Supporting information for:

A Lithiomethyl Trimethylammonium Reagent as Methylene Donor

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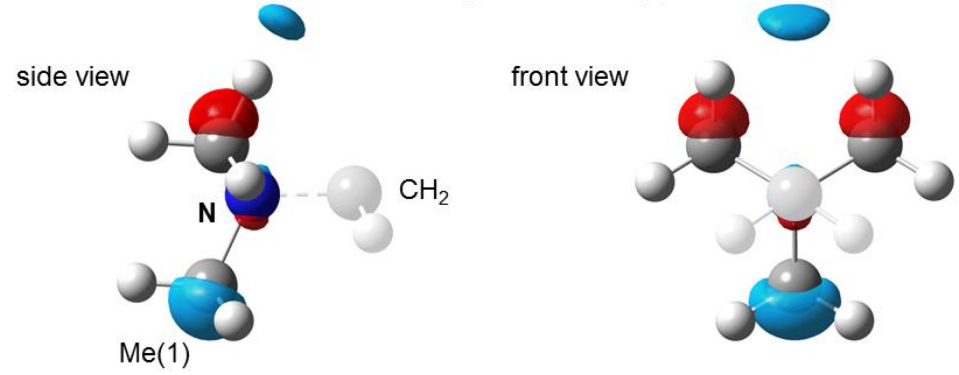
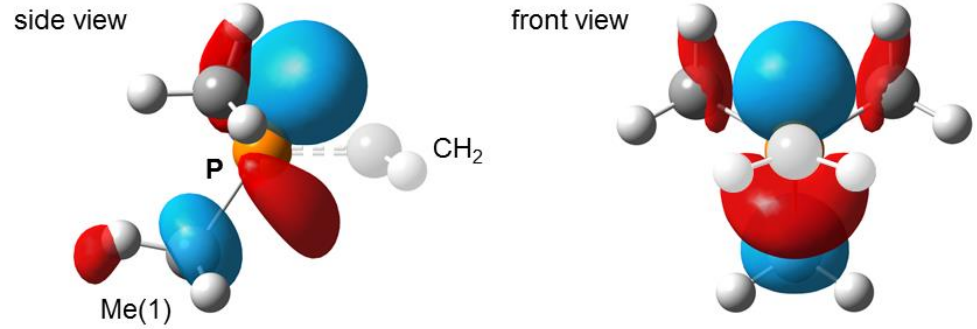
Table S1. Support for the reduced negative p,σ*-hyperconjugation in N–C ylides *vs.* P–C ylides as evidenced by the reduced electronic redistribution from the CH_2 or CH_2Li^+ fragment into the N–Me(1) *vs.* the P–Me(1) σ* antibonding Symmetrised Fragment Orbital (SFO)[a] of the NMe_3 and the PMe_3 fragment, respectively.

Structure	X = N (electrons[b])	X = P (electrons[b])
XMe_3CH_2	0.06	0.34
XMe_3CH_2 (Li^+ geometry)	0.05	0.20
$XMe_3CH_2Li^+$	0.01	0.08

Visualisation[c] of the σ* antibonding SFO in NMe_3 (for NMe_3CH_2, 0.06 electron)



Visualisation[c] of the σ* antibonding SFO in PMe_3 (for PMe_3CH_2, 0.34 electron)



[a] SFOs are obtained from the ETS bond analysis, for more information see ref 1. [b] Mulliken population. [c] 5% contours.

[1] a) T. Ziegler and A. Rauk, *Inorg. Chem.*, 1979, **18**, 1558; b) T. Ziegler and A. Rauk, *Inorg. Chem.*, 1979, **18**, 1755; c) F. M. Bickelhaupt and E. J. Baerends, in *Rev. Comput. Chem.*, ed. K. B. Lipkowitz and D. B. Boyd, Wiley, New York, 2000, vol. 15, pp. 1.

2. Experimental procedures

General procedures:

Warning: *to ensure a good reproducibility no traces of metals need to be present in the reaction mixture. We ensured this by cleaning all glassware, including self-made glass stir bars, using aqua regia.*

All reactions were conducted under an Ar atmosphere using standard Schlenk or glove-box techniques. Flash chromatography was performed over silica gel, or over neutral or basic aluminium oxide. Concentration of solutions was conducted using a rotary evaporator. ^{1}H NMR spectra were recorded at 400 MHz (Bruker AV400 spectrometer) or at 500 MHz (Varian DRX500 spectrometer) with $CDCl_3$, CD_3OD, or THF-D_8 as solvent. NOESY spectra were recorded at 500 MHz (Varian DRX500 spectrometer) with THF-D_8 as solvent. LED/DOSY spectra were recorded at 500 MHz (Varian DRX500 spectrometer) with THF-D_8 as solvent. ^{13}C NMR spectra were recorded at 101 MHz (Bruker AV400 spectrometer) or 126 MHz (Varian DRX500 spectrometer) with $CDCl_3$ or THF-D_8 as solvent. The nature of the carbon was determined from HSQC ^{1}H,^{13}C NMR experiments at 126 MHz (Varian DRX500 spectrometer) with THF-D_8 as solvent. ^{6}Li- and ^{1}H,^{6}Li HMBC spectra were recorded at 73.62 MHz, respectively 500 MHz (both on Bruker AV500 spectrometer) with THF-D_8 as solvent. ^{1}H,^{15}N HMBC spectra were recorded at 500 MHz (Varian DRX500 spectrometer) with THF-D_8 as solvent. ^{19}F NMR experiments were recorded at 376 MHz (Bruker AV400 spectrometer) with CD_3OD as solvent. Chemical shifts were determined relative to the residual solvent peaks ($CHCl_3$, δ = 7.26 for hydrogen atoms, δ = 77.0 for carbon atoms; THF-D_8 δ = 3.58 for hydrogen atoms, δ = 67.57 for carbon atoms; CD_3OD δ = 3.31 for hydrogen atoms, δ = 49.00 for carbon atoms) or not corrected (^{6}Li, ^{15}N and ^{19}F). The following abbreviations are used to indicate signal multiplicity: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. Elemental analysis was performed by the Mikroelementaranalytisches Laboratorium der ETHZ. Melting point was measured on a Büchi melting point apparatus.

CH_2Cl_2 (purum) was purchased from Sigma-Aldrich. Anhydrous CH_2Cl_2 was distilled from CaH under N_2 prior to use. Anhydrous Et_2O was distilled from Na/K under N_2 prior to use. Anhydrous THF-D_8 was distilled from CaH_2 under Ar and stored in the glove-box prior to use. Anhydrous THF was distilled from K or Na/benzophenone under N_2 prior to use.

Sodium tetrakis(3,5-bis(trifluoromethyl)phenyl)borate ($NaBAr^F$) was prepared according to the procedure described in ref 2; after washing the $NaBAr^F$ at low temperature with anhydrous CH_2Cl_2 the $NaBAr^F$ was left open to air in order to attract water as this enhances the solubility of $NaBAr^F$ in CH_2Cl_2.

NMe_4I, *n*BuLi (2.0 M in cyclohexane), $AgSO_3CF_3$ (99%), *n*BuLi (1.6 M in hexane), benzophenone, butyrophenone, 5-nonanone, benzylideneaniline and benzylidene-*tert*-butylamine were purchased from Sigma-Aldrich and used without further purification. 12-crown-4 was purchased from Sigma-Aldrich and stored in the glove box. NMe_4Cl was purchased from Acros Organics, dried under high vacuum and stored in the glove box. Cyclopropyl-4-mehoxyphenyl ketone was purchased from ABCR chemicals and used without further purification. 3-phenylpropionaldehyde was purchased from TCI-Deutschland and used without further purification.

Experimental data:

Tetramethylammonium BAr^F (**6**):[3]

In a round-bottom flask equipped with stir bar and open to air, $NaBAr^F$ (1 equiv., wet, open to air for a week) was dissolved in CH_2Cl_2 (40 mL/mmol $NaBAr^F$). Tetramethylammonium iodide (1.25 equiv.) was added. After stirring for 1 h the reaction was filtered over a glass filter. The CH_2Cl_2 was evaporated and the resulting powder was dissolved in Et_2O and filtered (to remove excess NMe_4I). The Et_2O was evaporated and the resulting powder was recrystalised from CH_2Cl_2 yielding the pure product. The product was then dried overnight under high vacuum.

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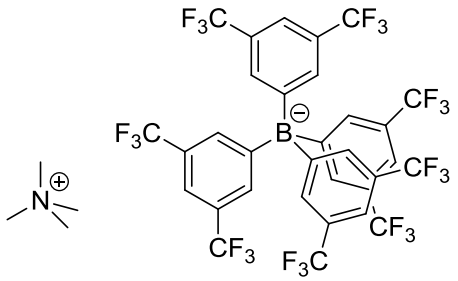
[2] N. A. Yakelis, R. G. Bergman, *Organometallics* **2005**, *24*, 3579-3581.

[3] P. N. Bartlett, D. C. Cook, M. W. George, J. Ke, W. Levason, G. Reid, W. Su, W. Zhang, *Phys. Chem. Chem. Phys.* **2010**, 12, 492-502.

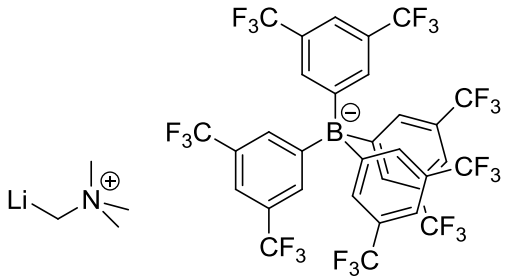
Characterisation:



Mp 249-250 °C (from CH_2Cl_2); Elemental analysis: found: C, 45.88; H, 2.56; N, 1.49; calc. for $C_{36}H_{24}BF_{24}N$: C, 46.13; H, 2.58; N, 1.49 %; ^{1}H NMR (400 MHz, THF-D_8) δ 7.80 (s, 8H), 7.59 (s, 4H), 3.31 – 3.14 (m, 12H); ^{13}C NMR (101 MHz, THF-D_8) δ 162.99 (dd, $^1J_{(C\text{-}B)}$ = 49.8 Hz, C), 135.78 (CH), 130.22 (qq, $^2J_{(C\text{-}F)}$ = 31.5 Hz, $^3J_{(C\text{-}B)}$ = 2.8 Hz, C), 125.71 (q, $^1J_{(C\text{-}F)}$ = 272.2 Hz, C), 118.38 (m, CH), 55.90 (t, $^3J_{(C\text{-}N)}$ = 4.0 Hz, CH_3).

Monolithiation of tetramethylammonium BAr^F for NMR studies:
In an NMR tube (closable with a screw cap with septum) under an Ar atmosphere, tetramethylammonium BAr^F (weighed in the glove box, 1 equiv) was dissolved in anhydrous THF-D_8 (8 mL/mmol NMe_4 BAr^F). The NMR tube was cooled to approximately -40 °C and *n*BuLi (2.0 M in cyclohexane, 1.05 equiv.) was added via microsyringe. The NMR tube was closed, shaken and cooled to approximately -60 °C and transferred into the NMR spectrometer.

Characterisation of lithiomethyl trimethylammonium BAr^F:

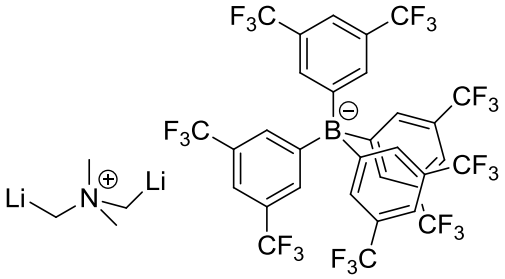


^{1}H NMR (500 MHz, THF-D_8, -30 °C) δ 7.84 (s, broad, 8H), 7.64 (s, broad, 4H), 2.95 (s, 9H), 2.27 (s, 2H); Residual peaks: 3.17 (s, NMe_4), 2.10 (s, NMe_3), 1.43 (s, broad, cyclohexane), 1.31 – 1.21 (m, Bu), 0.92 – 0.83 (m, Bu); ^{1}H NMR (500 MHz, THF-D_8, -60 °C) δ 7.88 (s, broad, 8H), 7.69 (s, broad, 4H), 2.95 (s, 9H), 2.25 (s, 2H); Residual peaks: 3.17 (s, NMe_4), 2.10 (s, NMe_3), 1.66 (s, broad, cyclohexane), 1.32 – 1.24 (m, Bu), 1.20 (s, broad, cyclohexane), 0.92 – 0.83 (m, Bu); NOESY (500 MHz, THF-D_8, -30 °C): there is a strong correlation between δ 2.95 and δ 2.27; there are weak correlations between δ 3.17 and δ 2.95 and between δ 3.17 and δ 2.27; NOESY (500 MHz, THF-D_8, -60 °C): there is correlation between δ 2.95 and δ 2.25; LED/DOSY (500 MHz, THF-D_8, -60 °C): the lithiomethyl trimethylammonium and BAr^F have different diffusion constants, thus the BAr^F is, even at -60 °C, not coordinating strongly to lithiomethyl trimethylammonium in solution; ^{13}C NMR (126 MHz, THF-D_8, -30 °C) δ 163.02 (q, $^1J_{(C\text{-}B)}$ = 49.6 Hz, C), 135.63 (s, CH), 130.13 (qq, $^2J_{(C\text{-}F)}$ = 31.5 Hz, $^3J_{(C\text{-}B)}$ = 2.7 Hz, C), 125.61 (q, $^1J_{(C\text{-}F)}$ = 272.3 Hz, C), 118.44 (m, CH), 76.82 (s, broad, CH_2), 60.16 (s, CH_3); Residual peaks: 55.73 – 55.00 (m, $^1J_{(C\text{-}N)}$, NMe_4), 48.20 (s, NMe_3), 32.98 (s, aliphatic), 27.87 (s, cyclohexane), 26.05 (s, Bu). 23.94 (s, aliphatic), 14.52 (s, Bu); ^{13}C NMR (126 MHz, THF-D_8, -60 °C) δ 163.11 (q, $^1J_{(C\text{-}B)}$ = 49.6 Hz, C), 135.56 (s, CH), 130.11 (qq, $^2J_{(C\text{-}F)}$ = 31.5 Hz, $^3J_{(C\text{-}B)}$ = 2.5 Hz, C), 125.58 (q, $^1J_{(C\text{-}F)}$ = 272.3 Hz, C), 118.52 (s, CH), 76.33 (q, $J_{(C\text{-}^7Li)}$ = 34.9 Hz, CH_2), 59.98 (s, CH_3); Residual peaks: 55.25 – 55.12 (m, $^1J_{(C\text{-}N)}$, NMe_4), 48.24 (s, NMe_3), 33.11 (s, aliphatic), 27.83 (s, cyclohexane), 26.16 (s, Bu), 14.70 (s, Bu); ^{6}Li NMR (73.61 MHz, THF-D_8, -30 °C) -1.04 (s); ^{6}Li NMR (73.61 MHz, THF-D_8, -60 °C) -0.94 (s); ^{1}H,^{6}Li HMBC (73.61 MHz,

THF-D_8, -30 °C) there is correlation between ^{1}H-δ 2.27 and ^{6}Li-δ -1.04; ^{1}H,^{6}Li HMBC (73.61 MHz, THF-D_8, -60 °C) there is correlation between ^{1}H-δ 2.25 and ^{6}Li-δ -0.94; ^{1}H,^{15}N HMBC (500 MHz, THF-D_8, -30 °C) there is correlation between ^{1}H-δ 2.95 and ^{15}N-δ 49.78 and between H-δ 2.27 and N-δ 49.78.

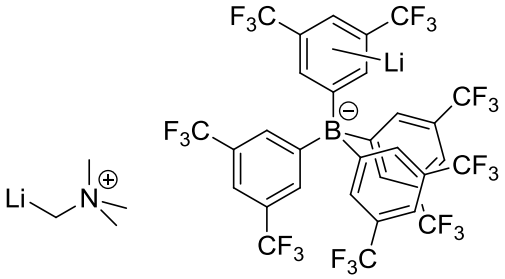
Double lithiation of tetramethylammonium BAr^F for NMR studies:
In an NMR tube (closable with a screw cap with septum) under an Ar atmosphere, tetramethylammonium BAr^F (weighed in the glove box, 1 equiv) was dissolved in anhydrous THF-D_8 (8 mL/mmol NMe_4 BAr^F). The NMR tube was cooled to ~ -40 °C and nBuLi (2.0 M in cyclohexane, 2.5 equiv.) was added via microsyringe. The NMR tube was closed, shaken and cooled to ~ -60 °C and transferred into the NMR spectrometer.

Characterisation of dilithiomethyl dimethylammonium BAr^F (**9**):



This compound slowly converts to lithiomethyl trimethylammonium LiBAr^F at -78 °C.
^{1}H NMR (500 MHz, THF-D_8, -78 °C) δ 7.90 (s, broad, 8H), 7.72 (s, broad, 4H), 3.00 (s, 6H), 2.11 (s, 4H); Residual peaks: 7.94 (s, LiBAr^F), 7.57 (s, LiBAr^F), 7.45 (s, LiBAr^F), 2.95 (s, lithiomethyl trimethylammonium BAr^F), 2.23 (s, lithiomethyl trimethylammonium BAr^F), 2.10 (s, NMe_3), 1.66 (s, broad, cyclohexane), 1.23 (m, cyclohexane, *n*BuLi and Bu), 0.93 – 0.78 (m, Bu), -0.97 – -1.23 (m, *n*BuLi); NOESY (500 MHz, THF-D_8, -78 °C): there is a strong correlation between δ 3.00 and δ 2.11; there are weak correlations between δ 3.17 and δ 2.95 and between δ 3.17 and δ 2.27; ^{13}C NMR (126 MHz, THF-D_8, -78 °C) δ 163.16 (q, $^1J_{(C\text{-}B)}$ = 49.6 Hz, C), 135.49 (s, CH), 130.08 (qq, $^2J_{(C\text{-}F)}$ = 31.4 Hz, $^3J_{(C\text{-}B)}$ = 2.7 Hz, C), 125.55 (q, $^1J_{(C\text{-}F)}$ = 272.4 Hz, C), 118.53 (s, CH), 73.42-71.87 (m, $J_{(C\text{-}^7Li)}$, CH_2), 59.85 (s, CH_3); Residual peaks: 135.97 (s, CH, LiBAr^F), 131.74 (s, CH, LiBAr^F), 130.86 (s, CH, LiBAr^F), 129.32 (q, $^2J_{(C\text{-}F)}$ = 31.1 Hz, C, LiBAr^F), 128.70 (s, CH, LiBAr^F), 125.80 (q, $^1J_{(C\text{-}F)}$ = 272.2 Hz, C, LiBAr^F), 117.45 (s, CH, LiBAr^F), 113.82 (s, CH, LiBAr^F), 48.26 (s, NMe_3), 45-10 (several alkanes and alkanelithium), 27.80 (s, Bu), 26.24 (s, cyclohexane), 14.83 (s, Bu); ^{6}Li NMR (74 MHz, THF-D_8, -78 °C) δ 0.79, -0.04 (*n*BuLi), -1.88; ^{1}H,^{6}Li HMBC (73.61 MHz, THF-D_8, -60 °C) no correlations were found, we attribute this to fast exchange processes between the different Li-species; ^{1}H,^{15}N HMBC (500 MHz, THF-D_8, -78 °C) there is correlation between ^{1}H-δ 3.00 and ^{15}N-δ 56.88 and between H-δ 2.11 and N-δ 56.88 and between ^{1}H-δ 2.95 and ^{15}N-δ 49.78, likely the concentration of NMe_3CH_2Li is too low to give the correlation between ^{1}H-δ 2.23 and ^{15}N-δ 49.78.

Characterisation of lithiomethyl trimethylammonium LiBAr^F:



^{1}H NMR (500 MHz, THF-D_8, -30 °C) δ 7.93 – 7.81 (m, 8H), 7.63 (s, broad), 7.51 (s, broad), 7.46 (s, broad), 7.39 (s, broad), 2.86 (s, 9H), 2.25 (s, 2H); Residual peaks: 2.11 (s, NMe_3), 1.43 (s, broad,

cyclohexane), 1.31 – 1.05 (m, Bu), 0.99 – 0.77 (m, Bu); ^{1}H NMR (500 MHz, THF-D_8, -60 °C) δ 7.95 – 7.83 (m, 8H), 7.68 (s, broad), 7.54 (s, broad), 7.44 (s, broad), 7.34 (s, broad), 2.85 (s, 9H), 2.20 (s, 2H); Residual peaks: 2.25 (s), 2.11 (s, NMe_3), 1.66 (s, broad, cyclohexane), 1.34 – 1.24 (m, Bu), 1.20 (s, broad, cyclohexane), 0.94 – 0.83 (m, Bu); NOESY (500 MHz, THF-D_8, -60 °C): there are no correlations with respect to either (Li)BAr^F or lithiomethyl trimethylammonium, we attribute this to fast exchange processes between the different Li-species; ^{13}C NMR (126 MHz, THF-D_8, -60 °C) δ 167.06 – 164.71 (m, broad, C), 163.10 (q, $^{1}J_{(C-B)}$ = 49.6 Hz, C), 151.70 – 149.30 (m, broad, C), 141.21 (s, C), 140.40 (q, $^{2}J_{(C-F)}$ = 24.4 Hz, C), 136.52 (s, CH), 136.00 (s, CH), 135.54 (s, CH), 133.13 (s, C), 132.51 (s, CH), 131.81 (s, CH), 130.96 (s, C), 130.09 (q, $^{2}J_{(C-F)}$ = 32.1 Hz, C), 129.33 (q, $^{2}J_{(C-F)}$ = 31.3 Hz, C), 125.82 (q, $^{1}J_{(C-F)}$ = 272.2 Hz, C), 125.56 (q, $^{1}J_{(C-F)}$ = 272.3 Hz, C), 126.10 (q, $^{1}J_{(C-F)}$ = 272.4 Hz, C), 118.46 (s, CH), 117.45 (s, CH), 116.49 (s, CH), 113.80 (s, C), 78.48 – 75.06 (m, broad, CH_2), 59.91 (s, CH_3); Residual peaks: 48.24 (s, NMe_3), 27.83 (s, Bu), 26.16 (s, cyclohexane), 14.72 (s, Bu); ^{6}Li NMR (74 MHz, THF-D_8, -30 °C) δ 2.0 – -2.0 (s, broad), 0.21 (s); ^{6}Li NMR (74 MHz, THF-D_8, -60 °C) δ 1.51 (s), 0.09 (s), -0.06 (s), -0.97 (s, NMe_3CH_2Li), -1.93 (s); ^{1}H,^{6}Li HMBC (73.61 MHz, THF-D_8, -60 °C) there is correlation between ^{1}H-δ 2.25 and ^{6}Li-δ -0.94.

Study of the formation of products of the degradation of lithiomethyl trimethylammonium BAr^F using NMR:

In an NMR tube (closable with a screw cap with septum) under an Ar atmosphere, tetramethylammonium BAr^F (weighed in the glove box, 1 equiv) was dissolved in anhydrous THF-D_8 (3 mL/mmol NMe_4 BAr^F). The NMR tube was cooled to ~ -40 °C and *n*BuLi (2.0 M in cyclohexane, 1.5 equiv.) was added via microsyringe. Consecutively, the solvent was evaporated at the Schlenk line under high vacuum at low temperature (up to ~-20 °C) leaving an off white powder on the walls of the NMR tube. Then slowly THF-D_8 (8 mL/mmol NMe_4 BAr^F) and THF-H_8 (20 equiv.) were added to the reaction mixture. The NMR tube was closed, shaken, cooled to ~ -60 °C and transferred into the NMR spectrometer (-20 °C). The NMR tube was then kept for 16 h at 10 °C. NMR spectra were recorded after 1 h and 16 h.

Results:

After 1 h and 16 h traces of ethylene (δ= 5.36 ppm), and substantial quantities of NMe_4 (δ= 3.16 ppm) and NMe_3 (δ= 2.10 ppm) formed.

12-crown-4 experiments:

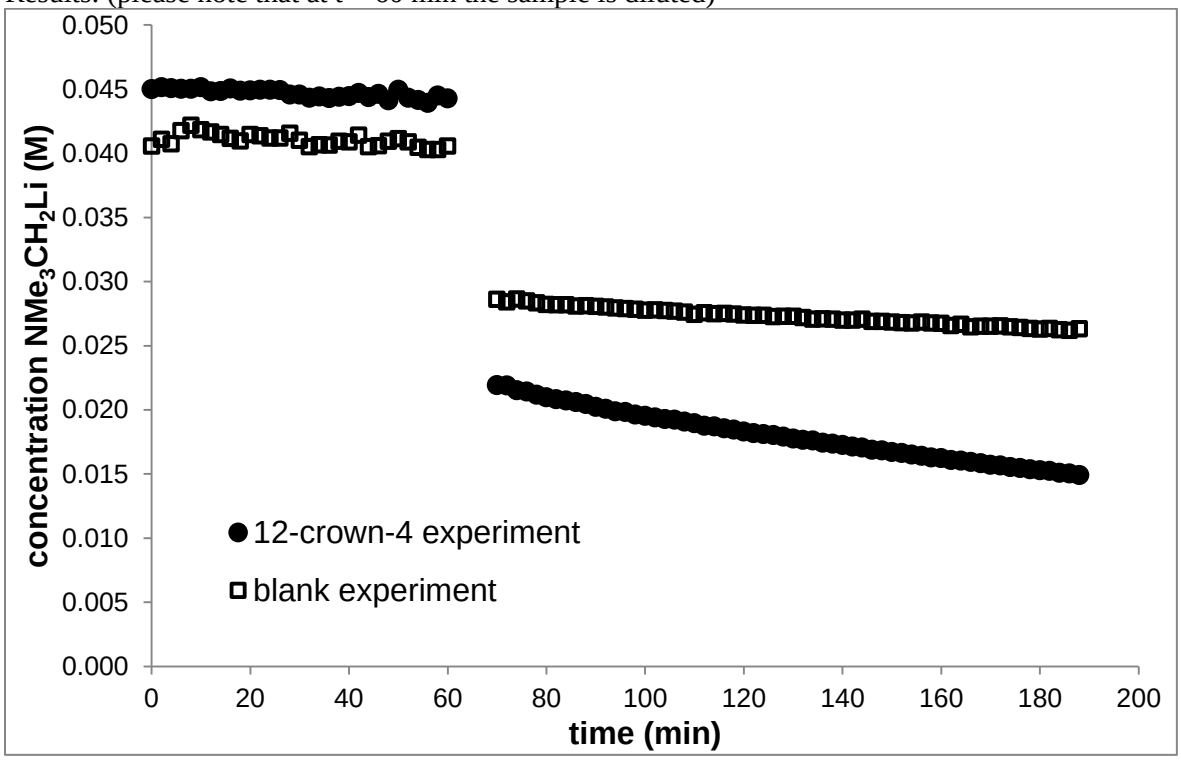
Blank experiment:

In an NMR tube (closable with a screw cap with septum) under an Ar atmosphere, tetramethylammonium BAr^F (weighed in the glove box, 1 equiv) was dissolved in anhydrous THF-D_8 (17 mL/mmol NMe_4 BAr^F). The NMR tube was cooled to ~ -40 °C and *n*BuLi (2.0 M in cyclohexane, 1.1 equiv.) was added via microsyringe. The NMR tube was closed, shaken and cooled to -60 °C and transferred into the NMR spectrometer (-30 °C). Spectra were recorded over 1 h showing only slight decomposition. Then the NMR tube was removed from the NMR spectrometer and cooled to -60 °C. Then anhydrous THF-D8 (3 mL/mmol NMe_4 BAr^F) was added. The NMR tube was shaken, cooled to ~ -60 °C and transferred into the NMR spectrometer (-30 °C). Spectra were recorded over the next 2 h.

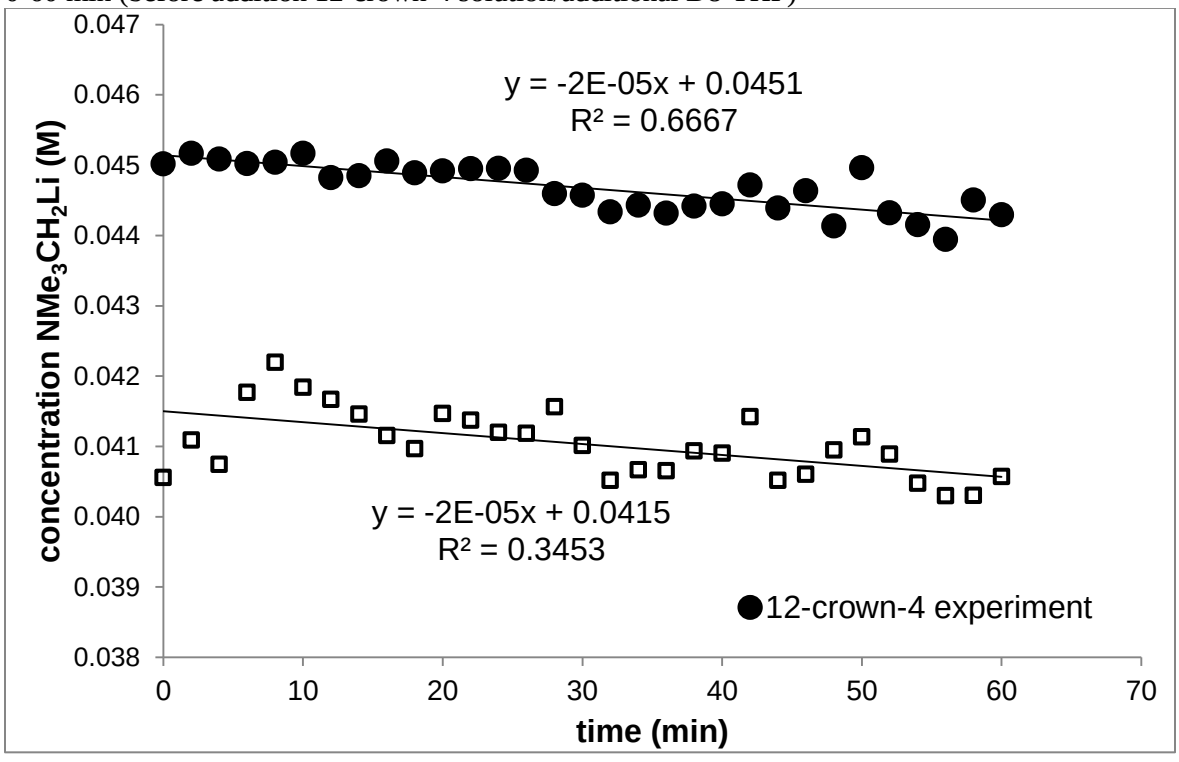
12-crown-4 experiment:

In an NMR tube (closable with a screw cap with septum) under an Ar atmosphere, tetramethylammonium BAr^F (weighed in the glove box, 1 equiv) was dissolved in anhydrous THF-D_8 (17 mL/mmol NMe_4 BAr^F). The NMR tube was cooled to ~ -40 °C and *n*BuLi (2.0 M in cyclohexane, 1.1 equiv.) was added via microsyringe. The NMR tube was closed, shaken and cooled to -60 °C and transferred into the NMR spectrometer (-30 °C). Spectra were recorded over 1 h showing only slight decomposition. Then the NMR tube was removed from the NMR spectrometer and cooled to -60 °C. Then 12-crown-4 (2 equiv.) in anhydrous THF-D8 (3 mL/mmol NMe_4 BAr^F) was added. The NMR tube was shaken, cooled to ~ -60 °C and transferred into the NMR spectrometer (-30 °C). Spectra were recorded over the next 2 h.

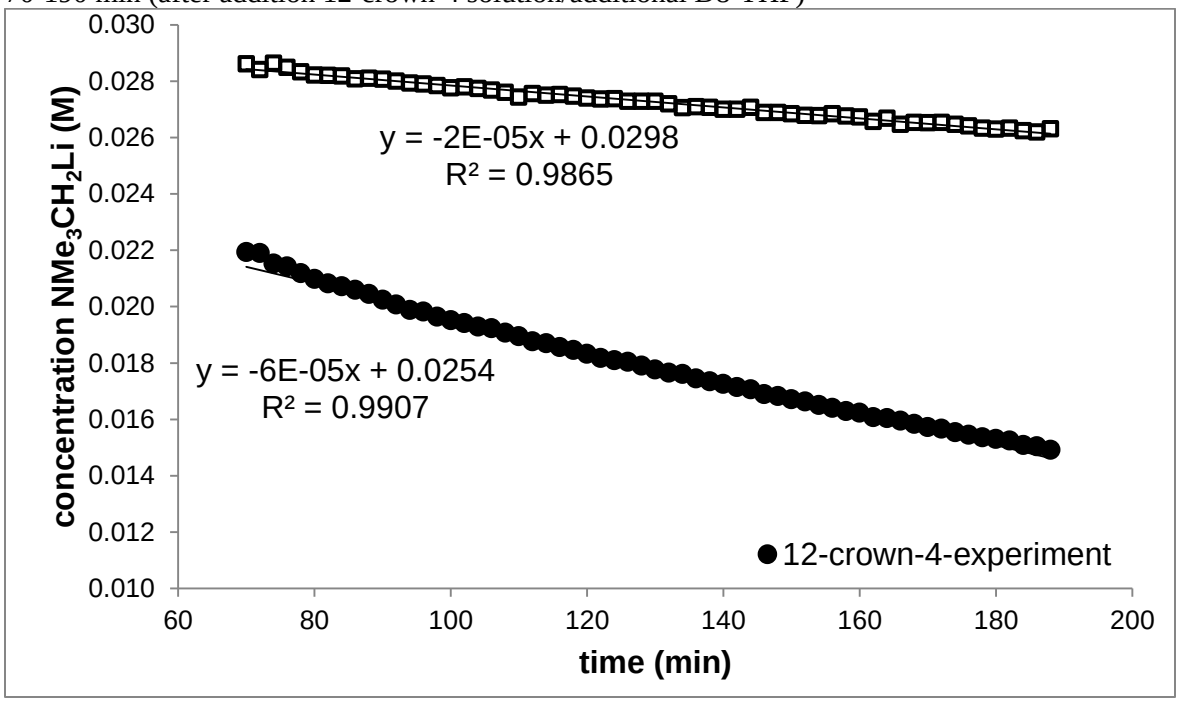
Results: (please note that at t = 60 min the sample is diluted)



Fits:
0-60 min (before addition 12-crown-4 solution/additional D8-THF)



70-190 min (after addition 12-crown-4 solution/additional D8-THF)

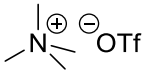


Tetramethylammonium OTf (**16**):

16 was prepared either following the procedure described by Martin and co-workers,[4] or by anion exchange according to the following procedure:

A 250 mL round bottom flask equipped with stir bar under air, was charged with tetramethylammonium chloride (2.2020 g, 20.09 mmol, 1 equiv) and 100 mL methanol. In another flask under air, silver trifluoromethanesulfonate (5.1622 g, 20.09 mmol, 1 equiv) was dissolved in 50 mL methanol. The AgOTf solution was added to the NMe_4 OTf solution under constant stirring. After 10 minutes the suspension was filtered to remove AgCl, and the solution was concentrated under reduced pressure. The crude salt was then recrystallised from anhydrous *iso*-propanol: the crude NMe_4 OTf was dissolved in *i*PrOH (approximately 60 mL per gram of salt), after keeping the solution at -20 °C for 20 h the crystals were filtered off, and rinsed with a small amount of chilled *i*PrOH. The product was dried under high vacuum ($5x10^{-2}$ mbar) for 16h. 3.7824 g (84%) of **16** was obtained as white powder.

Characterisation:[5]



Elemental analysis: Found: C, 26.95; H, 5.33; N, 6.22; F, 25.72; S, 14.29. Calc. for $C_5H_{12}NO_3F_3S$: C, 26.90; H, 5.42; N, 6.27; F, 25.53; S, 14.37 %; ^{1}H NMR (400 MHz, CD_3OD) δ 3.21-3.18 (m, 12H); ^{13}C NMR (101 MHz, CD_3OD) δ 123.3 (t, $^1J_{(C-F)}$ = 319 Hz), 55.9 (t, $^1J_{(C-N)}$ = 4 Hz); ^{19}F NMR (376 MHz, CD_3OD) δ -76.2.

Formation of epoxides and aziridines:

General procedure from methylenation of ketones and imines:

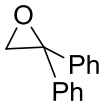
A dried 50 mL Schlenk flask equipped with a glass coated stir bar and a glass stopper under Ar, was charged with NMe_4 OTf (390 mg, 1.74 mmol). The salt was suspended in anhydrous THF (20 mL) and

[4] D. J. Sagl, J. C. Martin, *J. Am. Chem. Soc.* **1988**, *110*, 5827-5833.

[5] V. Beyl, H. Niederprüm, P. Voss, *Liebigs Ann. Chem.* **1970**, *731*, 58-66.

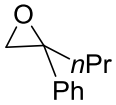
the flask was cooled down to 0 °C in an ice-water bath. *n*BuLi (1.00 mL, 1.6 M, 1.60 mmol) was added to the suspension and the flask was completely closed using the glass stopper and the Schlenk tap to prevent any gas exchange. The reaction mixture was stirred for 30 minutes at 0 °C. Then under an Ar counterflow at 0 °C, the ketone or imine substrate was added (1.45 mmol) either neat, or alternatively if the substrate is solid, dissolved in 2 mL of anhydrous THF. The flask was then again fully closed and the stirring was continued for 16 h during which the temperature was allowed to slowly reach room temperature. Then the reaction mixture was diluted with 30 mL of H_2O and transferred to a separation funnel. 20 mL of pentane was used to rinse the Schlenk flask and perform the first extraction of the aqueous phase. The aqueous phase was extracted using pentane (2x 10 mL). The combined organic extracts were washed with H_2O (4x 10 mL) and brine (10 mL), dried using $MgSO_4$, filtered and the solvent was concentrated under reduced pressure. The crude material was then purified by column chromatography on neutral aluminium oxide (epoxides), or basic aluminium oxide (aziridines).

2,2-diphenyloxirane (**19a**):
Benzophenone was used as substrate. **19a** was purified using column chromatography (neutral aluminium oxide) with a mixture of pentane/Et_2O (85/15) as eluent. 190 mg of **19a** (67 % yield) was obtained as a colorless oil.



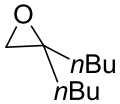
All experimental data was in agreement with data in ref 6.

2-phenyl-2-propyloxirane (**19b**):
Butyrophenone was used as substrate. **19b** was purified using column chromatography (neutral aluminium oxide) with a mixture of pentane/Et_2O (95/5) as eluent. 173 mg of **19b** (73 % yield) was obtained as a colorless oil.



All experimental data was in agreement with data in ref 7.

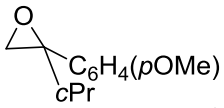
2,2-dibutyloxirane (**19c**):
Nonanone was used as substrate. **19c** was purified using column chromatography (neutral aluminium oxide) with a mixture of pentane/Et_2O (96/4) as eluent. 190 mg of **19c** (84 % yield) was obtained as a colorless oil.



All experimental data was in agreement with data in ref 8.

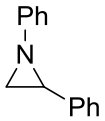
2-cyclopropyl-2-(4-methoxyphenyl)oxirane (**19d**):
Cyclopropyl-4-mehoxyphenyl ketone was used as substrate. All attempts to purify **19d** by traditional methods caused **19d** to decompose, therefore the crude product was characterised, the impurity consists of the ring-opened epoxide product: 2-cyclopropyl-2-(4-methoxyphenyl)acetaldehyde. 199 mg of a mixture of approximately 94% **19d** (corresponding to 68 % yield of **19d**) and 6% 2-cyclopropyl-2-(4-methoxyphenyl)acetaldehyde was obtained as a colorless oil.

