SUPPORTING INFORMATION

Sodium Hexamethyldisilazide: Using ^{15}N–^{29}Si Scalar Coupling to Determine Aggregation and Solvation States

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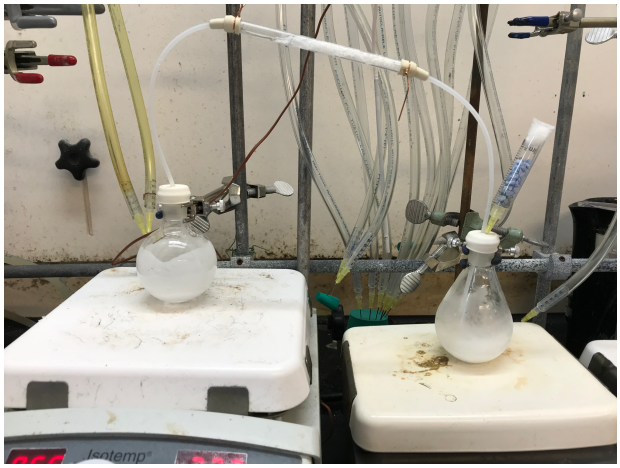
I. NMR Spectroscopic Data and Computed Free Energies

II. Computations: Coordinates and Energies

Reagents and solvents. Toluene, pentane, THF, MTBE, and 1,4-dioxane were distilled from blue or purple solutions containing sodium benzophenone ketyl. 1-(Trimethylsilyl)imidazole (96% purity) was purchased from Oakwood Chemical and used without further purification. Ammonium chloride (^{15}N, >99%) and toluene-d_8 (D, 99.94%) were purchased from Cambridge Isotope Laboratories. 1,1,3,3-Tetramethyldisilazane was purchased from Gelest and used without further purification.

NMR spectroscopic analyses. An NMR tube under vacuum was flame-dried on a Schlenk line, allowed to cool to room temperature, backfilled with argon, placed in a −78 °C dry ice/acetone bath, and charged with NaHMDS and solvents using stock solutions. The sample is mixed with a vortex mixer. Standard ^{1}H NMR spectra were recorded on a 500 MHz spectrometer at 500 MHz. Standard ^{1}H, ^{13}C, and ^{29}Si spectra were recorded on a 500 MHz spectrometer at 500, 125.79, and 99.36 MHz, respectively. The chemical shifts are referenced at −80 °C as follows: ^{1}H (Me_4Si, 0.0 ppm), ^{13}C (Me_4Si, 0.0 ppm), and ^{29}Si (Me_4Si, 0.0 ppm).



Picture 1. Experimental setup for [^{15}N]NH_3 generation.

[^{15}N]Hexamethyldisilazane. [^{15}N]NH_3 was generated by a known procedure[18] by mixing [^{15}N]ammonium chloride (3.0 g, 55.0 mmol, >99% ^{15}N isotopic purity) with 6.00 g (0.15 mol) of granular NaOH in a 25 mL one-neck round-bottom flask equipped with an NaOH-filled tube to transfer the ammonia gas to an empty 100 mL round-bottom flask cooled to –78 °C. The mixture was warmed with a heat gun for approximately 20 min. After the transfer of ammonia was complete, 1-(trimethylsilyl)imidazole (14.7 g, 15.3 mL, 105 mmol, 98% purity) was added to ammonia at –78 °C and stirred. HCl offgasses and imidazole precipitates immediately. Anhydrous diethyl ether (20 mL) is then added to the flask, and the mixture is held at 0 °C for 40 min. Cholesterol (3.0 g) was added to the [^{15}N]hexamethyldisilazane with stirring for 45 mins to remove excess 1-(trimethylsilyl)imidazole. Short path distillation at atm pressure removed the diethyl ether. Vacuum distillation (40 mm Hg, 20 °C) afforded 4.75 mL (47% yield) of $(Me_3Si)_2{}^{15}NH$.

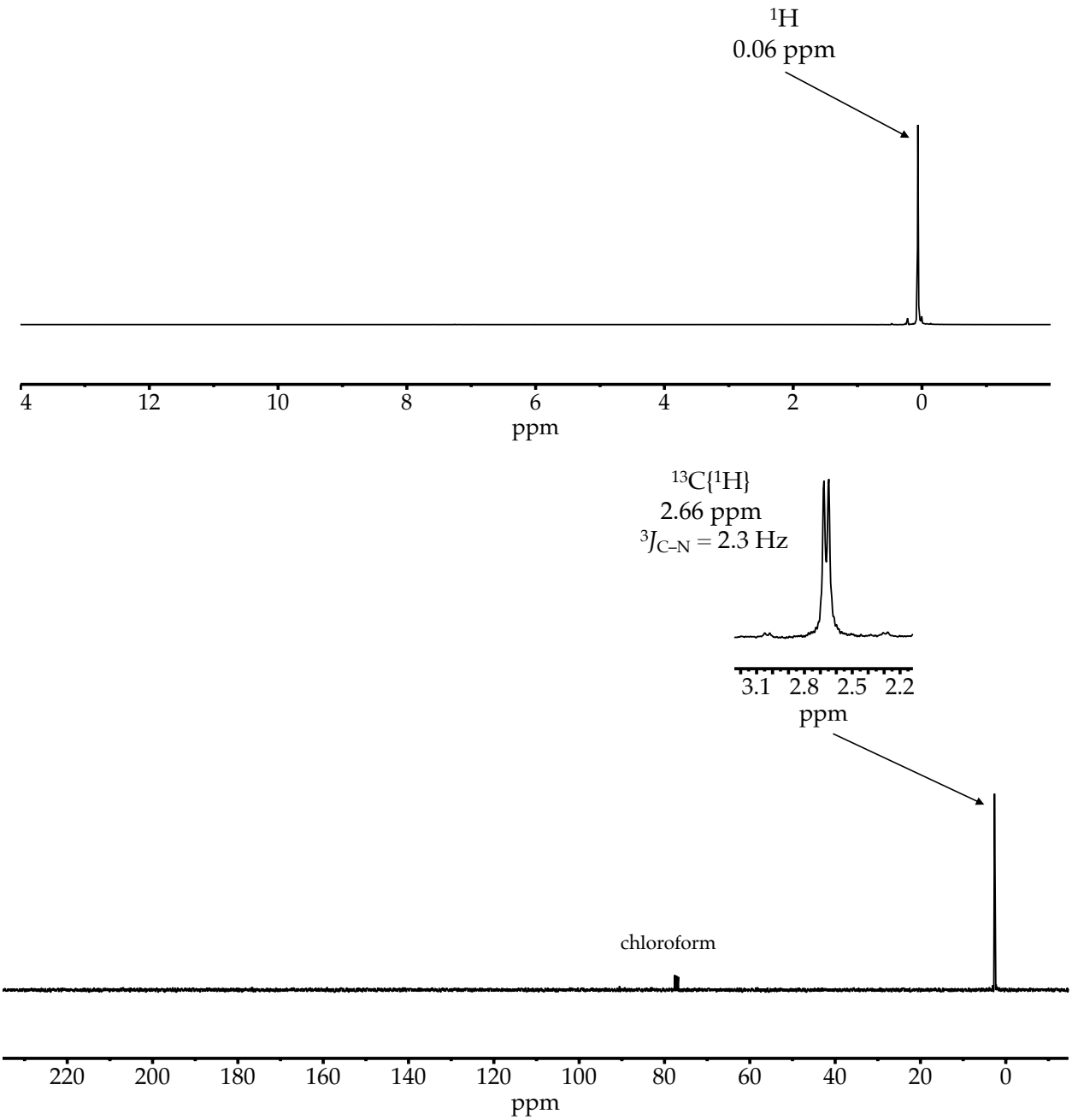
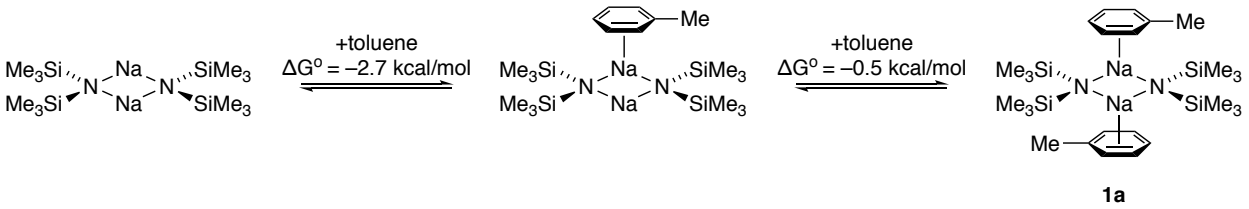
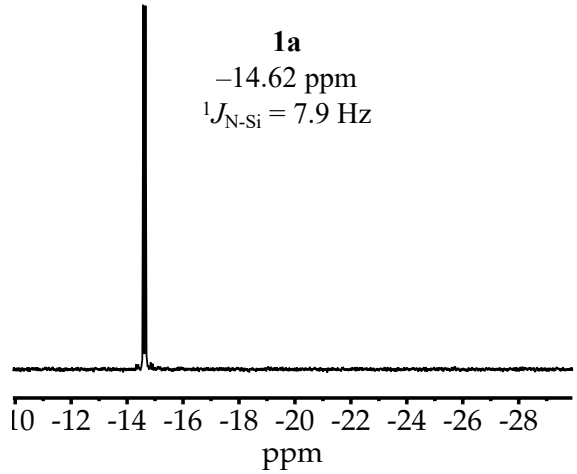


Figure S1. ^{1}H and ^{13}C{^{1}H} NMR spectra of [^{15}N]hexamethyldisilazane in $CDCl_3$ at room temperature.

Toluene:



^{29}Si{^{1}H} spectrum



^{13}C{^{1}H} spectrum

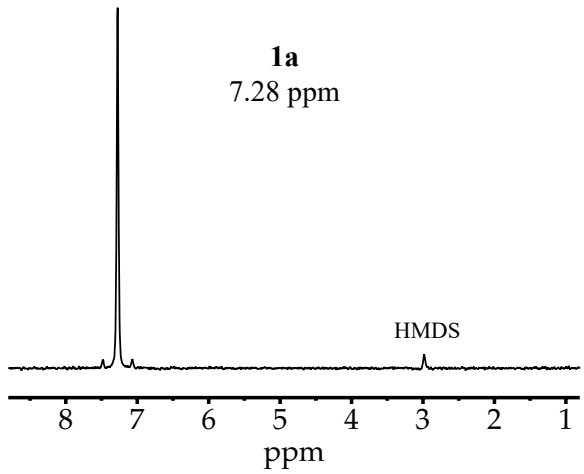
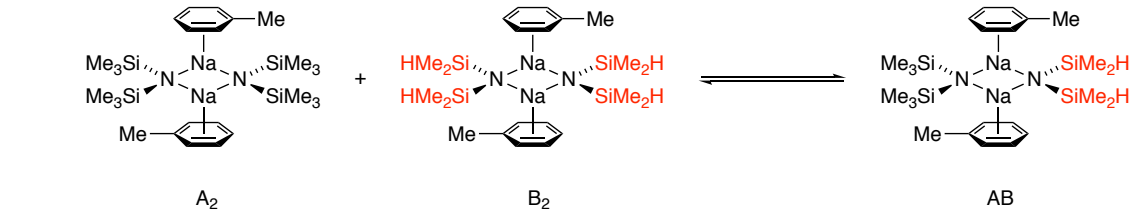
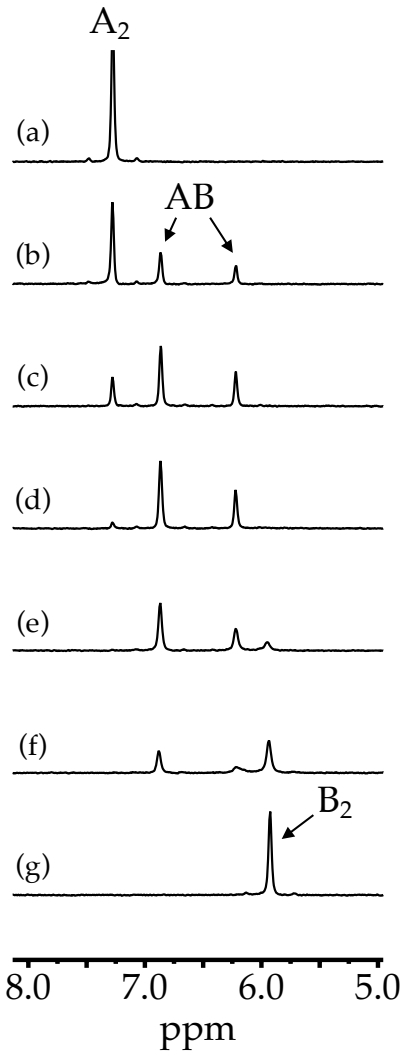


Figure S2. NMR spectra of [^{15}N]NaHMDS (^{29}Si spectrum) and NaHMDS (^{13}C spectrum) in neat toluene-d_8 at –80 °C.





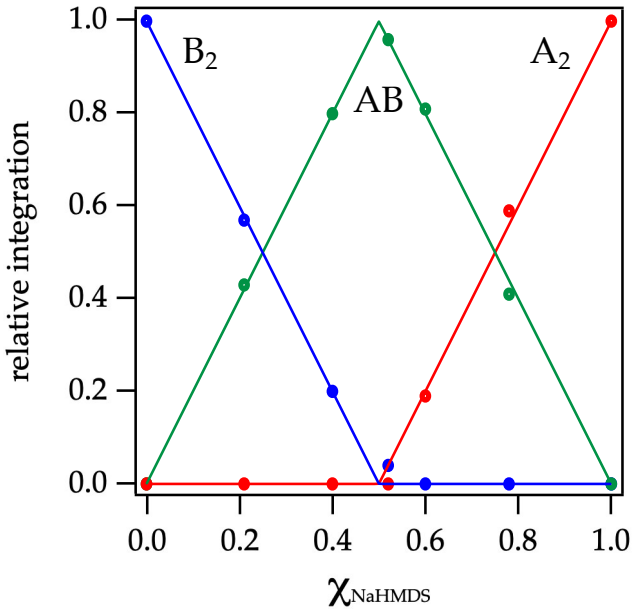


Figure S3. $^{13}C\{^{1}H\}$ NMR spectra and affiliated Job plot showing relative integrations of NaHMDS-derived homodimer (A_2, red), NaTMDS-derived homodimer (B_2, blue), and heterodimer (AB, green) versus the measured mole fraction of NaHMDS (X_{NaHMDS}) at 0.30 total molarity in neat toluene at –80 °C. The measured mole fractions, X_{NaHMDS}, in (a)–(g) are 1.00, 0.78, 0.60, 0.52, 0.40, 0.21, and 0.00, respectively.

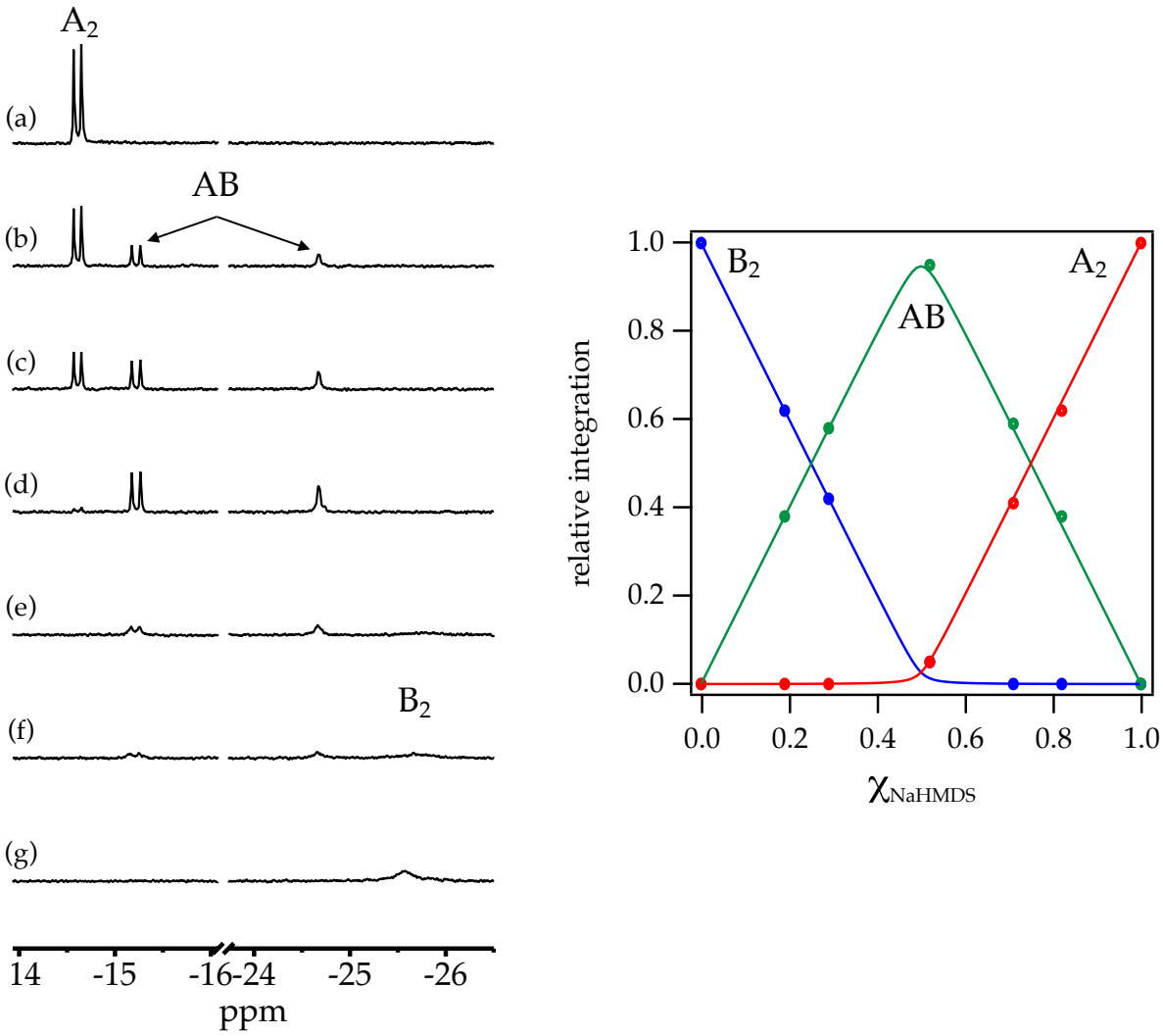


Figure S4. $^{29}Si\{^{1}H\}$ NMR spectra and affiliated Job plot showing relative integrations of NaHMDS-derived homodimer (A_2, red), NaTMDS-derived homodimer (B_2, blue), and heterodimer (AB, green) versus the measured mole fraction of NaHMDS (X_{NaHMDS}) at 0.20 total molarity in neat toluene at –80 °C. The measured mole fractions, X_{NaHMDS}, in (a)–(g) are 1.00, 0.81, 0.71, 0.52, 0.29, 0.19, and 0.00, respectively.

