Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

An anionic beryllium hydride dimer with an exceedingly short Be···Be distance

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1. Experimental methods and data

General considerations. All experiments and manipulations were carried out under dry oxygen free argon atmosphere using standard Schlenk techniques or in a MBraun inert atmosphere glovebox containing an atmosphere of high purity argon. THF was dried by distillation over a sodium/benzophenone mixture and stored over activated 4Å mol sieves. C_6D_6 was dried, degassed and stored over a potassium mirror. All other solvents were dried over activated 4Å mol sieves. [(^{i}Pr$_3$Si)(Dipp)NK] (L*; Dipp = 2,6-^{i}Pr$_2$-C$_6$H$_3$),[1] and [Br$_2$Be·(Et$_2$O)$_2$][2] were synthesized according to known literature procedures. All other reagents were used as received. NMR spectra were recorded on a Bruker AV 400 Spectrometer. The ^{1}H and ^{13}C{^{1}H} NMR spectra were referenced to the residual solvent signals as internal standards. ^{29}Si{^{1}H} NMR spectra were externally calibrated with SiMe4. ^{9}Be NMR spectra were externally calibrated with BeBr$_2$·(Et$_2$O)$_2$. Liquid Injection Field Desorption Ionization Mass Spectrometry (LIFDI-MS) was measured directly from an inert atmosphere glovebox with a Thermo Fisher Scientific Exactive Plus Orbitrap equipped with an ion source from Linden CMS.[3] Elemental analyses (C, H, N) were performed with a combustion analyzer (elementar vario EL, Bruker).

CAUTION: *Beryllium, most notably as fine powders, and beryllium compounds are regarded as highly toxic, and are potential carcinogens. A severe allergic reaction can also occur if inhaled, with the risk of causing chronic beryllium disease.[4] One should take care and use adequate safety measures (i.e. breathing apparatus, protective clothing, well-ventilated fume-hoods) for any manipulations involving beryllium and compounds containing this element.[5]*

[L*BeBr·Et$_2$O], 1. A solid mixture of [(^{i}Pr$_3$Si)(Dipp)NK] (2.35 g, 6.33 mmol) and [Br$_2$Be·(Et$_2$O)$_2$] (2.00 g, 6.33 mmol) was cooled to -80 °C with rapid stirring. Toluene (50 mL) was added to this rapidly stirred mixture, and the reaction allowed to slowly warm over the course of 16 h. All volatiles were subsequently removed *in-vacuo*, the oily residue extracted in heptane (~50 mL), and the suspension filtered. The filtrate was concentrated to ~15 mL, and stored at -40°C overnight, leading to the deposition of a large crops of colourless crystals, which were collected by filtration and dried under vacuum. Compound **1** was isolated as an off-white waxy crystalline powder (2.10 g, 67%). Crystals grown in this manner were suitable for X-ray diffraction analysis.

^{1}H NMR (C$_6$D$_6$, 400 MHz, 298 K): δ = 0.78 (t, 4H, $^3J_{HH}$ = 7.1 Hz, Et$_2$O-C*H*$_2$), 1.16 (d, 6H, $^3J_{HH}$ = 6.8 Hz, Dipp-^{i}Pr-C*H*$_3$), 1.32 (d, 18H, $^3J_{HH}$ = 7.6 Hz, ^{i}Pr$_3$Si-C*H*$_3$), 1.37 (d, 6H, $^3J_{HH}$ = 6.8 Hz, Dipp-^{i}Pr-C*H*$_3$), 1.67 (sept, 3H, $^3J_{HH}$ = 7.6 Hz, ^{i}Pr$_3$Si-C*H*), 3.02 (q, 6H, $^3J_{HH}$ = 7.1 Hz, Et$_2$O-C*H*$_3$), 3.90 (sept, 2H, $^3J_{HH}$ = 6.8 Hz, Dipp-^{i}Pr-C*H*), 7.02-7.09 (m, 3H, Ar-C*H*).

$^{13}C\{^1H\}$ NMR (C_6D_6, 101 MHz, 298 K): δ = 12.9 (Et_2O-*C*H_3), 14.9 ($^iPr_3Si$-*C*H), 20.2 ($^iPr_3Si$-*C*H_3), 24.9 (Dipp-^{i}Pr-*C*H_3), 26.3 (Dipp-^{i}Pr-*C*H_3), 27.3 (Dipp-^{i}Pr-*C*H), 69.8 (Et_2O-*C*H_2), 123.6, 124.4, 146.3, 146.4 (Ar-*C*).

$^{29}Si\{^1H\}$ NMR (C_6D_6, 99 MHz, 298 K): δ = 2.7.

^9Be NMR (C_6D_6, 58 MHz, 298 K): δ = 9.0.

MS/LIFDI-HRMS found (calcd.) m/z: 406.1996 (406.1980) for $[M\text{-}Cl]^+$.

Anal. calcd. for $C_{25}H_{48}BeBrNOSi$: C, 60.58%; H, 9.76%; N, 2.83%; found: C, 60.87%; H, 10.32%; N, 2.95%.

[L*Be(μ-H)$_3$BeL*][C], 2.

A = [(THF)$_3$·Li(μ-Br)Li·(THF)$_3$]$^+$, 2a. Compound **1** (200 mg, 0.40 mmol) was dissolved in heptane (5 mL), and a 1M THF solution of Li[HB^{s}Bu$_3$] added (0.8 mL, 0.80 mmol). The mixture was briefly shaken, and allowed to stand overnight, leading to a to formation of colourless crystals of **2a**, which were suitable for X-ray diffraction analysis. The solution was decanted, and the crystalline solid washed with a small amount of pentane (5 mL), and dried under vacuum, yielding a colourless crystalline solid (83 mg, 49 %).

^1H NMR (C_6D_6, 400 MHz, 298 K): δ = 1.23 (d, 12H, $^3J_{HH}$ = 6.8 Hz, Dipp-^{i}Pr-C*H*$_3$), 1.28 (m, 24H, THF-C*H*$_2$), 1.36 (overlapping d, 48H, Dipp-^{i}Pr-C*H*$_3$ and $^iPr_3Si$-C*H*$_3$), 1.53 (sept, 6H, $^3J_{HH}$ = 7.6 Hz, $^iPr_3Si$-C*H*), 2.67 (br s, 3H, Be-*H*-Be), 3.29 (m, 24H, THF-C*H*$_2$), 4.17 (sept, 4H, $^3J_{HH}$ = 6.8 Hz, Dipp-^{i}Pr-C*H*), 6.84 (m, 2H, *p*-Ar-C*H*), 7.02 (m, 4pH, *m*-Ar-C*H*).

$^{13}C\{^1H\}$ NMR (C_6D_6, 101 MHz, 298 K): δ = 14.8 ($^iPr_3Si$-*C*H), 19.8 ($^iPr_3Si$-*C*H_3), 23.4 (Dipp-^{i}Pr-*C*H_3), 25.4 (THF-*C*H_2), 25.7 (Dipp-^{i}Pr-*C*H_3), 27.3 (Dipp-^{i}Pr-*C*H), 68.3 (THF-*C*H_2), 121.9, 123.7, 146.3, 152.9 (Ar-*C*).

$^{29}Si\{^1H\}$ NMR (C_6D_6, 99 MHz, 298 K): δ = -1.0.

^9Be NMR (C_6D_6, 58 MHz, 298 K): δ = 4.5.

Anal. calcd. for $C_{66}H_{121}Be_2BrLi_2N_2O_6Si_2$: C, 65.69%; H, 10.11%; N, 2.32%; found: C, 62.43%; H, 10.45%; N, 2.20%.

N.B. Carbon values were found to be low after running several samples, possibly due to silicon carbide formation.

B = [(TMEDA)$_2$·Li]$^+$, 2b. Compound **1** (200 mg, 0.40 mmmol) dissolved in toluene (5 mL), and a 1M THF solution of Li[HB^{s}Bu$_3$] (0.8 mL, 0.80 mmol) was added. The reaction was stirred for 2 h at ambient temperature, filtered, and concentrated to ~2 mL. The solution was layered with heptane (~10 mL), and stored for 3 days, leading to the formation of a crop of large colourless crystals suitable for X-ray diffraction analysis (68 mg, 40 %).

^{1}H NMR (D_8-THF, 400 MHz, 298 K): δ = 1.01 (d, 36H, $^{3}J_{HH}$ = 7.6 Hz, $^{i}Pr_3Si$-C*H*$_3$), 1.07 (d, 12H, $^{3}J_{HH}$ = 6.8 Hz, Dipp-^{i}Pr-C*H*$_3$), 1.11 (d, 12H, $^{3}J_{HH}$ = 6.8 Hz, Dipp-^{i}Pr-C*H*$_3$), 1.20 (sept, 6H, $^{3}J_{HH}$ = 7.6 Hz, $^{i}Pr_3Si$-C*H*), 2.00 (br s, 3H, Be-*H*-Be), 2.15 (s, 24H, TMEDA-C*H*$_3$), 2.31 (s, 8H, TMEDA-CH_2), 3.99 (sept, 4H, $^{3}J_{HH}$ = 6.8 Hz, Dipp-^{i}Pr-C*H*), 6.60 (m, 2H, *p*-Ar-C*H*), 6.74 (m, 4H, *m*-Ar-C*H*).

^{13}C{^{1}H} NMR (D_8-THF, 101 MHz, 298 K): δ = 15.4 ($^{i}Pr_3Si$-*C*H), 20.4 ($^{i}Pr_3Si$-*C*H$_3$), 24.0 (Dipp-^{i}Pr-*C*H$_3$), 26.9 (Dipp-^{i}Pr-*C*H$_3$), 27.7 (Dipp-^{i}Pr-*C*H), 46.4 (TMEDA-*C*H$_3$), 59.1 (TMEDA-*C*H$_2$), 120.5, 122.6, 147.1, 152.6 (Ar-*C*).

^{29}Si{^{1}H} NMR (D_8-THF, 99 MHz, 298 K): δ = -5.1.

^{9}Be NMR (C_6D_6, 58 MHz, 298 K): δ = -4.2.

MS/LIFDI-HRMS found (calcd.) m/z: 685.6027 (685.6026) for [M-{(TMEDA)$_2$Li}]$^{+}$.

[L*Be(μ-H)$_3$BeL*]·[K(TMEDA)], 3. Compound **1** (200 mg, 0.40 mmol) was dissolved in heptane (10 mL), and neat TMEDA added (0.07 mL, 0.44 mmol), leading to the precipitation of what is presumably L*BeBr·TMEDA. The suspension was cooled to -80 °C with rapid stirring, and a THF solution of K[HB^{S}Bu$_3$] added (1M, 0.40 mL, 0.40 mmol). The reaction mixture was slowly warmed over the course of 4 h, leading the dissolution of the copious precipitate, and formation of a fine colourless precipitate. The reaction mixture was then allowed to settle, filtered, and concentrated to ~3 mL, whereby small crystals began to form. These were redissolved by mild heating, and the flask left at ambient temperature overnight, leading to a crop of colourless crystals suitable for single-crystal X-ray diffraction analysis (95 mg, 56%).

^{1}H NMR (C_6D_6, 400 MHz, 298 K): δ = 1.17 (d, 12H, $^{3}J_{HH}$ = 6.8 Hz, Dipp-^{i}Pr-C*H*$_3$), 1.36 (d, 12H, $^{3}J_{HH}$ = 6.8 Hz, Dipp-^{i}Pr-C*H*$_3$), 1.41 (d, 36H, $^{3}J_{HH}$ = 7.6 Hz, $^{i}Pr_3Si$-C*H*$_3$), 1.52 (sept, 6H, $^{3}J_{HH}$ = 7.6 Hz, $^{i}Pr_3Si$-C*H*), 1.71 (s, 12H, TMEDA-C*H*$_3$), 1.76 (s, 4H, TMEDA-CH_2), 2.19 (br s, 3H, Be-*H*-Be), 4.23 (sept, 4H, $^{3}J_{HH}$ = 6.8 Hz, Dipp-^{i}Pr-C*H*), 6.71 (m, 2H, *p*-Ar-C*H*), 6.91 (m, 4pH, *m*-Ar-C*H*).

^{13}C{^{1}H} NMR (C_6D_6, 101 MHz, 298 K): δ = 15.0 ($^{i}Pr_3Si$-*C*H), 20.0 ($^{i}Pr_3Si$-*C*H$_3$), 23.8 (Dipp-^{i}Pr-*C*H$_3$), 26.2 (Dipp-^{i}Pr-*C*H$_3$), 27.1 (Dipp-^{i}Pr-*C*H), 45.6 (TMEDA-*C*H$_3$), 57.2 (TMEDA-*C*H$_2$), 120.9, 123.3, 147.3, 153.1 (Ar-*C*).

^{29}Si{^{1}H} NMR (C_6D_6, 99 MHz, 298 K): δ = -4.1.

^{9}Be NMR (C_6D_6, 58 MHz, 298 K): δ = -3.4.

Anal. calcd. for $C_{48}H_{95}Be_2KN_4Si_2$: C, 68.50%; H, 11.38%; N, 6.66%; found: C, 63.11%; H, 10.95%; N, 6.09%.

N.B. Carbon values were found to be low after running several samples, possibly due to silicon carbide formation.

NMR and IR spectra:

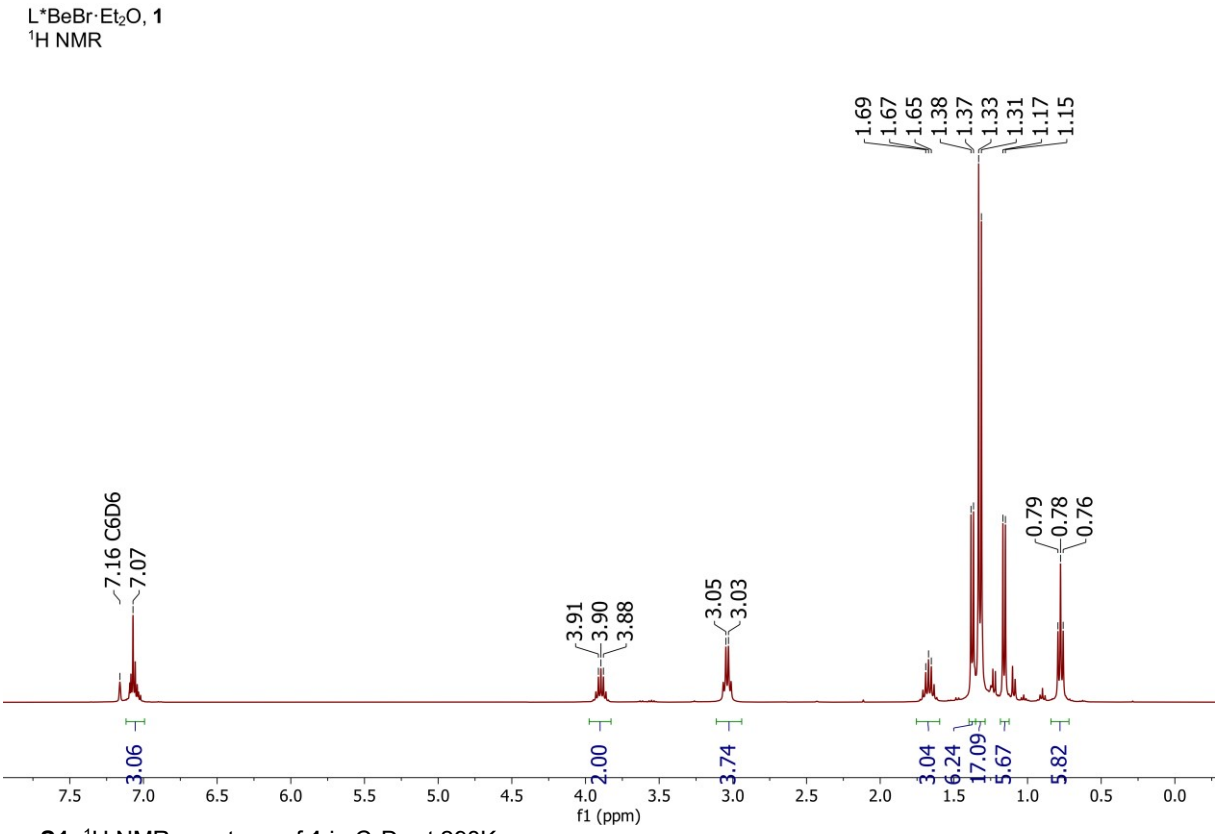

Figure S1. ^{1}H NMR spectrum of **1** in C_6D_6 at 298K.