[6] Y. H. Kim, B. C. Chung, *J. Org. Chem.* **1983**, *48*, 1564-1565.
[7] B. Wang, O. A. Wong, M.-X. Zhao, Y. Shi, *J. Org. Chem.* **2008**, *73*, 9539-9543.
[8] F.-L. Wu, B. P. Ross, R. P. McGeary, *Eur. J. Org. Chem.* **2010**, 1989-1998.



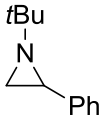
Characterisation: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42 – 7.35 (m, 2H), 6.91 – 6.85 (m, 2H), 3.81 (s, 3H), 2.86 (d, *J* = 5.4 Hz, 1H), 2.76 (d, *J* = 5.4 Hz, 1H), 1.50 (tt, *J* = 8.3, 5.2 Hz, 1H), 0.59 – 0.52 (m, 2H), 0.44 – 0.37 (m, 2H). ^{13}C NMR (75 MHz, CDCl3) δ 159.18, 132.91, 127.44, 113.74, 69.97, 55.42, 54.60, 14.44, 2.42, 1.94. MS(EI(+)) m/z 190.2 (M+, 6), 161.2 (100), 145.9 (18), 130.9 (14), 91 (32), 77.0 (14), 62.9 (5).

1,2-diphenylaziridine (**21a**):
Benzylideneaniline was used as substrate. **21a** was purified using column chromatography (basic aluminium oxide) with a mixture of pentane/ NEt_3 (95/5) as eluent. 135 mg of **21a** (46 % yield) was obtained as a colorless oil.



All experimental data was in agreement with data in ref 9.

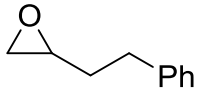
1-*tert* butyl-2-diphenylaziridine (**21b**):
Benzylidene-*tert*-butylamine was used as substrate. **21b** was purified using column chromatography (basic aluminium oxide) with a mixture of pentane/NEt_3 (98/2) as eluent. 185 mg of **21b** (73 % yield) was obtained as a colorless oil.



All experimental data was in agreement with data in ref 10.

2-phenethyloxirane (**23**):
A dried 50 mL Schlenk flask equipped with a glass coated stir bar and a glass stopper under Ar, was charged with NMe_4 OTf (390 mg, 1.74 mmol). The salt was suspended in anhydrous THF (20 mL) and the flask was cooled down to 0 °C in an ice-water bath. *n*BuLi (1.00 mL, 1.6 M, 1.60 mmol) was added to the suspension and the flask was completely closed using the glass stopper and the Schlenk tap to prevent any gas exchange. The reaction mixture was stirred for 30 minutes at 0 °C. Then under an Ar counterflow at 0 °C, 3-phenylpropionaldehyde (192 μL, 1.45 mmol) was added neat. The flask was then again fully closed and the stirring was continued for 30 min. The flask was then opened to the Ar line and the reaction mixture was stirred for 5 h at 65 °C. Then the reaction mixture was allowed to cool to room temperature with 30 mL of H_2O and transferred to a separation funnel. 20 mL of pentane was used to rinse the Schlenk flask and perform the first extraction of the aqueous phase. The aqueous phase was extracted using pentane (2x 10 mL). The combined organic extracts were washed with H_2O (4x 10 mL) and brine (10 mL), dried using $MgSO_4$, filtered and the solvent was concentrated under reduced pressure. The crude material was then purified by distillation under reduced pressure in a Kugelrohr apparatus. 125 mg of **23** (58 % yield) was obtained as a colorless oil.

Characterisation:

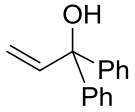


[9] W. Chamchaang, A. R. Pinhas, *J. Org. Chem.* **1990**, *55*, 2943-2950.
[10] Y. Da, Y. Wu, A.-H. Liu, L.-N. He, *J. Org. Chem.* **2008**, *73*, 4709-4712.

All experimental data was in agreement with data in ref 11.

1,1-diphenylprop-2-en-1-ol (**24**):
A dried 50 mL Schlenk flask equipped with a glass coated stir bar and a glass stopper under Ar, was charged with NMe_4 OTf (382 mg, 1.71 mmol). The salt was suspended in anhydrous THF (20 mL) and the flask was cooled down to 0 °C in an ice-water bath. *n*BuLi (1.00 mL, 1.6 M, 1.60 mmol) was added to the suspension and the flask was completely closed using the glass stopper and the Schlenk tap to prevent any gas exchange. The reaction mixture was stirred for 30 minutes at 0 °C. Then under an Ar counterflow at 0 °C, 2,2-diphenyloxirane (160 mg, 0.82 mmol) dissolved in 2 mL of anhydrous THF was added. The flask was then again fully closed and the stirring was continued for 18 h during which the temperature was allowed to slowly reach room temperature. Then the reaction mixture was diluted with 30 mL of H_2O and transferred to a separation funnel. 20 mL of pentane was used to rinse the Schlenk flask and perform the first extraction of the aqueous phase. The aqueous phase was extracted using pentane (2x 10 mL). The combined organic extracts were washed with H_2O (4x 10 mL) and brine (10 mL), dried using $MgSO_4$, filtered and the solvent was concentrated under reduced pressure. The crude material was then purified by column chromatography (silica gel) with a mixture of pentane/EtOAc (90/10) as eluent. 120 mg of **24** (70 % yield) was obtained as a colorless oil. The oil solidified slowly.

Characterisation:



All experimental data was in agreement with data in ref 12.

[11] D. Bernier, A. J. Blake, S. Woodward, *J. Org. Chem.* **2008**, *73*, 4229-4232.
[12] M. Hatano, S. Suzuki, K. Ishihara, *J. Am. Chem. Soc.* **2006**, *128*, 9998-9999.

3. Density-functional theory calculations

a) Influence of a Li cation on the stability of P-C and N-C ylides

A) Computational methods

Density functional theory (DFT) calculations were performed with the Gaussian 09 suite[13] employing the M06 density functional.[14] Geometry optimisations were performed with either the SDB-aug-cc-pVDZ basis set or the SDB-aug-cc-pVTZ basis set for all elements. The GEDIIS algorithm[15] was applied in combination with an ultrafine integration grid and tight SCF and geometry convergence criteria. Occasionally, when solvent molecules were incorporated, convergence problems arose in the geometry optimisations; these optimisations were performed using IOp(2/15=3), which turns off the use of symmetry and reorientation of the molecule. The nature of each stationary point was confirmed by a frequency analysis. For structures optimised with the SDB-aug-cc-pVDZ basis set, subsequent single-point energies were calculated with the SDB-aug-cc-pVTZ basis set, to which the SDB-aug-cc-pVDZ zero-point energy corrections were added.[16]

Furthermore, geometry optimisations were done including solvation effects by using the polarisable continuum model for THF with radii and non-electrostatic terms for the SMD model.[17] For structures optimised with the SDB-aug-cc-pVDZ basis set, subsequent single-point energies were calculated with the SDB-aug-cc-pVTZ basis set using the SMD(THF) model, to which the SDB-aug-cc-pVDZ/SMD(THF) zero-point energy corrections were added.[18] For all geometry optimisations using the polarisable solvent model IOp(2/15=3) was used since we encountered that otherwise problems with convergence occurred, and furthermore that the single-point energies were inconsistent due to reorientation of the molecule in the solvent cage.

Additionally, geometries were reoptimised with the Amsterdam Density Functional 2010 (ADF2010) suite[19] employing the BP86 density functional and an all-electron Slater-type basis set of triple-zeta quality with added polarisation functions (TZP).The auxiliary fit set was extended to QZ4P to obtain more accurate Coulomb interaction energies. The integration accuracy was set to 7.0, and geometry convergence criteria of 2×10^{-5} on the energy and 3×10^{-4} on the gradients were used. To remove eigenvectors corresponding to small eigenvalues from the valence space, thus reducing numerical

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[13] Gaussian 09, Revision A.1, 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**.

[14] Y. Zhao, D. G. Truhlar, *Theor. Chem. Account*, **2008**, *120*, 215-241.

[15] X. Li, M. J. Frisch, *J. Chem. Theory and Comput.*, **2006**, *2*, 835-839.

[16] Energies obtained from the calculations with the two basis sets differ by less than 1.05 kcal mol^{-1}.

[17] A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B*, **2009**, *113*, 6378-6396.

[18] Energies obtained from the calculations with the two basis sets using SMD(THF) differ by less than 0.57 kcal mol^{-1}.

[19] a) ADF2010, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com; b) C. Fonseca Guerra, J. G. Snijders, G. te Velde, E. J. Baerends, *Theor. Chem. Acc.* **1998**, *99*, 391-403; c) G. te Velde, F. M. Bickelhaupt, S. J. A. van Gisbergen, C. Fonseca Guerra, E. J. Baerends, J. G. Snijders, T. Ziegler, *J. Comput. Chem.* **2001**, *22*, 931-967.

problems, the key *dependency tolbas* = 1 x 10^{-4} was used. Extended Transition State[20] (ETS) bond analyses in terms of the separate fragments were performed with ADF2010[19] using the BP86/TZP electron densities.

According to the extended transition-state model,[20] the net bond energy (ΔE_{net}) between two fragments can be decomposed in three steps:

1) the two fragments are distorted from their equilibrium structures towards the (spatial and electronic) structures that the fragments possess in the total molecule – this requires a preparation energy ΔE_{prep};
2) the distorted fragments are brought from infinite separation to their molecule positions, without changing their electron densities – this affords the Pauli repulsion (ΔE_{Pauli}) and electrostatic attraction (ΔV_{elstat}) contributions;
3) the sum-of-fragments electron density is relaxed to the molecular density – this affords the total orbital interaction energy (ΔE_{oi}).

The last three interactions are usually summed to give the total interaction energy (ΔE_{int}). Furthermore, the net transfer of electron density between the fragments is indicated by their Hirshfeld charges.

B) Optimised Energies and Thermochemistry

1) Gaussian: M06/aug-cc-pVDZ

Table S1. M06/aug-cc-pVDZ results in Hartree (at 298.15 K, S_{tot} in kcal mol^{-1} K^{-1})[a]

Structure	$E_{aug\text{-}cc\text{-}pVDZ}$	*ZPE*	H_{corr}	S_{tot}	G_{corr}	$E_{aug\text{-}cc\text{-}pVTZ//aug\text{-}cc\text{-}pVDZ}$
THF	−232.307513265	0.115598	0.120532	0.121476	0.087483	−232.369102784
BuH	−158.320118842	0.129998	0.135878	0.136822	0.101899	−158.372861553
BuLi	−165.205210162	0.117860	0.125040	0.125985	0.087684	−165.255398999
$BuLi(THF)_2$	−629.882328532	0.352233	0.371944	0.372888	0.299787	−630.051580719
$BuLi(THF)_3$	−862.211603424	0.471065	0.496735	0.497679	0.412062	
NMe_4^+	−213.993522362	0.161497	0.168076	0.169020	0.134966	−214.062858812
NMe_3CH_2	−213.528020178	0.145883	0.152444	0.153389	0.117169	−213.593215811
$NMe_3CH_2Li^+$	−220.926436504	0.149676	0.157528	0.158473	0.118967	−220.993285762
$NMe_3CH_2Li(THF)_2^+$	−685.624260795	0.385748	0.405922	0.406866	0.335158	−685.810999050
$NMe_3CH_2Li(THF)_3^+$	−917.963513624	0.502026	0.528868	0.529812	0.441163	
PMe_4^+	−500.648207089	0.148973	0.157827	0.158771	0.119408	−500.723196548
PMe_3CH_2	−500.206811587	0.134870	0.143667	0.144612	0.103206	−500.280464887
$PMe_3CH_2Li^+$	−507.593647116	0.138091	0.148096	0.149040	0.104407	−507.667084239
$PMe_3CH_2Li(THF)_2^+$	−972.292989716	0.373710	0.396215	0.397159	0.318904	−972.486779045
$PMe_3CH_2Li(THF)_3^+$	−1204.633633490	0.490204	0.518221	0.519165	0.429780	

[a] Unscaled frequencies.

[20] a) T. Ziegler, A. Rauk, *Inorg. Chem.* **1979**, *18*, 1558-1565; b) T. Ziegler, A. Rauk, *Inorg. Chem.* **1979**, *18*, 1755-1759; c) F. M. Bickelhaupt, E. J. Baerends, in: Rev. Comput. Chem.; K. B. Lipkowitz, D. B. Boyd, Eds.; Wiley, New York, **2000**, Vol. 15, pp.1-86.

2) Gaussian: M06/aug-cc-pVDZ/SMD(THF)

Table S2. M06/aug-cc-pVDZ/SMD(THF) results in Hartree (at 298.15 K, S_{tot} in kcal mol^{-1} K^{-1})

Structure	$E_{aug\text{-}cc\text{-}pVDZ/SMD(THF)}$	*ZPE*	H_{corr}	S_{tot}	G_{corr}	$E_{aug\text{-}cc\text{-}pVTZ/SMD(THF)//aug\text{-}cc\text{-}pVDZ/SMD(THF)}$
THF	−232.314063211	0.115401	0.120357	0.121301	0.087129	−232.375517334
BuH	−158.323505961	0.129727	0.135525	0.136470	0.101778	−158.376282547
BuLi	−165.228215348	0.116918	0.124209	0.125153	0.086673	−165.278106883
$BuLi(THF)_2$	−629.902931770	0.352195	0.371797	0.372741	0.302294	−630.072534547
$BuLi(THF)_3$	−862.237630527	0.469294	0.494951	0.495895	0.411183	
NMe_4^+	−214.080817358	0.161590	0.168097	0.169041	0.132805	−214.150114819
NMe_3CH_2	−213.548874987	0.146204	0.152737	0.153681	0.117475	−213.614272877
$NMe_3CH_2Li^+$	−221.012870635	0.149409	0.157197	0.158141	0.118925	−221.079462114
$NMe_3CH_2Li(THF)_2^+$	−685.693811915	0.384043	0.404390	0.405334	0.332410	−685.880207918
$NMe_3CH_2Li(THF)_3^+$	−918.030637741	0.502400	0.528495	0.529439	0.445748	
PMe_4^+	−500.729234296	0.149692	0.158082	0.159026	0.118557	−500.804579404
PMe_3CH_2	−500.217127164	0.134856	0.143478	0.144422	0.103379	−500.290101062
$PMe_3CH_2Li^+$	−507.676264765	0.137327	0.147361	0.148305	0.103735	−507.749793614
$PMe_3CH_2Li(THF)_2^+$	−972.359028057	0.373132	0.395383	0.396327	0.320703	−972.552628690
$PMe_3CH_2Li(THF)_3^+$	−1204.696419020	0.490600	0.519028	0.519972	0.429336	

3) Gaussian: M06/aug-cc-pVTZ

Table S3. M06/aug-cc-pVTZ results in Hartree (at 298.15 K, S_{tot} in kcal mol^{-1} K^{-1})

Structure	$E_{aug\text{-}cc\text{-}pVTZ}$	*ZPE*	H_{corr}	S_{tot}	G_{corr}
BuH	−158.373330492	0.130708	0.136500	0.137445	0.103370
BuLi	−165.255848654	0.118445	0.125569	0.126513	0.088350
NMe_4^+	−214.063345642	0.162709	0.168959	0.169903	0.136618
NMe_3CH_2	−213.593725331	0.146349	0.152866	0.153810	0.117707
$NMe_3CH_2Li^+$	−220.993793260	0.150227	0.158025	0.158969	0.119632
PMe_4^+	−500.723934707	0.150650	0.159046	0.159990	0.121825
PMe_3CH_2	−500.281440281	0.136040	0.144633	0.145577	0.104754
$PMe_3CH_2Li^+$	−507.667926935	0.139214	0.149042	0.149986	0.105812

4) Gaussian: M06/aug-cc-pVTZ/SMD(THF)

Table S4. M06/aug-cc-pVTZ/SMD(THF) results in Hartree (at 298.15 K, S_{tot} in kcal mol^{-1} K^{-1})

Structure	$E_{aug\text{-}cc\text{-}pVTZ/SMD(THF)}$	*ZPE*	H_{corr}	S_{tot}	G_{corr}
BuH	−158.376744688	0.130514	0.136227	0.137171	0.102684
BuLi	−165.278569030	0.117618	0.124834	0.125779	0.087462
NMe_4^+	−214.150590375	0.162278	0.168680	0.169624	0.133662
NMe_3CH_2	−213.614775383	0.146858	0.153306	0.154250	0.118261
$NMe_3CH_2Li^+$	−221.080061061	0.149832	0.157684	0.158628	0.118830
PMe_4^+	−500.805293710	0.150867	0.159108	0.160052	0.119904
PMe_3CH_2	−500.291015792	0.135935	0.144408	0.145352	0.104701
$PMe_3CH_2Li^+$	−507.750640865	0.138665	0.148454	0.149398	0.105453

5) ADF: BP86/TZP

Table S5. ADF: BP86/TZP results in Hartree

Structure	E_{TZP}	*ZPE*
CH_2 carbene(singlet)	−0.412348372	
CH_2Li cation	−0.276093763	
CH_3 cation	−0.288530019	
NMe_3	−2.471758912	
NMe_4 cation	−2.972384262	0.158772
NMe_2CH_2 anion	−2.271573100	
NMe_3CH_2	−2.968209828	0.142705
NMe_2CH_2Li	−2.353016474	
NMe_3CH_2Li cation	−2.883003239	0.147025
$NMe_3CH_2Li(THF)_2$ cation	−8.159844866	0.376135
PMe_3	−2.374241950	
PMe_4 cation	−2.901553100	0.147743
PMe_2CH_2 anion	−2.205809443	
PMe_3CH_2	−2.926964160	0.133366
PMe_2CH_2Li	−2.261283335	
PMe_3CH_2Li cation	−2.826564294	0.136805
$PMe_3CH_2Li(THF)_2$ cation	−8.105178309	0.366169

C) Energy difference between M06/aug-cc-pVTZ and M06/aug-cc-pVTZ//aug-cc-pVDZ structures with and without SMD(THF)

Table S6. Energy difference between M06/aug-cc-pVTZ vs. M06/aug-cc-pVTZ//aug-cc-pVDZ results in kcal mol^{-1}, ZPE or G_{corr} (at 298.15 K) included in energies[a]

Structure	ΔE	ΔE + ΔZPE	ΔE + ΔG_{corr}	ΔE(SMD(THF))	ΔE(SMD(THF)) + ΔZPE	ΔE(SMD(THF)) + ΔG_{corr}
BuH	0.29	−0.15	−0.63	0.29	−0.20	−0.28
BuLi	0.28	−0.08	−0.14	0.29	−0.15	−0.21
NMe_4^+	0.31	−0.46	−0.73	0.30	−0.13	−0.24
NMe_3CH_2	0.32	0.03	−0.02	0.32	−0.10	−0.18
$NMe_3CH_2Li^+$	0.32	−0.03	−0.10	0.38	0.11	0.44
PMe_4^+	0.46	−0.59	−1.05	0.45	−0.29	−0.40
PMe_3CH_2	0.61	−0.12	−0.36	0.57	−0.10	−0.26
$PMe_3CH_2Li^+$	0.53	−0.18	−0.35	0.53	−0.31	−0.55

[a] ΔE = E(M06/aug-cc-pVTZ//aug-cc-pVDZ) - E(M06/aug-cc-pVTZ).

D) Solvation

Table S7. M06/aug-cc-pVDZ solvation energies in kcal mol^{-1}, G_{corr} (at 298.15 K) included in energies

Structure	Stabilisation[a]	Stabilisation 3 THF – 2 THF[b]
$BuLi(THF)_2$	−15.66	
$BuLi(THF)_3$	−13.76	+1.90
$NMe_3CH_2Li(THF)_2^+$	−26.09	
$NMe_3CH_2Li(THF)_3^+$	−34.38	−8.29
$PMe_3CH_2Li(THF)_2^+$	−28.10	
$PMe_3CH_2Li(THF)_3^+$	−34.21	−6.11

[a] Stabilisation= $E(G_{corr})$ $RLi(THF)_x$ – {$E(G_{corr})$ RLi + x[$E(G_{corr})$ THF]}. [b] Stabilisation= $E(G_{corr})$ $RLi(THF)_3$ – ($E(G_{corr})$ $RLi(THF)_2$ + $E(G_{corr})$ THF).

Table S8. M06/aug-cc-pVDZ/SMD(THF) solvation energies in kcal mol^{-1}, G_{corr} (at 298.15 K) included in energies

Structure	Stabilisation[a]	Stabilisation 3 THF – 2 THF[b]
$BuLi(THF)_2$	−3.28	
$BuLi(THF)_3$	−2.57	+0.71
$NMe_3CH_2Li(THF)_2^+$	−8.53	
$NMe_3CH_2Li(THF)_3^+$	−6.36	+2.16
$PMe_3CH_2Li(THF)_2^+$	−7.48	
$PMe_3CH_2Li(THF)_3^+$	−8.63	−1.14

[a] Stabilisation= $E(G_{corr})$ $RLi(THF)_x$ – {$E(G_{corr})$ RLi + x[$E(G_{corr})$ THF]}. [b] Stabilisation= $E(G_{corr})$ $RLi(THF)_3$ – ($E(G_{corr})$ $RLi(THF)_2$ + $E(G_{corr})$ THF).

E) Isodesmic reaction energies comparing the stabilisation of N-C and P-C ylides by a Li cation

Table S9. Gas-phase stabilisation of N-C and P-C ylides by a Li cation, results in kcal mol^{-1}, ZPE correction included in energies

	aug-cc-pVTZ	aug-cc-pVDZ	aug-cc-pVTZ//aug-cc-pVDZ	ADF:BP86/TZP
$E(NMe_3CH_2Li^+ + PMe_3CH_2)$	−452420.58	−452332.56	−452420.73	−3745.28
$E(PMe_3CH_2Li^+ + NMe_3CH_2)$	−452412.50	−452325.65	−452412.64	−3736.74
ΔE	−8.08	−6.91	−8.08	−8.53

Table S10. Gibbs free energy-corrected gas-phase stabilisation of N-C and P-C ylides by a Li cation, results in kcal mol^{-1}, G_{corr} (at 298.15 K) included in energies

	aug-cc-pVTZ	aug-cc-pVDZ	aug-cc-pVTZ//aug-cc-pVDZ
$E(NMe_3CH_2Li^+ + PMe_3CH_2)$	−452459.41	−452371.70	−452459.86
$E(PMe_3CH_2Li^+ + NMe_3CH_2)$	−452451.43	−452364.81	−452451.80
ΔE	−7.98	−6.89	−8.07

Table S11. Solution-phase stabilisation (taking into account the G_{corr} and the SMD(THF)) of N-C and P-C ylides by a Li cation, results in kcal mol^{-1}, G_{corr} (at 298.15 K) included in energies

	aug-cc-pVTZ	aug-cc-pVDZ	aug-cc-pVTZ//aug-cc-pVDZ
$E(NMe_3CH_2Li^+ + PMe_3CH_2)$	−452520.09	−452432.33	−452519.91
$E(PMe_3CH_2Li^+ + NMe_3CH_2)$	−452516.42	−452429.97	−452517.14
ΔE	−3.67	−2.36	−2.76

Table S12. Gibbs free energy-corrected gas-phase stabilisation of N-C and P-C ylides by a Li microsolvated cation, results in kcal mol^{-1}, G_{corr} (at 298.15 K) included in energies

	aug-cc-pVDZ	aug-cc-pVTZ//aug-cc-pVDZ
$E(NMe_3CH_2Li(THF)_2^+ + PMe_3CH_2)$	−743833.92	−743997.32
$E(PMe_3CH_2Li(THF)_2^+ + NMe_3CH_2)$	−743829.05	−743991.56
$\Delta E(THF)_2$	−4.88	−5.76
$E(NMe_3CH_2Li(THF)_3^+ + PMe_3CH_2)$	−889560.29	
$E(PMe_3CH_2Li(THF)_3^+ + NMe_3CH_2)$	−889553.23	
$\Delta E(THF)_3$	−7.06	
$\Delta E(THF)_0$	−6.89	−8.07
$\Delta E(THF)_2$	−4.88	−5.76
$\Delta E(THF)_3$	−7.06	

Table S13. Solution-phase stabilisation (taking into account the G_{corr} and SMD(THF)) of N-C and P-C ylides by a microsolvated Li cation, results in kcal mol^{-1}, G_{corr} (at 298.15 K) included in energies

	aug-cc-pVDZ	aug-cc-pVTZ//aug-cc-pVDZ
$E(NMe_3CH_2Li(THF)_2^+ + PMe_3CH_2)$	−743885.66	−744048.41
$E(PMe_3CH_2Li(THF)_2^+ + NMe_3CH_2)$	−743882.25	−744044.77
$\Delta E(THF)_2$	−3.40	−3.64
$E(NMe_3CH_2Li(THF)_3^+ + PMe_3CH_2)$	−889605.90	
$E(PMe_3CH_2Li(THF)_3^+ + NMe_3CH_2)$	−889605.80	
$\Delta E(THF)_3$	−0.10	
$\Delta E(THF)_0$	−2.36	−2.76
$\Delta E(THF)_2$	−3.40	−3.64
$\Delta E(THF)_3$	−0.10	

F) Isodesmic reaction energies comparing the deprotonation/lithiation of N- and P-quaternary salts by *n*BuLi

Table S14. Gas phase deprotonation/lithiation energies of N-C and P-C ylides by *n*BuLi, results in kcal mol^{-1}, ZPE correction included in energies

	aug-cc-pVTZ	aug-cc-pVDZ	aug-cc-pVTZ//aug-cc-pVDZ
$E(NMe_3CH_2Li^+ + BuH)$	−237876.58	−237801.72	−237876.76
$E(BuLi + NMe_4^+)$	−237846.37	−237771.91	−237846.91
ΔE (N)	−30.21	−29.81	−29.85
$E(PMe_3CH_2Li^+ + BuH)$	−417771.51	−417692.66	−417771.84
$E(BuLi + PMe_4^+)$	−417733.46	−417655.58	−417734.13
ΔE (P)	−38.06	−37.08	−37.71
ΔE (N) − ΔE (P)	7.84	7.27	7.86

Table S15. Gibbs free energy-corrected deprotonation/lithiation energies of N-C and P-C ylides by *n*BuLi, results in kcal mol^{-1}, G_{corr} (at 298.15 K) included in energies

	aug-cc-pVTZ	aug-cc-pVDZ	aug-cc-pVTZ//aug-cc-pVDZ
$E(NMe_3CH_2Li^+ + BuH)$	−237912.94	−237838.62	−237913.66
$E(BuLi + NMe_4^+)$	−237881.63	−237807.49	−237882.49
ΔE (N)	−31.31	−31.13	−31.17
$E(PMe_3CH_2Li^+ + BuH)$	−417809.63	−417731.43	−417810.61
$E(BuLi + PMe_4^+)$	−417770.43	−417693.07	−417771.62
ΔE (P)	−39.20	−38.36	−38.99
ΔE (N) − ΔE (P)	7.89	7.23	7.82

Table S16. Solution-phase deprotonation/lithiation energies of N-C and P-C ylides by *n*BuLi (taking into account the G_{corr} and SMD(THF)), results in kcal mol^{-1}, G_{corr} (at 298.15 K) included in energies

	aug-cc-pVTZ	aug-cc-pVDZ	aug-cc-pVTZ//aug-cc-pVDZ
$E(NMe_3CH_2Li^+ + BuH)$	−237970.15	−237895.09	−237969.99
$E(BuLi + NMe_4^+)$	−237953.04	−237878.70	−237953.49
ΔE (N)	−17.10	−16.39	−16.50
$E(PMe_3CH_2Li^+ + BuH)$	−417864.33	−417785.90	−417865.15
$E(BuLi + PMe_4^+)$	−417837.50	−417759.52	−417838.10
ΔE (P)	−26.83	−26.38	−27.05
ΔE (N) − ΔE (P)	9.72	9.99	10.55

Table S17. Solution-phase deprotonation/lithiation energies of N-C and P-C ylides by *n*BuLi (taking into account the G_{corr} and THF microsolvation), results in kcal mol^{-1}, G_{corr} (at 298.15 K) included in energies

	aug-cc-pVDZ	aug-cc-pVTZ//aug-cc-pVDZ
$E(NMe_3CH_2Li(THF)_2^+ + BuH)$	−529300.84	−529451.12
$E(BuLi(THF)_2 + NMe_4^+)$	−529259.29	−529409.00
ΔE (N) $(THF)_2$	−41.56	−42.12
$E(PMe_3CH_2Li(THF)_2^+ + BuH)$	−709195.67	−709350.37
$E(BuLi(THF)_2 + PMe_4^+)$	−709144.87	−709298.13
ΔE (P) $(THF)_2$	−50.81	−52.24
ΔE (N) − ΔE (P) $(THF)_2$	9.25	10.13
$E(NMe_3CH_2Li(THF)_3^+ + BuH)$	−675027.21	
$E(BuLi(THF)_3 + NMe_4^+)$	−674975.46	
ΔE (N) $(THF)_2$	−51.75	
$E(PMe_3CH_2Li(THF)_3^+ + BuH)$	−854919.85	
$E(BuLi(THF)_3 + PMe_4^+)$	−854861.03	
ΔE (P) $(THF)_3$	−58.82	
ΔE (N) − ΔE (P) $(THF)_3$	7.07	
ΔE (N) − ΔE (P) $(THF)_0$	7.23	7.82
ΔE (N) − ΔE (P) $(THF)_2$	9.25	10.13
ΔE (N) − ΔE (P) $(THF)_3$	7.07	

Table S18. Solution-phase deprotonation/lithiation energies of N-C and P-C ylides by *n*BuLi (taking into account the G_{corr}, THF microsolvation and SMD(THF)), results in kcal mol^{-1}, G_{corr} (at 298.15 K) included in energies

	aug-cc-pVDZ	aug-cc-pVTZ//aug-cc-pVDZ
$E(NMe_3CH_2Li(THF)_2^+ + BuH)$	−529348.41	−529498.49
$E(BuLi(THF)_2 + NMe_4^+)$	−529326.78	−529476.69
ΔE (N) $(THF)_2$	−21.64	−21.81
$E(PMe_3CH_2Li(THF)_2^+ + BuH)$	−709238.18	−709392.78
$E(BuLi(THF)_2 + PMe_4^+)$	−709207.60	−709361.31
ΔE (P) $(THF)_2$	−30.58	−31.48
ΔE (N) − ΔE (P) $(THF)_2$	8.95	9.67
$E(NMe_3CH_2Li(THF)_3^+ + BuH)$	−675068.65	
$E(BuLi(THF)_3 + NMe_4^+)$	−675048.47	
ΔE (N) $(THF)_2$	−20.18	
$E(PMe_3CH_2Li(THF)_3^+ + BuH)$	−854961.73	
$E(BuLi(THF)_3 + PMe_4^+)$	−854929.30	
ΔE (P) $(THF)_3$	−32.43	
ΔE (N) − ΔE (P) $(THF)_3$	12.25	
ΔE (N) − ΔE (P) $(THF)_0$	9.99	10.55
ΔE (N) − ΔE (P) $(THF)_2$	8.95	9.67
ΔE (N) − ΔE (P) $(THF)_3$	12.25	

G) Selected bond lengths and angles

Table S19. ADF/TZP results for the N-containing molecules, bond distances in Å, bond angles in °. (Y=lone pair or Li^+)

Feature	NMe_4^+	NMe_3CH_2	%[a]	$NMe_3CH_2Li^+$	%[a]	$NMe_3CH_2Li(THF)_2^+$	%[a]
NMe_3-CH_3 bond length	1.510						
NMe_3-CH_2Y bond length		1.531	101.4	1.530	101.3	1.533	101.6
NMe_2CH_2Y-CH_3 bond length (2x)[b]		1.496	99.1	1.501	99.5	1.499[c]	99.3
NMe_2CH_2Y-CH_3 bond length[d]		1.517	100.5	1.511	100.1	1.509	100.0
HC(Y)H angle[e]	110.1	106.4	96.7	104.2	94.6	104.6	95.0
out of plane angle[f]	124.3	114.1	91.8	113.0	91.0	112.5	90.6

[a] % of the corresponding feature in NMe_4. [b] Bonds out of the Me-N-C-Y plane. [c] Average of the two bond lengths. [d] Bond in the Me-N-C-Y plane. [e] In the CH_2Y group. [f] Out of plane angle= -centre of the H's of the CH_2Y group_C of the CH_2Y group_N-.

Table S20. ADF/TZP results for the P-containing molecules, bond distances in Å, bond angles in °. (Y=lone pair or Li^+)

Feature	PMe_4^+	PMe_3CH_2	%[a]	$PMe_3CH_2Li^+$	%[a]	$PMe_3CH_2Li(THF)_2^+$	%[a]
PMe_3-CH_3 bond length	1.809						
PMe_3-CH_2Y bond length		1.682	93.0	1.753	96.9	1.734	95.9
PMe_2CH_2Y-CH_3 bond length (2x)[b]		1.829	101.1	1.818	100.5	1.821	100.7
PMe_2CH_2Y-CH_3 bond length[c]		1.867	103.2	1.825	100.9	1.833	101.4
HC(Y)H angle[d]	109.1	115.8	106.1	106.3	97.5	107.9	98.9
out of plane angle[e]	125.8	148.3	117.9	119.0	94.6	122.4	97.3

[a] % of the corresponding feature in PMe_4. [b] Bonds out of the Me-P-C-Y plane. [c] Bond in the Me-P-C-Y plane. [d] In the CH_2Y group. [e] out of plane angle= -centre of the H's of the CH_2Y group_C of the CH_2Y group_P-.

H) ETS bond analyses

Table S21. Extended Transition State (ETS) analysis for the bond between XMe_3 and CH_2Y, results in kcal mol^{-1} (ADF: BP86/TZP level)

Parameter[Error! Bookmark not defined.]	NMe_3CH_2	$NMe_3CH_2Li^+$	$NMe_3CH_2\{Li\}$[a]	$NMe_3CH_2Li(THF)_2^+$	PMe_3CH_2	$PMe_3CH_2Li^+$	$PMe_3CH_2\{Li\}$[a]	$PMe_3CH_2Li(THF)_2^+$
Pauli Repulsion								
Kinetic (ΔT)	1005.66	721.97	1007.53	811.25	1632.24	824.03	1155.05	969.03
ΔV Pauli Coulomb	−512.38	−357.44	−516.42	−408.83	−808.78	−408.45	-602.91	-482.71
ΔV Pauli LDA-XC	−181.23	−147.91	−181.04	−161.01	−222.41	−145.88	-178.14	-163.42
ΔV Pauli GGA-XC	25.93	26.12	25.70	27.07	23.12	24.56	23.88	25.32
ΔV Pauli GGA-correlation	−10.86	−11.02	−10.72	−11.23	−9.18	−10.75	-10.27	-10.79
Total (ΔE Pauli)	327.12	231.72	325.06	257.25	614.99	283.51	387.61	337.43
Steric Interactions								
Pauli repulsion (ΔE Pauli)	327.12	231.72	325.06	257.25	614.99	283.51	387.61	337.43
Electrostatic Interaction (ΔV elstat)	−172.51	−139.81	−168.5	−147.36	−310.57	−154.88	-199.38	-179.45
Total Steric Interactions	154.61	91.91	156.55	109.89	304.41	128.63	188.22	157.98
Orbital Interactions								
A (ΔE oi)	−210.41	−199.39	−210.98	−198.66	−398.28	−268.41	-277.62	-279.21
Alternative Decomposition Orbital Interactions								
Kinetic	−937.03	−623.63	−941.34	−718.35	−1628.43	−831.38	-1192.07	-973.25
Coulomb	626.36	367.94	629.63	454.24	1114.95	517.8	828.25	639.69
XC	100.27	56.3	100.73	65.46	115.2	45.18	86.20	54.34
Total	−210.41	−199.39	−210.98	−198.66	−398.28	−268.41	-277.62	-279.21
Total Bonding Energy (ΔE int)	−55.79	−107.48	−54.43	−88.77	−93.87	−139.77	-89.40	-121.23
Summary of Bonding Energy								
Electrostatic Energy (ΔV elstat)	−172.51	−139.81	−168.5	−147.36	−310.57	−154.88	-199.38	-179.45
Kinetic Energy	68.63	98.34	66.19	92.89	3.81	−7.35	-37.02	-4.21
Coulomb (Steric +OrbInt) Energy	113.98	10.5	113.21	45.41	306.17	109.35	225.34	156.98
XC Energy	−65.89	−76.51	−65.32	−79.71	−93.28	−86.89	-78.33	-94.55
Total Bonding Energy (ΔE int)	−55.79	−107.48	−54.43	−88.77	−93.87	−139.77	-89.40	-121.23
difference in stabilisation (+Li)	51.69				45.90			
Deformation Energy XMe_3	2.48	2.43			2.61	5.40		
Deformation Energy CH_2Y	0.53	20.24			3.17	23.79		
Net Bonding Energy (ΔE net)	−52.77	−84.81			−88.08	−110.58		
difference in stabilisation (+Li)	−32.03				−22.50			

[a] {Li} means that the atomic coordinates of the XMe_3CH_2Li structure were used, but the Li cation was omitted.

