SUPPORTING INFORMATION

Aggregation and Solvation of Sodium Hexamethyldisilazide Across the Solvent Spectrum

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I. NMR Spectroscopic Data and Computed Free Energies

II. Computations: Coordinates and Energies

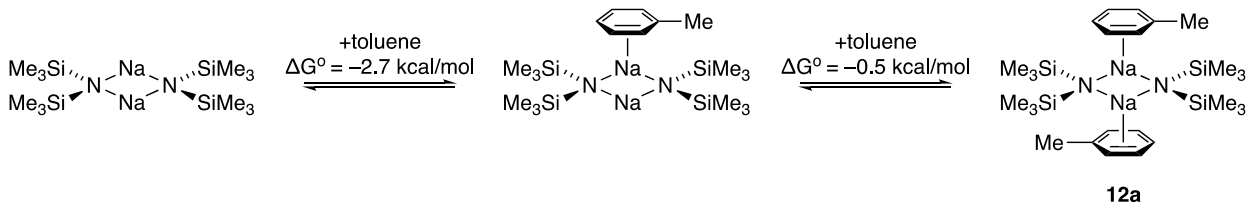
Table S1. Spectroscopic and computational data for NaHMDS dimers and monomers in different solvents.

Entry	Solvent	Structure (A_mS_n (#))	^{13}C-Si shifts (ppm)	^{15}N shifts (ppm)	^{29}Si shifts (ppm ($^1J_{N\text{-}Si}$))	Solvation Energy per S–Na (kcal/mol)
a	toluene	A_2S_2 (**12a**)	6.8	47.0	–14.4 (7.9)	–1.6
b	benzene	A_2S_2 (**12b**)	6.9	47.0	–14.2 (7.8)	–2.3
c	styrene	A_2S_2 (**12c**)	6.8	47.5	–14.3 (7.8)	–1.5
d	DMEA	A_2S_2 (**12d**)	6.5	46.2	–15.7 (8.7)	–5.9
e	Et_3N	A_2S_2 (**12e**)	6.5	46.6	–14.5 (7.6)	–4.1
f	*N*-Me-pyrrolidine	A_2S_2 (**12f**)	–	–	–15.5 (8.7)	–6.7
g	pyridine	A_2S_2 (**12g**)	6.6	44.4	–15.4 (8.8)	–7.3
		AS_3 (**13g**)	6.8	47.6	–20.7 (13.0)	–5.5
h	pyrrolidine	A_2S_2 (**12h**)	–	–	–15.5 (9.2)	–8.6
		AS_4 (**13h**)	–	–	–19.7 (11.1)	–7.4
i	Et_2O	A_2S_2 (**12i**)	6.4	49.4	–15.5 (8.3)	–5.0
j	MTBE	A_2S_2 (**12j**)	6.8	47.4	–15.6 (8.8)	–7.7
k	1,4-dioxane	A_2S_2 (**12k**)	–	–	–	–6.5
		AS_3 (**13k**)	–	–	–	–6.0
l	1,3-dioxolane	A_2S_2 (**12l**)	–	–	–16.0 (8.6)	–
		AS_4 (**13l**)	–	–	–21.1 (13.0)	–
m	THF	A_2S_2 (**12m**)	6.3	45.3	–15.8 (8.7)	–6.7
		AS_4 (**13m**)	6.5	49.0	–21.7 (13.3)	–5.5
n	HMPA	A_2S_2 (**12n**)	–	–	–16.5 (9.8)	–13.6
		AS_3 (**13n**)	–	–	–23.7 (13.4)	–11.46
o	DMPU	A_2S_2 (**12o**)	–	–	–16.4	–10.9
		AS_2 (**13o**)	–	–	–22.5 (13.6)	–13.1
p	DMF	A_2S_4 (**12p**)	–	–	–	–8.2
		AS_4 (**13p**)	–	–	–22.4 (13.7)	–9.3
q	DMSO	A_2S_4 (**12q**)	–	–	–	–6.5
		AS_3 (**13q**)	–	–	–20.0 (12.4)	–10.1
r	TMEDA	A_2S_2 (**12r**)	8.7	–	–14.2 (5.8)	–7.4
		AS_2 (**13r**)	8.1	–	–21.0 (11.3)	–9.5
s	(*R,R*)-TMCDA	A_2SS' (**15s**)	–	–	–15.7 (7.7) –14.7 (7.1)	–11.0
t	(–)-sparteine (**25**)	–	–	–	–	–

u	bipy	A_2S (**26u**)	–	–	–16.2 (8.8)	–
			–	–	–20.5 (12.5)	–
		A_2S_2 (**12u**)	–	–	–15.5 (7.8)	–13.2
v	DME	A_2S_2 (**12v**)	–	–	–14.8 (7.6)	–9.6
		AS_2 (**13v**)		46.5	–21.4 (13.7)	–11.7
w	PMDTA	AS **(13w)**	7.8	48.8	–22.7 (13.7)	–25.7
x	diglyme	AS (**13x**)	6.5	49.7	–21.3 (12.7)	–23.4
y	12-crown-4	AS (**13y**)	–	–	–22.4 (13.7)	–18.7
z	15-crown-5	AS (**13z**)	–	–	–22.1 (13.0)	–29.4
aa	18-crown-6	A_2S (**16aa**)	–	–	–22.3 (13.6)	–
		AS (**13aa**)	–	–	–21.6 (12.3)	–28.8
bb	TDA-1 (**31**)	A_2S (**16bb**)	–	–	–20.5 (13.5)	–
		AS (**13bb**)	–	–	–19.7 (12.8)	–23.8
cc	[2.2.2]crypt (**32**)	A_2S (**16cc**)	–	–	–20.5 (13.5)	–
		AS (**14cc**)	–	–	–27.2	–

I. NMR Spectroscopic Data and Computed Free Energies

Toluene (entry a):



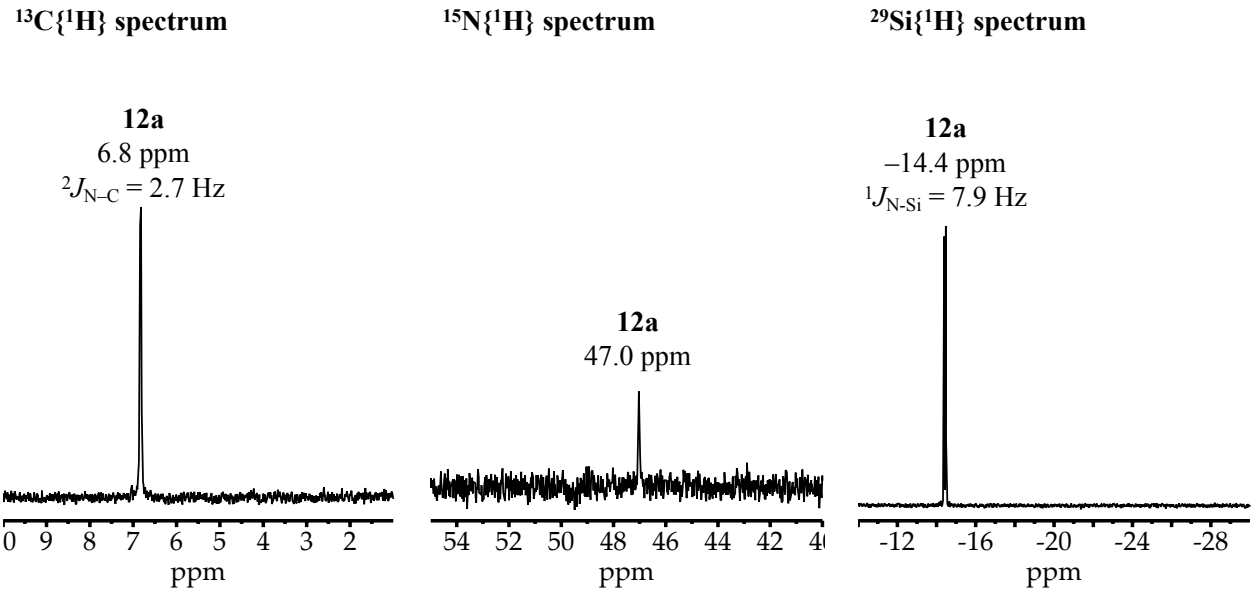
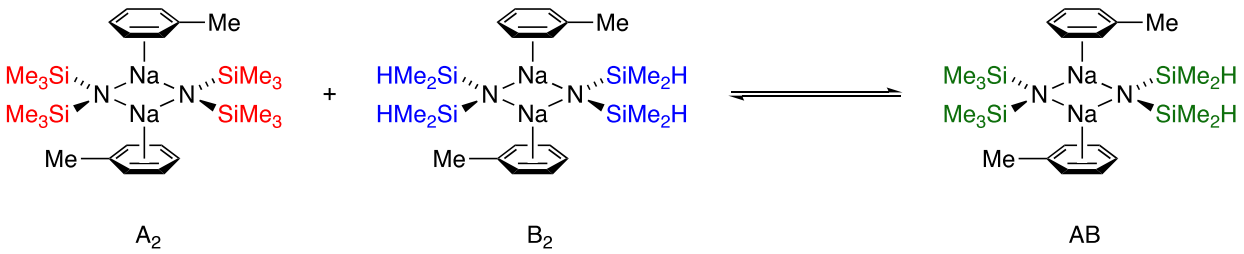


Figure S1. NMR spectra of 0.10 [^{15}N]NaHMDS in 2:1 pentane/toluene-d_8 at 25 °C. ^{13}C{^{1}H} and ^{29}Si spectra are referenced to a TMS internal standard (TMS chemical shift = 0.0 ppm for each). Standard ^{13}C, ^{15}N, and ^{29}Si spectra were recorded on a 500 MHz spectrometer at 125.79, 50.66, and 99.36 MHz, respectively.



A_2 B_2 AB

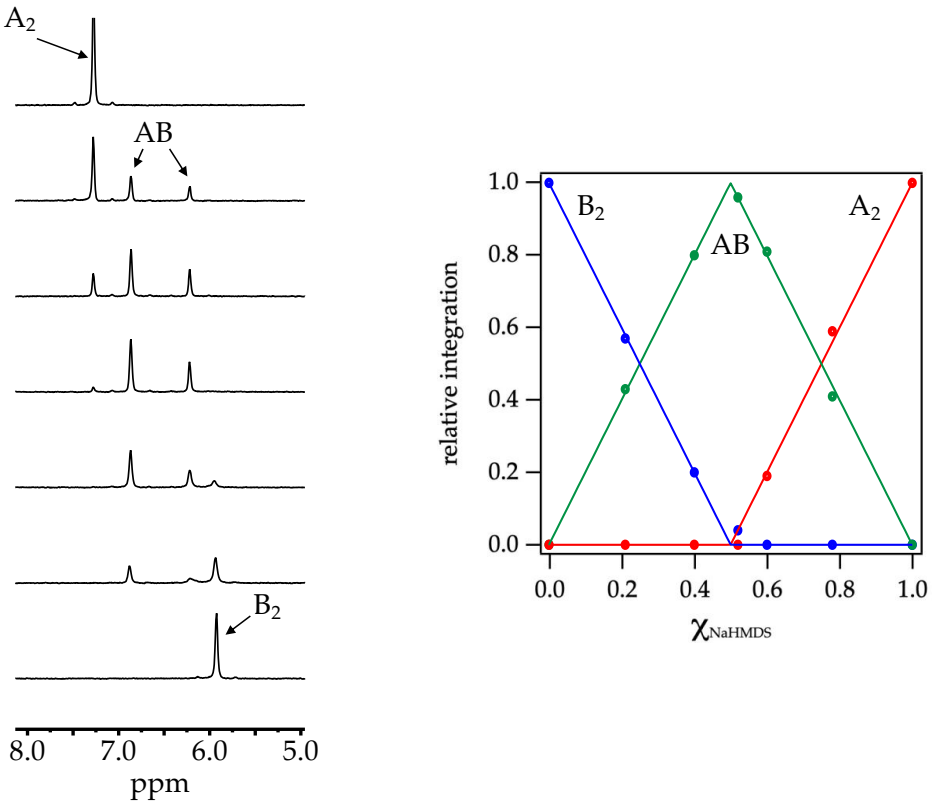


Figure S2. $^{13}C\{^1H\}$ NMR (125.79 MHz, toluene) spectra and affiliated Job plot showing relative integrations of NaHMDS-derived homodimer (A_2, red), NaTMDS-derived homodimer (B_2, blue), and heterodimer (AB, green) versus the measured mole fraction of NaHMDS (X_{NaHMDS}) at 0.30 total molarity in neat toluene at −80 °C.

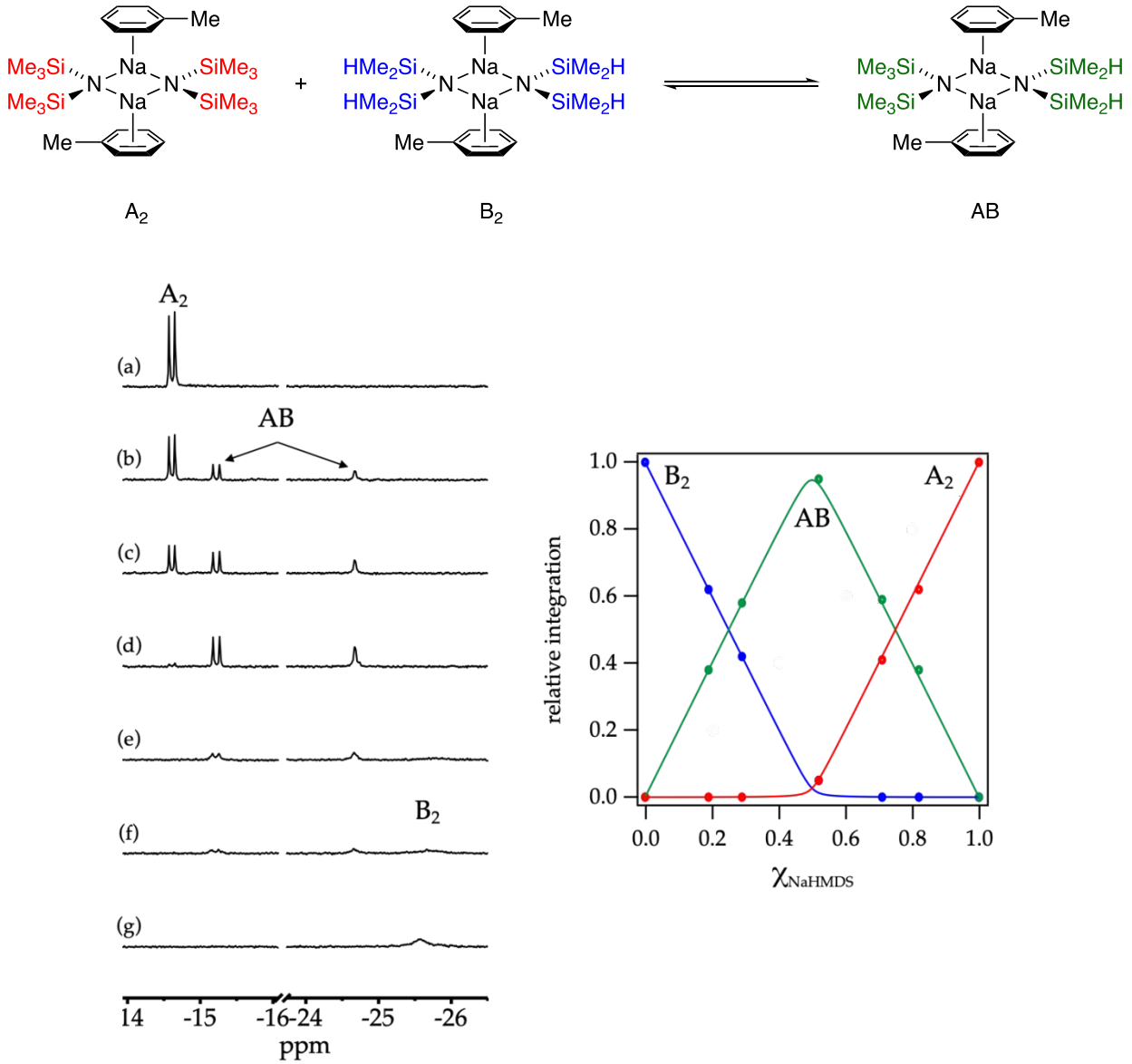
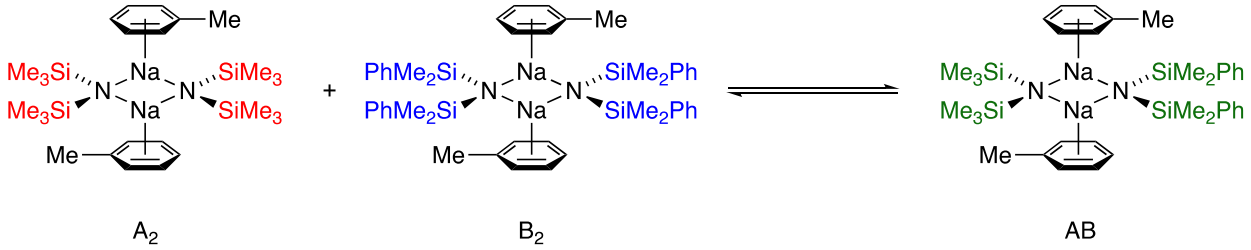
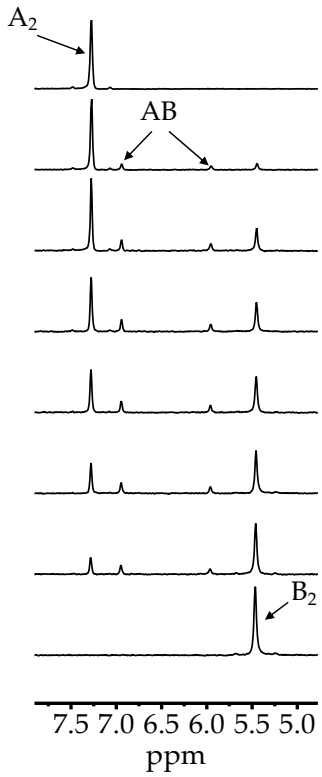


Figure S3. $^{29}Si\{^{1}H\}$ NMR (99.36 MHz, toluene) spectra and affiliated Job plot showing relative integrations of NaHMDS-derived homodimer (A_2, red), NaTMDS-derived homodimer (B_2, blue), and heterodimer (AB, green) versus the measured mole fraction of NaHMDS (X_{NaHMDS}) at 0.20 total molarity 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.



A_2 B_2 AB



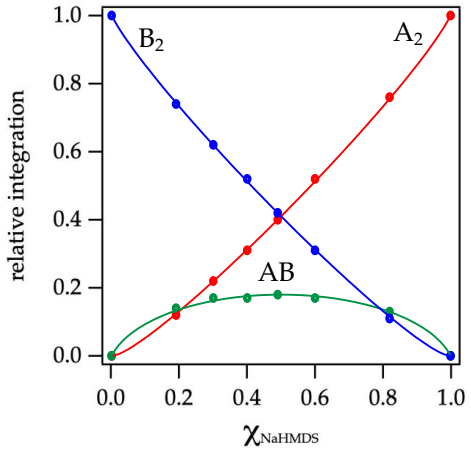
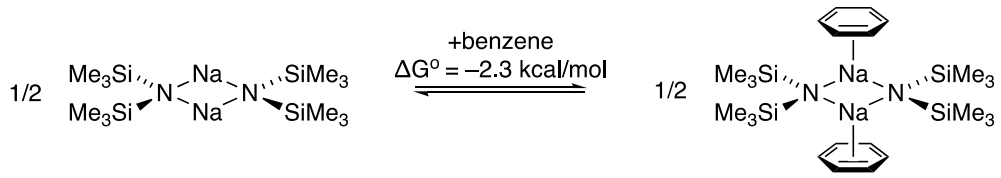


Figure S4. Job plot showing relative integrations of the $^{13}C\{^1H\}$ (125.79 MHz, toluene) resonances of NaHMDS homodimer (A_2, red), NaDPTMDS-derived homodimer (B_2, blue), and heterodimer (AB, green) versus the measured mole fraction of NaHMDS (X_{NaHMDS}) at 0.30 total molarity in neat toluene at −80 °C.

Benzene (entry b):



12b

$^{13}C\{^{1}H\}$ spectrum **$^{15}N\{^{1}H\}$ spectrum** **$^{29}Si\{^{1}H\}$ spectrum**

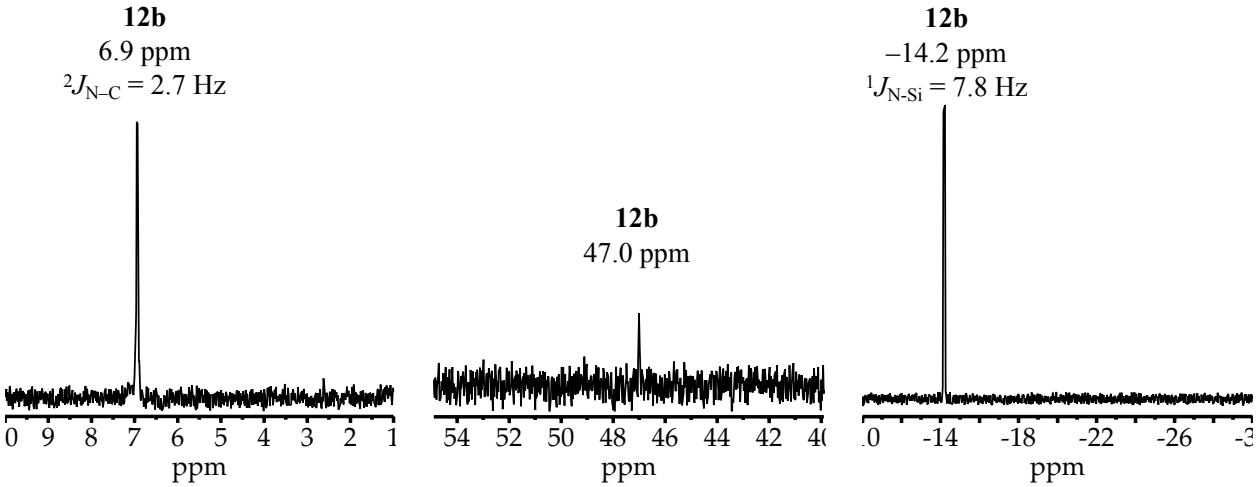


Figure S5. NMR spectra of 0.10 [^{15}N]NaHMDS in benzene at 25 °C. (TMS chemical shift = 0.0 ppm for each). Standard ^{13}C, ^{15}N, and ^{29}Si spectra were recorded on a 500 MHz spectrometer at 125.79, 50.66, and 99.36 MHz, respectively.

Styrene (entry c):

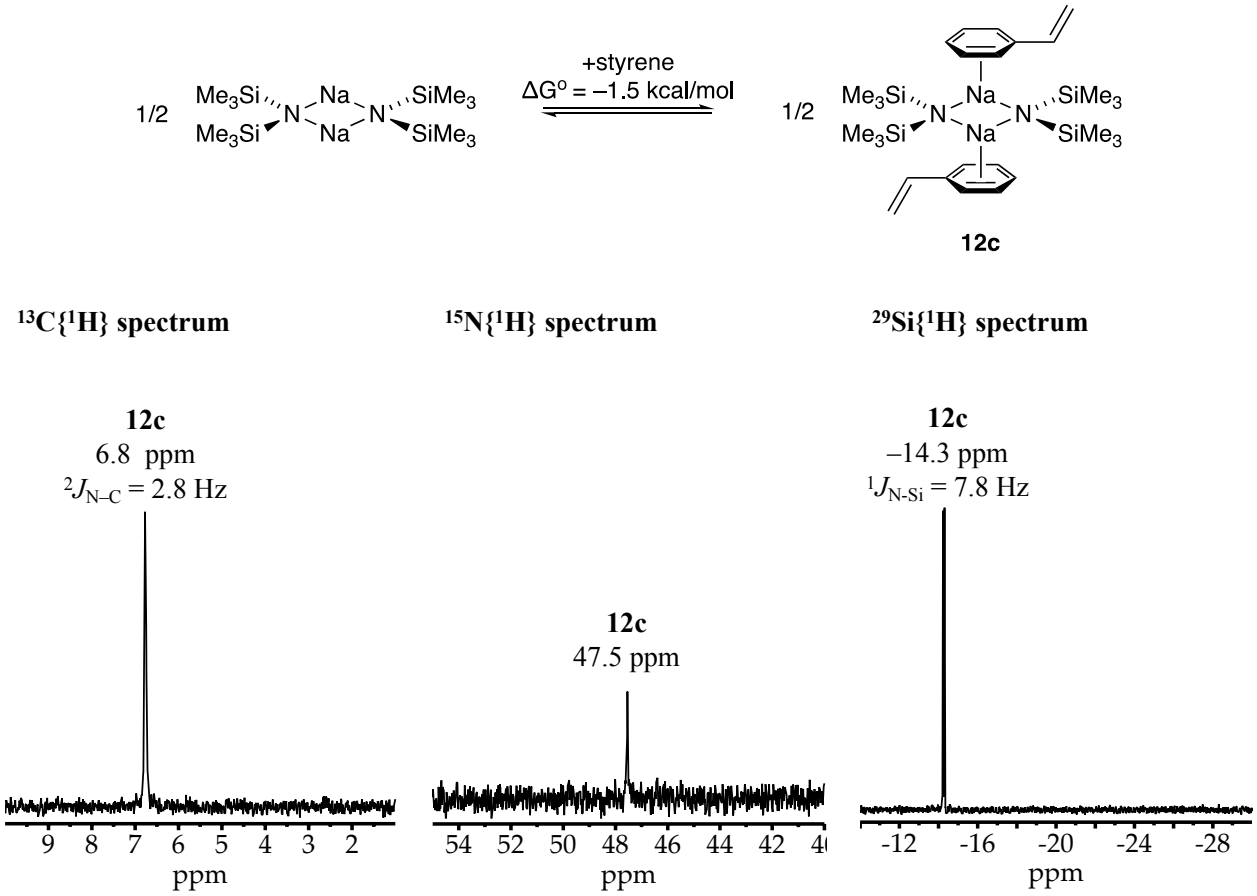
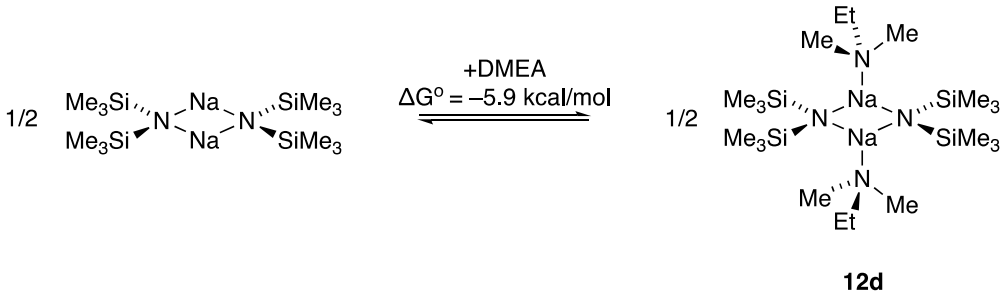


Figure S6. NMR spectra of 0.10 M [^{15}N]NaHMDS in styrene at 25 °C. (TMS chemical shift = 0.0 ppm for each). Standard ^{13}C, ^{15}N, and ^{29}Si spectra were recorded on a 500 MHz spectrometer at 125.79, 50.66, and 99.36 MHz, respectively.

DMEA (entry d):



12d

^{29}Si{^{1}H} spectrum **^{13}C{^{1}H} spectrum** **^{15}N{^{1}H} spectrum**

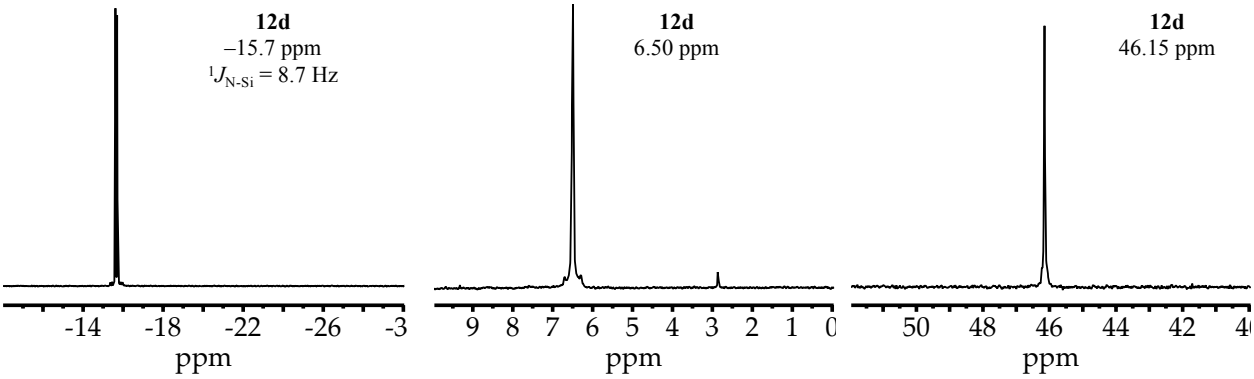
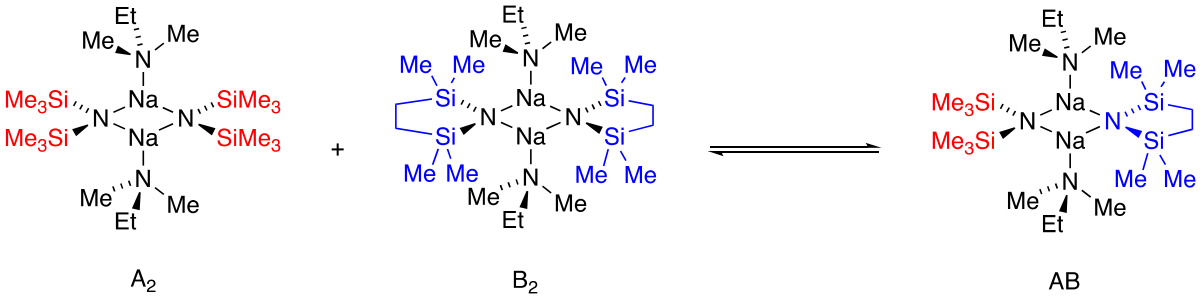


Figure S7. NMR spectra of [^{15}N]NaHMDS in neat DMEA at –120 °C. Concentrations vary from 0.20 M NaHMDS (^{15}N and ^{29}Si) to 0.30 M NaHMDS (^{13}C). ^{13}C{^{1}H} spectrum is referenced to cyclopentane internal standard (26.05 ppm). ^{15}N is referenced to DMEA (25.70 ppm). ^{29}Si is referenced to TMS internal standard (0.00 ppm). Standard ^{13}C, ^{15}N, and ^{29}Si spectra were recorded on a 500 MHz spectrometer at 125.79, 50.66, and 99.36 MHz, respectively.



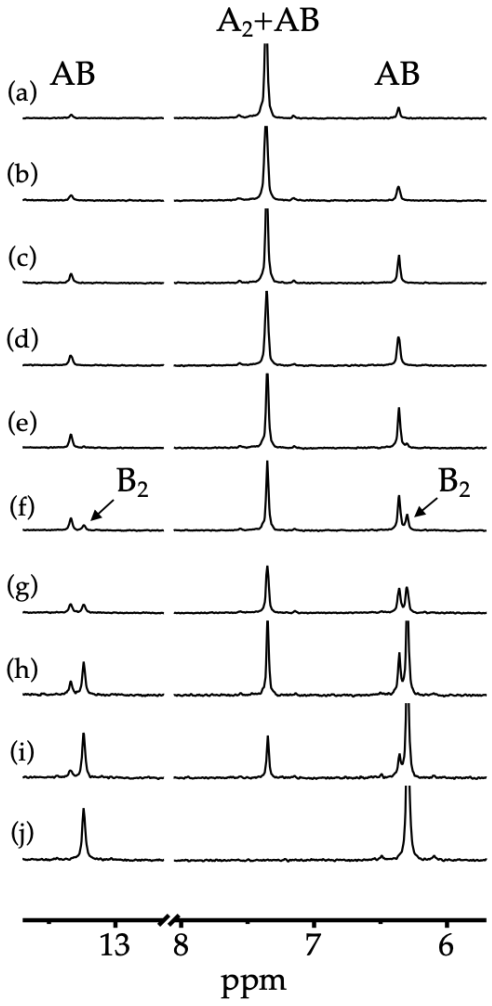


Figure S8. $^{13}C\{^{1}H\}$ NMR (125.79 MHz, toluene) spectra of with mixing NaHMDS and cyclopentyl-derived sodium disilazide **20** at 0.10 total molarity in 0.15 M DMEA in toluene-d_8 cosolvent at –80 °C. Addition of DMEA was necessary to dissolve **20** which is insoluble in neat toluene. $^{13}C\{^{1}H\}$ spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).

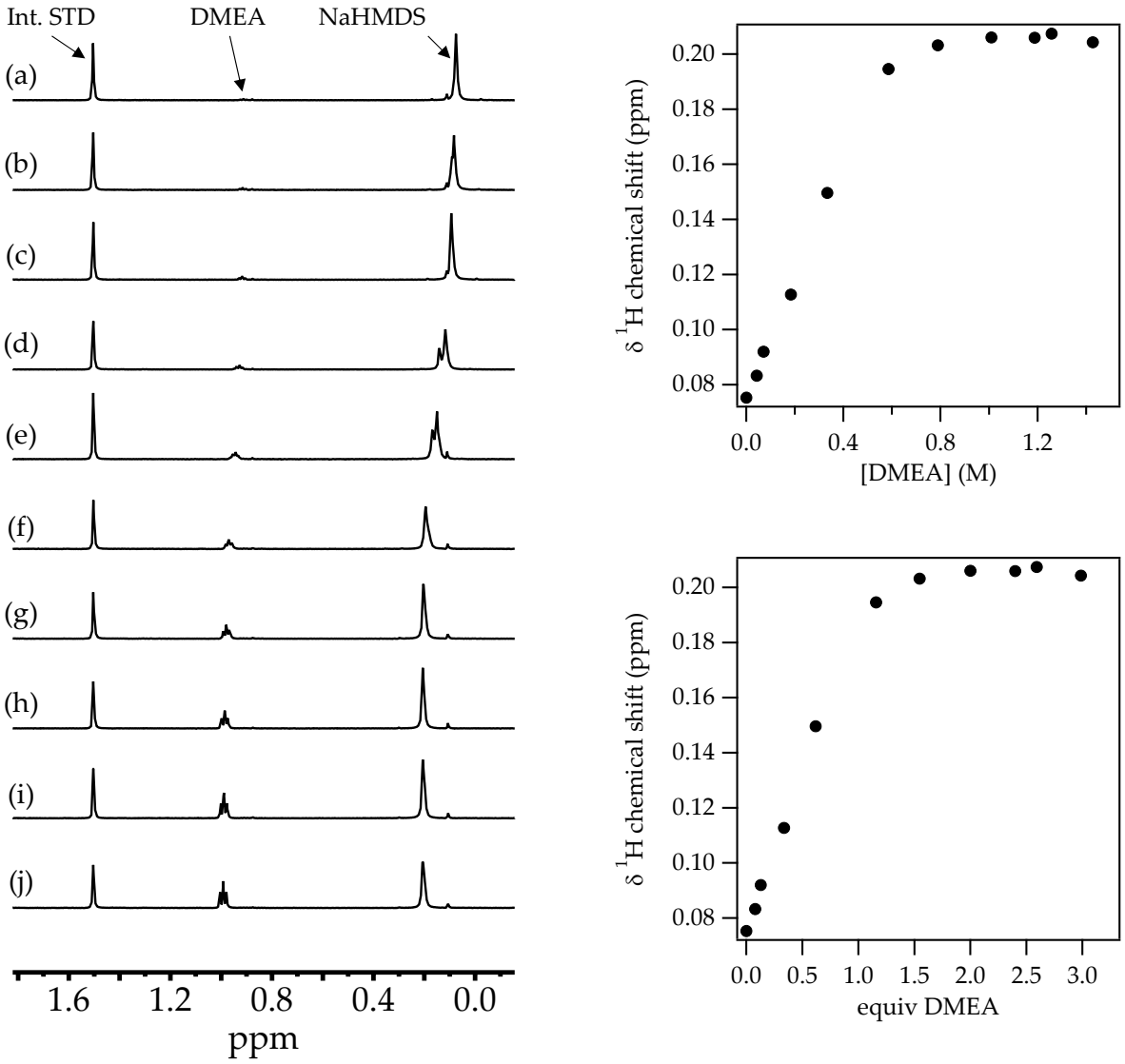
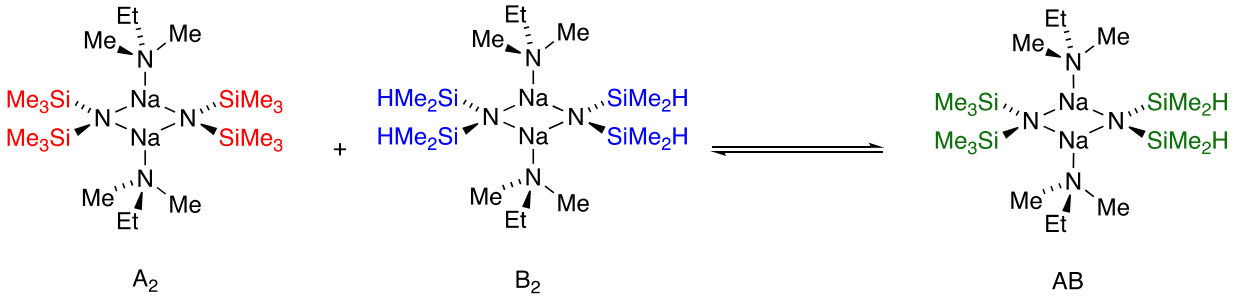


Figure S9. ^{1}H NMR (500 MHz, toluene) spectra for 0.56 M solutions of NaHMDS in toluene with cyclopentane internal standard varying DMEA at 25 °C. The equivalents of THF in (a)–(j) are 0.00, 0.08, 0.13, 0.34, 0.61, 1.15, 1.54, 2.00, 2.40, 2.59, and 2.98, respectively. Plots of chemical shift affiliated with 0.56 M solutions of NaHMDS in toluene with cyclopentane internal standard (1.51 ppm) varying DMEA at 25 °C.



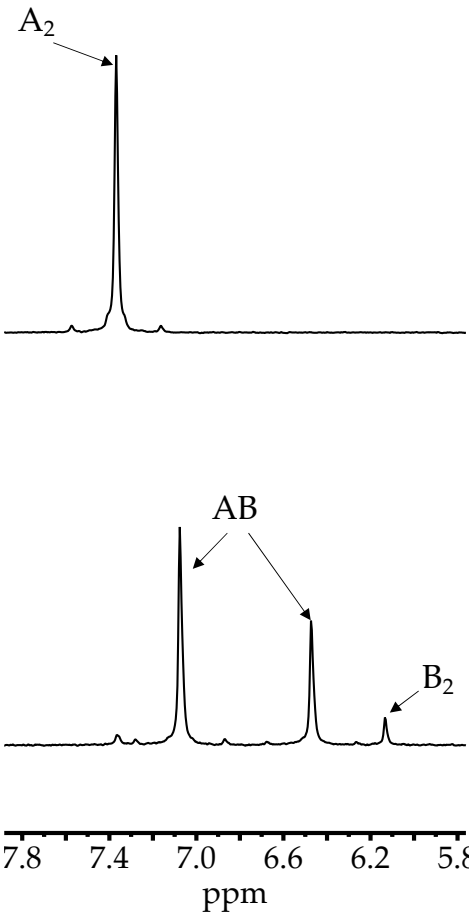
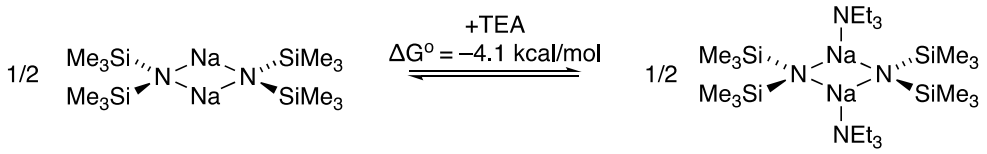


Figure S10. $^{13}C\{^{1}H\}$ NMR (125.79 MHz, toluene) spectra of mixing NaHMDS and NaTMDS at 0.20 total molarity in 0.50 M DMEA in toluene-d_8 cosolvent at –80 °C. The measured mole fractions, X_{NaHMDS}, in (a) and (b) are 1.00 and 0.51, respectively. $^{13}C\{^{1}H\}$ spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).

Triethylamine (entry e):



12e

^{29}Si{^{1}H} spectrum **^{13}C{^{1}H} spectrum** **^{15}N{^{1}H} spectrum**

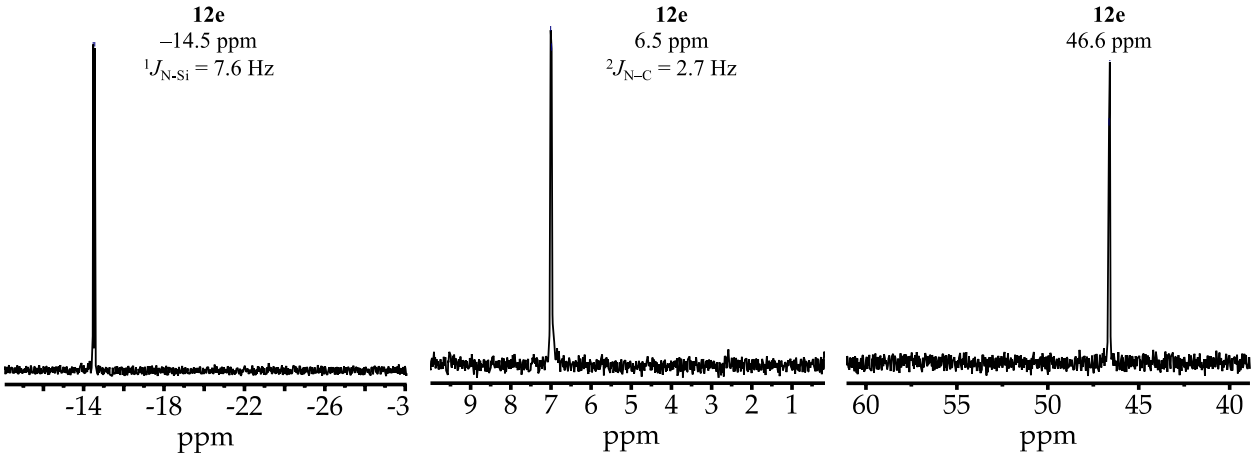


Figure S11. NMR spectra of 0.10 M [^{15}N]NaHMDS in neat triethylamine at 25 °C. ^{13}C{^{1}H} and ^{29}Si spectra are referenced to TMS internal standard (0.00 ppm). Standard ^{13}C, ^{15}N, and ^{29}Si spectra were recorded on a 500 MHz spectrometer at 125.79, 50.66, and 99.36 MHz, respectively.

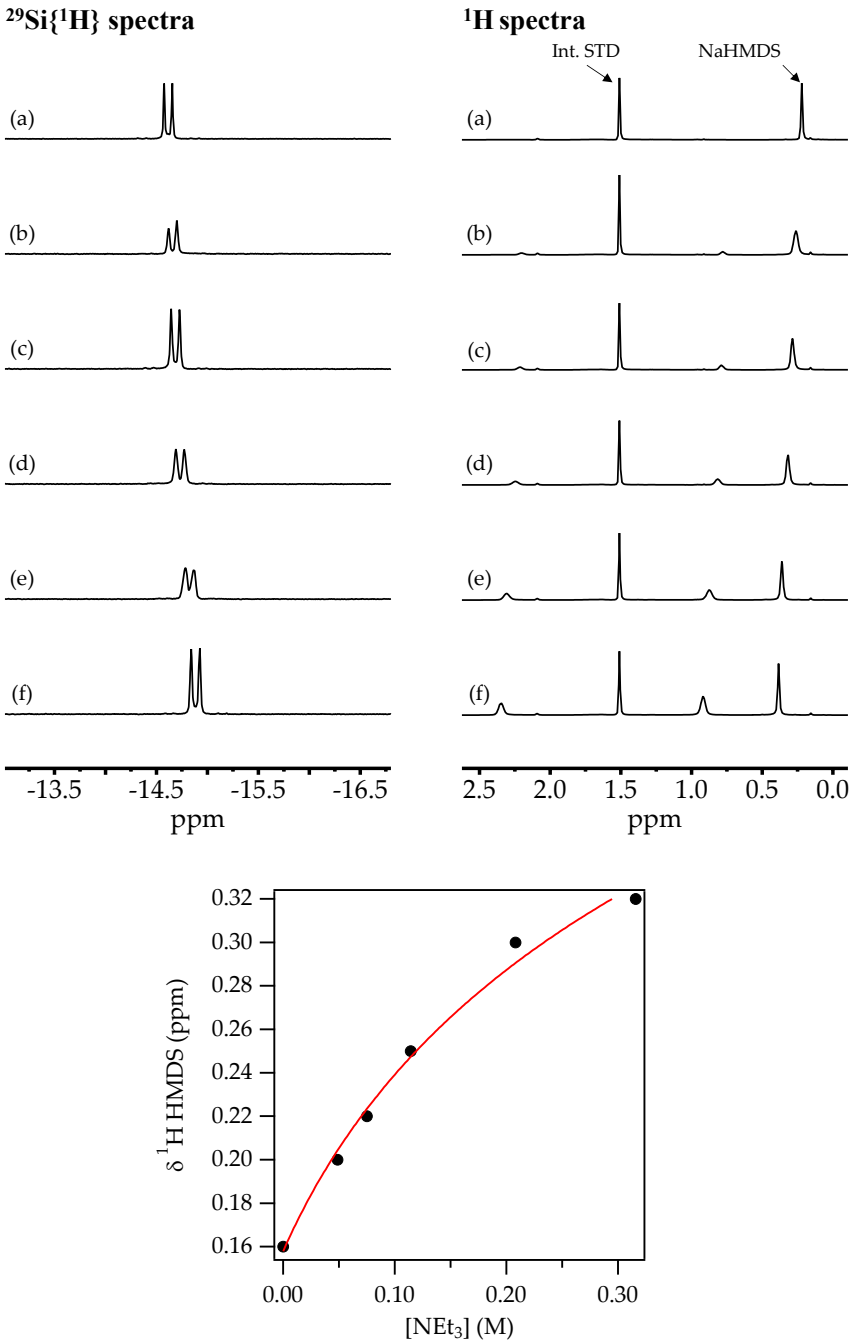


Figure S12. ^{1}H (500 MHz, toluene) and ^{29}Si NMR (99.36 MHz, toluene) spectra for 0.19 M solutions of NaHMDS in toluene with cyclopentane internal standard (1.51 ppm) varying triethylamine concentration at –80 °C. The concentration of triethylamine in (a)–(f) are 0.00, 0.05, 0.08, 0.11, 0.21, and 0.31, respectively. The plot shown corresponds to the spectra above.

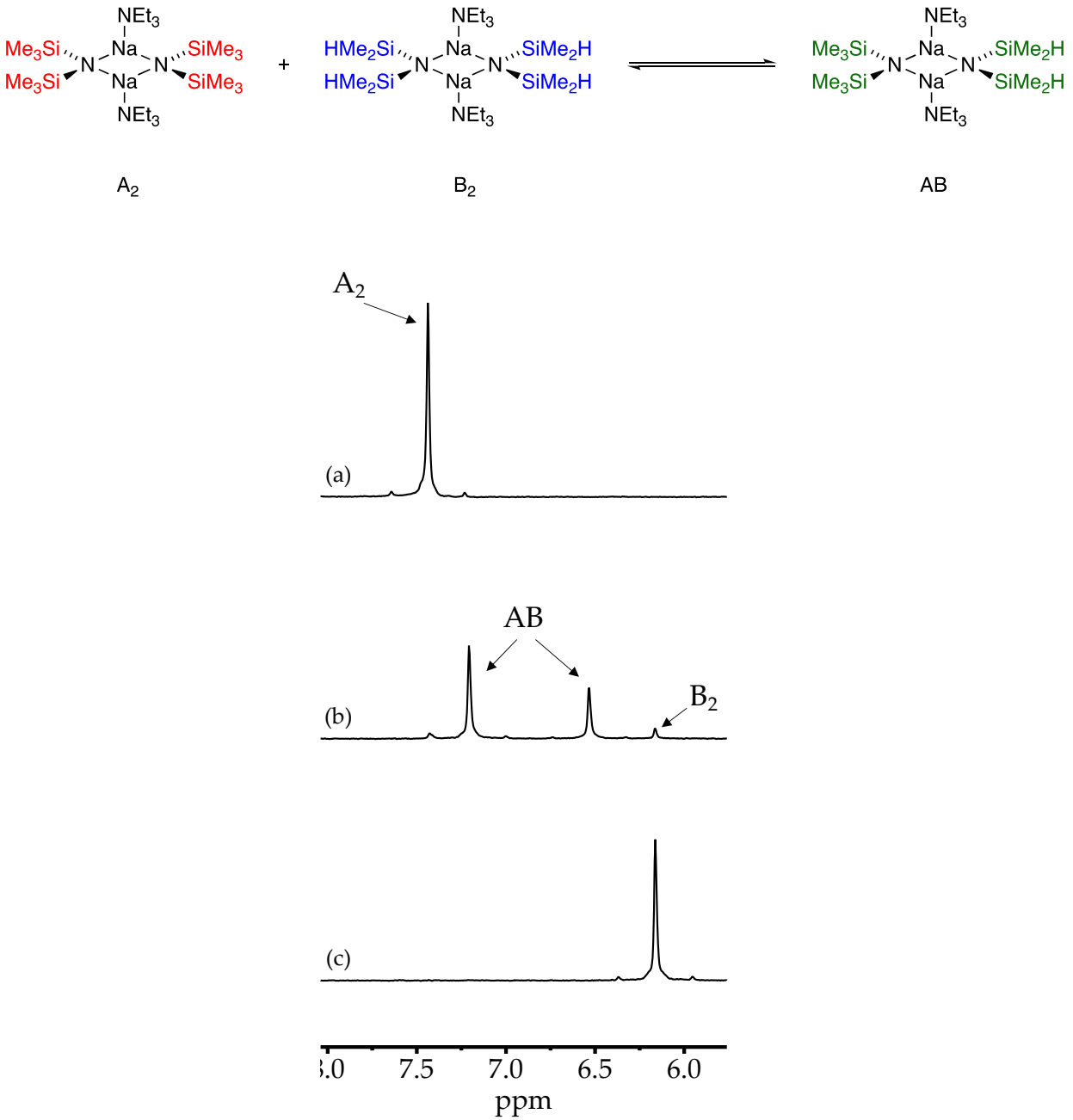


Figure S13. $^{13}C\{^1H\}$ NMR (125.79 MHz, toluene) spectra of with mixing NaHMDS and NaTMDS at 0.20 total molarity in 0.50 M triethylamine in toluene-d_8 cosolvent at –80 °C. The measured mole fractions, X_{NaHMDS}, in (a)–(c) are 1.00, 0.50, and 0.00, respectively. $^{13}C\{^1H\}$ spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).

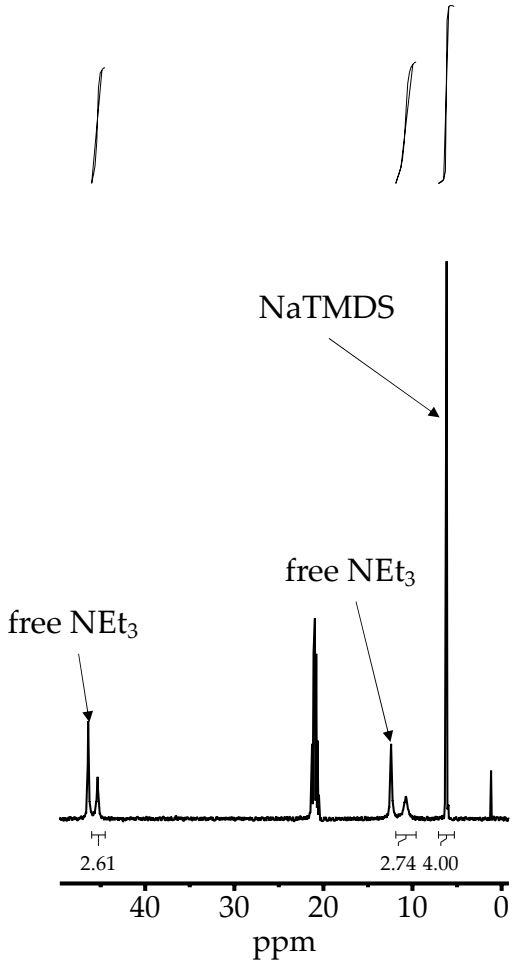


Figure S14. $^{13}C\{^{1}H\}$ NMR (125.79 MHz, toluene) spectra of NaTMDS at 0.20 total molarity in 0.50 M triethylamine in toluene-d_8 cosolvent at –100 °C. Free and bound triethylamine are observed at this temperature. Relative integrations so a 1:1 stoichiometry of triethylamine to NaTMDS. $^{13}C\{^{1}H\}$ spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).

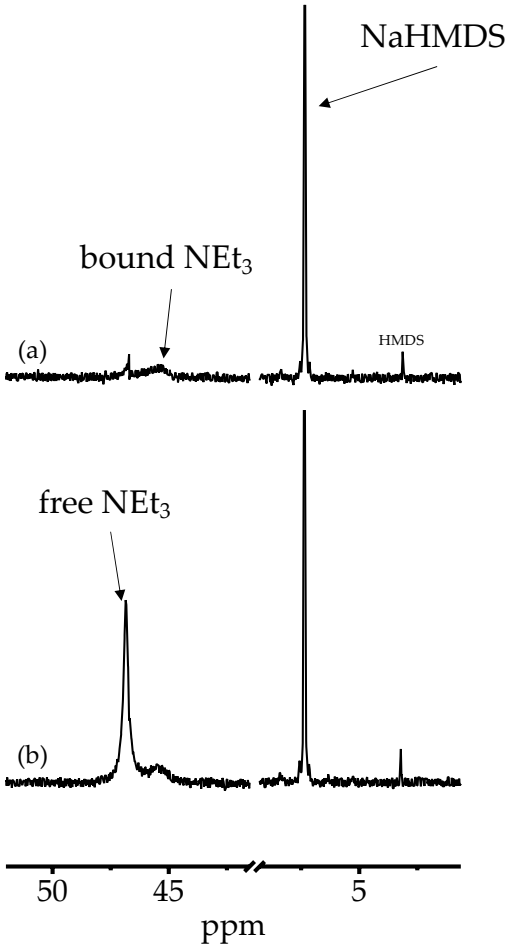
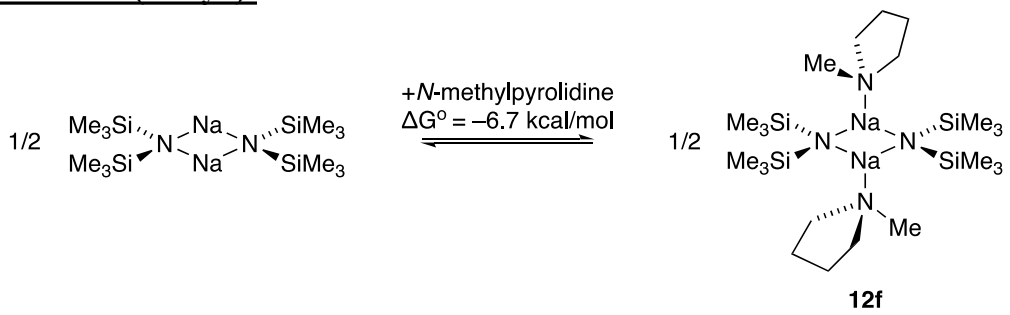


Figure S15. $^{13}C\{^{1}H\}$ NMR (125.79 MHz, toluene) spectra of [^{15}N]NaHMDS at 0.10 M in 2:1 pentane/toluene-d_8 cosolvent with varying amounts of triethylamine added at –120 °C. The concentration of triethylamine in (a) and (b) are 0.15 M and 0.44 M, respectively. Free and bound triethylamine are observed at this temperature. Accurate relative integrations between NaHMDS and bound triethylamine were unable to be obtained, but over 1.0 equiv of triethylamine added the peak corresponding to free triethylamine grows. $^{13}C\{^{1}H\}$ spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).

_N_-Me-pyrrolidine (entry f):



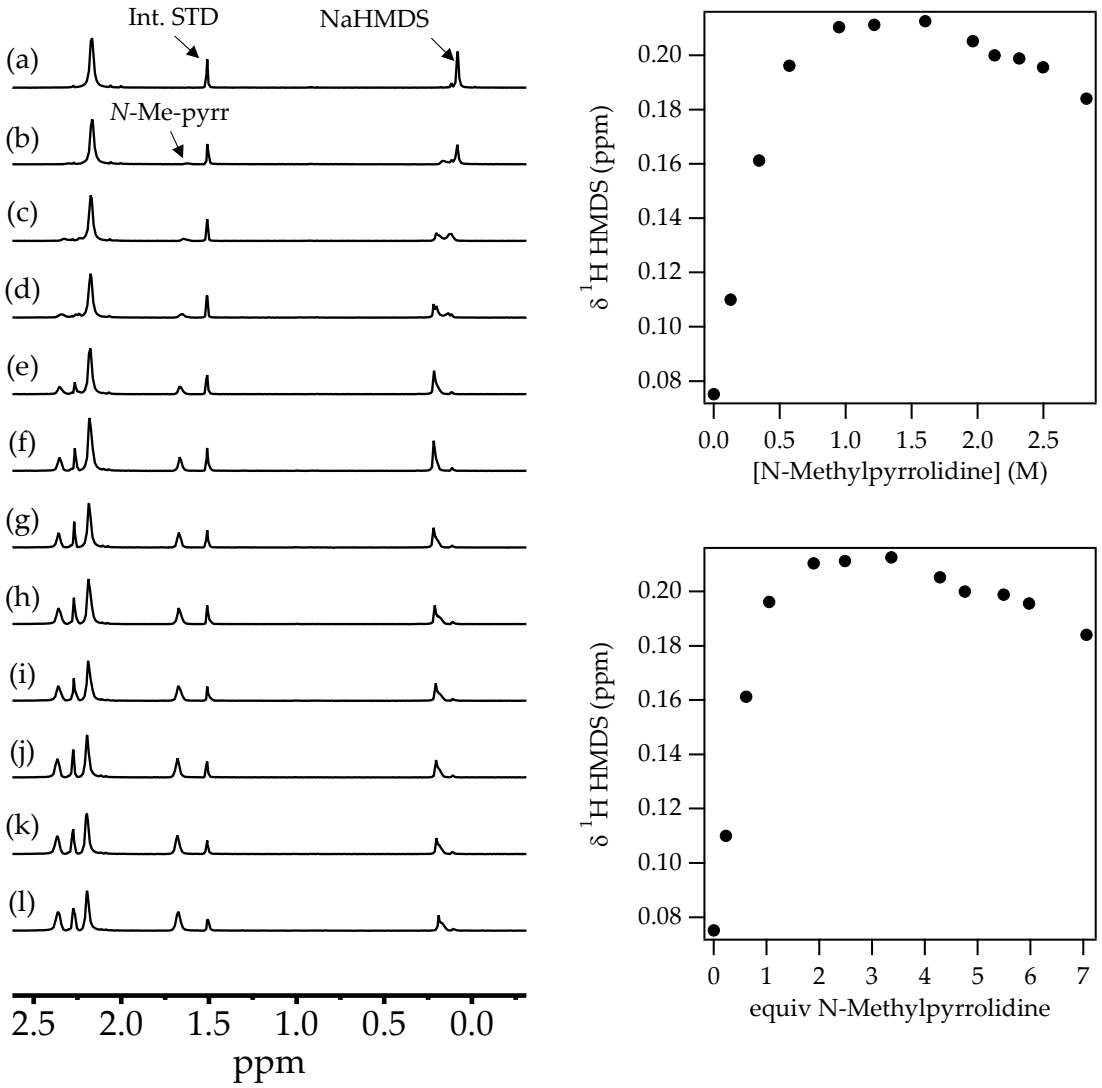


Figure S16. ^{1}H NMR (500 MHz, toluene)spectra for 0.55 M solutions of NaHMDS in toluene with cyclopentane internal standard (1.51 ppm) varying *N*-Me-pyrrolidine concentration at 25 °C. The concentrations of *N*-Me-pyrrolidine in (a)–(l) are 0.00, 0.13, 0.34, 0.57, 0.95, 1.21, 1.60, 1.96, 2.12, 2.31, 2.50, and 2.82, respectively. The plot shown corresponds to the spectra above.

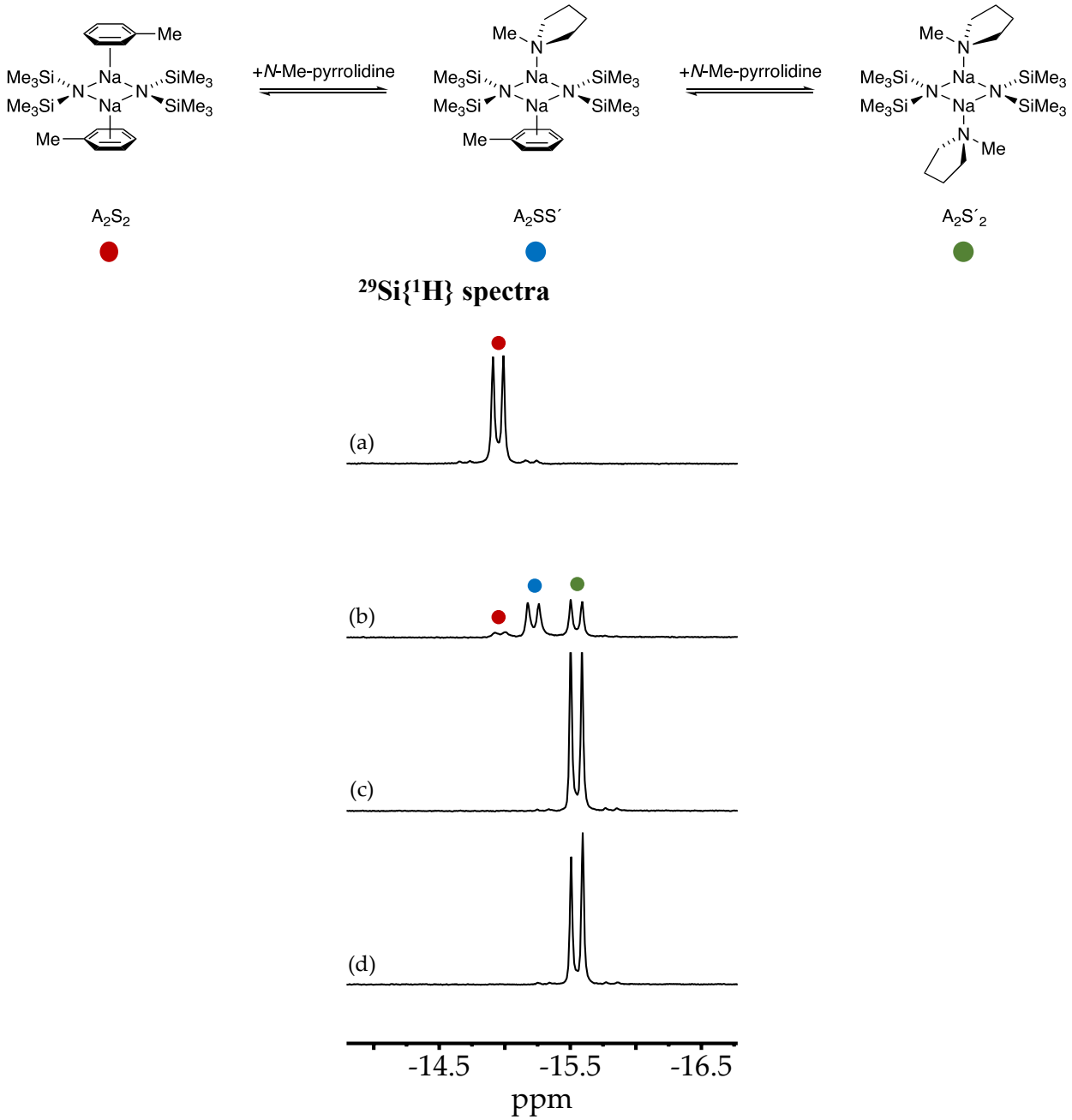
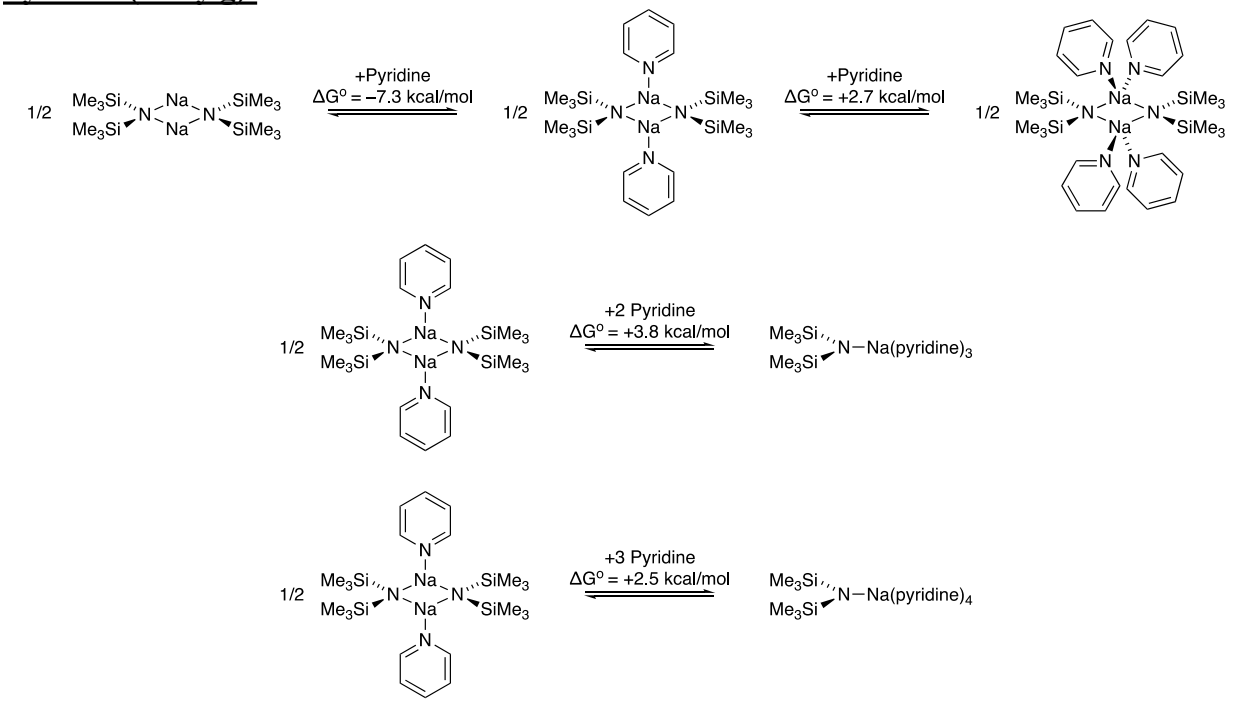


Figure S17. ^{29}Si NMR (99.36 MHz, toluene)spectra of 0.20 M [^{15}N]NaHMDS in 2:1 pentane/toluene-d_8 cosolvent with varying amounts of *N*-Me-pyrrolidine added at –120 °C. The equivalents of *N*-Me-pyrrolidine for (a)–(d) are as follows: 0.0, 0.75, 1.5, and 5.0 equiv, respectively. ^{29}Si spectra are referenced to a TMS internal standard (TMS chemical shift = 0.0 ppm for each).

Pyridine (entry g):



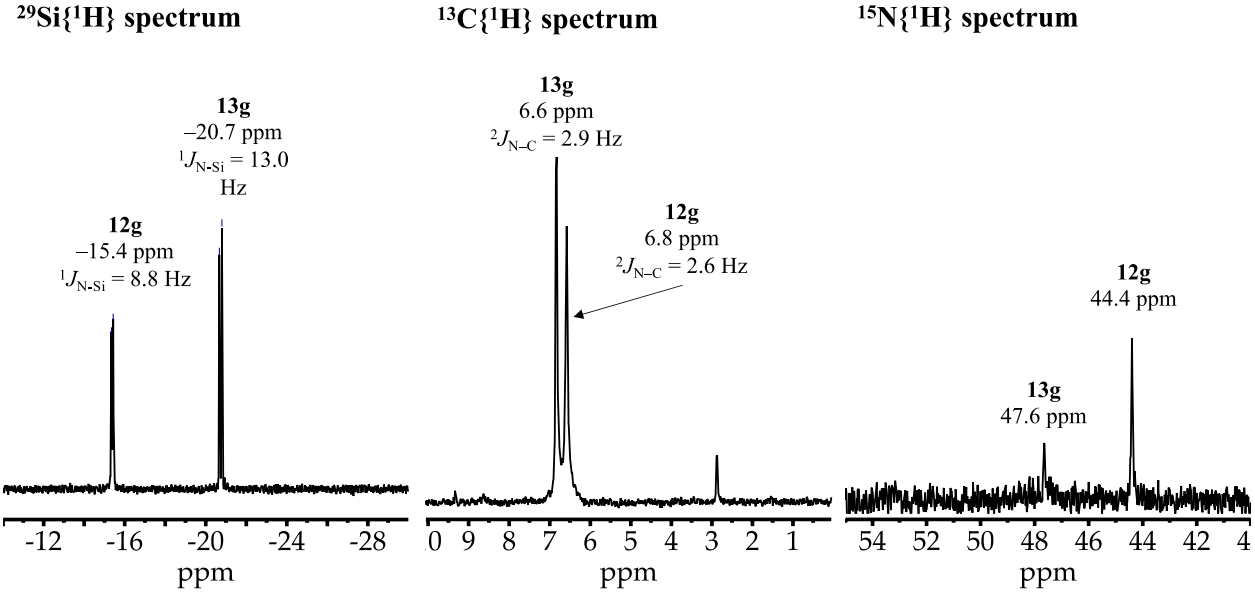


Figure S18. NMR spectra of [^{15}N]NaHMDS at intermediate concentrations of pyridine. Conditions vary on a per spectrum basis. Conditions in which each spectra where taken are delineated below. Standard ^{13}C, ^{15}N, and ^{29}Si spectra were recorded on a 500 MHz spectrometer at 125.79, 50.66, and 99.36 MHz, respectively.
^{29}Si and ^{13}C{^{1}H} spectra: 0.15 M [^{15}N]NaHMDS with 0.45 M pyridine in DMEA cosolvent at –120 °C. The ^{13}C{^{1}H} spectrum is referenced to cyclopentane (26.05 ppm).
^{15}N spectrum: 0.10 M [^{15}N]NaHMDS with 0.3 M pyridine in MTBE cosolvent at –110 °C.

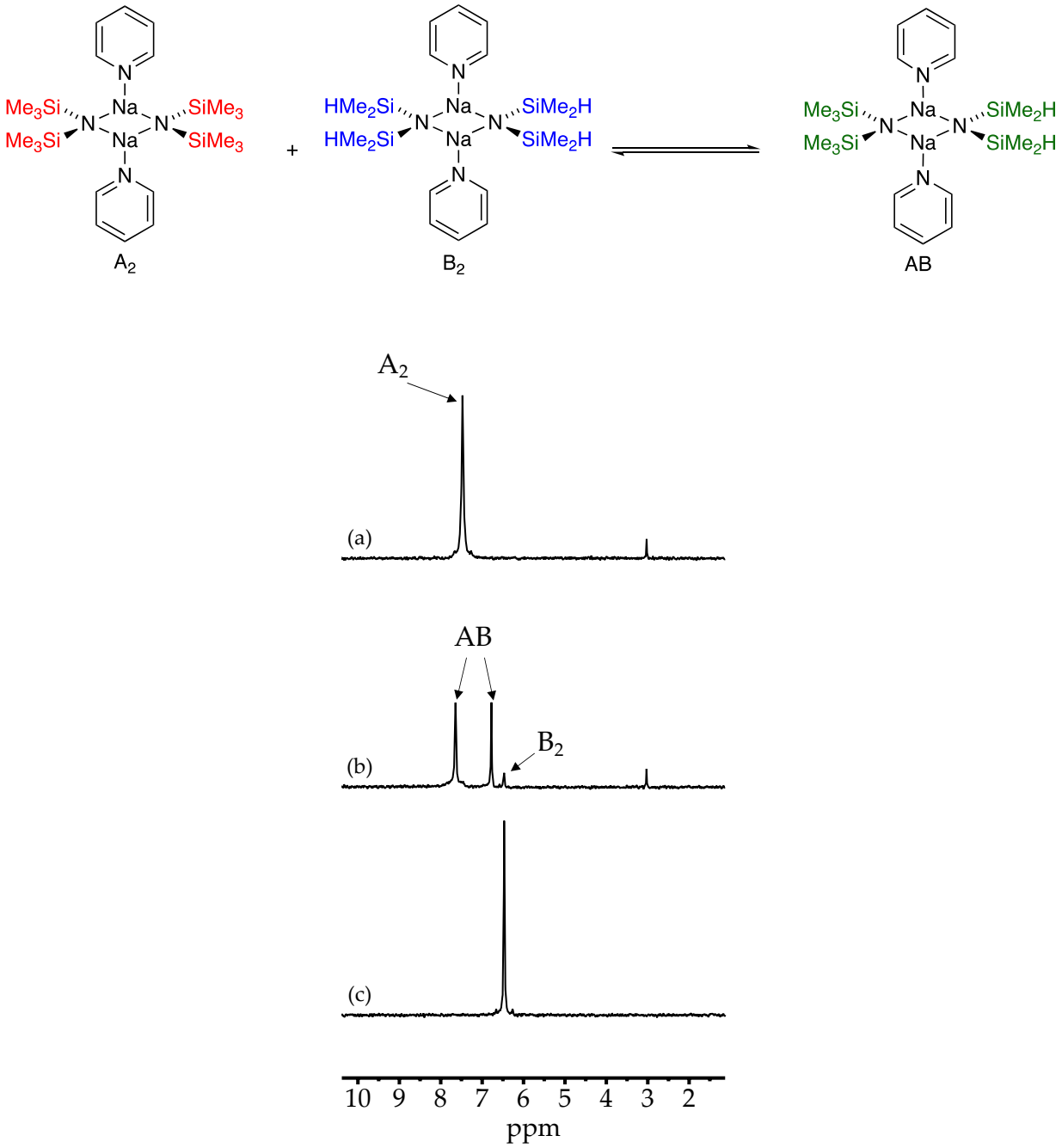


Figure S19. $^{13}C\{^{1}H\}$ NMR (125.79 MHz, toluene) spectra of with mixing NaHMDS and NaTMDS at 0.10 total molarity in 0.30 M pyridine in toluene-d_8 cosolvent at –80 °C. The measured mole fractions, X_{NaHMDS}, in (a)–(c) are 1.00, 0.52, and 0.00, respectively. $^{13}C\{^{1}H\}$ spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).

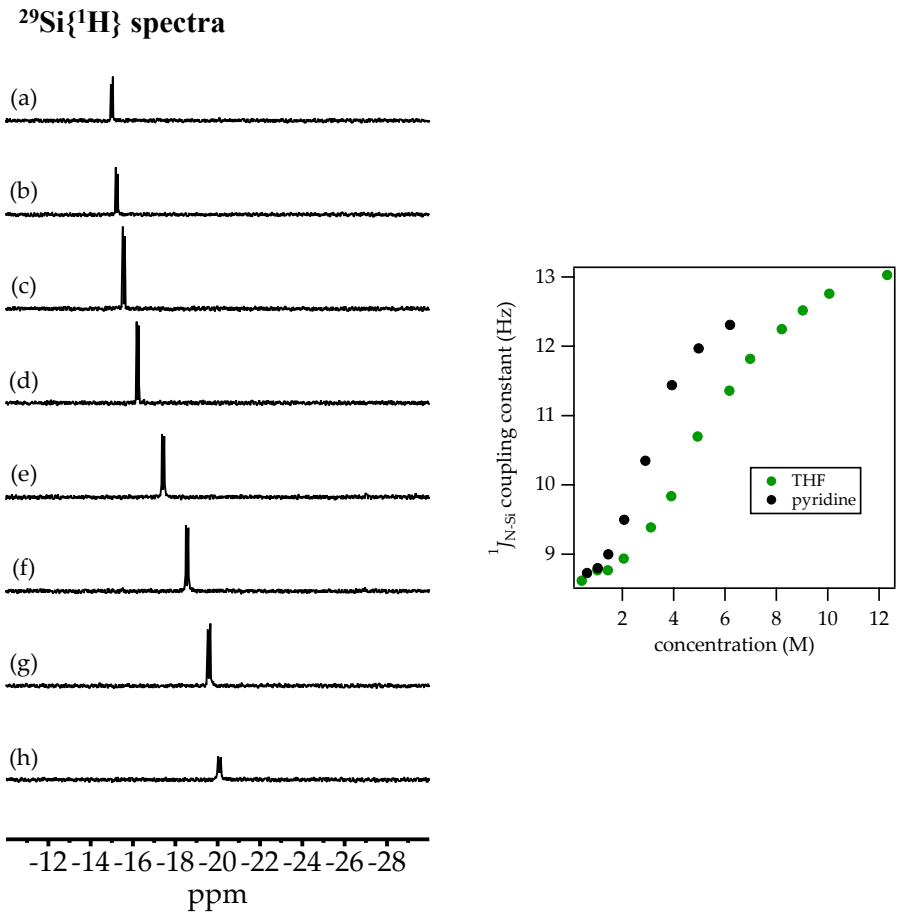


Figure S20. $^{29}Si\{^{1}H\}$ (99.36 MHz, toluene) NMR spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of pyridine at +50 °C. Pyridine concentrations for (a)–(h) are as follows: 0.62, 1.03, 1.44, 2.06, 2.89, 3.92, 4.96, and 6.19 M, respectively. Concentrations for THF are listed below. Data acquisition at higher concentrations was cut short due to coalescence severely hindered resolution of coupling constants.

[THF] (M)	$^{1}J_{N–Si}$ coupling constant (Hz)	[pyridine] (M)	$^{1}J_{N–Si}$ coupling constant (Hz)
0.41	8.62	0.62	8.73
1.02	8.77	1.03	8.80
1.43	8.77	1.44	9.00
2.05	8.94	2.06	9.50
3.10	9.39	2.89	10.35
3.90	9.84	3.92	11.44
4.92	10.7	4.96	11.97
6.16	11.36	6.19	12.31
6.97	11.82		
8.20	12.25		
9.02	12.52		
10.05	12.76		
12.31	13.03		

Pyrrolidine (entry h):

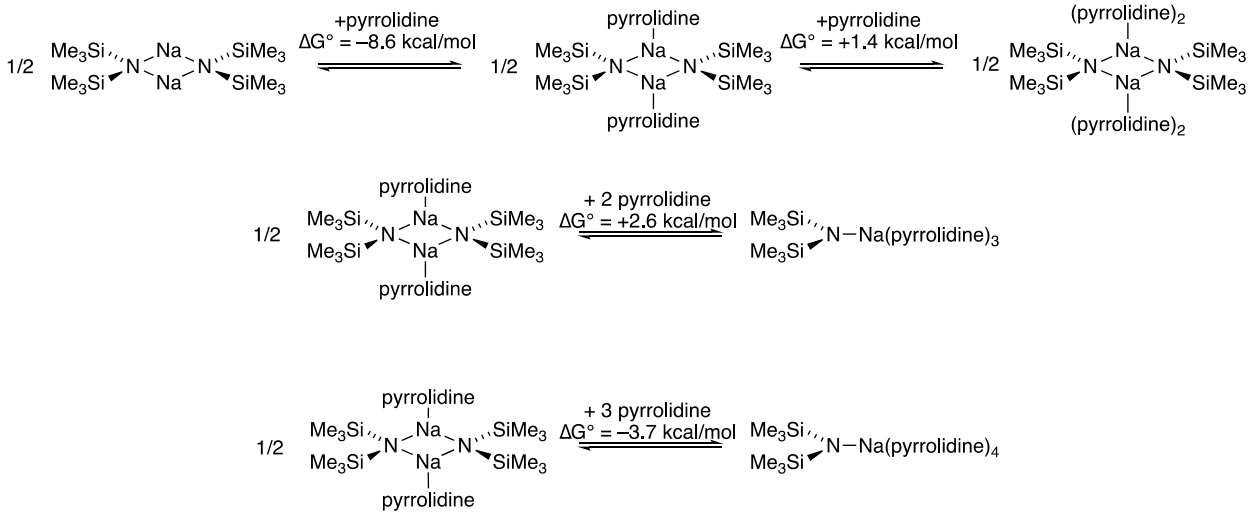


Figure S21. DFT computed energies or various NaHMDS pyrrolidine solvation states.

^{29}Si{^{1}H} spectra

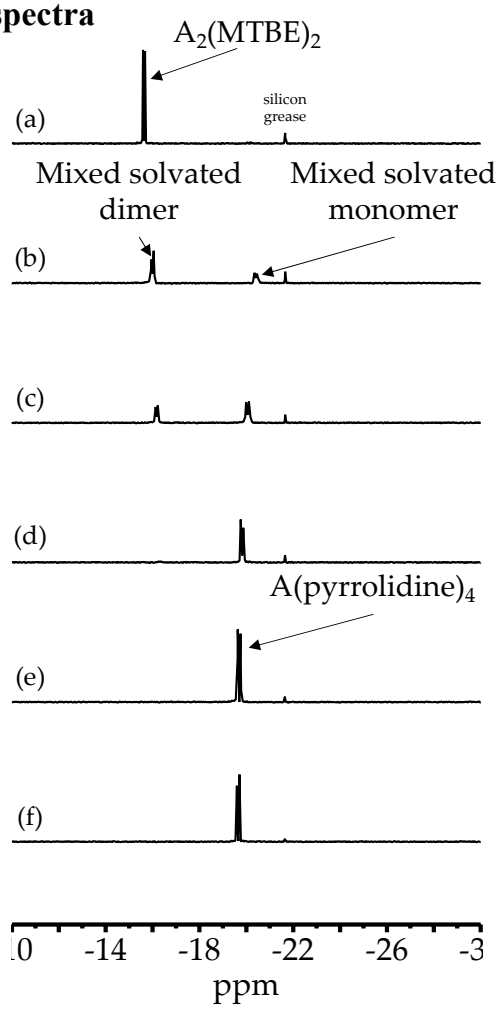
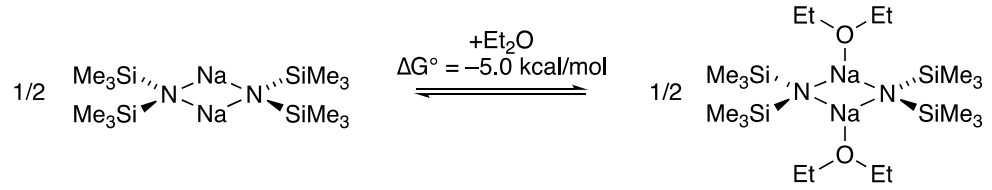


Figure S22. ^{29}Si NMR (99.36 MHz, MTBE) spectra of 0.20 M [^{15}N]NaHMDS in MTBE cosolvent with varying amounts of pyrrolidine added at –110 °C. The equivalents of pyrrolidine for (a)–(f) are as follows: 0.0, 1.0, 2.0, 3.0, 4.0, and 6.0 equiv, respectively. ^{29}Si spectra are referenced to a TMS internal standard (TMS chemical shift = 0.0 ppm for each).

Diethyl ether (entry i):



^{29}Si{^{1}H} spectrum **^{13}C{^{1}H} spectrum** **^{15}N{^{1}H} spectrum**

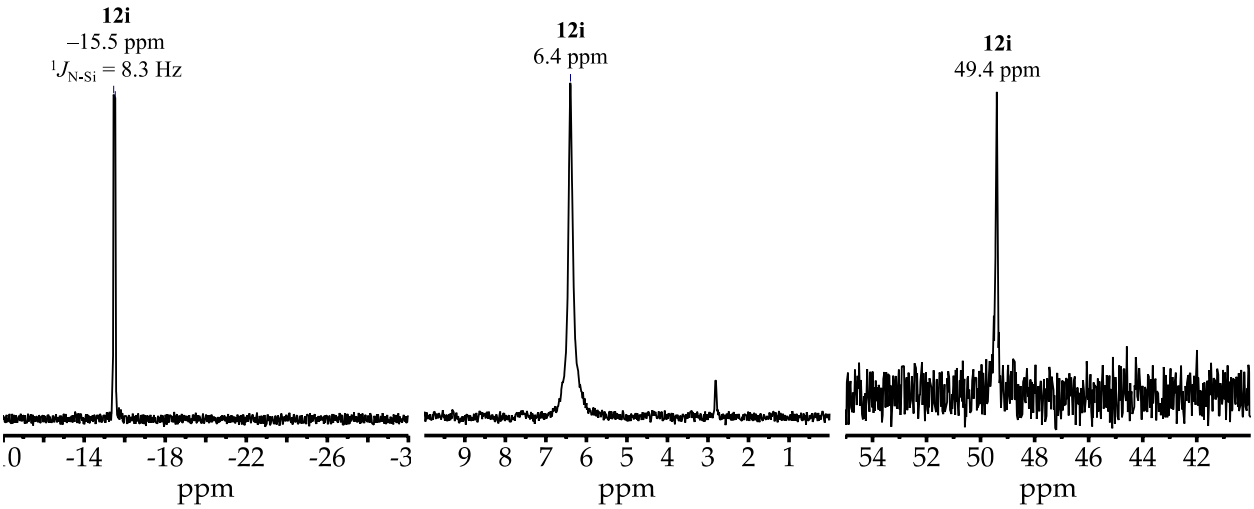
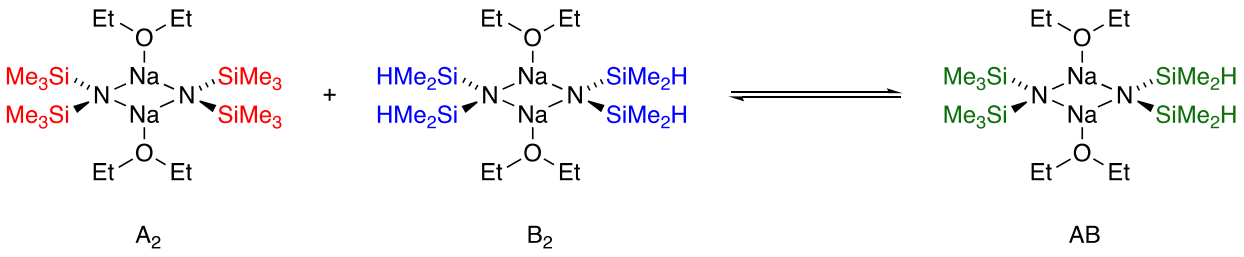


Figure S23. NMR spectra of [^{15}N]NaHMDS in various cosolvents with added diethyl ether. Conditions vary on a per spectrum basis. Conditions in which each spectra where taken are delineated below. Standard ^{13}C, ^{15}N, and ^{29}Si spectra were recorded on a 500 MHz spectrometer at 125.79, 50.66, and 99.36 MHz, respectively.
^{29}Si and ^{13}C{^{1}H} spectra: 0.15 M [^{15}N]NaHMDS with 4.5 M diethyl ether in DMEA cosolvent at –120 °C. Cyclopentane internal standard was used.
^{15}N spectrum: 0.10 M [^{15}N]NaHMDS in neat diethyl ether (9.60 M) at 25 °C. TMS internal standard was used.



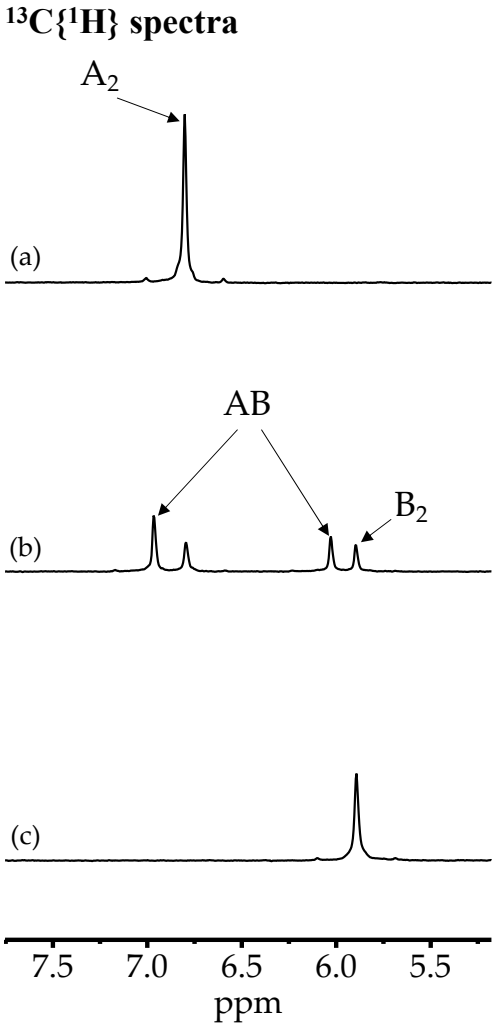


Figure S24. $^{13}C\{^1H\}$ NMR (125.79 MHz, toluene) spectra of with mixing NaHMDS and NaTMDS at 0.20 total molarity in 0.80 M diethyl ether in toluene-d_8 cosolvent at –80 °C. The measured mole fractions, X_{NaHMDS}, in (a)–(c) are 1.00, 0.50, and 0.00, respectively. $^{13}C\{^1H\}$ spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).

^{29}Si{^{1}H} spectra

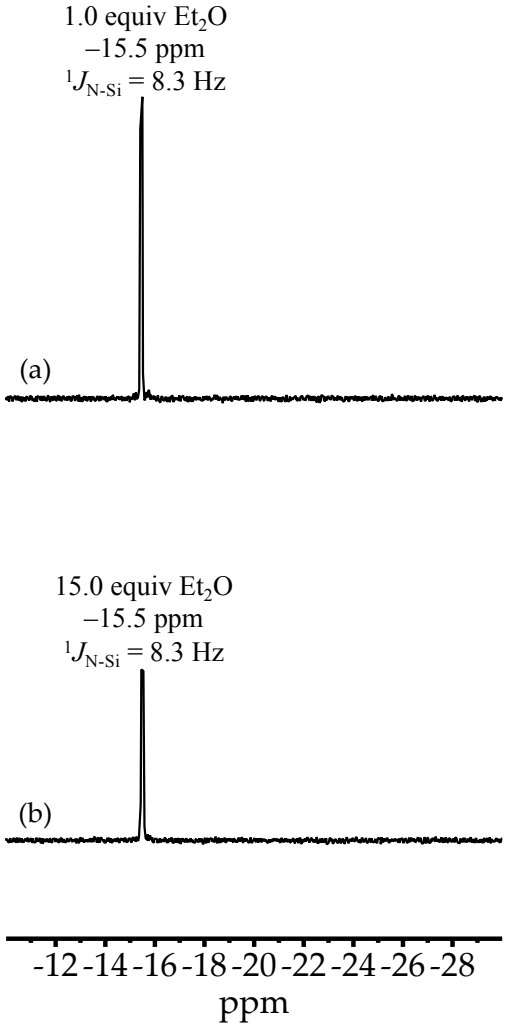
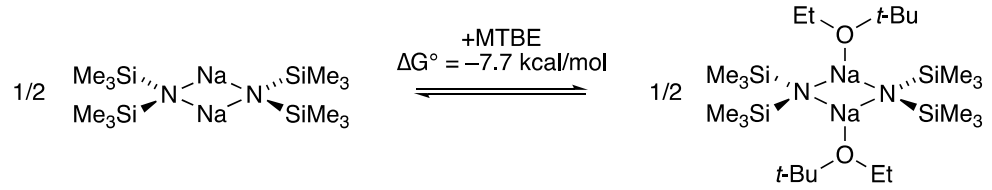


Figure S25. ^{29}Si NMR (99.36 MHz, DMEA) spectra of 0.15 M [^{15}N]NaHMDS in DMEA cosolvent with varying amounts of diethyl ether added at –120 °C. The equivalents of diethyl ether for (a) and (b) are as follows: 1.0 and 15.0 equiv, respectively.