THF:

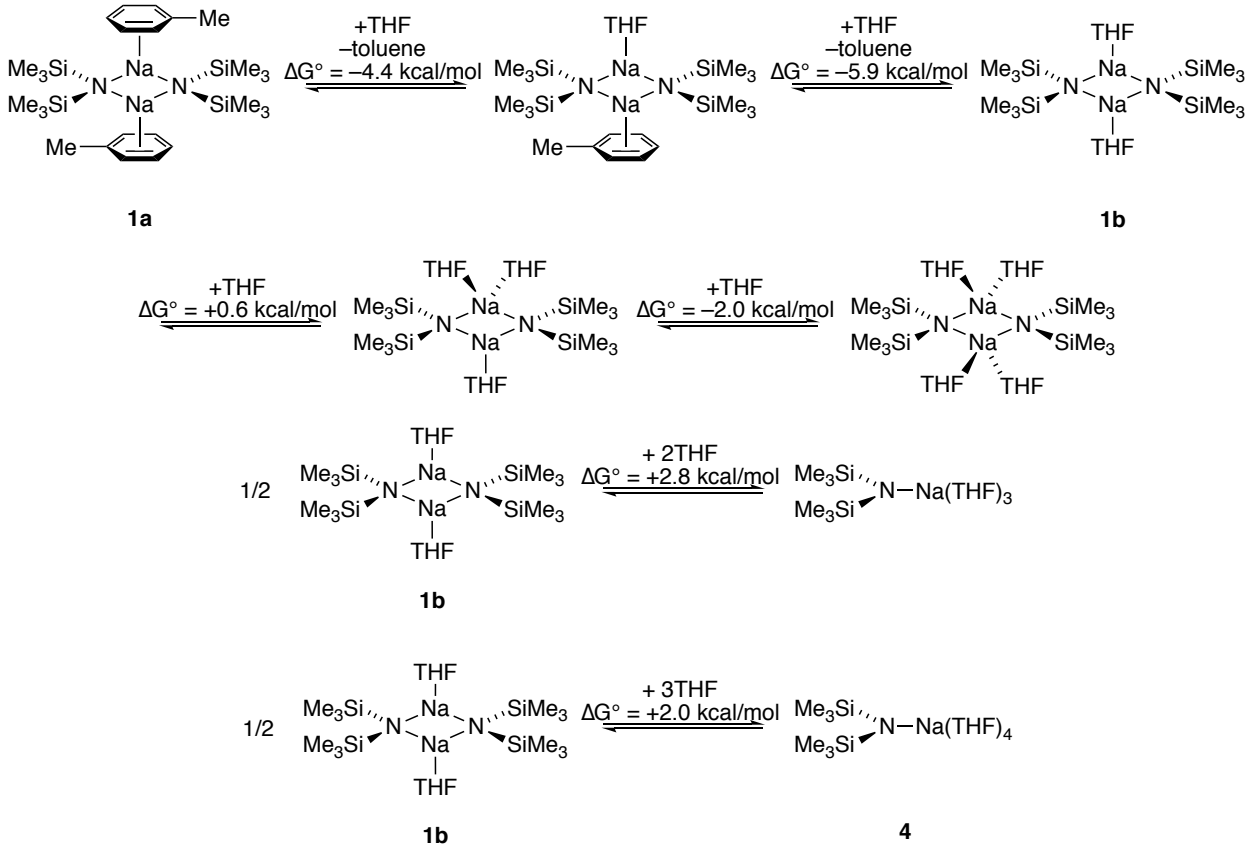


Figure S5. Computed free energies for the serial solvation of NaHMDS with THF.

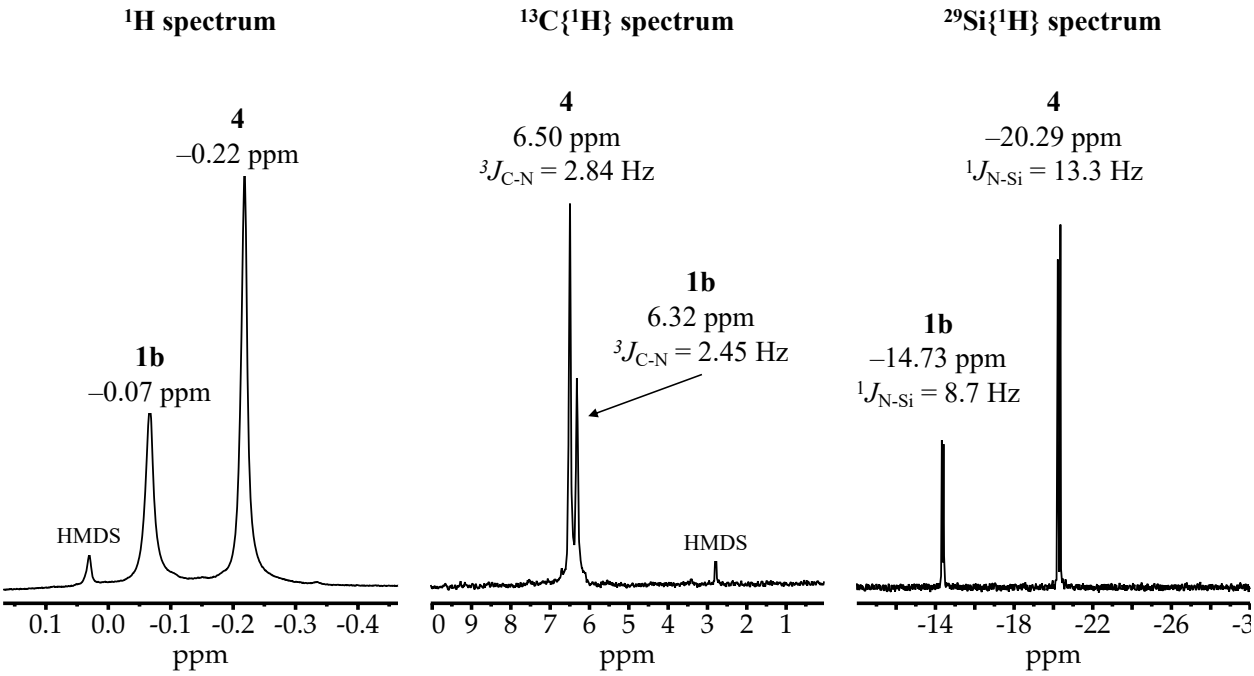


Figure S6. NMR spectra of 0.15 M [^{15}N]NaHMDS in 0.75 M THF with DMEA cosolvent at –120 °C.

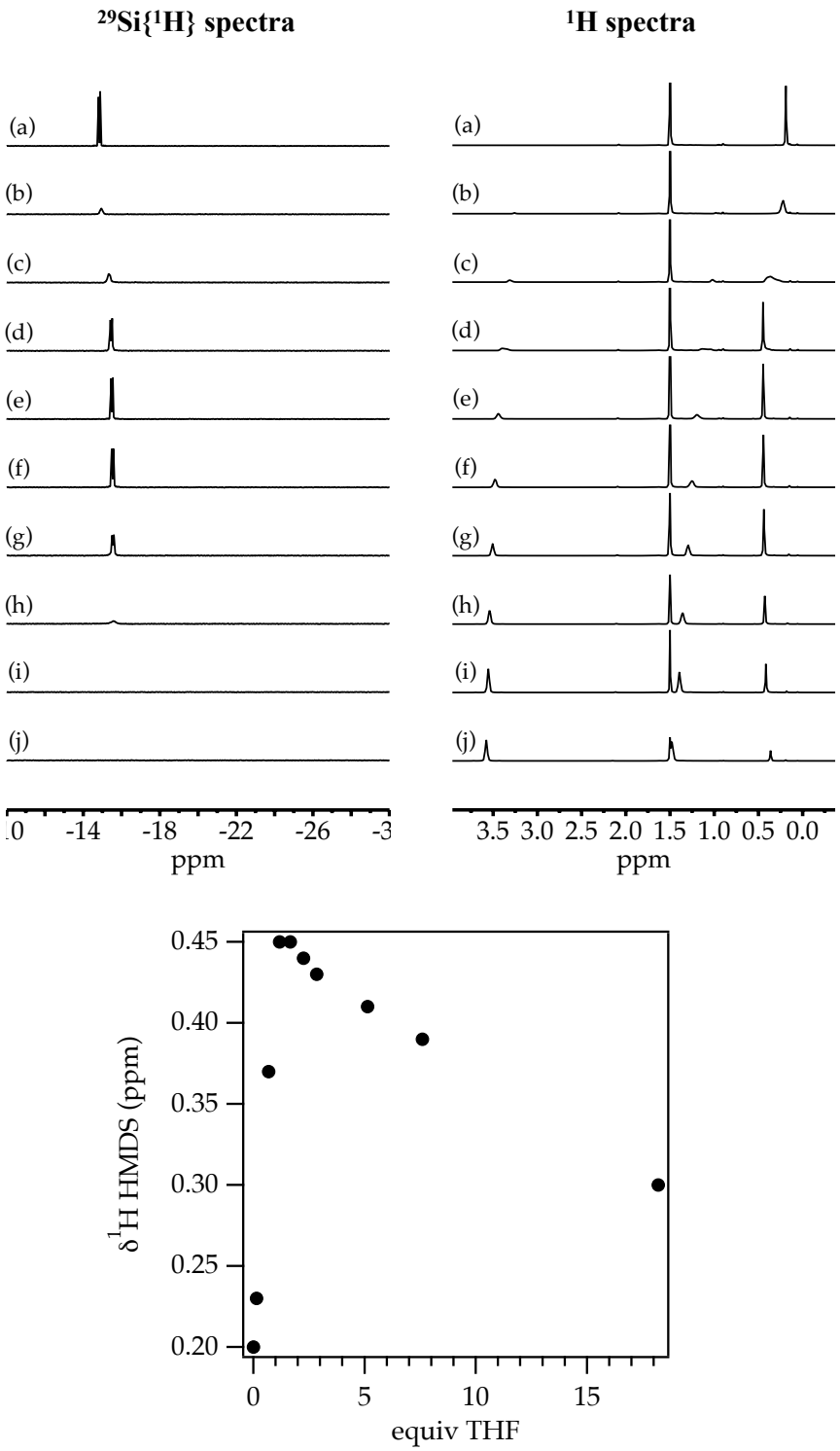


Figure S7. ^{1}H and ^{29}Si{^{1}H} NMR spectra for the titration of 0.23 M NaHMDS in toluene-d_8 with THF at –80 °C. Equiv of THF for (a)–(j) are as follows: 0.0, 0.1, 0.7, 1.2, 1.7, 2.3, 2.8, 5.1, 7.6, and 18.2, respectively.

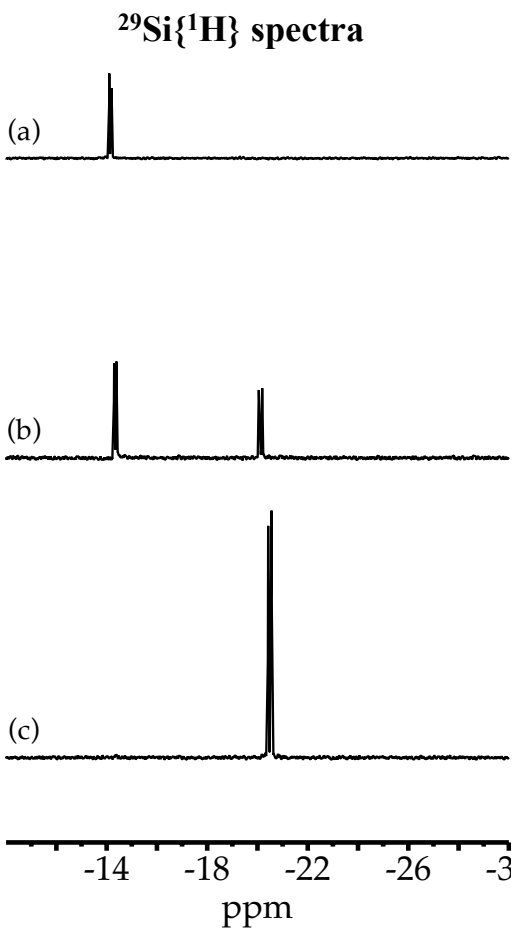


Figure S8. ^{29}Si{^{1}H} NMR spectra for the titration of 0.15 M NaHMDS in DMEA with THF at –120 °C. Equiv of THF for (a)–(c) are as follows: 0.0, 4.0, and 10.0, respectively.

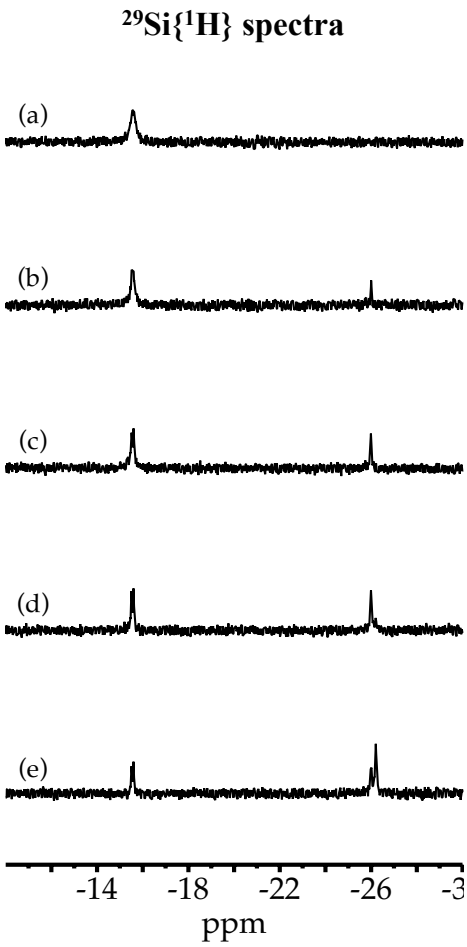


Figure S9. ^{29}Si{^{1}H} NMR spectra of NaHMDS-derived homodimer (A_2), NaTMDS-derived homodimer (B_2), and heterodimer (AB) at 0.20 total molarity with 5.0 equiv THF in toluene cosolvent at –80 °C. The mole fraction of NaHMDS for (a)–(e) are as follows: 1.0, 0.8, 0.7, 0.5, and 0.3, respectively. Due to the poor resolution, a formal Job plot was not obtained. However, based on the coupling constants of (b)–(e) dimer is present at this THF concentration.

