.32	586.09	-75.83	-56.88	-5675.54591	-5679.99028	-5679.14091	0.00	0.00	*0.00*	0.00
TS1	116i	664.54	709.87	604.94	-58.68	-45.07	-5675.56500	-5680.00736	-5679.11215	-11.98	-10.72	*18.05*	16.79
A + LiCl + THF	0	663.80	709.86	578.44	-93.30	-69.18	-5675.58330	-5680.03033	-5679.20974	-23.46	-25.13	*-43.19*	-41.52
Metalation of two sp2 C-H bonds are also exergonic													
A + MeLi.THF	0	684.52	731.51	607.79	-74.99	-56.79	-5255.21015	-5259.36042	-5258.47633	0.00	0.00	*0.00*	0.00
TS2	1121i	683.91	730.52	622.29	-57.92	-44.92	-5255.23568	-5259.38382	-5258.46071	-16.02	-14.68	*9.80*	8.46
B + CH_4 + THF	0	684.18	731.12	600.59	-71.10	-52.12	-5255.24184	-5259.39227	-5258.50919	-19.89	-19.98	*-20.62*	-20.53
..followed by metalation of a C-H bond and elimination of Et_2NLim													
MeLi.THF + **B**	0	677.99	725.65	600.84	-84.80	-64.42	-5262.15775	-5266.32428	-5265.46342	0.00	0.00	*0.00*	0.00
TS3	1557i	678.24	724.82	617.98	-62.89	-49.44	-5262.17606	-5266.33945	-5265.43042	-11.49	-9.52	*20.71*	18.74
C + CH_4 + THF	0	677.91	725.32	593.77	-70.63	-51.28	-5262.20180	-5266.36714	-5265.49360	-27.64	-26.90	*-18.94*	-19.68

MeLi.THF + **C**	0	671.72	719.86	594.01	-84.33	-63.58	-5269.11771	-5273.29915	-5272.44784	0.00	0.00	*0.00*	0.00
TS4	1273i	670.22	717.99	607.93	-65.97	-49.54	-5269.14431	-5273.31932	-5272.42646	-16.69	-12.65	*13.41*	9.38
D + CH_4	0	672.72	720.62	602.53	-66.34	-48.78	-5269.18617	-5273.36794	-5272.47947	-42.96	-43.17	*-19.85*	-19.64
TS5 + THF +CH_4	44i	670.95	718.04	587.96	-81.83	-59.46	-5269.10596	-5273.28941	-5272.43815	7.37	6.11	*6.08*	7.34
E + CH_4 + THF + Et_2NLim	0	672.01	718.86	581.51	-88.19	-62.31	-5269.12463	-5273.30544	-5272.46750	-4.35	-3.94	*-12.34*	-12.74
*Further quenching of **E** with PCl_3 is still highly exergonic.*													
E + PCl_3	0	489.70	528.65	421.94	-76.24	-54.96	-6497.28499	-6502.22421	-6501.63336	0.00	0.00	*0.00*	0.00
5 + 2 LiCl	0	488.09	528.32	411.12	-119.34	-89.10	-6497.34488	-6502.28694	-6501.76473	-37.58	-39.36	*-82.43*	-80.65

Table 2. TPSS-D3/def2-SVP + COSMO(THF) optimized Cartesian coordinates (in Å).

2c

111

Energy = -5392.702611235

C	1.0795385	-1.1235436	0.3328336
N	0.6151975	-3.0175749	-0.7608010
Ge	0.8566027	0.4795319	1.3867626
N	2.2268490	-1.9334438	0.2584399
C	1.9585749	-3.1090079	-0.4187928
C	-0.1200368	-4.0193982	-1.4827891
C	-0.4994610	1.6377791	0.6237480
N	0.3994759	0.0041756	3.0950725
C	3.5458854	-1.5523250	0.6931332
N	-2.3265718	2.9179067	0.4456596
S	3.0146503	-4.3668750	-0.7450631
C	0.0375707	-4.1048103	-2.8807248
C	-0.9820412	-4.8690445	-0.7614777
N	-0.5753047	2.2027592	-0.6642891
C	-0.4052156	-1.2080933	3.3139977
C	0.8084303	0.7871974	4.2672509
C	3.9519151	-1.8466977	2.0065307
C	4.3692954	-0.8673666	-0.2210180
C	-1.7004470	2.9965403	-0.7916664
C	-3.5736221	3.5604941	0.7637061
C	-0.7214469	-5.0713823	-3.5611612
C	1.0185437	-3.2157968	-3.6033367
C	-1.7190062	-5.8192530	-1.4875103
C	-1.0805786	-4.7720075	0.7434464
C	0.3379260	1.9645532	-1.7500861
C	-1.9121611	-1.0586584	3.0639972
H	-0.2276299	-1.5347639	4.3554212
H	-0.0222096	-2.0199096	2.6654619
C	-0.2717110	1.7016834	4.8596870
H	1.6848947	1.3935435	3.9799275
H	1.1592021	0.0789361	5.0446957
C	5.2209110	-1.3997065	2.4105463
C	3.0453689	-2.6081114	2.9409491
C	5.6288658	-0.4430875	0.2268773
C	3.8872784	-0.5987144	-1.6228336
S	-2.2091035	3.8559269	-2.1357562
C	-4.7652376	2.8287131	0.5987393
C	-3.5540756	4.8933391	1.2160886
C	-1.6076225	-5.9310816	-2.8858890
H	-0.6143986	-5.1546798	-4.6491605
H	2.0490636	-3.5670237	-3.4064504
H	0.8402375	-3.2280087	-4.6901860
H	0.9647542	-2.1741092	-3.2445775
H	-2.3903947	-6.4944888	-0.9441688
H	-1.5284674	-3.8130271	1.0630668
H	-1.7013053	-5.5863312	1.1483730
H	-0.0787492	-4.8312364	1.2051840
C	1.4781235	2.7844162	-1.8672347
C	0.0226064	0.9680843	-2.6963659
H	-2.3595650	-0.2874742	3.7138533
H	-2.4301161	-2.0149094	3.2590490
H	-2.1095006	-0.7748739	2.0141179
H	0.1177151	2.2216727	5.7533053
H	-0.5800767	2.4705286	4.1293163
H	-1.1661761	1.1307118	5.1641819
C	6.0669241	-0.6879879	1.5416108
H	5.5553514	-1.6153329	3.4323060
H	3.5682906	-2.8619543	3.8764256
H	2.1582833	-2.0025345	3.1966093
H	2.6930621	-3.5422464	2.4684502
H	6.2811736	0.0997662	-0.4673840
H	3.7031671	-1.5486129	-2.1573943
H	2.9384311	-0.0346036	-1.6179183
H	4.6290621	-0.0142873	-2.1888215
C	-5.9716345	3.4659625	0.9321928
C	-4.7312615	1.4244472	0.0435008
C	-4.7857501	5.4882558	1.5355595
C	-2.2522402	5.6511824	1.3087047
C	-2.4380569	-6.9374941	-3.6499475
C	2.3643039	2.5204836	-2.9248250
C	1.6766674	3.9598692	-0.9423568
C	0.9377254	0.7455645	-3.7382215
C	-1.3002888	0.2431717	-2.6580886
C	7.4066605	-0.1720372	2.0158017
C	-6.0014351	4.7903364	1.4080485
H	-6.9117854	2.9157394	0.8082819
H	-5.7455839	1.0012688	-0.0218767
H	-4.2854471	1.4249843	-0.9682298
H	-4.1172351	0.7529996	0.6712294
H	-4.7946714	6.5264599	1.8877484
H	-1.5083064	5.1081834	1.9188915
H	-1.8183340	5.7746399	0.2988536
H	-2.4052527	6.6480906	1.7507255
H	-3.3702504	-6.4707989	-4.0214197
H	-1.8930043	-7.3241150	-4.5276491
H	-2.7259601	-7.7888416	-3.0108999
C	2.1205821	1.4974734	-3.8587965
H	3.2623907	3.1404192	-3.0274675
H	1.6162044	3.6631822	0.1171944
H	2.6558930	4.4334473	-1.1144689
H	0.8856780	4.7107041	-1.1271856
H	0.7115057	-0.0240648	-4.4849693
H	-1.6896471	0.1497850	-1.6319266
H	-2.0494013	0.8247002	-3.2267027
H	-1.2260903	-0.7596657	-3.1087370
H	7.3164970	0.8737878	2.3668079
H	7.7951439	-0.7708453	2.8565487
H	8.1525413	-0.1810077	1.2028235
C	-7.3099221	5.4427160	1.7936408
C	3.1110106	1.1979118	-4.9599197
H	-8.1504806	5.0338874	1.2081960
H	-7.5337696	5.2636736	2.8626436
H	-7.2738809	6.5348149	1.6435986
H	3.7903151	2.0486106	-5.1337684
H	3.7326271	0.3224653	-4.6928193
H	2.5984862	0.9567125	-5.9068939
C	-1.6035504	2.1007436	1.2986364
H	-1.9298467	1.9120574	2.3182081
C	0.0836476	-1.8219614	-0.3012679
H	-0.9629309	-1.5754063	-0.4582769
Cl	2.7306547	1.6062011	1.5112217