Methyl *tert*-butyl ether (entry j):



^{29}Si{^{1}H} spectrum **^{13}C{^{1}H} spectrum** **^{15}N{^{1}H} spectrum**

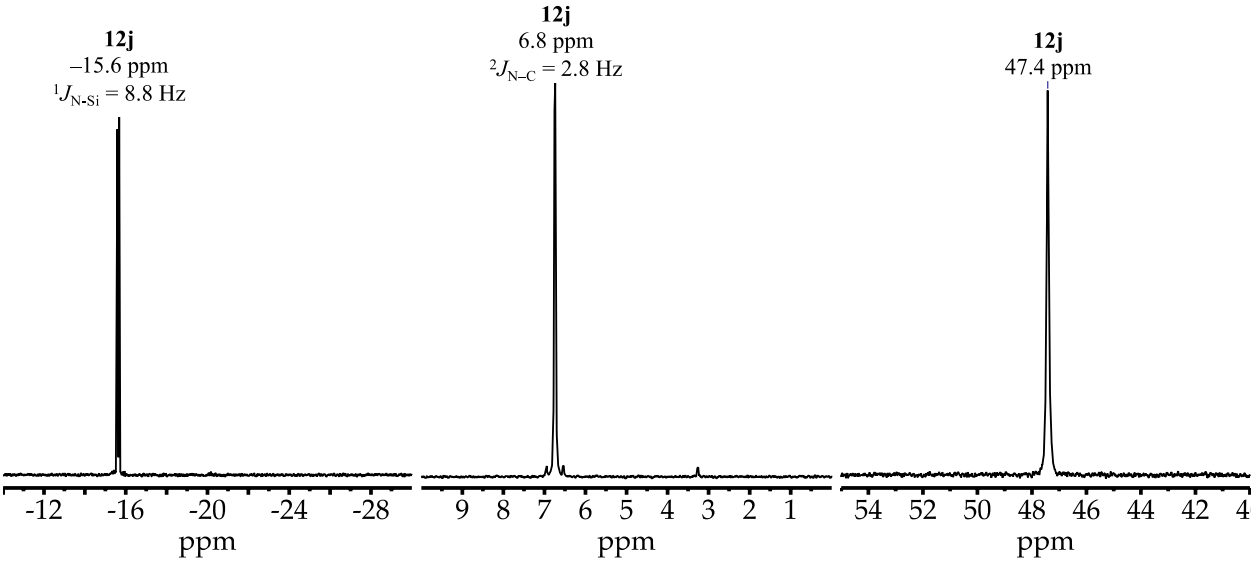


Figure S26. NMR spectra of [^{15}N]NaHMDS at intermediate concentrations of methyl *tert*-butyl ether. Conditions vary on a per spectrum basis. Conditions in which each spectra where taken are delineated below. Standard ^{13}C, ^{15}N, and ^{29}Si spectra were recorded on a 500 MHz spectrometer at 125.79, 50.66, and 99.36 MHz, respectively.
^{29}Si spectrum: 0.20 M [^{15}N]NaHMDS in neat MTBE at –110 °C. TMS internal standard was used.
^{13}C{^{1}H} spectrum: 0.30 M [^{15}N]NaHMDS with 5.55 M MTBE in toluene cosolvent at –80 °C. ^{13}C{^{1}H} spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).
^{15}N spectrum: 0.15 M [^{15}N]NaHMDS with 2.75 M MTBE in DMEA cosolvent at –110 °C. ^{15}N spectra are referenced to DMEA (25.7 ppm).

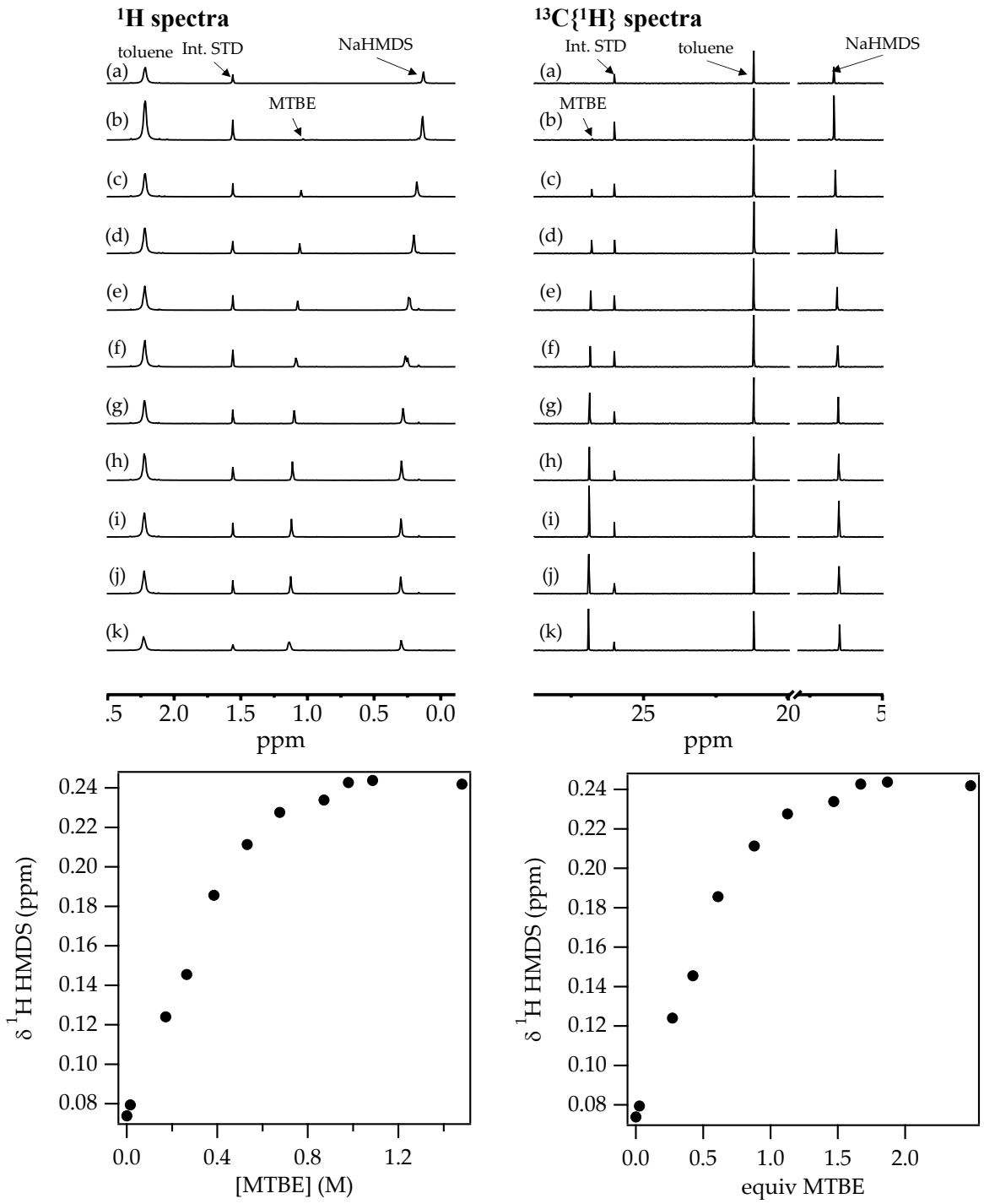
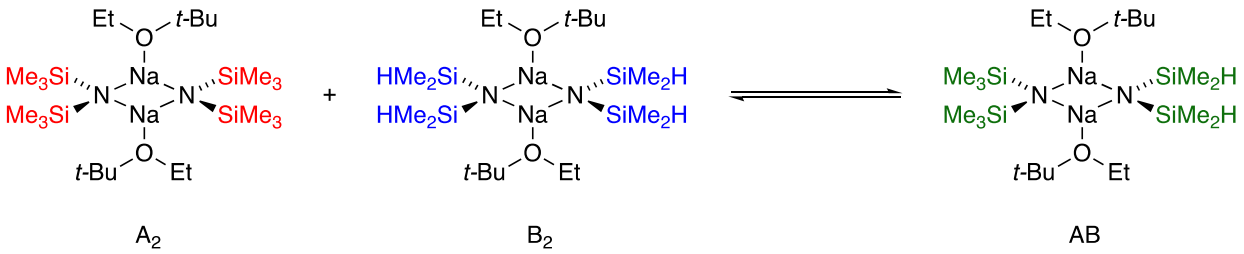


Figure S27. ^{1}H (500 MHz, toluene) and ^{13}C{^{1}H} NMR (125.79 MHz, toluene) spectra for 0.60 M solutions of NaHMDS in toluene with cyclopentane internal standard varying methyl *tert*-butyl ether concentration at 25 °C. The concentrations of methyl *tert*-butyl ether in (a)–(k) are 0.00, 0.02, 0.17, 0.26, 0.38, 0.53, 0.68, 0.87, 0.98, 1.10, and 1.50, respectively. The plot shown corresponds to the spectra above.



$^{13}C\{^{1}H\}$ spectra

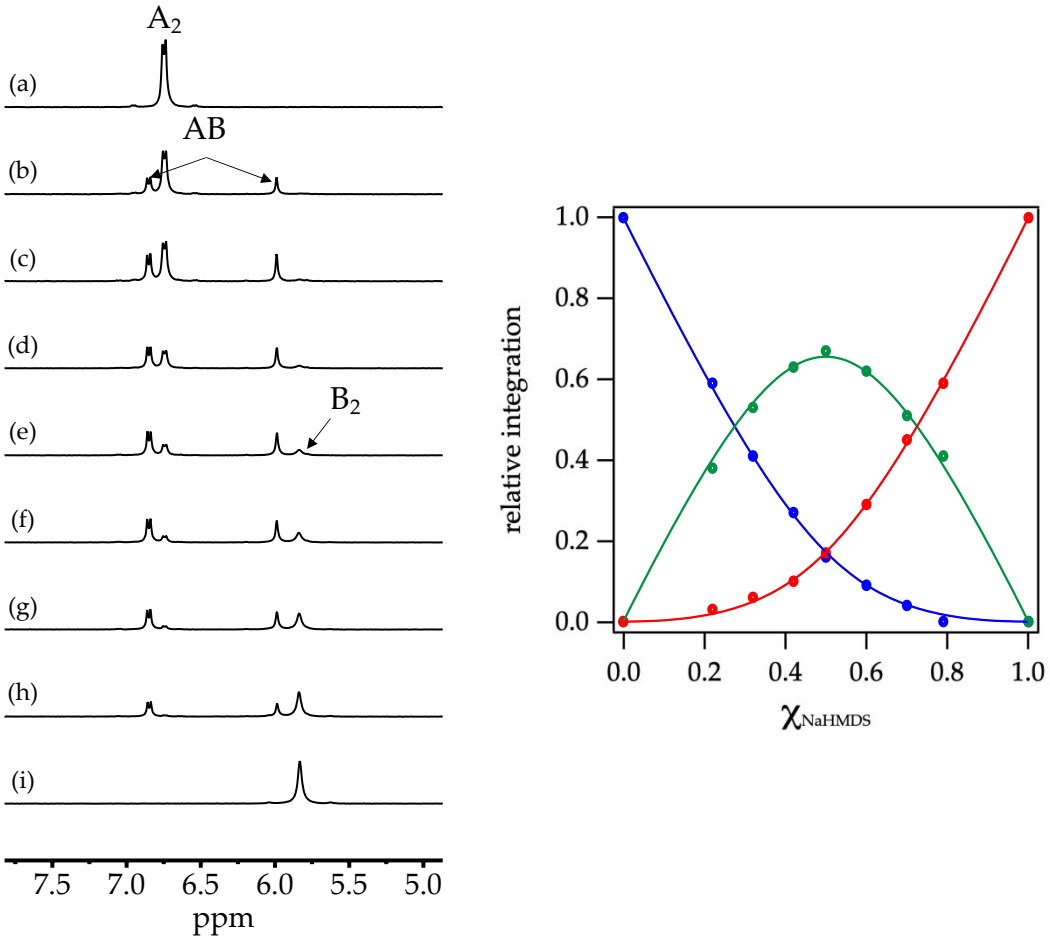


Figure S28. $^{13}C\{^{1}H\}$ (125.79 MHz, toluene) NMR spectra and affiliated Job plot showing relative integrations of NaHMDS-derived homodimer (A_2, red), NaTMDS-derived homodimer (B_2, blue), and heterodimer (AB, green) versus the measured mole fraction of NaHMDS (X_{NaHMDS}) at 0.30 total molarity in 5.50 M methyl tert-butyl ether in toluene cosolvent at −80 °C. The measured mole fractions, X_{NaHMDS}, in (a)–(g) are 1.00, 0.79, 0.70, 0.60, 0.50, 0.42, 0.32, 0.22, and 0.00, respectively.

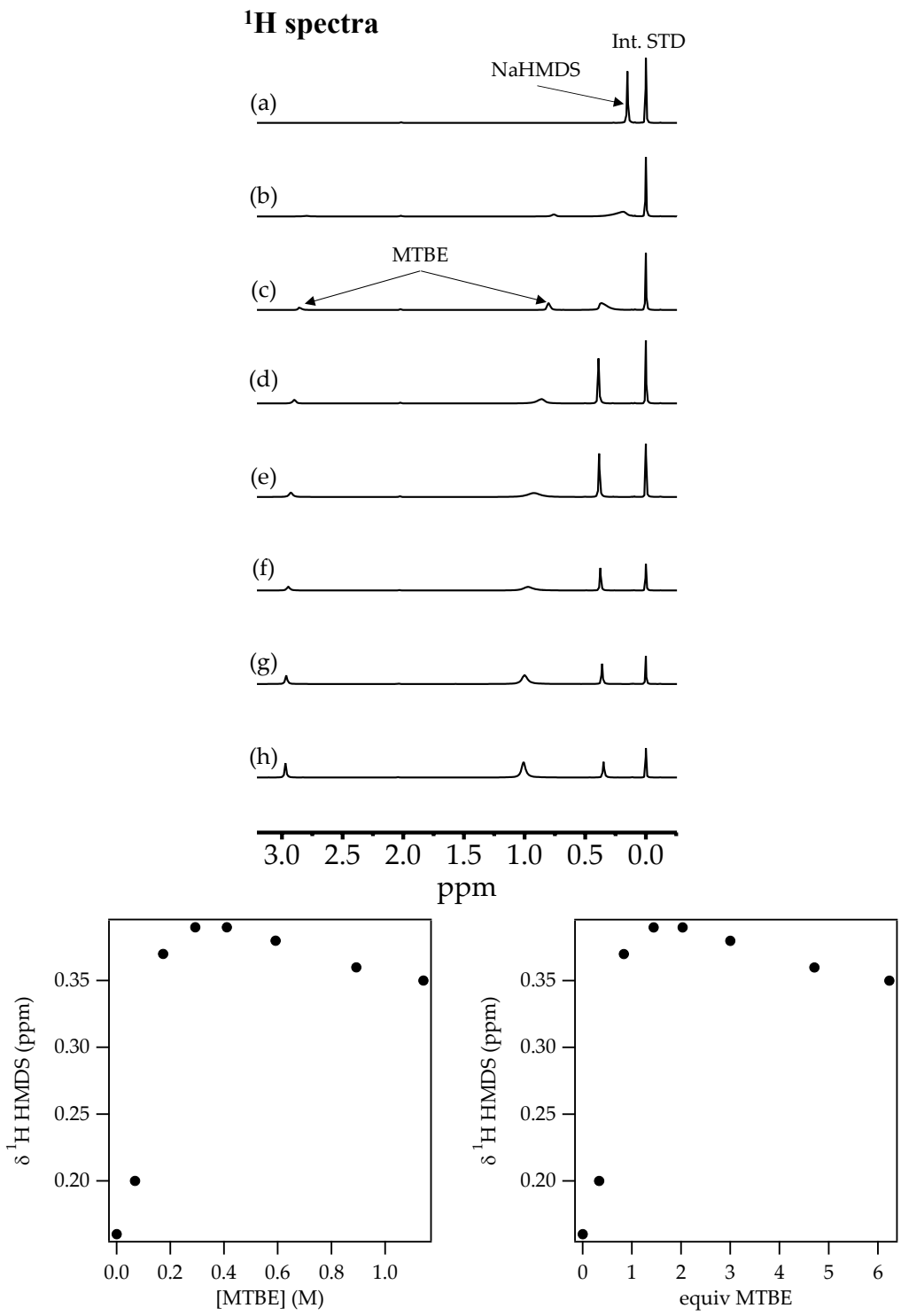


Figure S29. ^{1}H NMR (500 MHz, toluene) spectra for 0.20 M solutions of NaHMDS in toluene with TMS internal standard varying methyl *tert*-butyl ether concentration at –80 °C. The concentrations of methyl *tert*-butyl ether in (a)–(h) are 0.00, 0.07, 0.17, 0.29, 0.41, 0.59, 0.89, and 1.14, respectively. The plot shown corresponds to the spectra above.

1,4-dioxane (entry k):

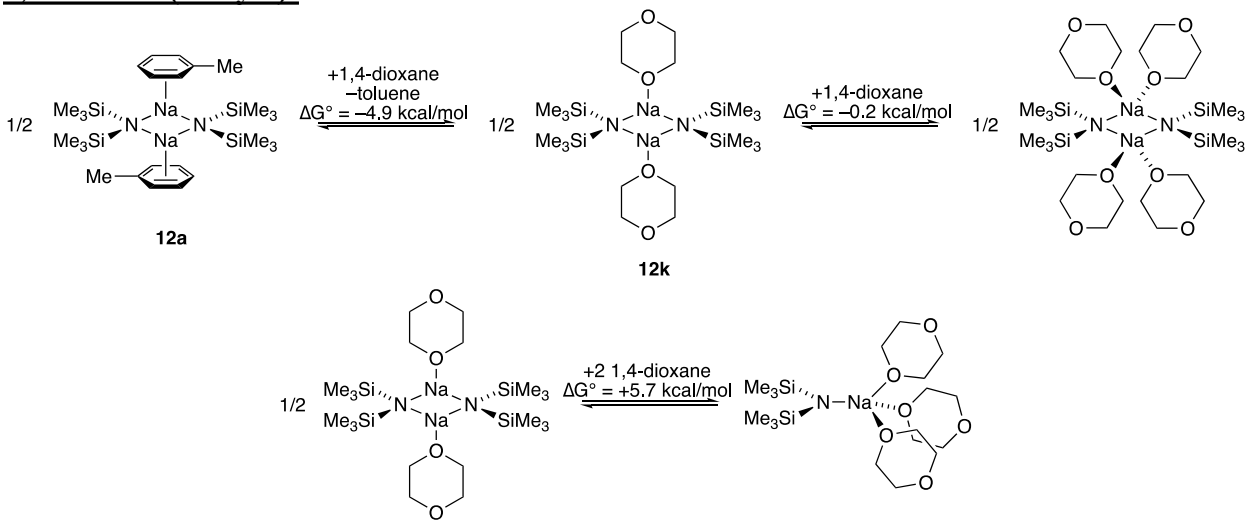


Figure S30. Computed free energies for the serial solvation of NaHMDS with 1,4-dioxane.

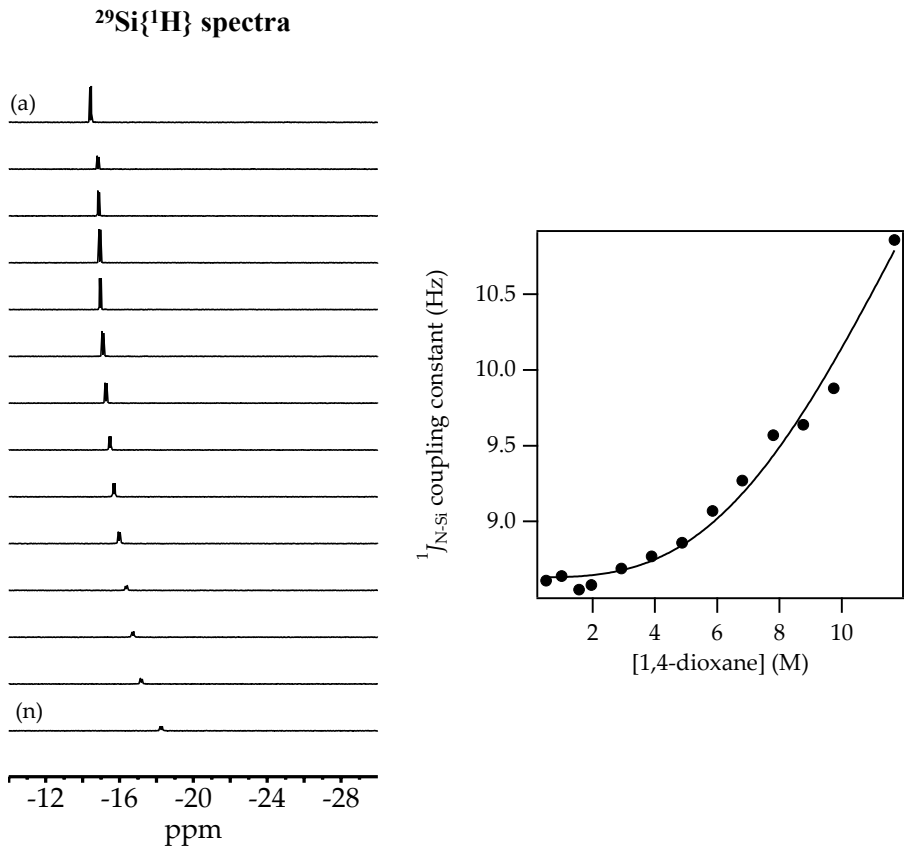


Figure S31. ^{29}Si NMR (99.36 MHz, toluene) spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of 1,4-dioxane at +20 °C. 1,4-Dioxane concentration for (a)–(n) are as follows: 0.50, 1.00, 1.56, 1.95, 2.92, 3.89, 4.87, 5.85, 6.80, 7.80, 8.76, 9.74, and 11.69, respectively. The curve is fit to the function described in the "Derivation" section of this Supporting Information on page S-117 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.

1,3-dioxolane (entry l):

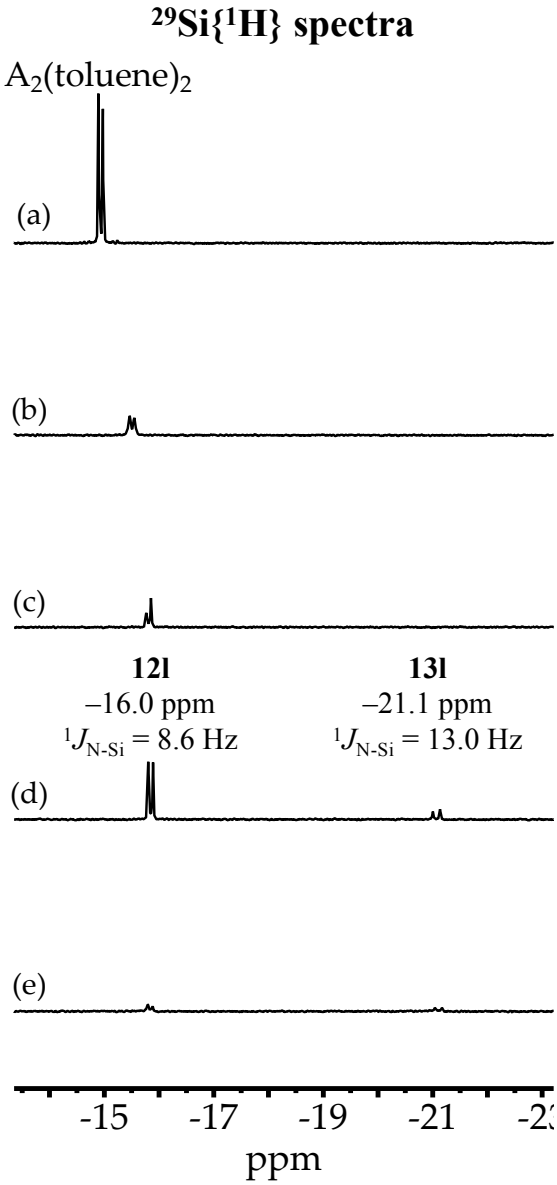
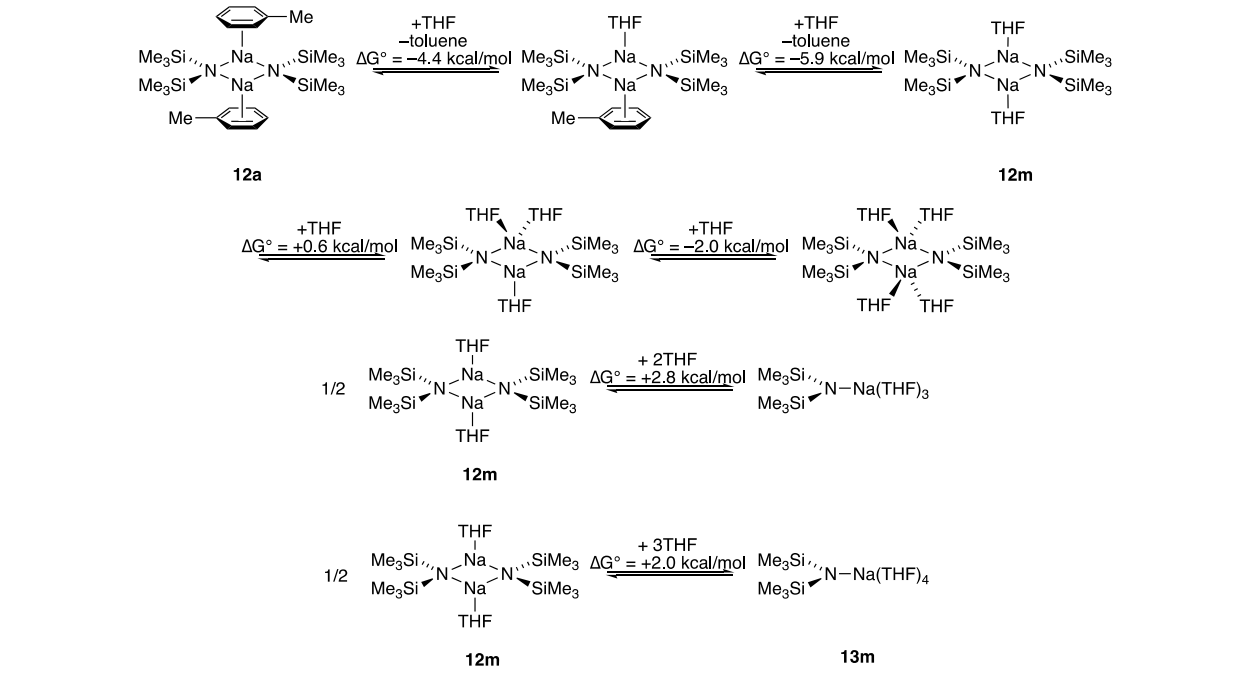


Figure S32. ^{29}Si NMR (99.36 MHz, toluene) spectra of 0.10 M [^{15}N]NaHMDS in 2:1 pentane/toluene cosolvent with varying amounts of 1,3-dioxolane added at –120 °C. The equivalents of dioxolane for (a)–(e) are as follows: 0.0, 0.5, 1.0, 3.0, and 5.0 equiv respectively. At 0.5 equiv a polymeric network was present at the bottom of the NMR tube.

Tetrahydrofuran (entry m):



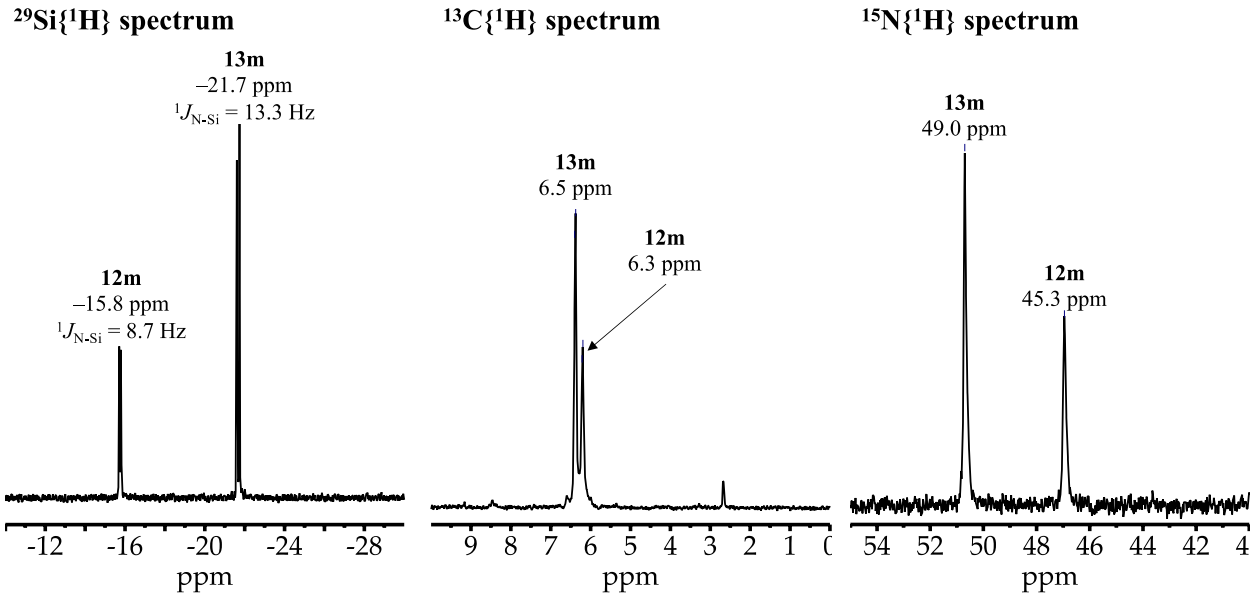


Figure S33. NMR spectra of 0.15 M [^{15}N]NaHMDS in 0.75 M THF with DMEA cosolvent at –120 °C. ^{13}C{^{1}H} spectra are referenced relative cyclopentane (26.05 ppm). ^{15}N spectra are referenced to DMEA (25.7 ppm). Standard ^{13}C, ^{15}N, and ^{29}Si spectra were recorded on a 500 MHz spectrometer at 125.79, 50.66, and 99.36 MHz, respectively.

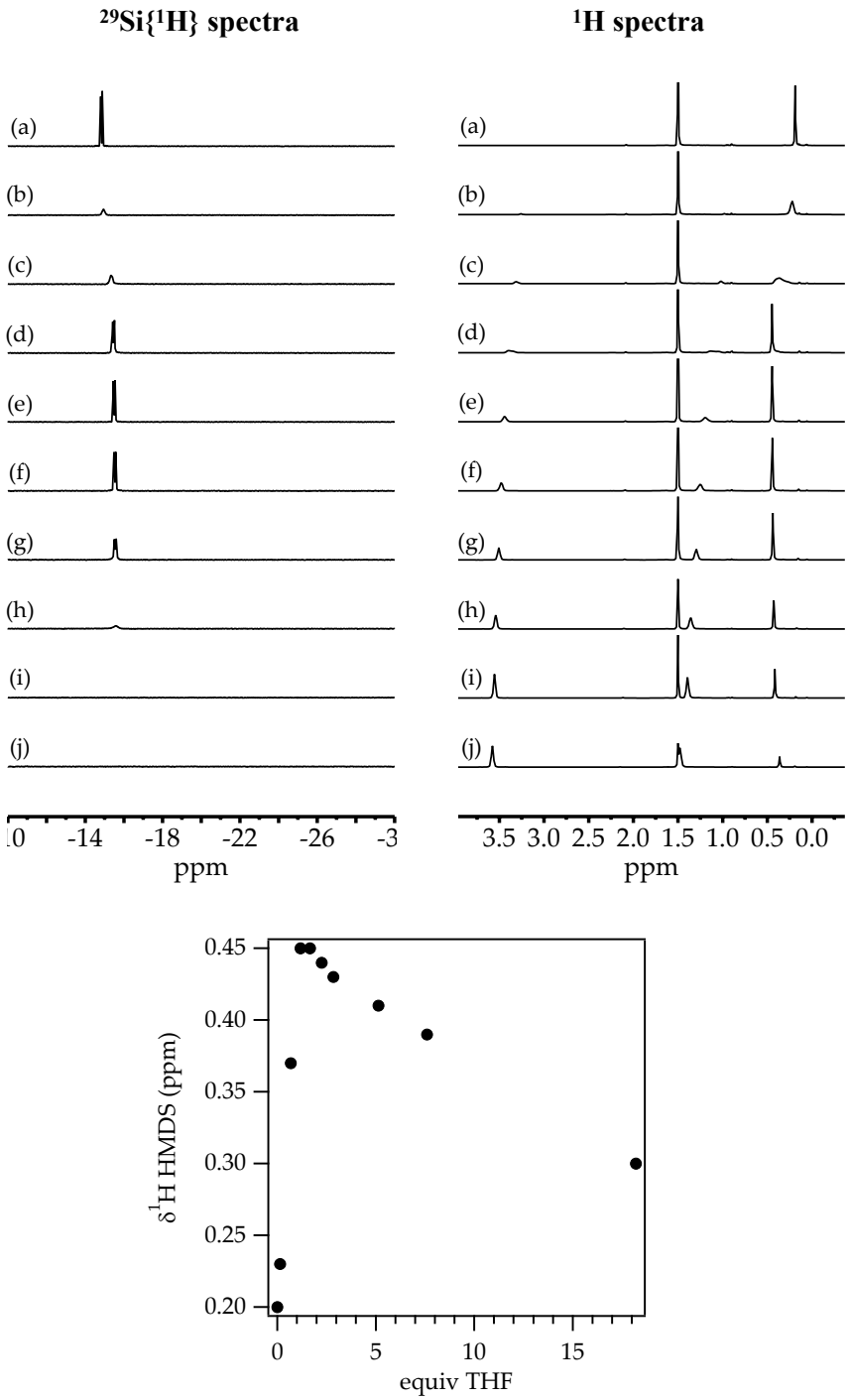


Figure S34. ^{1}H (500 MHz, toluene) and ^{29}Si{^{1}H} NMR (99.36 MHz, toluene) spectra for the titration of 0.23 M NaHMDS in toluene-d_8 with THF at –80 °C. Equiv of THF for (a)–(j) are as follows: 0.0, 0.1, 0.7, 1.2, 1.7, 2.3, 2.8, 5.1, 7.6, and 18.2, respectively. ^{1}H are referenced to cyclopentane (1.51 ppm).

^{29}Si{^{1}H} spectra

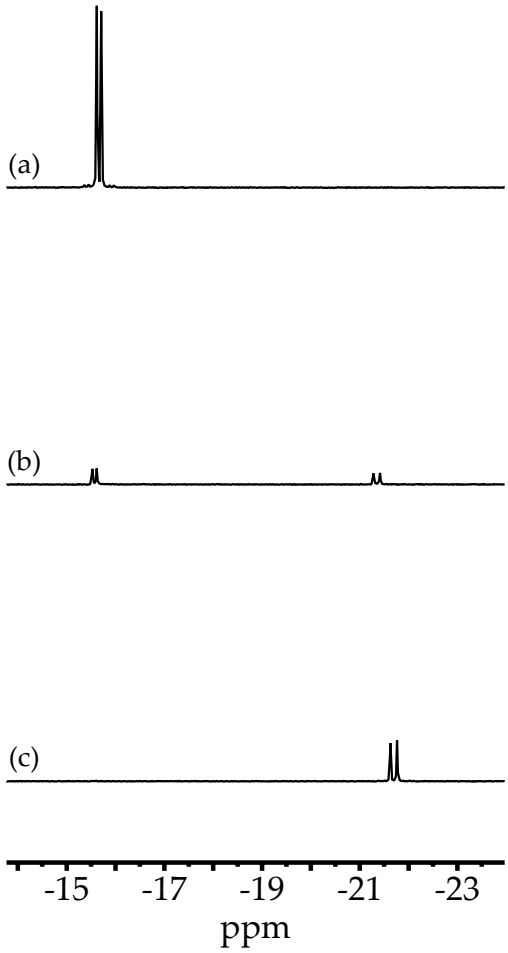


Figure S35. ^{29}Si{^{1}H} NMR (99.36 MHz, toluene) spectra for the titration of 0.15 M NaHMDS in DMEA with THF at –120 °C. Equiv of THF for (a)–(c) are as follows: 0.0, 4.0, and 10.0, respectively.

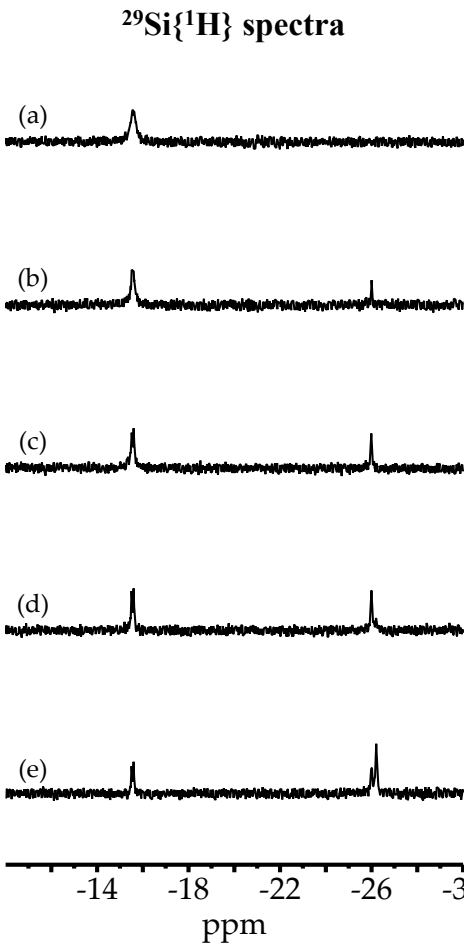


Figure S36. $^{29}Si\{^{1}H\}$ NMR (99.36 MHz, toluene) spectra of NaHMDS-derived homodimer (A_2), NaTMDS-derived homodimer (B_2), and heterodimer (AB) at 0.20 total molarity with 5.0 equiv THF in toluene cosolvent at −80 °C. The mole fraction of NaHMDS for (a)−(e) are as follows: 1.0, 0.8, 0.7, 0.5, 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.

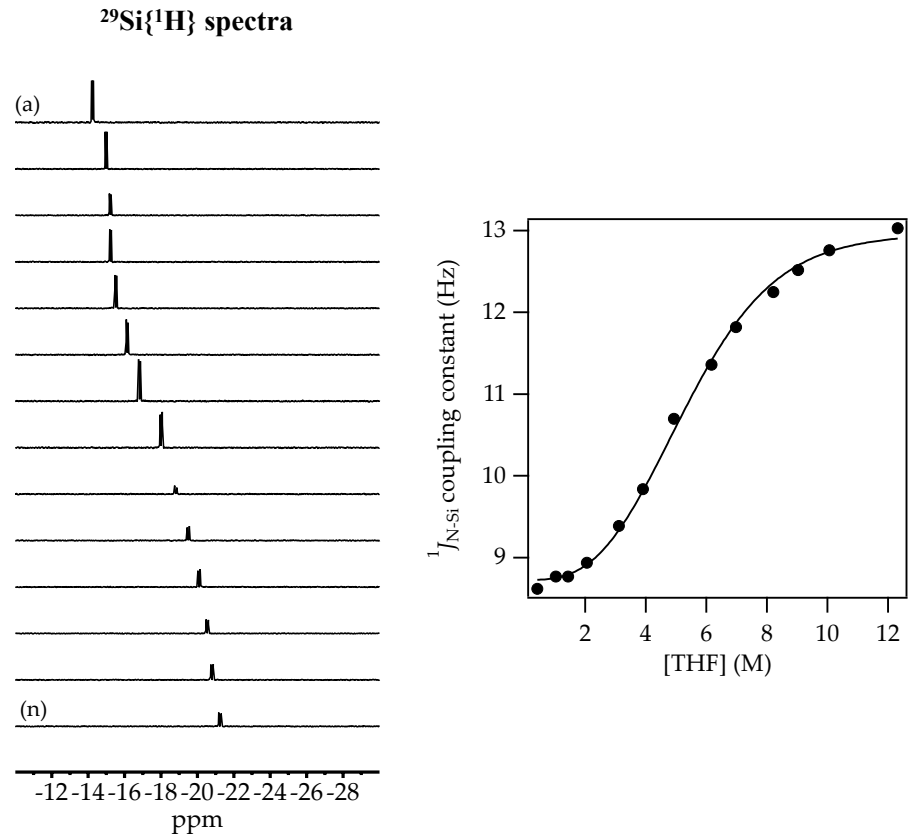


Figure S37. $^{29}Si\{^{1}H\}$ NMR (99.36 MHz, toluene) spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of THF at +50 °C. THF concentration for (a)–(n) are as follows: 0.00, 0.41, 1.02, 1.43, 2.05, 3.10, 3.90, 4.92, 6.16, 6.97, 8.2, 9.02, 10.05, and 12.31, respectively. The curve is fit to the function described in the "Derivation" section of this Supporting Information on page S-117 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

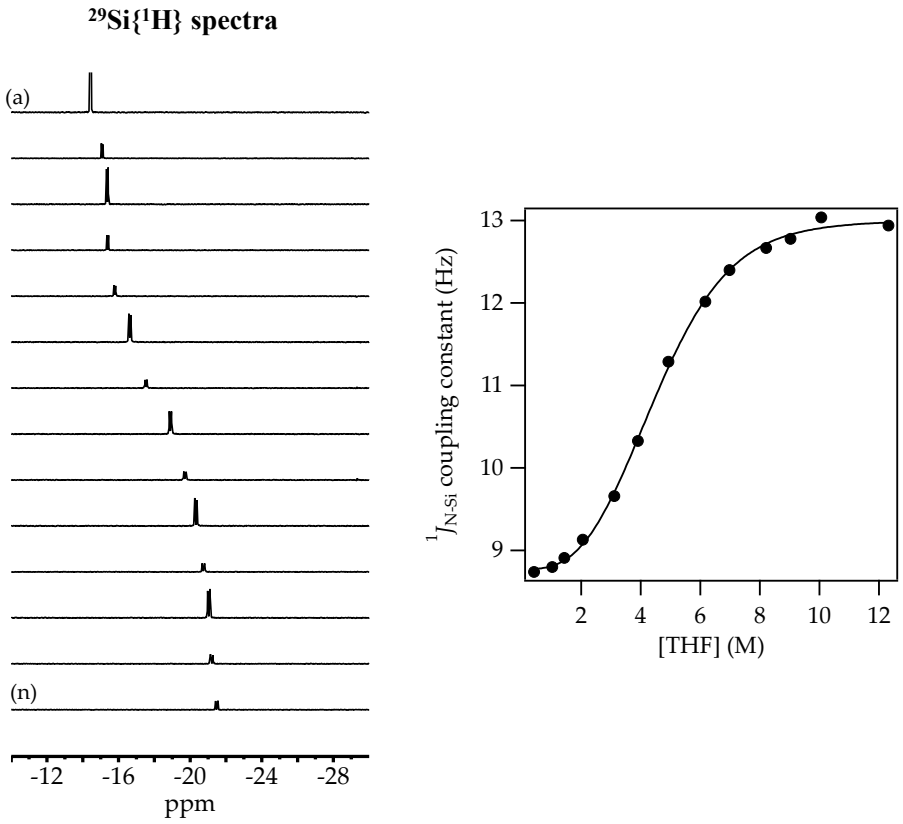


Figure S38. $^{29}Si\{^{1}H\}$ NMR (99.36 MHz, toluene) spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of THF at +20 °C. THF concentration for (a)–(n) are as follows: 0.00, 0.41, 1.02, 1.43, 2.05, 3.10, 3.90, 4.92, 6.16, 6.97, 8.2, 9.02, 10.05, and 12.31, respectively. The curve is fit to the function described in the "Derivation" section of this Supporting Information on page S-117 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

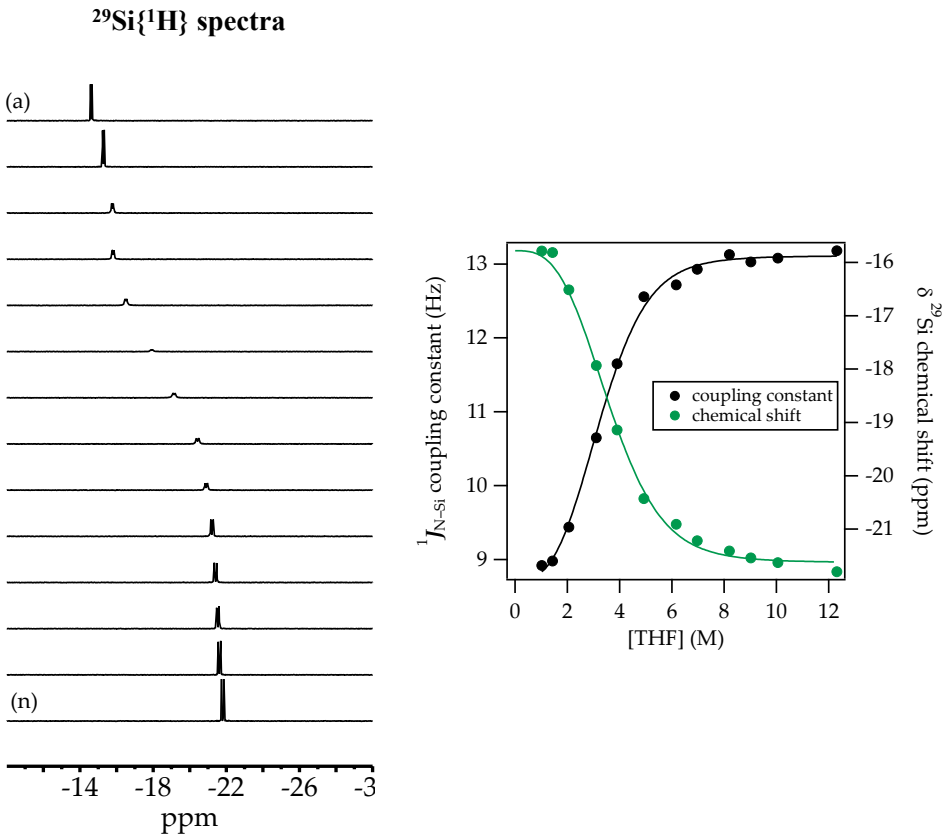


Figure S39. $^{29}Si\{^{1}H\}$ NMR (99.36 MHz, toluene) spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of THF at –20 °C. THF concentration for (a)–(n) are as follows: 0.41, 1.02, 1.43, 2.05, 3.10, 3.90, 4.92, 6.16, 6.97, 8.2, 9.02, 10.05, and 12.31, respectively. The curve is fit to the function described in the "Derivation" section of this Supporting Information on page S-117 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

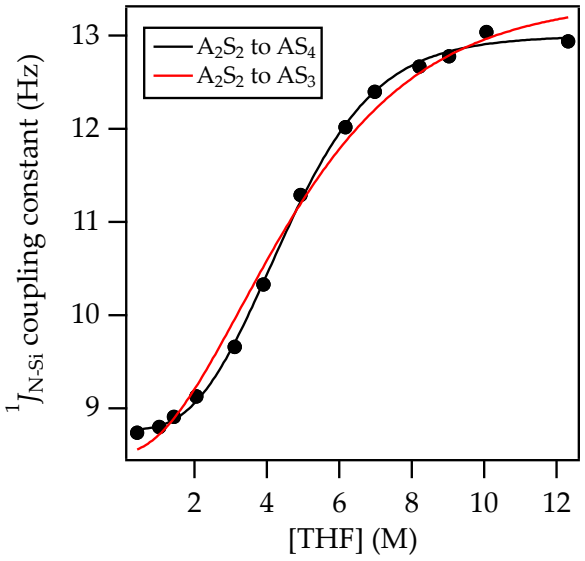


Figure S40. ^{29}Si NMR (99.36 MHz, toluene) spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of THF at +20 °C. THF concentration for (a)–(n) are as follows: 0.00, 0.41, 1.02, 1.43, 2.05, 3.10, 3.90, 4.92, 6.16, 6.97, 8.2, 9.02, 10.05, and 12.31, respectively. The difference 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

$^{13}C\{^1H\}$ spectra

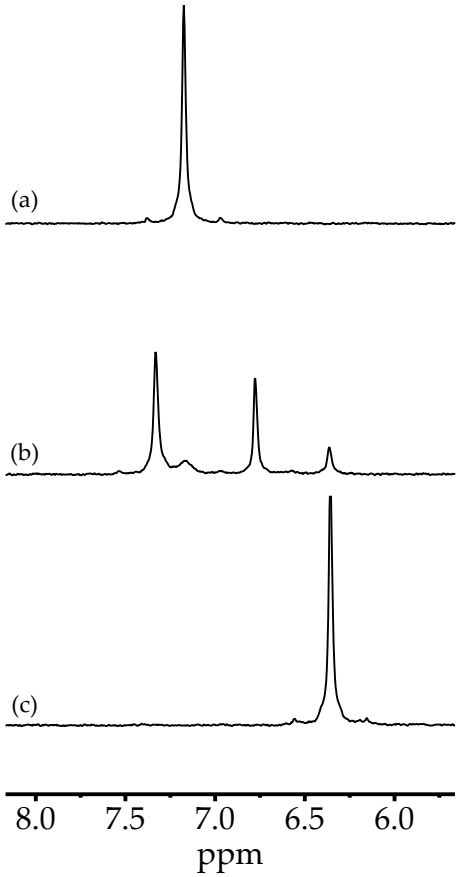


Figure S41. $^{13}C\{^1H\}$ NMR (125.79 MHz, toluene) spectra of with mixing NaHMDS and NaTMDS at 0.20 total molarity in 0.85 M THF in toluene-d_8 cosolvent at –80 °C. The measured mole fractions, X_{NaHMDS}, in (a)–(c) are 1.00, 0.50, and 0.00, respectively. $^{13}C\{^1H\}$ spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).

HMPA (entry n):

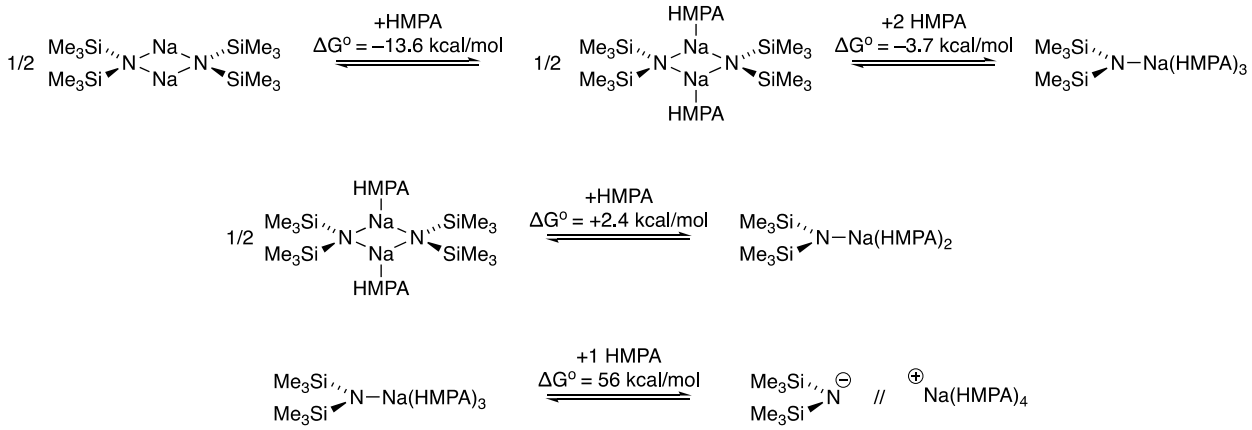
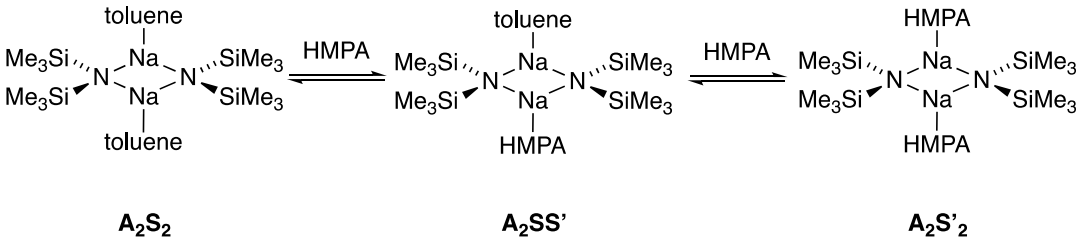


Figure S42. Computed free energies for the serial solvation of NaHMDS with HMPA.



^{29}Si{^{1}H} spectra

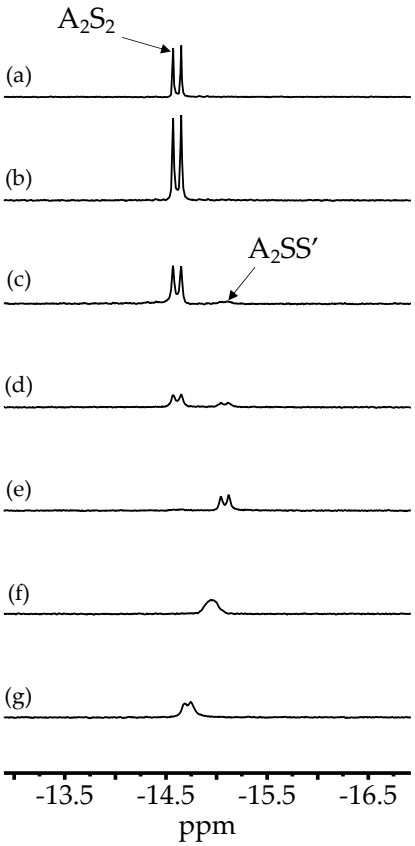


Figure S43. ^{29}Si{^{1}H} NMR (99.36 MHz, toluene) spectra for the titration of 0.10 M NaHMDS in toluene-d_8 with HMPA at –80 °C. Equiv of HMPA for (a)–(g) are as follows: 0.0, 0.03, 0.1, 0.15, 0.31, 0.5, and 1.0, respectively. Time averaged mixed solvate dimer and disolvated HMPA dimer average above 0.5 equiv, which is the reason for the broadening in (f) and (g). ^{29}Si spectra are referenced to trace HMDS present in tube (2.00 ppm).

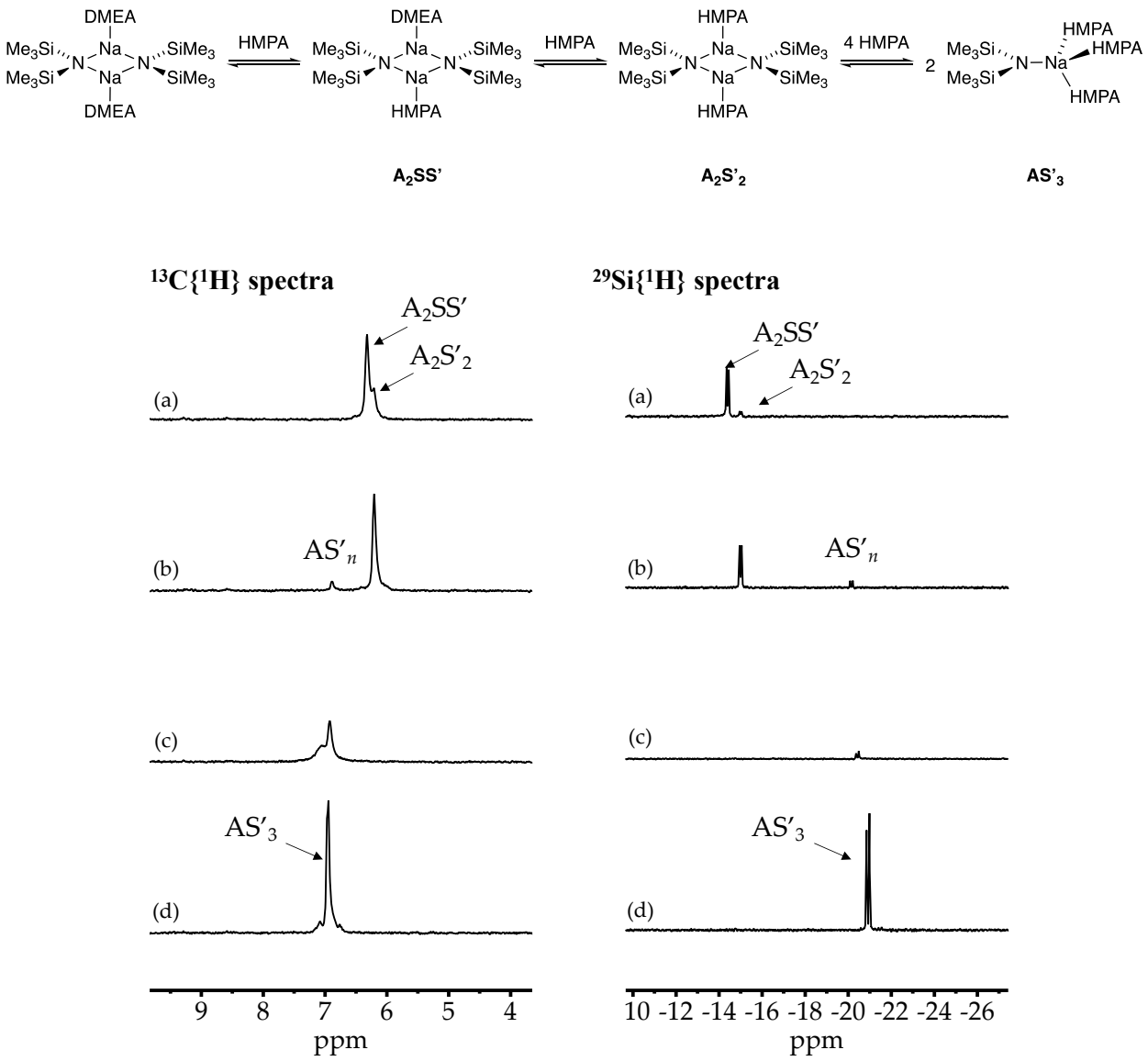
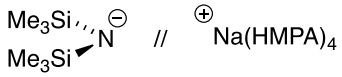


Figure S44. $^{13}C\{^1H\}$ (125.79 MHz, DMEA) and $^{29}Si\{^1H\}$ NMR (99.36 MHz, DMEA) spectra for the titration of 0.10 M NaHMDS in DMEA with HMPA at –120 °C. Equiv of HMPA for (a)–(d) are as follows: 0.6, 1.2, 3.0, and 5.0, respectively. The changing signal intensity from (c) to (d) in the ^{29}Si spectra is due to time averaged solvation states of the monomer. $^{13}C\{^1H\}$ spectra are referenced relative cyclopentane (26.01 ppm).



ion pair

$^{29}Si\{^{1}H\}$ spectra

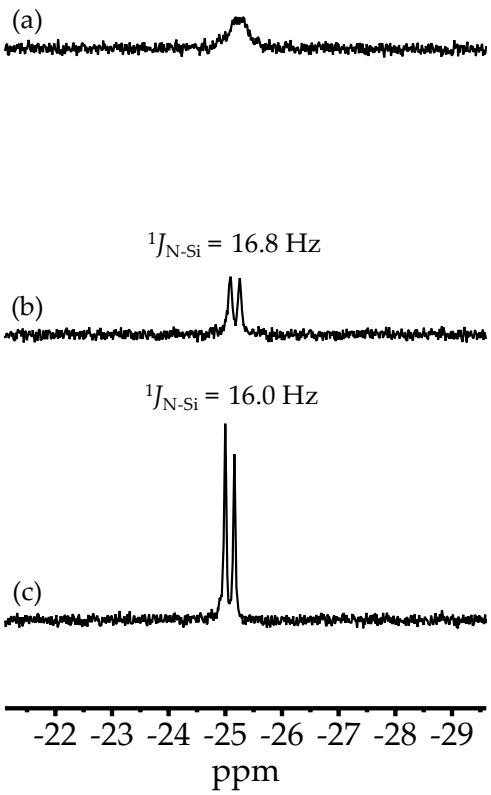
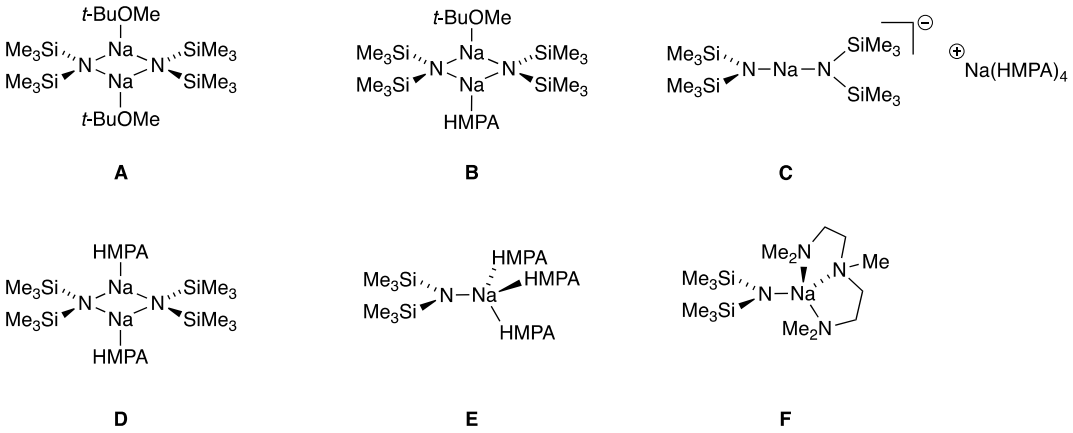


Figure S45. $^{29}Si\{^{1}H\}$ NMR (99.36 MHz, MTBE) spectra of 0.10 M NaHMDS in 2:1 HMPA:MTBE at various temperatures. Temperatures for (a)–(c) are as follows: 0 °C, 25 °C, and 40 °C, respectively. The large coupling constants in (b) and (c) suggest an ion pair. ^{29}Si spectra are referenced to TMS (0.00 ppm).



^{29}Si{^{1}H} spectra

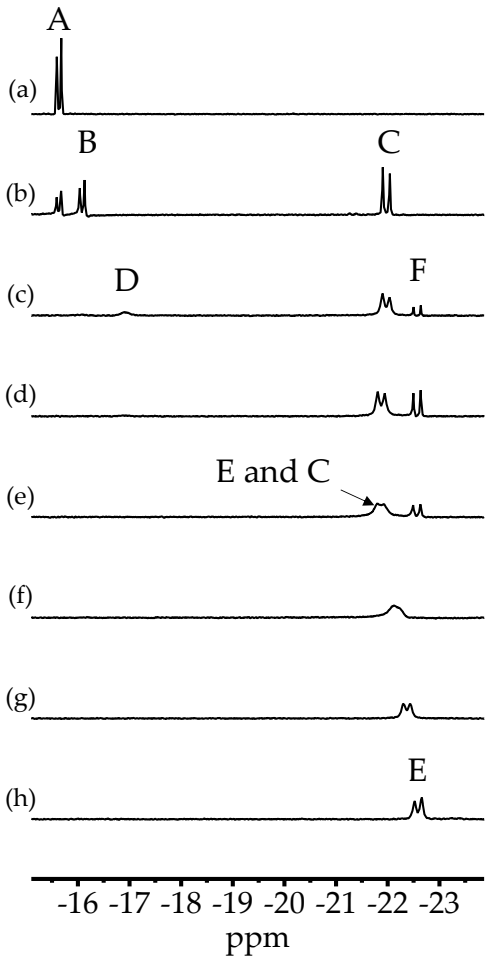
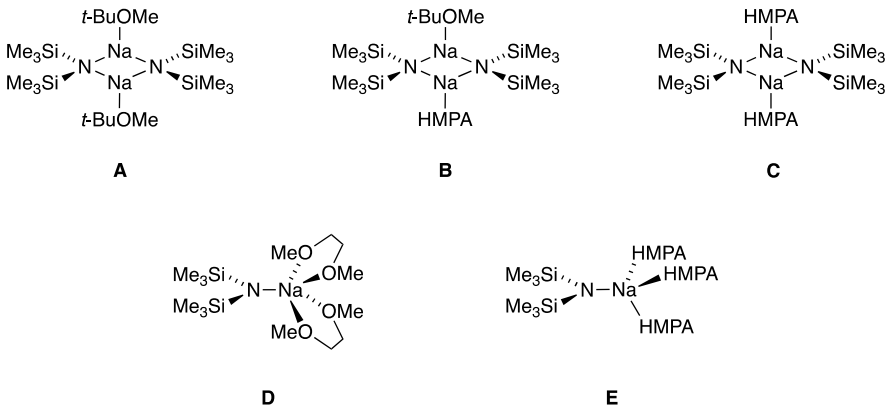


Figure S46. ^{29}Si NMR(99.36 MHz, MTBE) spectra of 0.20 M [^{15}N]NaHMDS in MTBE at –110 °C with incremental additions of 1:1 PMDTA/HMPA. The equiv of total added ligand for (a) to (h) are as follows:
0.0, 0.5, 1.0, 1.5, 2.0, 4.0, 6.0, and 10.0, respectively. ^{29}Si spectra are referenced to TMS internal standard (0.00 ppm).



^{29}Si{^{1}H} spectra

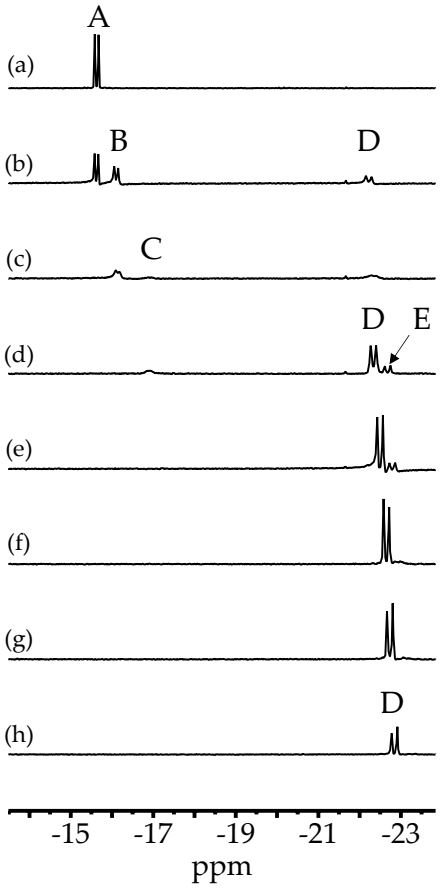


Figure S47. ^{29}Si NMR (99.36 MHz, MTBE) spectra of 0.20 M [^{15}N]NaHMDS in MTBE at –110 °C with incremental additions of 1:1 DME/HMPA. The equiv of total added ligand for (a) to (h) are as follows:
0.0, 0.5, 1.0, 2.0, 3.0, 4.0, 5.0, and 7.0, respectively. ^{29}Si spectra are referenced to TMS internal standard (0.00 ppm).

$^{31}P\{^{1}H\}$ spectra

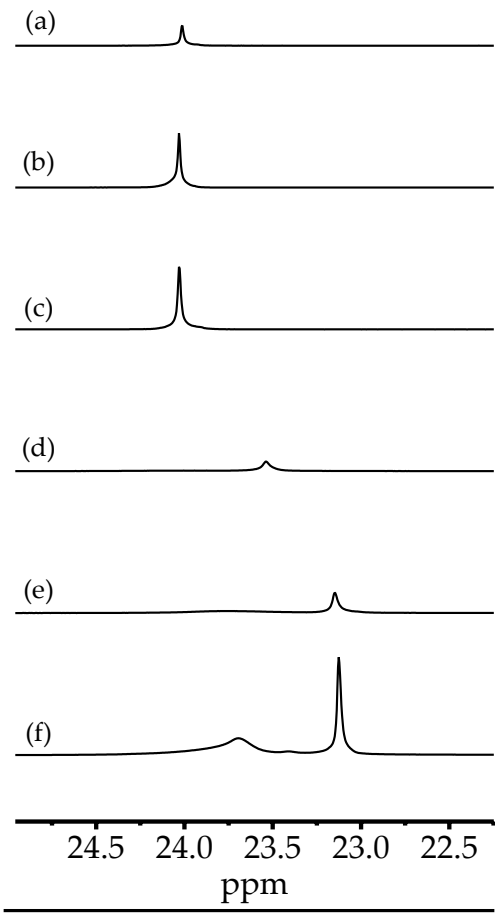


Figure S48. $^{31}P\{^{1}H\}$ (500 MHz, toluene) NMR spectra of 0.20 M [^{15}N]NaHMDS in 2:1 pentane/toluene with various quantities of HMPA at –80 °C. The equiv of HMPA for (a) to (f) are as follows:
0.3, 0.5, 0.8, 1.0, 2.0, 3.0, and 5.0 respectively.

DMPU (entry o):

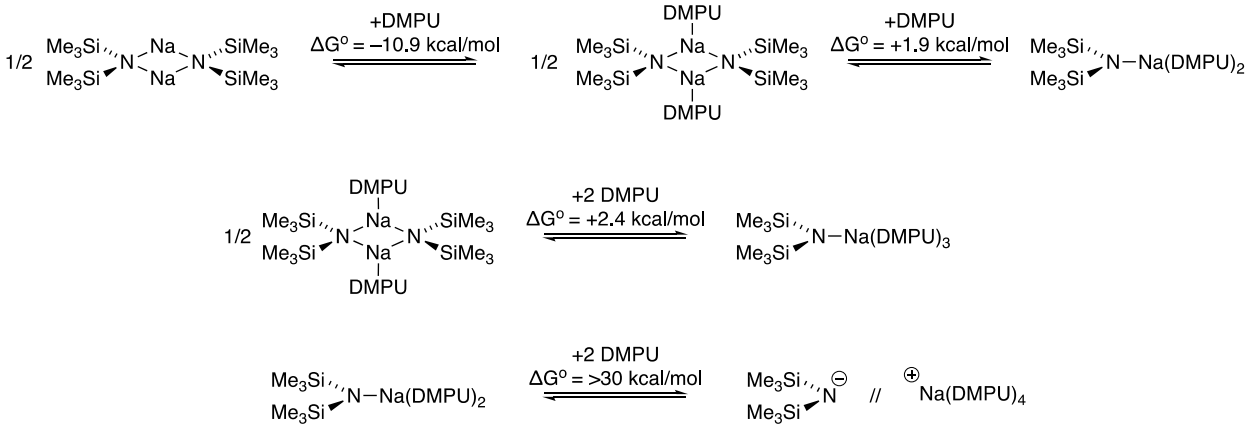
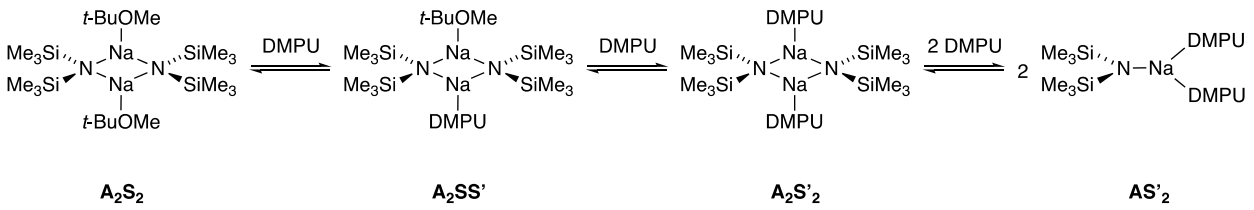


Figure S49. Computed free energies for the serial solvation of NaHMDS with DMPU.



^{29}Si{^{1}H} spectra

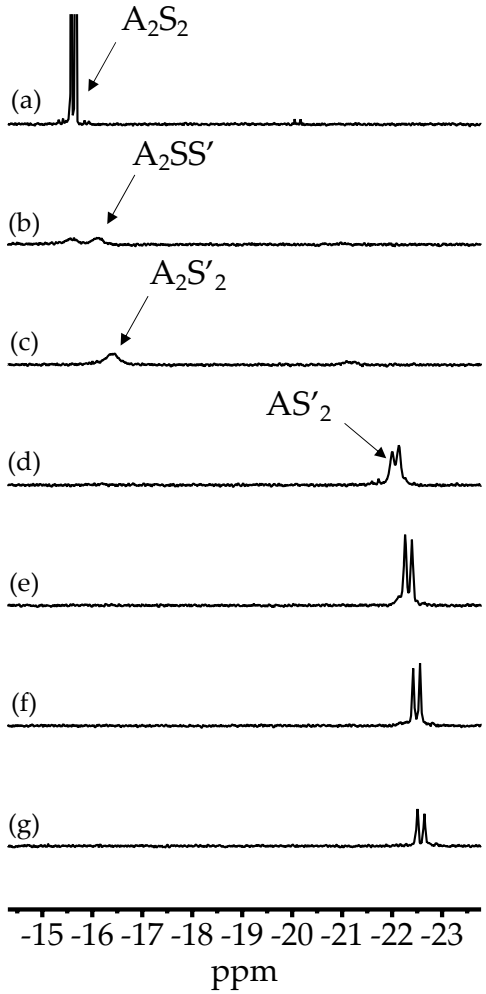
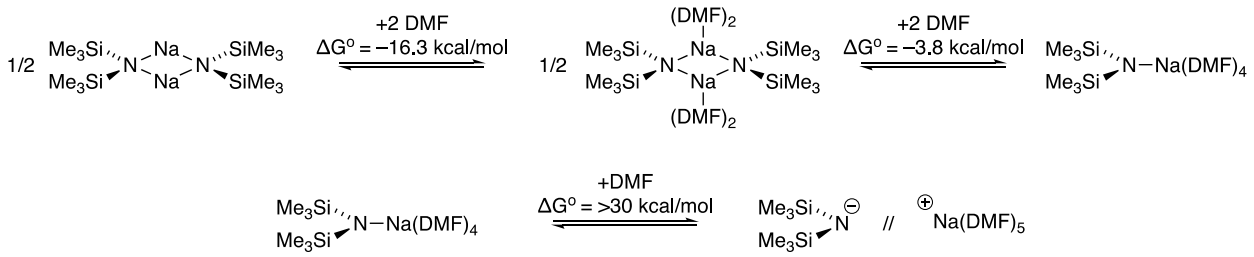


Figure S50^{29}Si{^{1}H} NMR (99.36 MHz, MTBE) spectra for the titration of 0.20 M NaHMDS in MTBE with DMPU at –110 °C. Equiv of DMPU for (a)–(g) are as follows: 0.0, 0.5, 1.0, 2.0, 3.0, 5.0 and 7.0, respectively. ^{29}Si spectra are referenced to TMS internal standard (0.00 ppm).

DMF (entry p):



^{29}Si{^{1}H} spectra

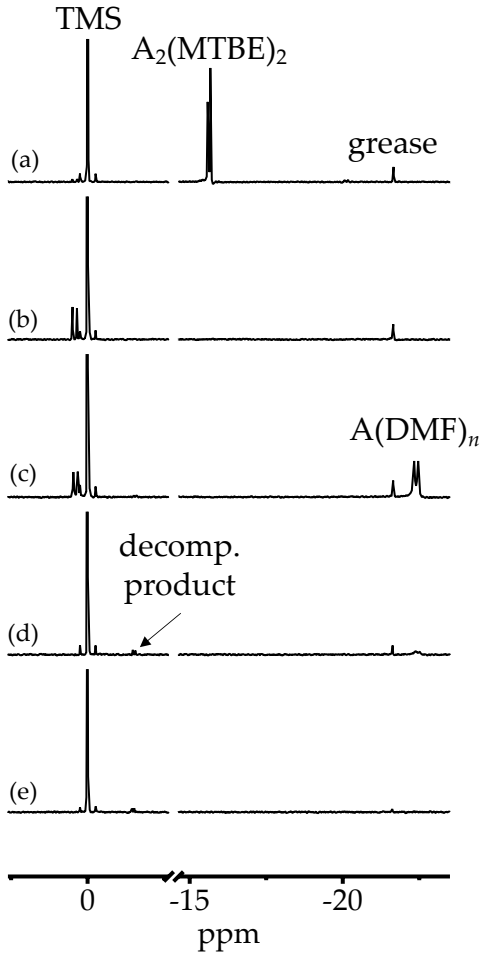
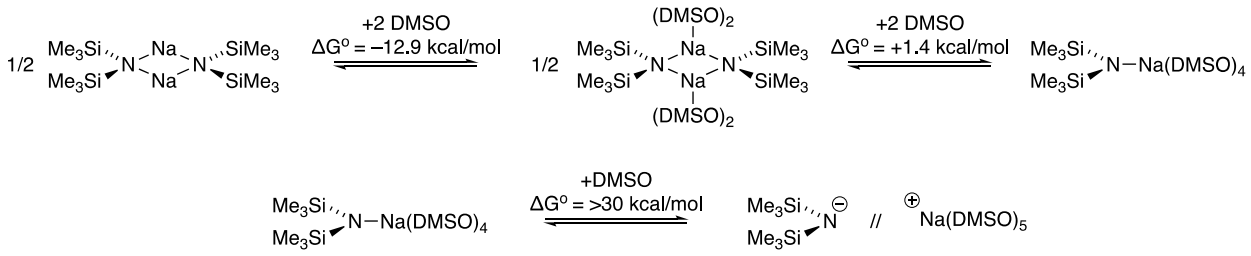


Figure S51. ^{29}Si{^{1}H} NMR (99.36 MHz, MTBE) spectra for the titration of 0.20 M NaHMDS in MTBE with DMF at –110 °C. Equiv of DMF for (a)–(e) are as follows: 0.0, 1.0, 2.0, 4.0, and 7.0, respectively. ^{9}Si spectra are referenced to TMS internal standard (0.00 ppm).

DMSO (entry q):



^{29}Si{^{1}H} spectra

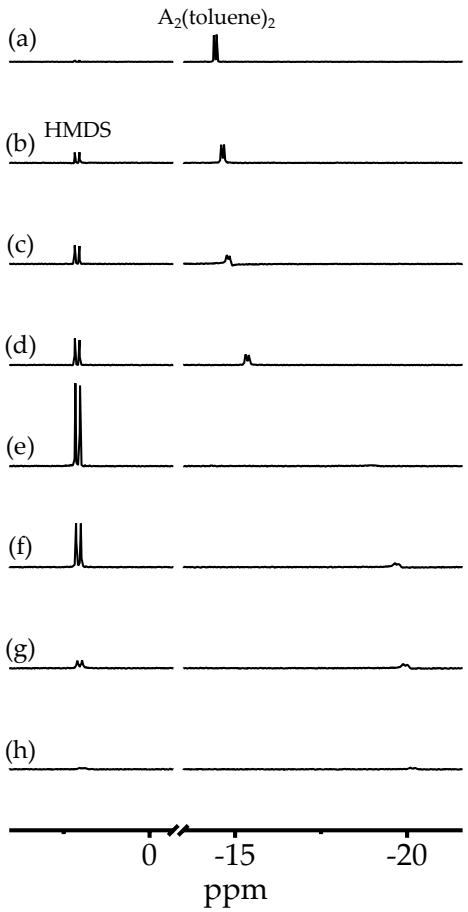
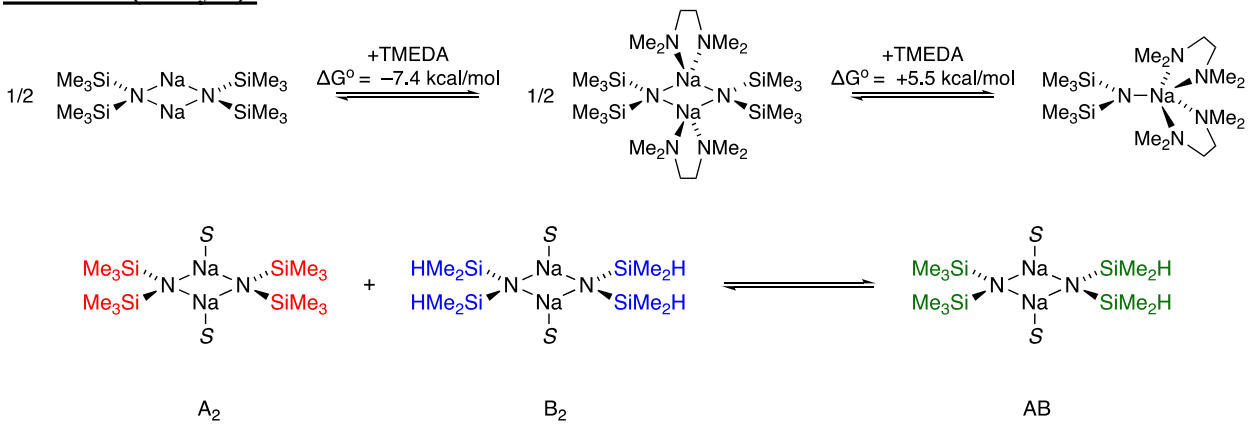


Figure S52. ^{29}Si{^{1}H} (99.36 MHz, toluene) NMR spectra for the titration of 0.10 M NaHMDS in toluene with DMSO at –80 °C. Equiv of DMSO for (a)–(h) are as follows: 0.0, 0.2, 0.4, 0.8, 0.9, 1.3, 2.0, and 3.0, respectively. The increasing intensity of the HMDS signal is most likely due to the formation of dimsyl sodium. ^{29}Si spectra are referenced to trace HMDS present in tube (1.78 ppm).

TMEDA (entry r):



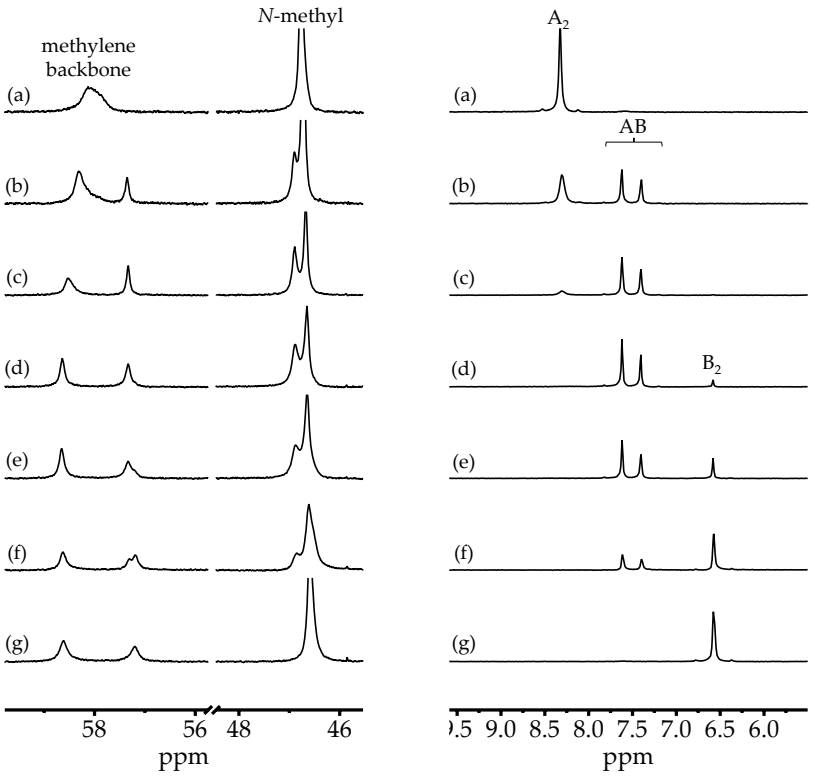


Figure S53. $^{13}C\{^1H\}$ NMR (125.79 MHz, toluene) relative integrations of NaHMDS-derived homodimer (A_2), NaTMDS-derived homodimer (B_2), and heterodimer (AB) versus the measured mole fraction of NaHMDS (X_{NaHMDS}) at 0.30 total molarity in 0.60 M TMEDA in toluene cosolvent at –100 °C. The measured mole fractions, X_{NaHMDS}, in (a)–(g) are 1.00, 0.80, 0.60, 0.50, 0.40, 0.20, and 0.00, respectively. Free and bound TMEDA is observable for both heterodimer AB and NaTMDS homodimer B_2 as evident in the 2 methylene signals. Integration of the more upfield methylene signal results in a 1:1 ratio of for both heterodimer AB and NaTMDS homodimer B_2. $^{13}C\{^1H\}$ spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).

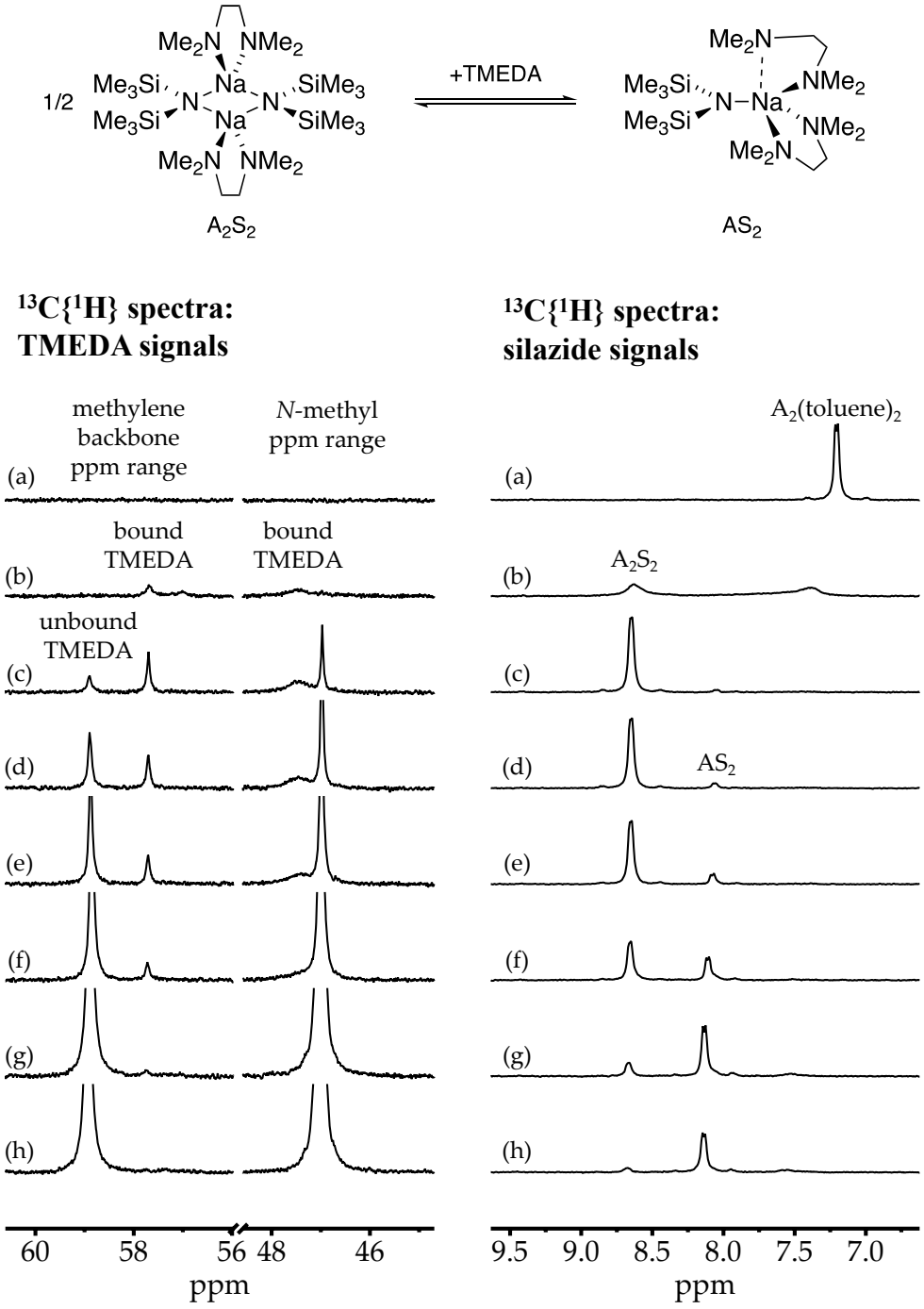


Figure S54. $^{13}C\{^{1}H\}$ NMR (125.79 MHz, toluene) spectra of 0.12 M [^{15}N]NaHMDS in 2:1 pentane/toluene-d_8 cosolvent with varying amounts of TMEDA added at –120 °C. The equivalents of TMEDA for (a)–(h) are as follows: 0.00, 0.68, 0.89, 1.26, 2.04, 4.00, 7.18, 8.76, and 14.59 equiv, respectively. $^{13}C\{^{1}H\}$ spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).

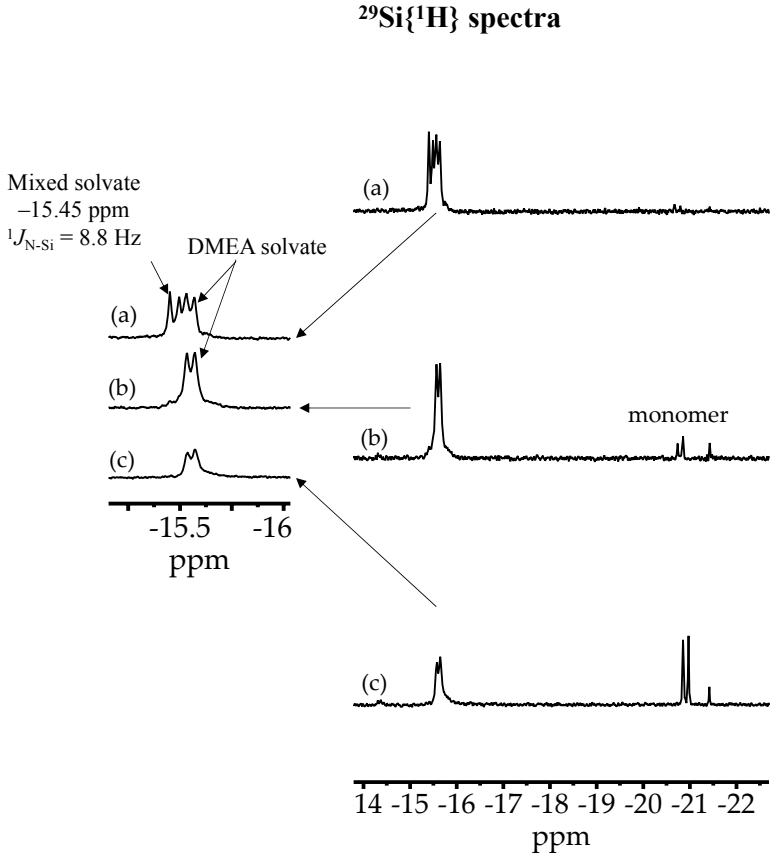


Figure S55. ^{29}Si NMR (99.36 MHz, DMEA) spectra of 0.15 M [^{15}N]NaHMDS in DMEA cosolvent with varying amounts of TMEDA added at –120 °C. The equivalents of TMEDA for (a)–(c) are as follows: 0.7, 1.2, and 3.0 equiv, respectively.

