Supporting information for:

Defluorosilylation of Trifluoromethane: Upgrading an Environmentally Damaging Fluorocarbon

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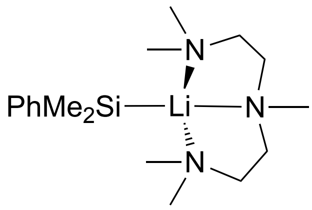
Contents

1. General Experimental

Standard Schlenk line and glovebox techniques were used for all manipulations under an inert atmosphere of dinitrogen or argon unless otherwise stated. NMR scale reactions were performed in J. Young NMR tubes equipped with internal standard capillaries of ferrocene (^{1}H NMR spectroscopy) and prepared in a glovebox. An MBraun Labmaster glovebox was utilised, operating at <0.1 ppm H_2O and <0.1 ppm O_2. ^{1}H, ^{13}C, ^{29}Si, ^{7}Li and ^{19}F NMR spectra were recorded on BRUKER 400 MHz or 500 MHz machines, and referenced against $SiMe_4$ (^{1}H, ^{13}C, ^{29}Si), $CFCl_3$ (^{19}F) or LiCl (^{7}Li) . Data were processed using the MestReNova software package. Solvents were dried over activated alumina from a solvent purification system (SPS) based upon the Grubbs design and de-gassed before use. Glassware was dried for >6 h prior to use at 120 °C. Benzene-d_6 and toluene-d_8 were de-gassed and stored over 3 Å molecular sieves before use. All reagents were acquired from Sigma Aldrich (Merck), Honeywell or Fluorochem and used without further purification unless specified. Trifluoromethane was acquired from CK special gases and used without further purification. Where liquids at 25 °C, reagents were dried over activated 3 Å molecular sieves and freeze-pump-thaw degassed prior to use.

2. Synthetic Procedures

2.1 Preparation of Silyl Lithium Reagents



Synthesis of compound 1·PMDETA ($PhMe_2SiLi$·PMDETA): Synthesis was carried out following literature procedures.[1,2] Lithium wire (450 mg, 66.8 mmol) was washed with *n*-hexane and added to a Schlenk flask. The atmosphere was evacuated and backfilled with argon 4 times. THF (50 mL) was added followed by $PhMe_2SiCl$ (3.00 mL, 17.6 mmol) and the reaction stirred for 24 hours where a colour change to dark red was observed. *n*-Hexane (80 mL) was added and the solution was stirred for a further 15 minutes, before the precipitate was allowed to settle. The solution was filtered *via* cannula filtration to a separate Schlenk flask then concentrated *in vacuo*. Toluene (20 mL) was added along with PMDETA (4.4 mL, 20.1 mmol), and the reaction was stirred for 15 minutes. *n*-Hexane (40 mL) was added and the Schlenk flask was placed in a -20°C freezer for 24 hours, allowing the product to crystallise. The product was isolated as brown crystals (3.90 g, 70 %, 12.4 mmol) and washed with *n*-hexane (3 x 5 mL).

δ_H (400 MHz, C_6D_6, 298K): 7.99 – 7.96 (m, 2H, *o*-C$\underline{H}$), 7.44 (apparent t, 2H, $^3J_{HH}$ = 7.5 Hz, *m*-C$\underline{H}$), 7.23 (tt, 1H, $^3J_{HH}$ = 7.3 Hz, $^4J_{HH}$ = 1.3 Hz, *p*-C$\underline{H}$), 1.89 (s, 3H, N(C$\underline{H}_3$)), 1.82 (br s, 12H, (N(C$\underline{H}_3)_2$), 1.57 (br m, 8H, (N(C$\underline{H})_2)_4$), 0.89 (s, 6H, C$\underline{H}_3$Si).

δ_C (100 MHz, C_6D_6, 298K): 165.3 (s, 1C, *i*-$\underline{C}^{IV}$Si), 133.9 (s, 2C, *o*-$\underline{C}$H), 127.0 (s, 2C, *m*-$\underline{C}$H), 123.3 (s, 1C, *p*-$\underline{C}$H), 57.0 (s, 2C, N$\underline{C}H_2$), 53.4 (s, 2C, N$\underline{C}H_2$), 45.8 (br s, 4C, N($\underline{C}H_3)_2$), 44.8 (s, 1C, N($\underline{C}H_3$)), 7.7 (s, 2C, Si($\underline{C}H_3)_2$)

δ_{Li} (100 MHz, C_6D_6, 298K): 1.43 (s).

δ_{Si} (79.5 MHz, C_6D_6, 298K): -27.5 (s).

$$PhMe_2Si{-}Li\cdot{}^{1.5}THF$$

Synthesis of compound 1·THF ($PhMe_2SiLi\cdot^{1.5}THF$): Synthesis was carried out following our previously published procedure.[1] Lithium wire, from paraffin oil, (328 mg, 47.2 mmol) was washed with n-hexane and added to an oven dried Schlenk flask. The lithium was stirred under vacuum for 10 minutes then backfilled with argon and this process repeated three times. Dry THF (40 mL) was added and the solution cooled to 0 °C, followed by the addition of $PhMe_2SiCl$ (3.00 mL, 17.8 mmol). The solution was stirred for 16 hours at 22 °C observing a colour change to deep red. The solvent was removed *in vacuo* then toluene (40 mL) was added and the solution stirred for 3 hours at 22 °C. The solution was transferred to another Schlenk flask via cannula filtration and the solvent removed *in vacuo* yielding a dark red oil as the target compound containing 2 THF molecules (2.59 g, 51 %, 9.0 mmol). *The number of THF molecules varied slightly batch to batch between of 1.5 – 2 THF.*

δ_H (400 MHz, C_6D_6, 298K): 7.74 (d, 2H, $^3J_{HH}$ = 7.0 Hz, *o*-C$\underline{H}$), 7.33 – 7.28 (m, 2H, *m*-C$\underline{H}$), 7.11 (tt, 1H, $^3J_{HH}$ = 7.4 Hz, *p*-C$\underline{H}$), 3.38 – 3.33 (m, 6H, $(C\underline{H}_2)_2O$), 1.24 – 1.17 (m, 6H, $(C\underline{H}_2)_2CH_2O$), 0.67 (s, 6H, $C\underline{H}_3Si$).

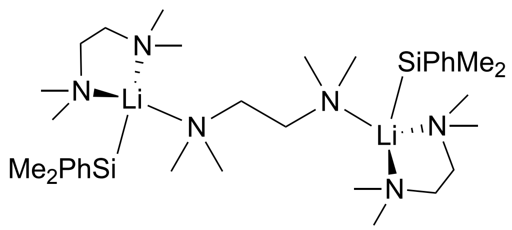
δ_C (100 MHz, C_6D_6, 298K): 160.2 (s, 1C, *i*-$\underline{C}^{IV}Si$), 133.8 (s, 2C, *o*-$\underline{C}H$), 127.6 (s, 2C, *m*-$\underline{C}H$), 124.7 (s, 1C, *p*-$\underline{C}H$), 68.6 (s, 4C, $O\underline{C}H_2$), 25.3 (s, 4C, $OCH_2(\underline{C}H_2)_2$), 6.3 (s, 1C, $Si(\underline{C}H_3)_2$).

δ_{Li} (100 MHz, C_6D_6, 298K): 1.27 (s).

δ_{Si} (79.5 MHz, C_6D_6, 298K): -29.8 (s).

Procedure for purity determination of 1·THF:

A batch of **1·THF** was synthesised according to our procedure above. Purity by mass was determined by ^1H NMR comparison to a known quantity of internal standard. Assuming 100 % purity, **$PhMe_2SiLi\cdot^{1.5}THF$** (25 mg, 0.10 mmol) was dissolved in C_6D_6 (0.6 mL) then mesitylene (13.9 µL, 0.10 mmol) was added. A ^1H NMR spectrum was recorded, and the silyl lithium measured to be 84 % pure upon integral comparison of mesitylene (s, 9H) to **$PhMe_2SiLi\cdot^{1.5}THF$** (s, 6H). Inspection of the ^1H NMR spectrum reveals the presence of between 1.5 – 2 THF molecules per lithium atom, which varied from batch to batch.



Synthesis of compound 1·TMEDA ($PhMe_2SiLi\cdot^{1.5}$TMEDA): Synthesis was carried out following our previously published procedure.[1] **1·THF** (33 mg, 0.134 mmol) was dissolved in C_6D_6 (0.6 mL) and added to a J. Young NMR tube before TMEDA (18.7 µL, 0.12 mmol) was added and a ^{1}H NMR spectrum recorded. The solvent was removed *in vacuo* and the product crystallised from a saturated pentane/toluene solution (0.5 mL, 10:1), yielding X-ray quality brown crystals (10 mg, 26 %, 0.032 mmol).

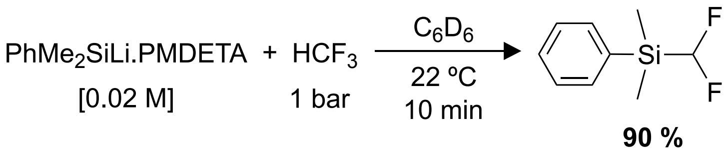
δ_H (400 MHz, C_6D_6, 298K): 7.98 – 7.96 (m, 2H, *o*-C<u>H</u>), 7.45 (apparent t, 2H, $^3J_{HH}$ = 7.4 Hz, *m*-C<u>H</u>), 7.21 (tt, 1H, $^3J_{HH}$ = 7.3 Hz, *p*-C<u>H</u>), 2.02 – 1.41 (br m, 23H, PMEDTA), 0.90 (s, 6H, C<u>H</u>$_3$Si).

δ_C (100 MHz, C_6D_6, 298K): 163.5 (s, 1C, *i*-<u>C</u>^{IV}Si), 134.0 (s, 2C, *o*-<u>C</u>H), 127.2 (s, 2C, *m*-<u>C</u>H), 123.8 (s, 1C, *p*-<u>C</u>H), 56.7 (s, 3C, (N(<u>C</u>H$_2$))$_3$), 45.5 (s, 6C, N(<u>C</u>H$_3$)$_6$), 7.4 (s, 2C, Si(<u>C</u>H$_3$)$_2$).

δ_{Li} (100 MHz, C_6D_6, 298K): 1.38 (s).

δ_{Si} (79.5 MHz, C_6D_6, 298K): -27.6 (s).

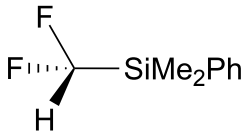
2.2 General Procedure for NMR scale reactions with HCF_3



Scheme S1: Optimised conditions for reaction of HCF_3 with **1·PMDETA**.

In an N_2 filled glovebox, 0.6 mL of a 0.02 M solution of $PhMe_2SiLi$·PMDETA (**1·PMDETA**) (0.012 mmol) in C_6D_6 was added to a J. Young NMR tube equipped with a ferrocene capillary internal standard, and a t=0 ^1H NMR spectrum was recorded. The solution was degassed once *via* freeze-pump-thaw and HCF_3 (1 bar, 22 °C, approx. 0.09 mmol, approx. 7.5 equiv.) was added. The J. Young tube was inverted multiple times then t=1 ^1H and ^{19}F NMR spectra recorded. The orange solution turned colourless within seconds of trifluoromethane addition. The yield of the desired product $PhMe_2SiCF_2H$ (**2**) was determined *in situ* upon integral comparison {δ 5.70 (t, 1H, $^2J_{HF}$ = 46.2 Hz, C$\underline{H}F_2$)} to the ferrocene internal standard in the ^1H NMR spectrum. Further ^1H and ^{19}F NMR spectra were recorded if required. Formation of the by-product $PhMe_2SiH$ (10 %) was observed in the ^1H NMR spectrum (δ 4.63, septet, 1H, $^3J_{HF}$ = 3.7 Hz, Si$\underline{H}$; δ 0.21, doublet, 6H, $^3J_{HH}$ = 3.7 Hz, Si$\underline{Me_2}$).[3]

2.3 Preparation of $PhMe_2SiCF_2H$ (Gram-Scale):



Compound 2, (difluoromethyl)dimethyl(phenyl)silane: Toluene (160 mL) was added to a Strauss flask under an argon atmosphere and moved into a glovebox where $PhMe_2SiLi·PMDETA$ (1.00 g, 3.17 mmol) was added. The solution was degassed once on a Schlenk line *via* freeze-pump-thaw technique then transferred to a room temperature water bath (in case of exotherm). Trifluoromethane (1 bar, 22 °C) was added whilst maintaining manual stirring (swirling of flask) observing a colour change from dark orange to pale yellow. The reaction was left for 10 minutes then the contents transferred to a round bottom flask and the solvent removed under reduced pressure. The product was extracted into n-hexane (50 mL) washing with 0.1 M HCl (2 x 25 mL) then brine (2 x 25 mL) then H_2O (2 x 25 mL). The organic layers were combined and dried over $MgSO_4$, then the solvent removed under reduced pressure yielding a yellow oil. The product was isolated *via* short path distillation (45 °C, 0.1 mbar) and collected into a flask in a cold bath (-78 °C) yielding the desired product (404 mg, 68 %, 2.17 mmol).

δ_H (400 MHz, C_6D_6, 298K): 7.41 – 7.37 (m, 2H, *o*-C$\underline{H}$), 7.20 – 7.11 (m, 3H, *m/p*-C$\underline{H}$), 5.70 (t, 1H, $^2J_{HF}$ = 46.2 Hz, C$\underline{H}F_2$), 0.20 (s, 6H, Si(C$\underline{H}_3$)$_2$).

δ_C (100 MHz, C_6D_6, 298K): 134.5 (s, 2C, *o*-$\underline{CH}$), 132.8 (m, 1C, *i*-$\underline{C}^{IV}$Si), 130.5 (s, 1C, *p*-$\underline{C}$H), 128.4 (s, 2C, *m*-$\underline{C}$H), 123.6 (t, 1C, $^1J_{CF}$ = 255 Hz, $\underline{C}HF_2$), -7.0 (s, 2C, Si($\underline{C}H_3$)$_2$).

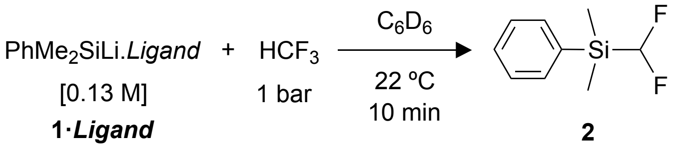
δ_F (376 MHz, C_6D_6, 298K): -137.7 (d, 2F, $^2J_{HF}$ = 46.2 Hz, CH$\underline{F_2}$)

δ_{Si} (79.5 MHz, C_6D_6, 298K): -7.9 (t, $^2J_{SiF}$ = 28.9 Hz,).

3. Optimisation of Reaction Conditions

3.1 Reagent, Solvent and Temperature Screen

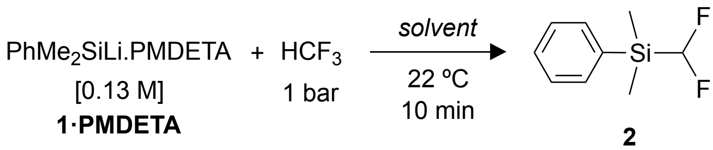
We began by adopting the conditions from our previous report for the defluorosilylation of fluoroolefins using silyl lithium reagents (0.13 M, C_6D_6, 22 °C, 15 min).[1] A ligand screen (Table S1) determined PMDETA to be crucial for formation of **2**.



Ligand	*Compound **2** Yield (%)*	*$PhMe_2SiH$ yield (%)*
THF (**1·THF**)	< 5	15
PMDETA (**1·PMDETA**)	30	10
TMEDA (**1·TMEDA**)	< 5	15

Table S1: Results of lithium ligand variation on the defluorosilylation of trifluoromethane. Yields were measured by ^1H NMR spectroscopy against a ferrocene internal standard in a capillary tube. PMDETA = pentamethyldiethylenetriamine, TMEDA = tetramethylethylenediamine.

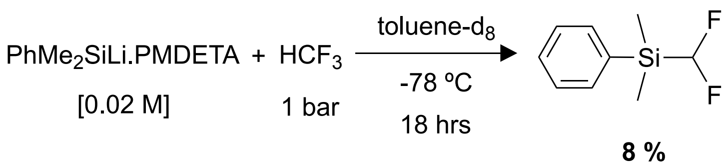
A solvent scope showed no improvement on our initial conditions with C_6D_6 (Table S2). A more polar solvent such as THF resulted in a decreased yield with new, unidentified signals observed in the ^{19}F NMR spectra suggesting a more complex process. Use of C_6H_6 resulted in a similar yield of compound **2** (27 %) and $PhMe_2SiH$ (14 %). This result suggests there is no significant deuterium incorporation into **2**. A more viscous solvent (mesitylene) had no discernible effect on the yield.



Solvent	*Compound **2** Yield (%)*	*Viscosity (cP, 298.15 K)*
C_6D_6	30	-
C_6H_6	27	0.60[4]
THF	10[a]	0.46[5]
Mesitylene	24[b]	0.66[4]

Table S2: Results of solvent screen. [a]PMDETA used as an internal standard, [b]1,2,4,5-tetrafluorobenzene used as an internal standard, added after reaction completion. [c]Fisher-Scientific, recorded at 293.15 K.