5

98

Energy = -5558.946991925

C	1.4102839	0.7944935	-0.0019470
C	0.2777203	1.5773004	0.0299359

P	1.6783031	-0.9813193	0.2476311
N	2.4524452	1.5986080	-0.4953794
Ge	-1.5742598	1.0154741	-0.1516896
N	0.6360998	2.8298246	-0.4733025
C	-0.0247842	-1.5429202	-0.0613392
Cl	1.7083091	-1.0658978	2.4180536
C	1.9816696	2.8496979	-0.8517620
C	3.7998296	1.1388235	-0.6962570
C	-1.2263942	-0.8944277	-0.2875965
C	-2.8238921	1.4945587	1.2664803
C	-0.3455964	3.8590868	-0.6804991
N	-0.2848668	-2.9213692	-0.1543090
S	2.8402824	4.0453272	-1.6478769
C	4.1353181	0.5583700	-1.9353323
C	4.7155974	1.2508335	0.3668012
N	-2.1774814	-1.8835109	-0.5099451
H	-2.8782869	2.5933117	1.3330233
H	-3.8219121	1.0918560	1.0284669
H	-2.4810269	1.0832948	2.2289699
C	-0.1825608	5.1312253	-0.0894188
C	-1.5380465	3.5049123	-1.3696005
C	-1.6166027	-3.1525663	-0.4471231
C	0.7111743	-3.9456481	0.0153961
C	5.4404806	0.0673678	-2.0906632
C	3.1147184	0.4878672	-3.0441492
C	6.0106491	0.7464280	0.1625047
C	4.3038398	1.9006293	1.6656490
C	-3.5549917	-1.5896024	-0.7980872
C	-1.1940428	6.0856903	-0.3031993
C	0.9898670	5.4549043	0.8010600
C	-2.5256006	4.4907167	-1.5283472
C	-1.8076584	2.0823179	-1.8136981
S	-2.3843528	-4.6162425	-0.7012551
C	1.5664570	-4.2359433	-1.0665885
C	0.8027905	-4.6041989	1.2579476
C	6.3885923	0.1469905	-1.0530404
H	5.7229957	-0.3899950	-3.0460758
H	2.8116721	1.5067374	-3.3486861
H	3.5178873	-0.0406157	-3.9220033
H	2.1997122	-0.0393700	-2.7140353
H	6.7421933	0.8250186	0.9752606
H	5.1513659	1.9484449	2.3671922
H	3.9371822	2.9277757	1.4868911
H	3.4860109	1.3354810	2.1485739
C	-4.4909929	-1.6314442	0.2559625
C	-3.8993914	-1.2099498	-2.1095428
C	-2.3607956	5.7957889	-1.0299352
H	-1.0737593	7.0793293	0.1438593
H	0.7716878	6.3418481	1.4168778
H	1.2227211	4.6073546	1.4700039
H	1.8976924	5.6411530	0.1987188
H	-3.4491275	4.2262369	-2.0559414
H	-1.0495422	1.7135544	-2.5277709
H	-2.8054470	1.9880354	-2.2671819
C	2.5638691	-5.2034593	-0.8659130
C	1.3965738	-3.5331469	-2.3910730
C	1.8134187	-5.5673205	1.4061632
C	-0.1728707	-4.2942649	2.3652629
C	7.7755853	-0.4272802	-1.2325880
C	-5.8078584	-1.2406909	-0.0313106
C	-4.0777752	-2.1047434	1.6274841
C	-5.2303593	-0.8216440	-2.3450156
C	-2.8803242	-1.2716183	-3.2225943
C	-3.4150988	6.8526004	-1.2644550
C	2.7077744	-5.8726703	0.3631321
H	3.2407209	-5.4438769	-1.6939535
H	2.0721817	-3.9563539	-3.1505478
H	0.3570089	-3.6228280	-2.7535052
H	1.6220708	-2.4534737	-2.3004172
H	1.9029571	-6.0933750	2.3638540
H	-0.1797640	-3.2140756	2.5935498
H	-1.1957174	-4.5809448	2.0577540
H	0.0873190	-4.8437417	3.2835624
H	7.7874864	-1.5018948	-0.9680707
H	8.1132963	-0.3435738	-2.2794038
H	8.5087935	0.0803592	-0.5838391
C	-6.1934727	-0.8223624	-1.3205652
H	-6.5512029	-1.2607190	0.7741740
H	-3.1806103	-1.5709771	1.9876999
H	-4.8888320	-1.9606350	2.3580070
H	-3.8199195	-3.1795084	1.5883265
H	-5.5209162	-0.5190895	-3.3576276
H	-1.9778333	-0.6789555	-2.9914049
H	-2.5490743	-2.3155192	-3.3735341
H	-3.3057488	-0.8999049	-4.1674865
H	-3.4015842	7.6164561	-0.4693090
H	-3.2368942	7.3711264	-2.2256570
H	-4.4247209	6.4106940	-1.3125408
C	3.8142279	-6.8822825	0.5677634
C	-7.6177202	-0.3932619	-1.5901913
H	4.1196972	-7.3436562	-0.3861529
H	4.7081186	-6.3948521	1.0016188
H	3.5065677	-7.6810278	1.2636039
H	-8.3259786	-1.2099727	-1.3611995
H	-7.8982151	0.4651735	-0.9532151
H	-7.7571896	-0.1013075	-2.6435857

A

114

Energy = -4972.479931886

C	1.0244805	-1.1800380	0.2361955
N	0.2555300	-3.0416628	-0.7488510
Ge	1.1374920	0.4729915	1.2646818
N	2.0784988	-2.0822460	-0.0029521
C	1.6217739	-3.2376152	-0.6092425
C	-0.6560315	-4.0042485	-1.3044303
C	-0.3233066	1.6044890	0.5883389
N	0.7540736	-0.0201470	3.0081510
C	3.4714589	-1.7935396	0.2150684
N	-2.2917089	2.6495655	0.3263341
S	2.5197977	-4.5797319	-1.0621476
C	-0.7403473	-4.1387563	-2.7046016
C	-1.4360339	-4.7760474	-0.4204670
N	-0.3392699	2.3457106	-0.6115399
C	-0.0442163	-1.2041075	3.3375563
C	1.1385966	0.8722185	4.1059550
C	4.0422500	-2.0405858	1.4770027
C	4.2072565	-1.2367800	-0.8511837
C	-1.5438892	2.9995265	-0.7847595
C	-3.6449562	3.0732114	0.5597059
C	-1.6604815	-5.0695022	-3.2142802
C	0.1568068	-3.3339280	-3.6113512
C	-2.3427484	-5.6922700	-0.9787856
C	-1.2743338	-4.6352326	1.0751792

C	0.7838928	2.5168354	-1.4917994
C	-1.5730067	-1.0585594	3.2865278
H	0.2554323	-1.5289079	4.3532925
H	0.2433535	-2.0244557	2.6535489
C	0.1200734	1.9611946	4.4819269
H	2.0952432	1.3607224	3.8409212
H	1.3521075	0.2455765	4.9949964
C	5.3845086	-1.6681767	1.6702994
C	3.2302523	-2.6648118	2.5838159
C	5.5420102	-0.8785225	-0.6099308
C	3.5665109	-1.0587731	-2.2034567
S	-1.9999523	3.9991902	-2.0537346
C	-4.6931196	2.2236077	0.1571822
C	-3.8706860	4.3194646	1.1751105
C	-2.4744185	-5.8481360	-2.3708608
H	-1.7407393	-5.1892200	-4.3012216
H	1.1988243	-3.6931915	-3.5139720
H	-0.1554136	-3.4273234	-4.6633793
H	0.1569647	-2.2660375	-3.3346789
H	-2.9546945	-6.3058008	-0.3070713
H	-1.6090911	-3.6434608	1.4294928
H	-1.8612379	-5.4007832	1.6063332
H	-0.2136805	-4.7419973	1.3651251
C	1.7322939	3.5104322	-1.1780965
C	0.8900728	1.7071528	-2.6389981
H	-1.9333722	-0.2536999	3.9496688
H	-2.0553592	-2.0010716	3.6033348
H	-1.9126708	-0.8384043	2.2590545
H	0.5101903	2.5849969	5.3067723
H	-0.0835835	2.6218007	3.6202106
H	-0.8382998	1.5235372	4.8103119
C	6.1448187	-1.0740944	0.6472397
H	5.8463112	-1.8499417	2.6478672
H	3.8766024	-2.9618225	3.4246945
H	2.4806390	-1.9459804	2.9617155
H	2.6909940	-3.5563244	2.2189306
H	6.1255595	-0.4358469	-1.4258400
H	3.3207429	-2.0461599	-2.6362584
H	2.6260795	-0.4872888	-2.1284963
H	4.2384535	-0.5261574	-2.8941583
C	-6.0089484	2.6450215	0.4112592
C	-4.3946233	0.9253711	-0.5551206
C	-5.2029669	4.6984981	1.4075702
C	-2.7106919	5.2182720	1.5278136
C	-3.4835762	-6.8143296	-2.9490420
C	2.8622066	3.6207484	-2.0053179
C	1.4987327	4.4553259	-0.0243280
C	2.0290801	1.8650962	-3.4452733
C	-0.2123286	0.7441624	-3.0000031
C	7.5716497	-0.6385301	0.8924121
C	-6.2831466	3.8739257	1.0400290
H	-6.8398531	1.9999907	0.1020364
H	-5.3241702	0.3941047	-0.8123839
H	-3.8313668	1.1195885	-1.4862359
H	-3.7744232	0.2546651	0.0676404
H	-5.4012351	5.6660828	1.8836509
H	-1.9594362	4.6890584	2.1413135
H	-2.2015011	5.5494441	0.6032622
H	-3.0517636	6.1071412	2.0813989
H	-4.4378487	-6.2971211	-3.1653210
H	-3.1251772	-7.2505776	-3.8967683
H	-3.7042611	-7.6341823	-2.2452251
C	3.0374697	2.7943950	-3.1306135
H	3.6200291	4.3763641	-1.7676261
H	1.2036967	3.9205060	0.8947137
H	2.3987664	5.0529951	0.1886953
H	0.6704628	5.1452543	-0.2725780
H	2.1328311	1.2400501	-4.3397036
H	-0.4044174	0.0316663	-2.1794896
H	-1.1492634	1.3021536	-3.1828241
H	0.0425404	0.1749432	-3.9075803
H	7.6188171	0.4510592	1.0799672
H	8.0026756	-1.1468512	1.7706676
H	8.2107346	-0.8461186	0.0170325
C	-7.7065675	4.2912492	1.3343583
C	4.2903944	2.8849676	-3.9709928
H	-8.4158131	3.8252324	0.6300749
H	-8.0005843	3.9805615	2.3551153
H	-7.8234060	5.3867915	1.2787206
H	4.7412767	3.8898605	-3.9176978
H	5.0485172	2.1628601	-3.6110203
H	4.0855079	2.6447436	-5.0278772
C	-1.5549964	1.8119461	1.1572922
H	-1.9698581	1.4420060	2.0907558
C	-0.1050289	-1.8002675	-0.2348125
H	-1.1410128	-1.4666588	-0.2389007
C	2.8814278	1.3480671	1.1787892
H	3.6305676	0.7093183	1.6729340
H	3.1692241	1.4930661	0.1263872
H	2.8448279	2.3293686	1.6773209