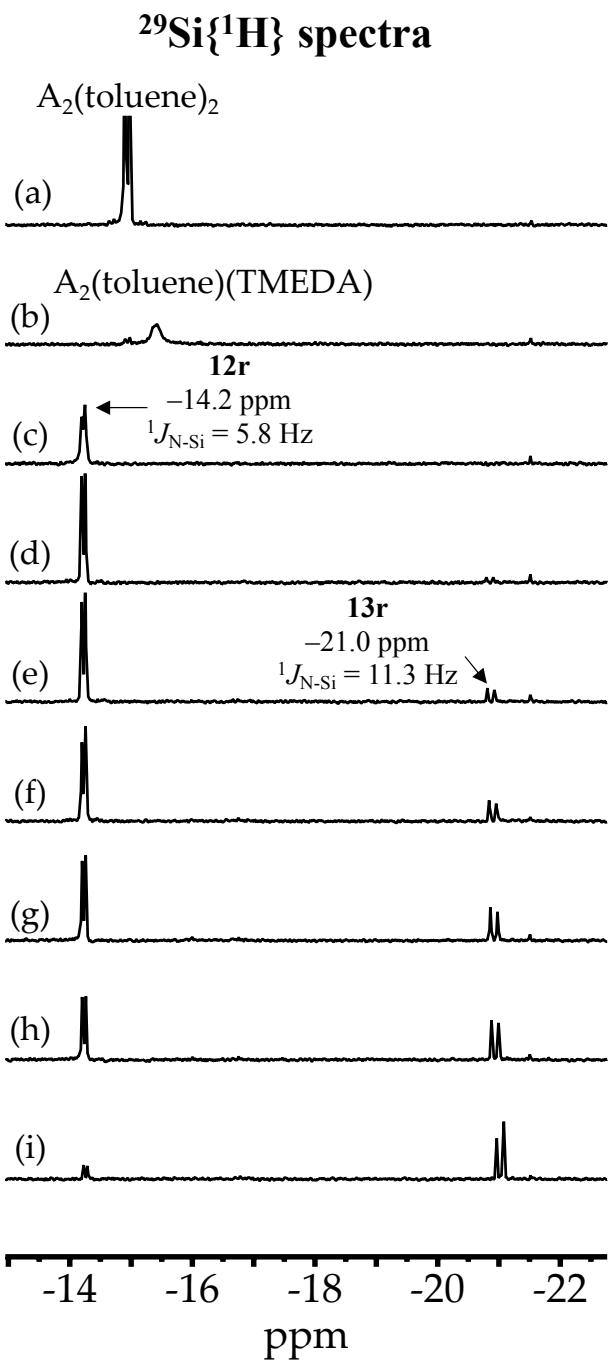


Figure S56. $^{29}Si\{^{1}H\}$ NMR (99.36 MHz, toluene) spectra of 0.10 M [^{15}N]NaHMDS in 2:1 pentane/toluene-d_8 cosolvent with varying amounts of TMEDA added at –120 °C. The equivalents of TMEDA for (a)–(i) are as follows: 0.00, 0.5, 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, and 10.0 equiv, respectively.

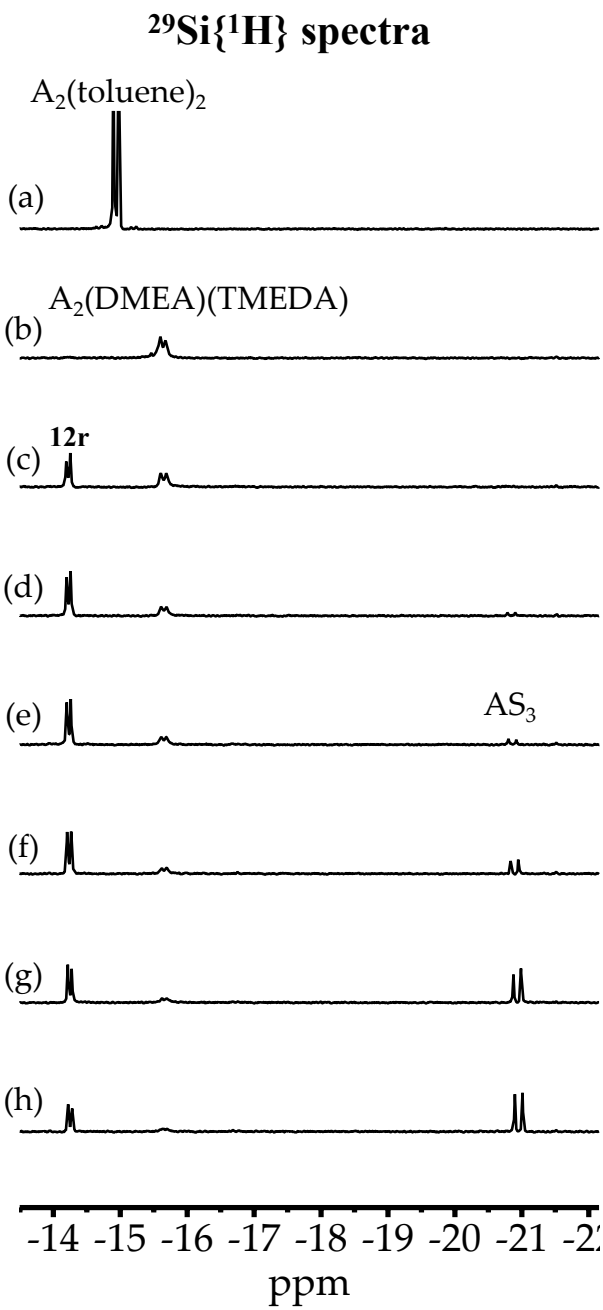


Figure S57 $^{29}Si\{^{1}H\}$ NMR(99.36 MHz, toluene) spectra of 0.10 M [^{15}N]NaHMDS in 2:1 pentane/toluene at –120 °C with incremental additions of 1:1 TMEDA/DMEA. The equiv of total added ligand from (a)-(h) are 0.0, 1.0, 2.0, 3.0, 4.0, 6.0, 10.0, and 14.0 equiv respectively.

^{29}Si{^{1}H} spectra

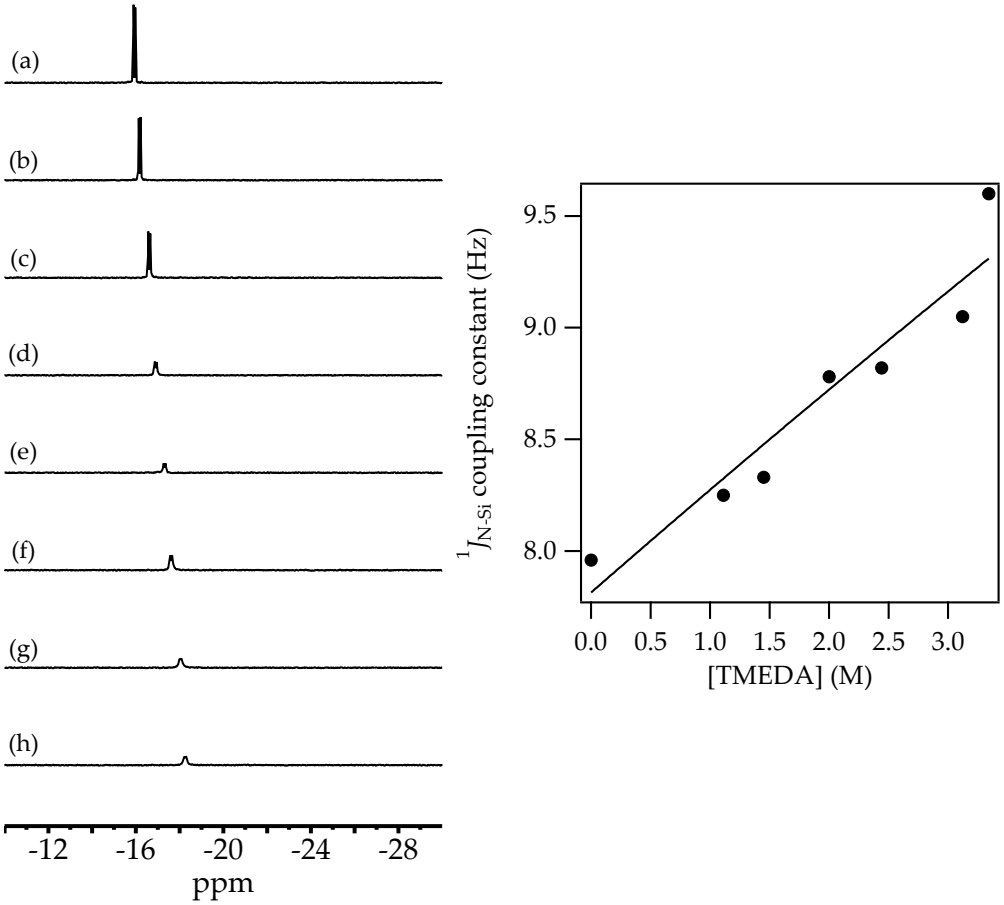


Figure S58. ^{29}Si{^{1}H} NMR (99.36 MHz, toluene) spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of TMEDA at –20 °C. TMEDA concentration for (a)–(h) are as follows: 0.00, 1.11, 1.45, 2.00, 2.44, 3.12, and 3.34, respectively. The curve is fit to the function described in the "Derivation" section of this Supporting Information on page S-117 with $n = 1$.

[TMEDA] (M)	$^{1}J_{N-Si}$ coupling constant (Hz)
0.00	7.96
1.11	8.25
1.45	8.33
2.00	8.78
2.44	8.82
3.12	9.05
3.34	9.60

(*R*, *R*)-TMCDA (entry s):

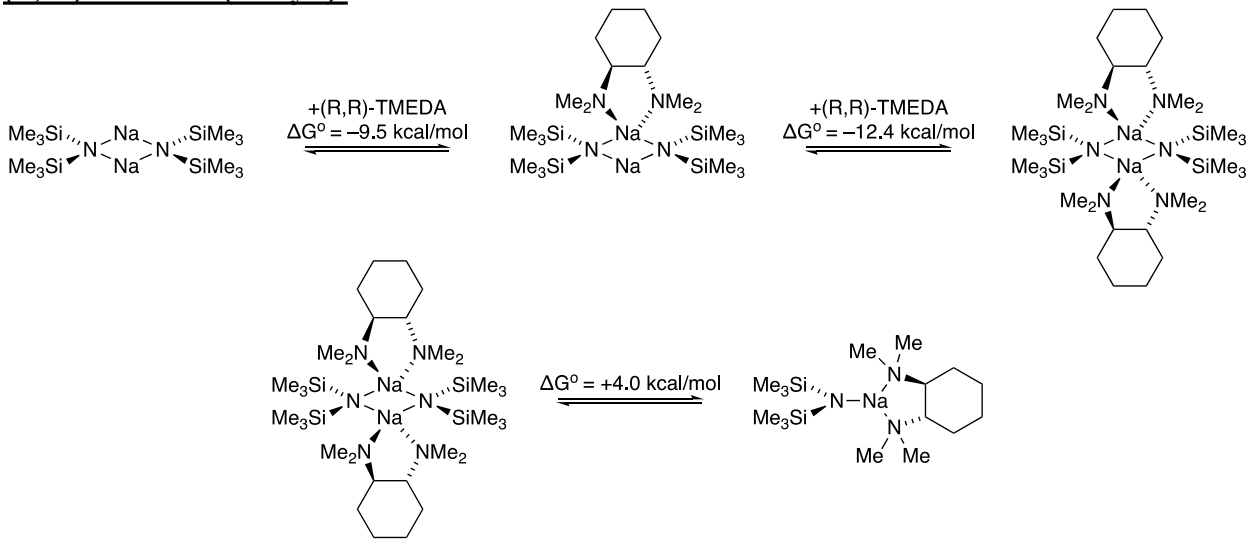


Figure S59. Computed free energies for the serial solvation of NaHMDS with TMCDA.

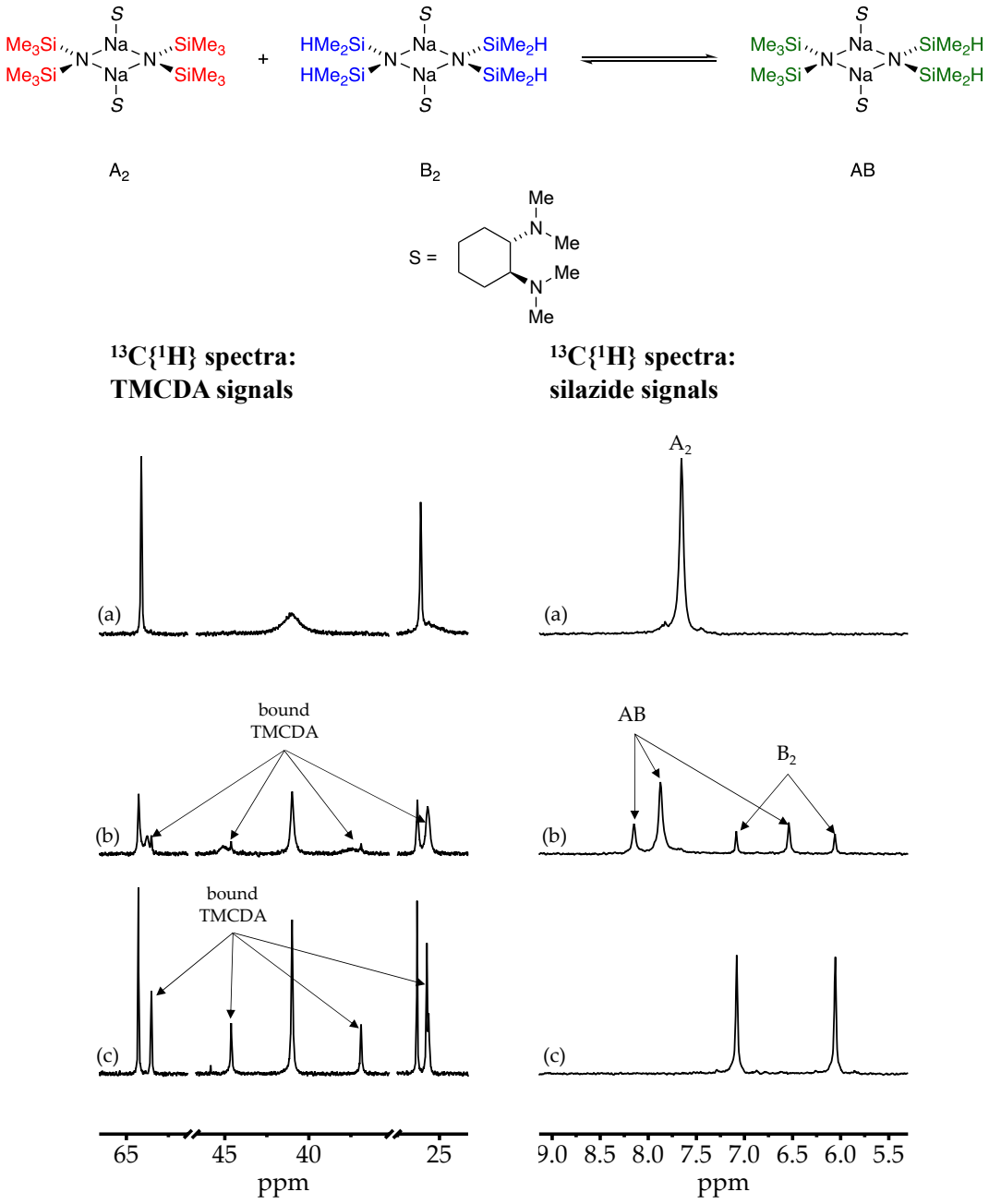


Figure S60. $^{13}C\{^1H\}$ NMR (125.79 MHz, toluene) relative integrations of NaHMDS-derived homodimer (A_2), NaTMDS-derived homodimer (B_2), and heterodimer (AB) versus the measured mole fraction of NaHMDS (X_{NaHMDS}) at 0.20 total molarity in 0.40 M (*R*,*R*)-TMCDA in toluene-d_8 cosolvent at −80 °C. The measured mole fractions, X_{NaHMDS}, in (a)–(c) are 1.00, 0.50, and 0.00, respectively. Free and bound TMCDA is observable for both heterodimer AB and NaTMDS homodimer B_2 as evident in the methylene and methyl signals noted above (methylene = red and blue; methyl = green). Integration of the these signals for the NaTMDS homodimer shows a 1:1 ratio of silazide to TMCDA.

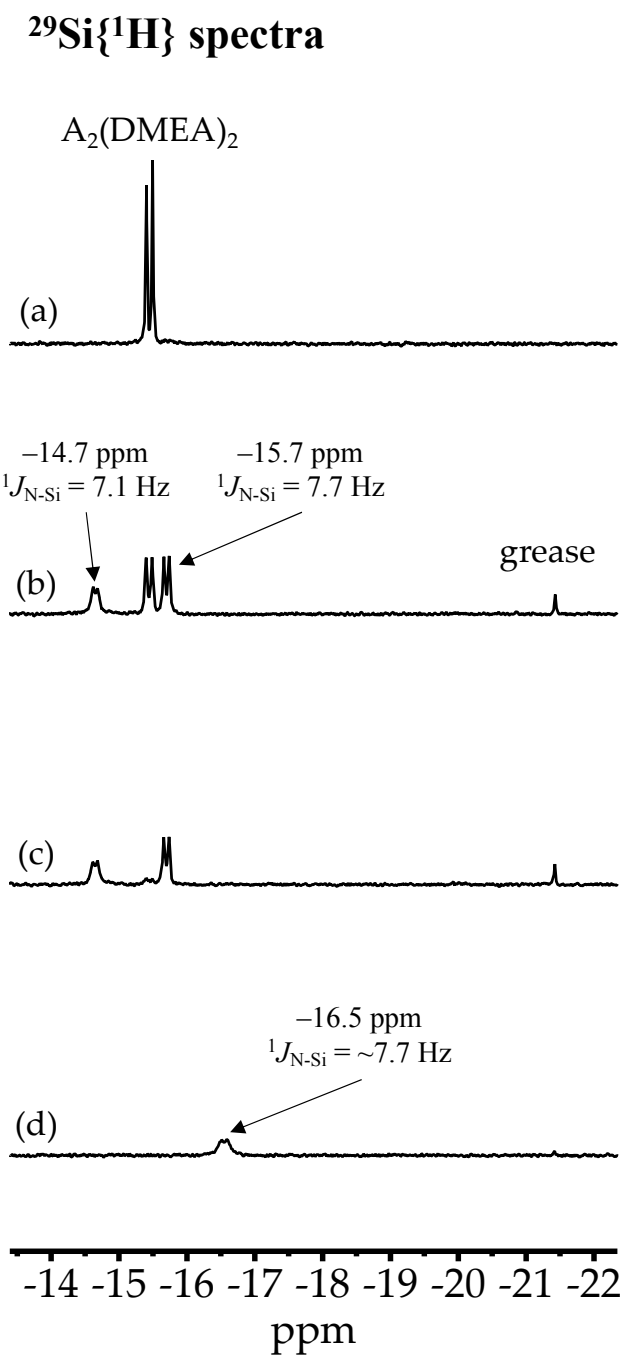


Figure S61. ^{29}Si NMR (99.36 MHz, DMEA) spectra of 0.15 M [^{15}N]NaHMDS in DMEA cosolvent with varying amounts of TMCDA added at –120 °C. The equivalents of TMCDA for (a)–(c) are as follows: 0.0, 0.5, and 3.0 equiv, respectively. Spectrum (d) consists of 0.15 M [^{15}N]NaHMDS in neat TMCDA at 25 °C.

(–)-sparteine (26):

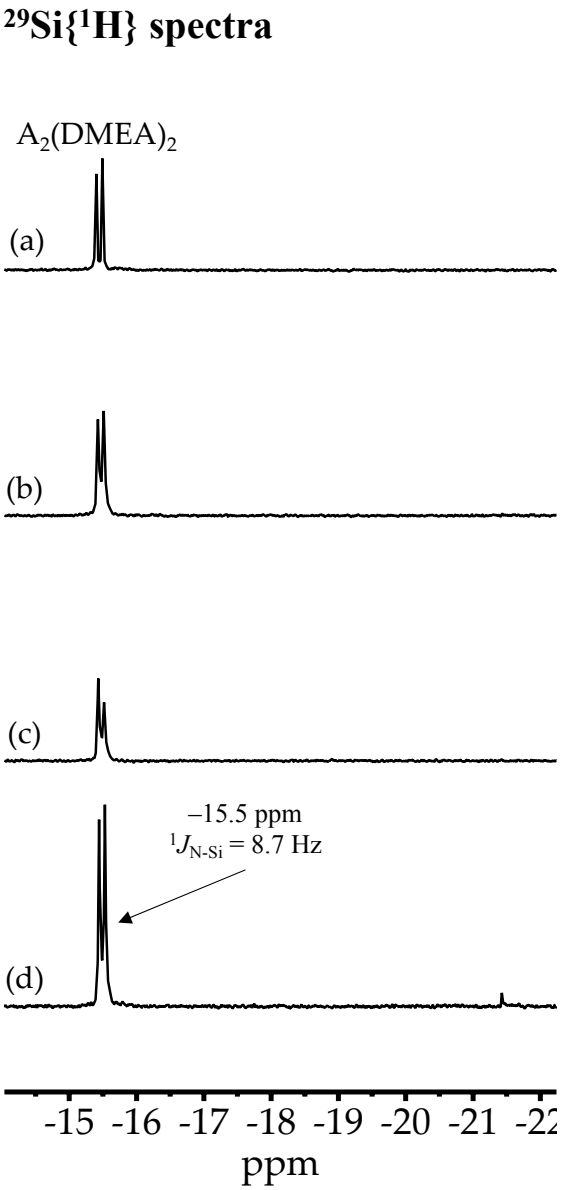


Figure S62. ^{29}Si NMR (99.36 MHz, DMEA) spectra of 0.15 M [^{15}N]NaHMDS in DMEA cosolvent with varying amounts of sparteine added at –120 °C. The equivalents of sparteine for (a)–(d) are as follows: 0.0, 0.5, 1.0, and 3.0 equiv, respectively. The shift and coupling constant even with 3.0 equivalents of sparteine indicate a lack of binding to NaHMDS even in trialkylamines.

bipy (entry u):

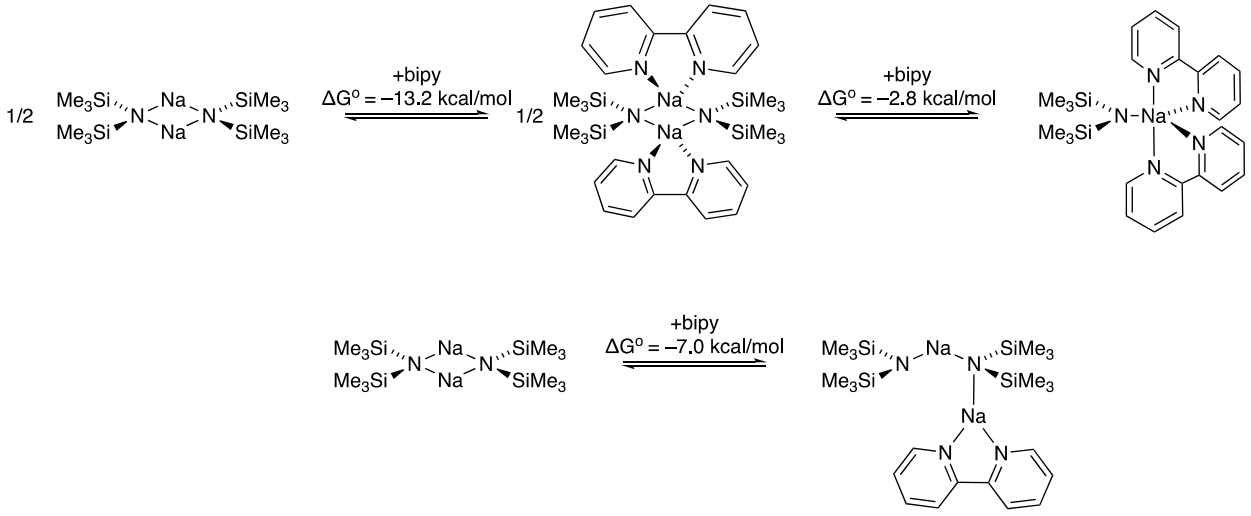


Figure S63. Computed free energies for the serial solvation of NaHMDS with bipy.

^{29}Si{^{1}H} spectra

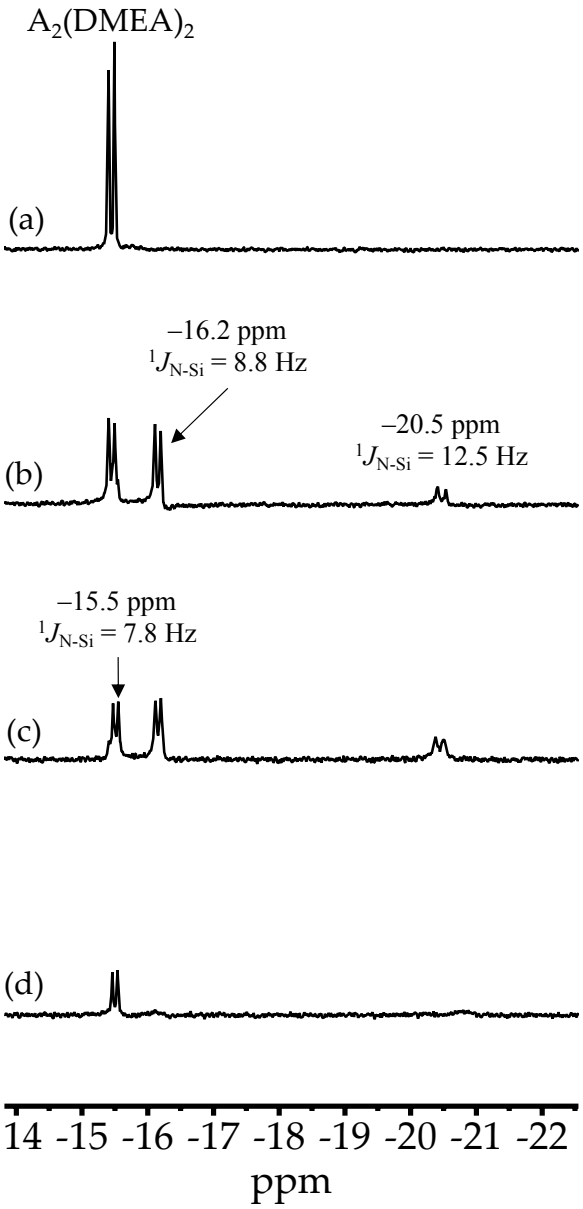


Figure S64. ^{29}Si NMR (99.36 MHz, DMEA) spectra of 0.10 M [^{15}N]NaHMDS in DMEA cosolvent with varying amounts of bipy added at –120 °C. The equivalents of bipy for (a)–(d) are as follows: 0.0, 0.5, 1.0, and 3.0 equiv, respectively. Spectra (b) and (c) show DMEA disolvated dimer, bipy disolvated dimer, and a proposed mixed solvated open dimer based on the two most upfield signals.

DME (entry v):

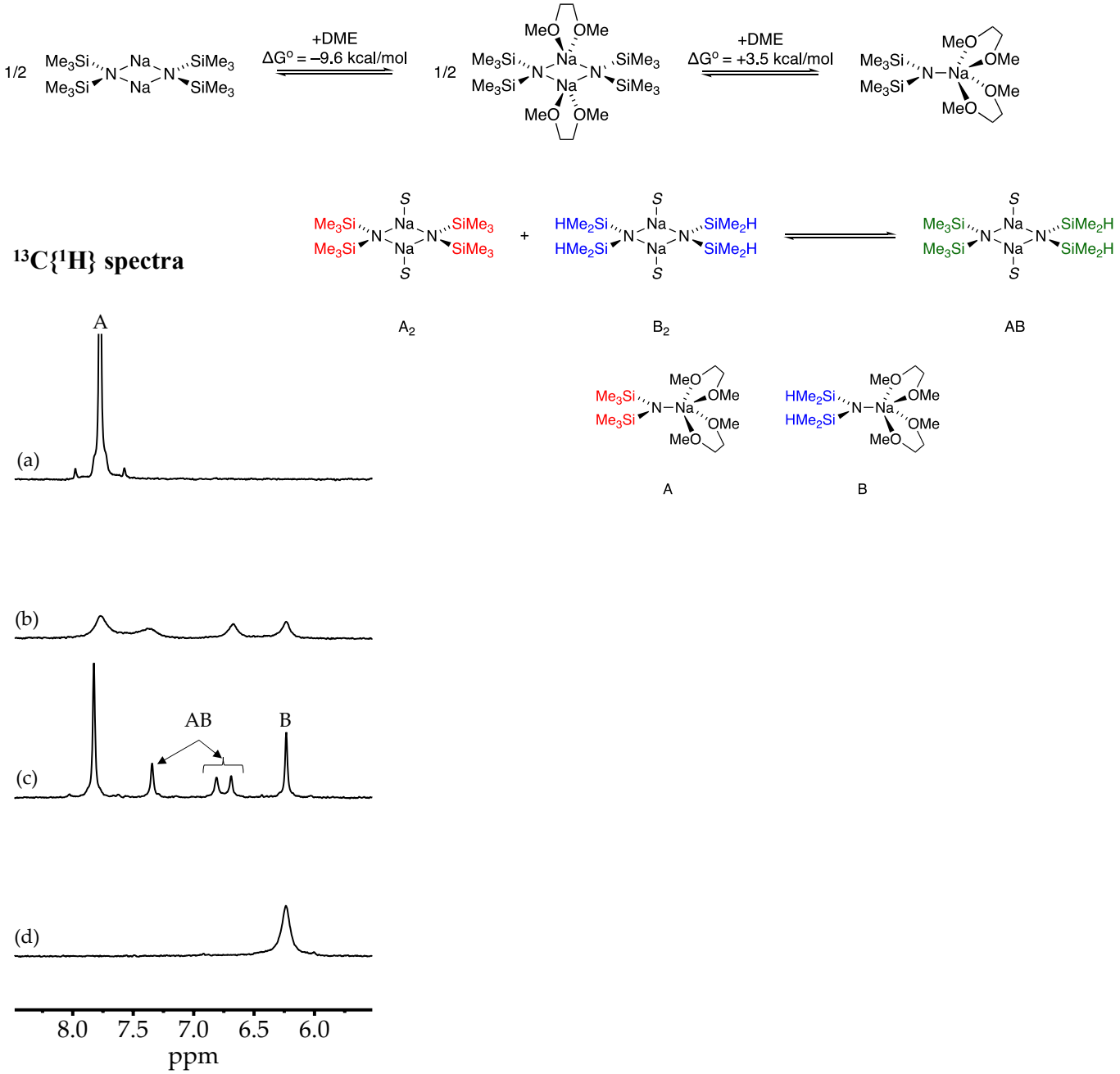


Figure S65. $^{13}C\{^{1}H\}$ NMR (125.79 MHz, toluene) relative integrations of NaHMDS-derived homodimer (A_2), NaTMDS-derived homodimer (B_2), and heterodimer (AB) versus the measured mole fraction of NaHMDS (X_{NaHMDS}) at 0.20 total molarity in 0.40 M DME in toluene cosolvent at −80 °C or −100 °C (only spectrum (c)). The measured mole fractions, X_{NaHMDS}, in (a)–(d) are 1.00, 0.50, 0.50, and 0.00, respectively.

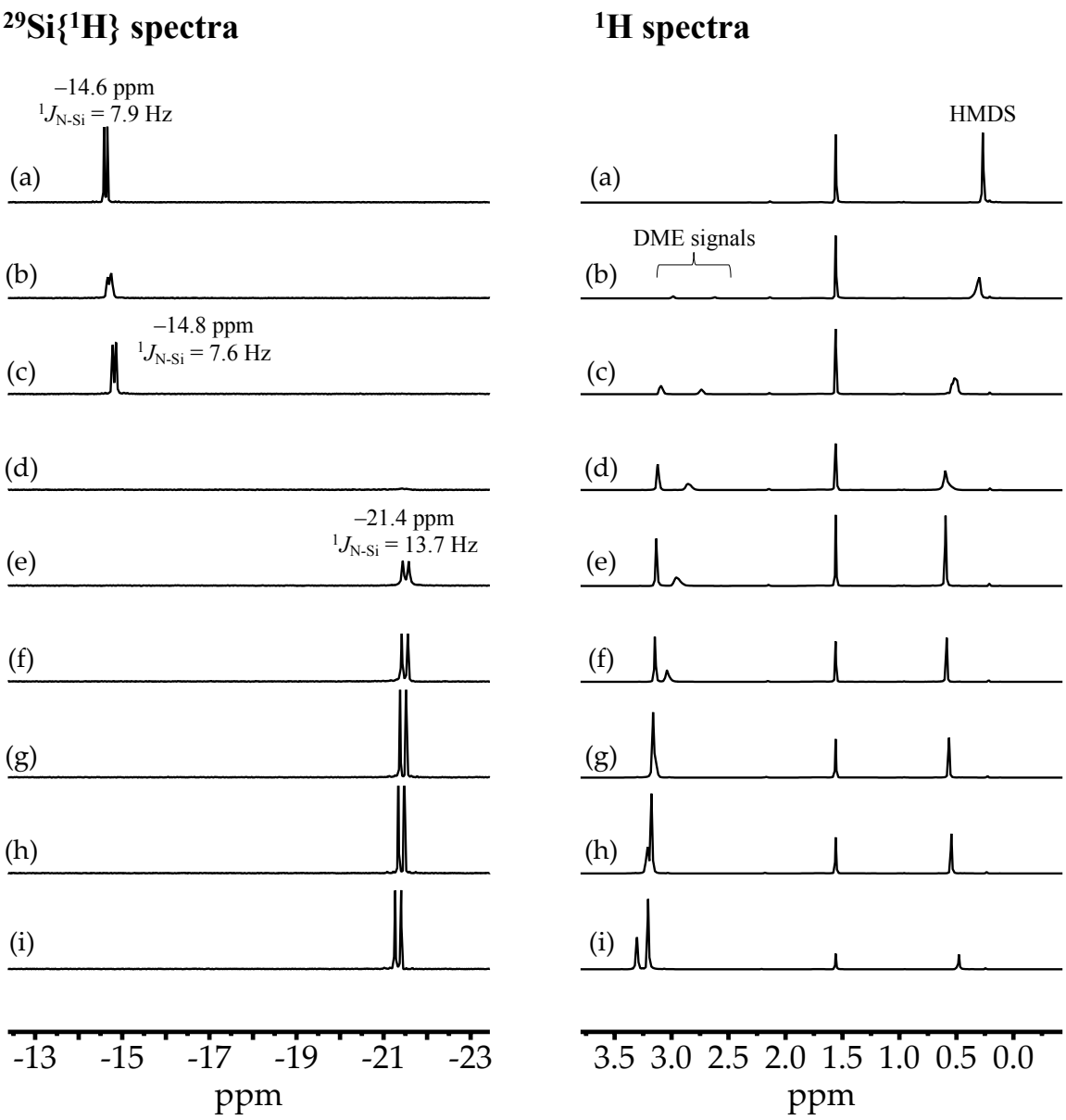


Figure S66. ^{1}H (500 MHz, toluene) and ^{29}Si{^{1}H} NMR (99.36 MHz, toluene) spectra for the titration of 0.20 M [^{15}N]NaHMDS in toluene-d_8 with DME at –80 °C. Equiv of DME for (a)–(i) are as follows: 0.0, 0.2, 0.9, 1.9, 2.8, 3.6, 5.4, 7.4, and 14.0, respectively.

^{29}Si{^{1}H} spectra

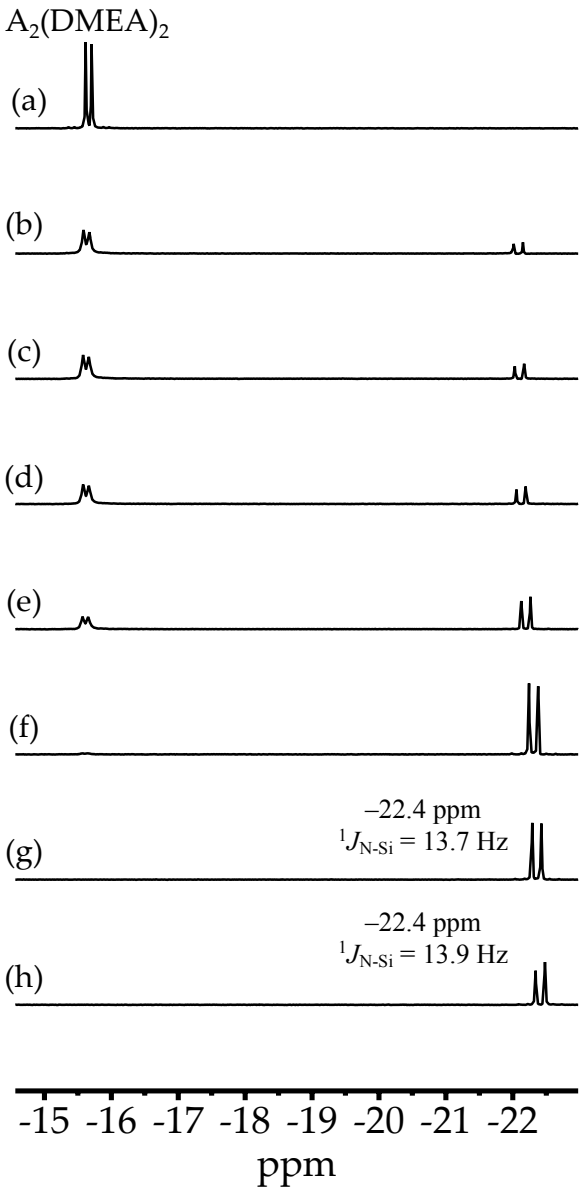


Figure S67. ^{29}Si NMR (99.36 MHz, DMEA) spectra of 0.20 M [^{15}N]NaHMDS in DMEA cosolvent with varying amounts of DME added at –120 °C. The equivalents of DME for (a)–(h) are as follows: 0.0, 0.5, 1.0, 1.5, 2.0, 3.0, 4.0, and 7.0 equiv, respectively.

^{29}Si{^{1}H} spectra

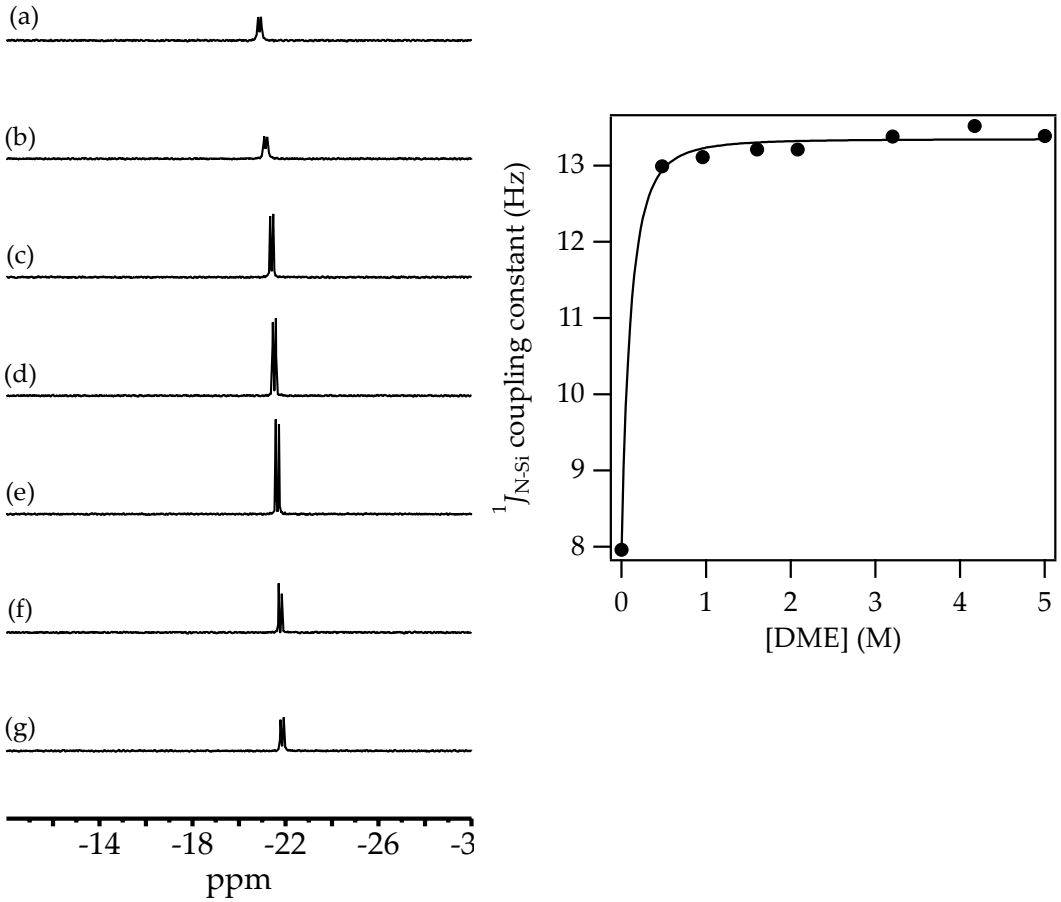


Figure S68. ^{29}Si{^{1}H} NMR (99.36 MHz, toluene) spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of DME at –20 °C. DME concentrations for (a)–(g) are as follows: 0.48, 0.96, 1.60, 2.08, 3.20, 4.17, and 5.00, respectively. The curve is fit to the function described in the "Derivation" section of this Supporting Information on page S-117 with $n = 1$.

[TMEDA] (M)	$^{1}J_{N–Si}$ coupling constant (Hz)
0.00	7.96
0.48	12.95
0.96	13.08
1.60	13.22
2.08	13.19
3.20	13.40
4.17	13.52
5.00	13.35

$^{29}Si\{^{1}H\}$ spectra

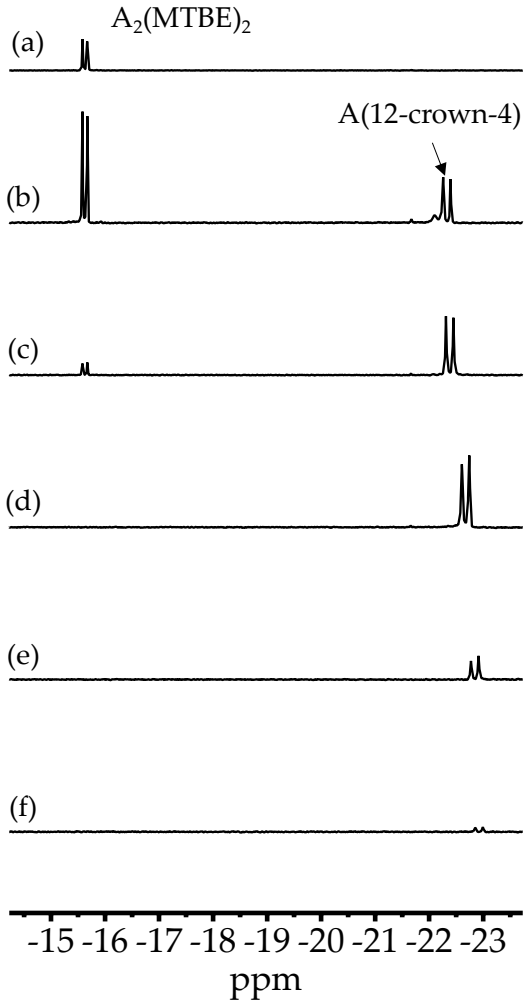


Figure S69. ^{29}Si NMR (99.36 MHz, MTBE) spectra of 0.20 M [^{15}N]NaHMDS in MTBE at –110 °C with incremental additions of 1:1 DME/12-crown-4. The equiv of total added ligand for (a)–(f) are as follows: 0.0, 0.5, 1.0, 2.0, 4.0, and 6.0 total equiv, respectively. Loss of signal in (f) is due to preferential crown binding and subsequent precipitation of this crown complex.

NIPA (26):

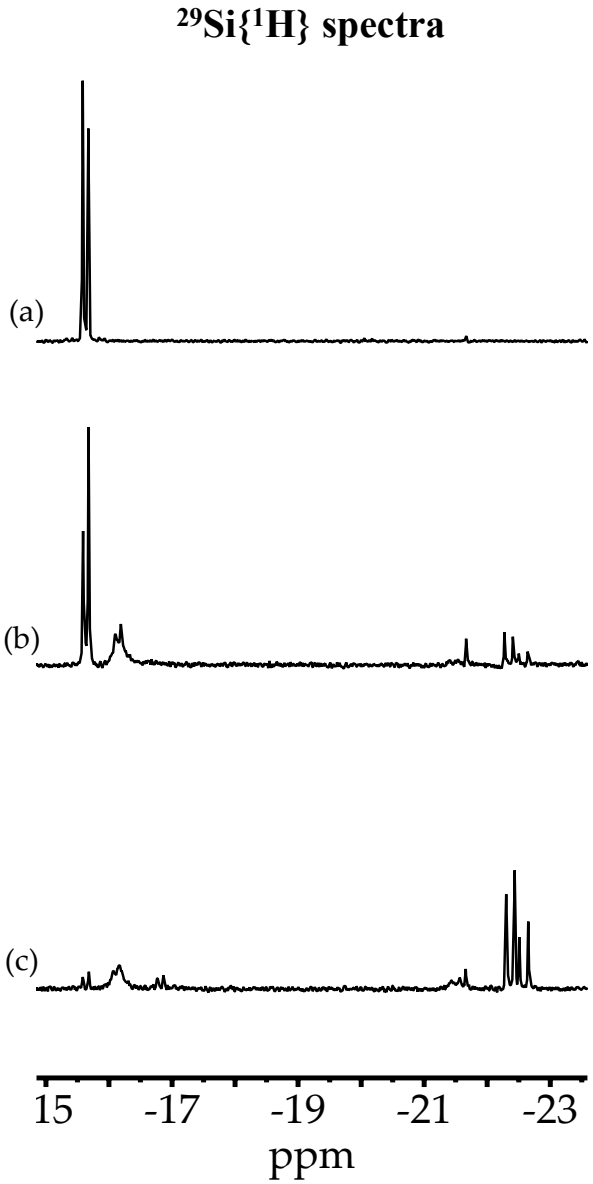
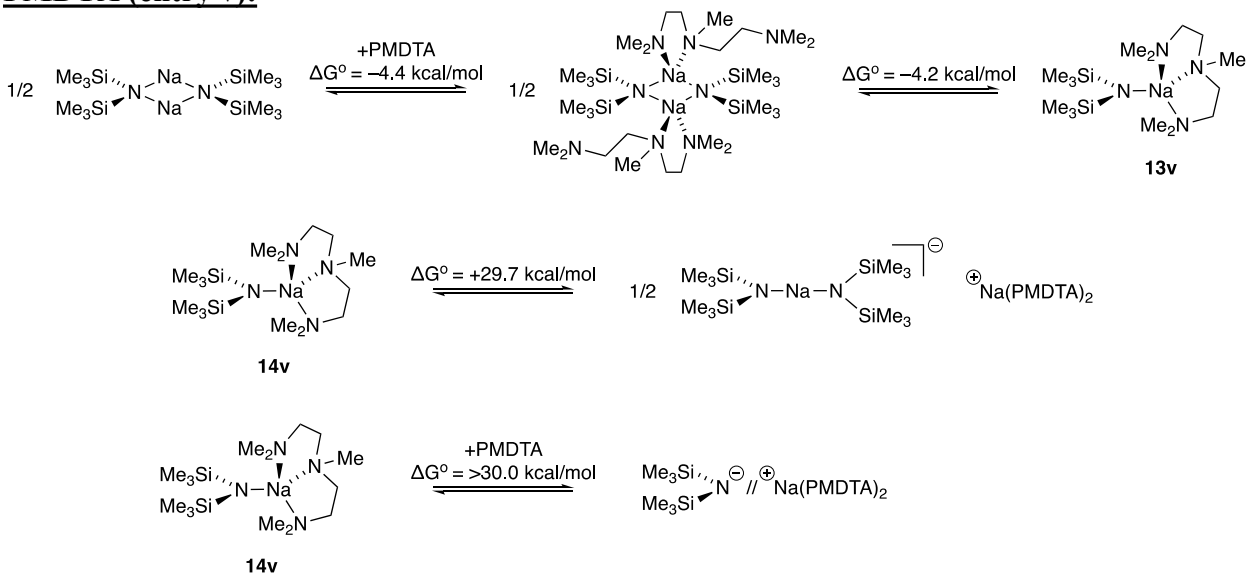


Figure S70. ^{29}Si NMR (99.36 MHz, MTBE) spectra of 0.20 M [^{15}N]NaHMDS in MTBE at –110 °C with incremental additions NIPA. The equiv of total NIPA for (a)–(c) are as follows: 0.0, 0.5, and 1.0 equiv, respectively. A white precipitate was present at the bottom of the NMR tube following the final addition of NIPA.

PMDTA (entry v):



^{29}Si{^{1}H} spectrum **^{13}C{^{1}H} spectrum** **^{15}N{^{1}H} spectrum**

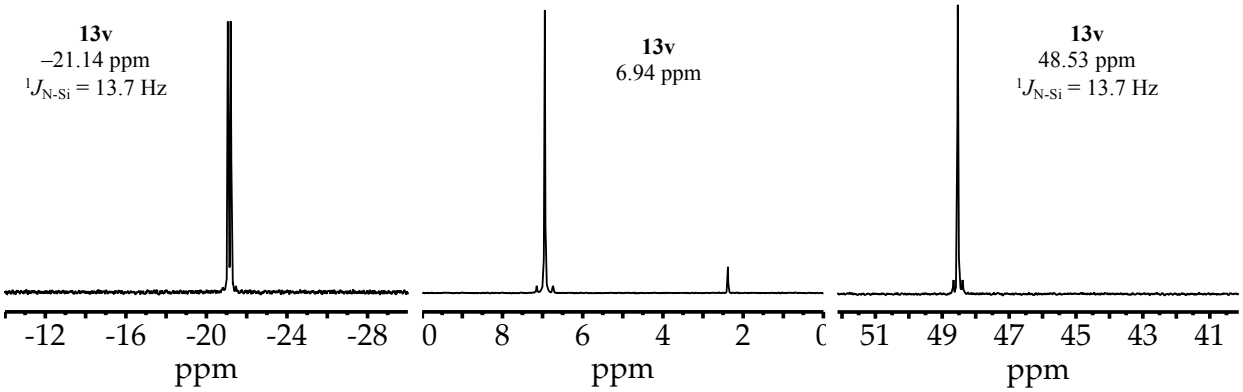


Figure S71. NMR spectra of [^{15}N]NaHMDS (^{29}Si and ^{15}N) and NaHMDS (^{13}C{^{1}H}) with at least 2 equiv PMDTA per sodium in toluene-d_8 cosolvent at –80 °C. Concentrations vary from 0.20 M NaHMDS (^{15}N) to 0.30 M NaHMDS (^{29}Si and ^{13}C{^{1}H}). Standard ^{13}C, ^{15}N, and ^{29}Si spectra were recorded on a 500 MHz spectrometer at 125.79, 50.66, and 99.36 MHz, respectively.

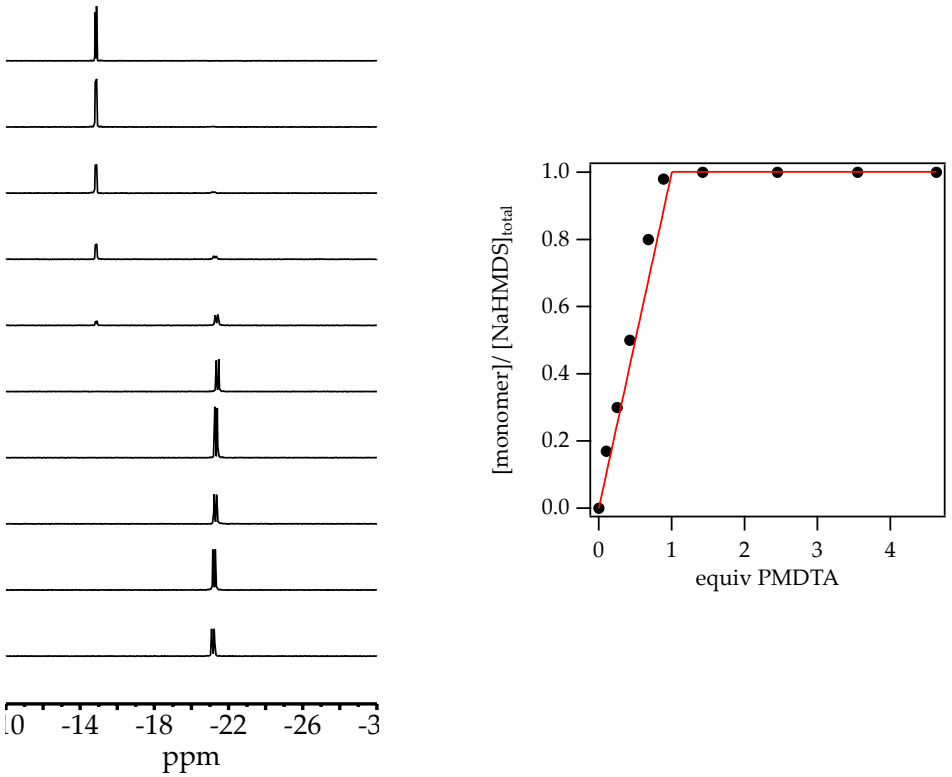


Figure S72. ^{29}Si NMR (99.36 MHz, toluene) spectra for 0.30 M solution of NaHMDS in toluene-d_8 with varying [PMDTA] at –80 °C and cyclopentane as an internal standard. The plot corresponds to the monomer concentration as a function equivalents of PMDTA added.

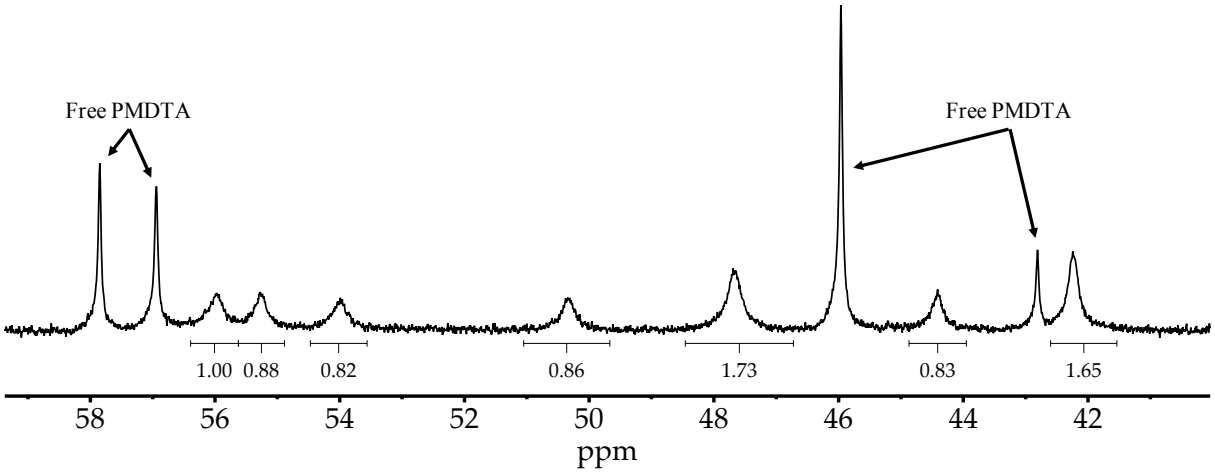


Figure S73. $^{13}C\{^{1}H\}$ NMR (125.79 MHz, toluene) spectrum highlighting PMDTA in the slow-exchange limit under the following conditions: 0.30 M NaHMDS in 1:1 pentane/toluene-d_8 cosolvent with 2.0 equiv of added PMDTA at –120 °C.

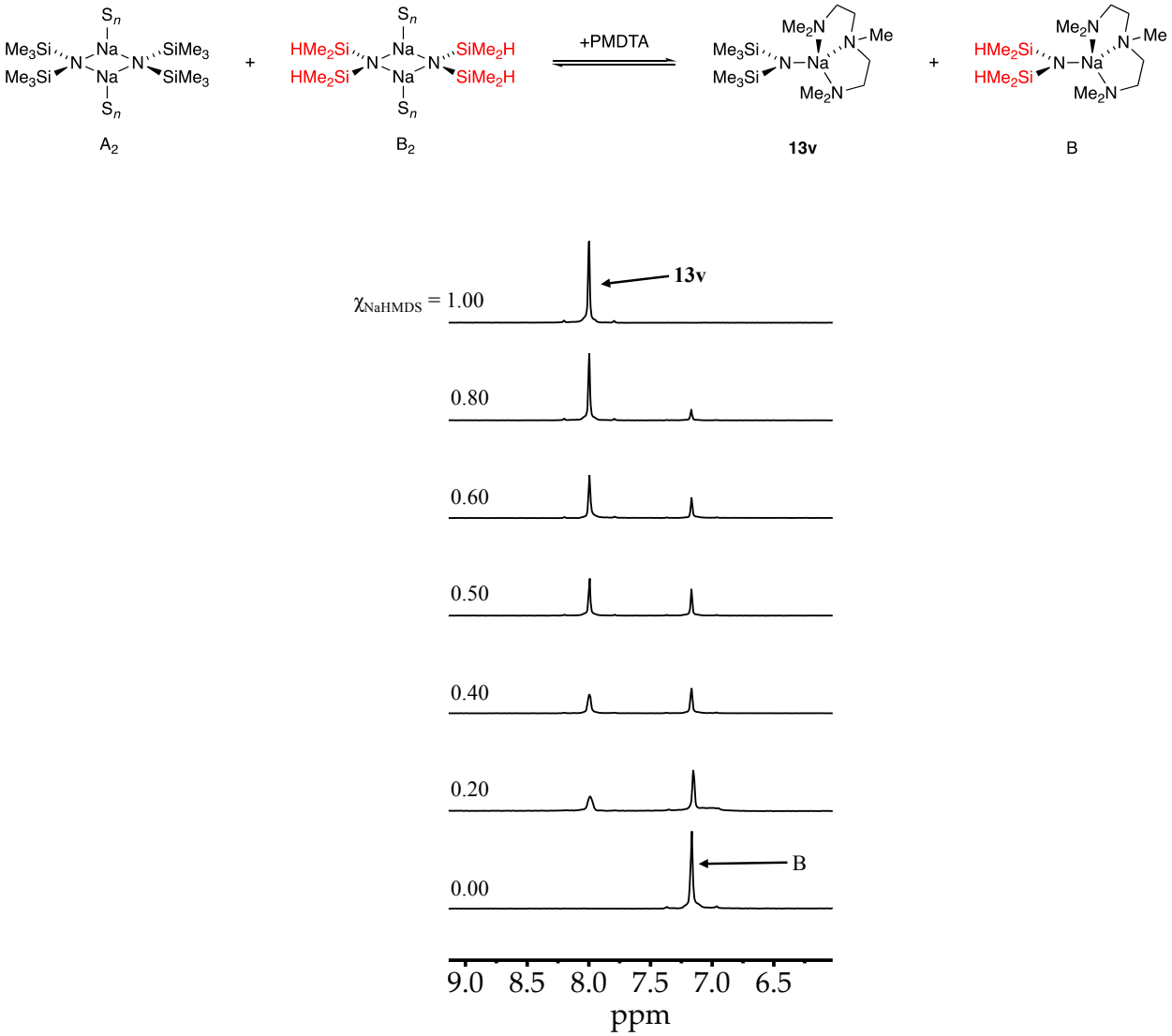


Figure S74. $^{13}C\{^{1}H\}$ NMR (125.79 MHz, toluene) spectra for 0.30 M solutions of NaHMDS and NaTMDS in toluene-d_8 with at the indicated mole fractions (χ_{NaHMDS}) at –80 °C.

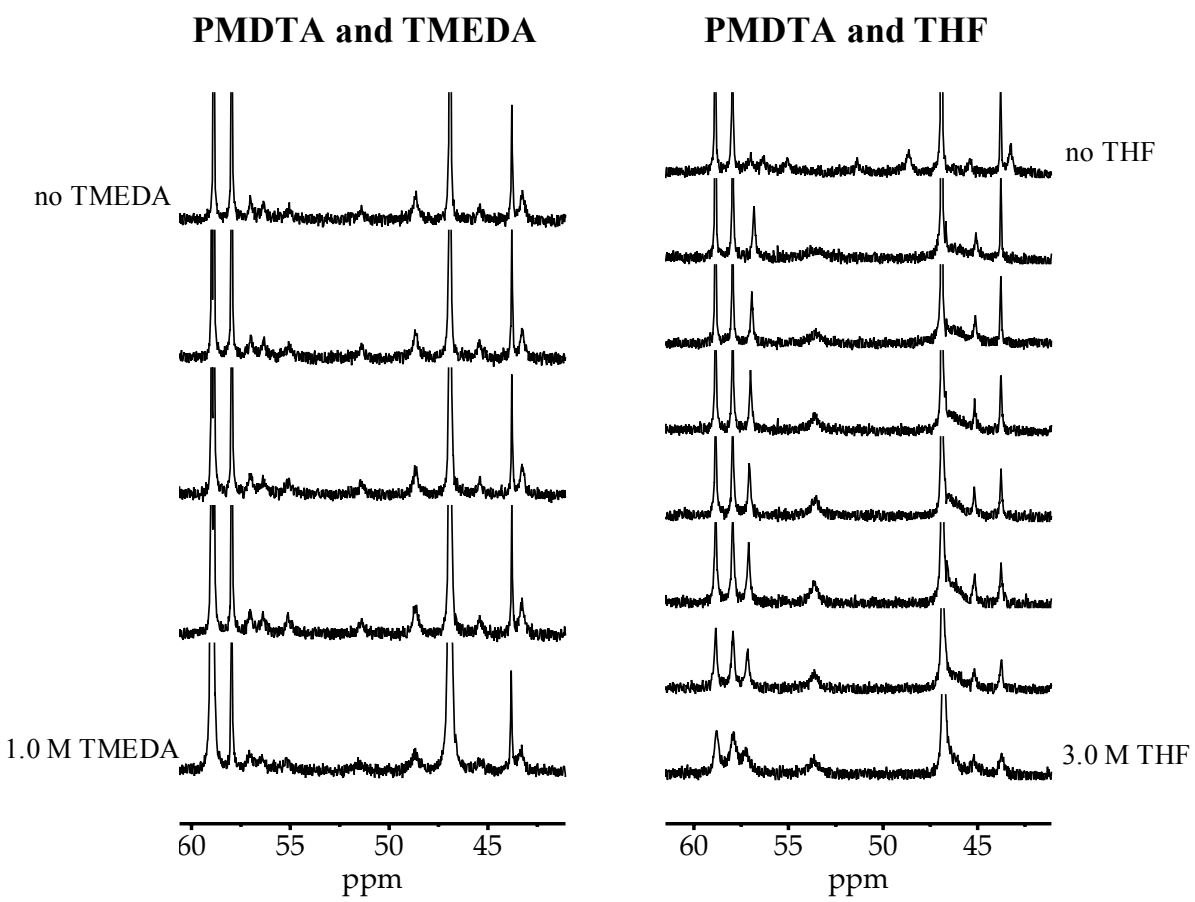


Figure S75. $^{13}C\{^{1}H\}$ NMR (500 MHz, toluene) spectra showing free and bound PMDTA resonances as TMEDA and THF were titrated into solutions. Both titrations were run under the following starting conditions: 0.10 M NaHMDS in 2:1 pentane/toluene-d_8 and 2.0 equiv of PMDTA at –120 °C. Bound PMDTA resonances are observed even at 1.0 M TMEDA concentrations whereas THF appears to catalyze exchange.

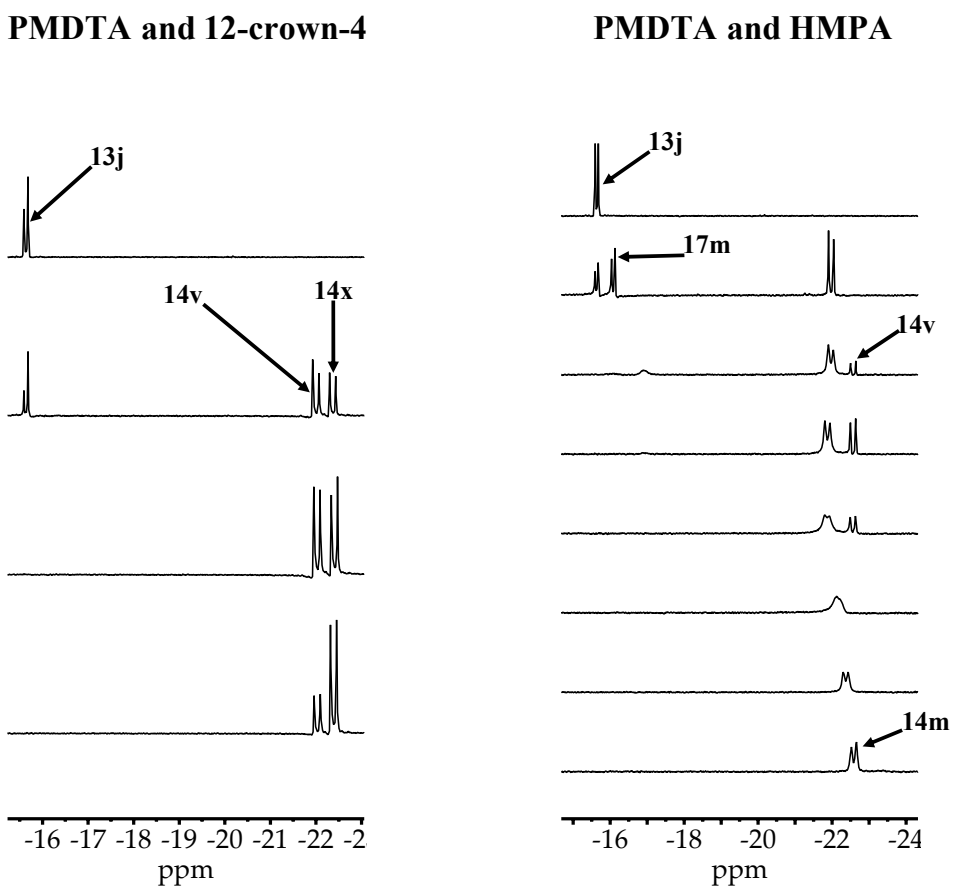


Figure S76. ^{29}Si NMR (99.36 MHz, MTBE) spectra of 0.20 M [^{15}N]NaHMDS in MTBE at –110 °C with incremental additions of 1:1 PMDTA/HMPA and 1:1 PMDTA/12-crown-4. The equiv of total added ligand from top to bottom are (A) PMDTA/12-crown-4: 0.0, 0.50, 1.0, and 1.5; and
(B) PMDTA/HMPA: 0.0, 0.50, 1.0, 1.5, 2.0, 3.0, 4.0, 6.0

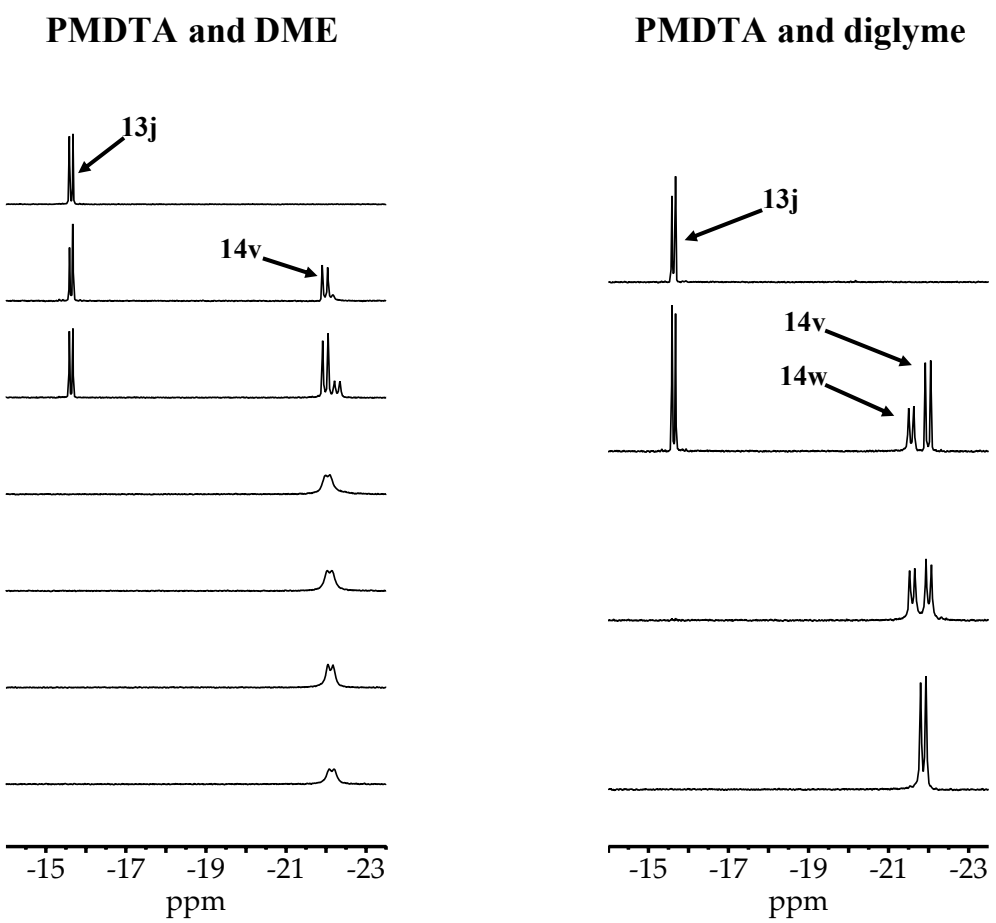
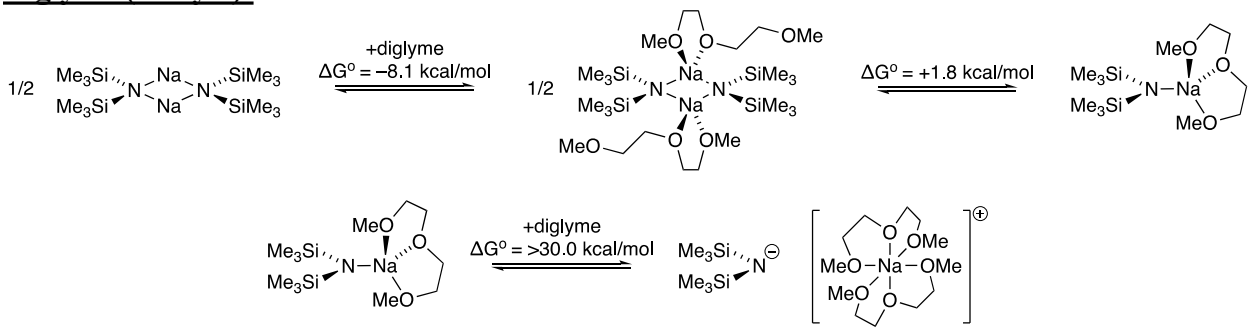


Figure S77. ^{29}Si NMR (99.36 MHz, MTBE) spectra of 0.20 M [^{15}N]NaHMDS in MTBE at –110 °C with incremental additions of 1:1 PMDTA/DME and 1:1 PMDTA/diglyme. The equiv of total added ligand are from top to bottom are (A) PMDTA/DME: 0.0, 0.50, 1.0, 2.0, 3.0, 4.0, and 6.0; and (B) PMDTA/diglyme: 0.0, 0.50, 1.0, and 2.0.

Diglyme (entry x):



^{29}Si{^{1}H} spectrum **^{13}C{^{1}H} spectrum** **^{15}N{^{1}H} spectrum**

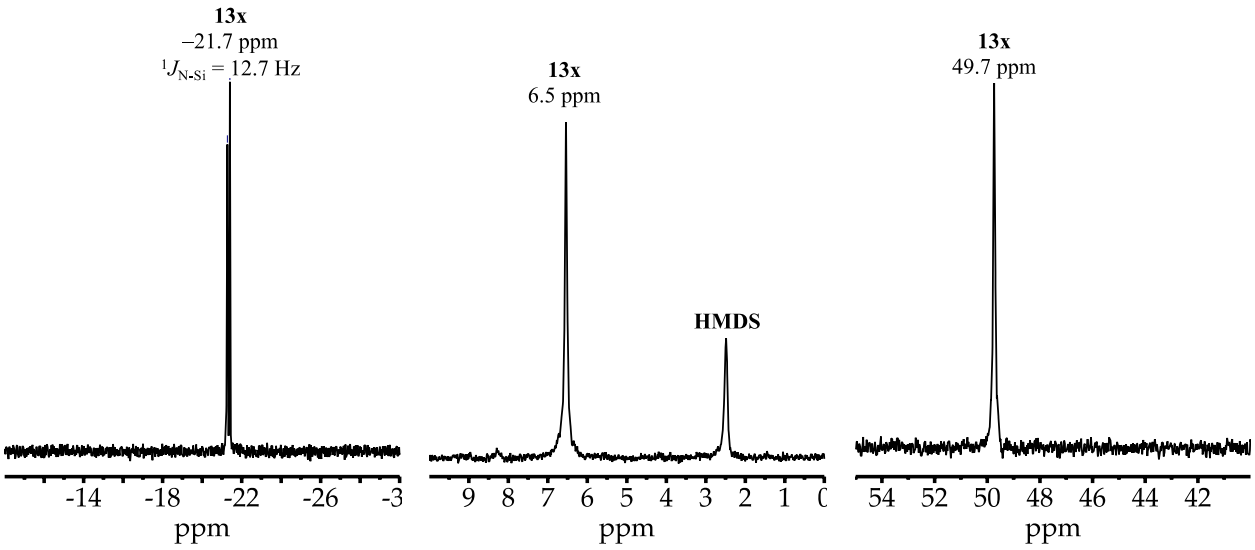


Figure S78. NMR spectra of 0.15 M [^{15}N]NaHMDS in 0.45 M diglyme with DMEA cosolvent at –120 °C. Standard ^{13}C, ^{15}N, and ^{29}Si spectra were recorded on a 500 MHz spectrometer at 125.79, 50.66, and 99.36 MHz, respectively.

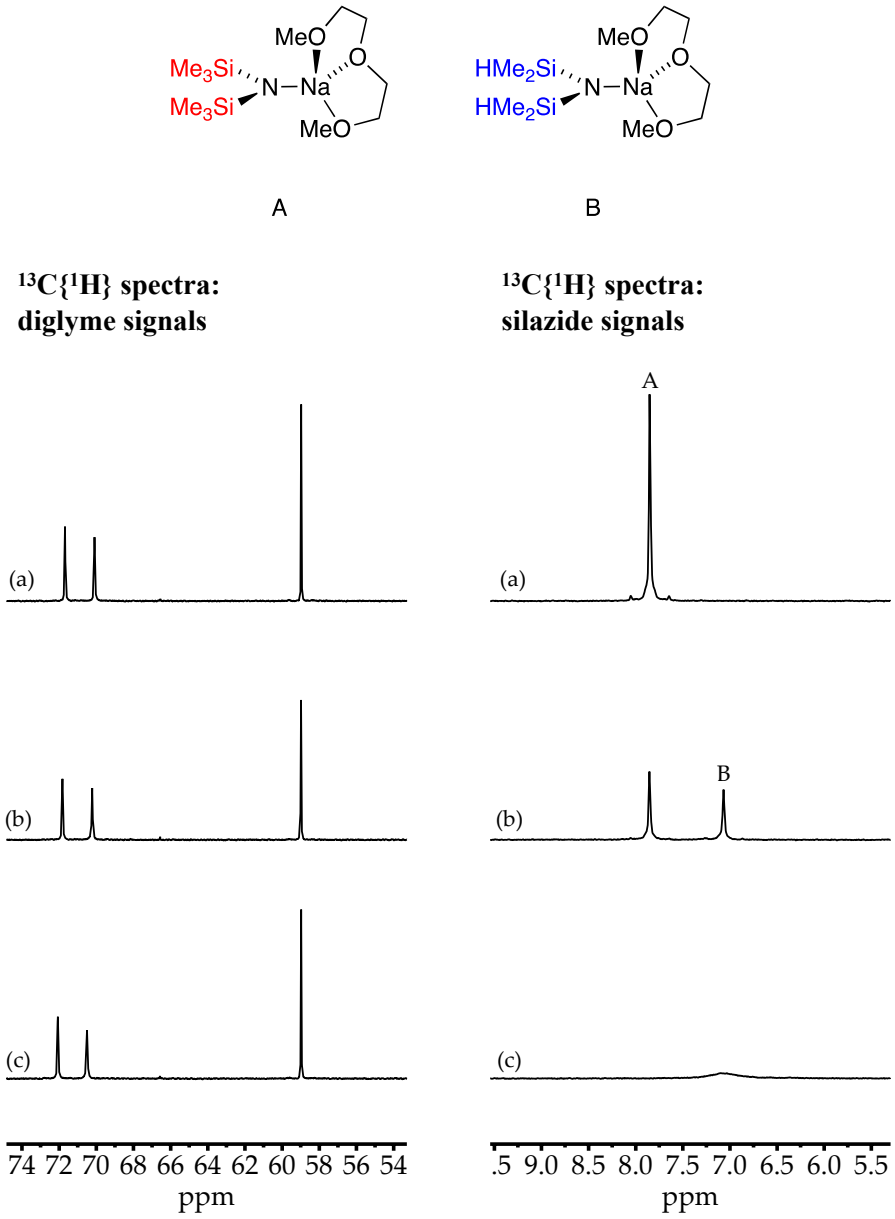


Figure S79. $^{13}C\{^{1}H\}$ NMR (125.79 MHz, toluene) relative integrations of NaHMDS-derived homodimer (A_2), NaTMDS-derived homodimer (B_2), and heterodimer (AB) versus the measured mole fraction of NaHMDS (X_{NaHMDS}) at 0.20 total molarity in 0.40 M diglyme in toluene-d_8 cosolvent at −80 °C. The measured mole fractions, X_{NaHMDS}, in (a)–(c) are 1.00, 0.50, and 0.00, respectively.

$^{29}Si\{^{1}H\}$ spectra

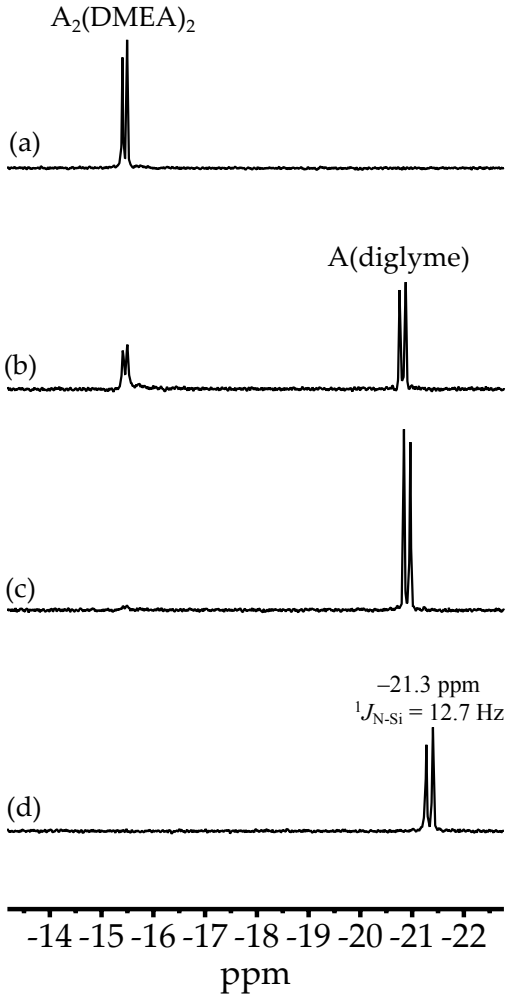


Figure S80. ^{29}Si NMR (99.36 MHz, DMEA) spectra of 0.15 M [^{15}N]NaHMDS in DMEA cosolvent with varying amounts of diglyme added at –120 °C. The equivalents of diglyme for (a)–(d) are as follows: 0.0, 0.7, 1.0, and 3.0 equiv, respectively.

12-crown-4 (entry y):

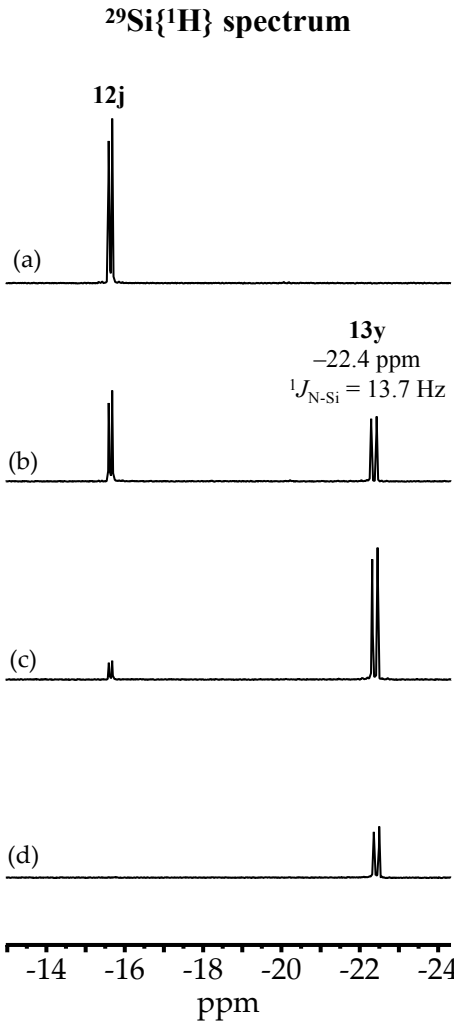


Figure S81. ^{29}Si NMR (99.36 MHz, MTBE) spectra of 0.20 M [^{15}N]NaHMDS in MTBE cosolvent with varying amounts of 12-crown-4 added at –110 °C. The equivalents of crown for (a)–(d) are as follows: 0.0, 0.3, 0.7, and 1.5 equiv, respectively.

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

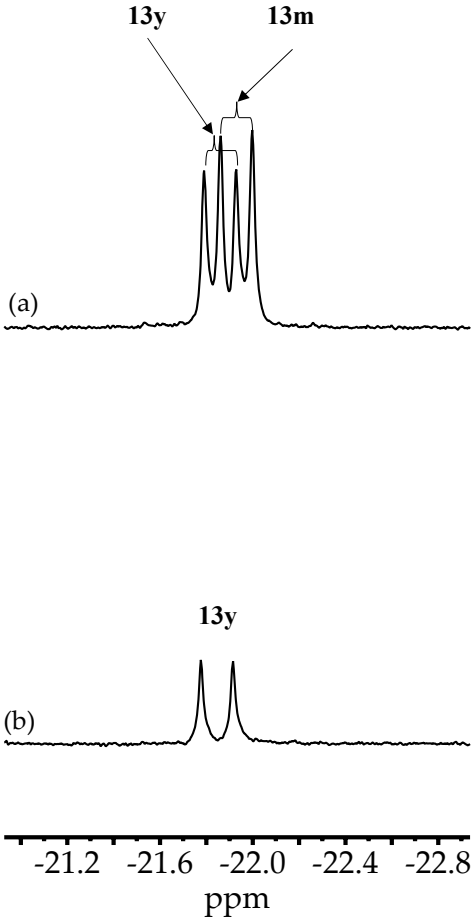


Figure S82. ^{29}Si NMR (99.36 MHz, THF) spectra of 0.15 M [^{15}N]NaHMDS in THF cosolvent with varying amounts of 12-crown-4 added at –105 °C. The equivalents of crown for (a) and (b) are as follows: 0.5 and 2.0 equiv, respectively.

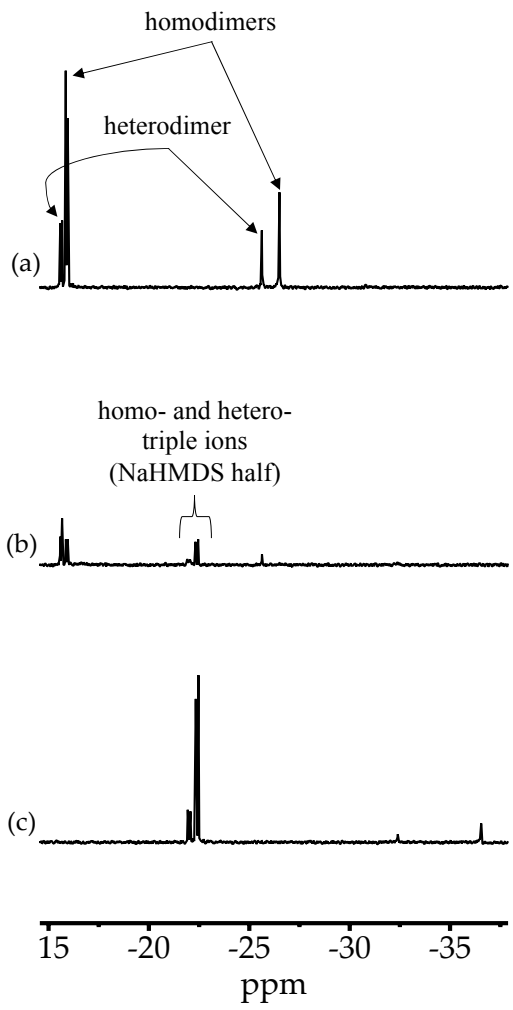


Figure S83. ^{29}Si NMR (99.36 MHz, THF) spectra for titration of 12-crown-4 to a tube containing a 1:1 mix of NaHMDS and NaTMDS in MTBE cosolvent at –110 °C. The equivalents of crown for (a)–(c) are as follows: 0.0, 0.4, and 1.5 equiv, respectively.

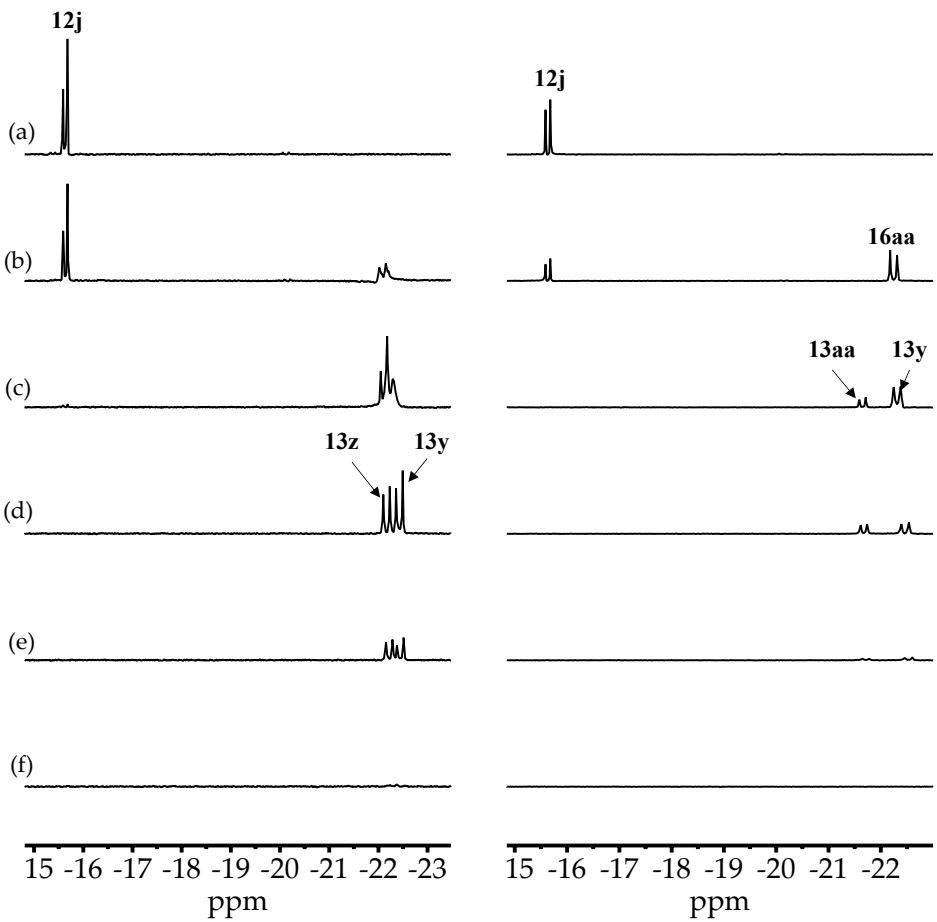


Figure S84. ^{29}Si NMR (99.36 MHz, MTBE) spectra of 0.20 M [^{15}N]NaHMDS in MTBE at –110 °C with incremental additions of 1:1 12-crown-4/15-crown-5 (left spectra) and 1:1 12-crown-4/18-crown-6 (right spectra). The equiv of total added ligand from (a)–(f) for each titration are as follows:
12-crown-4/15-crown-5: 0.0, 0.5, 1.0, 1.5, 2.0, and 2.5 equiv respectively.
12-crown-4/18-crown-6: 0.0, 0.5, 1.0, 1.5, 2.0, and 2.5 equiv respectively.

15-crown-5 (entry z):

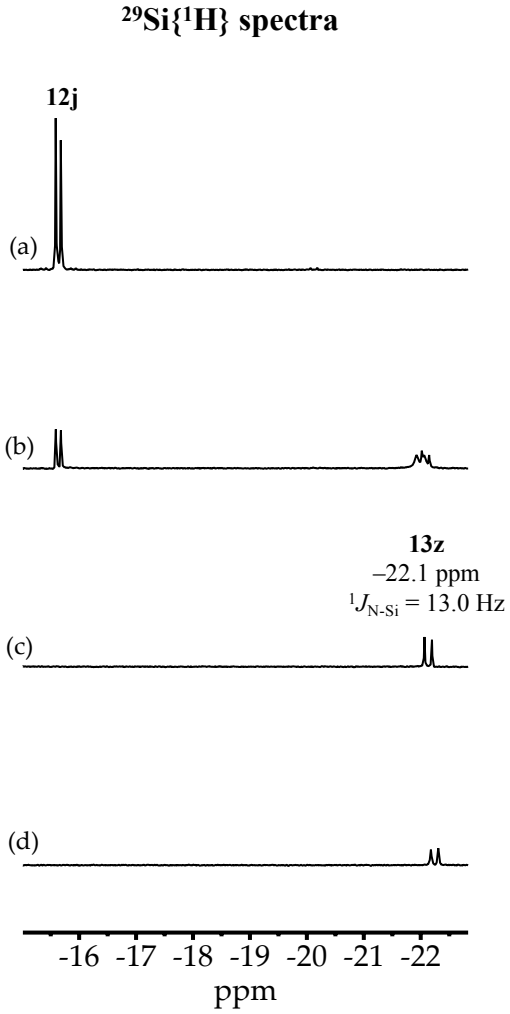


Figure S85. ^{29}Si NMR (99.36 MHz, MTBE) spectra of 0.20 M [^{15}N]NaHMDS in MTBE cosolvent with varying amounts of 15-crown-5 added at –110 °C. The equivalents of crown for (a)–(d) are as follows: 0.0, 0.3, 1.0, and 1.5 equiv, respectively.