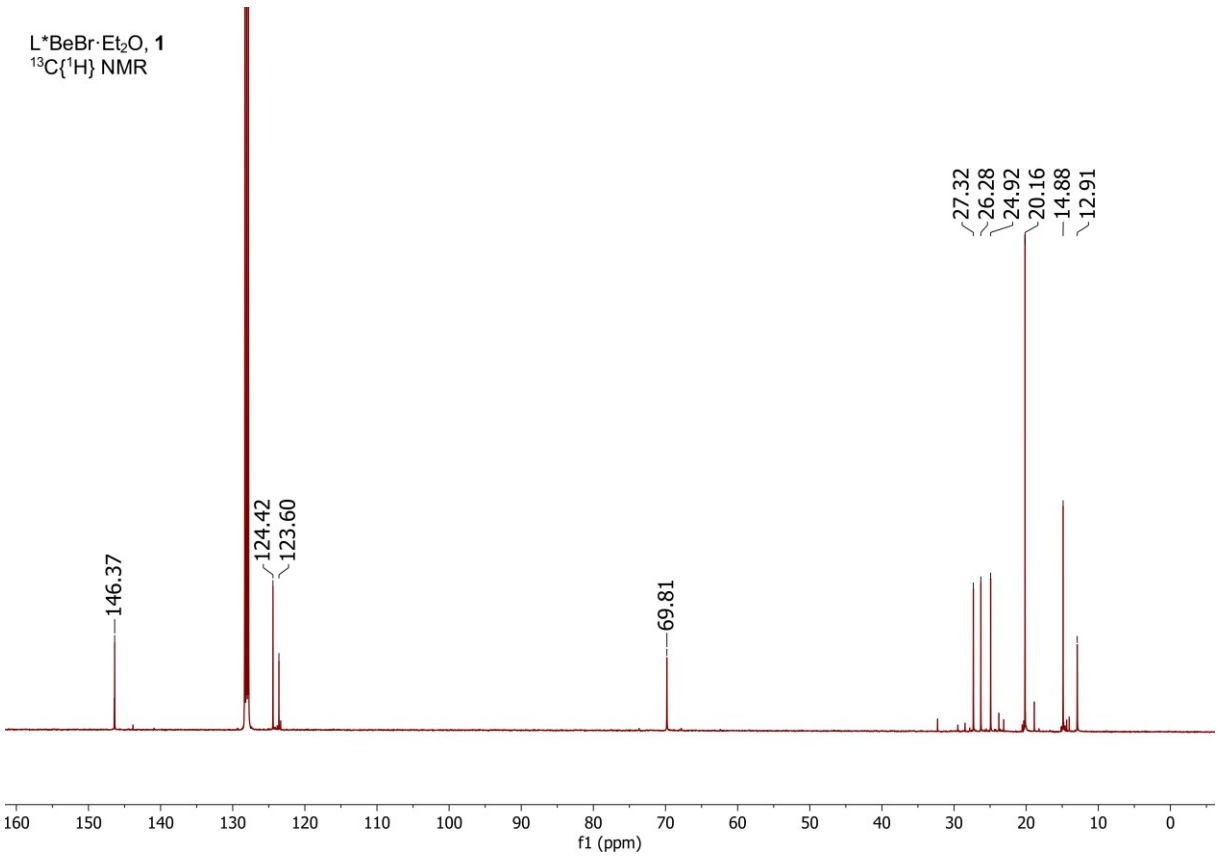

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **1** in C_6D_6 at 298K.

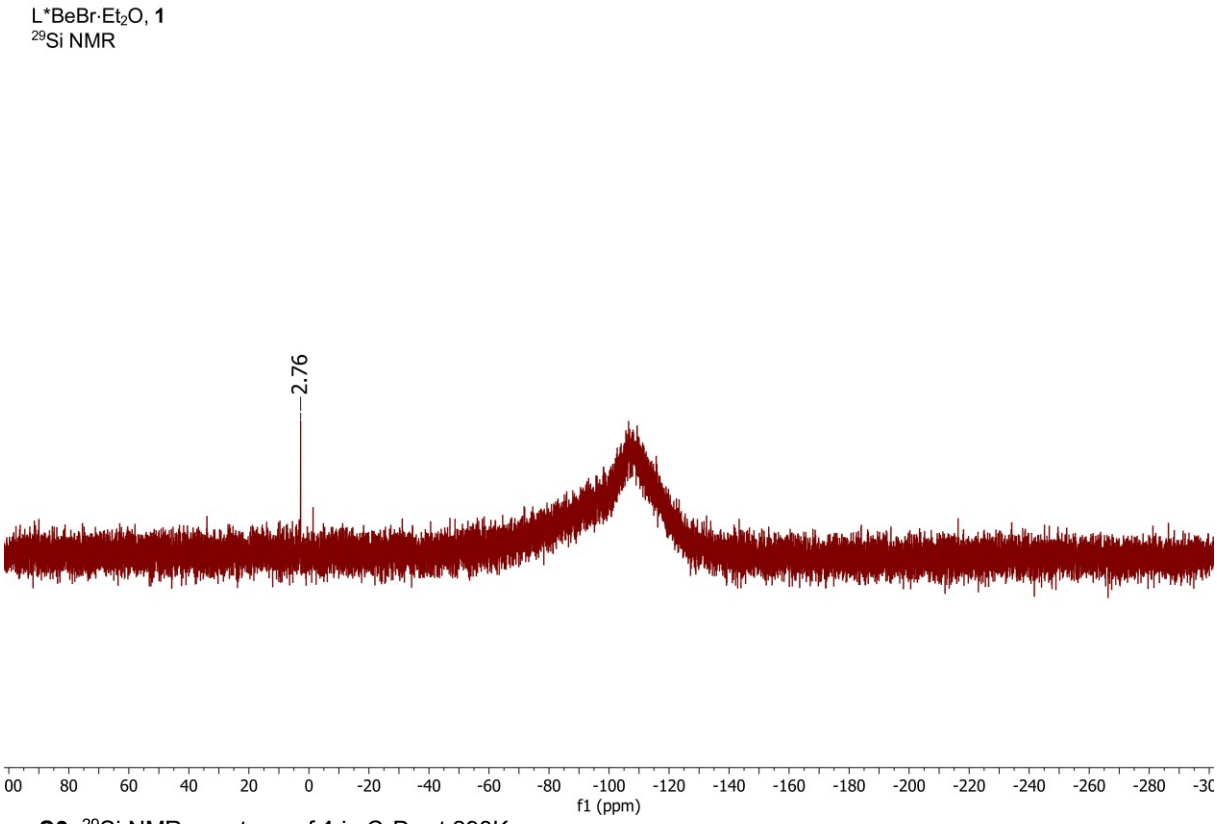

Figure S3. ^{29}Si NMR spectrum of **1** in C_6D_6 at 298K.

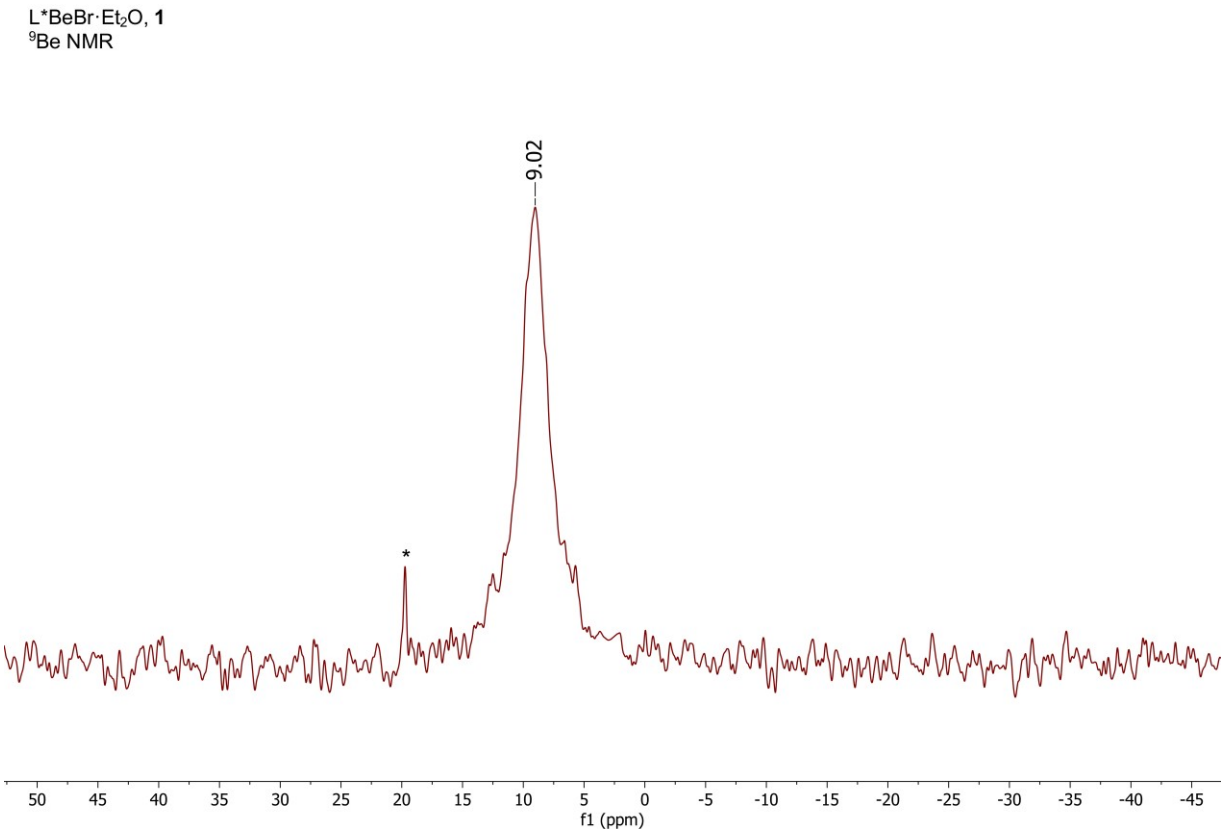

Figure S4. ^{9}Be NMR spectrum of **1** in C_6D_6 at 298K. **artifact of the NMR spectrometer*

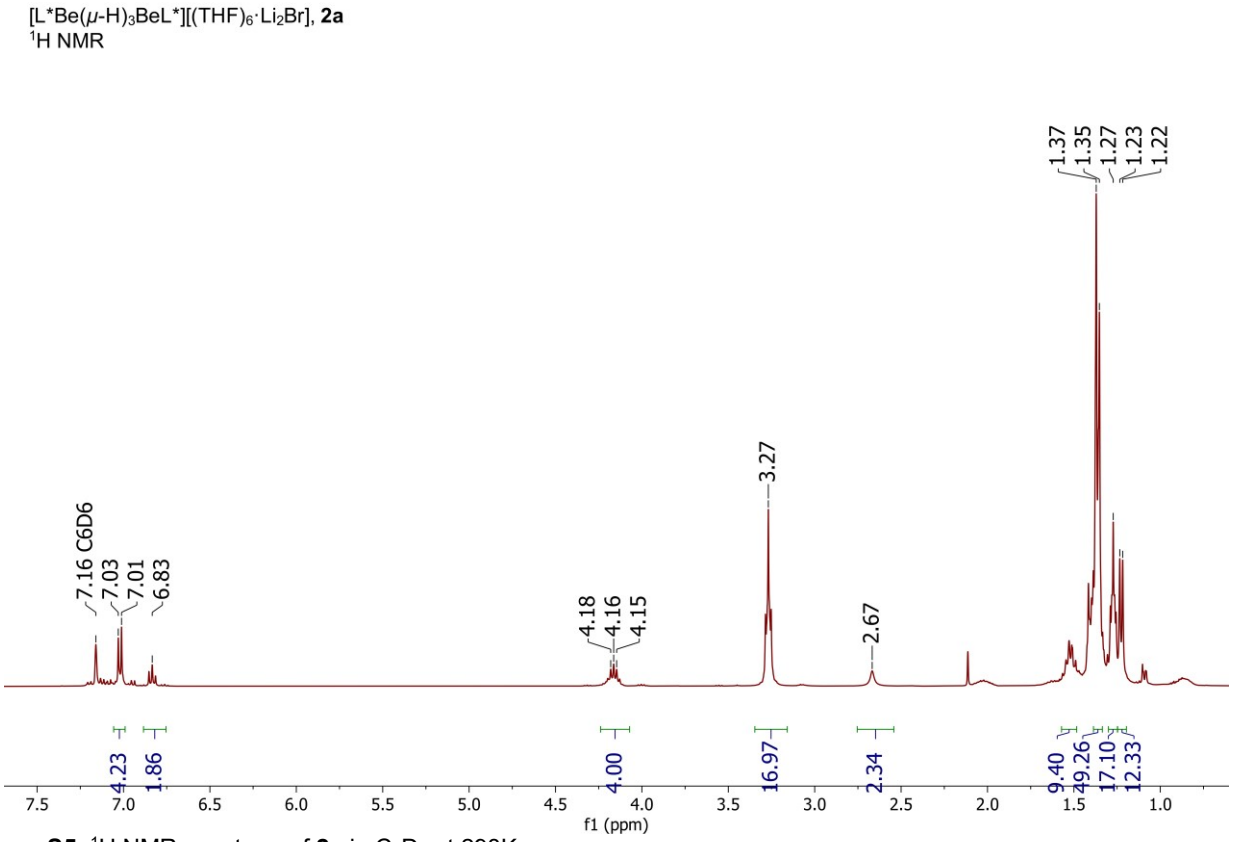

Figure S5. ^{1}H NMR spectrum of **2a** in C_6D_6 at 298K.

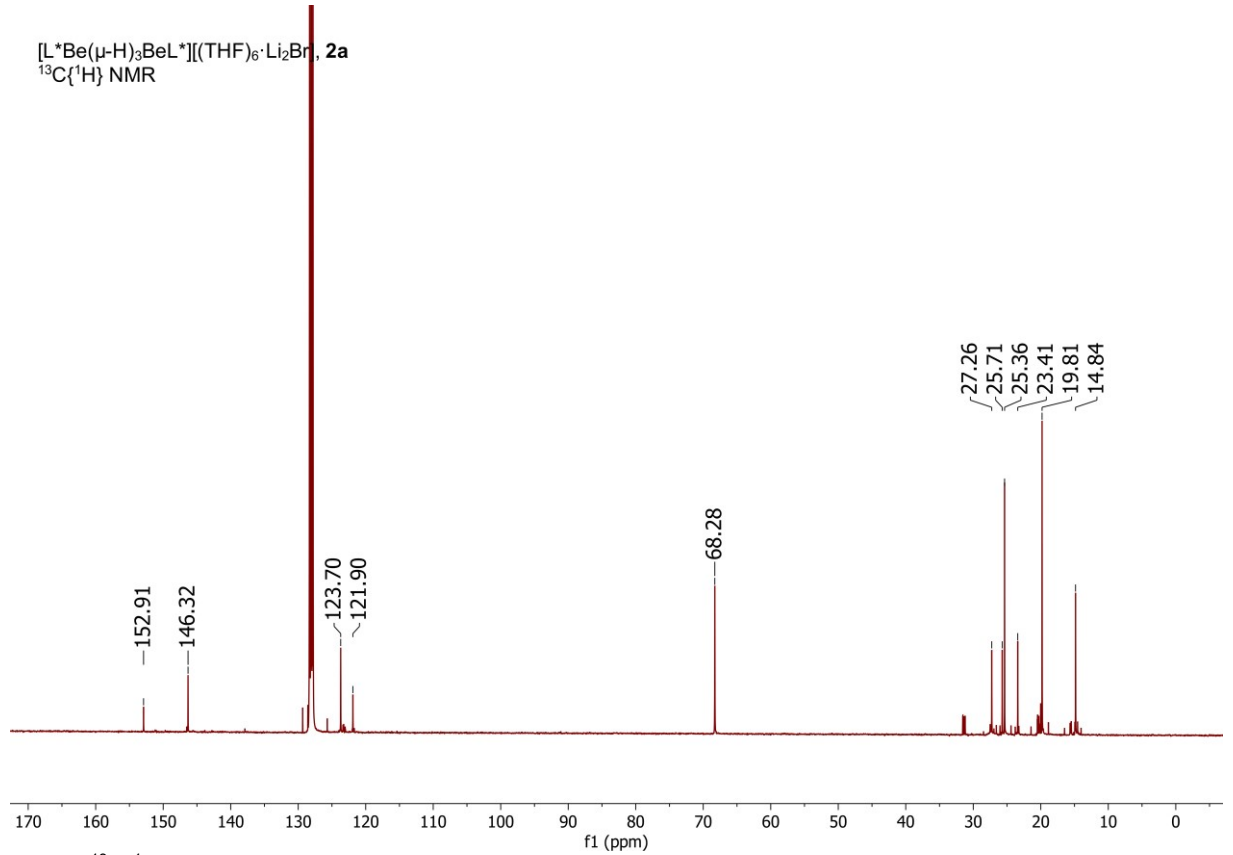

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of **2a** in C_6D_6 at 298K.