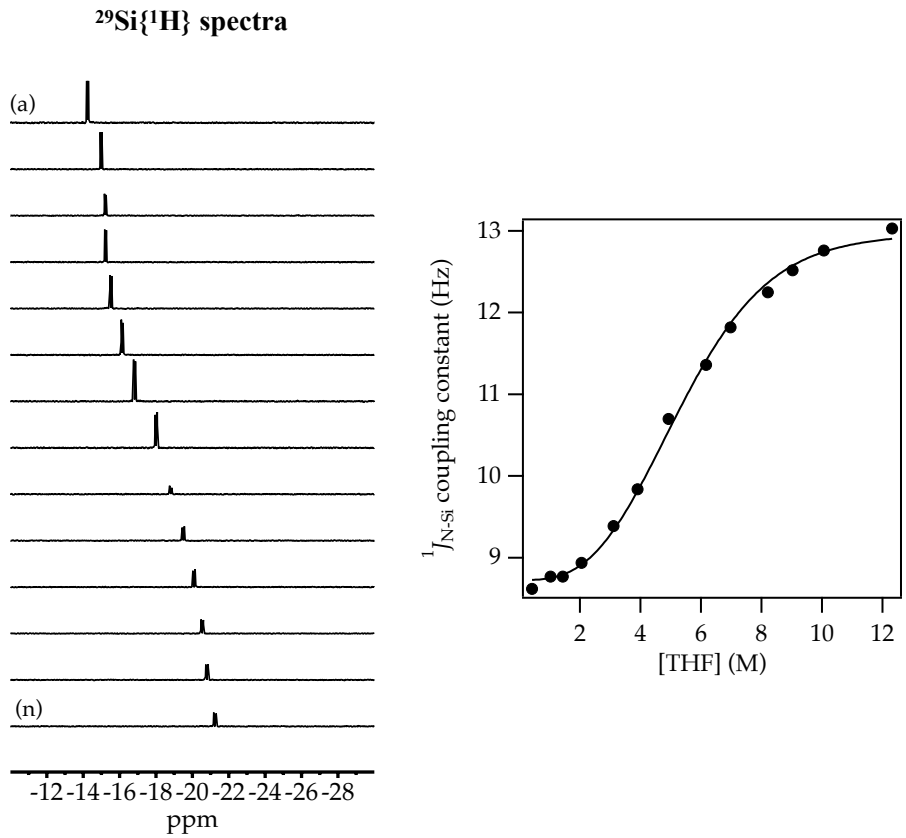


Figure S10. ^{29}Si{^{1}H} NMR spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of THF at +50 °C. THF concentration for (a)–(n) are as follows: 0.00, 0.41, 1.02, 1.43, 2.05, 3.10, 3.90, 4.92, 6.16, 6.97, 8.2, 9.02, 10.05, and 12.31, respectively. The curve is fit to the function described in the "Derivation" section of this Supporting Information on page S-21 with $n = 3$.

[THF] (M)	$^{1}J_{N–Si}$ coupling constant (Hz)
0.41	8.62
1.02	8.77
1.43	8.77
2.05	8.94
3.10	9.39
3.90	9.84
4.92	10.7
6.16	11.36
6.97	11.82
8.20	12.25
9.02	12.52
10.05	12.76
12.31	13.03

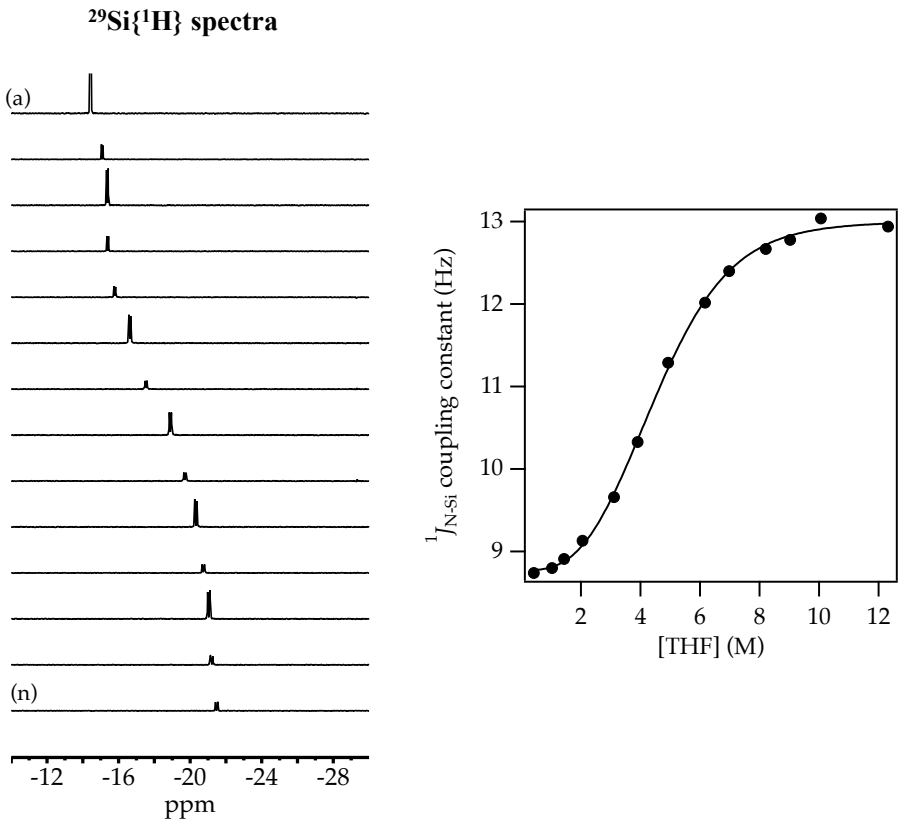


Figure S11. $^{29}Si\{^{1}H\}$ NMR spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of THF at +20 °C. THF concentration for (a)–(n) are as follows: 0.00, 0.41, 1.02, 1.43, 2.05, 3.10, 3.90, 4.92, 6.16, 6.97, 8.2, 9.02, 10.05, and 12.31, respectively. The curve is fit to the function described in the "Derivation" section of this Supporting Information on page S-21 with $n = 3$.

[THF] (M)	$^{1}J_{N–Si}$ coupling constant (Hz)
0.41	8.74
1.02	8.8
1.43	8.91
2.05	9.13
3.10	9.66
3.90	10.33
4.92	11.29
6.16	12.02
6.97	12.4
8.20	12.67
9.02	12.78
10.05	13.04
12.31	12.94

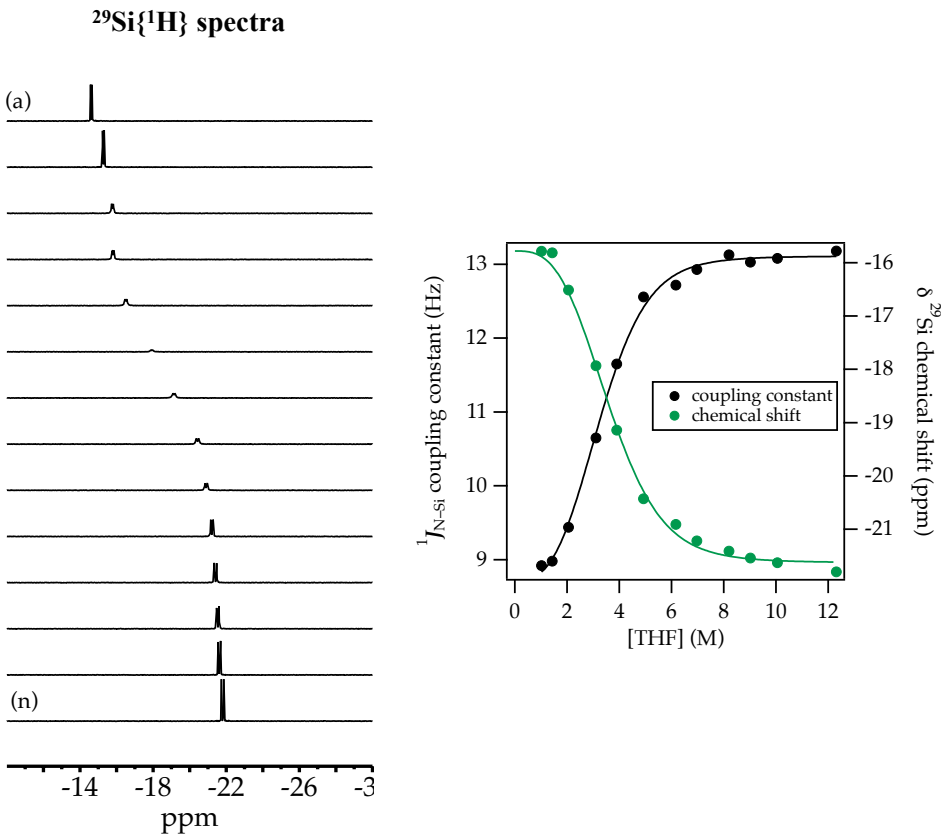


Figure S12. $^{29}Si\{^{1}H\}$ NMR spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of THF at –20 °C. THF concentration for (a)–(n) are as follows: 0.41, 1.02, 1.43, 2.05, 3.10, 3.90, 4.92, 6.16, 6.97, 8.2, 9.02, 10.05, and 12.31, respectively. The curve is fit to the function described in the "Derivation" section of this Supporting Information on page S-21 with $n = 3$.

[THF] (M)	$^{1}J_{N–Si}$ coupling constant (Hz)	^{29}Si chemical shift (ppm)
1.02	8.77	–15.78
1.43	8.91	–15.81
2.05	9.13	–16.51
3.10	9.66	–17.93
3.90	10.33	–19.14
4.92	11.29	–20.43
6.16	12.02	–20.91
6.97	12.4	–21.22
8.20	12.67	–21.41
9.02	12.78	–21.54
10.05	13.04	–21.63
12.31	12.94	–21.8

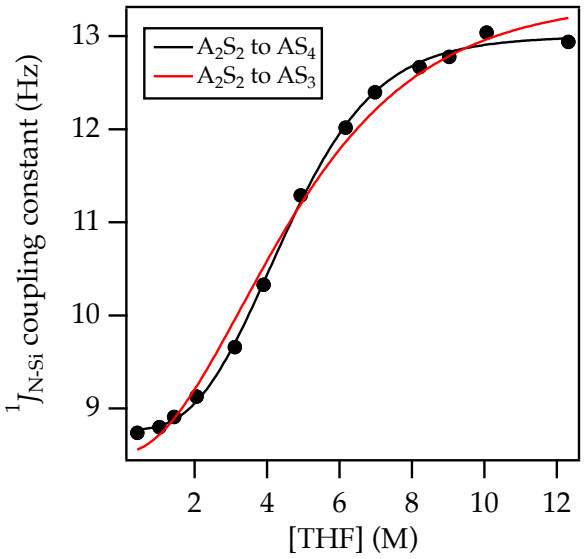


Figure S13. ^{29}Si NMR spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of THF at +20 °C. THF concentration for (a)–(n) are as follows: 0.00, 0.41, 1.02, 1.43, 2.05, 3.10, 3.90, 4.92, 6.16, 6.97, 8.2, 9.02, 10.05, and 12.31, respectively. The difference in curvature for n = 2 (red curve) versus n = 3 (black curve) confirms monomer solvation with a superior fit to the data.

[THF] (M)	$^1J_{N–Si}$ coupling constant (Hz)
0.41	8.74
1.02	8.8
1.43	8.91
2.05	9.13
3.10	9.66
3.90	10.33
4.92	11.29
6.16	12.02
6.97	12.4
8.20	12.67
9.02	12.78
10.05	13.04
12.31	12.94

1,4-dioxane:

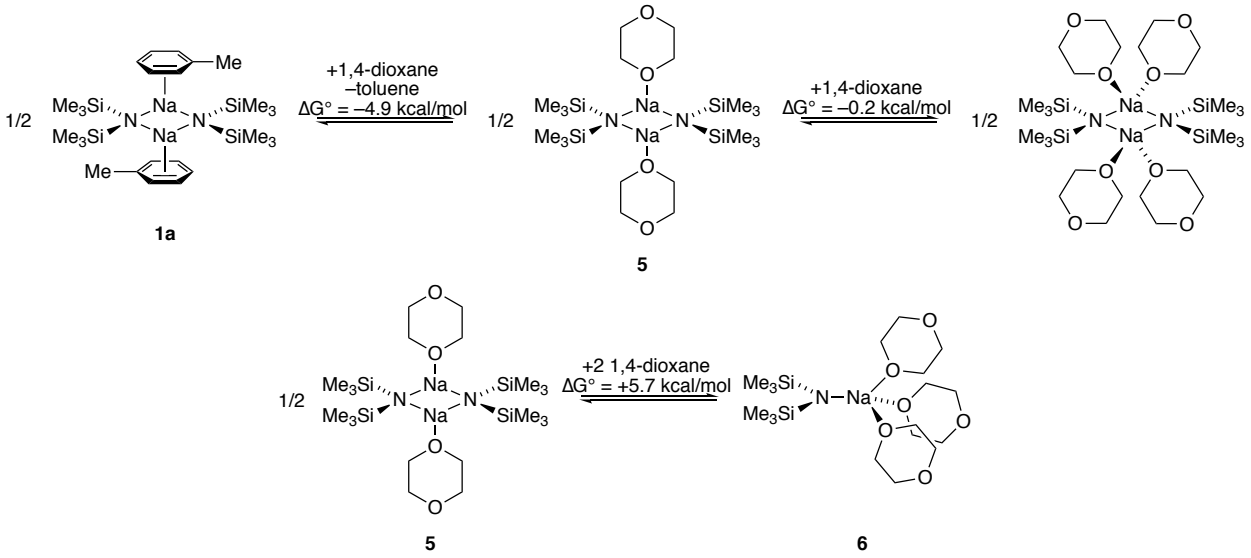


Figure S14. Computed free energies for the serial solvation of NaHMDS with 1,4-dioxane.

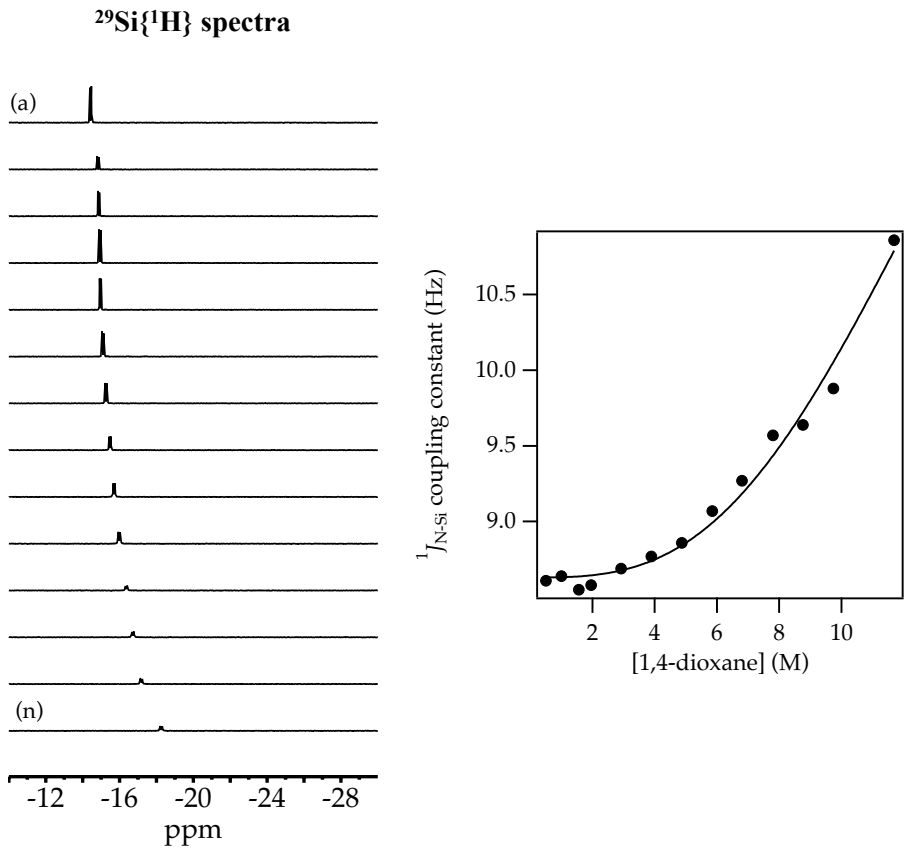


Figure S15. ^{29}Si NMR spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of 1,4-dioxane at +20 °C. 1,4-Dioxane concentration for (a)–(n) are as follows: 0.50, 1.00, 1.56, 1.95, 2.92, 3.89, 4.87, 5.85, 6.80, 7.80, 8.76, 9.74, and 11.69, respectively. The curve is fit to the function described in the "Derivation" section of this Supporting Information on page S-21 with $n = 3$.

[1,4-dioxane] (M)	$^{1}J_{N–Si}$ coupling constant (Hz)
0.50*	8.61
1.00*	8.64
1.56	8.55
1.95	8.58
2.92	8.69
3.89	8.77
4.87	8.86
5.85	9.07
6.80	9.27
7.80	9.57
8.76	9.64
9.74	9.88
11.69	10.86

* due to polymeric network at the bottom of the tube an accurate concentration was not obtained. 0.50 M and 1.00 M are idealized concentrations.