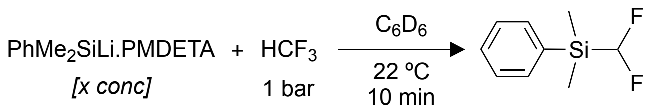
Low temperature reaction: In an N_2 filled glovebox, 0.6 mL of a 0.02 M solution of $PhMe_2SiLi.PMDETA$ (**1·PMDETA**) (0.012 mmol) in C_7D_8 (d_8-toluene) was added to a J. Young NMR tube equipped with a ferrocene capillary internal standard, and a t=0 ^1H NMR spectrum was recorded. The solution was degassed once *via* freeze-pump-thaw and cooled to -78 °C. HCF_3 (1 bar) was added and the temperature was maintained at -78 °C for 18 hours, before the reaction was warmed to 22 °C and ^1H and ^{19}F NMR spectra were recorded. The desired product $PhMe_2SiCF_2H$ (**2**) was formed in only an 8 % yield (Scheme S2). Instead, $PhMe_2SiH$ was formed (23 %) and a new product identified as H_2CF_2 was also formed in a 15 % yield (^1H NMR: δ 4.71 ppm, triplet, $^2J_{HF}$ = 50.3 Hz; ^{19}F NMR: δ = - 141.7 ppm, $^2J_{HF}$ = 50.3 Hz).[6] Another new signal was observed in the ^1H NMR spectrum at δ 0.30 ppm. This has been verified by independent synthesis to be the dimeric species $[PhMe_2Si]_2$, forming in an approximate 21% yield. This change in selectivity suggests an alternative pathway is likely operating at - 78 °C. As a result, we were unable to obtain a kinetic analysis at low temperature for the reaction to form $PhMe_2SiCF_2H$ (**2**).



Scheme S2: Effect of low temperature on reaction of HCF_3 with **1·PMDETA**.

3.2 Silyl Lithium Concentration Studies

1·PMDETA (x mmol) was dissolved in C_6D_6 (0.6 mL) and added to a J. Young NMR tube equipped with a ferrocene capillary internal standard, then a t=0 ^{1}H NMR spectrum recorded. The solution was degassed once *via* freeze-pump-thaw technique before trifluoromethane (1 bar, 22 °C) was added. The J. Young tube was inverted multiple times, observing a colour change from dark orange to pale yellow, then t=1 ^{1}H and ^{19}F NMR spectra recorded. The yield of the desired product $PhMe_2SiCF_2H$ (**2**) was determined *in situ* upon integral comparison {δ 5.70 (t, 1H, $^2J_{HF}$ = 46.2 Hz, C<u>H</u>F_2)} to the ferrocene internal standard in the ^{1}H NMR spectrum.



1·PMDETA **2**

*Concentration of **1.PMDETA** (M) {amount of **1.PMDETA** (mmol)}*	*Approx. equivalence of HCF_3 (headspace of NMR tube = 2.2 mL)*	*Yield of **2** (%)*
0.26 {0.16}	0.6	15
0.13[a] {0.079}	1	30
0.067 {0.040}	2	48
0.033 {0.019}	5	67
0.022 {0.013}	7	87
0.011 {0.007}	13	93

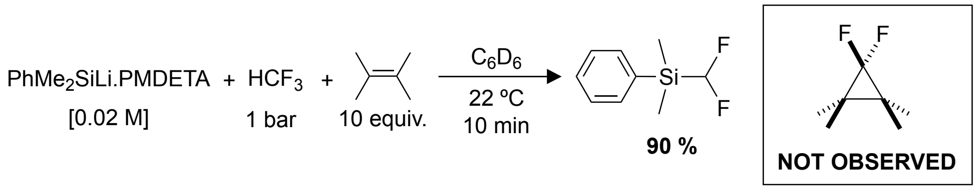
Table S3: Effect of HCF_3 equivalence/concentration of **1·PMDETA**. [a]Standard reaction conditions for previous optimisations.

A clear trend is shown with these results, that decreasing the concentration of **1·PMDETA** (and conversely increasing the equivalence of HCF_3) increases the yield. Previous reports utilising HCF_3 as a difluoromethyl source have also depended on a high equivalence of HCF_3.[7] There was only a very small difference in the yield of **2** between the silyl lithium concentrations 0.011 M and 0.022 M, therefore an optimal concentration of 0.02 M was selected, with consideration made to the quantity of solvent spared. It is noted that running the reaction with PhMe$_2$SiLi·TMEDA (**1·TMEDA**) at the new optimised concentration of 0.02 M still led to no product (**2**) being formed.

3.3 Carbene Trap Experiments

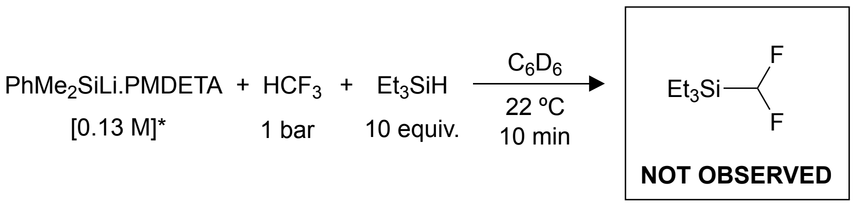
We sought to further explore the possible operation of an alternative difluorocarbene pathway. If deprotonation of HCF_3 by **1·PMDETA** to form $LiCF_3$ is the first step of the reaction, consistent with the observed formation of $PhMe_2SiH$, then a plausible next step is formation of $:CF_2$ from $LiCF_3$, and insertion of $:CF_2$ into the Si–H bond of $PhMe_2SiH$.

The reaction of **1·PMDETA** with HCF_3 was carried out in the presence of 10 equivalents of tetramethylethylene (TME), an electron-rich alkene known to undergo cyclopropanation with carbenes.[8] However, no product inhibition was observed, and the ^{19}F NMR spectrum displayed no sign of a difluorocyclopropane product. This result suggests there is no formation of difluorocarbene, although it does not necessarily rule it out on the basis that TME may not be nucleophilic enough to trap $:CF_2$ at room temperature.



Scheme S3: Tetramethylethylene trapping experiment. No inhibition of product **2** was observed, and no difluorocyclopropane trapping product was observed in the ^{1}H and ^{19}F NMR spectrum.

In a competition experiment, 10 equivalents of Et_3SiH were added to the reaction of **1·PMDETA** with HCF_3. We noted that **1·PMDETA** does not deprotonate Et_3SiH to form Et_3SiLi·PMDETA, and thus any formation of Et_3SiCF_2H must result from difluorocarbene insertion into the Si–H bond of Et_3SiH. However, the reaction produced only $PhMe_2SiCF_2H$ (**2**), with no formation of Et_3SiCF_2H, suggesting there is no occurrence of $:CF_2$ insertion into an Si–H bond.[9]



Scheme S4: Competition experiment. The cross-over product Et_3SiCF_2H was not observed, instead only $PhMe_2SiCF_2H$ (**2**) was observed. *Unoptimised concentration was used.

We also explored the potential of a solvent cage effect through the use of a more viscous solvent (mesitylene) in the reaction of HCF_3 with **1·PMDETA** (Table S2), as a more viscous solvent would lead to a higher product yield if a carbene insertion mechanism were operating within a solvent cage.[4,10] However this resulted in a largely unchanged yield of **2**, suggesting the reaction is unaffected by solvent viscosity. These experimental results cannot rule out a carbene mechanism entirely, but combined with the evidence obtained by the DFT studies they provide a strong basis that a carbene mechanism is not operating here.