B

114

Energy = -4979.433504866

C	1.6560612	-0.8806696	0.6102832
N	0.5884562	-2.6344993	-0.2970588
Ge	1.9389824	0.8794819	1.4261933
N	2.5627124	-1.9234429	0.3373397
C	1.9259387	-3.0045410	-0.2447225
C	-0.4750039	-3.4638381	-0.7961114
C	0.5244918	1.9819324	0.7407149
N	1.3267622	0.7178842	3.2413095
C	3.9827990	-1.8492817	0.5417624
N	-1.5245329	2.6285138	0.3126110
S	2.6253188	-4.4243559	-0.8005154
C	-1.0315541	-3.1726140	-2.0563069
C	-0.9398818	-4.5272803	0.0075960
N	0.5240486	2.7925725	-0.4153609
C	1.8137764	-0.4862165	3.9724516
C	1.5859526	1.9859687	3.9794383
C	4.5559978	-2.4675053	1.6695944
C	4.7545571	-1.1401121	-0.4028674
C	-0.7571361	3.2086225	-0.6843130
C	-2.9458635	2.8071386	0.3921311
C	-2.0936297	-3.9783904	-2.5047378
C	-0.5068406	-2.0350993	-2.8996829
C	-1.9978669	-5.3047018	-0.4866430
C	-0.3060375	-4.8188210	1.3451440
C	1.6945176	3.1456978	-1.1598106
C	0.7401674	-1.5719846	4.0510037
H	2.1094196	-0.1859503	4.9935395
H	2.7292443	-0.8930239	3.5001120
C	0.5842120	2.2067826	5.1158210
H	1.4954898	2.8183077	3.2573062

H	2.6216983	2.0090412	4.3754708
C	5.9343407	-2.2827292	1.8836155
C	3.7426942	-3.3655976	2.5676976
C	6.1259475	-0.9900826	-0.1502931
C	4.1150019	-0.5957228	-1.6557858
S	-1.2682750	4.2097827	-1.9453678
C	-3.7867709	1.8513681	-0.2092547
C	-3.4577758	3.9275732	1.0749445
C	-2.5912837	-5.0444356	-1.7371187
H	-2.5362744	-3.7688019	-3.4855177
H	0.5958379	-2.0028893	-2.8869039
H	-0.8443849	-2.1358463	-3.9431949
H	-0.8662393	-1.0594021	-2.5253382
H	-2.3702543	-6.1353015	0.1247855
H	-0.2703463	-3.9138749	1.9774058
H	-0.8648159	-5.5996111	1.8846010
H	0.7372272	-5.1575088	1.2015783
C	2.5230734	4.1751631	-0.6712151
C	2.0160550	2.4112534	-2.3190449
H	-0.1530848	-1.2002447	4.5884986
H	1.1073022	-2.4613263	4.5918385
H	0.4306678	-1.8905078	3.0398983
H	0.8236184	3.1279676	5.6744355
H	-0.4448003	2.3238701	4.7218223
H	0.5892495	1.3663030	5.8320406
C	6.7305549	-1.5344899	0.9992444
H	6.3973934	-2.7460050	2.7628464
H	4.1838017	-3.4340233	3.5750646
H	2.6994424	-3.0260744	2.6528408
H	3.7067934	-4.3795337	2.1273168
H	6.7379839	-0.4358221	-0.8715837
H	3.6492597	-1.4142783	-2.2339822
H	3.3189252	0.1332753	-1.4281908
H	4.8591562	-0.0931460	-2.2926195
C	-5.1767050	2.0273348	-0.0948593
C	-3.1912543	0.6925768	-0.9720934
C	-4.8529611	4.0649512	1.1666464
C	-2.5133062	4.9537510	1.6512381
C	-3.7415018	-5.8923851	-2.2314484
C	3.7247320	4.4328960	-1.3530393
C	2.0999573	4.9830082	0.5316546
C	3.2224453	2.7084732	-2.9732990
C	1.0677997	1.3536228	-2.8241604
C	8.2002362	-1.3110176	1.2745237
C	-5.7289631	3.1232778	0.5937086
H	-5.8445505	1.2932811	-0.5623528
H	-3.9764478	0.0489802	-1.3998277
H	-2.5504129	1.0629891	-1.7930056
H	-2.5528231	0.0764510	-0.3135709
H	-5.2661029	4.9338697	1.6937139
H	-1.7563075	4.4762592	2.2989824
H	-1.9662480	5.4565879	0.8314797
H	-3.0566386	5.7146860	2.2344530
H	-4.6347758	-5.7530548	-1.5946935
H	-4.0170555	-5.6318069	-3.2663611
H	-3.4864752	-6.9667305	-2.1996000
C	4.0973996	3.7029974	-2.4966658
H	4.3847875	5.2260271	-0.9819450
H	1.9053786	4.3340873	1.4043187
H	2.8695376	5.7219342	0.8051963
H	1.1554000	5.5156945	0.3176781
H	3.4890161	2.1414036	-3.8731440
H	0.8134627	0.6395027	-2.0217680
H	0.1220848	1.8267323	-3.1492934
H	1.5016133	0.7959463	-3.6692751
H	8.3659944	-0.3089569	1.7137632
H	8.5948720	-2.0558530	1.9851438
H	8.7943613	-1.3617603	0.3458602
C	-7.2277315	3.2766729	0.7343156
C	5.4168687	3.9617475	-3.1890408
H	-7.7637001	2.7416717	-0.0676721
H	-7.5774788	2.8630335	1.6997157
H	-7.5272755	4.3385412	0.7072953
H	5.8388926	4.9386601	-2.9004694
H	6.1578119	3.1847190	-2.9203461
H	5.3062121	3.9380050	-4.2869984
C	-0.7756561	1.8522839	1.2221118
C	0.4307928	-1.3451917	0.1991313
H	-0.5395319	-0.8518584	0.2295707
C	3.7845766	1.5241689	1.3704240
H	4.4660557	0.7845848	1.8200983
H	4.0874581	1.7107789	0.3283875
H	3.8438836	2.4721946	1.9293030
Li	-0.7244324	0.7872323	2.9436567

CH_4
5
Energy = -40.49605427542

C	-1.5718229	-1.0382342	-1.3553853
H	-1.2044016	-2.0774690	-1.3553938
H	-1.2043500	-0.5185956	-0.4554175
H	-1.2043592	-0.5186015	-2.2553603
H	-2.6741013	-1.0382303	-1.3553981

C
114
Energy = -4986.387310700

C	1.6758256	-1.0535586	0.4064154
N	0.4914419	-2.8228747	-0.1394865
Ge	2.0299462	0.6720168	1.2197044
N	2.5418105	-2.0946301	0.0195631
C	1.8014080	-3.2001786	-0.3552608
C	-0.6394394	-3.6395899	-0.4714519
C	0.6151164	1.8391168	0.5713446
N	1.2852550	0.3327759	2.9642866
C	3.9711110	-1.9893832	-0.0270587
N	-1.3982859	2.6511593	0.2167364
S	2.3582976	-4.6624273	-0.9848531
C	-1.2153165	-3.5074886	-1.7501767
C	-1.1688200	-4.5074631	0.5029210
N	0.7201235	3.0945122	-0.0530922
C	1.9670626	-0.7781891	3.6651595
C	1.1201891	1.5573603	3.7939817
C	4.7547604	-2.6586423	0.9375311
C	4.5502234	-1.1622885	-1.0135723
C	-0.5346858	3.6045649	-0.2985076
C	-2.8254111	2.7526775	0.1373139
C	-2.3754868	-4.2501380	-2.0317250
C	-0.5585586	-2.6355489	-2.7950495
C	-2.3244863	-5.2360572	0.1769353
C	-0.4778045	-4.6505615	1.8371253
C	1.9427118	3.6033420	-0.6024581
C	1.1213297	-1.4549085	4.7470419
H	2.9254593	-0.4334973	4.1096275

H	2.2221968	-1.5290899	2.8966222
C	-0.2816865	1.6976239	4.3967771
H	1.3043062	2.4426840	3.1568816
H	1.8907883	1.5776470	4.5904149
C	6.1439564	-2.4436729	0.9176599
C	4.1301938	-3.6043738	1.9316109
C	5.9421166	-0.9784807	-0.9911572
C	3.6960496	-0.4966912	-2.0648647
S	-0.9020911	5.0421405	-1.1007203
C	-3.5247291	1.9330903	-0.7699574
C	-3.5036414	3.6414078	1.0021558
C	-2.9485553	-5.1128470	-1.0795467
H	-2.8361673	-4.1590715	-3.0227659
H	0.4095763	-3.0772286	-3.0965116
H	-1.1934820	-2.5300193	-3.6886877
H	-0.3231776	-1.6262911	-2.4061701
H	-2.7483250	-5.9180985	0.9240752
H	-0.3759867	-3.6713612	2.3393642
H	-1.0303044	-5.3331587	2.5022183
H	0.5446649	-5.0456310	1.6909339
C	2.7331499	4.4879550	0.1525090
C	2.3413581	3.1256727	-1.8680222
H	0.9004574	-0.7728825	5.5854298
H	1.6615196	-2.3261810	5.1574287
H	0.1612877	-1.8140839	4.3314913
H	-0.3569834	2.6243922	4.9932582
H	-1.0347760	1.7539638	3.5886188
H	-0.5344349	0.8478620	5.0528217
C	6.7555584	-1.5984378	-0.0256798
H	6.7645662	-2.9541525	1.6638724
H	4.8397169	-3.8643681	2.7332231
H	3.2222106	-3.1728822	2.3858871
H	3.8102097	-4.5267340	1.4110503
H	6.4017885	-0.3379630	-1.7533764
H	2.9429343	-1.1953534	-2.4671707
H	3.1460239	0.3653771	-1.6481194
H	4.3168501	-0.1229056	-2.8944156
C	-4.9292097	2.0156497	-0.8049522
C	-2.8096495	0.9750291	-1.7003606
C	-4.9034747	3.6917659	0.9323193
C	-2.7312275	4.5058509	1.9666364
C	-4.2169459	-5.8768827	-1.3885450
C	3.9876788	4.8501909	-0.3673606
C	2.2196366	5.0306989	1.4628925
C	3.6057057	3.5071254	-2.3450042
C	1.3994220	2.2703746	-2.6825966
C	8.2463246	-1.3472854	0.0075934
C	-5.6369103	2.8885787	0.0362281
H	-5.4810908	1.3875751	-1.5144817
H	-3.2940226	0.9427948	-2.6891495
H	-1.7576102	1.2717976	-1.8651549
H	-2.8653168	-0.0724278	-1.3252632
H	-5.4388936	4.3761081	1.6015061
H	-2.0059240	3.9049678	2.5430718
H	-2.1514755	5.2626077	1.4052202
H	-3.4083866	5.0180258	2.6686360
H	-5.1004891	-5.3528609	-0.9765448
H	-4.3694610	-5.9803932	-2.4758135
H	-4.1979060	-6.8848977	-0.9397648
C	4.4498813	4.3539112	-1.6005516
H	4.6218332	5.5337640	0.2095335
H	1.9927684	4.2156185	2.1738376
H	2.9535990	5.7052525	1.9309514
H	1.2773466	5.5839114	1.2968613
H	3.9372267	3.1377701	-3.3226087
H	1.0637133	1.3853917	-2.1104991
H	0.4972774	2.8553927	-2.9415438
H	1.8769768	1.9230760	-3.6117075
H	8.4775516	-0.4508090	0.6142253
H	8.7881956	-2.1968526	0.4559112
H	8.6467725	-1.1701088	-1.0050339
C	-7.1455553	2.9774595	-0.0178280
C	5.8296012	4.7055774	-2.1096194
H	-7.5678195	2.2317600	-0.7111023
H	-7.5892703	2.8128392	0.9805494
H	-7.4696460	3.9794805	-0.3541967
H	6.1872188	5.6562772	-1.6805488
H	6.5584684	3.9207825	-1.8302755
H	5.8439117	4.7878975	-3.2097175
C	-0.7277031	1.5268427	0.7617214
C	0.3580337	-1.4958560	0.3268030
C	3.8618363	1.3514044	1.2610897
H	4.5419677	0.5493989	1.5903726
H	4.1621566	1.6945133	0.2583281
H	3.9214593	2.2012179	1.9600530
Li	-1.0555477	-0.1823319	-0.3706520
Li	-0.5136771	-0.2026986	2.0585513