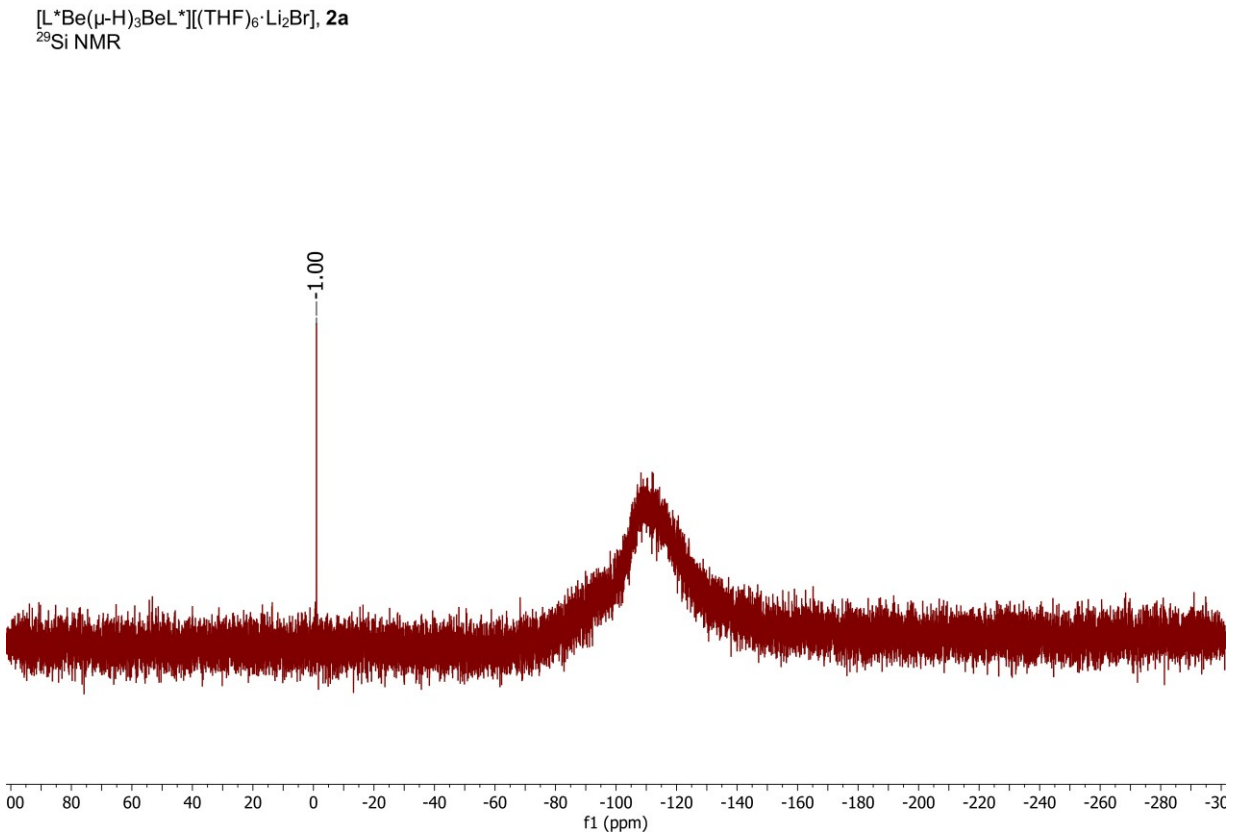

Figure S7. ^{29}Si NMR spectrum of **2a** in C_6D_6 at 298K.

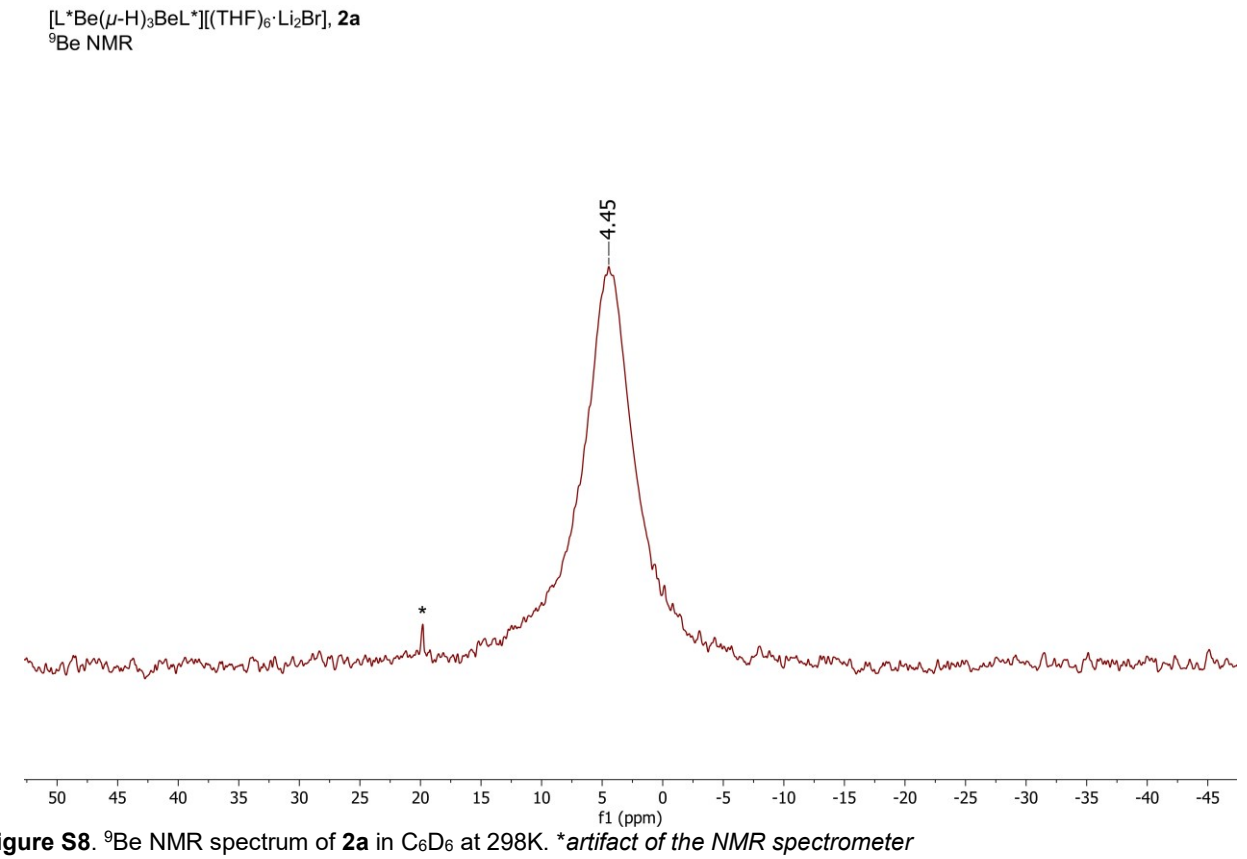

Figure S8. ^{9}Be NMR spectrum of **2a** in C_6D_6 at 298K. **artifact of the NMR spectrometer*

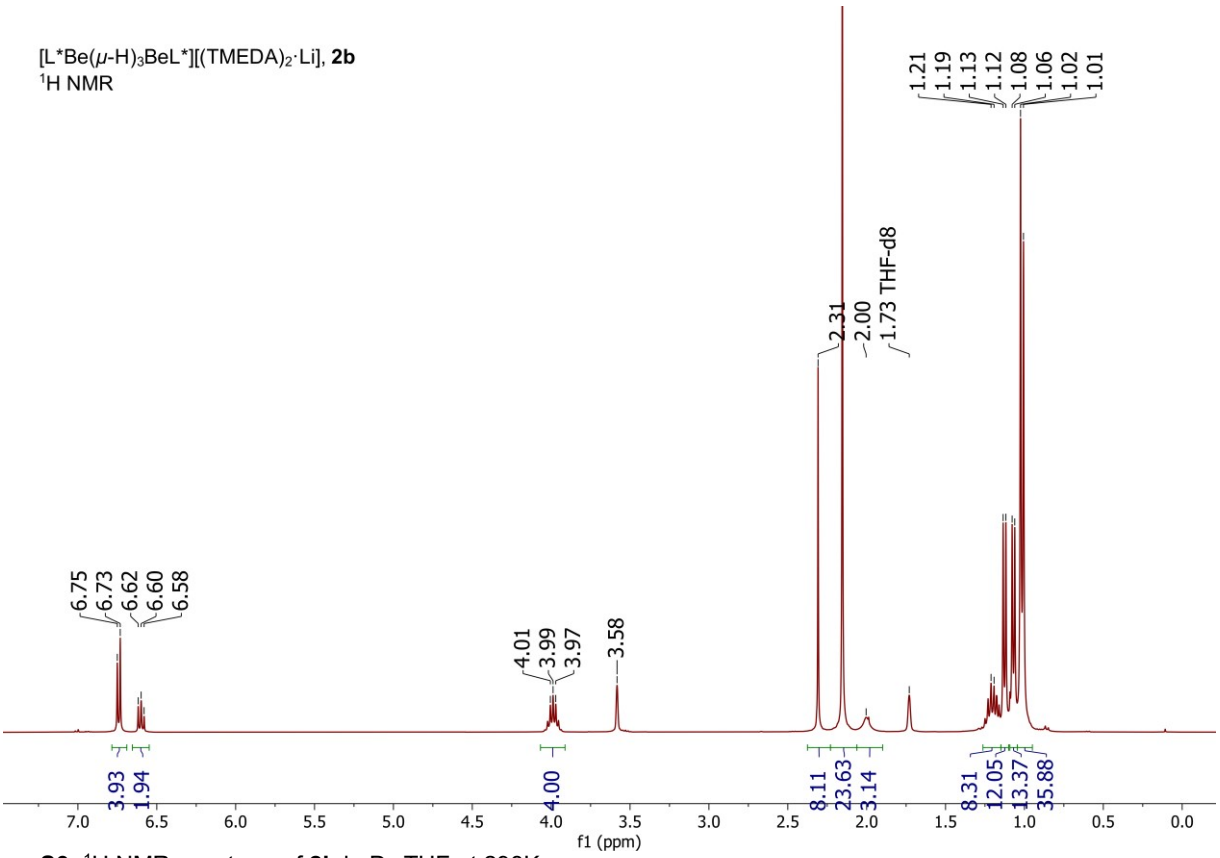

Figure S9. ^{1}H NMR spectrum of **2b** in D_8-THF at 298K.

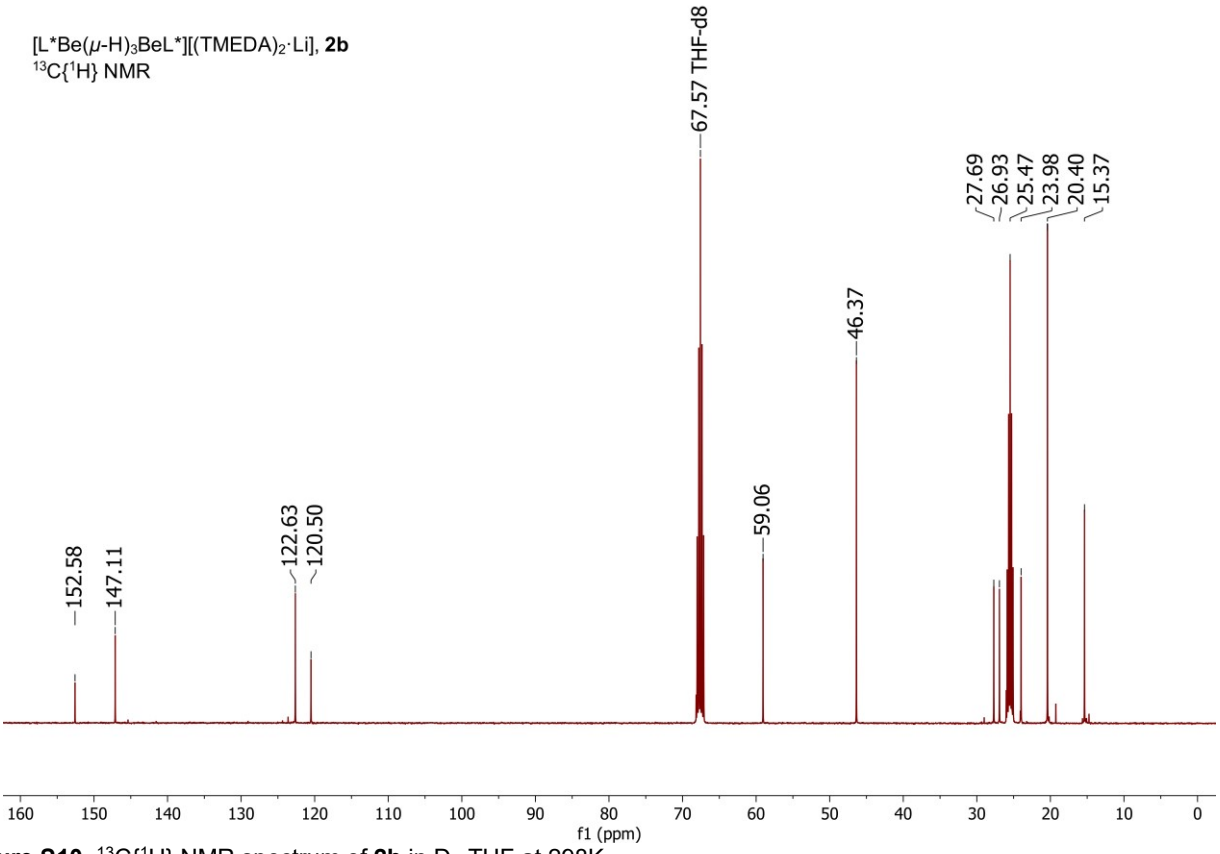

Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of **2b** in D_8-THF at 298K.

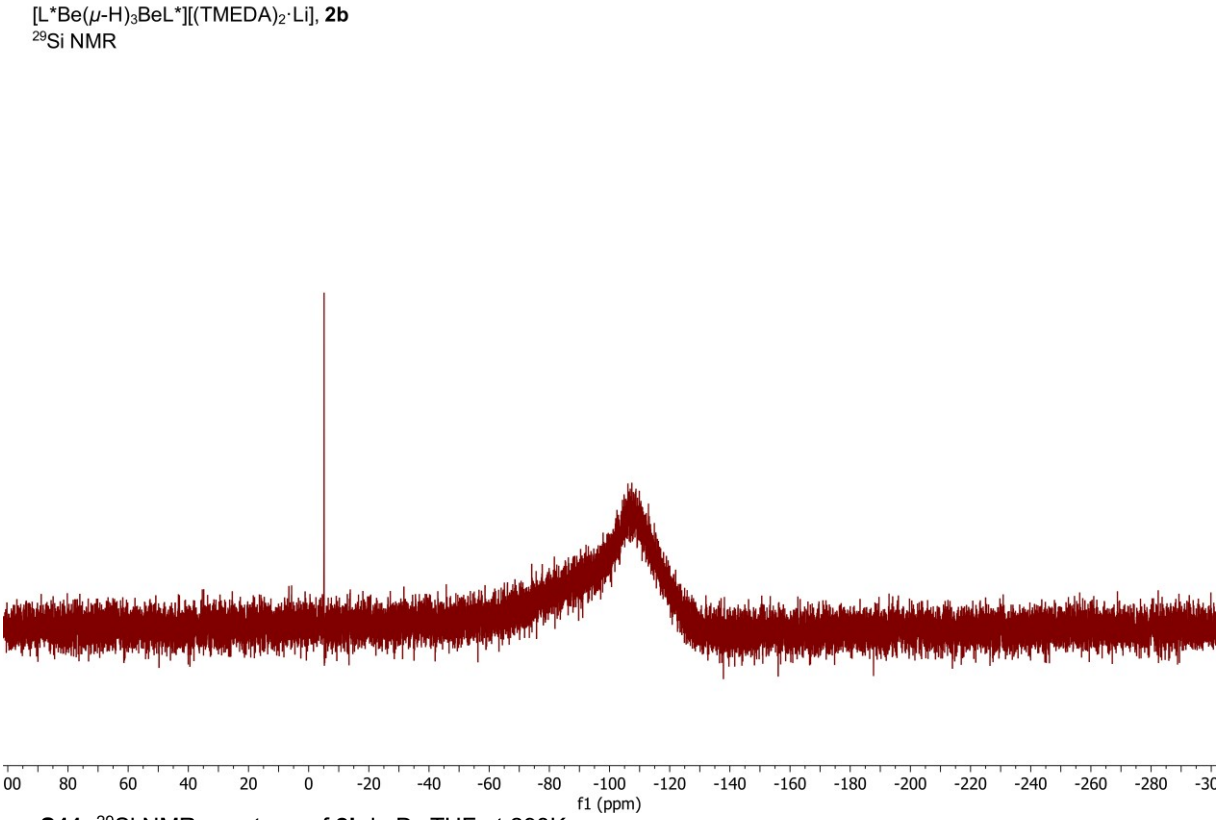

Figure S11. ^{29}Si NMR spectrum of **2b** in D_8-THF at 298K.