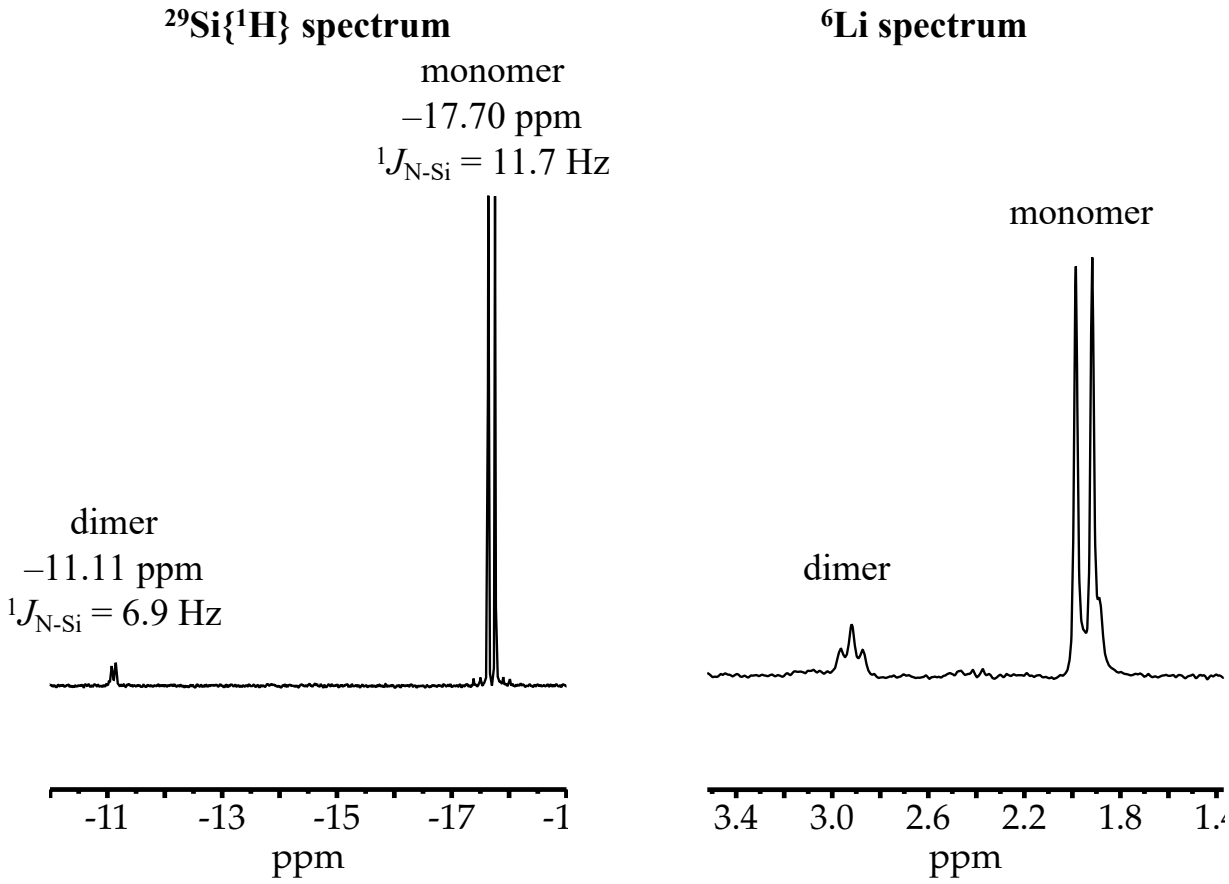
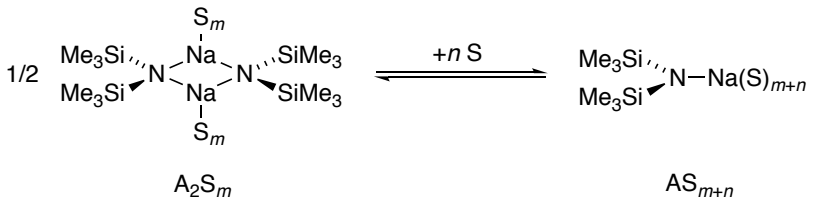


Figure S16. ^{29}Si and ^{6}Li NMR spectra of 0.10 M [^{6}Li,^{15}N]LiHMDS with 40.0 equiv THF in 2:1 pentane/toluene cosolvent at –100 °C.

Derivation for coupling constant fitting function:

To simplify the presentation, we introduce the following shorthand: A = a NaHMDS subunit, S = solvent, $[A]_T$ = total [NaHMDS], J_{obsd} = observed average coupling constant. As shown in eq 1 subscripts *m* corresponds to the number of solvent molecules bound in the dimer subunits whereas *n* corresponds to the additional solvent molecules to the monomer. With this simplified model only a single monomer solvation number is assumed to be present.



(1)

Given:

$$[A]_T = 2[A_2S_m] + [AS_{m+n}]$$

$$K_{eq} = \frac{[AS_{m+n}]}{[A_2S_m]^{1/2}[S]^n}$$

One can solve for $[AS_{m+n}]$ as a function of [S] by applying the quadratic equation:

$$[AS_{m+n}] = 0.125\left(4[A]_T + {K_{eq}}^2[S]^{2n} - \sqrt{8[A]_T{K_{eq}}^2[S]^{2n} + {K_{eq}}^4[S]^{4n}}\right)$$

Using the equation relating the observed coupling constant to the average of the dimer and monomer coupling constants and the equation solved above for $[A]_T$ one can solve for $[AS_{m+n}]$:

$$J_{obsd} = \frac{J_{A_2S_m}[A_2S_m] + J_{AS_{m+n}}[AS_{m+n}]}{[A_2S_m] + [AS]_{m+n}}$$

$$[AS_{m+n}] = \frac{[A]_T J_{obsd} - [A]_T J_{AS_{m+n}}}{J_{A_2S_m} - 2J_{AS_{m+n}} + J_{obsd}}$$

Setting each equation solved for in terms of $[AS_{m+n}]$ equal to one another gives:

$$\frac{[A]_T J_{obsd} - [A]_T J_{AS_{m+n}}}{J_{A_2S_m} - 2J_{AS_{m+n}} + J_{obsd}} = 0.125\left(4[A]_T + {K_{eq}}^2S^{2n} - \sqrt{8[A]_T{K_{eq}}^2S^{2n} + {K_{eq}}^4S^{4n}}\right)$$

Rearranging affords the equation used as the fitting function:

$$J_{obsd} = \frac{4[A]_T J_{A_2S_m} + J_{A_2S_m} K_{eq}{}^2[S]^{2n} - 2J_{AS_{m+n}} K_{eq}{}^2[S]^{2n} - J_{A_2S_m}\sqrt{8[A]_T K_{eq}{}^2[S]^{2n} + K_{eq}{}^4[S]^{4n}} + 2J_{AS_{m+n}}\sqrt{8[A]_T K_{eq}{}^2[S]^{2n} + K_{eq}{}^4[S]^{4n}}}{4[A]_T - K_{eq}{}^2[S]^{2n} + \sqrt{8[A]_T K_{eq}{}^2[S]^{2n} + K_{eq}{}^4[S]^{4n}}}$$

Below is the input file used for a non-linear least squares fit. A legend for the assigned variables *a–d* is also provided. The red highlighted terms in the equation below corresponds to the solvent order that must be adjusted manually.

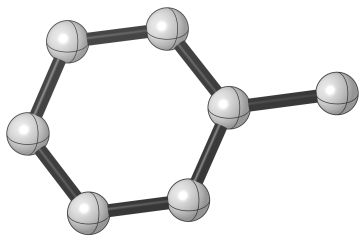
f(x) = J_{obs}
x = [S]
a = $[A]_T$
b = $J_{A_2S_m}$
c = $J_{AS_{m+n}}$
d = K_{eq}

f(x) = (4*a*b+b*(d^2)*(x^2n)-2*c*(d^2)*(x^2n)-
b*sqrt(8*a*(d^2)*(x^2n)+(d^4)*(x^4n))+2*c*sqrt(8*a*(d^2)*(x^2n)+(d^4)*(x^4n)))/(4*a-
(d^2)*(x^2n)+sqrt(8*a*(d^2)*(x^ 2n)+(d^4)*(x^ 4n)))

II. Computations

DFT calculations were performed with the Gaussian 09 program package.[9] Geometry optimizations and single point energies were computed at the M06-2X/def2-SVP level and of theory and M06-2X/def2-TZVP level of theory respectively.[7,10] A pruned (99,590) integration grid was used for all computations as well. CYLview Visualization Software was used for all ball-and-stick structures.[11] Energies are defined as follows: G is the sum of electronic and thermal free energies calculated at the M06-2X level of theory (Hartrees; T = 195 K). G_{SP} is derived from a single point calculation corresponding to the DFT-optimized geometry with the larger basis set (def2-TZVP) and includes a thermal correction from the optimization.

Table S1. Geometric coordinates and single point energies for toluene.

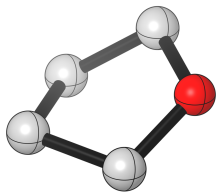


G = -271.014613 Hartrees

$\mathbf{G_{SP}}$ = -271.4240179 Hartrees

Atom	X	Y	Z
C	2.4199700	0.0001370	0.0094220
C	0.9133230	0.0003670	-0.0119040
C	0.1953080	-1.2010320	-0.0090820
C	-1.1984960	-1.2041830	0.0021120
C	-1.9016160	-0.0002670	0.0084730
C	-1.1991070	1.2038450	0.0021090
C	0.1948480	1.2013150	-0.0090800
H	0.7380160	2.1492950	-0.0181460
H	-1.7393190	2.1521350	0.0021330
H	-2.9926080	-0.0005390	0.0143450
H	-1.7383390	-2.1526870	0.0021330
H	0.7389200	-2.1487830	-0.0181610
H	2.7962350	-0.0161780	1.0442130
H	2.8258640	-0.8824340	-0.5032250
H	2.8258480	0.8981050	-0.4755900

Table S2. Geometric coordinates and single point energies for THF.

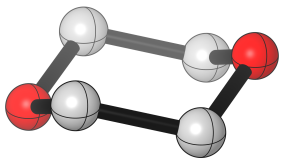


G = -231.959476

G_{SP} = -232.329161

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.1561140	-0.4302150	-0.1364250				
H	-1.5191120	-0.4680640	-1.1798190				
H	-1.9521560	-0.8248280	0.5124330				
C	-0.7265970	0.9879550	0.2364880				
H	-0.7694920	1.1264360	1.3276930				
H	-1.3464000	1.7629510	-0.2329060				
C	0.7269230	0.9876820	-0.2366390				
H	0.7698960	1.1257440	-1.3278950				
H	1.3469340	1.7626540	0.2325220				
C	1.1559260	-0.4304830	0.1367540				
H	1.9523400	-0.8254160	-0.5114370				
H	1.5181460	-0.4681940	1.1804400				
O	-0.0001230	-1.2351150	-0.0002630				

Table S3. Geometric coordinates and single point energies for 1,4-dioxane.

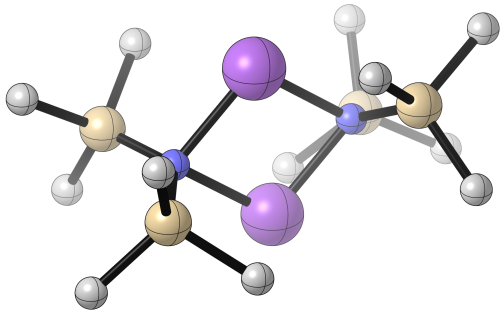


G = -307.076688

G_{SP} = -307.5433292

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.1608310	0.7357100	-0.1911120				
C	-1.1606400	-0.7359220	0.1911820				
H	-1.2091790	-0.8237820	1.2943440				
H	-2.0261940	-1.2563710	-0.2412660				
O	0.0001070	-1.3682410	-0.2936670				
C	1.1607560	-0.7357490	0.1911900				
C	1.1607130	0.7358800	-0.1911150				
H	2.0262260	1.2562490	0.2415040				
H	1.2094990	0.8237400	-1.2942700				
O	-0.0001030	1.3683450	0.2934790				
H	1.2092960	-0.8236230	1.2943500				
H	2.0263760	-1.2560740	-0.2412700				
H	-1.2096230	0.8235700	-1.2942630				
H	-2.0264220	1.2559460	0.2415130				

Table S4. Geometric coordinates and single point energies for NaHMDS unsolvated dimer.



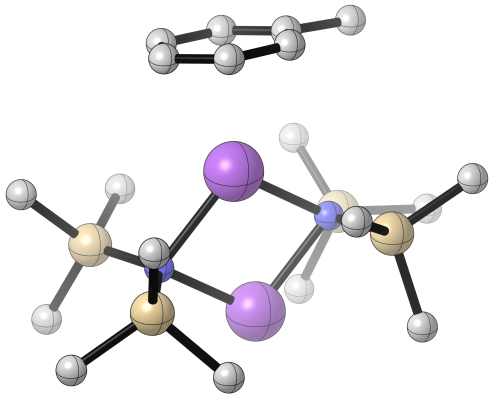
G = -2069.188949

G_{SP} = -2071.228693

Atom	X	Y	Z	Atom	X	Y	Z
N	-1.7952900	0.0000070	-0.0000210	H	3.7529040	2.0667410	1.6179880
Na	-0.0000350	-0.0000810	1.4474900	H	3.5015230	3.5140390	0.6117200
N	1.7952170	-0.0000090	-0.0000230	H	2.1526310	2.8394980	1.5571510
Na	-0.0000360	0.0000780	-1.4475440	C	4.1273480	1.1881550	-1.5406110
Si	2.5739460	-1.4436610	0.4883300	H	4.5537770	2.1490670	-1.8682580
C	4.1273740	-1.1880880	1.5405950	H	4.9093750	0.6493510	-0.9837050
H	4.5538290	-2.1489850	1.8682510	H	3.8935990	0.5966520	-2.4399500
H	4.9093840	-0.6492720	0.9836760	Si	-2.5739270	-1.4437020	-0.4883350
H	3.8936180	-0.5965800	2.4399290	C	-3.0366690	-2.5767690	0.9544610
C	1.3659910	-2.4280060	1.5989490	H	-3.5012860	-3.5141810	0.6117190
H	1.2145790	-1.9424860	2.5812390	H	-2.1523570	-2.8395940	1.5570580
H	0.3808220	-2.5807570	1.1238860	H	-3.7526740	-2.0669380	1.6180610
H	1.7643140	-3.4293200	1.8216880	C	-1.3659610	-2.4279120	-1.5990640
C	3.0369080	-2.5766680	-0.9544390	H	-1.7642030	-3.4292570	-1.8218030
H	2.1526590	-2.8395560	-1.5571020	H	-1.2146730	-1.9423410	-2.5813470
H	3.7529170	-2.0667680	-1.6179820	H	-0.3807380	-2.5805820	-1.1240840
H	3.5015790	-3.5140430	-0.6116710	C	-4.1274720	-1.1882880	-1.5404630
Si	2.5739210	1.4436720	-0.4883310	H	-4.9095500	-0.6497070	-0.9834150
C	1.3659460	2.4280300	-1.5989170	H	-3.8938950	-0.5966150	-2.4397330

H	1.2145460	1.9425400	-2.5812220
H	0.3807730	2.5807450	-1.1238510
H	1.7642490	3.4293590	-1.8216220
C	3.0368760	2.5766440	0.9544690
H	-4.9095520	0.6496290	0.9833940
C	-3.0367020	2.5767910	-0.9544310
H	-3.7527110	2.0669720	-1.6180370
H	-3.5013180	3.5141940	-0.6116650
H	-2.1523950	2.8396290	-1.5570300
C	-1.3659990	2.4278870	1.5990960
H	-1.2147040	1.9422860	2.5813630
H	-0.3807780	2.5805900	1.1241230
H	-1.7642590	3.4292180	1.8218680
H	-4.5537570	-2.1492280	-1.8682170
Si	-2.5739480	1.4436920	0.4883350
C	-4.1274930	1.1882280	1.5404500
H	-4.5538050	2.1491550	1.8682080
H	-3.8939060	0.5965560	2.4397200

Table S5. Geometric coordinates and single point energies for NaHMDS/toluene monosolvated dimer.



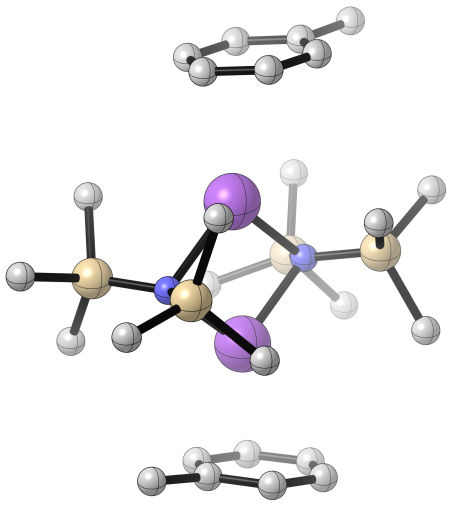
G = -2340.195978

G_{SP} = -2342.782403

Atom	X	Y	Z	Atom	X	Y	Z
N	1.9579580	-0.5249370	0.1468370	H	-2.9797510	1.3549480	2.4072830
Na	0.0485390	0.8123480	-0.2225590	H	-2.6582910	0.3103160	3.8078570
Na	0.2657820	-2.0458630	0.4237650	H	-1.3016950	0.9684390	2.8669850
N	-1.6631250	-0.7132320	0.1365080	C	-4.1881510	-1.5303060	1.6419350
Si	-2.2844200	-1.2090420	-1.3778500	H	-4.5388090	-1.7541960	2.6614990
C	-4.0496690	-0.6685000	-1.7975330	H	-4.8393220	-0.7437780	1.2297090
H	-4.2986210	-0.9572920	-2.8310300	H	-4.3271220	-2.4355170	1.0299020
H	-4.7927970	-1.1298180	-1.1311570	Si	2.7605790	0.1361620	1.5103160
H	-4.1567580	0.4248710	-1.7199080	C	1.4781170	0.7927990	2.7481430
C	-1.1970450	-0.5024240	-2.7696860	H	0.8506690	1.5949470	2.3260330
H	-1.4053620	0.5672870	-2.9248680	H	0.8041320	-0.0094520	3.0898190
H	-0.1191830	-0.6073150	-2.5654630	H	1.9727550	1.2074130	3.6404660
H	-1.3923230	-1.0137640	-3.7251730	C	3.8971920	1.5978530	1.0908400
C	-2.2521660	-3.1054580	-1.5722730	H	4.3619820	2.0253630	1.9930960
H	-1.2334630	-3.5243680	-1.4910280	H	4.7070060	1.2930970	0.4096590
H	-2.8677160	-3.5807250	-0.7912140	H	3.3298420	2.3974130	0.5884270
H	-2.6472130	-3.4262170	-2.5489010	C	3.7975730	-1.1186530	2.4802820

Si	-2.3815520	-0.9621680	1.6685400	H	4.6321480	-1.5039730	1.8761240
C	-1.4281370	-2.3364630	2.6101320	H	4.2203600	-0.6681720	3.3920100
H	-1.4332600	-3.2854130	2.0429640	H	3.1798060	-1.9788090	2.7860190
H	-0.3820690	-2.0599620	2.8377910	Si	2.7732990	-1.0642600	-1.2608330
H	-1.8971460	-2.5537900	3.5817680	C	1.9003490	-2.6273260	-1.9276770
C	-2.3207430	0.5610400	2.7898360	H	1.9937800	-3.4545070	-1.2003080
H	2.3714460	-2.9804250	-2.8578280	H	1.2094900	3.7969460	1.1611410
H	0.8323930	-2.4792780	-2.1586050	H	1.9985320	3.5731360	-1.1938140
C	2.7818850	0.2428780	-2.6357390	H	0.3553820	3.0531620	-2.9956020
H	3.2612280	-0.1226530	-3.5571510				
H	1.7647300	0.5767150	-2.8973340				
H	3.3441230	1.1250730	-2.2878850				
C	4.5751950	-1.5995740	-1.0206280				
H	5.1955950	-0.7913160	-0.6036370				
H	4.6429600	-2.4605030	-0.3376880				
H	5.0184830	-1.8974660	-1.9838020				
C	0.0212060	3.1466120	-1.9608400				
C	0.9434060	3.4387460	-0.9521260				
C	0.4988510	3.5618110	0.3666770				
C	-0.8516640	3.3727370	0.6762020				
C	-1.7860240	3.0687050	-0.3249550				
C	-1.3278890	2.9713530	-1.6469370				
H	-2.0447540	2.7498260	-2.4408080				
C	-3.2290600	2.8023380	0.0022560				
H	-3.8888430	3.1399080	-0.8083850				
H	-3.3768250	1.7173950	0.1316390				
H	-3.5295570	3.3021070	0.9324280				
H	-1.1873780	3.4575020	1.7124070				

Table S6. Geometric coordinates and single point energies for NaHMDS/toluene disolvated dimer.