4. Multinuclear NMR Data

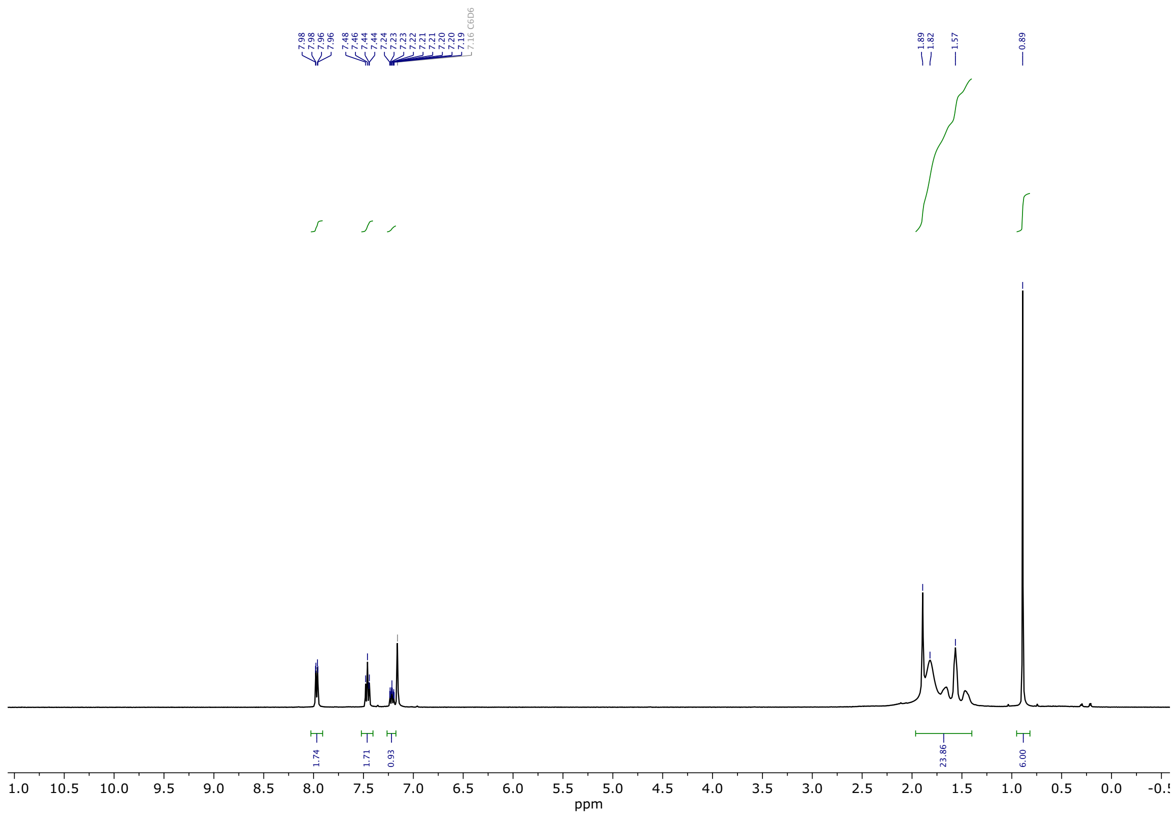


Figure S1: ^{1}H NMR spectrum of **1·PMDETA** in C_6D_6

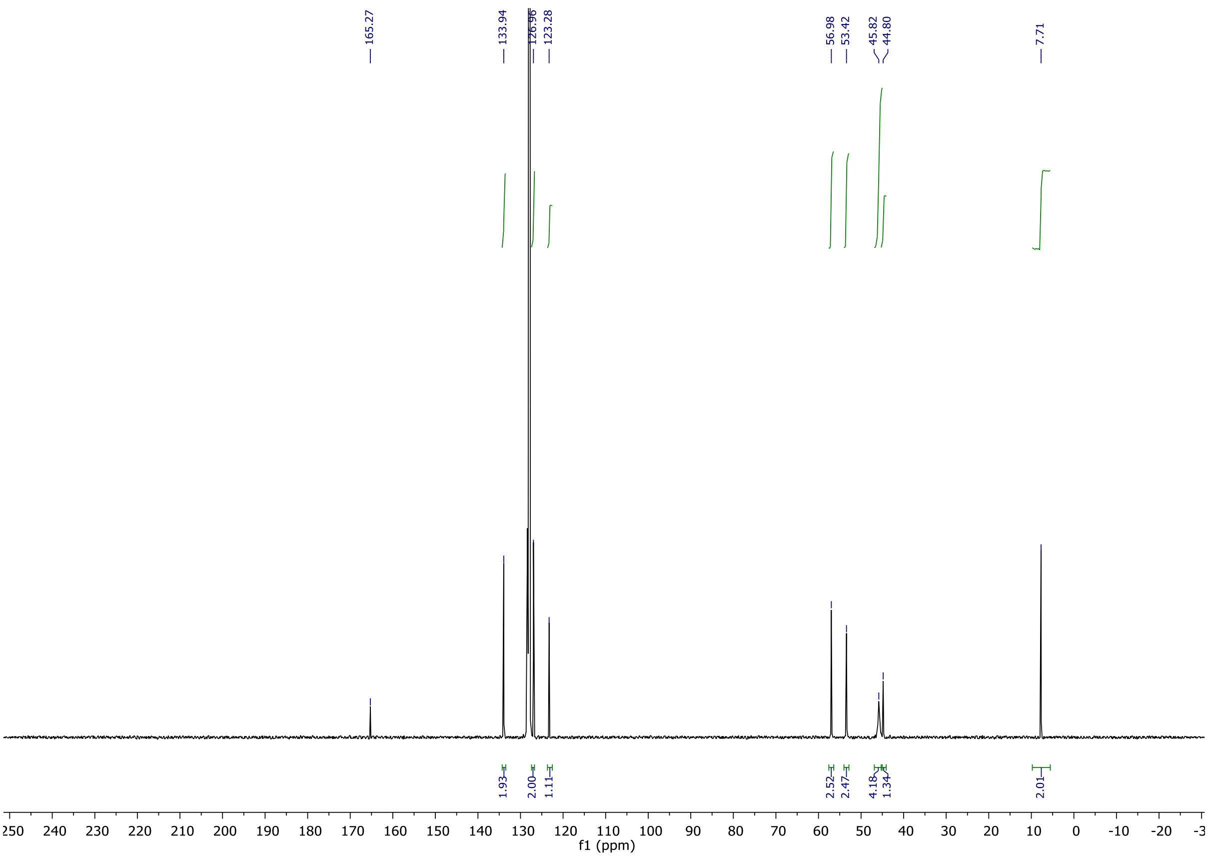


Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of **1·PMDETA** in C_6D_6

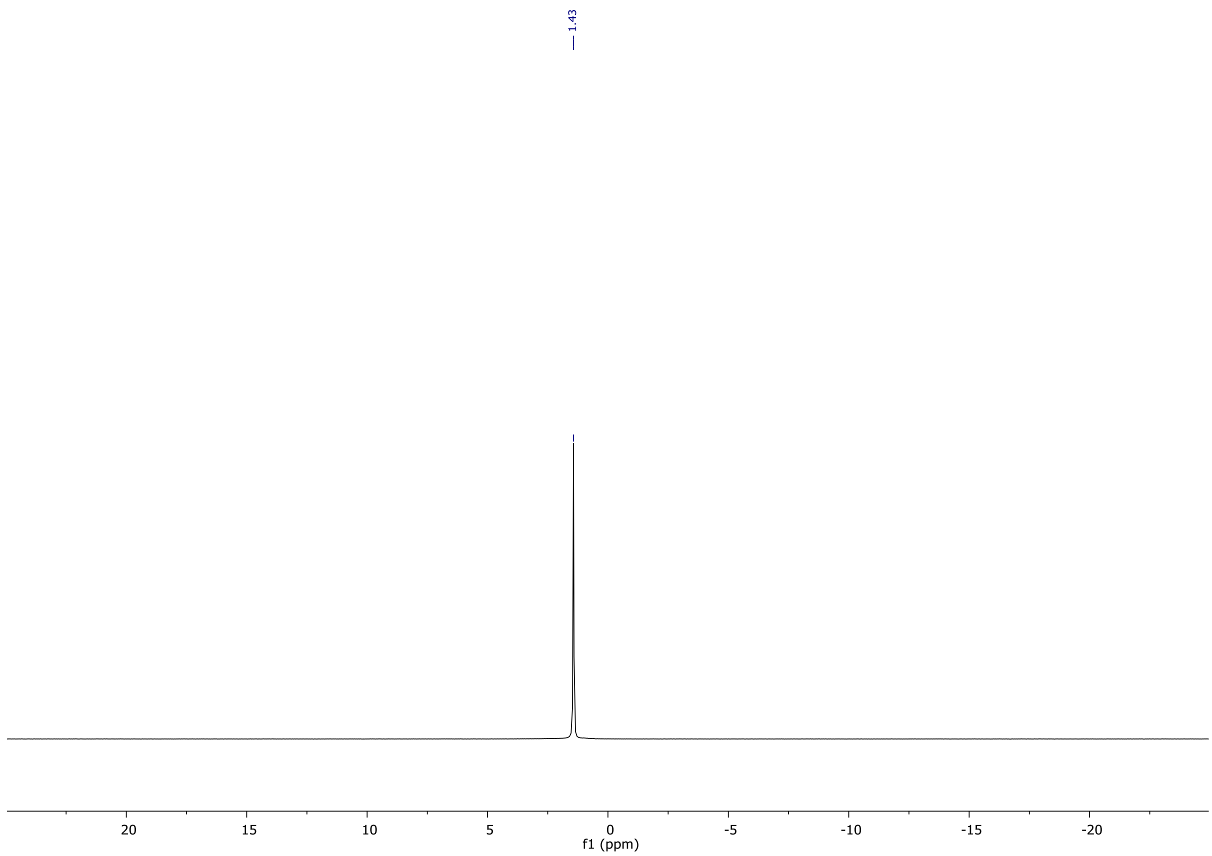


Figure S3: ^{7}Li NMR spectrum of **1·PMDETA** in C_6D_6

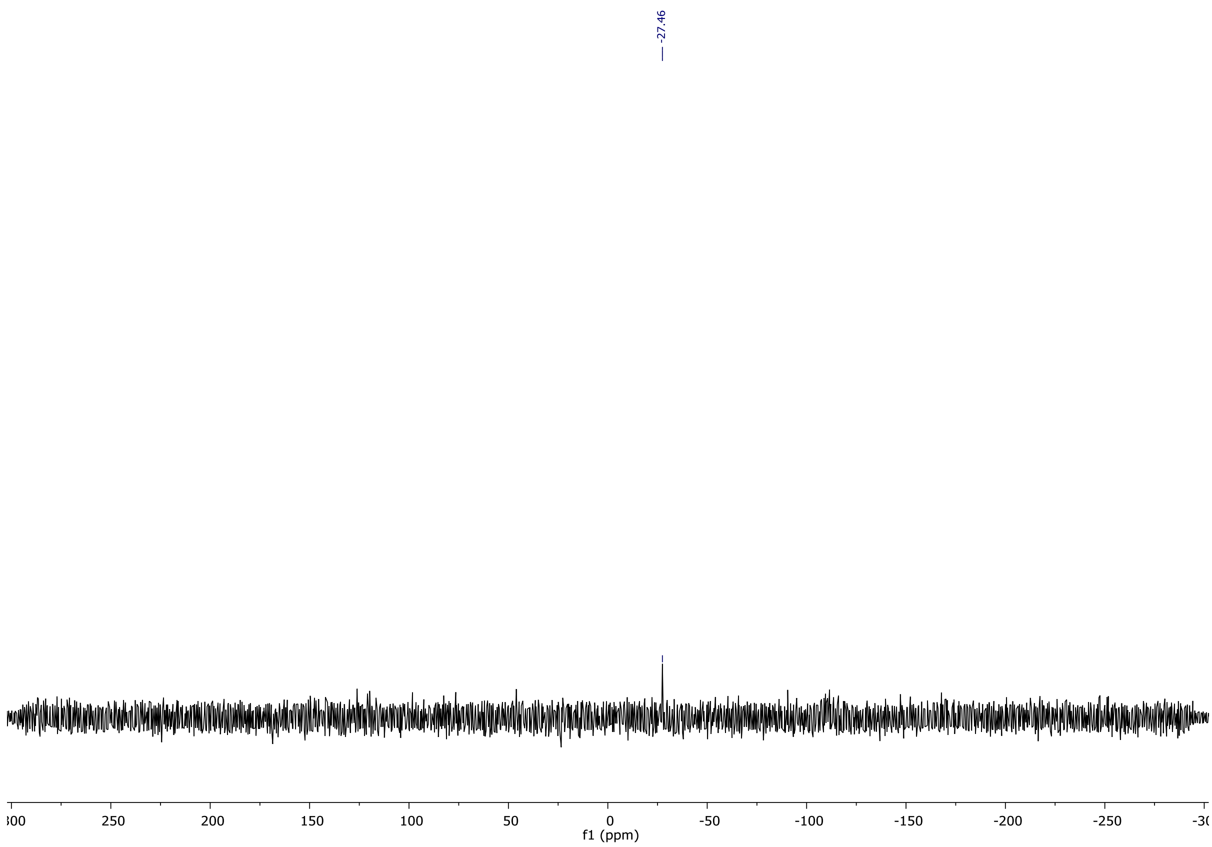


Figure S4: ^{29}Si NMR spectrum of **1·PMDETA** in C_6D_6

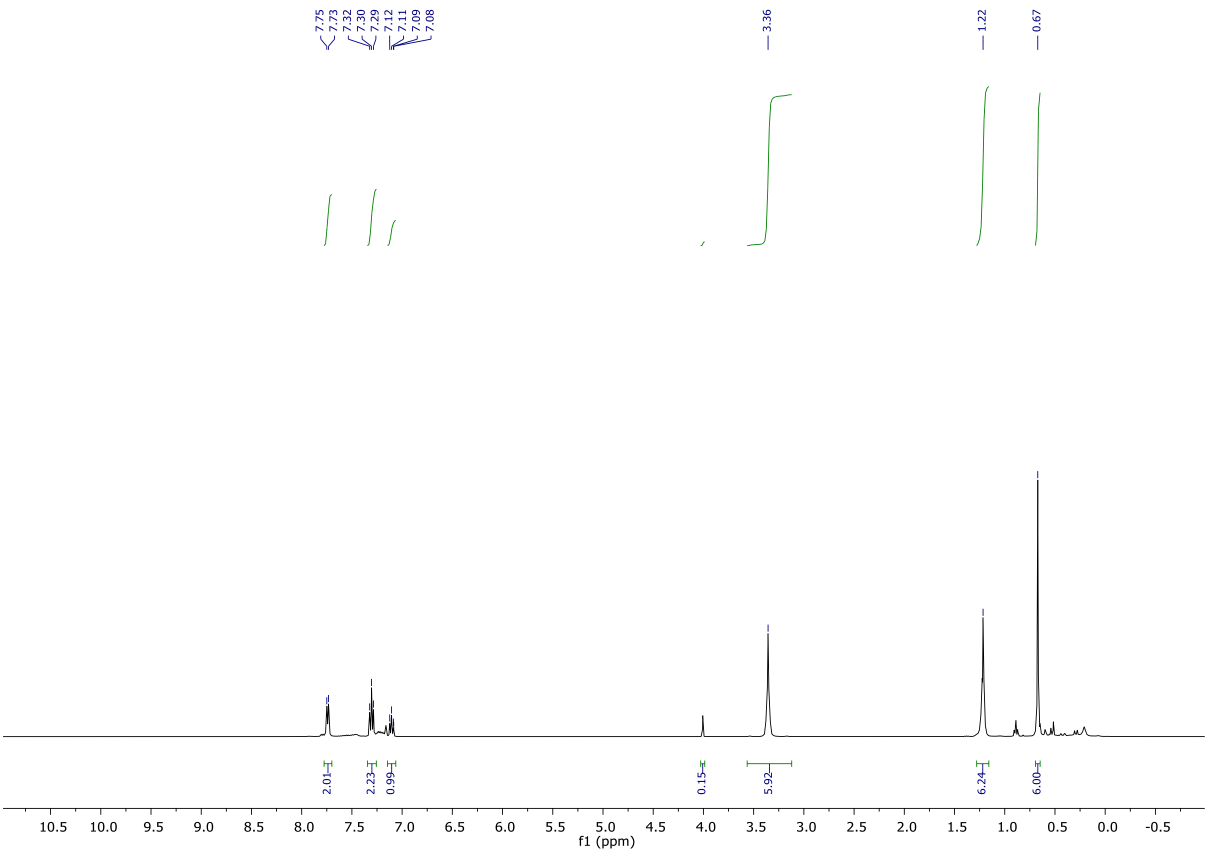


Figure S5: ^{1}H NMR spectrum of **1·THF** in C_6D_6

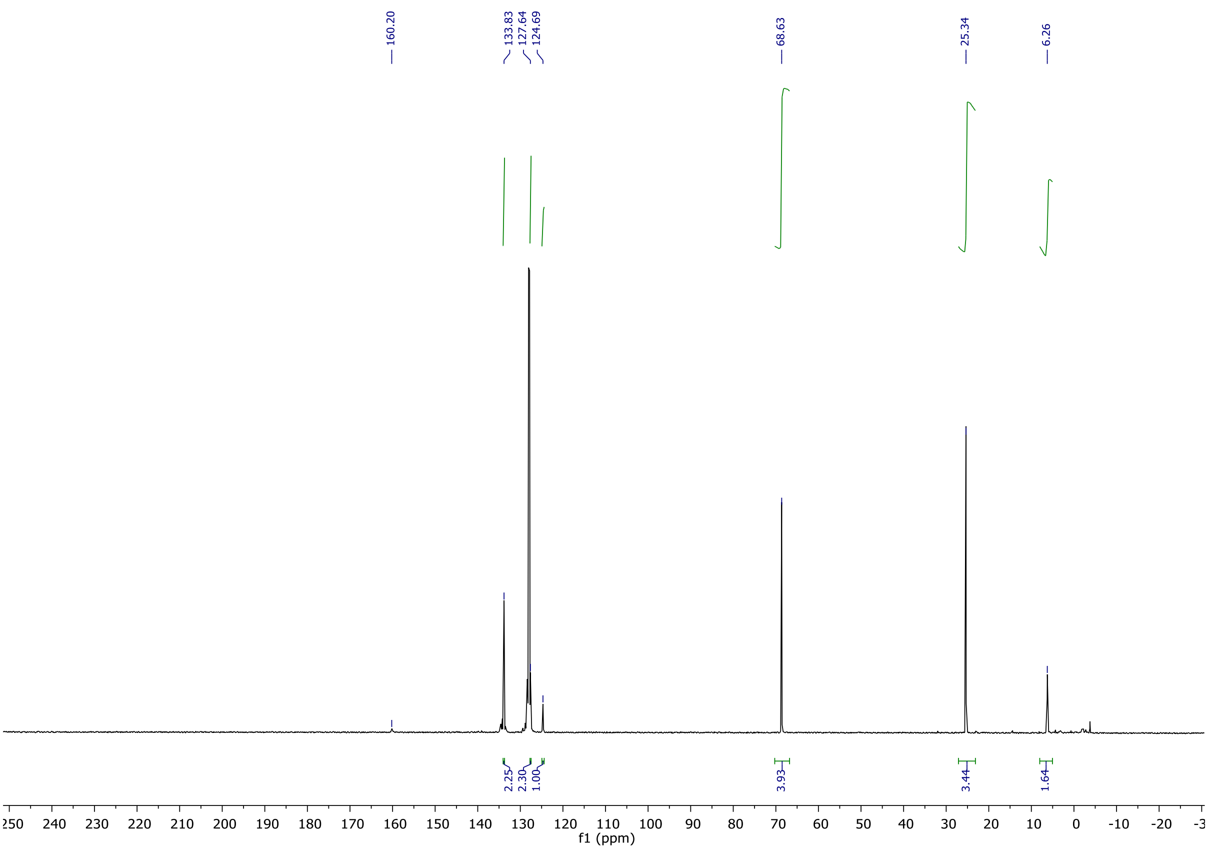


Figure S6: $^{13}C\{^{1}H\}$ NMR spectrum of **1·THF** in C_6D_6

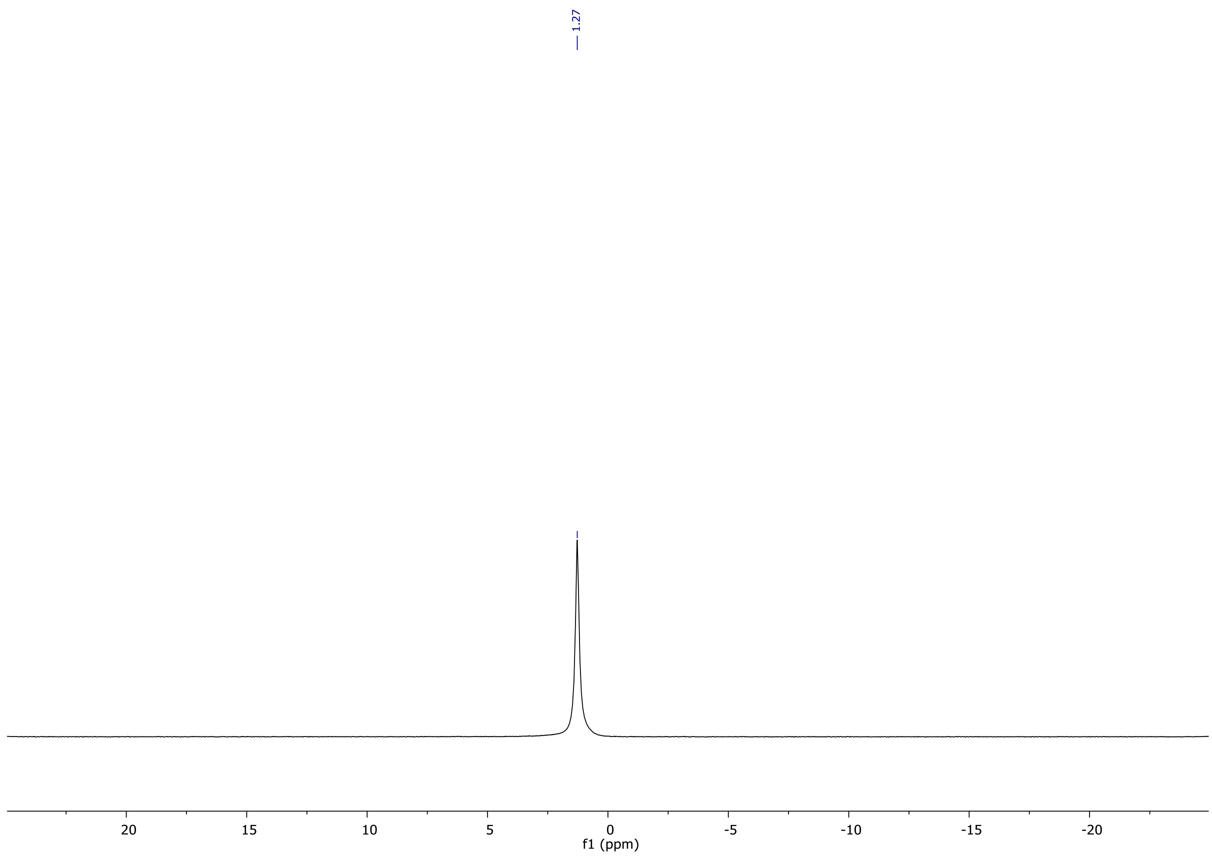


Figure S7: ^{7}Li NMR spectrum of **1·THF** in C_6D_6

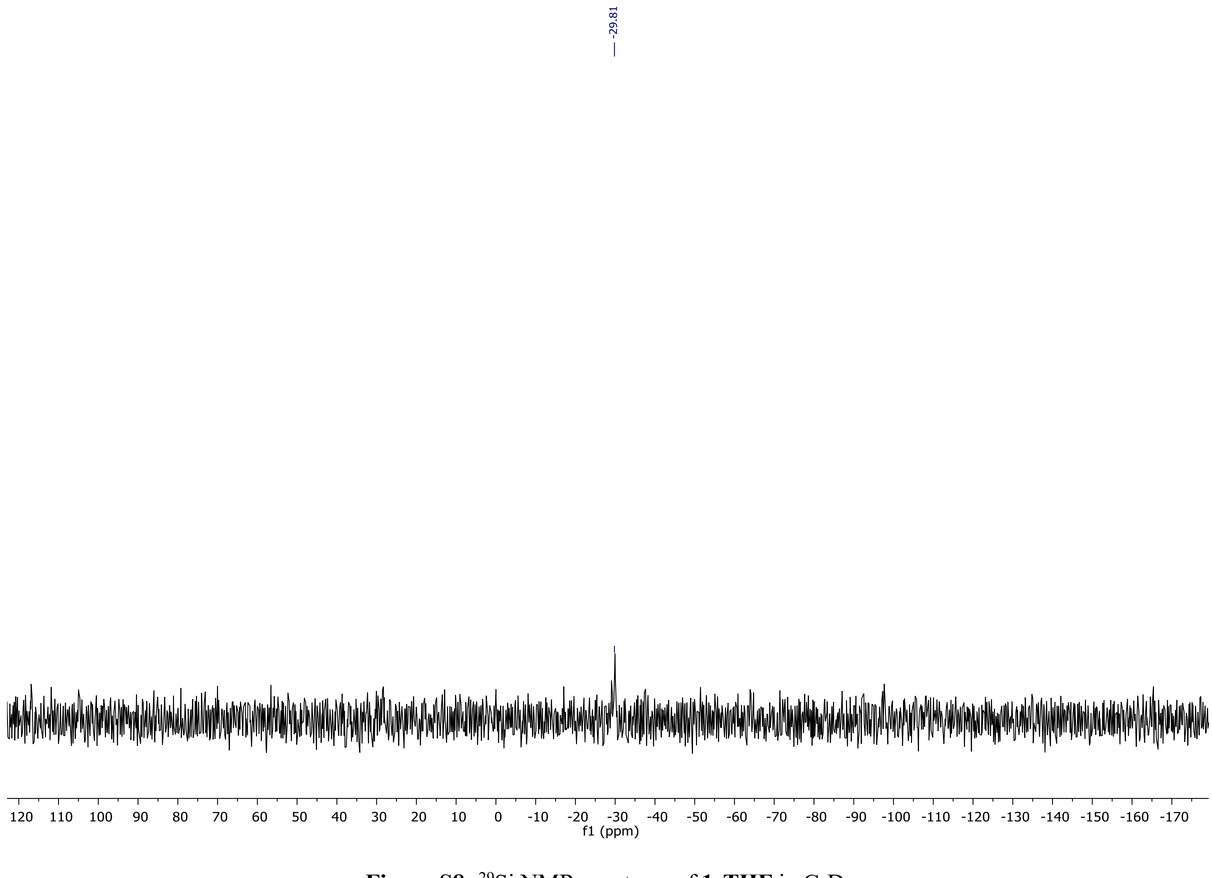


Figure S8: ^{29}Si NMR spectrum of **1·THF** in C_6D_6

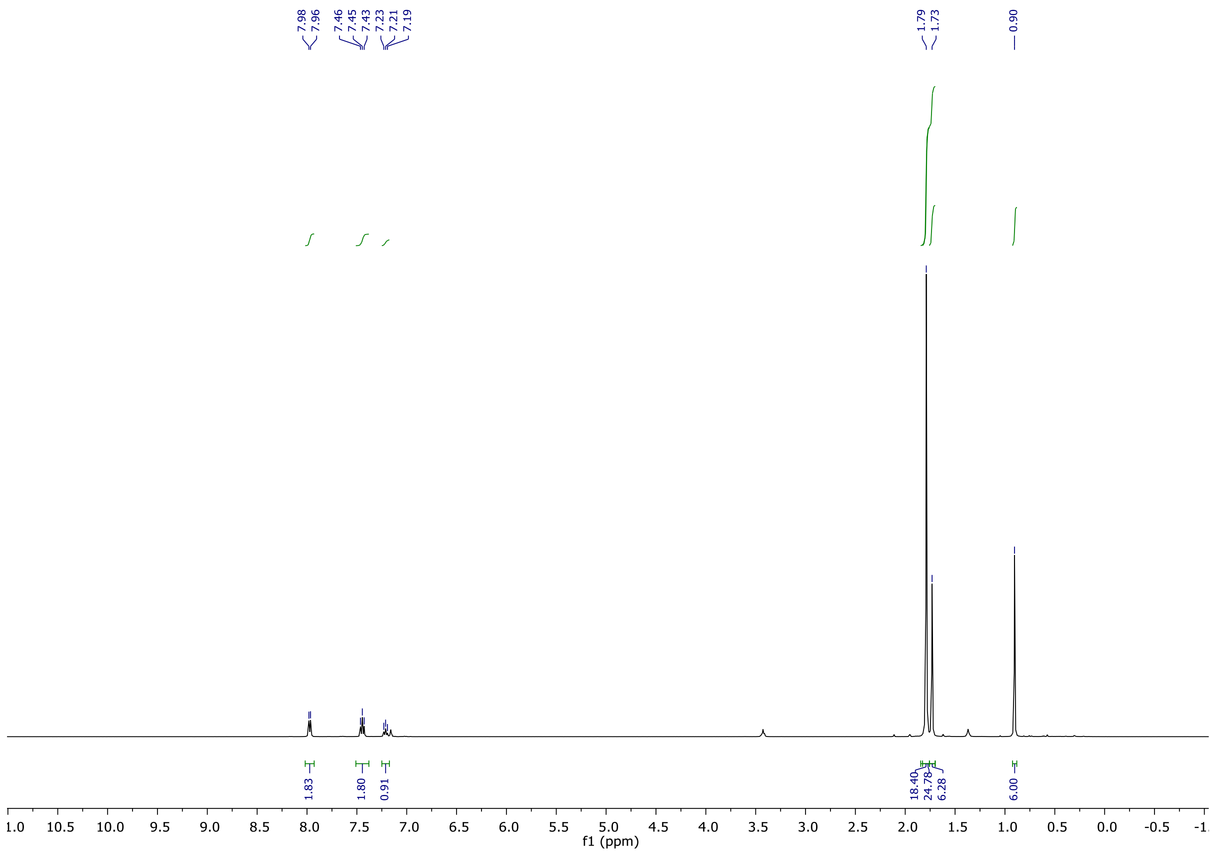


Figure S9: ^{1}H NMR spectrum of **1·TMEDA** in C_6D_6

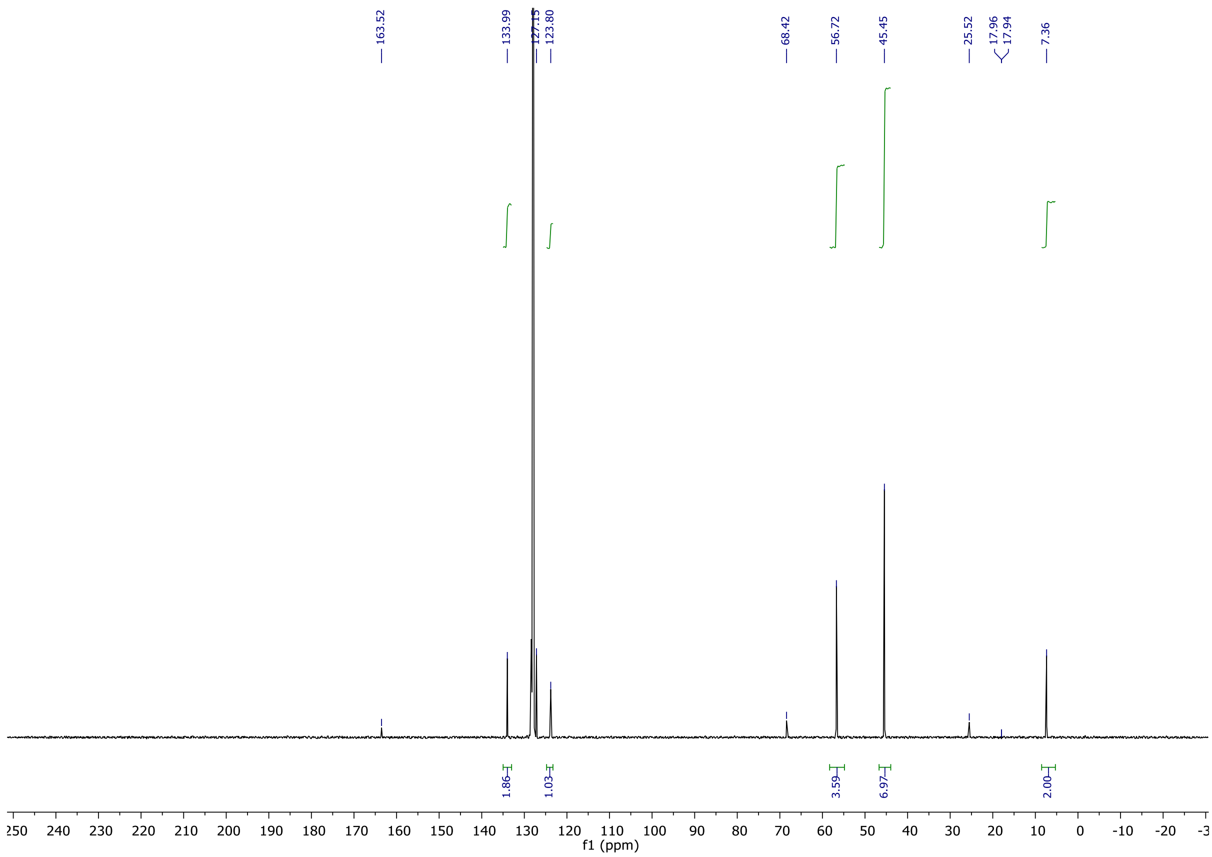


Figure S10: $^{13}C\{^{1}H\}$ NMR spectrum of **1·TMEDA** in C_6D_6

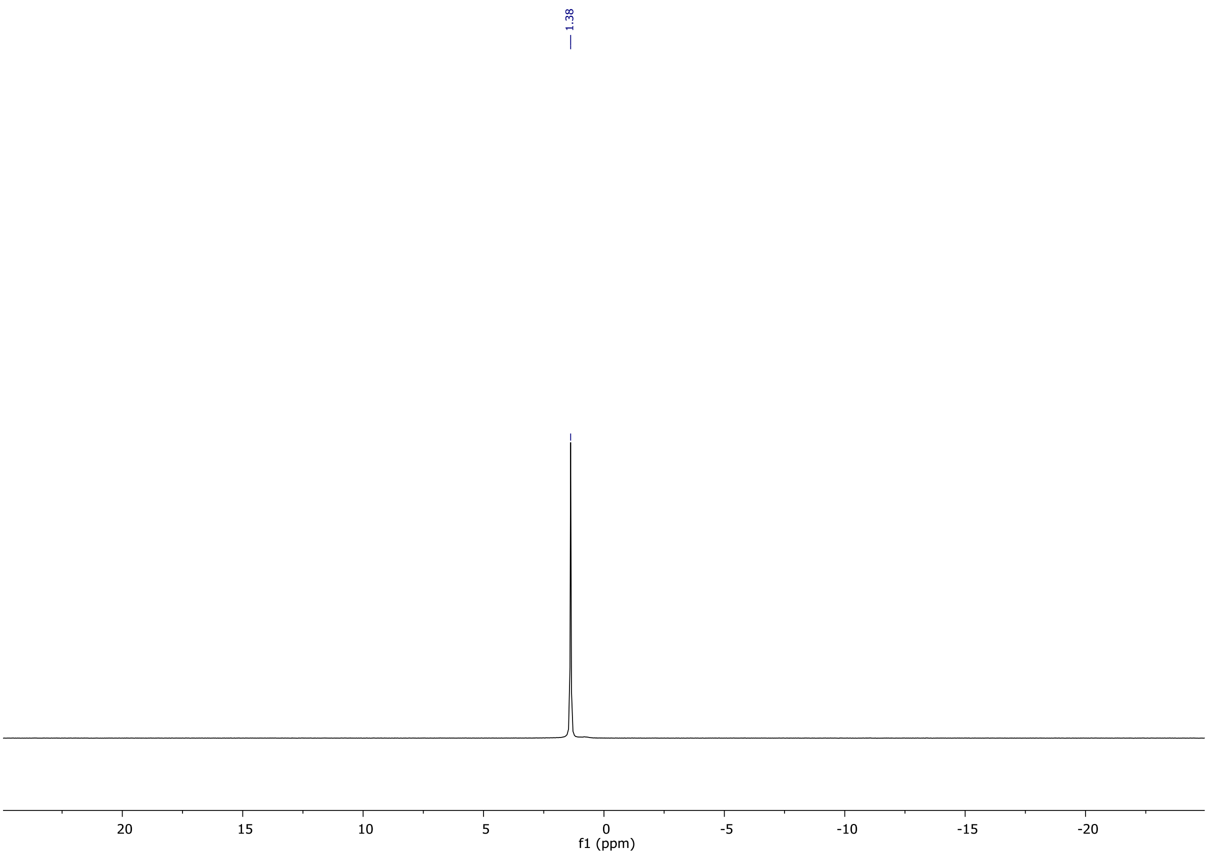


Figure S11: ^{7}Li NMR spectrum of **1·TMEDA** in C_6D_6

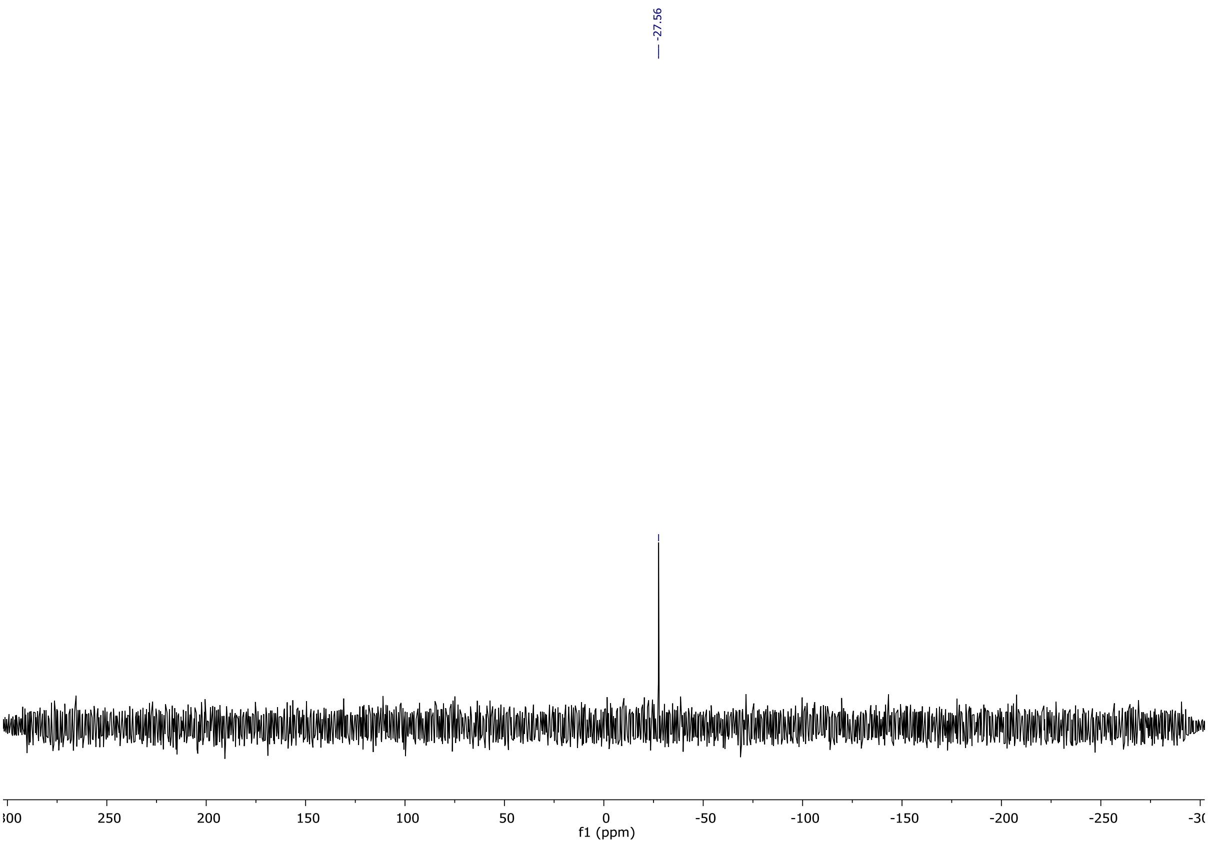


Figure S12: ^{29}Si NMR spectrum of **1·TMEDA** in C_6D_6

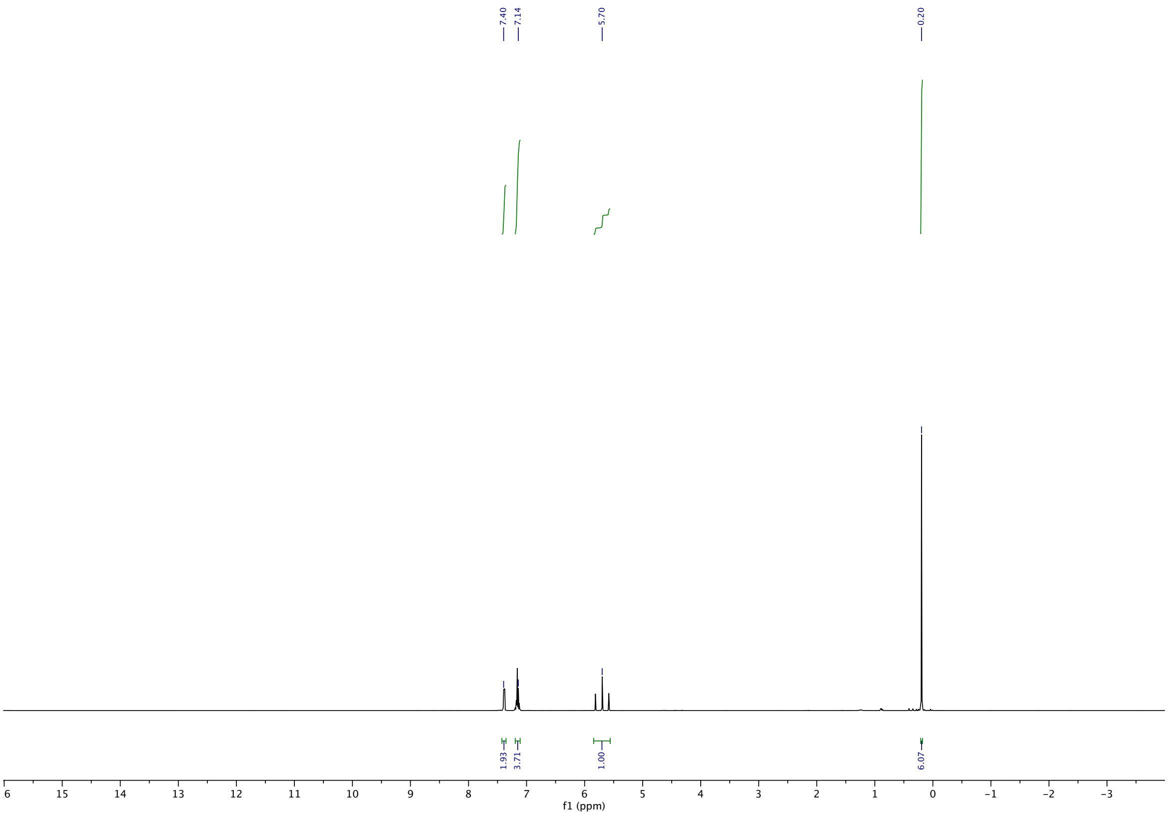


Figure S13: ^{1}H NMR spectrum of **2** in C_6D_6

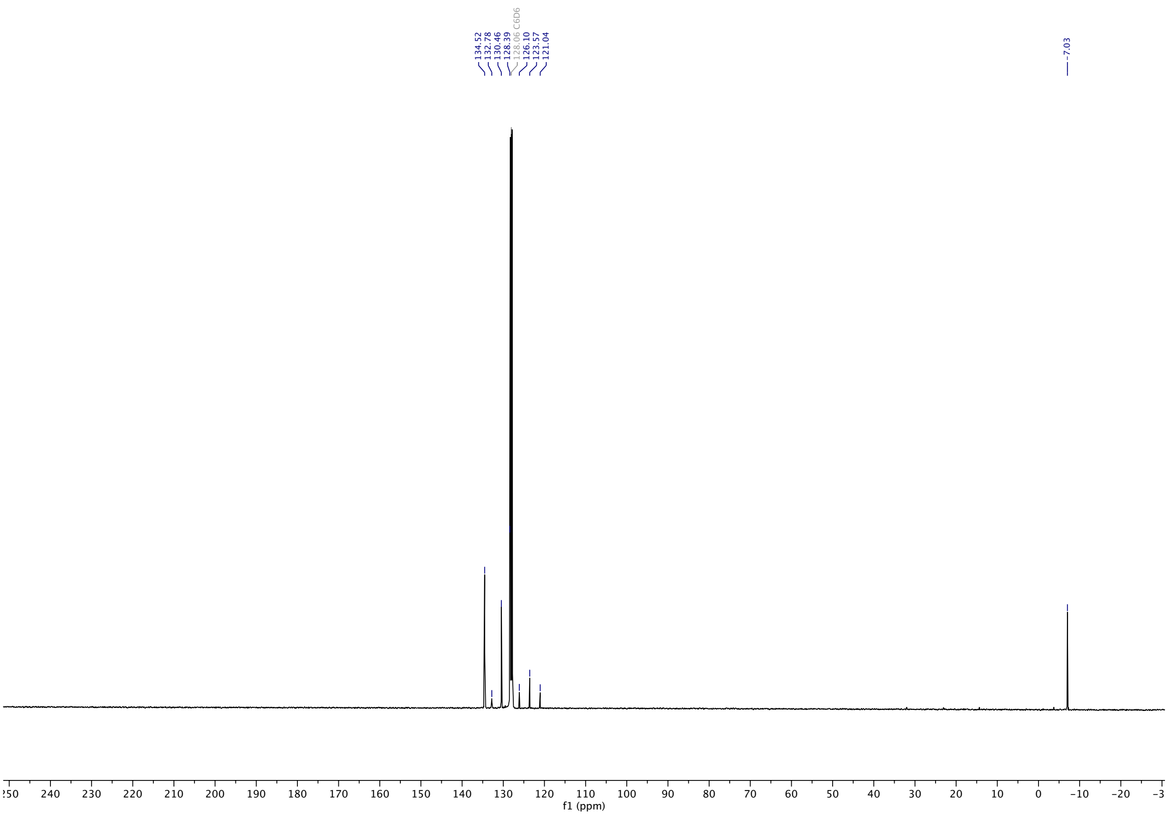


Figure S14: ^{13}C NMR spectrum of **2** in C_6D_6

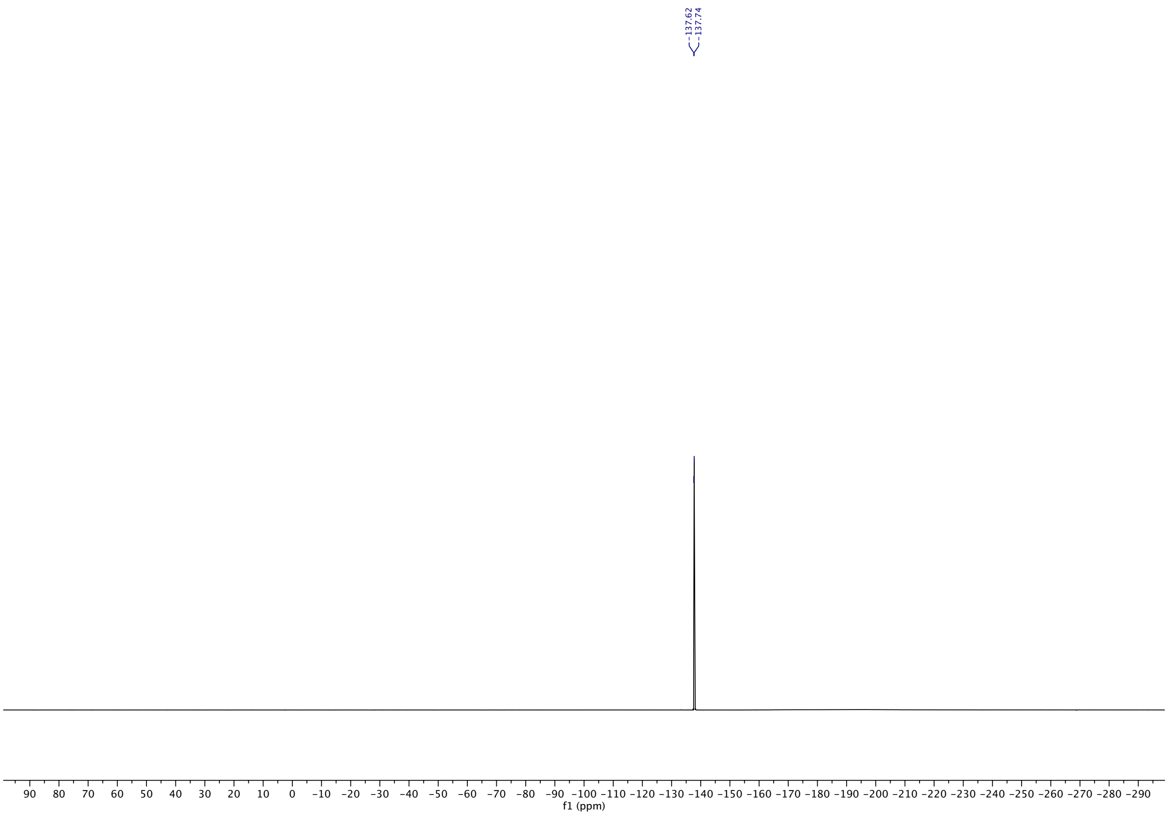


Figure S15: ^{19}F NMR spectrum of **2** in C_6D_6

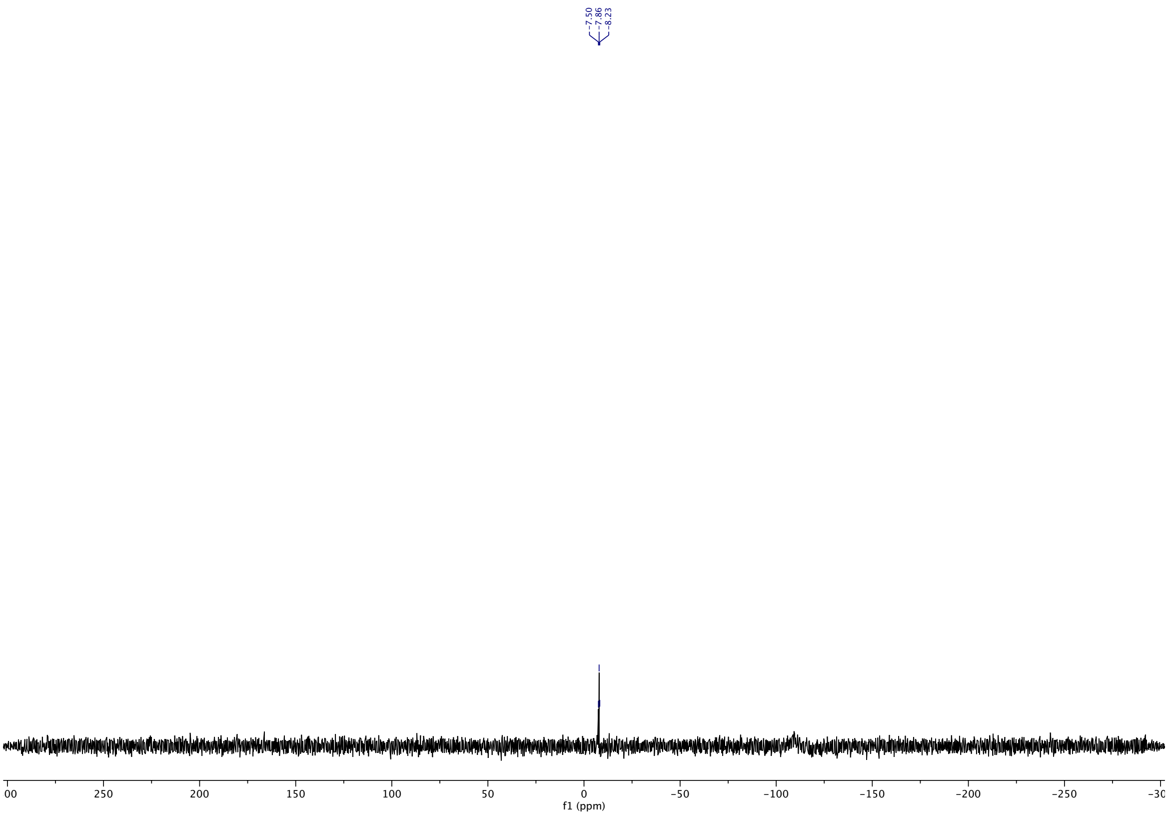


Figure S16: ^{29}Si NMR spectrum of **2** in C_6D_6

5. Computational Methods

DFT calculations were run using Gaussian 09 (Revision D.01)[11] using the B3PW91 density functional,[12–16] incorporating solvent and dispersion effects into the optimisation process. Solvent effects were treated by the polarised continuum model (PCM) with a dielectric constant of 2.2706 (benzene),[17] and dispersion effects were treated by Grimme's D3 correction.