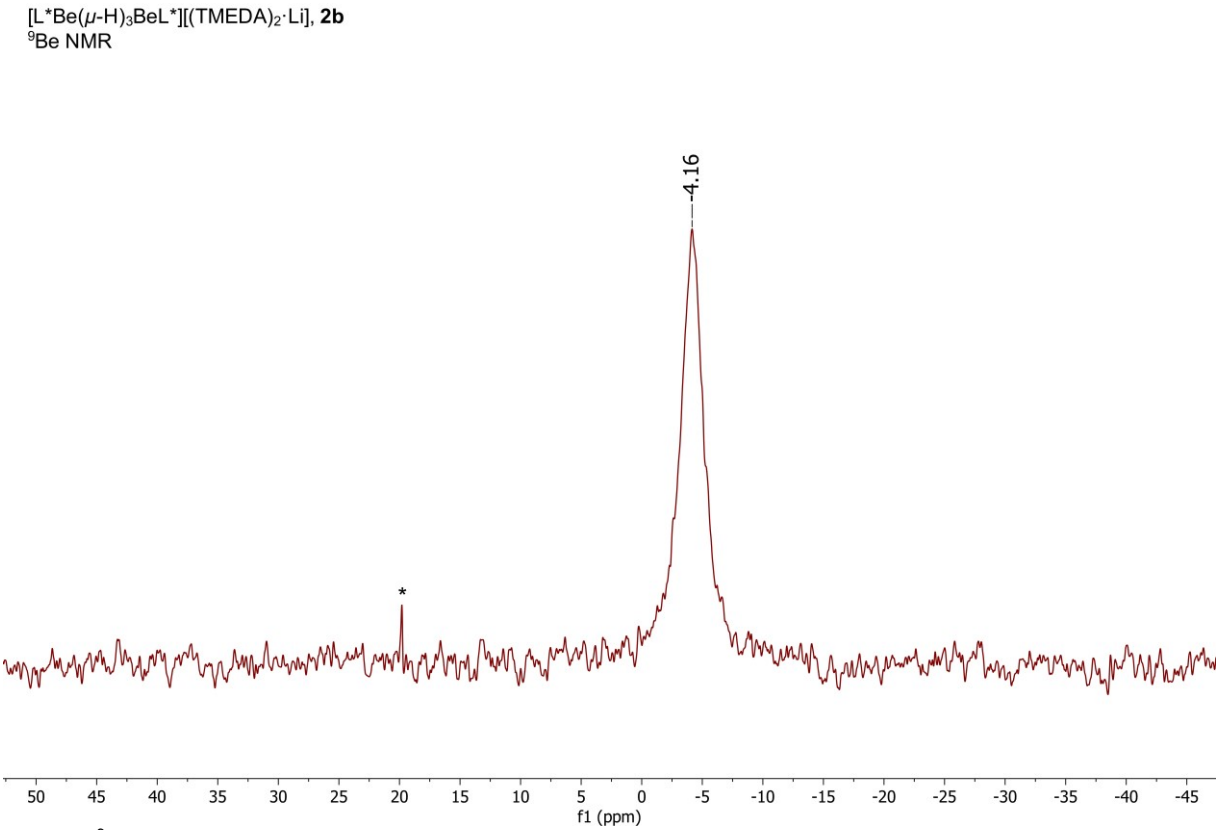

Figure S12. ^{9}Be NMR spectrum of **2b** in D_8-THF at 298K. **artifact of the NMR spectrometer*

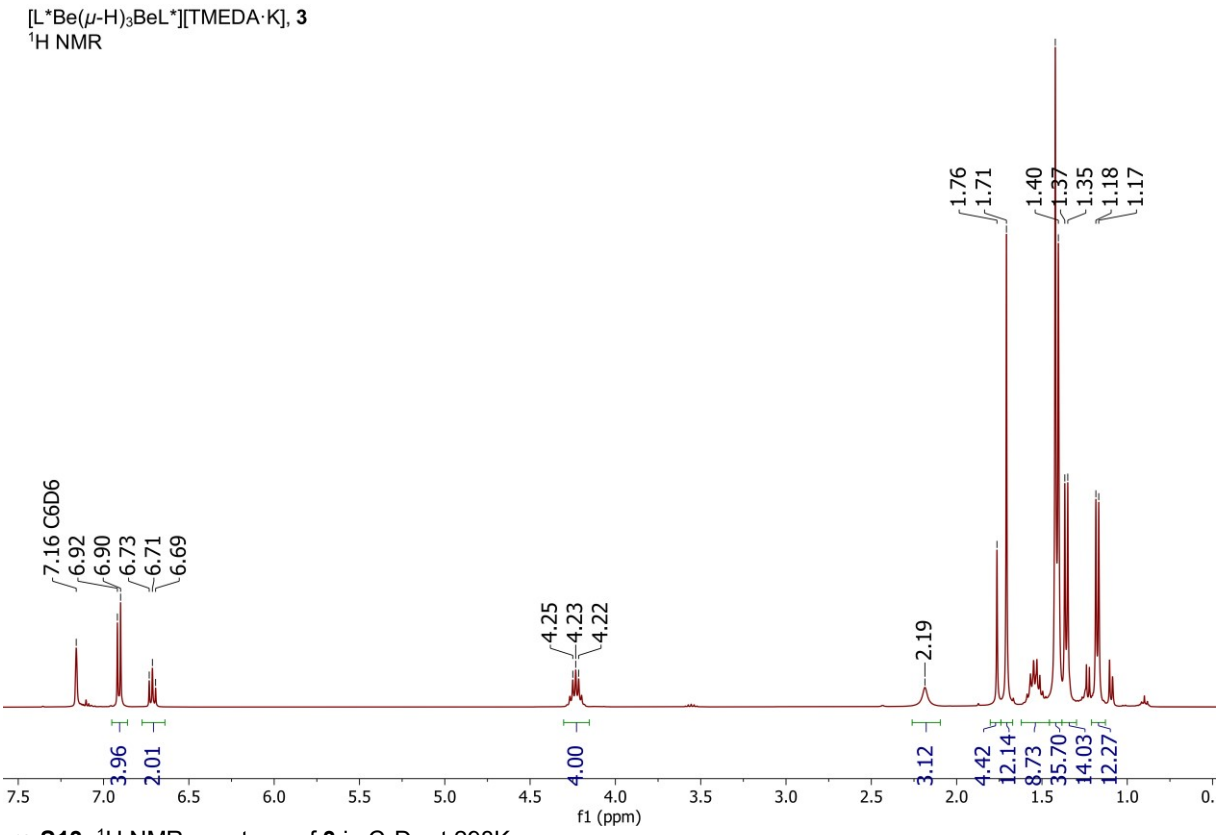

Figure S13. ^{1}H NMR spectrum of **3** in C_6D_6 at 298K.

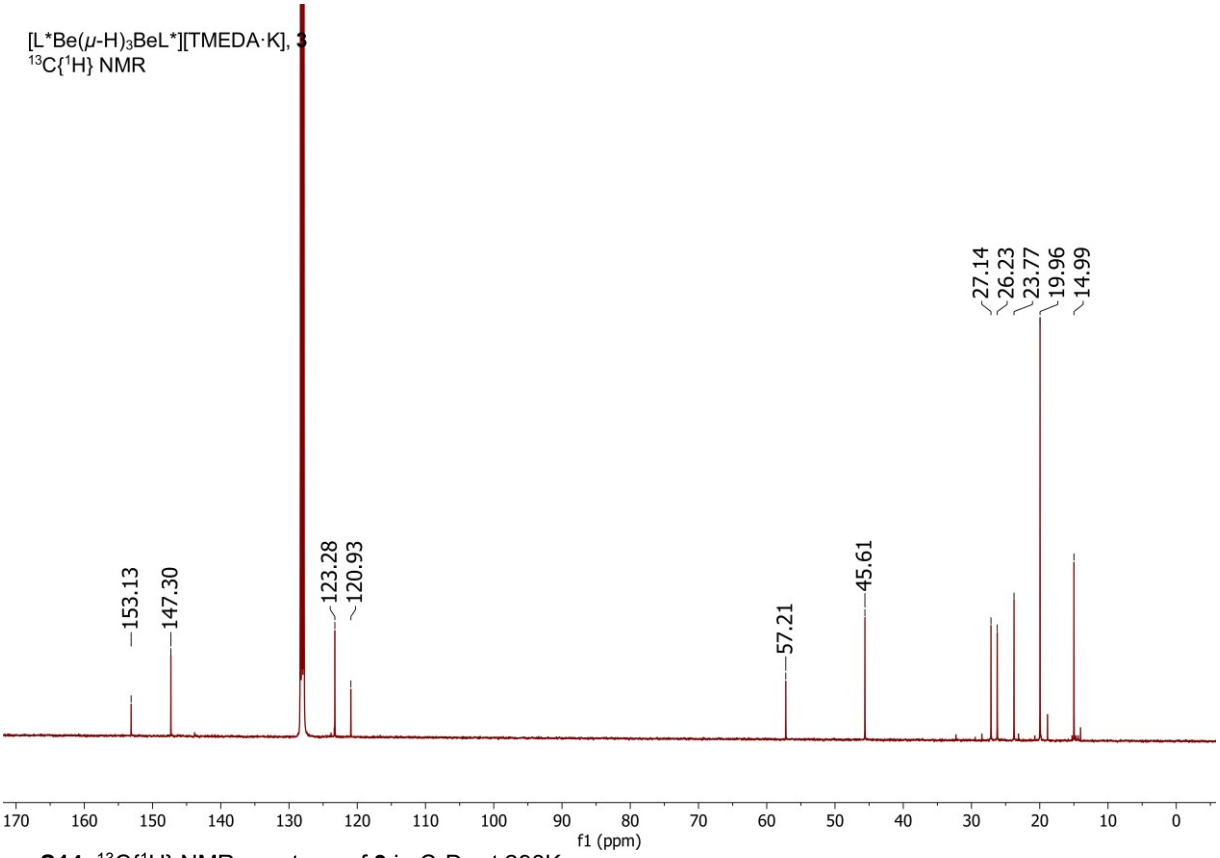

Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of **3** in C_6D_6 at 298K.

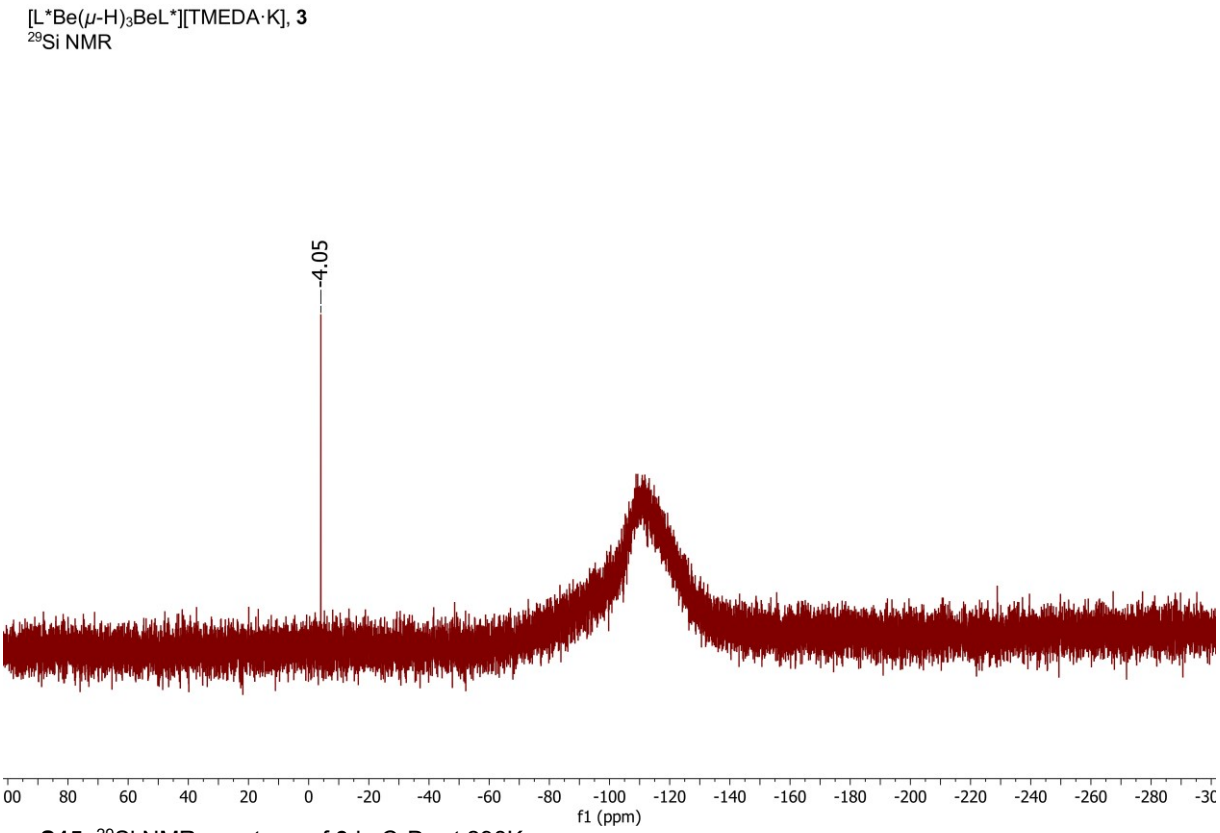

Figure S15. ^{29}Si NMR spectrum of **3** in C_6D_6 at 298K.

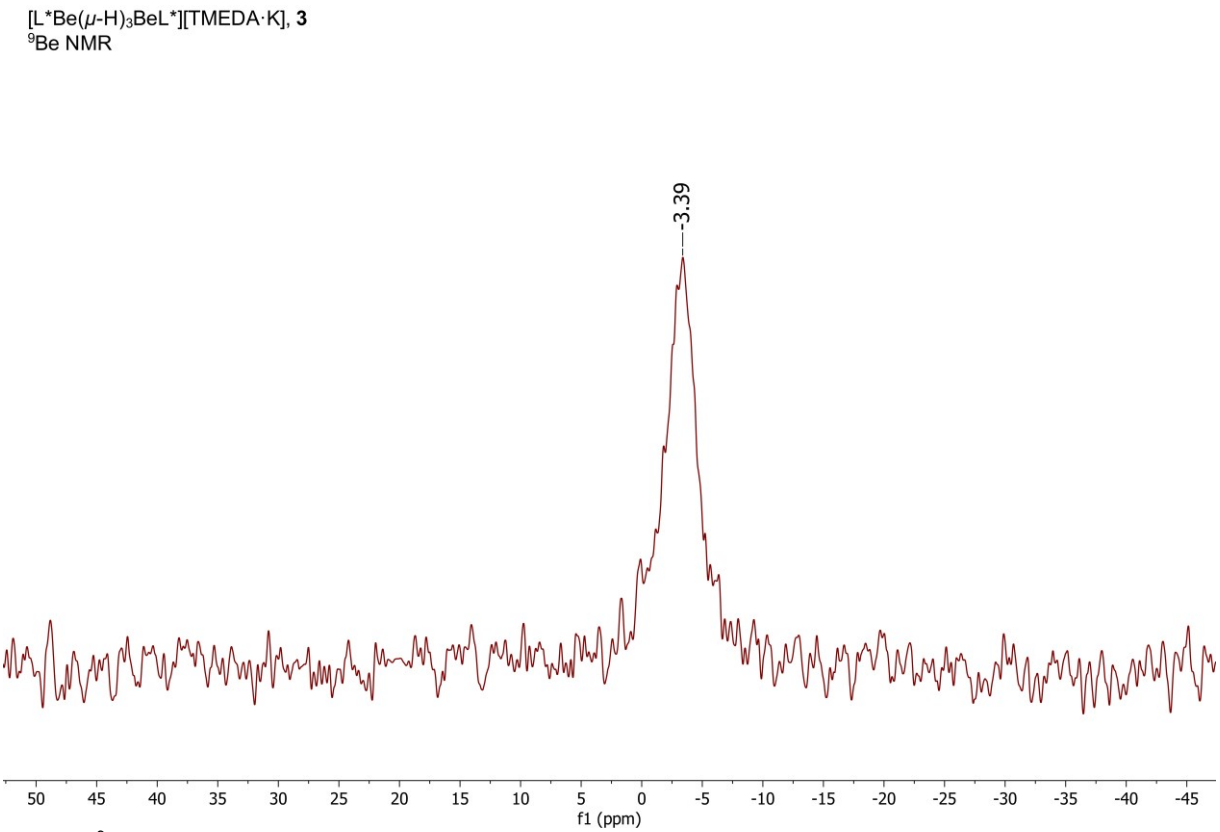

Figure S16. ^{9}Be NMR spectrum of **3** in C_6D_6 at 298K.

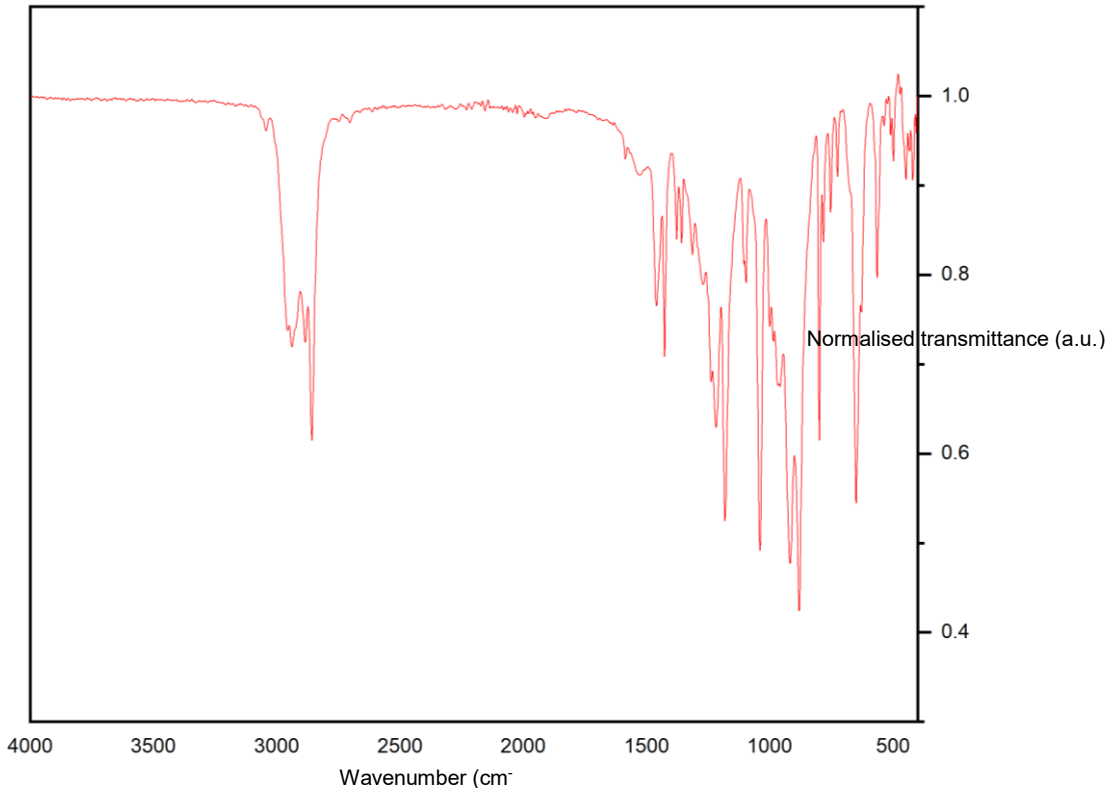

Figure S17. ATR-IR spectrum of compound **2a**.