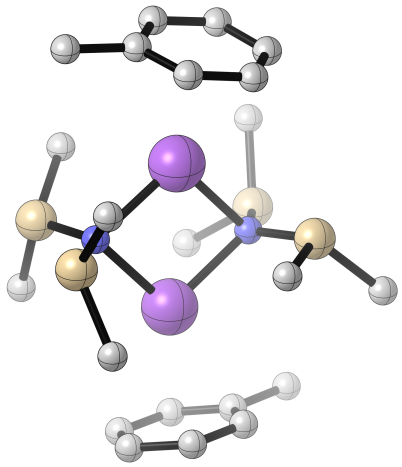
G = -2611.198378

G_{SP} = -2614.332947

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.4351020	-0.6963370	-0.0543420	H	0.3737860	3.7573610	1.8020980
N	0.8002690	-1.3637770	0.0182030	H	-0.2346090	3.2948340	3.4097760
Na	1.0694810	0.9456540	0.0465920	Si	-1.4082020	2.4382580	-1.5110870
N	-1.2183480	1.6297270	-0.0167260	C	0.2777220	2.6526970	-2.3784100
Si	-1.5592850	2.1876220	1.5613930	H	0.8891320	3.3732310	-1.8103020
C	-2.8997210	3.5138960	1.7524040	H	0.8544190	1.7162740	-2.4775190
H	-3.1240000	3.6526520	2.8222580	H	0.1560210	3.0576090	-3.3952340
H	-2.5862730	4.4860740	1.3460550	C	-2.5194000	1.4888560	-2.7207870
H	-3.8359390	3.2249930	1.2492730	H	-3.5465060	1.4229640	-2.3281110
C	-2.1694020	0.7526340	2.6558040	H	-2.5665640	1.9993880	-3.6955270
H	-3.2333290	0.5640420	2.4434340	H	-2.1515710	0.4668310	-2.9010480
H	-1.6232110	-0.1957280	2.5134680	C	-2.1145990	4.1943640	-1.4336430
H	-2.0894930	1.0082200	3.7242610	H	-2.1366840	4.6326280	-2.4440260
C	-0.0120860	2.9147660	2.4003430	H	-3.1407590	4.2076370	-1.0370520
H	0.7938090	2.1705820	2.5103180	H	-1.4988690	4.8489210	-0.7964140

C	3.5251640	2.1882260	1.2586670	H	1.7435860	-1.0585160	3.8030380
C	4.3892190	1.0934810	1.1565950	H	0.5023000	-0.1077520	2.9673240
C	4.8744280	0.6709520	-0.0847370	C	0.1513860	-3.2953950	2.2326820
C	4.4591690	1.3674030	-1.2303630	H	0.5434190	-3.7514820	3.1552250
C	3.5935540	2.4539780	-1.1387960	H	-0.8155690	-2.8247650	2.4765890
C	3.1222970	2.8727920	0.1112010	H	-0.0404410	-4.0989710	1.5039800
H	2.4569450	3.7353200	0.1904510	C	3.0670480	-2.7894440	1.4436720
H	3.2874260	2.9822890	-2.0429030	H	3.0951560	-3.6632290	0.7736910
H	4.8286290	1.0517070	-2.2089490	H	3.7974950	-2.0558370	1.0654290
C	5.8299920	-0.4848420	-0.2053540	H	3.3974110	-3.1202930	2.4408070
H	6.7834870	-0.1541420	-0.6430710	C	-3.3716840	-3.0272880	1.0861540
H	6.0391390	-0.9365070	0.7726620	C	-2.9338910	-3.5519780	-0.1302530
H	5.4147310	-1.2613260	-0.8639590	C	-3.1706460	-2.8407560	-1.3079720
H	4.6975410	0.5620510	2.0599440	C	-3.8228440	-1.6052230	-1.2658110
H	3.1707840	2.5124780	2.2392020	C	-4.2522760	-1.0565260	-0.0467530
Si	1.0981450	-2.1569140	-1.4725590	C	-4.0267260	-1.7956930	1.1240660
C	-0.0098300	-1.4129440	-2.8253990	H	-4.3710870	-1.3996260	2.0811320
H	-1.0791560	-1.6039040	-2.6352840	C	-4.8950710	0.3041040	0.0058930
H	0.1235030	-0.3227650	-2.9117720	H	-5.4990570	0.4248800	0.9150540
H	0.2217360	-1.8516170	-3.8085170	H	-4.1172330	1.0870610	0.0079390
C	0.7283350	-4.0188600	-1.4570230	H	-5.5379450	0.4754170	-0.8682280
H	0.9170480	-4.4720440	-2.4429450	H	-4.0025670	-1.0550330	-2.1921020
H	1.3517910	-4.5486790	-0.7195460	H	-2.8470180	-3.2508860	-2.2663290
H	-0.3249370	-4.2018000	-1.1934930	H	-2.4219570	-4.5145560	-0.1597890
C	2.8795240	-1.9743060	-2.0942660	H	-3.2039060	-3.5812330	2.0107960
H	3.5735890	-2.4879860	-1.4113140	Si	1.3416040	-2.0033040	1.5153920
H	3.0071390	-2.4062510	-3.0992410	C	1.4591970	-0.6341540	2.8271990
H	3.1666210	-0.9111420	-2.1359790	H	2.2256100	0.1127780	2.5647430

Table S7. Geometric coordinates and single point energies for NaTMDS/toluene disolvated dimer.



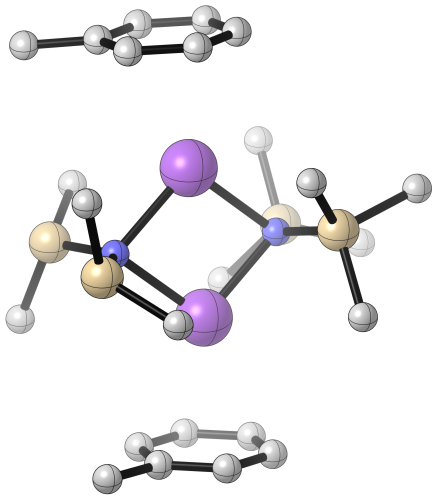
G = -2456.478908

G_{SP} = -2454.313636

Atom	X	Y	Z	Atom	X	Y	Z
Na	1.3560690	-0.5695680	0.0151840	C	1.9002420	3.1104830	2.3910580
N	0.4661130	1.5899940	0.1468950	H	1.7351520	3.4251460	3.4331770
Na	-1.5190960	0.3320020	-0.0906210	H	2.8419540	2.5427720	2.3526500
N	-0.6305460	-1.8131210	-0.2825150	H	2.0295390	4.0171350	1.7807310
Si	-0.7919530	-3.0782640	0.8637890	H	-0.7781250	2.9100280	2.1493580
C	0.7552100	-3.3023500	1.9382900	C	4.0776370	-1.7212330	-1.0369480
H	1.6224310	-3.5909180	1.3265160	C	3.8160960	-2.3050380	0.2019660
H	1.0019940	-2.3756830	2.4824960	C	3.7470660	-1.4969250	1.3416210
H	0.5947110	-4.0924150	2.6880680	C	3.9304510	-0.1174070	1.2351720
C	-2.2086530	-2.8534910	2.1013510	C	4.1913030	0.4856950	-0.0066110
H	-2.0823840	-1.9348280	2.6967510	C	4.2644890	-0.3402860	-1.1360110
H	-3.1839550	-2.8117660	1.5947800	H	4.4791330	0.1045480	-2.1100130
H	-2.2298620	-3.7034580	2.8010740	C	4.3657160	1.9751970	-0.1154570
H	-1.0321080	-4.4108810	0.2098290	H	4.7987850	2.2566840	-1.0841130
Si	-0.7481150	-2.1054390	-1.9642800	H	3.3935180	2.4834940	-0.0164390
C	-1.6183970	-0.6544320	-2.8348460	H	5.0173430	2.3558450	0.6835770

H	-2.6744010	-0.5920150	-2.5271640	H	3.8816570	0.5045010	2.1320670
H	-1.1378050	0.3181120	-2.6291180	H	3.5487370	-1.9467290	2.3160400
H	-1.6054080	-0.7852510	-3.9276070	H	3.6777140	-3.3838550	0.2827140
C	0.9458070	-2.3045860	-2.7965210	H	4.1373790	-2.3412060	-1.9325160
H	1.4905380	-3.1445850	-2.3359820	H	-0.4699030	-0.1507500	2.5705730
H	0.8516080	-2.5098590	-3.8740500	H	0.1648880	0.7930570	3.9375100
H	1.5667930	-1.3980760	-2.6895680	H	1.2855610	-0.0285290	2.8364260
H	-1.5415840	-3.3280590	-2.3244390	H	-1.5449320	2.6421930	-2.2713210
C	-3.8666550	2.2024530	-0.5039110	H	1.5927550	3.8359000	-0.8198760
C	-4.3068280	0.9367010	-0.8989240	Si	0.4316330	2.0839990	1.7842730
C	-4.3322230	-0.1363200	0.0029030	C	0.3372270	0.5354840	2.8814360
C	-3.9300850	0.1055820	1.3268540	H	-1.4168330	3.9554560	-1.0715470
C	-3.4753160	1.3653210	1.7228380	H	-0.6489460	4.1259700	-2.6709840
C	-3.4329860	2.4180270	0.8045740				
H	-3.0621990	3.3964460	1.1116420				
H	-3.1443990	1.5272450	2.7503130				
H	-3.9641470	-0.7089840	2.0513070				
C	-4.7266550	-1.5179740	-0.4464030				
H	-5.2813270	-2.0500950	0.3382950				
H	-5.3476690	-1.4814810	-1.3510020				
H	-3.8268420	-2.1137600	-0.6775920				
H	-4.6352160	0.7778600	-1.9285190				
H	-3.8518550	3.0201220	-1.2253820				
Si	0.7206920	2.6576970	-1.1672420				
C	1.5790380	1.7789560	-2.6079060				
H	2.5728360	1.4149160	-2.3074490				
H	0.9940580	0.9135090	-2.9589230				
H	1.7150630	2.4572510	-3.4640930				
C	-0.8727360	3.4141790	-1.8612990				

Table S8. Geometric coordinates and single point energies for mixed NaHMDS/NaTMDS dimer with toluene.



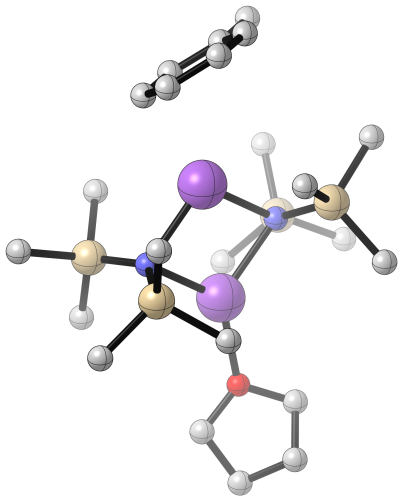
G = -2532.75828

G_{SP} = -2535.070267

Atom	X	Y	Z	Atom	X	Y	Z
Na	1.5322680	-0.0340290	0.0905760	H	1.1102570	3.8742310	-1.2073150
N	-0.0004910	1.7374800	-0.0039500	Si	-0.3613180	2.5878610	1.4376010
Na	-1.5290280	-0.0381270	-0.0925820	C	-1.4412730	1.5366040	2.5923450
N	0.0039970	-1.8006480	-0.0012620	H	-2.4262360	1.3075480	2.1573800
Si	-0.0715380	-2.5358340	1.5379280	H	-1.6242810	2.0653230	3.5405860
C	0.5494010	-4.3228520	1.6427400	H	-0.9493550	0.5819750	2.8400330
H	0.6578830	-4.6318680	2.6945250	C	1.1586900	3.0835440	2.4503070
H	-0.1440310	-5.0247230	1.1563100	H	0.8776990	3.6882320	3.3262550
H	1.5326000	-4.4272300	1.1554970	H	1.6902310	2.1881030	2.8128040
C	0.9882380	-1.5719780	2.7982990	H	1.8544560	3.6754500	1.8350540
H	2.0440900	-1.8723210	2.7156230	H	-1.1238900	3.8673760	1.2000830
H	0.9368480	-0.4766390	2.6701810	C	4.4623900	-0.9803180	-0.3688090
H	0.6675980	-1.7888110	3.8294900	C	4.1530520	-1.0876550	0.9869350
C	-1.8398140	-2.5505840	2.2342610	C	3.9393170	0.0743800	1.7364710
H	-2.2590480	-1.5342660	2.3307870	C	4.0253840	1.3267130	1.1281750

H	-2.4970630	-3.1247340	1.5609930	C	4.3277820	1.4491520	-0.2368450
H	-1.8815710	-3.0180760	3.2306730	C	4.5465690	0.2773110	-0.9719230
Si	0.0788510	-2.5299440	-1.5432540	H	4.7844440	0.3497150	-2.0357020
C	-0.9818480	-1.5605740	-2.7987620	C	4.3926080	2.8077890	-0.8810970
H	-2.0378300	-1.8605560	-2.7162430	H	4.7260100	2.7392240	-1.9246700
H	-0.9293450	-0.4657870	-2.6663860	H	3.4021750	3.2894910	-0.8720700
H	-0.6625420	-1.7734330	-3.8311880	H	5.0861840	3.4651060	-0.3376220
C	1.8463940	-2.5419510	-2.2414340	H	3.8546350	2.2281820	1.7193720
H	2.5043720	-3.1188270	-1.5712130	H	3.7004170	0.0032530	2.7991590
H	1.8868970	-3.0054840	-3.2397430	H	4.0850720	-2.0696320	1.4578440
H	2.2655910	-1.5252990	-2.3344580	H	4.6342360	-1.8775990	-0.9641910
C	-0.5421710	-4.3164930	-1.6549130	Si	0.3558060	2.5900140	-1.4454290
H	-0.6509220	-4.6213550	-2.7078820	C	1.4435570	1.5464800	-2.5996470
H	0.1515070	-5.0201810	-1.1714650	H	2.4288040	1.3232020	-2.1623480
H	-1.5251890	-4.4229140	-1.1677540	H	0.9582480	0.5890880	-2.8495590
C	-4.4635520	-0.9911150	0.3684030	H	1.6254310	2.0776370	-3.5467380
C	-4.5534630	0.2620620	0.9797960	C	-1.1670060	3.0775380	-2.4579180
C	-4.3355900	1.4395150	0.2535410	H	-1.8624080	3.6712580	-1.8440160
C	-4.0274340	1.3274270	-1.1110420	H	-0.8887010	3.6787290	-3.3371270
C	-3.9359650	0.0795480	-1.7277200	H	-1.6979800	2.1796800	-2.8152560
C	-4.1494050	-1.0882110	-0.9870230	H	-3.4206230	3.2823980	0.8964300
H	-4.0772840	-2.0667230	-1.4644990	H	-4.7947940	0.3265610	2.0433070
H	-3.6929610	0.0164020	-2.7900130	H	-4.6346840	-1.8929810	0.9570320
H	-3.8562880	2.2333050	-1.6953450				
C	-4.4074760	2.7935530	0.9066690				
H	-5.1080960	3.4491730	0.3701580				
H	-4.7362660	2.7160120	1.9510740				

Table S9. Geometric coordinates and single point energies for NaHMDS dimer with 1 THF and 1 toluene.