[18] A hybrid basis set was used (6-31g**(C, H)/6-311+g*(N, Si, Li, F). Geometry optimisation calculations were performed without symmetry constraints. The Gaussian 09 default optimisation criteria were tightened to 10^{-9} on the density matrix and 10^{-7} on the energy matrix. The default numerical integration grid was also improved using a pruned grid with 99 radial shells and 590 angular points per shell. Frequency analyses for all stationary points were performed using the enhanced criteria to confirm the nature of the structures as either minima (no imaginary frequency) or transition states (only one imaginary frequency). Intrinsic reaction coordinate (IRC) calculations followed by full geometry optimisations on final points were used to connect transition states and minima located on the potential energy surface allowing a full energy profile (calculated at 298.15 K, 1 atm) of the reaction to be constructed.[19,20] The graphical user interface used to visualise the various properties of the intermediates and transition states was GaussView 5.0.9.[21] Natural Bond Orbital analysis was carried out using NBO 6.0.[22]

An assessment of the computational methodology was carried out by a series of functional benchmarking calculations (Table S4). The functionals included were the hybrid GGA functional B3PW91,[12–16] the Minnesota hybrid-meta functional M06-2X,[23] and the long-range corrected functional ω-B97X-D with Grimme's D2 dispersion correction.[24] Throughout functional variation the same basis set was maintained, along with solvent corrections (PCM)[17] and dispersion corrections (GD3)[18] (apart from ω-B97X-D which includes D2 in the functional).

	B3PW91	**ωB97XD**	**M062X**
$\Delta G_1^{\ddagger}$	20.5	21.0	22.4
$\Delta G_2^{\ddagger}$	23.4	23.3	25.1
$\Delta G_3^{\ddagger}$	18.7	19.5	21.0

Table S4: Relative free-energy barriers for the 3 key bond forming steps calculated for various density functionals.

Consistent results were obtained across the different functionals. B3PW91 was the final functional choice as it has been previously established in describing bond activation mechanisms with bimetallic main group reagents,[25,26] including the C–F activation of fluoroalkenes using magnesium silyl reagents.[1]

5.1 NBO Data and Analysis

A full NBO analysis was carried out and the relevant NPA charges and Wiberg Bond Indices are tabulated below (Table S5 and S6).

	HCF_3	SiLi	INT1	TS1	INT2	$LiCF_3$	INT4	TS2	INT5	$SiCF_2Li$	INT7	TS3	INT8
Si1		0.61	0.59	0.93	1.36								
Li1		0.71	0.72	0.87	0.78	0.78	0.84	0.88	0.89				
C1	0.94		0.94	0.77	0.51	0.51	0.55	0.64	-0.21	-0.19	-0.22	-0.07	0.22
F1	-0.38		-0.39	-0.50	-0.47	-0.46	-0.53	-0.93	-0.94				
F2	-0.38		-0.38	-0.41	-0.46	-0.46	-0.45	-0.35	-0.46	-0.46	-0.47	-0.46	-0.41