D

114

Energy = -4993.337914179

C	-1.9853767	-0.9009371	0.1334074
N	-3.8043326	0.1700372	-0.4804151
Ge	-0.3212187	-1.1810631	1.0916529
N	-2.9088503	-1.8178554	-0.4050759
C	-4.0424688	-1.1456514	-0.8221837
C	-4.7029852	1.2456763	-0.7823833
C	0.7485719	0.3984974	0.6950861
N	-0.8917068	-0.6273818	2.8492815
C	-2.6766944	-3.2271614	-0.5334610
N	1.4477498	2.4808634	0.6262221
S	-5.3935953	-1.7685352	-1.6176101
C	-4.5598475	1.9249045	-2.0075639
C	-5.6686173	1.6181827	0.1730500
N	2.0806249	0.4250691	0.2632215
C	-2.0028944	-1.4505198	3.3746289
C	0.2411289	-0.4677275	3.8041068
C	-3.3692213	-4.1285430	0.3056830
C	-1.7106206	-3.6688622	-1.4625369
C	2.5214182	1.7184272	0.2245103
C	1.4438379	3.9151716	0.6504031
C	-5.3967975	3.0281995	-2.2523753
C	-3.5703792	1.4329769	-3.0378660
C	-6.4875971	2.7219896	-0.1146711
C	-5.8150934	0.8179363	1.4444758
C	2.7778510	-0.7342641	-0.2238324
C	-2.8175374	-0.7747374	4.4807031
H	-1.6289953	-2.4305648	3.7417802
H	-2.6719165	-1.6630379	2.5220603
C	0.2363207	0.8856115	4.5224908
H	1.1948557	-0.5626908	3.2509548
H	0.2266487	-1.2965548	4.5398440
C	-3.0385277	-5.4914118	0.2198006
C	-4.4558123	-3.6546188	1.2371989

C	-1.4158567	-5.0419036	-1.5098173
C	-1.0032601	-2.7001812	-2.3788815
S	4.0728952	2.2610119	-0.2609228
C	0.7141985	4.6108061	-0.3338151
C	2.1274379	4.5941409	1.6840437
C	-6.3603018	3.4457664	-1.3164385
H	-5.2989795	3.5679069	-3.2020700
H	-3.8841504	0.4409689	-3.4130514
H	-3.4962108	2.1279648	-3.8890247
H	-2.5603382	1.2915931	-2.6078883
H	-7.2462623	3.0235516	0.6178995
H	-4.8590548	0.7699383	1.9968964
H	-6.5830027	1.2523271	2.1041205
H	-6.0997633	-0.2230494	1.2038339
C	3.6236728	-1.4552758	0.6833508
C	2.5149968	-1.1365496	-1.5492349
H	-2.2162405	-0.6047845	5.3899361
H	-3.6752219	-1.4116539	4.7602699
H	-3.2133353	0.2009103	4.1418575
H	1.0985916	0.9655976	5.2085634
H	0.3151600	1.7048185	3.7837310
H	-0.6843633	1.0354577	5.1114986
C	-2.0570049	-5.9675324	-0.6688778
H	-3.5658322	-6.2008475	0.8689606
H	-4.7192031	-4.4346098	1.9693277
H	-4.1548382	-2.7432197	1.7807956
H	-5.3531843	-3.3840497	0.6493921
H	-0.6667066	-5.3951640	-2.2284663
H	-1.6679147	-1.8763352	-2.6862033
H	-0.1261782	-2.2496517	-1.8809487
H	-0.6333734	-3.2169216	-3.2790732
C	0.6875717	6.0165547	-0.2781890
C	-0.0397706	3.8913585	-1.4334980
C	2.0734566	5.9959034	1.6986345
C	2.8863919	3.8268277	2.7377237
C	-7.2315578	4.6532213	-1.5834089
C	4.1535046	-2.6800449	0.1445399
C	3.9828296	-0.9451690	1.9741066
C	3.0575654	-2.3459815	-2.0055101
C	1.6934607	-0.2435597	-2.4541477
C	-1.6886866	-7.4337482	-0.7037227
C	1.3627016	6.7275088	0.7266905
H	0.1299011	6.5677061	-1.0447083
H	0.0354608	4.4347626	-2.3887805
H	0.3492360	2.8715738	-1.6039033
H	-1.1310834	3.8543923	-1.2139968
H	2.5975757	6.5330858	2.4981970
H	2.2709699	3.0108078	3.1548044
H	3.7828923	3.3588727	2.2895032
H	3.2012269	4.4906989	3.5584305
H	-6.8697308	5.5319366	-1.0163423
H	-7.2296552	4.9217686	-2.6528362
H	-8.2745744	4.4723501	-1.2702490
C	3.8704466	-3.1303147	-1.1443118
H	4.7889143	-3.2933715	0.7965320
H	4.4221896	-1.6616690	2.6826030
H	3.3003545	-0.2117814	2.4319588
H	2.8584749	-2.6786182	-3.0305348
H	0.7006723	-0.0221505	-2.0196684
H	2.2064119	0.7256318	-2.6012045
H	1.5401237	-0.7111340	-3.4394859
H	-0.9025519	-7.6563769	0.0429970
H	-2.5560451	-8.0728825	-0.4665140
H	-1.2966664	-7.7264697	-1.6922926
C	1.3415860	8.2389996	0.7649796
C	4.4140449	-4.4551900	-1.6353827
H	0.6300433	8.6501176	0.0303690
H	1.0595363	8.6078104	1.7671227
H	2.3420727	8.6516874	0.5378388
H	5.0787768	-4.9224434	-0.8896913
H	3.5908279	-5.1622396	-1.8506171
H	4.9818264	-4.3309402	-2.5759508
C	0.3041134	1.6972286	0.9291623
C	-2.5373990	0.3774883	0.1102477
C	0.5420472	-2.9298227	1.0733603
H	-0.2035682	-3.7098451	1.2974609
H	0.9947331	-3.1206614	0.0873847
H	1.3410625	-2.9325759	1.8319299
Li	-1.3155975	1.9680819	-0.3326203
Li	-1.5000692	1.1903183	2.0349389
Li	5.1696546	0.3874143	0.7819523

Et_2NH
16
Energy = -213.6896743417

N	0.0000502	-0.9976893	0.3539354
C	1.2586173	-0.5428531	-0.2417401
C	1.7137048	0.9018568	0.0420825
H	1.1806152	-0.6987676	-1.3347189
H	2.0554091	-1.2273699	0.1101743
H	2.7330241	1.0670110	-0.3534376
H	1.0471837	1.6492561	-0.4200125
H	1.7392499	1.0946078	1.1307088
C	-1.2589116	-0.5431874	-0.2411741
C	-1.7134030	0.9020553	0.0409177
H	-2.0555459	-1.2269733	0.1124915
H	-1.1819948	-0.7007017	-1.3340025
H	-2.7331735	1.0667362	-0.3536307
H	-1.7375575	1.0965726	1.1292603
H	-1.0473494	1.6486201	-0.4232140
H	0.0002254	-0.8190123	1.3641706

Et_2NLi_2
32
Energy = -441.3242371202

Li	-0.1684899	-0.4742484	-1.8788025
N	1.5396458	-0.3237264	-0.9232168
C	2.0762710	1.0337767	-0.8259063
C	2.1019974	1.8577057	-2.1338372
H	3.1083744	1.0269459	-0.3970085
H	1.4667007	1.6267788	-0.1012044
H	2.4816957	2.8840696	-1.9605596
H	2.7349643	1.3805229	-2.9015703
H	1.0802419	1.9473811	-2.5519611
C	2.5680616	-1.3365367	-1.1163940
C	3.2316716	-1.4138627	-2.5105796
H	2.1169524	-2.3318116	-0.9119185
H	3.3961918	-1.2239533	-0.3685625
H	3.9248340	-2.2753160	-2.5774100
H	2.4637950	-1.5247088	-3.3003735
H	3.8121746	-0.5008595	-2.7338869
Li	0.1562926	-0.5012778	0.4377818
N	-1.5519740	-0.3303365	-0.5141052
C	-2.0881993	1.0292216	-0.5804197

C -2.1127013 1.8233325 0.7458203
H -3.1205304 1.0324811 -1.0087294
H -1.4788429 1.6383367 -1.2918433
H -2.4919016 2.8536048 0.5961972
H -2.7453825 1.3292044 1.5029995
H -1.0905953 1.9029201 1.1651314
C -2.5806993 -1.3469545 -0.3439256
C -3.2447790 -1.4552718 1.0480023
H -2.1297461 -2.3374763 -0.5705241
H -3.4086334 -1.2174698 -1.0892419
H -3.9383140 -2.3177195 1.0952649
H -2.4772329 -1.5841145 1.8353864
H -3.8251149 -0.5473158 1.2915057