$^{13}C\{^1H\}$ spectra

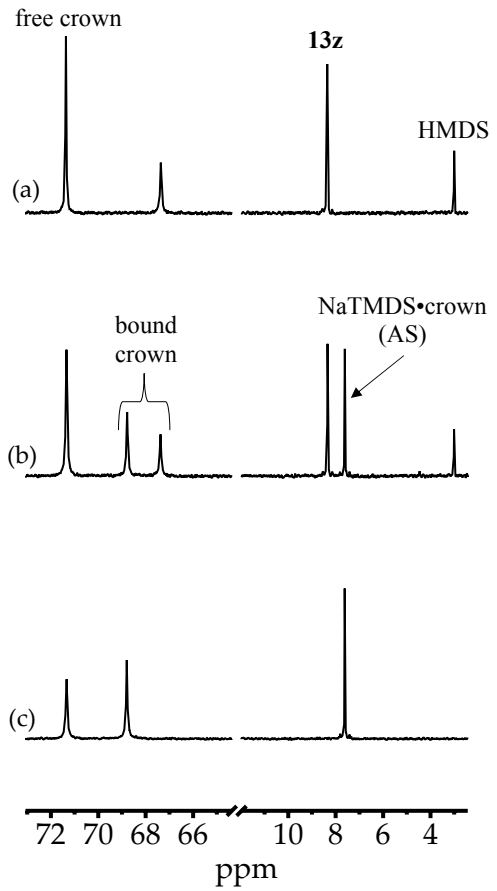


Figure S86. $^{13}C\{^1H\}$ NMR (125.79 MHz, toluene) spectra of with mixing NaHMDS and NaTMDS at 0.20 total molarity with 0.35 M15-crown-5 in toluene-d_8 cosolvent at –80 °C. The measured mole fractions, X_{NaHMDS}, in (a)–(c) are 1.00, 0.50, and 0.00, respectively. Show are the crown carbon signals which appear to be in the slow exchange limit.

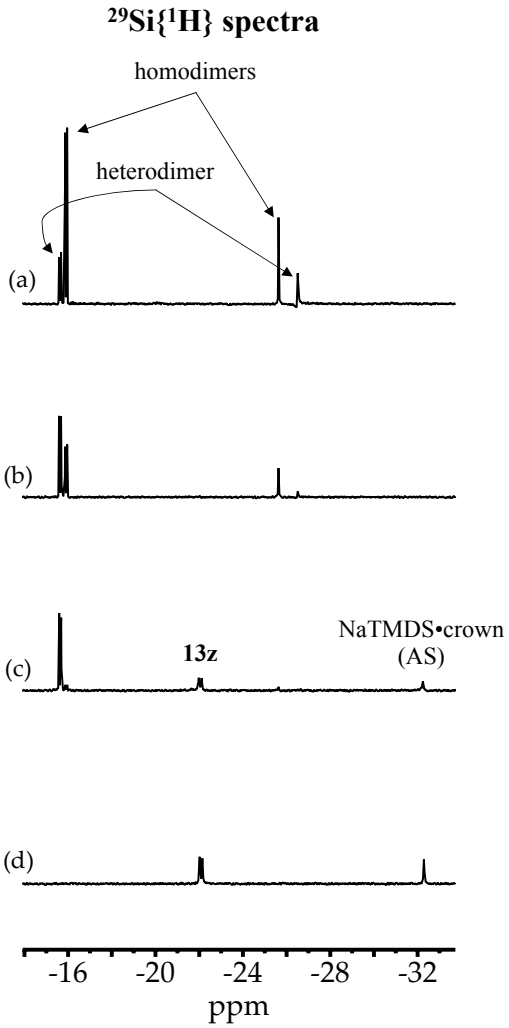


Figure S87. ^{29}Si NMR (99.36 MHz, MTBE) spectra for titration of 15-crown-5 to a tube containing a 1:1 mix of NaHMDS and NaTMDS in MTBE cosolvent at –110 °C. The equivalents of crown for (a)–(d) are as follows: 0.0, 0.3, 0.5 and 1.5 equiv, respectively.

$^{29}Si\{^{1}H\}$ spectra

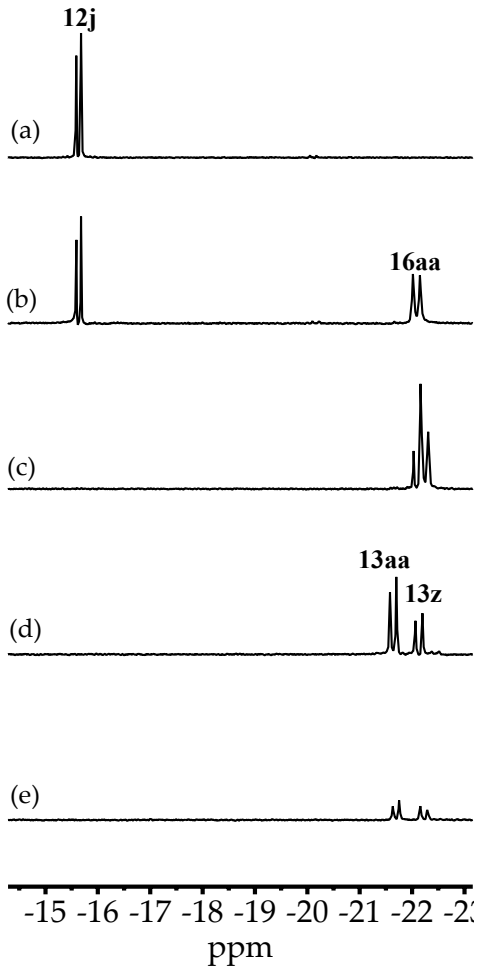
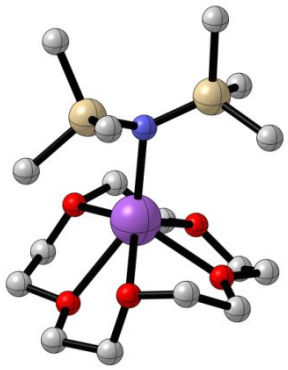


Figure S88. ^{29}Si NMR (99.36 MHz, MTBE) spectra of 0.20 M [^{15}N]NaHMDS in MTBE at –110 °C with incremental additions of 1:1 15-crown-5/18-crown-6. The equiv of total added ligand from (a)–(e) for each titration are as follows:
15-crown-5/18-crown-6: 0.0, 0.5, 1.0, 1.5, and 2.0 equiv respectively.

Table S2. Crystal structure for NaHMDS•15-crown5.
Owing to the low resolution of the crystal, only coordinates (xyz) are presented.



13z
crystal
structure

	X	Y	Z
Si	1.526694	8.150690	13.955027
Si	2.056675	5.715469	12.255062
Na	3.809574	5.810148	15.085720
O	4.894962	7.493565	16.536383
O	5.310636	3.855943	15.547027
O	2.859955	5.941554	17.252881
O	6.130063	6.141126	14.322110
O	2.555439	3.704031	15.786514
C	6.245870	7.668347	16.226228
C	6.490829	7.519347	14.795195
C	4.631154	2.608138	15.692289
N	2.394793	6.800571	13.462312
C	0.262917	7.807782	15.278095
C	4.614322	7.402933	17.943860
C	1.773234	5.088611	17.694558
C	3.248065	4.281517	12.288433
C	7.103296	5.196469	14.732378
C	2.642086	9.537823	14.551782
C	6.390006	3.801934	14.634228
C	3.158789	7.058132	18.067530
C	3.409069	2.830171	16.532457
C	0.331114	4.945509	12.384620
C	2.115940	6.441890	10.564911
C	0.443759	8.923576	12.582884
C	1.414068	4.190501	16.465715

18-crown-6 (entry aa):

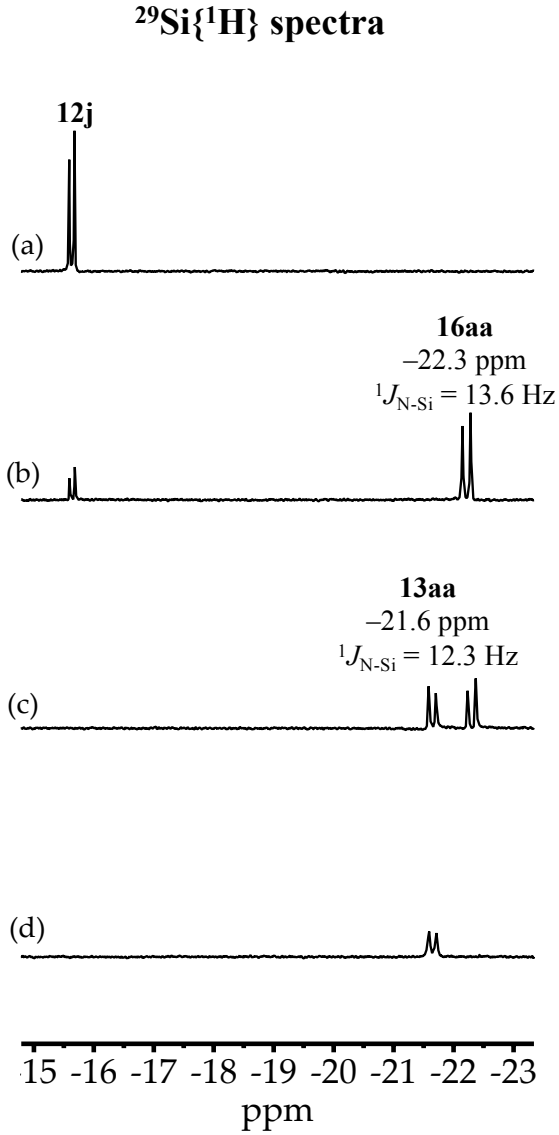


Figure S89. ^{29}Si NMR (99.36 MHz, MTBE) spectra of 0.20 M [^{15}N]NaHMDS in MTBE cosolvent with varying amounts of 18-crown-6 added at –110 °C. The equivalents of crown for (a)–(d) are as follows: 0.0, 0.5, 1.0, and 1.5 equiv, respectively.

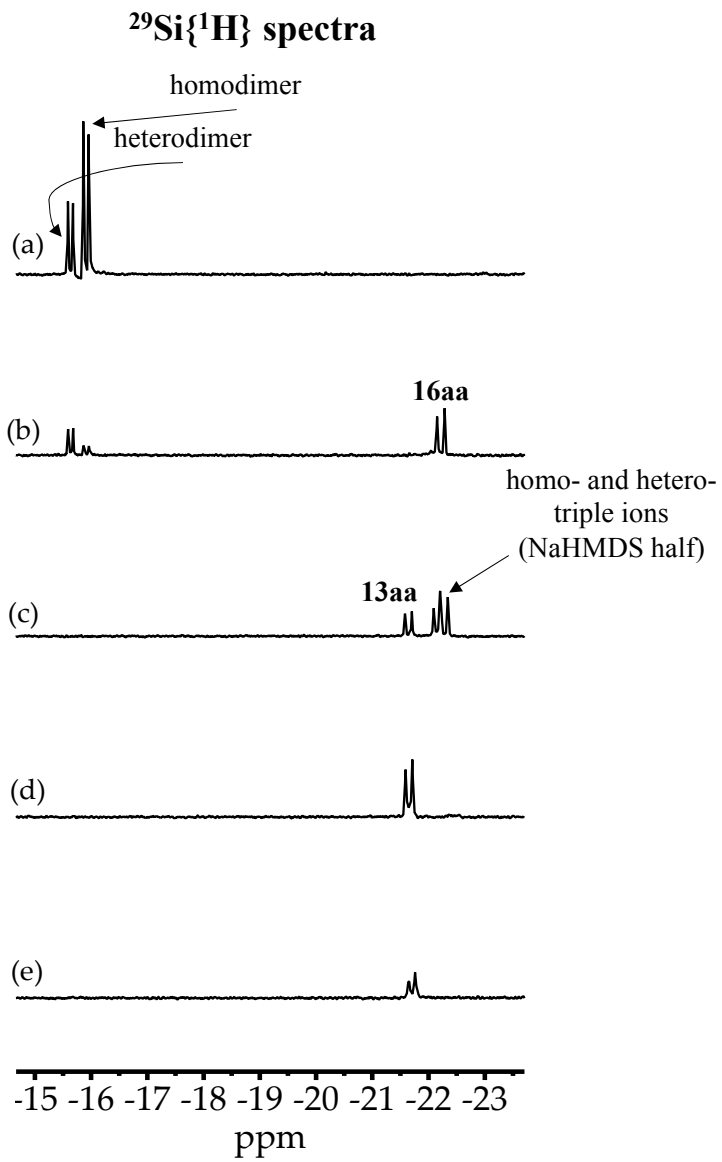


Figure S90. ^{29}Si NMR (99.36 MHz, MTBE) spectra for titration of 18-crown-6 to a tube containing a 1:1 mix of NaHMDS and NaTMDS in MTBE cosolvent at –110 °C. The equivalents of crown for (a)–(e) are as follows: 0.0, 0.5, 1.0, 1.5, and 2.0 equiv, respectively.

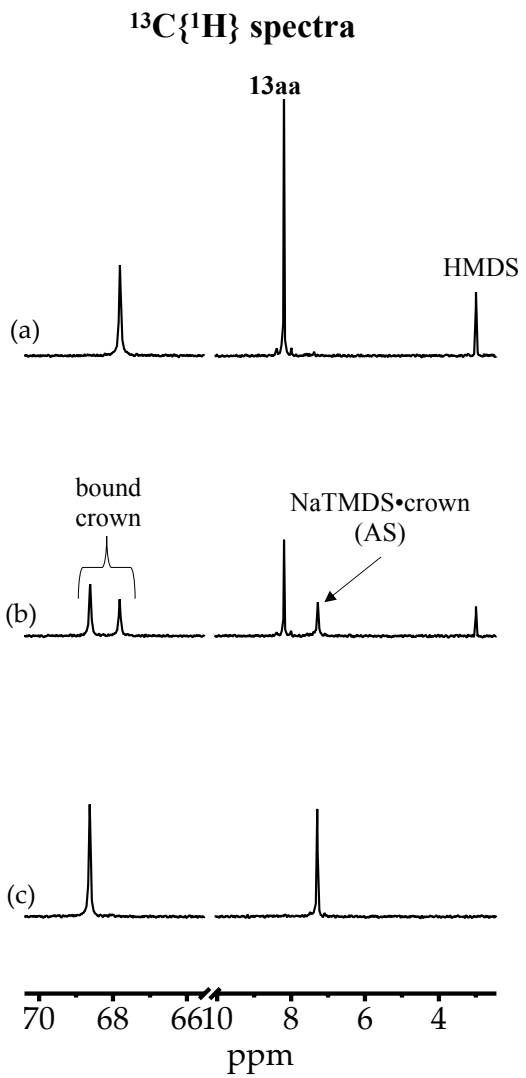


Figure S91. $^{13}C\{^{1}H\}$ NMR (125.79 MHz, toluene) spectra of with mixing NaHMDS and NaTMDS at 0.20 total molarity with 0.40 M 18-crown-6 in toluene-d_8 cosolvent at –80 °C. The measured mole fractions, X_{NaHMDS}, in (a)–(c) are 1.00, 0.50, and 0.00, respectively. Show are the crown carbon signals which appear to be in the slow exchange limit.

TDA-1 (entry bb):

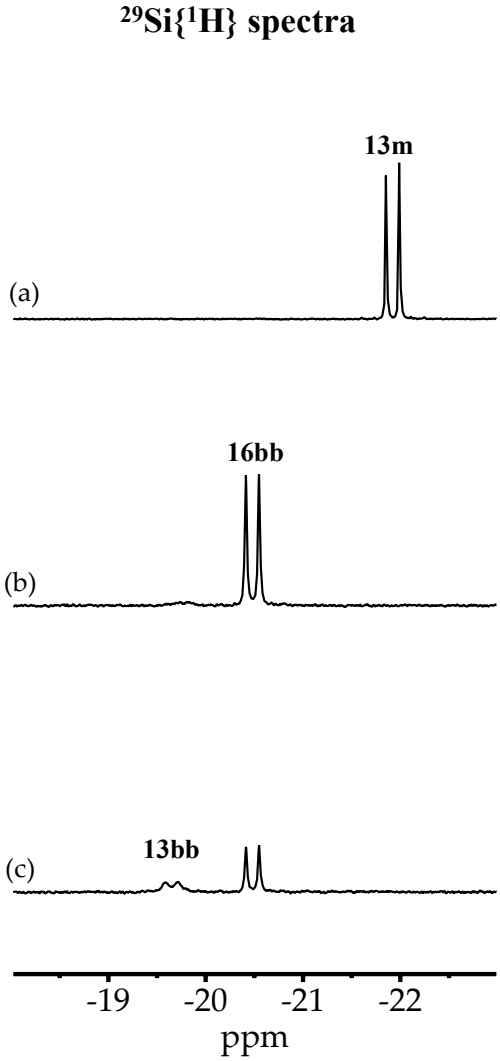


Figure S92. ^{29}Si NMR (99.36 MHz, THF) spectra of 0.20 M [^{15}N]NaHMDS in THF cosolvent with varying amounts of TDA-1 added at –105 °C. The equivalents of TDA-1 for (a)–(c) are as follows: 0.0, 0.5, and 1.5 equiv, respectively.

[2.2.2]cryptand (entry cc):

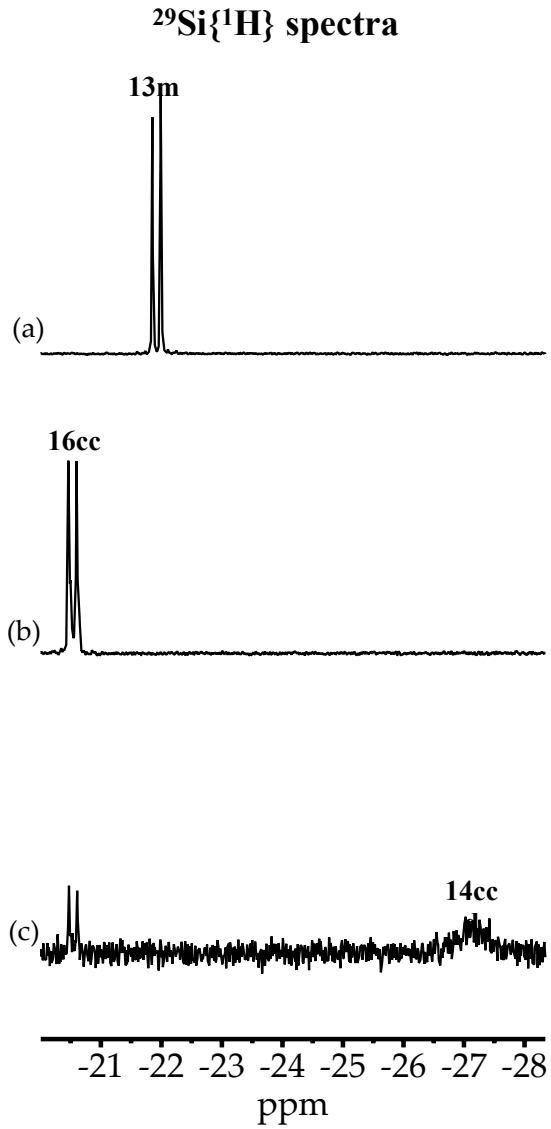
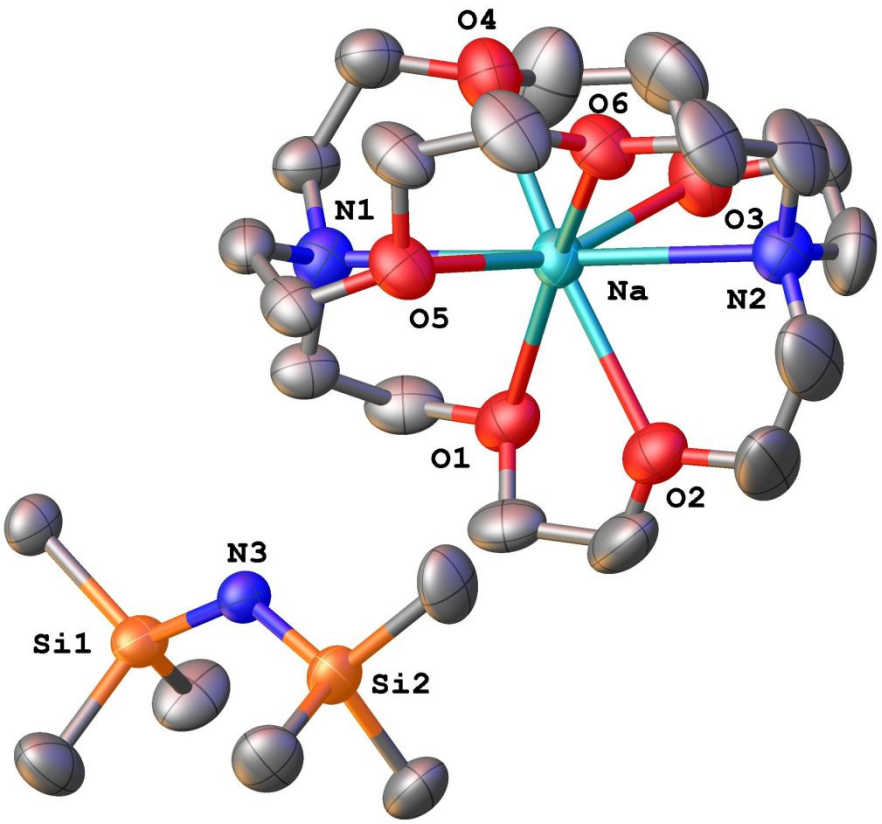


Figure S93. ^{29}Si NMR (99.36 MHz, THF) spectra of 0.20 M [^{15}N]NaHMDS in THF cosolvent with varying amounts of [2.2.2]cryptand added at –105 °C. The equivalents of cryptand for (a)–(c) are as follows: 0.0, 0.5, and 1.5 equiv, respectively.

Table S3. Crystal data and structure refinement for NaHMDS•cryptand complex. Our facility maintains a Rigaku XtaLAB Synergy diffractometer, equipped with a 4-circle Kappa goniometer, dual microfocus X-ray sources (Mo/Cu), a HyPix-6000HE Hybrid Photon Counting (HPC) detector and an Oxford Cryosystems 800 Series Cryostream. See Cornell facility website for more details.

Identification code	rraw4_abs7
Empirical formula	C24 H54 N3 Na O6 Si2
Formula weight	559.87
Temperature	100.02(10) K
Wavelength	1.54184 Å
Crystal system	Monoclinic
Space group	P 1 21/c 1
Unit cell dimensions	a = 14.12790(10) Å a= 90°.
	b = 19.22530(10) Å b= 117.6180(10)°.
	c = 13.27070(10) Å g = 90°.
Volume	3193.79(5) $Å^3$
Z	4
Density (calculated)	1.164 Mg/m^3
Absorption coefficient	1.455 mm^{-1}
F(000)	1224
Crystal size	0.231 x 0.14 x 0.073 mm^3
Theta range for data collection	3.531 to 77.972°.
Index ranges	-17<=h<=17, -24<=k<=24, -16<=l<=16
Reflections collected	131803
Independent reflections	6804 [R(int) = 0.0465]
Completeness to theta = 67.684°	99.9 %
Absorption correction	Gaussian
Max. and min. transmission	1.000 and 0.530
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6804 / 1329 / 374
Goodness-of-fit on F^2	1.083
Final R indices [I>2sigma(I)]	R1 = 0.0775, wR2 = 0.2088
R indices (all data)	R1 = 0.0809, wR2 = 0.2118
Extinction coefficient	n/a
Largest diff. peak and hole	0.779 and -0.631 e.$Å^{-3}$



Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for Rraw4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

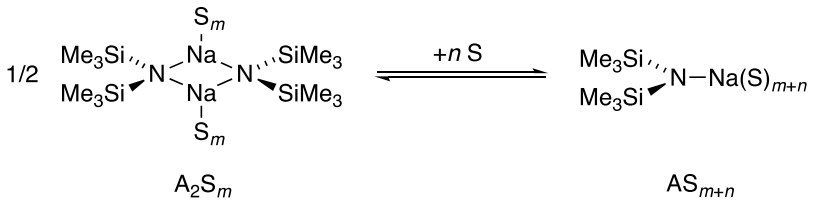
	x	y	z	U(eq)
Si(1)	7796(1)	5762(1)	3660(1)	44(1)
Si(2)	7016(1)	6752(1)	4848(1)	47(1)
N(3)	6945(2)	6042(1)	4109(2)	40(1)
C(19)	7685(4)	6238(2)	2358(4)	74(1)
C(20)	7600(3)	4816(2)	3231(3)	50(1)
C(21)	9263(3)	5840(2)	4709(4)	77(1)
C(22)	5777(3)	6885(2)	5024(3)	69(1)

C(23)	7208(3)	7592(2)	4229(4)	71(1)
C(24)	8147(3)	6767(2)	6358(3)	66(1)
Na	2568(1)	6109(1)	1667(1)	46(1)
O(1)	3834(2)	6564(1)	846(2)	58(1)
O(4)	1600(2)	5080(1)	228(2)	70(1)
O(5)	3760(2)	5412(1)	3443(2)	57(1)
N(1)	3921(2)	5066(1)	1399(2)	52(1)
C(1)	4745(2)	5443(2)	1242(2)	51(1)
C(2)	4287(3)	6043(2)	435(3)	60(1)
C(3)	4636(3)	6975(2)	1731(3)	64(1)
C(4)	4090(4)	7556(2)	1979(4)	83(1)
C(9)	391(4)	5892(3)	-966(4)	98(1)
C(10)	1162(5)	5355(3)	-877(4)	109(2)
C(11)	2199(3)	4472(2)	345(3)	62(1)
C(12)	3279(3)	4621(2)	427(3)	56(1)
C(13)	4413(2)	4649(2)	2441(3)	50(1)
C(14)	4675(2)	5076(2)	3478(2)	51(1)
C(15)	3067(3)	4936(2)	3603(3)	65(1)
C(16)	2274(3)	5343(3)	3799(3)	81(1)
O(2)	3346(4)	7335(2)	2193(4)	58(1)
O(3)	985(6)	6456(4)	-120(5)	70(1)
O(6)	1734(4)	5827(3)	2937(4)	57(1)
N(2)	1209(4)	7092(3)	1702(5)	52(1)
C(5)	2776(8)	7875(5)	2399(12)	114(4)
C(6)	1843(8)	7631(6)	2465(9)	96(3)
C(7)	673(8)	7412(5)	575(8)	84(2)
C(8)	111(7)	6910(6)	-338(11)	87(3)
C(17)	1098(7)	6296(6)	3185(7)	83(2)
C(18)	525(7)	6738(6)	2096(9)	86(3)
O(2')	3451(5)	7215(3)	2584(5)	58(1)
O(3')	905(8)	6417(5)	-346(6)	70(1)
O(6')	1513(5)	5576(4)	2625(5)	57(1)
N(2')	1347(5)	7038(3)	2159(6)	52(1)
C(5')	3002(11)	7740(9)	2997(13)	113(5)
C(6')	2126(11)	7462(8)	3077(12)	99(4)
C(7')	710(15)	7325(9)	1027(10)	111(4)

C(8')	491(16)	7055(10)	-89(13)	121(6)
C(17')	640(10)	5970(6)	2544(15)	96(3)
C(18')	746(15)	6707(7)	2642(16)	98(4)

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.

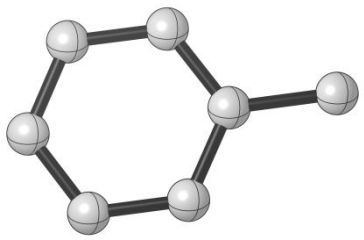
$f(x) = J_{obs}$
$x = [S]$
$a = [A]_T$
$b = J_{A_2S_m}$
$c = J_{AS_{m+n}}$
$d = K_{eq}$

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. Geometry optimizations and single point energies were computed at the M06-2X/def2-SVP level of theory and M06-2X/def2-TZVP level of theory respectively. A pruned (99,590) integration grid was used for all computations as well. CYLview Visualization Software was used for all ball-and-stick structures. 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. Hydrogens have been removed from ball-and-stick models to improve clarity. All structures computed are group state structures and contain zero imaginary frequencies.

Table S4. Geometric coordinates and single point energies for toluene.

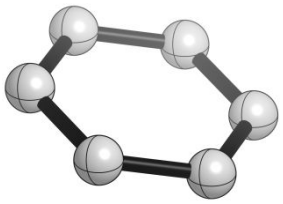


G = -271.12497 Hartrees

$\mathbf{G_{SP}}$ = -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 S5. Geometric coordinates and single point energies for benzene.

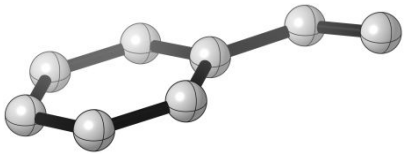


G = -231.883978 Hartrees

$\mathbf{G_{SP}}$ = -232.1392645 Hartrees

Atom	X	Y	Z
C	0.3386370	-1.3529650	0.0000010
C	-1.0024190	-0.9697130	0.0000240
C	-1.3410280	0.3832200	-0.0000220
C	-0.3385860	1.3529780	0.0000030
C	1.0023830	0.9697500	0.0000210
C	1.3410130	-0.3832700	-0.0000200
H	2.3904480	-0.6831270	-0.0000280
H	1.7868900	1.7285520	0.0000130
H	-0.6035830	2.4117590	-0.0000090
H	-2.3904260	0.6832060	-0.0000270
H	-1.7868330	-1.7286110	0.0000070
H	0.6035010	-2.4117780	-0.0000060

Table S6. Geometric coordinates and single point energies for styrene.

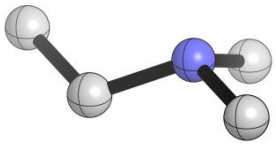


G = -309.15983 Hartrees

G_{SP} = -309.5005756 Hartrees

Atom	X	Y	Z
C	-2.2590310	0.2665490	0.0000690
C	-1.7811140	-1.0419690	0.0000780
C	-0.4085590	-1.2823770	-0.0000010
C	0.5122130	-0.2256220	-0.0000790
C	0.0154680	1.0873750	-0.0001150
C	-1.3536640	1.3300170	-0.0000310
H	-1.7200000	2.3578530	-0.0000730
H	0.7078000	1.9305760	-0.0002330
C	1.9550980	-0.5353920	-0.0001260
H	2.1930840	-1.6039590	-0.0003950
C	2.9640690	0.3396710	0.0001720
H	3.9992410	-0.0037250	0.0001010
H	2.8015950	1.4195030	0.0005270
H	-0.0367420	-2.3094970	0.0000120
H	-2.4792220	-1.8804630	0.0001510
H	-3.3326370	0.4602020	0.0001250

Table S7. Geometric coordinates and single point energies for dimethylethylamine.

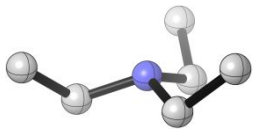


G = -213.373821 Hartrees

G_{SP} = -213.6201404 Hartrees

Atom	X	Y	Z
N	0.4572520	-0.0032570	-0.3159140
C	0.6019050	1.3750890	0.0939050
H	1.4864430	1.8140140	-0.3891340
H	-0.2701570	1.9680140	-0.2120010
H	0.7248790	1.4840390	1.1955680
C	1.6656120	-0.7524300	-0.0601070
H	1.5599020	-1.7797790	-0.4373950
H	2.5158730	-0.2856190	-0.5778930
H	1.9161600	-0.8104610	1.0230840
C	-0.6984810	-0.6508520	0.2775880
H	-0.6810680	-1.7051230	-0.0402510
H	-0.6237550	-0.6591910	1.3906980
C	-2.0240790	-0.0323280	-0.1423630
H	-2.8604340	-0.6584920	0.1972410
H	-2.1698380	0.9693930	0.2850800
H	-2.0684990	0.0491280	-1.2377430

Table S8. Geometric coordinates and single point energies for triethylamine.

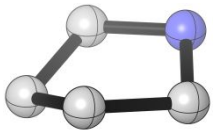


G = -291.846611 Hartrees

G_{SP} = -292.1796866 Hartrees

Atom	X	Y	Z
C	-1.3428320	0.3788900	0.4447400
N	-0.0000020	0.0000430	0.0292400
C	0.9994960	0.9736150	0.4445480
H	0.5444500	1.9733820	0.3945760
H	1.2837780	0.8208640	1.5097520
C	2.2391170	0.9658090	-0.4391700
H	2.9555350	1.7322610	-0.1111940
H	2.7564110	-0.0038350	-0.4130810
H	1.9555780	1.1682290	-1.4810810
C	0.3434160	-1.3523100	0.4445960
H	1.4367600	-1.4581300	0.3945980
H	0.0690520	-1.5221110	1.5098200
C	-0.2830800	-2.4219900	-0.4391340
H	0.0223940	-3.4256490	-0.1110670
H	-1.3814650	-2.3851970	-0.4132420
H	0.0341600	-2.2777240	-1.4810030
H	-1.9811410	-0.5150910	0.3952010
H	-1.3525000	0.7017650	1.5098560
C	-1.9561180	1.4559910	-0.4392370
H	-2.9781020	1.6931880	-0.1112760
H	-1.3751730	2.3889020	-0.4135900
H	-1.9897120	1.1088200	-1.4810100

Table S9 Geometric coordinates and single point energies for pyrrolidine.

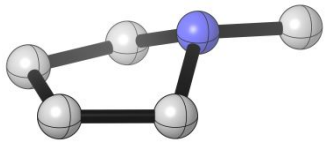


G = -212.198736 Hartrees

G_{SP} = -212.4417845 Hartrees

Atom	X	Y	Z
C	-1.2104140	-0.3884390	-0.0305730
H	-1.7496930	-0.4859390	-0.9863720
H	-1.9229270	-0.6568000	0.7652560
C	-0.6873410	1.0525510	0.1602300
C	0.7772530	0.9603480	-0.2733970
C	1.1490190	-0.4360340	0.2330290
H	2.0354620	-0.8647750	-0.2548040
H	1.3649270	-0.3915720	1.3150740
N	-0.0305750	-1.2668570	-0.0081100
H	0.0624900	-1.7463610	-0.8972140
H	0.8537260	0.9920680	-1.3726000
H	1.4061330	1.7633410	0.1355160
H	-0.7388980	1.3350670	1.2227840
H	-1.2682960	1.7924150	-0.4065990

Table S10. Geometric coordinates and single point energies for *N*-methylpyrrolidine.

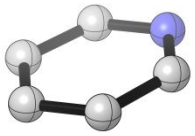


G = -251.434505 Hartrees

G_{SP} = -251.7201927 Hartrees

Atom	X	Y	Z
C	1.4901110	0.7748660	-0.0609950
C	1.4900710	-0.7748880	-0.0611920
C	0.0193280	-1.1475600	0.1659610
H	-0.2861150	-2.0695200	-0.3511270
H	-0.1768080	-1.2931000	1.2537670
N	-0.7082770	-0.0000270	-0.3412410
C	0.0193050	1.1475940	0.1658100
H	-0.2860370	2.0694460	-0.3515290
H	-0.1770120	1.2933840	1.2535470
C	-2.1135040	-0.0000060	-0.0308810
H	-2.5965150	0.8891530	-0.4613250
H	-2.5965170	-0.8892230	-0.4612040
H	-2.3076690	0.0000720	1.0655690
H	2.1407370	-1.2002850	0.7139060
H	1.8355240	-1.1586150	-1.0300260
H	2.1405140	1.1999960	0.7144700
H	1.8359790	1.1588490	-1.0295790

Table S11. Geometric coordinates and single point energies for pyridine.

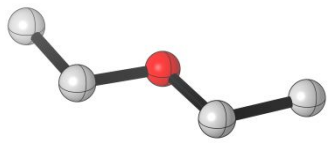


G = -247.915535 Hartrees

G_{SP} = -248.192147 Hartrees

Atom	X	Y	Z
C	1.1393060	-0.7235290	0.0000880
N	-0.0000890	-1.4116930	0.0000850
C	-1.1394220	-0.7233660	-0.0003330
C	-1.1967860	0.6710370	0.0000760
C	0.0001040	1.3828730	0.0000030
C	1.1968750	0.6708920	-0.0000960
H	2.1606160	1.1811570	-0.0000870
H	0.0001490	2.4743850	0.0000870
H	-2.1604290	1.1814880	0.0004000
H	-2.0628690	-1.3111810	0.0004310
H	2.0626940	-1.3114430	0.0001460

Table S12. Geometric coordinates and single point energies for diethylether.

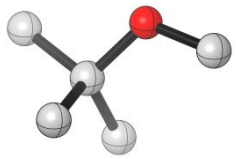


G = -233.241254 Hartrees

G_{SP} = -233.5145333 Hartrees

Atom	X	Y	Z
C	2.3647570	-0.4147040	-0.0000180
H	2.3411230	-1.0583010	-0.8897860
H	3.3042780	0.1541970	0.0000890
H	2.3410760	-1.0585850	0.8895410
C	1.1716650	0.5163730	0.0000840
H	1.1949610	1.1784720	-0.8889100
H	1.1949700	1.1780420	0.8893920
O	0.0000080	-0.2509080	-0.0001010
C	-1.1717300	0.5164040	-0.0000290
H	-1.1949930	1.1784530	0.8890060
H	-1.1955140	1.1782300	-0.8892430
C	-2.3646970	-0.4147780	0.0001130
H	-3.3042740	0.1539820	-0.0001850
H	-2.3405190	-1.0583710	-0.8896790
H	-2.3411470	-1.0586310	0.8896780

Table S13. Geometric coordinates and single point energies for methyl *t*-butylether.

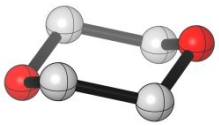


G = -272.479744 Hartrees

G_{SP} = -272.7967012 Hartrees

Atom	X	Y	Z
C	2.0151930	-0.0000340	-0.1524300
H	2.1680520	0.8953560	0.4757110
H	2.1676800	-0.8949840	0.4764320
O	0.7780070	-0.0000200	-0.8005840
C	-0.3938030	0.0000030	0.0075160
C	-1.5345800	0.0008250	-1.0039380
H	-2.5104760	0.0007890	-0.4988920
H	-1.4610540	0.8911200	-1.6436950
H	-1.4614830	-0.8888250	-1.6446410
C	-0.4602520	1.2589600	0.8759730
H	0.3119580	1.2598530	1.6586670
H	-0.3261930	2.1527210	0.2493820
H	-1.4374530	1.3240370	1.3750840
C	-0.4610360	-1.2597340	0.8747900
H	-1.4381980	-1.3245860	1.3740070
H	-0.3277170	-2.1529850	0.2473180
H	0.3112990	-1.2619400	1.6573560
H	2.7863910	-0.0005120	-0.9335200

Table S14. Geometric coordinates and single point energies for methyl 1,4-dioxane.

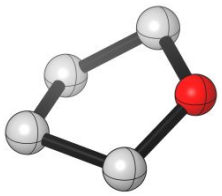


G = -307.183426 Hartrees

G_{SP} = -307.5433292 Hartrees

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 S15. Geometric coordinates and single point energies for THF.

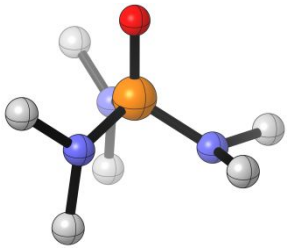


G = -232.060313 Hartrees

$\mathbf{G_{SP}}$ = -232.329161 Hartrees

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 S16. Geometric coordinates and single point energies for HMPA.

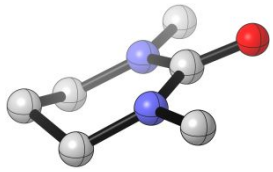


G = -819.403088 Hartrees

G_{SP} = -820.1003633 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
P	-0.0001830	0.0482870	0.4993850	H	1.2531460	-2.8277850	1.0650930
O	-0.0009080	0.3119180	1.9630360	C	-1.2076620	-2.3307060	0.0791780
N	-1.3995700	0.6572820	-0.2069790	H	-2.0942820	-1.6942340	-0.0217860
C	-1.6815450	0.5466420	-1.6208580	H	-1.2389230	-3.1075940	-0.7012690
H	-1.1627870	-0.3224270	-2.0459800	H	-1.2491530	-2.8299320	1.0638460
H	-2.7643060	0.4035290	-1.7768150	N	0.0014620	-1.5368390	-0.0710920
H	-1.3794360	1.4492790	-2.1845060	C	1.2117490	-2.3286680	0.0803610
C	-2.1513630	1.6808570	0.4933420	H	1.2450520	-3.1055370	-0.7000210
H	-1.9625840	2.6879400	0.0777020	H	2.0974290	-1.6907510	-0.0197420
H	-3.2322010	1.4779590	0.4104680				
H	-1.8677450	1.6727490	1.5517080				
N	1.3985320	0.6597380	-0.2061980				
C	2.1469030	1.6860220	0.4938700				
H	1.9561870	2.6921180	0.0767270				
H	1.8619770	1.6784870	1.5518890				
H	3.2283400	1.4856770	0.4126500				
C	1.6826780	0.5483040	-1.6195820				
H	1.3791630	1.4496340	-2.1845810				
H	2.7660040	0.4076820	-1.7738750				
H	1.1666020	-0.3224140	-2.0445660				

Table S17. Geometric coordinates and single point energies for DMPU.

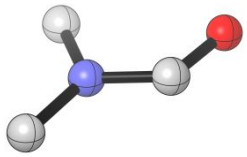


G = -419.945815 Hartrees

G_{SP} = -420.4209791 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	0.0000560	1.9923990	0.3658860				
C	1.2338520	1.3144390	-0.1969130				
H	1.3336000	1.5383760	-1.2778980				
H	2.1415790	1.7025400	0.2913850				
N	1.1759320	-0.1132290	0.0327330				
C	-0.0000280	-0.8406920	0.0624080				
O	-0.0000400	-2.0564720	0.1348890				
N	-1.1759610	-0.1131790	0.0328340				
C	-1.2337830	1.3144960	-0.1968940				
H	-1.3334820	1.5383930	-1.2778900				
H	-2.1414920	1.7026880	0.2913590				
C	-2.4261000	-0.8309680	-0.0667020				
H	-2.8769650	-0.7121270	-1.0677000				
H	-2.2368910	-1.8929250	0.1143310				
H	-3.1426690	-0.4537730	0.6799980				
C	2.4260570	-0.8310520	-0.0666670				
H	2.2367500	-1.8930320	0.1141360				
H	2.8771170	-0.7120280	-1.0675550				
H	3.1425130	-0.4540420	0.6802390				
H	0.0000490	1.8994910	1.4624190				
H	0.0000980	3.0613380	0.1123860				

Table S18 Geometric coordinates and single point energies for DMF.

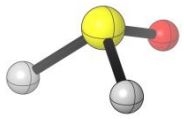


G = -248.116542 Hartrees

G_{SP} = -248.4052246 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.6436700	-0.6743900	0.0000520				
N	-0.3639330	0.0073100	-0.0000990				
C	0.7924140	-0.7023160	-0.0000120				
O	1.8955630	-0.2092570	0.0000470				
H	0.6210950	-1.8053300	-0.0001360				
C	-0.2488520	1.4540610	-0.0000030				
H	0.3010290	1.8021710	0.8870370				
H	0.3053980	1.8016000	-0.8845050				
H	-1.2503850	1.8986610	-0.0025750				
H	-1.7735890	-1.3050040	0.8933550				
H	-2.4461590	0.0717520	0.0000920				
H	-1.7737210	-1.3050980	-0.8931670				

Table S19. Geometric coordinates and single point energies for DMSO.

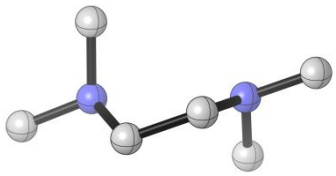


G = -552.775442 Hartrees

G_{SP} = -553.126551 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	1.3548720	-0.7986380	0.1864640				
S	-0.0000010	0.2297450	-0.4529670				
O	-0.0000420	1.4684330	0.3923000				
C	-1.3548360	-0.7986990	0.1864590				
H	-2.2813170	-0.2614300	-0.0483980				
H	-1.3550120	-1.7870120	-0.2912290				
H	-1.2347960	-0.8713350	1.2753970				
H	1.3551540	-1.7869040	-0.2913220				
H	2.2813230	-0.2612730	-0.0482960				
H	1.2347870	-0.8713990	1.2753890				

Table S20. Geometric coordinates and single point energies for *N,N,N',N'*-tetramethylethylenediamine (TMEDA).

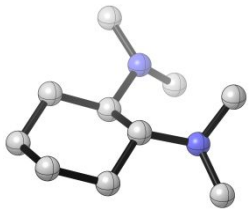


G = -347.098997 Hartrees

G_{SP} = -347.4956942 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.7069220	-0.2873500	0.9881320	H	-0.4568220	1.6871550	-0.8389580
H	-1.2314030	0.1316480	1.8791130	H	-2.0665940	1.4462310	-1.5474710
H	-0.6634400	-1.3778250	1.1455440	H	-1.9342340	2.0004390	0.1464540
C	0.7069200	0.2873500	0.9881310	H	-3.2859930	-0.5139240	-1.1202870
H	0.6634390	1.3778260	1.1455410	H	-2.7063940	-1.6921760	0.0813540
H	1.2314020	-0.1316450	1.8791130	C	-1.4765480	1.3414990	-0.6259160
N	1.4485050	0.0487120	-0.2313130				
C	1.4765500	-1.3415010	-0.6259140				
H	2.0665920	-1.4462320	-1.5474720				
H	1.9342410	-2.0004380	0.1464540				
H	0.4568250	-1.6871590	-0.8389530				
C	2.7719550	0.6196250	-0.1542410				
H	3.4050460	0.1394960	0.6255900				
H	3.2859950	0.5139200	-1.1202840				
H	2.7063920	1.6921780	0.0813480				
N	-1.4485050	-0.0487130	-0.2313130				
C	-2.7719560	-0.6196240	-0.1542410				
H	-3.4050490	-0.1394900	0.6255850				

Table S21. Geometric coordinates and single point energies for *(1R,2R)-N,N,N',N'*-tetramethylcyclohexane-1,2-diamine ((R,R)-TMCDA).

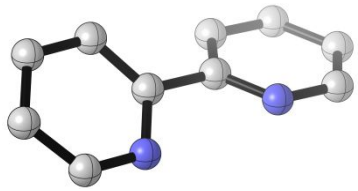


G = -502.865558 Hartrees

G_{SP} = -503.4291549 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	0.1791590	0.7242740	0.2795520	H	3.5991680	1.2533800	-0.1192610
C	1.4437220	1.4481450	-0.1965420	H	2.7645600	0.7269580	1.3480470
C	2.7095080	0.7189340	0.2461000	H	1.4305010	1.5153780	-1.2983280
C	2.7083270	-0.7233460	-0.2461350	H	1.4567010	2.4773460	0.1879840
C	1.4413910	-1.4504990	0.1965400	H	0.2618800	0.6304220	1.3849360
C	0.1779500	-0.7245480	-0.2795170	N	-1.0630290	1.4398430	-0.0394690
H	0.2609650	-0.6307140	-1.3848810	C	-2.0570620	1.3093190	1.0080180
N	-1.0653700	-1.4381000	0.0393240	H	-3.0369110	1.6525400	0.6413470
C	-2.0590870	-1.3061450	-1.0082650	H	-2.1415890	0.2585220	1.3064400
H	-1.8019980	-1.9118890	-1.9057340	H	-1.7990060	1.9143440	1.9056850
H	-3.0395630	-1.6475930	-0.6416020	C	-0.9665200	2.8149540	-0.4756850
H	-2.1417970	-0.2552760	-1.3069470	H	-0.6134610	3.5135310	0.3143290
C	-0.9712380	-2.8132070	0.4760260	H	-0.3073240	2.9192760	-1.3459700
H	-0.6192110	-3.5126670	-0.3136880	H	-1.9672820	3.1530940	-0.7826840
H	-0.3123510	-2.9183720	1.3464420				
H	-1.9726020	-3.1496100	0.7829760				
H	1.4526520	-2.4797030	-0.1880320				
H	1.4280980	-1.5177540	1.2983240				
H	2.7633270	-0.7314530	-1.3480850				
H	3.5971320	-1.2592500	0.1191800				

Table S22. Geometric coordinates and single point energies for 2,2'-bipyridine (bipy).

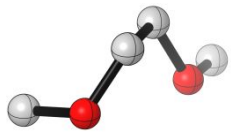


G = -494.662501 Hartrees

G_{SP} = -495.2079865 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.7479110	0.0013160	0.0003520				
C	-1.4628240	1.1541000	0.3549010				
C	-2.8535720	1.1128720	0.3421420				
C	-3.4832600	-0.0727670	-0.0237520				
C	-2.6808090	-1.1664690	-0.3555200				
H	-3.1410330	-2.1158240	-0.6473670				
N	-1.3539440	-1.1360400	-0.3436700				
H	-4.5698930	-0.1566930	-0.0493300				
H	-3.4356710	1.9922550	0.6225350				
H	-0.9353470	2.0582330	0.6603200				
C	0.7479110	0.0013150	-0.0003540				
C	1.4628240	1.1541000	-0.3549020				
C	2.8535720	1.1128720	-0.3421420				
C	3.4832600	-0.0727660	0.0237540				
C	2.6808090	-1.1664690	0.3555210				
H	3.1410330	-2.1158230	0.6473720				
N	1.3539440	-1.1360410	0.3436680				
H	4.5698930	-0.1566920	0.0493350				
H	3.4356720	1.9922560	-0.6225320				
H	0.9353470	2.0582330	-0.6603210				

Table S23. Geometric coordinates and single point energies for 1,2-dimethoxyethane (DME).

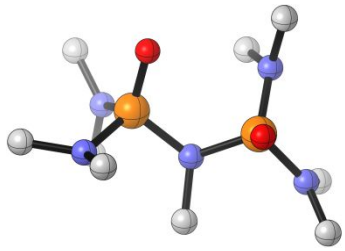


G = -308.347018 Hartrees

G_{SP} = -308.7116513 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	0.8545320	1.0807780	-0.0333880				
H	1.4082410	1.5961330	0.7787710				
H	0.6933360	1.8015900	-0.8470190				
C	-0.4922100	0.6499760	0.5210180				
H	-0.3631990	0.0258080	1.4291910				
H	-1.0482120	1.5558250	0.8379540				
O	-1.1877530	-0.0582110	-0.4594400				
C	-2.4357060	-0.5086350	-0.0274660				
H	-3.0965540	0.3302800	0.2617460				
H	-2.3453150	-1.1869650	0.8423880				
H	-2.9043750	-1.0569690	-0.8538690				
O	1.6140040	0.0440770	-0.5803980				
C	1.8299410	-1.0406890	0.2708620				
H	2.5777850	-1.6888460	-0.2031870				
H	2.2191200	-0.7216180	1.2575770				
H	0.9098240	-1.6307360	0.4289980				

Table S24. Geometric coordinates and single point energies for *N,N,N′,N″,N″*-nonamethylimidodiphosphoramide (NIPA).



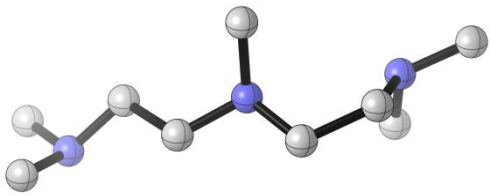
G = -1464.665262 Hartrees

G_{SP} = -1465.855078 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.0047680	0.3528710	1.8834350	H	2.7533190	2.9113670	1.2325640
N	-2.7876000	-0.4771510	0.7234100	C	2.2771890	0.4399120	2.3130710
P	-1.6030490	-0.1432410	-0.4146260	H	1.4414450	-0.2218190	2.5712780
N	-1.5979910	1.4900890	-0.7003370	H	3.2235960	-0.1053700	2.4922420
C	-1.7948540	1.9273580	-2.0759290	H	2.2457140	1.2954020	3.0067580
H	-0.8181520	2.1577370	-2.5326030	N	2.1725470	-1.3661610	-0.4499200
H	-2.2697620	1.1271930	-2.6542700	C	3.6229940	-1.3527880	-0.4594830
H	-2.4382720	2.8211730	-2.0953520	H	4.0041040	-0.6780390	0.3182410
C	-0.9289620	2.4702520	0.1342300	H	4.0000970	-2.3653420	-0.2478020
H	-1.6091330	3.3071260	0.3677510	H	4.0339900	-1.0317390	-1.4342740
H	-0.5899400	2.0182140	1.0756700	C	1.5804260	-2.2909970	-1.4116710
H	-0.0392100	2.8609750	-0.3863190	H	1.7754460	-3.3309640	-1.1047800
O	-1.7876450	-1.0052720	-1.6127800	H	0.4934890	-2.1323650	-1.4800510
N	-0.1327290	-0.4662770	0.4297720	H	1.9981690	-2.1368530	-2.4215870
P	1.3349920	0.0766480	-0.2395450	C	-0.2003040	-1.6886900	1.2423490
O	1.1385000	0.9238540	-1.4458080	H	-0.7450690	-1.5042830	2.1807500
N	2.1527190	0.9145840	0.9543730	H	-0.7101010	-2.4995600	0.6958850
C	2.9894020	2.0431260	0.5946730	H	0.8119510	-2.0388060	1.4718840
H	4.0640600	1.8128260	0.7163460	C	-3.4776430	-1.7502430	0.7084390
H	2.7987640	2.3129410	-0.4509070	H	-3.1654680	-2.4020110	1.5464410

H	-4.5660260	-1.5922910	0.7890290
H	-3.2697360	-2.2582790	-0.2407850
H	-4.0799090	0.3802520	2.1225200
H	-2.4701820	-0.0118810	2.7826690
H	-2.6886640	1.3842410	1.6842110

Table S25. Geometric coordinates and single point energies for *N,N,N′,N″,N″*-pentamethyldiethlylenetriamine (PMDTA).

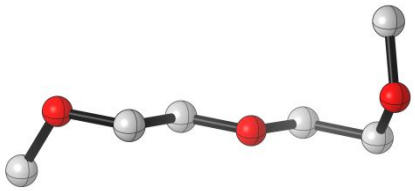


G = -520.058617 Hartrees

G_{SP} = -520.6513216 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	2.6833450	-0.8495710	-0.3928530	C	-4.0405990	-0.7597630	-0.6056820
H	3.2989410	-1.1266260	-1.2809410	H	-4.3430170	-1.3218340	0.3069280
H	2.9230330	-1.5917790	0.3863840	H	-4.9514370	-0.5176710	-1.1715430
C	1.2199890	-0.9883810	-0.8035260	H	-3.4300690	-1.4267990	-1.2291420
H	1.0584520	-0.4875470	-1.7719120	N	3.0391550	0.4562450	0.1189160
H	1.0318590	-2.0728530	-0.9818120	C	4.4337430	0.5068040	0.4880520
N	0.2743120	-0.4290910	0.1413170	H	5.1158940	0.3797300	-0.3824810
C	0.4679140	-0.9189630	1.4894820	H	4.6644970	1.4719280	0.9613350
H	-0.2552300	-0.4486120	2.1684550	H	4.6612410	-0.2905080	1.2111100
H	0.3415250	-2.0227500	1.5663810	C	2.6697610	1.5398530	-0.7636740
H	1.4706880	-0.6420920	1.8383050	H	2.9828230	2.4947980	-0.3181560
C	-1.0837670	-0.6057560	-0.3358280	H	3.1471210	1.4607710	-1.7666180
H	-1.3630530	-1.6846760	-0.3455120	H	-3.6248230	2.3434830	0.5592770
H	-1.1321730	-0.2510200	-1.3779180	H	1.5790210	1.5664120	-0.8838500
C	-2.1054390	0.2081860	0.4552410	H	-4.5308690	1.0320940	1.3711990
H	-2.3377160	-0.2858710	1.4269520				
H	-1.6367970	1.1773270	0.6878120				
N	-3.3218030	0.4562360	-0.2956520				
C	-4.1714280	1.4056090	0.3862310				
H	-5.0526770	1.6322550	-0.2309760				

Table S26. Geometric coordinates and single point energies for 1-methoxy-2-(2-methoxyethoxy)ethane (diglyme).

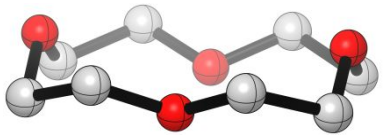


G = -461.935402 Hartrees

G_{SP} = -462.4788181 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	2.5518820	0.9555020	-0.3165470	H	3.6327440	-2.1081760	0.0188110
H	3.3256950	1.4871730	0.2751590	H	3.7306280	-0.7839770	1.2167830
H	2.4105220	1.5000100	-1.2605470	H	2.1446870	-1.5229410	0.8110630
C	1.2557620	0.9885800	0.4744360				
H	1.3991070	0.5585950	1.4860960				
H	0.9567660	2.0461690	0.6189120				
O	0.2766470	0.2742170	-0.2198280				
C	-0.9563050	0.2246470	0.4374950				
H	-1.3617120	1.2453200	0.5877830				
H	-0.8605200	-0.2394720	1.4385500				
C	-1.9023340	-0.6098980	-0.4127050				
H	-1.9658070	-0.1670870	-1.4242990				
H	-1.4794720	-1.6190270	-0.5186280				
O	-3.1662040	-0.7330100	0.1769020				
C	-4.0359690	0.3285350	-0.0920210				
H	-4.2227440	0.4324610	-1.1767160				
H	-4.9885380	0.1150090	0.4086460				
H	-3.6567330	1.2958290	0.2841660				
O	2.9805500	-0.3258760	-0.6693740				
C	3.1215370	-1.2144540	0.3981120				

Table S27. Geometric coordinates and single point energies for 12-crown-4.

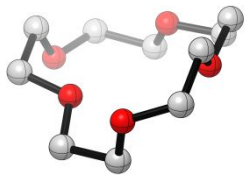


G = -614.356638 Hartrees

G_{SP} = -615.070846 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	0.2505660	2.3482010	1.2081860	H	1.3360610	2.2584590	-1.0302090
H	0.0718640	3.2832680	1.7681530	H	0.1796140	1.2991110	-3.0896610
H	1.3360610	2.2584590	1.0302090	H	-1.2985940	1.1604510	-2.0906590
C	-0.1923090	1.1734570	2.0516710	H	-1.2985990	-1.1604470	-2.0906430
H	0.1796140	1.2991110	3.0896610	H	0.1796000	-1.2991070	-3.0896580
H	-1.2985940	1.1604510	2.0906590	H	0.0718690	-3.2832620	-1.7681620
O	0.2990340	0.0000030	1.4794900	H	1.3360640	-2.2584560	-1.0302110
C	-0.1923130	-1.1734530	2.0516650				
H	0.1796000	-1.2991070	3.0896580				
H	-1.2985990	-1.1604470	2.0906430				
C	0.2505680	-2.3481990	1.2081860				
H	0.0718690	-3.2832620	1.7681620				
H	1.3360640	-2.2584560	1.0302110				
O	-0.4586510	-2.3790310	0.0000000				
C	0.2505680	-2.3481990	-1.2081860				
C	-0.1923130	-1.1734530	-2.0516650				
O	0.2990340	0.0000030	-1.4794900				
C	-0.1923090	1.1734570	-2.0516710				
C	0.2505660	2.3482010	-1.2081860				
O	-0.4586560	2.3790110	0.0000000				
H	0.0718640	3.2832680	-1.7681530				

Table S28. Geometric coordinates and single point energies for 15-crown-5.

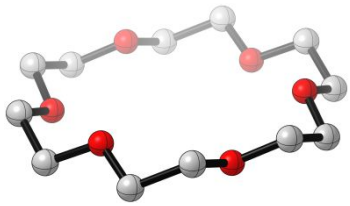


G = -767.952198 Hartrees

G_{SP} = -768.844353 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	0.4305190	-0.6200380	-2.4999700	C	0.9068120	-2.5208980	-1.2221400
H	0.3717800	-1.1171900	-3.4885590	O	0.0000000	-1.4898330	-1.4924220
H	1.4817020	-0.3153580	-2.3382540	H	1.1287510	-3.0989190	-2.1431310
C	-0.4305190	0.6200380	-2.4999700	H	1.8596800	-2.1044590	-0.8434060
H	-0.3717800	1.1171900	-3.4885590	H	0.9983560	-4.3234560	-0.0831100
H	-1.4817020	0.3153580	-2.3382540	H	-0.6557410	-3.8194210	-0.5134400
O	0.0000000	1.4898330	-1.4924220	H	-1.6699100	-2.8270100	1.8550430
C	-0.9068120	2.5208980	-1.2221400	H	-1.3877640	-1.7499120	0.4425430
H	-1.1287510	3.0989190	-2.1431310	H	-1.5432300	-0.6160170	2.7507000
H	-1.8596800	2.1044590	-0.8434060	H	0.0502040	-1.3600880	3.0832910
C	-0.3313070	3.4523910	-0.1755290	H	-0.0502040	1.3600880	3.0832910
H	0.6557410	3.8194210	-0.5134400	H	1.5432300	0.6160170	2.7507000
H	-0.9983560	4.3234560	-0.0831100	H	1.6699100	2.8270100	1.8550430
O	-0.2505450	2.8522540	1.0851460	H	1.3877640	1.7499120	0.4425430
C	0.9410100	2.1547810	1.3636740				
C	0.6171430	0.9981180	2.2769900				
O	0.0000000	0.0000000	1.5195940				
C	-0.6171430	-0.9981180	2.2769900				
C	-0.9410100	-2.1547810	1.3636740				
O	0.2505450	-2.8522540	1.0851460				
C	0.3313070	-3.4523910	-0.1755290				

Table S29 Geometric coordinates and single point energies for 18-crown-6.

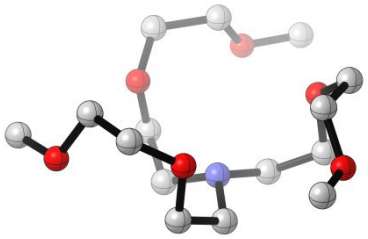


G = -921.537616 Hartrees

G_{SP} = -922.6124367 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.1661250	3.4073030	0.2966740	C	3.5338730	-0.6937570	0.2966740
H	-1.2275390	4.4932020	0.0781630	C	3.5338730	0.6937570	-0.2966740
H	-1.1904630	3.2834960	1.3965600	O	2.4777930	1.4305540	0.2417800
C	-2.3677480	2.7135460	-0.2966740	C	2.3677480	2.7135460	-0.2966740
H	-3.2774570	3.3096810	-0.0781630	C	1.1661250	3.4073030	0.2966740
H	-2.2483600	2.6727190	-1.3965600	O	0.0000000	2.8611090	-0.2417800
O	-2.4777930	1.4305540	0.2417800	H	1.2275390	4.4932020	0.0781630
C	-3.5338730	0.6937570	-0.2966740	H	1.1904630	3.2834960	1.3965600
H	-4.5049960	1.1835210	-0.0781630	H	3.2774570	3.3096810	-0.0781630
H	-3.4388230	0.6107770	-1.3965600	H	2.2483600	2.6727190	-1.3965600
C	-3.5338730	-0.6937570	0.2966740	H	4.5049960	1.1835210	-0.0781630
H	-4.5049960	-1.1835210	0.0781630	H	3.4388230	0.6107770	-1.3965600
H	-3.4388230	-0.6107770	1.3965600	H	4.5049960	-1.1835210	0.0781630
O	-2.4777930	-1.4305540	-0.2417800	H	3.4388230	-0.6107770	1.3965600
C	-2.3677480	-2.7135460	0.2966740	H	2.2483600	-2.6727190	1.3965600
H	-3.2774570	-3.3096810	0.0781630	H	3.2774570	-3.3096810	0.0781630
H	-2.2483600	-2.6727190	1.3965600	H	1.2275390	-4.4932020	-0.0781630
C	-1.1661250	-3.4073030	-0.2966740	H	1.1904630	-3.2834960	-1.3965600
H	-1.2275390	-4.4932020	-0.0781630	C	1.1661250	-3.4073030	-0.2966740
H	-1.1904630	-3.2834960	-1.3965600	C	2.3677480	-2.7135460	0.2966740
O	0.0000000	-2.8611090	0.2417800	O	2.4777930	-1.4305540	-0.2417800

Table S30. Geometric coordinates and single point energies for TDA-1.



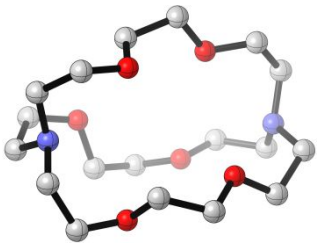
G = -1095.676597 Hartrees

G_{SP} = -1096.938665 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-4.3924890	0.6252980	-0.1800840	H	1.1864310	-0.8895640	2.7840680
O	-3.3981500	1.6113960	-0.1125500	H	0.7613040	-1.9308170	1.4028460
C	-2.5515540	1.5997520	-1.2381230	C	-1.3113120	-0.4585050	1.6766010
C	-1.5410210	2.7283080	-1.1494230	C	-1.7728790	-1.7586310	1.0398060
O	-0.4234850	2.4305540	-0.3554660	O	-1.8945140	-1.5818480	-0.3544490
C	-0.6368110	2.4139760	1.0389400	C	-1.5930550	-2.6980210	-1.1488220
C	0.2588220	1.3647090	1.6758860	C	-0.1102460	-3.0078390	-1.2379610
N	0.0000790	-0.0003160	1.2529630	O	0.3035090	-3.7474270	-0.1129620
C	1.0528270	-0.9068740	1.6762320	C	1.6544940	-4.1159210	-0.1814910
C	2.4094990	-0.6559930	1.0394980	H	1.8367120	-4.7985190	-1.0332420
O	2.3174920	-0.8492370	-0.3548840	H	1.9079660	-4.6417900	0.7480630
C	3.1340890	-0.0302070	-1.1487830	H	2.3014180	-3.2293440	-0.2969720
C	2.6619630	1.4091980	-1.2377750	H	0.4571840	-2.0606670	-1.3017800
O	3.0949230	2.1366840	-0.1121170	H	0.0779590	-3.5984890	-2.1575790
C	2.7378060	3.4907780	-0.1798580	H	-1.9608230	-2.4576800	-2.1569390
H	3.0658440	3.9728200	0.7501330	H	-2.1278390	-3.6010800	-0.7975780
H	3.2378700	3.9907190	-1.0311000	H	-2.7595460	-2.0165910	1.4714880
H	1.6465080	3.6072290	-0.2957940	H	-1.0926500	-2.5924960	1.2621580
H	1.5580510	1.4279240	-1.3026630	H	-2.0522390	0.3060860	1.4035140
H	3.0804500	1.8675820	-2.1568690	H	-1.3627670	-0.5829450	2.7844440

H	4.1834130	-0.0424570	-0.7971160
H	3.1099740	-0.4685970	-2.1570160
H	2.7911660	0.3500890	1.2622130
H	3.1264850	-1.3813390	1.4710100
H	-2.0549200	3.6432990	-0.7979140
H	-1.1492830	2.9262910	-2.1577120
H	-3.1576810	1.7326080	-2.1573350
H	-2.0156400	0.6344640	-1.3024850
H	-5.0755870	0.8084890	-1.0312130
H	-4.9737910	0.6685310	0.7500070
H	-3.9479090	-0.3781230	-0.2959570
H	0.1770910	1.4720330	2.7837000
H	1.2912940	1.6241520	1.4024620
H	-1.6989210	2.2415570	1.2617710
H	-0.3670690	3.3976760	1.4702270

Table S31. Geometric coordinates and single point energies for [2.2.2]-cryptand.



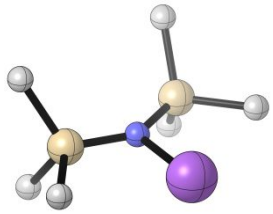
G = -1266.283094 Hartrees

G_{SP} = -1267.734192 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.5119160	-0.5856540	-1.2605280	H	-1.5351590	-1.1268220	3.2719780
N	-3.1056950	0.0009780	-0.0004380	H	0.6321260	-2.4750470	2.7139630
C	-3.5125540	1.3854160	0.1210400	H	0.7007460	-1.0859880	3.8368940
C	-2.7087100	2.1867200	1.1420120	H	2.6842050	-2.2795680	1.3899730
O	-1.3260500	2.1436020	0.9605130	H	3.0338690	-1.5738970	2.9891940
C	-0.8863200	2.5745710	-0.3077600	H	4.7417480	-0.8113570	1.4626450
C	0.5302730	3.0977860	-0.2036910	H	3.7136730	0.5404440	1.9785520
O	1.4511990	2.0577750	-0.3461760	C	3.7263310	-0.9901270	-0.9986030
C	2.7111350	2.3596820	0.1707270	C	2.7110460	-1.0312160	-2.1263180
C	3.7253480	1.3619400	-0.3588290	O	1.4524920	-1.3311400	-1.6049240
N	3.4187740	0.0010670	0.0004500	C	0.5307190	-1.7286980	-2.5757520
C	3.7253690	-0.3682260	1.3585620	C	-0.8855500	-1.5544630	-2.0706450
C	2.7117520	-1.3272640	1.9562360	O	-1.3236160	-0.2404650	-2.3341480
O	1.4514970	-0.7295390	1.9525290	C	-2.7059470	-0.1033610	-2.4640670
C	0.5301460	-1.3751050	2.7798350	H	-3.0733310	-0.6603790	-3.3514300
C	-0.8863690	-1.0217420	2.3797020	H	-2.8889770	0.9637090	-2.6607830
O	-1.3277500	-1.9042490	1.3726600	H	-1.5355900	-2.2742190	-2.6068930
C	-2.7105460	-2.0820580	1.3204050	H	-0.9159750	-1.7691380	-0.9873850
C	-3.5134470	-0.7965590	1.1373900	H	0.6335300	-1.1266080	-3.4985020
H	-4.5940020	-1.0668190	1.0916080	H	0.6998980	-2.7903340	-2.8483810

H	-3.3931560	-0.1878220	2.0445450
H	-2.8961580	-2.7854600	0.4948310
H	-3.0780250	-2.5712030	2.2468660
H	-0.9156850	0.0245440	2.0262390
H	3.7154930	1.4440310	-1.4558410
H	4.7411790	1.6739330	-0.0257030
H	3.0340810	3.3771000	-0.1328180
H	2.6824610	2.3467890	1.2785850
H	0.7007390	3.8662250	-0.9850470
H	0.6327590	3.5938050	0.7802170
H	-0.9165130	1.7452890	-1.0370390
H	-1.5354300	3.3999630	-0.6621010
H	-3.0765630	3.2335240	1.1029500
H	-2.8931580	1.8232450	2.1641060
H	-3.3926910	1.8661930	-0.8599830
H	-4.5928850	1.4815650	0.3786470
H	-4.5917590	-0.4092020	-1.4738580
H	-3.3936680	-1.6757630	-1.1861670
H	2.6795170	-0.0644730	-2.6673300
H	3.0345210	-1.8011480	-2.8571530
H	4.7416270	-0.8558310	-1.4359880
H	3.7182650	-1.9813170	-0.5214070

Table S32. Geometric coordinates and single point energies for NaHMDS unsolvated monomer.

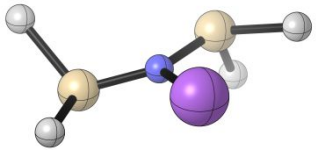


G = -1034.7736 Hartrees

G_{SP} = -1035.375722 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	-1.5699080	-0.2392140	0.0001360	H	-3.8262110	0.9556380	0.0054040
N	0.0000010	0.3957450	0.0000670	H	-2.6198020	1.8800110	0.9061000
Si	1.5699100	-0.2392170	-0.0001170	H	-2.6220470	1.8839020	-0.8940440
C	2.0109970	-1.2712870	1.5253290	C	-2.0107950	-1.2715990	-1.5251550
H	3.0686840	-1.5782380	1.5244400	H	-1.8147000	-0.7058580	-2.4490660
H	1.8150410	-0.7053390	2.4491440	H	-1.3956320	-2.1844240	-1.5610690
H	1.3958090	-2.1840850	1.5615240	H	-3.0684910	-1.5785200	-1.5243390
C	2.7674060	1.2565060	-0.0053120	H	-1.3936180	-2.1935460	1.5495390
H	2.6221810	1.8840600	0.8935240	C	-2.7674050	1.2565090	0.0048820
H	3.8262120	0.9556380	-0.0059290				
H	2.6196650	1.8798440	-0.9066190				
C	2.0075550	-1.2800860	-1.5205290				
H	1.3934660	-2.1939060	-1.5490620				
H	1.8079770	-0.7201730	-2.4472350				
H	3.0656180	-1.5857260	-1.5209830				
Na	0.0000020	2.5420030	0.0000060				
C	-2.0077610	-1.2797720	1.5207020				
H	-1.8083720	-0.7196430	2.4473180				
H	-3.0658060	-1.5854780	1.5210480				

Table S33. Geometric coordinates and single point energies for NaTMDS unsolvated monomer.

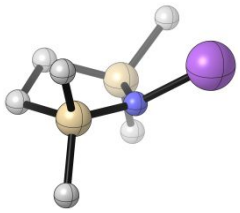


G = -956.273505 Hartrees

G_{SP} = -956.7823872 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	1.5300110	-0.4910960	-0.3144320	C	2.7320710	0.9769090	-0.5480500
N	0.0000190	0.1628100	-0.0008810	H	2.4195530	1.6214430	-1.3894220
Si	-1.5297690	-0.4908860	0.3140890	H	2.7854420	1.5865020	0.3727880
C	-2.2460350	-1.5707570	-1.0612680	H	3.7596760	0.6515590	-0.7696090
H	-3.2543070	-1.9349150	-0.8106860	H	1.6343230	-1.2960730	-1.5810620
H	-2.3028170	-1.0078400	-2.0058020				
H	-1.6031020	-2.4468590	-1.2368230				
C	-2.7312370	0.9772930	0.5496520				
H	-2.7853920	1.5873330	-0.3708460				
H	-3.7587020	0.6520880	0.7720710				
H	-2.4177220	1.6213580	1.3910100				
H	-1.6327870	-1.2964380	1.5804660				
Na	0.0002450	2.3084540	-0.0003770				
C	2.2444300	-1.5717680	1.0612600				
H	1.6010850	-2.4477930	1.2356900				
H	3.2528970	-1.9360650	0.8116650				
H	2.3002750	-1.0092930	2.0061140				

Table S34 Geometric coordinates and single point energies for NaCPTMDS unsolvated monomer.

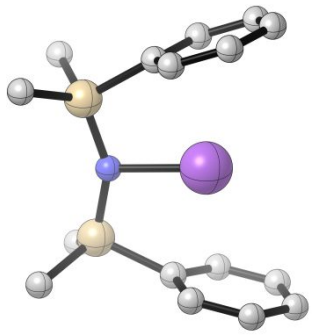


G = -1033.579549 Hartrees

G_{SP} = -1034.175637 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	-1.4586700	-0.1068820	0.0509860	H	-1.5625470	-2.1439690	-1.5176200
C	-0.8892310	-1.7623000	-0.7327070	C	-2.6264540	-0.4344900	1.5020220
C	0.5590940	-1.5482890	-1.2420200	H	-2.9627390	0.5084270	1.9614250
H	0.5375670	-1.0456900	-2.2254210	H	-3.5215550	-0.9923360	1.1848710
H	1.1052900	-2.4949440	-1.3828800	H	-2.1119210	-1.0198050	2.2789640
Si	1.3433300	-0.3360980	0.0049440	C	-2.4516460	0.9179710	-1.2080360
N	0.0227370	0.6490570	0.4779970	H	-3.3995900	0.4315800	-1.4866620
Na	0.5294680	2.7119600	0.3712720	H	-2.7052750	1.9101960	-0.7958080
C	2.1860990	-1.2898800	1.4058280	H	-1.8658270	1.0706030	-2.1286150
H	3.0255380	-1.9024740	1.0411040				
H	2.5714920	-0.6032060	2.1758800				
H	1.4610090	-1.9589800	1.8942560				
C	2.7114620	0.7349650	-0.7926940				
H	3.1291440	1.4584300	-0.0673580				
H	3.5634640	0.1333610	-1.1450570				
H	2.3222290	1.2891870	-1.6641200				
H	-0.8907860	-2.5214780	0.0696920				

Table S35. Geometric coordinates and single point energies for NaDPTMDS unsolvated monomer.



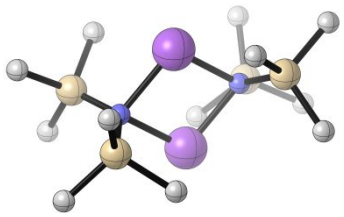
G = -1417.731619 Hartrees

G_{SP} = -1418.74092 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	-1.6196610	-1.5579560	0.0000410	H	3.2029510	2.7442600	2.1534450
N	0.0000030	-1.1216560	-0.0011250	H	3.5121180	3.9585220	-0.0004670
Si	1.6196680	-1.5579510	0.0000440	H	3.2100570	2.7416040	-2.1538680
C	2.2291420	-2.4944140	-1.5238280	H	2.5595130	0.3546870	-2.1542780
H	3.3241850	-2.6085320	-1.5318570	Na	-0.0000010	1.1305910	-0.0018390
H	1.7826660	-3.5011520	-1.5374180	C	-2.2270860	-2.4938770	1.5250730
H	-1.7827120	-3.5010660	-1.5375300	H	-1.9185070	-1.9912170	2.4542910
C	-2.2291500	-2.4943120	-1.5238910	H	-3.3220580	-2.6085510	1.5342600
H	-1.9211730	-1.9923010	-2.4536580	H	-1.7800650	-3.5003750	1.5387920
H	-3.3241970	-2.6083920	-1.5319440	C	-2.4976440	0.1617570	0.0002930
H	1.9212000	-1.9924430	-2.4536280	C	-2.6952400	0.8711460	1.1993150
C	2.2271120	-2.4937690	1.5251340	C	-3.0562670	2.2221950	1.2059280
H	1.7801350	-3.5002850	1.5388930	C	-3.2326170	2.9036730	-0.0000890
H	3.3220890	-2.6083970	1.5343460	C	-3.0609590	2.2205840	-1.2058510
H	1.9184920	-1.9910780	2.4543220	C	-2.6998910	0.8695370	-1.1988630
C	2.4976450	0.1617640	0.0001860	H	-2.5601300	0.3545770	-2.1541590
C	2.6995450	0.8696040	-1.1989970	H	-3.2106830	2.7414890	-2.1536760
C	3.0606030	2.2206520	-1.2060250	H	-3.5121370	3.9585100	-0.0002500

C	3.2326030	2.9036830	-0.0002770
C	3.0566030	2.2221460	1.2057550
C	2.6955800	0.8710950	1.1991820
H	2.5523780	0.3573480	2.1546320
H	-2.5517610	0.3574450	2.1547480
H	-3.2023500	2.7443530	2.1536350

Table S36. Geometric coordinates and single point energies for NaHMDS unsolvated dimer.



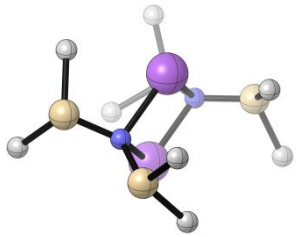
G = -2069.611626 Hartrees

G_{SP} = -2070.806016 Hartrees

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	-4.5537570	-2.1492280	-1.8682170
H	0.3807730	2.5807450	-1.1238510	Si	-2.5739480	1.4436920	0.4883350

H	1.7642490	3.4293590	-1.8216220
C	3.0368760	2.5766440	0.9544690
H	-1.7642590	3.4292180	1.8218680
H	-3.8939060	0.5965560	2.4397200
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
C	-4.1274930	1.1882280	1.5404500
H	-4.5538050	2.1491550	1.8682080
H	-4.9095520	0.6496290	0.9833940

Table S37. Geometric coordinates and single point energies for NaTMDS unsolvated dimer.



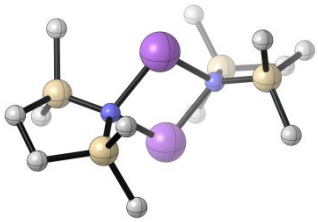
G = -1912.612565 Hartrees

G_{SP} = -1913.621594 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.0000980	0.0001240	1.4641640	H	1.9317280	3.4477920	-1.7966210
Si	-2.5860740	1.4592200	0.3825700	H	3.9036500	1.2678280	-1.0774470
N	-1.7786530	-0.0001200	-0.0003030	C	2.9203400	-2.5580260	-1.1172150
Si	-2.5854460	-1.4598990	-0.3828400	H	3.4395350	-3.4874520	-0.8380740
C	-2.9195090	-2.5584900	1.1173920	H	1.9842020	-2.8359010	-1.6285950
H	-3.4384730	-3.4880980	0.8384250	H	3.5531840	-2.0208760	-1.8404450
H	-1.9832710	-2.8360450	1.6287640	H	3.9036310	-1.2669710	1.0780570
H	-3.5524590	-2.0214020	1.8405770	H	1.9320880	-3.4474560	1.7966230
C	-1.4957440	-2.4599640	-1.5859400	H	1.3890880	-1.9582130	2.5646530
H	-0.4901730	-2.6414580	-1.1663090	H	-1.9310990	-3.4480800	-1.7963310
H	0.4909440	-2.6413830	1.1663930	H	-3.9032990	-1.2681170	-1.0780390
C	1.4964380	-2.4595100	1.5860420	C	-2.9200560	2.5582500	-1.1173560
Si	2.5858750	-1.4592990	0.3828220	H	-3.5526830	2.0212700	-1.8409020
N	1.7786490	0.0001720	0.0000210	H	-3.4393010	3.4876480	-0.8382090
Na	0.0000940	0.0000800	-1.4644170	H	-1.9837370	2.8361820	-1.6283720
H	-1.3885940	-1.9588010	-2.5646410	C	-1.4969980	2.4592900	1.5862460
Si	2.5856360	1.4598130	-0.3826160	H	-1.3897100	1.9578090	2.5647700
C	2.9193270	2.5586770	1.1175030	H	-0.4914790	2.6414000	1.1667540
H	3.5520910	2.0217380	1.8409600	H	-1.9328080	3.4471340	1.7969710
H	3.4383340	3.4882550	0.8385170	H	-3.9040400	1.2667040	1.0773450

H	1.9829370	2.8362900	1.6285660
C	1.4962320	2.4597690	-1.5860850
H	1.3890890	1.9584460	-2.5647040
H	0.4906580	2.6414740	-1.1665470

Table S38. Geometric coordinates and single point energies for NaCPTMDS unsolvated dimer.



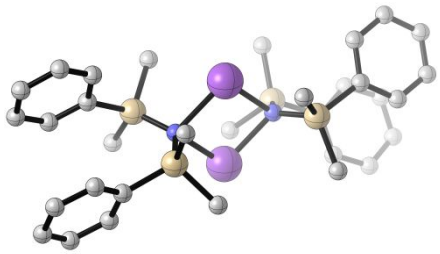
G = -2067.238754 Hartrees

G_{SP} = -2068.420947 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	-2.7385720	-1.3576540	-0.3787250	H	5.3070200	1.3143980	-0.2739980
C	-4.4905810	-0.6075410	-0.4811890	H	4.6400600	0.2549510	-1.5205110
C	-4.4905100	0.6055410	0.4837920	C	2.2095270	2.1467870	-2.0264530
H	-4.6400080	0.2552630	1.5205440	H	2.2514350	1.4103550	-2.8469770
H	-5.3068720	1.3147840	0.2740410	H	1.1838590	2.5525920	-1.9660950
Si	-2.7395320	1.3576650	0.3783870	H	2.8593350	2.9877120	-2.3129510
N	-1.7459200	0.0005440	-0.0007930	C	2.6644240	2.7319710	0.9222210
Na	-0.0005520	0.0009550	1.4681670	H	1.6339290	3.1084990	1.0340630
Na	0.0005540	0.0009370	-1.4681000	H	2.9951370	2.3510850	1.9015210
N	1.7459210	0.0005840	0.0008500	H	3.3033610	3.5894380	0.6604300
Si	2.7396880	1.3575780	-0.3783850	C	-2.6641110	2.7319950	-0.9222800
C	4.4905830	0.6052450	-0.4837610	H	-3.3029490	3.5895480	-0.6605270
C	4.4905090	-0.6078350	0.4812210	H	-1.6335740	3.1084030	-1.0341400
H	4.6421330	-0.2577390	1.5177240	H	-2.9948700	2.3511060	-1.9015630
H	5.3056220	-1.3181280	0.2701630	C	-2.2092600	2.1468920	2.0264120
Si	2.7384180	-1.3577410	0.3787310	H	-1.1835540	2.5525960	1.9660180
C	2.6589560	-2.7318940	-0.9219310	H	-2.8589780	2.9878970	2.3128820
H	3.2970080	-3.5903980	-0.6613870	H	-2.2512300	1.4105040	2.8469740
H	1.6276850	-3.1068510	-1.0320040	H	-5.3057690	-1.3177430	-0.2701190
H	2.9885680	-2.3514150	-1.9017690	H	-4.6421840	-0.2574280	-1.5176900
C	2.2098670	-2.1463520	2.0275320	C	-2.2101300	-2.1462550	-2.0275640

H	1.1837200	-2.5511590	1.9686860
H	2.8592790	-2.9878960	2.3131170
H	2.2536000	-1.4098540	2.8478780
C	-2.6592770	-2.7318670	0.9218800
H	-3.2974310	-3.5902830	0.6612930
H	-1.6280510	-3.1069480	1.0319450
H	-2.9888510	-2.3513910	1.9017320
H	-1.1840260	-2.5511710	-1.9687490
H	-2.8596390	-2.9877130	-2.3131800
H	-2.2537920	-1.4097120	-2.8478750

Table S39. Geometric coordinates and single point energies for NaDPTMDS unsolvated dimer with phenyl rings pulled back away from sodium.



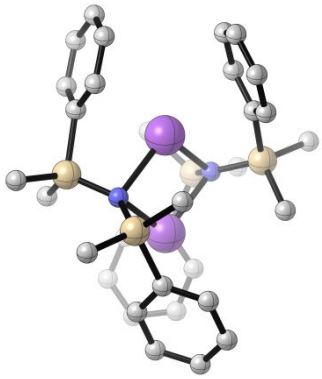
G = -2835.522747 Hartrees

G_{SP} = -2837.509341 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
N	1.7830540	0.0000050	-0.0000050	C	5.6910080	0.3210040	-2.8364510
Na	0.0000580	-0.0042530	1.4670460	C	6.8410390	0.7466580	-2.1705200
N	-1.7829270	-0.0000040	-0.0000030	C	6.7248200	1.4382890	-0.9658370
Na	0.0000560	0.0042550	-1.4670590	C	5.4641870	1.6965120	-0.4263590
Si	-2.5728780	1.4877650	0.3149660	H	5.3978250	2.2213560	0.5303450
C	-1.5174670	2.4588900	1.5712630	H	7.6207130	1.7675920	-0.4360490
H	-1.4593560	1.9440340	2.5474570	H	7.8263740	0.5394260	-2.5919620
H	-0.4926880	2.6248990	1.1937310	H	5.7744410	-0.2170370	-3.7828220
H	-1.9453340	3.4516880	1.7745220	H	3.5445110	0.2377400	-2.8221890
C	-2.7664040	2.6011930	-1.2017010	Si	2.5732370	-1.4893860	0.3068840
H	-1.7922020	2.7985040	-1.6776030	C	2.7681330	-2.5940040	-1.2160640
H	-3.4175760	2.1258220	-1.9512560	H	3.4201390	-2.1141630	-1.9620090
H	-3.2067440	3.5750590	-0.9367780	H	3.2080870	-3.5694830	-0.9565140
C	-4.2945880	1.2671230	1.0783980	H	1.7943630	-2.7882810	-1.6940930
C	-4.4369820	0.5739680	2.2911450	C	1.5175050	-2.4684460	1.5567090
C	-5.6923390	0.3066730	2.8363760	H	1.4583990	-1.9598330	2.5361120
C	-6.8418930	0.7360910	2.1720510	H	0.4931170	-2.6327680	1.1774130
C	-6.7248630	1.4338640	0.9709840	H	1.9458840	-3.4622250	1.7540210
C	-5.4638850	1.6946410	0.4335620	C	4.2944030	-1.2725740	1.0727140
H	-5.3968420	2.2244510	-0.5203550	C	4.4359670	-0.5857480	2.2891680

H	-7.6204070	1.7660130	0.4423830	C	5.6909430	-0.3209900	2.8364870
H	-7.8275090	0.5269160	2.5918800	C	6.8409900	-0.7466660	2.1705960
H	-5.7764260	-0.2362330	3.7799060	C	6.7247990	-1.4383150	0.9659200
H	-3.5458370	0.2228740	2.8227620	C	5.4641800	-1.6965350	0.4264100
Si	-2.5728780	-1.4877680	-0.3149950	H	5.3978400	-2.2213940	-0.5302870
C	-1.5174890	-2.4588540	-1.5713410	H	7.6207040	-1.7676350	0.4361640
H	-1.4594150	-1.9439750	-2.5475250	H	7.8263150	-0.5394370	2.5920630
H	-0.4926960	-2.6248580	-1.1938440	H	5.7743540	0.2170650	3.7828510
H	-1.9453480	-3.4516540	-1.7746100	H	3.5444480	-0.2377050	2.8221590
C	-2.7663690	-2.6012280	1.2016520	Si	2.5732410	1.4893900	-0.3069180
H	-3.4175260	-2.1258700	1.9512290	C	2.7680990	2.5940390	1.2160130
H	-3.2067150	-3.5750890	0.9367200	H	3.2080640	3.5695120	0.9564560
H	-1.7921590	-2.7985470	1.6775330	H	1.7943180	2.7883280	1.6940160
C	-4.2946050	-1.2671230	-1.0783880	H	3.4200850	2.1142090	1.9619820
C	-5.4638880	-1.6946230	-0.4335160	C	1.5175350	2.4684150	-1.5567930
C	-6.7248790	-1.4338450	-0.9709080	H	1.9459090	3.4621940	-1.7541150
C	-6.8419360	-0.7360870	-2.1719810	H	1.4584650	1.9597770	-2.5361860
C	-5.6923960	-0.3066870	-2.8363420	H	0.4931330	2.6327360	-1.1775320
C	-4.4370260	-0.5739830	-2.2911410	C	4.2944250	1.2725720	-1.0727040
H	-3.5458930	-0.2229040	-2.8227870	C	4.4360180	0.5857660	-2.2891650
H	-5.7765040	0.2362070	-3.7798770				
H	-7.8275610	-0.5269110	-2.5917880				
H	-7.6204110	-1.7659810	-0.4422790				
H	-5.3968240	-2.2244200	0.5204070				

Table S40. Geometric coordinates and single point energies for NaDPTMDS unsolvated dimer with phenyl rings over sodium.