F3	-0.38		-0.38	-0.42	-0.46	-0.46	-0.44	-0.34	-0.47	-0.46	-0.47	-0.46	-0.41
H1	0.19		0.20	0.004	-0.18								
Si2							0.57	0.64	1.51	1.50	1.51	1.51	1.52
Li2							0.72	0.72	0.82	0.79	0.80	0.88	0.78
H2											0.22	0.21	0.23
C2											0.94	0.84	0.50
F6											-0.38	-0.40	-0.45
F5											-0.39	-0.40	-0.46
F4											-0.39	-0.49	-0.46

Table S5: NPA charges of key stationary points.

	HCF_3	SiLi	INT1	TS1	INT2	$LiCF_3$	INT4	TS2	INT5	$SiCF_2Li$	INT7	TS3	INT8
Si1-Li1		0.29	0.26	0.01	0.003								
C1-F1	0.88		0.85	0.71	0.78	0.79	0.67	0.02	0.001				
C1-F2	0.88		0.88	0.85	0.79	0.79	0.80	0.98	0.76	0.77	0.76	0.79	0.84
C1-F3	0.88		0.87	0.84	0.80	0.80	0.81	1.00	0.76	0.77	0.76	0.79	0.84
C1-H1	0.91		0.87	0.38	0.001								
Si1-H1			0.03	0.55	0.90								
Li1-C1			0.001	0.01	0.16	0.18	0.05	0.01	0.01				
Li1-F1			0.004	0.03	0.01		0.03	0.03	0.03				
Si2-Li1							0.01	0.01	0.001				
Si2-Li2							0.19	0.17	0.01		0.01	0.002	0.0004
Si2-C1							0.02	0.17	0.91	0.90	0.89	0.90	0.81
C1-Li2							0.09	0.11	0.10	0.15	0.12	0.008	0.0003
C1-H2											0.002	0.31	0.90
C2-H2											0.89	0.61	0.001
Li2-C2											0.001	0.01	0.16
Li2-F4											0.01	0.02	0.02

Table S6: Wiberg Bond Indices of key stationary points.

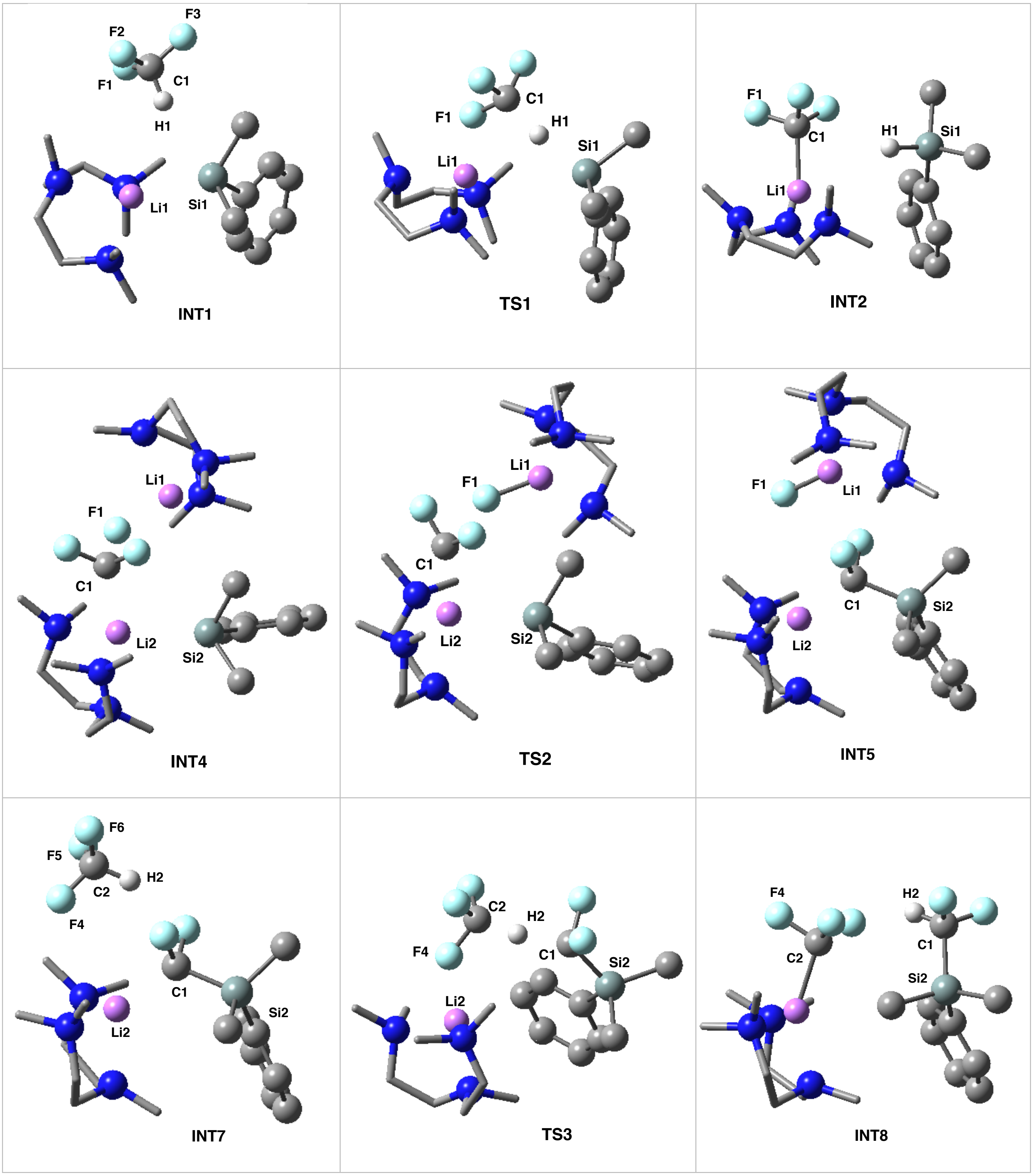


Figure S17: Calculated structures of **INT1, TS1, INT2, INT4, TS2, INT5, INT7, TS3** and **INT8**, relevant for NBO analysis.

5.2 Additional Mechanistic Discussion

In the calculated pathway (Figure 3, manuscript), the CF_3^- anion formed in **TS1** from deprotonation primarily interacts with the lithium cation through a fluorine lone pair, reflected by an interaction of 8 kcal mol^{-1} identified by second-order perturbation analysis. A similar geometry is observed later where there is an isomerisation of PMDETA·$LiCF_3$ from a tetrahedral shape (**INT3**) to a geometry with strong coordination of one fluorine atom to the lithium cation (**INT4**), which is again reflected by an interaction of 8 kcal mol^{-1}. This 8 kcal mol^{-1} interaction is observed again in **TS3** in the protonation of $PhMe_2SiCF_2Li$·PMDETA by HCF_3 (Figure S18). Various equilibrium isomers of $LiCF_3$ have previously been calculated with similar geometries.[27]

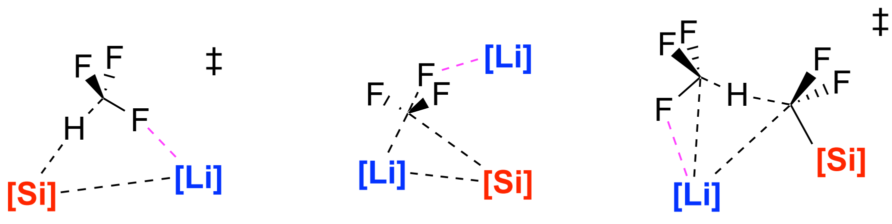


Figure S18: **TS1, INT4** and **TS3**, displaying Li···F interactions (labelled in pink).