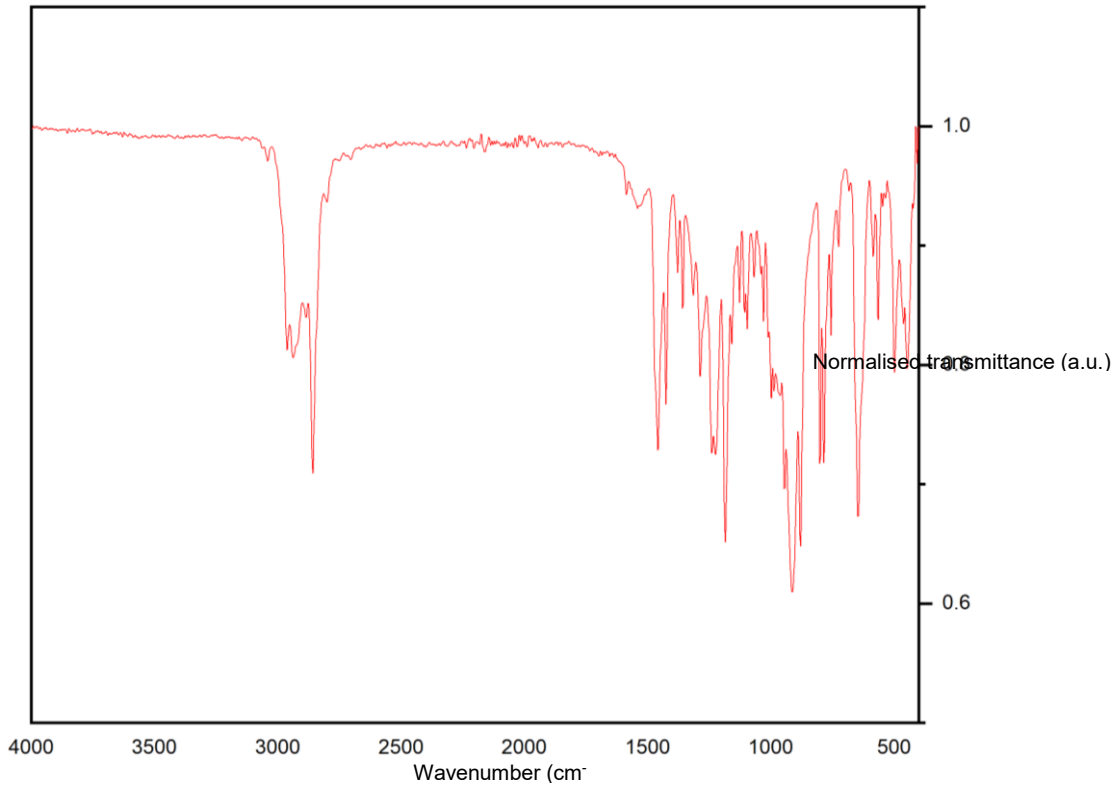

Figure S18. ATR-IR spectrum of compound **2b**.

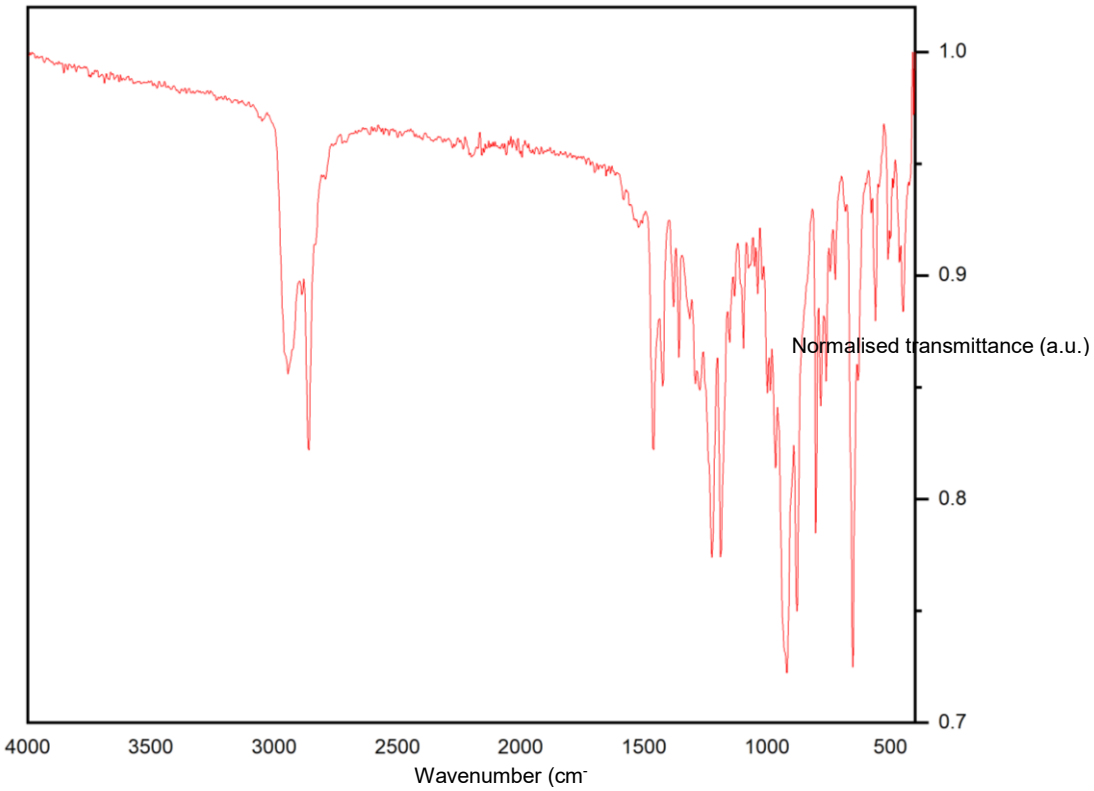

Figure S19. ATR-IR spectrum of compound **3**.

2. X-ray crystallographic details

Single crystals of **1**, **2b**, and **3** suitable for X-ray structural analysis were mounted in perfluoroalkyl ether oil on a nylon loop and positioned in a 150 K cold N_2 gas stream. Data collection was performed with a STOE StadiVari diffractometer (MoKα radiation) equipped with a DECTRIS PILATUS 300K detector. Structures were solved by Direct Methods (SHELXS-2018)[6] and refined by full-matrix least-squares calculations against F^2 (SHELXL-2018).[7] The positions of the hydrogen atoms, aside from those in the $[Be_2H_3]$ moieties of **2b** and **3**, were calculated and refined using a riding model. All non-hydrogen atoms and the hydride ligands in **2b** and **3** were treated with anisotropic displacement parameters. Crystal data, details of data collections, and refinements for all structures can be found in their CIF files, which are available free of charge *via* www.ccdc.cam.ac.uk/data_request/cif, and are summarized in Table S1.

Table S1. Summary of X-ray crystallographic data for **1**, **2b**, and **3**.

	1	**2b**	**3**
empirical form.	$C_{21}H_{38}BeBrNSi{\cdot}Et_2O$	$C_{42}H_{79}Be_2N_2Si_2{\cdot}\ C_{12}H_{32}LiN_4$	$C_{48}H_{95}Be_2KN_4Si_2$
formula wt	495.65	925.62	841.57
crystal syst.	orthorhombic	triclinic	orthorhombic
space group	$P2_12_12_1$	*P-1*	$Pna2_1$
a (Å)	10.508(2)	13.849(3)	26.540(5)
b (Å)	14.060(3)	15.592(3)	10.950(2)
c (Å)	18.959(4)	16.930(3)	90
α (deg.)	90	85.77(3)	90
β (δεγ)	90	67.48(3)	90
γ (deg.)	90	67.01(3)	79.94(3)
vol (Å^3)	2800.9(10)	3096.1(14)	5588.5(19)
Z	4	2	4
ρ(calc) (g.cm^{-3})	1.175	0.993	1.000
μ (mm^{-1})	1.526	0.093	0.169
F(000)	1064	1032	1864
T (K)	150(2)	150(2)	150(2)
reflns collect.	26524	93689	52410
unique reflns	5459	12159	10054
R_{int}	0.0524	0.0278	0.1004
R1 [$I>2\sigma(I)$]	0.0417	0.0460	0.0504
*w*R2 (all data)	0.0928	0.1293	0.1158
CCDC No.	2303227	2303228	2303229

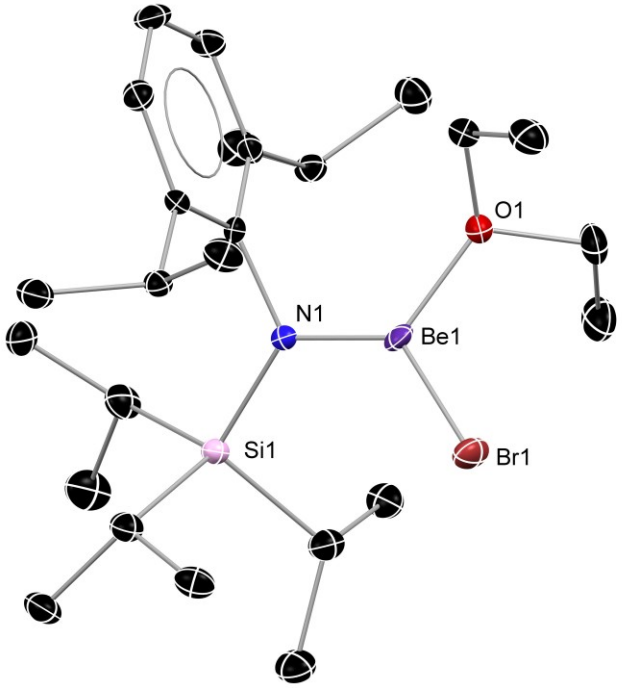

Figure S20. Molecular structure of **1**, with thermal ellipsoids at 30% probability, and hydrogen atoms omitted. Selected bond lengths (Å) and angles (°): Be1-N1 1.565(7); Be1-Br1 2.088(6); Be1-O1 1.565(7); Br1-Be1-O1 109.3(3); N1-Be1-O1 120.0(4); Br1-Be1-N1 130.6(4).

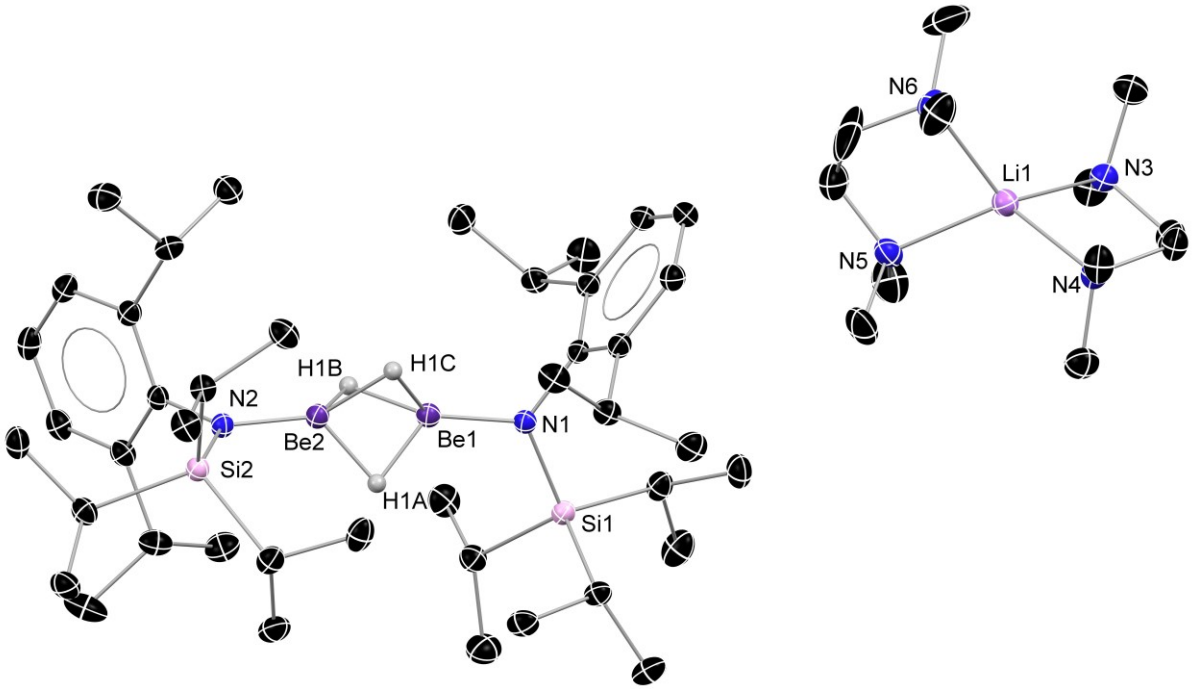

Figure S21. Molecular structure of **2b** including the [(TMEDA)$_2$Li] counterion, with thermal ellipsoids at 30% probability, hydrogen atoms omitted. For metrical parameters, see the main text.

3. Computational methods and details

Computational experiments were performed using the Gaussian 16 program.[8] Geometry optimization was carried out at the B97 or B3LYP level, with the def2-TZVP basis set for Be, N, and Si, and the def2-SVP basis set for all other atoms.[9] Stationary points were confirmed as true minima by vibrational frequency analysis (no negative eigenvalues). Dispersion corrections were implemented with Grimme's D3 model.[9(d)] Solvent effects were considered using the SMD model, for THF and benzene. Hydride ion affinity was calculated for the model complex [{(Me$_3$Si)(Xyl)NBe(μ-H)}$_2$], through isodesmic anchoring to the Me$_3$SiH/[Me$_3$Si]$^+$ couple (HIA_{Me3Si+} = 959 kJ·mol^{-1}),[10] with geometry optimization at the B3LYP level, using the def2-TZVP basis set for Be, N, and Si, and the def2-SVP basis set for all other atoms. The QTAIM and Mayer Bond Order analysis were executed using the Multiwfn program.[11]

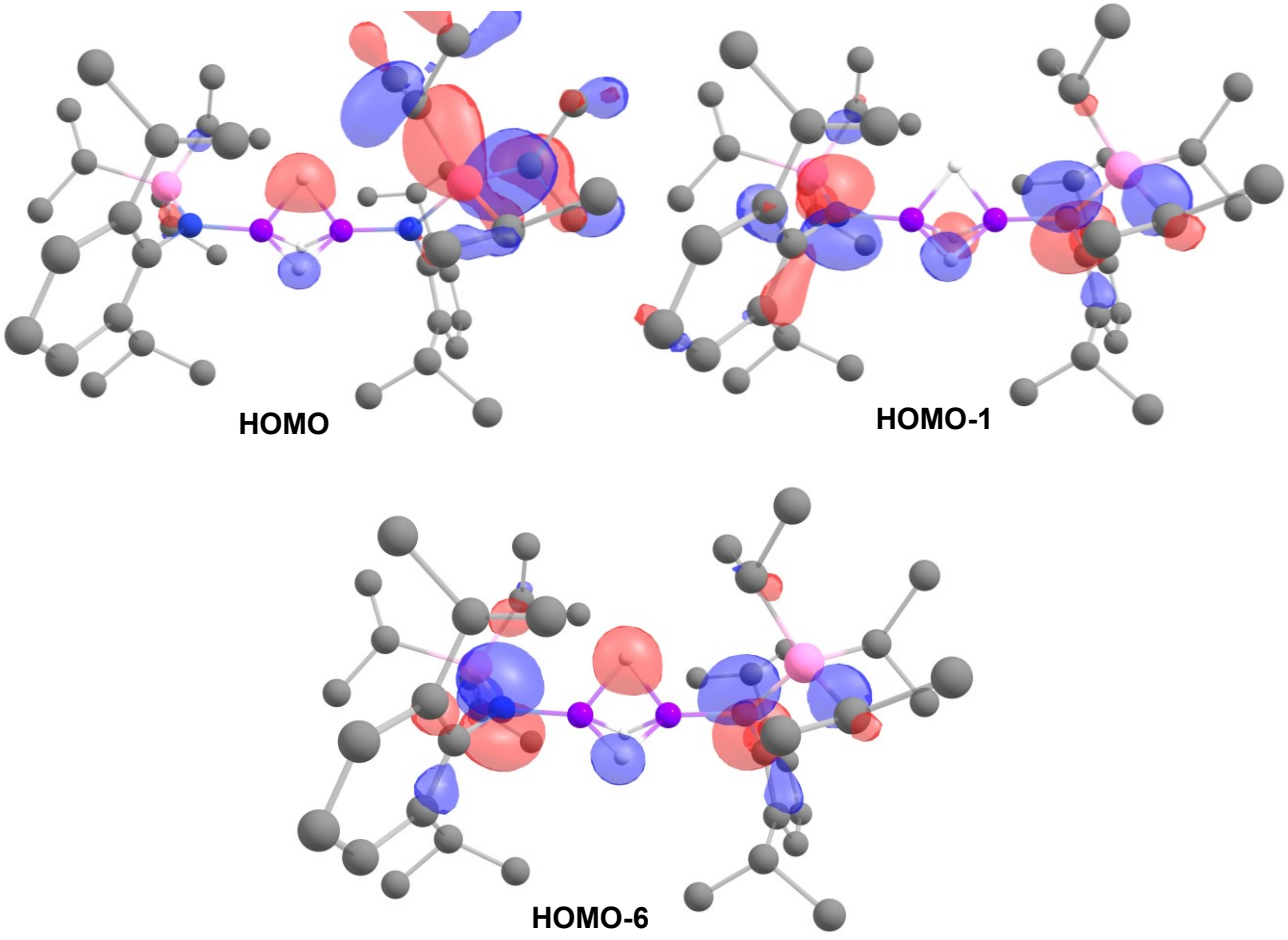

Figure S22. Selected frontier orbitals for calculated anion **2**.