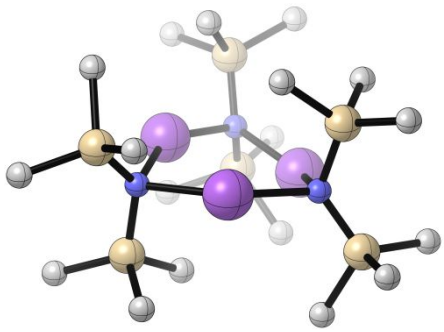
G = -2835.500531 Hartrees

G_{SP} = -2837.529058 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.4989850	0.0007790	-0.0009190	C	-2.2629700	-1.8252280	-1.8369280
Si	0.5168100	-2.5410350	1.4648630	C	-2.5926410	-1.1419050	-3.0177170
N	-0.0004450	-1.8447720	-0.0000140	C	-3.8609360	-0.5875280	-3.2124790
Si	-0.5186920	-2.5417400	-1.4642130	C	-4.8375360	-0.7133200	-2.2259280
C	-0.7310740	-4.4174370	-1.5153020	C	-4.5413760	-1.3959140	-1.0443920
H	-1.1196760	-4.7140400	-2.5018450	C	-3.2696810	-1.9392010	-0.8575990
H	0.2202830	-4.9438730	-1.3487120	H	-3.0483260	-2.4613540	0.0809030
H	-1.4479230	-4.7614100	-0.7545100	H	-5.2988960	-1.4995060	-0.2651880
C	0.5805350	-2.0490710	-2.9219020	H	-5.8284890	-0.2812900	-2.3767790
H	1.6023040	-2.4279960	-2.7569420	H	-4.0854740	-0.0539230	-4.1378680
Na	1.4992050	-0.0007340	-0.0010080	H	-1.8430370	-1.0333910	-3.8061800
N	0.0007010	1.8448400	-0.0007800	C	0.7288730	-4.4167840	1.5167640
Si	0.5187750	2.5412710	-1.4652970	H	1.4452280	-4.7613800	0.7558020
C	0.7314180	4.4169210	-1.5169600	H	1.1178850	-4.7129520	2.5032800
H	1.4482030	4.7610790	-0.7561960	H	-0.2227250	-4.9430770	1.3509880
H	1.1201510	4.7131780	-2.5035550	C	-0.5827440	-2.0479460	2.9221160
H	-0.2199230	4.9434740	-1.3506280	H	-0.6523200	-0.9522610	3.0167450

C	-0.5806730	2.0484120	-2.9227530	H	-1.6047830	-2.4257530	2.7562730
H	-0.6514760	0.9527260	-3.0164380	H	-0.2276920	-2.4528640	3.8825770
H	-1.6023540	2.4275740	-2.7577990	C	2.2612340	-1.8249670	1.8378480
H	-0.2247290	2.4519870	-3.8834560	C	2.5907220	-1.1414100	3.0185450
C	2.2629190	1.8243470	-1.8378830	C	3.8591910	-0.5875780	3.2136860
C	2.5924530	1.1406920	-3.0185140	C	4.8361470	-0.7141160	2.2275790
C	3.8605600	0.5858170	-3.2130760	C	4.5401860	-1.3969730	1.0461510
C	4.8370990	0.7113800	-2.2264370	C	3.2683240	-1.9397530	0.8589980
C	4.5410760	1.3942680	-1.0450360	H	3.0471540	-2.4622420	-0.0793720
C	3.2695730	1.9380780	-0.8584580	H	5.2980010	-1.5011920	0.2673160
H	3.0483110	2.4604330	0.0799530	H	5.8272200	-0.2824530	2.3786960
H	5.2985500	1.4976570	-0.2657590	H	4.0835900	-0.0537770	4.1389930
H	5.8278960	0.2789290	-2.3771150	H	1.8408090	-1.0322850	3.8066370
H	4.0849960	0.0519890	-4.1383600	C	-2.2611540	1.8258630	1.8370010
H	1.8428770	1.0323330	-3.8070270	C	-2.5907910	1.1429300	3.0180250
Si	-0.5166780	2.5416420	1.4638000	C	-3.8593860	0.5894750	3.2134080
C	-0.7285490	4.4174380	1.5150490	C	-4.8363230	0.7157950	2.2272490
H	-1.1174460	4.7140110	2.5014900	C	-4.5401900	1.3979950	1.0454870
H	0.2230430	4.9436340	1.3489710	C	-3.2681850	1.9403500	0.8580680
H	-1.4449810	4.7617680	0.7540340	H	-3.0468690	2.4622760	-0.0805810
C	0.5827550	2.0488560	2.9212510	H	-5.2979860	1.5020630	0.2666170
H	1.6048030	2.4266140	2.7553440	H	-5.8275080	0.2844680	2.3785830
H	0.2277040	2.4539610	3.8816310	H	-4.0839130	0.0561580	4.1389650
H	0.6523360	0.9531900	3.0160920	H	-1.8409300	1.0340330	3.8061950
H	0.2245970	-2.4529300	-3.8824880				
H	0.6511330	-0.9533980	-3.0158440				

Table S41. Geometric coordinates and single point energies for NaHMDS unsolvated trimer.



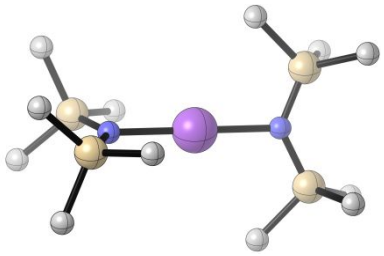
G = -3104.42812 Hartrees

G_{SP} = -3106.215009 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.4298660	1.8070580	0.2686480	H	-0.8259350	0.7977680	-3.6343250
Na	1.2877420	-1.2947880	-0.4529550	H	0.2849700	1.4716900	-2.4315090
Na	-2.2012700	-0.5163530	0.2575060	H	-0.5683190	-0.0614760	-2.1068110
N	-0.7664070	-2.2921050	0.0737470	N	2.4334230	0.6680560	-0.0363170
Si	-0.4705920	-2.6946560	1.7180260	Si	3.3157620	0.7897580	-1.5102850
C	-1.1045220	-4.3752330	2.3059140	C	5.1756730	0.4614580	-1.3602660
H	-0.6855700	-5.2043360	1.7153330	H	5.6587630	0.5457530	-2.3463640
H	-0.8285590	-4.5401490	3.3590470	H	5.6748110	1.1726650	-0.6845340
H	-2.2013840	-4.4302040	2.2320860	H	5.3655330	-0.5536660	-0.9779430
C	1.3924000	-2.6406600	2.1002170	C	2.7013520	-0.5411910	-2.7342770
H	1.6058640	-2.9186060	3.1436250	H	3.2140600	-0.4297420	-3.7017690
H	1.9423940	-3.3486590	1.4559930	H	2.9431140	-1.5620220	-2.3843410
H	1.8221860	-1.6353950	1.9535320	H	1.6215300	-0.4779470	-2.9455930
C	-1.3038530	-1.4069860	2.8468860	C	3.1311670	2.4793140	-2.3470010
H	-1.0872120	-0.3632050	2.5559130	H	3.5581420	3.2589340	-1.6962500
H	-2.3988910	-1.5457470	2.8516170	H	3.6624580	2.5187610	-3.3104760
H	-0.9703450	-1.5135050	3.8905920	H	2.0790630	2.7445060	-2.5372720
Si	-1.0231960	-3.4641000	-1.1625030	Si	3.1526740	1.0957830	1.4693660
C	-1.1465540	-2.6384370	-2.8630400	C	1.7703320	1.2591180	2.7740560

H	-1.9541240	-1.8901410	-2.9091950	H	1.0712980	0.4063300	2.7607960
H	-0.2109020	-2.1342360	-3.1553370	H	2.2013400	1.3039670	3.7860150
H	-1.3570420	-3.3997850	-3.6305050	H	1.1836320	2.1886930	2.6636990
C	-2.6108020	-4.4709970	-0.9485290	C	4.4244790	-0.1329380	2.1372160
H	-2.7726260	-5.1398520	-1.8080450	H	5.2937780	-0.1882450	1.4652270
H	-2.5837880	-5.0894920	-0.0398100	H	4.7856470	0.1827390	3.1285260
H	-3.4850880	-3.8037820	-0.8751860	H	4.0102080	-1.1475290	2.2348430
C	0.4283970	-4.6845200	-1.2921810	C	3.9886340	2.7993030	1.4412280
H	0.5806510	-5.2385440	-0.3525790	H	3.2767030	3.5797080	1.1253070
H	0.2684820	-5.4222470	-2.0936990	H	4.3662140	3.0754850	2.4382200
H	1.3719810	-4.1587960	-1.5216930	H	4.8390560	2.8296480	0.7428550
N	-1.8292810	1.7764300	-0.0283130	H	-2.1820940	3.5522680	-3.5632490
Si	-2.8234990	2.4758520	1.1842560	H	-3.0434780	4.1655580	-2.1316490
C	-1.7884850	2.9794270	2.6859040	H	-1.2664580	4.1779110	-2.1703970
H	-1.0443540	3.7466770	2.4133660	C	-3.7063600	0.9806940	-2.2428900
H	-2.4154590	3.4025740	3.4857810	H	-4.5851640	1.4593730	-1.7814300
H	-1.2506060	2.1169280	3.1121330	H	-3.8450120	1.0117140	-3.3347490
C	-4.0997630	1.2017050	1.8094280	H	-3.7238500	-0.0860350	-1.9548810
H	-4.8183360	1.6562550	2.5086240	C	-0.6746500	0.9421910	-2.5533200
H	-4.6860690	0.7850710	0.9718280				
H	-3.6218650	0.3712760	2.3565250				
C	-3.8141990	3.9896420	0.6346970				
H	-4.5106990	3.7405050	-0.1817530				
H	-4.4087850	4.3889170	1.4709570				
H	-3.1497340	4.7910570	0.2769110				
Si	-2.1060430	1.8680610	-1.7195940				
C	-2.1591640	3.6029560	-2.4634960				

Table S42. Geometric coordinates and single point energies for $(SiMe_3)_2$–N–Na–$N(SiMe_3)_2$ anion piece of triple ion.



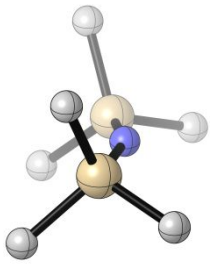
G = -1907.397903 Hartrees

G_{SP} = -1908.549853 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	2.9412810	-1.2641930	-0.8686230	H	-2.9546240	-3.0429690	-0.8978080
N	2.2374350	-0.0001890	0.0001610	H	-4.1270800	-3.4536450	0.3856720
Si	2.9399640	1.2645550	0.8689470	H	-4.5239930	-2.2139500	-0.8355620
C	4.3192330	0.7359710	2.0734250	C	-1.6140950	-2.1339050	1.9231340
H	3.9546440	-0.0466140	2.7573820	H	-1.1490730	-1.4235630	2.6266000
H	5.1738650	0.3177680	1.5160890	H	-2.0301580	-2.9666450	2.5122780
H	4.6909260	1.5801180	2.6768790	H	-0.8128190	-2.5516540	1.2893770
C	1.6125690	2.1342280	1.9221380	Si	-2.9404850	1.2641310	-0.8691420
H	2.0278750	2.9675440	2.5109980	C	-4.3226400	0.7358040	-2.0704280
H	0.8114030	2.5511060	1.2876730	H	-3.9598380	-0.0469700	-2.7551190
H	1.1475630	1.4240580	2.6257950	H	-5.1760000	0.3178490	-1.5109530
C	3.7121260	2.6269760	-0.2157450	H	-4.6955890	1.5799320	-2.6731260
H	4.5238120	2.2134460	-0.8352910	C	-1.6145300	2.1321560	-1.9254750
H	2.9540020	3.0415110	-0.8990860	H	-2.0304270	2.9654210	-2.5139930
H	4.1255190	3.4539050	0.3847070	H	-0.8118320	2.5488680	-1.2928330
Na	0.0000200	-0.0012530	-0.0005350	H	-1.1513950	1.4212200	-2.6295770
N	-2.2374390	-0.0006620	-0.0008910	C	-3.7093400	2.6278020	0.2163290
Si	-2.9406360	-1.2644470	0.8686930	H	-4.5200630	2.2152010	0.8377610
C	-4.3202740	-0.7341790	2.0720150	H	-2.9494890	3.0420760	0.8979130
H	-5.1739850	-0.3154310	1.5136640	H	-4.1233270	3.4547780	-0.3836520

H	-4.6933250	-1.5776310	2.6755980
H	-3.9555320	0.0484350	2.7558570
C	-3.7128840	-2.6274350	-0.2152220
H	1.1486300	-1.4259880	-2.6251230
H	2.0309140	-2.9683270	-2.5104330
H	0.8142190	-2.5533970	-1.2868490
H	3.9543320	0.0479900	-2.7573120
C	3.7151780	-2.6257070	0.2159740
H	2.9576460	-3.0411100	0.8994440
H	4.1293770	-3.4521640	-0.3845780
H	4.5265210	-2.2112910	0.8353720
C	1.6147020	-2.1355070	-1.9215090
C	4.3197910	-0.7341690	-2.0733380
H	5.1740040	-0.3150310	-1.5160570
H	4.6923590	-1.5779550	-2.6767570

Table S43. Geometric coordinates and single point energies for $(SiMe_3)_2N$ anion piece of separated ion pair.

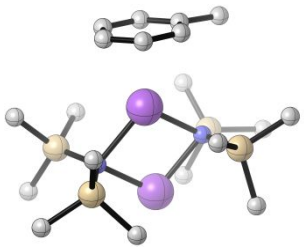


G = -872.551192 Hartrees

G_{SP} = -873.1101533 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	-1.6059210	0.0133710	0.0725470	C	-2.0651380	-1.0629820	-1.4469740
N	0.0000000	0.0807800	0.4430140	H	-1.5766780	-0.6709100	-2.3542010
Si	1.6059140	0.0133600	0.0725510	H	-1.7081740	-2.0957880	-1.3025990
C	2.0649960	-1.0616790	-1.4479440	H	-3.1529610	-1.0958170	-1.6292310
H	1.7075810	-2.0944870	-1.3047190	H	-3.7487310	-0.7125510	1.2445420
H	1.5768870	-0.6684620	-2.3548680	H	-2.3569730	-1.7250210	1.7280120
H	3.1528410	-1.0947530	-1.6300200	C	-2.4092280	1.7122440	-0.3002140
C	2.4095610	1.7124070	-0.2986540	H	-3.4916120	1.6352460	-0.5000410
H	2.2633060	2.3929140	0.5557570	H	-2.2628660	2.3935110	0.5535720
H	3.4919380	1.6353660	-0.4985040	H	-1.9287300	2.1770350	-1.1766570
H	1.9291920	2.1781060	-1.1746840				
C	2.6735310	-0.6978050	1.4910440				
H	3.7485460	-0.7140150	1.2439530				
H	2.5370910	-0.0953990	2.4036520				
H	2.3565740	-1.7266390	1.7264860				
C	-2.6737180	-0.6963360	1.4916370				
H	-2.5371700	-0.0931340	2.4037030				

Table S44. Geometric coordinates and single point energies for NaHMDS monosolvated toluene dimer.



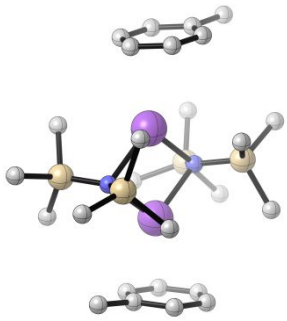
G = -2340.744069 Hartrees

G_{SP} = -2342.234312 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
N	1.9579580	-0.5249370	0.1468370	C	-2.3207430	0.5610400	2.7898360
Na	0.0485390	0.8123480	-0.2225590	H	-2.9797510	1.3549480	2.4072830
Na	0.2657820	-2.0458630	0.4237650	H	-2.6582910	0.3103160	3.8078570
N	-1.6631250	-0.7132320	0.1365080	H	-1.3016950	0.9684390	2.8669850
Si	-2.2844200	-1.2090420	-1.3778500	C	-4.1881510	-1.5303060	1.6419350
C	-4.0496690	-0.6685000	-1.7975330	H	-4.5388090	-1.7541960	2.6614990
H	-4.2986210	-0.9572920	-2.8310300	H	-4.8393220	-0.7437780	1.2297090
H	-4.7927970	-1.1298180	-1.1311570	H	-4.3271220	-2.4355170	1.0299020
H	-4.1567580	0.4248710	-1.7199080	Si	2.7605790	0.1361620	1.5103160
C	-1.1970450	-0.5024240	-2.7696860	C	1.4781170	0.7927990	2.7481430
H	-1.4053620	0.5672870	-2.9248680	H	0.8506690	1.5949470	2.3260330
H	-0.1191830	-0.6073150	-2.5654630	H	0.8041320	-0.0094520	3.0898190
H	-1.3923230	-1.0137640	-3.7251730	H	1.9727550	1.2074130	3.6404660
C	-2.2521660	-3.1054580	-1.5722730	C	3.8971920	1.5978530	1.0908400
H	-1.2334630	-3.5243680	-1.4910280	H	4.3619820	2.0253630	1.9930960
H	-2.8677160	-3.5807250	-0.7912140	H	4.7070060	1.2930970	0.4096590
H	-2.6472130	-3.4262170	-2.5489010	H	3.3298420	2.3974130	0.5884270
Si	-2.3815520	-0.9621680	1.6685400	C	3.7975730	-1.1186530	2.4802820
C	-1.4281370	-2.3364630	2.6101320	H	4.6321480	-1.5039730	1.8761240
H	-1.4332600	-3.2854130	2.0429640	H	4.2203600	-0.6681720	3.3920100

H	-0.3820690	-2.0599620	2.8377910	H	3.1798060	-1.9788090	2.7860190
H	-1.8971460	-2.5537900	3.5817680	Si	2.7732990	-1.0642600	-1.2608330
C	1.9003490	-2.6273260	-1.9276770	H	1.9937800	-3.4545070	-1.2003080
H	3.3441230	1.1250730	-2.2878850	H	2.3714460	-2.9804250	-2.8578280
C	4.5751950	-1.5995740	-1.0206280	H	0.8323930	-2.4792780	-2.1586050
H	5.1955950	-0.7913160	-0.6036370	C	2.7818850	0.2428780	-2.6357390
H	4.6429600	-2.4605030	-0.3376880	H	3.2612280	-0.1226530	-3.5571510
H	5.0184830	-1.8974660	-1.9838020	H	1.7647300	0.5767150	-2.8973340
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				
H	1.2094900	3.7969460	1.1611410				
H	1.9985320	3.5731360	-1.1938140				
H	0.3553820	3.0531620	-2.9956020				

Table S45 Geometric coordinates and single point energies for NaHMDS disolvated toluene dimer.



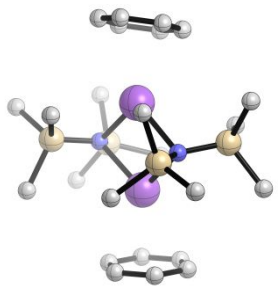
G = -2611.872211 Hartrees

G_{SP} = -2613.659114 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.4351020	-0.6963370	-0.0543420	C	2.8795240	-1.9743060	-2.0942660
N	0.8002690	-1.3637770	0.0182030	H	3.5735890	-2.4879860	-1.4113140
Na	1.0694810	0.9456540	0.0465920	H	3.0071390	-2.4062510	-3.0992410
N	-1.2183480	1.6297270	-0.0167260	H	3.1666210	-0.9111420	-2.1359790
Si	-1.5592850	2.1876220	1.5613930	Si	1.3416040	-2.0033040	1.5153920
C	-2.8997210	3.5138960	1.7524040	C	1.4591970	-0.6341540	2.8271990
H	-3.1240000	3.6526520	2.8222580	H	2.2256100	0.1127780	2.5647430
H	-2.5862730	4.4860740	1.3460550	H	1.7435860	-1.0585160	3.8030380
H	-3.8359390	3.2249930	1.2492730	H	0.5023000	-0.1077520	2.9673240
C	-2.1694020	0.7526340	2.6558040	C	0.1513860	-3.2953950	2.2326820
H	-3.2333290	0.5640420	2.4434340	H	0.5434190	-3.7514820	3.1552250
H	-1.6232110	-0.1957280	2.5134680	H	-0.8155690	-2.8247650	2.4765890
H	-2.0894930	1.0082200	3.7242610	H	-0.0404410	-4.0989710	1.5039800
C	-0.0120860	2.9147660	2.4003430	C	3.0670480	-2.7894440	1.4436720
H	0.7938090	2.1705820	2.5103180	H	3.0951560	-3.6632290	0.7736910
H	0.3737860	3.7573610	1.8020980	H	3.7974950	-2.0558370	1.0654290
H	-0.2346090	3.2948340	3.4097760	H	3.3974110	-3.1202930	2.4408070
Si	-1.4082020	2.4382580	-1.5110870	C	-3.3716840	-3.0272880	1.0861540

C	0.2777220	2.6526970	-2.3784100	C	-2.9338910	-3.5519780	-0.1302530
H	0.8891320	3.3732310	-1.8103020	C	-3.1706460	-2.8407560	-1.3079720
H	0.8544190	1.7162740	-2.4775190	C	-3.8228440	-1.6052230	-1.2658110
H	0.1560210	3.0576090	-3.3952340	C	-4.2522760	-1.0565260	-0.0467530
C	-2.5194000	1.4888560	-2.7207870	C	-4.0267260	-1.7956930	1.1240660
H	-3.5465060	1.4229640	-2.3281110	H	-4.3710870	-1.3996260	2.0811320
H	-2.5665640	1.9993880	-3.6955270	C	-4.8950710	0.3041040	0.0058930
H	-2.1515710	0.4668310	-2.9010480	H	-5.4990570	0.4248800	0.9150540
C	-2.1145990	4.1943640	-1.4336430	H	-4.1172330	1.0870610	0.0079390
H	-2.1366840	4.6326280	-2.4440260	H	-5.5379450	0.4754170	-0.8682280
H	-3.1407590	4.2076370	-1.0370520	H	-4.0025670	-1.0550330	-2.1921020
H	-1.4988690	4.8489210	-0.7964140	H	-2.8470180	-3.2508860	-2.2663290
C	3.5251640	2.1882260	1.2586670	H	-2.4219570	-4.5145560	-0.1597890
C	4.3892190	1.0934810	1.1565950	H	-3.2039060	-3.5812330	2.0107960
C	4.8744280	0.6709520	-0.0847370	Si	1.0981450	-2.1569140	-1.4725590
C	4.4591690	1.3674030	-1.2303630	C	-0.0098300	-1.4129440	-2.8253990
C	3.5935540	2.4539780	-1.1387960	H	-1.0791560	-1.6039040	-2.6352840
C	3.1222970	2.8727920	0.1112010	H	0.1235030	-0.3227650	-2.9117720
H	2.4569450	3.7353200	0.1904510	H	0.2217360	-1.8516170	-3.8085170
H	3.2874260	2.9822890	-2.0429030	C	0.7283350	-4.0188600	-1.4570230
H	4.8286290	1.0517070	-2.2089490	H	0.9170480	-4.4720440	-2.4429450
C	5.8299920	-0.4848420	-0.2053540	H	1.3517910	-4.5486790	-0.7195460
H	6.7834870	-0.1541420	-0.6430710	H	-0.3249370	-4.2018000	-1.1934930
H	6.0391390	-0.9365070	0.7726620				
H	5.4147310	-1.2613260	-0.8639590				
H	4.6975410	0.5620510	2.0599440				
H	3.1707840	2.5124780	2.2392020				

Table S46. Geometric coordinates and single point energies for NaHMDS disolvated benzene dimer.



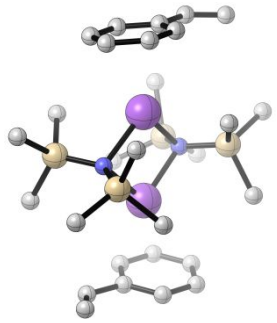
G = -2533.391992 Hartrees

G_{SP} = -2535.091764 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.3573950	1.4165280	0.0562670	H	-4.1487450	2.7388850	-0.3776600
Na	-0.4239510	-1.4052120	-0.1060170	H	-2.6240140	3.4414430	-0.9469860
N	1.7270020	-0.4632380	0.0492570	C	-0.0770710	-4.1216880	-1.0679710
Si	2.5961400	-1.0210050	-1.3197840	C	0.0741880	-4.1854820	0.3199880
C	1.4406920	-1.2510360	-2.8102910	C	-1.0227030	-3.9445750	1.1529720
H	0.5673510	-1.8942690	-2.6145440	C	-2.2685100	-3.6402490	0.5977160
H	1.0622130	-0.2753120	-3.1520870	C	-2.4193580	-3.5745930	-0.7893060
H	1.9912700	-1.7029850	-3.6506440	C	-1.3232360	-3.8133700	-1.6222220
C	3.4716570	-2.6843970	-1.0280580	H	-1.4391830	-3.7566840	-2.7060220
H	3.9379150	-3.0632370	-1.9512030	H	-3.3922060	-3.3334770	-1.2186460
H	4.2661480	-2.5857750	-0.2711320	H	-3.1249590	-3.4480670	1.2456250
H	2.7677210	-3.4480390	-0.6616080	H	-0.9032650	-3.9857900	2.2371000
C	3.9333850	0.1619400	-1.9672250	H	1.0486710	-4.4123570	0.7552710
H	4.6323290	0.4664580	-1.1737830	H	0.7813250	-4.3003000	-1.7179720
H	4.5180400	-0.3135550	-2.7707020	C	0.9980650	4.2592470	0.8883760
H	3.4714820	1.0690570	-2.3880690	C	2.2633230	3.7693660	0.5534300
Si	2.4398940	-0.4505830	1.6102420	C	2.5201390	3.3205030	-0.7434530
C	1.5896300	0.8381740	2.7241250	C	1.5132640	3.3747180	-1.7119690
H	1.8110870	1.8638260	2.3871700	C	0.2499970	3.8749990	-1.3812200

H	1.9648030	0.7559690	3.7562160	C	-0.0092610	4.3113760	-0.0782670
H	0.4965560	0.7200860	2.7731820	H	-0.9980720	4.6896120	0.1856830
C	2.3001960	-2.1186170	2.5069810	H	-0.5384770	3.9137720	-2.1350600
H	2.7371400	-2.0767900	3.5169850	H	1.7124030	3.0218320	-2.7259220
H	1.2481760	-2.4316630	2.6105280	H	3.5016150	2.9186680	-0.9973400
H	2.8311260	-2.8996520	1.9396280	H	3.0503440	3.7262040	1.3080630
C	4.2767500	0.0271180	1.6457560	H	0.7932210	4.5960170	1.9060270
H	4.9000110	-0.6695260	1.0637950	H	-2.4782050	2.3153670	3.4391520
H	4.4225630	1.0350270	1.2243190	Si	-2.6658960	0.9545600	-1.3476940
H	4.6584010	0.0343220	2.6788520	C	-1.5351190	0.9574570	-2.8733180
N	-1.7930030	0.4490120	0.0384360	H	-2.0423650	1.4163230	-3.7367580
Si	-2.4451280	0.5552260	1.6204650	H	-0.5893380	1.5015220	-2.7159000
C	-4.3206120	0.3073800	1.7560400	H	-1.2747130	-0.0749480	-3.1569410
H	-4.6416570	0.3736910	2.8077040	C	-4.1073210	-0.1789450	-1.8325130
H	-4.8851540	1.0609400	1.1853520	H	-4.8413010	-0.2791780	-1.0193990
H	-4.6092900	-0.6859240	1.3769600	H	-4.6326200	0.2076260	-2.7201880
C	-1.7071950	-0.7875040	2.7595310	H	-3.7302630	-1.1840270	-2.0784260
H	-2.3176370	-1.7021780	2.7091720	C	-3.4019170	2.7001960	-1.1865650
H	-0.6684840	-1.0631990	2.5121300	H	-3.9009150	3.0167840	-2.1159510
H	-1.7038320	-0.4562250	3.8101010				
C	-2.0849550	2.2470280	2.4126150				
H	-1.0050980	2.4668100	2.4586990				
H	-2.5623180	3.0389760	1.8124990				

Table S47. Geometric coordinates and single point energies for NaHMDS disolvated styrene dimer.



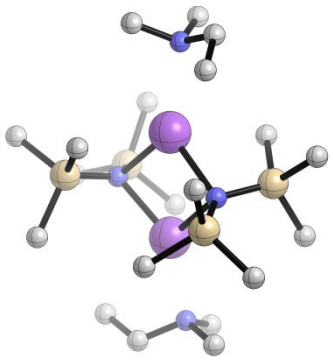
G = -2687.942165 Hartrees

G_{SP} = -2689.812106 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	1.5006870	-0.2799530	-0.0754230	H	1.3596410	-4.4064780	0.9689800
N	-0.2706880	-1.7628830	0.0677630	C	-1.9498340	-2.6338600	2.3884110
Na	-1.4783440	0.2671830	0.0694990	H	-2.6615220	-3.1694420	1.7403240
N	0.3088720	1.7475570	0.0681380	H	-1.9278130	-3.1370350	3.3680310
Si	0.6783010	2.5161370	-1.4129650	H	-2.3405460	-1.6133570	2.5470210
C	1.7595690	4.0682360	-1.2885040	Si	-0.6892730	-2.4468980	-1.4426640
H	2.1378820	4.3627990	-2.2804450	C	-1.6619830	-1.1553330	-2.4523170
H	1.1922760	4.9198380	-0.8835370	H	-2.6461630	-0.9728390	-1.9907100
H	2.6254640	3.8920420	-0.6313750	H	-1.8484350	-1.4998430	-3.4812200
C	1.6442240	1.2962150	-2.5160740	H	-1.1294250	-0.1912000	-2.5283950
H	2.6369090	1.0931120	-2.0804790	C	0.8079390	-2.9118730	-2.5121390
H	1.1176620	0.3344850	-2.6461470	H	0.4891390	-3.3037330	-3.4910930
H	1.8135360	1.7053520	-3.5240220	H	1.4684580	-2.0484390	-2.6957090
C	-0.8569670	3.0211550	-2.4051460	H	1.4050600	-3.6909170	-2.0122640
H	-1.5151990	2.1590530	-2.6019030	C	-1.7800010	-3.9968000	-1.3843720
H	-1.4409480	3.7655330	-1.8407610	H	-1.2002780	-4.8844200	-1.0892950
H	-0.5836810	3.4662550	-3.3749340	H	-2.6049730	-3.8742550	-0.6660290
Si	0.3129380	2.4532130	1.6246080	H	-2.2175500	-4.2009340	-2.3747830

C	-0.8014270	1.4481160	2.8040440	C	4.4064670	-0.1146250	0.0636790
H	-1.8516440	1.7653470	2.7291830	C	4.0290040	-0.9463590	1.1312860
H	-0.7559860	0.3635590	2.6143370	C	3.6872550	-2.2837200	0.9148870
H	-0.4941480	1.5960040	3.8513320	C	3.7170030	-2.8134940	-0.3730780
C	2.0391070	2.4714750	2.4150010	C	4.0992940	-2.0009400	-1.4443010
H	2.7355960	3.0503680	1.7879710	C	4.4443410	-0.6705170	-1.2286250
H	2.0294420	2.9157550	3.4227180	H	4.7595520	-0.0562670	-2.0731840
H	2.4410000	1.4477520	2.5049220	H	4.1283630	-2.4106720	-2.4549180
C	-0.3384190	4.2330250	1.7082380	H	3.4486710	-3.8568350	-0.5433870
H	-0.5201280	4.5404720	2.7504570	H	3.3961890	-2.9135160	1.7559060
H	0.3743250	4.9470610	1.2692390	H	4.0059650	-0.5376550	2.1446370
H	-1.2871170	4.3220960	1.1542900	C	4.7423690	1.2974410	0.3315290
C	-4.4807590	0.7367170	-1.1959920	H	4.8217250	1.5606560	1.3903190
C	-4.1908710	2.0855440	-1.3713120	C	4.9296120	2.2532050	-0.5836540
C	-3.8540810	2.8843270	-0.2745690	H	4.8409990	2.0676450	-1.6568130
C	-3.8139110	2.3207880	0.9981420	H	5.1725930	3.2725480	-0.2802920
C	-4.0953930	0.9632230	1.1733510	H	-3.6292040	3.9424630	-0.4139070
C	-4.4285270	0.1464010	0.0806200	H	-4.2264770	2.5209300	-2.3709070
C	-4.7056260	-1.2850240	0.3110950	H	-4.7588510	0.1336110	-2.0613350
H	-4.7362170	-1.5856130	1.3626310	Si	-0.2335120	-2.5677040	1.5757210
C	-4.8983250	-2.2169530	-0.6273590	C	0.8925980	-1.6632880	2.8399270
H	-5.0961560	-3.2528780	-0.3485550	H	1.7544590	-2.2846950	3.1264110
H	-4.8618640	-1.9939220	-1.6963610	H	1.2827960	-0.6942550	2.4859680
H	-4.0628390	0.5253500	2.1744680	H	0.3344680	-1.4481960	3.7647230
H	-3.5616650	2.9405480	1.8599380	C	0.4015900	-4.3545500	1.5114590
H	-0.3103370	-5.0167860	0.9968070	H	0.5600880	-4.7564000	2.5248420

Table S48. Geometric coordinates and single point energies for NaHMDS disolvated DMEA dimer.



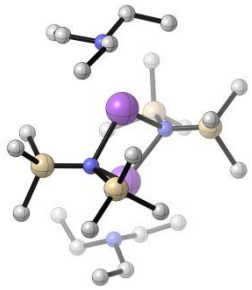
G = -2496.387851 Hartrees

G_{SP} = -2498.065172 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
N	0.2843140	1.8296480	0.1303500	H	-3.7818240	2.5875320	0.5510970
Na	-1.5035340	0.3048570	-0.0225370	C	-4.5824090	-0.5922280	-0.2197540
N	-0.2733280	-1.7262930	0.0745760	H	-4.4511860	-1.1571880	-1.1563650
Na	1.4715660	-0.1648410	-0.1138520	H	-5.6774190	-0.4695010	-0.0795610
N	3.8076260	-0.8247340	-0.5197340	C	-3.9820580	-1.3921890	0.9251600
C	3.9539130	-2.2290110	-0.1532590	H	-4.0656420	-0.8738820	1.8915540
H	5.0108610	-2.5583420	-0.2203180	H	-4.5017720	-2.3550990	1.0279010
H	3.6060420	-2.3982160	0.8745820	H	-2.9188420	-1.6187380	0.7438230
H	3.3502560	-2.8517060	-0.8285030	Si	0.4802660	2.7525380	-1.2897030
C	4.2841500	-0.6433350	-1.8860630	C	-1.1734480	3.0631470	-2.1693310
H	4.1355360	0.3874250	-2.2261430	H	-1.0582460	3.6674060	-3.0827790
H	5.3622170	-0.8916770	-1.9709260	H	-1.6529310	2.1129720	-2.4583020
H	3.7255780	-1.3054600	-2.5621130	H	-1.8592670	3.5985120	-1.4915780
C	4.5363660	0.0280270	0.4245590	C	1.5819260	1.8043320	-2.5205440
H	4.2010590	-0.2439070	1.4388550	H	1.5758100	2.2725510	-3.5169860
H	5.6224230	-0.2035020	0.3816330	H	2.6218950	1.8174320	-2.1591160
C	4.3129410	1.5176900	0.2078120	H	1.2786480	0.7512020	-2.6576650
H	3.2402490	1.7734560	0.2231750	C	1.3071780	4.4438180	-1.0747670

H	4.7957160	2.0846690	1.0153860	H	0.6387220	5.1560680	-0.5684130
H	4.7390290	1.8687310	-0.7425260	H	2.2283470	4.3611490	-0.4752820
Si	-0.6766830	-2.4315040	-1.4271550	H	1.5764990	4.8742980	-2.0522360
C	-1.9401920	-3.8436920	-1.3523880	Si	0.1475860	2.3555090	1.7483390
H	-2.1799590	-4.2206950	-2.3590320	C	-0.4578060	4.1360100	1.9919510
H	-1.5671060	-4.6915360	-0.7576340	H	-0.7219760	4.3158350	3.0462080
H	-2.8778320	-3.5010470	-0.8861900	H	0.3159300	4.8667360	1.7128000
C	-1.4722270	-1.0923050	-2.5255100	H	-1.3509760	4.3403840	1.3792820
H	-2.4459150	-0.7784540	-2.1135440	C	1.7734410	2.2291830	2.7201340
H	-0.8345540	-0.1961330	-2.6167560	H	2.4903290	2.9747450	2.3403750
H	-1.6618420	-1.4615380	-3.5448140	H	1.6207570	2.4270020	3.7928680
C	0.8307320	-3.0700360	-2.3880120	H	2.2413710	1.2355400	2.6274820
H	1.5684560	-2.2600690	-2.5208480	C	-1.1486360	1.2733840	2.6425160
H	1.3214090	-3.8886640	-1.8381000	H	-2.1599740	1.5723500	2.3216360
H	0.5613680	-3.4451160	-3.3876210	H	-1.0258970	0.1952520	2.4446990
Si	0.1168740	-2.6063630	1.4901210	H	-1.1108020	1.4065500	3.7346990
C	1.3225620	-1.6071990	2.5787740	H	0.3082520	-4.9557330	0.6015400
H	2.2512970	-1.3294990	2.0510970	H	1.8957930	-4.1623670	0.6033640
H	0.8659210	-0.6781430	2.9519620	N	-3.9573850	0.7222070	-0.4078250
H	1.6282600	-2.1969700	3.4572100	C	-4.3472760	1.2800210	-1.6979120
C	-1.3668270	-2.9917650	2.6066090	H	-5.4496600	1.3686470	-1.7805590
H	-2.1110990	-3.5988470	2.0667570	H	-3.9091380	2.2784910	-1.8221900
H	-1.0502580	-3.5585040	3.4963420	H	-3.9876600	0.6424910	-2.5175170
H	-1.8676120	-2.0741600	2.9534920	C	-4.3524780	1.6516320	0.6450320
C	0.9620110	-4.2789480	1.1737840	H	-5.4336860	1.8922170	0.5872890
H	1.2065920	-4.7799170	2.1237420	H	-4.1522610	1.2272440	1.6362880

Table S49. Geometric coordinates and single point energies for NaHMDS disolvated triethylamine dimer.



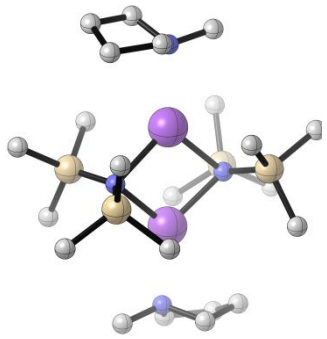
G = -2653.325993 Hartrees

G_{SP} = -2655.178414 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.4658810	-0.9428330	-3.1031770	H	-2.2612200	3.4163620	-2.9169340
C	-3.8025220	-1.7030440	-1.8268230	Si	0.6873490	-2.0120520	2.0084050
N	-3.7759630	-0.8808980	-0.6108570	C	1.5276890	-0.4778670	2.7688710
C	-4.1438690	-1.6753740	0.5710010	H	2.5940040	-0.4446130	2.4970900
H	-5.2325770	-1.8972810	0.5454100	H	1.0569810	0.4622310	2.4401030
H	-3.9785910	-1.0496200	1.4622450	H	1.4770390	-0.4892310	3.8687940
C	-3.3668130	-2.9727640	0.7302580	C	1.8091120	-3.4814230	2.4417260
H	-3.5504860	-3.3871960	1.7304830	H	1.8615620	-3.6000350	3.5357420
H	-3.6686560	-3.7308480	-0.0046820	H	1.4210180	-4.4235110	2.0239580
H	-2.2803950	-2.8144060	0.6339290	H	2.8359240	-3.3492810	2.0703490
C	-4.6759870	0.2714880	-0.7300760	C	-0.8969490	-2.3293720	3.0119630
H	-4.4676640	0.7708950	-1.6834060	H	-1.2669990	-3.3475280	2.8137020
H	-5.7289220	-0.0805790	-0.7790130	H	-0.6919820	-2.2521130	4.0916470
C	-4.5099320	1.2974280	0.3779770	H	-1.7133310	-1.6257560	2.7818920
H	-5.1185980	2.1852230	0.1560080	C	2.3900210	-3.4552200	-1.1852210
H	-4.8200640	0.9245760	1.3640620	H	2.4485290	-4.2026640	-1.9922630
H	-3.4604990	1.6266180	0.4360460	H	2.9886130	-2.5825200	-1.4930680
H	-3.0651420	-2.5081550	-1.6972640	H	2.8579290	-3.8872800	-0.2874280
H	-4.7937290	-2.1948900	-1.9347720	C	-0.3787270	-4.5487920	-0.5664060

H	-3.2292970	-1.6568030	-3.9036210	H	-0.3175170	-4.8756340	0.4835420
H	-4.2927590	-0.3126450	-3.4557380	H	-1.4449830	-4.4275860	-0.8117220
H	-2.5833820	-0.2994240	-2.9592100	H	0.0125160	-5.3636430	-1.1955260
H	-1.0309840	-1.8530140	-2.4744990	H	-0.0766270	-3.1104720	-3.2861020
C	-0.0239160	-2.2929860	-2.5496850	H	0.6455250	-1.5221040	-2.9626090
Si	0.5892630	-2.9390350	-0.8734500	N	3.8780980	0.6572240	-0.6057130
N	0.4042070	-1.7399360	0.3373000	C	4.5744880	0.2292390	0.6164570
Na	1.4327010	0.3450580	-0.0463710	H	5.6364160	0.5551210	0.5782590
N	-0.4453970	1.8408250	0.2342980	H	4.1186010	0.7621640	1.4620520
Na	-1.4606110	-0.2889920	0.1094240	C	4.4956490	-1.2672720	0.8883170
Si	-0.8628200	2.6053560	1.7167740	H	5.1833870	-1.8541970	0.2654180
C	-1.6537440	1.3638480	2.9224760	H	4.7523100	-1.4680540	1.9379860
H	-2.5708870	0.9196710	2.4988930	H	3.4755230	-1.6420550	0.7101890
H	-0.9743560	0.5444750	3.1986180	C	3.9781920	2.1156170	-0.7571060
H	-1.9496690	1.8717680	3.8539960	H	5.0486350	2.4070830	-0.8181120
C	0.6155990	3.3832350	2.6187410	H	3.5265750	2.3862570	-1.7227090
H	1.0481990	4.1931420	2.0091720	C	3.2900860	2.9157580	0.3395580
H	0.2997700	3.8188810	3.5797820	H	3.3498150	3.9868570	0.1017170
H	1.4150250	2.6553340	2.8265510	H	2.2183050	2.6700250	0.4247680
C	-2.1283140	4.0196160	1.5725220	H	3.7549300	2.7812440	1.3253130
H	-2.2825560	4.4794460	2.5616200	C	4.4630480	-0.0110940	-1.7757740
H	-1.7870300	4.8127930	0.8896420	H	4.5773030	-1.0741110	-1.5321360
H	-3.1080610	3.6709340	1.2132880	H	5.4871120	0.3830220	-1.9500640
Si	-0.5177980	2.6708170	-1.2627110	C	3.6421400	0.0829780	-3.0511730
C	0.3173780	4.3748430	-1.3186580	H	3.5101600	1.1135670	-3.4076990
H	0.1691820	4.8430990	-2.3045880	H	4.1464290	-0.4786180	-3.8497950
H	-0.0867510	5.0611730	-0.5592650	H	2.6463910	-0.3616640	-2.9068950
H	1.4008250	4.2912920	-1.1465580	H	1.4716300	1.5635100	-2.3182780
C	0.3960210	1.6199730	-2.5550890	H	0.0042960	0.5892810	-2.5975730
H	-2.7754770	1.9443330	-2.0598310	H	0.3193930	2.0426430	-3.5686700
H	-2.8844360	3.5261640	-1.2501010	C	-2.2743950	2.9173390	-1.9352030

Table S50. Geometric coordinates and single point energies for NaHMDS disolvated *N*-methylpyrrolidine dimer.



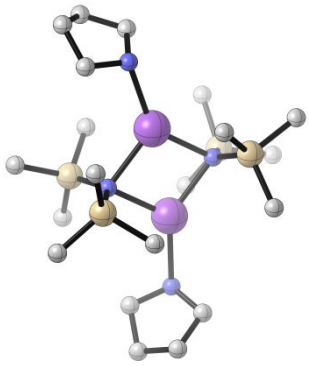
G = -2572.513393 Hartrees

G_{SP} = -2574.267725 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	1.3759790	0.6067660	0.0348540	H	3.0425660	-3.7133410	2.3800170
N	0.7288910	-1.6419830	-0.0909870	H	2.4139740	-4.4202330	0.8762400
Na	-1.3760200	-0.6067850	0.0349890	H	3.5371500	-3.0450490	0.8037510
N	-0.7289740	1.6419590	-0.0909820	C	-0.1776850	-3.1461600	2.3442460
Si	-0.7117870	2.4346280	-1.6032240	H	-0.5027790	-4.0347170	1.7794860
C	-0.4517490	4.3133880	-1.5322390	H	0.1262740	-3.4765020	3.3497690
H	-0.2835820	4.7251450	-2.5400960	H	-1.0518860	-2.4822380	2.4607880
H	-1.3283760	4.8256050	-1.1075190	Si	0.7118500	-2.4346980	-1.6032130
H	0.4197320	4.5732260	-0.9102910	C	-0.7396110	-1.7755790	-2.6547100
C	0.7396650	1.7753020	-2.6545950	H	-1.6930020	-2.2172140	-2.3217450
H	1.6931480	2.2164290	-2.3212200	H	-0.6222680	-2.0503690	-3.7143990
H	0.8379230	0.6775850	-2.6160290	H	-0.8383300	-0.6779130	-2.6158120
H	0.6227080	2.0505080	-3.7142170	C	2.2894790	-2.1688570	-2.6227100
C	-2.2893660	2.1689140	-2.6228280	H	2.2007220	-2.6183430	-3.6242320
H	-2.5192060	1.0989000	-2.7545570	H	2.5192700	-1.0988240	-2.7543700
H	-3.1502350	2.6374070	-2.1195450	H	3.1503390	-2.6373280	-2.1193900
H	-2.2005170	2.6184430	-3.6243230	C	0.4520080	-4.3134830	-1.5321930

Si	-1.2272550	2.2690800	1.4159120	H	1.3286620	-4.8256010	-1.1074100
C	-1.7976100	0.8267150	2.5247630	H	-0.4194850	-4.5734000	-0.9102950
H	-2.6879400	0.3407530	2.0957840	H	0.2839430	-4.7252770	-2.5400510
H	-1.0237670	0.0531990	2.6561830	N	3.5811180	1.6696290	0.1826070
H	-2.0770230	1.1768390	3.5304070	C	4.4977890	1.3588310	1.2883350
C	0.1776780	3.1460670	2.3442400	C	5.0622460	-0.0431440	0.9731380
H	0.5028290	4.0346040	1.7794770	C	4.5533150	-0.3487960	-0.4498080
H	-0.1262310	3.4764310	3.3497700	C	4.1899530	1.0311500	-0.9864710
H	1.0518320	2.4820790	2.4607550	H	3.4944580	1.0102240	-1.8396840
C	-2.6904650	3.4737670	1.3640600	H	5.0990800	1.5840710	-1.3067670
H	-3.0425030	3.7136380	2.3798860	H	5.2882890	-0.8715750	-1.0751850
H	-2.4138130	4.4204010	0.8760880	H	3.6462050	-0.9743380	-0.4119400
H	-3.5371230	3.0453230	0.8036430	H	6.1595170	-0.0247010	1.0064090
N	-3.5811040	-1.6695710	0.1827140	H	4.7307520	-0.8025990	1.6937840
C	-4.4980630	-1.3587780	1.2881980	H	3.9716610	1.4235700	2.2526510
C	-5.0625150	0.0431520	0.9728050	H	5.3179620	2.1039860	1.3081760
C	-4.5532820	0.3487580	-0.4500440	C	3.3502140	3.0963130	0.0396780
C	-4.1896800	-1.0311870	-0.9865500	H	2.6418630	3.2938320	-0.7773180
H	-3.4939650	-1.0102370	-1.8395840	H	2.9149590	3.4963430	0.9660180
H	-5.0986780	-1.5841920	-1.3070640	H	4.2911540	3.6438470	-0.1723970
H	-5.2881560	0.8714360	-1.0756240	H	-4.2908480	-3.6438600	-0.1725080
H	-3.6462310	0.9743750	-0.4120080	Si	1.2271720	-2.2690300	1.4159380
H	-6.1597920	0.0246650	1.0058390	C	1.7972700	-0.8265570	2.5247790
H	-4.7312110	0.8026530	1.6934880	H	2.6875340	-0.3404640	2.0958110
H	-3.9721670	-1.4234470	2.2526470	H	1.0232920	-0.0531680	2.6561350
H	-5.3182020	-2.1039770	1.3078700	H	2.0767140	-1.1765930	3.5304450
C	-3.3500380	-3.0962400	0.0399150	C	2.6905240	-3.4735490	1.3641740
H	-2.6413430	-3.2937220	-0.7767930				
H	-2.9151030	-3.4962050	0.9664340				

Table S51. Geometric coordinates and single point energies for NaHMDS disolvated pyrrolidine dimer.



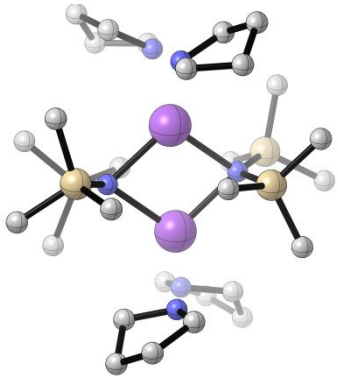
G = -2494.048679 Hartrees

G_{SP} = -2495.71708 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	1.4548970	0.2970370	-0.2723700	C	-0.9870990	1.8109160	2.7599890
N	0.0008980	2.1058510	0.0000480	H	-0.8866160	2.1809020	3.7917740
Na	-1.4550350	0.2985250	0.2722890	H	-2.0570760	1.8725070	2.4964120
N	-0.0010160	-1.5232270	0.0001990	H	-0.6939470	0.7468210	2.7717170
Si	0.5371410	-2.2595150	1.4396140	C	-0.6706650	4.6006920	1.6325120
C	1.3738590	-3.9519510	1.2454640	H	-0.0017750	5.3336330	1.1572180
H	1.8437500	-4.2683070	2.1901990	H	-1.6487300	4.6591770	1.1285970
H	0.6396430	-4.7230430	0.9665860	H	-0.8094610	4.9069150	2.6814790
H	2.1531040	-3.9390760	0.4669620	Si	-0.0437640	2.8486310	-1.5350890
C	1.8187370	-1.1147610	2.2667600	C	0.6740990	4.6003520	-1.6322960
H	2.7115790	-0.9840790	1.6309190	H	0.8129590	4.9065640	-2.6812580
H	1.3931900	-0.1171500	2.4667380	H	0.0057990	5.3337270	-1.1568430
H	2.1678360	-1.5162130	3.2304370	H	1.6522810	4.6581000	-1.1285220
C	-0.8493310	-2.5092630	2.7117330	C	-1.8017040	2.9592590	-2.2447910
H	-1.3682090	-1.5606470	2.9292910	H	-2.4366000	3.5506640	-1.5651160
H	-1.5955310	-3.2175650	2.3168740	H	-1.8208040	3.4438500	-3.2335640
H	-0.4715870	-2.9115820	3.6647940	H	-2.2631210	1.9643690	-2.3546860

Si	-0.5391140	-2.2590850	-1.4394530	C	0.9885200	1.8104620	-2.7599760
C	-1.8194530	-1.1133020	-2.2670670	H	2.0585400	1.8713150	-2.4964060
H	-2.7123690	-0.9818890	-1.6314840	H	0.6946580	0.7465630	-2.7718080
H	-1.3930270	-0.1160420	-2.4669140	H	0.8882540	2.1806190	-3.7917210
H	-2.1685890	-1.5144770	-3.2308470	N	3.7475700	-0.0657900	-0.8240560
C	0.8477600	-2.5098640	-2.7109510	C	4.6998070	0.4296750	0.2045510
H	1.5932120	-3.2187810	-2.3157860	H	5.3685110	1.1845020	-0.2355450
H	0.4701680	-2.9118110	-3.6642300	H	4.1679950	0.9165510	1.0361870
H	1.3674990	-1.5616410	-2.9281900	C	5.4921960	-0.8009340	0.6783460
C	-1.3772660	-3.9508530	-1.2457150	C	5.4059950	-1.7602570	-0.5095530
H	-1.8466210	-4.2670050	-2.1907840	C	3.9792840	-1.5159390	-0.9989990
H	-0.6438780	-4.7224620	-0.9660910	H	3.8044230	-1.8067720	-2.0430580
H	-2.1571550	-3.9372390	-0.4678690	H	3.2586240	-2.0801870	-0.3825710
N	-3.7481930	-0.0624580	0.8232840	H	6.1277040	-1.4713560	-1.2905760
C	-4.7004970	0.4318610	-0.2058070	H	5.5967860	-2.8073980	-0.2396750
H	-5.3695320	1.1867750	0.2336390	H	5.0027880	-1.2523360	1.5548580
H	-4.1687710	0.9182890	-1.0377530	H	6.5203030	-0.5473070	0.9677260
C	-5.4923910	-0.7993990	-0.6787280	H	3.9385450	0.4046550	-1.7048790
C	-5.4060310	-1.7577430	0.5099470	H	-3.9393630	0.4086880	1.7036890
C	-3.9794850	-1.5125370	0.9994310	Si	0.0459830	2.8484740	1.5352510
H	-3.8047260	-1.8024240	2.0437720	C	1.8039230	2.9578190	2.2451380
H	-3.2585000	-2.0770710	0.3836400	H	1.8232680	3.4425030	3.2338610
H	-6.1279700	-1.4684860	1.2906250	H	2.2645410	1.9625780	2.3552010
H	-5.5964010	-2.8051670	0.2408700	H	2.4393620	3.5486560	1.5654770
H	-5.0027140	-1.2513410	-1.5548100				
H	-6.5205460	-0.5463570	-0.9684510				

Table S52. Geometric coordinates and single point energies for NaHMDS tetrasolvated pyrrolidine dimer.



G = -2918.449045 Hartrees

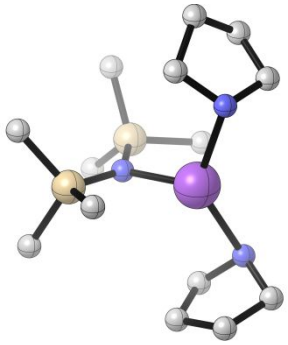
G_{SP} = -2920.596227 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.4538810	-0.0012290	0.0013050	H	4.5852400	4.0893070	-0.9952020
N	0.0186560	1.8048980	0.5683640	H	3.3622840	3.5397630	-2.9988550
Na	1.5167780	0.0000370	-0.0010170	H	4.9404890	2.8853790	-3.4596170
N	0.0183270	-1.8060570	-0.5683710	H	4.1877170	0.3286250	-1.1057090
Si	0.2105150	-1.7246720	-2.2677320	Si	0.2087780	1.7232720	2.2679120
C	-1.0427740	-2.7250260	-3.2917280	C	0.0176870	-0.0894320	2.7870890
H	-0.9206420	-2.5237090	-4.3683650	H	-0.9715640	-0.4821400	2.5072130
H	-0.9235790	-3.8086470	-3.1387060	H	0.7568830	-0.7261890	2.2766860
H	-2.0766860	-2.4669690	-3.0128220	H	0.1451560	-0.2392650	3.8716990
C	0.0232510	0.0883250	-2.7872290	C	-1.0441210	2.7256480	3.2904600
H	-0.9643130	0.4836710	-2.5052210	H	-0.9230010	2.5247280	4.3672890
H	0.7652880	0.7233350	-2.2787560	H	-0.9231750	3.8090130	3.1369790
H	0.1490650	0.2373610	-3.8721450	H	-2.0782580	2.4690660	3.0110390
C	1.9379400	-2.2313650	-2.8804720	C	1.9361010	2.2276810	2.8826190
H	2.6905550	-1.5329330	-2.4778930	H	2.2063600	3.2438880	2.5573140
H	2.2071050	-3.2475520	-2.5542120	H	1.9996600	2.1892970	3.9819540
H	2.0022830	-2.1938970	-3.9798000	H	2.6883330	1.5289560	2.4798900

Si	-0.2794590	-3.3164620	0.1829670	Si	-0.2763640	3.3154590	-0.1836590
C	0.1987130	-3.3994790	2.0183730	C	0.2050320	3.3979290	-2.0181990
H	1.2422040	-3.0862730	2.1787740	H	1.2487850	3.0844080	-2.1762890
H	-0.4324230	-2.7658400	2.6570200	H	0.1101710	4.4381230	-2.3688700
H	0.1028100	-4.4396950	2.3687010	H	-0.4248600	2.7643010	-2.6580450
C	-2.1203380	-3.7986630	0.1219070	C	-2.1166020	3.8003580	-0.1251400
H	-2.4696700	-3.8745810	-0.9202160	H	-2.3110640	4.7638320	-0.6222110
H	-2.3172150	-4.7612810	0.6196870	H	-2.7221250	3.0316980	-0.6329530
H	-2.7253380	-3.0283640	0.6278760	H	-2.4674720	3.8757980	0.9165020
C	0.6636250	-4.7812850	-0.5930040	C	0.6676180	4.7790710	0.5936450
H	0.3757820	-5.7240660	-0.1012630	H	0.4624810	4.8894160	1.6696160
H	0.4603130	-4.8910180	-1.6693790	H	1.7577090	4.6620280	0.4781490
H	1.7536840	-4.6660990	-0.4753790	H	0.3823520	5.7222560	0.1011790
N	3.4051020	-0.9620720	1.2924090	N	-3.4152730	-0.5462890	1.4996470
C	3.4948740	-1.3786950	2.7118450	C	-3.3993000	-1.2653610	2.7884340
H	4.0939110	-0.6458540	3.2701030	H	-4.2794150	-1.9246960	2.8959570
H	2.4952160	-1.3828800	3.1676650	H	-2.5010850	-1.8937000	2.8755410
C	4.1191570	-2.7973590	2.7346700	C	-3.4579340	-0.1509250	3.8275550
C	4.5898640	-3.0333140	1.2937440	C	-4.4380970	0.8343880	3.1892620
C	3.6098930	-2.1798980	0.4886100	C	-4.0762300	0.7654760	1.6983760
H	3.9590990	-1.9247940	-0.5223280	H	-4.9719820	0.8690300	1.0636430
H	2.6423250	-2.6930490	0.3674550	H	-3.3821710	1.5796950	1.4239160
H	5.6154840	-2.6554610	1.1518030	H	-5.4705640	0.4860290	3.3449910
H	4.5792160	-4.0926010	1.0037680	H	-4.3612930	1.8523850	3.5941140
H	3.3548850	-3.5398350	3.0055930	H	-2.4671410	0.3156740	3.9348200
H	4.9326820	-2.8847870	3.4667730	H	-3.7779150	-0.5090130	4.8146290
H	4.1846340	-0.3321190	1.1089610	H	-3.8987290	-1.1005550	0.7986380
N	3.4093870	0.9599300	-1.2896300	N	-3.4084170	0.5490370	-1.5036410
C	3.5019550	1.3781870	-2.7084660	C	-3.3904260	1.2693720	-2.7915450
H	4.1021910	0.6460000	-3.2663080	H	-4.2695940	1.9299770	-2.8993920
H	2.5032530	1.3828520	-3.1663870	H	-2.4912700	1.8965440	-2.8772410

C	4.1262750	2.7968210	-2.7284170
C	4.5956010	3.0304320	-1.2866930
C	3.6142990	2.1764550	-0.4838020
H	3.9625660	1.9196050	0.5270120
H	2.6469810	2.6901090	-0.3626030
H	5.6208470	2.6517760	-1.1442190
H	-4.3563290	-1.8461830	-3.6002990
H	-2.4592780	-0.3124350	-3.9373650
H	-3.7672820	0.5149720	-4.8188360
H	-3.8894310	1.1041340	-0.8016150
C	-3.4494550	0.1557620	-3.8314750
C	-4.4323930	-0.8281830	-3.1953180
C	-4.0737270	-0.7603120	-1.7035260
H	-4.9715940	-0.8603590	-1.0711930
H	-3.3834250	-1.5769970	-1.4270030
H	-5.4639910	-0.4782370	-3.3531660

Table S53 Geometric coordinates and single point energies for NaHMDS disolvated pyrrolidine monomer.



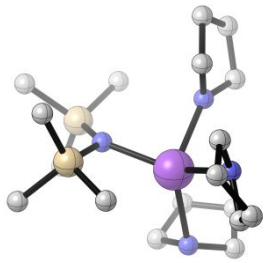
G = -1459.214564 Hartrees

G_{SP} = -1460.29046 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	-0.8028940	-1.2404540	-1.5973970	H	3.6048970	0.5007000	-2.0266480
N	-0.0633190	-0.9718990	-0.1035490	H	2.1696300	-0.3099930	-1.2982760
Si	0.2139420	-1.9439060	1.2495330	H	4.6724700	-0.2847660	-0.0584150
C	-1.2875110	-2.9466720	1.8389040	H	3.1576750	-0.3561480	0.8459290
H	-1.0818840	-3.4912320	2.7740770	H	3.4599910	1.8083820	1.6633700
H	-2.1583410	-2.2927620	2.0063960	H	5.0379510	1.9006250	0.8728160
H	-1.5741290	-3.6881550	1.0756040	H	1.9421800	2.1703180	-1.8011270
C	0.6889480	-0.8019980	2.7128720	N	-1.5242660	2.2887810	1.1785920
H	-0.1193390	-0.0784100	2.9194820	C	-2.1039600	3.0737710	0.0595040
H	0.8636030	-1.3663160	3.6418670	H	-2.4452240	4.0599730	0.4133820
H	1.6153560	-0.2344820	2.5105530	H	-1.3598620	3.2544560	-0.7331070
C	1.6352640	-3.1862330	1.0544460	C	-3.2909550	2.2468100	-0.4440970
H	1.3949950	-3.9111120	0.2606420	C	-3.7837800	1.5552680	0.8263710
H	2.5686710	-2.6801490	0.7614550	C	-2.4647330	1.1796700	1.4998270
H	1.8264450	-3.7494260	1.9816640	H	-2.5436380	1.0497990	2.5880530
Na	0.4088160	1.1393930	0.3944630	H	-2.0726960	0.2404980	1.0740960
N	2.2981060	1.7819570	-0.9283920	H	-4.3537460	2.2629820	1.4499960
C	3.3657540	2.6070390	-0.3564950	H	-4.4213730	0.6832900	0.6276780

H	4.1272030	2.8652630	-1.1169620
H	2.9698350	3.5444920	0.0590330
C	3.9770520	1.6788680	0.7007200
C	3.7373810	0.2544080	0.1390880
C	2.9308010	0.4694190	-1.1506830
H	-3.1408140	-1.6423530	-2.4880430
H	-2.8662210	-2.4995040	-0.9510870
C	-0.5700470	0.3128920	-2.6880180
H	-1.1473340	0.2570870	-3.6241710
H	-0.8853520	1.2338920	-2.1652670
H	0.4921160	0.4273260	-2.9623100
C	-0.0852390	-2.6871720	-2.5939210
H	1.0014660	-2.5667770	-2.7285840
H	-0.2473470	-3.6357230	-2.0568860
H	-0.5472380	-2.7805720	-3.5895090
H	-2.9447970	1.4892220	-1.1646160
H	-4.0500040	2.8645740	-0.9414450
H	-1.4181480	2.8895940	1.9908690
C	-2.6756560	-1.5595140	-1.4928310
H	-3.1922010	-0.7580900	-0.9401780

Table S54. Geometric coordinates and single point energies for NaHMDS trisolvated pyrrolidine monomer.



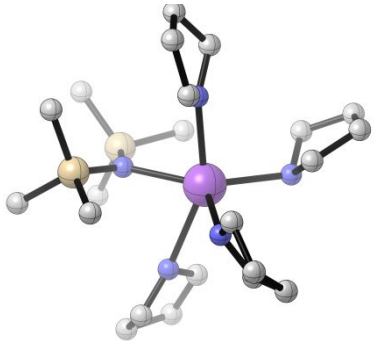
G = -1671.423598 Hartrees

G_{SP} = -1672.737941 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.7645690	-0.0143960	-0.3708800	H	1.2610440	-2.3292750	3.2866880
N	1.3424160	0.7254590	0.1942640	H	1.6791080	-4.1454450	1.8900240
Si	2.9531650	0.1848680	0.0775710	H	0.1362380	-4.9081980	2.3010670
C	4.1445040	0.9811460	1.3279180	H	0.7419730	-1.5530820	0.6417780
H	3.8073040	0.7862950	2.3584640	N	-3.0651460	-0.1329450	0.3570390
H	5.1645980	0.5793490	1.2214300	C	-3.3384330	0.3575670	1.7297100
H	4.2015550	2.0737590	1.1990460	H	-3.7692890	-0.4462770	2.3477490
C	3.1339320	-1.6868850	0.4099160	H	-2.4132860	0.6892990	2.2262170
H	4.1949240	-1.9698580	0.3249500	C	-4.3416940	1.5075630	1.5636460
H	2.8069780	-1.9425740	1.4312910	C	-5.1028030	1.1211600	0.2956360
H	2.5759690	-2.3191770	-0.3006210	C	-3.9738440	0.5659770	-0.5728550
C	3.7335920	0.4562680	-1.6368980	H	-4.3170240	-0.1143720	-1.3645330
H	3.2135670	-0.1301730	-2.4111990	H	-3.4333160	1.3960570	-1.0588060
H	3.6738150	1.5177160	-1.9250340	H	-5.8377600	0.3302620	0.5161500
H	4.7945300	0.1597440	-1.6495890	H	-5.6341070	1.9616580	-0.1702330
Si	0.9697600	2.3536620	0.5126330	H	-3.8041780	2.4538050	1.3975440
C	1.1210710	2.8702150	2.3327870	H	-4.9819380	1.6345410	2.4461760
H	0.7990320	3.9113040	2.4942040	H	-3.2227750	-1.1362430	0.3137140
H	0.5018560	2.2166220	2.9683520	N	-1.0891800	0.1237960	-2.7545020

H	2.1612100	2.7779230	2.6804960	C	0.3314930	0.0569450	-3.1237500
C	-0.8637210	2.6974780	0.0668260	H	0.4797320	0.2629590	-4.2007450
H	-1.5608150	2.1067960	0.6856560	H	0.9251380	0.7683730	-2.5311140
H	-1.1061640	3.7571380	0.2403720	C	0.6887430	-1.4027590	-2.8020470
H	-1.0745590	2.4843070	-0.9960940	C	-0.6549640	-2.1704400	-2.8985010
C	1.9500010	3.6247650	-0.5057550	C	-1.6732430	-1.0971250	-3.3089910
H	3.0302550	3.5524840	-0.3033550	H	-1.7517550	-1.0488560	-4.4124650
H	1.8051410	3.4505210	-1.5842570	H	-2.6801620	-1.2768180	-2.9049890
H	1.6356660	4.6563280	-0.2810820	H	-0.6252540	-2.9990880	-3.6175090
N	-0.1622310	-2.0182900	0.7719470	H	-0.9251070	-2.5902660	-1.9180320
C	0.0090710	-3.4640390	0.6451040	H	1.1005070	-1.4622640	-1.7830680
H	-0.9790810	-3.9213390	0.4700300	H	1.4541440	-1.7929280	-3.4849610
H	0.6390520	-3.7016410	-0.2240060	H	-1.5384520	0.9661590	-3.1086570
C	0.6000940	-3.9635600	1.9861610				
C	0.3217580	-2.8116440	2.9806820				
C	-0.5307560	-1.8134590	2.1730880				
H	-1.6054920	-2.0346390	2.2986440				
H	-0.3586250	-0.7639530	2.4549090				
H	-0.1846940	-3.1491650	3.8949170				

Table S55. Geometric coordinates and single point energies for NaHMDS tetrasolvated pyrrolidine monomer.



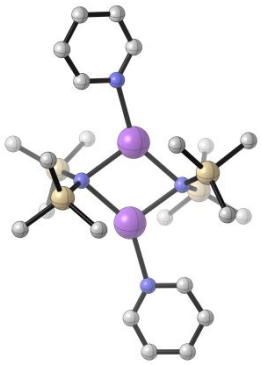
G = -1883.637203 Hartrees

G_{SP} = -1885.189714 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.5174560	-0.2439810	-0.2898570	H	3.7914450	-0.9209470	-0.3289880
N	-1.6698000	0.5509190	0.0736100	C	4.6246020	0.6041160	-1.7264620
Si	-2.4144350	1.0657820	-1.3680880	C	3.9309150	1.0369790	-3.0391720
C	-3.2905100	2.7460030	-1.2480410	C	2.4381450	0.7779620	-2.7725400
H	-2.5922630	3.5227670	-0.8954600	H	1.9758010	1.6521310	-2.2889210
H	-3.6968110	3.0678200	-2.2198290	H	1.8542690	0.5459980	-3.6727230
H	-4.1270420	2.7041300	-0.5320520	H	4.1282470	2.0847740	-3.3017460
C	-1.0925330	1.2623310	-2.7243000	H	4.2774740	0.4206230	-3.8817290
H	-1.5347680	1.5737560	-3.6834570	H	5.4218590	-0.1258230	-1.9236630
H	-0.3511390	2.0234110	-2.4327620	H	5.0865260	1.4507970	-1.2011140
H	-0.5431710	0.3229190	-2.9053930	H	2.6043320	-1.1970740	-2.3017520
C	-3.6918910	-0.1673970	-2.0453480	N	0.9591980	2.1293840	0.2325690
H	-3.2289600	-1.1516650	-2.2241390	C	1.2641870	3.4438670	-0.3246920
H	-4.5093530	-0.3133210	-1.3218990	H	2.3416330	3.4984450	-0.5683770
H	-4.1337620	0.1744160	-2.9947230	H	0.7022290	3.6159080	-1.2538830
Si	-2.3574510	0.6200410	1.6282280	C	0.9211160	4.4329640	0.7955650
C	-2.3374580	2.3638300	2.3846780	C	1.3797290	3.6864930	2.0599440
H	-2.7360230	2.3750040	3.4115380	C	1.3970460	2.1912390	1.6321800

H	-1.3119160	2.7671980	2.4161640	H	2.4178770	1.7821030	1.7224910
H	-2.9438600	3.0535550	1.7769050	H	0.7413930	1.5596820	2.2495300
C	-1.3917510	-0.4854380	2.8446200	H	2.3856710	4.0105720	2.3627080
H	-0.3447510	-0.1568360	2.9484770	H	0.7103590	3.8679530	2.9116220
H	-1.8451480	-0.4652250	3.8477480	H	-0.1694850	4.5843790	0.8148780
H	-1.3885970	-1.5329080	2.5004380	H	1.3966520	5.4160490	0.6763460
C	-4.1563880	0.0153160	1.7117750	H	-0.0605420	1.9785990	0.2144130
H	-4.8135410	0.6503260	1.0958620	N	1.5961090	-1.5615810	1.4107980
H	-4.2379660	-1.0144370	1.3264350	C	2.5131550	-1.2382500	2.5107470
H	-4.5483360	0.0263440	2.7410120	H	3.3007710	-0.5529810	2.1512210
N	-0.9552280	-2.3717000	-0.2978870	H	1.9755490	-0.7234260	3.3195410
C	-1.6803750	-3.4905240	0.2962940	C	3.1373210	-2.5723900	2.9228100
H	-0.9902240	-4.3382250	0.4651250	C	3.3207150	-3.2462270	1.5614600
H	-2.1073970	-3.2083770	1.2691110	C	2.0676580	-2.8129040	0.7761310
C	-2.7371210	-3.8727100	-0.7469970	H	2.2887660	-2.6561600	-0.2923640
C	-1.9795550	-3.6952550	-2.0723140	H	1.2757070	-3.5739130	0.8214610
C	-0.8447780	-2.6887580	-1.7257600	H	4.2305640	-2.8542510	1.0791610
H	0.1400830	-3.1406140	-1.9360590	H	3.4240750	-4.3378540	1.6184350
H	-0.9098210	-1.7622650	-2.3171410	H	2.4257830	-3.1434560	3.5404730
H	-1.5529770	-4.6515830	-2.4075920	H	4.0725330	-2.4654490	3.4889570
H	-2.6310100	-3.3296560	-2.8776680	H	0.6610670	-1.7251340	1.7805240
H	-3.5734480	-3.1588140	-0.6853810				
H	-3.1440710	-4.8844710	-0.6132880				
H	-1.5087650	-1.5080030	-0.1816310				
N	2.3884100	-0.3292840	-1.8092950				
C	3.4883610	-0.0223630	-0.8832110				
H	3.1044980	0.7080030	-0.1531370				

Table S56. Geometric coordinates and single point energies for NaHMDS disolvated pyridine dimer.



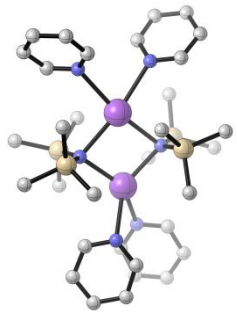
G = -2565.477035 Hartrees

G_{SP} = -2567.213588 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	1.2621910	-0.7352430	-0.1978580	C	-0.5155930	-4.3559180	1.0346890
N	-0.9262910	-1.5789060	-0.1307180	H	-0.4270870	-4.8891360	1.9943890
Na	-1.2621920	0.7347690	-0.1971920	H	-1.3275830	-4.8297880	0.4619290
N	0.9263370	1.5784970	-0.1310030	H	0.4205460	-4.5122850	0.4747750
Si	1.5570740	2.1147390	-1.6273530	C	-2.3414420	-2.3512290	2.4255100
C	3.1635770	3.1217590	-1.5123830	H	-3.2385200	-2.7312520	1.9090240
H	3.4999530	3.4407390	-2.5114920	H	-2.2179730	-2.9338850	3.3516700
H	3.0301770	4.0274050	-0.9007450	H	-2.5308970	-1.3030330	2.7083800
H	3.9768080	2.5305310	-1.0620820	Si	-1.5571880	-2.1157390	-1.6267690
C	1.9766160	0.5996270	-2.7042790	C	-1.9772120	-0.6009990	-2.7040090
H	2.8058310	0.0133500	-2.2727750	H	-2.8062340	-0.0146710	-2.2721940
H	1.1110340	-0.0723860	-2.8359320	H	-2.2945990	-0.9095040	-3.7118060
H	2.2935130	0.9079200	-3.7122960	H	-1.1117590	0.0710750	-2.8361620
C	0.3255790	3.1679010	-2.6139240	C	-0.3256750	-3.1690520	-2.6131440
H	-0.6223670	2.6267740	-2.7718190	H	-0.7185250	-3.4516810	-3.6022680
H	0.0938260	4.0939820	-2.0645170	H	0.6220130	-2.6276970	-2.7717930
H	0.7181110	3.4497310	-3.6034020	H	-0.0933850	-4.0946810	-2.0631970
Si	0.8180320	2.5019320	1.3040570	C	-3.1635070	-3.1230300	-1.5113480

C	-0.6810210	1.9165830	2.3303050	H	-3.0298890	-4.0285570	-0.8995870
H	-1.6337240	2.2416930	1.8772880	H	-3.9768250	-2.5318910	-1.0610940
H	-0.7187840	0.8203320	2.4485240	H	-3.4999030	-3.4422350	-2.5103800
H	-0.6540300	2.3480620	3.3426360	N	3.5613620	-1.2258210	0.0885860
C	2.3421450	2.3536940	2.4241770	C	4.3204430	-2.3221920	0.0455650
H	3.2390040	2.7332850	1.9069980	C	5.6802860	-2.3118310	0.3484130
H	2.2187230	2.9375200	3.3496090	C	6.2704230	-1.1037190	0.7150060
H	2.5319100	1.3059200	2.7083920	C	5.4806720	0.0419540	0.7637500
C	0.5147150	4.3561690	1.0322550	C	4.1293230	-0.0685400	0.4402990
H	0.4261680	4.8902380	1.9914760	H	3.4675890	0.8044490	0.4649760
H	1.3262750	4.8299680	0.4588190	H	5.8936840	1.0101010	1.0474210
H	-0.4216550	4.5114930	0.4724300	H	7.3327550	-1.0574030	0.9602590
N	-3.5612730	1.2260060	0.0890760	H	6.2588290	-3.2340110	0.2970290
C	-4.3199240	2.3227010	0.0466810	H	3.8209600	-3.2515730	-0.2428280
C	-5.6799190	2.3125700	0.3488680				
C	-6.2706900	1.1043550	0.7140840				
C	-5.4813910	-0.0416580	0.7621790				
C	-4.1298500	0.0686240	0.4394780				
H	-3.4684570	-0.8046370	0.4637040				
H	-5.8949080	-1.0099040	1.0447740				
H	-7.3331580	1.0582210	0.9587750				
H	-6.2580910	3.2350140	0.2980310				
H	-3.8200130	3.2521900	-0.2406460				
Si	-0.8178040	-2.5012900	1.3049910				
C	0.6820850	-1.9159960	2.3300910				
H	1.6343150	-2.2423230	1.8769600				
H	0.7208520	-0.8196780	2.4473760				
H	0.6551200	-2.3466150	3.3427920				

Table S57. Geometric coordinates and single point energies for NaHMDS tetrasolvated pyridine dimer.



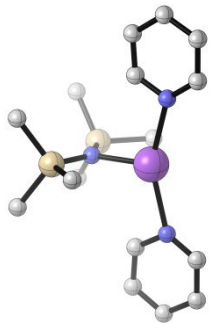
G = -3061.307522 Hartrees

G_{SP} = -3063.5893 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.6723430	0.0024250	-0.0015520	H	-2.2467950	0.7042010	2.3589280
N	-0.0277380	1.8054640	0.1988120	H	-0.7967890	-0.3220980	2.4576940
Na	1.4731760	-0.0038890	0.0037950	H	-1.1941820	0.7740420	3.7852960
N	-0.0334530	-1.8065800	-0.1980360	C	-0.6688590	3.7189300	2.5182440
Si	-0.0921090	-2.0214720	-1.8847900	H	-0.9872240	3.6605610	3.5717110
C	-0.6726770	-3.7190580	-2.5190720	H	0.1570550	4.4446540	2.4598380
H	-0.9891210	-3.6597000	-3.5730640	H	-1.5014380	4.1265500	1.9242680
H	0.1521370	-4.4459460	-2.4596390	C	1.5994400	1.7440980	2.7292850
H	-1.5067910	-4.1259120	-1.9267650	H	2.3259600	2.5115980	2.4145270
C	-1.1942380	-0.6795760	-2.6893620	H	1.5098240	1.8005750	3.8259350
H	-2.2463440	-0.7010130	-2.3611060	H	2.0215020	0.7526790	2.4886880
H	-0.7939840	0.3221450	-2.4591770	Si	-0.0452870	2.9888950	-1.0353050
H	-1.1927580	-0.7737160	-3.7864800	C	1.0127670	2.5106270	-2.5484630
C	1.5986500	-1.7474570	-2.7255930	H	2.0445140	2.8806810	-2.4554480
H	2.0205160	-0.7559670	-2.4850900	H	0.5824050	2.9634500	-3.4560820
H	2.3242080	-2.5148400	-2.4083720	H	1.0734680	1.4239490	-2.7129180
H	1.5113070	-1.8051680	-3.8223680	C	-1.7698140	3.3275700	-1.7595470
Si	-0.0534290	-2.9899550	1.0360960	H	-1.7048510	4.0910710	-2.5514840
C	1.0078150	-2.5145140	2.5479180	H	-2.2018250	2.4190720	-2.2101750
H	2.0398860	-2.8826130	2.4511750	H	-2.4693880	3.6940680	-0.9915910

H	1.0672610	-1.4282570	2.7158290	C	-4.6322290	3.6567500	0.9264110
H	0.5804710	-2.9708330	3.4552060	C	-5.4251090	3.6591600	-0.2181290
C	-1.7774870	-3.3236940	1.7637450	C	-5.3404420	2.5761640	-1.0888030
H	-2.4800170	-3.6918640	0.9992610	C	-4.4624930	1.5390570	-0.7777850
H	-1.7117910	-4.0846600	2.5580780	N	-3.6944700	1.5335570	0.3132930
H	-2.2071260	-2.4132040	2.2125870	C	-3.7835120	2.5723990	1.1451840
C	0.5878090	-4.7060150	0.5124320	H	-3.1429490	2.5478840	2.0302870
H	0.7226470	-5.3444060	1.4004590	H	-4.3694650	0.6699690	-1.4357670
H	-0.1158480	-5.2153630	-0.1627340	H	-5.9367490	2.5307410	-1.9999170
H	1.5599390	-4.6459620	-0.0046770	H	-6.0969550	4.4927940	-0.4291040
N	3.4662890	-1.0096830	1.0648640	H	-4.6585480	4.4797450	1.6407730
C	4.5244600	-0.4388240	1.6381950	C	0.6008280	4.7032580	-0.5118670
C	5.8115520	-0.9684510	1.5508870	H	-0.1013850	5.2141990	0.1636230
C	5.9970700	-2.1468280	0.8309100	H	1.5730480	4.6409810	0.0047830
C	4.8913530	-2.7503720	0.2364930	H	0.7367140	5.3413950	-1.3999200
C	3.6446660	-2.1427820	0.3844420	C	-4.4662370	-1.5346000	0.7766660
H	2.7447690	-2.5799960	-0.0625940	C	-5.3462240	-2.5707970	1.0849850
H	4.9834150	-3.6762760	-0.3314900	C	-5.4299670	-3.6533750	0.2137000
H	6.9897960	-2.5906980	0.7376930	C	-4.6342400	-3.6514430	-0.9288790
H	6.6455320	-0.4620230	2.0369580	C	-3.7838490	-2.5679190	-1.1450940
H	4.3379270	0.4905960	2.1859800	H	-3.1412510	-2.5436440	-2.0286850
C	3.6410150	2.1364940	-0.3809660	N	-3.6957570	-1.5294340	-0.3126840
C	4.8859850	2.7488100	-0.2383160	H	-4.6596180	-4.4741800	-1.6435730
C	5.9915950	2.1490550	-0.8368010	H	-6.1032950	-4.4863130	0.4226950
C	5.8076370	0.9695840	-1.5553530	H	-5.9447360	-2.5250600	1.9946390
C	4.5221430	0.4351700	-1.6374060	H	-4.3736430	-0.6659280	1.4352620
N	3.4641700	1.0024430	-1.0602540	H	4.9768360	3.6753780	0.3287900
H	4.3368460	-0.4951250	-2.1841360	H	2.7412100	2.5703760	0.0694550
H	6.6415890	0.4659910	-2.0444140	Si	-0.0895650	2.0203870	1.8854510
H	6.9830170	2.5966970	-0.7478040	C	-1.1950650	0.6803290	2.6881370

Table S58. Geometric coordinates and single point energies for NaHMDS disolvated pyridine monomer.



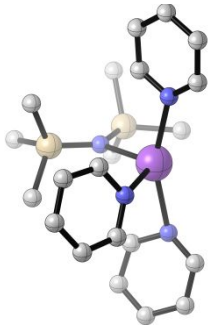
G = -1530.645531 Hartrees

G_{SP} = -1531.790063 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	-0.0098660	-1.6839690	1.5673380	H	2.2988800	-0.2884610	0.0101570
N	0.0000240	-1.0509310	0.0000220	Si	0.0097990	-1.6839860	-1.5672880
Na	0.0000390	1.1924550	-0.0000070	C	1.5406010	-2.7251040	-1.9939550
N	-2.3074040	1.7783660	-0.0042770	H	1.5271680	-3.0651190	-3.0416420
C	-3.0382390	2.8956280	-0.0014340	H	2.4658100	-2.1467440	-1.8386720
C	-4.4306890	2.8931110	-0.0025450	H	1.5949400	-3.6168870	-1.3498930
C	-5.0918770	1.6661980	-0.0067490	C	0.0031470	-0.2152110	-2.7860950
C	-4.3351510	0.4983080	-0.0097490	H	0.8940740	0.4203180	-2.6361730
C	-2.9439770	0.6000050	-0.0084360	H	0.0085730	-0.5365750	-3.8390180
H	-2.2988560	-0.2884160	-0.0104460	H	-0.8967210	0.4086780	-2.6413000
H	-4.8040140	-0.4857860	-0.0129820	C	-1.5009060	-2.7499010	-2.0034730
H	-6.1823730	1.6235980	-0.0076500	H	-1.5390730	-3.6473180	-1.3660680
H	-4.9794230	3.8348260	-0.0000720	H	-2.4367580	-2.1900270	-1.8443250
H	-2.4893640	3.8414870	0.0019010	H	-1.4802750	-3.0819960	-3.0535680
N	2.3074850	1.7783230	0.0042840	C	1.5008080	-2.7498840	2.0036290
C	2.9440250	0.5999430	0.0082670	H	2.4366690	-2.1900020	1.8445620
C	4.3351970	0.4982100	0.0095190	H	1.4800970	-3.0819970	3.0537170
C	5.0919540	1.6660800	0.0066470	H	1.5390280	-3.6472910	1.3662120
C	4.4307990	2.8930120	0.0026200	C	-0.0032750	-0.2151800	2.7861280

C	3.0383490	2.8955650	0.0015500
H	2.4894990	3.8414400	-0.0016540
H	4.9795580	3.8347120	0.0002470
H	6.1824490	1.6234500	0.0075030
H	4.8040340	-0.4858970	0.0125970
H	-1.5949760	-3.6168940	1.3498990
H	-1.5273420	-3.0650470	3.0416260
H	-0.0087450	-0.5365290	3.8390550
H	0.8966000	0.4087050	2.6413620
H	-0.8941940	0.4203500	2.6361600
C	-1.5406960	-2.7250800	1.9939230
H	-2.4659010	-2.1467390	1.8385410

Table S59. Geometric coordinates and single point energies for NaHMDS trisolvated pyridine monomer.



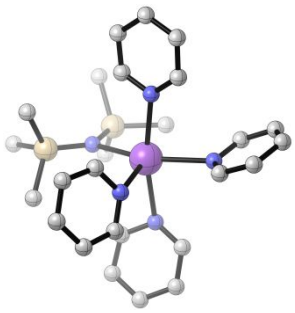
G = -1778.568232 Hartrees

G_{SP} = -1779.985009 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.0115690	0.2830760	-1.1430790	N	1.0427110	2.1509140	0.0098140
N	-0.4969390	-1.3223280	0.4087100	C	2.3472230	2.3251560	0.2320680
Si	-1.1131530	-2.6094690	-0.5095440	C	2.8464690	2.9513780	1.3725440
C	-2.9300890	-3.0509610	-0.1506910	C	1.9436180	3.4077090	2.3301860
H	-3.5918340	-2.1905390	-0.3420280	C	0.5820170	3.2291260	2.1038260
H	-3.2787460	-3.8872190	-0.7775130	C	0.1824730	2.5986240	0.9261830
H	-3.0613250	-3.3439430	0.9031510	H	-0.8785920	2.4359600	0.7144380
C	-1.0601680	-2.1232970	-2.3556150	H	-0.1648810	3.5581230	2.8261560
H	-1.4415120	-2.9341040	-2.9951040	H	2.2973680	3.8896100	3.2430370
H	-1.6839820	-1.2345540	-2.5569410	H	3.9222040	3.0636230	1.5066070
H	-0.0268270	-1.9104880	-2.6803120	H	3.0303220	1.9387900	-0.5309740
C	-0.1366690	-4.2319030	-0.3737340	N	-2.1240700	1.3853500	-1.3634970
H	0.9268860	-4.0626510	-0.6065910	C	-2.9334010	0.8079010	-0.4670800
H	-0.1953060	-4.6385180	0.6476630	C	-4.2484050	1.2273920	-0.2628720
H	-0.5200240	-4.9983640	-1.0659770	C	-4.7386970	2.2855750	-1.0226700
Si	-0.3751590	-1.1886250	2.0950080	C	-3.8966160	2.8873740	-1.9562910
C	-1.7149820	-0.0536610	2.8409980	C	-2.5976970	2.4012080	-2.0877730
H	-1.5975030	0.0557130	3.9310330	H	-1.9085850	2.8519740	-2.8076750
H	-1.6940120	0.9546770	2.3968810	H	-4.2351510	3.7192850	-2.5738920

H	-2.7155780	-0.4779860	2.6523010
C	1.3036260	-0.4689930	2.6346760
H	1.5611120	0.4466630	2.0793680
H	1.3127630	-0.2269800	3.7096290
H	2.1060590	-1.2037830	2.4539630
C	-0.5267950	-2.8256580	3.0517250
H	-1.4743530	-3.3407470	2.8268100
H	0.2950270	-3.5090560	2.7857280
H	-0.4861230	-2.6572600	4.1398050
N	2.2468250	-0.3253960	-1.8015780
C	2.6498680	-0.9623300	-0.6961820
C	3.9981500	-1.1127750	-0.3669330
C	4.9596240	-0.5853030	-1.2240300
C	4.5398580	0.0686600	-2.3819450
C	3.1712990	0.1718380	-2.6247100
H	2.8056000	0.6837680	-3.5195370
H	5.2552700	0.4935480	-3.0861910
H	6.0226860	-0.6832650	-0.9967950
H	-5.7628590	2.6388430	-0.8904980
H	-4.8654190	0.7245510	0.4820720
H	-2.4910200	-0.0161220	0.1070580
H	4.2755210	-1.6328350	0.5500570
H	1.8479980	-1.3493880	-0.0525820

Table S60. Geometric coordinates and single point energies for NaHMDS tetrasolvated pyridine monomer.



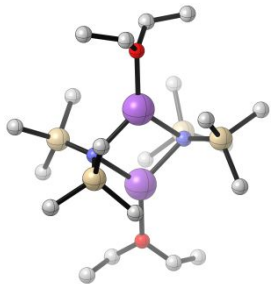
G = -2026.490481 Hartrees

G_{SP} = -2028.179273 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.3952000	-0.1675690	-0.3604390	C	-0.1253000	-0.4896400	2.6863110
N	-1.5467300	1.0990280	-0.5904780	H	0.3330240	0.4894060	2.5167820
Si	-1.3033660	1.7926990	-2.1174030	H	-1.0240720	0.0534330	4.5704380
C	-1.2623670	3.6969390	-2.1425220	H	-2.0484250	-2.2270930	4.8759760
H	-0.4564280	4.0816160	-1.4964550	H	-1.6699790	-3.9548570	3.0837360
H	-1.0945400	4.0888640	-3.1585400	H	-0.3103610	-3.3329770	1.0875700
H	-2.2127460	4.1147120	-1.7741640	N	1.7699510	1.6435020	0.6557170
C	0.4093270	1.2538970	-2.7797440	C	1.0006620	2.7302330	0.7851420
H	0.6045050	1.6821720	-3.7749790	C	1.4975710	3.9560630	1.2308620
H	1.2127400	1.6025650	-2.1068860	C	2.8487350	4.0536480	1.5502750
H	0.4716210	0.1550180	-2.8714470	C	3.6519770	2.9228850	1.4129580
C	-2.5542110	1.2728190	-3.4482010	C	3.0647030	1.7420830	0.9619120
H	-2.5911330	0.1749560	-3.5329400	H	3.6673590	0.8354610	0.8420680
H	-3.5652920	1.6241160	-3.1899850	H	4.7159260	2.9495060	1.6488160
H	-2.2955290	1.6836890	-4.4371810	H	3.2724630	4.9967600	1.9000810
Si	-2.8343650	1.3334340	0.4852170	H	0.8264650	4.8108770	1.3183610
C	-2.3731350	2.4432040	1.9688130	H	-0.0518000	2.5936710	0.5091320
H	-3.2097910	2.5348480	2.6799210	N	2.6347160	-1.0567830	-0.8239240
H	-1.5012780	2.0563400	2.5205440	C	3.4658590	-0.5247770	-1.7204820
H	-2.1195220	3.4579690	1.6182740	C	4.8523820	-0.6608190	-1.6424440

C	-3.4737440	-0.3036010	1.2234480	C	5.3907270	-1.3869120	-0.5826570
H	-2.6501480	-0.9646110	1.5352140	C	4.5241990	-1.9478790	0.3533740
H	-4.1203180	-0.1275510	2.0983430	C	3.1523120	-1.7528550	0.1895490
H	-4.0725150	-0.8499160	0.4753990	H	2.4337880	-2.1562320	0.9099640
C	-4.3827950	2.1491430	-0.2636970	H	4.8981360	-2.5233350	1.2002810
H	-4.1501190	3.1285120	-0.7111560	H	6.4705140	-1.5138480	-0.4871610
H	-4.8116490	1.5145530	-1.0553630	H	5.4896300	-0.2030200	-2.3990220
H	-5.1609470	2.3048990	0.5008170	H	3.0023830	0.0432690	-2.5326280
N	-0.4695820	-2.1696550	-1.4314520				
C	0.1661060	-3.3298550	-1.5926720				
C	-0.4818750	-4.5639450	-1.5394190				
C	-1.8561760	-4.5798210	-1.3014690				
C	-2.5224210	-3.3684550	-1.1373280				
C	-1.7870720	-2.1835860	-1.2145900				
H	-2.2471560	-1.1975080	-1.0816150				
H	-3.5951980	-3.3293330	-0.9470720				
H	-2.3986770	-5.5255810	-1.2473390				
H	0.0810260	-5.4871450	-1.6791200				
H	1.2453980	-3.2679460	-1.7640660				
N	0.0730570	-1.4036900	1.7349120				
C	-0.4772070	-2.6093800	1.8927700				
C	-1.2392060	-2.9566590	3.0068760				
C	-1.4457390	-1.9973250	3.9958020				
C	-0.8793490	-0.7363510	3.8333680				

Table S61. Geometric coordinates and single point energies for NaHMDS disolvated Et_2O dimer.