5.3 High-Energy Transition States of Alternative Mechanisms

Alternative mechanisms were explored and ruled out on the basis of finding transition states that were prohibitively high in energy. **TS4** represents a direct S_N2 attack of **1·PMDETA** at HCF_3, and **TS5** represents a 'frontside' nucleophilic attack at the fluorine atom of HCF_3 by **1·PMDETA**.

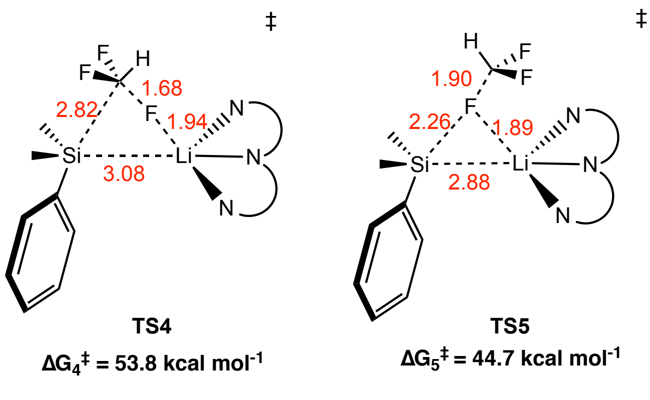


Figure S19: High-energy transition states of alternative mechanistic pathways, annotated with bond lengths (Å).

5.4 DFT Coordinates and Energies

CF3LiPMDETA

SCF (B3PW91) = -866.146814499
E(SCF)+ZPE(0 K)= -865.804330
H(298 K)= -865.782678
G(298 K)= -865.853522
Lowest Frequency = 27.4982cm-1

N	-5.51770500	4.10470100	0.86426000
Li	-4.19591100	2.46493400	0.60918300
C	-6.20201900	2.40254900	2.52205900
C	-6.02013200	3.88935200	2.22651300
H	-6.65903300	2.27295800	3.51908600
H	-6.90080100	1.97424600	1.79643200
H	-6.97615100	4.41522400	2.38837800
H	-5.31174300	4.32165600	2.93986000
C	-3.26826500	5.06111500	1.28089800
C	-4.67833300	5.29929500	0.74372800
H	-2.66377700	5.97178500	1.11750100
H	-3.30605000	4.90560100	2.36544000
H	-5.11783300	6.17168500	1.25753600
H	-4.62643500	5.56415500	-0.31645400
C	-6.60251500	4.10214700	-0.11721800
H	-7.28172000	4.96181500	0.01355700
H	-6.18447500	4.11637900	-1.12595700
H	-7.18223100	3.18099300	-0.02966900
N	-2.62932500	3.87973200	0.68902900
N	-4.93819100	1.66021900	2.41111200
C	-5.19166400	0.22770500	2.22929100
H	-4.23954200	-0.30098300	2.12791600
H	-5.74098100	-0.20599900	3.08237600
H	-5.76316000	0.07064800	1.31173000
C	-4.08039300	1.87568500	3.57438200
H	-3.12914300	1.35591700	3.42959000
H	-3.86355500	2.93911100	3.70415500
H	-4.54254500	1.50366300	4.50522500
C	-2.31902700	4.08028600	-0.73055200
H	-1.66646000	4.95644900	-0.88735800
H	-1.81533900	3.19193700	-1.11871400
H	-3.23418500	4.20495500	-1.31253900
C	-1.41512000	3.53214300	1.42530600
H	-1.65646600	3.34521000	2.47567700
H	-0.98061000	2.62015600	1.00634800
H	-0.65500400	4.33094000	1.37971600
C	-4.65660000	1.41417200	-1.13185400
F	-5.92904800	0.79956500	-1.07989300
F	-4.78302600	2.21237600	-2.28783800
F	-3.85511000	0.36446300	-1.59873300

HCF3

SCF (B3PW91) = -338.215834929
E(SCF)+ZPE(0 K)= -338.190714
H(298 K)= -338.186298
G(298 K)= -338.216833
Lowest Frequency = 504.8451cm-1

C	-0.555488	-0.056957	0.000000
H	-1.649379	-0.056937	-0.000006
F	-0.082883	-1.309893	0.000003
F	-0.082863	0.569523	-1.085067
F	-0.082872	0.569521	1.085070

INT1

SCF (B3PW91) = -1467.62895838
E(SCF)+ZPE(0 K)= -1467.106567
H(298 K)= -1467.073073
G(298 K)= -1467.171353
Lowest Frequency = 16.3386cm-1

Si	0.163539	-1.990027	0.338770
C	1.567105	-2.003812	-0.972425
C	2.930410	-2.141900	-0.650266
C	1.272278	-1.712757	-2.320286
C	3.937523	-1.970710	-1.602836
H	3.217769	-2.376205	0.372830
C	2.267326	-1.547042	-3.283103
H	0.232282	-1.595139	-2.623261
C	3.612784	-1.664479	-2.924744
H	4.980621	-2.076889	-1.312172
H	1.996675	-1.322113	-4.312915
H	4.394620	-1.526326	-3.666971
C	0.945220	-2.944700	1.821208
H	0.195984	-3.099429	2.608376
H	1.300262	-3.934430	1.501345
H	1.793582	-2.428299	2.285380
C	-1.007203	-3.358729	-0.361567
H	-0.475999	-4.317503	-0.436362
H	-1.880054	-3.508710	0.286695
H	-1.378509	-3.113817	-1.364589
N	-1.623571	2.351595	0.583306
Li	-0.684394	0.505458	-0.169404
C	0.650291	3.056381	-0.115757
C	-0.828348	3.413169	-0.053455
H	1.212963	3.906672	-0.542068
H	1.032223	2.904553	0.898601
H	-0.952447	4.371163	0.478826
H	-1.206798	3.579178	-1.065895
C	-3.109189	1.694627	-1.289992
C	-3.004358	2.342359	0.086289
H	-4.167956	1.697514	-1.607264
H	-2.565720	2.294711	-2.028707
H	-3.428884	3.360184	0.044183
H	-3.616837	1.786649	0.802489
C	-1.598551	2.483566	2.041068
H	-2.124273	3.391144	2.383639
H	-2.066582	1.609381	2.501841
H	-0.568434	2.534019	2.396157
N	-2.547682	0.340624	-1.311355
N	0.901223	1.821855	-0.870242
C	2.263715	1.349140	-0.601130
H	2.467367	0.454038	-1.188445
H	3.014196	2.118898	-0.851708
H	2.364605	1.091974	0.455707
C	0.738242	2.019124	-2.311218
H	0.925450	1.071347	-2.822653
H	-0.278734	2.341799	-2.548631
H	1.438600	2.776041	-2.705853
C	-3.381598	-0.587310	-0.541206
H	-4.425480	-0.589953	-0.900885
H	-2.973668	-1.594204	-0.624096
H	-3.375139	-0.324578	0.519107
C	-2.423037	-0.136113	-2.688172
H	-1.752324	0.517875	-3.252633
H	-1.998337	-1.142704	-2.686532
H	-3.396323	-0.172434	-3.207360
C	1.117002	0.262799	3.299382
H	0.719638	-0.279799	2.426511
F	1.581303	1.476482	2.930124
F	2.126620	-0.394128	3.881190
F	0.161687	0.460609	4.221424

INT2

SCF (B3PW91) = -1467.64521356
E(SCF)+ZPE(0 K)= -1467.127727
H(298 K)= -1467.093750
G(298 K)= -1467.193402
Lowest Frequency = 19.1646cm-1

Si	0.312632	-3.117828	0.080108
C	1.417535	-2.312262	-1.222782
C	2.696360	-1.833552	-0.891756
C	1.006175	-2.192848	-2.562090
C	3.528140	-1.257390	-1.853497
H	3.051714	-1.908889	0.133220
C	1.830519	-1.615566	-3.528282
H	0.029865	-2.564094	-2.865612
C	3.096175	-1.145768	-3.174564
H	4.511783	-0.893170	-1.569355
H	1.488314	-1.537152	-4.556989
H	3.741755	-0.697326	-3.924720
C	1.344361	-3.769669	1.500906
H	0.710856	-4.320739	2.204191
H	2.131969	-4.443332	1.146073
H	1.801354	-2.941263	2.049781
C	-0.691627	-4.488399	-0.732611
H	-0.035510	-5.247281	-1.172913
H	-1.331430	-4.980048	0.008614
H	-1.341669	-4.104633	-1.526705
N	-1.562898	3.008664	0.476611
Li	-0.589087	1.087376	0.468087
C	0.765420	3.470283	-0.226336
C	-0.710964	3.799063	-0.419977
H	1.377014	4.115043	-0.882744
H	1.055339	3.704638	0.802667
H	-0.869563	4.881137	-0.270611
H	-0.998151	3.589406	-1.454814
C	-2.904364	1.704184	-1.142720
C	-2.902199	2.794520	-0.075025
H	-3.941104	1.546140	-1.492148
H	-2.331038	2.036523	-2.016021
H	-3.329960	3.718930	-0.500759
H	-3.562482	2.504352	0.747654
C	-1.616982	3.587562	1.818377
H	-2.097712	4.581190	1.822856
H	-2.168836	2.919030	2.483383
H	-0.610124	3.678427	2.228996
N	-2.303373	0.450503	-0.673863
N	1.049275	2.049049	-0.452263
C	2.310403	1.668924	0.187045
H	2.482944	0.602374	0.038982
H	3.166627	2.225427	-0.233040
H	2.247817	1.854105	1.261356
C	1.079745	1.707867	-1.872703
H	1.230762	0.631723	-1.987892
H	0.132269	1.970013	-2.352294
H	1.891391	2.231456	-2.407998
C	-3.131190	-0.196267	0.349341
H	-4.153759	-0.395421	-0.016032
H	-2.668586	-1.140384	0.643744
H	-3.189156	0.423068	1.246812
C	-2.100084	-0.456582	-1.801386
H	-1.412744	-0.008415	-2.524361
H	-1.652174	-1.384923	-1.443132
H	-3.045628	-0.701583	-2.315941
C	-0.020808	0.376325	2.350910
H	-0.641716	-2.097774	0.591890
F	0.482564	1.423335	3.162528
F	1.049389	-0.538135	2.396108
F	-0.946444	-0.225258	3.214863

INT4

SCF (B3PW91) = -1995.56143599
E(SCF)+ZPE(0 K)= -1994.722638
H(298 K)= -1994.671984
G(298 K)= -1994.805467
Lowest Frequency = 17.4659cm-1

Si	1.621983	-1.456048	0.248657
C	1.168618	-2.861351	-1.021419
C	2.038419	-3.276005	-2.047912
C	-0.092262	-3.479769	-0.991334
C	1.666186	-4.225663	-2.999985
H	3.031426	-2.833006	-2.114738
C	-0.482809	-4.434949	-1.933361
H	-0.796452	-3.184873	-0.213170
C	0.396956	-4.807054	-2.949093
H	2.363359	-4.514592	-3.784337
H	-1.472910	-4.883530	-1.879014
H	0.100504	-5.544377	-3.691337
C	2.412302	-0.150091	-0.955601
H	2.818188	0.675638	-0.359501
H	3.224372	-0.556031	-1.577421
H	1.666898	0.281671	-1.634987
C	3.285832	-2.203600	0.930492
H	3.993965	-2.414828	0.115078
H	3.785722	-1.513104	1.623286
H	3.122290	-3.145628	1.468335
N	-1.705022	2.991997	-2.795405
Li	-0.243963	1.785954	-1.818110
C	0.406713	4.255992	-3.052448
C	-0.911198	3.837638	-3.696007
H	0.954052	4.927148	-3.738304
H	0.201170	4.834333	-2.145466
H	-1.473120	4.737692	-3.997275
H	-0.709331	3.284130	-4.617250
C	-1.773890	0.874044	-4.091030
C	-2.563799	2.047684	-3.516978
H	-2.478039	0.175670	-4.578487
H	-1.100623	1.228255	-4.880120
H	-3.124313	2.539487	-4.331008
H	-3.312638	1.676557	-2.810640
C	-2.477374	3.798437	-1.850421
H	-3.250424	4.401272	-2.356678
H	-2.949113	3.146321	-1.112692
H	-1.814635	4.473007	-1.303401
N	-0.953643	0.187693	-3.085874
N	1.231470	3.102922	-2.664061
C	2.288114	3.529090	-1.740598
H	2.879377	2.660632	-1.444394
H	2.955820	4.274997	-2.204804
H	1.842780	3.954013	-0.839237
C	1.841840	2.461526	-3.830660
H	2.412473	1.587960	-3.505126
H	1.076024	2.120891	-4.530904
H	2.518974	3.147727	-4.367984
C	-1.782658	-0.571684	-2.144208
H	-2.337118	-1.379656	-2.650672
H	-1.141311	-1.013171	-1.378048
H	-2.493241	0.088532	-1.645097
C	-0.019682	-0.730351	-3.746095
H	0.659685	-0.172163	-4.395591
H	0.570210	-1.260843	-2.997742
H	-0.550474	-1.481974	-4.353852
C	-0.361527	1.694575	1.126423
F	0.798172	2.271146	0.597671
F	-1.151019	1.595329	-0.132620

F	-0.979347	2.808662	1.691524
N	-0.304947	-2.387648	3.521411
Li	-0.097014	-0.307522	2.047965
C	1.477239	-0.951488	4.479814
C	0.302560	-1.886454	4.751436
H	1.974792	-0.712373	5.439730
H	2.213765	-1.471018	3.857579
H	0.652457	-2.716937	5.392629
H	-0.455146	-1.357848	5.336728
C	-2.595443	-1.451130	3.730871
C	-1.719968	-2.697515	3.668893
H	-3.653664	-1.772974	3.798375
H	-2.387016	-0.894654	4.652171
H	-1.924621	-3.315826	4.564463
H	-2.016262	-3.307856	2.809324
C	0.427941	-3.531939	3.000051
H	0.335631	-4.420555	3.653493
H	0.069457	-3.782090	1.998162
H	1.484780	-3.282761	2.900791
N	-2.389566	-0.536324	2.611593
N	1.093071	0.268543	3.768017
C	2.284268	0.965633	3.285430
H	1.986857	1.853725	2.724285
H	2.947861	1.271477	4.115128
H	2.840251	0.313273	2.607956
C	0.296261	1.168816	4.595817
H	0.016741	2.045079	4.006116
H	-0.627696	0.682006	4.916239
H	0.843892	1.501178	5.497145
C	-2.804076	-1.121314	1.341424
H	-3.863727	-1.440929	1.349735
H	-2.664105	-0.379524	0.553681
H	-2.178742	-1.982653	1.094439
C	-3.116354	0.706323	2.847532
H	-2.749974	1.183664	3.760889
H	-2.941958	1.397179	2.021801
H	-4.204831	0.538552	2.952297

INT5

SCF (B3PW91) = -1995.63172889
E(SCF)+ZPE(0 K)= -1994.792060
H(298 K)= -1994.741345
G(298 K)= -1994.875103
Lowest Frequency = 4.9863cm-1

Si	2.522427	-1.372800	-0.436512
C	1.515721	-2.956141	-0.663777
C	2.086097	-4.235470	-0.564885
C	0.126326	-2.877919	-0.861869
C	1.303877	-5.388558	-0.647817
H	3.157120	-4.339432	-0.401475
C	-0.663780	-4.024886	-0.946920
H	-0.343450	-1.901136	-0.922812
C	-0.075409	-5.285599	-0.834705
H	1.768252	-6.367670	-0.560361
H	-1.737385	-3.934059	-1.094482
H	-0.686953	-6.182200	-0.892845
C	3.335515	-0.869627	-2.066285
H	3.890671	0.065688	-1.931000
H	4.035282	-1.635793	-2.420519
H	2.585626	-0.707676	-2.845604
C	3.888327	-1.694392	0.825107
H	4.566055	-2.492368	0.501746
H	4.483621	-0.785410	0.965705
H	3.471603	-1.978937	1.796611
N	-2.207552	3.321310	-3.232838
Li	-1.284756	1.980095	-1.706070
C	-0.298395	4.644328	-2.402787
C	-1.134720	4.236128	-3.613564
H	0.490849	5.350300	-2.721420
H	-0.932145	5.187472	-1.694460
H	-1.526482	5.143252	-4.110094
H	-0.490833	3.740889	-4.346304
C	-1.642302	1.352819	-4.628297
C	-2.647416	2.458530	-4.323531
H	-2.051961	0.715909	-5.435923
H	-0.717683	1.790423	-5.022523
H	-2.847800	3.025487	-5.252214
H	-3.601339	2.011408	-4.026415
C	-3.332814	4.012678	-2.615988
H	-3.883827	4.641403	-3.339545
H	-4.002592	3.276300	-2.167585
H	-2.982651	4.650064	-1.801541
N	-1.283734	0.559511	-3.452990
N	0.264627	3.489838	-1.700713
C	0.609289	3.835740	-0.322324
H	1.019082	2.956766	0.177236
H	1.356109	4.649621	-0.274415
H	-0.292392	4.153544	0.209911
C	1.427150	2.940234	-2.394883
H	1.776374	2.054788	-1.861027
H	1.154067	2.639466	-3.410389
H	2.252560	3.672637	-2.461730
C	-2.404714	-0.253752	-2.980633
H	-2.818516	-0.893314	-3.781869
H	-2.059330	-0.895691	-2.167683
H	-3.189538	0.382823	-2.566322
C	-0.137225	-0.288584	-3.759707
H	0.708638	0.332032	-4.069607
H	0.160890	-0.836536	-2.866089
H	-0.354413	-1.011437	-4.567112
C	1.340379	-0.088500	0.314708
F	2.168619	1.101253	0.449645
F	-2.555312	1.810230	-0.536763
F	0.433165	0.313624	-0.758357
N	-0.016780	-2.393205	3.231444
Li	0.180873	-0.480867	2.076660
C	1.611857	-1.031129	4.508872
C	0.450393	-2.015036	4.571705
H	2.008377	-0.859635	5.526759
H	2.426664	-1.473530	3.925616
H	0.754897	-2.904275	5.149460
H	-0.377287	-1.565368	5.126996
C	-2.295629	-1.407890	3.269392
C	-1.455246	-2.679154	3.206685
H	-3.365865	-1.687960	3.258709
H	-2.125601	-0.893993	4.222907
H	-1.751648	-3.354986	4.028958
H	-1.668306	-3.213470	2.275614
C	0.744609	-3.530455	2.718493
H	0.604838	-4.434247	3.337927
H	0.440760	-3.751418	1.694341
H	1.810519	-3.292501	2.697673
N	-1.982361	-0.470903	2.190652
N	1.237270	0.230420	3.861624
C	2.434391	0.975166	3.466897
H	2.142948	1.887345	2.942700
H	3.056316	1.242864	4.339766
H	3.026177	0.381205	2.769007
C	0.412119	1.063029	4.733920
H	0.123595	1.972786	4.200684
H	-0.503770	0.541791	5.021148
H	0.946752	1.353004	5.656253
C	-2.470108	-0.965860	0.897822
H	-3.554312	-1.177977	0.935852