E
98
Energy = -4772.653515327
C 1.5714090 0.7943911 0.4012806
C 0.5576078 1.5161011 -0.2154398
N 2.7074356 1.6312051 0.2536415
Ge -1.1617110 0.9770102 -0.9662722
N 1.0835122 2.7440005 -0.6993664
C -0.0790090 -1.7875183 -0.4234781
C 2.4482903 2.7831533 -0.4735231
C 4.0091296 1.2697437 0.7296197
C -1.0826025 -0.9734988 -0.9528999
C -2.7518015 1.7476070 -0.1183489
C 0.2762686 3.7461192 -1.3277617
N -0.5553014 -3.0947883 -0.6661348
S 3.5862679 3.8666422 -1.0870160
C 4.6644928 0.1549040 0.1674153
C 4.5911023 2.0033539 1.7886129
N -2.1002621 -1.7933141 -1.4752114
H -2.6547338 2.8460242 -0.1252500
H -3.6541872 1.4573425 -0.6808867
H -2.8422118 1.3961004 0.9223456
C 0.2680853 5.0739184 -0.8364978
C -0.6305707 3.3378094 -2.3452119
C -1.7786300 -3.1212413 -1.3051752
C 0.1647602 -4.2738823 -0.2787675
C 5.9239099 -0.2141615 0.6708903
C 4.0436062 -0.6419653 -0.9579872
C 5.8516829 1.6011604 2.2579832
C 3.8744569 3.1831699 2.3946162
C -3.2806637 -1.2976314 -2.1199164
C -0.5732926 6.0078046 -1.4690551
C 1.0655862 5.4898121 0.3729104
C -1.4683600 4.3079130 -2.9207768
C -0.8028289 1.8826817 -2.7097075
S -2.6775599 -4.4613810 -1.7901860
C 1.2084943 -4.7363016 -1.1054456
C -0.1663167 -4.9099757 0.9326662
C 6.5383235 0.4994737 1.7132504
H 6.4400553 -1.0751865 0.2296370
H 4.8121294 -1.1047069 -1.5964461
H 3.4272203 -1.4794272 -0.5613125
H 3.4341236 0.0174155 -1.6040998
H 6.3083508 2.1638534 3.0812423
H 4.3624987 3.5043259 3.3286536
H 3.8744046 4.0267174 1.6787164
H 2.8183769 2.9403950 2.6071940
C -4.4566512 -1.1355144 -1.3600798
C -3.2054716 -0.9382328 -3.4798483
C -1.4346853 5.6550801 -2.5209998
H -0.5755815 7.0395669 -1.0973683
H 0.6555073 6.4185790 0.8016687
H 1.0494108 4.7023354 1.1470107
H 2.1278593 5.6434009 0.1072894
H -2.1713754 3.9923884 -3.7006884
H 0.1298937 1.4354708 -3.1013506
H -1.6001865 1.7543112 -3.4571596
C 1.9461664 -5.8516252 -0.6778318
C 1.4960921 -4.0575986 -2.4234196
C 0.5971005 -6.0252375 1.3208990
C -1.3261896 -4.4129444 1.7603858
C 7.9096232 0.1143338 2.2211922
C -5.5657314 -0.5468962 -1.9886482
C -4.5033756 -1.6085797 0.0715577
C -4.3380456 -0.3458249 -4.0649343
C -1.9616740 -1.2441674 -4.2793845
C -2.3063835 6.6888150 -3.1967679
C 1.6580111 -6.5078765 0.5342225
H 2.7619147 -6.2209921 -1.3109770
H 2.2503981 -4.6146490 -3.0009707
H 0.5756509 -3.9736832 -3.0277919
H 1.8777422 -3.0281422 -2.2789846
H 0.3546405 -6.5295496 2.2641266
H -1.2507641 -3.3268281 1.9502500
H -2.2719681 -4.5761281 1.2100312
H -1.3808305 -4.9386380 2.7269020
H 7.9700630 0.2047068 3.3195945
H 8.1673087 -0.9202102 1.9401060
H 8.6850843 0.7797051 1.7964717
C -5.5200966 -0.1297001 -3.3331493
H -6.4880986 -0.4081089 -1.4121593
H -3.6696181 -1.1873670 0.6608916
H -5.4534518 -1.3284398 0.5532202
H -4.3963544 -2.7090732 0.1017693
H -4.2973895 -0.0549232 -5.1212990
H -1.0524109 -0.8599663 -3.7853170
H -1.8387321 -2.3395031 -4.3700643
H -2.0219140 -0.8120606 -5.2905846
H -2.5391524 7.5251797 -2.5163247
H -1.7940650 7.1146207 -4.0806397
H -3.2545541 6.2480707 -3.5491473
C 2.4563041 -7.7197904 0.9611004
C -6.7120612 0.5504551 -3.9681441
H 3.5398989 -7.5521701 0.8306825
H 2.2675547 -7.9735457 2.0172877
H 2.1889561 -8.6022320 0.3496768
H -7.6606263 0.1106416 -3.6154045
H -6.7332903 1.6252619 -3.7050985
H -6.6785603 0.4782352 -5.0678942
Li 1.5771009 -0.7200901 -1.0802933
Li 0.8730305 -0.9440047 1.2877237

LiCl.THF
15
Energy = -700.0683375162
Li 0.0130014 0.2640754 -1.4976079
C 0.2266671 1.2724680 1.3039122
O -0.0272569 0.1885014 0.3613165
C -0.2581210 -1.0622634 1.0795416
C 0.1848319 -0.7793244 2.5135064

C -0.1680133 0.7092780 2.6681156
H 1.3008592 1.5300896 1.2590188
H -0.3686535 2.1453178 0.9898332
H -1.3349876 -1.3046096 1.0201719
H 0.3193596 -1.8555201 0.5776150
H -0.3279849 -1.4271129 3.2423210
H 1.2736831 -0.9310115 2.6179389
H -1.2523972 0.8328948 2.8365600
H 0.3703124 1.2024184 3.4932259
Cl 0.0486999 -0.7852018 -3.3461969

LiCl
2
Energy = -467.7066057978
Li -0.1106700 0.0000000 0.0000000
Cl 2.0106700 0.0000000 0.0000000

Me_4Li_4
20
Energy = -189.7559215054
Li 1.0478936 0.5693525 0.9016384
C -1.5284428 -0.8289242 -1.3140000
H -1.2149561 -0.9862575 -2.3759716
H -1.9214722 -1.8335541 -1.0188618
H -2.4593969 -0.2177189 -1.4170296
Li 0.5580379 -0.1528868 -1.3778033
C 0.6263232 1.9483497 -0.7521567
H 1.0614321 1.9480325 -1.7824928
H -0.1804835 2.7196689 -0.8228113
H 1.4134691 2.4657750 -0.1492076
Li -1.1763374 0.9212372 -0.0388055
C 1.7160682 -1.3428319 0.0563934
H 2.5632365 -1.0110174 0.7067741
H 1.5065972 -2.3766289 0.4282275
H 2.2145447 -1.5281838 -0.9274279
Li -0.4287954 -1.3347131 0.5149456
C -0.8143234 0.2237277 2.0098046
H -1.7042606 0.8955648 2.0962741
H -1.1683816 -0.7217205 2.4910804
H -0.1105458 0.6428208 2.7713110

MeLi.THF
18
Energy = -279.7618695899
Li 3.1235053 -4.3720731 -0.3976219
C 4.7033281 -5.4457651 -1.1893768
H 5.2792467 -4.8195326 -1.9163392
H 5.4824642 -5.8086788 -0.4734603
H 4.4353279 -6.3592240 -1.7767098
C 0.6984763 -2.6416075 -0.8065917
O 2.1093698 -2.7756107 -0.4574310
C 2.7825591 -1.4882876 -0.5881703
C 1.8379042 -0.6384330 -1.4335077
C 0.4623529 -1.1379172 -0.9617578
H 0.5227711 -3.1866652 -1.7519739
H 0.0989063 -3.1053292 -0.0061750
H 2.9284368 -1.0608880 0.4214183
H 3.7672586 -1.6670161 -1.0501809
H 1.9888703 0.4410385 -1.2722761
H 1.9823664 -0.8547886 -2.5068656
H 0.2035833 -0.6852703 0.0116877
H -0.3498786 -0.9169520 -1.6726441

PCl_3
4
Energy = -1721.568629861
P -1.0556397 0.7745770 0.0000022
Cl -0.0831217 1.7020392 1.6060682
Cl -0.0831201 1.7020406 -1.6060704
Cl -0.0831886 -1.0800910 0.0000000

THF
13
Energy = -232.3344032647
C -0.0049910 0.2873596 0.4804847
O 1.3084094 0.3903545 1.0388996
C 1.8584727 1.5811759 0.4682024
C 0.7105682 2.6132070 0.4923295
C -0.5677759 1.7269508 0.4762453
H 0.0518755 -0.1115781 -0.5556425
H -0.5814540 -0.4206395 1.0974543
H 2.7381752 1.8695526 1.0658363
H 2.1877276 1.3877881 -0.5761345
H 0.7532074 3.2182160 1.4131633
H 0.7624776 3.3018360 -0.3671621
H -1.1811466 1.9097329 1.3739420
H -1.2006263 1.9112930 -0.4076353

TS1
129
Energy = -5672.474766524
C 1.0820993 0.6872383 -0.4932970
N 1.3401835 2.9109076 -0.6955213
Ge 0.2045999 -1.0776137 -0.6271480
N 2.4504108 1.0318565 -0.5044606
C 2.6249746 2.3968790 -0.6346765
C 1.0059840 4.2999457 -0.8310689
C -1.6055620 -0.6497379 -0.0637349
N 0.3807122 -1.5731390 -2.3940818
C 3.5571477 0.1209570 -0.3878008
N -3.8345545 -0.4621275 0.0042902
S 4.0789426 3.2328699 -0.7286465
C 1.1634768 5.1566870 0.2788550
C 0.4905098 4.7483116 -2.0642452
N -2.0222107 -0.2062487 1.2103975
C -0.1053787 -0.6204072 -3.3960234
C 1.3086475 -2.6213706 -2.8230286
C 4.0875795 -0.4538408 -1.5573577
C 4.0550561 -0.1766130 0.8937030
C -3.4009404 -0.1060644 1.2706270
C -5.2106631 -0.4486769 -0.4112718
C 0.7727138 6.4971830 0.1261406
C 1.7538137 4.6533926 1.5718355
C 0.1134757 6.0980510 -2.1652417
C 0.3593772 3.8074778 -3.2403468
C -1.1592508 0.1672539 2.2994269
C -1.1799795 -1.1674875 -4.3460882
H 0.7454297 -0.2365877 -4.0013109
H -0.5111242 0.2594241 -2.8604040
C 0.6781098 -3.9365059 -3.3075884
H 1.9995894 -2.8372400 -1.9858160
H 1.9497841 -2.2095113 -3.6281063
C 5.0952574 -1.4214913 -1.4124039
C 3.6235769 0.0201620 -2.9110752