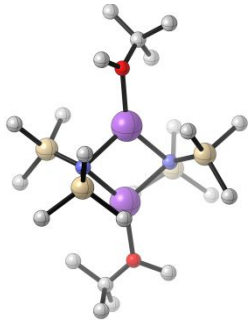
G = -2536.125652 Hartrees

G_{SP} = -2537.851147 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.4500330	-0.0002120	-0.0014070	H	5.2584730	-2.0852410	0.7172080
N	0.0000150	-1.8251740	-0.0007060	H	3.7222350	-2.6762420	0.0319310
Na	1.4500510	-0.0003040	-0.0000820	H	5.3690070	-0.3436990	-1.1366700
N	0.0000100	1.8247590	-0.0007400	H	3.8356950	-0.9629570	-1.7793930
Si	-0.3060890	2.5654940	1.5056620	Si	-0.3057990	-2.5656860	-1.5073050
C	-1.0981500	4.2870050	1.4330400	C	-1.5000010	-1.4592560	-2.5012720
H	-1.4647980	4.5926010	2.4256490	H	-2.4865960	-1.3961050	-2.0097560
H	-0.3687080	5.0415480	1.1016760	H	-1.1017300	-0.4354650	-2.6131670
H	-1.9485150	4.3148100	0.7333990	H	-1.6658310	-1.8485380	-3.5173090
C	-1.5018530	1.4600350	2.4988530	C	-1.0999850	-4.2861840	-1.4348590
H	-2.4881170	1.3972310	2.0066410	H	-1.4660640	-4.5917620	-2.4276800
H	-1.1041210	0.4360740	2.6111300	H	-0.3720070	-5.0416170	-1.1023170
H	-1.6682300	1.8495230	3.5147250	H	-1.9511080	-4.3121870	-0.7360660
C	1.2581900	2.7547770	2.5657700	C	1.2589920	-2.7566580	-2.5663200
H	1.7173590	1.7764740	2.7832620	H	2.0018670	-3.3701290	-2.0308070
H	2.0024650	3.3665980	2.0303010	H	1.0503390	-3.2448260	-3.5312790
H	1.0496140	3.2440440	3.5301890	H	1.7199260	-1.7789300	-2.7826660
Si	0.3069740	2.5652120	-1.5071340	Si	0.3049340	-2.5659210	1.5059310
C	1.5019790	1.4587510	-2.5001160	C	1.4999620	-1.4605170	2.5000520
H	2.4882130	1.3956370	-2.0078730	H	2.4865800	-1.3977590	2.0085440

H	1.1038080	0.4349440	-2.6122180	H	1.6655790	-1.8500430	3.5160320
H	1.6685590	1.8479620	-3.5160580	H	1.1021980	-0.4365400	2.6120840
C	-1.2569730	2.7561600	-2.5673890	C	-1.2601930	-2.7551270	2.5648130
H	-1.9998470	3.3705430	-2.0329260	H	-1.0526010	-3.2452870	3.5289890
H	-1.0473510	3.2434090	-3.5326030	H	-1.7188770	-1.7767000	2.7827760
H	-1.7183610	1.7785360	-2.7832350	H	-2.0044840	-3.3660290	2.0283160
C	1.1009240	4.2858140	-1.4342370	C	1.0971390	-4.2873750	1.4338390
H	1.4676270	4.5913530	-2.4268410	H	0.3680500	-5.0420020	1.1018970
H	0.3725530	5.0411370	-1.1023010	H	1.9479990	-4.3149370	0.7347900
H	1.9515580	4.3121490	-0.7348640	H	1.4631330	-4.5929830	2.4266840
O	3.6753330	-0.0002890	0.0009460	O	-3.6753240	-0.0007810	-0.0015880
C	4.4256250	0.8418080	0.8624330	C	-4.4252630	0.8458250	-0.8589560
H	5.3659620	0.3376080	1.1447240	H	-3.8366490	0.9623160	-1.7816070
H	3.8324050	0.9622920	1.7816110	H	-5.3703880	0.3475260	-1.1356350
C	4.6864070	2.1890580	0.2169970	C	-4.6736800	2.1948200	-0.2122790
H	5.2452810	2.8448940	0.8989540	H	-5.2318750	2.8543230	-0.8912540
H	5.2681430	2.0790680	-0.7100110	H	-5.2510550	2.0887420	0.7179170
H	3.7316170	2.6756680	-0.0302570	H	-3.7143390	2.6751110	0.0297680
C	4.4259140	-0.8447360	-0.8579890	C	-4.4262500	-0.8408630	0.8613100
C	4.6796380	-2.1930120	-0.2118800	H	-3.8313860	-0.9633670	1.7791570
H	5.2385580	-2.8507480	-0.8919710	H	-5.3644620	-0.3339260	1.1457780
H	-5.2757260	-2.0751950	-0.7096810	C	-4.6924980	-2.1871710	0.2161460
H	-3.7397440	-2.6767440	-0.0330460	H	-5.2521030	-2.8413430	0.8990990

Table S62. Geometric coordinates and single point energies for NaHMDS disolvated MTBE dimer.



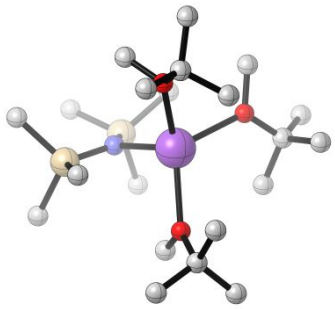
G = -2614.610773 Hartrees

G_{SP} = -2616.424086 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.4433530	-0.1752760	-0.0241910	Si	0.7975900	-2.4548750	1.5279820
N	0.2241610	-1.8108020	0.0521650	C	1.7061740	-1.0858470	2.4973810
Na	1.4425570	0.1778430	-0.0251580	H	2.6419180	-0.7784860	2.0000320
N	-0.2243980	1.8130770	0.0515340	H	1.9791570	-1.4338230	3.5053340
Si	-0.7965060	2.4574130	1.5277250	H	1.0810110	-0.1856840	2.6249790
C	-2.0504610	3.8719140	1.3434880	C	-0.5752260	-3.1028490	2.6650990
H	-2.3960470	4.2281650	2.3267700	H	-0.1695680	-3.5215970	3.5993460
H	-1.6130010	4.7315660	0.8120280	H	-1.2784250	-2.2987750	2.9362030
H	-2.9359200	3.5488410	0.7728250	H	-1.1455350	-3.8981290	2.1585200
C	-1.7077890	1.0895910	2.4963820	C	2.0541390	-3.8669610	1.3424110
H	-2.6444600	0.7849160	1.9991240	H	1.6179250	-4.7269430	0.8104270
H	-1.0848670	0.1877170	2.6230670	H	2.9388030	-3.5419530	0.7715940
H	-1.9795240	1.4373470	3.5047450	H	2.4007620	-4.2234400	2.3252420
C	0.5778110	3.1020940	2.6649230	O	-3.6034500	-0.7769910	0.1528330
H	1.2802000	2.2968260	2.9345870	C	-4.6892360	0.0039960	-0.3761330
H	1.1487680	3.8972230	2.1588110	C	-5.5782180	-0.8522550	-1.2754040
H	0.1733760	3.5203460	3.5999180	H	-6.1452420	-1.5985730	-0.7009890
Si	0.1769640	2.7293310	-1.3342940	H	-6.3030000	-0.2109580	-1.7955410
C	1.3973280	1.7292950	-2.4085500	H	-4.9711610	-1.3723450	-2.0312890

H	2.3824020	1.6558840	-1.9167060	C	-3.9945300	1.0888060	-1.1910600
H	1.0321790	0.7064040	-2.6120060	H	-3.2863630	1.6549580	-0.5642840
H	1.5567710	2.2129720	-3.3842240	H	-3.4391890	0.6386490	-2.0277060
C	-1.3034150	3.1385730	-2.4443110	H	-4.7229310	1.8002120	-1.6037260
H	-2.0780330	3.6783560	-1.8764160	C	-5.4911120	0.6225610	0.7673930
H	-1.0076980	3.7674690	-3.2986400	H	-5.9582360	-0.1463180	1.3991580
H	-1.7584950	2.2188550	-2.8451460	H	-4.8422490	1.2490980	1.3961290
C	1.0609500	4.3683090	-0.9647210	H	-6.2950410	1.2533680	0.3628360
H	1.3315660	4.8965400	-1.8925180	C	-3.8944740	-1.9948100	0.7979080
H	0.4292150	5.0445620	-0.3677710	H	-4.6016020	-1.8606980	1.6324300
H	1.9865390	4.1900600	-0.3946290	H	-4.2974930	-2.7418850	0.0954050
O	3.6038850	0.7758080	0.1508790	H	-2.9453590	-2.3743950	1.2013830
C	3.8979140	1.9914600	0.7986440	H	4.8333820	-1.2569960	1.3935110
H	4.6005210	1.8529750	1.6362800	Si	-0.1774270	-2.7275240	-1.3332890
H	4.3077490	2.7373710	0.0988840	C	-1.3984920	-1.7281240	-2.4073140
H	2.9488180	2.3752440	1.1981850	H	-2.3834370	-1.6551090	-1.9152010
C	4.6879190	-0.0084090	-0.3769690	H	-1.0337590	-0.7050670	-2.6107190
C	5.5816230	0.8457790	-1.2735110	H	-1.5579020	-2.2117300	-3.3830250
H	6.1508610	1.5888670	-0.6971040	C	-1.0603300	-4.3668830	-0.9627860
H	6.3045410	0.2024130	-1.7936920	H	-1.3309320	-4.8957230	-1.8902370
H	4.9776920	1.3695130	-2.0293900	H	-0.4278420	-5.0424090	-0.3657880
C	3.9908590	-1.0896690	-1.1945720	H	-1.9857830	-4.1890600	-0.3923540
H	3.2786130	-1.6533190	-0.5701480	C	1.3023600	-3.1368960	-2.4441000
H	3.4395360	-0.6365410	-2.0322710	H	2.0774500	-3.6763960	-1.8765770
H	4.7173200	-1.8038650	-1.6058530	H	1.0059220	-3.7663180	-3.2977990
C	5.4854390	-0.6312840	0.7672560	H	1.7570950	-2.2174270	-2.8458750
H	6.2883680	-1.2637960	0.3633720	H	5.9534660	0.1351660	1.4013120

Table S63. Geometric coordinates and single point energies for NaHMDS trisolvated MTBE monomer.



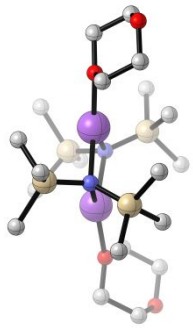
G = -1852.25893 Hartrees

G_{SP} = -1853.793235 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	-2.7373720	0.1223940	1.2572650	H	-1.0157300	2.4006650	0.5074600
N	-1.9239530	0.2649910	-0.2249920	H	-0.5695740	3.1834480	2.0580010
Si	-2.6082040	0.3747730	-1.7730880	C	2.0383360	2.4833830	1.8421600
C	-2.8736570	-1.3235710	-2.5987650	C	2.4015550	3.9458710	1.5840710
H	-3.3559070	-1.2311960	-3.5849450	H	2.5243900	4.1306560	0.5063270
H	-1.9187140	-1.8556920	-2.7430400	H	3.3519420	4.1810040	2.0827670
H	-3.5137790	-1.9605860	-1.9667940	H	1.6391200	4.6337490	1.9745320
C	-1.4541550	1.3338860	-2.9400800	C	3.1716690	1.5777090	1.3741810
H	-0.4614050	0.8564720	-2.9459760	H	4.0862330	1.7707210	1.9520420
H	-1.8317250	1.3668600	-3.9742210	H	2.8945840	0.5239930	1.5136640
H	-1.3236840	2.3700110	-2.5865530	H	3.3819240	1.7417540	0.3079790
C	-4.2953120	1.2456170	-1.8492010	C	1.7458040	2.2476430	3.3237010
H	-5.0504510	0.7010040	-1.2591980	H	1.5150650	1.1874560	3.5019520
H	-4.2270900	2.2664120	-1.4411180	H	2.6161500	2.5264800	3.9347360
H	-4.6656160	1.3151570	-2.8843770	H	0.8894010	2.8467620	3.6646090
Na	0.3253520	0.0493940	0.0659480	O	0.4122760	-2.2756160	0.6836320
O	1.7313440	0.6251330	-1.7231470	C	1.2747670	-3.0870470	1.4919630
C	2.3481970	-0.3315950	-2.6036060	C	0.5184730	-3.6462440	2.6983040
C	2.2376960	0.0932400	-4.0676410	H	0.0427110	-2.8328700	3.2637340
H	1.1922010	0.3056370	-4.3336740	H	1.2183070	-4.1719730	3.3632030

H	2.5973330	-0.7241470	-4.7076170	H	-0.2564250	-4.3656930	2.4007470
H	2.8464480	0.9813160	-4.2874250	C	2.3580840	-2.1240120	1.9584150
C	1.5678890	-1.6193700	-2.3752900	H	3.0829630	-2.6297570	2.6108530
H	1.9725900	-2.4363360	-2.9893830	H	2.8968660	-1.7135890	1.0904790
H	1.6230860	-1.9183970	-1.3187160	H	1.9009630	-1.2951990	2.5206710
H	0.5087740	-1.4706060	-2.6379450	C	1.8869050	-4.2192730	0.6664850
C	3.8098820	-0.5021310	-2.1916570	H	2.3871180	-3.8217280	-0.2291030
H	3.8701880	-0.8274310	-1.1425630	H	2.6320880	-4.7582010	1.2682170
H	4.3044620	-1.2552120	-2.8215310	H	1.1257390	-4.9457210	0.3492390
H	4.3670180	0.4407240	-2.2954550	C	-0.6507490	-2.9213020	0.0081570
C	1.9428590	1.9894780	-2.0041850	H	-0.2824340	-3.5201960	-0.8422860
H	1.5387800	2.5484930	-1.1520810	H	-1.3160210	-2.1256140	-0.3576390
H	1.4141120	2.3008450	-2.9181060	H	-1.2242050	-3.5728520	0.6857240
H	3.0168820	2.2248500	-2.1076720	C	-3.9143910	-1.3675340	1.3826830
O	0.9042220	2.0841640	1.0590320	H	-3.3828360	-2.3152840	1.2039940
C	-0.2205650	2.9442940	1.0394910	H	-4.3966000	-1.4281540	2.3713950
H	0.0033120	3.8828760	0.5065620	H	-4.7114560	-1.2889230	0.6254840
H	-0.7854730	0.7897030	2.7008700	C	-1.4464640	-0.0911910	2.6445770
C	-3.7879670	1.6279420	1.7556010	H	-1.9129590	-0.2255390	3.6329400
H	-3.1899630	2.5528100	1.7567610	H	-0.8211510	-0.9745690	2.4364090
H	-4.6214510	1.7738480	1.0516260				
H	-4.2151150	1.4989460	2.7631480				

Table S64. Geometric coordinates and single point energies for NaHMDS disolvated 1,4-dioxane dimer.



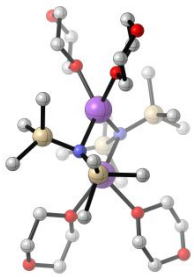
G = -2684.014117 Hartrees

G_{SP} = -2685.913388 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.3707820	-0.4811800	0.3953470	H	3.3252690	-1.2696570	-0.3247720
N	0.6066370	-1.7173920	0.2881920	H	4.8842750	-0.9108960	0.4975870
Na	1.3711110	0.4819420	0.3954630	H	4.0782180	-0.0409110	-2.3388850
N	-0.6063920	1.7181060	0.2881260	H	5.3325000	-1.2487780	-1.9212250
Si	-1.1648180	2.3760010	1.7641190	H	5.3042640	1.4459210	1.0696430
C	-2.5543860	3.6575490	1.6042740	H	4.0358930	2.6263360	0.6024650
H	-2.8872920	4.0047880	2.5949840	Si	0.3376470	-2.5600530	-1.1731650
H	-2.2252770	4.5407430	1.0357600	C	-1.0656680	-1.7028700	-2.1461170
H	-3.4299500	3.2358360	1.0861890	H	-2.0419990	-1.8607610	-1.6554940
C	-1.8779400	0.9653300	2.8306330	H	-0.9105000	-0.6153650	-2.2509540
H	-2.7779040	0.5216180	2.3710140	H	-1.1525750	-2.1168280	-3.1623740
H	-1.1426500	0.1584590	2.9969750	C	-0.2489080	-4.3521120	-0.9673230
H	-2.1729140	1.3321510	3.8254790	H	-0.4407710	-4.8236530	-1.9440190
C	0.2178570	3.1855630	2.7783450	H	0.4918080	-4.9705270	-0.4377960
H	1.0386100	2.4736470	2.9678790	H	-1.1849610	-4.3855320	-0.3867910
H	0.6381520	4.0420880	2.2277650	C	1.8546540	-2.5984650	-2.3106820
H	-0.1386440	3.5519030	3.7535780	H	2.6880410	-3.1253440	-1.8173050
Si	-0.3376420	2.5603520	-1.1735000	H	1.6444140	-3.1167830	-3.2589400
C	1.0667180	1.7039010	-2.1456330	H	2.1917110	-1.5774410	-2.5531780

H	2.0427160	1.8628640	-1.6546970	Si	1.1645470	-2.3753500	1.7643630
H	0.9125830	0.6162070	-2.2501480	C	1.8777910	-0.9648170	2.8309590
H	1.1536380	2.1175460	-3.1620170	H	2.7778960	-0.5213110	2.3714220
C	-1.8543310	2.5970110	-2.3115090	H	2.1725660	-1.3316690	3.8258520
H	-2.6881560	3.1237980	-1.8187670	H	1.1426420	-0.1577920	2.9971790
H	-1.6441030	3.1147690	-3.2600750	C	-0.2185950	-3.1845320	2.7782740
H	-2.1907610	1.5756300	-2.5533700	H	0.1375380	-3.5508180	3.7536610
C	0.2473250	4.3530010	-0.9683850	H	-1.0392790	-2.4724430	2.9674720
H	0.4394000	4.8240900	-1.9452560	H	-0.6388790	-4.0410450	2.2276680
H	-0.4942560	4.9711140	-0.4397220	C	2.5538040	-3.6572810	1.6048550
H	1.1829830	4.3875640	-0.3872860	H	2.2247540	-4.5401500	1.0357960
O	3.5923520	0.6792670	0.2088110	H	3.4298020	-3.2356380	1.0874470
C	4.5616300	1.7113090	0.2961050	H	2.8860270	-4.0050070	2.5956220
C	5.2538990	1.8889990	-1.0449080	O	-3.5918310	-0.6796450	0.2084260
H	4.5227000	2.2555980	-1.7916080	C	-4.5606660	-1.7120620	0.2962170
H	6.0663050	2.6235170	-0.9630800	C	-5.2532170	-1.8902880	-1.0445750
O	5.8171370	0.6745510	-1.4725290	H	-4.5220580	-2.2567240	-1.7913950
C	4.8359770	-0.3292330	-1.5841880	H	-6.0653020	-2.6251220	-0.9624070
C	4.1529790	-0.5480210	-0.2475430	O	-5.8170700	-0.6761460	-1.4722630
H	-4.0787260	0.0399250	-2.3392800	C	-4.8363730	0.3280360	-1.5843940
H	-5.3334040	1.2473090	-1.9214260	C	-4.1530620	0.5473380	-0.2479920
H	-5.3031900	-1.4468080	1.0699050	H	-3.3256510	1.2692770	-0.3256050
H	-4.0344670	-2.6268050	0.6026240	H	-4.8842660	0.9100880	0.4972890

Table S65 Geometric coordinates and single point energies for NaHMDS tetrasolvated 1,4-dioxane dimer.



G = -3298.392461 Hartrees

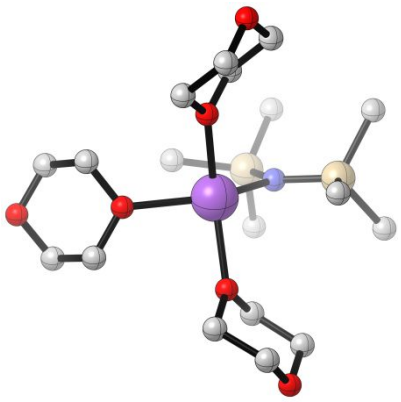
G_{SP} = -3301.000578 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	0.7553370	-2.7621160	1.2851670	H	-0.2809900	-5.0577840	1.1252730
N	-0.0005390	-1.9158720	0.0000310	H	0.4598260	-4.7888990	2.7164770
Na	-1.4480080	0.0002580	0.0000410	C	4.3077290	-0.1642070	1.7281560
Na	1.4476780	-0.0001920	-0.0001530	O	3.2200890	0.6445490	1.3126900
N	0.0005870	1.9157590	0.0001590	C	2.9345170	1.6737960	2.2510300
Si	-0.7553360	2.7604130	1.2863370	C	4.1740230	2.5145690	2.4909420
C	-0.9725800	1.6177460	2.7867180	H	4.4503700	3.0375610	1.5547840
H	-1.5453840	0.7098990	2.5352080	H	3.9852000	3.2656810	3.2694560
H	-1.5113950	2.1313420	3.5987130	O	5.2391550	1.7032130	2.9296550
H	0.0019530	1.2899690	3.1806640	C	5.5294330	0.7001670	1.9909560
C	0.1401870	4.3117980	1.9274470	H	5.8693800	1.1574940	1.0393410
H	-0.4610660	4.7860380	2.7192590	H	6.3501540	0.0917940	2.3944990
H	1.1315310	4.0942740	2.3540570	H	2.6042280	1.2171880	3.2030310
H	0.2798640	5.0564500	1.1285060	H	2.1118930	2.2622920	1.8228050
C	-2.5010540	3.3550680	0.8189060	H	4.4915180	-0.8887000	0.9228110
H	-2.4503920	4.1103590	0.0174420	H	4.0268870	-0.7129150	2.6464590
H	-3.1020480	2.5120100	0.4419300	H	-2.1148970	-2.2672240	1.8165420
H	-3.0314330	3.8024740	1.6745320	C	-2.9359330	-1.6783420	2.2472140
Si	0.7568600	2.7621880	-1.2846170	O	-3.2209740	-0.6467240	1.3112980
C	0.9741130	1.6214490	-2.7864710	C	-4.3071400	0.1626930	1.7292690

H	1.5448360	0.7121630	-2.5355140	C	-5.5297880	-0.7004930	1.9915800
H	-0.0007480	1.2959470	-3.1815700	O	-5.2399970	-1.7057410	2.9280650
H	1.5144550	2.1350440	-3.5974320	C	-4.1764500	-2.5177200	2.4867260
C	2.5024630	3.3560430	-0.8157560	H	-4.4544510	-3.0384480	1.5497760
H	3.0332290	3.8043680	-1.6706720	H	-3.9879300	-3.2706720	3.2635330
H	2.4516460	4.1104250	-0.0134420	H	-5.8712680	-1.1555170	1.0394070
H	3.1031850	2.5124410	-0.4395820	H	-6.3492850	-0.0917700	2.3970650
C	-0.1387780	4.3141390	-1.9240500	H	-4.4907330	0.8889000	0.9254080
H	-0.2786620	5.0581280	-1.1245440	H	-4.0247480	0.7094030	2.6482930
H	0.4620450	4.7891320	-2.7157320	H	-2.6036650	-1.2242510	3.1997280
H	-1.1300250	4.0960820	-2.3505630	C	-4.3080610	-0.1616660	-1.7275480
Si	-0.7553770	-2.7602010	-1.2869070	O	-3.2204280	0.6471560	-1.3121530
C	-0.9708630	-1.6176310	-2.7876140	C	-2.9353650	1.6769990	-2.2499740
H	-1.5441970	-0.7098080	-2.5372330	C	-4.1752290	2.5174080	-2.4893860
H	0.0043280	-1.2897020	-3.1798590	H	-4.4515400	3.0399970	-1.5529830
H	-1.5080680	-2.1314340	-3.6005200	H	-3.9867910	3.2688560	-3.2676690
C	0.1397990	-4.3122750	-1.9268480	O	-5.2402020	1.7059090	-2.9281330
H	0.2771660	-5.0571710	-1.1277230	C	-5.5300120	0.7025360	-1.9896340
H	-0.4609550	-4.7856920	-2.7195540	H	-5.8696960	1.1595220	-1.0377630
H	1.1321090	-4.0963490	-2.3519850	H	-6.3507780	0.0941630	-2.3930800
C	-2.5016020	-3.3545930	-0.8209550	H	-2.6047660	1.2210760	-3.2021870
H	-3.0313300	-3.8022120	-1.6768720	H	-2.1131400	2.2658160	-1.8214340
H	-2.4515350	-4.1097250	-0.0192870	H	-4.4913500	-0.8863970	-0.9223140
H	-3.1029920	-2.5115250	-0.4446380	H	-4.0275210	-0.7100500	-2.6461460
C	2.5010740	-3.3560240	0.8169050	C	4.3075950	0.1636610	-1.7275980
H	3.0317840	-3.8039700	1.6720510	O	3.2203410	-0.6456280	-1.3121470
H	2.4504960	-4.1106740	0.0148310	C	2.9352110	-1.6748140	-2.2506270
H	3.1017370	-2.5124600	0.4405190	C	4.1750450	-2.5151080	-2.4904930
C	0.9724130	-1.6212540	2.7868870	H	4.4515220	-3.0379850	-1.5542910
H	1.5447510	-0.7129550	2.5360180	H	3.9865600	-3.2663080	-3.2690010
H	-0.0022040	-1.2942400	3.1812740	O	5.2398820	-1.7033510	-2.9291480

H	1.5115670	-2.1354070	3.5982980	C	5.5296820	-0.7001380	-1.9905020
C	-0.1407530	-4.3137810	1.9246940	H	5.8698900	-1.1572610	-1.0388780
H	-1.1318710	-4.0950080	2.3511420	H	6.3500860	-0.0913660	-2.3940880
H	2.1127870	-2.2637880	-1.8226870	H	2.6048390	-1.2182250	-3.2026110
H	4.4911830	0.8881190	-0.9221850				
H	4.0263730	0.7123590	-2.6457680				

Table S66. Geometric coordinates and single point energies for NaHMDS trisolvated monomer with 3 1,4-dioxane.



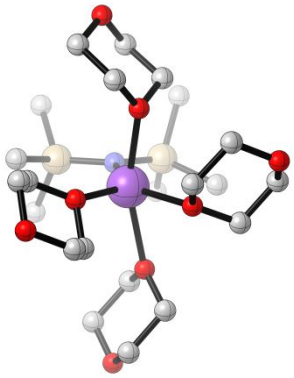
G = -1956.372468 Hartrees

$\mathbf{G_{SP}}$ = -1958.034321 Hartrees

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 S67. Geometric coordinates and single point energies for NaHMDS tetrasolvated monomer with four 1,4-dioxane.



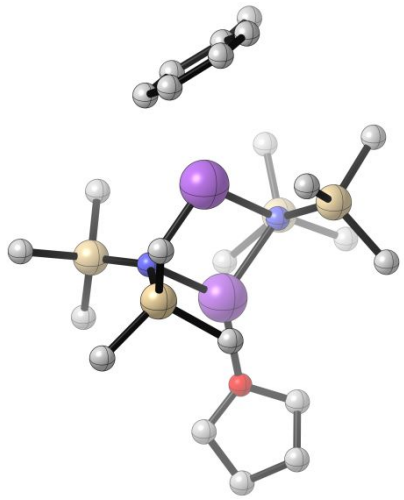
G = -2263.560388 Hartrees

$\mathbf{G_{SP}}$ = -2265.576913 Hartrees

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				

Table S68. Geometric coordinates and single point energies for NaHMDS dimer with 1 THF and 1 toluene.



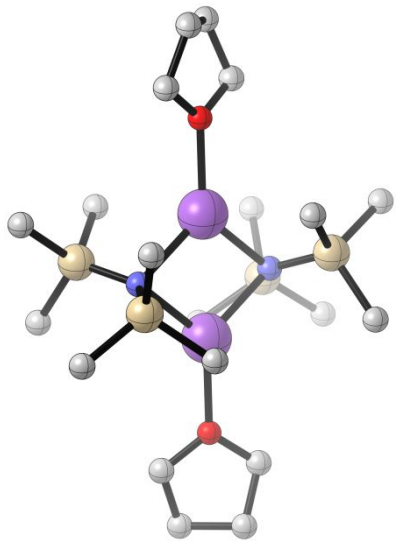
G = -2572.819764 Hartrees

$\mathbf{G_{SP}}$ = -2574.571273 Hartrees

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 S69. Geometric coordinates and single point energies for NaHMDS disolvated dimer with 2 THF



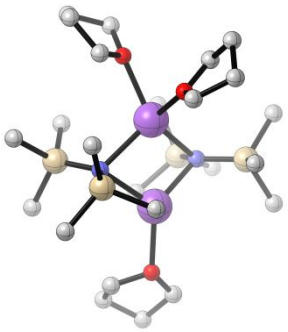
G = -2533.768605 Hartrees

$\mathbf{G_{SP}}$ = -2535.485816 Hartrees

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 S70. Geometric coordinates and single point energies for NaHMDS trisolvated dimer with 3 THF.



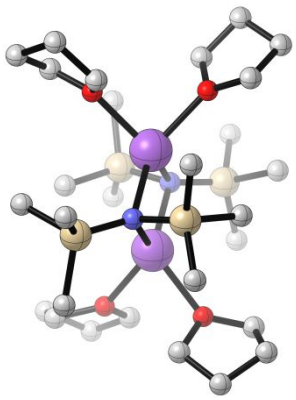
G = -2765.831427 Hartrees

$\mathbf{G_{SP}}$ = -2767.813944 Hartrees

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 S71. Geometric coordinates and single point energies for NaHMDS tetrasolvated dimer with 4 THF



G = -2997.89965 Hartrees

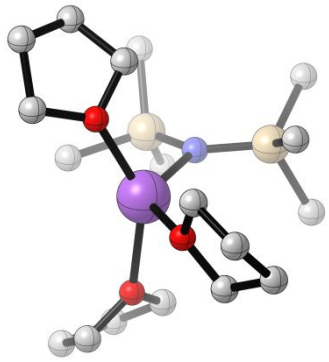
$\mathbf{G_{SP}}$ = -3000.146223 Hartrees

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 S72. Geometric coordinates and single point energies for NaHMDS trisolvated monomer with 3 THF.



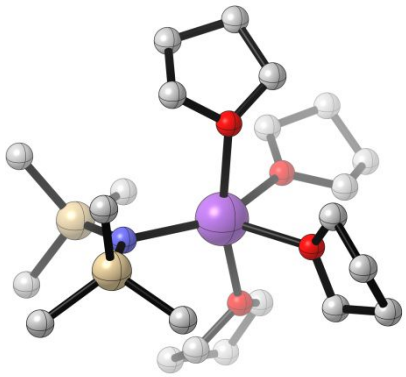
G = -1731.006704 Hartrees

$\mathbf{G_{SP}}$ = -1732.396722 Hartrees

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 S73. Geometric coordinates and single point energies for NaHMDS tetrasolvated monomer with 4 THF.



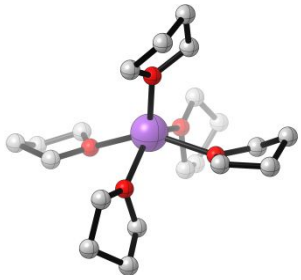
G = -1963.073823 Hartrees

G_{SP} = -1964.727222 Hartrees

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 S74. Geometric coordinates and single point energies for sodium cation with 5 THF's bound.



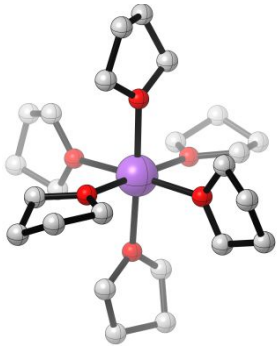
G = -1322.459668 Hartrees

G_{SP} = -1323.825501 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.1201990	0.0299590	0.3364380	H	4.3053350	0.5856310	3.1798120
O	1.5192360	0.6582040	-1.1095080	H	4.0258760	-1.4319580	1.7887400
C	2.0095210	1.9668980	-1.4066140	H	3.8005550	-2.0828510	3.4292240
H	1.6183170	2.2925000	-2.3862330	O	-2.3021520	-0.4851570	0.6390730
H	1.6383710	2.6571770	-0.6354810	C	-2.6990100	-1.8507960	0.8044480
C	3.5262880	1.8293060	-1.4510050	H	-2.9305030	-2.2785150	-0.1859850
C	3.6835060	0.4190080	-2.0205210	H	-1.8597590	-2.4158420	1.2350310
C	2.5293920	-0.3251590	-1.3527810	C	-3.9301520	-1.8166920	1.7045430
H	2.1067500	-1.1259240	-1.9770400	C	-4.5420080	-0.4634390	1.3434290
H	2.8242250	-0.7665100	-0.3838480	C	-3.2945630	0.3939750	1.1761370
H	3.5464490	0.4348490	-3.1116660	H	-3.4276120	1.2393030	0.4863900
H	4.6591320	-0.0354680	-1.8083290	H	-2.9451910	0.7891420	2.1454070
H	3.9510540	1.8870970	-0.4371740	H	-5.0890810	-0.5309200	0.3912670
H	4.0042100	2.6046120	-2.0624420	H	-5.2267760	-0.0728140	2.1061250
O	-0.1311340	-1.8863390	-0.8924960	H	-3.6306300	-1.8275560	2.7629010
C	-0.6961510	-1.5318650	-2.1599090	H	-4.6033390	-2.6652630	1.5315150
H	-1.7750490	-1.3393550	-2.0241230	O	-0.8983860	2.1393920	0.0469280
H	-0.2133460	-0.6047720	-2.5060760	C	-1.0316120	3.3940720	0.7191970
C	-0.4473750	-2.7317910	-3.0673730	H	-1.7938710	3.3019820	1.5114110
C	-0.4959460	-3.8873780	-2.0676810	H	-0.0707330	3.6475980	1.1891310

C	0.2057430	-3.2733780	-0.8620370	C	-1.4658840	4.3814950	-0.3567890
H	-0.1194550	-3.6983570	0.0987120	C	-2.3156480	3.4890740	-1.2620610
H	1.3020460	-3.3825890	-0.9385290	C	-1.5192100	2.1885460	-1.2418520
H	-1.5390610	-4.1331750	-1.8177740	H	-2.1380920	1.2857590	-1.3650980
H	-0.0053050	-4.8010570	-2.4248960	H	-0.7343910	2.1829070	-2.0173070
H	0.5509960	-2.6662480	-3.5261630	H	-3.3127410	3.3384320	-0.8206240
H	-1.1872710	-2.8141040	-3.8728810	H	-2.4490670	3.8873140	-2.2752590
O	1.4232490	-0.3793150	1.9111000	H	-0.5899790	4.7584450	-0.9062010
C	1.9408120	-1.6377200	2.3524800	H	-2.0107470	5.2417190	0.0509540
H	1.3757260	-1.9722840	3.2378500				
H	1.8021690	-2.3742720	1.5475590				
C	3.4021180	-1.3729110	2.6941100				
C	3.3390920	0.0669820	3.2044780				
C	2.3153050	0.6837870	2.2575340				
H	1.7372900	1.5014750	2.7111750				
H	2.7891790	1.0593170	1.3336300				
H	2.9647050	0.0886650	4.2383070				

Table S75. Geometric coordinates and single point energies for sodium cation with 6 THF's bound.



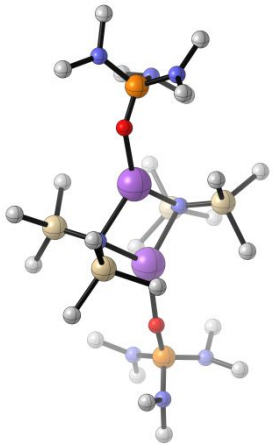
G = -1554.536592 Hartrees

G_{SP} = -1556.165596 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.0455590	0.0002590	-0.0013920	O	-1.2573120	-1.7887500	-0.4826960
O	1.3007950	1.8457170	0.3907730	C	-1.1469920	-3.0451750	0.1806870
C	2.4165340	1.9036730	1.2769300	H	-0.4161460	-3.6820520	-0.3501520
H	2.0557450	2.0735690	2.3071920	H	-0.7702600	-2.8645390	1.1978260
H	2.9367860	0.9342740	1.2483220	C	-2.5434330	-3.6479500	0.1142730
C	3.2564090	3.0791540	0.7912920	C	-3.0029100	-3.1693820	-1.2639550
C	2.1712960	4.0291210	0.2834740	C	-2.4093870	-1.7617820	-1.3229480
C	1.1885010	3.0554730	-0.3602640	H	-2.1118580	-1.4608650	-2.3398390
H	0.1428210	3.3957990	-0.3339440	H	-3.1129290	-1.0037590	-0.9375850
H	1.4543510	2.8498990	-1.4115580	H	-2.5632450	-3.8033980	-2.0481920
H	1.6972480	4.5493810	1.1293290	H	-4.0921170	-3.1756110	-1.3935450
H	2.5406480	4.7861930	-0.4191810	H	-3.1811060	-3.2192940	0.9028300
H	3.9103750	2.7671840	-0.0375640	H	-2.5461500	-4.7394080	0.2241990
H	3.8856270	3.5090890	1.5803200	O	1.3204520	-1.2412050	1.4032670
O	-1.2787740	1.2894300	-1.3070800	C	1.2028760	-1.2031150	2.8261900
C	-2.4380770	1.9907010	-0.8618460	H	1.4462780	-0.1854310	3.1770500
H	-3.1384370	1.2685660	-0.4078960	H	0.1606870	-1.4189010	3.1038560
H	-2.1491400	2.7161430	-0.0849480	C	2.2050150	-2.2289970	3.3475610
C	-3.0315500	2.6493800	-2.1071530	C	3.2907190	-2.1719330	2.2725460

C	-2.5632210	1.7058290	-3.2161540	C	2.4494640	-2.0187370	1.0111020
C	-1.1658500	1.3519250	-2.7264780	H	2.9616220	-1.4995760	0.1869620
H	-0.7831320	0.3849880	-3.0837660	H	2.1062600	-3.0019360	0.6422290
H	-0.4388330	2.1358330	-3.0064140	H	3.9278890	-1.2860890	2.4185330
H	-3.1952470	0.8048900	-3.2472680	H	3.9367180	-3.0582120	2.2499280
H	-2.5660990	2.1634770	-4.2131120	H	1.7499930	-3.2305450	3.3734860
H	-2.5970320	3.6491740	-2.2552610	H	2.5683900	-1.9930920	4.3553370
H	-4.1215420	2.7583600	-2.0501000	O	1.3294020	-0.5745660	-1.7811120
O	-1.2840250	0.4661640	1.7738190	C	1.2287770	-1.8296860	-2.4552760
C	-1.1917130	1.6667330	2.5358470	H	1.4777490	-2.6372590	-1.7454900
H	-0.4752120	1.5252930	3.3654470	H	0.1897560	-1.9756980	-2.7853420
H	-0.8061520	2.4606140	1.8798630	C	2.2353550	-1.7614220	-3.6001780
C	-2.5987210	1.9034770	3.0667710	C	3.3085050	-0.8446590	-3.0119010
C	-3.0571730	0.4681580	3.3298850	C	2.4526380	0.1644220	-2.2555870
C	-2.4385670	-0.2819950	2.1498830	H	2.9554790	0.6272520	-1.3929500
H	-2.1397550	-1.3118820	2.4017580	H	2.1034390	0.9695940	-2.9266830
H	-3.1268500	-0.3299920	1.2885690	H	3.9492150	-1.4045350	-2.3133000
H	-2.6335250	0.1058010	4.2783110	H	3.9524150	-0.3772340	-3.7670230
H	-4.1470170	0.3541500	3.3798100	H	1.7789860	-1.2913550	-4.4842480
H	-3.2244720	2.3720550	2.2914480	H	2.6108770	-2.7491720	-3.8945800
H	-2.6195040	2.5418130	3.9586520				

Table S76. Geometric coordinates and single point energies for NaHMDS disolvated HMPA dimer.



G = -3708.476029 Hartrees

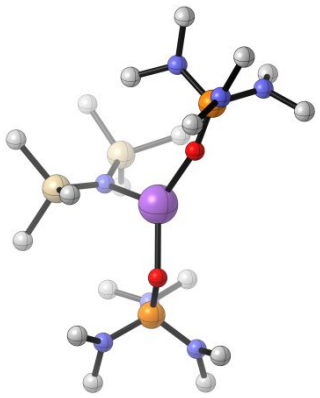
G_{SP} = -3711.050065 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.5664420	0.4046260	-0.0754600	H	1.9687200	3.7063750	2.0476130
N	0.0794330	2.0635710	-0.0229720	H	0.9515430	3.6187890	3.5104620
Na	1.3683670	0.1372210	-0.1452490	H	1.6986510	2.1427120	2.8544820
N	-0.2803510	-1.5687600	0.0969770	Si	0.5672310	2.8924880	-1.4341090
Si	-0.5191320	-2.3430870	-1.4036640	C	1.2547620	1.6462450	-2.7000100
C	-1.2035670	-4.1142020	-1.3280980	H	2.1850360	1.1698690	-2.3473040
H	-1.5405440	-4.4477580	-2.3225330	H	1.4847900	2.1457500	-3.6541780
H	-0.4286990	-4.8171480	-0.9865660	H	0.5238760	0.8499880	-2.9203460
H	-2.0548480	-4.1966660	-0.6342600	C	-0.8448430	3.8040360	-2.3123970
C	-1.7527430	-1.3360910	-2.4498560	H	-0.5125170	4.2667060	-3.2551090
H	-2.7411100	-1.2780260	-1.9640080	H	-1.6616140	3.1008430	-2.5436370
H	-1.4076230	-0.3023120	-2.6264130	H	-1.2609720	4.5957980	-1.6710490
H	-1.8952450	-1.7960590	-3.4403680	C	1.9623950	4.1463190	-1.1326060
C	1.0825420	-2.4662680	-2.4234490	H	1.6419460	4.9452810	-0.4447870
H	1.5477570	-1.4783930	-2.5781240	H	2.8222350	3.6342660	-0.6702390
H	1.8108680	-3.0997620	-1.8900070	H	2.3040570	4.6221750	-2.0655550
H	0.9114110	-2.9139230	-3.4153540	O	-3.7033190	0.7862920	-0.3032940

Si	0.2491720	-2.2584220	1.5629730	P	-4.9565970	-0.0192950	-0.1016750
C	1.5948160	-1.1519250	2.3483620	N	-6.1138480	0.9425730	0.6197980
H	2.5119540	-1.1025530	1.7355090	C	-7.4661070	0.4631400	0.8125190
H	1.2267980	-0.1206210	2.4926790	H	-7.4818290	-0.6348190	0.8369750
H	1.8898490	-1.5291910	3.3402800	H	-7.8598460	0.8254920	1.7763390
C	-1.0955170	-2.4230540	2.8930450	H	-8.1494260	0.8093010	0.0155170
H	-1.8942870	-3.1047950	2.5599260	C	-5.9328240	2.3785240	0.7348170
H	-0.6749190	-2.8316390	3.8257810	H	-6.5608680	2.9248920	0.0091690
H	-1.5545730	-1.4508130	3.1308610	H	-6.2103040	2.7132300	1.7478080
C	0.9989660	-4.0013130	1.4200330	H	-4.8824210	2.6316810	0.5526380
H	1.5777180	-4.2574840	2.3220520	N	-5.4543000	-0.6744580	-1.5573850
H	0.2044790	-4.7557210	1.3100760	C	-5.1554230	0.0367300	-2.7893700
H	1.6645020	-4.0957770	0.5475540	H	-6.0402180	0.5761860	-3.1723660
O	3.5091180	0.2468120	-0.4827130	H	-4.3444200	0.7534010	-2.6147130
P	4.8979120	-0.2094040	-0.1372430	H	-4.8243810	-0.6777310	-3.5600330
N	5.9981850	0.6384310	-1.0641540	C	-6.4884960	-1.6828210	-1.6743370
C	7.4170730	0.5203010	-0.7980630	H	-7.4628950	-1.2465150	-1.9603150
H	7.6422180	-0.4608280	-0.3581940	H	-6.2062480	-2.4137970	-2.4499820
H	7.9825110	0.6038530	-1.7400670	H	-6.6067650	-2.2200850	-0.7251980
H	7.7814390	1.3073510	-0.1122150	N	-4.8753710	-1.3648590	0.8909880
C	5.5965610	1.8330740	-1.7873100	C	-4.0262520	-2.4662350	0.4385610
H	5.8816090	2.7531320	-1.2465570	H	-4.2867030	-3.3746570	1.0030760
H	6.0835950	1.8512680	-2.7754490	H	-4.1863240	-2.6640150	-0.6288730
H	4.5100780	1.8334810	-1.9276320	H	-2.9513850	-2.2545340	0.5962330
N	5.1618820	-0.0535930	1.5059780	C	-4.7865500	-1.1471480	2.3309410
C	4.4848890	1.0095980	2.2318180	H	-5.4586130	-0.3367530	2.6358130
H	5.1796590	1.8291300	2.4874090	H	-5.0837990	-2.0694750	2.8518250
H	3.6661630	1.4180920	1.6270350	H	-3.7595800	-0.8920100	2.6460180
H	4.0550410	0.6140020	3.1665600	H	6.1699810	-3.1465320	-1.7724570
C	6.2798800	-0.6480310	2.2109490	H	4.5935560	-2.4959980	-2.3073020
H	7.0728080	0.0916690	2.4233610	Si	-0.2925350	2.8020930	1.4683900

H	5.9355350	-1.0578930	3.1751730	C	-1.4649560	1.6637600	2.4553520
H	6.7113090	-1.4679410	1.6237380	H	-2.4557880	1.5952580	1.9723110
N	5.2934530	-1.8122590	-0.4158770	H	-1.0479490	0.6456930	2.5445070
C	4.5920660	-2.8186440	0.3739370	H	-1.6259650	2.0396180	3.4773680
H	5.1758350	-3.7514410	0.3760470	C	-1.1915370	4.4678580	1.3296880
H	4.4676140	-2.4822040	1.4105430	H	-1.4395710	4.8757630	2.3223510
H	3.5911720	-3.0346830	-0.0399990	H	-0.5764320	5.2153610	0.8036260
C	5.5349670	-2.2478420	-1.7859220	H	-2.1284580	4.3484510	0.7626510
H	6.0490710	-1.4607320	-2.3487870	C	1.2206640	3.0963600	2.5788130

Table S77. Geometric coordinates and single point energies for NaHMDS disolvated HMPA monomer.



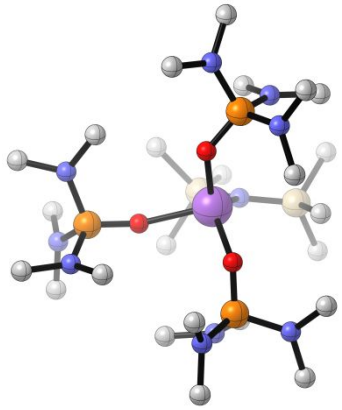
G = -2673.639552 Hartrees

G_{SP} = -2675.621637 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	0.7159340	2.3287170	-1.5443030	H	3.0638500	-4.6861030	0.9571380
N	0.4156400	1.8645770	0.0524560	H	2.4421850	-3.7983080	-0.4604650
Si	-0.1397610	2.6338400	1.4489300	N	4.3499940	-0.7552390	-1.1507200
C	1.2195900	3.1517460	2.6811830	C	3.9930150	-0.7937390	-2.5567680
H	0.7843960	3.6952390	3.5354040	H	4.4513060	-1.6595980	-3.0684600
H	1.7797200	2.2929360	3.0820450	H	2.9041310	-0.8576700	-2.6563740
H	1.9451660	3.8207000	2.1902620	H	4.3371110	0.1265250	-3.0556190
C	-1.2822800	1.4506350	2.4187640	C	5.7681470	-0.6641310	-0.8747510
H	-0.7533370	0.5197820	2.6894530	H	6.3189570	-1.5540790	-1.2317930
H	-1.6588350	1.8992930	3.3520180	H	6.1918070	0.2218740	-1.3753890
H	-2.1484710	1.1676730	1.7982740	H	5.9431880	-0.5546480	0.2041160
C	-1.1319350	4.2358710	1.1819920	N	3.4806510	-0.1964880	1.2744010
H	-0.4715930	5.0416000	0.8241600	C	3.7171050	1.2261020	1.0255690
H	-1.9310240	4.1130110	0.4358380	H	4.1626160	1.6640260	1.9324990
H	-1.5894420	4.5749000	2.1254540	H	4.4177480	1.3587950	0.1935430
Na	0.0602480	-0.3747380	-0.1584380	H	2.7758150	1.7506010	0.7895470
O	-1.9885610	-1.0710050	-0.2315900	C	2.6797080	-0.4353170	2.4685010

P	-3.4820850	-1.0394450	-0.0978040	H	2.5094570	-1.5113270	2.6047280
N	-4.0433910	0.5320070	-0.1781630	H	3.2088920	-0.0476850	3.3533770
C	-5.4694010	0.7884680	-0.2367360	H	1.7045760	0.0800380	2.4034560
H	-6.0234540	0.0097980	0.3046850	C	2.5507760	2.6356090	-1.9399720
H	-5.6896750	1.7557560	0.2415520	H	3.1334260	1.7225230	-1.7371760
H	-5.8451260	0.8307470	-1.2759160	H	2.6987060	2.9117310	-2.9965000
C	-3.2157270	1.5809920	-0.7576690	H	2.9635320	3.4422080	-1.3128060
H	-3.3773640	1.6827800	-1.8468080	C	0.2050510	0.9179640	-2.7337070
H	-3.4737440	2.5394260	-0.2816120	H	0.3850750	1.1967470	-3.7839180
H	-2.1503260	1.3916210	-0.5686230	H	0.7802720	-0.0046710	-2.5424780
N	-4.1528600	-2.0446010	-1.2610200	H	-0.8675770	0.6793050	-2.6335020
C	-3.4346000	-2.2804520	-2.5012430	C	-0.2272250	3.8617780	-2.1534150
H	-3.8492230	-1.6847690	-3.3341930	H	-1.3149240	3.7305460	-2.0357660
H	-2.3774670	-2.0235350	-2.3717780	H	0.0597820	4.7598100	-1.5851480
H	-3.5054830	-3.3453650	-2.7768580	H	-0.0211630	4.0541980	-3.2185220
C	-5.5565750	-2.3995150	-1.3003300	H	-3.3805960	-0.9015810	3.1422200
H	-6.1194970	-1.7959200	-2.0353480	O	1.9203810	-1.4792180	-0.5727320
H	-5.6648840	-3.4597100	-1.5851340	P	3.2875520	-1.2809060	0.0250810
H	-6.0131630	-2.2648770	-0.3119520	N	3.7745650	-2.7223940	0.7385190
N	-4.1803340	-1.6212510	1.3062310	C	4.9201170	-2.8385590	1.6168240
C	-4.0648430	-3.0417970	1.5987050	H	5.1478860	-1.8672810	2.0726720
H	-4.9726370	-3.3916640	2.1159470	H	4.6971250	-3.5542470	2.4257620
H	-3.9477030	-3.6128500	0.6699550	H	5.8195390	-3.2027790	1.0862040
H	-3.1966140	-3.2500960	2.2478270	C	3.3296220	-3.9753050	0.1575480
C	-4.2739880	-0.7971200	2.5023770	H	4.1153740	-4.4429300	-0.4639900
H	-4.3763580	0.2597400	2.2333440				
H	-5.1568790	-1.1045170	3.0849670				

Table S78. Geometric coordinates and single point energies for NaHMDS trisolvated HMPA monomer.



G = -3493.059983 Hartrees

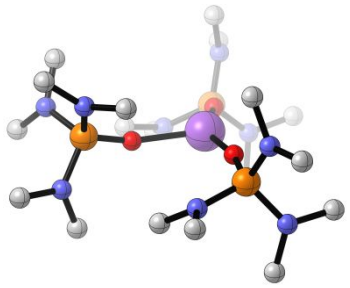
G_{SP} = -3495.731653 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	-1.7636420	-1.4221760	2.9051490	H	3.2441910	2.9330130	2.6825800
N	-0.7323880	-0.1655500	2.4585580	C	4.8411490	1.6533750	0.9733160
Si	0.1309330	0.9508520	3.3897880	H	5.0230130	0.9646790	0.1397630
C	0.0031520	2.7160070	2.6848410	H	5.7536290	2.2474170	1.1463170
H	0.6181050	3.4323880	3.2542840	H	4.6354640	1.0639190	1.8842220
H	0.3373690	2.7220260	1.6341640	O	-1.5779610	0.9244320	-1.3802620
H	-1.0395120	3.0710210	2.7156850	P	-3.0751780	1.0062780	-1.4254580
C	1.9987350	0.5661170	3.4432930	N	-3.5637040	2.4678450	-2.0798080
H	2.3973260	0.6410610	2.4170740	C	-4.7766730	3.1720070	-1.7333030
H	2.5540380	1.2600540	4.0963280	H	-5.2635670	2.6888890	-0.8768680
H	2.1770530	-0.4575740	3.8100540	H	-4.5531820	4.2172650	-1.4587840
C	-0.4368100	1.0853560	5.2020740	H	-5.4922060	3.1945370	-2.5767030
H	-1.4919370	1.3987870	5.2527880	C	-2.8361600	2.9986760	-3.2144480
H	-0.3530140	0.1156540	5.7187880	H	-3.4195880	2.9181240	-4.1500420
H	0.1620900	1.8197040	5.7644900	H	-2.5992640	4.0636340	-3.0513210
Na	-0.3315080	-0.0845210	0.1783880	H	-1.8918910	2.4524100	-3.3316190
O	0.1610190	-1.8150260	-1.2164940	N	-3.6994570	-0.2175150	-2.3727470

P	1.2081800	-2.8625940	-0.9640370	C	-3.0320270	-1.5052540	-2.4451000
N	0.4697280	-4.3336590	-0.6488980	H	-2.9709100	-1.8316500	-3.4971810
C	1.1892650	-5.5041080	-0.1909960	H	-2.0092400	-1.4261810	-2.0491390
H	2.1578610	-5.2136870	0.2342050	H	-3.5788970	-2.2816350	-1.8774460
H	0.6097010	-6.0151740	0.5960380	C	-5.0065630	-0.1488760	-2.9837800
H	1.3622410	-6.2294120	-1.0071530	H	-4.9455310	-0.4310710	-4.0484690
C	-0.8597390	-4.6000650	-1.1660470	H	-5.7317020	-0.8279020	-2.4979210
H	-0.8278430	-5.2572570	-2.0546150	H	-5.4042980	0.8729030	-2.9276390
H	-1.4705220	-5.0938030	-0.3928280	N	-3.8197010	0.9445340	0.0563210
H	-1.3461270	-3.6542370	-1.4301390	C	-4.8272540	-0.0141580	0.4595070
N	2.2399600	-2.9333190	-2.2911920	H	-5.7895180	0.4854720	0.6761670
C	1.7338460	-2.5223870	-3.5875960	H	-4.9876190	-0.7563440	-0.3322880
H	1.3241960	-3.3746910	-4.1622880	H	-4.5074320	-0.5524840	1.3647090
H	0.9438710	-1.7743740	-3.4519810	C	-3.3454300	1.8529260	1.0953540
H	2.5490970	-2.0773720	-4.1814450	H	-2.7256240	2.6419980	0.6451790
C	3.3025460	-3.9160920	-2.3441680	H	-4.2029450	2.3321190	1.5981990
H	2.9766730	-4.8638970	-2.8132030	H	-2.7221320	1.3197590	1.8335950
H	4.1456970	-3.5212930	-2.9347210	C	-3.3463780	-0.8919450	3.8353720
H	3.6694950	-4.1338460	-1.3325590	H	-3.8182830	0.0045770	3.4060240
N	2.2557820	-2.6901540	0.3202820	H	-4.0977800	-1.6984950	3.8645930
C	3.3463750	-1.7226680	0.2461860	H	-3.0826740	-0.6482780	4.8772870
H	4.1508880	-2.0411420	0.9277790	C	-2.2742900	-2.3497860	1.3173100
H	3.7456310	-1.6720740	-0.7742630	H	-3.0634550	-3.1024790	1.4764010
H	3.0059680	-0.7159070	0.5403010	H	-2.6234040	-1.6420660	0.5447800
C	1.6872880	-2.7917970	1.6664020	H	-1.3886350	-2.8619370	0.9050020
H	0.9190570	-3.5743290	1.6938050	C	-1.0381100	-2.7494590	4.0677680
H	2.4875310	-3.0630500	2.3725370	H	-0.1359300	-3.2252480	3.6554720
H	1.2246490	-1.8429580	1.9963360	H	-0.7587650	-2.2934430	5.0311920
O	1.5176300	1.0845420	-0.0246840	H	-1.7745130	-3.5427150	4.2772000
P	2.5508690	2.0872220	-0.4305520	H	2.5499720	5.0195260	-2.1613650
N	3.4621230	1.4387740	-1.6876290	H	2.1376640	5.6003460	-0.5263810

C	4.4973310	2.2228190	-2.3284500	H	3.6194030	4.6463070	-0.7775830
H	4.9867790	2.8803980	-1.5976070	N	3.7327440	2.5418040	0.6602270
H	5.2639230	1.5518960	-2.7485260	C	3.4221160	3.4714070	1.7376930
H	4.1046260	2.8452040	-3.1550350	H	4.2632770	4.1699550	1.8814170
C	2.8503250	0.4372480	-2.5443840	H	2.5184660	4.0452440	1.5026670
H	2.4145430	0.8863660	-3.4569830	H	-0.0769420	2.6471020	-0.9854370
H	3.6110540	-0.2986180	-2.8564620	H	-0.0802840	4.3681970	-0.4991150
H	2.0566480	-0.0914750	-2.0008460	C	2.5729730	4.7559300	-1.0885990
N	1.8297090	3.5432250	-0.8212900				
C	0.4131890	3.6167890	-1.1395910				
H	0.2682100	3.9149700	-2.1933310				

Table S79. Geometric coordinates and single point energies for sodium cation solvated by 3 HMPA molecules.



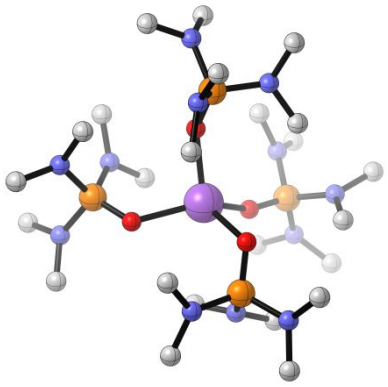
G = -2620.387829 Hartrees

G_{SP} = -2622.510303 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.2493170	-0.7882380	0.3399500	P	3.8096600	-1.1970790	0.0843670
O	-1.7719650	-1.5157450	0.3672720	N	4.1820980	0.1139440	-0.8881150
P	-3.2147330	-1.8297560	0.0616690	C	5.5074130	0.2940910	-1.4555420
N	-4.0372710	-2.2551680	1.4407070	H	6.0060820	-0.6743700	-1.5852220
C	-5.2401020	-3.0673260	1.4865400	H	5.4230290	0.7685130	-2.4462470
H	-5.4610160	-3.4776550	0.4945010	H	6.1455990	0.9387340	-0.8249340
H	-5.1078130	-3.9047010	2.1913680	C	3.4129760	1.3422440	-0.7809390
H	-6.1076660	-2.4756010	1.8270530	H	3.9209500	2.0825140	-0.1344390
C	-3.6888600	-1.6122190	2.6960900	H	3.3032570	1.7922860	-1.7815720
H	-4.4458860	-0.8658170	2.9942340	H	2.4099230	1.1448420	-0.3817620
H	-3.6173660	-2.3662480	3.4956000	N	4.7280530	-1.2942810	1.4739450
H	-2.7141820	-1.1195180	2.6030380	C	4.1719480	-0.9317350	2.7657480
N	-3.9259610	-0.4949130	-0.6447740	H	4.5091180	0.0691880	3.0883000
C	-3.1617170	0.4334150	-1.4573500	H	3.0785250	-0.9393350	2.7123590
H	-3.4461950	1.4711560	-1.2130430	H	4.4935400	-1.6596730	3.5274530
H	-2.0899570	0.3279220	-1.2452400	C	6.1780640	-1.3505530	1.4304950
H	-3.3378120	0.2773930	-2.5380600	H	6.6364660	-0.3615870	1.6076230
C	-5.3665170	-0.3833670	-0.7643050	H	6.5475720	-2.0384490	2.2079290
H	-5.6783730	0.6511670	-0.5499490	H	6.5195740	-1.7272380	0.4579230

H	-5.7258070	-0.6425640	-1.7769410	N	4.3573370	-2.4835060	-0.8223100
H	-5.8660570	-1.0409330	-0.0422740	C	4.6060920	-3.7802500	-0.2087410
N	-3.4932080	-3.1269410	-0.9521290	H	5.4932490	-4.2441130	-0.6674720
C	-3.5810550	-2.9529480	-2.3917920	H	4.7842040	-3.6674250	0.8662710
H	-4.2174100	-3.7439480	-2.8161910	H	3.7500500	-4.4613250	-0.3520620
H	-4.0356050	-1.9856270	-2.6363630	C	4.0623510	-2.5681620	-2.2451400
H	-2.5923960	-3.0123790	-2.8811100	H	3.8397190	-1.5741550	-2.6491740
C	-2.9984850	-4.4333320	-0.5402310	H	4.9303540	-2.9813150	-2.7826680
H	-2.9296930	-4.4828340	0.5541090	H	3.1981100	-3.2275650	-2.4354860
H	-3.6889400	-5.2200660	-0.8814340	H	-2.4921710	1.6011960	2.6698320
H	-1.9992470	-4.6407700	-0.9604570	C	-1.9519500	4.1152690	1.9326830
O	-0.0348950	1.3064850	-0.1114160	H	-2.9879140	4.4320130	1.7204690
P	-0.5209500	2.7276060	0.0134250	H	-1.8598860	3.9792550	3.0231970
N	-1.1799100	3.2040850	-1.4411640	H	-1.2684930	4.9147740	1.6237310
C	-1.9932230	4.3977170	-1.5570260	N	0.6250150	3.8758360	0.4125450
H	-2.3360910	4.7300110	-0.5694330	C	1.3117830	3.7587810	1.6900100
H	-1.4448190	5.2313780	-2.0315820	H	1.5057150	4.7598930	2.1058770
H	-2.8844100	4.1873230	-2.1702410	H	0.6909270	3.2022250	2.4038100
C	-0.7755960	2.5985550	-2.6960020	H	2.2767640	3.2330590	1.5852290
H	-1.6645440	2.3127930	-3.2824060	C	1.3753440	4.5969190	-0.6006110
H	-0.1754720	3.2939720	-3.3102680	H	0.7971480	4.6698350	-1.5292130
H	-0.1826670	1.6983350	-2.4963650	H	1.5867770	5.6180130	-0.2475670
N	-1.6302460	2.8780360	1.2442380	H	2.3401220	4.1090900	-0.8257550
C	-2.4941950	1.7582080	1.5783210	O	2.3529010	-1.1398980	0.4619300
H	-3.5376160	1.9393310	1.2635480				
H	-2.1387010	0.8398360	1.0939850				

Table S80. Geometric coordinates and single point energies for sodium cation solvated by 4 HMPA molecules.



G = -3439.817587 Hartrees

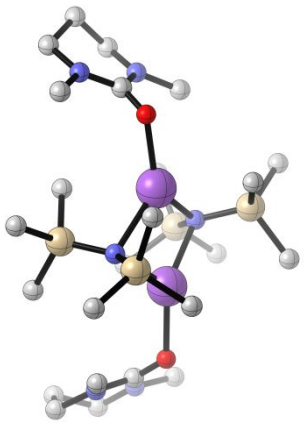
G_{SP} = -3442.626722 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.0631850	-0.3487530	0.0856390	H	0.5678010	-3.0268830	-0.8068320
O	1.6354010	0.5101470	-0.9815750	H	1.5855720	-1.9005610	-1.7470920
P	2.6520390	1.5418740	-1.3833220	C	3.7726720	-2.0884680	-0.3148200
N	1.9368440	2.8222380	-2.1747480	H	4.3630210	-1.8960630	0.5884790
C	2.5819180	3.6483320	-3.1770890	H	4.3067520	-2.8273520	-0.9352870
H	3.5445770	3.2134120	-3.4710080	H	3.6790860	-1.1508490	-0.8899130
H	1.9457700	3.7270330	-4.0740110	O	-1.5838490	-1.8951700	-0.3648600
H	2.7591020	4.6723820	-2.8023480	P	-2.6795380	-1.6737300	-1.3824520
C	0.6856380	3.3553770	-1.6620560	N	-2.6786030	-2.9340270	-2.4690040
H	0.8438590	4.2997930	-1.1078350	C	-3.3741570	-2.8636000	-3.7390420
H	0.0001540	3.5643790	-2.4999570	H	-3.6419340	-1.8237280	-3.9638510
H	0.1940960	2.6305950	-0.9987620	H	-2.7231650	-3.2350920	-4.5466250
N	3.4619880	2.1026810	-0.0398780	H	-4.2945980	-3.4748530	-3.7402140
C	3.6523040	1.2596280	1.1284080	C	-2.2069980	-4.2520660	-2.0856380
H	3.4817800	1.8547140	2.0407090	H	-3.0397740	-4.9722900	-1.9959650
H	2.9278050	0.4331500	1.1219750	H	-1.5042610	-4.6384230	-2.8416790
H	4.6783960	0.8503030	1.1811110	H	-1.6859120	-4.1888130	-1.1227090

C	4.2060600	3.3456350	-0.0480250	N	-4.2188830	-1.5396100	-0.7424900
H	3.9528900	3.9445940	0.8425500	C	-4.4084270	-0.5884750	0.3411470
H	5.2981060	3.1785470	-0.0396330	H	-4.3535080	-1.0819640	1.3278580
H	3.9568090	3.9390840	-0.9370480	H	-3.6303120	0.1879150	0.3071980
N	3.7921460	0.9916050	-2.4691210	H	-5.3942070	-0.1028610	0.2511000
C	5.1995240	0.8059010	-2.1797920	C	-5.1315740	-2.6688650	-0.7103850
H	5.8245570	1.3271730	-2.9241940	H	-5.0097220	-3.2760150	0.2047860
H	5.4439130	1.1992730	-1.1860620	H	-6.1687700	-2.3015460	-0.7382200
H	5.4701290	-0.2641080	-2.2012500	H	-4.9788530	-3.3157340	-1.5819600
C	3.3279150	0.3835320	-3.7037660	N	-2.4879660	-0.2858950	-2.2828910
H	2.2629350	0.6049370	-3.8571190	C	-3.4113660	0.8300400	-2.3358670
H	3.8901990	0.7784500	-4.5658240	H	-3.4103090	1.2558460	-3.3521810
H	3.4548020	-0.7132270	-3.6806080	H	-4.4294510	0.4922710	-2.1096750
O	1.0832200	-1.0695570	1.8427660	H	-3.1153170	1.6192440	-1.6207590
P	1.7835170	-2.3728240	1.5471160	C	-1.1496330	0.0111720	-2.7672710
N	3.0976430	-2.5254190	2.5711750	H	-0.5171580	-0.8865810	-2.7149880
C	3.8336890	-3.7758490	2.6154080	H	-1.1934650	0.3303200	-3.8215470
H	3.8695010	-4.2348920	1.6181050	H	-0.6698490	0.8090680	-2.1760740
H	4.8692980	-3.5836300	2.9351560	O	-1.4185560	1.3680220	0.2289400
H	3.3869750	-4.5001240	3.3209250	P	-1.8698700	2.3059740	1.3171800
C	3.1465930	-1.7490410	3.7995120	N	-2.4687550	1.4120610	2.6016740
H	2.7521530	-2.3158670	4.6618770	C	-2.7500350	2.1057240	3.8491230
H	4.1901850	-1.4757220	4.0212450	H	-3.1383210	3.1132790	3.6467550
H	2.5546140	-0.8352820	3.6781050	H	-3.5164190	1.5546600	4.4145240
N	0.6903310	-3.6278910	1.6502910	H	-1.8528430	2.1965390	4.4885160
C	-0.5865530	-3.4539620	2.3227750	C	-1.9932840	0.0420430	2.7726740
H	-0.6912790	-4.1753220	3.1500670	H	-0.9744800	-0.0071840	3.1985510
H	-0.6545830	-2.4368590	2.7236050	H	-2.6813630	-0.4843160	3.4515760
H	-1.4153550	-3.5921320	1.6089890	H	-1.9925520	-0.4914100	1.8129470
C	0.9347220	-4.9662590	1.1523310	N	-0.6089380	3.3195260	1.7527210
H	0.9740250	-5.7009920	1.9745290	C	0.7383140	2.7716050	1.7960930

H	0.1258690	-5.2715050	0.4655260	H	1.0210790	2.4630850	2.8190070
H	1.8811420	-5.0079310	0.5999530	H	0.8312560	1.9035190	1.1310650
N	2.4586360	-2.5979620	0.0366210	H	1.4608320	3.5302510	1.4515700
C	1.5982100	-2.8097740	-1.1203750	C	-0.7826050	4.5178500	2.5561430
H	1.9723480	-3.6510610	-1.7278230	H	-0.5248460	4.3432970	3.6155380
C	-2.8381330	4.4355830	-0.0075210	H	-0.1245900	5.3167410	2.1768540
H	-3.3736960	5.3506580	0.2899000	H	-1.8190480	4.8715090	2.5025810
H	-1.7649690	4.6582800	-0.0516800	N	-3.0966750	3.3748510	0.9573040
H	-3.1791430	4.1501410	-1.0181030				
C	-4.4979710	2.9896230	1.0340020				
H	-4.6353270	2.1949810	1.7758640				
H	-5.1012670	3.8610070	1.3316740				
H	-4.8729870	2.6308580	0.0586620				

Table S81. Geometric coordinates and single point energies for NaHMDS disolvated DMPU dimer.



G = -2909.549901 Hartrees

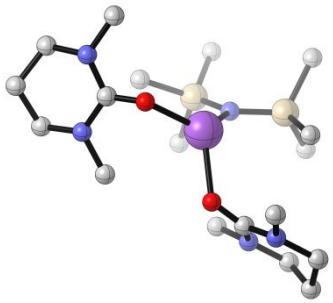
G_{SP} = -2911.682836 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.4607820	-0.0881610	0.8339100	C	5.2543000	-1.6807570	-1.6525160
Na	1.4775260	0.3319650	0.9096860	N	4.5595620	-1.1951310	-0.4725040
N	0.2763570	-1.6762770	0.7213570	C	4.0515840	-2.1515030	0.4982390
Si	0.4383010	-2.4175920	2.2488360	H	4.4675120	-1.9561400	1.4971530
C	1.4723710	-1.2725810	3.3671900	H	2.9526050	-2.1105670	0.5629970
H	2.4815670	-1.1032890	2.9545890	H	4.3493100	-3.1578930	0.1795710
H	0.9903690	-0.2874910	3.4981780	H	6.3048910	-1.9295280	-1.4131700
H	1.5973320	-1.6953370	4.3757360	H	4.7608400	-2.6073290	-1.9805380
C	1.2865400	-4.1151310	2.2589290	H	4.1547060	-0.5468560	-3.1095660
H	1.4960560	-4.4431390	3.2892820	H	5.8149350	-0.9572700	-3.6068610
H	0.6399590	-4.8741700	1.7925600	H	6.7497410	0.6646380	-1.9967730
H	2.2393510	-4.1018280	1.7070590	H	5.5130820	1.4846430	-2.9707560
C	-1.2300630	-2.6710250	3.1194120	C	4.7858600	2.4633640	-0.7334520
H	-1.8516630	-3.3713890	2.5381550	H	4.2806940	2.5811660	0.2299320
H	-1.1080590	-3.0892910	4.1310060	H	5.7837860	2.9266240	-0.6765850
H	-1.7986240	-1.7311460	3.2157720	H	4.1999720	2.9816130	-1.5104210
Si	0.0332980	-2.3520220	-0.8203120	O	-3.6408050	-0.4650310	0.7607920

C	-1.2647020	-1.3258340	-1.7803530	C	-4.3061380	-0.3992600	-0.2807040
H	-2.2669950	-1.5323030	-1.3706930	N	-4.5750290	0.8123840	-0.8461080
H	-1.2869800	-1.5936230	-2.8484630	C	-5.1731940	0.9525500	-2.1624190
H	-1.0855310	-0.2386340	-1.7178310	C	-6.1568410	-0.1776760	-2.4025820
C	1.6138960	-2.3999370	-1.8821310	C	-5.4583560	-1.5051490	-2.1788250
H	1.3897160	-2.5722120	-2.9468740	N	-4.7918290	-1.5246080	-0.8898940
H	2.1854630	-1.4614170	-1.7945480	C	-4.4190220	-2.8297090	-0.3842010
H	2.2620940	-3.2223660	-1.5369800	H	-3.8119910	-3.3728690	-1.1281800
C	-0.6401510	-4.1277700	-0.8401550	H	-3.8346560	-2.7089340	0.5333300
H	0.1267910	-4.8478240	-0.5160260	H	-5.3188940	-3.4253000	-0.1650710
H	-1.5012650	-4.2285610	-0.1601910	H	-4.7259770	-1.6985530	-2.9859460
H	-0.9660180	-4.4198310	-1.8517180	H	-6.1852280	-2.3314490	-2.1984120
N	-0.2453440	1.9061780	0.5554580	H	-6.9997800	-0.0817100	-1.7017120
Si	0.2434360	2.6406250	-0.9066670	H	-6.5554430	-0.1276650	-3.4247270
C	1.2474030	4.2393890	-0.6854260	H	-4.3957760	0.9594150	-2.9488920
H	1.5903560	4.6359720	-1.6547480	H	-5.6862140	1.9234060	-2.2043350
H	0.6598280	5.0286600	-0.1913050	C	-4.0198810	1.9803220	-0.1803310
H	2.1347310	4.0497780	-0.0609510	H	-2.9171900	1.9953530	-0.2040140
C	1.3909610	1.4797890	-1.8917870	H	-4.3870760	2.8788290	-0.6910960
H	2.3416830	1.3020860	-1.3615170	H	-4.3391060	2.0083030	0.8706000
H	0.9256750	0.5024020	-2.0930450	C	0.7793850	3.3308480	3.0002470
H	1.6489960	1.9293060	-2.8644940	H	1.3729730	4.0669090	2.4356880
C	-1.1899320	3.0694220	-2.0778220	H	0.4692030	3.7993350	3.9474260
H	-1.7729230	2.1708360	-2.3387840	H	1.4457640	2.4870680	3.2458420
H	-1.8737100	3.7903910	-1.6017920	C	-1.7970400	4.2781180	1.6867370
H	-0.8211380	3.5180030	-3.0136690	H	-2.0596970	4.7572070	2.6430480
Si	-0.7044340	2.7505110	1.9705710	H	-1.2826230	5.0295460	1.0678940
C	-1.7079070	1.5809260	3.0919120	H	-2.7353860	4.0131170	1.1755130
H	-2.6459620	1.2391170	2.6208620	O	3.6811550	0.4593620	0.7836900
H	-1.1233660	0.6887990	3.3777410	C	4.3563770	0.1239970	-0.1999890
H	-1.9859550	2.0841080	4.0305230	N	4.9080330	1.0531630	-1.0371360

C	5.1937430	-0.6432620	-2.7573810	C	5.6667380	0.6944550	-2.2204940

Table S82. Geometric coordinates and single point energies for NaHMDS disolvated DMPU monomer.



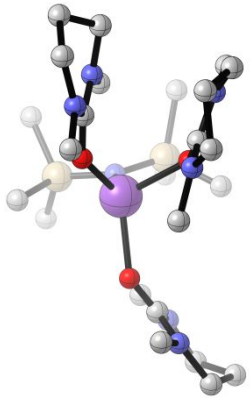
G = -1874.71751 Hartrees

G_{SP} = -1876.259356 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	-0.8308590	-2.4437700	0.7623100	C	-3.1331000	1.3572000	-0.6287390
N	0.2943330	-1.6546310	-0.2261640	N	-4.2957150	0.8630110	-1.1529250
Si	1.7345400	-2.2613640	-0.8744210	C	-5.4661490	0.5929240	-0.3379950
C	2.9680500	-2.8961540	0.4313400	C	-5.5852530	1.6208860	0.7696560
H	3.9430380	-3.1682560	-0.0043250	C	-4.2835970	1.6631340	1.5455470
H	3.1368210	-2.1397600	1.2150730	N	-3.1636510	1.8692900	0.6432300
H	2.5627910	-3.7923520	0.9292910	C	-1.8960810	2.2266610	1.2506420
C	2.6464820	-0.8768050	-1.8252990	H	-1.2343090	2.7023190	0.5195160
H	2.9507890	-0.0620640	-1.1488670	H	-2.0847180	2.9313030	2.0710810
H	3.5560220	-1.2575500	-2.3166940	H	-1.3753830	1.3430740	1.6676560
H	2.0070780	-0.4454890	-2.6156020	H	-4.1485350	0.7252530	2.1178760
C	1.5314930	-3.6711690	-2.1287800	H	-4.2925600	2.4902290	2.2706050
H	1.0823070	-4.5576840	-1.6555470	H	-5.7873830	2.6106290	0.3332090
H	0.8656930	-3.3611690	-2.9494840	H	-6.4175820	1.3658850	1.4392100
H	2.4979100	-3.9716290	-2.5643390	H	-6.3495320	0.6243200	-0.9929940
Na	-0.1377850	0.4610770	-0.8191360	H	-5.4050510	-0.4277630	0.0857320
O	1.2067470	2.0253960	0.0157330	C	-4.2542360	0.2090060	-2.4441190
C	2.4213110	1.8993960	0.2239320	H	-5.1520880	0.4779070	-3.0195550
N	2.8752400	1.1860640	1.2920550	H	-3.3632000	0.5352350	-2.9869480

C	4.2695360	0.8024750	1.4421720	H	-4.2235780	-0.8890080	-2.3349830
C	5.1711580	1.8897960	0.8902070	C	-0.3973360	-2.3695770	2.6164690
C	4.7619640	2.1932410	-0.5377760	H	-0.3966380	-1.3276580	2.9776680
N	3.3418840	2.4867580	-0.6075050	H	-1.1127370	-2.9372680	3.2328820
C	2.8715080	3.0674700	-1.8471820	H	0.6084170	-2.7832200	2.7949100
H	1.8383240	3.4040540	-1.7227860	C	-2.5362850	-1.5949360	0.6373250
H	3.5043520	3.9276480	-2.1074720	H	-3.3038370	-2.1325740	1.2174320
H	2.9140910	2.3368530	-2.6749370	H	-2.4734280	-0.5694360	1.0377120
H	5.0083430	1.3393830	-1.1983800	H	-2.8686570	-1.5312890	-0.4118310
H	5.3092650	3.0679540	-0.9206160	C	-1.1098900	-4.2793320	0.3654120
H	5.0716490	2.7979020	1.5037880	H	-1.3934750	-4.4139080	-0.6901080
H	6.2205990	1.5677580	0.9231210	H	-0.1875770	-4.8578570	0.5376960
H	4.4660820	0.6439900	2.5119650	H	-1.9009760	-4.7167270	0.9949700
H	4.4647370	-0.1572700	0.9278050				
C	1.8772770	0.5008200	2.1030020				
H	1.1037600	1.2128150	2.4199480				
H	1.3952810	-0.3229230	1.5482060				
H	2.3743410	0.0983910	2.9944480				
O	-2.0882600	1.3691450	-1.2872360				

Table S83. Geometric coordinates and single point energies for NaHMDS trisolvated DMPU monomer.



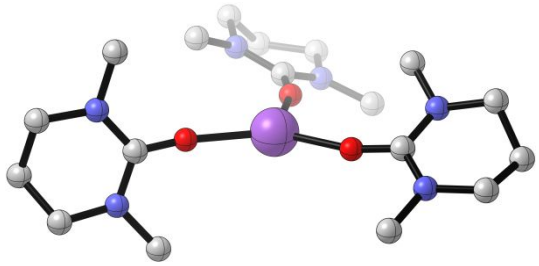
G = -2294.669544 Hartrees

G_{SP} = -2296.679577 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	1.9647340	2.3106830	1.6766360	H	4.3882080	-4.8297250	-1.0420620
N	1.6055870	2.0459240	0.0470500	C	1.6706460	-4.2444360	-1.4359420
Si	1.8984760	3.0017990	-1.3149440	H	1.0842440	-4.9130230	-0.7844160
C	1.0497630	4.7085890	-1.2960460	H	1.0107590	-3.4873790	-1.8688530
H	1.2261480	5.2678960	-2.2289740	H	2.1012150	-4.8530450	-2.2496450
H	-0.0386600	4.6197320	-1.1521550	O	-1.5542450	0.0031750	-1.5804960
H	1.4427260	5.3132150	-0.4621110	C	-2.6887880	0.3817970	-1.2900990
C	1.2650280	2.0818390	-2.8600100	N	-3.8066440	-0.3050610	-1.7196720
H	0.1877570	1.8512580	-2.8001300	C	-5.1598820	0.2260040	-1.7292420
H	1.4298380	2.6602060	-3.7826180	C	-5.2170110	1.6480990	-1.1958480
H	1.8010910	1.1230390	-2.9687850	C	-4.2421060	1.7723270	-0.0360440
C	3.7313590	3.3792380	-1.6689510	N	-2.9095050	1.4825160	-0.5188210
H	4.1752320	3.9725650	-0.8546000	C	-1.7563620	2.2437100	-0.0636470
H	4.3147790	2.4492320	-1.7587770	H	-1.0647340	2.4244170	-0.8954440
H	3.8516210	3.9458990	-2.6065040	H	-2.0987320	3.2123470	0.3220940
Na	0.4973120	0.1384630	-0.5428070	H	-1.1908770	1.7229260	0.7226530
O	-0.7331630	-0.6612840	1.2017410	H	-4.5278870	1.0796810	0.7812030

C	-1.8493660	-1.1603340	1.3172730	H	-4.2458510	2.7893100	0.3766100
N	-2.1756960	-2.2985800	0.6263330	H	-4.9186910	2.3637440	-1.9757450
C	-3.3825510	-3.0570880	0.8919530	H	-6.2435550	1.8897630	-0.8883310
C	-4.5125820	-2.1091450	1.2457940	H	-5.5533470	0.1846390	-2.7595250
C	-4.0857760	-1.2280940	2.4038980	H	-5.8087420	-0.4330700	-1.1215490
N	-2.8091320	-0.5989630	2.1263940	C	-3.6282000	-1.5590190	-2.4122330
C	-2.4479170	0.5174750	2.9759350	H	-3.7631980	-1.4475220	-3.5018170
H	-1.3893050	0.7576500	2.8321730	H	-2.6193420	-1.9374260	-2.2213410
H	-3.0535960	1.4073050	2.7344000	H	-4.3735610	-2.2864580	-2.0479380
H	-2.6161580	0.2600350	4.0344400	C	0.6483420	3.3394700	2.6016230
H	-4.0292770	-1.8185280	3.3389780	H	-0.3311460	2.8344140	2.6030500
H	-4.8293960	-0.4332860	2.5776760	H	0.9318480	3.5285140	3.6497020
H	-4.7277310	-1.4789360	0.3697650	H	0.5137490	4.3133360	2.1032860
H	-5.4203430	-2.6693640	1.5078890	C	2.0880560	0.6616800	2.6180080
H	-3.6340860	-3.6313900	-0.0117090	H	2.3209780	0.8139640	3.6841890
H	-3.2254480	-3.7883150	1.7086170	H	1.1405120	0.1042450	2.5441540
C	-1.0962890	-2.9169700	-0.1234960	H	2.8768710	0.0234220	2.1856320
H	-1.4806950	-3.8305830	-0.5954320	C	3.6022390	3.2315420	1.9936500
H	-0.7296760	-2.2341750	-0.9027480	H	4.4434650	2.7202770	1.4984970
H	-0.2419410	-3.1718670	0.5238750	H	3.5575070	4.2566290	1.5904850
O	1.8711470	-1.5370750	-1.1499160	H	3.8291280	3.3035120	3.0695860
C	2.7971660	-2.2120250	-0.6966020	H	3.2080960	0.3522430	-0.3624730
N	2.7209330	-3.5896180	-0.6905990	H	4.7970500	0.1628880	0.4029030
C	3.7702420	-4.4617170	-0.1999230	H	4.6436090	-0.0321680	-1.3682340
C	4.6360520	-3.7396590	0.8115450	H	5.7606440	-2.5918360	-0.6407730
C	5.0809090	-2.4189420	0.2164530	H	5.6413590	-1.8310050	0.9571040
N	3.9269240	-1.6375280	-0.1858310	H	4.0584190	-3.5471610	1.7281970
C	4.1480340	-0.2154710	-0.3989140	H	5.5048130	-4.3567770	1.0773700
H	3.2957100	-5.3456750	0.2559330				

Table S84. Geometric coordinates and single point energies for sodium cation solvated by 3 DMPU molecules.



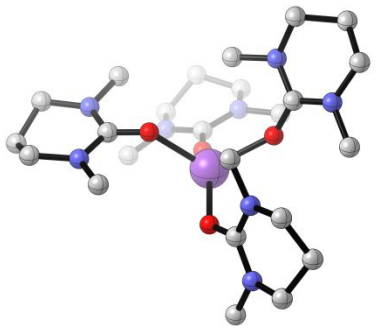
G = -1422.00152 Hartrees

G_{SP} = -1423.46305 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.1289250	-0.5187300	0.0073490	N	3.9522940	-2.6301550	-0.2648860
O	-1.9203650	-1.1661830	0.1142330	C	3.1887710	-3.7499780	-0.7769400
C	-3.0675050	-1.6386750	0.0416890	H	3.4435940	-4.6627450	-0.2163120
N	-3.4934120	-2.2379440	-1.1057780	H	2.1208470	-3.5474120	-0.6654980
C	-4.7618560	-2.9473900	-1.1887530	H	3.4165130	-3.9223460	-1.8406370
C	-5.7989290	-2.2379220	-0.3399000	H	5.6096500	-3.4907180	0.7039710
C	-5.2794970	-2.1142560	1.0783300	H	5.7127520	-3.3920520	-1.0627090
N	-3.9318970	-1.5627270	1.0929820	H	6.0860040	-0.9885810	-1.0098570
C	-3.4887340	-1.0300250	2.3647920	H	7.1836670	-1.7068800	0.1900390
H	-3.6456980	-1.7751690	3.1603580	H	5.6034610	-1.1503700	2.0179110
H	-2.4248850	-0.7848750	2.3113790	H	5.9345950	0.3125320	1.0705630
H	-4.0569170	-0.1229950	2.6261730	C	3.3772530	0.6237280	1.3141710
H	-5.2864190	-3.0976040	1.5825290	H	2.4926300	0.8954950	0.7269480
H	-5.9249060	-1.4463830	1.6684730	H	3.0621350	0.4152610	2.3510810
H	-5.9888900	-1.2382490	-0.7583450	H	4.0640350	1.4801480	1.3284610
H	-6.7459430	-2.7929610	-0.3466870	O	0.2350450	1.6262140	-0.1347430
H	-4.6473020	-3.9973200	-0.8627150	C	-0.1033790	2.8193940	-0.1928190
H	-5.0722680	-2.9652520	-2.2421280	N	-1.2964600	3.2292440	0.3282210
C	-2.5342900	-2.3946540	-2.1829550	C	-1.6585440	4.6340140	0.4472870

H	-1.9909030	-1.4564780	-2.3455300	C	-1.0833770	5.4190380	-0.7148700
H	-1.8026650	-3.1928290	-1.9760430	C	0.4105110	5.1752530	-0.7877780
H	-3.0780660	-2.6476000	-3.1005770	N	0.6977780	3.7487630	-0.7886350
O	2.0801820	-1.3925510	0.0614440	C	2.0068790	3.3621610	-1.2741930
C	3.3115730	-1.5081720	0.1677040	H	2.8030540	3.7313310	-0.6060340
N	4.0612940	-0.5069180	0.7165120	H	2.0684070	2.2723760	-1.3364650
C	5.4721270	-0.6830060	1.0242430	H	2.1703430	3.7892680	-2.2742040
C	6.1280280	-1.5267410	-0.0511660	H	0.9263590	5.6670200	0.0573910
C	5.3887310	-2.8444460	-0.1648080	H	0.8267040	5.6037450	-1.7111910
H	-1.3023940	5.0485820	1.4084960	H	-1.5592950	5.0897830	-1.6505300
H	-2.7553150	4.7017710	0.4520870	H	-1.2866520	6.4905290	-0.5899300
C	-2.0939340	2.2624860	1.0589730				
H	-2.0679960	1.2856210	0.5616060				
H	-1.7430350	2.1382400	2.0981580				
H	-3.1324240	2.6166120	1.0844980				

Table S85 Geometric coordinates and single point energies for sodium cation solvated by 4 DMPU molecules.