H	-2.298974	-0.192996	0.143014
H	-1.948867	-1.884473	0.620706
C	-2.582454	0.841454	2.455261
H	-2.139470	1.278693	3.355485
H	-2.412158	1.488751	1.588691
H	-3.673516	0.762332	2.609834

INT7

SCF (B3PW91) = -1705.40715988
E(SCF)+ZPE(0 K)= -1704.874640
H(298 K)= -1704.837483
G(298 K)= -1704.944502
Lowest Frequency = 19.8236cm-1

Si	1.836994	-0.594818	-1.603110
C	0.922338	-2.241959	-1.746171
C	1.537865	-3.473273	-1.468610
C	-0.445509	-2.255933	-2.071393
C	0.817551	-4.668538	-1.493588
H	2.593799	-3.503249	-1.207809
C	-1.175259	-3.445650	-2.090166
H	-0.945877	-1.318010	-2.298049
C	-0.544856	-4.655862	-1.794907
H	1.315786	-5.608373	-1.269332
H	-2.234265	-3.429468	-2.336669
H	-1.110685	-5.583743	-1.804578
C	2.471766	-0.063901	-3.297286
H	2.977440	0.905651	-3.227518
H	3.177213	-0.793504	-3.711538
H	1.636690	0.039772	-3.998236
C	3.286055	-0.805851	-0.414497
H	4.022150	-1.528706	-0.783146
H	3.795548	0.154743	-0.282505
H	2.942300	-1.144746	0.569133
C	0.629990	0.633344	-0.790875
F	1.409951	1.866285	-0.693694
F	-0.342304	1.006798	-1.821515
N	-0.651570	-1.651269	2.148085
Li	-0.407256	0.229506	1.031392
C	0.952429	-0.290013	3.455215
C	-0.214248	-1.270546	3.498263
H	1.322544	-0.107237	4.480406
H	1.781691	-0.740411	2.898526
H	0.073001	-2.158866	4.085677
H	-1.053317	-0.814596	4.031366
C	-2.943945	-0.695893	2.111499
C	-2.084348	-1.956300	2.088954
H	-4.006996	-0.988122	2.028864
H	-2.839301	-0.190272	3.078253
H	-2.398339	-2.622153	2.912023
H	-2.265172	-2.509208	1.162054
C	0.136925	-2.771541	1.638198
H	0.014394	-3.679073	2.254935
H	-0.159323	-2.996176	0.613059
H	1.197532	-2.510238	1.619473
N	-2.570329	0.263224	1.067868
N	0.592892	0.963121	2.782674
C	1.794470	1.701933	2.386332
H	1.504648	2.607213	1.850501
H	2.411344	1.978917	3.259185
H	2.390728	1.096768	1.701008
C	-0.246985	1.809884	3.628329
H	-0.528638	2.708352	3.074944
H	-1.164807	1.288914	3.911807
H	0.273471	2.114637	4.553374
C	-2.930157	-0.226446	-0.265569
H	-4.019774	-0.376374	-0.364876
H	-2.590362	0.488593	-1.017350
H	-2.427454	-1.172998	-0.472109
C	-3.217982	1.551923	1.309668
H	-2.897219	1.958747	2.272316
H	-2.931891	2.259556	0.530232
H	-4.318730	1.466664	1.313853
C	-0.740975	3.998962	-0.548174
H	-0.276747	3.182212	-1.102536
F	-0.095606	5.158690	-0.738108
F	-2.023596	4.177560	-0.915499
F	-0.735036	3.739649	0.773678

INT8

SCF (B3PW91) = -1705.42581734
E(SCF)+ZPE(0 K)= -1704.892968
H(298 K)= -1704.856155
G(298 K)= -1704.960721
Lowest Frequency = 26.1105cm-1

Si	2.324319	-0.460759	-2.048282
C	0.939200	-1.727090	-2.119835
C	1.236192	-3.100474	-2.102884
C	-0.413849	-1.343892	-2.139858
C	0.224460	-4.060818	-2.090863
H	2.272373	-3.431976	-2.096317
C	-1.427815	-2.303594	-2.152020
H	-0.688132	-0.292221	-2.139302
C	-1.112010	-3.662615	-2.118182
H	0.478315	-5.117227	-2.070092
H	-2.467219	-1.990070	-2.198449
H	-1.903615	-4.407037	-2.123218
C	3.877424	-1.107037	-2.872118
H	4.643817	-0.325351	-2.889200
H	4.287571	-1.968310	-2.333812
H	3.674667	-1.410126	-3.904009
C	2.641218	0.078386	-0.281813
H	3.089102	-0.736234	0.297531
H	3.316695	0.939164	-0.252501
H	1.697439	0.375889	0.183722
C	1.767192	1.101594	-3.036850
F	2.815089	2.007453	-3.064795
F	1.506695	0.767561	-4.354909
N	-0.601082	-1.536263	2.105488
Li	-0.821157	0.522109	1.404098
C	0.908245	-0.176490	3.530143
C	-0.090328	-1.328496	3.469604
H	1.335168	-0.110575	4.547042
H	1.742803	-0.384017	2.851305
H	0.383489	-2.245876	3.856805
H	-0.929905	-1.118247	4.137750
C	-3.014098	-1.027253	2.453333
C	-1.965878	-2.078657	2.094727
H	-4.016903	-1.485392	2.374113
H	-2.897547	-0.724590	3.500188
H	-2.068958	-2.939335	2.778339
H	-2.156516	-2.461785	1.087157
C	0.297737	-2.402053	1.341865
H	0.355693	-3.417041	1.771052
H	-0.044964	-2.474635	0.309040
H	1.303734	-1.978218	1.326405
N	-2.902937	0.177013	1.627589
N	0.303841	1.094421	3.114856
C	1.332595	2.086300	2.790224
H	0.855967	2.997587	2.422893
H	1.953984	2.334075	3.667953
H	1.978024	1.709779	1.994643
C	-0.585514	1.637560	4.141217

H	-1.060999	2.546666	3.763926
H	-1.375148	0.924823	4.390552
H	-0.041412	1.884082	5.069477
C	-3.306737	-0.079184	0.243173
H	-4.345654	-0.447841	0.181701
H	-3.215684	0.839314	-0.338654
H	-2.646087	-0.817892	-0.214367
C	-3.697207	1.274187	2.179227
H	-3.391236	1.476127	3.209236
H	-3.521116	2.175812	1.587819
H	-4.777247	1.047534	2.175793
C	-0.614871	2.003207	-0.087135
H	0.892436	1.637346	-2.654566
F	0.605493	2.621197	-0.381036
F	-1.158354	1.841230	-1.382555
F	-1.375454	3.090461	0.394992

LiFPMDETA

SCF (B3PW91) = -628.431790127
E(SCF)+ZPE(0 K)= -628.099720
H(298 K)= -628.081291
G(298 K)= -628.143590
Lowest Frequency = 39.4374cm-1

C	3.374459	3.996875	0.854093
H	2.521392	3.817765	1.514112
H	3.639759	3.044006	0.387607
H	3.053712	4.695570	0.060860
C	5.669706	4.692659	0.731256
H	5.494308	5.475982	-0.026919
H	5.890169	3.753859	0.215455
H	6.543969	4.946428	1.335296
C	4.187872	5.743891	2.322760
H	3.644851	6.454998	1.674086
H	5.131255	6.227176	2.597107
C	3.375584	5.477225	3.587719
H	3.082967	6.437286	4.046654
H	2.442292	4.971958	3.320975
C	5.019514	5.426405	5.367006
H	5.690064	6.014638	4.736492
H	5.646983	4.759399	5.962961
H	4.477379	6.113210	6.040657
C	3.248840	3.770409	5.331164
H	2.364588	4.305137	5.720389
H	3.815711	3.443557	6.208154
C	2.784839	2.549553	4.537980
H	2.171489	1.906378	5.196052
H	2.128888	2.869882	3.720124
C	3.409293	0.842436	2.961592
H	2.762217	0.071230	3.415749
H	4.257570	0.342613	2.485402
H	2.837403	1.358767	2.185335
C	4.711900	1.130277	4.953892
H	4.116854	0.418847	5.553630
H	5.175962	1.856763	5.624164
H	5.522652	0.588641	4.461628
Li	5.267791	3.323380	3.242955
N	4.514151	4.504639	1.609506
N	4.116248	4.637956	4.534486
N	3.898221	1.806952	3.942610
F	6.968137	3.249005	3.373572

PhMe2SiCF2H

SCF (B3PW91) = -839.260733147
E(SCF)+ZPE(0 K)= -839.072686
H(298 K)= -839.058048
G(298 K)= -839.114301
Lowest Frequency = 23.7360cm-1

C	-2.01365500	-0.72050100	-0.70618400
H	-3.11038500	-0.66305000	-0.65308200
Si	-1.07254700	0.53827900	0.42385300
F	-1.67327300	-0.54776800	-2.03278800
F	-1.67229600	-2.01955300	-0.37612600
C	-1.62353800	0.16202500	2.17532600
H	-1.35258200	-0.85916500	2.46188300
H	-1.14626300	0.84906200	2.88203200
H	-2.70902200	0.26641800	2.27986500
C	-1.58648300	2.24846300	-0.14078500
H	-1.35270100	2.40250200	-1.19912600
H	-2.66428200	2.39158800	-0.00904500
H	-1.07190800	3.02196600	0.43919600
C	0.76070400	0.24322800	0.19525800
C	1.57465800	1.16677900	-0.48048800
C	1.35832000	-0.93053700	0.68733400
C	2.93753500	0.92969200	-0.65716800
H	1.14432200	2.08384200	-0.87617500
C	2.71910300	-1.17236400	0.51032900
H	0.75481000	-1.66968900	1.20904500
C	3.51094400	-0.24085100	-0.16199700
H	3.55097000	1.65720100	-1.18189700
H	3.16213800	-2.08685900	0.89533000
H	4.57254400	-0.42759600	-0.29978200

PhMe2SiCF2LiPMDETA

SCF (B3PW91) = -1367.17295106
E(SCF)+ZPE(0 K)= -1366.666831
H(298 K)= -1366.635164
G(298 K)= -1366.728055
Lowest Frequency = 19.9723cm-1

Si	-3.63593000	0.23369700	-2.37134900
C	-4.17704400	-0.05841300	-4.15524500
C	-3.80721200	0.85116300	-5.16302600
C	-5.01920800	-1.12261400	-4.52039800
C	-4.24860300	0.69991500	-6.47662700
H	-3.16920400	1.69673200	-4.91508700
C	-5.46562800	-1.28024400	-5.83298600
H	-5.33411500	-1.84367900	-3.76872500
C	-5.07925600	-0.36900700	-6.81568800
H	-3.94732500	1.41657800	-7.23693100
H	-6.11436500	-2.11442500	-6.08953200
H	-5.42467000	-0.48969800	-7.83931000
C	-1.78634200	0.61051800	-2.35575700
H	-1.42802800	0.72432400	-1.32597200
H	-1.21291200	-0.19407700	-2.82907300
H	-1.57187700	1.54102000	-2.89244600
C	-3.96751600	-1.31902300	-1.35437100
H	-3.51854800	-2.20494800	-1.81715300
H	-3.54348400	-1.21096300	-0.35027700
H	-5.04277700	-1.49567200	-1.24495800
N	-5.35811400	4.25550800	0.68252600
Li	-4.21110900	2.48231500	0.40445500
C	-6.50322900	2.47812600	1.95934800
C	-6.11205200	3.95196100	1.90376600
H	-7.15560700	2.29598000	2.83218800
H	-7.08568500	2.22836900	1.06683600
H	-7.01923500	4.57528500	1.97867200
H	-5.49863800	4.20347400	2.77463300
C	-3.12050400	4.83347600	1.57457900
C	-4.37972300	5.32869300	0.86627000
H	-2.39626600	5.66609800	1.64190800

H	-3.36163700	4.54790700	2.60536100
H	-4.79694000	6.18352800	1.42666900
H	-4.11560800	5.71231500	-0.12356200
C	-6.24868200	4.51921800	-0.44801800
H	-6.83626600	5.44226400	-0.30339700
H	-5.66100500	4.59039100	-1.36505600
H	-6.93250700	3.67954200	-0.58515000
N	-2.52963400	3.66187800	0.91896700
N	-5.32799300	1.59599400	1.97767400
C	-5.70196200	0.23652300	1.58040000
H	-4.81642300	-0.40449000	1.59551600
H	-6.45614400	-0.19959100	2.25843400
H	-6.09199600	0.25123700	0.56024900
C	-4.68099600	1.57899200	3.28685700
H	-3.78485300	0.95328200	3.24417500
H	-4.37074000	2.58542500	3.57935900
H	-5.34556200	1.18211700	4.07429300
C	-1.98829000	3.99413300	-0.40280500
H	-1.25896300	4.82136700	-0.35051700
H	-1.49285400	3.11503900	-0.81946100
H	-2.79158100	4.25702400	-1.09387800
C	-1.49108000	3.07333100	1.76076600
H	-1.91205000	2.79499800	2.73145800
H	-1.10220900	2.16853800	1.28462500
H	-0.64735300	3.76418500	1.93239600
C	-4.50156100	1.69200600	-1.51843500
F	-5.93189900	1.42928800	-1.56742500
F	-4.36860700	2.82539000	-2.42191000

PhMe2SiH

SCF (B3PW91) = -601.483716817
E(SCF)+ZPE(0 K)= -601.310055
H(298 K)= -601.298670
G(298 K)= -601.346994
Lowest Frequency = 16.6147cm-1

Si	-1.63990700	-0.44843700	-0.01645000
H	-1.87090100	-1.92311100	-0.00797600
C	-2.40698900	0.31856300	1.51982800
H	-3.49363800	0.17953000	1.52966100
H	-1.99543900	-0.12934400	2.43023200
H	-2.20398700	1.39487800	1.55402300
C	-2.40219900	0.30283500	-1.56267000
H	-2.19782100	1.37847200	-1.60830400
H	-1.98925400	-0.15556100	-2.46717800
H	-3.48903300	0.16562100	-1.57346800
C	0.22139400	-0.18461700	-0.01601000
C	1.11811900	-1.26400200	0.02780900
C	0.75839700	1.11420900	-0.05699500
C	2.49817700	-1.05743300	0.03119700
H	0.73434300	-2.28194900	0.05925900
C	2.13566700	1.32725100	-0.05385200
H	0.09392000	1.97628000	-0.09251900
C	3.00870900	0.23923300	-0.00961500
H	3.17424100	-1.90784400	0.06528300
H	2.52940700	2.33985600	-0.08610900
H	4.08308600	0.40282500	-0.00727500

SiLiPMDETA

SCF (B3PW91) = -1129.40474783
E(SCF)+ZPE(0 K)= -1128.909222
H(298 K)= -1128.880894
G(298 K)= -1128.965316
Lowest Frequency = 26.0518cm-1

C	9.274737	3.570845	2.395720
H	10.196234	2.972667	2.416928
H	9.541335	4.613116	2.613251
H	8.884355	3.545116	1.371042
C	9.032098	2.704112	5.255309
H	8.450113	2.275964	6.081507
H	9.396052	3.682040	5.595350
H	9.907717	2.059815	5.089374
C	7.724085	1.105361	3.067877
C	7.270460	0.839972	1.757868
H	7.184350	1.664374	1.050771
C	6.923047	-0.439857	1.329222
H	6.583219	-0.597764	0.307437
C	7.008735	-1.521391	2.210756
H	6.729151	-2.520604	1.887195
C	7.470147	-1.299514	3.508508
H	7.557783	-2.133222	4.202409
C	7.827026	-0.012779	3.920463
H	8.195703	0.122430	4.935967
C	3.956376	3.157927	0.955457
H	3.106663	2.884589	1.585688
H	4.549123	2.254492	0.786208
H	3.564569	3.512963	-0.013764
C	5.915913	4.520351	0.756001
H	5.585283	5.010801	-0.176262
H	6.475726	3.620379	0.494198
H	6.596374	5.184253	1.294410
C	4.022242	5.364188	1.974557
H	3.403493	5.717419	1.130176
H	4.741961	6.161194	2.188886
C	3.137036	5.142540	3.196107
H	2.558570	6.059557	3.400390
H	2.401365	4.363738	2.976349
C	4.495958	5.895072	5.053647
H	5.094610	6.483888	4.354414
H	5.164731	5.557966	5.849940
H	3.721494	6.550866	5.487903
C	3.142818	3.902573	5.293693
H	2.140584	4.324069	5.484465
H	3.661369	3.897748	6.257191
C	2.999449	2.470966	4.782537
H	2.438411	1.879882	5.529567
H	2.395392	2.460791	3.867840
C	4.108753	0.620275	3.707195
H	3.546586	-0.137319	4.280665
H	5.083529	0.207846	3.439470
H	3.560644	0.829978	2.784637
C	5.060989	1.576893	5.684136
H	4.498858	0.930647	6.381628
H	5.327885	2.503507	6.197926
H	5.989751	1.074918	5.408528
Li	5.428415	3.437644	3.537742
N	4.786578	4.163686	1.616063
N	3.920435	4.736867	4.370875
N	4.291827	1.856934	4.468719
Si	7.971689	2.922223	3.662419