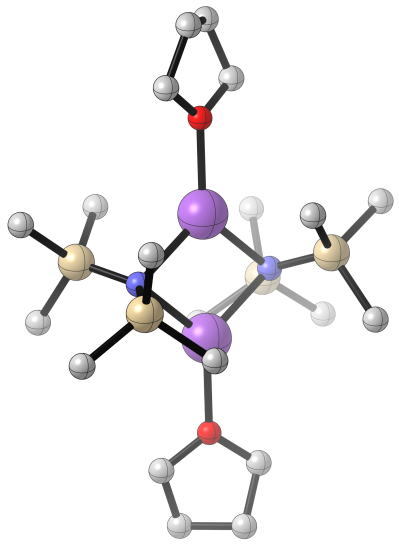
G = -2574.571273

$\mathbf{G_{SP}}$ = -2572.158453

Atom	X	Y	Z	Atom	X	Y	Z
N	0.5757890	1.8175990	0.1670690	H	2.3458790	2.5400290	3.6114050
Na	-1.3032570	0.4768320	0.0643620	H	2.4889610	1.0438810	2.6638700
Na	1.5079220	-0.3178060	0.2366070	Si	1.1266060	2.4192230	-1.3303500
N	-0.3864080	-1.6627080	0.1025330	C	1.9662830	1.0005690	-2.3002630
Si	-1.0054930	-2.2566180	-1.3765980	H	2.9070080	0.6991140	-1.8074760
C	-2.5023840	-3.4067140	-1.1888680	H	2.2210630	1.3042000	-3.3272210
H	-2.8880060	-3.7352860	-2.1667270	H	1.3238090	0.1061340	-2.3778940
H	-2.2603740	-4.3071390	-0.6029540	C	-0.2862280	3.0805640	-2.4079050
H	-3.3136590	-2.8759180	-0.6640830	H	0.0644190	3.4314730	-3.3910540
C	-1.6331420	-0.7900090	-2.4196560	H	-1.0612090	2.3155630	-2.5789120
H	-2.5257940	-0.3181380	-1.9719640	H	-0.7643070	3.9307590	-1.8939160
H	-0.8619140	-0.0150370	-2.5623830	C	2.4207220	3.8013580	-1.2338470
H	-1.9386700	-1.1243990	-3.4230690	H	1.9759570	4.7361080	-0.8602520
C	0.2874860	-3.1515130	-2.4362800	H	3.2467540	3.5294270	-0.5570240
H	1.0958080	-2.4593670	-2.7247260	H	2.8496840	4.0100430	-2.2266400

H	0.7378930	-3.9845250	-1.8741730	C	-4.6684750	1.3573320	-1.7712860
H	-0.1470410	-3.5599900	-3.3619400	C	-3.8673110	2.3290510	-1.1750290
Si	-0.1745930	-2.6129280	1.5090680	C	-3.4730110	2.1690760	0.1564400
C	1.1509370	-1.8156540	2.6230030	C	-3.8709840	1.0380170	0.8745240
H	2.1533050	-1.8446190	2.1602580	C	-4.6664580	0.0452750	0.2791070
H	0.9137370	-0.7670400	2.8700190	C	-5.0600100	0.2273420	-1.0509540
H	1.2292800	-2.3566680	3.5784490	H	-5.6779900	-0.5338030	-1.5320690
C	-1.7502660	-2.7557210	2.5528800	C	-5.0979400	-1.1610940	1.0695160
H	-2.5384160	-3.2637660	1.9744590	H	-5.6015720	-1.8968810	0.4296570
H	-1.5898270	-3.3249510	3.4816220	H	-4.2356330	-1.6497940	1.5448500
H	-2.1221910	-1.7549330	2.8292270	H	-5.7956360	-0.8708070	1.8693660
C	0.4454480	-4.3754980	1.1781440	H	-3.5677130	0.9223640	1.9195650
H	0.5716860	-4.9400530	2.1152420	H	-2.8497460	2.9299650	0.6333970
H	-0.2491220	-4.9406740	0.5371170	H	-3.5491620	3.2068540	-1.7383660
H	1.4210640	-4.3474340	0.6664710	H	-4.9822420	1.4718670	-2.8099290
O	3.6601980	-0.9017540	0.1613600	C	0.4306650	4.3908600	1.7996930
C	4.7865940	-0.0294340	0.2956580	H	0.3105130	4.7334980	2.8395270
H	4.5288120	0.9432720	-0.1562520	H	1.2971060	4.9176480	1.3722680
H	4.9930980	0.1298920	1.3632220	H	-0.4628480	4.7002170	1.2337630
C	5.9335340	-0.7170930	-0.4469810	C	2.3062500	2.1294880	2.5902500
C	5.1882220	-1.5779030	-1.4693590	H	3.1380640	2.5708260	2.0171880
C	3.9844800	-2.0283660	-0.6541980	Si	0.6590070	2.5120720	1.7213220
H	3.1015890	-2.2866580	-1.2579280	C	-0.7256830	1.7789090	2.8101580
H	4.2324410	-2.8901240	-0.0109070	H	-1.7000760	2.2227690	2.5472430
H	4.8567810	-0.9664550	-2.3223150	H	-0.8093370	0.6819050	2.7136340
H	5.7819530	-2.4173010	-1.8525110	H	-0.5556910	1.9937460	3.8765660
H	6.5055680	-1.3577520	0.2401720				
H	6.6276120	0.0009300	-0.9012860				

Table S10. Geometric coordinates and single point energies for NaHMDS disolvated dimer with 2 THF



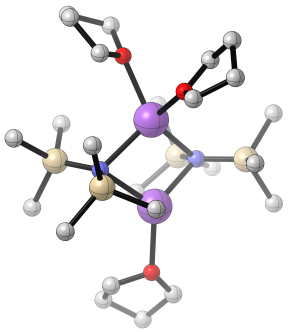
G = -2535.485816

G_{SP} = -2533.120241

Atom	X	Y	Z	Atom	X	Y	Z
N	-0.0000990	1.8127690	0.0001650	H	6.0456910	0.1584590	1.5271390
Na	1.4548150	0.0001210	0.0002980	H	6.6856030	1.3212710	0.3387610
N	0.0001880	-1.8127540	0.0002100	Si	-0.4395480	2.5768140	1.4618550
Na	-1.4548180	-0.0001050	0.0002430	C	1.0530760	3.0245010	2.5417840
O	-3.6905860	-0.0001820	0.0000450	H	0.7589210	3.4987030	3.4910110
C	-4.4998460	1.1243270	-0.3531840	H	1.6419750	2.1239750	2.7819770
H	-4.4520190	1.8696970	0.4587740	H	1.7118680	3.7229560	2.0014740
H	-4.0933470	1.5783020	-1.2678470	C	-1.5234920	1.3872380	2.4899620
C	-5.9091770	0.5656220	-0.5153740	H	-1.7235180	1.8022840	3.4896650
C	-5.9095760	-0.5661810	0.5136120	H	-2.5043630	1.2122210	2.0141210
C	-4.5000320	-1.1247360	0.3527070	H	-1.0390020	0.4072430	2.6412530
H	-4.0942910	-1.5785640	1.2677790	C	-1.4819590	4.1488030	1.2554450
H	-4.4514080	-1.8701910	-0.4591250	H	-0.9345770	4.9304920	0.7064750
H	-6.0455740	-0.1598930	1.5270250	H	-2.4005360	3.9280760	0.6883640

H	-6.6855530	-1.3216340	0.3376340	H	-1.7768350	4.5685120	2.2300820
H	-6.0442030	0.1593260	-1.5289130	Si	0.4391680	2.5768530	-1.4615600
H	-6.6854000	1.3209860	-0.3400950	C	1.4808790	4.1493170	-1.2552580
Si	0.4395190	-2.5768660	1.4619030	H	1.7755150	4.5691100	-2.2299320
C	1.4814860	-4.1491520	1.2555300	H	0.9331650	4.9307840	-0.7063030
H	1.7761390	-4.5689760	2.2301850	H	2.3995860	3.9290420	-0.6882120
H	0.9339240	-4.9306610	0.7064830	C	-1.0535900	3.0238270	-2.5416090
H	2.4001880	-3.9286820	0.6885510	H	-1.7126090	3.7221710	-2.0014280
C	1.5238260	-1.3875500	2.4899230	H	-0.7595880	3.4979590	-3.4909180
H	2.5046570	-1.2127460	2.0139260	H	-1.6421980	2.1230690	-2.7816460
H	1.0395780	-0.4074490	2.6413120	C	1.5236920	1.3876400	-2.4894730
H	1.7239020	-1.8026670	3.4895860	H	2.5045360	1.2130170	-2.0134350
C	-1.0532120	-3.0241350	2.5418630	H	1.0396020	0.4074530	-2.6408020
H	-1.6419820	-2.1234840	2.7819070	H	1.7237310	1.8027200	-3.4891590
H	-1.7120930	-3.7225630	2.0016230	H	-2.3998940	-3.9284050	-0.6881710
H	-0.7591760	-3.4982570	3.4911660	O	3.6906000	0.0001750	0.0001370
Si	-0.4391060	-2.5767750	-1.4615380	C	4.5000810	1.1243870	0.3538020
C	-1.5232020	-1.3873070	-2.4896110	H	4.4514100	1.8706040	-0.4573270
H	-2.5041120	-1.2124640	-2.0137870	H	4.0944080	1.5773590	1.2693270
H	-1.0388570	-0.4072290	-2.6408220	C	5.9096290	0.5656670	0.5141040
H	-1.7231340	-1.8023240	-3.4893440	C	5.9091530	-0.5652040	-0.5159070
C	1.0536130	-3.0241750	-2.5414600	C	4.4998180	-1.1240280	-0.3541520
H	1.7125130	-3.7225380	-2.0011630	H	4.0932720	-1.5771570	-1.2692130
H	0.7595510	-3.4983960	-3.4907060	H	4.4520100	-1.8701380	0.4571260
H	1.6423610	-2.1235410	-2.7816210	H	6.0441350	-0.1579930	-1.5290850
C	-1.4812750	-4.1489420	-1.2552580	H	6.6853690	-1.3207420	-0.3413540
H	-1.7760720	-4.5686230	-2.2299310	H	-0.9337780	-4.9305870	-0.7063410

Table S11. Geometric coordinates and single point energies for NaHMDS trisolvated dimer with 3 THF.



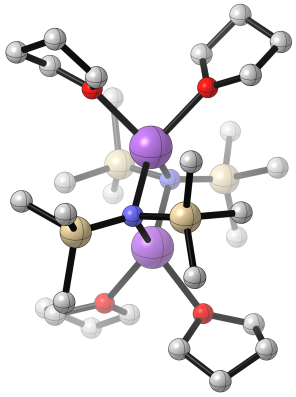
G = -2765.063137

G_{SP} = -2767.813944

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.1033070	0.2467200	-0.2782560	H	-0.1710980	4.8965630	-1.6442560
Na	1.6792540	0.1252170	0.5484880	H	-1.6049050	4.1903160	-0.8847580
N	0.1802100	-1.6814170	0.3739910	O	3.8067910	-0.1602120	1.1526610
Si	-0.0058500	-2.0307640	2.0387620	C	4.9210170	0.6747060	0.8290410
C	0.5102150	-0.4887080	3.0356350	H	4.5892580	1.4064570	0.0756700
H	1.6060430	-0.3464200	3.0262740	H	5.2375240	1.2274300	1.7260240
H	0.0420310	0.4305180	2.6432970	C	6.0181200	-0.2618410	0.2991040
H	0.2186710	-0.5758740	4.0937800	C	5.2482110	-1.5432260	-0.0386350
C	1.0752480	-3.4451190	2.7021990	C	4.1695280	-1.5344300	1.0333440
H	0.9192460	-3.5851010	3.7836890	H	3.2659480	-2.1043510	0.7696660
H	0.8444660	-4.4004830	2.2056070	H	4.5548220	-1.9068020	1.9994120
H	2.1447300	-3.2366170	2.5419900	H	4.7819340	-1.4707330	-1.0328130
C	-1.7859320	-2.4552320	2.5408020	H	5.8716410	-2.4458250	-0.0118420
H	-2.0917220	-3.4099230	2.0844080	H	6.7604090	-0.4640860	1.0845700
H	-1.8974230	-2.5491300	3.6327580	H	6.5477590	0.1636270	-0.5625540
H	-2.4822230	-1.6809770	2.1868640	O	-2.7068440	0.9684230	1.2627700
Si	0.2262340	-2.9269640	-0.8032470	C	-3.0600210	0.8819040	2.6443660
C	-0.2869790	-2.2967540	-2.5173070	H	-3.7320300	0.0188110	2.7954900
H	-1.2552280	-1.7762620	-2.4516590	H	-2.1459590	0.7147410	3.2318620

H	-0.4002910	-3.1384650	-3.2191800	C	-3.7742280	2.1898170	2.9619870
H	0.4400080	-1.5944590	-2.9510090	C	-4.4873400	2.4690950	1.6387960
C	1.9448160	-3.7130450	-1.0139570	C	-3.4365290	2.0244330	0.6262330
H	1.9258860	-4.5149050	-1.7688440	H	-3.8544050	1.6378830	-0.3142060
H	2.6896300	-2.9687770	-1.3397520	H	-2.7346650	2.8427380	0.3934660
H	2.2925710	-4.1519490	-0.0647070	H	-5.3916590	1.8470090	1.5544010
C	-0.9452740	-4.3892360	-0.4541600	H	-4.7782760	3.5188180	1.5068040
H	-0.7329780	-4.8680470	0.5146810	H	-3.0399520	2.9809290	3.1747310
H	-2.0016680	-4.0750770	-0.4418000	H	-4.4527670	2.1022370	3.8200800
H	-0.8373770	-5.1589480	-1.2348480	O	-3.0222500	-0.4105930	-1.3917980
N	0.6595530	1.8769690	-0.5421320	C	-3.5870180	-0.4928840	-2.6970240
Si	1.2434420	1.6701230	-2.1367920	H	-4.4131790	0.2349750	-2.7915580
C	2.2214830	3.1118990	-2.8863330	H	-2.8089010	-0.2347620	-3.4283550
H	2.4855710	2.8862850	-3.9316840	C	-4.0972700	-1.9232050	-2.8126150
H	1.6480260	4.0515480	-2.8807620	C	-4.6032370	-2.1800250	-1.3920180
H	3.1570050	3.2858290	-2.3324250	C	-3.5990580	-1.4053780	-0.5345830
C	2.4651640	0.2012350	-2.1904300	H	-4.0632870	-0.9063030	0.3294290
H	3.3904360	0.4755040	-1.6549270	H	-2.7811890	-2.0423180	-0.1597360
H	2.0599980	-0.7165450	-1.7327970	H	-5.6146980	-1.7653460	-1.2688830
H	2.7508440	-0.0550380	-3.2227850	H	-4.6388450	-3.2448160	-1.1282120
C	-0.1737700	1.2999070	-3.3436780	H	-3.2639830	-2.5999200	-3.0534270
H	-0.7721060	0.4429720	-2.9972280	H	-4.8725290	-2.0380940	-3.5809170
H	-0.8399290	2.1765210	-3.3998970	C	-0.1641620	3.1708060	1.9948450
H	0.1783470	1.0667460	-4.3607300	H	-1.0309230	2.4935520	1.9988890
Si	0.5198380	3.3932330	0.2376660	H	0.6039130	2.7334120	2.6534970
H	2.0351330	5.2050830	1.1001290	H	-0.4675300	4.1346360	2.4337820
H	2.8965150	3.6515260	0.9876090	C	2.1692080	4.3052610	0.4785520
C	-0.6132170	4.6200580	-0.6739750	H	2.6093980	4.6210600	-0.4788370
H	-0.7564980	5.5484860	-0.0986750				

Table S12. Geometric coordinates and single point energies for NaHMDS tetrasolvated dimer with 4 THF



G = -3000.146223

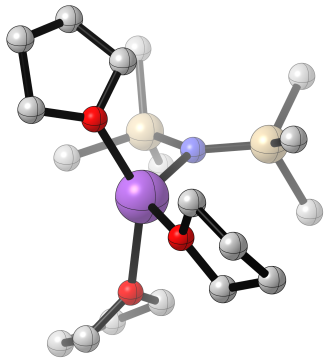
G_{SP} = -2997.013147

Atom	X	Y	Z	Atom	X	Y	Z
Na	1.4480640	0.0000100	0.0000010	H	1.0225970	-0.4524160	2.6765620
N	0.0221590	-1.9137850	0.0587160	H	-0.7071080	-0.1135080	2.5380700
Na	-1.3941310	-0.0000040	-0.0000070	H	-0.1131850	-1.1323370	3.8687650
N	0.0221430	1.9137880	-0.0587160	C	1.0619010	-3.7090250	2.3155740
Si	-0.1787690	2.4119440	-1.6848660	H	0.8939020	-3.9217890	3.3836710
C	1.0618600	3.7090600	-2.3155650	H	0.9787170	-4.6605920	1.7683190
H	0.8938620	3.9218120	-3.3836650	H	2.0983810	-3.3540120	2.2010980
H	0.9786370	4.6606280	-1.7683190	C	-1.9123040	-3.0919560	2.0695800
H	2.0983520	3.3540880	-2.2010790	H	-2.1213780	-4.0137890	1.5060370
C	0.0222030	0.8953770	-2.8010240	H	-2.0323110	-3.3130410	3.1426130
H	1.0226360	0.4524560	-2.6765680	H	-2.6760800	-2.3481150	1.7895110
H	-0.7070620	0.1135010	-2.5380900	Si	0.2361460	-3.0861750	-1.1733670
H	-0.1131570	1.1323590	-3.8687700	C	-0.3493850	-2.5149360	-2.8860120
C	-1.9123260	3.0919290	-2.0695980	H	-1.3452840	-2.0486730	-2.8136010
H	-2.6760970	2.3480780	-1.7895410	H	-0.4215650	-3.3822560	-3.5613520
H	-2.1214220	4.0137590	-1.5060600	H	0.3237220	-1.7796030	-3.3493360
H	-2.0323220	3.3130110	-3.1426330	C	2.0593040	-3.5899060	-1.3752060