C	5.0741521	-1.1381246	0.9904370
C	3.4898435	0.5162126	2.1064749
S	-4.3512648	0.3421201	2.5784434
C	-5.7348823	0.7400246	-0.9548209
C	-5.9771796	-1.6198556	-0.2617472
C	0.2448042	6.9864493	-1.0829226
H	0.8801121	7.1764028	0.9803335
H	2.8498447	4.5500390	1.4616978
H	1.5393118	5.3457453	2.4016117
H	1.3690168	3.6527546	1.8309168
H	-0.2892903	6.4640379	-3.1170174
H	-0.4856784	3.1059452	-3.1093922
H	0.1860365	4.3692703	-4.1716743
H	1.2695682	3.1945359	-3.3608068
C	-0.5855021	-0.8485808	3.0913695
C	-0.9419387	1.5372624	2.5645307
H	-0.7746184	-1.9552308	-5.0023164
H	-1.5638933	-0.3568171	-4.9911952
H	-2.0254180	-1.6014448	-3.7844233
H	1.4741347	-4.6609359	-3.5588282
H	0.0318840	-4.3746664	-2.5302582
H	0.0605747	-3.7828803	-4.2071671
C	5.5921706	-1.7851215	-0.1462529
H	5.5098258	-1.8925168	-2.3118145
H	4.0059000	-0.6262353	-3.7164778
H	2.5238488	0.0505932	-2.9687888
H	3.9865343	1.0510609	-3.0817536
H	5.4630335	-1.3983344	1.9820661
H	3.7047870	1.5998011	2.0587216
H	2.3937043	0.4000858	2.1592372
H	3.9264692	0.1098806	3.0324118
C	-7.0723918	0.7276077	-1.3823373
C	-4.8830542	1.9842491	-1.0324682
C	-7.3106731	-1.5836716	-0.7037059
C	-5.3816347	-2.8464514	0.3851560
C	-0.1432681	8.4414155	-1.2216372
C	0.3125509	-0.4647185	4.1015426
C	-1.0000554	-2.2890125	2.9237688
C	-0.0468420	1.8684337	3.5950257
C	-1.7049003	2.6224086	1.8453361
C	6.6881410	-2.8198729	-0.0203335
C	-7.8743077	-0.4237265	-1.2668525
H	-7.4986792	1.6414030	-1.8129666
H	-5.4233949	2.8039962	-1.5309710
H	-4.6049623	2.3132943	-0.0140315
H	-3.9431422	1.7993258	-1.5836923
H	-7.9252154	-2.4859073	-0.6009444
H	-4.4563408	-3.1712111	-0.1244269
H	-5.1099932	-2.6213403	1.4333828
H	-6.0987549	-3.6824173	0.3800216
H	-0.5902347	8.8275023	-0.2895430
H	0.7454008	9.0636311	-1.4402209
H	-0.8629393	8.5893223	-2.0438858
C	0.6096649	0.8849961	4.3565508
H	0.7810234	-1.2445093	4.7131640
H	-1.0198913	-2.6012062	1.8665434
H	-0.3203997	-2.9581280	3.4753443
H	-2.0228304	-2.4246228	3.3237552
H	0.1349628	2.9267785	3.8143398
H	-2.0649816	2.2929233	0.8592164
H	-2.6036289	2.8839550	2.4329186
H	-1.0935492	3.5302925	1.7176182
H	6.5025787	-3.6833021	-0.6829507
H	7.6666463	-2.3934527	-0.3111355
H	6.7774961	-3.1875611	1.0149925
C	-9.3215511	-0.4018023	-1.7055573
C	1.6154821	1.2760152	5.4145786
H	-9.4704031	0.2716621	-2.5665428
H	-9.6733153	-1.4098382	-1.9818750
H	-9.9709759	-0.0371985	-0.8868909
H	1.7881005	0.4550637	6.1300413
H	2.5883000	1.5253940	4.9503230
H	1.2843896	2.1673018	5.9748258
C	-2.7546090	-0.8013692	-0.7993026
H	-2.8978379	-1.1507510	-1.8179228
C	0.4123770	1.8764707	-0.6226762
H	-0.6543303	2.0757637	-0.6645157
Cl	1.6263751	-2.1893388	0.7465153
Li	0.5922340	-4.0900609	-0.0652585
C	-1.3573538	-3.6621216	-0.4946549
H	-1.4126322	-4.7825510	-0.5622845
H	-1.7113598	-3.2791264	-1.4693662
H	-2.0981847	-3.3680605	0.2732736
C	1.9750354	-6.4765119	0.9305318
O	1.9694505	-5.3934086	-0.0314889
C	3.3663304	-5.0533105	-0.2271098
C	3.9947223	-5.1370672	1.1753240
C	3.0289814	-6.0629382	1.9702830
H	0.9521682	-6.5791251	1.3250491
H	2.2551064	-7.4112352	0.4095875
H	3.8093749	-5.7886197	-0.9242222
H	3.4077903	-4.0494445	-0.6754293
H	5.0188912	-5.5391363	1.1275084
H	4.0434703	-4.1356558	1.6316707
H	3.5379489	-6.9412823	2.3977350
H	2.5556092	-5.5097293	2.7979400

TS2

132

Energy = -5252.258813555

C	-1.7336839	0.1514619	0.4955929
N	-2.6161292	2.1971832	0.2544648
Ge	-0.4314523	-1.2986346	0.6128098
N	-3.1322127	0.1127893	0.6848176
C	-3.6919616	1.3654827	0.5262409
C	-2.7219676	3.6163090	0.0461805
C	1.0564269	-0.7718818	-0.5089777
N	0.3630057	-1.2170123	2.3686201
C	-3.9057620	-1.0779569	0.9057736
N	2.9610647	0.1453136	-1.1693159
S	-5.3131987	1.7868179	0.6211705
C	-3.0365879	4.0920943	-1.2413114
C	-2.5121553	4.4737879	1.1432918
N	1.3789882	-1.2188610	-1.8062781
C	-0.5367799	-0.6514426	3.4074526
C	0.9064609	-2.5341888	2.7974637
C	-4.3086716	-1.4168321	2.2116861
C	-4.2371174	-1.8699210	-0.2138644
C	2.5604051	-0.6481389	-2.2299282
C	4.1975928	0.8733595	-1.1394558
C	-3.1086124	5.4830511	-1.4214860
C	-3.3221526	3.1266450	-2.3654805
C	-2.5957917	5.8572321	0.9135646
C	-2.2325291	3.9093242	2.5155666

C	0.5437608	-2.0584720	-2.6169971
C	0.2126625	-0.1248687	4.6360159
H	-1.2915209	-1.4013560	3.7249296
H	-1.0847553	0.1859799	2.9444391
C	2.0565832	-3.0298041	1.9229717
H	0.1023800	-3.2999640	2.8385646
H	1.2706152	-2.4250652	3.8346601
C	-4.9744802	-2.6438187	2.3893658
C	-4.1257895	-0.4596145	3.3627618
C	-4.9108446	-3.0789180	0.0120704
C	-3.9066179	-1.3935046	-1.6059442
S	3.3277229	-0.8627522	-3.7139796
C	4.1838372	2.2537453	-1.4158433
C	5.3796829	0.1842220	-0.8025564
C	-2.8834074	6.3801685	-0.3607254
H	-3.3520235	5.8743797	-2.4163692
H	-4.2442745	2.5574292	-2.1428078
H	-3.4572175	3.6587597	-3.3201938
H	-2.5073716	2.3915780	-2.4849275
H	-2.4385978	6.5425708	1.7548712
H	-1.2705054	3.3645221	2.5360062
H	-2.1874459	4.7122125	3.2681232
H	-3.0248147	3.1968841	2.8089459
C	0.8013688	-3.4415519	-2.6798254
C	-0.5343107	-1.4631981	-3.3037782
H	0.7762634	-0.9177901	5.1565763
H	-0.5073499	0.2972066	5.3581325
H	0.9173895	0.6795065	4.3579272
H	2.4486105	-3.9803709	2.3215988
H	1.7379580	-3.2065882	0.8827599
H	2.8794057	-2.2955788	1.8887458
C	-5.2654894	-3.4958595	1.3097082
H	-5.2845017	-2.9327317	3.4006075
H	-4.9710480	0.2533828	3.3740770
H	-4.0999355	-0.9902058	4.3281168
H	-3.2099988	0.1406773	3.2570858
H	-5.1670493	-3.7097928	-0.8472449
H	-4.4553237	-0.4592145	-1.8256871
H	-2.8325345	-1.1715134	-1.7196322
H	-4.1809930	-2.1485436	-2.3585955
C	5.3969733	2.9553928	-1.3121149
C	2.9022710	2.9338787	-1.8329415
C	6.5711778	0.9245542	-0.7225638
C	5.3458398	-1.3018815	-0.5452528
C	-2.9287320	7.8740241	-0.5908054
C	-0.1045537	-4.2450407	-3.3929325
C	2.0370626	-4.0188492	-2.0378864
C	-1.4092103	-2.3049218	-4.0092412
C	-0.6985310	0.0375382	-3.3090835
C	-5.9399319	-4.8305795	1.5319504
C	6.5978008	2.3114349	-0.9597477
H	5.4040353	4.0318541	-1.5210610
H	3.0790513	3.9937081	-2.0755092
H	2.4752915	2.4341170	-2.7211780
H	2.1448300	2.8812635	-1.0313084
H	7.5016517	0.4038548	-0.4659872
H	4.5696357	-1.5569594	0.1981310
H	5.0899150	-1.8390350	-1.4775992
H	6.3197156	-1.6655379	-0.1808601
H	-1.9356152	8.2499859	-0.9028023
H	-3.6443670	8.1365875	-1.3881762
H	-3.2117142	8.4142056	0.3282344
C	-1.2258854	-3.6998373	-4.0444955
H	0.0723739	-5.3260897	-3.4397716
H	2.1474393	-3.6798855	-0.9941175
H	2.0197637	-5.1199678	-2.0532700
H	2.9325609	-3.6639847	-2.5819779
H	-2.2546146	-1.8580974	-4.5453101
H	-0.7941802	0.4394414	-2.2848993
H	0.1904010	0.5126559	-3.7628224
H	-1.5884925	0.3336946	-3.8862455
H	-5.1933041	-5.6473488	1.5406889
H	-6.4733031	-4.8568756	2.4965559
H	-6.6593635	-5.0555148	0.7259464
C	7.8826718	3.0961190	-0.8156260
C	-2.2223521	-4.5886409	-4.7534997
H	7.9074607	3.9578456	-1.5039734
H	7.9838629	3.4941012	0.2123141
H	8.7646783	2.4636877	-1.0122795
H	-1.7757777	-5.5592850	-5.0257349
H	-3.0922527	-4.7939214	-4.1004692
H	-2.6088526	-4.1092239	-5.6690485
C	2.0580996	0.0851892	-0.0980979
H	1.9136633	1.0459179	0.7854116
C	-1.4366271	1.4651959	0.2286471
H	-0.4742272	1.9381503	0.0465983
C	-1.1822823	-3.0689671	0.2482132
H	-1.9812156	-3.2978981	0.9712223
H	-1.5996623	-3.0873833	-0.7701738
H	-0.3918638	-3.8326617	0.3150113
Li	1.9807811	0.1102421	2.2050462
C	1.5211820	2.1971109	1.8640252
H	0.5661051	2.1491853	2.4344779
H	2.2971433	2.5824107	2.5630472
H	1.3754032	2.9962382	1.1080377
C	4.7308852	0.8596905	2.6538965
O	3.6858186	-0.0753760	3.0461590
C	4.2336577	-0.9387600	4.0630150
C	5.6553465	-1.2047942	3.5737674
C	6.0704483	0.1678146	2.9955820
H	4.5954273	1.0617834	1.5810970
H	4.5950316	1.8002221	3.2161881
H	4.2239494	-0.4170426	5.0407712
H	3.5941776	-1.8318203	4.1261416
H	6.3242384	-1.5532014	4.3769480
H	5.6349593	-1.9732279	2.7818315
H	6.6259027	0.7563323	3.7441413
H	6.7105594	0.0646499	2.1055574