Table S21. Extended Transition State (ETS) analysis for one of the two shortened bonds between XMe_2CH_2Y and CH_3, results in kcal mol^{-1} (ADF: BP86/TZP level)

Parameter[Error! Bookmark not defined.]	NMe_3CH_2	$NMe_3CH_2Li^+$	$NMe_3CH_2Li(THF)_2^+$	PMe_3CH_2	$PMe_3CH_2Li^+$	$PMe_3CH_2Li(THF)_2^+$
Pauli Repulsion						
Kinetic (ΔT)	607.51	583.33	593.24	643.51	614.7	627.85
ΔV Pauli Coulomb	−278.17	−267.77	−272.02	−301.15	-289.59	-295.21
ΔV Pauli LDA-XC	−133.72	−129.08	−131.05	−122.38	-118.15	-120.38
ΔV Pauli GGA-XC	25.4	25.05	25.33	21.51	21.71	21.91
ΔV Pauli GGA-correlation	−10.6	−10.43	−10.52	−9.11	-9.32	-9.31
Total (ΔE Pauli)	210.42	201.1	204.99	232.38	219.35	224.86
Steric Interactions						
Pauli repulsion (ΔE Pauli)	210.42	201.1	204.99	232.38	219.35	224.86
Electrostatic Interaction (ΔV elstat)	−244.74	−156.29	−170.16	−242.25	-154.92	-167.69
Total Steric Interactions	−34.32	44.81	34.83	−9.87	64.43	57.17
Orbital Interactions						
A (ΔE oi)	−250.91	−235.5	−242.53	−303.41	-283.45	-292.34
Alternative Decomposition Orbital Interactions						
Kinetic	−352.92	−372.11	−365.42	−542.86	-553.72	-550.25
Coulomb	121.17	145.13	132.87	260.27	277.94	268.2
XC	−19.15	−8.51	−9.98	−20.82	-7.67	-10.29
Total	−250.91	−235.5	−242.53	−303.41	-283.45	-292.34
Total Bonding Energy (ΔE int)	−285.23	−190.69	−207.7	−313.28	-219.02	-235.17
Summary of Bonding Energy						
Electrostatic Energy (ΔV elstat)	−244.74	−156.29	−170.16	−242.25	-154.92	-167.69
Kinetic Energy	254.59	211.22	227.83	100.65	60.98	77.6
Coulomb (Steric +OrbInt) Energy	−157	−122.65	−139.15	−40.88	-11.65	-27.01
XC Energy	−138.07	−122.97	−126.21	−130.79	-113.42	-118.07
Total Bonding Energy (ΔE int)	−285.23	−190.69	−207.7	−313.28	-219.02	-235.17
Difference in Stabilisation (+Li)	94.54			94.26		
Deformation Energy XMe_2CH_2Y	3.62	12.60		12.94	15.82	
Deformation Energy CH_3	25.51	26.57		28.86	29.54	
Net Bonding Energy (ΔE net)	−256.09	−151.51		−271.47	-173.66	
Difference in Stabilisation (+Li)	104.57			97.81		

Table S22. Extended Transition State (ETS) analysis for the longer bond between XMe_2CH_2Y and CH_3, results in kcal mol^{-1} (ADF: BP86/TZP level)

Parameter[Error! Bookmark not defined.]	NMe_3CH_2	$NMe_3CH_2Li^+$	$NMe_3CH_2Li(THF)_2^+$	PMe_3CH_2	$PMe_3CH_2Li^+$	$PMe_3CH_2Li(THF)_2^+$
Pauli Repulsion						
Kinetic (ΔT)	589.24	546.92	570.73	618.43	543.11	593.62
ΔV Pauli Coulomb	−272.81	−249.58	−262.38	−288.69	-247.75	-278.54
ΔV Pauli LDA-XC	−130.28	−121.26	−126.49	−116.69	-104.59	-114.03
ΔV Pauli GGA-XC	24.45	24.87	24.93	20.56	21.33	21.46
ΔV Pauli GGA-correlation	−10.18	−10.38	−10.39	−8.51	-9.17	-9.15
Total (ΔE Pauli)	200.43	190.57	196.39	225.10	202.93	213.36
Steric Interactions						
Pauli repulsion (ΔE Pauli)	200.43	190.57	196.39	225.10	202.93	213.36
Electrostatic Interaction (ΔV elstat)	−237.45	−141.72	−164.39	−233.53	-133.51	-161.15
Total Steric Interactions	−37.02	48.85	32.00	−8.43	69.41	52.21
Orbital Interactions						
A (ΔE oi)	−249.16	−237.17	−240.02	−311.73	-288.02	-290.72
Alternative Decomposition Orbital Interactions						
Kinetic	−347.54	−336.26	−353.34	−510.05	-479.1	-524.21
Coulomb	118.49	128.08	129.64	237.78	231.32	255.49
XC	−20.12	−28.99	−16.32	−39.46	-40.24	-21.99
Total	−249.16	−237.17	−240.02	−311.73	-288.02	-290.72
Total Bonding Energy (ΔE int)	−286.19	−188.32	−208.01	−320.16	-218.60	-238.50
Summary of Bonding Energy						
Electrostatic Energy (ΔV elstat)	−237.45	−141.72	−164.39	−233.53	-133.51	-161.15
Kinetic Energy	241.71	210.66	217.39	108.38	64.01	69.41
Coulomb (Steric +OrbInt) Energy	−154.32	−121.50	−132.74	−50.91	-16.43	-23.06
XC Energy	−136.12	−135.76	−128.27	−144.1	-132.68	-123.70
Total Bonding Energy (ΔE int)	−286.19	−188.32	−208.01	−320.16	-218.60	-238.50
Difference in Stabilisation (+Li)	97.87			101.56		
Deformation Energy XMe_2CH_2Y	3.40	10.39		18.87	15.50	
Deformation Energy CH_3	26.70	26.42		29.81	29.43	
Net Bonding Energy (ΔE net)	−256.09	−151.51		−271.47	-173.66	
Difference in Stabilisation (+Li)	104.57			97.81		

I) Hirsfeld charges

Table S23. Hirsfeld charges in electrons of different fragments, results in kcal mol^{-1} (ADF: BP86/TZP level)

Fragment	NMe_3CH_2|	$NMe_3CH_2Li^+$	$NMe_3CH_2\{Li\}^a$	$NMe_3CH_2Li(THF)_2^+$	PMe_3CH_2|	$PMe_3CH_2Li^+$	$PMe_3CH_2\{Li\}^a$	$PMe_3CH_2Li(THF)_2^+$
				Fragmentation 1				
XMe_3	0.3197	0.3633	0.3222	0.3639	0.2359	0.2919	0.2009	0.2807
CH_2Y	−0.3197	0.6367	−0.3222	0.6361	−0.2359	0.7081	−0.2009	0.7193
				Fragmentation 2 (short XMe_2CH_2Y-CH_3 bonds)				
XMe_2CH_2Y	0.5806	0.6028		0.5963	0.5882	0.6039		0.5995
CH_3	−0.5806	0.3972		0.4037	−0.5882	0.3961		0.4005
				Fragmentation 3 (long XMe_2CH_2Y-CH_3 bond)				
XMe_2CH_2Y	0.561	0.5858		0.5829	0.5601	0.5638		0.5731
CH_3	−0.561	0.4142		0.4171	−0.5601	0.4363		0.4269

[a] {Li} means that the atomic coordinates of the XMe_3CH_2Li structure were used, but the Li cation was omitted.

b) Possibility of Stevens rearrangement of the lithiomethyl trimethylammonium cation/ trimethylammonium methylide via a radical mechanism

A) Computational methods

Density functional theory (DFT) calculations were performed with the Gaussian 09 suite[13] employing the M06, M052-X (when explicit solvent molecules are included).[14] Ab initio calculations were performed with the Gaussian 09 suite[13] employing MP2. Geometry optimisations were performed with either the SDB-aug-cc-pVTZ basis set (M06 and MP2), or the 6-311+G** (M052-X) basis set for all elements. The GEDIIS algorithm[15] was applied in combination with an ultrafine integration grid and tight SCF and geometry convergence criteria. The nature of each stationary point was confirmed by a frequency analysis. For structures optimised with MP2/SDB-aug-cc-pVTZ, subsequent single-point energies were calculated on the CCSD(T)/SDB-aug-cc-pVTZ level, to which the MP2/SDB-aug-cc-pVTZ zero-point energy corrections were added.

Furthermore, geometry optimisations were done at the M052-X/6-311+G** level including solvation effects by using the polarisable continuum model for THF with radii and non-electrostatic terms for the SMD model.[17] For all geometry optimisations using the solvation model IOp(2/15=3) was used, which turns off the use of symmetry and reorientation of the molecule since we have encountered that otherwise problems with convergence occurred, and furthermore that the single-point energies were inconsistent due to reorientation of the molecule in the solvent cage.

B) Optimised Energies and Thermochemistry

1) Gaussian: M06/aug-cc-pVTZ

Table S24. M06/aug-cc-pVTZ results in Hartree (at 298.15 K, S_{tot} in kcal mol^{-1} K^{-1})[a]

Structure	$E_{aug\text{-}cc\text{-}pVTZ}$	*ZPE*	H_{corr}	S_{tot}	G_{corr}
NMe_3CH_2	−213.593725331	0.146349	0.153810	0.152866	0.117707
$NMe_3CH_2Li^+$	−220.993793260	0.150227	0.158969	0.158025	0.119632
NMe_3 radical cation	−174.111406106	0.117237	0.124579	0.123634	0.087225
CH_2 radical anion	− 39.151539397	0.015673	0.019463	0.018518	−0.002685
CH_2Li radical	− 46.718665425	0.117237	0.124579	0.123634	0.087225

[a] Unscaled frequencies.

2) Gaussian: M05-2X/6-311+G**

Table S25. M05-2X/6-311+G** results in Hartree (at 298.15 K, S_{tot} in kcal mol^{-1} K^{-1})[a]

Structure	$E_{6\text{-}311+G^{**}}$	*ZPE*	H_{corr}	S_{tot}	G_{corr}
NMe_3CH_2	−213.7033772	0.150717	0.158019	0.157075	0.122170
$NMe_3CH_2Li^+$	−221.1037552	0.154407	0.163038	0.162093	0.123847
$NMe_3CH_2Li(THF)_2^+$	−686.1504655	0.39571	0.417231	0.416287	0.340731
NMe_3 radical cation	−174.197364	0.120413	0.127769	0.126825	0.090309
CH_2 radical anion	− 39.16799053	0.015871	0.019660	0.018716	−0.002477
CH_2Li radical	− 46.73624185	0.021022	0.025402	0.024458	−0.001328
$CH_2Li(THF)_2$ radical	−511.7570761	0.262811	0.279287	0.278342	0.216476

[a] Unscaled frequencies.

3) Gaussian: MP2/aug-cc-pVTZ

Table S26. MP2/aug-cc-pVTZ results in Hartree (at 298.15 K, S_{tot} in kcal mol^{-1} K^{-1})[a]

Structure	$E_{MP2/\text{aug-cc-pVTZ}}$	*ZPE*	H_{corr}	S_{tot}	G_{corr}	$E_{CCSD(T)/\text{aug-cc-pVTZ//MP2/aug-cc-pVTZ}}$
NMe_3CH_2	−213.2301608	0.149236	0.155724	0.156668	0.120599	−213.3223282
$NMe_3CH_2Li^+$	−220.5760634	0.153043	0.161755	0.160811	0.122475	−220.6685727
NMe_3 radical cation	−173.8047149	0.120082	0.127493	0.126549	0.089819	−173.8870283
CH_2 radical anion	− 39.0753566	0.016102	0.019889	0.018945	−0.002245	− 39.1003395
CH_2Li radical	− 46.5853591	0.020847	0.025273	0.024329	−0.000890	− 46.6100350

[a] Unscaled frequencies.

4) Gaussian: M05-2X/6-311+G**/SMD(THF)

Table S27. M05-2X/6-311+G**/SMD(THF) results in Hartree (at 298.15 K, S_{tot} in kcal mol^{-1} K^{-1})[a]

Structure	$E_{6\text{-}311+G^{**}}$	*ZPE*	H_{corr}	S_{tot}	G_{corr}
NMe_3CH_2	−213.7275166	0.150880	0.157263	0.158207	0.122266
$NMe_3CH_2Li^+$	−221.190207	0.153864	0.161582	0.162526	0.123399
$NMe_3CH_2Li(THF)_2^+$	−686.2201663	0.395089	0.415381	0.416325	0.343094
NMe_3 radical cation	−174.2875379	0.120521	0.126843	0.127788	0.090714
CH_2 radical anion	− 39.26858563	0.016473	0.019315	0.020259	−0.002503
CH_2Li radical	− 46.75640002	0.020183	0.023811	0.024755	−0.002357
$CH_2Li(THF)_2$ radical	−511.7799934	0.261875	0.277749	0.278693	0.215315

[a] Unscaled frequencies.

C) Reaction energies for the homolytic cleavage of the Me_3N-$CH_2(Li)$ bond in lithiomethyl trimethylammonium cation / trimethylammonium methylide

Table S28. Gas-phase reaction energies for the homolytic cleavage of the Me_3N-CH2(Li) bond, results in kcal mol^{-1}, ZPE corrections included in energy differences

Reaction energy	M05-2X/ 6-311+G**	M06/ aug-cc-pVTZ	MP2/ aug-cc-pVTZ	CCSD(T)/aug-cc-pVTZ// MP2/aug-cc-pVTZ
ΔE([NMe_3 radical cation + CH_2 radical anion] - NMe_3CH_2)	−203.05	−199.13	−164.94	−202.00
ΔE([NMe_3 radical cation + CH_2Li radical] - $NMe_3CH_2Li^+$)	− 98.63	− 94.805	−109.11	−100.02
ΔE([NMe_3 radical cation + $CH_2Li(THF)_2$ radical] - $NMe_3CH_2Li(THF)_2^+$)	−115.17			

Table S29. Solution-phase reaction energies for the homolytic cleavage of the Me_3N-CH2(Li) bond, results in kcal mol^{-1}, G_{corr} (at 298.15 K)[a] included in energy differences

Reaction energy	M05-2X/ 6-311+G**	M05-2X/ 6-311+G**/ SMD(THF)	M06/ aug-cc-pVTZ	MP2/ aug-cc-pVTZ	CCSD(T)/aug-cc-pVTZ// MP2/aug-cc-pVTZ
ΔE([NMe_3 radical cation + CH_2 radical anion] - NMe_3CH_2)	−190.56	− 86.18	−186.75	−198.96	−189.46
ΔE([NMe_3 radical cation + CH_2Li radical] - $NMe_3CH_2Li^+$)	− 84.89	− 69.79	− 81.11	− 95.66	− 86.57
ΔE([NMe_3 radical cation + $CH_2Li(THF)_2$ radical] - $NMe_3CH_2Li(THF)_2^+$)	−101.70	− 72.52			

[a] Unscaled frequencies.

D) Conclusions

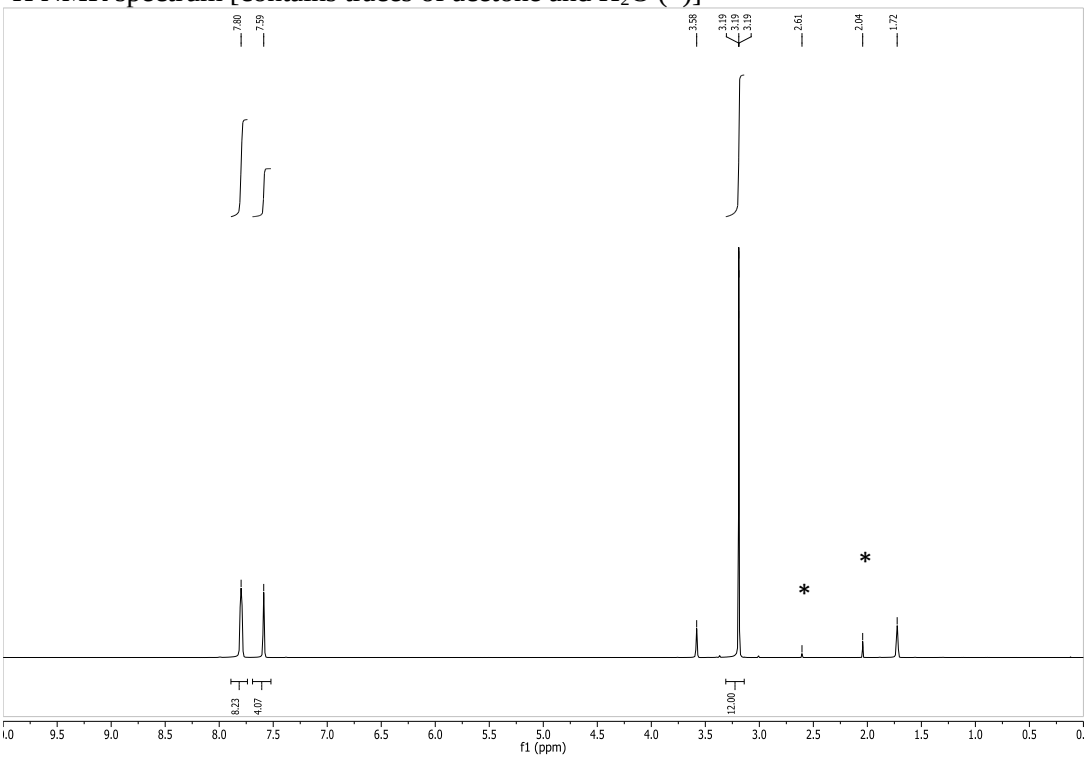
Assuming that the Stevens rearrangement proceeds via a radical mechanism,[21] the Stevens rearrangement for the lithiomethyl trimethylammonium reagent would require an activation energy of around 70 kcal mol^{-1}. Thus, it is unlikely that the Stevens rearrangement takes place for the lithiomethyl trimethylammonium reagent. However, the presence of the Li cation does lower the reaction barrier with around 15 kcal mol^{-1} as compared to the homolysis of the trimethylammonium methylide.

[21] a) W. D. Ollis, M. Rey, I. O. Sutherland, *J. Chem. Soc. Perkin Trans. 1* **1983**, 1009-1027; b) S. Bhakat, *J. Chem. Pharm. Res.* **2011**, *3*, 115-121.

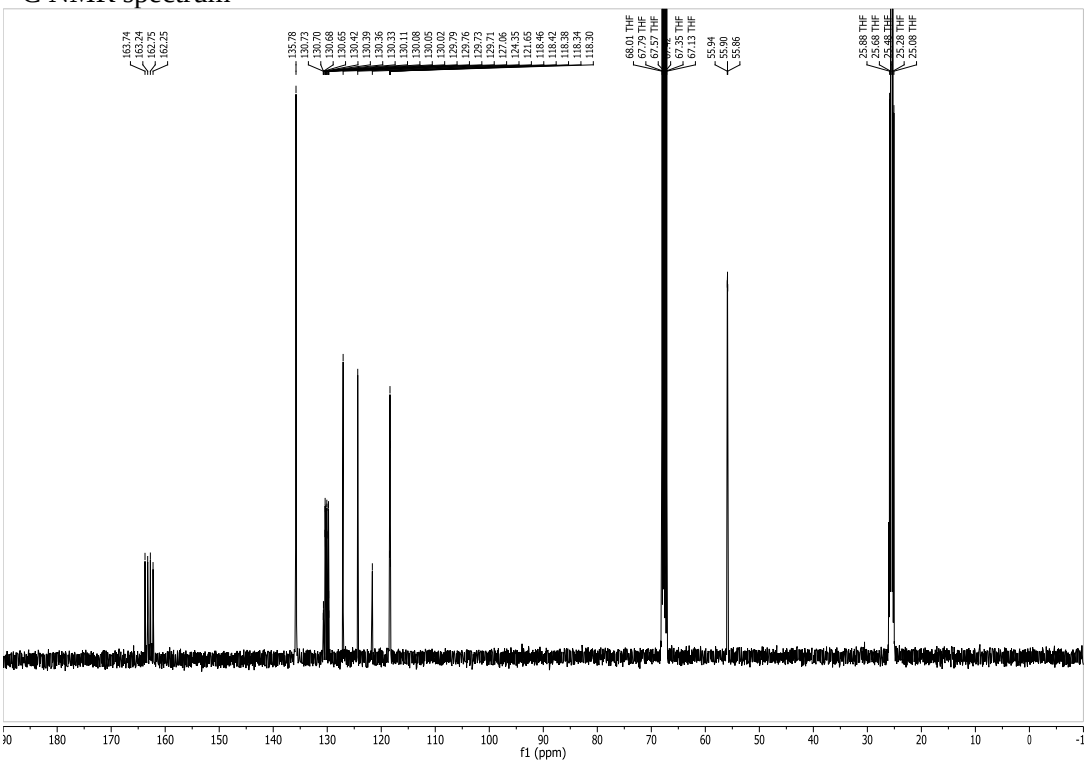
3. Spectra

Tetramethylammonium BAr^F (**6**):

^{1}H NMR spectrum [contains traces of acetone and H_2O (*)]

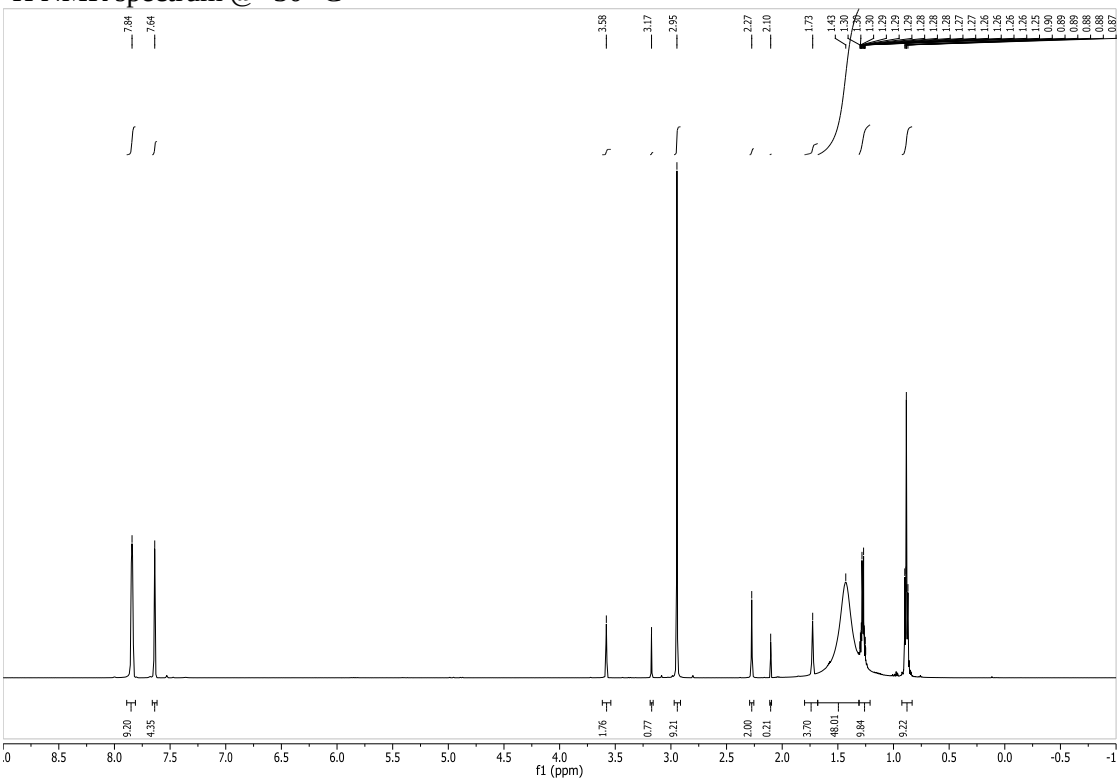


^{13}C NMR spectrum

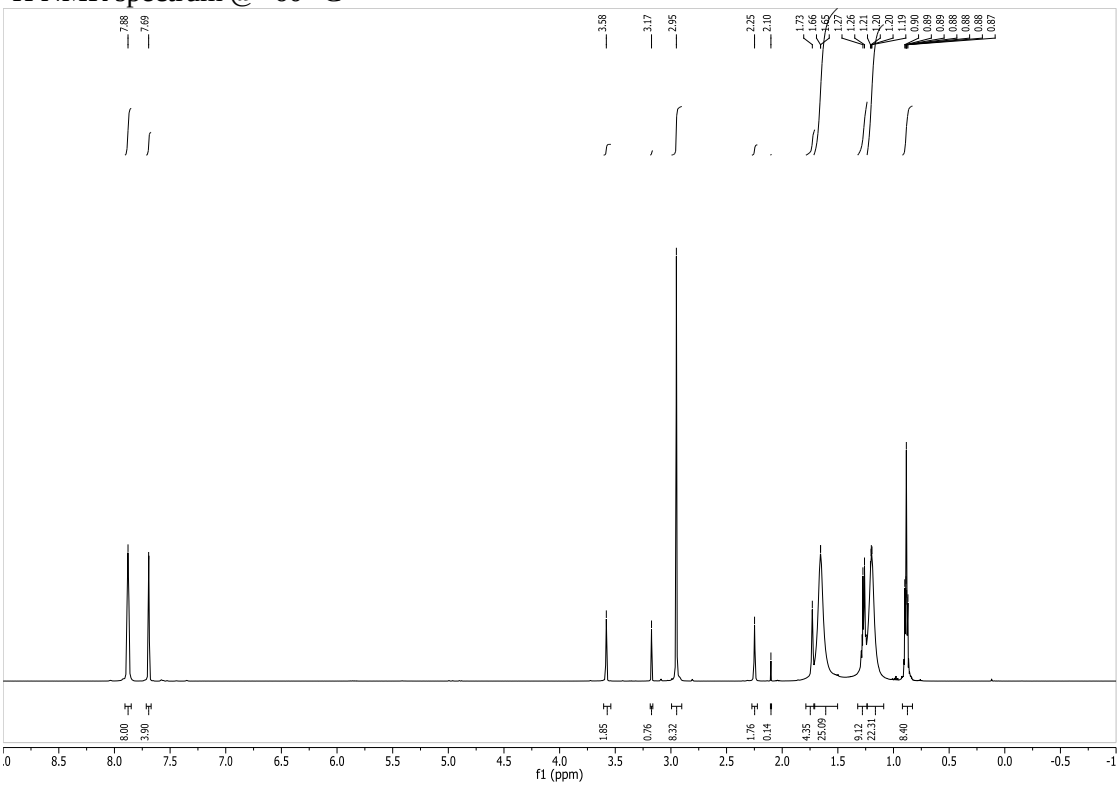


Lithiomethyl trimethylammonium BAr^F (**8**):