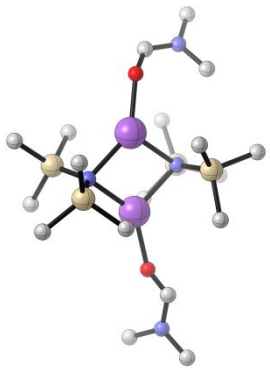
G = -1841.966869 Hartrees

G_{SP} = -1843.897348 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.1079340	0.3340000	-0.6929780	H	-3.8913590	-3.1838440	-0.8492170
O	1.7815940	-0.5104380	-1.3781030	H	-3.7000570	-3.4603100	2.6270720
C	2.8079200	-1.1890010	-1.5028590	H	-3.6777280	-4.6483450	1.3116860
N	2.7591180	-2.5551060	-1.5161610	H	-1.3491380	-5.1930720	1.6902030
C	3.9221280	-3.3998860	-1.7399280	H	-2.1159890	-5.1619530	3.2934330
C	5.1912860	-2.7001230	-1.2971700	H	-1.2832600	-2.8415950	3.6616230
C	5.2417690	-1.3218390	-1.9263440	H	0.0730380	-3.9042960	3.2354370
N	4.0325580	-0.5845390	-1.5970150	C	0.7080220	-1.8676440	1.7216740
C	4.0793850	0.8598080	-1.7218080	H	1.1068320	-1.7514660	0.7057710
H	4.0125230	1.1842630	-2.7738970	H	0.5545030	-0.8576810	2.1383590
H	3.2526740	1.3094910	-1.1614840	H	1.4472050	-2.4024070	2.3317970
H	5.0315950	1.2202290	-1.3074090	O	0.6801500	1.4627720	1.0319090
H	5.3679510	-1.3997930	-3.0222640	C	1.4934340	2.3724960	1.2393060
H	6.1002760	-0.7523100	-1.5428650	N	1.0959650	3.6770610	1.2577200
H	5.1992320	-2.6009560	-0.2010650	C	1.9662190	4.7603920	1.6871410
H	6.0700760	-3.2891090	-1.5903810	C	3.4034830	4.4575390	1.3104180
H	3.9860040	-3.6797910	-2.8077130	C	3.7869190	3.0958740	1.8554110
H	3.7765870	-4.3318770	-1.1734190	N	2.8223840	2.0933660	1.4332450

C	1.4778990	-3.2350020	-1.5529970	C	3.2192990	0.7047950	1.5547210
H	0.6632450	-2.5159170	-1.4208820	H	3.1584850	0.3479590	2.5978330
H	1.3489200	-3.7572320	-2.5152770	H	2.5723940	0.0867870	0.9227400
H	1.4248710	-3.9818490	-0.7450590	H	4.2575460	0.5983170	1.2099010
O	-1.8039430	1.6729870	-1.1395260	H	3.8575450	3.1266830	2.9588720
C	-3.0348160	1.5525780	-1.0838550	H	4.7758350	2.7942830	1.4790480
N	-3.6537080	1.1078050	0.0549200	H	3.5025000	4.4570400	0.2143080
C	-5.0951340	0.9846650	0.1910660	H	4.0733190	5.2295840	1.7111610
C	-5.7436160	0.7405780	-1.1564680	H	1.8787320	4.9222210	2.7775990
C	-5.2733550	1.8030100	-2.1294200	H	1.6267990	5.6832210	1.1961570
N	-3.8216040	1.8541960	-2.1581670	C	-0.3236140	3.9573700	1.1300290
C	-3.2242800	2.4163570	-3.3529020	H	-0.7827030	3.2640920	0.4150520
H	-3.6338030	3.4204540	-3.5471650	H	-0.8465940	3.8701290	2.0976070
H	-2.1428010	2.4917650	-3.2149960	H	-0.4439790	4.9835030	0.7597670
H	-3.4378570	1.7801050	-4.2256410	H	-1.8431170	1.1817230	1.1210570
H	-5.6897050	2.7906140	-1.8574030	H	-3.3041730	1.5762200	2.0686720
H	-5.6227700	1.5761420	-3.1472600	H	-2.9677760	-0.1204390	1.6194480
H	-5.4566450	-0.2534310	-1.5329360	O	-1.2140240	-1.4706230	-0.1152260
H	-6.8372030	0.7635510	-1.0625310	C	-1.4662240	-2.2909710	0.7750700
H	-5.5147110	1.8919620	0.6645220	N	-0.5175090	-2.6468030	1.6934010
H	-5.2974210	0.1460370	0.8756040	C	-0.8544250	-3.4593770	2.8497780
C	-2.8964840	0.9258570	1.2772020	C	-1.8327630	-4.5414210	2.4332370
C	-3.7459690	-2.4465810	-0.0424080	C	-3.0664730	-3.8952970	1.8330900
H	-4.6939040	-2.3501190	0.5098450	N	-2.7046250	-2.8596770	0.8759150
H	-3.4806480	-1.4793600	-0.4842890				

Table S86. Geometric coordinates and single point energies for NaHMDS disolvated DMF dimer.



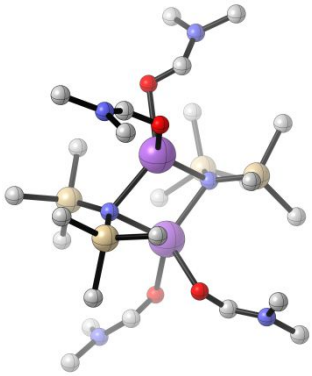
G = -2565.894022 Hartrees

G_{SP} = -2567.653526 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.4340150	0.9481630	-0.4634510	H	6.6108770	-0.9107850	1.4181050
N	0.5709310	2.0958760	-0.1118930	H	4.9145460	-0.7607910	1.9765470
Na	1.2573970	-0.1017850	0.2495400	H	5.9111250	-2.1595570	2.4899330
N	-0.7905500	-1.2761240	-0.0759210	H	3.7676780	-2.5845710	-0.8951160
Si	-0.6789340	-2.0331380	-1.5948990	Si	0.2089160	3.0746550	1.2447200
C	-1.7239120	-3.5977850	-1.8565010	C	-1.3048120	2.3652060	2.1563560
H	-1.6855170	-3.9079710	-2.9129270	H	-2.2223020	2.4259620	1.5456210
H	-1.3397540	-4.4309390	-1.2486990	H	-1.1528730	1.3113660	2.4413040
H	-2.7809660	-3.4502550	-1.5875400	H	-1.4997100	2.9269000	3.0831830
C	-1.2201100	-0.7937020	-2.9359230	C	-0.2546240	4.8657990	0.8215500
H	-2.2784330	-0.5127280	-2.8008930	H	-0.5063390	5.4399360	1.7271840
H	-0.6205770	0.1324240	-2.9077120	H	0.5637540	5.3928110	0.3070640
H	-1.1169300	-1.2080350	-3.9505240	H	-1.1313650	4.8816540	0.1545520
C	1.0972490	-2.5834580	-2.0116190	C	1.6169070	3.1382310	2.5148280
H	1.8073230	-1.7406890	-1.9933450	H	2.5166650	3.5874760	2.0664280
H	1.4221830	-3.3213310	-1.2586090	H	1.3470310	3.7291710	3.4040980
H	1.1624280	-3.0555790	-3.0046050	H	1.8842680	2.1227520	2.8507630

Si	-1.0663490	-1.9069490	1.4818360	Si	1.5154520	2.6331530	-1.4329750
C	0.3253420	-1.3562170	2.6660350	C	2.3040800	1.1393620	-2.3135060
H	1.2978720	-1.7638430	2.3407020	H	3.0059060	0.6050540	-1.6498460
H	0.4177860	-0.2579520	2.7313560	H	2.8774300	1.4638570	-3.1958410
H	0.1463630	-1.7173160	3.6904830	H	1.5473300	0.4196650	-2.6647530
C	-2.6958720	-1.2967640	2.2539540	C	0.5014410	3.5587300	-2.7408480
H	-3.5591560	-1.8108110	1.8017620	H	1.1123530	3.8615450	-3.6056190
H	-2.7230020	-1.4947690	3.3372150	H	-0.3238770	2.9298850	-3.1132490
H	-2.8328100	-0.2131310	2.1072580	H	0.0546070	4.4654970	-2.3038890
C	-1.1199810	-3.7994770	1.6008150	C	2.9785300	3.7483490	-0.9609040
H	-1.2014230	-4.1253450	2.6498740	H	2.6505940	4.6641040	-0.4450920
H	-1.9841290	-4.2062180	1.0530070	H	3.6630430	3.2124230	-0.2840020
H	-0.2098180	-4.2512280	1.1743360	H	3.5507620	4.0521620	-1.8516990
O	3.2043890	-1.1474120	0.4310480	O	-3.6272640	1.1874980	-0.4175490
C	4.0036960	-1.9608490	-0.0083310	C	-4.7058620	0.8332130	0.0360460
N	5.2221560	-2.1954070	0.5051910	N	-5.2150050	-0.4014420	-0.0690420
C	6.1120860	-3.1766230	-0.0735960	C	-6.5198150	-0.7344370	0.4575260
H	7.0483750	-2.7029740	-0.4063030	H	-7.1863110	-1.0866770	-0.3443890
H	6.3595420	-3.9579020	0.6613320	H	-6.4383640	-1.5245150	1.2193900
H	5.6306500	-3.6485440	-0.9391590	H	-6.9691420	0.1532370	0.9202910
C	5.6926960	-1.4649490	1.6647080	C	-4.4609510	-1.4374890	-0.7522060
H	-4.7219720	-2.4127320	-0.3191590	H	-4.6892140	-1.4545850	-1.8304410
H	-5.3629240	1.5384660	0.5861040	H	-3.3842240	-1.2667090	-0.6096570

Table S87. Geometric coordinates and single point energies for NaHMDS tetrasolvated DMF dimer.



G = -3062.152163 Hartrees

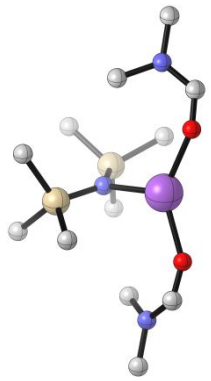
G_{SP} = -3064.478895 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.3746360	0.3435970	0.0620200	H	4.2236260	0.5481030	-0.1043360
N	-0.4873010	-1.8623790	0.2998600	Si	-0.9685370	-2.7380420	-1.0838020
Na	1.4204690	-0.4857560	0.2253580	C	-1.1277210	-1.5858370	-2.5782120
N	0.5256380	1.7428580	0.2361890	H	-1.8897920	-0.8011410	-2.4391030
Si	0.5176280	2.3491780	1.8327450	H	-0.1689780	-1.0743660	-2.7597400
C	0.4180900	4.2383940	2.0232550	H	-1.3911230	-2.1478400	-3.4889610
H	0.3456860	4.5019920	3.0907650	C	-2.6487190	-3.6187680	-0.8856180
H	1.3119950	4.7362070	1.6150420	H	-2.9846580	-4.0850540	-1.8255420
H	-0.4626020	4.6541950	1.5092990	H	-2.5963490	-4.4057180	-0.1161250
C	-0.9895360	1.6927880	2.7863950	H	-3.4182420	-2.9001360	-0.5634930
H	-1.9129830	2.1590080	2.4058120	C	0.2450200	-4.1048420	-1.6213900
H	-1.1260240	0.6029790	2.6994720	H	0.2989530	-4.9088350	-0.8723910
H	-0.9157650	1.9272320	3.8601820	H	-0.0548380	-4.5533210	-2.5832660
C	2.0824540	1.8751390	2.8129420	H	1.2574400	-3.6864410	-1.7328720
H	2.2628250	0.7883270	2.8191630	Si	-0.5350240	-2.5615990	1.8634130
H	2.9572860	2.3592280	2.3452860	C	0.7229920	-1.7361420	3.0197060
H	2.0241540	2.2157010	3.8594660	H	1.7525870	-1.8694790	2.6481440

Si	1.0334820	2.6023940	-1.1506980	H	0.6710760	-2.1815690	4.0258950
C	0.5699830	1.6928910	-2.7437080	H	0.5411380	-0.6565960	3.1326400
H	1.1390170	0.7525820	-2.8031620	C	-2.2443410	-2.3956610	2.6788840
H	-0.5039080	1.4514000	-2.7742540	H	-2.2804200	-2.8617420	3.6765130
H	0.8190350	2.3008090	-3.6288500	H	-2.5208980	-1.3339710	2.7779540
C	0.2973760	4.3539310	-1.3276580	H	-3.0038980	-2.8801650	2.0414860
H	0.7309510	5.0671700	-0.6121220	C	-0.1046580	-4.4140450	1.9249740
H	0.4817200	4.7411520	-2.3434780	H	-0.8073010	-5.0263290	1.3379660
H	-0.7900750	4.3279580	-1.1561700	H	0.9077600	-4.5900850	1.5278630
C	2.9237920	2.8463850	-1.2488380	H	-0.1291120	-4.7807560	2.9635450
H	3.2038930	3.5831860	-2.0185280	O	-2.6816940	1.3710420	-1.5643380
H	3.3295230	3.1905500	-0.2824320	C	-3.0199150	2.4630170	-1.1296700
H	3.3966220	1.8870420	-1.5155180	N	-3.1329100	3.5837150	-1.8646600
O	2.6524120	-0.7554870	-1.6916780	C	-3.4958710	4.8484370	-1.2674560
C	3.2142750	-1.8341510	-1.8202720	H	-3.6839150	4.7099890	-0.1950220
N	3.1931170	-2.5831260	-2.9361280	H	-2.6800060	5.5788320	-1.3870270
C	3.7922490	-3.8978930	-2.9758240	H	-4.4044620	5.2550180	-1.7381630
H	4.3347730	-4.0848970	-2.0404020	C	-2.7718520	3.5848270	-3.2671840
H	3.0155570	-4.6711090	-3.0897880	H	-1.8369680	4.1482360	-3.4180450
H	4.4974690	-3.9765620	-3.8169980	H	-2.6230170	2.5498710	-3.5928510
C	2.3876080	-2.1822230	-4.0720580	H	-3.5724520	4.0505160	-3.8610320
H	1.4701420	-2.7914750	-4.1231610	H	-3.2755210	2.6010010	-0.0573690
H	2.1086640	-1.1289730	-3.9581340	O	-3.4595340	0.3648480	1.0798170
H	2.9610440	-2.3153800	-5.0007240	C	-4.1790810	-0.4314900	0.4941840
H	3.7995170	-2.2794760	-0.9877620	N	-5.1562710	-1.1557820	1.0689200
O	3.5114510	-0.8872770	1.1483650	C	-5.9362990	-2.1120760	0.3176150
C	4.2262990	0.0755360	0.8993050	H	-5.6609540	-2.0631780	-0.7435090
N	5.0655470	0.6607640	1.7695310	H	-5.7490400	-3.1362760	0.6773090
C	5.8052780	1.8494360	1.4118390	H	-7.0111490	-1.8943830	0.4161840
H	5.4804780	2.7042320	2.0269310	C	-5.4197110	-1.0473340	2.4887870
H	6.8847090	1.6978730	1.5662860	H	-5.1917020	-1.9973970	2.9956210

H	5.6245910	2.0933520	0.3570270	H	-4.7809590	-0.2599540	2.9026480
C	5.1353130	0.2147860	3.1448420	H	-6.4781880	-0.7946000	2.6563320
H	4.7538860	1.0001170	3.8161810	H	-4.0756550	-0.6087980	-0.5982780
H	4.5148680	-0.6813500	3.2538840				
H	6.1761690	-0.0177660	3.4169690				

Table S88 Geometric coordinates and single point energies for NaHMDS disolvated DMF monomer.



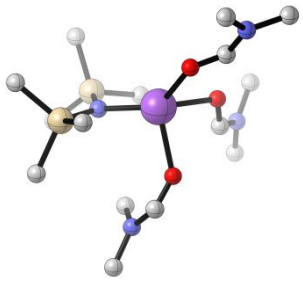
G = -1531.066646 Hartrees

G_{SP} = -1532.233946 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	0.6165410	1.3591270	-1.3945640	H	5.8906690	-1.1318130	1.1427690
N	0.0000090	0.6185400	-0.0000960	C	3.3344990	-0.1130730	0.9675190
Si	-0.6164400	1.3585300	1.3947150	H	2.2566820	-0.0776580	0.7485580
C	0.7298200	1.9123160	2.6189430	H	3.4900160	-0.1290770	2.0581780
H	0.3084160	2.4303960	3.4950400	H	3.7976130	0.7971470	0.5611230
H	1.3005280	1.0433980	2.9845390	H	3.8309540	-3.1470800	-0.4738830
H	1.4388670	2.5976850	2.1270040	O	-2.0171180	-2.4678650	-0.1417610
C	-1.7076530	0.1265830	2.3563820	C	-3.2233180	-2.3416290	0.0095470
H	-1.1521410	-0.7961220	2.5984240	N	-3.9502460	-1.2726300	-0.3437160
H	-2.0568750	0.5543360	3.3093480	C	-5.3861090	-1.2504620	-0.1718400
H	-2.5974530	-0.1609640	1.7723000	H	-5.7227610	-2.1897120	0.2848800
C	-1.6979200	2.8918450	1.0800740	H	-5.6831710	-0.4146640	0.4792420
H	-1.1167090	3.6830540	0.5798310	H	-5.8906780	-1.1310010	-1.1429550
H	-2.5509310	2.6506010	0.4264350	C	-3.3345690	-0.1125430	-0.9671100
H	-2.0953910	3.3108140	2.0181490	H	-2.2566880	-0.0774170	-0.7484280
Na	-0.0000510	-1.6223650	-0.0004390	H	-3.4903880	-0.1278470	-2.0577370
O	2.0169940	-2.4679370	0.1412980	H	-3.7974120	0.7975060	-0.5600160

C	3.2231850	-2.3417030	-0.0100890	H	-3.8311610	-3.1471840	0.4729330
N	3.9501620	-1.2728730	0.3435670	C	1.6976100	2.8925640	-1.0791470
C	5.3860180	-1.2506480	0.1716200	H	2.5506370	2.6510930	-0.4256070
H	5.7226000	-2.1896200	-0.2857240	H	2.0950530	3.3121450	-2.0169570
H	5.6830540	-0.4144570	-0.4789660	H	1.1162340	3.6833720	-0.5784640
H	2.5976510	-0.1601870	-1.7719180	C	1.7082580	0.1277810	-2.3564160
H	1.1528240	-0.7947360	-2.5993580	H	2.0581270	0.5560830	-3.3088950
C	-0.7297760	1.9128120	-2.6187670				
H	-1.2999370	1.0437320	-2.9848390				
H	-1.4392850	2.5975480	-2.1266110				
H	-0.3085390	2.4315340	-3.4945650				

Table S89. Geometric coordinates and single point energies for NaHMDS trisolvated DMF monomer.



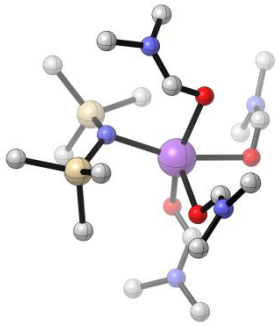
G = -1779.193206 Hartrees

G_{SP} = -1780.64386 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	1.8156620	0.4025630	-2.0770990	N	2.0883570	0.3967620	2.9645700
N	1.2876580	-0.6262580	-0.8411840	C	3.0875970	0.1656200	3.9839710
Si	1.9684150	-2.1152960	-0.4062160	H	2.6631510	-0.4516440	4.7862190
C	2.4846680	-3.2272370	-1.8580640	H	3.9560980	-0.3595120	3.5578880
H	2.8600490	-4.2042460	-1.5142200	H	3.4299060	1.1176350	4.4183840
H	1.6313580	-3.4027390	-2.5318090	C	2.4536970	1.1896660	1.8009910
H	3.2826170	-2.7506110	-2.4505670	H	1.9376840	0.7912370	0.9103400
C	0.7166060	-3.1237860	0.6201960	H	2.2095710	2.2548510	1.9542120
H	-0.1953240	-3.3387900	0.0389330	H	3.5358780	1.0961710	1.6403970
H	1.1415960	-4.0892120	0.9366260	H	0.6985910	-0.7237750	3.9757040
H	0.4136730	-2.5875540	1.5363270	C	1.3938980	-0.1827290	-3.8342570
C	3.5123220	-1.9727970	0.7070980	H	0.3073380	-0.3323890	-3.9355210
H	4.2749670	-1.3303020	0.2383480	H	1.7154320	0.5407670	-4.6006520
H	3.2384500	-1.5262180	1.6765370	H	1.8813210	-1.1464790	-4.0487980
H	3.9672170	-2.9565940	0.9050500	C	0.9988810	2.1179470	-1.9064500
Na	-0.7333650	-0.5235900	0.2000190	H	1.3526840	2.8185860	-2.6797370
O	-2.7436140	-1.5440780	0.1302730	H	-0.0951140	2.0211040	-2.0007900
C	-3.8037630	-0.9422020	0.0860170	H	1.2231600	2.5549760	-0.9181490
N	-5.0163390	-1.5312190	0.0408930	C	3.6943740	0.7240720	-2.0702020

C	-6.2319680	-0.7555580	-0.0176840	H	4.0186890	1.1422700	-1.1032950
H	-5.9871050	0.3140970	-0.0102950	H	4.2487590	-0.2162580	-2.2240090
H	-6.7968830	-0.9799010	-0.9362840	H	3.9982710	1.4254220	-2.8637090
H	-6.8786710	-0.9735000	0.8469070	H	-0.8941350	5.5746890	0.8114610
C	-5.1368040	-2.9733840	0.0388940	C	-2.0926950	3.9986710	-1.1220080
H	-4.1317280	-3.4052350	0.0882370	H	-1.4516160	4.2389400	-1.9855480
H	-5.7248600	-3.3111230	0.9063060	H	-2.7169240	3.1340580	-1.3701190
H	-5.6382480	-3.3162900	-0.8794330	H	-2.7306860	4.8667550	-0.8976150
H	-3.8386450	0.1663420	0.0779300	H	-0.4905500	2.2451320	1.3000030
O	-1.8853690	1.4677780	0.0446830	O	-0.0672530	0.1186290	2.2867300
C	-1.2176420	2.3974840	0.4760990	C	0.8448050	-0.0920340	3.0733420
N	-1.2772770	3.6636520	0.0247430				
C	-0.3542920	4.6691420	0.4954080				
H	0.2090240	4.2793550	1.3530050				
H	0.3599260	4.9412830	-0.2988020				

Table S90. Geometric coordinates and single point energies for NaHMDS tetrasolvated DMF monomer.



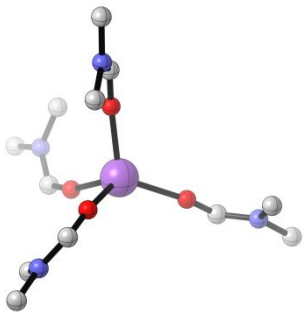
G = -2027.320541 Hartrees

G_{SP} = -2029.056022 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.1126930	0.6707300	0.0350670	H	4.9705760	0.2376930	-1.1039720
N	-0.9250750	-1.3034210	-0.6323590	H	5.4121460	1.7668110	-1.9201980
Si	0.1195620	-2.6242200	-0.7990910	H	4.5613250	1.7972160	-0.3447240
C	1.7224200	-2.1834210	-1.7275790	C	3.2694150	0.5989370	-3.2454430
H	2.2348810	-1.3659530	-1.1913480	H	3.5721300	-0.4541510	-3.1451290
H	2.4170050	-3.0347290	-1.8185590	H	2.2279770	0.6368850	-3.5831960
H	1.4771240	-1.8258470	-2.7402770	H	3.9184960	1.0922740	-3.9859380
C	0.7075200	-3.2957210	0.8901350	H	2.4870850	2.2700000	-0.3949590
H	1.4820770	-4.0667670	0.7472810	O	2.1742900	0.0807600	0.9144130
H	1.1444060	-2.4921320	1.5046200	C	1.9704090	0.0241620	2.1193750
H	-0.1130480	-3.7573050	1.4633980	N	2.6065860	-0.8119590	2.9641570
C	-0.6414230	-4.1236780	-1.6882650	C	2.2706510	-0.8575450	4.3677080
H	-1.5430720	-4.4681210	-1.1559360	H	1.9051520	-1.8588410	4.6454980
H	-0.9456240	-3.8577690	-2.7135970	H	3.1475690	-0.6229870	4.9914350
H	0.0597690	-4.9708900	-1.7539250	H	1.4804180	-0.1258870	4.5791060
Si	-1.9587670	-0.6521350	-1.8043870	C	3.6079060	-1.7378120	2.4791620
C	-1.2282100	-0.5763700	-3.5580300	H	3.3198060	-2.7712110	2.7256510
H	-1.9144040	-0.1023130	-4.2781020	H	3.6758940	-1.6372170	1.3901380

H	-0.2995750	0.0161520	-3.5238960	H	4.5872960	-1.5225110	2.9351880
H	-0.9803810	-1.5811820	-3.9367040	H	1.2074970	0.6663200	2.6047380
C	-2.3117120	1.1782110	-1.3573860	O	0.5409910	2.7175900	1.0738720
H	-1.4397900	1.7896580	-1.6470540	C	-0.5445110	3.1971820	1.3676730
H	-3.1845230	1.5790060	-1.8972270	N	-1.2801800	3.9921130	0.5692470
H	-2.4878270	1.3077350	-0.2754170	C	-2.5785350	4.4745870	0.9764410
C	-3.6468790	-1.5154280	-1.9931470	H	-2.7890910	4.1473560	2.0027870
H	-3.4988310	-2.5913400	-2.1809140	H	-2.6160570	5.5746610	0.9429580
H	-4.2819550	-1.4198590	-1.0985770	H	-3.3623390	4.0767920	0.3123500
H	-4.2082770	-1.0986730	-2.8446860	C	-0.8153140	4.3523610	-0.7562100
O	1.1314380	1.7013100	-1.7975220	H	0.0178940	3.6962880	-1.0372010
C	2.2737820	1.7747890	-1.3626350	H	-1.6320310	4.2141760	-1.4790360
N	3.3656000	1.2757680	-1.9695360	H	-0.4911470	5.4054480	-0.7820970
C	4.6456120	1.2713510	-1.3038660	H	-1.0277120	2.9880460	2.3429600
H	-3.3066400	-2.5907420	0.5639400	O	-1.1690740	0.4917550	2.0496090
H	-2.2670630	-3.0881340	1.9139500	C	-1.5454350	-0.6778070	2.0113160
C	-3.8831320	-0.1118820	1.7600330	N	-2.8256290	-1.0793520	1.9450100
H	-4.7488930	-0.3786210	2.3842100	C	-3.1256260	-2.4617010	1.6424810
H	-3.5092600	0.8760210	2.0520850	H	-4.0044670	-2.7917000	2.2156150
H	-4.2020660	-0.0754150	0.7054980				
H	-0.8350990	-1.5219450	2.0830220				

Table S91. Geometric coordinates and single point energies for sodium cation solvated by 4 DMF molecules.



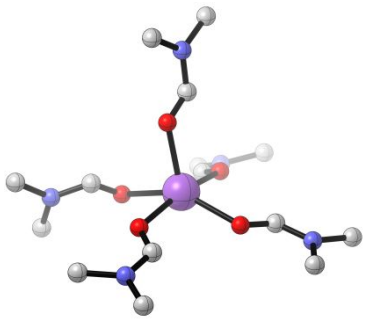
G = -1154.656055 Hartrees

G_{SP} = -1155.838722 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.2593880	-0.1058410	0.0416360	N	1.2501780	3.4371100	1.5894050
O	0.4210560	0.7981020	-1.8556000	C	1.6525620	4.5794210	2.3846840
C	0.7805190	0.9274670	-3.0190440	H	1.6808700	4.3039840	3.4460520
N	1.3406980	-0.0250040	-3.7752310	H	2.6519320	4.9261030	2.0827330
C	1.7082430	0.2209280	-5.1550070	H	0.9417210	5.4090440	2.2549160
H	1.4729450	1.2577530	-5.4247950	C	1.1525570	3.6315330	0.1549070
H	2.7853840	0.0531940	-5.3023470	H	0.9129250	2.6798390	-0.3330240
H	1.1552640	-0.4520570	-5.8271300	H	0.3682370	4.3687740	-0.0752880
C	1.5768180	-1.3589540	-3.2557930	H	2.1100550	4.0096980	-0.2328340
H	1.3410270	-1.3876780	-2.1858610	H	1.0815660	2.2625290	3.2563670
H	0.9504900	-2.0908150	-3.7885890	O	1.0186280	-1.9015190	0.2117960
H	2.6323260	-1.6308170	-3.4040080	C	1.7094690	-2.8030650	0.6693200
H	0.6650190	1.8934150	-3.5527100	N	2.2831190	-2.8121390	1.8790700
O	-2.4231860	-0.4729890	0.1914570	C	3.0627290	-3.9431420	2.3400440
C	-3.4744940	-1.0818030	0.3435200	H	3.0981480	-4.7144750	1.5609700
N	-4.6987370	-0.5425840	0.2811440	H	4.0910010	-3.6316390	2.5759860
C	-5.8927160	-1.3399290	0.4732080	H	2.6134880	-4.3774870	3.2455550
H	-5.6162970	-2.3836020	0.6670610	C	2.1247750	-1.6997000	2.7970110

H	-6.4736710	-0.9641500	1.3284820	H	1.6021020	-0.8769420	2.2960530
H	-6.5289110	-1.3040760	-0.4236000	H	1.5499040	-2.0147130	3.6813620
C	-4.8796520	0.8713380	0.0156930	H	3.1141800	-1.3534450	3.1302850
H	-3.8965720	1.3364450	-0.1063420	H	1.9216320	-3.7199210	0.0813760
H	-5.4697560	1.0121680	-0.9020100	C	0.9586680	2.2583260	2.1536270
H	-5.4115980	1.3488520	0.8518850				
H	-3.4889680	-2.1710930	0.5528040				
O	0.5953950	1.2513020	1.5592120				

Table S92. Geometric coordinates and single point energies for sodium cation solvated by 5 DMF molecules.



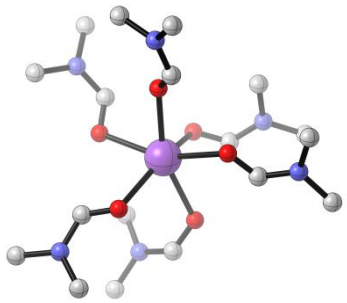
G = -1402.789499 Hartrees

G_{SP} = -1404.256287 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.0509710	0.1844940	-0.0838240	C	2.5878120	-3.0585090	-2.7417350
O	2.2707970	0.5532900	-0.0053140	H	2.5062420	-4.1194960	-3.0230390
C	2.8112340	1.6420800	0.1314750	H	1.7572590	-2.4971990	-3.1812000
N	4.1389820	1.8472790	0.1170670	H	3.5404270	-2.6667470	-3.1288920
C	4.7078470	3.1646350	0.2994950	H	1.6297950	-2.1627140	0.3876610
H	3.9033380	3.8983920	0.4336790	O	-0.2334670	-1.0697720	1.7652330
H	5.3573750	3.1887710	1.1876790	C	-1.3244570	-1.3888970	2.2180660
H	5.3066290	3.4548470	-0.5771240	N	-1.5204010	-2.0287420	3.3822380
C	5.0557320	0.7426000	-0.0756660	C	-2.8458450	-2.3763650	3.8460020
H	4.4707480	-0.1672120	-0.2470090	H	-3.5932320	-2.0427390	3.1153670
H	5.7030940	0.9337880	-0.9446440	H	-2.9397870	-3.4654330	3.9738840
H	5.6922110	0.6096550	0.8125080	H	-3.0581180	-1.8942650	4.8122760
H	2.2135870	2.5652260	0.2762230	C	-0.4007980	-2.3911810	4.2281300
O	-0.2946440	2.4172480	0.0349480	H	0.5209530	-2.0278320	3.7627980
C	-1.3983240	2.9167860	-0.1485130	H	-0.5138550	-1.9347220	5.2227960
N	-1.6838080	4.2236070	-0.0362690	H	-0.3484660	-3.4838830	4.3485780
C	-3.0160260	4.7320410	-0.2831230	H	-2.2639400	-1.1576370	1.6732950
H	-3.6835980	3.9039430	-0.5517220	O	-2.1339620	-0.1205570	-0.7081330

H	-3.4141690	5.2297040	0.6140110	C	-2.3677240	-0.9727220	-1.5623370
H	-3.0072710	5.4593430	-1.1089840	N	-3.5767060	-1.2187730	-2.0897390
C	-0.6640110	5.1847340	0.3309660	C	-3.7642320	-2.2286390	-3.1104980
H	0.2714480	4.6490470	0.5201510	H	-2.8056280	-2.7149760	-3.3284790
H	-0.5127020	5.9132420	-0.4799100	H	-4.4803900	-2.9927390	-2.7727630
H	-0.9640570	5.7283510	1.2391600	H	-4.1493550	-1.7764700	-4.0368790
H	-2.2690750	2.2900080	-0.4300370	C	-4.7435350	-0.4666660	-1.6765920
O	0.6266930	-1.6624730	-1.3117150	H	-4.4561800	0.2136000	-0.8683440
C	1.5478920	-2.2099770	-0.7174430	H	-5.1468020	0.1140620	-2.5203020
N	2.5342460	-2.9095790	-1.3019350	H	-5.5281750	-1.1500810	-1.3190880
C	3.5766760	-3.5432580	-0.5254020	H	-1.5591220	-1.6169670	-1.9605550
H	3.5703620	-4.6333620	-0.6781130				
H	4.5661100	-3.1596280	-0.8181720				
H	3.4206940	-3.3357270	0.5406170				

Table S93. Geometric coordinates and single point energies for sodium cation solvated by 6 DMF molecules.



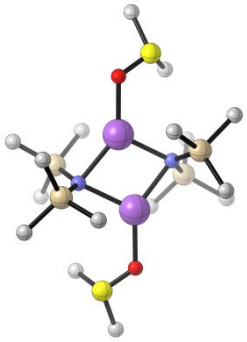
G = -1650.920751 Hartrees

G_{SP} = -1652.669205 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.1329780	-0.1186070	0.0697210	H	-3.0311850	-2.2140430	2.6590990
O	0.9775840	1.8861480	0.3857050	H	-4.4570380	-1.6652090	3.5918770
C	1.7177430	2.1583550	1.3194630	H	-4.6836790	-2.7525540	2.1954160
N	1.9554890	3.4026310	1.7712280	H	-3.2749470	0.6820490	0.5498890
C	2.8471760	3.6539230	2.8818000	H	-1.7703560	-3.7755960	0.3647610
H	3.6798880	4.3047370	2.5743140	C	-1.5647400	-2.9342100	-0.3309640
H	2.3110700	4.1436930	3.7088820	O	-0.4474830	-2.4519260	-0.4427910
H	3.2588410	2.7043050	3.2458830	N	-2.6542120	-2.5423930	-1.0121530
C	1.3052710	4.5432360	1.1595280	C	-3.9460160	-3.1525610	-0.7948710
H	2.0524840	5.2299570	0.7326560	H	-3.8577940	-3.9614180	-0.0579690
H	0.6431120	4.1790710	0.3652470	H	-4.6654020	-2.4072090	-0.4182320
H	0.7151730	5.0923750	1.9090690	H	-4.3406180	-3.5737600	-1.7319310
H	2.2572170	1.3621410	1.8727500	C	-2.5843750	-1.4513280	-1.9661280
O	1.8581690	-0.8929590	0.9957840	H	-1.5377520	-1.1601090	-2.1202210
C	2.2597060	-2.0382790	0.8464890	H	-3.0266960	-1.7683340	-2.9223200
N	3.4855200	-2.4785430	1.1992300	H	-3.1306740	-0.5703080	-1.5938590
C	3.8514080	-3.8722780	1.0646520	O	-1.6500670	1.4350000	-0.8695230
H	3.0521520	-4.4148870	0.5439880	C	-1.0127320	2.2397850	-1.5348770
H	4.7829970	-3.9756590	0.4867810	N	-1.2747240	3.5600200	-1.6087950

H	4.0064660	-4.3352590	2.0516690	C	-0.5079750	4.4323130	-2.4698860
C	4.4366270	-1.6056800	1.8548390	H	-1.1456000	4.8750420	-3.2508570
H	4.0242660	-0.5914060	1.8787270	H	-0.0549620	5.2519180	-1.8901320
H	4.6276220	-1.9436090	2.8853470	H	0.2936170	3.8599210	-2.9530480
H	5.3924070	-1.6020570	1.3084200	C	-2.3670690	4.1480530	-0.8646740
H	1.6158120	-2.8146570	0.3867860	H	-3.1476000	4.5245820	-1.5441950
O	-1.9343270	-0.5972890	1.3808020	H	-2.7947240	3.3838500	-0.2076300
C	-3.0735960	-0.1998780	1.1914000	H	-2.0019310	4.9896640	-0.2560920
N	-4.1808740	-0.7712840	1.7071120	H	-0.1417960	1.9221710	-2.1399090
C	-5.4968990	-0.2189660	1.4735980	O	0.7127210	-0.2392140	-2.0797370
H	-5.4225150	0.6365020	0.7903190	C	1.5003990	-1.1500060	-2.2808500
H	-6.1613800	-0.9727470	1.0223470	N	2.8241190	-1.0926240	-2.0448840
H	-5.9535860	0.1205700	2.4160870	C	3.7022860	-2.1975930	-2.3537810
C	-4.0831010	-1.9167180	2.5873460	H	4.4447600	-1.9109880	-3.1144390
H	2.6232670	0.7835420	-1.1684790	H	4.2398650	-2.5205520	-1.4479320
H	4.0396850	-0.1637870	-0.6217810	H	3.1165610	-3.0426510	-2.7383090
H	4.0606360	0.6013270	-2.2406700	C	3.4220260	0.1057810	-1.4925450
H	1.1682400	-2.1323730	-2.6765420				

Table S94. Geometric coordinates and single point energies for NaHMDS disolvated DMSO dimer.



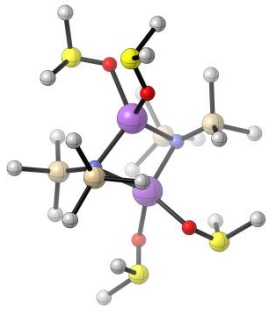
G = -3175.219833 Hartrees

G_{SP} = -3177.089036 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
N	1.2135850	-1.3797500	0.0396810	C	-0.9788080	4.1771320	-1.1191040
Na	-1.1065510	-0.9527140	0.3439810	H	-0.8493670	4.7119990	-2.0732280
N	-1.2139620	1.3790060	0.0392710	H	-1.9081640	4.5420200	-0.6531700
Na	1.1056330	0.9513040	0.3432500	H	-0.1417950	4.4541050	-0.4589930
O	3.0354260	2.0006150	0.4579470	O	-3.0369620	-2.0000370	0.4567720
S	4.3875390	1.3123560	0.2907060	S	-4.3888320	-1.3108290	0.2910640
C	4.2070470	0.3004760	-1.1861500	C	-4.2086230	-0.2974790	-1.1847960
H	5.1522430	-0.2122810	-1.4101830	H	-5.1536460	0.2161250	-1.4076300
H	3.4213560	-0.4307830	-0.9410050	H	-3.4222340	0.4329510	-0.9393700
H	3.8808600	0.9412050	-2.0169940	H	-3.8834410	-0.9375450	-2.0165440
C	5.4552120	2.5997130	-0.3845660	C	-5.4576180	-2.5968910	-0.3849020
H	5.5761500	3.3526300	0.4030680	H	-5.5785770	-3.3505000	0.4020630
H	6.4278660	2.1682230	-0.6536730	H	-6.4301540	-2.1645700	-0.6530990
H	4.9507520	3.0387760	-1.2548350	H	-4.9538400	-3.0353870	-1.2558500
Si	-2.0013330	1.9080020	1.4642830	Si	2.0029480	-1.9093160	1.4634660
C	-3.7957080	2.4802130	1.1997350	C	1.0993580	-3.3070510	2.3713930
H	-4.2110550	2.9328890	2.1136400	H	1.5695150	-3.5253610	3.3431140
H	-3.8634280	3.2272270	0.3926410	H	0.0485970	-3.0307400	2.5618020

H	-4.4452070	1.6314850	0.9303760	H	1.0958790	-4.2346230	1.7798820
C	-2.0955470	0.4700260	2.7104110	C	2.0973330	-0.4722030	2.7105170
H	-2.6979820	-0.3784420	2.3480780	H	2.5552980	-0.8134450	3.6516190
H	-1.0941320	0.0840380	2.9672830	H	2.6982990	0.3771640	2.3478090
H	-2.5519170	0.8114420	3.6522260	H	1.0957900	-0.0874510	2.9687080
C	-1.0957920	3.3043350	2.3724570	C	3.7974390	-2.4798730	1.1962760
H	-0.0449250	3.0275200	2.5615270	H	3.8647470	-3.2267540	0.3890260
H	-1.0926340	4.2324020	1.7817060	H	4.4457820	-1.6305150	0.9261420
H	-1.5648610	3.5220420	3.3448440	H	4.2144550	-2.9322180	2.1095890
Si	-1.0157030	2.2999370	-1.3918870	Si	1.0154100	-2.3001620	-1.3918670
C	0.6613570	1.8868410	-2.2101440	C	0.9790700	-4.1775430	-1.1201590
H	1.5045850	2.3341950	-1.6553130	H	0.8494760	-4.7115400	-2.0747600
H	0.8324290	0.7990940	-2.2857640	H	1.9087300	-4.5425670	-0.6549350
H	0.6985010	2.2966840	-3.2311590	H	0.1423850	-4.4554470	-0.4600320
C	-2.3243990	2.0082150	-2.7391110	C	2.3241690	-2.0078460	-2.7389600
H	-3.3299350	2.2916830	-2.3886670	H	3.3298540	-2.2903280	-2.3881530
H	-2.0944190	2.6282510	-3.6198880	H	2.0949420	-2.6284400	-3.6195380
H	-2.3582950	0.9585320	-3.0705590	H	2.3572960	-0.9582650	-3.0708450
H	-0.8323950	-0.7990470	-2.2854120	C	-0.6615790	-1.8868480	-2.2100670
H	-0.6986050	-2.2963990	-3.2312020	H	-1.5050390	-2.3341280	-1.6555370

Table S95. Geometric coordinates and single point energies for NaHMDS tetrasolvated DMSO dimer.



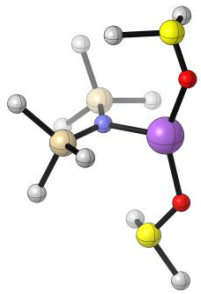
G = -4280.807505 Hartrees

G_{SP} = -4283.353401 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Symbol	X	Y	Z	C	-2.1434550	-2.6520600	2.2750430
Na	-1.2890680	0.3272850	-0.1293630	H	-2.5570860	-3.5050200	1.7132830
N	0.4881110	1.8371020	-0.7444510	H	-2.2221270	-2.8832250	3.3499240
Na	1.6227730	-0.1128830	-0.0156030	H	-2.7561140	-1.7617190	2.0667080
N	-0.1700940	-1.7971110	0.1495010	C	0.6413120	-3.8459130	2.2987640
Si	-0.2077350	-2.8978000	-1.1579960	H	0.0266200	-4.4914350	2.9459330
C	-1.1544370	-4.5256260	-0.8317170	H	0.9561680	-4.4523480	1.4350250
H	-1.0957750	-5.1710970	-1.7234110	H	1.5450940	-3.5821400	2.8702810
H	-0.7233170	-5.0851930	0.0129000	O	3.6004440	-0.9166230	-0.8790060
H	-2.2206830	-4.3682720	-0.6079720	S	4.5441170	-1.6136780	0.1005290
C	-1.0619010	-2.1382370	-2.6926060	C	3.4830890	-2.5088100	1.2507020
H	-2.0580410	-2.5813110	-2.8563720	H	4.0660850	-3.2727170	1.7821890
S	-4.0312380	-0.6966080	-1.8303560	H	3.0955140	-1.7559770	1.9483810
O	-3.3680710	0.4474550	-1.0670740	H	2.6681210	-2.9533810	0.6639920
C	-3.9521760	-2.1003030	-0.7002290	C	5.1680490	-3.0311600	-0.8300800
H	-4.3458450	-2.9990270	-1.1939410	H	5.7326590	-2.6201410	-1.6752330
H	-2.8858260	-2.2293280	-0.4610970	H	5.8236530	-3.6345590	-0.1890530
H	-4.5038780	-1.8577010	0.2171840	H	4.3093410	-3.6092720	-1.1951550
C	-5.7988810	-0.3512350	-1.6819710	O	3.1084770	0.5482800	1.6235270

H	-5.9951250	0.5543300	-2.2684930	S	4.2351420	1.5498260	1.3629160
H	-6.3765970	-1.1951220	-2.0808610	C	4.0119190	2.1237780	-0.3346170
H	-6.0225110	-0.1794170	-0.6204920	H	4.6381390	3.0107600	-0.5003580
H	-1.1845380	-1.0453570	-2.6117950	H	4.3121270	1.2895610	-0.9808610
H	-0.4797080	-2.3195960	-3.6095720	H	2.9392090	2.3346220	-0.4791590
C	1.5054770	-3.4983400	-1.7270730	C	3.7375670	3.0579990	2.2202970
H	2.2067460	-2.6566900	-1.8431780	H	3.6756260	2.8003040	3.2844800
H	1.9195240	-4.2049920	-0.9865900	H	4.5017760	3.8291550	2.0563620
H	1.4343130	-4.0346020	-2.6868130	H	2.7565080	3.3780760	1.8488690
Si	-0.3382360	-2.2764610	1.7860580	Si	0.5981900	1.8468930	-2.4519810
C	0.2051040	-0.8953390	2.9571070	C	-1.0919170	1.8572120	-3.3281850
H	1.2295050	-0.5343310	2.7634050	H	-0.9863160	1.6804500	-4.4106190
H	-0.4773830	-0.0365410	2.8592750	H	-1.7839150	1.1049920	-2.9184520
H	0.1646590	-1.2402850	4.0033200	H	-1.5760640	2.8373380	-3.1888150
H	0.9520150	4.2650150	-3.0770320	C	1.5481120	0.3133740	-3.0398020
H	2.5070620	3.4854530	-2.7061350	H	1.5100630	0.2197320	-4.1367170
H	1.7048390	3.1797440	-4.2670630	H	2.6069980	0.3602230	-2.7397710
Si	0.1231800	3.1931250	0.2256700	H	1.1396120	-0.6205350	-2.6217400
C	-1.6320580	3.8613020	-0.0837940	C	1.5288780	3.3339040	-3.1902800
H	-1.9395580	4.6029980	0.6718140	H	-0.7581910	2.2211260	2.3344580
H	-1.7087910	4.3310670	-1.0773670	H	1.0053160	2.0269520	2.2825530
H	-2.3428130	3.0202030	-0.0571870	H	0.2890300	3.6119440	2.7122810
C	1.2506580	4.7187140	-0.0256490	O	-2.5112710	0.7756910	1.7066210
H	0.9967520	5.2296030	-0.9665910	S	-4.0209590	0.6170570	1.7646900
H	1.1011160	5.4411810	0.7936980	C	-4.3881070	0.7731790	3.5254920
H	2.3243900	4.4811460	-0.0740330	H	-5.4737220	0.7824400	3.6879770
C	0.1826200	2.7262380	2.0641350	H	-3.9357870	-0.1010380	4.0097900
H	-4.4926320	2.2371580	0.1358490	H	-3.9135410	1.6919290	3.8931620
H	-5.7843860	2.2116670	1.4066200	C	-4.7034220	2.1914470	1.2114350
H	-4.1789700	2.9995180	1.7381260				

Table S96. Geometric coordinates and single point energies for NaHMDS disolvated DMSO monomer.



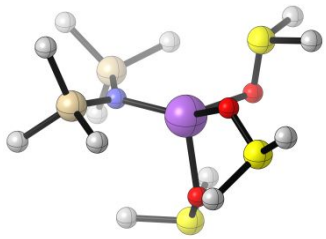
G = -2140.395238 Hartrees

G_{SP} = -2141.674509 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.0396930	1.6126480	-0.1515750	H	-3.1291000	-1.5644060	-1.1292490
N	-0.1149770	-0.6656670	0.0289360	H	-2.6070770	-3.1109420	-1.8278910
Si	0.3002350	-1.0373460	1.6344690	O	-1.8781810	2.6199800	0.0881630
C	1.9784810	-1.9118190	1.8460780	S	-3.2979950	2.0736090	0.1653660
H	2.8124260	-1.2496850	1.5647060	C	-3.5747030	1.3039650	-1.4447010
H	2.1378440	-2.2117760	2.8941350	H	-4.5531450	0.8062500	-1.4594100
H	2.0351950	-2.8173770	1.2219550	H	-3.5463260	2.1129040	-2.1845540
C	0.4490340	0.5853260	2.6235340	H	-2.7613800	0.5869340	-1.6214120
H	0.6859390	0.3943650	3.6815230	C	-3.1874790	0.5559590	1.1373500
H	1.2584130	1.2212240	2.2240860	H	-3.0117850	0.8589980	2.1772820
H	-0.4840910	1.1727350	2.5954030	H	-4.1341010	0.0039580	1.0606810
C	-0.9519870	-2.1409480	2.5456510	H	-2.3320730	-0.0268510	0.7520190
H	-1.9682550	-1.7167550	2.5201610	O	2.1633210	2.0642580	-0.3866930
H	-0.9982780	-3.1347230	2.0707220	S	3.2677970	1.0828100	-0.0110450
H	-0.6721950	-2.2885960	3.6007080	C	3.1103880	-0.2894620	-1.1659760
Si	-0.5885410	-1.7349450	-1.2008190	H	3.9233750	-1.0079570	-0.9956520
C	0.4616890	-3.3165970	-1.3190110	H	2.1316430	-0.7347470	-0.9266530
H	0.1547040	-3.9457900	-2.1694320	H	3.1218010	0.1108760	-2.1885440
H	1.5319590	-3.0840950	-1.4403160	C	4.7603510	1.8385430	-0.6886830

H	0.3569350	-3.9192460	-0.4020040	H	4.9350810	2.7564440	-0.1152880
C	-0.4489170	-0.8811200	-2.8953340	H	5.6081880	1.1504810	-0.5780080
H	0.6046250	-0.6480150	-3.1183480	H	4.5686330	2.0810860	-1.7417540
H	-0.8307590	-1.5152640	-3.7105810	H	-2.5259230	-2.8520520	-0.0676730
H	-1.0027710	0.0717990	-2.9269180				
C	-2.3806800	-2.3678120	-1.0467270				

Table S97. Geometric coordinates and single point energies for NaHMDS trisolvated DMSO monomer.



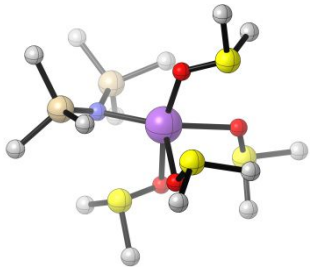
G = -2693.187629 Hartrees

G_{SP} = -2694.803643 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.5022200	0.1122760	0.1269820	C	-3.0278720	2.8852130	0.0925800
N	1.7548910	0.1332950	0.4203770	H	-2.1488970	2.8881010	-0.5641620
Si	2.0457750	1.5219630	1.3537820	H	-3.8506370	3.4608550	-0.3519400
C	3.4966470	2.5886630	0.7353290	H	-2.7783230	3.2393190	1.1014680
H	3.3429860	2.9120370	-0.3067250	O	-1.0286820	1.4161700	-1.6156470
H	3.6393850	3.4898400	1.3527400	S	-0.1961260	1.2453120	-2.8896600
H	4.4340570	2.0095380	0.7652320	C	1.4402650	1.8859770	-2.4773560
C	0.4971610	2.6360770	1.3011140	H	2.1184630	1.6999950	-3.3213780
H	0.6712120	3.5901130	1.8229410	H	1.3246690	2.9645890	-2.3126570
H	0.2074650	2.8599260	0.2609730	H	1.7719540	1.3702560	-1.5567700
H	-0.3620650	2.1462260	1.7924400	C	0.2496460	-0.5030220	-2.9452790
C	2.3781760	1.2098470	3.1972540	H	-0.6866360	-1.0732590	-2.9690020
H	1.5684210	0.6021600	3.6313230	H	0.8522360	-0.6845540	-3.8453070
H	3.3224180	0.6647250	3.3473890	H	0.8090260	-0.7470740	-2.0310520
H	2.4385300	2.1547870	3.7609200	O	-1.3074930	-1.8612760	-0.6657370
Si	2.8221010	-1.1485970	0.1247960	S	-1.5188280	-2.7438760	0.5587210
C	3.8257030	-0.9155900	-1.4815160	C	-3.2990040	-2.6970430	0.8480690
H	4.5374730	-1.7400970	-1.6470730	H	-3.5718690	-3.4061490	1.6402670
H	3.1731360	-0.8565290	-2.3677010	H	-3.4903520	-1.6632650	1.1609500
H	4.3999650	0.0240200	-1.4312850	H	-3.8074080	-2.9237460	-0.0982910

C	1.8772570	-2.7909530	-0.0844140	C	-1.3944260	-4.4312050	-0.0690430
H	1.0915490	-2.6922140	-0.8503230	H	-0.3396880	-4.5841930	-0.3282530
H	2.5451390	-3.6208830	-0.3649780	H	-1.7046210	-5.1411190	0.7084930
H	1.3900190	-3.0467430	0.8723750	H	-2.0265690	-4.5042560	-0.9635190
C	4.1140600	-1.4747710	1.4790680	S	-3.5286120	1.1575500	0.2102650
H	4.7659810	-0.5983400	1.6258620	C	-4.9438550	1.3959990	1.3120690
H	3.6239620	-1.6898540	2.4415580	H	-5.7121190	1.9993020	0.8115320
H	4.7566790	-2.3319220	1.2218840	H	-5.3415420	0.4011120	1.5463600
O	-2.4985850	0.4790720	1.1141670	H	-4.5815070	1.8814370	2.2274500

Table S98. Geometric coordinates and single point energies for NaHMDS tetrasolvated DMSO monomer.



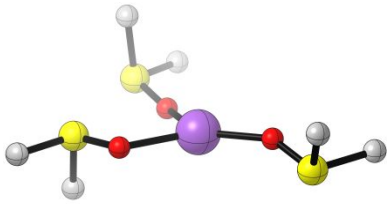
G = -3245.975952 Hartrees

G_{SP} = -3247.927531 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.0887620	0.1423070	-0.0969850	C	2.7374890	3.9915630	1.0862290
N	-2.2386230	0.4157640	-0.0777250	H	2.6948920	3.7832290	2.1618840
Si	-2.7173490	0.7493970	1.5021650	H	3.7066820	4.4313450	0.8172020
C	-4.0042000	-0.4929470	2.1696600	H	1.9019340	4.6442530	0.8021250
H	-3.5774090	-1.5091740	2.2098940	O	2.1032590	-0.0358720	-1.3470360
H	-4.3368960	-0.2335580	3.1877000	S	1.8542960	-1.2085280	-2.3038630
H	-4.8923540	-0.5260600	1.5181680	C	3.2474770	-1.1080720	-3.4540480
C	-1.2450590	0.5976390	2.7117890	H	3.2718310	-2.0072830	-4.0837850
H	-1.5576520	0.7804410	3.7528230	H	3.0837170	-0.2206430	-4.0773980
H	-0.8178170	-0.4171810	2.6480190	H	4.1737860	-0.9999750	-2.8744850
H	-0.4554390	1.3234890	2.4517340	C	2.3888090	-2.6681110	-1.3906880
C	-3.4554120	2.4756660	1.7976810	H	1.8224080	-2.6106590	-0.4518360
H	-2.7343570	3.2498410	1.4894990	H	2.1099610	-3.5648220	-1.9590800
H	-4.3749040	2.6225630	1.2100490	H	3.4725110	-2.6179740	-1.2189880
H	-3.6990050	2.6360170	2.8603780	O	-0.4402330	-1.9929970	-0.9132450
Si	-2.5046690	1.0354760	-1.6208860	S	-1.3304460	-2.3387230	0.2864120
C	-3.0254080	-0.2943070	-2.8785780	C	-2.9333030	-2.7494460	-0.4168790
H	-3.0534940	0.1127400	-3.9022270	H	-3.5371850	-3.2733530	0.3359720
H	-2.2909070	-1.1160110	-2.8511350	H	-3.3752670	-1.7760850	-0.6622740

H	-4.0209990	-0.7120490	-2.6568200	H	-2.7716930	-3.3604930	-1.3147740
C	-0.8865300	1.7454460	-2.3622330	C	-0.7818620	-4.0151360	0.6987750
H	-0.1330430	0.9517330	-2.5143870	H	0.2216280	-3.8933830	1.1255810
H	-1.0550730	2.2267210	-3.3388890	H	-1.4557140	-4.4612420	1.4421830
H	-0.4614280	2.4901800	-1.6700050	H	-0.7455260	-4.6133620	-0.2214080
C	-3.7803430	2.4380310	-1.7536650	O	1.1929040	-1.3200490	1.3881300
H	-4.7634180	2.1026670	-1.3859760	S	2.1567470	-0.4542020	2.1892210
H	-3.4775990	3.3055570	-1.1468510	C	2.4078260	-1.3738370	3.7231130
H	-3.9038500	2.7722960	-2.7963860	H	3.2146100	-0.9156050	4.3098450
O	1.0796820	2.0270110	0.5868250	H	1.4590450	-1.3125770	4.2703700
S	2.5090360	2.4056080	0.2476770	H	2.6342130	-2.4170700	3.4670210
C	2.4796410	3.0259600	-1.4458910	C	3.7618180	-0.7634810	1.4197760
H	3.4748230	3.4086140	-1.7092420	H	3.6369110	-0.4076480	0.3864070
H	2.2137010	2.1543040	-2.0550180	H	4.5461940	-0.1991760	1.9416580
H	1.7096500	3.8043810	-1.5216480	H	3.9600840	-1.8439690	1.4383000

Table S99. Geometric coordinates and single point energies for sodium cation solvated by 3 DMSO molecules.

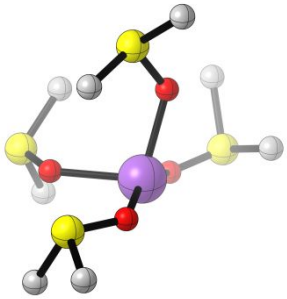


G = -1820.502293 Hartrees

G_{SP} = -1821.570515 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.6108080	0.0915100	0.0733800	S	-2.2038360	1.6812570	-0.1425140
O	-1.1788710	-1.1242040	0.3765970	C	-2.6282660	1.5290110	1.6036030
S	-2.5399530	-1.7363210	0.0543350	H	-3.7191490	1.5414830	1.7260460
C	-2.5840610	-1.8785960	-1.7418980	H	-2.2117930	0.5651520	1.9214390
H	-3.4876660	-2.4237880	-2.0441770	H	-2.1517110	2.3558920	2.1460500
H	-2.6142360	-0.8541370	-2.1325310	C	-2.7979130	3.3588250	-0.4198760
H	-1.6740030	-2.3943260	-2.0749190	H	-2.5199290	3.6233770	-1.4468320
C	-2.3640280	-3.4824960	0.4594090	H	-3.8882950	3.3928120	-0.2998250
H	-2.2210480	-3.5370740	1.5450310	H	-2.2895840	4.0224330	0.2909770
H	-3.2770000	-4.0193160	0.1713120	C	4.8510880	0.8782820	-1.1437920
H	-1.4815360	-3.8747880	-0.0617690	H	4.3071620	1.7943090	-1.4031310
O	2.7201850	-0.1739040	0.0025740	H	5.9134330	1.1040790	-0.9849580
S	4.1296270	0.2657660	0.3899780	H	4.7103750	0.1162050	-1.9209280
C	5.0564940	-1.2741630	0.5170170	O	-0.6854980	1.8156320	-0.1753730
H	6.1189590	-1.0514700	0.6789970				
H	4.6493900	-1.8142640	1.3798480				
H	4.8979000	-1.8498070	-0.4037680				

Table S100. Geometric coordinates and single point energies for sodium cation solvated by 4 DMSO molecules.



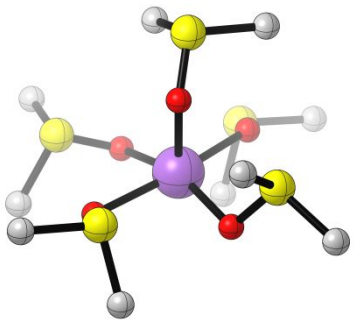
G = -2373.308057 Hartrees

G_{SP} = -2374.711214 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.0729290	0.1166760	-0.8421200	H	-1.6362570	-2.2155700	0.5444660
O	-2.1122770	-0.5282360	-1.2684920	C	0.5550670	-3.9282400	1.1238180
S	-3.3807440	-0.1258790	-0.5156270	H	1.6045310	-4.2155010	0.9892470
C	-3.5708100	1.6457090	-0.7798950	H	0.1142380	-4.4929190	1.9553090
H	-4.5469730	1.9668990	-0.3939520	H	-0.0063210	-4.0762160	0.1923460
H	-2.7547910	2.1055360	-0.2104120	O	-0.8954450	1.2933690	0.8700470
H	-3.4763680	1.8474880	-1.8549260	S	-0.0988030	2.2260180	1.7948000
C	-4.7140790	-0.6966130	-1.5868830	C	1.4081980	1.3082390	2.1726170
H	-4.6654100	-1.7917580	-1.5961270	H	2.1092220	1.9664870	2.7029960
H	-5.6800840	-0.3638690	-1.1860770	H	1.1223910	0.4715080	2.8233290
H	-4.5365240	-0.3027550	-2.5956850	H	1.8151430	0.9479720	1.2169170
O	1.0518510	-1.4907830	0.2366710	C	0.6324030	3.4647350	0.7063130
S	0.5425140	-2.1696350	1.5144110	H	-0.2016650	4.0348940	0.2792910
C	-1.2406980	-1.9071810	1.5221730	H	1.2635170	4.1318780	1.3083470
H	-1.6826890	-2.4750020	2.3515690	H	1.2066020	2.9482760	-0.0775960
H	-1.3947970	-0.8260580	1.6555410	O	1.8594520	1.1384970	-1.1687150
H	3.2415870	-0.8200890	0.2268070	S	3.1800140	0.5669380	-1.6968780
C	2.7305970	-0.9756580	-2.5216220	C	3.9832760	-0.1688060	-0.2568740

H	2.1104280	-0.7033570	-3.3848800	H	4.8731160	-0.7209010	-0.5869090
H	3.6445010	-1.4748450	-2.8696920	H	4.2843280	0.6578980	0.3981230
H	2.1744340	-1.5983840	-1.8059800				

Table S101. Geometric coordinates and single point energies for sodium cation solvated by 5 DMSO molecules.



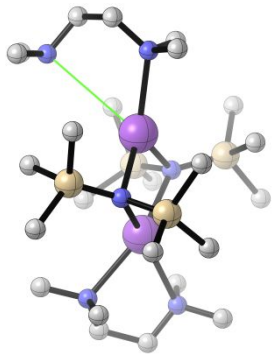
G = -2926.111957 Hartrees

G_{SP} = -2927.852845 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.0363420	-0.0136200	-0.4566180	H	-2.4503520	4.3376190	-0.4184360
O	1.4335160	-1.7807080	-0.4854950	C	-3.2252920	1.9677000	-1.7460050
S	2.9099230	-1.6955660	-0.8817910	H	-3.0061230	0.9881290	-2.1880990
C	3.2997460	-3.3711170	-1.4283340	H	-4.3046330	2.0944170	-1.5872260
H	4.3140140	-3.3995780	-1.8468780	H	-2.8104940	2.7827530	-2.3529640
H	3.2409910	-4.0160890	-0.5436380	O	-1.9244160	-0.8162020	-1.2143490
H	2.5490940	-3.6757300	-2.1687150	S	-2.4158120	-2.0018410	-0.3827620
C	2.9361480	-0.8952590	-2.4967570	C	-3.6994320	-1.3220360	0.6831790
H	2.6622760	0.1493220	-2.3077790	H	-4.1982430	-2.1367960	1.2248050
H	3.9479920	-0.9634430	-2.9172480	H	-3.1661490	-0.6556570	1.3721830
H	2.1995720	-1.3945890	-3.1400550	H	-4.4119550	-0.7658230	0.0592040
O	2.0080970	1.0938510	-0.3543290	C	-3.4755800	-2.9138320	-1.5232520
S	1.9587910	2.4266430	0.3974420	H	-2.8203340	-3.3156650	-2.3050340
C	3.6969510	2.7917970	0.7199660	H	-3.9773170	-3.7331970	-0.9924140
H	3.7927750	3.7876730	1.1714760	H	-4.2000660	-2.2156160	-1.9616530
H	4.0559770	2.0253640	1.4175230	O	-0.8623020	-0.4229290	1.5772650
H	4.2478520	2.7262580	-0.2270430	S	-0.1099720	-1.0180650	2.7673730
C	1.6573780	3.6753240	-0.8633500	C	0.2164820	-2.7334550	2.3095790

H	0.6330950	3.4851150	-1.2061230	H	0.8142480	-3.2090990	3.0983590
H	1.7437540	4.6727930	-0.4128140	H	-0.7626460	-3.2222540	2.2363660
H	2.3872660	3.5348890	-1.6710150	H	0.7245430	-2.7289860	1.3340940
O	-0.8903160	2.0343020	-0.5124590	C	1.5778160	-0.3925130	2.6131140
S	-2.3765370	1.9570640	-0.1568960	H	1.5297700	0.6796770	2.8440930
C	-2.7774100	3.6390980	0.3625720	H	2.2252850	-0.9060690	3.3360660
H	-3.8558120	3.7248770	0.5484130	H	1.8982340	-0.5518190	1.5732790
H	-2.2221350	3.8188280	1.2908700				

Table S102. Geometric coordinates and single point energies for NaHMDS TMEDA disolvated dimer. The green bond indicates a minor N–Na contact. This contact is an angstrom longer than the other N–Na bonds.



G = -2763.842314 Hartrees

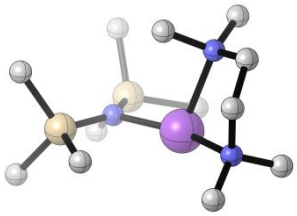
G_{SP} = -2765.821037 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
N	0.2894380	1.8569280	0.0388730	H	-0.6427280	5.0783660	0.1551780
Na	1.7377060	-0.0981030	-0.1733730	H	-1.9749690	4.1378710	0.8462750
Na	-1.3054120	0.1157010	0.4197330	H	-0.9459960	5.1337020	1.9018090
N	0.1844440	-1.7404070	0.6075800	N	-3.6728600	0.4986390	1.2226660
Si	0.7675580	-1.9289830	2.2063620	C	-3.6926060	-0.0062020	2.5918350
C	1.4443530	-3.6487050	2.6421990	H	-3.6970140	-1.1051010	2.5906820
H	1.8945710	-3.6358180	3.6474910	H	-2.8017320	0.3295580	3.1384310
H	0.6413320	-4.4029420	2.6492060	H	-4.5885500	0.3480840	3.1420420
H	2.2138340	-3.9846190	1.9297930	C	-4.8902030	0.0454580	0.5487680
C	2.2024680	-0.7161240	2.5230000	C	-5.0134900	0.3934500	-0.9274660
H	3.1088800	-1.0125360	1.9729030	N	-4.1531620	-0.3710100	-1.8117440
H	1.9506580	0.3176890	2.2304320	C	-4.5116040	-1.7790070	-1.8189650
H	2.4626490	-0.6939410	3.5927750	H	-3.9517280	-2.2947750	-2.6081870
C	-0.5184530	-1.5481960	3.5513630	H	-4.2556450	-2.2659800	-0.8692360
H	-0.7871040	-0.4807700	3.5451800	H	-5.5963680	-1.9234970	-2.0154000
H	-1.4365480	-2.1377850	3.4022440	C	-4.2167020	0.1574550	-3.1627050
H	-0.1247360	-1.7791880	4.5539720	H	-3.9725670	1.2277170	-3.1641600

Si	-0.6928940	-2.9516530	-0.2197400	H	-3.4859840	-0.3618450	-3.7996100
C	-1.2423070	-2.3471080	-1.9335270	H	-5.2248820	0.0298860	-3.6125320
H	-1.8517990	-1.4280870	-1.8884020	H	-4.8025710	1.4630800	-1.0805180
H	-0.3814990	-2.1467030	-2.5876960	H	-6.0818800	0.2483010	-1.2077540
H	-1.8491360	-3.1255500	-2.4225900	H	-4.9653430	-1.0442300	0.6817500
C	0.1891240	-4.6052300	-0.5430020	H	-5.7705470	0.4820350	1.0685600
H	0.5835640	-5.0507270	0.3816210	C	-3.6022510	1.9559180	1.2385390
H	-0.5264910	-5.3194320	-0.9812050	H	-2.7575610	2.2805530	1.8592770
H	1.0264060	-4.5088960	-1.2513450	H	-3.4396520	2.3532610	0.2282890
C	-2.2909940	-3.4139380	0.7130910	H	-4.5274350	2.4056550	1.6559850
H	-2.9309200	-4.1076190	0.1445840	N	4.2255150	0.7172960	-0.1100640
H	-2.0541940	-3.8894380	1.6789450	C	4.8563070	1.0618930	1.1532290
H	-2.8786890	-2.5044690	0.9313070	H	4.1686360	1.6626510	1.7627140
Si	0.0860090	2.2983340	-1.6024060	H	5.1006570	0.1507500	1.7167870
C	-1.7442840	2.5483500	-2.0527510	H	5.7899190	1.6431960	1.0037500
H	-2.3242550	1.6481710	-1.7813010	C	5.0941540	-0.1442540	-0.8997310
H	-2.1625390	3.4078450	-1.5048440	C	4.3784280	-0.8495650	-2.0443960
H	-1.8876170	2.7269930	-3.1304170	N	3.1800540	-1.5626590	-1.6287830
C	0.6761810	0.8763950	-2.7222140	C	3.4551170	-2.5696940	-0.6145860
H	1.7690360	0.7355080	-2.6883200	H	2.5161210	-3.0682760	-0.3400610
H	0.2080020	-0.0784270	-2.4312710	H	4.1818760	-3.3304410	-0.9711120
H	0.4073450	1.0643580	-3.7733350	H	3.8573470	-2.1057510	0.2960950
C	0.9995630	3.8559060	-2.1881650	C	2.5367900	-2.1776120	-2.7767640
H	0.8204430	4.0244760	-3.2619450	H	1.6200030	-2.6861330	-2.4520080
H	0.6567390	4.7525900	-1.6499870	H	2.2664500	-1.4126270	-3.5184980
H	2.0867460	3.7752120	-2.0373160	H	3.1954910	-2.9254490	-3.2663430
Si	0.2773920	3.0277880	1.2904320	H	5.1062200	-1.5403640	-2.5250800
C	-0.1637510	2.2618380	2.9747380	H	4.0860730	-0.1236950	-2.8209460
H	-1.1001340	1.6820770	2.9559100	H	5.9498100	0.4267740	-1.3203320
H	-0.2893610	3.0541510	3.7296550	H	5.5318370	-0.8952670	-0.2257820
H	0.6254720	1.5848840	3.3344980	C	3.8699770	1.9269650	-0.8370620

C	1.9340280	3.9079610	1.5929950	H	3.4075770	1.6771180	-1.8012780
H	1.8240450	4.6613320	2.3889890	H	3.1374870	2.5070200	-0.2607600
H	2.7186010	3.2043720	1.9104770	H	4.7577820	2.5633990	-1.0376900
H	2.2855880	4.4273870	0.6872710				
C	-0.9417060	4.4694590	1.0228540				

Table S103. Geometric coordinates and single point energies for NaHMDS TMEDA monosolvated monomer.



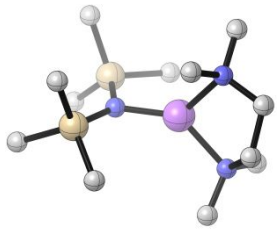
G = -1381.908281 Hartrees

G_{SP} = -1382.900732 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	3.2668390	0.8802470	1.0446370	H	-3.2824980	-3.6157140	-0.1571140
Na	0.7280570	0.0315630	-0.7263800	N	1.8482010	1.2113230	1.0654780
N	-1.3998540	-0.1369700	-0.1886050	C	1.6336330	2.6441380	1.2009940
Si	-2.2265060	1.2791450	-0.5813690	H	2.0557450	3.0393500	2.1474400
C	-2.7208780	2.3365340	0.9190330	H	2.0991580	3.1806750	0.3613430
H	-1.8481160	2.5759660	1.5481470	H	0.5553540	2.8551720	1.1899070
H	-3.1980080	3.2845020	0.6238300	C	1.1319500	0.4979300	2.1197400
H	-3.4327220	1.7823750	1.5513250	H	1.4768750	0.8099470	3.1264720
C	-1.0555920	2.3666170	-1.6367690	H	0.0526600	0.6791050	2.0172240
H	-1.5089080	3.3286260	-1.9214300	H	1.2826780	-0.5870860	2.0258860
H	-0.1217500	2.6040260	-1.0953510	N	3.0231030	-0.7058350	-0.8828430
H	-0.7904340	1.8423340	-2.5716580	C	3.5601760	-0.4989650	0.4616750
C	-3.8019970	1.0496790	-1.6101750	H	3.1368490	-1.2814070	1.1107840
H	-3.5947080	0.4490580	-2.5094030	H	4.6613230	-0.6483550	0.4677230
H	-4.5696050	0.5171880	-1.0267590	C	3.5768590	0.2365340	-1.8453410
H	-4.2300380	2.0135240	-1.9281430	H	3.2703840	1.2660810	-1.6090950
Si	-1.7634560	-1.6770410	0.3934470	H	4.6853250	0.2028090	-1.8740090
C	-2.1878040	-1.7471590	2.2437870	H	3.2034380	-0.0028400	-2.8508330
H	-2.3854790	-2.7756670	2.5852490	C	3.2558080	-2.0790150	-1.3110960
H	-1.3688980	-1.3370170	2.8560350	H	2.7884340	-2.7752330	-0.6014910

H	-3.0861650	-1.1440130	2.4504340	H	2.8047750	-2.2457100	-2.2992610
C	-0.2029340	-2.7693240	0.1749550	H	4.3375160	-2.3128660	-1.3775150
H	0.6607420	-2.3511400	0.7244140	H	3.7900040	1.6475190	0.4541600
H	-0.3498000	-3.7956260	0.5455990	H	3.7074220	0.9252410	2.0628170
H	0.0706790	-2.8422530	-0.8924710				
C	-3.1617710	-2.5804090	-0.5133530				
H	-4.1198410	-2.0585390	-0.3630820				
H	-2.9674360	-2.6071570	-1.5968130				

Table S104. Geometric coordinates and single point energies for LiHMDS TMEDA monosolvated monomer.



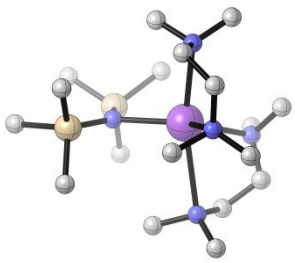
G = -1227.22675 Hartrees

G_{SP} = -1228.175576 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	-1.8625680	1.4667750	-0.2308920	H	2.8119630	1.9180000	-0.1930850
N	-1.0443340	0.0220390	0.1301950	H	4.2825040	1.2386510	0.5282370
Si	-1.6486850	-1.5374270	0.4144440	C	2.1378010	1.5724710	2.2257430
C	-2.8545790	-1.7089640	1.8651180	H	3.0568030	1.9389240	2.7245990
H	-3.1011140	-2.7644400	2.0618060	H	1.6573830	2.4095520	1.7032740
H	-2.4197690	-1.2785820	2.7805840	H	1.4407060	1.2076800	2.9920540
H	-3.7949140	-1.1744370	1.6618350	C	3.0234820	-0.6421740	1.9591940
C	-0.1419910	-2.6332050	0.8696200	H	4.0380090	-0.4113880	2.3420770
H	0.3182820	-2.2947070	1.8150210	H	2.3904760	-0.9308790	2.8088740
H	-0.4371740	-3.6829330	1.0188810	H	3.0915810	-1.5092070	1.2865820
H	0.6347690	-2.6356540	0.0837100	C	-3.5365100	1.6472440	0.6421090
C	-2.4803360	-2.3467960	-1.0861350	H	-3.4308890	1.5094010	1.7294520
H	-3.3881020	-1.7855420	-1.3609440	H	-3.9826560	2.6378390	0.4609610
H	-1.8106650	-2.3338150	-1.9608590	H	-4.2488510	0.8893600	0.2772580
H	-2.7764960	-3.3896650	-0.8919310	C	-0.8111830	2.9643020	0.2888740
Li	0.7933120	-0.2570730	0.2625170	H	-1.2746420	3.9170290	-0.0110510
N	2.4279370	0.5018210	1.2789010	H	-0.6818140	2.9782370	1.3827380
C	3.2608590	0.9833880	0.1774390	H	0.1917030	2.9263950	-0.1716500
C	3.3613350	-0.0323640	-0.9567210	C	-2.2234330	1.6989660	-2.0841820
N	2.0448050	-0.4874830	-1.3972210	H	-1.2988040	1.8299690	-2.6682070

C	1.3715870	0.5024830	-2.2354670	H	-2.7491110	0.8178780	-2.4854470
H	1.2621460	1.4568250	-1.7003720	H	-2.8565620	2.5824320	-2.2638830
H	1.9313160	0.6849040	-3.1744540	H	3.9403560	0.4111310	-1.7917950
H	0.3577600	0.1512210	-2.4673040	H	1.0967070	-2.1013400	-2.3391680
C	2.1131250	-1.7672190	-2.0885000	H	2.7018020	-1.7013810	-3.0249580
H	2.5743330	-2.5243820	-1.4385040	H	3.9307700	-0.9101620	-0.6172990

Table S105. Geometric coordinates and single point energies for NaHMDS TMEDA disolvated monomer.



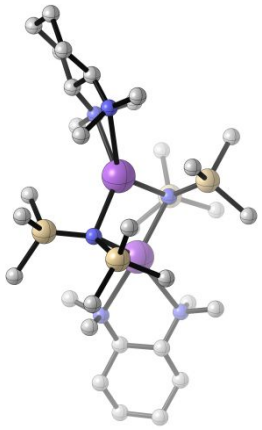
G = -1729.011139 Hartrees

G_{SP} = -1730.397455 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.7932070	2.3183800	1.3684070	H	-0.2474570	3.0177790	0.4454610
Si	-2.7528500	0.4136820	1.2077110	H	0.6357370	4.3171890	-0.3627140
N	-1.6979470	-0.1468230	-0.0035590	C	-0.7330300	2.5746980	-1.9326990
Si	-2.1014710	-1.0643830	-1.3743310	H	-1.0139120	3.6410400	-2.0599790
C	-3.8392750	-0.8494080	-2.1119010	H	-0.7557130	2.0941110	-2.9179300
H	-3.8725630	-1.3201120	-3.1080950	H	-1.4624550	2.0654270	-1.2862370
H	-4.6246410	-1.3093150	-1.4957210	C	1.5987560	2.8823600	-2.3189540
H	-4.0855470	0.2178060	-2.2338570	H	1.5185080	2.2771430	-3.2332450
C	-1.9167830	-2.9463480	-1.1243470	H	1.4590070	3.9480620	-2.5994170
H	-2.5279670	-3.2828010	-0.2711620	H	2.6164770	2.7631220	-1.9238530
H	-2.2446800	-3.5025420	-2.0172210	N	2.4020790	-1.2223570	-1.3786770
H	-0.8752360	-3.2404730	-0.9150530	C	2.9930610	-2.0159110	-0.3022580
C	-0.9630070	-0.6440380	-2.8619760	C	1.9367050	-2.7745720	0.4977490
H	-1.4597010	0.1046990	-3.4980050	N	1.4448540	-1.9918590	1.6251450
H	0.0184860	-0.2284610	-2.5778610	C	0.1150270	-2.4256800	2.0379140
H	-0.7866200	-1.5342620	-3.4865630	H	-0.1711400	-1.8929780	2.9543090
Na	0.6145730	0.1040710	-0.1754120	H	-0.6292870	-2.1726720	1.2684450
N	0.6030360	2.4449360	-1.3562500	H	0.0866890	-3.5149570	2.2507940
C	0.6663010	3.2303690	-0.1284820	C	2.3650360	-2.0941580	2.7442570

C	1.8944960	2.9655450	0.7298550	H	2.0754170	-1.3998550	3.5469180
N	1.9541230	1.6155700	1.2784710	H	2.3807330	-3.1203460	3.1677590
C	3.2776100	1.3346740	1.8041600	H	3.3910550	-1.8492040	2.4339840
H	3.3066090	0.3109970	2.1989230	H	2.3323930	-3.7532470	0.8423800
H	4.0350490	1.4275020	1.0119900	H	1.0852650	-2.9986690	-0.1607500
H	3.5547530	2.0287510	2.6250990	H	3.5227780	-1.3294430	0.3762800
C	0.9540220	1.4098080	2.3186320	H	3.7532150	-2.7111210	-0.7159640
H	1.0099540	0.3712830	2.6721040	C	3.2959580	-0.1525490	-1.7909070
H	1.1035670	2.0957320	3.1783170	H	4.2858390	-0.5330360	-2.1183420
H	-0.0602520	1.5634910	1.9266180	H	2.8458160	0.3992330	-2.6267390
H	1.9188100	3.7189120	1.5466440	H	3.4448070	0.5499000	-0.9571270
H	2.8066870	3.1292110	0.1354450	C	2.0821530	-2.0740320	-2.5172180
H	-5.0423480	0.3945220	0.1255540	H	1.6633610	-1.4724540	-3.3324280
C	-2.3406110	-0.1871810	2.9698830	H	2.9854750	-2.5991290	-2.8906830
H	-3.0287970	0.2840940	3.6900370	H	1.3292200	-2.8261210	-2.2432540
H	-2.4705410	-1.2780780	3.0500870	C	-4.5820280	-0.0680580	1.0110920
H	-1.3140420	0.0550170	3.2847160	H	-4.7011690	-1.1597930	0.9207750
H	-1.8725870	2.7417310	1.8019710	H	-5.1490010	0.2589600	1.8973370
H	-2.9611190	2.8021090	0.3930730	H	-3.6188610	2.6166380	2.0342400

Table S106 Geometric coordinates and single point energies for NaHMDS (R,R)-TMCDA disolvated dimer.



G = -3075.385111 Hartrees

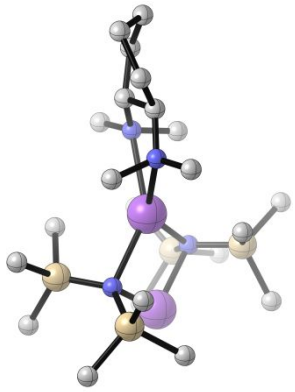
G_{SP} = -3077.699253 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	1.5988980	-0.1281490	-0.0283950	H	5.3039760	-3.0361640	0.2825190
N	-0.0101300	-1.9520580	-0.2816790	H	4.5983840	-2.1100120	1.6384630
Na	-1.5205070	-0.0276390	-0.1702010	H	3.5555580	-3.0911840	0.6042160
N	-0.0234350	1.8474340	-0.3993980	H	5.0025660	-2.2593210	-2.0057870
Si	0.4836080	2.2835070	-1.9805710	H	3.2510170	-2.4600910	-1.7320280
C	1.4448130	3.9209550	-2.1310130	H	3.8740730	-0.9029770	-2.3162510
H	1.7525850	4.0730030	-3.1780540	H	1.5144130	-3.8234440	-2.6407110
H	0.8144080	4.7788840	-1.8490900	C	-1.5594540	-4.1636630	-1.7275650
H	2.3503350	3.9560650	-1.5080300	H	-0.9932950	-5.0066100	-1.3017650
C	1.6705630	0.9430630	-2.6334490	H	-2.4713520	-4.0362110	-1.1252890
H	2.6203840	0.9745470	-2.0706610	H	-1.8676770	-4.4568750	-2.7438840
H	1.2453590	-0.0706160	-2.5455370	H	-1.8501390	-1.6153460	-3.7002470
H	1.9245640	1.0989700	-3.6929310	H	-1.0451860	-0.3290960	-2.7840050
C	-0.9039350	2.5041820	-3.2612860	H	-4.1403790	-2.8169000	1.1249520
H	-1.5401240	1.6163230	-3.3901400	H	-3.8052450	-1.9822110	-0.4320650
H	-1.5511230	3.3437880	-2.9599880	H	-2.4639690	-2.5138420	0.5957040

H	-0.4752720	2.7532210	-4.2450400	H	-5.3719920	-0.8004090	3.2202750
H	-3.9040160	0.4255170	-3.1789060	H	-6.0492420	-1.6946080	1.8509550
C	-4.7389850	0.2250500	-2.4921720	H	-6.7791010	1.1623110	2.7022050
N	-4.3064210	0.4579080	-1.1286170	H	-7.7901130	-0.2710610	2.9143350
C	-5.3067130	0.0722830	-0.1363350	H	-8.4805310	1.0813750	0.9005990
C	-6.5428210	0.9858890	-0.0737650	H	-7.9657890	-0.5489360	0.4520750
C	-7.6080830	0.4126030	0.8588290	H	-6.2414860	1.9841500	0.2869530
C	-7.0369470	0.1864180	2.2558680	H	-6.9549900	1.1224440	-1.0849790
C	-5.7820020	-0.6845590	2.2063780	H	-5.6656110	-0.9261250	-0.4440370
C	-4.7137930	-0.0798660	1.2775150	H	-5.0349470	-0.8274410	-2.6194240
H	-4.4951830	0.9334100	1.6657230	H	-5.5886260	0.8674370	-2.8006290
N	-3.4321730	-0.7933990	1.2681170	Si	0.5102960	-3.0197190	0.9539200
C	-2.8468300	-0.9181160	2.5953400	C	1.4761440	-2.0077780	2.2467940
H	-3.3073710	-1.7280590	3.1946960	H	2.3564410	-1.4998000	1.8208200
H	-1.7723720	-1.1437530	2.5053130	H	0.8139920	-1.2351680	2.6756800
H	-2.9529030	0.0255600	3.1474590	H	1.8337070	-2.6334400	3.0793680
C	-3.4773360	-2.0925020	0.6100880	C	1.5711690	-4.4802180	0.3322890
H	-2.5242700	-1.1019960	-2.1441040	H	2.1658580	-4.9244420	1.1470290
C	-1.5815610	-1.2864970	-2.6846970	H	0.9032120	-5.2700820	-0.0461920
Si	-0.5069930	-2.5798460	-1.8032790	H	2.2539810	-4.2144660	-0.4866680
C	0.8801650	-3.0106310	-3.0272120	C	-0.8168420	-3.9498530	1.9549300
H	0.4411460	-3.3574450	-3.9764650	H	-1.4679680	-4.5397460	1.2902700
H	1.5274270	-2.1503350	-3.2544490	H	-0.3076170	-4.6585050	2.6284250
C	4.0850860	-1.7489340	-1.6466580	H	-1.4574000	-3.3072830	2.5744010
N	4.1863390	-1.2945520	-0.2696680	H	-0.8098400	1.4780590	2.6201160
C	5.1567330	-0.2060830	-0.0882540	H	-1.7670220	2.9509110	2.9102540
C	4.8610200	0.5876960	1.1996750	C	-1.7416640	4.3686310	-0.0500910
C	5.9214830	1.6743070	1.4490290	H	-2.1629700	4.9914370	0.7555890
C	7.3455700	1.1288170	1.4349140	H	-1.1731280	5.0415700	-0.7119760
C	7.6207510	0.4507110	0.0965370	H	-2.5773470	3.9652850	-0.6367090
C	6.6210660	-0.6801340	-0.1229560	H	1.3540770	4.6857010	0.7515050

H	6.8159480	-1.1954110	-1.0762600	H	0.2229230	4.9384060	2.0972360
H	6.7740410	-1.4243190	0.6755440	H	1.8624570	1.5055570	2.4596160
H	7.5335530	1.1945930	-0.7140440	H	3.0545850	0.3562670	3.1130760
H	8.6476430	0.0582320	0.0574620	H	3.4130650	2.1148630	3.0909670
H	8.0624000	1.9425100	1.6193200	C	3.3277400	2.3309050	0.4217950
H	7.4788040	0.3962630	2.2495990	H	3.7403330	3.2237820	0.9323460
H	5.8460860	2.4386790	0.6591800	H	3.8233860	2.2348600	-0.5550970
H	5.7028910	2.1828250	2.4013880	H	2.2600960	2.5077190	0.2456620
H	4.9199380	-0.1254540	2.0397660	H	5.0085900	0.4843250	-0.9388350
N	3.4870070	1.1085510	1.1973550	C	4.4307080	-2.4345170	0.6027760
C	2.9386080	1.2816030	2.5319880	H	-2.3804030	1.6912750	1.8193360
H	1.4252860	3.6358650	2.1854280	H	-3.4949170	1.9760810	0.0790330
C	0.7430180	4.1668710	1.5067260	C	-3.7882690	1.7999620	-0.9647500
Si	-0.5735460	3.0562020	0.6905600	H	-4.5109370	2.5929840	-1.2500650
C	-1.4702120	2.2210640	2.1413410	H	-2.8905110	1.9326550	-1.5872020

Table S107. Geometric coordinates and single point energies for NaHMDS (R,R)-TMCDA monosolvated dimer. The starting geometry for this computation started as a monosolvated open dimer but collapsed to a closed dimer.



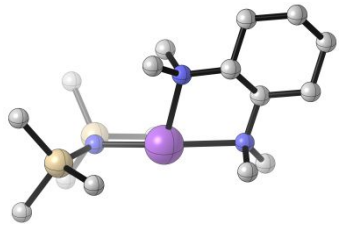
G = -2572.497021 Hartrees

G_{SP} = -2574.25027 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.6380980	0.2869740	-0.6929680	H	0.1949330	-4.2603770	1.5595810
Na	-0.2067990	0.0248270	-0.0239540	H	1.3830400	-4.2851770	2.8852870
C	-3.6496980	-0.2793310	0.7339290	C	3.2962860	-4.1843530	0.3819640
N	-2.3785740	-0.9171940	1.0982830	H	4.1651870	-3.7668170	-0.1505140
C	-2.3482010	-1.2740820	2.5075290	H	3.6749060	-4.7894520	1.2207340
H	-1.3284090	-1.5617680	2.7948470	H	2.7762810	-4.8639640	-0.3109310
H	-2.6398970	-0.4081330	3.1199360	C	3.2803580	-1.7580740	2.1619750
H	-3.0235530	-2.1178970	2.7514010	H	2.7587470	-0.8875490	2.5940480
C	-2.0184060	-2.0629690	0.2744460	H	3.6386630	-2.3617910	3.0097270
H	-2.0185820	-1.7862860	-0.7899260	H	4.1914540	-1.4040690	1.6434620
H	-0.9986500	-2.3881970	0.5299440	N	1.3822150	1.8538910	0.1452130
H	-2.6896270	-2.9347550	0.4034520	Si	2.0864450	2.8175050	-1.0787500
H	-3.7536690	0.5798850	1.4191520	C	2.7009190	4.5268260	-0.5351750
C	-4.8823360	-1.1961520	0.9453890	H	3.3530210	4.4793660	0.3502950
H	-5.1673320	-1.1544470	2.0076190	H	3.2696850	5.0056580	-1.3476280
H	-4.6029090	-2.2408110	0.7429430	H	1.8520040	5.1844500	-0.2924800

C	-6.0880830	-0.8087640	0.0797660	C	0.9775140	3.1470650	-2.5782450
C	-6.1189400	0.7021520	-0.1164400	H	0.7131290	2.2214260	-3.1117790
C	-4.9061410	1.1439100	-0.9452730	H	0.0453080	3.6531560	-2.2816130
H	-4.6826210	2.2010660	-0.7381370	H	1.4981990	3.8027590	-3.2938410
H	-5.1559420	1.0868530	-2.0155220	C	3.6196630	1.9153180	-1.7963720
H	-6.1047010	1.1896000	0.8723470	H	4.4050540	1.7677550	-1.0318590
H	-7.0479650	1.0247250	-0.6075160	H	3.3606140	0.9363990	-2.2404080
H	-6.0212320	-1.2941450	-0.9078600	H	4.0849150	2.5005920	-2.6038500
H	-7.0163860	-1.1732820	0.5419810	Si	1.2854880	2.2620080	1.8035600
N	-2.3872600	0.9883010	-1.0104700	C	2.9845800	2.3215770	2.6618780
C	-2.3412400	1.3832120	-2.4102660	H	2.8862690	2.5514820	3.7346330
H	-1.3319420	1.7337860	-2.6602000	H	3.5260410	1.3626620	2.5887840
H	-2.5739000	0.5205270	-3.0519000	H	3.6246630	3.0970690	2.2130030
H	-3.0543240	2.1968580	-2.6491550	C	0.4286470	3.9011480	2.2092900
C	-2.1009090	2.1310990	-0.1519810	H	0.2748900	4.0043960	3.2950400
H	-1.1008050	2.5204450	-0.3945010	H	1.0297090	4.7590780	1.8733360
H	-2.8273040	2.9600750	-0.2604310	H	-0.5550480	3.9667070	1.7185850
H	-2.0830420	1.8230910	0.9032350	C	0.2967520	0.9089860	2.7068020
H	-3.6764670	-0.5733490	-1.3840420	H	0.6624080	-0.1060770	2.4690180
Na	2.8230310	0.0458770	0.0553540	H	0.3616820	1.0297470	3.7991490
N	1.4894000	-1.7936190	-0.1924370	H	-0.7712020	0.9464560	2.4389100
Si	1.2305200	-2.2896840	-1.8112620	H	-0.7573590	-3.8151580	-1.5321350
C	0.2682540	-0.9209680	-2.7164790	H	0.0760730	-4.1323740	-3.0729210
H	0.7623270	0.0577290	-2.5839180	C	2.8257940	-2.5308480	-2.8113970
H	0.2130330	-1.1164850	-3.7982360	H	2.6049740	-2.7565530	-3.8666220
H	-0.7682110	-0.8243370	-2.3543130	H	3.4535030	-1.6243960	-2.7910420
C	0.2316610	-3.8909990	-2.0096260	H	3.4255000	-3.3607500	-2.4085660
H	0.7558240	-4.7430590	-1.5492040	Si	2.1598900	-2.8031260	1.0156590
H	0.2934280	-2.8939080	2.6976300	C	0.8889230	-3.6366710	2.1453460

Table S108. Geometric coordinates and single point energies for NaHMDS (R,R)-TMCDA monosolvated monomer.