TS3

132

Energy = -5259.202965407

C	-1.1660479	-0.6677408	0.1582221
N	-2.8477243	0.1865156	-1.0138103
Ge	0.4448443	-0.8615632	1.2537745
N	-1.8255412	-1.6845582	-0.5570075
C	-2.8660748	-1.1655503	-1.2992278
C	-3.8116591	1.1300110	-1.5019399
C	2.0172591	-0.1385496	0.4007590
N	0.1093785	0.5605915	2.5349841
C	-1.5412087	-3.0876972	-0.4409365
N	3.4141690	1.4235956	-0.2479562
S	-3.9085541	-2.0116722	-2.3178259
C	-3.4070236	2.0696469	-2.4724798

C	-5.1208739	1.1109022	-0.9751371
N	3.1885128	-0.7431576	-0.1271219
C	-1.1542488	0.3562125	3.2829397
C	1.2677701	0.7448160	3.4666205
C	-2.1074119	-3.7987268	0.6358752
C	-0.6887206	-3.6957173	-1.3797048
C	4.0672371	0.2355155	-0.5266099
C	3.9675582	2.7172953	-0.5238062
C	-4.3458139	3.0296145	-2.8904414
C	-2.0235225	2.0035057	-3.0755790
C	-6.0303806	2.0749163	-1.4423807
C	-5.5299974	0.0701298	0.0362388
C	3.3848938	-2.1465266	-0.3273461
C	-1.6232652	1.5760087	4.0865156
H	-1.0669355	-0.5036829	3.9809067
H	-1.9290471	0.0643765	2.5466362
C	1.6703200	2.2110182	3.6645227
H	2.1399729	0.2099192	3.0507419
H	1.0341485	0.2743337	4.4423752
C	-1.7355072	-5.1420615	0.8012029
C	-3.1005370	-3.1271510	1.5532107
C	-0.3360327	-5.0395341	-1.1702161
C	-0.2373425	-2.9247518	-2.5912613
S	5.6098372	0.0248709	-1.1905508
C	3.5141627	3.4131344	-1.6632111
C	4.9072762	3.2727567	0.3648496
C	-5.6593777	3.0511272	-2.3859173
H	-4.0458471	3.7685959	-3.6427081
H	-1.8949306	2.7787685	-3.8472750
H	-1.2357511	2.1342935	-2.3140617
H	-1.8570311	1.0141419	-3.5387912
H	-7.0552306	2.0676698	-1.0520981
H	-4.7640983	-0.0489879	0.8227886
H	-6.4912451	0.3262228	0.5089857
H	-5.6233046	-0.9131321	-0.4623791
C	3.7431659	-2.9526532	0.7712126
C	3.1855223	-2.6846286	-1.6164734
H	-2.6189615	1.3824901	4.5200748
H	-0.9369857	1.8010692	4.9183485
H	-1.6870993	2.4939318	3.4686031
H	2.4894342	2.2872546	4.4007744
H	2.0542196	2.6350234	2.7163554
H	0.8335375	2.8322722	4.0247815
C	-0.8324517	-5.7718648	-0.0766507
H	-2.1580796	-5.7092884	1.6390745
H	-3.4110317	-3.8025957	2.3657091
H	-2.6814199	-2.2086847	2.0023468
H	-3.9980180	-2.8241269	0.9829907
H	0.3414071	-5.5235473	-1.8825556
H	-1.1128581	-2.7143183	-3.2340480
H	0.1970285	-1.9520821	-2.3092083
H	0.5070854	-3.4910548	-3.1698669
C	4.0177979	4.7035148	-1.8938941
C	2.5320092	2.7611806	-2.6070990
C	5.3883793	4.5660264	0.0928483
C	5.3870338	2.4804165	1.5558021
C	-6.6418210	4.1156468	-2.8197318
C	3.8028314	-4.3432636	0.5779265
C	4.1353271	-2.3194195	2.0849708
C	3.2686119	-4.0787453	-1.7651471
C	2.9646526	-1.7700740	-2.7949813
C	-0.3948821	-7.1989314	0.1645946
C	4.9530097	5.2990171	-1.0256215
H	3.6752599	5.2552511	-2.7781805
H	2.2746076	3.4351415	-3.4400814
H	2.9594400	1.8309696	-3.0243347
H	1.6065106	2.4726136	-2.0769871
H	6.1228617	5.0115324	0.7751816
H	4.5354410	2.0953417	2.1445329
H	5.9622255	1.6011265	1.2083726
H	6.0263542	3.0933498	2.2117771
H	-7.6689289	3.7166289	-2.8745252
H	-6.6541458	4.9531723	-2.0957749
H	-6.3738258	4.5346799	-3.8037474
C	3.5473121	-4.9260196	-0.6768614
H	4.0669742	-4.9853341	1.4268990
H	3.4436156	-1.5113615	2.3752396
H	4.1747437	-3.0652941	2.8948095
H	5.1346380	-1.8555674	1.9868967
H	3.1097703	-4.5145332	-2.7589932
H	2.2089553	-0.9973760	-2.5720865
H	3.9081623	-1.2339217	-3.0125459
H	2.6518877	-2.3325381	-3.6885183
H	0.4438027	-7.2306495	0.8859977
H	-1.2127609	-7.8056797	0.5891964
H	-0.0500755	-7.6778619	-0.7668881
C	5.4597069	6.7012280	-1.2844582
C	3.5569161	-6.4279152	-0.8502102
H	5.7153962	6.8454929	-2.3490864
H	4.6883757	7.4536323	-1.0320031
H	6.3543442	6.9233196	-0.6791457
H	4.2442776	-6.9132889	-0.1368042
H	2.5479001	-6.8448057	-0.6708670
H	3.8527961	-6.7142373	-1.8736090
C	2.1437770	1.2429369	0.3283747
C	-1.8148406	0.5244958	-0.1128416
H	-1.3223996	1.8576425	0.0595017
C	0.5962641	-2.5993567	2.1454724
H	-0.3478427	-2.8478215	2.6539540
H	0.8225528	-3.3826557	1.4047236
H	1.4078428	-2.5596239	2.8887965
Li	0.5537543	2.1573306	1.1897003
Li	-2.3590168	2.0092778	1.3665989
C	-0.9823647	3.3201463	0.2601406
H	-0.0152560	3.4837278	-0.2587267
H	-1.7418978	3.7847518	-0.3940898
H	-0.9577436	3.9398637	1.1888198
C	-4.3492359	4.0635987	1.0216431
O	-3.9433267	2.8827433	1.7914974
C	-4.9738087	2.5380650	2.7582160
C	-6.2428785	3.1840755	2.2139091
C	-5.6995860	4.4881539	1.6062701
H	-3.5664791	4.8310067	1.1294339
H	-4.4221782	3.7555892	-0.0341836
H	-5.0175739	1.4394930	2.8242049
H	-4.6928377	2.9512933	3.7448066
H	-6.6879491	2.5479798	1.4311550
H	-6.9962930	3.3526084	2.9995846
H	-6.3629539	4.9114875	0.8351317
H	-5.5588267	5.2482587	2.3938902