TS1

SCF (B3PW91) = -1467.59902721
E(SCF)+ZPE(0 K)= -1467.084733
H(298 K)= -1467.051149
G(298 K)= -1467.149488
Lowest Frequency = -1127.6293cm-1

Si	-4.266035	-0.931793	-2.857746
C	-3.185537	-0.325258	-4.313777
C	-1.894544	0.190822	-4.076085
C	-3.623601	-0.317477	-5.653044

C	-1.095963	0.695390	-5.102268
H	-1.499860	0.191421	-3.060693
C	-2.836471	0.193586	-6.687059
H	-4.596963	-0.735509	-5.902141
C	-1.567361	0.707215	-6.416606
H	-0.104293	1.081131	-4.876824
H	-3.210088	0.179816	-7.708697
H	-0.950786	1.103128	-7.219130
C	-3.104192	-2.082639	-1.866503
H	-3.649852	-2.541593	-1.032869
H	-2.693907	-2.887150	-2.490606
H	-2.263159	-1.528941	-1.433031
C	-5.545345	-2.124772	-3.637912
H	-5.055910	-2.881079	-4.266297
H	-6.081819	-2.651396	-2.839049
H	-6.302286	-1.621227	-4.250415
N	-6.179158	4.890068	-2.728922
Li	-5.193220	3.015204	-2.804238
C	-3.882168	5.391834	-3.502937
C	-5.373071	5.668434	-3.679677
H	-3.303563	6.013106	-4.207710
H	-3.573665	5.693646	-2.496916
H	-5.563076	6.750051	-3.575379
H	-5.673825	5.401887	-4.697047
C	-7.557733	3.541548	-4.288531
C	-7.537756	4.629447	-3.218167
H	-8.604684	3.332075	-4.569878
H	-7.060989	3.901757	-5.196676
H	-8.016059	5.540782	-3.615887
H	-8.142295	4.313276	-2.362541
C	-6.205478	5.515346	-1.406571
H	-6.721262	6.490105	-1.419482
H	-6.708254	4.853054	-0.698076
H	-5.187896	5.667613	-1.040221
N	-6.861994	2.320887	-3.863310
N	-3.564048	3.965173	-3.660222
C	-2.302114	3.637270	-2.990696
H	-2.087867	2.575778	-3.126292
H	-1.457270	4.215673	-3.400652
H	-2.386350	3.842763	-1.919912
C	-3.502522	3.570028	-5.070608
H	-3.349638	2.490721	-5.146694
H	-4.439435	3.819654	-5.576587
H	-2.680138	4.077667	-5.601579
C	-7.613455	1.586209	-2.837708
H	-8.611468	1.287521	-3.199446
H	-7.053094	0.688032	-2.562185
H	-7.733202	2.190697	-1.936051
C	-6.617431	1.448253	-5.011675
H	-6.004267	1.964238	-5.754981
H	-6.066594	0.568896	-4.677947
H	-7.555478	1.120093	-5.490220
C	-5.028248	1.264517	-0.439702
H	-4.812342	0.318611	-1.598619
F	-5.040087	2.620473	-0.948616
F	-4.011868	1.304581	0.463787
F	-6.168714	1.228410	0.311728

TS2

SCF (B3PW91) = -1995.53724489
E(SCF)+ZPE(0 K)= -1994.699426
H(298 K)= -1994.648839
G(298 K)= -1994.781613
Lowest Frequency = -77.4019cm-1

Si	-3.378342	1.074312	-0.412817
C	-3.925738	-0.402221	-1.553828
C	-3.055556	-0.959504	-2.510254
C	-5.230048	-0.920392	-1.529841
C	-3.465327	-1.954755	-3.397532
H	-2.031271	-0.595347	-2.576011
C	-5.660953	-1.914586	-2.412013
H	-5.937440	-0.518735	-0.806935
C	-4.776639	-2.434396	-3.355314
H	-2.764529	-2.356193	-4.126862
H	-6.685744	-2.277049	-2.366020
H	-5.101955	-3.205795	-4.048980
C	-2.777433	2.318660	-1.763579
H	-2.131177	3.074498	-1.302738
H	-2.206643	1.831739	-2.566790
H	-3.625387	2.844124	-2.215551
C	-1.655574	0.440387	0.212382
H	-1.031804	0.037455	-0.598930
H	-1.097426	1.270591	0.665004
H	-1.756646	-0.344585	0.972577
N	-7.133419	5.101174	-4.057434
Li	-5.732420	4.073622	-2.760882
C	-5.136342	6.558437	-3.971458
C	-6.284478	6.019467	-4.819594
H	-4.560239	7.297801	-4.557579
H	-5.546413	7.094065	-3.108975
H	-6.868653	6.864778	-5.224411
H	-5.878743	5.488171	-5.685619
C	-6.778811	2.967118	-5.258423
C	-7.759501	4.079400	-4.895170
H	-7.317327	2.194979	-5.839859
H	-5.997331	3.361064	-5.919120
H	-8.187233	4.502719	-5.821500
H	-8.600805	3.657313	-4.337083
C	-8.106921	5.810641	-3.234948
H	-8.849022	6.358914	-3.842468
H	-8.623678	5.099618	-2.586165
H	-7.596616	6.520669	-2.580900
N	-6.114010	2.388313	-4.089763
N	-4.271878	5.490670	-3.458753
C	-3.492501	5.968469	-2.316346
H	-2.849736	5.164907	-1.953703
H	-2.860786	6.835266	-2.580261
H	-4.168459	6.244667	-1.503777
C	-3.385305	4.961690	-4.492024
H	-2.795909	4.139953	-4.076859
H	-3.964621	4.565222	-5.330025
H	-2.695892	5.731830	-4.882071
C	-7.052395	1.664745	-3.230827
H	-7.580715	0.864288	-3.778936
H	-6.499299	1.213607	-2.406937
H	-7.785361	2.349271	-2.797782
C	-5.037002	1.495023	-4.516727
H	-4.291280	2.059945	-5.083971
H	-4.548290	1.058344	-3.645127
H	-5.409962	0.669409	-5.147292
C	-4.332359	4.041449	1.148299
F	-3.178750	4.367891	0.608801
F	-6.159390	4.120730	-1.101033
F	-5.015098	5.154285	1.141947
N	-5.411335	-0.132697	2.725540
Li	-4.845679	1.901000	1.670074
C	-3.660666	0.779033	4.215253
C	-4.999373	0.058883	4.115614
H	-3.342826	0.814008	5.274347
H	-2.899603	0.204605	3.677350
H	-4.929321	-0.906138	4.649769
H	-5.764773	0.637821	4.639977
C	-7.551767	1.126785	2.698859
C	-6.863450	-0.230199	2.583895

H	-8.643575	0.979357	2.590878
H	-7.397771	1.538230	3.703963
H	-7.305614	-0.923083	3.323653
H	-7.072006	-0.661483	1.599979
C	-4.744783	-1.293994	2.144483
H	-5.040797	-2.235098	2.643487
H	-4.973562	-1.365128	1.080183
H	-3.661232	-1.186442	2.226135
N	-7.051014	2.103982	1.733852
N	-3.695500	2.120133	3.627301
C	-2.332744	2.607377	3.425437
H	-2.357256	3.605471	2.982026
H	-1.767193	2.664846	4.372805
H	-1.804606	1.944377	2.736530
C	-4.440087	3.057331	4.463653
H	-4.460799	4.038180	3.981246
H	-5.475774	2.730745	4.583748
H	-3.992631	3.167487	5.468187
C	-7.460469	1.782216	0.363724
H	-8.563167	1.742046	0.272882
H	-7.055372	2.547909	-0.309468
H	-7.056331	0.813323	0.067177
C	-7.534436	3.443472	2.066205
H	-7.129428	3.762142	3.032377
H	-7.202264	4.138111	1.292685
H	-8.637959	3.479125	2.122092

TS3

SCF (B3PW91) = -1705.37851914
E(SCF)+ZPE(0 K)= -1704.851099
H(298 K)= -1704.814458
G(298 K)= -1704.918563
Lowest Frequency = -705.1223cm-1

Si	3.079633	-1.476788	-0.525915
C	1.586666	-2.633510	-0.673878
C	1.754283	-4.027672	-0.607395
C	0.283682	-2.145475	-0.870906
C	0.670812	-4.899878	-0.714453
H	2.749453	-4.445495	-0.463044
C	-0.806440	-3.011859	-0.985330
H	0.119549	-1.074522	-0.956628
C	-0.616833	-4.391887	-0.899310
H	0.828364	-5.973837	-0.655811
H	-1.800295	-2.608862	-1.162071
H	-1.463344	-5.067451	-0.990528
C	4.239657	-1.835266	-1.968726
H	5.137895	-1.211625	-1.899657
H	4.550676	-2.886628	-1.984697
H	3.743573	-1.610227	-2.918304
C	3.979022	-1.868696	1.086708
H	4.182491	-2.940445	1.189772
H	4.932797	-1.331857	1.122355
H	3.392501	-1.548663	1.952957
C	2.400257	0.292063	-0.428286
F	3.439631	1.131354	0.095132
F	2.246571	0.761160	-1.777498
N	-0.134754	-2.510889	3.373632
Li	-0.459679	-0.654385	2.388274
C	1.499562	-0.934625	4.374027
C	0.510399	-2.068980	4.621164
H	1.993989	-0.661062	5.322043
H	2.290266	-1.280654	3.701859
H	1.027545	-2.907370	5.115903
H	-0.262294	-1.733767	5.319049
C	-2.513601	-1.987575	3.857619
C	-1.470452	-3.074931	3.612947
H	-3.506869	-2.457629	3.966274
H	-2.307966	-1.478037	4.805768
H	-1.471288	-3.779463	4.461432
H	-1.745381	-3.658916	2.729370
C	0.706402	-3.466533	2.649622
H	0.852826	-4.400054	3.218262
H	0.250132	-3.704409	1.687074
H	1.685826	-3.032248	2.443425
N	-2.509030	-0.971311	2.799481
N	0.856783	0.230312	3.749020
C	1.858132	1.102163	3.119859
H	1.364529	1.980432	2.699480
H	2.615353	1.442125	3.844896
H	2.358313	0.583984	2.298745
C	0.076983	0.998312	4.722566
H	-0.441614	1.813782	4.211606
H	-0.676013	0.366937	5.201694
H	0.715707	1.428453	5.511948
C	-3.042162	-1.499905	1.539940
H	-4.084184	-1.844739	1.647714
H	-3.007052	-0.717704	0.777903
H	-2.434242	-2.335586	1.185556
C	-3.273579	0.209958	3.203152
H	-2.862535	0.622299	4.128602
H	-3.196556	0.973359	2.425203
H	-4.338884	-0.022284	3.367815
C	-0.084629	1.534618	0.222203
H	1.029653	0.928119	0.050379
F	-0.049472	2.772330	0.767487
F	-0.887335	1.618404	-0.859950
F	-0.862294	0.784029	1.148890

TS4

SCF (B3PW91) = -1467.55509067
E(SCF)+ZPE(0 K)= -1467.035065
H(298 K)= -1467.001986
G(298 K)= -1467.096364
Lowest Frequency = -438.0414cm-1

Si	-4.686813	-0.451905	-2.648536
C	-3.901551	-0.419017	-4.392529
C	-2.676496	0.236498	-4.634416
C	-4.525103	-1.008414	-5.512016
C	-2.110927	0.311990	-5.906105
H	-2.143602	0.687755	-3.800600
C	-3.966259	-0.942273	-6.789614
H	-5.466308	-1.539210	-5.383551
C	-2.757377	-0.275497	-6.996491
H	-1.159703	0.820944	-6.047382
H	-4.475808	-1.413497	-7.627133
H	-2.321651	-0.220446	-7.990414
C	-3.215725	-0.879298	-1.507532
H	-2.701467	-1.794292	-1.830518
H	-2.482211	-0.065452	-1.487380
H	-3.568714	-1.022417	-0.480881
C	-5.803283	-2.003307	-2.685294
H	-5.271157	-2.875071	-3.090444
H	-6.134844	-2.242659	-1.669747
H	-6.703553	-1.843873	-3.290739
N	-6.019059	4.485627	-2.624947
Li	-4.919260	2.606154	-2.979559
C	-3.637957	4.938820	-2.092331
C	-4.934736	5.475226	-2.687593
H	-2.891292	5.752403	-2.048646
H	-3.821511	4.615868	-1.062802
H	-5.216772	6.403362	-2.161925
H	-4.769005	5.760116	-3.729923

C	-6.413879	4.151578	-5.047820
C	-6.981748	4.633729	-3.718877
H	-7.192079	4.250843	-5.826569
H	-5.590117	4.804236	-5.357616
H	-7.325695	5.677680	-3.829596
H	-7.866998	4.043581	-3.461524
C	-6.693176	4.537286	-1.329654
H	-7.198770	5.504539	-1.164314
H	-7.437611	3.739160	-1.272425
H	-5.970595	4.374143	-0.527834
N	-5.892777	2.782771	-4.985942
N	-3.111546	3.777909	-2.824461
C	-2.101813	3.101882	-2.005521
H	-1.689124	2.253600	-2.556053
H	-1.269124	3.777109	-1.742704
H	-2.566391	2.720778	-1.094234
C	-2.524572	4.160101	-4.107684
H	-2.219181	3.259916	-4.648358
H	-3.255669	4.685987	-4.725585
H	-1.646016	4.816995	-3.982319
C	-6.980631	1.802400	-4.911015
H	-7.651736	1.874144	-5.785417
H	-6.553678	0.798014	-4.874407
H	-7.567555	1.942118	-4.001945
C	-5.080511	2.514391	-6.174159
H	-4.244787	3.216161	-6.222493
H	-4.675368	1.505267	-6.123728
H	-5.670984	2.611552	-7.102309
C	-6.164521	1.102576	-0.825095
H	-6.462144	1.788028	-0.030069
F	-4.857171	2.127329	-1.100650
F	-7.217999	1.103752	-1.691766
F	-6.007885	-0.090912	-0.200522

TS5

SCF (B3PW91) = -1467.56540964
E(SCF)+ZPE(0 K)= -1467.047117
H(298 K)= -1467.013411
G(298 K)= -1467.110948
Lowest Frequency = -338.9024cm-1

Si	-4.129684	-0.142574	-2.996850
C	-3.134456	-0.255530	-4.615373
C	-1.741675	-0.020009	-4.637884
C	-3.759109	-0.408070	-5.872474
C	-1.029117	0.098976	-5.830734
H	-1.198055	0.068019	-3.698846
C	-3.054290	-0.298003	-7.068988
H	-4.824080	-0.624880	-5.918750
C	-1.683077	-0.028155	-7.057060
H	0.042702	0.283542	-5.803282
H	-3.573676	-0.427060	-8.016288
H	-1.131968	0.067025	-7.988800
C	-2.914188	-0.654953	-1.627315
H	-3.471230	-0.827430	-0.700084
H	-2.370187	-1.573918	-1.882110
H	-2.178302	0.129619	-1.417581
C	-5.446622	-1.517168	-3.082495
H	-4.977719	-2.509484	-3.128592
H	-6.083337	-1.480787	-2.191440
H	-6.099072	-1.421462	-3.957980
N	-6.041787	4.620446	-2.547524
Li	-5.177636	2.535009	-2.886208
C	-3.678512	5.031792	-3.161635
C	-5.133522	5.431571	-3.367623
H	-3.023777	5.712010	-3.734949
H	-3.411507	5.159486	-2.107644
H	-5.255902	6.507256	-3.150301
H	-5.394909	5.301793	-4.421303
C	-7.481904	3.697257	-4.349532
C	-7.395216	4.580604	-3.109135
H	-8.531988	3.669792	-4.693811
H	-6.903574	4.140762	-5.168067
H	-7.765657	5.590934	-3.359968
H	-8.062786	4.191629	-2.334266
C	-6.074102	5.111750	-1.170126
H	-6.445601	6.150077	-1.111293
H	-6.716500	4.469988	-0.566238
H	-5.075557	5.076181	-0.730041
N	-6.957267	2.350421	-4.117671
N	-3.440171	3.629710	-3.518868
C	-2.226068	3.137438	-2.868152
H	-2.058800	2.099290	-3.157196
H	-1.337150	3.726942	-3.153299
H	-2.344998	3.177043	-1.781614
C	-3.340343	3.445707	-4.968576
H	-3.225770	2.382585	-5.194926
H	-4.249632	3.801556	-5.461148
H	-2.482201	3.995171	-5.393211
C	-7.842992	1.565363	-3.253746
H	-8.847806	1.451221	-3.697032
H	-7.405109	0.577760	-3.096966
H	-7.938585	2.033017	-2.272739
C	-6.761757	1.655384	-5.386968
H	-6.030787	2.187921	-6.001765
H	-6.365659	0.658677	-5.188665
H	-7.701634	1.555643	-5.957960
C	-5.874082	1.681774	0.174455
F	-5.167293	1.227110	-1.526545
F	-5.096774	2.643473	0.700205
F	-7.128301	2.164319	0.045588
H	-5.853748	0.767378	0.770371

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