Table S2. Selected Mayer Bond Order values for **2**

Element centres		Mayer Bond Order
Be123	Be124	0.532
Be123	H125	0.508
Be123	H126	0.282
Be123	H127	0.428
Be124	H125	0.414
Be124	H126	0.654
Be124	H127	0.521
Mean (Be-H)		**0.468**

Table 2. The B97D3(def2-TZVP//def2-SVP) Cartesian coordinates for anion **2** in the gas phase.

Atom	x-Coordinate	y-Coordinate	z-Coordinate
Si	3.32235	1.21878	-0.60456
Si	-3.43073	-0.93874	-1.1186
N	-2.57326	-0.05112	0.09713
N	2.4811	-0.13623	0.08763
C	3.1702	-1.21221	0.70215
C	-3.72939	0.45607	2.22972
C	-3.20469	0.87687	0.96651
C	3.58647	2.58743	0.71633
H	4.02084	2.02278	1.5636
C	3.43242	-1.21612	2.10798
C	3.6003	-2.33735	-0.07247
C	-3.3007	2.25994	0.61604
C	-2.54973	-3.46059	0.05062
H	-2.84885	-4.40063	0.5579
H	-2.02751	-2.82668	0.78614
H	-1.80316	-3.72801	-0.71654
C	-5.12707	-0.07491	-1.40585
H	-4.88406	0.99993	-1.30269
C	-3.54383	-0.98553	2.68072
H	-3.45408	-1.58362	1.76405
C	-3.76947	-2.74857	-0.56204
H	-4.51173	-2.62782	0.25331
C	4.17422	-2.2658	2.67935
H	4.37495	-2.25286	3.7584
C	-4.34809	1.39128	3.07721
H	-4.74402	1.05973	4.04476
C	-3.92988	3.16186	1.49292
H	-3.99417	4.22135	1.21362
C	3.89264	0.5176	3.93068
H	3.45207	1.38075	4.46434
H	4.7657	0.87864	3.35762
H	4.26606	-0.18843	4.6966

C	2.20489	1.89245	-2.00293
H	1.22149	1.97613	-1.50117
C	-5.75041	-0.26902	-2.79853
H	-5.99574	-1.3291	-2.99726
H	-5.08373	0.06886	-3.61052
H	-6.69788	0.30135	-2.89163
C	-2.65954	2.77474	-0.66456
H	-2.43191	1.88421	-1.26538
C	2.85039	-0.13536	3.00859
H	2.45035	0.64183	2.34175
C	-2.17725	0.39339	-3.36461
H	-1.36088	0.84904	-2.77852
H	-3.03529	1.0881	-3.34274
H	-1.82848	0.32567	-4.41524
C	-4.43208	-3.6145	-1.64717
H	-3.76308	-3.75922	-2.51573
H	-5.36745	-3.16573	-2.02607
H	-4.68367	-4.62462	-1.26242
C	-4.71594	-1.55386	3.49282
H	-4.57127	-2.63714	3.66404
H	-5.67715	-1.41585	2.96503
H	-4.80583	-1.07834	4.48789
C	-4.46257	2.73916	2.7152
H	-4.95271	3.45559	3.3871
C	5.03611	0.63858	-1.24299
H	4.81913	-0.33457	-1.71905
C	4.34309	-3.36227	0.53847
H	4.67602	-4.21556	-0.06538
C	-2.52122	-0.99913	-2.80698
H	-3.28641	-1.44789	-3.47529
C	5.66785	1.53215	-2.32423
H	5.8644	2.5555	-1.95685
H	5.02343	1.62278	-3.2155
H	6.6408	1.11805	-2.66176
C	3.16697	-2.48177	-1.52568
H	2.88522	-1.47474	-1.86791
C	4.26209	-3.01428	-2.46224
H	5.19295	-2.42498	-2.37481
H	3.92352	-2.96729	-3.51439
H	4.51389	-4.07041	-2.24925
C	1.65797	-0.69259	3.80833
H	0.90905	-1.13018	3.12821
H	1.16079	0.10703	4.38921
H	1.98352	-1.4811	4.51363
C	-6.15186	-0.4019	-0.30513
H	-7.06815	0.21329	-0.41657
H	-5.74715	-0.20782	0.70191
H	-6.46719	-1.46178	-0.34538

C	-1.27952	-1.90574	-2.86591
H	-0.82375	-1.885	-3.8771
H	-1.51553	-2.95755	-2.63496
H	-0.50866	-1.57382	-2.15283
C	6.03477	0.36393	-0.10243
H	6.96578	-0.09613	-0.49307
H	5.62095	-0.32075	0.65583
H	6.32868	1.2961	0.41463
C	4.6524	-3.3271	1.90356
H	5.24076	-4.13238	2.36207
C	4.57944	3.71449	0.38285
H	4.25685	4.31012	-0.48953
H	5.59009	3.33108	0.16059
H	4.67776	4.41994	1.2343
C	1.89708	-3.35239	-1.60254
H	2.11065	-4.38354	-1.26152
H	1.51072	-3.4032	-2.63791
H	1.10319	-2.93773	-0.95925
C	2.24042	3.16204	1.19152
H	2.36237	3.78331	2.10204
H	1.50711	2.36988	1.42176
H	1.78283	3.8059	0.41869
C	2.01854	0.87496	-3.14078
H	1.31191	1.25586	-3.90546
H	1.60316	-0.07247	-2.76082
H	2.97038	0.64627	-3.657
C	-2.20862	-1.13435	3.43375
H	-1.3721	-0.76848	2.81635
H	-2.00939	-2.19231	3.69024
H	-2.21887	-0.5462	4.37102
C	-1.31419	3.45992	-0.36053
H	-1.4591	4.37124	0.25067
H	-0.79821	3.7508	-1.29542
H	-0.65176	2.77713	0.1944
C	-3.57782	3.68263	-1.49677
H	-3.79241	4.63999	-0.98484
H	-4.54544	3.19221	-1.70813
H	-3.10107	3.92841	-2.46446
C	2.54988	3.28887	-2.54607
H	3.54533	3.32542	-3.0245
H	2.53702	4.05597	-1.75351
H	1.81129	3.60219	-3.31228
Be	0.86732	-0.15576	0.16276
Be	-0.95932	-0.11093	0.19109
H	-0.07526	0.59466	1.16133
H	-0.03445	0.33431	-0.91172
H	-0.03855	-1.33794	0.34532

Table 3. The B97D3(def2-TZVP//def2-SVP) Cartesian coordinates for anion **2** with the SMD-Benzene model.

Atom	x-Coordinate	y-Coordinate	z-Coordinate
Si	3.33472	1.21706	-0.60671
Si	-3.45073	-0.94087	-1.11288
N	-2.57216	-0.05131	0.09322
N	2.49428	-0.13998	0.09232
C	3.18692	-1.21724	0.70232
C	-3.72591	0.47274	2.22767
C	-3.19704	0.8845	0.962
C	3.62322	2.57762	0.71759
H	4.06568	2.00698	1.55704
C	3.45713	-1.2212	2.10766
C	3.61197	-2.34317	-0.07533
C	-3.28384	2.26854	0.60714
C	-2.61666	-3.47353	0.0716
H	-2.9362	-4.37749	0.62954
H	-2.0398	-2.83685	0.76344
H	-1.91038	-3.80919	-0.70717
C	-5.12831	-0.04741	-1.41338
H	-4.86618	1.02348	-1.31735
C	-3.55829	-0.96894	2.6876
H	-3.45093	-1.56878	1.77447
C	-3.82471	-2.73539	-0.53266
H	-4.55279	-2.58563	0.29037
C	4.20345	-2.27073	2.67453
H	4.41189	-2.25859	3.752
C	-4.33644	1.41682	3.07258
H	-4.73578	1.09214	4.04096
C	-3.90422	3.17897	1.48243
H	-3.96182	4.23782	1.20011
C	3.90403	0.50018	3.95141
H	3.46111	1.36716	4.47725
H	4.79204	0.85679	3.3985
H	4.25777	-0.20628	4.72623
C	2.19181	1.89998	-1.9801
H	1.21902	1.98856	-1.4581
C	-5.75023	-0.23649	-2.80719
H	-6.01591	-1.29165	-3.00617
H	-5.07835	0.08928	-3.6202
H	-6.68667	0.35098	-2.90576
C	-2.64346	2.77718	-0.67712
H	-2.44327	1.88572	-1.28655
C	2.87335	-0.14274	3.01076
H	2.48448	0.64009	2.34394
C	-2.16461	0.34198	-3.36994
H	-1.3334	0.7847	-2.7947
H	-3.00472	1.0585	-3.35186

H	-1.82415	0.25872	-4.42245
C	-4.52384	-3.59817	-1.59664
H	-3.87106	-3.78016	-2.47096
H	-5.45129	-3.13157	-1.97337
H	-4.80155	-4.59398	-1.19295
C	-4.75023	-1.5304	3.47481
H	-4.61941	-2.61629	3.64197
H	-5.7022	-1.38418	2.93201
H	-4.85619	-1.06275	4.47204
C	-4.43886	2.76469	2.70706
H	-4.92268	3.48718	3.37689
C	5.03437	0.63543	-1.27813
H	4.8068	-0.33415	-1.75641
C	4.35848	-3.36861	0.53175
H	4.6893	-4.22186	-0.07308
C	-2.53883	-1.03666	-2.79867
H	-3.31242	-1.47466	-3.464
C	5.65234	1.53127	-2.36528
H	5.86597	2.55123	-1.99786
H	4.99648	1.63109	-3.24741
H	6.61571	1.11186	-2.723
C	3.17354	-2.48698	-1.52811
H	2.90115	-1.47801	-1.87303
C	4.25879	-3.03571	-2.46598
H	5.20344	-2.46871	-2.37554
H	3.92458	-2.97298	-3.5189
H	4.48819	-4.09899	-2.26388
C	1.66904	-0.7006	3.79158
H	0.93456	-1.1475	3.1015
H	1.15608	0.09905	4.35894
H	1.98155	-1.48395	4.50871
C	-6.16414	-0.34716	-0.3157
H	-7.06051	0.2975	-0.42342
H	-5.75754	-0.1712	0.69422
H	-6.51534	-1.39558	-0.35927
C	-1.31761	-1.97127	-2.84981
H	-0.84995	-1.95462	-3.85587
H	-1.57916	-3.02037	-2.63319
H	-0.54477	-1.66495	-2.12768
C	6.05283	0.35226	-0.15804
H	6.96941	-0.12271	-0.56489
H	5.64967	-0.32511	0.61298
H	6.37237	1.28071	0.35045
C	4.6754	-3.33308	1.89547
H	5.26668	-4.13819	2.35032
C	4.61796	3.701	0.37801
H	4.28776	4.30977	-0.48263
H	5.62433	3.3165	0.13884

H	4.73475	4.39795	1.23423
C	1.89399	-3.34285	-1.60015
H	2.09451	-4.37863	-1.26477
H	1.49983	-3.38683	-2.63296
H	1.10773	-2.92433	-0.94937
C	2.28875	3.15951	1.21548
H	2.42598	3.76482	2.13482
H	1.54944	2.37245	1.44487
H	1.82793	3.82141	0.45959
C	1.98215	0.89108	-3.12108
H	1.24983	1.27013	-3.86232
H	1.59143	-0.0685	-2.74443
H	2.92023	0.6813	-3.66987
C	-2.24037	-1.12285	3.46937
H	-1.39035	-0.76131	2.86827
H	-2.04882	-2.1813	3.73024
H	-2.26358	-0.53565	4.40724
C	-1.27927	3.42632	-0.37885
H	-1.3957	4.34217	0.23209
H	-0.75852	3.7046	-1.31485
H	-0.63394	2.72763	0.17736
C	-3.54297	3.71548	-1.49503
H	-3.71809	4.68075	-0.98294
H	-4.53075	3.26098	-1.69484
H	-3.0732	3.94685	-2.46982
C	2.52903	3.29737	-2.52496
H	3.51374	3.335	-3.02508
H	2.53267	4.0647	-1.73249
H	1.77624	3.61539	-3.27562
Be	0.88021	-0.16733	0.1675
Be	-0.95822	-0.11996	0.18677
H	-0.0683	0.63529	1.12134
H	-0.02771	0.25852	-0.93432
H	-0.02791	-1.34137	0.41688

Table 4. The B97D3(def2-TZVP//def2-SVP) Cartesian coordinates for anion **2** with the SMD-THF model.

Atom	**x-Coordinate**	**y-Coordinate**	**z-Coordinate**
Si	3.35775	1.20229	-0.60426
Si	-3.49229	-0.98851	-1.06896
N	-2.58092	-0.05548	0.08177
N	2.49376	-0.15296	0.0768
C	3.16748	-1.22806	0.71013
C	-3.71561	0.60739	2.18748
C	-3.17051	0.9414	0.90458
C	3.62563	2.55742	0.72747

H	4.04616	1.98285	1.57557
C	3.3885	-1.23319	2.12452
C	3.62225	-2.35284	-0.05388
C	-3.20137	2.31115	0.48899
C	-2.63025	-3.45908	0.21894
H	-2.93234	-4.38808	0.74486
H	-2.11886	-2.81198	0.95138
H	-1.87507	-3.74481	-0.53387
C	-5.17615	-0.10699	-1.35806
H	-4.91631	0.9676	-1.29776
C	-3.60313	-0.81839	2.7111
H	-3.5849	-1.47004	1.82718
C	-3.84425	-2.76289	-0.42046
H	-4.58214	-2.59938	0.3911
C	4.11412	-2.28408	2.71699
H	4.28493	-2.27198	3.80107
C	-4.29282	1.61111	2.98652
H	-4.70694	1.34668	3.96673
C	-3.79106	3.28326	1.31959
H	-3.80851	4.32958	0.98841
C	3.79928	0.50051	3.96231
H	3.34511	1.36764	4.47803
H	4.69275	0.85923	3.4196
H	4.14434	-0.20274	4.74365
C	2.24056	1.88377	-1.99774
H	1.25786	1.96823	-1.49425
C	-5.82471	-0.34079	-2.73305
H	-6.09061	-1.40268	-2.89105
H	-5.16972	-0.03958	-3.56881
H	-6.7645	0.24107	-2.83071
C	-2.5442	2.74334	-0.8149
H	-2.2919	1.81646	-1.34717
C	2.78452	-0.15077	3.00974
H	2.4056	0.6268	2.33122
C	-2.27515	0.2116	-3.40878
H	-1.4217	0.67994	-2.88755
H	-3.11504	0.92746	-3.38186
H	-1.97878	0.08858	-4.47063
C	-4.52083	-3.67074	-1.46185
H	-3.85291	-3.88191	-2.31751
H	-5.44446	-3.22387	-1.87073
H	-4.79942	-4.65132	-1.02342
C	-4.77245	-1.26991	3.59601
H	-4.6908	-2.35218	3.80975
H	-5.74711	-1.09495	3.10455
H	-4.78796	-0.74944	4.57195
C	-4.34441	2.94509	2.55959
H	-4.8032	3.71437	3.19395

C	5.06693	0.61543	-1.24301
H	4.84869	-0.35082	-1.73195
C	4.34676	-3.37946	0.57845
H	4.70066	-4.23125	-0.01511
C	-2.6212	-1.14486	-2.77053
H	-3.40779	-1.61567	-3.39655
C	5.70732	1.51637	-2.31311
H	5.91468	2.53384	-1.93597
H	5.06763	1.62066	-3.20641
H	6.67652	1.09664	-2.65392
C	3.24398	-2.48939	-1.52404
H	3.00775	-1.47593	-1.88123
C	4.35674	-3.06155	-2.41391
H	5.30653	-2.51073	-2.285
H	4.06754	-2.99496	-3.47964
H	4.5568	-4.12805	-2.19934
C	1.57129	-0.70606	3.77917
H	0.84876	-1.16971	3.08687
H	1.04573	0.09856	4.32761
H	1.87867	-1.47532	4.51346
C	-6.19089	-0.38213	-0.23436
H	-7.09206	0.25534	-0.34393
H	-5.76923	-0.18052	0.76448
H	-6.53736	-1.43278	-0.24558
C	-1.39402	-2.07125	-2.81442
H	-0.96286	-2.10836	-3.8363
H	-1.63521	-3.10786	-2.52603
H	-0.59882	-1.71507	-2.14037
C	6.06228	0.32657	-0.10349
H	6.98172	-0.15797	-0.49189
H	5.63862	-0.34328	0.6636
H	6.38026	1.25418	0.40712
C	4.61414	-3.34581	1.95373
H	5.18852	-4.15161	2.42852
C	4.63481	3.67351	0.40638
H	4.3248	4.28142	-0.46235
H	5.64284	3.28139	0.18861
H	4.73776	4.37115	1.26365
C	1.95101	-3.31754	-1.65173
H	2.1164	-4.35912	-1.31515
H	1.59821	-3.34845	-2.69991
H	1.14759	-2.88612	-1.03102
C	2.287	3.15283	1.19721
H	2.40975	3.74849	2.1248
H	1.53074	2.37513	1.40088
H	1.85747	3.82807	0.4347
C	2.05685	0.87897	-3.1469
H	1.33127	1.25541	-3.89654

H	1.67281	-0.08868	-2.78259
H	3.00521	0.68345	-3.68266
C	-2.2531	-1.0099	3.4271
H	-1.4168	-0.73736	2.7629
H	-2.11116	-2.06137	3.74145
H	-2.18986	-0.37081	4.32851
C	-1.22012	3.48019	-0.54034
H	-1.39318	4.43904	-0.01494
H	-0.68796	3.7028	-1.48453
H	-0.556	2.86427	0.08728
C	-3.46515	3.57282	-1.72276
H	-3.71122	4.55598	-1.27863
H	-4.41752	3.04875	-1.92237
H	-2.97563	3.76708	-2.69583
C	2.58637	3.28385	-2.52997
H	3.57905	3.32096	-3.01385
H	2.57939	4.046	-1.7326
H	1.84613	3.6064	-3.291
Be	0.88134	-0.16885	0.13317
Be	-0.96754	-0.12986	0.15041
H	-0.07767	0.64451	1.07116
H	-0.03229	0.22964	-0.97913
H	-0.02946	-1.34314	0.4015

Table 5. The B3LYP(def2-TZVP//def2-SVP) Cartesian coordinates for anion **2** in the gas phase.