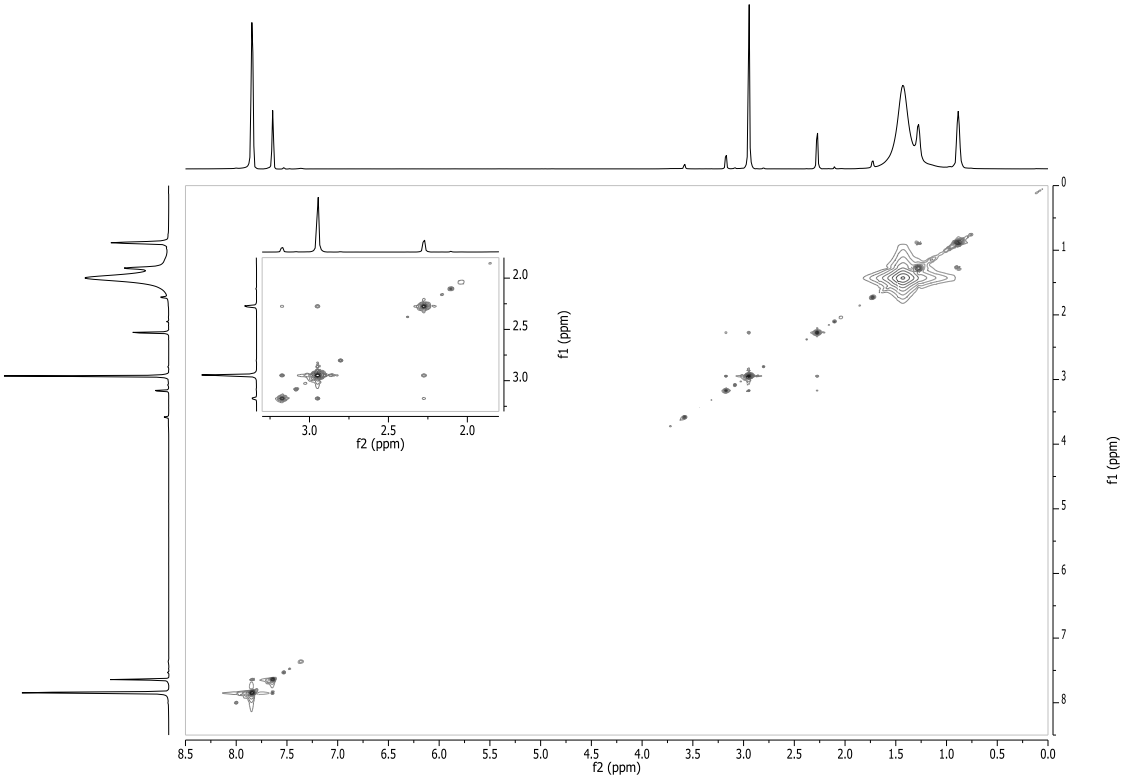
^{1}H NMR spectrum @ -30 °C



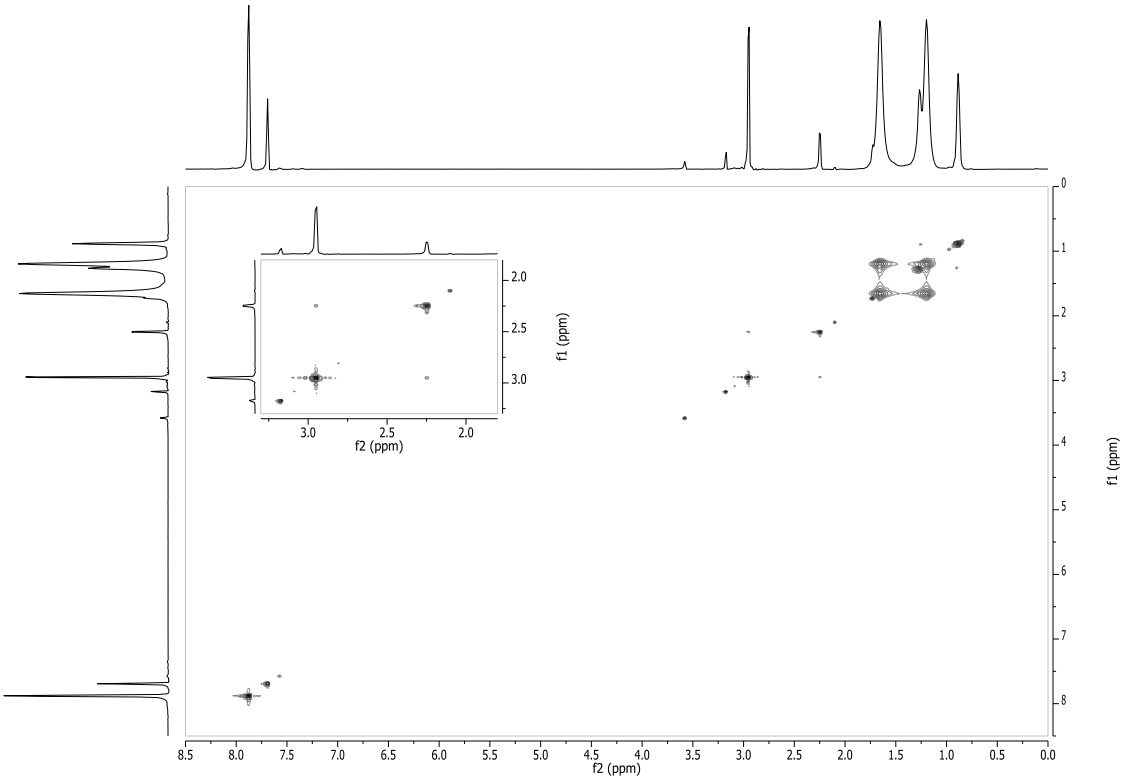
^{1}H NMR spectrum @ -60 °C



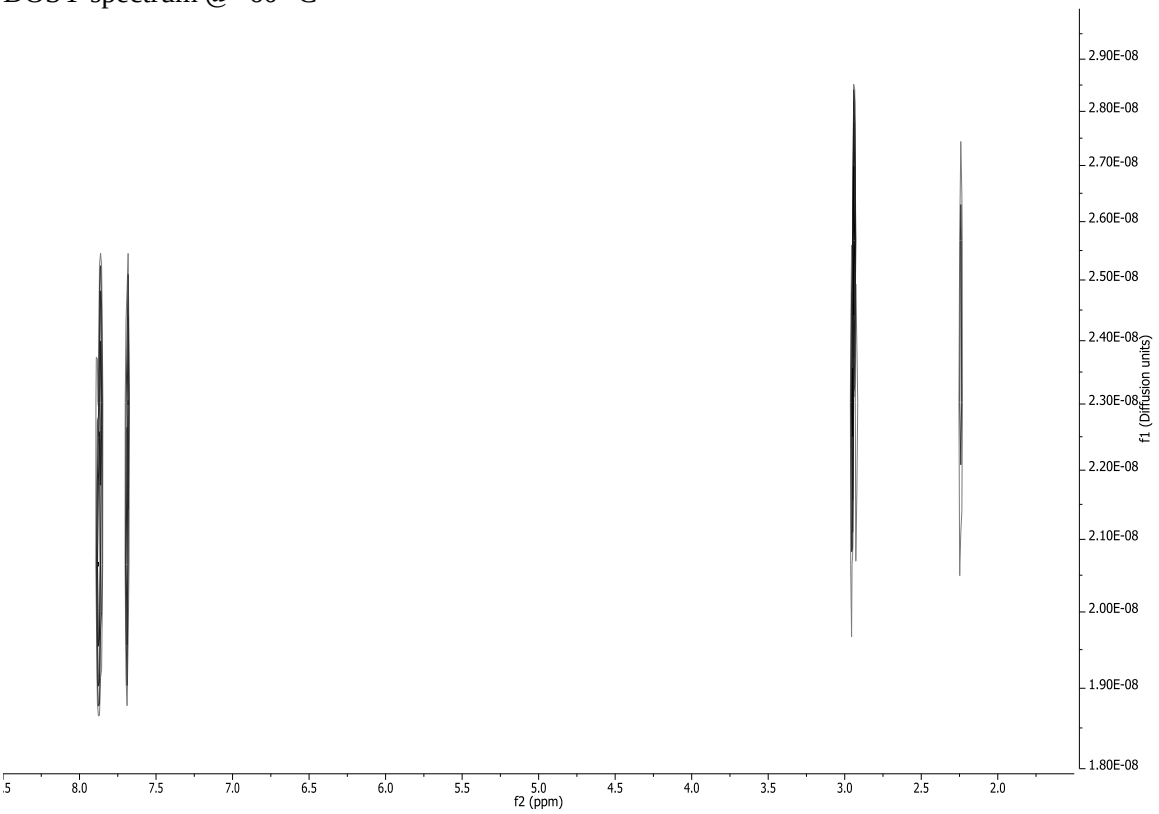
NOESY spectrum @ -30 °C



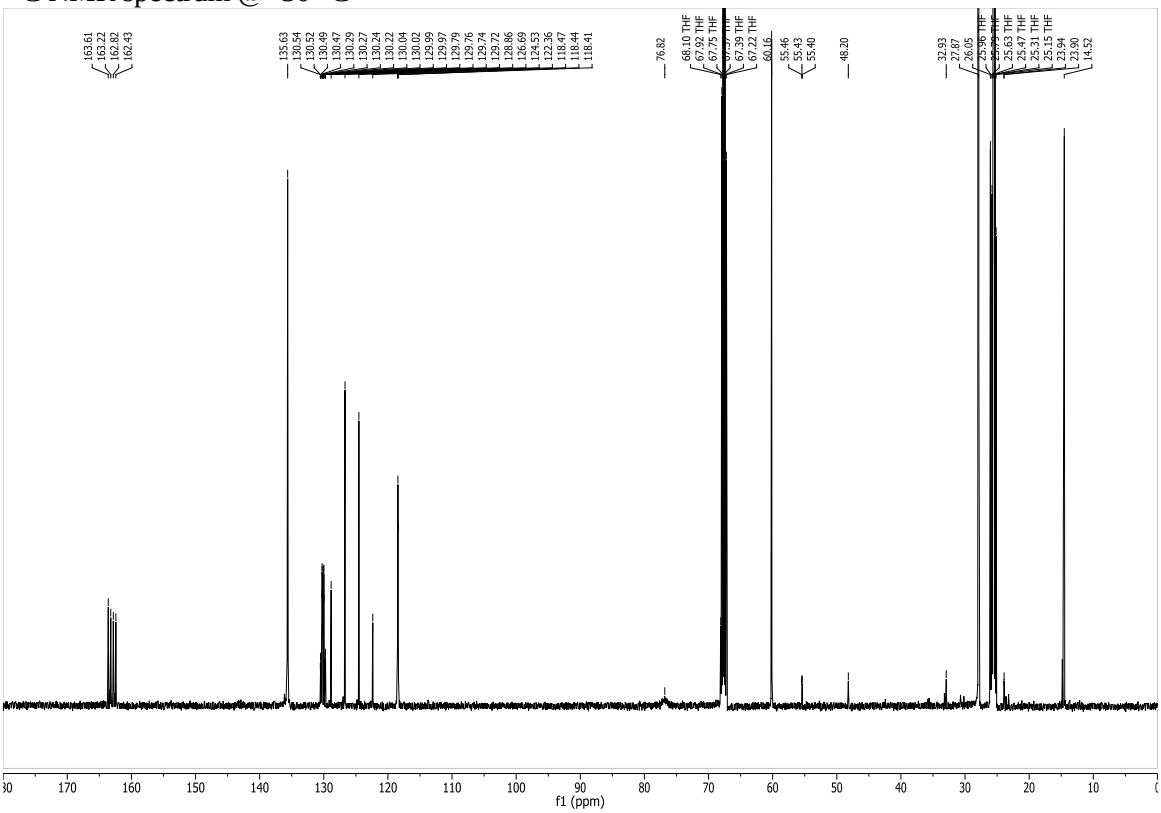
NOESY spectrum @ -60 °C



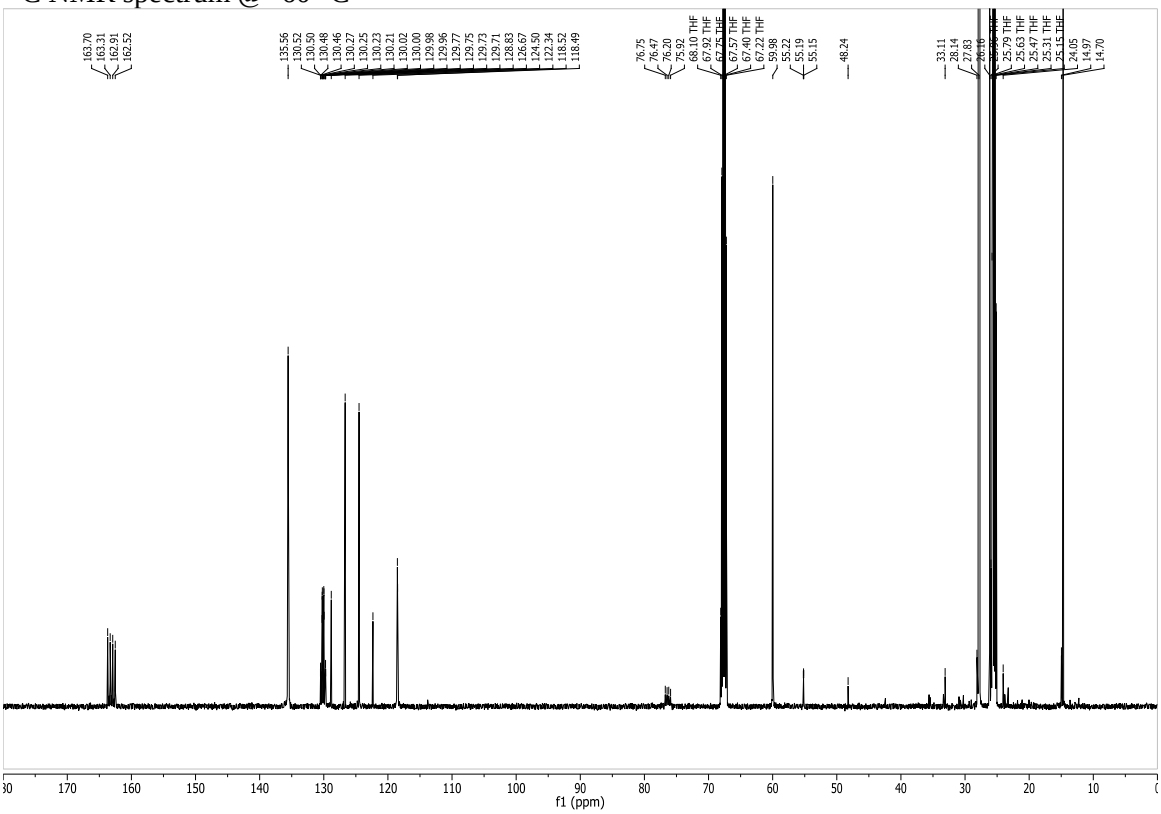
DOSY spectrum @ -60 °C



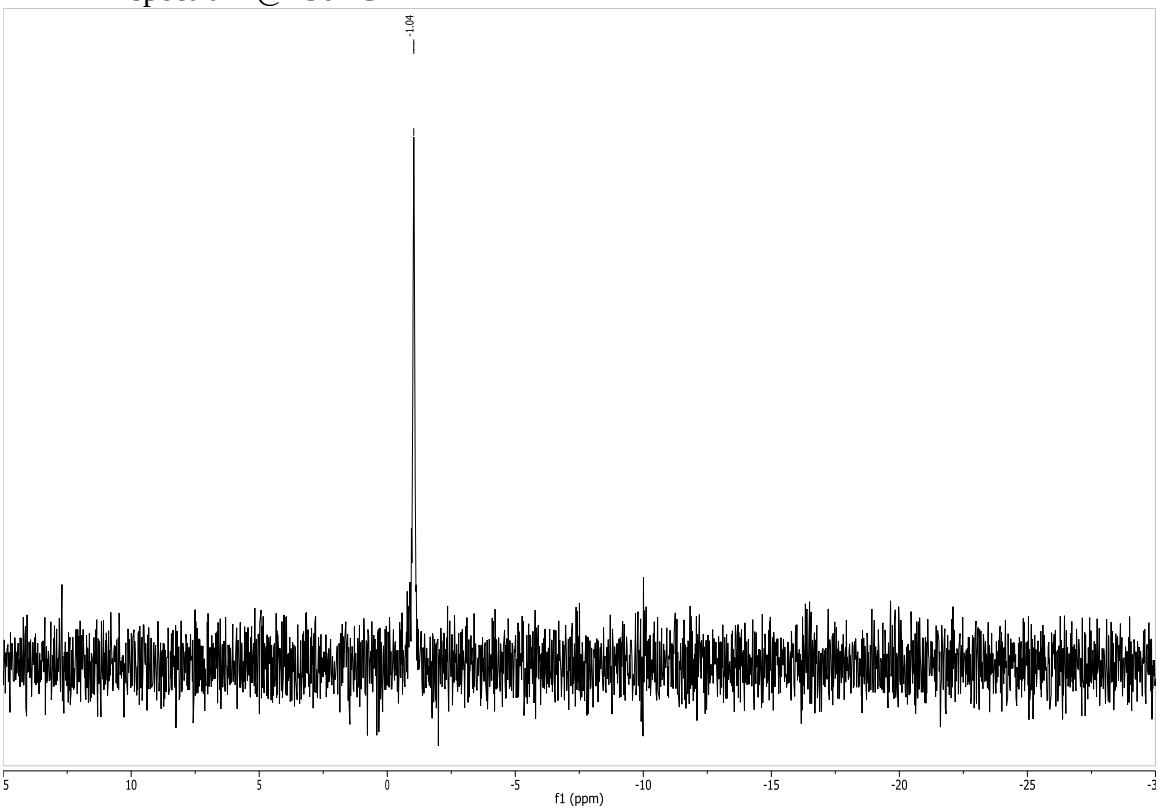
^{13}C NMR spectrum @ -30 °C



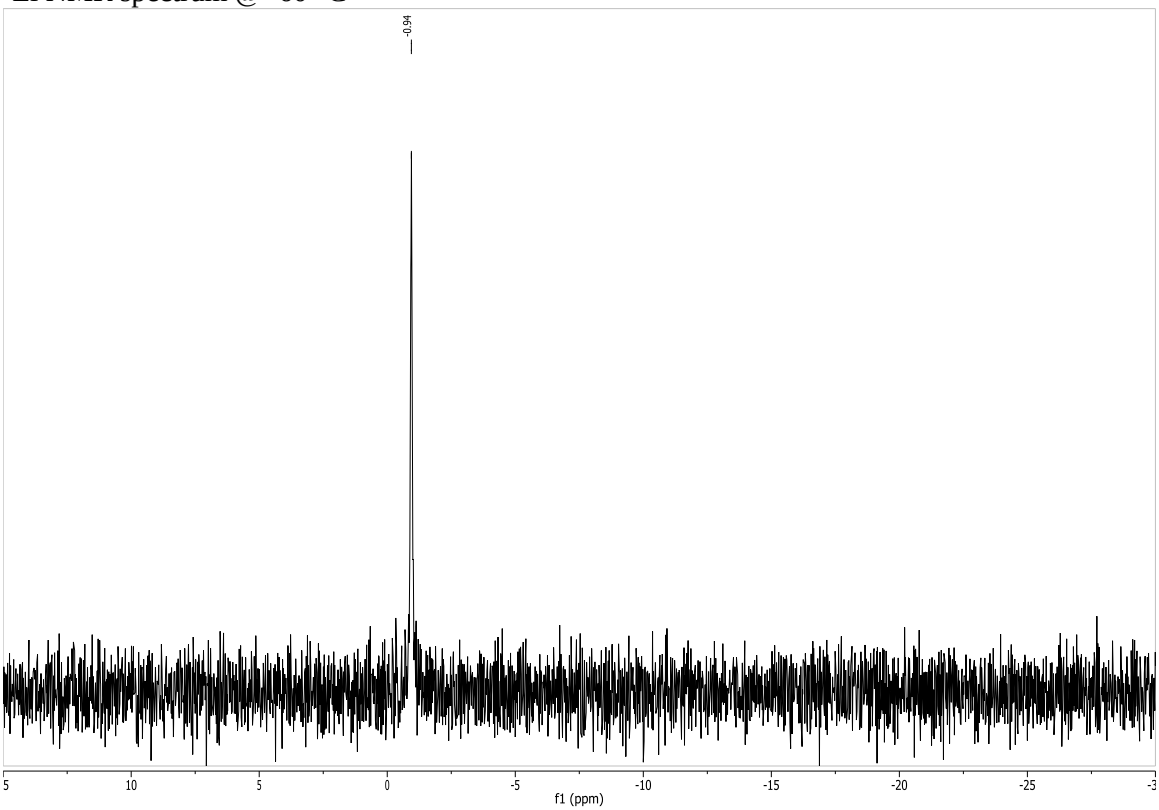
^{13}C NMR spectrum @ -60 °C



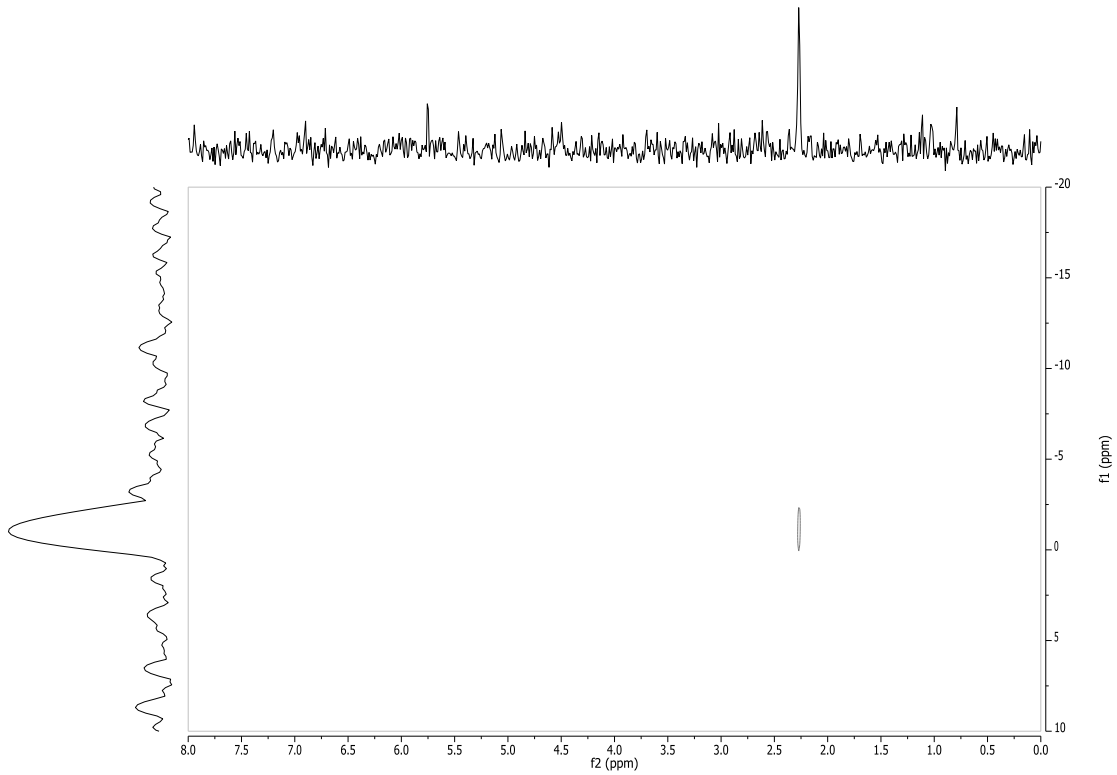
^{6}Li NMR spectrum @ -30 °C



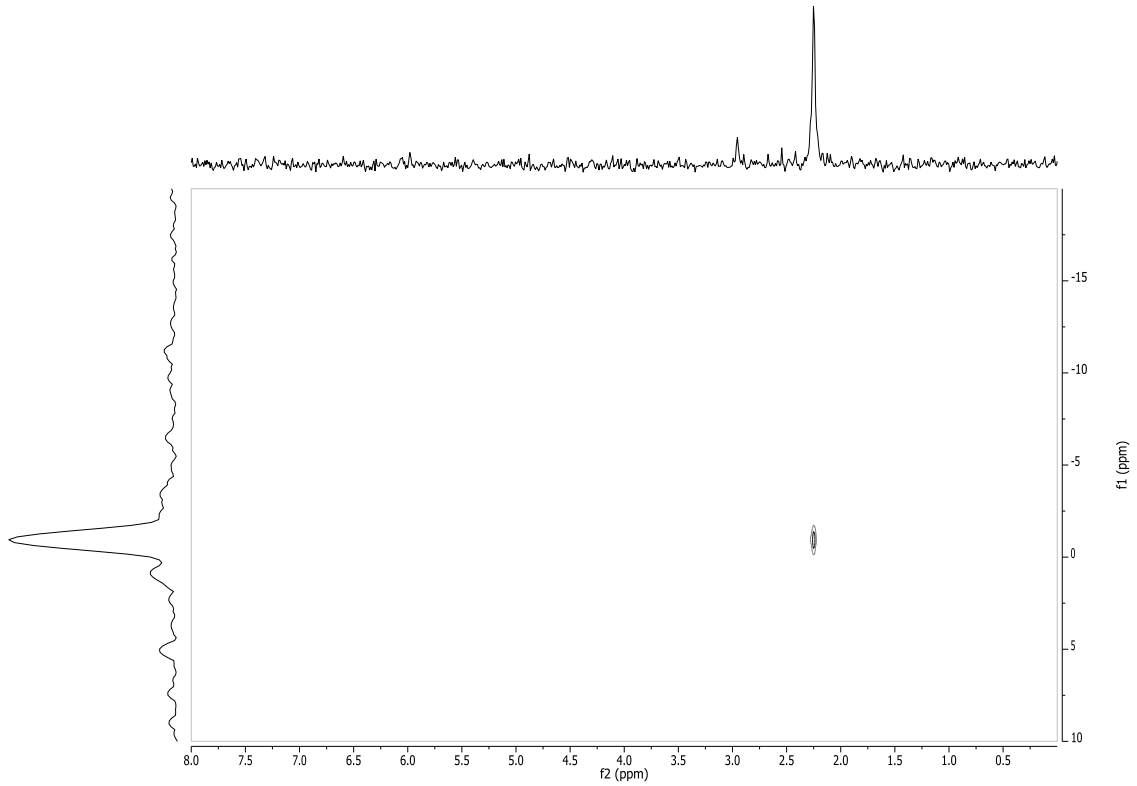
^{6}Li NMR spectrum @ -60 °C



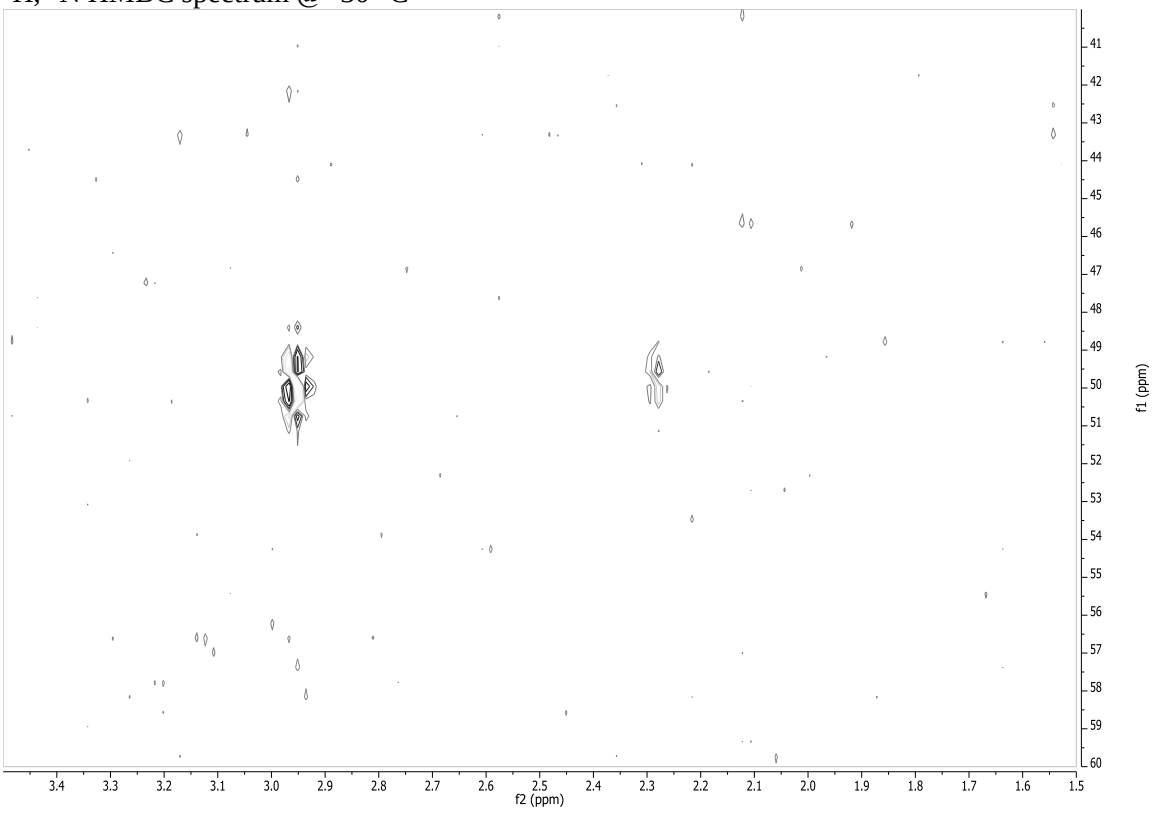
^{1}H,^{6}Li HMBC spectrum @ -30 °C



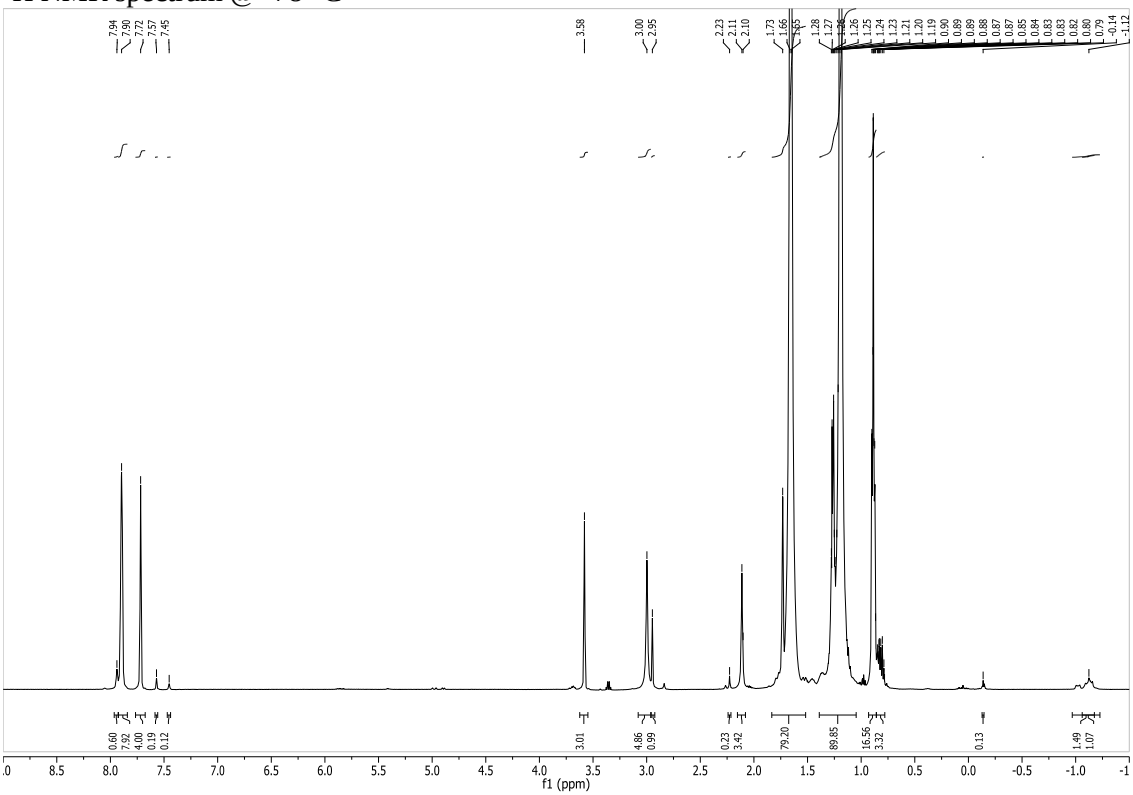
$^{1}H,^{6}Li$ HMBC spectrum @ -60 °C



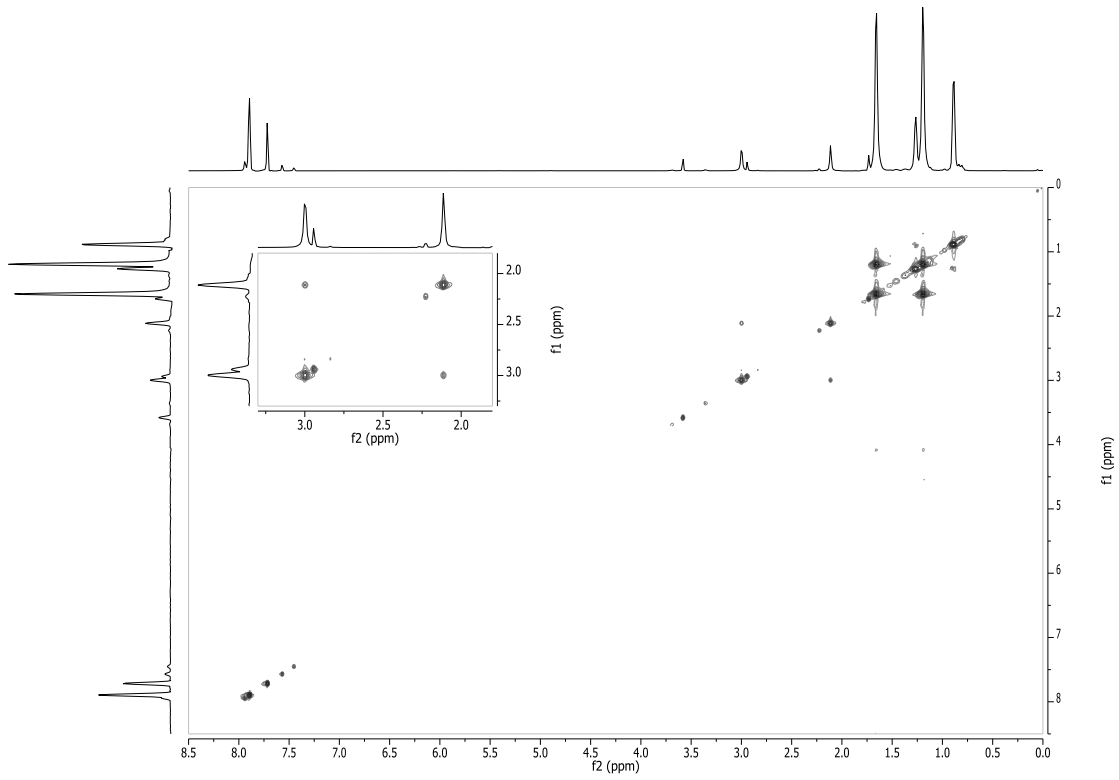
$^{1}H,^{15}N$ HMBC spectrum @ -30 °C



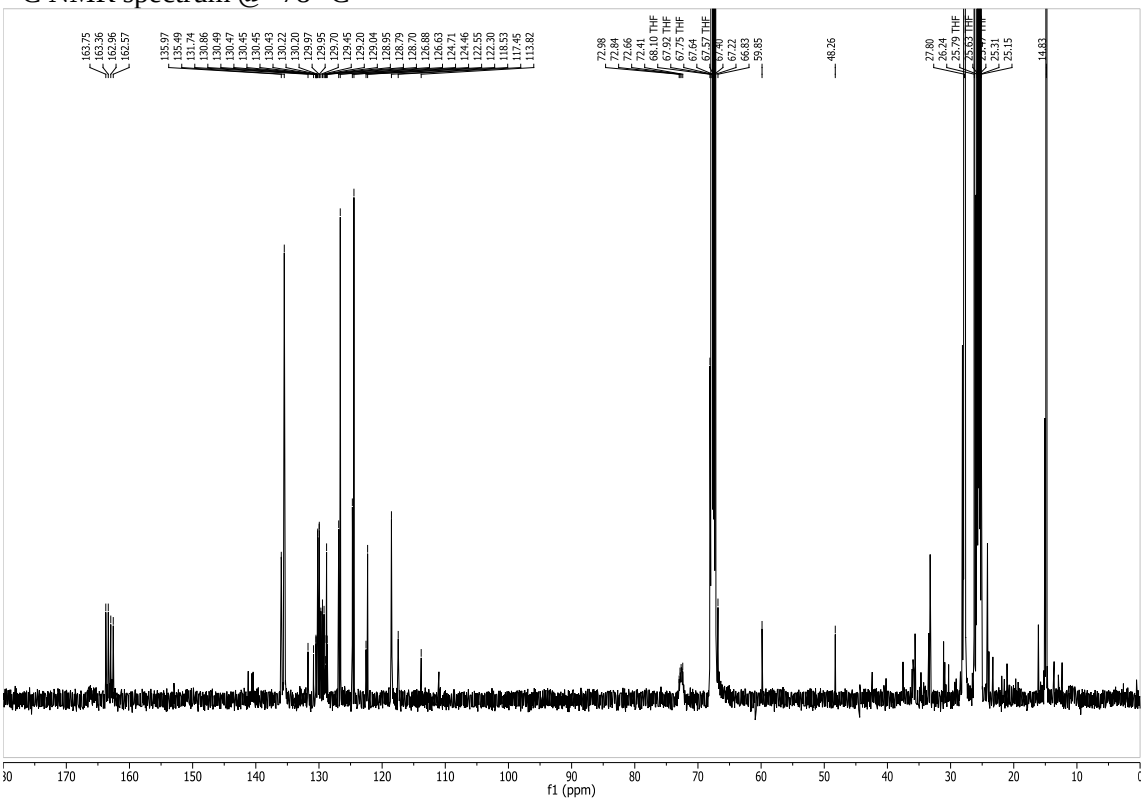
Dilithiomethyl dimethylammonium BAr^F (**9**):
^{1}H NMR spectrum @ -78 °C



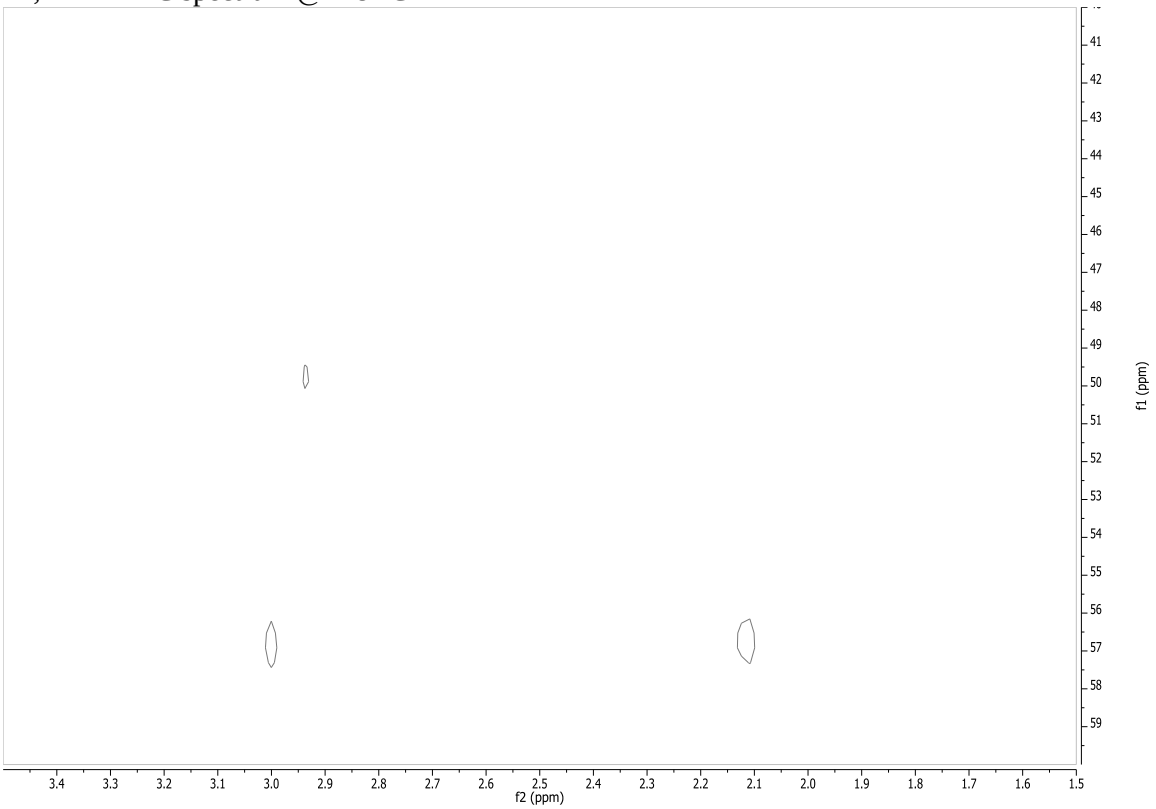
NOESY spectrum @ -78 °C



^{13}C NMR spectrum @ -78 °C

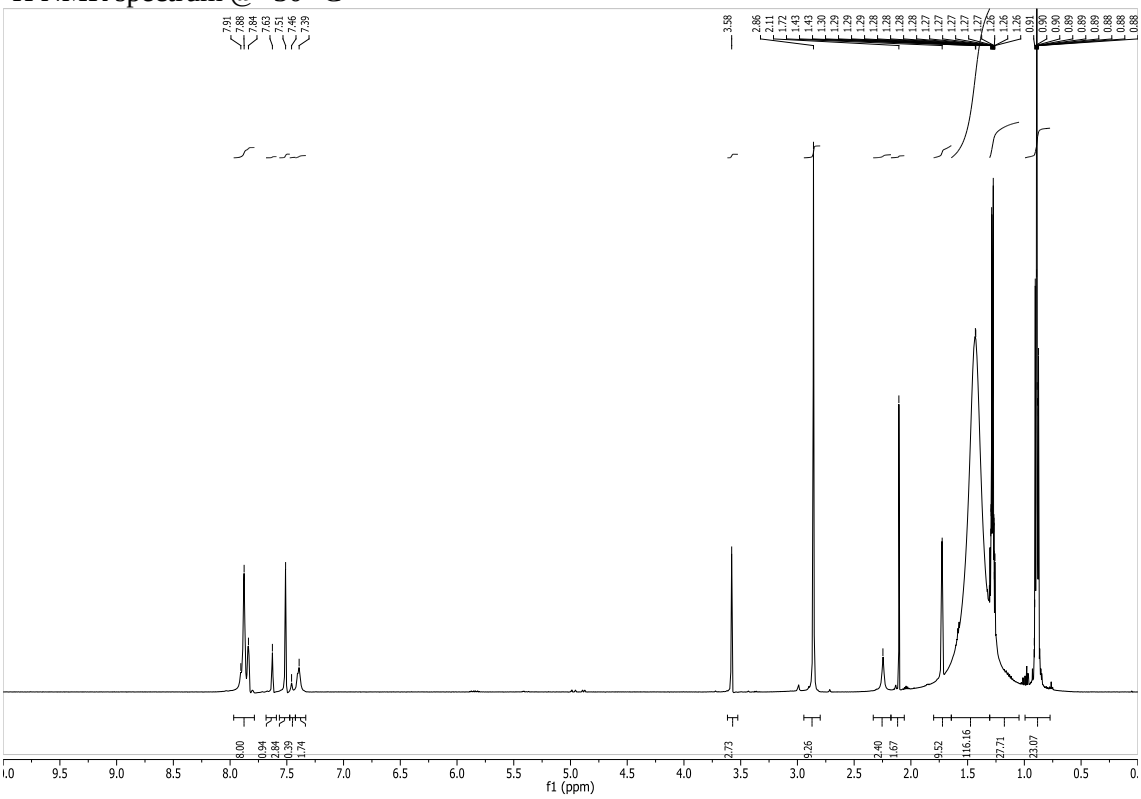


^{1}H,^{15}N HMBC spectrum @ -78 °C

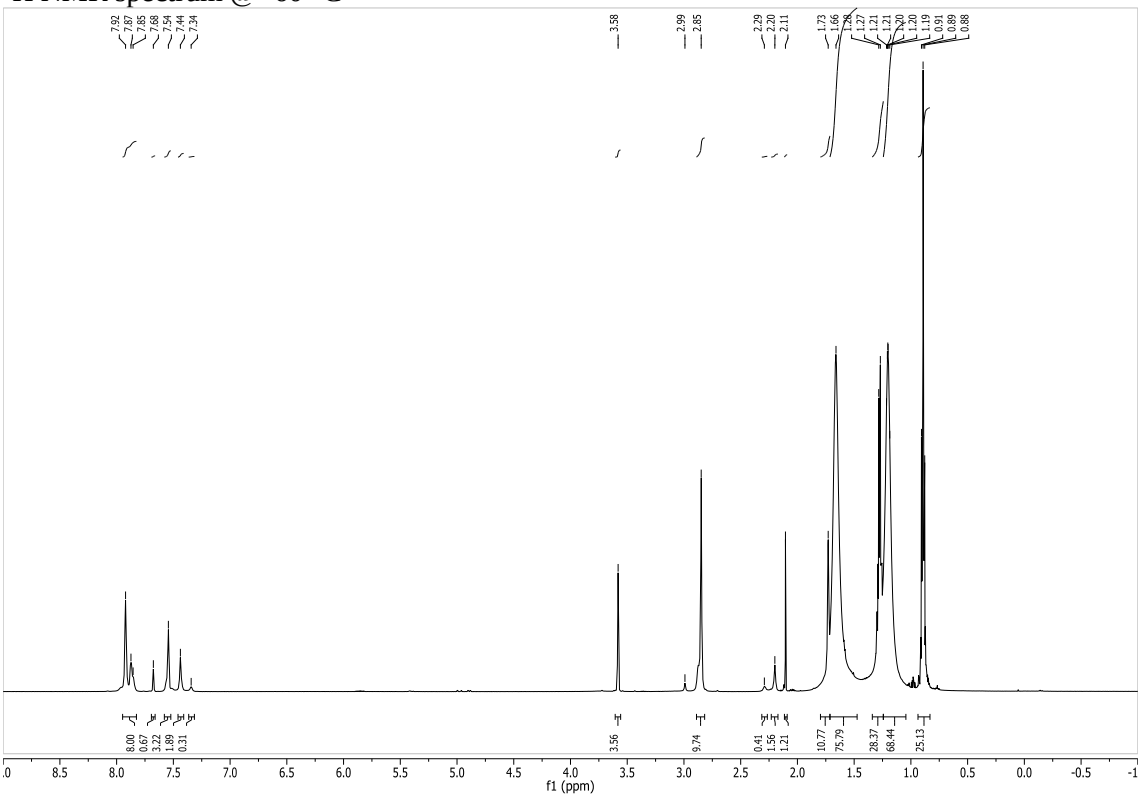


Lithiomethyl trimethylammonium LiBAr^F:

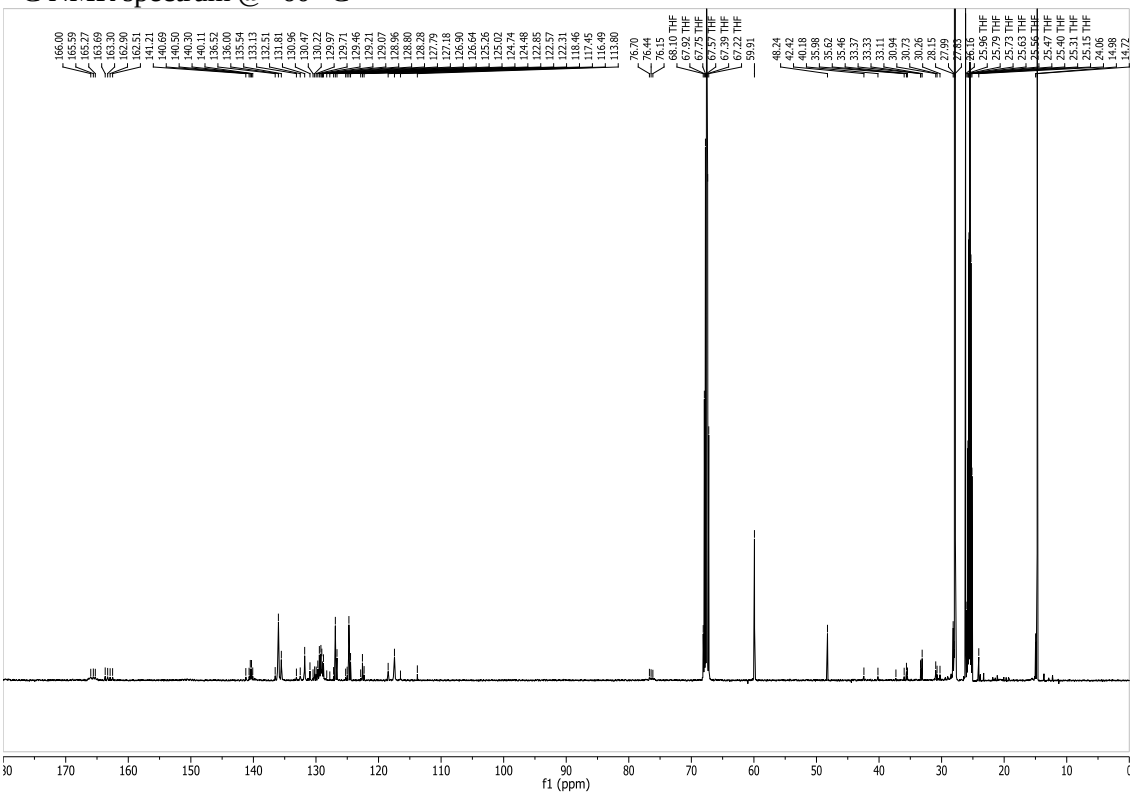
^{1}H NMR spectrum @ -30 °C



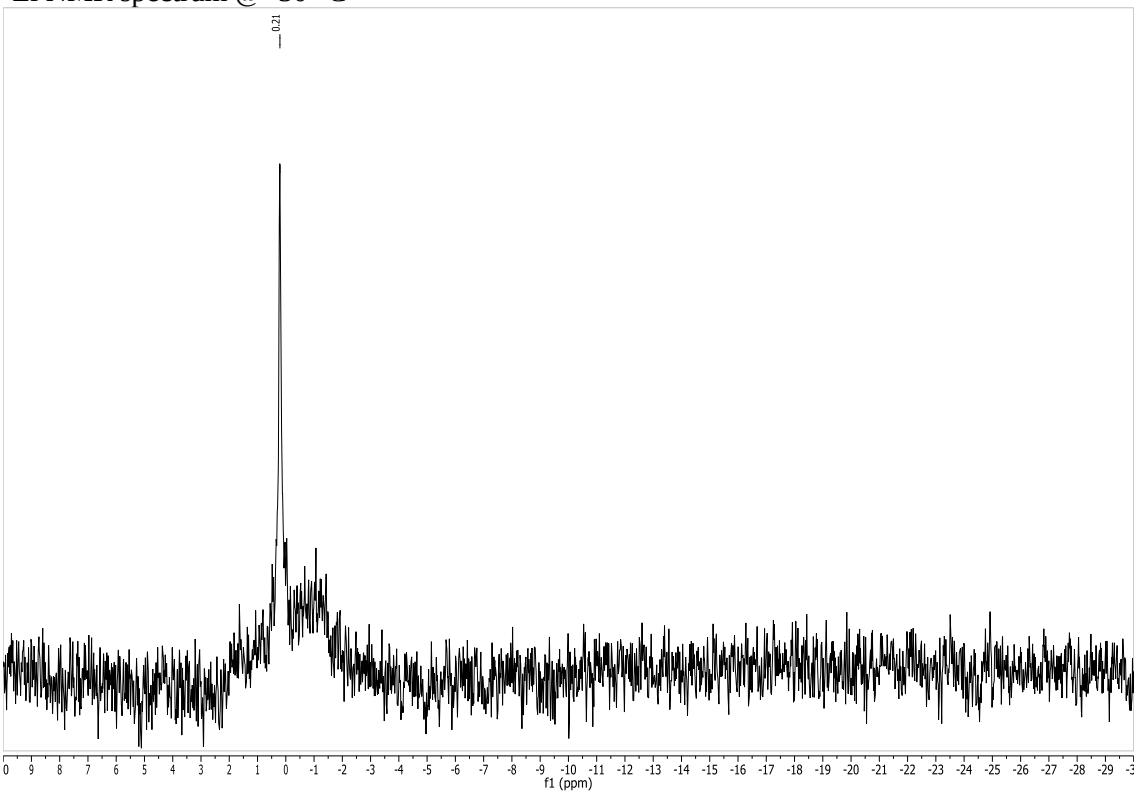
^{1}H NMR spectrum @ -60 °C



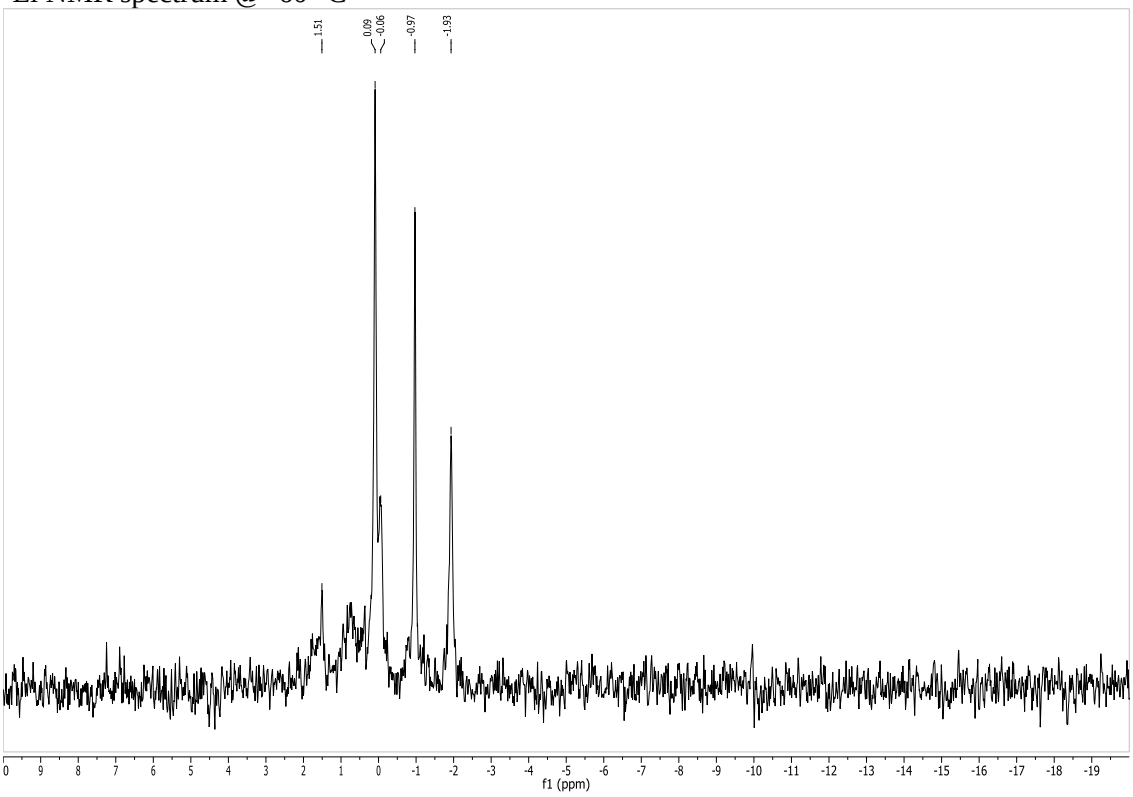
^{13}C NMR spectrum @ -60 °C



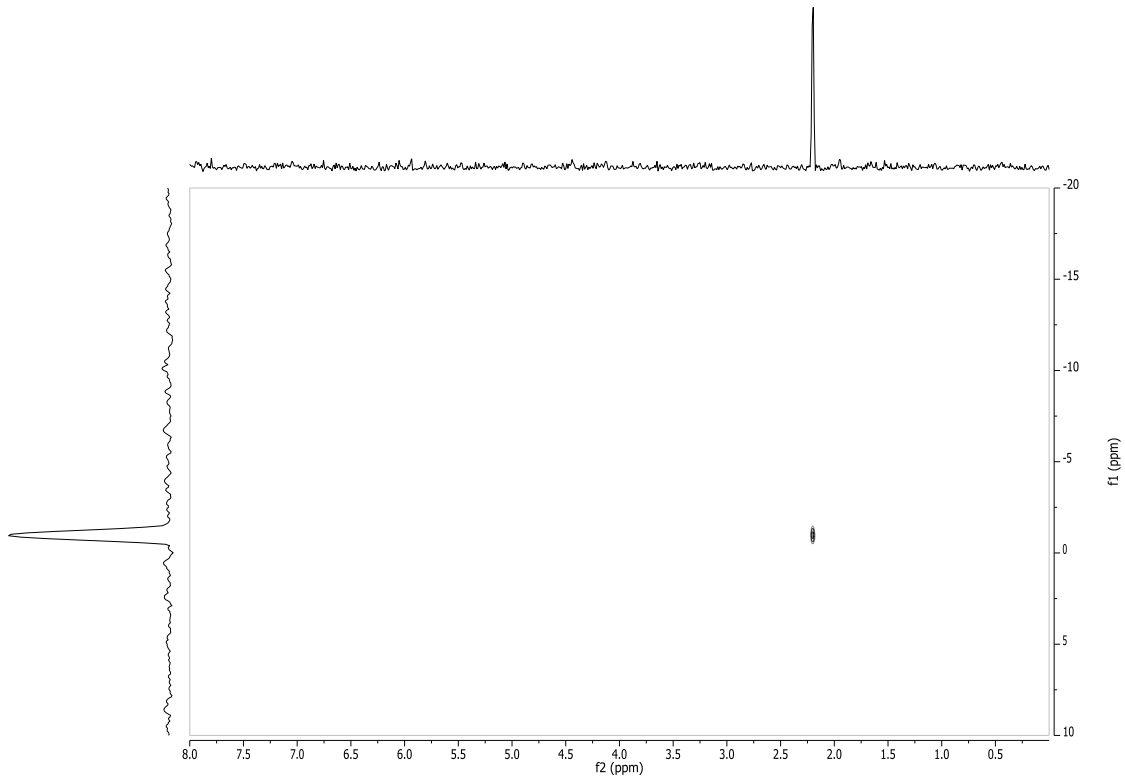
^{6}Li NMR spectrum @ -30 °C



^{6}Li NMR spectrum @ -60 °C

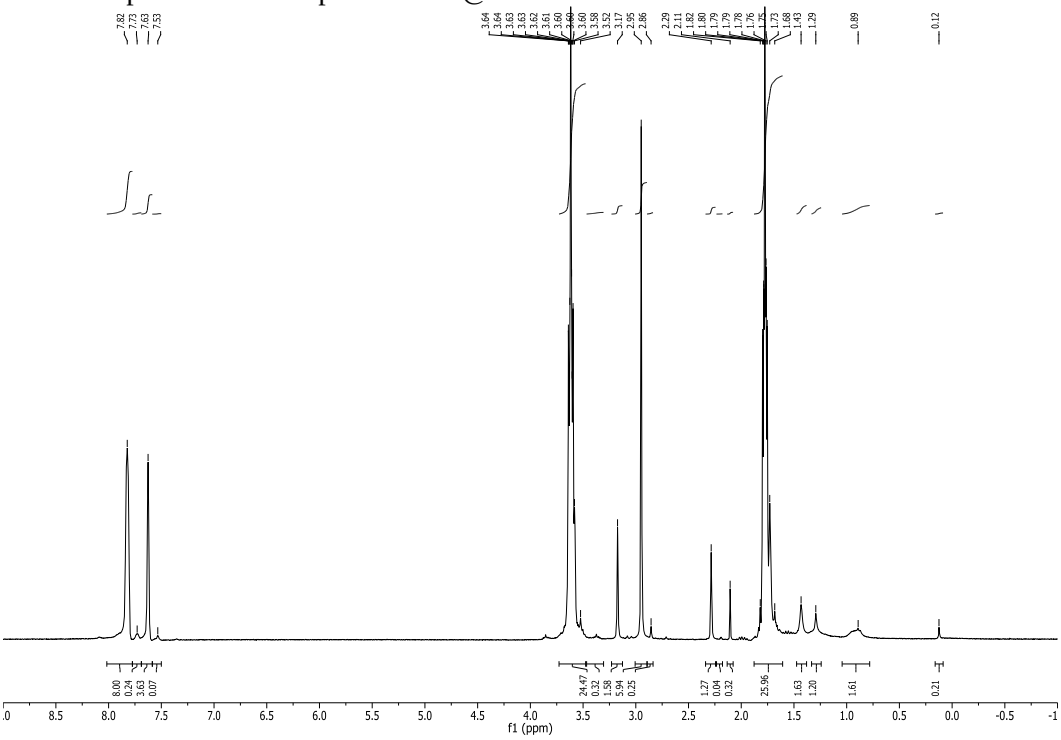


^{1}H,^{6}Li HMBC spectrum @ -60 °C



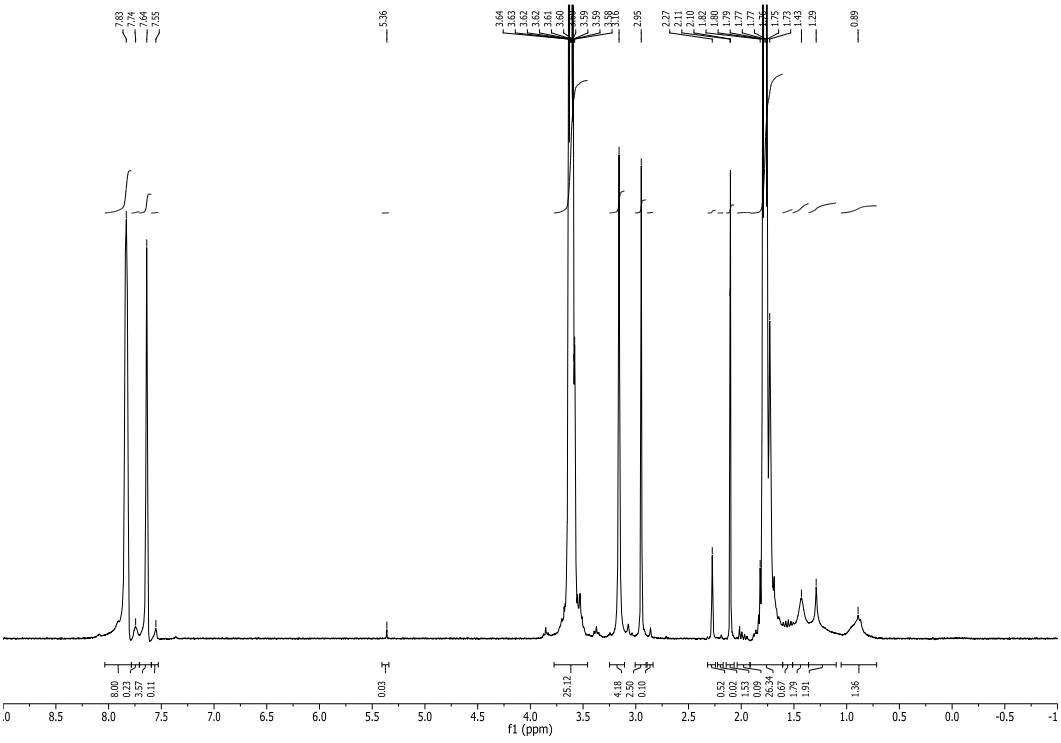
Study of the formation of products of the degradation of lithiomethyl trimethylammonium BAr^F

^{1}H NMR spectrum after deprotonation @ -20 °C

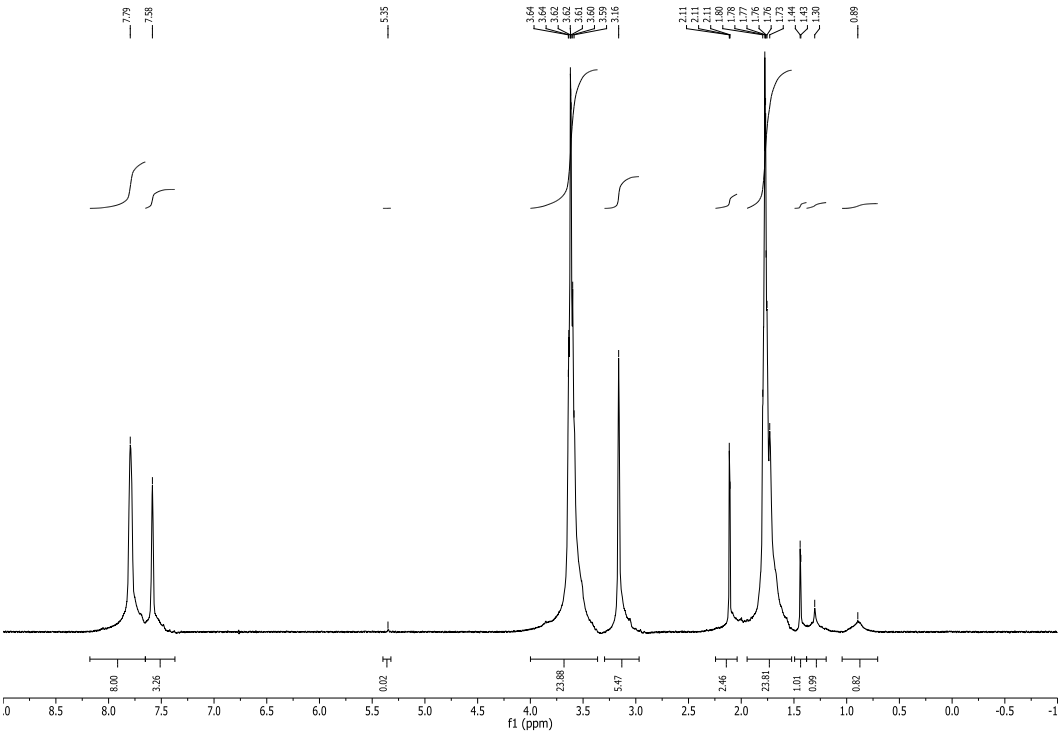


^{1}H NMR spectrum after 1 h at 10 °C @ -20 °C

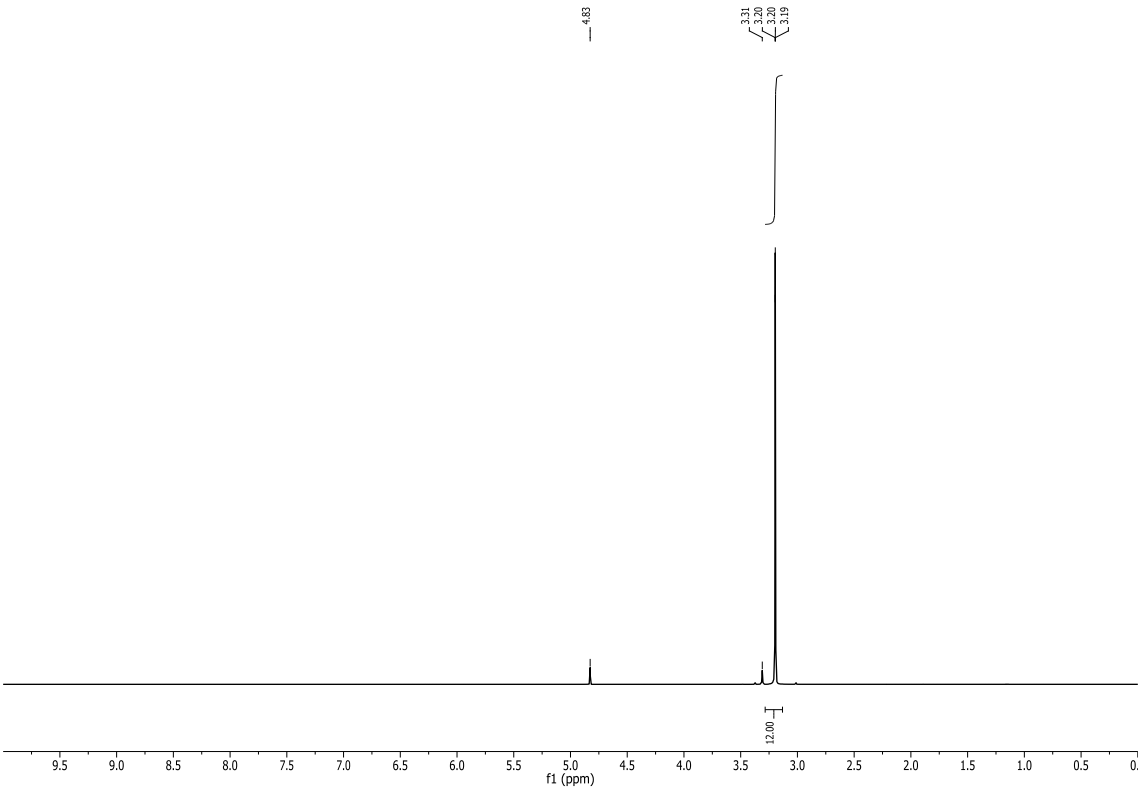
Traces of ethylene (δ= 5.36 ppm), and substantial quantities of NMe_4^+ (δ= 3.16 ppm) and NMe_3 (δ= 2.10 ppm) formed.



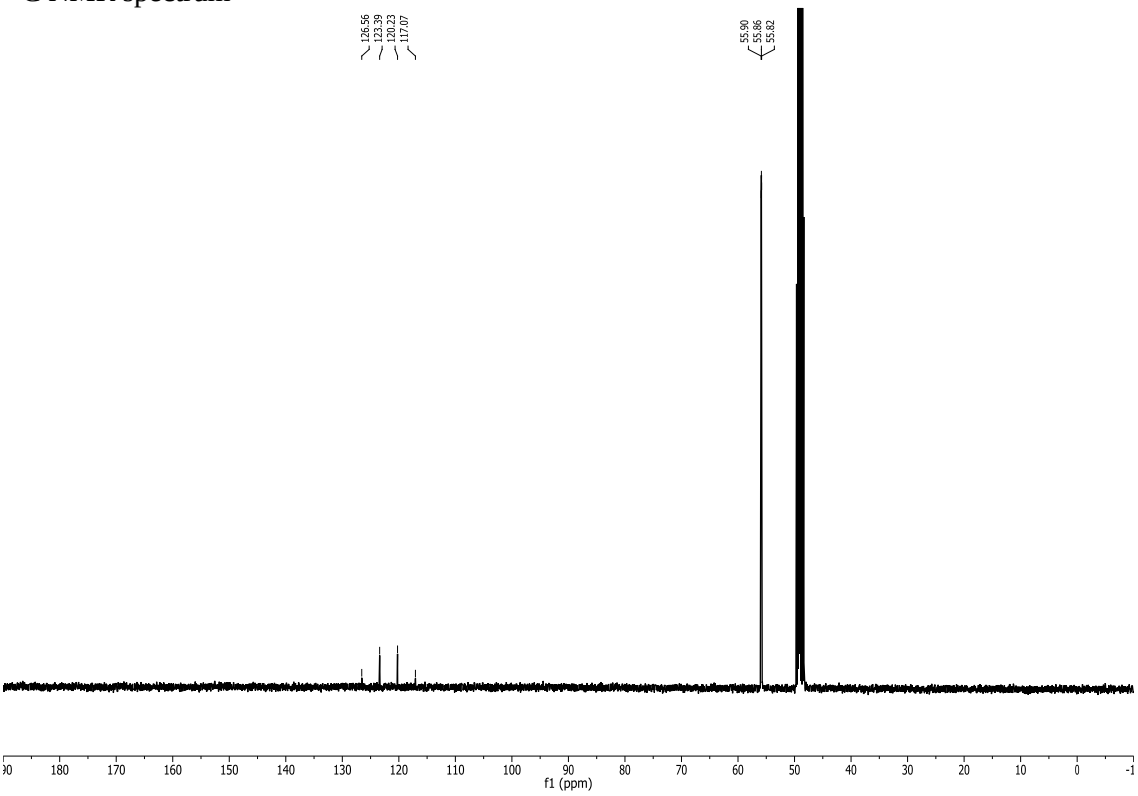
^{1}H NMR spectrum after 16 h at 10 °C @ -20 °C
Traces of ethylene (δ= 5.36 ppm), and substantial quantities of NMe_4^+ (δ= 3.16 ppm) and NMe_3 (δ= 2.10 ppm) formed.



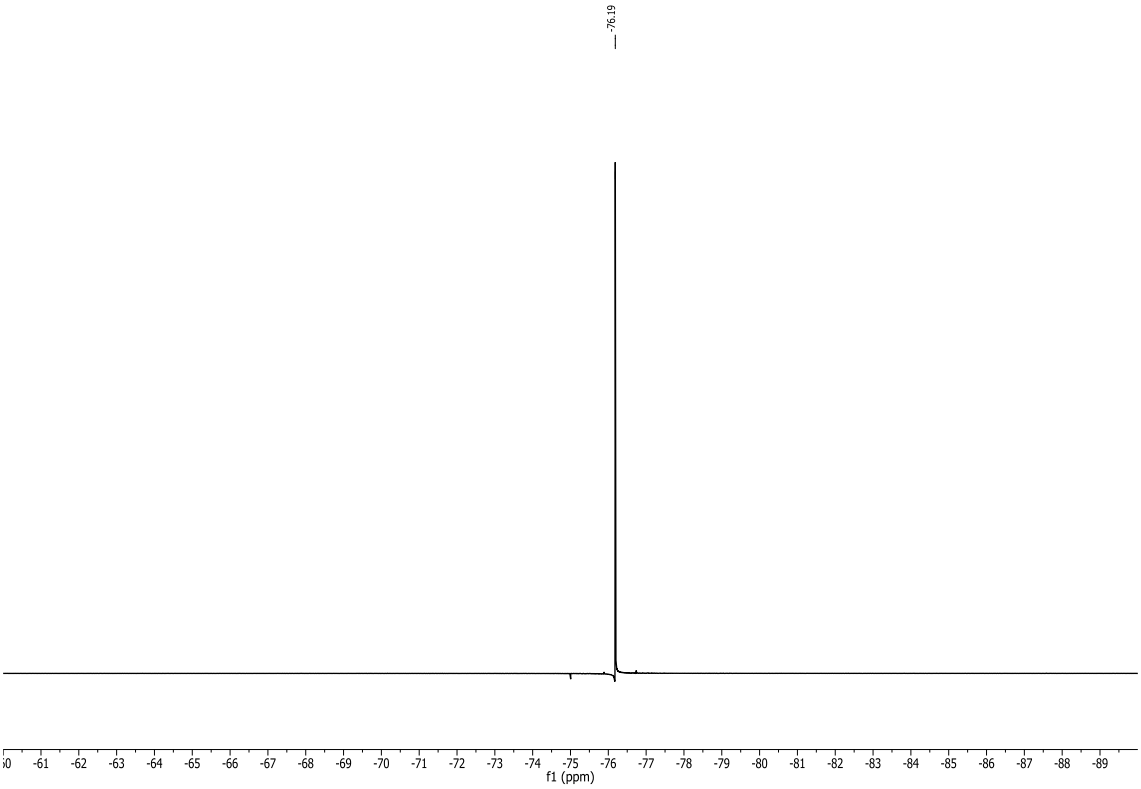
Tetramethylammonium OTf (**16**):
^{1}H NMR spectrum



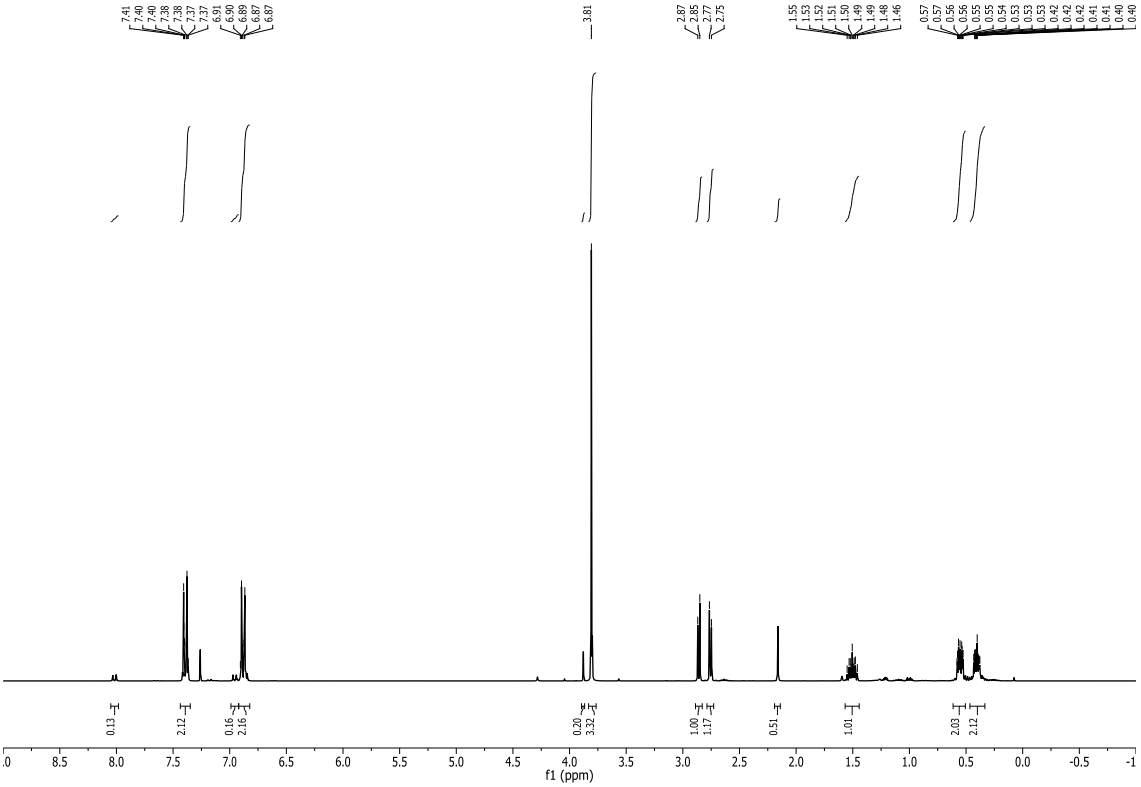
^{13}C NMR spectrum



^{19}F NMR spectrum



2-Cyclopropyl-2-(4-methoxyphenyl)oxirane (**19d**):
^{1}H NMR spectrum

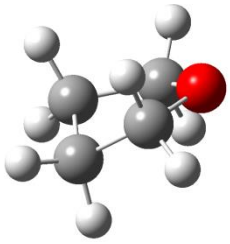


5. Optimised geometries

a) Influence of a Li cation on the stability of P-C and N-C ylides

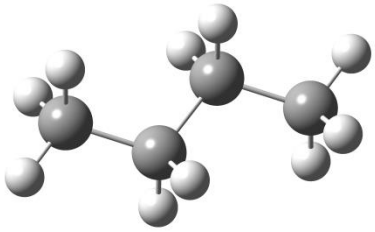
1) Gaussian: M06/aug-cc-pVDZ

THF (C_2, N_{imag} = 0)



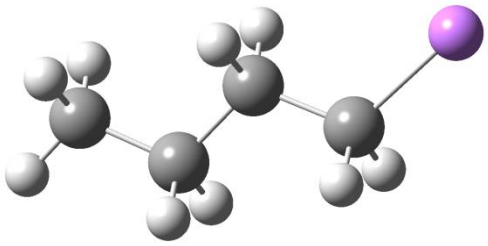
C	0.724753442820	0.986468299477	0.234402195280
C	-0.724972914704	0.986272307927	-0.234506606175
C	-1.157265000035	-0.423036776281	0.134670777042
C	1.157395535747	-0.422845235647	-0.134423077359
H	1.342818470228	1.759952308699	-0.240163105851
H	0.771022219227	1.129656117353	1.325299929373
H	-0.771298553658	1.129161663610	-1.325441368910
H	-1.343185447906	1.759742639043	0.239889759734
H	-1.517026375297	-0.466307180923	1.179622391900
H	-1.950062844792	-0.823511168835	-0.514734911957
H	1.949988328744	-0.823074842104	0.515392302276
H	1.517616725987	-0.466238123971	-1.179201889297
O	0.000097413639	-1.240433008347	-0.000106396055

Bu (C_{2h}, N_{imag} = 0)



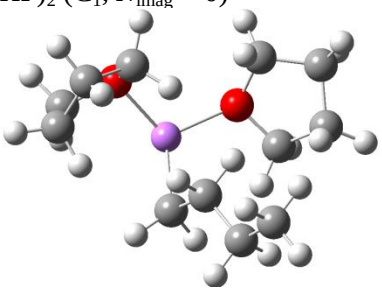
C	-2.505146118051	0.093858144557	0.003580897249
H	-2.157274747078	-0.950442385961	-0.029478626060
H	-2.156951848787	0.585414596172	-0.918270996727
H	-3.603905939702	0.080653957848	-0.019591634805
C	-1.970841456936	0.805205980980	1.232942148000
H	-2.352640328621	1.840740506439	1.264822462700
H	-2.352721118868	0.316904672975	2.146629196521
C	-0.452122123445	0.834388690697	1.283506656980
H	-0.070242448313	1.322689600226	0.369819397333
H	-0.070323264898	-0.201145850475	1.251626791949
C	0.082182539604	1.545737045324	2.512867607070
H	-0.266012560032	1.054181563800	3.434719710087
H	-0.265687997000	2.590037878008	2.545926185546
H	1.180942361359	1.558940348968	2.536040646418

BuLi (C_S, N_{imag} = 0)



C	-2.522510865427	0.094625869871	0.004805204825
H	-2.178959233313	-0.951955278189	-0.032386327596
H	-2.178418511744	0.583583806440	-0.921084090316
H	-3.622636801735	0.084257157643	-0.013743811287
C	-1.970866138966	0.803536971718	1.230017458716
H	-2.343580200059	1.842613963515	1.267710351027
H	-2.343928042763	0.318635827467	2.149637064025
C	-0.445726492324	0.831632246942	1.279096930385
H	-0.089812761941	1.303409211562	0.340676608443
H	-0.090071718224	-0.217162781762	1.220643627752
C	0.154936712878	1.536447958999	2.497269558437
H	-0.263238696947	1.052948765529	3.406971571357
H	-0.263102831206	2.566173818598	2.531359417108
Li	2.127189370599	1.627964741281	2.654418167764

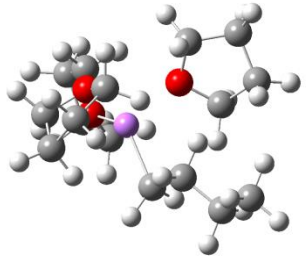
BuLi(THF)$_2$ (C_1, N_{imag} = 0)



C	-1.041833135717	3.472674504890	-1.580224543576
H	-1.897462672496	3.043234456953	-2.125910898830
H	-0.125837100002	3.119509705765	-2.083102922749
H	-1.085211876609	4.565235976981	-1.701040527865
C	-1.059962093041	3.045670467858	-0.122273615700
H	-0.219390977087	3.514222201371	0.421612893406
H	-1.975099249687	3.407698420995	0.376816812439
C	-0.971833881990	1.534030555308	0.073779101277
H	-0.057539139775	1.205719441819	-0.480101176807
H	-1.803672996489	1.072792816495	-0.498720689966
C	-0.986192981858	1.018628488877	1.517520760115
H	-2.029154785073	1.062011095810	1.889096196854
H	-0.450253744897	1.761508092828	2.148469565254
Li	0.109377781921	-0.681891542183	1.336668803988
O	1.945863681977	-0.394492223765	0.674543774069
C	2.431916991897	0.935697160944	0.954250584143
C	2.405875324736	-0.820985111461	-0.614521520046
C	2.948389252990	1.461591639431	-0.369059044138
H	1.598824160942	1.512407789484	1.378920087494
H	3.238432091187	0.859205282901	1.702755438156
C	3.461936571203	0.186696166031	-1.029001511371
H	2.777856932105	-1.851539674970	-0.527514333730
H	1.554978533274	-0.812605407152	-1.317996156897
H	3.721364375776	2.229516966008	-0.240576785019

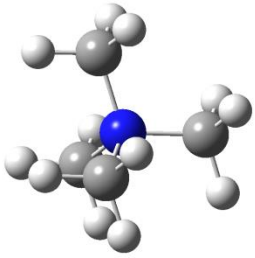
H	2.121317162724	1.895084390652	-0.951986424089
H	4.442240541915	-0.090942067116	-0.612072060632
H	3.560895436260	0.263403354274	-2.118964177089
O	-0.739853134491	-2.277138663835	0.514849180402
C	-1.948104644417	-2.540359987834	1.249174490077
C	-1.070874316057	-1.999908382525	-0.859739411158
C	-3.042935900625	-1.860362136460	0.458766299926
H	-2.100324968688	-3.632196815013	1.313444018462
H	-1.821679063431	-2.132112257562	2.262010766268
C	-2.583994056617	-2.116865068382	-0.972651757800
H	-0.731527082846	-0.977789477738	-1.095844935702
H	-0.528931832054	-2.711196340310	-1.500626094113
H	-3.034760026663	-0.784605888078	0.686745245559
H	-4.038001366764	-2.269558438045	0.674346090199
H	-2.996279462584	-1.401383187009	-1.695352400090
H	-2.870934051783	-3.130535445378	-1.291289734155

$BuLi(THF)_3$ (IOp(2/15=3), N_{imag} = 0)



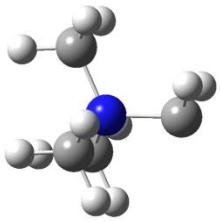
C	4.677913000158	1.416800020984	-0.887553789416
H	5.211118054707	0.603655795876	-0.368976863702
H	4.308893953591	2.109299600494	-0.112398736134
H	5.414620158480	1.962715564620	-1.495733249291
C	3.527097833607	0.868131786583	-1.714499225952
H	3.023823580468	1.690268921767	-2.255942918515
H	3.901613898151	0.183803973147	-2.495230333823
C	2.478481749943	0.128374298757	-0.885712593971
H	2.161102537480	0.839429558604	-0.084936166347
H	3.001058662213	-0.678457082867	-0.330635890004
C	1.277216132321	-0.457115435969	-1.630941227064
H	1.627488054408	-1.347309167596	-2.192314027852
H	0.997501405442	0.262478356570	-2.435690111665
Li	-0.298924333920	-0.488045759914	-0.299533141765
O	-2.198346166389	-0.906353099885	-0.761848681433
C	-2.590172829715	-0.306279099116	-1.993958136845
C	-3.228292375847	-0.574391444524	0.162038815253
C	-4.089971856904	-0.565228881402	-2.093365162966
H	-2.373990327336	0.778152750819	-1.950494456444
H	-1.980502764777	-0.751006882400	-2.788905751517
C	-4.530655660360	-0.721589041923	-0.623516921979
H	-3.131850269149	-1.245596548526	1.025058212013
H	-3.080292639139	0.467028051020	0.504035118033
H	-4.285589516163	-1.485183946558	-2.659483847333
H	-4.608605707060	0.255238925108	-2.605852990866
H	-4.980381020412	-1.708337430853	-0.452566648006
H	-5.267962595973	0.033685590994	-0.321660319381
O	-0.146367209869	-1.627121995460	1.396538721089
C	1.130762488417	-1.466915097362	2.040057852609
C	-0.252862607555	-2.975529234854	0.920767759815
C	1.912101598062	-2.756399877272	1.800974022617
H	1.630454207261	-0.599408882136	1.583149070918
H	0.966369402966	-1.260864366552	3.109392349891
C	1.172280188067	-3.389600740547	0.626221033534
H	-0.707254110340	-3.608246332368	1.705807358695
H	-0.913803390944	-2.965266172517	0.043425326516
H	1.858866330983	-3.410913649849	2.684296786620
H	2.969961314653	-2.558072533880	1.587555789940
H	1.297850497742	-4.478600039699	0.571850359653
H	1.487841776951	-2.934333088450	-0.324287123877
O	-0.596378140724	1.418730568780	0.392938475829
C	-0.122886821020	2.467151477886	-0.471559932904
C	-0.422248219840	1.797996087836	1.761162659586
C	0.649670141584	3.415212124681	0.424183086929
H	0.475389845968	2.001616075091	-1.266119893482
H	-0.997491297678	2.967661105930	-0.923702609633
C	-0.109184867908	3.282691983478	1.740360821870
H	-1.337610348046	1.537812193007	2.313335485453
H	0.416119897804	1.223097906319	2.191486656498
H	0.671093563894	4.439319645738	0.031030185300
H	1.687377128541	3.065568598044	0.538106919186
H	-1.039289643868	3.871173359736	1.705735815040
H	0.467605668240	3.601827388683	2.617512837564

NMe_4 cation (T_D, N_{imag} = 0)



C	0.000000001872	0.000000002340	1.493889758614
H	0.000000000886	1.037109429625	1.847877185971
H	-0.898163106975	-0.518554711627	1.847877189775
H	0.898163113036	-0.518554709150	1.847877187524
C	0.000000001318	-1.408452773296	-0.497963251376
H	-0.898163107524	-1.915046893810	-0.127060986803
H	-0.000000000072	-1.396492181760	-1.593755205691
H	0.898163112486	-1.915046891334	-0.127060989054
C	-1.219755882355	0.704226383331	-0.497963253486
H	-1.209397705564	1.735355513948	-0.127060992699
H	-1.209397705972	0.698246084747	-1.593755207782
H	-2.107560813425	0.179691372697	-0.127060988895
C	1.219755879166	0.704226386694	-0.497963256542
H	2.107560812611	0.179691378508	-0.127060994176
H	1.209397700053	0.698246088082	-1.593755210813
H	1.209397700461	1.735355517283	-0.127060995730
N	0.000000000000	-0.000000000233	-0.000000000698

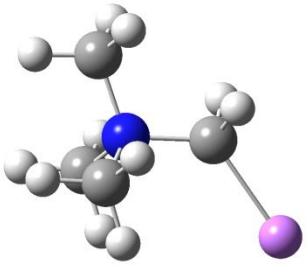
NMe_3CH_2 (C_S, N_{imag} = 0)



C	-2.019929250045	4.234374152247	-1.497354994077
H	-2.416070526267	5.254854414550	-1.480027569402
H	-2.340393597860	3.661065799378	-0.614568380655
H	-0.925296123788	4.279610970695	-1.540058188154
C	-3.982407703119	3.541052344535	-2.698926833595
H	-4.333997511972	3.075361846258	-3.627155509757
H	-4.326230088750	2.959453093915	-1.830467188324
H	-4.345221305132	4.573295469185	-2.661137475659
C	-1.986377341023	2.190554302378	-2.776236386135
H	-0.892122182407	2.238805324373	-2.806234693509
H	-2.316665166036	1.607205046538	-1.899617304928
H	-2.350042900261	1.723605965063	-3.698360226295

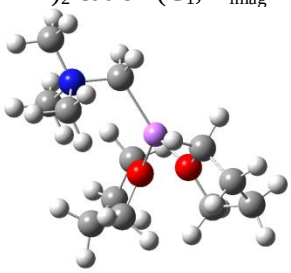
N	-2.505787475135	3.584755008177	-2.732407540937
C	-2.091799475745	4.471046468488	-3.919911825679
H	-2.431842348754	3.888591018475	-4.801899359776
H	-0.983783375244	4.399736008543	-3.915581885103

NMe_3CH_2Li cation (C_S, N_{imag} = 0)



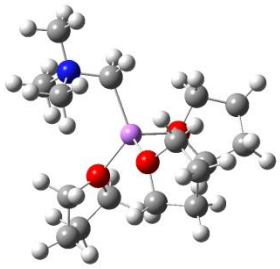
C	-1.976702017505	4.239315184991	-4.063381466586
H	-2.409950791946	3.744632384725	-4.941778677731
H	-2.301069844897	5.285410922023	-4.027296256777
H	-0.883324539060	4.191913305836	-4.109688829020
C	-1.857462405517	4.260788978468	-1.607226358813
H	-2.341258571573	5.255876554713	-1.628724426461
H	-2.340412551613	3.744010107445	-0.756116662335
C	-3.928163391569	3.566330061167	-2.810264528839
H	-4.318455837070	3.052948187989	-3.698986278689
H	-4.268791097030	3.057475137759	-1.902081808106
H	-4.268621824630	4.607310115562	-2.797433389829
C	-1.976850107862	2.144383793287	-2.853902534035
H	-0.883424823759	2.127818353553	-2.917404829043
H	-2.301847656766	1.652457148189	-1.930205184181
H	-2.409606134978	1.631230861857	-3.721875903488
N	-2.434625342237	3.556123665410	-2.827726598259
Li	0.118882613791	4.532950940697	-1.138355274616

$NMe_3CH_2Li(THF)_2$ cation (C_1, N_{imag} = 0)



C	2.951998767776	-0.778207360070	0.356953975279
H	3.652550403174	-0.982277187347	1.177027880562
H	3.508139246906	-0.516203836779	-0.550362632696
H	2.276843712427	0.043675123572	0.623244866355
C	1.142188607319	-1.663158770461	-1.043306674757
H	1.794572499336	-1.495771011692	-1.920985547431
H	0.656582813361	-2.637736126511	-1.239698419725
C	3.054946767350	-3.106177664906	-0.272503945010
H	3.755193670022	-3.302250377940	0.551927917109
H	2.449172359036	-3.996730757800	-0.472046465714
H	3.606216856998	-2.831748370758	-1.178327814784
C	1.387052767636	-2.352776253294	1.299552791113
H	0.740732977600	-1.513946321170	1.581412636646
H	0.771725266792	-3.232043723598	1.078235425440
H	2.087095349153	-2.583659857223	2.113117723910
Li	-0.218246543982	-0.090868038182	-0.737662607565
O	-1.976730003140	-0.326914996330	-0.021004679339
C	-2.947250493397	0.708098900487	0.234186674471
C	-2.631171522536	-1.615687193071	-0.034666779442
C	-4.289607659817	0.071333277335	-0.051943452659
H	-2.866636242447	1.016981410566	1.290292358369
H	-2.704339837805	1.566657344169	-0.407021829125
C	-4.054537481956	-1.358268828653	0.422239892650
H	-2.594033963252	-2.010641935859	-1.062465142320
H	-2.069868658984	-2.295174995179	0.621526763142
H	-4.502491254411	0.092506029474	-1.131037148268
H	-5.111909787482	0.574085475743	0.470792316213
H	-4.763192474719	-2.080374186402	0.000025336947
H	-4.124459808788	-1.412597583739	1.518757067248
O	0.319623234046	1.730380467838	-0.399910136734
C	1.252922865324	2.471413219391	-1.215821714712
C	0.171090600480	2.373552120144	0.879778852709
C	1.536830572430	3.750789595928	-0.452312500690
H	2.160016713503	1.857682372108	-1.346630126980
H	0.798743386930	2.636195755203	-2.201864106447
C	1.357654037231	3.306517423904	0.994928751111
H	-0.782537017611	2.927188224905	0.893948642787
H	0.131617125402	1.590549325891	1.651839477855
H	0.797340595752	4.523488603847	-0.708378416421
H	2.534442234991	4.151442494343	-0.666605579958
H	1.173196816728	4.136177531610	1.687427944284
H	2.246743168811	2.759769955049	1.345441895862
N	2.138232973811	-1.984248404541	0.076942370715