Si	0.2360770	3.0861790	1.1733750	H	2.2080210	-4.2848320	-2.2168120
C	-0.3494780	2.5149210	2.8860050	H	2.6886770	-2.7013990	-1.5491150
H	-1.3453600	2.0486260	2.8135710	H	2.4253460	-4.0827870	-0.4596370
H	0.3236440	1.7796080	3.3493400	C	-0.7189360	-4.7123570	-0.8941250
H	-0.4216990	3.3822360	3.5613470	H	-0.4731560	-5.1902270	0.0665520
C	2.0592230	3.5899420	1.3752440	H	-1.8085290	-4.5455810	-0.9099490
H	2.4252640	4.0828300	0.4596780	H	-0.4822670	-5.4315010	-1.6943850
H	2.2079210	4.2848710	2.2168520	O	3.2021100	0.1282720	-1.4633690
H	2.6886100	2.7014460	1.5491570	C	3.5224250	-0.2619260	-2.7912740
C	-0.7190250	4.7123480	0.8941250	H	4.4221020	-0.9046670	-2.7903430
H	-0.4823750	5.4314880	1.6943940	H	2.6802600	-0.8439130	-3.1908320
H	-0.4732340	5.1902280	-0.0665440	C	3.7792550	1.0516550	-3.5155670
H	-1.8086170	4.5455630	0.9099310	C	4.5224440	1.8457230	-2.4374660
O	-3.0521740	0.4364430	1.5062010	C	3.8750250	1.3500030	-1.1362140
C	-3.5484920	0.1256310	2.8057720	H	4.6095400	1.1589000	-0.3382390
H	-4.2880190	-0.6918500	2.7313320	H	3.1231920	2.0511580	-0.7408680
H	-2.7101450	-0.2217290	3.4256890	H	5.5932120	1.5954860	-2.4537890
C	-4.1962590	1.4123290	3.3031760	H	4.4288470	2.9326970	-2.5602730
C	-4.7589760	1.9922700	2.0044110	H	2.8188010	1.5325330	-3.7572470
C	-3.6785270	1.6181900	0.9909400	H	4.3539040	0.9290880	-4.4425350
H	-4.0756360	1.3932950	-0.0105100	O	3.2021070	-0.1282220	1.4633910
H	-2.9080490	2.4014110	0.8886400	C	3.5223910	0.2619550	2.7913090
H	-5.7101910	1.5005600	1.7507750	H	4.4220680	0.9046960	2.7904070
H	-4.9341770	3.0746160	2.0466860	H	2.6802180	0.8439390	3.1908550
H	-3.4326350	2.0826020	3.7245630	C	3.7792080	-1.0516340	3.5155910
H	-4.9603390	1.2320500	4.0701620	C	4.5224190	-1.8456870	2.4374950
O	-3.0521540	-0.4364780	-1.5062280	C	3.8750170	-1.3499570	1.1362390
C	-3.5484680	-0.1256790	-2.8058040	H	4.6095410	-1.1588540	0.3382710
H	-4.2880070	0.6917920	-2.7313730	H	3.1231840	-2.0511050	0.7408820
H	-2.7101210	0.2216910	-3.4257170				
C	-4.1962120	-1.4123880	-3.3032080				

C	-4.7589310	-1.9923290	-2.0044430
C	-3.6784910	-1.6182340	-0.9909690
H	-4.0756050	-1.3933460	0.0104800
H	-2.9080020	-2.4014440	-0.8886680
H	-5.7101520	-1.5006280	-1.7508150
H	-4.9341210	-3.0746780	-2.0467150
H	-3.4325750	-2.0826520	-3.7245850
H	-4.9602880	-1.2321230	-4.0702010
Si	-0.1787560	-2.4119400	1.6848660
C	0.0221750	-0.8953630	2.8010170
H	5.5931850	-1.5954400	2.4538380
H	4.4288290	-2.9326630	2.5602890
H	2.8187510	-1.5325180	3.7572460
H	4.3538390	-0.9290780	4.4425730

Table S13. Geometric coordinates and single point energies for NaHMDS trisolvated monomer with 3 THF.



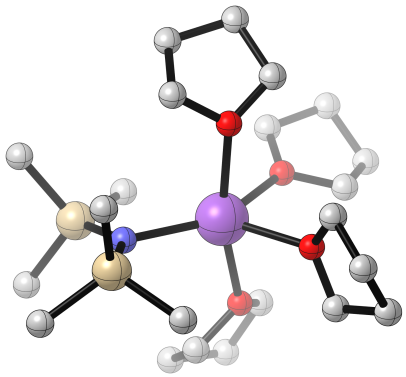
G = -1730.462204

G_{SP} = -1732.396722

Atom	X	Y	Z	Atom	X	Y	Z
Si	2.6181760	0.2198260	-0.0778390	H	-3.5535860	-2.1291220	-0.2596750
N	1.2072890	0.0326850	0.8292400	H	-2.2725350	-1.9994080	0.9781560
Si	0.9450640	-0.2339740	2.4778750	C	-4.2180570	-1.1415070	1.5773900
C	0.9476500	-2.0787690	2.9487980	C	-4.8333850	0.1196310	0.9687970
H	0.8029420	-2.2354240	4.0296130	C	-3.5989450	0.8113210	0.4001290
H	0.1441020	-2.6180490	2.4200530	H	-3.8065580	1.4524490	-0.4674540
H	1.9036260	-2.5464050	2.6620720	H	-3.0892950	1.4161750	1.1695190
C	-0.7829020	0.4112840	2.9548240	H	-5.5309890	-0.1458330	0.1598890
H	-1.5381780	-0.0392400	2.2889110	H	-5.3693130	0.7415830	1.6969480
H	-1.0583720	0.1723070	3.9940650	H	-3.7476170	-0.9038560	2.5431930
H	-0.8382780	1.5052070	2.8285600	H	-4.9389570	-1.9541090	1.7332540
C	2.1920930	0.6121940	3.6327700	O	-0.9050840	2.2096630	-1.0871480
H	3.2085490	0.2240630	3.4556870	C	-0.2212400	3.0480970	-0.1465210
H	2.2156630	1.6981500	3.4494930	H	-0.9630190	3.5510360	0.4995990
H	1.9503210	0.4482670	4.6948250	H	0.4231590	2.4018360	0.4696350
Na	-0.5695990	0.0244650	-0.5599900	C	0.5235380	4.0552170	-1.0096980
O	-2.7344970	-0.2461180	-0.0112950	C	-0.4824540	4.2837000	-2.1392880
C	-3.1491880	-1.4933770	0.5460960	C	-1.0667510	2.8823130	-2.3342300

H	-1.6133480	-3.5328620	-2.4092490	H	-2.1328400	2.8974330	-2.6071440
H	-1.4341820	-1.9495460	-3.2235340	H	-0.5188550	2.3218740	-3.1104070
C	0.3978770	-3.2096090	-3.2088340	H	-1.2653740	4.9837760	-1.8114850
C	1.2918110	-3.4414160	-1.9676670	H	-0.0328050	4.6814290	-3.0579830
C	0.4275310	-2.9506500	-0.7946880	H	1.4488230	3.6035090	-1.3992240
H	-0.0923210	-3.7946630	-0.3057780	H	0.7888710	4.9706070	-0.4654860
H	0.9660530	-2.3652900	-0.0358310	O	-0.5442310	-2.0920150	-1.3857020
H	1.5731420	-4.4948330	-1.8426960	C	-0.9168940	-2.6972090	-2.6077540
H	2.2179860	-2.8560150	-2.0380590				
H	0.8377570	-2.4476650	-3.8664280				
H	0.2468640	-4.1186620	-3.8049840				
C	3.8684700	-1.2056140	0.0771410				
H	3.3997710	-2.1818730	-0.1248030				
H	4.7263990	-1.0889020	-0.6041310				
H	4.2610370	-1.2421530	1.1065950				
C	2.1189960	0.3340910	-1.9208540				
H	2.9831450	0.4383290	-2.5948380				
H	1.5565030	-0.5634760	-2.2318360				
H	1.4658690	1.2105970	-2.0789060				
C	3.6084720	1.7988420	0.2958920				
H	2.9728670	2.6952830	0.2157890				
H	3.9989130	1.7670500	1.3252850				
H	4.4640330	1.9231060	-0.3871570				

Table S14. Geometric coordinates and single point energies for NaHMDS tetrasolvated monomer with 4 THF.



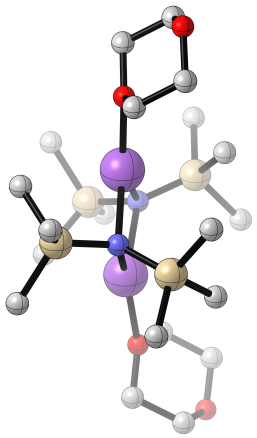
G = -1962.411746

G_{SP} = -1964.727222

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.2720600	-0.0111720	0.0803480	H	-3.7613210	2.0696920	2.8906150
N	-2.0170340	0.1189060	-0.0625900	H	-2.1536430	2.4736830	2.2402500
Si	-2.4618490	0.0729410	-1.6876270	H	-3.5970940	2.6556960	1.2147610
C	-3.3094710	1.6454530	-2.3463720	C	-1.9747930	-0.6463120	2.7777320
H	-2.6641450	2.5306570	-2.2246320	H	-0.9462140	-0.2511650	2.8288730
H	-3.5689330	1.5606150	-3.4138630	H	-2.4490440	-0.4981190	3.7608280
H	-4.2403770	1.8365570	-1.7879140	H	-1.9095340	-1.7305300	2.5887320
C	-0.8650260	-0.1098500	-2.7246020	C	-4.6464450	-0.5151970	1.2957540
H	-1.0566410	-0.2219500	-3.8030850	H	-5.2697780	0.0207480	0.5612480
H	-0.2428030	0.7924000	-2.5899690	H	-4.6015880	-1.5708670	0.9838410
H	-0.2686060	-0.9761650	-2.3892710	H	-5.1582150	-0.4661780	2.2700320
C	-3.6265080	-1.3519880	-2.1711380	O	1.5023480	-0.2997290	1.9895600
H	-3.2742380	-2.3176550	-1.7759410	C	1.6688760	0.7596220	2.9301230
H	-4.6272550	-1.1749590	-1.7461590	H	2.6413130	1.2527810	2.7477890
H	-3.7368360	-1.4447170	-3.2636040	H	0.8715130	1.4990420	2.7686930
Si	-2.9042240	0.2396680	1.3698350	C	1.6351910	0.0943620	4.3029900
C	-3.1293510	2.0262530	1.9891950	C	2.2404100	-1.2754110	3.9934520

C	1.6338570	-1.5699760	2.6251780	H	2.2288740	3.8523470	-1.8526920
H	2.2533750	-2.2211640	1.9915160	H	1.7467050	5.0479180	-0.6424440
H	0.6362810	-2.0306740	2.7171840	O	2.2793230	0.0693820	-1.0340420
H	3.3365820	-1.2015010	3.9206160	C	3.4553060	-0.3707210	-0.3654930
H	1.9952420	-2.0432310	4.7382510	H	3.7431340	0.3693620	0.4033560
H	0.5943590	-0.0206710	4.6404120	H	3.2294720	-1.3145070	0.1483110
H	2.1874200	0.6613030	5.0634330	C	4.5134160	-0.4796810	-1.4564920
O	0.5775490	-2.3113920	-0.2180660	C	4.1154500	0.6809890	-2.3700460
C	-0.6500470	-3.0326200	-0.0781970	C	2.5912190	0.6003960	-2.3183910
H	-0.5807050	-3.7167340	0.7880520	H	2.0942180	1.5767590	-2.4300530
H	-1.4484670	-2.2944690	0.0918820	H	2.1894660	-0.0732360	-3.0944770
C	-0.7823300	-3.8106820	-1.3794300	H	4.4636560	1.6344470	-1.9424040
C	0.6725340	-4.1984990	-1.6474710	H	4.5101760	0.5997450	-3.3906600
C	1.4344110	-2.9658430	-1.1467690	H	4.4105630	-1.4370960	-1.9908390
H	2.3820280	-3.2380940	-0.6523630	H	5.5376900	-0.4076480	-1.0690670
H	1.6648630	-2.2586630	-1.9612300	H	-0.6458180	3.8821870	0.7096380
H	0.9429830	-5.0840690	-1.0532930	H	-1.3458030	2.5097980	-0.2207280
H	0.8822270	-4.4203140	-2.7017620	H	-0.4410450	4.7414660	-1.5914720
H	-1.1601040	-3.1472810	-2.1718820	H	-0.0274020	3.1219380	-2.1969730
H	-1.4589910	-4.6712230	-1.2979850				
O	0.6108770	2.2795930	0.3042880				
C	1.8142520	3.0076400	0.1502200				
H	2.0573390	3.5306640	1.0925620				
H	2.6151280	2.2863340	-0.0629870				
C	1.5668140	4.0223770	-0.9925200				
C	0.0822470	3.8090200	-1.3440600				
C	-0.4548730	3.1369880	-0.0859380				

Table S15. Geometric coordinates and single point energies for NaHMDS disolvated dimer with 2 1,4-dioxane.



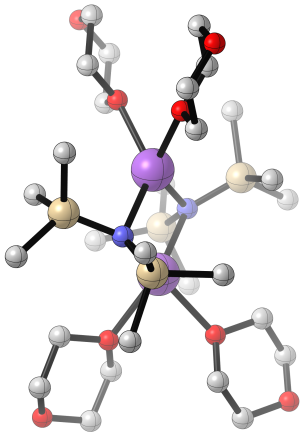
G = -2683.352611

G_{SP} = -2685.913388

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.3707820	-0.4811800	0.3953470	H	-0.9105000	-0.6153650	-2.2509540
N	0.6066370	-1.7173920	0.2881920	H	-1.1525750	-2.1168280	-3.1623740
Na	1.3711110	0.4819420	0.3954630	C	-0.2489080	-4.3521120	-0.9673230
N	-0.6063920	1.7181060	0.2881260	H	-0.4407710	-4.8236530	-1.9440190
Si	-1.1648180	2.3760010	1.7641190	H	0.4918080	-4.9705270	-0.4377960
C	-2.5543860	3.6575490	1.6042740	H	-1.1849610	-4.3855320	-0.3867910
H	-2.8872920	4.0047880	2.5949840	C	1.8546540	-2.5984650	-2.3106820
H	-2.2252770	4.5407430	1.0357600	H	2.6880410	-3.1253440	-1.8173050
H	-3.4299500	3.2358360	1.0861890	H	1.6444140	-3.1167830	-3.2589400
C	-1.8779400	0.9653300	2.8306330	H	2.1917110	-1.5774410	-2.5531780
H	-2.7779040	0.5216180	2.3710140	Si	1.1645470	-2.3753500	1.7643630
H	-1.1426500	0.1584590	2.9969750	C	1.8777910	-0.9648170	2.8309590
H	-2.1729140	1.3321510	3.8254790	H	2.7778960	-0.5213110	2.3714220
C	0.2178570	3.1855630	2.7783450	H	2.1725660	-1.3316690	3.8258520
H	1.0386100	2.4736470	2.9678790	H	1.1426420	-0.1577920	2.9971790
H	0.6381520	4.0420880	2.2277650	C	-0.2185950	-3.1845320	2.7782740

H	-0.1386440	3.5519030	3.7535780	H	0.1375380	-3.5508180	3.7536610
Si	-0.3376420	2.5603520	-1.1735000	H	-1.0392790	-2.4724430	2.9674720
C	1.0667180	1.7039010	-2.1456330	H	-0.6388790	-4.0410450	2.2276680
H	2.0427160	1.8628640	-1.6546970	C	2.5538040	-3.6572810	1.6048550
H	0.9125830	0.6162070	-2.2501480	H	2.2247540	-4.5401500	1.0357960
H	1.1536380	2.1175460	-3.1620170	H	3.4298020	-3.2356380	1.0874470
C	-1.8543310	2.5970110	-2.3115090	H	2.8860270	-4.0050070	2.5956220
H	-2.6881560	3.1237980	-1.8187670	O	-3.5918310	-0.6796450	0.2084260
H	-1.6441030	3.1147690	-3.2600750	C	-4.5606660	-1.7120620	0.2962170
H	-2.1907610	1.5756300	-2.5533700	C	-5.2532170	-1.8902880	-1.0445750
C	0.2473250	4.3530010	-0.9683850	H	-4.5220580	-2.2567240	-1.7913950
H	0.4394000	4.8240900	-1.9452560	H	-6.0653020	-2.6251220	-0.9624070
H	-0.4942560	4.9711140	-0.4397220	O	-5.8170700	-0.6761460	-1.4722630
H	1.1829830	4.3875640	-0.3872860	C	-4.8363730	0.3280360	-1.5843940
O	3.5923520	0.6792670	0.2088110	C	-4.1530620	0.5473380	-0.2479920
C	4.5616300	1.7113090	0.2961050	H	-3.3256510	1.2692770	-0.3256050
C	5.2538990	1.8889990	-1.0449080	H	-4.8842660	0.9100880	0.4972890
H	4.5227000	2.2555980	-1.7916080	H	-4.0787260	0.0399250	-2.3392800
H	6.0663050	2.6235170	-0.9630800	H	-5.3334040	1.2473090	-1.9214260
O	5.8171370	0.6745510	-1.4725290	H	-5.3031900	-1.4468080	1.0699050
C	4.8359770	-0.3292330	-1.5841880	H	-4.0344670	-2.6268050	0.6026240
C	4.1529790	-0.5480210	-0.2475430	Si	0.3376470	-2.5600530	-1.1731650
H	3.3252690	-1.2696570	-0.3247720	C	-1.0656680	-1.7028700	-2.1461170
H	4.8842750	-0.9108960	0.4975870	H	-2.0419990	-1.8607610	-1.6554940
H	4.0782180	-0.0409110	-2.3388850				
H	5.3325000	-1.2487780	-1.9212250				
H	5.3042640	1.4459210	1.0696430				
H	4.0358930	2.6263360	0.6024650				

Table S16. Geometric coordinates and single point energies for NaHMDS disolvated dimer with 4 1,4-dioxane.