Atom	**x-Coordinate**	**y-Coordinate**	**z-Coordinate**
Si	3.30891	1.18868	-0.62053
Si	-3.38781	-0.98124	-1.08386
N	-2.5571	-0.04464	0.10418
N	2.44395	-0.13011	0.09578
C	3.10464	-1.20231	0.74844
C	-3.74254	0.60384	2.17813
C	-3.17497	0.94487	0.9133
C	3.59007	2.58101	0.6641
H	4.01174	2.0343	1.52575
C	3.34401	-1.17442	2.15323
C	3.51942	-2.35379	0.01376
C	-3.20348	2.30954	0.50406
C	-2.47371	-3.41524	0.21636
H	-2.75368	-4.36019	0.71804
H	-2.0291	-2.74822	0.96852
H	-1.67256	-3.65316	-0.49944
C	-5.09443	-0.16399	-1.41636
H	-4.87485	0.9159	-1.34242
C	-3.63678	-0.82418	2.69627
H	-3.66527	-1.48028	1.81993

C	-3.69043	-2.7745	-0.47331
H	-4.46733	-2.65195	0.30391
C	4.05804	-2.21739	2.76008
H	4.24139	-2.18141	3.83789
C	-4.33923	1.5983	2.96387
H	-4.77397	1.3319	3.93004
C	-3.8088	3.27218	1.32436
H	-3.81883	4.31708	1.00033
C	3.7922	0.58391	3.95512
H	3.35061	1.454	4.46936
H	4.67652	0.93034	3.39676
H	4.14391	-0.11393	4.73381
C	2.20714	1.85226	-2.02997
H	1.23578	1.98298	-1.52279
C	-5.70053	-0.41377	-2.807
H	-5.91851	-1.48191	-2.97505
H	-5.0397	-0.08471	-3.62302
H	-6.65765	0.12857	-2.92294
C	-2.52009	2.75066	-0.78206
H	-2.26098	1.83591	-1.32226
C	2.76115	-0.06925	3.02346
H	2.38185	0.70245	2.34486
C	-2.16052	0.27676	-3.39128
H	-1.33133	0.76206	-2.85455
H	-3.01812	0.96758	-3.37471
H	-1.84389	0.16479	-4.44459
C	-4.27793	-3.70788	-1.54438
H	-3.57189	-3.86966	-2.3757
H	-5.20885	-3.31064	-1.97969
H	-4.51255	-4.70402	-1.12457
C	-4.78399	-1.25382	3.61875
H	-4.71376	-2.33352	3.83148
H	-5.76694	-1.05897	3.15986
H	-4.75619	-0.73228	4.59023
C	-4.38451	2.92862	2.54486
H	-4.85576	3.69107	3.17196
C	5.01217	0.57356	-1.24386
H	4.78659	-0.40842	-1.6899
C	4.23439	-3.37021	0.66074
H	4.55737	-4.24435	0.089
C	-2.47374	-1.0917	-2.76275
H	-3.22625	-1.58986	-3.40436
C	5.65032	1.42847	-2.35122
H	5.85213	2.45976	-2.01922
H	5.01126	1.49298	-3.24484
H	6.6182	0.99905	-2.6718
C	3.09498	-2.54269	-1.43722
H	2.82637	-1.55212	-1.8228

C	4.1887	-3.12042	-2.34593
H	5.12133	-2.53738	-2.28018
H	3.85448	-3.11367	-3.39695
H	4.43058	-4.1658	-2.09054
C	1.5491	-0.59585	3.81069
H	0.79823	-1.01506	3.12592
H	1.06632	0.21501	4.38191
H	1.84796	-1.38694	4.51976
C	-6.12974	-0.48277	-0.32373
H	-7.0497	0.11502	-0.46086
H	-5.74908	-0.26633	0.68507
H	-6.4294	-1.54463	-0.35002
C	-1.20951	-1.96657	-2.78518
H	-0.76928	-1.99464	-3.79929
H	-1.40816	-3.00616	-2.48812
H	-0.44167	-1.57217	-2.10621
C	6.01463	0.32338	-0.10178
H	6.94142	-0.14215	-0.48606
H	5.60841	-0.34541	0.67075
H	6.30996	1.26264	0.39449
C	4.52673	-3.30309	2.02295
H	5.0923	-4.10313	2.50943
C	4.59759	3.68697	0.3086
H	4.28675	4.26579	-0.57531
H	5.60206	3.28925	0.09966
H	4.70083	4.40761	1.14181
C	1.82033	-3.40447	-1.49264
H	2.02353	-4.42254	-1.11823
H	1.43927	-3.48539	-2.52448
H	1.02824	-2.96438	-0.86991
C	2.25081	3.18744	1.1158
H	2.37797	3.83252	2.0045
H	1.50705	2.41581	1.36728
H	1.8054	3.81217	0.32454
C	1.97693	0.8059	-3.13159
H	1.27144	1.18069	-3.89547
H	1.54184	-0.1151	-2.71864
H	2.91138	0.53571	-3.6534
C	-2.27233	-1.04819	3.37018
H	-1.45091	-0.78828	2.68868
H	-2.14573	-2.10173	3.67212
H	-2.17339	-0.41701	4.26945
C	-1.19598	3.4701	-0.4769
H	-1.36747	4.408	0.07871
H	-0.65773	3.71681	-1.40807
H	-0.54338	2.8271	0.12886
C	-3.41901	3.5922	-1.69836
H	-3.67481	4.56634	-1.24802

H	-4.36333	3.07112	-1.92391
H	-2.90783	3.79665	-2.65423
C	2.58451	3.21867	-2.62305
H	3.57258	3.21399	-3.11056
H	2.59925	4.01126	-1.86041
H	1.84881	3.52437	-3.39001
Be	0.84355	-0.13373	0.163
Be	-0.95517	-0.0895	0.19622
H	-0.08444	0.60356	1.16345
H	-0.04266	0.3674	-0.8945
H	-0.05434	-1.30284	0.33353

Table 6. The B3LYP(def2-TZVP//def2-SVP) Cartesian coordinates for anion **2** with the SMD-Benzene model.

Atom	x-Coordinate	y-Coordinate	z-Coordinate
Si	3.31998	1.18391	-0.61257
Si	-3.40846	-0.96221	-1.09608
N	-2.56269	-0.04267	0.10039
N	2.44566	-0.14974	0.07981
C	3.07887	-1.23171	0.74279
C	-3.7159	0.63371	2.18432
C	-3.14681	0.96008	0.91787
C	3.5957	2.54414	0.70962
H	4.03488	1.9792	1.55168
C	3.29417	-1.22368	2.15456
C	3.51651	-2.36831	0.00089
C	-3.10955	2.33236	0.52443
C	-2.51764	-3.43324	0.16772
H	-2.816	-4.37435	0.66682
H	-2.04944	-2.78468	0.92534
H	-1.72956	-3.68957	-0.55695
C	-5.10786	-0.12702	-1.41085
H	-4.88141	0.94849	-1.3014
C	-3.68025	-0.80874	2.67987
H	-3.80441	-1.44782	1.79804
C	-3.7244	-2.7587	-0.50408
H	-4.49345	-2.63817	0.28003
C	4.02014	-2.26465	2.75435
H	4.18808	-2.24487	3.83496
C	-4.25584	1.64966	2.98554
H	-4.6981	1.39646	3.95126
C	-3.6503	3.31692	1.36423
H	-3.61088	4.36497	1.05191
C	3.67896	0.48773	4.01992
H	3.21777	1.34378	4.54115
H	4.58129	0.85285	3.50307
H	4.00885	-0.22584	4.79379

C	2.20946	1.88972	-2.00183
H	1.24778	2.05338	-1.4762
C	-5.7103	-0.33032	-2.80994
H	-5.93121	-1.39104	-3.01756
H	-5.04829	0.02594	-3.61396
H	-6.6656	0.21784	-2.91237
C	-2.43514	2.7489	-0.7755
H	-2.235	1.82465	-1.32083
C	2.6811	-0.14614	3.04028
H	2.31235	0.63888	2.37333
C	-2.16287	0.3012	-3.39692
H	-1.31532	0.76589	-2.8694
H	-3.00471	1.0114	-3.36748
H	-1.85848	0.19369	-4.45485
C	-4.33123	-3.66199	-1.58926
H	-3.63263	-3.824	-2.42786
H	-5.25711	-3.24178	-2.01402
H	-4.58424	-4.66183	-1.18925
C	-4.80087	-1.17724	3.6605
H	-4.79478	-2.26331	3.85155
H	-5.79469	-0.90984	3.26559
H	-4.68327	-0.68006	4.63749
C	-4.23338	2.98687	2.58539
H	-4.65921	3.76395	3.22677
C	5.01882	0.58138	-1.26392
H	4.79422	-0.39475	-1.72035
C	4.25183	-3.37631	0.6378
H	4.59637	-4.23716	0.05929
C	-2.49941	-1.0668	-2.78026
H	-3.26131	-1.54388	-3.42724
C	5.63984	1.45125	-2.36885
H	5.84885	2.47836	-2.02973
H	4.99151	1.52474	-3.25473
H	6.60302	1.02615	-2.70926
C	3.08099	-2.5476	-1.44942
H	2.79743	-1.55854	-1.82807
C	4.16492	-3.11437	-2.37569
H	5.10344	-2.54087	-2.30717
H	3.8246	-3.08237	-3.42444
H	4.4011	-4.1673	-2.14739
C	1.45884	-0.70651	3.78448
H	0.73395	-1.13282	3.07688
H	0.94368	0.08674	4.35284
H	1.7512	-1.50013	4.49327
C	-6.15005	-0.4733	-0.33351
H	-7.05899	0.14667	-0.44371
H	-5.76939	-0.30731	0.68501
H	-6.47162	-1.52693	-0.40211

C	-1.24957	-1.96313	-2.81103
H	-0.77658	-1.94833	-3.81035
H	-1.47374	-3.01323	-2.57528
H	-0.50064	-1.62027	-2.08729
C	6.04192	0.33598	-0.13961
H	6.95587	-0.14493	-0.5358
H	5.65055	-0.31652	0.65458
H	6.35998	1.27848	0.33713
C	4.52692	-3.32432	2.00495
H	5.10372	-4.11925	2.48638
C	4.58784	3.66722	0.3692
H	4.25973	4.2719	-0.49158
H	5.59208	3.28483	0.13339
H	4.70255	4.3637	1.22126
C	1.80837	-3.41402	-1.48603
H	2.02645	-4.44134	-1.14752
H	1.38919	-3.47239	-2.50651
H	1.03799	-2.9942	-0.82075
C	2.25114	3.13466	1.19348
H	2.38689	3.7752	2.08402
H	1.52124	2.35253	1.45326
H	1.78482	3.75992	0.41296
C	1.93054	0.85671	-3.10351
H	1.221	1.25306	-3.85298
H	1.479	-0.05602	-2.68732
H	2.84612	0.56362	-3.64614
C	-2.30319	-1.13366	3.27805
H	-1.49807	-0.92977	2.55955
H	-2.23447	-2.19447	3.5737
H	-2.11066	-0.51771	4.17338
C	-1.06742	3.39422	-0.50403
H	-1.16521	4.34212	0.05276
H	-0.53729	3.61122	-1.44784
H	-0.43794	2.71559	0.09054
C	-3.31668	3.63436	-1.66529
H	-3.50964	4.62022	-1.20928
H	-4.29467	3.16364	-1.85944
H	-2.82929	3.81341	-2.63868
C	2.61889	3.25072	-2.58439
H	3.59993	3.22751	-3.08323
H	2.66145	4.03624	-1.81426
H	1.88491	3.58684	-3.34039
Be	0.84738	-0.14371	0.14075
Be	-0.96009	-0.09762	0.18369
H	-0.08042	0.53609	1.1845
H	-0.04777	0.42669	-0.8803
H	-0.05215	-1.31658	0.23783

Table 7. The B3LYP(def2-TZVP//def2-SVP) Cartesian coordinates for anion **2** with the SMD-THF model.

Atom	x-Coordinate	y-Coordinate	z-Coordinate
Si	3.33218	1.19152	-0.60799
Si	-3.41863	-0.9828	-1.08524
N	-2.56117	-0.04868	0.09557
N	2.45345	-0.13708	0.08979
C	3.10457	-1.21631	0.74152
C	-3.72965	0.61905	2.17627
C	-3.16113	0.95061	0.90739
C	3.60255	2.5646	0.69723
H	4.0137	2.00608	1.55685
C	3.3135	-1.20692	2.15294
C	3.53888	-2.3581	-0.00023
C	-3.16884	2.31751	0.49835
C	-2.51802	-3.4282	0.21155
H	-2.80557	-4.37397	0.70773
H	-2.06802	-2.77484	0.9732
H	-1.72046	-3.67227	-0.50708
C	-5.1184	-0.15112	-1.39985
H	-4.89465	0.92694	-1.31218
C	-3.65954	-0.8131	2.69185
H	-3.7226	-1.46672	1.81521
C	-3.72894	-2.772	-0.47201
H	-4.50231	-2.64572	0.30783
C	4.01358	-2.25916	2.76268
H	4.17462	-2.23717	3.8444
C	-4.30193	1.62542	2.96726
H	-4.73705	1.36771	3.93559
C	-3.75131	3.29171	1.32388
H	-3.74771	4.33648	0.99928
C	3.73867	0.53303	3.98014
H	3.29234	1.40255	4.49167
H	4.63548	0.88141	3.44274
H	4.07245	-0.1703	4.76163
C	2.23124	1.86672	-2.01217
H	1.26064	1.99448	-1.50239
C	-5.72993	-0.37688	-2.79216
H	-5.95693	-1.44036	-2.97678
H	-5.07218	-0.03742	-3.60677
H	-6.68342	0.17393	-2.89672
C	-2.49975	2.75138	-0.79867
H	-2.23127	1.83334	-1.32857
C	2.72117	-0.10818	3.02624
H	2.35518	0.67117	2.3492
C	-2.19666	0.26572	-3.40372
H	-1.35318	0.74854	-2.88608

H	-3.04671	0.96515	-3.37556
H	-1.90052	0.14994	-4.46278
C	-4.32732	-3.69719	-1.54402
H	-3.62091	-3.87721	-2.37155
H	-5.24936	-3.28669	-1.98585
H	-4.58325	-4.68728	-1.12241
C	-4.80202	-1.20942	3.63389
H	-4.76283	-2.29219	3.83943
H	-5.78843	-0.98449	3.19598
H	-4.74075	-0.69561	4.6077
C	-4.32348	2.95806	2.54983
H	-4.77605	3.7286	3.18074
C	5.03586	0.5835	-1.22973
H	4.8169	-0.39265	-1.69113
C	4.23871	-3.38442	0.65042
H	4.57826	-4.24999	0.07545
C	-2.51286	-1.09816	-2.76779
H	-3.27246	-1.59202	-3.40364
C	5.67747	1.45402	-2.32288
H	5.87985	2.4808	-1.97776
H	5.04442	1.52859	-3.22019
H	6.64631	1.02843	-2.64535
C	3.16299	-2.52412	-1.46839
H	2.92219	-1.52599	-1.8525
C	4.27882	-3.10941	-2.34386
H	5.22245	-2.55125	-2.2307
H	3.98875	-3.07164	-3.40738
H	4.48592	-4.16566	-2.10392
C	1.49882	-0.63897	3.79449
H	0.7624	-1.07427	3.10313
H	0.99832	0.17194	4.35071
H	1.78891	-1.42001	4.51834
C	-6.15339	-0.48346	-0.31122
H	-7.06113	0.13815	-0.42124
H	-5.76571	-0.313	0.70421
H	-6.478	-1.53654	-0.3698
C	-1.25625	-1.98353	-2.7979
H	-0.81954	-2.01238	-3.81387
H	-1.46263	-3.02312	-2.50534
H	-0.47974	-1.59959	-2.12226
C	6.03558	0.32389	-0.0879
H	6.95663	-0.15419	-0.47052
H	5.62519	-0.33858	0.68882
H	6.34407	1.25932	0.40729
C	4.49758	-3.3365	2.02135
H	5.0512	-4.14359	2.50989
C	4.61661	3.67154	0.36465
H	4.31384	4.26794	-0.51061

H	5.62185	3.27539	0.15685
H	4.71821	4.37785	1.21031
C	1.87968	-3.36596	-1.58254
H	2.05249	-4.39463	-1.22166
H	1.53432	-3.42498	-2.62858
H	1.07021	-2.92848	-0.98018
C	2.2634	3.17385	1.14461
H	2.38399	3.7956	2.05097
H	1.5081	2.40539	1.37027
H	1.83649	3.82404	0.3633
C	2.00345	0.83681	-3.12983
H	1.29286	1.2189	-3.88589
H	1.58075	-0.09989	-2.73742
H	2.9378	0.58683	-3.66173
C	-2.2924	-1.07897	3.34437
H	-1.47307	-0.84849	2.64963
H	-2.19421	-2.13484	3.64849
H	-2.15754	-0.45136	4.24195
C	-1.18721	3.50097	-0.51703
H	-1.37051	4.45207	0.01203
H	-0.657	3.73351	-1.45641
H	-0.51774	2.89005	0.10451
C	-3.41924	3.56742	-1.71751
H	-3.68616	4.54292	-1.27673
H	-4.3577	3.03077	-1.93166
H	-2.92005	3.76978	-2.68029
C	2.60844	3.24009	-2.58827
H	3.59207	3.23864	-3.0846
H	2.63173	4.02356	-1.81637
H	1.86863	3.55966	-3.34597
Be	0.85603	-0.1382	0.15067
Be	-0.96143	-0.09725	0.18023
H	-0.09026	0.61031	1.1439
H	-0.03941	0.34612	-0.90937
H	-0.04647	-1.30829	0.34337

Table 8. The B3LYP(def2-TZVP//def2-SVP) Cartesian coordinates for anion $[\{(Xyl)(Me_3Si)NBe\}_2H_3]^-$ in the gas phase.