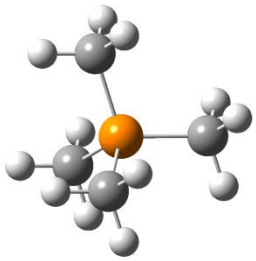
$NMe_3CH_2Li(THF)_3$ cation (IOp(2/15=3), N_{imag} = 0)



C	3.639634206717	-0.442547433762	-0.946238967101
H	4.662145160753	-0.142158248018	-0.681920858056
H	3.627120150074	-0.875493896910	-1.952676787851
H	2.956821900709	0.413026457226	-0.914786324703
C	1.695995417521	-1.799563055064	-0.339563048997
H	1.779412637634	-2.254734098194	-1.345033115756
H	1.462815455705	-2.648150059794	0.333412143935
C	4.056008127940	-2.644229891879	-0.050307729594
H	5.088561743435	-2.353129805006	0.191461511011
H	3.697965512175	-3.390036967874	0.667653225390
H	4.009284605998	-3.061892686952	-1.061761680991
C	3.194178212436	-0.903998805539	1.380470199578
H	2.559475951721	-0.012660372731	1.416389916456
H	2.802046918936	-1.655635844432	2.074830332761
H	4.228656943093	-0.652123964843	1.649049580578
N	3.151211378955	-1.463598513751	0.009829394585
Li	0.240472747119	-0.238401663580	-0.226197357864
O	-1.340296823624	-0.706164870745	-1.288582119615
C	-1.443479204894	-2.031558866852	-1.851306748079
C	-2.636120049641	-0.098743800641	-1.255445340220
C	-2.909469092073	-2.223612124083	-2.208074192629
H	-0.769777676052	-2.099640781628	-2.716529735742
H	-1.101391027665	-2.750665244693	-1.089767903075
C	-3.610719988818	-1.255450762165	-1.261126628933
H	-2.688308241230	0.537719588340	-0.360621439356
H	-2.767125846917	0.538816155447	-2.147841457666
H	-3.233464157793	-3.264147722455	-2.088780554805
H	-3.094735521159	-1.929014999457	-3.251321025314
H	-3.695655011101	-1.687113254420	-0.251342197845
H	-4.613234659392	-0.965042783769	-1.597144309015
O	0.649249653387	1.673079811921	-0.609679312460
C	-0.102857109494	2.448834463273	-1.561533666958

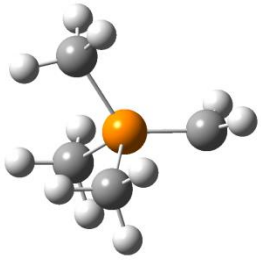
C	1.367782198132	2.550026727780	0.273265621525
C	0.430893849727	3.861772126368	-1.443728589992
H	0.025764993406	1.994552997104	-2.552770528816
H	-1.172105626940	2.400144929723	-1.290261944514
C	0.792145864980	3.931741712637	0.035749805519
H	1.243140454690	2.182153026901	1.302194426888
H	2.441179995962	2.514861032539	0.015730598136
H	-0.303897860436	4.614835117377	-1.751688629532
H	1.330383608467	3.985691316302	-2.064899596971
H	-0.111687131603	4.081085506406	0.646108768277
H	1.503079858538	4.730323501231	0.278254805425
O	-0.504375609421	-0.005555433918	1.620435233668
C	-1.056547679930	-1.227295150286	2.141829207088
C	-1.308404910483	1.108667571616	2.036364323719
C	-2.084925574836	-0.805469503049	3.172617364734
H	-1.518676052404	-1.786384337622	1.308715156948
H	-0.234458219571	-1.830740658048	2.549894292670
C	-2.586854663367	0.512107872106	2.592931837648
H	-0.760648935913	1.674453439155	2.809512148982
H	-1.456994051741	1.767255007008	1.166552758617
H	-1.603744955007	-0.635754747331	4.147125039596
H	-2.875245104325	-1.553451126274	3.308012554176
H	-3.065142599223	1.163236160054	3.334156073342
H	-3.312646833156	0.324704865249	1.786384931200

PMe_4 cation (T_D, N_{imag} = 0)



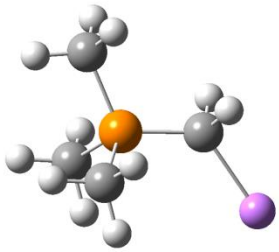
P	0.000000000000	0.000000000000	0.000000001765
C	-0.000000000887	0.000000000376	1.803964052264
H	-0.000000000573	1.033575823618	2.175060413187
H	-0.895102920917	-0.516787910699	2.175060413069
H	0.895102918280	-0.516787911560	2.175060413950
C	-0.000000000522	-1.700793617625	-0.601321348047
H	-0.895102920550	-2.222929258892	-0.237787819804
H	0.000000000016	-1.706141348044	-1.699484766333
H	0.895102918647	-2.222929259753	-0.237787818924
C	-1.472930478645	0.850396809333	-0.601321349303
H	-1.477561748523	1.886646497671	-0.237787820947
H	-1.477561748301	0.853070674201	-1.699484767593
H	-2.372664668867	0.336282763353	-0.237787821064
C	1.472930480054	0.850396807917	-0.601321347855
H	2.372664669424	0.336282761073	-0.237787818730
H	1.477561750793	0.853070672781	-1.699484766140
H	1.477561750571	1.886646496251	-0.237787819494

PMe_3CH_2 (C_S, N_{imag} = 0)



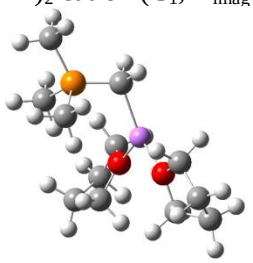
C	-1.854351753901	4.358906364102	-1.314242521914
H	-2.298909050556	5.355233824948	-1.199615352979
H	-2.118976506195	3.723378290472	-0.457967635513
H	-0.761587031896	4.467007594117	-1.355999849647
C	-4.245829949116	3.513882434357	-2.778255522542
H	-4.627317253359	3.099563590259	-3.721860525169
H	-4.557046481367	2.862985725299	-1.949633399045
H	-4.660754101225	4.520868371372	-2.646872669408
C	-1.929759400302	1.852430858563	-2.673800817400
H	-0.832444762839	1.794647226785	-2.652779496917
H	-2.336359189876	1.406680732181	-1.752743352931
H	-2.285762696610	1.281437420720	-3.542756606687
C	-1.970010930015	4.598671238882	-4.192570711195
H	-2.426505902066	4.342141482504	-5.153551700766
H	-0.912197812366	4.877209522517	-4.226198945781
P	-2.430141784658	3.628326696293	-2.881089088461

PMe_3CH_2Li cation (C_S, N_{imag} = 0)



C	-1.886446453984	4.396018731944	-4.295105114741
H	-2.351468592105	3.905022193418	-5.160286436350
H	-2.188593861552	5.452074162770	-4.281404467649
H	-0.794545452641	4.337782649523	-4.393168429415
C	-1.741489963644	4.405893038191	-1.355748595903
H	-2.168485809559	5.426943199478	-1.357171292905
H	-2.167718723228	3.893693150794	-0.472129405217
C	-4.237000713759	3.552263937826	-2.834588014535
H	-4.580130341551	3.029821517714	-3.738350558156
H	-4.625807064035	3.035159100014	-1.947072445372
H	-4.625508033396	4.579546184431	-2.839847199369
C	-1.886476920733	1.865328137221	-2.834220587107
H	-0.794540975897	1.809475639781	-2.933285648684
H	-2.188935298210	1.348994910802	-1.912975237188
H	-2.351234915796	1.361711932202	-3.692256581125
Li	0.227501292728	4.655767293673	-0.925044831240
P	-2.420802505442	3.595324068424	-2.759704150428

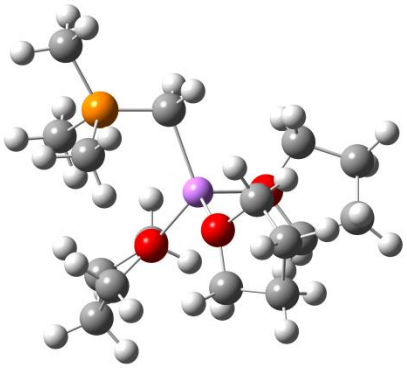
$PMe_3CH_2Li(THF)_2$ cation (C_1, N_{imag} = 0)



C	2.990716302531	0.285782559108	0.564796743952
H	3.641822119270	0.248397490994	1.447653360918
H	3.544012938598	0.747158151883	-0.264697973507
H	2.103204521118	0.895699991988	0.784063731266
C	1.359193238178	-1.305800319203	-1.255974324992
H	1.882399038985	-0.856278832614	-2.116596677293
H	1.056290250225	-2.330844373421	-1.526452644397
C	4.024161842779	-2.323955552516	-0.095137801630
H	4.626495094289	-2.275039327372	0.823136454851
H	3.790223860223	-3.373168500240	-0.320667823658

H	4.602556366267	-1.910367903327	-0.932248598866
C	1.654980326095	-2.112227824794	1.534180374201
H	0.784032001692	-1.504540476985	1.815583905315
H	1.315520148605	-3.127955602212	1.289586245408
H	2.351700619382	-2.165912558675	2.380875379645
P	2.467968470156	-1.385691727958	0.081673414343
Li	-0.326943664182	-0.135697784346	-0.825917392326
O	-1.959918791971	-0.836755061925	-0.135639219528
C	-3.143741505347	-0.086733735474	0.204778441796
C	-2.285430666648	-2.241921711947	-0.238746291090
C	-4.301410498295	-1.018689016750	-0.080721593051
H	-3.095966537287	0.181437541822	1.273692692500
H	-3.146091194434	0.834583518558	-0.394242712603
C	-3.702081725770	-2.371571856122	0.285314992454
H	-2.210627055714	-2.537815030677	-1.297472749055
H	-1.543018743816	-2.811043644492	0.337487443439
H	-4.564937840251	-0.988040116593	-1.148298887698
H	-5.195410748601	-0.765722098729	0.501397096467
H	-4.234128811042	-3.219630974273	-0.161400141034
H	-3.699645777448	-2.505993723841	1.377170681117
O	-0.207353854701	1.747653189214	-0.424252626742
C	0.479002547775	2.709730282898	-1.255091288068
C	-0.605181566587	2.366286898294	0.814846256931
C	0.270100379493	4.050588726277	-0.579812838344
H	1.545807333767	2.433045301570	-1.299070374655
H	0.061242313644	2.653060760160	-2.269096930206
C	0.185355791208	3.655854961236	0.890217372882
H	-1.690687003126	2.557202335048	0.784258490727
H	-0.397047585045	1.660250268819	1.632815783948
H	-0.675931986825	4.504084446141	-0.909925372699
H	1.080066168413	4.756794344852	-0.796258926904
H	-0.304343044681	4.409664248950	1.517746469113
H	1.190392569078	3.471487116673	1.299541317071

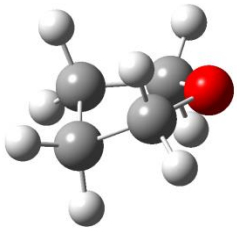
$PMe_3CH_2Li(THF)_3$ cation (C, N_{imag} = 1, -20.467)[20]



C	3.585315123013	0.304154142344	-1.067870321212
H	4.544710791747	0.710996880918	-0.723555677099
H	3.681589590928	0.003492928457	-2.119989786677
H	2.801784672976	1.068089218587	-0.989274362969
C	1.531184939738	-1.685372068932	-0.577817420531
H	1.559640703673	-1.908001323988	-1.656728967880
H	1.266987111926	-2.602353144105	-0.026647064485
C	4.544820579466	-2.257239810197	-0.168163415802
H	5.458150320762	-1.759473395280	0.188096875538
H	4.353562589011	-3.146800049933	0.447149702248
H	4.688391424776	-2.579292799685	-1.208354364369
C	3.065774619341	-0.605177528886	1.658771529850
H	4.036738976160	-0.187211781101	1.955161939937
H	2.274525926115	0.141725788345	1.806411108324
H	2.845462143392	-1.472241787390	2.296431868448
Li	0.036402549222	-0.198892372744	-0.159824283526
O	-1.569920196367	-0.540839258763	-1.227951843476
C	-1.814328877557	-1.808058008616	-1.873577379132
C	-2.819284249907	0.106241562510	-0.962712917514
C	-3.327369543635	-1.944192922559	-1.978045509170
H	-1.308326836256	-1.811661228931	-2.849199778636
H	-1.363998908997	-2.596773849537	-1.250849702527
C	-3.825419909187	-1.019223817877	-0.871643464792
H	-2.701197400372	0.698828410305	-0.044722240067
H	-3.065480598744	0.792111522709	-1.792422922125
H	-3.660102889529	-2.982387334518	-1.862589653654
H	-3.681184866751	-1.583647560505	-2.954741024503
H	-3.758971905683	-1.511754207570	0.111504241632
H	-4.858155241506	-0.681227378842	-1.018446473642
O	0.440440442412	1.700576013499	-0.476760593352
C	0.316361930810	2.158029632322	-1.839135860604
C	0.953852417064	2.756872936126	0.350786314898
C	1.065272182525	3.474389459382	-1.893764790795
H	0.723215530659	1.377237255393	-2.498734813095
H	-0.753646144505	2.282624315401	-2.070223953778
C	0.846270481967	4.016548506146	-0.485576418348
H	0.369930662171	2.786312989986	1.280980749230
H	2.004044857104	2.531730191126	0.609611884693
H	0.687974528979	4.137395632182	-2.681162872322
H	2.137011847212	3.303999809211	-2.078315260679
H	-0.160151220230	4.451075472412	-0.394208265504
H	1.575852569911	4.779759022808	-0.190537976671
O	-0.606553008582	-0.229954689191	1.715175490739
C	-1.086186899478	-1.525782034173	2.121555979726
C	-1.344238735446	0.796710680147	2.395928463583
C	-2.038393541235	-1.274657913106	3.275917586611
H	-1.596995673827	-1.990625366567	1.260526529297
H	-0.221890255167	-2.149278398913	2.388853501087
C	-2.577114195257	0.114029137862	2.951905756663
H	-0.715617772808	1.214281419016	3.200898462247
H	-1.562364640392	1.596410842387	1.672636917821
H	-1.489949602424	-1.257208573005	4.229091716855
H	-2.819290888689	-2.041255937912	3.347457298821
H	-2.989269612149	0.636654164691	3.823103162914
H	-3.364933881930	0.056502177179	2.185055454424
P	3.099630073549	-1.139127418628	-0.078630476645

2) Gaussian: M06/aug-cc-pVDZ/SMD(THF)

THF (IOp(2/15=3), N_{imag} = 0)

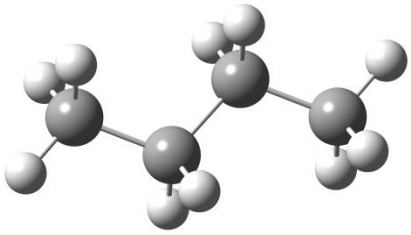


C	0.723945612051	0.985037513403	0.236285657953
C	-0.724169256599	0.984841460542	-0.236393150109
C	-1.159313188859	-0.420363451850	0.135427008944
C	1.159445149182	-0.420173118153	-0.135178633309
H	1.343155398817	1.758297401197	-0.237092708899
H	0.767458363317	1.124984106123	1.327786306510

[20] Apparently the potential energy surface is relatively flat for this molecule. Multiple minimal energy structures within 0.5 kcal mol^{-1} were obtained.

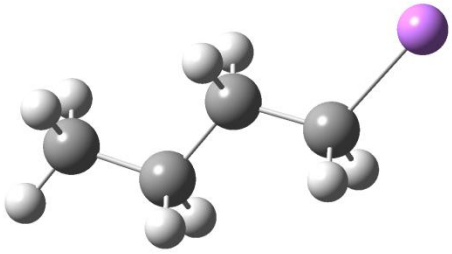
H	-0.767742256285	1.124484222687	-1.327931414393
H	-1.343526321975	1.758088451024	0.236814270272
H	-1.516364208533	-0.462061018751	1.181138590495
H	-1.954616374303	-0.820742361533	-0.511459464101
H	1.954511619252	-0.820323202101	0.512149155009
H	1.517003744742	-0.461982964226	-1.180703459401
O	0.000092719193	-1.244280038362	-0.000142158971

Bu (IOp(2/15=3), N_{imag} = 0)



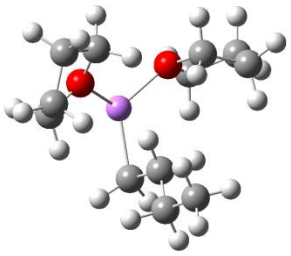
C	-2.504771088510	0.093674009111	0.003231222008
H	-2.160222721389	-0.952414597883	-0.029659986440
H	-2.157817592780	0.584553965710	-0.920163164545
H	-3.604443323642	0.082156232405	-0.018960323248
C	-1.970810647985	0.804506079661	1.232476980455
H	-2.353687616638	1.839864395247	1.262994384730
H	-2.353186338647	0.313466535664	2.144815054910
C	-0.452152932315	0.835065628588	1.283985112191
H	-0.069777235853	1.326104741185	0.371646802675
H	-0.069275972470	-0.200292700660	1.253468192342
C	0.081807508084	1.545898269302	2.513230542010
H	-0.265146836337	1.055019353339	3.436625168791
H	-0.262739993506	2.591987187005	2.546120722055
H	1.181479742798	1.557415164162	2.535422601852

BuLi (IOp(2/15=3), N_{imag} = 0)



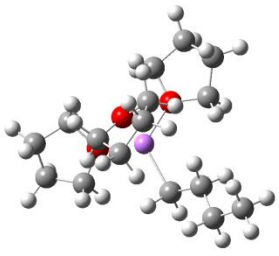
C	-2.524453405043	0.092340610104	-0.001698106983
H	-2.184743070851	-0.956099418440	-0.034612457844
H	-2.175913998899	0.578907155955	-0.927663218210
H	-3.625064165182	0.083427562408	-0.027231241359
C	-1.981679739468	0.803012513925	1.226359907264
H	-2.359312378670	1.841384897015	1.256619267227
H	-2.365224104029	0.315932705755	2.141567465908
C	-0.455455379955	0.835105845364	1.290383404091
H	-0.095144975243	1.303931728632	0.351376496308
H	-0.099027726006	-0.214097195807	1.233224623160
C	0.157814128525	1.537551727365	2.505592679081
H	-0.256504597694	1.049088365591	3.417829589410
H	-0.265781454005	2.567843450133	2.545438725134
Li	2.199749525850	1.638315216132	2.638244168462

$BuLi(THF)_2$ (IOp(2/15=3), N_{imag} = 0)



C	-0.068143149534	3.381555884189	-1.698589582802
H	-0.725713861306	2.635379612809	-2.175480851013
H	0.947295693560	3.227300390141	-2.098942170384
H	-0.405226304801	4.375844207170	-2.028697228215
C	-0.085854027635	3.234892513500	-0.187017117865
H	0.565228788186	3.995662327809	0.278909952393
H	-1.103350898832	3.429459117970	0.198546775557
C	0.354551680229	1.852030200891	0.291335867554
H	1.367158640904	1.660126321607	-0.119662592576
H	-0.298311129968	1.126735912246	-0.251712921990
C	0.358463425725	1.589755749749	1.801664066454
H	-0.536802516796	2.077271487136	2.246296740506
H	1.225589157439	2.119008818808	2.246515294631
Li	0.080368051567	-0.414418098153	1.368776940068
O	1.472648716237	-1.485046432485	0.502423476033
C	2.727671018321	-1.508939205028	1.212975092393
C	1.721266586582	-1.344205222820	-0.910466576000
C	3.781444020529	-1.769949919867	0.159420058170
H	2.877896511081	-0.530779818216	1.701882952194
H	2.666181102028	-2.284016077187	1.988958063550
C	3.198882884745	-1.034226340155	-1.040369477624
H	1.457505750543	-2.293161882127	-1.406242226260
H	1.072270925492	-0.548009973590	-1.303894297200
H	3.857764410229	-2.848096664199	-0.049315180959
H	4.769565426977	-1.401918471674	0.462088106382
H	3.608131607517	-1.366126349404	-2.002648756366
H	3.371175150575	0.048559090721	-0.942253541217
O	-1.681806671638	-0.901068347385	0.673567926573
C	-2.776809434043	-0.005269958518	0.960380652199
C	-1.874462667774	-1.500724355644	-0.619663775092
C	-3.544520035790	0.128921526695	-0.338309258030
H	-3.394928414686	-0.457319446487	1.753163567681
H	-2.361033342103	0.940072388274	1.336874881008
C	-3.322413472313	-1.238319096447	-0.973118066210
H	-1.198574536525	-1.016030648702	-1.345944172427
H	-1.610755766204	-2.564956780598	-0.548711806599
H	-3.102448225537	0.918531782917	-0.966083479124
H	-4.601651593784	0.370313756945	-0.172102288267
H	-3.495608372930	-1.254396621289	-2.056312458286
H	-3.974146576267	-1.990385619603	-0.502606498839

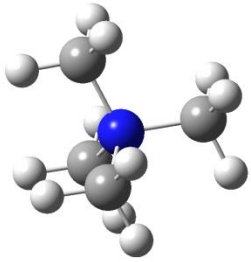
$BuLi(THF)_3$ (IOp(2/15=3), N_{imag} = 0)



C	1.513782619855	-1.023124162482	-1.261967989048
H	1.742376058389	-1.359830807768	-2.298253926490
H	1.306758554183	-1.971602218132	-0.710404784469

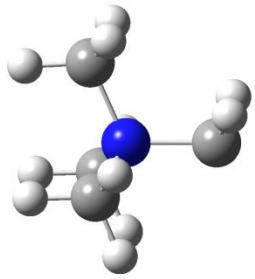
C	4.005127867315	-1.323597711613	-0.515100230098
H	3.709993545178	-2.208468550094	0.078095820965
H	4.292904055736	-1.709449981750	-1.509743581192
Li	-0.235100780716	0.070478844118	-0.780088444874
O	-2.007505276599	-0.774315333337	-1.186808074405
C	-2.053736215689	-2.076113926480	-1.794394122348
C	-3.254130097768	-0.494226847898	-0.534810452963
C	-3.510638137748	-2.492084312518	-1.752675904058
H	-1.637346543727	-2.000725490745	-2.808260123436
H	-1.419409145884	-2.766355995744	-1.212286119702
C	-3.985469453587	-1.819911917717	-0.469988404387
H	-3.039000661665	-0.051908535581	0.448305513686
H	-3.814537477977	0.242608279948	-1.136167943610
H	-3.632713038176	-3.582348036348	-1.749953953073
H	-4.051154179780	-2.082928863992	-2.620089632274
H	-3.655816573739	-2.396585281962	0.408512844999
H	-5.074159914706	-1.694264663712	-0.414123028666
O	-0.420568496390	2.005809167817	-1.172000408961
C	-1.528976859648	2.780719831667	-0.693031972295
C	0.743607839749	2.838197487668	-1.298332557826
C	-1.090366564552	4.228860238215	-0.794823276390
H	-2.409005794180	2.543404729525	-1.307715634718
H	-1.741150921866	2.491175210997	0.350613113072
C	0.410755623655	4.117256089048	-0.557224336210
H	1.607856887214	2.293408894265	-0.890414649511
H	0.930695964170	3.026781465551	-2.368961642898
H	-1.604413468819	4.872607496502	-0.070117390939
H	-1.287071075413	4.616921360900	-1.805817495522
H	0.621686420068	4.005213436755	0.517665015232
H	0.979795011542	4.976493681670	-0.933794405602
O	-0.525314329448	0.205187522617	1.245674648561
C	-0.584732063686	-1.082433207508	1.864837211466
C	0.426498444894	1.013748917413	1.954635343661
C	0.807368749674	-1.311866811984	2.411499044214
H	-1.339546260816	-1.073000186805	2.673100742156
H	-0.897314221046	-1.805670258116	1.099014969616
C	1.176469448002	0.083875171014	2.909473400586
H	1.089958990927	1.478434165656	1.209482743224
H	-0.105912926174	1.815740941026	2.490339686914
H	1.477513164154	-1.630636237493	1.599680079442
H	0.829492336140	-2.070522526776	3.203931009696
H	2.258563539559	0.269798639568	2.897142986574
H	0.821024152528	0.226041456849	3.940308474461
C	5.188879870571	-0.635811886030	0.143265755772
H	4.923451972479	-0.281281372437	1.153682257903
H	6.060467424317	-1.300287419372	0.246394979339
H	5.510181045941	0.244002562397	-0.438282892030
C	2.785981215511	-0.413706772204	-0.673698855834
H	3.099741381443	0.456916081671	-1.286177344103
H	2.580753416605	0.019498053740	0.329131806392

NMe_4 cation (IOp(2/15=3), N_{imag} = 0)



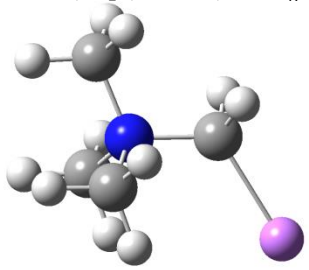
C	0.000000002047	0.000712344671	1.489640471278
H	0.000000001017	1.038078557342	1.841420015204
H	-0.898873647257	-0.519755363069	1.838907746706
H	0.898873653546	-0.519755360898	1.838907744393
C	0.000000001174	-1.403455643621	-0.496381530760
H	-0.898733234834	-1.906704791412	-0.123734605605
H	0.000000000459	-1.385731240833	-1.591938331524
H	0.898733238714	-1.906704789614	-0.123734606900
C	-1.215854323693	0.701804513256	-0.496453981147
H	-1.200852884512	1.732159578720	-0.124461201451
H	-1.202665683418	0.692343641805	-1.592052084485
H	-2.101333147242	0.175098579753	-0.123610259431
C	1.215854320525	0.701804516964	-0.496453984155
H	2.101333146621	0.175098585902	-0.123610265029
H	1.202665677684	0.692343645397	-1.592052087492
H	1.200852879101	1.732159582419	-0.124461204534
N	0.000000000068	0.000503639266	0.000068153072

NMe_3CH_2 (IOp(2/15=3), N_{imag} = 0)



C	-2.021386676070	4.239273502675	-1.495760340732
H	-2.433242320702	5.252677356761	-1.442565114577
H	-2.336674683475	3.646807802307	-0.626168794384
H	-0.926806077760	4.290370180319	-1.534218203574
C	-3.985275164630	3.545305425778	-2.699851111220
H	-4.342383260814	3.083928006390	-3.628235296646
H	-4.311664290400	2.948824829799	-1.837069722460
H	-4.368600069565	4.568602048397	-2.628676234670
C	-1.985477487245	2.207336782276	-2.786183901985
H	-0.890497636703	2.249271629883	-2.808046131167
H	-2.320681503821	1.638857559823	-1.905650736611
H	-2.353986225352	1.731170671631	-3.701772735222
N	-2.506791007889	3.600477478501	-2.739374142865
C	-2.077405666468	4.455026340177	-3.931083296188
H	-2.415627074512	3.863115244439	-4.806895610146
H	-0.971492123836	4.362313630649	-3.928409096769

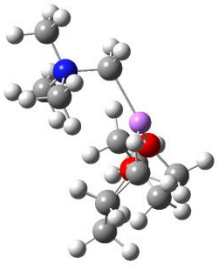
NMe_3CH_2Li cation (IOp(2/15=3), N_{imag} = 0)



C	0.226046234429	-0.835540555653	1.205903086971
H	1.177477067385	-1.382465836231	1.214883380802
H	0.152646034492	-0.198587071193	2.094847173133
H	-0.612242332921	-1.541061857764	1.183989924108
C	-1.158780457875	0.789131151698	-0.001287791894
H	-1.068559875140	1.462431613587	0.873212935904
H	-1.068188599474	1.460254733611	-0.877412209351
C	1.335680371096	0.932698568227	-0.000349193914
H	2.264817740479	0.346959270358	0.000284080670
H	1.289026883476	1.560229974441	-0.897353877140
H	1.288572856770	1.561437009096	0.895789991671
C	0.227138371474	-0.837767856325	-1.204342766151
H	-0.611647581243	-1.542692997510	-1.182343762249
H	0.155359906144	-0.202396458891	-2.094553464033
H	1.178256188579	-1.385273013601	-1.211053408133

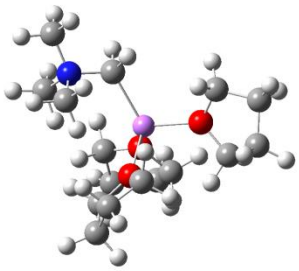
N	0.157527837978	0.022337854059	-0.000041191618
Li	-2.985768645650	-0.187210527908	0.000112091224

$NMe_3CH_2Li(THF)_2$ cation (IOp(2/15=3), N_{imag} = 0)



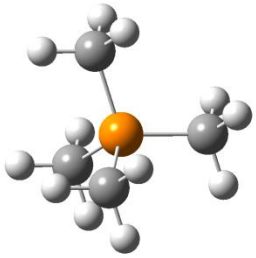
C	2.122899402878	-2.073448830479	-1.363904310968
H	2.751517004578	-2.068924957594	-2.263599155426
H	1.755880389478	-3.088034053117	-1.171698779517
H	1.278072534590	-1.387856514889	-1.494181480098
C	2.044076838328	-1.648940906011	1.052315910503
H	1.825662315351	-2.725359818635	1.194461083608
H	2.755442347080	-1.399959999284	1.863656316067
C	4.111453747724	-2.514948010545	-0.079477149773
H	4.713479412792	-2.467395714324	-0.997762144535
H	4.705739147312	-2.181214379282	0.778318221112
H	3.762802035724	-3.540169865023	0.088123868630
C	3.387253193027	-0.244009262874	-0.443710455464
H	2.508055338075	0.398798723648	-0.562262978598
H	3.976882103316	0.084952744702	0.419747642381
H	4.005591095414	-0.218192921764	-1.349908780176
Li	0.321733330600	-0.430192837818	1.013509750684
O	-1.426221516877	-1.023783250522	0.460794439241
C	-1.605044377328	-1.985687932789	-0.596299722193
C	-2.676949081844	-0.365697057573	0.741160167699
C	-3.103195071367	-2.144984558409	-0.744063220539
H	-1.150390239504	-1.586418837246	-1.519733927097
H	-1.079605567125	-2.908230153477	-0.313496775985
C	-3.598722670586	-0.746043314982	-0.398266750301
H	-3.055911137221	-0.731663174214	1.709293007917
H	-2.490031453972	0.714635335878	0.826571051958
H	-3.483357448826	-2.876327203875	-0.015027033924
H	-3.388872003816	-2.474908143382	-1.750357038945
H	-4.654984454497	-0.715615057496	-0.104169104772
H	-3.456139254174	-0.067561023071	-1.253453661829
O	0.375517269301	1.401214457713	0.371283980683
C	1.196439179412	2.480041094279	0.857408562797
C	-0.139976437540	1.724727955425	-0.933952399868
C	1.477651248995	3.345677528284	-0.352082885673
H	0.634918855576	3.032458320004	1.628692724129
H	2.093375275872	2.046730319924	1.323312290251
C	0.188255234836	3.188655278993	-1.149470070832
H	0.359888511399	1.083415823311	-1.680905180080
H	-1.216644136276	1.504082578722	-0.949244140666
H	2.333638384709	2.950020706476	-0.920392468092
H	1.696637046835	4.384470678997	-0.076598657900
H	0.295367859774	3.437174373882	-2.212268658202
H	-0.602670793420	3.822909403291	-0.722022311320
N	2.922553101396	-1.629436584854	-0.199328574888

$NMe_3CH_2Li(THF)_3$ cation (IOp(2/15=3), N_{imag} = 0)



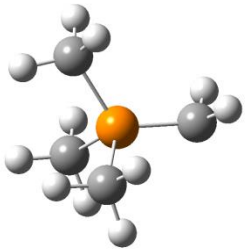
C	3.492988854146	0.588567234799	-0.626440289789
H	4.479610885335	0.599754785340	-0.145781093524
H	3.555808786113	1.055401358782	-1.615998611315
H	2.765878247360	1.122908614912	-0.005605871362
C	1.679550790051	-0.816507107467	-1.497154538641
H	1.921138975980	-0.440747575609	-2.511159211942
H	1.481790148679	-1.897110751663	-1.642911598115
C	4.082945814875	-1.565422328141	-1.526552453244
H	5.029824321033	-1.546261681649	-0.968325117677
H	3.740523082933	-2.598905856747	-1.649357116112
H	4.217272079166	-1.100614717038	-2.509800690887
C	2.875982426016	-1.411060126813	0.554876219397
H	2.119578219580	-0.833784146523	1.096196098149
H	2.540176663998	-2.448060765157	0.438417552768
H	3.835223505947	-1.386623353096	1.087549767327
N	3.036533061813	-0.809876490252	-0.788694752994
Li	-0.007451709607	0.169618735355	-0.596625508171
O	-1.687773763990	-0.739412244932	-1.063690834010
C	-1.684129886576	-2.015086192798	-1.729613529194
C	-2.958739044215	-0.525646688551	-0.428901181994
C	-3.127770367645	-2.473925273356	-1.734424337240
H	-1.251829750124	-1.882002829873	-2.731216665492
H	-1.043655471128	-2.711526102283	-1.161719400324
C	-3.642860291791	-1.876515863370	-0.430932651132
H	-2.779376533914	-0.112799414381	0.573904855799
H	-3.531161579575	0.213749178148	-1.014963443968
H	-3.217234237094	-3.565993383809	-1.784813006788
H	-3.665254298268	-2.039648291025	-2.591135887194
H	-3.304250333600	-2.479863341644	0.426115444331
H	-4.735630143700	-1.791058515897	-0.386395967850
O	-0.301306211143	2.122614421673	-0.899368350552
C	-1.600240594194	2.726096867610	-0.818839150922
C	0.712905191144	3.137050469166	-0.811378439447
C	-1.381054733765	4.181700676317	-1.168810284477
H	-2.266395629721	2.192684069646	-1.510297344215
H	-1.993011497676	2.617505309917	0.208240867422
C	-0.018384169008	4.439567555542	-0.538134625489
H	1.420242099936	2.865586704495	-0.013453260150
H	1.259390637030	3.163015567804	-1.768318141569
H	-2.173926782579	4.831466224047	-0.778179799880
H	-1.331623015294	4.306130391580	-2.261169718377
H	-0.127914470834	4.598839921906	0.545432969034
H	0.505754275538	5.305484588107	-0.960818954175
O	-0.168767302541	0.149738290507	1.375584587282
C	-0.491486372786	-1.046945246240	2.100415668436
C	0.382150324498	1.132577981062	2.264849255179
C	0.245108411396	-0.927971847409	3.418114061079
H	-1.583811724337	-1.089671866660	2.254097408015
H	-0.191451917636	-1.911651126897	1.489975692926
C	0.187830686870	0.575822262923	3.663169615274
H	1.452469694286	1.267607615876	2.025940763267
H	-0.134903670449	2.087953200055	2.094595078192
H	1.287881746230	-1.263579294534	3.306779067583
H	-0.225234123843	-1.518686005939	4.213656737265
H	0.949318074578	0.937136781583	4.364897558202
H	-0.802288187499	0.858882452599	4.050840881283

PMe_4 cation (IOp(2/15=3), N_{imag} = 0)



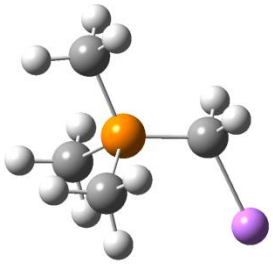
P	-0.000000000020	-0.000238457859	0.001099176125
C	-0.000000000943	0.000480521989	1.799480624752
H	-0.000000000748	1.036225028758	2.163777665384
H	-0.896665707473	-0.517377897189	2.164988311510
H	0.896665704888	-0.517377897791	2.164988312331
C	-0.000000000540	-1.695136145036	-0.601452803922
H	-0.896122628355	-2.212909531009	-0.234616112782
H	-0.000000000518	-1.693663252895	-1.699616040609
H	0.896122626971	-2.212909531506	-0.234616112723
C	-1.467889475741	0.847483021183	-0.598452663821
H	-1.466219956629	1.883455929743	-0.234696749460
H	-1.466689205859	0.844943811471	-1.696753899383
H	-2.364659439838	0.330570822313	-0.232113185968
C	1.467889477197	0.847483019675	-0.598452662243
H	2.364659440406	0.330570819923	-0.232113183483
H	1.466689208461	0.844943809993	-1.696753897815
H	1.466219958740	1.883455928237	-0.234696747894

PMe_3CH_2 (IOp(2/15=3), N_{imag} = 0)



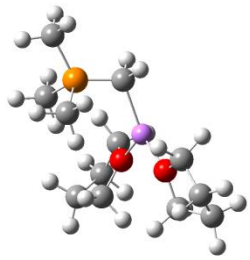
C	1.378716760442	-0.474676346450	0.993674240249
H	1.619237813039	0.295679475568	1.738077870541
H	1.091209095637	-1.405502728208	1.501827729132
H	2.269970661534	-0.662885468097	0.378135366587
C	-1.418786260741	0.353914421577	0.989541515229
H	-2.249547884218	0.741265586434	0.382554507528
H	-1.723792342339	-0.596385094088	1.449336514817
H	-1.182594591632	1.085967614772	1.773020757659
C	-0.406447045141	-1.376366306010	-1.052619024951
H	0.433348907222	-1.631542601727	-1.714752884128
H	-0.634221673338	-2.236891430227	-0.405471581611
H	-1.283662901135	-1.148701211178	-1.675412781906
C	0.472828867962	1.592108340510	-0.834371990810
H	-0.351444205449	2.015021692170	-1.428103140515
H	1.402978824193	1.496365713678	-1.414788275451
P	0.032697105125	0.112653071742	-0.071111578945

PMe_3CH_2Li cation (IOp(2/15=3), N_{imag} = 0)



C	-1.882874708330	4.408352627598	-4.262096998683
H	-2.308436899272	3.900750894454	-5.138304446730
H	-2.211339776674	5.457003942826	-4.259323042846
H	-0.786427782338	4.376877931903	-4.320778559042
C	-1.770460388915	4.412017050925	-1.340210424003
H	-2.164902069412	5.444843606706	-1.341592088150
H	-2.167124319047	3.901575377939	-0.443664187327
C	-4.251409249490	3.540448579593	-2.859087430933
H	-4.569338560669	3.018674903885	-3.772956864166
H	-4.649939956574	3.013055437598	-1.981191413420
H	-4.647053169228	4.565573858331	-2.866327480231
C	-1.887894343880	1.881338813144	-2.809841068727
H	-0.794392061259	1.842401261042	-2.905117374907
H	-2.187695964357	1.366406543461	-1.886391016465
H	-2.346832386475	1.371965090085	-3.668169647799
Li	0.283033456111	4.545970464678	-1.136565843643
P	-2.438596137703	3.603387560352	-2.740639567606

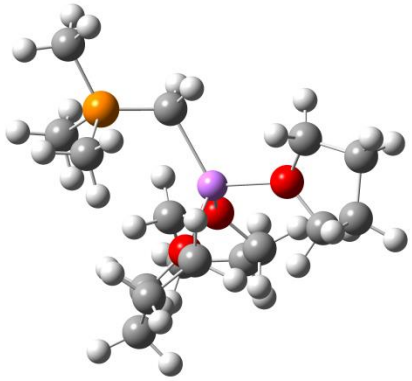
$PMe_3CH_2Li(THF)_2$ cation (IOp(2/15=3), N_{imag} = 0)