TS4

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Energy = -5266.163868049

C	-1.9877595	-0.8942727	0.1863495
N	-3.8052567	0.1707406	-0.4414582
Ge	-0.3266545	-1.1802387	1.1491031
N	-2.8959952	-1.8110147	-0.3768699
C	-4.0286979	-1.1426132	-0.8017302
C	-4.7002426	1.2454734	-0.7577039
C	0.7585024	0.3826023	0.7311939
N	-0.8971849	-0.6075549	2.8983692
C	-2.6436245	-3.2140931	-0.5324911
N	1.4287406	2.4710673	0.5907825
S	-5.3634611	-1.7688182	-1.6217090
C	-4.5405877	1.9208838	-1.9830709
C	-5.6782090	1.6214019	0.1837063
N	2.0740736	0.4177040	0.2462521
C	-2.0188641	-1.4149519	3.4273033
C	0.2312241	-0.4447860	3.8578664
C	-3.3228460	-4.1421853	0.2860840
C	-1.6681225	-3.6204456	-1.4681380
C	2.4937355	1.7150768	0.1517582
C	1.4251262	3.9047542	0.6165356
C	-5.3744834	3.0231002	-2.2429159
C	-3.5378892	1.4260378	-2.9991309
C	-6.4934936	2.7239748	-0.1188537
C	-5.8411085	0.8257898	1.4560621
C	2.7702343	-0.7437981	-0.2361297
C	-2.8302916	-0.7197989	4.5236475
H	-1.6558242	-2.3947827	3.8055946
H	-2.6870914	-1.6284622	2.5741263
C	0.2347641	0.9178934	4.5583379
H	1.1859957	-0.5533782	3.3099814
H	0.2065938	-1.2643166	4.6034988
C	-2.9710254	-5.4982880	0.1717676
C	-4.4139461	-3.6997843	1.2276210
C	-1.3509241	-4.9864131	-1.5439186
C	-0.9802012	-2.6155370	-2.3594321
S	3.9898702	2.2746648	-0.4507775
C	0.6553721	4.6053538	-0.3321472
C	2.1578071	4.5777812	1.6204977
C	-6.3507279	3.4433578	-1.3215988
H	-5.2639307	3.5597690	-3.1929285
H	-3.8550305	0.4397031	-3.3864420
H	-3.4416796	2.1257281	-3.8442159
H	-2.5371364	1.2708189	-2.5524347
H	-7.2617576	3.0280086	0.6025880
H	-4.8923719	0.7803946	2.0211379
H	-6.6180202	1.2621822	2.1037281
H	-6.1222245	-0.2162041	1.2157405
C	3.5559554	-1.5013318	0.6788992
C	2.5400729	-1.1308145	-1.5722109
H	-2.2302759	-0.5461172	5.4329742
H	-3.6948586	-1.3455667	4.8069717
H	-3.2159484	0.2560108	4.1736101
H	1.0916378	0.9972873	5.2510713
H	0.3293101	1.7263479	3.8095757
H	-0.6893719	1.0847468	5.1372832
C	-1.9804514	-5.9398085	-0.7241174
H	-3.4881944	-6.2296049	0.8045186
H	-4.6939183	-4.5095836	1.9200131
H	-4.1061730	-2.8192053	1.8167538
H	-5.3021127	-3.3917275	0.6440923
H	-0.5938211	-5.3121776	-2.2672276
H	-1.6928600	-1.8653417	-2.7414143
H	-0.1941972	-2.0676804	-1.8103935
H	-0.4952372	-3.1167953	-3.2119989
C	0.6345142	6.0110253	-0.2708311
C	-0.1458108	3.8901967	-1.4007119
C	2.1082902	5.9794542	1.6419432
C	2.9605383	3.8027390	2.6359061
C	-7.2199440	4.6485290	-1.6049916
C	4.0692680	-2.7311858	0.1705922
C	3.9177398	-0.9890515	1.9974521
C	3.0745099	-2.3511860	-2.0138319
C	1.7615491	-0.2194229	-2.4944690
C	-1.5873427	-7.3984831	-0.7902673
C	1.3556283	6.7162219	0.7056716
H	0.0454023	6.5665870	-1.0101583
H	-0.1128666	4.4364373	-2.3567067
H	0.2400878	2.8726852	-1.5936103
H	-1.2268100	3.8504939	-1.1349656
H	2.6701569	6.5128306	2.4180610
H	2.3544231	2.9993049	3.0899912
H	3.8250676	3.3161969	2.1467824
H	3.3283081	4.4655120	3.4352112
H	-6.8760738	5.5262351	-1.0254372
H	-7.1930491	4.9213238	-2.6729796
H	-8.2696242	4.4620184	-1.3183629
C	3.8286188	-3.1676157	-1.1354968
H	4.6585223	-3.3641909	0.8453967
H	4.1529522	-1.7808679	2.7270490
H	5.1013611	-0.2927423	1.9956355
H	3.2031835	-0.2612099	2.4144691
H	2.8987265	-2.6730154	-3.0466514
H	0.7723322	0.0360286	-2.0711266
H	2.3065486	0.7329570	-2.6363257
H	1.6051367	-0.6879157	-3.4787219
H	-0.7388613	-7.6050535	-0.1101276
H	-2.4201331	-8.0546011	-0.4862789
H	-1.2689791	-7.6832946	-1.8074824
C	1.3365984	8.2274864	0.7534420
C	4.3747641	-4.4923796	-1.6207679
H	0.6281285	8.6441424	0.0190233
H	1.0495341	8.5895928	1.7568660
H	2.3384701	8.6408489	0.5348740
H	4.9218864	-5.0200825	-0.8223072
H	3.5612664	-5.1514663	-1.9755667
H	5.0652269	-4.3514497	-2.4735322
C	0.3090462	1.6805425	0.9582055
C	-2.5481868	0.3803549	0.1698958
C	0.5029268	-2.9460973	1.1321761
H	-0.2629528	-3.7120633	1.3353443
H	0.9658900	-3.1385408	0.1514024
H	1.2886548	-2.9771732	1.9036531
Li	-1.3259140	1.9645156	-0.2888101
Li	-1.4983977	1.2073712	2.0774313
Li	5.4331677	0.4790192	0.3419346
C	6.4465560	0.4524646	2.2339899
H	7.0387938	1.1563938	1.5992538
H	6.1716591	1.0130480	3.1494212
H	7.1342012	-0.3667985	2.5276158
C	5.9794777	-0.0886274	-2.5015039
O	6.3489794	-0.3123165	-1.1118240
C	7.2425157	-1.4521673	-0.9998329
C	7.6861701	-1.7530108	-2.4319708
C	6.4479004	-1.3381375	-3.2440412

H	4.8921461	0.0774677	-2.5349357
H	6.4959683	0.8226405	-2.8569841
H	8.0664173	-1.1752527	-0.3220608
H	6.6774571	-2.2929228	-0.5581770
H	8.5546981	-1.1283841	-2.7070326
H	7.9642636	-2.8107618	-2.5688859
H	6.6687735	-1.1370972	-4.3048404
H	5.6702577	-2.1189215	-3.1895762

TS5

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Energy = -4993.299559069

C	-1.7075592	-0.0195160	0.5207160
N	-2.7568004	1.8225708	-0.0698902
Ge	-0.3376782	-1.2295464	1.2513043
N	-2.7217047	-0.3325240	-0.4146319
C	-3.3784040	0.8150955	-0.7972469
C	-3.0875232	3.2117690	-0.2066911
C	1.2724997	-0.5900501	0.4191813
N	-0.2026303	-0.4014127	2.9942932
C	-2.8157976	-1.6026117	-1.0715623
N	2.8690082	0.8290732	-0.0360515
S	-4.5973876	0.9488460	-1.9532106
C	-2.2005545	4.0564365	-0.9025676
C	-4.2712752	3.7055719	0.3816614
N	2.3945718	-1.3061309	-0.0062216
C	-1.4403354	-0.4168852	3.8049843
C	1.0566729	-0.0896725	3.7052990
C	-3.7687392	-2.5462013	-0.6488178
C	-1.8634862	-1.8905524	-2.0713743
C	3.4126722	-0.4241745	-0.2909759
C	3.5486802	2.0594793	-0.3212430
C	-2.5196888	5.4215752	-1.0085034
C	-0.9271110	3.5233254	-1.5221010
C	-4.5511477	5.0745925	0.2502945
C	-5.1993231	2.7768403	1.1236102
C	2.3489694	-2.7361792	-0.1468723
C	-1.5086661	-1.5937462	4.7856150
H	-2.2887016	-0.4528387	3.0991876
H	-1.5454429	0.5346126	4.3582246
C	1.0633901	1.2901158	4.3753955
H	1.8673492	-0.1512120	2.9619940
H	1.3118405	-0.8324224	4.5017790
C	-3.7033820	-3.8345094	-1.2073649
C	-4.8078417	-2.1608588	0.3740774
C	-1.8248199	-3.1923304	-2.5931976
C	-0.9252761	-0.8115948	-2.5607906
S	4.9745346	-0.7542286	-0.8315920
C	3.4300692	2.6131199	-1.6113560
C	4.2752075	2.6974783	0.7006948
C	-3.6911768	5.9499554	-0.4407446
H	-1.8391576	6.0855358	-1.5545821
H	-1.1213045	2.5815960	-2.0765581
H	-0.5071610	4.2333959	-2.2505121
H	-0.1414436	3.3686038	-0.7504217
H	-5.4680930	5.4694220	0.7043896
H	-5.9865926	3.3401650	1.6495050
H	-5.6726956	2.0750705	0.4112238
H	-4.6433666	2.1678159	1.8586058
C	2.2137234	-3.4962593	1.0529035
C	2.2567225	-3.3009571	-1.4351863
H	-1.4919138	-2.5656714	4.2503014
H	-2.4446374	-1.5833554	5.3684576
H	-0.6787661	-1.5700597	5.5166649
H	2.0272504	1.4500477	4.8858359
H	0.9605627	2.1196781	3.6470476
H	0.2614967	1.4020372	5.1230670
C	-2.7227260	-4.1845240	-2.1545564
H	-4.4272561	-4.5899563	-0.8796496
H	-5.4346785	-3.0223958	0.6530344
H	-4.3362048	-1.7554672	1.2880329
H	-5.4532858	-1.3607306	-0.0334105
H	-1.0752474	-3.4384716	-3.3537605
H	-0.4386570	-1.1039849	-3.5029677
H	-1.4795288	0.1291999	-2.7370290
H	-0.1148897	-0.6312503	-1.8242122
C	4.0369915	3.8556527	-1.8569286
C	2.7066859	1.8554115	-2.6984648
C	4.8696287	3.9377994	0.4121576
C	4.4211553	2.0340157	2.0483581
C	-4.0288124	7.4186673	-0.5683544
C	1.9686931	-4.8874334	0.8726137
C	2.2298660	-2.8647359	2.3660016
C	2.0106111	-4.6803506	-1.5427989
C	2.4359211	-2.4496307	-2.6683587
C	-2.6118134	-5.5991737	-2.6755753
C	4.7532830	4.5377394	-0.8553853
H	3.9523630	4.2988100	-2.8565279
H	3.2337952	0.9081313	-2.9151900
H	1.6793130	1.5780086	-2.3920674
H	2.6372480	2.4466016	-3.6247077
H	5.4415215	4.4462885	1.1979109
H	3.4341284	1.8547306	2.5109492
H	4.9088022	1.0485397	1.9342240
H	5.0225092	2.6512684	2.7345945
H	-4.1595506	7.8838965	0.4254968
H	-3.2374493	7.9678598	-1.1041925
H	-4.9771789	7.5599096	-1.1183731
C	1.8490301	-5.4793780	-0.3901978
H	1.8589218	-5.5135158	1.7683731
H	2.9014198	-1.9889070	2.4134837
H	2.5113727	-3.5906164	3.1583888
H	1.9336708	-5.1337096	-2.5381740
H	1.8785683	-1.5013792	-2.5885492
H	3.4995223	-2.1696233	-2.7856324
H	2.0970359	-2.9831985	-3.5714037
H	-1.7852452	-6.1311435	-2.1667202
H	-3.5379826	-6.1699665	-2.4980967
H	-2.3902500	-5.6139846	-3.7565171
C	5.3638317	5.8940982	-1.1302407
C	1.5148917	-6.9499426	-0.5251106
H	5.7097156	5.9756016	-2.1748580
H	4.6209592	6.6984346	-0.9672665
H	6.2179762	6.0936125	-0.4615427
H	1.7889510	-7.5134512	0.3830439
H	0.4280395	-7.0906101	-0.6863923
H	2.0315037	-7.4056726	-1.3879643
C	1.5330941	0.7771108	0.4146522
C	-1.7115693	1.3506161	0.7626495
C	-0.9972637	-3.0787930	1.2574045
H	-2.0640840	-3.0767508	1.5299600
H	-0.8899081	-3.4774974	0.2350980
H	-0.4237356	-3.7405936	1.9257855
Li	-0.1278819	1.3382088	-0.6684710

Li	0.0281339	1.5603434	1.8594757
Li	0.5768340	-2.4380435	3.5436684