Atom	x-Coordinate	y-Coordinate	z-Coordinate
Si	3.04628	1.74873	-1.15272
Si	-3.04616	-1.74843	-1.15342
N	-2.46374	-0.44239	-0.20817
N	2.46376	0.44245	-0.20786
C	3.30277	-0.42361	0.5207
C	-3.61913	0.14665	1.87648
C	-3.30282	0.42347	0.52053
C	2.36266	3.40117	-0.55607

C	3.61898	-0.14711	1.87674
C	3.81454	-1.60472	-0.07804
C	-3.81457	1.60471	-0.07798
C	-4.92913	-1.80004	-1.06877
C	-3.03848	-1.08064	2.52976
C	-2.36259	-3.40102	-0.55713
C	4.44982	-1.02217	2.58956
H	4.6872	-0.79693	3.63469
C	-4.45005	1.02154	2.58944
H	-4.68752	0.79605	3.63449
C	-4.64266	2.45786	0.6643
H	-5.032	3.36538	0.19078
C	2.51034	1.58542	-2.95263
C	-3.44398	1.92739	-1.50273
C	3.0383	1.08004	2.53025
C	-4.96928	2.17198	1.99162
H	-5.61574	2.84722	2.56004
C	4.92925	1.8003	-1.06788
C	4.64255	-2.45805	0.66411
H	5.0319	-3.36548	0.19041
C	-2.51004	-1.58465	-2.95324
C	3.44405	-1.92707	-1.5029
C	4.96907	-2.17249	1.99152
H	5.61547	-2.84788	2.55984
Be	0.88789	0.16428	-0.16168
Be	-0.88788	-0.16421	-0.16179
H	-0.13995	1.03684	-0.77294
H	0.14003	-1.03667	-0.77311
H	-0.00005	-0.00007	1.04552
H	5.27086	1.92284	-0.02729
H	5.33654	2.63403	-1.66414
H	5.36716	0.86184	-1.44436
H	1.41446	1.47543	-2.99447
H	2.95166	0.69455	-3.42717
H	2.78987	2.47042	-3.54955
H	2.71386	3.64248	0.45992
H	1.26236	3.34843	-0.52397
H	2.64773	4.23074	-1.22578
H	2.35145	-1.88692	-1.63735
H	3.80775	-2.92356	-1.79869
H	3.86367	-1.1878	-2.20469
H	3.27477	1.1153	3.60524
H	1.94454	1.10566	2.40067
H	3.42047	2.00282	2.0643
H	-3.80767	2.92394	-1.79832
H	-3.86354	1.18828	-2.20472
H	-2.35137	1.88729	-1.63712
H	-3.27506	-1.11615	3.60471

H	-1.94471	-1.10619	2.40028
H	-3.42058	-2.00331	2.06355
H	-1.41416	-1.47463	-2.99494
H	-2.95133	-0.69367	-3.42758
H	-2.7895	-2.4695	-3.55041
H	-5.27084	-1.92286	-0.02825
H	-5.33636	-2.63361	-1.6653
H	-5.36701	-0.86148	-1.44504
H	-2.71389	-3.6426	0.45876
H	-1.26229	-3.34828	-0.5249
H	-2.64757	-4.23042	-1.22708

Table 9. The B3LYP(def2-TZVP//def2-SVP) Cartesian coordinates for anion $[\{(Xyl)(Me_3Si)NBe\}_2H_3]^-$ with the SMD-THF model.

Atom	x-Coordinate	y-Coordinate	z-Coordinate
Si	3.11416	1.70983	-1.19551
Si	-3.11396	-1.70951	-1.19621
N	-2.46808	-0.43261	-0.23981
N	2.4681	0.4327	-0.23954
C	3.26437	-0.44074	0.53261
C	-3.5452	0.14345	1.8932
C	-3.26447	0.4406	0.53248
C	2.46711	3.38829	-0.63945
C	3.54506	-0.14389	1.89341
C	3.76542	-1.64627	-0.02818
C	-3.7656	1.64621	-0.02808
C	-4.99075	-1.71532	-1.08114
C	-2.99886	-1.12081	2.50367
C	-2.46701	-3.3881	-0.64043
C	4.32215	-1.03141	2.65279
H	4.53316	-0.79189	3.69998
C	-4.3224	1.03074	2.65273
H	-4.53343	0.79098	3.69987
C	-4.53927	2.51079	0.76119
H	-4.92112	3.43656	0.31887
C	2.6033	1.52287	-2.99797
C	-3.45893	1.98243	-1.46479
C	2.99881	1.12027	2.50412
C	-4.82379	2.20991	2.09553
H	-5.42753	2.89341	2.69943
C	4.99092	1.71559	-1.08009
C	4.53897	-2.51109	0.76094
H	4.92075	-3.4368	0.31844
C	-2.60275	-1.52209	-2.99852
C	3.4588	-1.98214	-1.46498
C	4.82346	-2.21051	2.09536
H	5.42711	-2.8942	2.69914

Be	0.89605	0.17535	-0.21776
Be	-0.89605	-0.17519	-0.21783
H	-0.13913	1.03723	-0.82989
H	0.1392	-1.03707	-0.82985
H	-0.00008	0.0001	0.98721
H	5.32994	1.85879	-0.04068
H	5.41891	2.53162	-1.68745
H	5.42268	0.76736	-1.44037
H	1.50439	1.46279	-3.07589
H	3.01676	0.60411	-3.44527
H	2.9361	2.3796	-3.60937
H	2.80573	3.64129	0.37867
H	1.3641	3.38814	-0.63166
H	2.79721	4.19512	-1.31694
H	2.37666	-1.92189	-1.66331
H	3.8104	-2.99182	-1.727
H	3.93571	-1.2681	-2.1563
H	3.21153	1.1726	3.58286
H	1.90926	1.19118	2.3547
H	3.42935	2.01645	2.0286
H	-3.81057	2.99216	-1.72658
H	-3.93576	1.26853	-2.1563
H	-2.37677	1.92229	-1.66307
H	-3.21168	-1.17342	3.58237
H	-1.90929	-1.19155	2.35434
H	-3.42925	-2.01691	2.02788
H	-1.50382	-1.46203	-3.07622
H	-3.0161	-0.6032	-3.44566
H	-2.93546	-2.37866	-3.61021
H	-5.32995	-1.85883	-0.04183
H	-5.41861	-2.5312	-1.6888
H	-5.42245	-0.767	-1.44123
H	-2.80582	-3.64135	0.37756
H	-1.364	-3.38795	-0.63244
H	-2.79698	-4.19477	-1.31819

Table 10. The B3LYP(def2-TZVP//def2-SVP) Cartesian coordinates for neutral {(Xyl)(Me_3Si)NBeH}$_2$ in the gas phase.

Atom	**x-Coordinate**	**y-Coordinate**	**z-Coordinate**
Si	-2.98726	-2.25056	0.00406
Si	2.98708	2.2505	0.00434
N	2.46424	0.54301	-0.00753
N	-2.46426	-0.54313	-0.00752
C	-3.4299	0.51281	-0.00504
C	3.89033	-1.04929	1.22692
C	3.42996	-0.51282	-0.00508
C	-2.27059	-3.11887	1.52764

C	-3.89049	1.04908	1.22696
C	-3.9159	1.03225	-1.23443
C	3.91633	-1.03193	-1.23446
C	4.87303	2.29906	0.02344
C	3.36525	-0.51129	2.53495
C	2.26991	3.11854	1.52784
C	-4.84251	2.08516	1.20884
H	-5.19946	2.49679	2.16143
C	4.84248	-2.08525	1.20881
H	5.19925	-2.49703	2.16141
C	4.86799	-2.06827	-1.21074
H	5.24468	-2.46683	-2.16129
C	-2.2985	-3.13261	-1.52437
C	3.41928	-0.4754	-2.54564
C	-3.36579	0.51078	2.53501
C	5.33509	-2.593	0.00046
H	6.07755	-3.39982	0.00263
C	-4.87322	-2.29901	0.02254
C	-4.86744	2.0687	-1.21073
H	-5.24385	2.46751	-2.16129
C	2.2986	3.13263	-1.52416
C	-3.41852	0.47599	-2.5456
C	-5.33477	2.59322	0.00047
H	-6.07714	3.40013	0.00263
Be	-0.96755	-0.19912	-0.0145
Be	0.96754	0.19888	-0.01447
H	-0.22268	1.07174	-0.01636
H	0.22267	-1.072	-0.01643
H	-5.27606	-1.78569	0.91386
H	-5.23576	-3.34347	0.0319
H	-5.29411	-1.79539	-0.86592
H	-1.19549	-3.05277	-1.55293
H	-2.69225	-2.69929	-2.46087
H	-2.5544	-4.20882	-1.51034
H	-2.648	-2.67742	2.4671
H	-1.16729	-3.03834	1.536
H	-2.52608	-4.19526	1.52775
H	-2.31416	0.49096	-2.60169
H	-3.81731	1.04945	-3.39892
H	-3.7163	-0.58043	-2.67743
H	-3.756	1.08884	3.38918
H	-2.26075	0.53808	2.57305
H	-3.65004	-0.54731	2.68189
H	3.81806	-1.04885	-3.39897
H	3.71735	0.58097	-2.67731
H	2.31492	-0.49007	-2.60189
H	3.75537	-1.08943	3.38911
H	2.26022	-0.53876	2.57274

H	3.6493	0.54682	2.68205
H	1.1956	3.05264	-1.55283
H	2.69247	2.69937	-2.46064
H	2.55436	4.20886	-1.51006
H	5.2756	1.78564	0.91482
H	5.23549	3.34355	0.03309
H	5.29427	1.79562	-0.86495
H	2.64734	2.67712	2.46732
H	1.16664	3.03769	1.53605
H	2.52509	4.195	1.52808
H	-2.79698	-4.19477	-1.31819

Table 11. The B3LYP(def2-TZVP//def2-SVP) Cartesian coordinates for neutral {(Xyl)(Me_3Si)NBeH}$_2$ with the SMD-THF model.

Atom	x-Coordinate	y-Coordinate	z-Coordinate
Si	-2.98021	2.23522	0.01244
Si	2.98024	-2.23522	0.01188
N	2.45543	-0.56578	0.02202
N	-2.45543	0.56576	0.02239
C	-3.38929	-0.51079	0.00243
C	3.79545	1.07566	-1.23292
C	3.38928	0.51079	0.00215
C	-2.27718	3.11752	-1.48806
C	-3.79557	-1.07548	-1.23269
C	-3.89319	-1.03991	1.21702
C	3.89326	1.03975	1.21678
C	4.85032	-2.30078	-0.01725
C	3.24621	0.53387	-2.52734
C	2.27715	-3.11736	-1.48868
C	-4.70963	-2.13993	-1.23411
H	-5.02309	-2.57013	-2.1901
C	4.7095	2.14012	-1.23426
H	5.02287	2.57046	-2.19022
C	4.80545	2.10518	1.17593
H	5.19372	2.50863	2.116
C	-2.31794	3.12337	1.52766
C	3.44891	0.46056	2.53495
C	-3.24641	-0.53353	-2.52707
C	5.21886	2.65411	-0.03978
H	5.93114	3.48358	-0.05609
C	-4.8503	2.30081	-0.01659
C	-4.8054	-2.10533	1.17609
H	-5.19361	-2.50891	2.11613
C	2.31806	-3.12356	1.52703
C	-3.44872	-0.46092	2.53525
C	-5.21892	-2.65408	-0.03966
H	-5.93121	-3.48353	-0.05604

Be	-0.96256	0.2145	0.03868
Be	0.96256	-0.21453	0.03847
H	-0.23598	-1.06175	0.0409
H	0.23598	1.06172	0.04087
H	-5.25818	1.80363	-0.91158
H	-5.19843	3.34765	-0.02482
H	-5.28766	1.80751	0.86633
H	-1.21804	3.04434	1.57005
H	-2.71982	2.69998	2.46208
H	-2.57158	4.19704	1.50425
H	-2.65868	2.69357	-2.43089
H	-1.17696	3.0341	-1.50437
H	-2.52735	4.19218	-1.47324
H	-2.3494	-0.4366	2.61379
H	-3.84479	-1.04102	3.38182
H	-3.7865	0.58143	2.65318
H	-3.59115	-1.12511	-3.38803
H	-2.14371	-0.53209	-2.52682
H	-3.55264	0.51247	-2.68936
H	3.84502	1.04055	3.38158
H	3.78673	-0.5818	2.65271
H	2.34959	0.43618	2.61357
H	3.59089	1.12557	-3.38824
H	2.14352	0.53242	-2.52702
H	3.55244	-0.5121	-2.68979
H	1.21816	-3.04455	1.56949
H	2.71998	-2.70027	2.46148
H	2.57172	-4.19722	1.50348
H	5.25815	-1.8035	-0.9122
H	5.19848	-3.34761	-0.02562
H	5.28773	-1.80758	0.86571
H	2.65859	-2.69329	-2.43148
H	1.17692	-3.03397	-1.50493
H	2.52735	-4.19202	-1.47401

Table 12. The B3LYP(def2-TZVP//def2-SVP) Cartesian coordinates for cation $[Me_3Si]^+$ in the gas phase.

Atom	**x-Coordinate**	**y-Coordinate**	**z-Coordinate**
Si	-0.00009	-0.00006	-0.00038
C	1.23567	-1.34409	-0.00186
H	1.03456	-2.03727	-0.83928
H	1.11802	-1.94291	0.92173
H	2.27123	-0.98	-0.06442
C	-1.78202	-0.398	0.0003
H	-2.26134	0.06554	-0.88257
H	-2.2627	0.06447	0.88274
H	-1.98434	-1.47867	-0.00128

C	0.54635	1.74201	0.00159
H	1.14057	1.93616	-0.91175
H	1.23238	1.91667	0.85107
H	-0.28716	2.45742	0.04888

Table 13. The B3LYP(def2-TZVP//def2-SVP) Cartesian coordinates for neutral $[Me_3Si]^+$ with the SMD-THF model.

Atom	x-Coordinate	y-Coordinate	z-Coordinate
Si	0.00039	-0.00019	0.00247
C	-1.19824	1.37123	-0.0031
H	-0.97075	2.05434	-0.84176
H	-1.06282	1.96179	0.92347
H	-2.2419	1.0302	-0.06815
C	1.78697	0.35093	-0.00064
H	2.24734	-0.1266	-0.88531
H	2.25443	-0.12159	0.88269
H	2.01052	1.42715	-0.00535
C	-0.59001	-1.72238	0.00069
H	-1.18528	-1.88817	-0.9176
H	-1.27817	-1.87809	0.85177
H	0.22884	-2.45503	0.04407

Table 14. The B3LYP(def2-TZVP//def2-SVP) Cartesian coordinates for neutral Me_3SiH in the gas phase.

Atom	x-Coordinate	y-Coordinate	z-Coordinate
Si	0.00004	-0.00004	0.37905
C	-1.27143	-1.24294	-0.22223
H	-1.30099	-1.27136	-1.32454
H	-2.28267	-0.98662	0.13295
H	-1.03807	-2.25993	0.13237
C	-0.44085	1.72248	-0.22216
H	-0.45147	1.76207	-1.32447
H	0.28699	2.47016	0.13234
H	-1.43802	2.02885	0.13315
C	1.71223	-0.47948	-0.22232
H	1.75165	-0.49048	-1.32464
H	1.99608	-1.48347	0.13248
H	2.4761	0.23118	0.13253
H	0.00009	-0.00011	1.87133

Table 15. The B3LYP(def2-TZVP//def2-SVP) Cartesian coordinates for neutral Me_3SiH with the SMD-THF model.

Atom	x-Coordinate	y-Coordinate	z-Coordinate
Si	0.0001	0.00008	-0.37532

C	-1.17832	1.33067	0.22016
H	-1.20532	1.3607	1.32313
H	-2.20638	1.14732	-0.13497
H	-0.87213	2.32927	-0.13431
C	-0.56351	-1.68566	0.22012
H	-0.57683	-1.72382	1.32311
H	0.10947	-2.48453	-0.13421
H	-1.58119	-1.91958	-0.1352
C	1.74171	0.3549	0.22018
H	1.78112	0.36284	1.32314
H	2.09735	1.33696	-0.13443
H	2.45309	-0.40983	-0.13459
H	0.00012	0.00015	-1.86998

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