C	1.630008710884	-2.149887957510	-1.476046323258
H	2.246836557023	-2.220312505509	-2.382211893964
H	1.268880192345	-3.153385146037	-1.211502610474
H	0.768937768316	-1.496480005814	-1.674872106380
C	1.655339649568	-1.448048326837	1.354840264899
H	1.385282619095	-2.486053466907	1.615244680680
H	2.277296052541	-1.029519865169	2.165427189107
C	4.157062375014	-2.427113427195	-0.115274922068
H	4.669870040450	-2.338085310253	-1.083859498361
H	4.813623370589	-2.049702585587	0.681243718241
H	3.934232989053	-3.484632613584	0.084836658815
C	3.072853816240	0.202477317998	-0.590804238669
H	2.161977211536	0.797843594059	-0.734639422749
H	3.684878833600	0.661108599272	0.198014020985
H	3.647816239348	0.183850031092	-1.526045133784
Li	-0.074724554227	-0.262061115238	1.169408855174
O	-1.800782102894	-0.861630758592	0.561397333247
C	-2.003631415092	-1.770698931466	-0.537439110910
C	-3.050358018991	-0.233323355176	0.913351818805
C	-3.503954518295	-1.937473546125	-0.648444253897
H	-1.582700761770	-1.320724353589	-1.453215509245
H	-1.464028489185	-2.702502698052	-0.318041399375
C	-4.000424512092	-0.562671085856	-0.218443714569
H	-3.396840614621	-0.655959596974	1.870449821212
H	-2.871974490105	0.842971206511	1.051757642703

H	-3.855783843727	-2.707916350554	0.054016108234
H	-3.815523644645	-2.220032631594	-1.661359292925
H	-5.048121655815	-0.557346299779	0.105942632458
H	-3.887095626806	0.160283283112	-1.041115157330
O	0.010072582515	1.567675340926	0.542101267871
C	0.869040379304	2.619887317799	1.023542450036
C	-0.542947431823	1.928452569722	-0.737901290783
C	1.107065295741	3.522909249865	-0.168247792610
H	0.351755863935	3.151761964902	1.838665195102
H	1.781331193926	2.159476702925	1.429804215646
C	-0.211318913013	3.395528494082	-0.923055360707
H	-0.070996134415	1.303959756323	-1.516771609423
H	-1.620859998303	1.713895417125	-0.724665737304
H	1.941759146214	3.144346443896	-0.778632857102
H	1.338446870239	4.551928584821	0.132539534667
H	-0.139753386417	3.674005024373	-1.981448898395
H	-0.982390504551	4.021893411234	-0.450203419923
P	2.603908829311	-1.477220626640	-0.105772863678

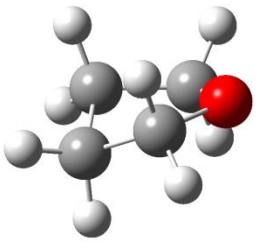
$PMe_3CH_2Li(THF)_3$ cation (IOp(2/15=3), N_{imag} = 0)



C	3.878523639584	0.912077091528	-0.545646678030
H	4.875881959177	0.838640586227	-0.091561955859
H	3.964287457400	1.428989485557	-1.511387274313
H	3.225192867728	1.493289944812	0.118232774885
C	1.666625448524	-0.682222034418	-1.617745597630
H	1.788746156351	-0.129290826795	-2.564486599630
H	1.356003784099	-1.716861326656	-1.844273705721
C	4.555460018304	-1.690398726830	-1.569844714201
H	5.461248634585	-1.676067938859	-0.946321529152
H	4.230809708793	-2.730417000901	-1.715615387750
H	4.781875198832	-1.253349250248	-2.552756337337
C	3.003109964630	-1.481732250834	0.846222699815
H	2.348525934432	-0.837440025484	1.447183661323
H	2.543981141989	-2.475839632501	0.751160848525
H	3.976170062550	-1.584082388728	1.344592278917
Li	-0.025564742931	0.159093497368	-0.598953048206
O	-1.684883068277	-0.783574462818	-1.052398429901
C	-1.699252066148	-2.081988365356	-1.673921818127
C	-2.955157357206	-0.527778686313	-0.430820354054
C	-3.145170579681	-2.534196108836	-1.640824050457
H	-1.286839463379	-1.987554817772	-2.687968999637
H	-1.051837015542	-2.761283230166	-1.093137478366
C	-3.647511944351	-1.872089357877	-0.363969670681
H	-2.773319491106	-0.066412358282	0.550199335213
H	-3.521312393696	0.185544800920	-1.053973395875
H	-3.238484958022	-3.627040413479	-1.636493137167
H	-3.689246530994	-2.141532548520	-2.513180155669
H	-3.305847885138	-2.434732691773	0.519134686596
H	-4.739350298093	-1.777817849230	-0.316496617159
O	-0.321401951260	2.077523042842	-0.941413720291
C	-1.600095135833	2.719621697273	-0.846838693493
C	0.725622932542	3.050552426926	-0.790732623776
C	-1.328811350152	4.175527919112	-1.154667855292
H	-2.279283252725	2.225357878148	-1.554481998010
H	-1.999944461967	2.595845647258	0.175938888473
C	0.032354913427	4.370403032794	-0.497807361149
H	1.396468649389	2.730005409428	0.020816582533
H	1.302160121048	3.082500730133	-1.729508750089
H	-2.105019510748	4.841003160225	-0.757197171327
H	-1.259943930574	4.326260811136	-2.242650295542
H	-0.089752154312	4.506078097019	0.587671460239
H	0.591494481492	5.228621454313	-0.889932373910
O	-0.120318912403	0.118353412667	1.364849227282
C	-0.484781074852	-1.071244074845	2.083029820464
C	0.383656336087	1.109904312277	2.271817955215
C	0.145397822289	-0.924996951217	3.452697711863
H	-1.585095825134	-1.124494198186	2.150991579770
H	-0.126599441330	-1.941162483440	1.513125476093
C	0.077937886219	0.584015086283	3.661259630660
H	1.470582776031	1.223098476359	2.109162494711
H	-0.103273177068	2.069472610093	2.044863270764
H	1.191058785128	-1.268885080012	3.434280415092
H	-0.391406311063	-1.495161284688	4.220672400231
H	0.784709436920	0.956773494637	4.412533414990
H	-0.938120867324	0.879602961511	3.963343435533
P	3.197824493759	-0.747107001779	-0.798884461386

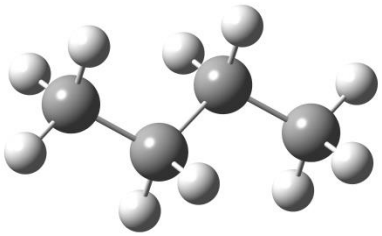
3) Gaussian: M06/aug-cc-pVTZ

THF (IOp(2/15=3), N_{imag} = 0)



C	0.721797307135	0.983939070857	0.237256879323
C	-0.722037310756	0.983757522508	-0.237359799276
C	-1.151769596213	-0.420919903119	0.136097490120
C	1.151851826091	-0.420752851450	-0.135851234786
H	1.338222036819	1.753220010852	-0.225484431278
H	0.761705537722	1.118775491453	1.321074287606
H	-0.761996877096	1.118295876517	-1.321212879395
H	-1.338592772595	1.753036675665	0.225211241462
H	-1.505726797094	-0.456735346746	1.175082593644
H	-1.944150280086	-0.817911683459	-0.502097958464
H	1.944018233508	-0.817518961053	0.502760306562
H	1.506275912495	-0.456693283269	-1.174663186376
O	0.000063903896	-1.234685618938	-0.000113309142

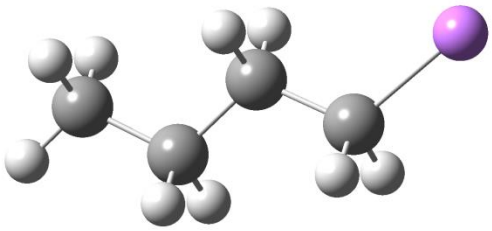
Bu (C_{2H}, N_{imag} = 0)



C	-2.501755065168	0.096428900642	0.008000829985

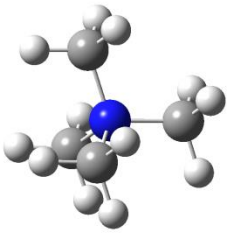
H	-2.154510252829	-0.938948521373	-0.024761930941
H	-2.154351754825	0.583843571359	-0.905999521739
H	-3.591714687570	0.081581015167	-0.017852582599
C	-1.969089965936	0.806138738508	1.234486135286
H	-2.346499155672	1.834254108713	1.266556633645
H	-2.346656583190	0.321746862859	2.141842398367
C	-0.453873612799	0.833455706414	1.281962799841
H	-0.076306995545	1.317847582064	0.374606536760
H	-0.076464423063	-0.194659663790	1.249892301482
C	0.078791486433	1.543165544281	2.508448105142
H	-0.268611823910	1.055750873563	3.422448456866
H	-0.268453325906	2.578542966296	2.541210866068
H	1.168751108835	1.558013429756	2.534301517726

BuLi (C_S, N_{imag} = 0)



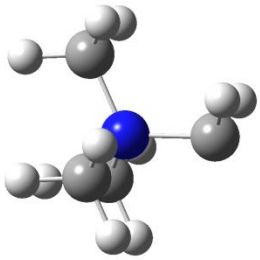
C	-2.518883801177	0.096267825130	0.007721848462
H	-2.174141230164	-0.940770247274	-0.028227849860
H	-2.173943643685	0.581732450743	-0.909299508826
H	-3.610048632109	0.082784661078	-0.015821926727
C	-1.972571759326	0.804163148511	1.231096216103
H	-2.342404156794	1.835184981209	1.268245629536
H	-2.342600437856	0.322741170848	2.143496214525
C	-0.451171994601	0.831719153632	1.279054517492
H	-0.097335928737	1.299793209577	0.348123624935
H	-0.097531699164	-0.208715900035	1.221097200287
C	0.148179772799	1.534108828304	2.492926950759
H	-0.256712316803	1.054479650611	3.398657235609
H	-0.256517133937	2.558461307103	2.528303695437
Li	2.114956752963	1.624762036701	2.650017876905

NMe_4 cation (T_D, N_{imag} = 0)



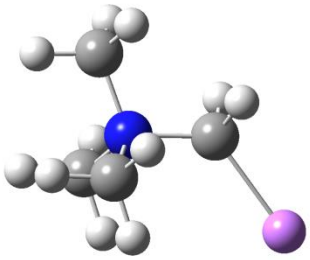
C	0.000000001870	0.000000002337	1.492116287730
H	0.000000000891	1.029499808740	1.843355426092
H	-0.891572981993	-0.514749901187	1.843355429868
H	0.891572988032	-0.514749898729	1.843355427634
C	0.000000001316	-1.406780728911	-0.497372094418
H	-0.891572982542	-1.909515467549	-0.129140943206
H	-0.000000000063	-1.394765565927	-1.585073533031
H	0.891572987483	-1.909515465090	-0.129140945441
C	-1.218307849441	0.703390361142	-0.497372096525
H	-1.207902412394	1.726882585161	-0.129140949071
H	-1.207902412799	0.697382776855	-1.585073535120
H	-2.099475395278	0.182632875234	-0.129140945295
C	1.218307846255	0.703390364502	-0.497372099578
H	2.099475394451	0.182632881023	-0.129140950557
H	1.207902406904	0.697382780186	-1.585073538147
H	1.207902407309	1.726882588492	-0.129140952099
N	0.000000000000	-0.000000000233	-0.000000000698

NMe_3CH_2 (C_S, N_{imag} = 0)



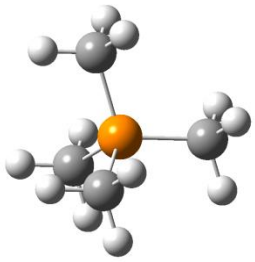
C	-2.019069858603	4.233309529960	-1.500400708821
H	-2.413069861132	5.245708021829	-1.484039369540
H	-2.337442576541	3.664654707726	-0.624030670796
H	-0.932566618741	4.277618803187	-1.542485177215
C	-3.979719587209	3.540647149265	-2.700780600252
H	-4.328748453320	3.077808678772	-3.621749169346
H	-4.321133576996	2.963852258980	-1.838517252982
H	-4.338616814643	4.565446821932	-2.662928086519
C	-1.987085413469	2.188901750034	-2.774202571435
H	-0.901092925652	2.235573387985	-2.802360057723
H	-2.316949577136	1.613046217311	-1.903127043874
H	-2.348428425232	1.724255717023	-3.688470618167
N	-2.504699345782	3.583171838203	-2.733297873131
C	-2.091078403767	4.463214485356	-3.916705086914
H	-2.435594198016	3.898247004866	-4.795162550550
H	-0.992673047942	4.408005165329	-3.911754612763

NMe_3CH_2Li cation (C_S, N_{imag} = 0)



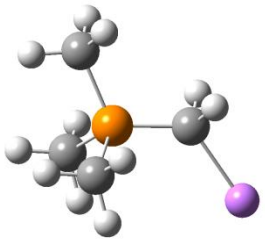
C	-1.978200754146	4.238384095184	-4.062252278923
H	-2.406692356996	3.745010091335	-4.933580022614
H	-2.302079880547	5.276220515981	-4.028137975246
H	-0.892739418394	4.193307746856	-4.106581867073
C	-1.859835739016	4.258850142704	-1.610765661648
H	-2.328656686108	5.250490262285	-1.631500064200
H	-2.328604504199	3.745091902663	-0.762307312379
C	-3.927382398097	3.566261169298	-2.810200237010
H	-4.313718163561	3.056698281239	-3.692714948214
H	-4.264995127364	3.060788347574	-1.908853603381
H	-4.265032562718	4.599575085831	-2.797330774534
C	-1.978149193963	2.145960684816	-2.854115212730
H	-0.892688628020	2.130145540701	-2.915339135819
H	-2.301990864522	1.656623622425	-1.938232108040
H	-2.406640077234	1.637993252882	-3.717017106564
N	-2.435294493525	3.556123411500	-2.827822084455
Li	0.101016550435	4.533273330093	-1.135595753257

PMe_4 cation (T_D, N_{imag} = 0)



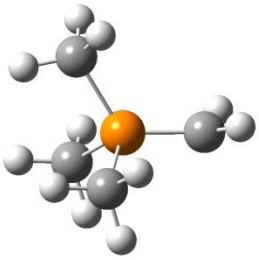
P	0.000000000000	0.000000000000	0.000000001765
C	-0.000000000881	0.000000000373	1.792210439007
H	-0.000000000569	1.025849244275	2.160172369499
H	-0.888411506914	-0.512924621035	2.160172369383
H	0.888411504296	-0.512924621889	2.160172370257
C	-0.000000000518	-1.689712204774	-0.597403476964
H	-0.888411506550	-2.207604913471	-0.236467483006
H	0.000000000015	-1.694680292287	-1.687237396243
H	0.888411504660	-2.207604914324	-0.236467482132
C	-1.463333693611	0.844856102904	-0.597403478212
H	-1.467636183093	1.873189390449	-0.236467484141
H	-1.467636182872	0.847340146322	-1.687237397494
H	-2.356047689437	0.334415525139	-0.236467484258
C	1.463333695011	0.844856101497	-0.597403476772
H	2.356047689991	0.334415522874	-0.236467481940
H	1.467636185346	0.847340144911	-1.687237396051
H	1.467636185126	1.873189389038	-0.236467482698

PMe_3CH_2Li cation (C_S, N_{imag} = 0)



C	-1.890851336646	4.393225301624	-4.284662002940
H	-2.353772331556	3.908135721047	-5.143654553402
H	-2.189327253908	5.441500841059	-4.267613980567
H	-0.807440999938	4.333125281361	-4.380976909271
C	-1.752269582113	4.398205985299	-1.369327711470
H	-2.152819088105	5.418864839368	-1.366597610882
H	-2.152790341577	3.890233102540	-0.484037630080
C	-4.227701484631	3.550149354435	-2.838117537307
H	-4.562872621271	3.031368661385	-3.736657029345
H	-4.614933061860	3.035311396897	-1.959128112607
H	-4.614961899433	4.568784555976	-2.844483302633
C	-1.890803997964	1.875933071664	-2.831296009926
H	-0.807393788551	1.822602090163	-2.931519040481
H	-2.189250622922	1.366554532594	-1.914931873343
H	-2.353724686508	1.374552068724	-3.680882660287
Li	0.201929150109	4.646885674412	-0.938667476561
P	-2.422697624987	3.595322842602	-2.759933910605

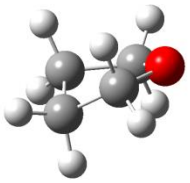
PMe_3CH_2 (C_S, N_{imag} = 0)



C	-1.852867030976	4.353575648401	-1.322759771370
H	-2.291610760067	5.342731464276	-1.206970014750
H	-2.113588120372	3.723145720211	-0.472491828679
H	-0.768416515978	4.456689951256	-1.369665664019
C	-4.236900287178	3.511154523605	-2.782228205088
H	-4.609035984521	3.099586668771	-3.720840227090
H	-4.547009181805	2.863260050466	-1.962204976398
H	-4.651195430395	4.508947394198	-2.651455275706
C	-1.936121434450	1.862661721440	-2.668992185876
H	-0.847642947031	1.804709991235	-2.646207506131
H	-2.341851613154	1.425518138205	-1.753899204445
H	-2.290602144748	1.294825379462	-3.529554981220
C	-1.960349488630	4.558144589893	-4.185285348480
H	-2.439230062843	4.359417972199	-5.136032852399
H	-0.930679052898	4.892474023300	-4.212529948139
P	-2.430917670573	3.626505815793	-2.878858837410

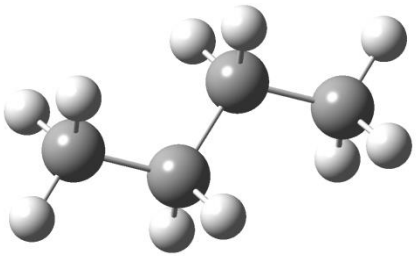
4) Gaussian: M06/aug-cc-pVTZ/SMD(THF)

THF (IOp(2/15=3), N_{imag} = 0)



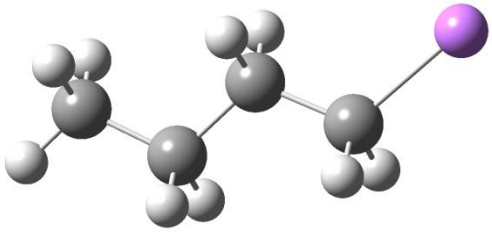
C	0.721143950421	0.982594628206	0.238877735711
C	-0.721363469207	0.982398332312	-0.238979920688
C	-1.153852973402	-0.418337081874	0.136740062561
C	1.153982226722	-0.418146944345	-0.136491896586
H	1.338493121562	1.751721346186	-0.223005815723
H	0.758716124789	1.114606436090	1.323262081160
H	-0.758989632181	1.114111096119	-1.323400101531
H	-1.338858989158	1.751511987875	0.222730498232
H	-1.505382404758	-0.453124514995	1.176363080656
H	-1.948370119767	-0.815261338783	-0.499372897439
H	1.948290788904	-0.814839166971	0.500034984216
H	1.505977648589	-0.453048856318	-1.175944571460
O	0.000094727484	-1.238378923504	-0.000113239109

Bu (IOp(2/15=3), N_{imag} = 0)



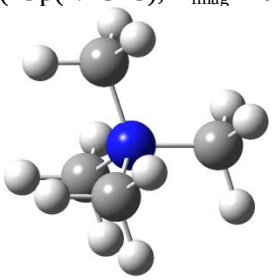
C	-2.501411194091	0.096237856701	0.007624653131
H	-2.157380096795	-0.940933880751	-0.025084941972
H	-2.155269938124	0.582969998692	-0.907969817203
H	-3.592353809235	0.082984787206	-0.017238969114
C	-1.969084021286	0.805447004117	1.233996326965
H	-2.347561472699	1.833426834409	1.264755896931
H	-2.347193115754	0.318453747563	2.140080073866
C	-0.453879557944	0.834124515628	1.282465874987
H	-0.075770464520	1.321117769880	0.376382126491
H	-0.075402107387	-0.193855314962	1.251706304593
C	0.078447616310	1.543333664638	2.508837547302
H	-0.267693638618	1.056601523369	3.424432018414
H	-0.265583480903	2.580505402171	2.541547142034
H	1.169390231473	1.556586734175	2.533701168257

BuLi (IOp(2/15=3), N_{imag} = 0)



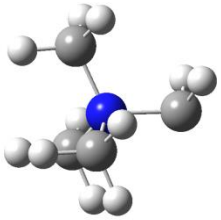
C	-2.521904046303	0.094291317244	0.001361171345
H	-2.181328582881	-0.944747602410	-0.031003585350
H	-2.172887539543	0.577479568011	-0.915844418419
H	-3.613625662873	0.082787808014	-0.028237821397
C	-1.983019443475	0.803293178547	1.227282075421
H	-2.356900662694	1.833894320586	1.257849408205
H	-2.362903640938	0.320009363979	2.135683654963
C	-0.460488584351	0.834026582824	1.289207693823
H	-0.102707905377	1.299004739615	0.357506789145
H	-0.106756827382	-0.207007545036	1.232653518465
C	0.152881042092	1.533675158017	2.499107858291
H	-0.248037948080	1.050217210884	3.407955827573
H	-0.256491571287	2.559036673707	2.540275251421
Li	2.183430030827	1.640684384238	2.641633867944

NMe_4 cation (IOp(2/15=3), N_{imag} = 0)



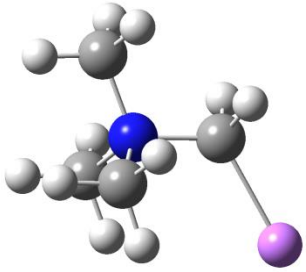
C	0.000000001953	0.000688337870	1.487879607288
H	0.000000001905	1.030509906347	1.836929304517
H	-0.892350038195	-0.515973748987	1.834583111893
H	0.892350043468	-0.515973748259	1.834583109552
C	0.000000001155	-1.401815586039	-0.495963355226
H	-0.892264587625	-1.901191223098	-0.125953266610
H	-0.000000000416	-1.383959734393	-1.583549940602
H	0.892264591996	-1.901191221366	-0.125953269197
C	-1.214487097683	0.700958389893	-0.495802753250
H	-1.199671928173	1.723906131749	-0.126719415751
H	-1.201371447918	0.691262832017	-1.583404647949
H	-2.093364363315	0.178073602069	-0.125380410376
C	1.214487094646	0.700958393655	-0.495802756482
H	2.093364362926	0.178073609698	-0.125380414502
H	1.201371443124	0.691262834450	-1.583404651154
H	1.199671922004	1.723906135963	-0.126719420293
N	0.000000000147	0.000505084478	0.000059156281

NMe_3CH_2 (IOp(2/15=3), N_{imag} = 0)



C	-2.020744639733	4.237581566872	-1.498044627028
H	-2.428523836961	5.243917639884	-1.447105859983
H	-2.335698281515	3.650405420744	-0.634955273337
H	-0.934123117285	4.286549182706	-1.535329989031
C	-3.982819241894	3.544364670242	-2.700973183515
H	-4.337216793314	3.083475968956	-3.621106913700
H	-4.306606005635	2.955070564380	-1.842539989734
H	-4.362194847971	4.560648183341	-2.633534826482
C	-1.986158298869	2.206209804883	-2.784559095292
H	-0.899296357526	2.247012341981	-2.805227439603
H	-2.320921774555	1.644808821346	-1.909652100306
H	-2.352279359325	1.732895683702	-3.692806580501
N	-2.505932430570	3.598863136611	-2.739795958312
C	-2.076530460509	4.447895588257	-3.928500742915
H	-2.418925138955	3.872827222397	-4.800630908294
H	-0.979936401579	4.370862472849	-3.925145350599

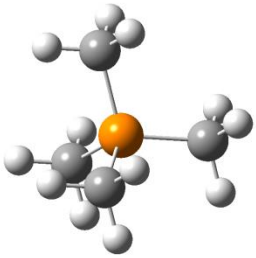
NMe_3CH_2Li cation (IOp(2/15=3), N_{imag} = 0)



C	0.262293033202	-0.537459256147	1.265549387098
H	1.187565198561	-1.109712176412	1.322966049495
H	0.219955853276	0.183677638726	2.079362784111
H	-0.596205888944	-1.203299589927	1.319511459588
C	-1.090908150247	0.969532745586	-0.105247748674
H	-1.022700209512	1.698945333587	0.712178746958
H	-0.989731002120	1.558078772376	-1.026297704304
C	1.401182516671	1.087161183377	-0.098710218679
H	2.315471346764	0.497242519622	-0.029667535210
H	1.369869029787	1.616909169089	-1.048021616994

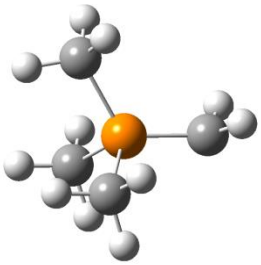
H	1.353054784792	1.798901613433	0.722319895727
C	0.280266684784	-0.775825919574	-1.132949295055
H	-0.557551119156	-1.464556603680	-1.047669345053
H	0.216016801075	-0.231691998468	-2.072977385356
H	1.221427867370	-1.322387553609	-1.083895813163
N	0.213389829530	0.196069144228	-0.018579229920
Li	-2.901252555834	-0.008645812206	-0.075674030570

PMe_4 cation (IOp(2/15=3), N_{imag} = 0)



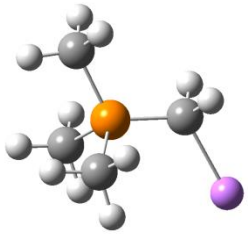
P	-0.000000001231	-0.000139957915	0.001126339237
C	-0.000000001946	0.000301168662	1.788379438403
H	-0.000000009720	1.028206222738	2.150070168219
H	-0.889958114753	-0.513792663716	2.150884240926
H	0.889958121703	-0.513792645401	2.150884239552
C	-0.000000000126	-1.684426743247	-0.597540798133
H	-0.889532082705	-2.198073715846	-0.233558310112
H	0.000000001850	-1.682545346168	-1.687469999630
H	0.889532081132	-2.198073716094	-0.233558306917
C	-1.458874530595	0.842231825477	-0.594786855480
H	-1.457091749964	1.870536984940	-0.234103989745
H	-1.457592010047	0.839237105552	-1.684836430508
H	-2.348740419792	0.329162794788	-0.230881217962
C	1.458874531480	0.842231820260	-0.594786854184
H	2.348740418427	0.329162785322	-0.230881217046
H	1.457592011261	0.839237101416	-1.684836429277
H	1.457091755027	1.870536979233	-0.234103987344

PMe_3CH_2 (IOp(2/15=3), N_{imag} = 0)



C	1.373501111715	-0.474751954531	0.983261704616
H	1.602869473108	0.282454063111	1.732116971599
H	1.096270165692	-1.408054088169	1.474190434582
H	2.259843661996	-0.644247885220	0.370161463929
C	-1.413179294895	0.354684531558	0.978930342188
H	-2.236149045442	0.732458896891	0.370498093034
H	-1.714967948064	-0.585746833902	1.441248905607
H	-1.180767766450	1.087442606304	1.750823029863
C	-0.407071789473	-1.375803149773	-1.040246931543
H	0.426316381149	-1.632674809356	-1.695620301997
H	-0.632480137625	-2.224984662364	-0.391899745195
H	-1.278157048955	-1.152232003483	-1.657966872944
C	0.465446642848	1.560768668318	-0.841872307036
H	-0.345809311604	2.026433953759	-1.398931792798
H	1.402778473212	1.504921750542	-1.393109335864
P	0.032047563948	0.109355646780	-0.072046414614

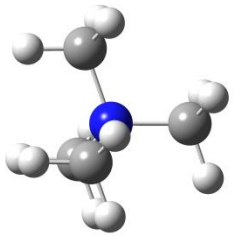
PMe_3CH_2Li cation (IOp(2/15=3), N_{imag} = 0)



C	-1.887832015675	4.405342348047	-4.252953312126
H	-2.316729200727	3.905685272989	-5.121669627052
H	-2.208713635650	5.447567343749	-4.245301675788
H	-0.800230421094	4.367953034716	-4.314568298975
C	-1.781657583566	4.404096619903	-1.353474839018
H	-2.148212426395	5.435967646485	-1.347452606346
H	-2.147662402813	3.896176616811	-0.455288556870
C	-4.241192071137	3.538077717494	-2.862964974313
H	-4.550441434919	3.018058284298	-3.770658419492
H	-4.638483699778	3.014510370548	-1.992850729253
H	-4.636281022767	4.554267610631	-2.873733938674
C	-1.892772826529	1.891786748868	-2.807153446815
H	-0.807610282275	1.853327288326	-2.900893723392
H	-2.191537775107	1.382997710932	-1.889918456946
H	-2.348399152652	1.386248893732	-3.658878499043
Li	0.255345059426	4.544491005409	-1.143991916050
P	-2.439273417851	3.604026212037	-2.740467943261

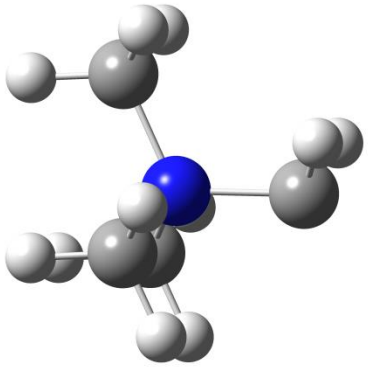
5) ADF: BP86/TZP

NMe_4 cation (T_D, N_{imag}=0)



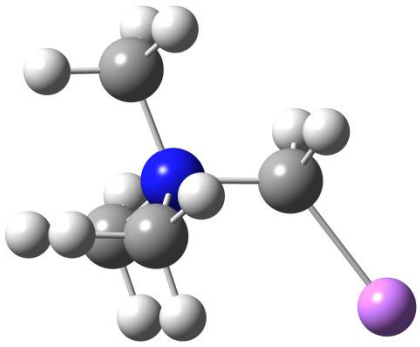
C	0.87158811	-0.87158811	0.87158811
H	1.49856613	-0.22920346	1.49856613
H	0.22920346	-1.49856613	1.49856613
H	1.49856613	-1.49856613	0.22920346
C	-0.87158811	-0.87158811	-0.87158811
H	-1.49856613	-1.49856613	-0.22920346
H	-1.49856613	-0.22920346	-1.49856613
H	-0.22920346	-1.49856613	-1.49856613
C	-0.87158811	0.87158811	0.87158811
H	-0.22920346	1.49856613	1.49856613
H	-1.49856613	1.49856613	0.22920346
H	-1.49856613	0.22920346	1.49856613
C	0.87158811	0.87158811	-0.87158811
H	1.49856613	0.22920346	-1.49856613
H	0.22920346	1.49856613	-1.49856613
H	1.49856613	1.49856613	-0.22920346
N	0.00000000	0.00000000	0.00000000

NMe_3CH_2 (C_S, N_{imag} = 0)



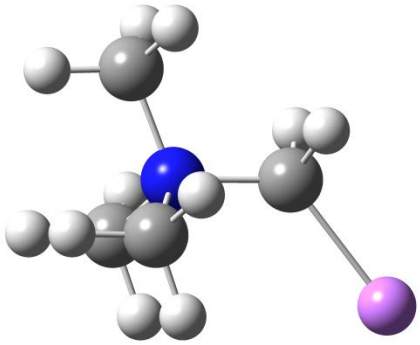
C	-0.56927459	4.75283233	1.21459063
H	-0.95223846	5.77734982	1.19278097
H	-1.38118381	4.01190753	1.22354815
H	0.06544331	4.62815501	2.09874328
C	-0.56927459	4.75283233	-1.21459063
H	0.06544331	4.62815501	-2.09874328
H	-1.38118381	4.01190753	-1.22354815
H	-0.95223846	5.77734982	-1.19278097
C	0.82507672	3.15452758	0.00000000
H	1.44855405	3.04234007	0.89214373
H	0.01902719	2.40112113	0.00000000
H	1.44855405	3.04234007	-0.89214373
N	0.28453107	4.57230204	0.00000000
C	1.33659972	5.68403833	0.00000000
H	1.96287175	5.46476051	-0.88766660
H	1.96287175	5.46476051	0.88766660

NMe_3CH_2Li cation (C_S, N_{imag} = 0)



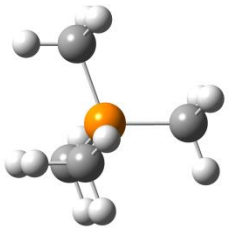
C	-1.97340233	-1.40954650	-1.22284745
H	-2.40709715	-2.41634465	-1.23086722
H	-2.29796893	-0.85517095	-2.10952663
H	-0.88070263	-1.47066137	-1.20261060
C	-1.85130463	0.74322362	0.00000000
H	-2.32746753	1.22748012	-0.87274224
H	-2.32746753	1.22748012	0.87274224
C	-3.94632230	-0.64678252	0.00000000
H	-4.33977209	-1.67089921	0.00000000
H	-4.28135012	-0.11265785	0.89406856
H	-4.28135012	-0.11265785	-0.89406856
C	-1.97340233	-1.40954650	1.22284745
H	-0.88070263	-1.47066137	1.20261060
H	-2.29796893	-0.85517095	2.10952663
H	-2.40709715	-2.41634465	1.23086722
N	-2.43512481	-0.67083190	0.00000000
Li	0.10695558	1.30156682	0.00000000

$NMe_3CH_2Li(THF)_2$ cation (C_1, N_{imag} = 0)



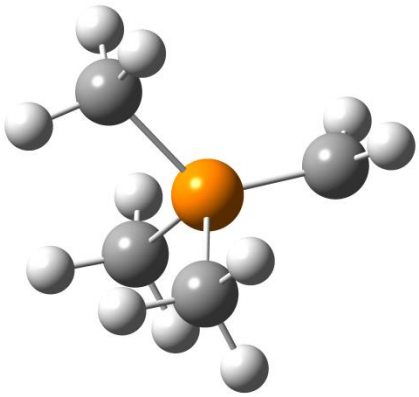
C	2.96175265	-1.76344510	-1.17832795
H	4.04363889	-1.94418048	-1.17751646
H	2.49781765	-2.26785141	-2.03237163
H	2.74975300	-0.69143935	-1.22636482
C	0.84569380	-2.03029241	0.06813181
H	0.47728347	-2.64031746	-0.77829894
H	0.47950175	-2.55657487	0.97070340
C	2.67772734	-3.77574960	0.17363978
H	3.76472310	-3.93289600	0.17854590
H	2.23545346	-4.16404642	1.09591511
H	2.22659035	-4.27852833	-0.68696755
C	2.96936473	-1.60559121	1.25563721
H	2.75504760	-0.53657412	1.16561201
H	2.51104578	-1.99673794	2.17004264
H	4.05140136	-1.78529958	1.27184402
Li	-0.11676101	-0.13802645	0.01666801
O	-2.03380229	-0.23147590	-0.17500612
C	-3.00096997	0.87090383	-0.21957086
C	-2.75162245	-1.50707353	-0.31683516
C	-4.30705433	0.25647084	-0.71278632
H	-3.10392297	1.28050237	0.79799686
H	-2.59836572	1.64761488	-0.88256153
C	-4.22923476	-1.17007973	-0.14639738
H	-2.53596269	-1.91030692	-1.31834012
H	-2.36258125	-2.19797200	0.44192207
H	-4.33425540	0.23618468	-1.81167226
H	-5.18388999	0.81251136	-0.35925023
H	-4.87692258	-1.87856262	-0.67695718
H	-4.50911824	-1.18035695	0.91672319
O	0.52153719	1.69827368	0.21360545
C	1.02595547	2.56023258	-0.86279707
C	0.35006895	2.50100702	1.43260665
C	0.86984160	3.99043016	-0.35585334
H	2.08276532	2.30514509	-1.04140355
H	0.44677854	2.34597058	-1.77102286
C	1.06095004	3.82256558	1.15996533
H	-0.72860223	2.64480993	1.60217669
H	0.77280457	1.93385268	2.27249953
H	-0.13611917	4.37327806	-0.57954922
H	1.60147813	4.67050680	-0.80865717
H	0.63235152	4.64823304	1.74076727
H	2.12888679	3.74746303	1.41002907
N	2.35425959	-2.30434680	0.08063748

PMe_4 cation (T_D, N_{imag}=0)



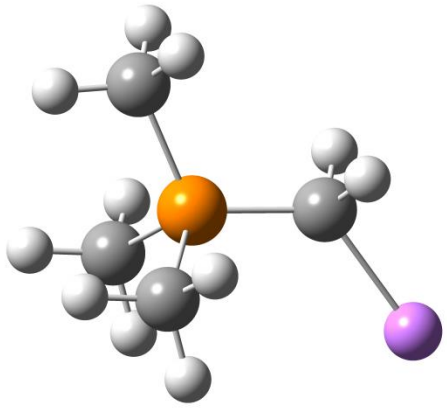
P	0.00000000	0.00000000	0.00000000
C	1.04422997	-1.04422997	1.04422997
H	1.68079547	-0.41592479	1.68079547
H	0.41592479	-1.68079547	1.68079547
H	1.68079547	-1.68079547	0.41592479
C	-1.04422997	-1.04422997	-1.04422997
H	-1.68079547	-1.68079547	-0.41592479
H	-1.68079547	-0.41592479	-1.68079547
H	-0.41592479	-1.68079547	-1.68079547
C	-1.04422997	1.04422997	1.04422997
H	-0.41592479	1.68079547	1.68079547
H	-1.68079547	1.68079547	0.41592479
H	-1.68079547	0.41592479	1.68079547
C	1.04422997	1.04422997	-1.04422997
H	1.68079547	0.41592479	-1.68079547
H	0.41592479	1.68079547	-1.68079547
H	1.68079547	1.68079547	-0.41592479

PMe_3CH_2 (C_S, N_{imag} = 0)



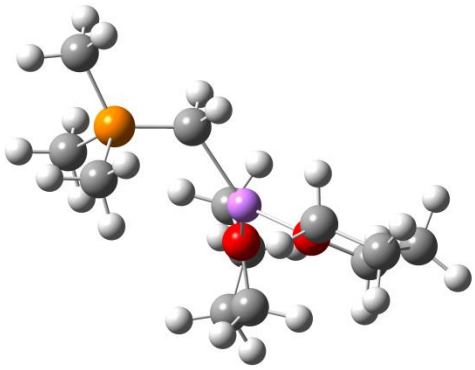
C	-0.63710798	4.79170190	1.47600210
H	-1.13494961	5.76794188	1.45889133
H	-1.38290752	3.98726620	1.51812866
H	-0.00641741	4.73741039	2.37327523
C	-0.63710798	4.79170190	-1.47600210
H	-0.00641741	4.73741039	-2.37327523
H	-1.38290752	3.98726620	-1.51812866
H	-1.13494961	5.76794188	-1.45889133
C	0.81599868	2.80998596	0.00000000
H	1.41996055	2.58095024	0.88824427
H	-0.08443850	2.17686593	0.00000000
H	1.41996055	2.58095024	-0.88824427
C	1.61088768	5.83678853	0.00000000
H	2.17471208	5.97570224	-0.92523909
H	2.17471208	5.97570224	0.92523909
P	0.43185349	4.63661542	0.00000000

PMe_3CH_2Li cation (C_S, N_{imag} = 0)