G = -3297.480615

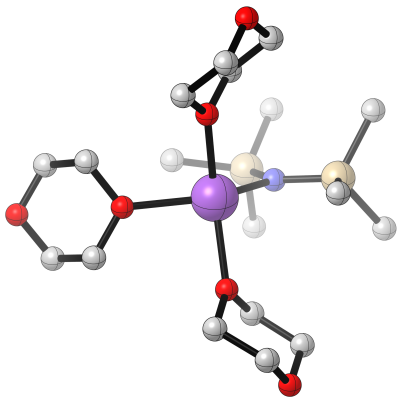
G_{SP} = -3301.000578

Atom	X	Y	Z	Atom	X	Y	Z
Si	0.7553370	-2.7621160	1.2851670	H	3.1017370	-2.5124600	0.4405190
N	-0.0005390	-1.9158720	0.0000310	C	0.9724130	-1.6212540	2.7868870
Na	-1.4480080	0.0002580	0.0000410	H	1.5447510	-0.7129550	2.5360180
Na	1.4476780	-0.0001920	-0.0001530	H	-0.0022040	-1.2942400	3.1812740
N	0.0005870	1.9157590	0.0001590	H	1.5115670	-2.1354070	3.5982980
Si	-0.7553360	2.7604130	1.2863370	C	-0.1407530	-4.3137810	1.9246940
C	-0.9725800	1.6177460	2.7867180	H	-1.1318710	-4.0950080	2.3511420
H	-1.5453840	0.7098990	2.5352080	H	-0.2809900	-5.0577840	1.1252730
H	-1.5113950	2.1313420	3.5987130	H	0.4598260	-4.7888990	2.7164770
H	0.0019530	1.2899690	3.1806640	C	4.3077290	-0.1642070	1.7281560
C	0.1401870	4.3117980	1.9274470	O	3.2200890	0.6445490	1.3126900
H	-0.4610660	4.7860380	2.7192590	C	2.9345170	1.6737960	2.2510300
H	1.1315310	4.0942740	2.3540570	C	4.1740230	2.5145690	2.4909420
H	0.2798640	5.0564500	1.1285060	H	4.4503700	3.0375610	1.5547840
C	-2.5010540	3.3550680	0.8189060	H	3.9852000	3.2656810	3.2694560
H	-2.4503920	4.1103590	0.0174420	O	5.2391550	1.7032130	2.9296550

H	-3.1020480	2.5120100	0.4419300	C	5.5294330	0.7001670	1.9909560
H	-3.0314330	3.8024740	1.6745320	H	5.8693800	1.1574940	1.0393410
Si	0.7568600	2.7621880	-1.2846170	H	6.3501540	0.0917940	2.3944990
C	0.9741130	1.6214490	-2.7864710	H	2.6042280	1.2171880	3.2030310
H	1.5448360	0.7121630	-2.5355140	H	2.1118930	2.2622920	1.8228050
H	-0.0007480	1.2959470	-3.1815700	H	4.4915180	-0.8887000	0.9228110
H	1.5144550	2.1350440	-3.5974320	H	4.0268870	-0.7129150	2.6464590
C	2.5024630	3.3560430	-0.8157560	H	-2.1148970	-2.2672240	1.8165420
H	3.0332290	3.8043680	-1.6706720	C	-2.9359330	-1.6783420	2.2472140
H	2.4516460	4.1104250	-0.0134420	O	-3.2209740	-0.6467240	1.3112980
H	3.1031850	2.5124410	-0.4395820	C	-4.3071400	0.1626930	1.7292690
C	-0.1387780	4.3141390	-1.9240500	C	-5.5297880	-0.7004930	1.9915800
H	-0.2786620	5.0581280	-1.1245440	O	-5.2399970	-1.7057410	2.9280650
H	0.4620450	4.7891320	-2.7157320	C	-4.1764500	-2.5177200	2.4867260
H	-1.1300250	4.0960820	-2.3505630	H	-4.4544510	-3.0384480	1.5497760
Si	-0.7553770	-2.7602010	-1.2869070	H	-3.9879300	-3.2706720	3.2635330
C	-0.9708630	-1.6176310	-2.7876140	H	-5.8712680	-1.1555170	1.0394070
H	-1.5441970	-0.7098080	-2.5372330	H	-6.3492850	-0.0917700	2.3970650
H	0.0043280	-1.2897020	-3.1798590	H	-4.4907330	0.8889000	0.9254080
H	-1.5080680	-2.1314340	-3.6005200	H	-4.0247480	0.7094030	2.6482930
C	0.1397990	-4.3122750	-1.9268480	H	-2.6036650	-1.2242510	3.1997280
H	0.2771660	-5.0571710	-1.1277230	C	-4.3080610	-0.1616660	-1.7275480
H	-0.4609550	-4.7856920	-2.7195540	O	-3.2204280	0.6471560	-1.3121530
H	1.1321090	-4.0963490	-2.3519850	C	-2.9353650	1.6769990	-2.2499740
C	-2.5016020	-3.3545930	-0.8209550	C	-4.1752290	2.5174080	-2.4893860
H	-3.0313300	-3.8022120	-1.6768720	H	-4.4515400	3.0399970	-1.5529830
H	-2.4515350	-4.1097250	-0.0192870	H	-3.9867910	3.2688560	-3.2676690
H	-3.1029920	-2.5115250	-0.4446380	O	-5.2402020	1.7059090	-2.9281330
C	2.5010740	-3.3560240	0.8169050	C	-5.5300120	0.7025360	-1.9896340
H	3.0317840	-3.8039700	1.6720510	H	-5.8696960	1.1595220	-1.0377630
H	2.4504960	-4.1106740	0.0148310	H	-6.3507780	0.0941630	-2.3930800

H	-2.6047660	1.2210760	-3.2021870
H	-2.1131400	2.2658160	-1.8214340
H	-4.4913500	-0.8863970	-0.9223140
H	-4.0275210	-0.7100500	-2.6461460
C	4.3075950	0.1636610	-1.7275980
O	3.2203410	-0.6456280	-1.3121470
C	2.9352110	-1.6748140	-2.2506270
C	4.1750450	-2.5151080	-2.4904930
H	4.4515220	-3.0379850	-1.5542910
H	3.9865600	-3.2663080	-3.2690010
O	5.2398820	-1.7033510	-2.9291480
C	5.5296820	-0.7001380	-1.9905020
H	5.8698900	-1.1572610	-1.0388780
H	6.3500860	-0.0913660	-2.3940880
H	2.6048390	-1.2182250	-3.2026110
H	2.1127870	-2.2637880	-1.8226870
H	4.4911830	0.8881190	-0.9221850
H	4.0263730	0.7123590	-2.6457680

Table S17. Geometric coordinates and single point energies for NaHMDS trisolvated monomer with 3 1,4-dioxane.



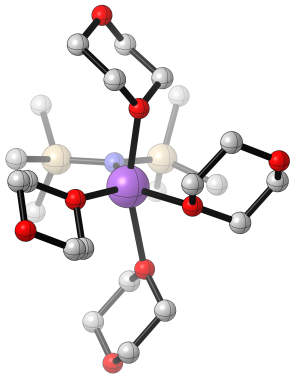
G = -1955.809722

G_{SP} = -1958.034321

Atom	X	Y	Z	Atom	X	Y	Z
Si	2.8447250	0.2469980	-0.0088110	H	1.0119880	-2.2965960	-0.5546940
N	1.4386920	0.1531010	-0.9415870	H	2.2104250	-4.3954060	0.3151990
Si	1.1463650	0.2374380	-2.6047710	H	2.3085420	-2.9899590	1.4150160
C	2.0495170	1.6425310	-3.5067410	H	-1.5174270	-3.7938500	1.6138840
H	1.7366600	1.7236730	-4.5597410	H	-1.4277080	-2.3618950	2.6932080
H	1.8614410	2.6117740	-3.0177100	O	-0.7194430	2.0765170	1.0541430
H	3.1380610	1.4721970	-3.4931080	C	0.0350850	3.0540490	0.3384540
C	-0.7228380	0.5229890	-2.8583170	C	0.8424740	3.8955070	1.3086630
H	-1.0408290	1.4504830	-2.3499900	H	1.3537620	4.7088860	0.7768490
H	-1.0111840	0.6015820	-3.9181730	H	1.6081840	3.2628710	1.7969030
H	-1.2913790	-0.3136730	-2.4171670	O	0.0043490	4.4798040	2.2810640
C	1.5608020	-1.3580260	-3.5504850	C	-0.6957240	3.4966390	2.9968320
H	2.6250750	-1.6137770	-3.4261360	C	-1.5389070	2.6599160	2.0495900
H	0.9690120	-2.2055870	-3.1681240	H	-2.2992890	3.3056200	1.5706690
H	1.3579800	-1.2662050	-4.6293110	H	-2.0490540	1.8406970	2.5765800
Na	-0.3930820	-0.0597720	0.3463490	H	-1.3324060	4.0064120	3.7327920
O	-0.2833460	-2.2470120	1.0138290	H	0.0103350	2.8357460	3.5373210

C	-0.8412880	-3.0338350	2.0499950	H	-0.6637090	3.6995550	-0.2261600
C	0.2563870	-3.7357500	2.8312510	H	0.6797470	2.4961660	-0.3580560
H	-0.1777260	-4.3975000	3.5932240	O	-2.6480080	-0.2317550	0.0481390
H	0.8870910	-2.9791600	3.3381000	C	-3.3834970	-1.4447910	0.0508160
O	1.0338120	-4.5239250	1.9694610	C	-4.1529080	-1.6017250	-1.2488910
C	1.6228120	-3.7310720	0.9626660	H	-4.7833390	-2.5005290	-1.2146070
C	0.5616320	-3.0112160	0.1515670	H	-3.4399510	-1.7022720	-2.0898930
H	-0.0589770	-3.7471620	-0.3928960	O	-4.9950820	-0.4953860	-1.4529940
H	-2.8029600	1.7645260	-0.2828110	C	-4.2464440	0.6955480	-1.5102050
H	-4.9504290	1.5244310	-1.6632360	C	-3.4704760	0.8945670	-0.2198870
H	-3.5402030	0.6657790	-2.3604230	H	-4.1755290	1.0365670	0.6208690
H	-4.0912580	-1.4414470	0.9008410				
H	-2.6548810	-2.2548240	0.1862270				
C	3.8100420	1.8775740	-0.1714440				
H	3.1701050	2.7518230	0.0281240				
H	4.6635750	1.9178200	0.5240370				
H	4.2030850	1.9898960	-1.1939710				
C	2.3443580	0.1097160	1.8294760				
H	3.2073850	0.1448220	2.5120160				
H	1.6699710	0.9408380	2.1000970				
H	1.8011590	-0.8311990	2.0198270				
C	4.1206680	-1.1188010	-0.3581470				
H	3.6643960	-2.1210810	-0.3379590				
H	4.5434650	-0.9776290	-1.3662020				
H	4.9561620	-1.1075890	0.3596990				

Table S18. Geometric coordinates and single point energies for NaHMDS tetrasolvated monomer with four 1,4-dioxane.



G = -2262.873732

G_{SP} = -2265.576913

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.1379700	-0.0711340	-0.0513110	C	1.2668190	-4.4568020	-0.1095780
N	-2.1502000	0.1134270	0.1806310	C	1.0395830	-3.3239270	-1.0987110
Si	-2.7325440	0.0667450	1.7726150	H	0.6462820	-3.7369630	-2.0472420
C	-3.4534610	-1.6134180	2.3143110	H	1.9728070	-2.7838570	-1.3126750
H	-2.6762220	-2.3951620	2.3270160	H	1.9246420	-5.2219710	-0.5445480
H	-3.8763730	-1.5556850	3.3299840	H	1.7550250	-4.0506030	0.7988590
H	-4.2527920	-1.9460100	1.6342060	H	-1.5515250	-3.4552660	-1.1821060
C	-1.2799430	0.3638940	2.9636610	H	-1.7853570	-2.2505830	0.1317860
H	-1.5777180	0.3286590	4.0228960	O	1.8088180	-0.2255750	-1.6877160
H	-0.5124330	-0.4126750	2.8020870	C	2.9461270	0.6121020	-1.5700730
H	-0.8185870	1.3454200	2.7692700	C	2.8817020	1.7447540	-2.5789690
C	-4.0761290	1.3466080	2.1794980	H	3.8018910	2.3440510	-2.5460860
H	-3.7418450	2.3719740	1.9559660	H	2.0205950	2.3921820	-2.3283000
H	-4.9795450	1.1562600	1.5771850	O	2.7502480	1.2354400	-3.8829100
H	-4.3688330	1.3077840	3.2406660	C	1.5920470	0.4442220	-3.9937810
Si	-3.0869560	0.0565250	-1.2312630	C	1.6434110	-0.7115710	-3.0105360
C	-4.5152880	-1.1993320	-1.2057210	H	2.4939030	-1.3717990	-3.2671710

H	-5.0347750	-1.2381020	-2.1763300	H	0.7115480	-1.2921510	-3.0224740
H	-4.1570180	-2.2145210	-0.9712090	H	1.5388520	0.0706580	-5.0250360
H	-5.2596290	-0.9264910	-0.4399830	H	0.6912120	1.0570000	-3.7958200
C	-1.9794040	-0.4389530	-2.7028690	H	3.8594320	0.0107040	-1.7477800
H	-1.5476170	-1.4386350	-2.5311830	H	2.9517630	0.9902690	-0.5388680
H	-2.5307070	-0.4583200	-3.6556980	O	1.9733090	-0.0543190	1.4893070
H	-1.1425510	0.2707800	-2.8175810	C	2.1167900	0.4609260	2.8048750
C	-3.8989660	1.7077380	-1.7231640	C	3.5761790	0.7680630	3.0872860
H	-4.4884320	2.1079270	-0.8829070	H	3.7046530	1.1071340	4.1237720
H	-3.1595660	2.4744300	-2.0040500	H	3.9262170	1.5737940	2.4098760
H	-4.5777890	1.5775290	-2.5811280	O	4.3649270	-0.3825380	2.9143020
O	0.6501460	2.2007600	-0.2554230	C	4.2332910	-0.8937280	1.6123580
C	1.4282240	3.1234090	0.4784580	C	2.7791990	-1.2069040	1.3017770
C	0.5503450	3.9106480	1.4387620	H	2.4222710	-2.0127910	1.9695480
H	1.1378130	4.6855510	1.9508290	H	2.6477010	-1.5165600	0.2561150
H	0.1346320	3.2219280	2.2007210	H	4.8441320	-1.8043290	1.5488720
O	-0.4877100	4.5478650	0.7453820	H	4.6188760	-0.1618150	0.8751840
C	-1.2723150	3.6156370	0.0293070	H	1.7446930	-0.2798170	3.5345510
C	-0.4067600	2.8511680	-0.9517200	H	1.4879350	1.3576590	2.8764900
H	0.0258310	3.5418030	-1.7010380	C	-0.8707200	-4.1448390	0.7412490
H	-0.9896320	2.0711610	-1.4562200	H	-1.8014760	-4.6855640	0.9575620
H	-2.0569400	4.1772100	-0.4942160	H	-0.4895080	-3.7114510	1.6877920
H	-1.7487270	2.8845790	0.7090250	O	0.0555080	-5.0774740	0.2279290
H	1.9269710	3.8227980	-0.2208130				
H	2.1965480	2.5460840	1.0134360				
O	0.1162860	-2.3909920	-0.5749280				
C	-1.1184250	-3.0324990	-0.2563730				