C	-1.88677716	-1.52388686	-1.46821044
H	-2.35102382	-2.51816966	-1.48232538
H	-2.18681658	-0.98067726	-2.37397346
H	-0.79570183	-1.63850982	-1.46608464
C	-1.74231149	1.01921708	0.00000000
H	-2.15166503	1.54061487	-0.88509480
H	-2.15166503	1.54061487	0.88509480
C	-4.24600338	-0.67750723	0.00000000
H	-4.59946656	-1.71720295	0.00000000
H	-4.63177533	-0.16462671	0.89047765
H	-4.63177533	-0.16462671	-0.89047765
C	-1.88677716	-1.52388686	1.46821044
H	-0.79570183	-1.63850982	1.46608464
H	-2.18681658	-0.98067726	2.37397346
H	-2.35102382	-2.51816966	1.48232538
Li	0.21030953	1.53984702	0.00000000
P	-2.42314646	-0.59567139	0.00000000

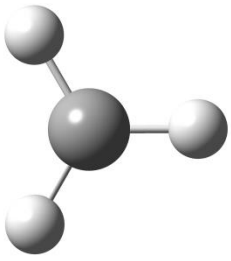
$PMe_3CH_2Li(THF)_2$ cation (C_1, N_{imag} = 0)



C	3.63712542	-0.11108965	0.54242820
H	4.53894556	-0.35640683	1.11747191
H	3.93507032	0.41635909	-0.37322246
H	2.99176679	0.54585483	1.13769166
C	1.30680900	-1.24214526	-0.82123704
H	1.61805870	-0.74473221	-1.75593680
H	0.80213531	-2.18530689	-1.09048980
C	3.98808770	-2.70675995	-0.68244982
H	4.84531567	-2.88153155	-0.01796806
H	3.52631991	-3.66961216	-0.93692581
H	4.34009188	-2.23877140	-1.61096465
C	2.29198200	-2.46841663	1.64750621
H	1.65609626	-1.81751735	2.25964619
H	1.73992193	-3.38886225	1.41646698

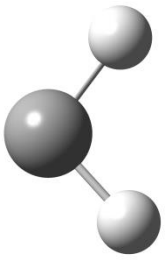
H	3.19486611	-2.73104222	2.21319299
P	2.72898877	-1.62419288	0.09451633
Li	-0.30626628	-0.00353528	-0.16926773
O	-2.07895531	-0.72153005	0.05422531
C	-3.32656586	-0.02367586	-0.28174921
C	-2.36544541	-2.15274461	0.23827983
C	-4.31038123	-1.11593668	-0.68281658
H	-3.66795591	0.52266619	0.61181638
H	-3.10449295	0.69315635	-1.08279917
C	-3.88676896	-2.27936223	0.22737506
H	-1.90105721	-2.70052920	-0.59578773
H	-1.90463953	-2.47091816	1.18258170
H	-4.18151393	-1.38245426	-1.74162328
H	-5.35242659	-0.80937284	-0.53053070
H	-4.21433802	-3.25752078	-0.14503739
H	-4.29399841	-2.14511305	1.23951362
O	-0.27077005	1.92540033	-0.08494192
C	0.49627185	2.76217769	-1.01941700
C	-0.97897575	2.79267170	0.86674107
C	-0.00226687	4.18702651	-0.80179451
H	1.56426948	2.65949600	-0.77226455
H	0.32321839	2.38211225	-2.03471567
C	-0.37233665	4.18056090	0.68976191
H	-2.05006295	2.78076632	0.61183656
H	-0.84337737	2.37284395	1.87211129
H	-0.88907043	4.38571211	-1.42032092
H	0.76183577	4.93301077	-1.05183928
H	-1.07771905	4.97543705	0.96072892
H	0.52616999	4.29345400	1.31313630

Me cation (D_{3H}, $N_{imag} = 0$)



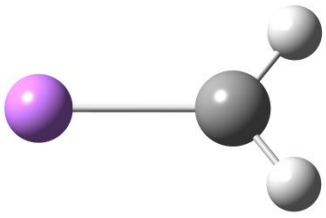
C	0.00000000	0.00000000	0.00000000
H	-0.55026034	0.95307887	0.00000000
H	1.10052069	0.00000000	0.00000000
H	-0.55026034	-0.95307887	0.00000000

CH_2 carbene, singlet (C_S, $N_{imag} = 0$)



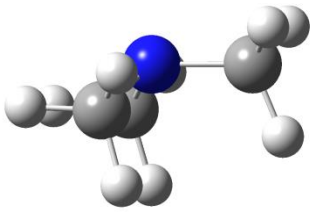
C	1.32920054	5.68662902	0.00000000
H	2.00692212	5.44933707	-0.86413459
H	2.00692212	5.44933707	0.86413459

CH_2Li cation (C_{2V}, $N_{imag} = 0$)



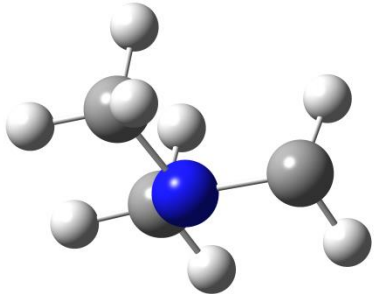
H	0.00000000	0.88128925	-1.13189369
H	0.00000000	-0.88128925	-1.13189369
Li	0.00000000	0.00000000	1.67097049
C	0.00000000	0.00000000	-0.45818041

NMe_3 (C_{3V}, $N_{imag} = 0$)



C	-0.69416735	1.20233312	-0.06281690
H	-0.74108656	1.28359958	-1.17320495
H	-0.18152563	2.09445530	0.32286737
H	-1.72308868	1.20443346	0.32286737
C	1.38833470	0.00000000	-0.06281690
H	1.48217313	0.00000000	-1.17320495
H	1.90461431	-0.89002185	0.32286737
H	1.90461431	0.89002185	0.32286737
C	-0.69416735	-1.20233312	-0.06281690
H	-1.72308868	-1.20443346	0.32286737
H	-0.18152563	-2.09445530	0.32286737
H	-0.74108656	-1.28359958	-1.17320495
N	0.00000000	0.00000000	0.38728100

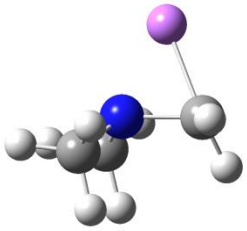
NMe_2CH_2 anion (C_1, $N_{imag} = 0$)



C	-0.55932919	4.73843242	-1.18728761
H	0.00498188	4.61054539	-2.15432750
H	-1.38357441	3.99846696	-1.19156019
H	-0.96950654	5.75863182	-1.18141432
C	0.81817486	3.20882241	-0.00834777
H	1.44656399	3.08009394	0.88274285
H	0.00380778	2.44508885	0.02213012
H	1.46697461	2.99368948	-0.90261913
N	0.29610491	4.57614649	-0.03051027
C	1.32362869	5.64015090	0.00974016
H	2.04653652	5.46089431	-0.84779765

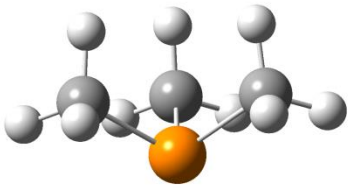
H	1.91551000	5.47944592	0.94002250

NMe_2CH_2Li (C_1, N_{imag} = 0)



C	-2.01634094	1.03524783	0.39880614
H	-2.70775563	1.59883085	-0.25247593
H	-2.27470731	1.28706814	1.44366817
C	-3.62874172	-0.76306506	-0.31757252
H	-3.71282672	-1.83391368	-0.56980382
H	-4.38370508	-0.51801241	0.45675586
H	-3.86138172	-0.17751525	-1.21643938
C	-1.94353853	-1.22660825	1.33031333
H	-0.92340869	-0.97921934	1.66830958
H	-2.62695349	-0.99171283	2.17355751
H	-2.00216855	-2.30459885	1.11804431
N	-2.27029944	-0.44192913	0.13793134
Li	-0.62741060	0.19325383	-0.63806245

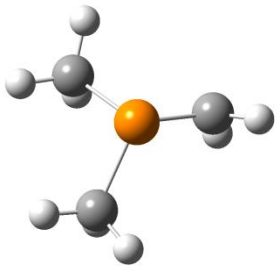
PMe_3 (C_{3V}, N_{imag} = 0)



C	0.81940911	1.41925821	-0.27986807
H	0.76345838	1.32234870	-1.37499631
H	1.87476674	1.47430023	0.02022316
H	0.33939808	2.36074574	0.02022316
C	0.81940911	-1.41925821	-0.27986807
H	0.76345838	-1.32234870	-1.37499631
H	0.33939808	-2.36074574	0.02022316
H	1.87476674	-1.47430023	0.02022316
C	-1.63881822	0.00000000	-0.27986807
H	-2.21416482	0.88644551	0.02022316
H	-2.21416482	-0.88644551	0.02022316
H	-1.52691676	0.00000000	-1.37499631

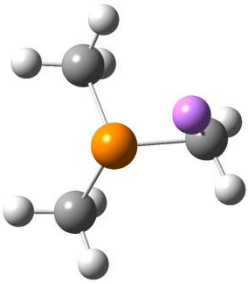
P	0.00000000	0.00000000	0.60422539

PMe_2CH_2 anion (C_1, N_{imag} = 0)



C	-0.58390151	4.74536270	-1.52114995
H	0.11189725	4.58438739	-2.36583715
H	-1.38481481	3.98719236	-1.57376356
H	-1.02801135	5.74514242	-1.62978325
C	0.88402429	2.84974474	-0.12041117
H	1.52136626	2.56922868	0.73162987
H	0.02661865	2.15060011	-0.16292496
H	1.47978400	2.74079052	-1.04630190
C	1.68401356	5.75565972	-0.11070951
H	2.40956654	5.56213879	-0.92000754
H	2.12748805	6.15841979	0.80800562
P	0.33432241	4.67986588	0.13334635

PMe_2CH_2Li (C_1, N_{imag} = 0)



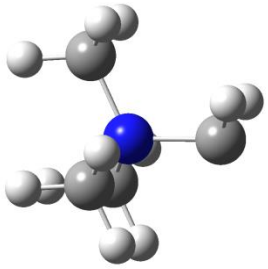
C	-1.86970106	1.21739506	0.31533331
H	-2.23082014	1.83070347	-0.53623714
H	-2.25479494	1.64766683	1.25149554
C	-4.11340982	-0.82545666	-0.15445433
H	-4.31424455	-1.90295576	-0.25575644
H	-4.65258330	-0.43431520	0.72204797
H	-4.48684986	-0.31873970	-1.05389657
C	-1.97165707	-1.30535166	1.64874983
H	-0.92208011	-1.16689268	1.94131904
H	-2.60945239	-0.85625573	2.42630044
H	-2.17946005	-2.38275594	1.59665188
Li	-0.28264319	0.60608743	-0.70462716
P	-2.27572355	-0.50517557	0.00229496

b) Possibility of Stevens rearrangement of the lithiomethyl trimethylammonium cation/ trimethylammonium methylide via a radical mechanism

A) Optimised geometries

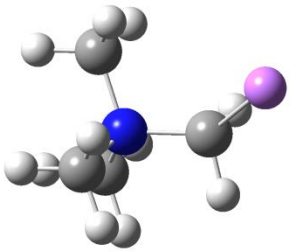
1) Gaussian: M06/aug-cc-pVTZ

NMe_3CH_2 (C_S, N_{imag} = 0)



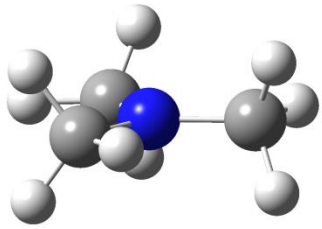
C	-2.019069858603	4.233309529960	-1.500400708821
H	-2.413069861132	5.245708021829	-1.484039369540
H	-2.337442576541	3.664654707726	-0.624030670796
H	-0.932566618741	4.277618803187	-1.542485177215
C	-3.979719587209	3.540647149265	-2.700780600252
H	-4.328748453320	3.077808678772	-3.621749169346
H	-4.321133576996	2.963852258980	-1.838517252982
H	-4.338616814643	4.565446821932	-2.662928086519
C	-1.987085413469	2.188901750034	-2.774202571435
H	-0.901092925652	2.235573387985	-2.802360057723
H	-2.316949577136	1.613046217311	-1.903127043874
H	-2.348428425232	1.724255717023	-3.688470618167
N	-2.504699345782	3.583171838203	-2.733297873131
C	-2.091078403767	4.463214485356	-3.916705086914
H	-2.435594198016	3.898247004866	-4.795162550550
H	-0.992673047942	4.408005165329	-3.911754612763

NMe_3CH_2Li cation (C_1, N_{imag} = 0)



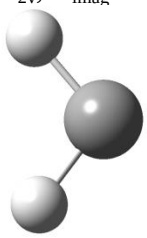
C	-1.978200754146	4.238384095184	-4.062252278923
H	-2.406692356996	3.745010091335	-4.933580022614
H	-2.302079880547	5.276220515981	-4.028137975246
H	-0.892739418394	4.193307746856	-4.106581867073
C	-1.859835739016	4.258850142704	-1.610765661648
H	-2.328656686108	5.250490262285	-1.631500064200
H	-2.328604504199	3.745091902663	-0.762307312379
C	-3.927382398097	3.566261169298	-2.810200237010
H	-4.313718163561	3.056698281239	-3.692714948214
H	-4.264995127364	3.060788347574	-1.908853603381
H	-4.265032562718	4.599575085831	-2.797330774534
C	-1.978149193963	2.145960684816	-2.854115212730
H	-0.892688628020	2.130145540701	-2.915339135819
H	-2.301990864522	1.656623622425	-1.938232108040
H	-2.406640077234	1.637993252882	-3.717017106564
N	-2.435294493525	3.556123411500	-2.827822084455
Li	0.101016550435	4.533273330093	-1.135595753257

NMe_3 radical cation (C_1, N_{imag} = 0)



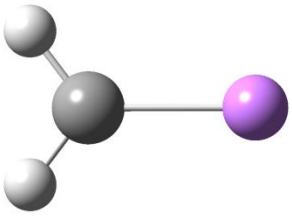
C	-0.268346423329	-0.889670542722	-1.239964775390
H	-0.833051932102	-0.465026239935	-2.064613976921
H	0.805735039285	-0.752072987499	-1.401815823503
H	-0.444435984936	-1.968163049824	-1.171935155108
C	-1.637576562064	0.755860926411	0.018313118732
H	-2.568391270367	0.361294864520	-0.401980027296
H	-1.801089752741	1.114674724488	1.030130201000
H	-1.318069259786	1.577394952790	-0.631124020114
C	-0.013488846402	-0.686431655940	1.221626785841
H	0.714796318523	-1.469867280166	1.034348556371
H	0.468007294718	0.178806805381	1.688797482917
H	-0.781703289289	-1.037836087140	1.918128995394
N	-0.639817016316	-0.273394228343	-0.000010489943

CH_2 radical anion (C_{2v}, N_{imag} = 0)



C	-0.000075893818	0.371559474156	1.531246064644
H	-0.873875042630	1.064894194795	1.626785215866
H	0.874203806113	1.064254314934	1.627030095512

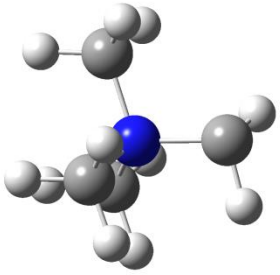
CH_2Li radical (C_1, N_{imag} = 0)



C	0.969973542950	-1.583939959592	-1.337166551212
H	1.928128897094	-1.504377656915	-1.867407585863
H	0.781443264897	-2.660749649411	-1.234772396794
Li	-0.135724000021	-0.151219663129	-0.722486747431

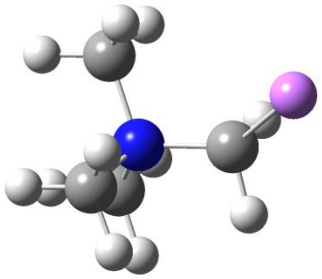
2) Gaussian: M05-2X/6-311+G**

NMe_3CH_2 (C_S, N_{imag} = 0)



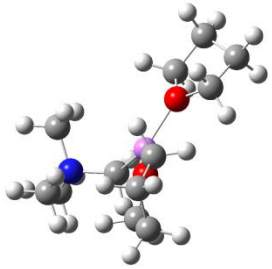
C	-2.018375777890	4.235231224718	-1.498428209036
H	-2.421893736141	5.242203705939	-1.485315894486
H	-2.331967690645	3.660808486561	-0.625938647412
H	-0.933755414764	4.286685165831	-1.548732453004
C	-3.982467151767	3.541352972481	-2.700915198801
H	-4.327522513292	3.087728124349	-3.626518057355
H	-4.319590237002	2.958617093169	-1.842832262621
H	-4.332979332216	4.567051444229	-2.655350851195
C	-1.986294386227	2.185289121905	-2.773409985472
H	-0.901500440006	2.234779079699	-2.801564402730
H	-2.319733311215	1.617665728394	-1.901245834485
H	-2.348567874364	1.723556111371	-3.687510844057
N	-2.503418425854	3.582333221950	-2.734906161802
C	-2.089548224752	4.455481958709	-3.914742470527
H	-2.436757622900	3.897417590396	-4.793077511837
H	-0.993596539562	4.407260514977	-3.909522678325

NMe_3CH_2Li cation (C_S, N_{imag} = 0)



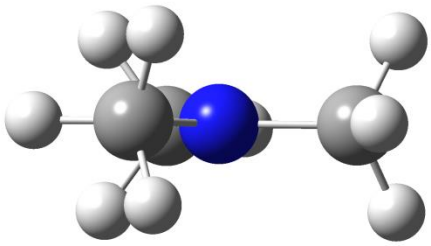
C	-1.975982008747	4.240352741562	-4.063821717579
H	-2.409507984560	3.748654192229	-4.932229384777
H	-2.295210585985	5.278303470129	-4.022589934632
H	-0.892076771086	4.186584163236	-4.103715313699
C	-1.866756306689	4.257634628166	-1.612853941081
H	-2.328697236646	5.250239957933	-1.631229741777
H	-2.328632426529	3.745413913765	-0.762387702384
C	-3.931806131284	3.565534045372	-2.811411445019
H	-4.312541528304	3.055606001456	-3.694573505372
H	-4.265662586564	3.059949525860	-1.909872823605
H	-4.265728873270	4.599060474098	-2.798509952329
C	-1.975891706746	2.143630674262	-2.853236424978
H	-0.891988457630	2.136034107191	-2.919788374452
H	-2.295054768190	1.660370248977	-1.933702325042
H	-2.409417055087	1.637362852063	-3.713232225039
N	-2.436960941163	3.556339776476	-2.827447336184
Li	0.100396846171	4.529659046028	-1.141857006462

$NMe_3CH_2Li(THF)_2$ cation (C_1, N_{imag} = 0)



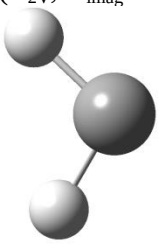
C	3.165572792092	-1.221647231643	0.469452753004
H	3.915423396484	-1.711806221483	1.088206401856
H	3.636429878401	-0.755270992620	-0.392135563928
H	2.622255820536	-0.474661675004	1.040846167263
C	1.148283602356	-1.526639332213	-0.878925313754
H	1.714470908316	-1.173102998837	-1.748274564146
H	0.521078794218	-2.343309559368	-1.253888328274
C	2.930148330955	-3.282520097744	-0.771467079839
H	3.665795090246	-3.757475627062	-0.123159368620
H	2.209091303302	-4.013931109494	-1.124976349797
H	3.420215796310	-2.814495476472	-1.620344551743
C	1.518717887741	-2.853915727829	1.142514145249
H	1.016394282136	-2.073310071343	1.706118469212
H	0.788521303755	-3.567911716124	0.770411778667
H	2.257487919695	-3.360051192229	1.761677257552
Li	-0.099801487985	0.047006364601	-0.201426555824
O	-1.936572476927	-0.225169314089	0.171722179596
C	-3.007224327948	0.751725207895	0.114010940609
C	-2.493122833618	-1.561181887364	0.284960050684
C	-4.270588684737	-0.056364505367	-0.137811497924
H	-3.048121465510	1.270227125156	1.072634251892
H	-2.775141059946	1.461137787833	-0.677054295048
C	-3.964083556539	-1.353968221308	0.611743287019
H	-2.359303884829	-2.066948961623	-0.671580510952
H	-1.941681030974	-2.091604879749	1.057993645147
H	-4.390318885884	-0.252005348935	-1.203603166276
H	-5.161149726023	0.450504344136	0.225543194820
H	-4.577497761979	-2.191773183007	0.289448513502
H	-4.100225403356	-1.214089783109	1.684383885333
O	0.437834672199	1.860432864338	-0.023413323479
C	1.611735712587	2.378511503185	-0.703182979037
C	-0.183637497146	2.913293488668	0.757340002450
C	1.540671176988	3.888480867092	-0.530751324912
H	2.494965631094	1.961665705926	-0.217720108823
H	1.577731840468	2.050285293179	-1.739219574862
C	0.858908312697	4.016861411662	0.832580954960
H	-1.078207779463	3.248829705569	0.231640142819
H	-0.461698510024	2.498003504262	1.723235108013
H	0.918771077128	4.331402670327	-1.308888690389
H	2.523624978389	4.351687186226	-0.566615591716
H	0.411485929139	4.993530871806	0.999753944108
H	1.569151057782	3.816327749814	1.635261205897
N	2.190062517874	-2.225737667662	-0.021993700306

NMe_3 radical cation (C_1, N_{imag} = 0)



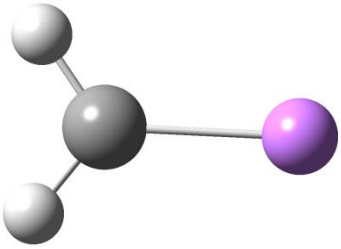
C	-0.274248685025	-0.897634711144	-1.249537219288
H	-1.185283763272	-1.092110422827	-1.821832393420
H	0.341919239580	-0.198596206568	-1.821380800214
H	0.265482799584	-1.820259832954	-1.063191309260
C	-1.368901587909	0.972765958199	-0.001692818724
H	-2.308994964266	0.827473084653	0.537247037528
H	-0.781768609157	1.720963952383	0.537576861627
H	-1.557131206704	1.294883622466	-1.020558824002
C	-0.276252795875	-0.895401137314	1.251223716172
H	0.811308908071	-1.002323615758	1.284402605708
H	-0.627855639284	-0.294909043395	2.083727284028
H	-0.715858449430	-1.895900450126	1.283968830367
N	-0.639817241250	-0.273436207297	-0.000013085392

CH_2 radical anion (C_{2V}, N_{imag} = 0)



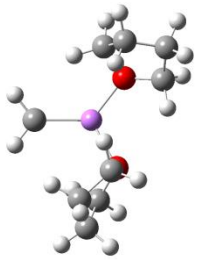
C	-0.000074905772	0.374409246382	1.531639438281
H	-0.872706683495	1.063468880817	1.626588692785
H	0.873034458932	1.062829856668	1.626833244953

CH_2Li radical (C_1, N_{imag} = 0)



C	0.974112938751	-1.589065171347	-1.339031464369
H	1.929690661778	-1.501838027693	-1.866082896078
H	0.780133336427	-2.661155345946	-1.231722820813
Li	-0.140092936956	-0.148228455014	-0.724955818740

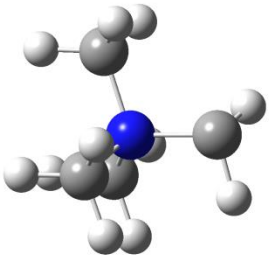
$CH_2Li(THF)_2$ radical (C_1, N_{imag} = 0)



C	1.108085270423	-0.857660950135	-0.829151673986
H	2.152847504260	-0.555993621907	-0.653295430109
H	1.127522531796	-1.954345895080	-0.743040557183
Li	-0.444461147845	0.320779303526	-1.317477990588
O	-2.279739806283	-0.178834801920	-1.079239509269
C	-3.398213882256	0.669975469072	-0.749815889794
C	-2.437554960667	-1.470036270553	-0.451094893449
C	-4.286000874367	-0.150203622111	0.190837973004
H	-3.003186747978	1.565581337717	-0.271077253470
H	-3.905166365271	0.954580100047	-1.670125271443
C	-3.309396669964	-1.184195252763	0.758996680912
H	-2.935716802103	-2.144198246389	-1.151368264347
H	-1.439243426060	-1.836136385189	-0.224845686715
H	-5.071954900825	-0.653535113358	-0.372626005684
H	-4.753911445349	0.468194223145	0.953674983322
H	-3.803683017697	-2.075295109344	1.140066421668
H	-2.704439149934	-0.749486569855	1.556012023993
O	-0.244269341519	2.188060801147	-0.797004196371
C	1.022369117189	2.708400841466	-1.276339883516
C	-0.244333709194	2.165043823556	0.648594337431
C	1.738955179809	3.245615520720	-0.043606494562
H	1.573751418119	1.879824186022	-1.722479532546
H	0.809823507776	3.467432011337	-2.025934659481
C	1.212767591977	2.317714412005	1.053006139192
H	-0.858427359901	2.995016247100	1.005470360464
H	-0.675248385584	1.217020090543	0.969670279140
H	1.443382999195	4.277203319618	0.153779673086
H	2.820298615661	3.206820452738	-0.155015533532
H	1.324600754763	2.726208620937	2.055480411512
H	1.700194501829	1.344724077907	0.993617442321

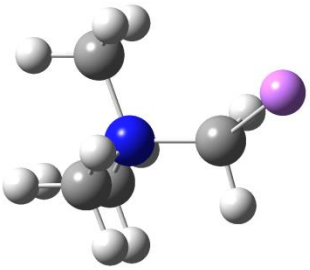
3) Gaussian: MP2/aug-cc-pVTZ

NMe_3CH_2 (C_S, N_{imag} = 0)



C	-2.017464182175	4.235618825103	-1.499574604205
H	-2.421496695309	5.242600366145	-1.484362641172
H	-2.332425564659	3.659653160522	-0.628683413657
H	-0.932632081686	4.283703372577	-1.549250506173
C	-3.982017885219	3.541577240266	-2.702344648423
H	-4.326069432364	3.084862825096	-3.626834227097
H	-4.316651999145	2.958661552538	-1.843497807708
H	-4.334077035330	4.566920038211	-2.655312733589
C	-1.986476290018	2.185869303780	-2.773447657329
H	-0.901783924277	2.236229267655	-2.800313304195
H	-2.321150183322	1.620040172833	-1.900301715391
H	-2.350178087489	1.724537589821	-3.687072016380
N	-2.502887560504	3.584393955908	-2.736962372431
C	-2.092139197663	4.455660316727	-3.910613403985
H	-2.436377472540	3.896808655963	-4.792214554960
H	-0.994141087690	4.406324901155	-3.909225854935

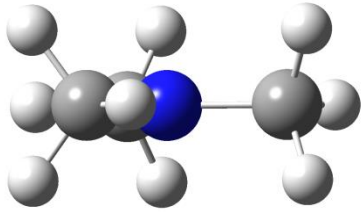
NMe_3CH_2Li cation (C_s, N_{imag} = 0)



C	-1.978153150195	4.239049331945	-4.065278005182

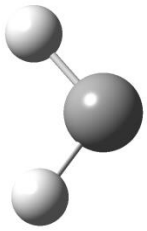
H	-2.413529683646	3.745695869018	-4.931824905677
H	-2.299233565138	5.276411040912	-4.024157437814
H	-0.894484002398	4.185666187914	-4.107361568936
C	-1.863852739169	4.256058517009	-1.615583967013
H	-2.331723465167	5.247855408652	-1.635617550506
H	-2.331658645425	3.742805910374	-0.766646495322
C	-3.930332885572	3.565820456985	-2.810915492758
H	-4.310808337547	3.055790604648	-3.694253903707
H	-4.262684145916	3.060023457015	-1.908950524629
H	-4.262750462255	4.599822451143	-2.797984910694
C	-1.978062878072	2.143021000636	-2.855093255219
H	-0.894395612236	2.133335110563	-2.922406320677
H	-2.299077811118	1.659958632905	-1.936124805927
H	-2.413438960359	1.639191971719	-3.715591873820
N	-2.436042506316	3.556153386281	-2.827770230716
Li	0.118710310987	4.544070485604	-1.116897897986

NMe_3 radical cation (C_1, $N_{imag} = 0$)



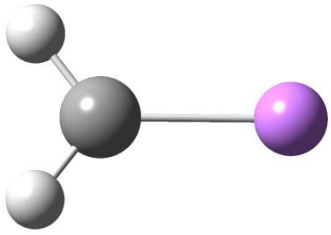
C	-0.277161264669	-0.894251469044	-1.249408628102
H	-0.716856290123	-1.893754236016	-1.279712894821
H	-0.627676949463	-0.294761094017	-2.082352887688
H	0.809478746050	-1.001664843478	-1.279966818375
C	-1.367149331385	0.971112087276	0.002017278906
H	-2.305414333500	0.824536099970	-0.537825878107
H	-1.555815952435	1.294192935217	1.019892925562
H	-0.779057127401	1.716587598430	-0.538048779067
C	-0.275091801224	-0.897128429549	1.247332744598
H	0.264078566788	-1.819701773459	1.062403194559
H	0.339703713659	-0.197077406379	1.817606623885
H	-1.186637931470	-1.089150162682	1.817832128208
N	-0.639802034728	-0.273424325485	-0.000017710223

CH_2 radical anion (C_{2V}, $N_{imag} = 0$)



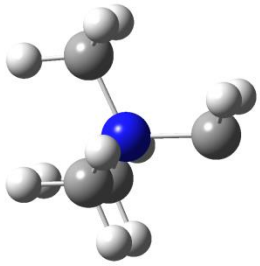
C	-0.000074915747	0.374380475386	1.531635466823
H	-0.872664860218	1.063483250821	1.626590684346
H	0.872992645630	1.062844257287	1.626835224799

CH_2Li radical (C_{2V}, $N_{imag} = 0$)



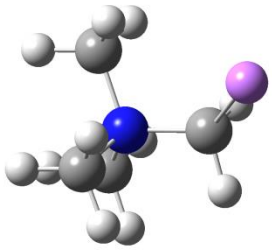
C	0.975059756205	-1.590530114693	-1.339993626404
H	1.930839434970	-1.506826950426	-1.868914490946
H	0.783230018745	-2.664129942138	-1.235767634775
Li	-0.145309251119	-0.138799468591	-0.717158349565

4) Gaussian: M05-2X/6-311+G**/SMD(THF)
NMe_3CH_2 (IOp(2/15=3), $N_{imag} = 0$)



C	-2.020150685507	4.240483154420	-1.496147114863
H	-2.437169265573	5.241752149131	-1.447735905645
H	-2.331571740311	3.646312204236	-0.638162403232
H	-0.935123766274	4.294666899824	-1.541365322340
C	-3.986164387487	3.545771770943	-2.700779398300
H	-4.336581859875	3.093569789895	-3.625523220305
H	-4.303183897345	2.949336851682	-1.846330547854
H	-4.357896810443	4.562809609708	-2.624042707430
C	-1.985795984336	2.203468621699	-2.783945467849
H	-0.900035754853	2.248145395142	-2.803650502335
H	-2.324816892618	1.650051588998	-1.907760005926
H	-2.353433104766	1.733925141574	-3.692402816193
N	-2.505398904566	3.599342911721	-2.741269235971
C	-2.074042049134	4.438512165475	-3.928406339559
H	-2.416608233044	3.867283579538	-4.799189827285
H	-0.979995342463	4.368029710693	-3.923300648059

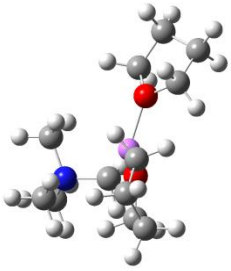
NMe_3CH_2Li cation (IOp(2/15=3), $N_{imag} = 0$)



C	-1.966872253628	4.247937580376	-4.036928114405
H	-2.383480751706	3.753948321615	-4.912652106771
H	-2.291536464125	5.284741718594	-3.998572807705
H	-0.881493294049	4.196507768498	-4.053151361411
C	-1.891143328694	4.265138600537	-1.592078544191
H	-2.368348905507	5.251120089452	-1.606645314579
H	-2.338581553378	3.733790200374	-0.744958288451
C	-3.938587777886	3.561106245932	-2.826244700858

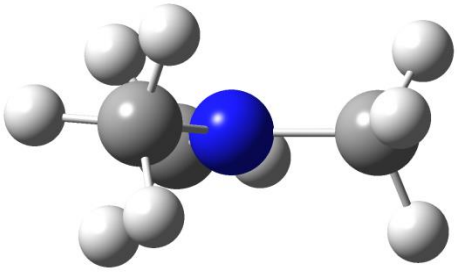
H	-4.296109292446	3.042370820485	-3.714695111344
H	-4.284119091438	3.055039845775	-1.928714542866
H	-4.279218944042	4.592878901850	-2.827320919014
C	-1.975175023130	2.156721984227	-2.830971197954
H	-0.888812156917	2.161393716911	-2.858999031672
H	-2.323166173191	1.666459059788	-1.925369920577
H	-2.376971154356	1.655237237568	-3.709126261202
N	-2.448465671683	3.562778199057	-2.812562069137
Li	0.150563313865	4.463559527767	-1.353468862274

$NMe_3CH_2Li(THF)_2$ cation (IOp(2/15=3), N_{imag} = 0)



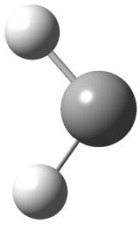
C	3.018576640498	-1.216550103113	0.612004588889
H	3.663022176994	-1.745612712837	1.312160801517
H	3.617503234509	-0.714377213437	-0.143749357877
H	2.395318477605	-0.496310769053	1.135235592601
C	1.219198364426	-1.448541251342	-1.027697994902
H	1.904947111967	-1.023211370011	-1.770380244711
H	0.678194281922	-2.246311048642	-1.550003505346
C	2.979309001938	-3.204072937041	-0.756338860502
H	3.624851404647	-3.698643869589	-0.031381291460
H	2.322045486812	-3.926734514828	-1.232457185986
H	3.575359951117	-2.692869504062	-1.507587201861
C	1.306232438430	-2.879422744809	0.952631636588
H	0.750601526021	-2.126152861344	1.504492172770
H	0.620433251189	-3.551563759890	0.442486376804
H	1.956694556939	-3.440046090226	1.621847009878
Li	-0.080273504334	0.031234674908	-0.239146915291
O	-1.868563215551	-0.240469590372	0.334153489629
C	-2.935752593772	0.724146374284	0.150789471032
C	-2.428117437029	-1.567018693445	0.521220881435
C	-4.170135947154	-0.108453060447	-0.151149011628
H	-3.052669730366	1.289023152145	1.076499978983
H	-2.651049904220	1.397038358712	-0.655098034825
C	-3.922311169924	-1.348768458411	0.707855328620
H	-2.214237326791	-2.155396964593	-0.371790296382
H	-1.944407987731	-2.022672216497	1.382213243669
H	-4.195431447495	-0.376806062382	-1.208099606746
H	-5.088001806633	0.417203143765	0.103257272634
H	-4.501592112479	-2.214610741999	0.394839350248
H	-4.146196200214	-1.133510553444	1.753360633290
O	0.392777316729	1.863937220083	-0.119254359873
C	1.551551562288	2.381017879993	-0.824093538133
C	-0.156197381346	2.887594572120	0.748348561528
C	1.528872462087	3.881388077557	-0.578520607178
H	2.443606484177	1.918165411937	-0.400097797554
H	1.463776888975	2.105717670794	-1.872647973954
C	0.918687646987	3.959885923785	0.821397476748
H	-1.069773014090	3.271594249501	0.293353500863
H	-0.389804747428	2.431353290162	1.707838311112
H	0.878153018738	4.374008493897	-1.301986527827
H	2.522572743441	4.319214425235	-0.642520995734
H	0.503637239486	4.937264431426	1.057421473769
H	1.663528116948	3.699988184596	1.574669339189
N	2.131517781688	-2.190627573089	-0.069029344024

NMe_3 radical cation (IOp(2/15=3), N_{imag} = 0)



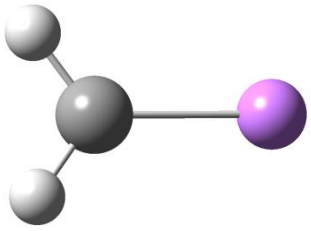
C	-0.249860374804	-0.881367411761	-1.243413995796
H	-1.165620260484	-1.129295000460	-1.787463160893
H	0.310670498921	-0.155627143191	-1.836690175409
H	0.339584135772	-1.771807374376	-1.053143541335
C	-1.373150204865	0.963544431889	-0.003011836883
H	-2.298170331019	0.802255148391	0.555497920842
H	-0.788710397913	1.725644467673	0.518934545120
H	-1.582099284963	1.267212507576	-1.023212915368
C	-0.285651472473	-0.897055230253	1.246449357594
H	0.783292681652	-1.117092624379	1.249164879270
H	-0.557716131238	-0.253494668684	2.076325999294
H	-0.829341753972	-1.845203974832	1.300140072493
N	-0.620629099550	-0.262198137274	0.000362736206

CH_2 radical anion (IOp(2/15=3), N_{imag} = 0)



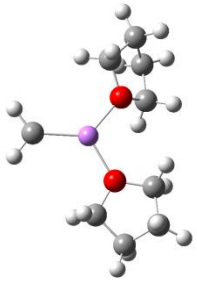
C	-0.000072109497	0.381834622657	1.532664414022
H	-0.869260088265	1.059755014926	1.626076699574
H	0.869585067427	1.059118346284	1.626320262424

CH_2Li radical (IOp(2/15=3), N_{imag} = 0)



C	0.982096698278	-1.599304021271	-1.341139559431
H	1.940741734225	-1.520897830927	-1.873026714431
H	0.796011828984	-2.677955583086	-1.241327631106
Li	-0.175006261487	-0.102129564717	-0.706299095031

$CH_2Li(THF)_2$ radical (IOp(2/15=3), N_{imag} = 0)



C	0.958119777510	-1.468053374680	-1.580846958824
H	1.991380229077	-1.405787848758	-1.959199974341
H	0.697231606303	-2.534842023252	-1.677410492953
Li	-0.256568240002	0.017385534071	-0.843563814171
O	-2.014884369049	-0.306427749162	-0.197521793339
C	-3.060035428633	0.635935015058	0.137083223258
C	-2.553961527850	-1.651469783968	-0.249401708752
C	-4.359432161701	-0.142546614376	-0.005718592098
H	-2.907245157610	0.969277912496	1.164630911812
H	-2.981498440727	1.486523544283	-0.536635376307
C	-3.924418168775	-1.551566238426	0.401244904402
H	-2.625604191620	-1.952244794329	-1.295295830959
H	-1.863074052451	-2.312050740258	0.268704995901
H	-4.692401100349	-0.135826088374	-1.044378882751
H	-5.149630028281	0.265137557778	0.621325203567
H	-4.599220369604	-2.330158001998	0.051759300152
H	-3.834761125989	-1.621400738539	1.486249698736
O	0.192932538836	1.845748299549	-0.492510906297
C	1.356314519374	2.434077399188	-1.130002636129
C	-0.040798517002	2.477575190627	0.787971921192
C	1.684156013615	3.667894410040	-0.302466999183
H	2.164479441589	1.702378831206	-1.102908553895
H	1.100661466281	2.653222282300	-2.164183957758
C	1.241781878036	3.233465076076	1.095446866896
H	-0.889580497138	3.156249996456	0.689849202875
H	-0.277087240947	1.702268572210	1.514078283178
H	1.091103966900	4.519763770961	-0.637954980605
H	2.738915634256	3.927774772986	-0.360894630497
H	1.073376264304	4.066369583890	1.774898177681
H	1.979398281647	2.559599246943	1.533321399210