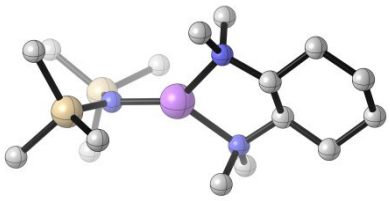
G = -1537.683691 Hartrees

G_{SP} = -1538.843276 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.9416610	0.5781630	0.3213690	H	-1.9697670	-1.1372520	2.1790610
Na	0.2119820	0.1406970	0.7537170	H	-1.2579060	0.1004840	3.2361710
N	2.2671080	0.0610370	-0.0337670	C	-1.9989470	2.2109360	1.8706810
Si	3.0395280	-1.3381660	0.5053470	H	-2.9161580	2.4751000	2.4314240
C	4.6840790	-1.0722040	1.4115730	H	-1.1411390	2.3880050	2.5368710
H	4.5644530	-0.3516400	2.2355720	H	-1.9036880	2.8910500	1.0125060
H	5.0750270	-2.0134540	1.8295670	N	-1.3005020	-1.0116530	-0.7029580
H	5.4451170	-0.6674840	0.7261620	C	-2.7103060	-0.7803550	-0.3745810
C	1.8821300	-2.1979610	1.7682320	H	-2.9861120	-1.5678220	0.3490570
H	2.2985860	-3.1423000	2.1514670	C	-3.6674530	-0.9205740	-1.5694900
H	1.7152400	-1.5403790	2.6399480	H	-3.4877880	-1.8845350	-2.0698530
H	0.9004200	-2.4418350	1.3237440	H	-3.4432230	-0.1317320	-2.3068260
C	3.3859440	-2.6176840	-0.8546260	C	-0.9695940	-2.4205410	-0.8501530
H	2.4667110	-2.8878760	-1.3982480	H	-1.2653470	-2.9767540	0.0516600
H	4.0869960	-2.1972470	-1.5930120	H	-1.4581610	-2.8901380	-1.7271790
H	3.8302550	-3.5422870	-0.4533280	H	0.1183030	-2.5231230	-0.9757510
Si	2.6997280	1.5473530	-0.7048380	C	-0.8108090	-0.2558120	-1.8532980
C	4.2732510	2.3374900	-0.0015820	H	-1.0976010	0.8031790	-1.7683300
H	4.4331260	3.3514260	-0.4013720	H	0.2896500	-0.3076080	-1.8710760
H	4.2205190	2.4031070	1.0963010	H	-1.2006010	-0.6412290	-2.8146220

H	5.1584300	1.7331470	-0.2544300	H	-2.7509960	1.3696640	-0.4261430
C	1.2815850	2.7864940	-0.3463660	C	-4.4155440	0.6934520	0.7464890
H	1.1537400	2.9209590	0.7423470	H	-4.5866740	1.6625200	1.2385470
H	1.4695180	3.7822530	-0.7768640	H	-4.6395610	-0.0889190	1.4917550
H	0.3222920	2.4336300	-0.7674400	C	-5.3666010	0.5320600	-0.4381450
C	2.9042050	1.5278340	-2.5924810	C	-5.1286250	-0.7992080	-1.1448060
H	3.7034200	0.8262890	-2.8793980	H	-5.3826350	-1.6265860	-0.4602140
H	1.9794860	1.1934120	-3.0891180	H	-5.7884560	-0.8986850	-2.0189770
H	3.1642450	2.5209850	-2.9917940	H	-5.2017880	1.3567530	-1.1524720
N	-1.9831900	0.8301570	1.4098440	H	-6.4093960	0.6131840	-0.0982200
C	-2.0766200	-0.0993140	2.5271460				
H	-3.0240240	-0.0159780	3.0928990				

Table S109. Geometric coordinates and single point energies for LiHMDS (R,R)-TMCDA monosolvated monomer.



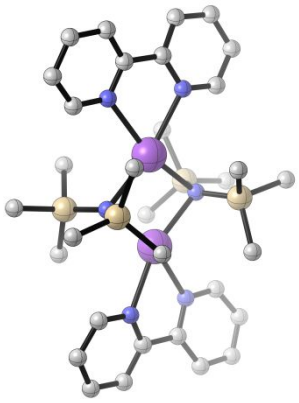
G = -1383.003398 Hartrees

G_{SP} = -1384.11993 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	2.6676500	-1.3661320	0.6801560	H	-3.9457900	1.9922760	1.5024400
N	1.9104010	-0.0014610	0.0002620	H	-3.9362620	0.2877470	1.9845480
Si	2.6722040	1.3619940	-0.6769560	C	-5.2172690	0.7052520	0.2991880
C	3.3074670	2.5942540	0.6201400	C	-5.2180020	-0.7095710	-0.2761180
H	3.7667360	3.4827290	0.1585500	H	-5.2638090	-1.4381190	0.5513330
H	2.4882720	2.9335420	1.2742700	H	-6.1136700	-0.8760990	-0.8920140
H	4.0625820	2.1156080	1.2631190	H	-5.2730960	1.4337240	-0.5277140
C	1.4220560	2.3121250	-1.7555030	H	-6.1074570	0.8691850	0.9236680
H	0.4963390	2.5313300	-1.1959330	C	-1.1993230	0.3737480	2.2022040
H	1.8295170	3.2748250	-2.1013470	H	-1.8822550	0.7202480	3.0002540
H	1.1500460	1.7242820	-2.6468660	H	-1.3188870	-0.7139120	2.0866310
C	4.1466800	0.9547960	-1.7988850	H	-0.1648750	0.5600020	2.5279400
H	4.9460330	0.4543670	-1.2287350	C	-1.2075980	2.4908500	1.0771310
H	3.8409590	0.2742590	-2.6090140	H	-1.8663520	2.9450240	1.8420230
H	4.5775420	1.8605010	-2.2540080	H	-0.1633090	2.6732950	1.3694270
Li	0.0623010	0.0020350	-0.0098540	H	-1.3866920	2.9959860	0.1178460
N	-1.4212470	1.0571910	0.9304010	C	4.1358860	-0.9600950	1.8106990
C	-2.6898340	0.7240010	0.2670350	H	3.8256540	-0.2799450	2.6194540
C	-2.6902710	-0.7211090	-0.2683670	H	4.5640260	-1.8660970	2.2677810
N	-1.4271470	-1.0505700	-0.9441040	H	4.9385500	-0.4594540	1.2453980

C	-1.2126760	-2.4835600	-1.0966390	C	1.4115800	-2.3177690	1.7502680
H	-1.3852400	-2.9917590	-0.1378090	H	1.8162940	-3.2820550	2.0949150
H	-1.8756750	-2.9362110	-1.8587410	H	1.1360450	-1.7324200	2.6421460
H	-0.1700110	-2.6640350	-1.3958800	H	0.4882980	-2.5338030	1.1854620
C	-1.2176010	-0.3630900	-2.2156900	C	3.3099110	-2.5970630	-0.6147270
H	-1.3343530	0.7243490	-2.0951950	H	2.4939480	-2.9361330	-1.2729770
H	-0.1871240	-0.5499800	-2.5533540	H	4.0681540	-2.1179320	-1.2536340
H	-1.9091000	-0.7058310	-3.0079680	H	3.7670210	-3.4857060	-0.1513030
H	-2.7419210	-1.3957310	0.6047090	H	-3.9544970	-0.2888280	-1.9738590
C	-3.9567580	-0.9638960	-1.1013250	H	-2.7521610	1.3984210	-0.6054890
H	-3.9545970	-1.9932580	-1.4912380	C	-3.9488790	0.9630110	1.1122600

Table S110. Geometric coordinates and single point energies for NaHMDS bipy disolvated dimer.



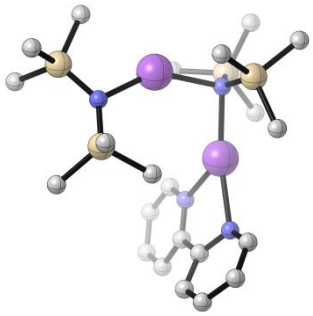
G = -3058.995001 Hartrees

G_{SP} = -3061.263951 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.5692120	-0.0002550	0.0004140	H	-1.0292540	-2.0215070	-3.7715650
N	-0.0001240	-1.8222230	-0.0004040	C	-0.2448520	-4.3464440	-1.7184640
Na	1.5688640	-0.0002920	-0.0015480	H	-0.1873290	-4.6503240	-2.7760210
N	-0.0002450	1.8215170	-0.0004420	H	0.5088650	-4.9248360	-1.1619530
Si	0.0907390	2.4775550	1.5681380	H	-1.2347060	-4.6471140	-1.3402840
C	-0.2410260	4.3453790	1.7185450	C	1.7860310	-2.2683930	-2.4203810
H	-0.1815950	4.6490660	2.7760520	H	2.5035280	-3.0285860	-2.0743500
H	0.5122230	4.9232920	1.1609040	H	1.6703310	-2.3980950	-3.5085000
H	-1.2312810	4.6468130	1.3420250	H	2.2540400	-1.2827350	-2.2609180
C	-1.1292810	1.6196480	2.7507810	Si	-0.0892820	-2.4795970	1.5677590
H	-2.1789600	1.7467730	2.4465290	C	1.1304350	-1.6212890	2.7503460
H	-0.9336980	0.5367340	2.8113120	H	2.1799960	-1.7458300	2.4445910
H	-1.0255870	2.0199660	3.7717120	H	1.0287640	-2.0235530	3.7707160
C	1.7884280	2.2652260	2.4184080	H	0.9327740	-0.5388780	2.8128430
H	2.2557790	1.2794200	2.2579780	C	-1.7867270	-2.2697750	2.4190840
H	2.5061970	3.0252830	2.0726470	H	-1.6711260	-2.3999290	3.5071620
H	1.6733000	2.3941320	3.5066840	H	-2.2548090	-1.2840960	2.2599630

Si	-0.0901570	2.4785680	-1.5686570	H	-2.5040960	-3.0299010	2.0726460
C	1.1295230	1.6204830	-2.7515260	C	0.2445550	-4.3472100	1.7165330
H	2.1791920	1.7451570	-2.4462130	H	-0.5086600	-4.9254850	1.1592290
H	0.9319850	0.5380290	-2.8138980	H	1.2347410	-4.6474860	1.3389080
H	1.0274090	2.0225990	-3.7719110	H	0.1863830	-4.6516290	2.7739000
C	-1.7877270	2.2677240	-2.4194880	C	-4.8146310	-0.7456470	-0.0352380
H	-2.5051700	3.0280560	-2.0736530	C	-5.9864310	-1.4915090	0.1420610
H	-1.6723200	2.3968710	-3.5077060	C	-5.9198560	-2.8787950	0.0566690
H	-2.2556180	1.2821270	-2.2593590	C	-4.6915210	-3.4807160	-0.1973050
C	0.2426990	4.3463200	-1.7177670	C	-3.5755500	-2.6574040	-0.3438780
H	0.1837180	4.6507050	-2.7750980	H	-2.5814510	-3.0792140	-0.5202050
H	-0.5105080	4.9241810	-1.1600060	N	-3.6365780	-1.3315710	-0.2668830
H	1.2329220	4.6471700	-1.3407100	H	-4.5879380	-4.5630300	-0.2701310
C	4.8142200	0.7471490	-0.0358740	H	-6.8185150	-3.4814960	0.1960900
C	5.9853950	1.4936750	0.1427420	H	-6.9313100	-0.9987600	0.3670200
C	5.9180950	2.8809300	0.0574160	C	-4.8140140	0.7478140	0.0370490
C	4.6896640	3.4821360	-0.1977850	C	-5.9853530	1.4946240	-0.1393340
C	3.5743230	2.6581810	-0.3455410	C	-5.9175870	2.8818520	-0.0539690
H	2.5801560	3.0794750	-0.5227030	C	-4.6885740	3.4827760	0.1990980
N	3.6360440	1.3323750	-0.2686290	C	-3.5731550	2.6585660	0.3448100
H	4.5855130	4.5643970	-0.2706160	H	-2.5785590	3.0795390	0.5203590
H	6.8162440	3.4841560	0.1978430	N	-3.6353310	1.3327810	0.2678470
H	6.9303110	1.0014260	0.3686570	H	-4.5840710	4.5650060	0.2718730
C	4.8144190	-0.7463070	0.0361970	H	-6.8158670	3.4852810	-0.1926830
C	5.9862810	-1.4924260	-0.1396120	H	-6.9308050	1.0026460	-0.3635760
C	5.9192310	-2.8797100	-0.0545680	H	6.8179240	-3.4826190	-0.1928650
C	4.6903950	-3.4813640	0.1976380	H	6.9315830	-0.9998510	-0.3631860
C	3.5744410	-2.6577980	0.3428850	Si	0.0887520	-2.4788670	-1.5688810
H	2.5799960	-3.0793330	0.5179040	C	-1.1313030	-1.6201710	-2.7508680
N	3.6359220	-1.3319650	0.2661890	H	-2.1808510	-1.7455160	-2.4454080
H	4.5864490	-4.5636650	0.2701500	H	-0.9342280	-0.5375990	-2.8124680

Table S111. Geometric coordinates and single point energies for NaHMDS bipy monosolvated open dimer.



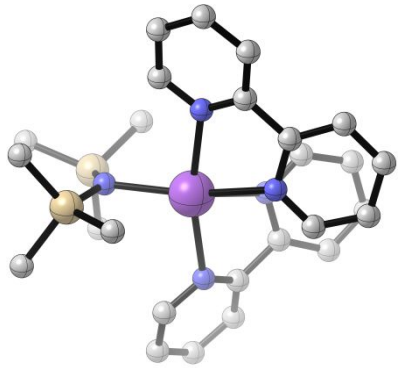
G = -2564.291623 Hartrees

G_{SP} = -2566.02517 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	1.4412770	1.0025880	0.3084450	C	0.8419280	2.1875220	2.8702300
N	-0.4789970	2.2986740	0.2169780	H	0.9316820	1.0871040	2.8823560
Na	-2.0659500	0.6676880	-0.1847540	H	1.7778090	2.6190160	2.4714940
N	-2.4559820	-1.5032270	-0.0400030	H	0.7621000	2.5060860	3.9209330
Si	-1.4117090	-2.5002500	0.8303860	C	-2.1637370	1.8545210	2.6124780
C	0.2434660	-1.5649370	1.0623330	H	-3.1020140	2.1615570	2.1197160
H	0.0421780	-0.6229720	1.6046500	H	-2.0770060	0.7576550	2.5202850
H	0.9985120	-2.1294500	1.6337930	H	-2.2740850	2.0801810	3.6842490
H	0.6575330	-1.3421090	0.0632710	Si	-0.2904010	3.2091280	-1.2126700
C	-0.9681030	-4.1434650	-0.0122150	C	-1.1864610	4.8720310	-1.2802360
H	-1.8624370	-4.7822520	-0.0948470	H	-1.1174080	5.3076170	-2.2895140
H	-0.5930740	-3.9683240	-1.0327990	H	-2.2536400	4.7512160	-1.0362020
H	-0.2057810	-4.7075770	0.5488080	H	-0.7586980	5.5951330	-0.5702790
C	-1.9981780	-2.9387930	2.5817560	C	1.5429280	3.5910570	-1.5685030
H	-1.2602580	-3.5461010	3.1301380	H	1.6756260	4.1296940	-2.5199580
H	-2.1949420	-2.0250560	3.1646160	H	1.9380320	4.2359080	-0.7658170
H	-2.9405170	-3.5070630	2.5380020	H	2.1849190	2.6947230	-1.6129880
Si	-3.9479660	-1.8253770	-0.7733240	C	-0.9650730	2.1837100	-2.6692540

C	-3.8345990	-2.8419080	-2.3721620	H	-2.0687380	2.1977160	-2.6706390
H	-3.1697990	-2.3460030	-3.0967840	H	-0.6468290	2.5813740	-3.6458780
H	-3.4137660	-3.8386540	-2.1659610	H	-0.6508890	1.1268640	-2.6190420
H	-4.8193720	-2.9806720	-2.8460220	C	3.4413980	-1.0021080	-1.1579690
C	-5.2071430	-2.7090870	0.3371860	C	4.1728060	-1.7225870	-2.1093840
H	-5.3449120	-2.1619480	1.2827680	C	3.9407000	-1.4875200	-3.4609920
H	-6.1894020	-2.8141470	-0.1499690	C	2.9908340	-0.5397720	-3.8265470
H	-4.8482990	-3.7206140	0.5885200	C	2.3207070	0.1424050	-2.8123560
C	-4.7287680	-0.1536310	-1.2734650	H	1.5744720	0.9041020	-3.0559460
H	-4.0994850	0.3738030	-2.0130070	N	2.5399230	-0.0799380	-1.5177450
H	-5.7185750	-0.2775950	-1.7386860	H	2.7711810	-0.3222030	-4.8711700
H	-4.8670820	0.5007510	-0.3945090	H	4.5020290	-2.0361060	-4.2185550
Si	-0.6759050	2.7517360	1.8516120	H	4.9299940	-2.4407650	-1.7980720
C	-0.8792170	4.6001820	2.1860750	C	3.6447710	-1.2308300	0.3067410
H	-1.7715770	5.0001610	1.6814060	C	4.1419150	-2.4496280	0.7819930
H	-0.9850560	4.7909040	3.2653740	C	4.3202620	-2.6188340	2.1515030
H	-0.0065700	5.1678990	1.8259660	C	4.0063570	-1.5676230	3.0062420
H	4.1307210	-1.6509110	4.0853940	C	3.5012680	-0.3954670	2.4455550
H	4.6925970	-3.5658920	2.5443620	H	3.2214290	0.4473420	3.0837570
H	4.3543050	-3.2673960	0.0948170	N	3.3181810	-0.2327630	1.1369510

Table S112. Geometric coordinates and single point energies for NaHMDS bipy disolvated monomer.



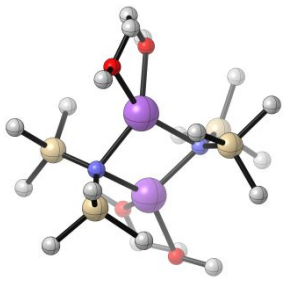
G = -2024.16868 Hartrees

G_{SP} = -2025.844374 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.0644860	0.1567170	-0.2862580	C	-0.0499610	4.5419710	0.9558760
N	-1.5316400	-1.2785170	0.9713630	C	0.2313990	3.1837690	0.7860420
C	-1.6108710	-2.5320700	0.5175970	H	1.2065250	2.7414900	1.0237320
C	-2.7516780	-3.3202780	0.7125330	H	0.7103950	5.2120980	1.3565070
C	-3.8325530	-2.7742140	1.3984730	H	-1.5619440	6.0649870	0.6960800
C	-3.7396880	-1.4696530	1.8774360	H	-3.2240770	4.4590900	-0.2570730
C	-2.5603610	-0.7644210	1.6381020	N	2.2554880	0.5339610	0.1679640
H	-2.4377280	0.2637690	1.9940090	Si	2.8063770	-0.1733810	1.5980590
H	-4.5592790	-1.0029430	2.4234880	C	1.5049690	0.0359040	2.9712200
H	-4.7391940	-3.3611180	1.5541350	H	0.5455910	-0.4089140	2.6560880
H	-2.7956480	-4.3326330	0.3101260	H	1.8077600	-0.4498990	3.9124190
C	-0.4179220	-3.0438680	-0.2222930	H	1.3273150	1.1031600	3.1815200
C	-0.0147800	-4.3793590	-0.1268660	C	3.0871570	-2.0544530	1.4602720
C	1.1332170	-4.7787380	-0.8072140	H	3.4937420	-2.4852380	2.3895870
C	1.8362680	-3.8389330	-1.5533490	H	2.1358760	-2.5688610	1.2385890
C	1.3571290	-2.5288350	-1.5875390	H	3.7888450	-2.2820560	0.6409180
H	1.8915920	-1.7503360	-2.1388810	C	4.4291620	0.5579290	2.2680380
N	0.2556520	-2.1470700	-0.9481760	H	5.2465770	0.4220980	1.5412070

H	2.7503930	-4.1005510	-2.0856800	H	4.3186790	1.6403330	2.4416040
H	1.4836920	-5.8094820	-0.7371760	H	4.7388180	0.0892790	3.2157520
H	-0.5682110	-5.0801920	0.4986090	Si	3.0288540	1.1351620	-1.2011940
N	-0.6662000	2.3332770	0.2957820	C	3.8093880	2.8560860	-0.9781680
C	-1.8736730	2.7725700	-0.0645490	H	3.0448740	3.5956760	-0.6894030
C	-2.7947570	1.7381350	-0.6284960	H	4.5658770	2.8289710	-0.1776700
C	-4.1856230	1.8375570	-0.4953700	H	4.2980280	3.2161050	-1.8977590
C	-4.9824560	0.8153930	-1.0020110	C	4.4257920	0.0421310	-1.9006380
C	-4.3730100	-0.2681240	-1.6299830	H	4.0784750	-0.9819200	-2.1131990
C	-2.9810930	-0.2759330	-1.7200580	H	4.8544690	0.4562430	-2.8272990
N	-2.2161210	0.6955010	-1.2320950	H	5.2396420	-0.0416290	-1.1620590
H	-2.4544370	-1.1097690	-2.1952450	C	1.7397320	1.3408390	-2.5969380
H	-4.9565440	-1.0929480	-2.0384850	H	2.1787320	1.7555460	-3.5177410
H	-6.0678710	0.8613670	-0.8995610	H	1.2607740	0.3827780	-2.8663970
H	-4.6304840	2.6867630	0.0235530	H	0.9397340	2.0292540	-2.2728850
C	-2.2424410	4.1145600	0.0688020	C	-1.3089810	5.0088020	0.5903240

Table S113. Geometric coordinates and single point energies for NaHMDS DME disolvated dimer.



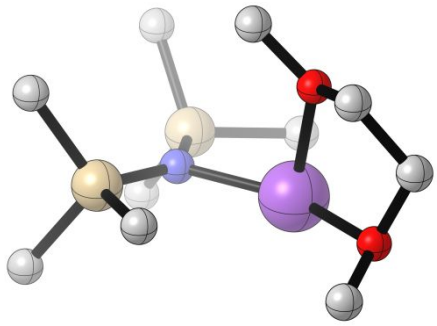
G = -2686.355084 Hartrees

G_{SP} = -2688.26002 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.7605140	1.1748110	-0.0715200	H	2.5402270	-2.6736220	2.5183330
N	-1.6319750	-1.0221470	0.2204460	H	3.9933070	-3.4214590	1.7798350
Na	0.7323680	-1.3435810	0.0480250	C	3.1894350	-3.0359980	-0.6636700
N	1.5677660	0.8488440	0.3950940	C	2.2950250	-3.4214990	-1.8166830
Si	1.5930320	1.4843380	1.9883070	H	1.8876440	-4.4382730	-1.6698630
C	2.3135570	3.2337890	2.1634420	H	2.8989510	-3.4201200	-2.7424880
H	2.2049840	3.5788640	3.2042280	O	1.2447340	-2.4912380	-1.9147890
H	3.3859850	3.2654620	1.9138660	C	0.6429170	-2.4605790	-3.1869700
H	1.7963720	3.9519750	1.5087340	H	0.2738650	-3.4593870	-3.4751650
C	-0.1955910	1.6501220	2.6290070	H	-0.2098090	-1.7733810	-3.1402150
H	-0.6910880	2.5025210	2.1308430	H	1.3608920	-2.1025240	-3.9453400
H	-0.8019420	0.7474720	2.4466740	H	3.6695570	-2.0600780	-0.8686260
H	-0.2198290	1.8557410	3.7100600	H	3.9875030	-3.7934960	-0.5530540
C	2.5599020	0.4617300	3.2622630	Si	-2.6204480	-1.1360000	-1.1672210
H	2.1591290	-0.5529950	3.3975220	C	-2.5862770	-2.8408330	-2.0174710
H	3.6137520	0.3728910	2.9520970	H	-1.6078360	-3.3277490	-1.8867520
H	2.5418990	0.9617820	4.2436600	H	-3.3408710	-3.5035600	-1.5670580
Si	2.7249450	1.3302100	-0.7698440	H	-2.8047710	-2.7737400	-3.0955710
C	2.4263280	0.4403440	-2.4310820	C	-2.0545960	0.1731810	-2.4401860

H	2.8293130	-0.5835200	-2.4123960	H	-2.4028110	1.1666590	-2.1122570
H	1.3539270	0.3530200	-2.6735210	H	-0.9581690	0.2232010	-2.5630170
H	2.9192350	0.9778430	-3.2566550	H	-2.4886310	-0.0153500	-3.4344530
C	2.7335210	3.2012160	-1.1450150	C	-4.4557000	-0.7437220	-0.8809930
H	3.4004810	3.7310320	-0.4485200	H	-5.0446170	-0.8724630	-1.8032480
H	3.0913260	3.4086200	-2.1665890	H	-4.8885350	-1.4053420	-0.1133490
H	1.7282530	3.6343150	-1.0297180	H	-4.5783430	0.2969020	-0.5422620
C	4.5237240	0.9313440	-0.2959070	Si	-1.9342490	-1.9491010	1.6282910
H	5.2296050	1.2568840	-1.0767980	C	-0.2854120	-2.3009050	2.5135720
H	4.7970940	1.4504440	0.6372180	H	0.3188100	-3.0231250	1.9382990
H	4.6785840	-0.1466470	-0.1292130	H	-0.4505960	-2.7380800	3.5100570
O	2.4222940	-2.9522990	0.5096500	H	0.3029080	-1.3786730	2.6557430
C	3.2047700	-2.6610360	1.6467080	C	-3.0729960	-1.1530260	2.9253870
H	3.6663520	-1.6628830	1.5594440	H	-3.1980780	-1.8366900	3.7800920
O	-2.6995920	2.3901940	0.2817040	H	-2.6788850	-0.2017560	3.3143650
C	-3.4821940	2.1009650	1.4172140	H	-4.0738890	-0.9641650	2.5044730
H	-3.4879500	1.0106110	1.5280480	C	-2.7024210	-3.6564640	1.3079910
H	-3.0506120	2.5562640	2.3255000	H	-3.7160100	-3.5734490	0.8839010
H	-4.5141270	2.4680260	1.2812720	H	-2.0918400	-4.2418460	0.6031030
H	-1.7279060	4.9671200	-1.5663170	H	-2.7815470	-4.2263500	2.2474440
H	-2.7049870	3.5591820	-2.0894630	O	-0.7883630	3.1227340	-1.4682620
C	-0.2517090	3.1330710	-2.7706710	C	-1.9500690	3.9045570	-1.3572380
H	0.6246530	2.4748480	-2.7792080	C	-2.5040670	3.7586310	0.0397410
H	-0.9939780	2.7642330	-3.4999900	H	-3.4580970	4.3117550	0.1117250
H	0.0654510	4.1510610	-3.0555530	H	-1.8026080	4.1848720	0.7832440

Table S114. Geometric coordinates and single point energies for NaHMDS DME monosolvated monomer.



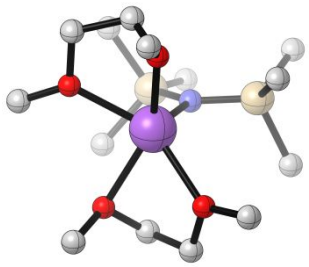
G = -1343.157151 Hartrees

G_{SP} = -1344.114079 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.8972420	-0.7077310	-0.8289060	H	4.3648070	-1.7858270	-1.4994780
N	1.0868680	0.0435050	-0.2460310	H	3.3207820	-0.7160320	-2.4761940
Si	1.0693660	1.6983560	0.0802280	C	1.3705640	-2.7907950	-0.8195710
C	1.5825830	2.1807720	1.8454320	H	0.5469810	-3.0469850	-0.1286130
H	0.9887170	1.6475370	2.6038930	H	0.9553490	-2.6809670	-1.8375430
H	2.6393630	1.9203180	2.0156230	H	2.0469750	-3.6588830	-0.8446530
H	1.4722080	3.2625450	2.0223140	C	-3.3087250	-0.5284320	1.1821930
C	2.1263180	2.7656120	-1.0774420	C	-3.8713040	-0.9885030	-0.1487990
H	1.8652870	2.5714540	-2.1294100	H	-4.9498180	-0.7678830	-0.2155870
H	1.9988390	3.8421800	-0.8816360	H	-3.7372800	-2.0768330	-0.2368790
H	3.1938790	2.5244410	-0.9539480	O	-3.1757270	-0.4011930	-1.2318010
C	-0.7322860	2.3102900	-0.1496020	C	-3.7069490	0.8350890	-1.6614340
H	-0.8677050	3.3648790	0.1358880	H	-3.0925030	1.1879560	-2.4980830
H	-1.0286110	2.2196700	-1.2096190	H	-4.7454920	0.7072130	-2.0085870
H	-1.4325800	1.7076600	0.4567340	H	-3.6770410	1.5929450	-0.8616640
Si	2.2465700	-1.1844500	-0.2622860	H	-3.4438110	0.5629420	1.3163700
C	3.0118080	-1.5684000	1.4331360	H	-3.8395690	-1.0378920	2.0079030
H	3.7213120	-2.4096710	1.3849460	O	-1.9444800	-0.8485970	1.1785030

H	3.5549460	-0.6911760	1.8187360	C	-1.2378100	-0.4676490	2.3412620
H	2.2322790	-1.8238820	2.1687560	H	-1.5572810	-1.0730090	3.2059810
C	3.6920740	-0.9146080	-1.4587900	H	-0.1714530	-0.6176530	2.1295450
H	4.2888610	-0.0418950	-1.1496990	H	-1.4049400	0.6007390	2.5619680

Table S115. Geometric coordinates and single point energies for NaHMDS DME disolvated monomer.



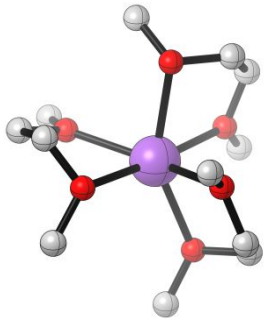
G = -1651.524745 Hartrees

G_{SP} = -1652.836119 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.9540170	-0.1797570	-0.2030820	H	0.2984960	-3.4634990	1.7463840
N	-1.2844070	0.1294900	-0.0112860	O	1.3093150	-2.4855800	0.2187450
Si	-1.8667250	1.3877680	0.9593030	C	1.4495280	-3.6366920	-0.5759360
C	-1.5237960	3.1097020	0.2163590	H	0.5270910	-4.2417450	-0.5581580
H	-0.4375080	3.2798060	0.1569800	H	1.6404440	-3.3151960	-1.6066830
H	-1.9385060	3.1860530	-0.8020480	H	2.2945280	-4.2551190	-0.2256330
H	-1.9586580	3.9182820	0.8250700	H	0.8156760	-1.6332920	3.3964900
C	-3.7321590	1.3615760	1.3235350	H	-0.1290430	-1.0821070	1.9679180
H	-4.0445370	0.3826710	1.7222820	C	3.1004850	-0.7159890	2.4036190
H	-3.9960720	2.1303450	2.0675390	H	3.6850340	0.1989620	2.2429420
H	-4.3210450	1.5557310	0.4140130	H	3.1296300	-0.9721210	3.4772340
C	-1.0208550	1.4240330	2.6673710	H	3.5671910	-1.5339240	1.8284140
H	-1.2515640	2.3535020	3.2123460	O	1.5780620	0.4958210	-2.3461680
H	-1.3622840	0.5804110	3.2899230	C	0.9935660	1.7804970	-2.2567770
H	0.0740390	1.3428130	2.5692130	C	1.7491820	2.6657270	-1.2823990
Si	-2.0923440	-1.0630320	-0.8978510	H	1.2094940	3.6241820	-1.1756160
C	-3.8176700	-0.6130620	-1.5533870	H	2.7748330	2.8943980	-1.6326110
H	-4.1829560	-1.3800360	-2.2550760	O	1.8001980	1.9793740	-0.0564310
H	-4.5488920	-0.5290550	-0.7353580	C	2.2527910	2.7466180	1.0279100

H	-3.7959940	0.3524380	-2.0838320	H	2.2337710	2.0982550	1.9126630
C	-2.3126460	-2.6883770	0.0746510	H	3.2802570	3.1139090	0.8545590
H	-2.8648280	-2.5091700	1.0112930	H	1.5881080	3.6097670	1.2054130
H	-2.8489730	-3.4614010	-0.4986020	H	-0.0284960	1.6219200	-1.8737820
H	-1.3217100	-3.0904750	0.3416670	H	0.9413340	2.2546080	-3.2524630
C	-1.0776190	-1.5532390	-2.4355520	C	2.7103860	0.4131180	-3.1693610
H	-0.9667750	-0.6986610	-3.1217760	H	3.0293100	-0.6362820	-3.1912200
H	-0.0614290	-1.8787060	-2.1591080	H	2.4717520	0.7311370	-4.1987120
H	-1.5537240	-2.3788720	-2.9883160	H	3.5465950	1.0282890	-2.7940410
O	1.7869050	-0.4589700	1.9823030	C	1.1444730	-2.7704070	1.5881210
C	0.8471530	-1.4660230	2.3048280	H	2.0562860	-3.2632730	1.9777730

Table S116. Geometric coordinates and single point energies for sodium cation with 3 DME molecules.



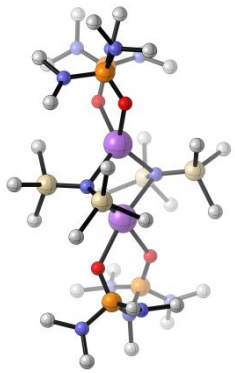
G -1087.214075 Hartrees

G_{SP} = -1088.328026 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.0145960	-0.0325590	-0.1256840	H	-0.3176540	3.2286020	2.2310550
O	1.8612670	-0.6650050	-1.3451520	H	1.2519770	3.7629090	0.3608800
C	2.9522310	-0.2822390	-0.5258510	H	-0.4300700	3.7195380	-0.2218410
C	2.8248810	-0.8763770	0.8617590	H	1.4540910	1.6388190	-2.5466560
H	2.7783970	-1.9818110	0.8135010	H	0.4312450	3.1183060	-2.4831270
H	3.7049090	-0.6037100	1.4719850	O	-0.8522770	-2.0731230	0.6480290
O	1.6433740	-0.3669680	1.4313160	C	-2.2051680	-1.7399790	0.8660620
C	1.3197280	-0.9199570	2.6876770	C	-2.9012930	-1.3167580	-0.4155010
H	2.1265460	-0.7378610	3.4166570	H	-3.9163380	-0.9505810	-0.1735460
H	0.4003240	-0.4293380	3.0320010	H	-3.0161420	-2.1626910	-1.1182610
H	1.1377700	-2.0041630	2.6051320	O	-2.1316270	-0.2972460	-1.0105990
H	3.9084570	-0.5756540	-0.9887710	C	-2.7390730	0.2872170	-2.1399640
H	2.9202320	0.8140730	-0.4455720	H	-2.0512300	1.0454810	-2.5337640
C	2.0908980	-1.8265390	-2.1132100	H	-2.9323220	-0.4659990	-2.9215260
H	1.1593780	-2.0676340	-2.6396890	H	-3.6930220	0.7697030	-1.8680130
H	2.8865050	-1.6538960	-2.8557670	H	-2.1974010	-0.8986700	1.5753130
H	2.3770400	-2.6844940	-1.4819120	H	-2.7484090	-2.5805110	1.3313810
H	2.0960130	3.1495100	-1.8221890	C	-0.6367510	-3.3501710	0.0920950

C	1.1963340	2.5252360	-1.9542150	H	0.4466570	-3.5210470	0.0728610
O	0.7148930	2.0681630	-0.7105720	H	-1.1076120	-4.1314160	0.7110710
C	0.3854510	3.0980970	0.1926550	H	-1.0265500	-3.4257580	-0.9369290
C	-0.0059600	2.4531710	1.5101150	H	-3.0232590	1.1971770	1.1238100
O	-1.0217920	1.4825930	1.3505540	H	-2.5712740	2.7668850	1.8532060
C	-2.2991380	2.0201720	1.0891030	H	0.8619800	1.9164620	1.9167390
H	-2.3532180	2.4873670	0.0915400				

Table S117 Geometric coordinates and single point energies for NaHMDS NIP disolvated dimer.



G = -4999.021698 Hartrees

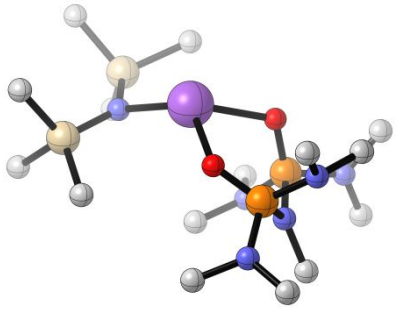
G_{SP} = -5002.574597 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.5880630	-0.0268000	0.2337810	H	1.1265980	-4.9592130	-0.1443490
N	-0.0970000	-1.7896990	-0.3336780	H	2.4462270	-3.7546660	-0.1079700
Na	1.4831100	-0.0052670	0.0843710	H	2.0202690	-4.6834670	1.3676200
N	-0.1006490	1.7086550	0.8316110	Si	-0.2924760	-2.2444210	-1.9598850
Si	-0.1446230	2.0518440	2.4972510	C	-0.5556820	-4.1153830	-2.2596610
C	-0.8036060	3.7816480	2.9679240	H	-1.0750880	-4.2982410	-3.2146650
H	-0.7873200	3.9151100	4.0619410	H	0.4149170	-4.6332320	-2.3094020
H	-0.1914890	4.5834110	2.5261170	H	-1.1394450	-4.5901260	-1.4547480
H	-1.8411120	3.9323320	2.6308190	C	1.2021870	-1.7976860	-3.0490800
C	-1.3013980	0.8520350	3.4137490	H	2.1075760	-2.2301700	-2.5969110
H	-2.3440100	1.0493740	3.1152470	H	1.0948060	-2.1688370	-4.0811170
H	-1.1075950	-0.2076350	3.1850240	H	1.3374970	-0.7045520	-3.0880300
H	-1.2302360	0.9828920	4.5054690	C	-1.7701090	-1.3532730	-2.7723260
C	1.5756760	1.9870250	3.3098270	H	-2.6798750	-1.4169070	-2.1556810
H	2.1114120	1.0617220	3.0475440	H	-1.5621290	-0.2785160	-2.8998690
H	2.1679240	2.8307000	2.9190020	H	-1.9782570	-1.7745580	-3.7701540
H	1.5297690	2.0749070	4.4071620	O	-3.3011320	-0.9695460	1.3504400
Si	0.1536560	2.8542120	-0.3953560	P	-4.6246990	-1.2700360	0.7309630

C	0.6889560	1.9448630	-1.9845610	N	-5.5864960	-2.0654510	1.8386860
H	1.7064770	1.5288020	-1.8768820	C	-6.7237690	-2.8756110	1.4675600
H	0.0003600	1.1111400	-2.1992190	H	-6.6585700	-3.8677220	1.9445010
H	0.6921530	2.6071880	-2.8651630	H	-7.6798460	-2.4141480	1.7771470
C	-1.4227330	3.8189850	-0.8419420	H	-6.7506430	-3.0251240	0.3802460
H	-1.7303060	4.4304780	0.0232180	C	-5.3911480	-1.8630560	3.2624160
H	-1.2945210	4.4896230	-1.7069880	H	-6.2333990	-1.3075230	3.7151920
H	-2.2235950	3.0950930	-1.0638690	H	-5.3112440	-2.8363710	3.7730020
C	1.4924160	4.1703690	-0.0675340	H	-4.4586370	-1.3103950	3.4282610
H	1.6659110	4.7941690	-0.9606020	N	-4.5724030	-2.2010790	-0.6416750
H	1.2039700	4.8420230	0.7560630	C	-3.7011590	-3.3675270	-0.6267980
H	2.4304960	3.6672500	0.2130360	H	-3.2863230	-3.5192370	-1.6340970
O	3.2627450	1.3709160	0.3836260	H	-2.8568910	-3.1922840	0.0538410
P	4.5638510	1.5181870	-0.3351420	H	-4.2400510	-4.2841110	-0.3236530
N	5.4132760	2.8174850	0.2665180	C	-5.4534040	-2.0956920	-1.7840880
C	6.4580900	3.5352370	-0.4333420	H	-6.1174810	-2.9759090	-1.8674220
H	6.1653830	4.5871400	-0.5968290	H	-6.0743040	-1.1928860	-1.7151520
H	7.3952430	3.5350470	0.1508420	H	-4.8559230	-2.0315270	-2.7094180
H	6.6522680	3.0742700	-1.4093460	N	-5.4800520	0.1337100	0.2608310
C	5.0885850	3.3359050	1.5866640	P	-4.7170720	1.2602060	-0.7740640
H	5.9563530	3.2585670	2.2639060	O	-3.3189640	0.8059570	-1.0315750
H	4.7944670	4.3963940	1.5171240	N	-5.5690250	1.4065260	-2.1969790
H	4.2447070	2.7757600	2.0069060	C	-4.9984310	0.9285610	-3.4459740
N	4.6019540	1.7667870	-1.9835820	H	-4.9246540	1.7532640	-4.1745680
C	4.0857960	3.0235250	-2.5135940	H	-3.9950510	0.5228120	-3.2651470
H	3.0974990	2.8848210	-2.9787780	H	-5.6303250	0.1374340	-3.8850980
H	3.9734230	3.7608790	-1.7080080	C	-6.9375250	1.8722210	-2.2760190
H	4.7799210	3.4265320	-3.2697950	H	-7.2496610	2.3258020	-1.3267350
C	4.5636550	0.6581670	-2.9273620	H	-7.0341010	2.6383330	-3.0642280
H	4.9803140	1.0005470	-3.8867120	H	-7.6337850	1.0493370	-2.5197960
H	5.1792450	-0.1751840	-2.5663130	N	-4.9794630	2.6979410	0.0251490

H	3.5400790	0.2829610	-3.0983990	C	-5.0178480	3.9762280	-0.6726990
N	5.4850910	0.1029810	-0.1209640	H	-5.2488760	3.8286870	-1.7341720
P	4.7095800	-1.4046910	0.0445750	H	-5.7953430	4.6178540	-0.2273040
O	3.3232920	-1.3263450	-0.5073260	H	-4.0487670	4.4944340	-0.6042730
N	5.5952220	-2.5557970	-0.7758690	C	-4.4319600	2.7859810	1.3772480
C	5.1517730	-3.0216650	-2.0796310	H	-5.0096100	3.5176280	1.9620050
H	5.0090550	-4.1150420	-2.0653510	H	-4.4899200	1.8086180	1.8746030
H	4.1944490	-2.5536550	-2.3352730	H	-3.3729470	3.0945900	1.3555610
H	5.8950550	-2.7809130	-2.8594230	C	-6.8547680	0.3598420	0.7012520
C	6.8300820	-3.1496140	-0.3082110	H	-7.5973940	-0.0552270	-0.0024360
H	7.0535540	-2.8196710	0.7131960	H	-7.0165770	-0.0990210	1.6845330
H	6.7444010	-4.2499220	-0.3023720	H	-7.0291880	1.4396010	0.8022430
H	7.6790060	-2.8804270	-0.9611910	H	5.2258600	0.1945080	2.3099160
N	4.9780460	-1.7893600	1.6438880	H	3.9786660	-0.7268310	3.1887660
C	4.6873370	-3.1411970	2.1037380	C	6.9396010	0.1315450	-0.2037840
H	4.6242420	-3.8320450	1.2533710	H	7.3081520	-0.1853370	-1.1942540
H	5.4863900	-3.4843600	2.7816550	H	7.3029610	1.1457490	0.0017750
H	3.7260910	-3.1789030	2.6409530	H	7.3741930	-0.5303300	0.5598880
C	4.9680420	-0.7940910	2.7062300	Si	0.4027350	-2.7948840	0.9455230
H	5.7113530	-1.0737600	3.4698650	C	-1.0144890	-3.6362620	1.8943340
H	1.4990320	-2.3481360	3.1790380	H	-0.6555890	-4.0900000	2.8320810
H	2.3410260	-1.4901120	1.8655490	H	-1.8019670	-2.9028710	2.1335930
H	0.8122040	-0.8491190	2.5285210	H	-1.4653100	-4.4407090	1.2902430
C	1.6131400	-4.1874580	0.4706340	C	1.3475040	-1.7706860	2.2526310

Table S118. Geometric coordinates and single point energies for NaHMDS NIPA monosolvated monomer.



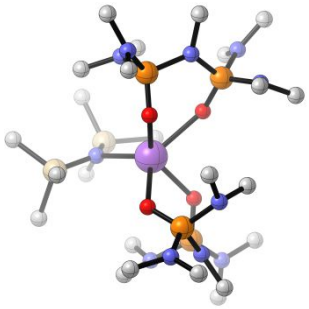
G = -2499.495146 Hartrees

G_{SP} = -2501.276167 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.8220350	0.3383910	1.3594530	H	1.5326640	-2.7694120	-1.0765020
P	-2.2578910	1.2638880	0.2754780	C	0.3862960	-0.5635760	-2.0698680
N	-3.4365670	1.0322700	1.4359270	H	0.5861490	-0.8131970	-3.1233630
C	-3.5548670	2.0927130	2.4278080	H	-0.2701370	0.3153030	-2.0364490
H	-2.9289580	1.8949720	3.3147100	H	1.3345760	-0.3117840	-1.5598780
H	-3.2396640	3.0509300	1.9934910	C	-3.1301430	-0.3375430	-1.7993590
H	-4.6035030	2.1858020	2.7501660	H	-4.0316480	-0.9252680	-1.5577180
C	-3.8153130	-0.2835370	1.9215320	H	-3.4388060	0.6445310	-2.1760320
H	-4.8198180	-0.2198880	2.3669280	H	-2.5828550	-0.8454330	-2.6070680
H	-3.8565460	-1.0005020	1.0917980	N	2.8076200	0.3432200	0.3382990
H	-3.1128980	-0.6689780	2.6801390	Si	3.7165840	-1.0553750	0.6357920
N	-2.8726480	2.4816690	-0.6732250	C	5.3060720	-0.7856740	1.6426550
C	-4.2809640	2.7511420	-0.8785510	H	6.0060180	-0.1365830	1.0914970
H	-4.5192550	3.7880390	-0.5869600	H	5.0803950	-0.2906830	2.6003800
H	-4.5608500	2.6305120	-1.9404150	H	5.8260900	-1.7328850	1.8582830
H	-4.8902660	2.0702460	-0.2726230	C	2.6672420	-2.2779970	1.6568390
C	-1.9624060	3.2994860	-1.4609420	H	2.5143510	-1.8794470	2.6749470
H	-2.1013150	3.1191710	-2.5414860	H	1.6681880	-2.4470010	1.2216510

H	-2.1492090	4.3674510	-1.2647450	H	3.1602370	-3.2569850	1.7652570
H	-0.9233170	3.0774050	-1.1889970	C	4.2942070	-1.9662060	-0.9376330
O	-0.8851150	1.6185000	0.7523100	H	4.6872760	-2.9710910	-0.7134120
N	-2.2557130	-0.1724540	-0.6410190	H	3.4896200	-2.0675620	-1.6826890
P	-1.3109780	-1.5077730	-0.1588070	H	5.1010430	-1.3914250	-1.4190090
O	-0.7870010	-1.2450670	1.2220120	Si	3.3593190	1.8106710	-0.3142630
N	-2.2383610	-2.8913160	-0.1710190	C	4.5836570	1.6129530	-1.7563310
C	-2.6301940	-3.5282660	1.0754810	H	4.8500280	2.5845140	-2.2022320
H	-2.2593800	-4.5665910	1.1029820	H	5.5160800	1.1352530	-1.4136770
H	-2.1959270	-2.9825680	1.9203410	H	4.1571600	0.9763810	-2.5482240
H	-3.7284230	-3.5543380	1.1806920	C	4.2197520	2.9323800	0.9560270
C	-2.6630340	-3.5846020	-1.3715200	H	5.0939630	2.4223830	1.3903940
H	-2.2331920	-3.1103120	-2.2615100	H	4.5625260	3.8801360	0.5107910
H	-2.3224340	-4.6340510	-1.3463710	H	3.5336080	3.1736030	1.7837810
H	-3.7625300	-3.5878190	-1.4647940	C	1.8953420	2.8250950	-0.9875030
N	-0.2698300	-1.7090740	-1.4332240	H	1.4176110	2.3022880	-1.8326220
C	0.5267900	-2.9311180	-1.4943390	H	1.1324400	2.9675090	-0.2046380
H	0.0418070	-3.7365570	-0.9280690	H	2.2171030	3.8174470	-1.3413970
H	0.6308060	-3.2508740	-2.5433140				

Table S119. Geometric coordinates and single point energies for NaHMDS NIPA disolvated monomer.



G = -3964.183624 Hartrees

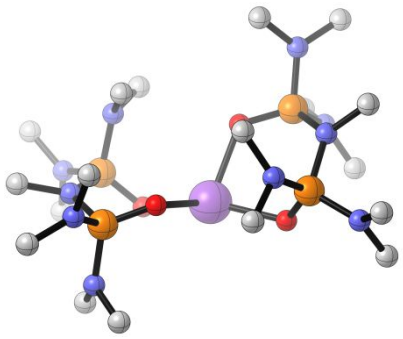
G_{SP} = -3967.14406 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.1640580	0.5050770	0.0024380	H	3.2056550	-1.5286090	-4.6613800
N	0.4379380	2.8637880	0.0463760	H	3.1643780	-0.3050050	-3.3665610
Si	0.9814740	3.6547150	-1.3530110	H	4.6610120	-1.2512760	-3.6638880
C	2.7925710	4.2632710	-1.2926710	C	3.4214600	-3.6593780	-3.0323260
H	2.9576430	4.8956150	-0.4055820	H	2.9413200	-4.3473850	-2.3262670
H	3.5134380	3.4337780	-1.2461720	H	3.0686610	-3.9068690	-4.0484700
H	3.0313490	4.8639580	-2.1856290	H	4.5135100	-3.8229910	-3.0063490
C	0.8585080	2.5171720	-2.8660640	N	1.2022170	-3.0783280	-1.0590220
H	1.4403980	1.5973460	-2.6973630	C	0.1655310	-3.2242530	-2.0773410
H	-0.1831710	2.1995240	-3.0335350	H	0.5772690	-2.9866290	-3.0676990
H	1.2226350	3.0117060	-3.7808920	H	-0.1888260	-4.2675100	-2.0922150
C	0.0239340	5.2516380	-1.7874880	H	-0.6792630	-2.5401110	-1.8815520
H	0.3534850	5.6623430	-2.7558210	C	0.7178290	-3.3489420	0.2891190
H	-1.0643600	5.0899460	-1.8408020	H	0.3496670	-4.3878730	0.3226810
H	0.2039990	6.0240360	-1.0213160	H	1.5324060	-3.2478460	1.0152980
Si	0.1510770	3.5713210	1.5586810	H	-0.0914910	-2.6575730	0.5882610
C	-1.3780460	4.7170560	1.6373590	C	4.3821620	-2.8726200	0.0310420
H	-1.5402380	5.0932450	2.6609240	H	5.1787250	-2.6675420	-0.7039390
H	-1.2202430	5.5879940	0.9813390	H	4.8270110	-2.8965430	1.0336010

H	-2.3040580	4.2253790	1.3067830	H	3.9700380	-3.8732630	-0.1731560
C	1.5261530	4.7163690	2.2285510	O	-1.5020760	-0.2672780	-1.4863890
H	1.2739230	5.0779040	3.2389470	P	-2.9307060	0.1126890	-1.2697500
H	2.5073060	4.2201730	2.2832780	N	-3.7796820	0.0113860	-2.7021390
H	1.6366340	5.6001030	1.5786150	C	-4.9925720	0.7438140	-3.0024380
C	-0.0857480	2.2095460	2.8638980	H	-4.8305180	1.4307150	-3.8511380
H	-0.7906150	1.4409750	2.5061460	H	-5.8135300	0.0576330	-3.2775290
H	0.8665250	1.6810000	3.0297150	H	-5.3002120	1.3374220	-2.1336850
H	-0.4448490	2.6012520	3.8292420	C	-3.2626780	-0.7955390	-3.7923050
P	3.1208090	-0.6632100	1.1868840	H	-3.9503250	-1.6235460	-4.0390170
N	3.9243100	-1.1668200	2.5593430	H	-3.1346710	-0.1764210	-4.6958310
C	5.3382100	-0.9809000	2.8050160	H	-2.2821500	-1.2006250	-3.5173510
H	5.4954110	-0.4063810	3.7339070	N	-3.3261050	1.6146860	-0.6838550
H	5.8590860	-1.9493490	2.9177590	C	-2.7794200	2.7623480	-1.4119710
H	5.7924400	-0.4250830	1.9764660	H	-1.8110470	3.0669540	-0.9793990
C	3.1963580	-1.8696990	3.5989760	H	-2.6278560	2.4984500	-2.4683520
H	3.5280130	-2.9204070	3.6861650	H	-3.4930860	3.6000540	-1.3604140
H	3.3596000	-1.3792140	4.5728590	C	-3.5338740	1.8686130	0.7336700
H	2.1231180	-1.8394890	3.3765860	H	-4.0933350	2.8104950	0.8376070
N	3.9967370	0.6428260	0.6513140	H	-4.1320630	1.0685820	1.1879240
C	3.6916580	1.8928110	1.3526480	H	-2.5848280	1.9690260	1.2858970
H	2.8052960	2.3851740	0.9157700	N	-3.6632790	-0.9547650	-0.1463810
H	3.4912990	1.6863620	2.4142740	P	-2.8025020	-1.4280630	1.2401540
H	4.5600240	2.5664830	1.2885680	O	-1.5149000	-0.6842570	1.3393750
C	4.3904220	0.8288940	-0.7364690	N	-3.7221260	-1.1743340	2.6129040
H	5.2421920	1.5258540	-0.7657150	C	-3.3783350	-0.1166930	3.5507250
H	4.7141440	-0.1248270	-1.1741260	H	-3.2255400	-0.5423370	4.5567900
H	3.5694190	1.2376120	-1.3466850	H	-2.4497240	0.3749940	3.2402910
O	1.6655170	-0.4818740	1.4729400	H	-4.1827980	0.6357710	3.6160450
N	3.3287640	-1.8685500	-0.0086530	C	-4.8782160	-1.9605130	2.9885870
P	2.2647990	-1.8161840	-1.3316140	H	-5.0152580	-2.8024330	2.2994370

O	1.7126150	-0.4378410	-1.4783090	H	-4.7472590	-2.3699770	4.0056390
N	3.0782510	-2.2914150	-2.7066500	H	-5.7989750	-1.3515400	2.9883690
C	3.5577050	-1.2900640	-3.6440810	N	-2.8141780	-3.0954340	1.1077090
H	-3.0889120	-3.1380820	-0.9740160	C	-2.4079940	-3.8984980	2.2467920
H	-1.9055020	-4.3169070	-0.3572520	H	-2.3512550	-3.2781030	3.1502100
C	-5.0935300	-1.2290940	-0.2050730	H	-3.1344140	-4.7097250	2.4248900
H	-5.6781340	-0.5564540	0.4463950	H	-1.4170400	-4.3536170	2.0798370
H	-5.4468410	-1.1157740	-1.2371890	C	-2.8668970	-3.8210150	-0.1456730
H	-5.2921610	-2.2678210	0.0991670	H	-3.6491700	-4.5988010	-0.1031780

Table S120. Geometric coordinates and single point energies for sodium cation solvated by 2 NIPA molecules.



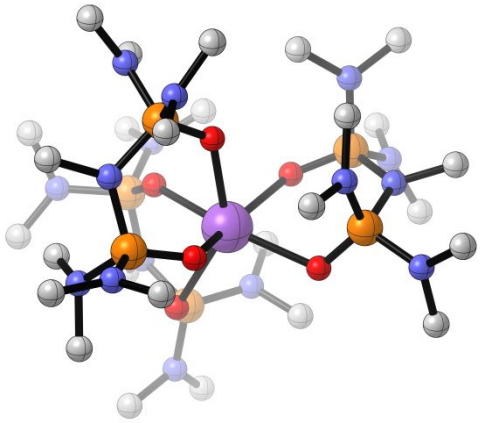
G = -3091.536447 Hartrees

G_{SP} = -3093.945049 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.0001000	0.0005780	-1.1242790	H	-5.3702960	2.3331110	-2.3548760
P	2.7519390	-1.4780410	-0.3829990	H	-4.1967560	3.6420030	-2.6640630
N	3.8780800	-2.5912640	-0.8699670	H	-3.6894730	1.9453600	-2.8558100
C	4.5300490	-3.5559490	-0.0019080	N	-2.0099340	2.1935220	0.9203920
H	4.3303220	-4.5821230	-0.3525700	C	-1.2540260	3.4169570	0.6621380
H	5.6235660	-3.4089760	0.0012710	H	-0.1830670	3.1889550	0.5343710
H	4.1553750	-3.4600050	1.0239000	H	-1.6238470	3.9043880	-0.2499700
C	4.3098590	-2.6235300	-2.2601460	H	-1.3829720	4.1157520	1.5035520
H	5.3695590	-2.3328540	-2.3551110	C	-1.5293200	1.4432450	2.0724200
H	4.1962300	-3.6419190	-2.6643510	H	-1.4889950	2.1218760	2.9382850
H	3.6886380	-1.9453430	-2.8559360	H	-2.2166750	0.6240130	2.3145580
N	2.0095850	-2.1934180	0.9204630	H	-0.5235180	1.0294730	1.8892620
C	1.2535170	-3.4167650	0.6622820	O	-1.9059770	1.0376330	-1.5442960
H	0.1825750	-3.1886220	0.5346500	N	-3.5300530	0.1082180	0.2630890
H	1.6231410	-3.9042030	-0.2499000	P	-2.7663520	-1.4062160	0.1655330
H	1.3825040	-4.1155960	1.5036610	O	-1.2718310	-1.2455430	0.2304750
C	1.5291090	-1.4430880	2.0725150	N	-3.2930150	-2.3540920	1.4235700
H	1.4888470	-2.1216740	2.9384180	C	-2.5384770	-2.3995870	2.6657880

H	2.2164950	-0.6238510	2.3145460	H	-2.3917380	-3.4463130	2.9766130
H	0.5233260	-1.0292680	1.8893850	H	-1.5535570	-1.9412570	2.5192100
O	1.9055350	-1.0372970	-1.5441620	H	-3.0678610	-1.8740280	3.4796480
N	3.5300220	-0.1083690	0.2631100	C	-4.5749360	-3.0356910	1.4634090
P	2.7666750	1.4062240	0.1655470	H	-5.0590100	-2.9917850	0.4807910
O	1.2721370	1.2458780	0.2307640	H	-4.4280410	-4.0946750	1.7308650
N	3.2937370	2.3540890	1.4234340	H	-5.2472500	-2.5860760	2.2141880
C	2.5393040	2.3999710	2.6657040	N	-3.4193590	-2.1240710	-1.1838660
H	2.3929710	3.4467780	2.9764430	C	-2.9198490	-3.4533240	-1.5156990
H	1.5542100	1.9419800	2.5192320	H	-2.5826030	-3.9673390	-0.6055310
H	3.0685570	1.8742960	3.4795770	H	-3.7254900	-4.0499310	-1.9692620
C	4.5759520	3.0351380	1.4631130	H	-2.0753980	-3.4070360	-2.2242770
H	5.0598380	2.9911040	0.4804060	C	-3.9231200	-1.3702050	-2.3236530
H	4.4295420	4.0941580	1.7306820	H	-4.6486380	-1.9964100	-2.8632600
H	5.2482290	2.5851870	2.2137270	H	-4.4364810	-0.4627020	-1.9855880
N	3.4196140	2.1238360	-1.1840060	H	-3.1201580	-1.0754750	-3.0192260
C	2.9205840	3.4532770	-1.5157740	C	-4.8188900	0.2049450	0.9479350
H	2.5833520	3.9673010	-0.6056070	H	-4.7197270	0.0543800	2.0347220
H	3.7264740	4.0496900	-1.9691570	H	-5.2547890	1.1949760	0.7701010
H	2.0762290	3.4073320	-2.2244880	H	-5.5257920	-0.5398530	0.5529020
C	3.9231100	1.3698060	-2.3237990	H	5.5263620	0.5383860	0.5520300
H	4.6486450	1.9958680	-2.8635490	P	-2.7523240	1.4780840	-0.3830330
H	4.4363950	0.4622610	-1.9857290	N	-3.8787530	2.5911220	-0.8697610
H	3.1200250	1.0751270	-3.0192490	C	-4.5308090	3.5555770	-0.0015150
C	4.8188600	-0.2054040	0.9479140	H	-4.3312850	4.5818320	-0.3520530
H	4.7198740	-0.0535940	2.0345350	H	-5.6243020	3.4084200	0.0017380
H	5.2539100	-1.1959970	0.7711540	H	-4.1560340	3.4595450	1.0242490
				C	-4.3105470	2.6236020	-2.2599280

Table S121. Geometric coordinates and single point energies for sodium cation solvated by 3 NIPA molecules.



G = -4556.22629 Hartrees

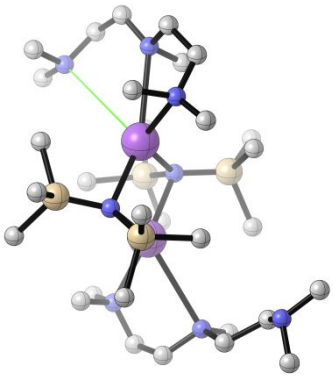
G_{SP} = -4559.81512 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.0816630	-0.0709330	-0.6016480	H	-4.6406690	0.7003170	2.7558480
P	-0.9148330	-2.7284660	1.4172570	H	-5.5304980	3.2397260	1.0119870
N	-1.4922720	-2.4571970	2.9572900	H	-4.4958710	2.6956840	-0.3416460
C	-2.0607750	-3.4646540	3.8290580	C	-3.4983900	-3.3063900	0.8443970
H	-1.4609590	-3.5671840	4.7501840	H	-3.4519330	-4.4051950	0.9387950
H	-3.0888310	-3.1951400	4.1276800	H	-3.7449250	-2.8785830	1.8255270
H	-2.0899070	-4.4385050	3.3258270	H	-4.3130340	-3.0509040	0.1554570
C	-1.4391330	-1.1166380	3.5166380	O	1.9805620	-0.1609190	-1.9344070
H	-2.4461240	-0.7990500	3.8384880	P	3.1680920	-0.8563240	-1.3626620
H	-0.7780490	-1.0912720	4.4007470	N	4.2655190	-1.2145450	-2.5640460
H	-1.0715280	-0.4081570	2.7624830	C	5.2380290	-2.2851270	-2.4980600
N	-0.4502180	-4.3350690	1.4705860	H	5.1480500	-2.9388120	-3.3814310
C	0.5774030	-4.7189150	2.4226170	H	6.2717030	-1.8961010	-2.4710990
H	1.5253680	-4.9589160	1.9111570	H	5.0719210	-2.8944440	-1.6006920
H	0.7659830	-3.8994790	3.1300350	C	4.3750670	-0.3424320	-3.7196340
H	0.2616620	-5.6062850	2.9967030	H	5.3234650	0.2251820	-3.7132630

C	-0.7203400	-5.3284640	0.4508100	H	4.3420000	-0.9371350	-4.6464450
H	-1.0241780	-6.2774110	0.9233480	H	3.5301370	0.3561010	-3.7316060
H	-1.5274710	-4.9964550	-0.2128240	N	2.9035200	-2.2862590	-0.5707560
H	0.1723270	-5.5293030	-0.1681210	C	2.0941700	-3.2872650	-1.2473600
O	0.1319620	-1.7224770	1.0679710	H	1.1817840	-3.4742510	-0.6591310
N	-2.2428790	-2.7377680	0.3499080	H	1.7670050	-2.9146380	-2.2269670
P	-2.0931310	-2.4068340	-1.3208800	H	2.6613850	-4.2263930	-1.3765430
O	-0.7005470	-1.9741090	-1.6276930	C	3.2134570	-2.5986600	0.8079840
N	-2.4725730	-3.7647190	-2.2194780	H	3.7722510	-3.5498810	0.8657700
C	-1.4271940	-4.5123030	-2.8978340	H	3.8244280	-1.8110840	1.2644170
H	-1.6097990	-4.5251850	-3.9854490	H	2.2802850	-2.6867610	1.3858190
H	-0.4568000	-4.0376410	-2.7144270	N	4.0031010	0.1141200	-0.2168450
H	-1.3947410	-5.5581320	-2.5464110	P	3.1609910	1.0224580	0.9472800
C	-3.8098990	-4.2968350	-2.3950810	O	1.6998250	1.0362810	0.6397980
H	-4.5582070	-3.5877810	-2.0215810	N	3.4134280	0.4429090	2.4894620
H	-4.0093550	-4.4666030	-3.4664860	C	2.3655770	-0.3094790	3.1668390
H	-3.9379560	-5.2613540	-1.8725250	H	2.0376520	0.2230060	4.0764840
N	-3.3854240	-1.4018540	-1.6082280	H	1.5061890	-0.4618430	2.4987760
C	-3.6204650	-1.0226440	-2.9980440	H	2.7463580	-1.2992070	3.4725450
H	-3.2954100	-1.8243450	-3.6734210	C	4.6839030	0.4859220	3.1869840
H	-4.6970780	-0.8519480	-3.1548900	H	5.3747900	1.1832920	2.6975080
H	-3.0576220	-0.1065180	-3.2405640	H	4.5319100	0.8307490	4.2232770
C	-3.8497680	-0.4011970	-0.6613650	H	5.1595060	-0.5102430	3.2308260
H	-4.9530340	-0.4009570	-0.6450170	N	4.0095910	2.4647280	0.9434220
H	-3.4606150	-0.5976360	0.3452780	C	3.8635780	3.4044510	2.0435340
H	-3.4813420	0.5920410	-0.9622420	H	3.4204700	2.9088370	2.9160830
H	-5.4732600	1.5157970	0.5627670	H	4.8474590	3.8091610	2.3317950
C	-4.8686490	2.4324610	0.6544610	H	3.2169800	4.2534350	1.7596690
N	-3.7696670	2.2340660	1.5817730	C	4.5043810	3.0739570	-0.2806000
P	-2.1491430	2.2207970	1.1782560	H	5.5106170	3.4906470	-0.1119250
N	-2.1183520	3.1950570	-0.2156380	H	4.5608680	2.3316440	-1.0856190

P	-1.2413110	2.7249400	-1.6104660	H	3.8453180	3.8948440	-0.6137290
N	-1.8019470	3.6933190	-2.8462700	C	5.4522660	-0.0578130	-0.0893210
C	-1.3067380	5.0231200	-3.1342670	H	5.7231420	-1.0187330	0.3807100
H	-1.0219660	5.1033690	-4.1962170	H	5.9259760	-0.0109850	-1.0791830
H	-2.0691790	5.7962760	-2.9299140	H	5.8683510	0.7549190	0.5194030
H	-0.4207020	5.2405830	-2.5245590	O	-1.4170080	1.2799400	-1.9399160
C	-2.9686940	3.2863780	-3.6064840	C	-2.6092260	4.5729890	-0.1360890
H	-3.8409050	3.9299710	-3.3893990	H	-1.7897690	5.3058190	-0.0450980
H	-2.7616140	3.3491790	-4.6867730	H	-3.1989040	4.8209010	-1.0294390
H	-3.2206890	2.2458990	-3.3683880	H	-3.2642180	4.6838460	0.7374710
N	0.3122090	3.2147140	-1.3138120	O	-1.4569290	0.9229740	0.9236760
C	1.3321850	2.8680270	-2.2923010	N	-1.4416210	2.9948380	2.4776150
H	2.1200790	2.2719550	-1.8074160	C	-0.1031460	2.6213050	2.9107230
H	0.9044050	2.2341970	-3.0800400	H	-0.1307870	2.2307690	3.9432870
H	1.7655560	3.7771590	-2.7469820	H	0.3167960	1.8582490	2.2412870
C	0.7913330	3.9726350	-0.1792700	H	0.5630690	3.5021150	2.8999670
H	1.1693070	4.9641810	-0.4931290	C	-2.0282460	4.1019180	3.2068410
H	-0.0028240	4.1172810	0.5629440	H	-3.0832530	4.2318040	2.9363410
H	1.6027750	3.4129950	0.3103350	H	-1.9776800	3.9072990	4.2913250
H	-3.3062790	1.5980770	3.5323790	H	-1.4939970	5.0482030	3.0101580
H	-4.9071590	2.3634630	3.3510810	C	-4.1750680	1.6948710	2.8689360

Table S122. Geometric coordinates and single point energies for NaHMDS PMDTA disolvated dimer.



G = -3109.752278 Hartrees

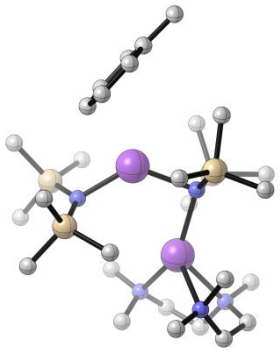
G_{SP} = -3112.122829 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	1.0860950	0.9365320	-0.4400130	H	5.5726660	-2.4314220	3.5620320
N	-0.5952840	1.1383610	1.2736340	C	6.6445960	-2.3750130	1.0475360
Si	-1.1172110	2.7121110	0.8611710	H	7.3976830	-1.9523800	1.7499510
C	-2.6684160	3.3717690	1.7355270	H	6.8096530	-3.4597400	0.9847420
H	-3.5384010	2.7332720	1.5247500	H	6.8326750	-1.9532580	0.0507030
H	-2.9045220	4.3865360	1.3753740	H	5.6626590	-0.2032500	2.3024960
H	-2.5395530	3.4204630	2.8264420	H	3.9647280	-0.5919880	1.9486350
C	-1.5840250	2.7195990	-0.9819390	H	6.1433690	0.2336420	-0.0257800
H	-0.8361390	2.2478290	-1.6429040	H	4.7211460	-0.7032110	-0.5552530
H	-1.7922590	3.7308730	-1.3666950	C	4.5910430	2.1584000	1.1840660
H	-2.5103330	2.1290440	-1.0777650	H	3.8985760	3.0102470	1.1664360
C	0.2180440	4.0239550	1.2111250	H	4.4673410	1.6767380	2.1597310
H	0.2990520	4.1726680	2.3006520	H	5.6320570	2.5418980	1.1073200
H	1.2054170	3.6908280	0.8518470	H	5.6159540	2.1206010	-1.2617590
H	-0.0106790	5.0010130	0.7567300	H	4.3839360	1.0709860	-1.9652680
Si	0.0147570	0.7768080	2.8324740	H	4.1647220	3.5138720	-2.4457350
C	1.8438520	1.2552990	2.9938660	H	3.8914120	3.8393070	-0.7320120

H	2.4003410	0.8443300	2.1357660	C	1.6594010	4.1940780	-1.8042110
H	1.9724380	2.3488070	2.9764520	H	0.5689370	4.0766730	-1.8553110
H	2.3055840	0.8675650	3.9165060	H	1.8951350	4.8186860	-0.9338050
C	-0.0724210	-1.0929210	3.2069250	H	2.0019960	4.7223130	-2.7181400
H	-0.5411290	-1.6301960	2.3702470	H	2.4392460	2.5619360	-3.7836450
H	0.9293860	-1.5247340	3.3583840	H	2.3852360	1.0764280	-2.7853140
H	-0.6640780	-1.2970540	4.1140610	H	0.7420770	0.3969540	-4.7485910
C	-0.8740530	1.6397850	4.2733410	H	-0.8744130	0.1690220	-5.4527450
H	-0.4535690	1.3027890	5.2343200	Si	1.4265990	-1.9776800	-1.5484720
H	-0.7572500	2.7339880	4.2248420	C	2.0818080	-1.7798900	0.2227040
H	-1.9533090	1.4176830	4.2799800	H	2.4964920	-0.7687300	0.3789970
Na	-1.5681090	-0.6477820	0.0562810	H	1.2938590	-1.9325040	0.9766780
N	0.1064130	-0.9046320	-1.7531670	H	2.9164070	-2.4684590	0.4327050
Si	-0.8120540	-0.8835150	-3.2023360	C	1.1332990	-3.8372940	-1.8712560
C	-0.8177690	-2.5204110	-4.1736650	H	1.3297800	-4.0668020	-2.9292030
H	-1.5043420	-2.4368410	-5.0312440	H	1.8400600	-4.4310700	-1.2686600
H	0.1812440	-2.7591070	-4.5723230	H	0.1182220	-4.1928880	-1.6479320
H	-1.1431860	-3.3766580	-3.5633500	C	2.9253250	-1.6268790	-2.6738370
C	-2.6371480	-0.5171080	-2.8416430	H	3.6853940	-2.4170340	-2.5599550
H	-3.1176040	-1.3444610	-2.2978150	H	2.6257640	-1.5967750	-3.7343940
H	-2.7795020	0.4027150	-2.2525400	H	3.4130650	-0.6695460	-2.4378000
H	-3.1909450	-0.3901520	-3.7857310	N	-2.0286870	-3.0597990	0.8587380
C	-0.3352580	0.4041450	-4.5211290	C	-2.9916130	-3.2268750	1.9399570
H	-0.6246030	1.4260950	-4.2306040	C	-4.3114840	-2.4961100	1.7438860
H	0.9220240	2.0381310	-3.0036290	N	-4.2005860	-1.0862810	1.3984170
C	2.0073140	2.1041420	-2.8685210	C	-5.5423790	-0.5668210	1.1645950
N	2.3005600	2.8904030	-1.6784340	C	-5.6342680	0.8556040	0.6346490
C	3.7372470	3.0823790	-1.5141680	N	-5.0239800	1.0745260	-0.6633380
C	4.5423380	1.8345550	-1.1888490	C	-5.1637530	2.4648720	-1.0514740
N	4.2804300	1.2266960	0.1103910	H	-4.6983240	3.1175710	-0.2997600
C	5.0800690	0.0046340	0.2093960	H	-4.6573770	2.6386440	-2.0116800

C	4.9900730	-0.6968790	1.5638430	H	-6.2293970	2.7643080	-1.1604520
N	5.2857450	-2.1127870	1.4673930	C	-5.5983650	0.2093930	-1.6740940
C	4.9674100	-2.7941100	2.7021450	H	-6.7082350	0.2891950	-1.7072510
H	3.9046050	-2.6460770	2.9448840	H	-5.2046100	0.4818590	-2.6606550
H	5.1467830	-3.8730050	2.5915150	H	-5.3270450	-0.8397130	-1.4946480
H	-3.2377430	-4.3030540	2.0765120	H	-6.7207780	1.1053570	0.5998620
H	-2.5031540	-2.9029050	2.8726130	H	-5.1874540	1.5567500	1.3551650
C	-2.5927160	-3.3894310	-0.4419480	H	-6.1286850	-0.5980560	2.1104610
H	-1.8289750	-3.2333870	-1.2185810	H	-6.0557240	-1.2487210	0.4702360
H	-2.9375840	-4.4439880	-0.4926430	C	-3.5330910	-0.3360640	2.4508210
H	-3.4440700	-2.7315680	-0.6649170	H	-2.5509540	-0.7726180	2.6664950
C	-0.8674830	-3.8992120	1.1230950	H	-3.3507470	0.6989800	2.1376280
H	-0.0794100	-3.7014190	0.3878800	H	-4.1263060	-0.3321950	3.3918460
H	-0.4685720	-3.6887460	2.1242700	H	-4.9014020	-2.6296000	2.6785500
H	-1.1305280	-4.9764940	1.0746360	H	-4.8890770	-2.9921270	0.9486170

Table S123. Geometric coordinates and single point energies for NaHMDS PMDTA/toluene mixed disolvated open dimer.



G = -2860.817235 Hartrees

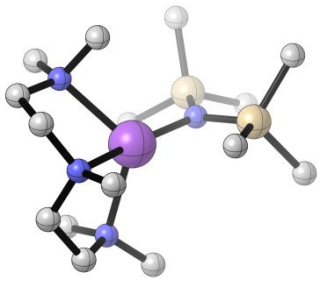
G_{SP} = -2862.894435 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.9847120	-0.2245020	0.0750880	C	-0.5469580	-4.3153440	1.3253130
Na	1.4742940	0.0906500	-0.1416620	H	-1.3249790	-4.0876530	2.0676090
N	1.1065740	2.3068110	0.0996460	H	-1.0406420	-4.7047750	0.4211980
Si	0.6538180	2.6288470	1.6981830	H	0.0705360	-5.1269530	1.7416230
C	-0.6030870	1.3145260	2.2909130	C	1.0702060	-2.0248010	2.5428050
H	-0.2805210	0.2974270	2.0079010	H	1.7672570	-1.1825840	2.3896480
H	-0.6991940	1.3329040	3.3885210	H	0.2200910	-1.6415140	3.1273870
H	-1.6071020	1.4938020	1.8737970	H	1.5944420	-2.7636920	3.1694910
C	-0.1608920	4.3188770	1.9981450	Si	-0.0921540	-1.9773550	-1.8925440
H	0.5925210	5.1213050	1.9508740	C	1.6195400	-1.9308190	-2.7283100
H	-0.9232680	4.5462900	1.2357720	H	1.5041570	-2.0420180	-3.8186400
H	-0.6353940	4.3670430	2.9914400	H	2.1397000	-0.9705400	-2.5654070
C	2.0692320	2.5069250	2.9653140	H	2.2851430	-2.7313070	-2.3740060
H	1.7386340	2.8036010	3.9735210	C	-0.8639380	-3.6319270	-2.4042280
H	2.4490820	1.4737580	3.0331440	H	-1.0095420	-3.6967150	-3.4937790
H	2.9121910	3.1570700	2.6807660	H	-0.2036150	-4.4620940	-2.1058680
Si	1.7873050	3.3449790	-1.0630470	H	-1.8347970	-3.7990240	-1.9131190
C	0.8652520	4.9854810	-1.3426590	C	-1.0078960	-0.5432550	-2.7360880

H	-0.1931330	4.8333400	-1.6031620	H	-0.4302160	0.3829210	-2.5750420
H	0.8994990	5.6185010	-0.4427500	H	-1.0989450	-0.6925240	-3.8232490
H	1.3352440	5.5490640	-2.1646480	H	-2.0194440	-0.3767860	-2.3378000
C	3.5712540	3.8928180	-0.6869920	N	-3.0059820	1.8388410	-0.8810520
H	4.2856530	3.0573680	-0.6324860	C	-4.0800630	1.4413220	-1.7832910
H	3.9381610	4.5957420	-1.4519700	C	-5.0161320	0.3975760	-1.1933180
H	3.6019750	4.4138550	0.2842380	N	-4.3624770	-0.8807090	-0.9098090
C	1.8004510	2.4863250	-2.7620470	C	-5.0611230	-1.6202960	0.1367780
H	0.7702730	2.3864750	-3.1407340	C	-4.9617020	-1.0015740	1.5238340
H	2.3721940	3.0633350	-3.5057010	N	-3.6017080	-0.7697370	1.9865310
H	2.2339320	1.4722480	-2.7291510	C	-3.6311160	-0.0827690	3.2686810
N	-0.0821990	-1.6816840	-0.2021580	H	-4.1173560	0.8981210	3.1617920
Si	0.5688590	-2.8343770	0.8972170	H	-4.1866540	-0.6647850	4.0326490
C	2.1673620	-3.6335870	0.2498640	H	-2.6079450	0.0803890	3.6272910
H	2.8871630	-2.8636260	-0.0694950	C	-2.8517900	-2.0111000	2.0948880
H	2.6473400	-4.2404860	1.0347290	H	-2.7148230	-2.4838870	1.1113650
H	1.9710040	-4.2916520	-0.6123620	H	-1.8488320	-1.7975220	2.4895620
H	-2.6898980	2.9769710	0.8487090	H	-3.3450110	-2.7430810	2.7694600
H	-4.2344520	3.3282340	0.0270350	H	-5.5045430	-1.6717650	2.2264760
C	4.9095890	-1.0269890	-1.0214860	H	-5.4954540	-0.0387570	1.5558780
C	4.3299280	0.1899430	-0.6568640	H	-4.6486200	-2.6401420	0.1578560
C	4.1346510	0.5028500	0.6911370	H	-6.1387130	-1.7338510	-0.1102870
C	4.5251500	-0.4167810	1.6680240	C	-4.3016090	-1.6985610	-2.1155710
C	5.1096170	-1.6263230	1.2979640	H	-3.8777950	-1.1266780	-2.9503320
C	5.3106370	-1.9507740	-0.0501920	H	-3.6573510	-2.5727590	-1.9496540
C	5.8874530	-3.2843420	-0.4423390	H	-5.3091130	-2.0497840	-2.4188320
H	6.6208700	-3.6352030	0.2960760	H	-5.4475930	0.7952300	-0.2658340
H	5.0864850	-4.0389580	-0.5019120	H	-5.8697640	0.2495920	-1.8862280
H	6.3765080	-3.2360650	-1.4241840	H	-3.6220570	1.0543990	-2.7066810
H	5.4140250	-2.3385260	2.0685560	H	-4.6861350	2.3251680	-2.0795670
H	4.3819720	-0.1809540	2.7244110	C	-2.0542980	2.7042460	-1.5720960

H	3.6819430	1.4579160	0.9680980	H	-1.1622590	2.8511690	-0.9445410
H	4.0425420	0.9112480	-1.4266580	H	-1.7332450	2.2263030	-2.5077560
H	5.0556530	-1.2616700	-2.0784640	H	-2.5044030	3.6873210	-1.8215500
H	-4.0276200	1.8156530	0.9764820	C	-3.5230890	2.5205140	0.2987200

Table S124. Geometric coordinates and single point energies for NaHMDS PMDTA monosolvated monomer.



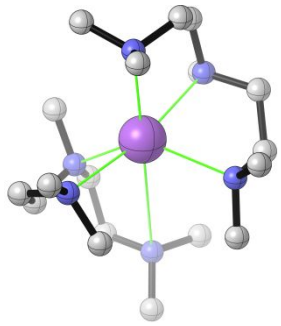
G = -1554.884204 Hartrees

G_{SP} = -1556.068039 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Symbol	X	Y	Z	H	-1.2397320	4.1677740	0.4232550
Si	2.6891480	0.9874910	-0.6808380	H	0.1148840	3.1481360	-0.1583110
N	1.6217800	-0.1072420	0.0473230	C	-0.8257520	1.9766180	1.9758090
Si	1.9838610	-1.4142930	1.0565060	H	-1.1234300	1.0555260	2.4993620
C	2.8576040	-2.8770490	0.2197320	H	0.2648090	1.9341630	1.8372340
H	3.8527290	-2.5767000	-0.1429740	H	-1.0803570	2.8398850	2.6246460
H	2.9903530	-3.7259920	0.9092590	H	-3.3029450	2.8977840	1.3567830
H	2.2807570	-3.2271670	-0.6509900	H	-3.3051420	2.2160850	-0.2745000
C	3.0052540	-0.9837930	2.5983140	H	-3.2365920	0.6917370	2.3886690
H	2.5137670	-0.1849450	3.1764590	H	-4.6089230	0.8323670	1.2903690
H	3.1533310	-1.8506980	3.2615800	C	-3.2688750	-1.6153520	1.5163840
H	4.0003130	-0.6119890	2.3047710	H	-2.8776200	-2.5262650	1.0452860
C	0.3305660	-2.1324720	1.7177570	H	-2.7476240	-1.4961130	2.4759840
H	-0.3210640	-2.4765260	0.8932980	H	-4.3504160	-1.7622870	1.7159920
H	0.4971090	-3.0003620	2.3737800	C	4.3658890	0.2419820	-1.1752220
H	-0.2245280	-1.3839830	2.3118540	H	4.9050640	-0.1351940	-0.2907420
Na	-0.6057500	-0.0843110	0.0706470	H	4.2257110	-0.6053730	-1.8649950
N	-3.0270010	-0.4558270	0.6694850	H	5.0132530	0.9830110	-1.6704360
C	-3.6320490	-0.6345170	-0.6502710	C	1.9528820	1.6968780	-2.2864070

C	-2.8514420	-1.5757600	-1.5660940	H	0.9581800	2.1412680	-2.1172470
N	-1.5126280	-1.0938980	-1.8628660	H	2.5963030	2.4753020	-2.7258620
C	-0.6136020	-2.1409660	-2.3234870	H	1.8417560	0.8936710	-3.0336040
H	0.4081100	-1.7381930	-2.3828560	C	3.1094590	2.4811880	0.4245210
H	-0.6035160	-2.9696500	-1.6011070	H	2.2137440	3.0638200	0.6952200
H	-0.9075970	-2.5420050	-3.3150840	H	3.5650530	2.1309090	1.3646910
C	-1.5051400	0.0355570	-2.7775290	H	3.8198850	3.1688210	-0.0615700
H	-2.0888530	0.8743170	-2.3696600	H	-4.6716880	-1.0123130	-0.5527300
H	-0.4736160	0.3875400	-2.9152380	C	-3.5010750	0.7621220	1.3234820
H	-1.9251700	-0.2284190	-3.7704760	C	-2.9211310	2.0509640	0.7450150
H	-2.7575290	-2.5615910	-1.0861020	N	-1.4695810	2.0601370	0.6717550
H	-3.4441650	-1.7351190	-2.4925230	C	-0.9785440	3.2089230	-0.0703230
H	-3.7101670	0.3490720	-1.1340370	H	-1.4055600	3.2142280	-1.0838850

Table S125. Geometric coordinates and single point energies for sodium cation solvated by 2 equivalents of PMDTA. The green bonds indicate N–Na contacts that are longer than those observed in the dimeric and monomeric species.



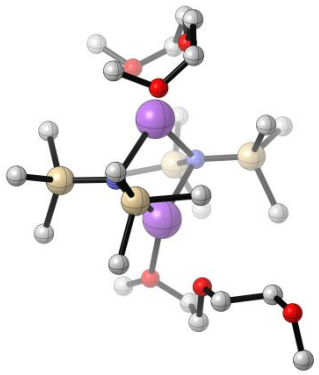
G = -1202.270772 Hartrees

G_{SP} = -1203.491449 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.4940170	-0.1996320	0.1123120	C	0.2495330	-1.5280930	-2.3040120
N	1.2943170	-1.1613720	-1.3580710	H	-0.5675980	-2.0549330	-1.7941590
C	1.8726960	-2.3509430	-0.7398090	H	-0.1680800	-0.6220870	-2.7663850
C	0.8857040	-3.1742040	0.0740940	H	0.6258020	-2.1817730	-3.1168440
N	0.1714890	-2.4001780	1.0867160	N	-1.4186380	1.7510820	-1.1499810
C	-0.7222840	-3.2821440	1.8257180	C	-1.5335630	2.8029730	-0.1322420
H	-1.2937800	-2.7078230	2.5676650	C	-0.3883960	2.7964840	0.8692520
H	-1.4282250	-3.7673840	1.1364950	N	-0.3754470	1.6431990	1.7739980
H	-0.1659480	-4.0782280	2.3591260	C	0.8853930	1.6452180	2.5135520
C	1.0949280	-1.7403920	2.0039150	H	0.8751130	0.8620890	3.2821070
H	1.6697280	-0.9546350	1.4873310	H	1.7177530	1.4461650	1.8239700
H	0.5193390	-1.2709960	2.8135230	H	1.0550090	2.6148490	3.0226010
H	1.8072420	-2.4554030	2.4643840	C	-1.4915560	1.6843420	2.7121710
H	0.1404380	-3.6570990	-0.5765340	H	-2.4541120	1.6622400	2.1844640
H	1.4591080	-3.9980580	0.5493690	H	-1.4518550	0.8073880	3.3737340
H	2.6843410	-2.0349270	-0.0731990	H	-1.4663220	2.5949100	3.3433720
H	2.3285750	-3.0156560	-1.5041440	H	0.5680200	2.7972740	0.3242190
C	2.3074900	-0.3598900	-2.0523540	H	-0.4206570	3.7396550	1.4536490

C	3.5410570	0.0027030	-1.2351380	H	-2.4864730	2.6966070	0.4008190
N	3.2685040	0.7924460	-0.0410750	H	-3.2877330	-0.4945330	1.8081890
C	4.2788320	0.5803100	0.9829450	C	-3.5301610	-1.1944540	0.9958450
H	4.3102670	-0.4806060	1.2716730	N	-2.9480100	-0.7341810	-0.2609880
H	5.2933670	0.8790120	0.6493590	C	-3.5506990	0.5399450	-0.6532560
H	4.0331840	1.1687460	1.8791060	C	-2.7270600	1.3325470	-1.6586150
C	3.1717610	2.2031600	-0.3707060	H	-3.3215830	2.2075090	-1.9920950
H	2.4042680	2.3651040	-1.1409840	H	-2.5554180	0.7208290	-2.5580630
H	2.8949870	2.7890180	0.5178780	H	-3.6980880	1.1366950	0.2591180
H	4.1292370	2.6074690	-0.7590530	H	-4.5645680	0.3811310	-1.0739610
H	4.0726240	-0.9122130	-0.9407440	C	-3.1604000	-1.7476390	-1.2882560
H	4.2387940	0.5358620	-1.9134650	H	-2.7608620	-1.4156970	-2.2554300
H	2.6624790	-0.8983550	-2.9566250	H	-2.6468230	-2.6788750	-1.0070750
H	1.8135120	0.5573360	-2.4111900	H	-4.2368520	-1.9746280	-1.4207690
H	0.3966700	2.5415280	-1.8749210	H	-4.6324910	-1.2855860	0.9316740
H	-0.4348360	1.4363010	-2.9943700	H	-3.1234360	-2.1793620	1.2544720
H	-1.0465240	3.0961650	-2.7639700	H	-1.5736050	3.7989550	-0.6143100
				C	-0.5874930	2.2292410	-2.2497080

Table S126. Geometric coordinates and single point energies for NaHMDS diglyme disolavted dimer.



G = -2993.531565 Hartrees

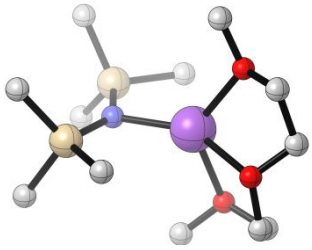
G_{SP} = -2995.78937 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.7622180	3.8076740	-0.6780900	H	1.5275570	3.3473570	-3.3648470
Si	-1.1180060	2.8715390	-0.9178130	H	2.8405550	2.4048460	-4.1590010
N	-0.6658440	1.7224390	0.2689530	Si	-0.1848090	2.2177750	1.8364960
Na	1.0208450	0.3546640	-0.7953820	C	1.6668110	2.6511430	1.9275950
Na	-1.6666790	-0.4804180	0.3222480	H	2.2803870	1.8481910	1.4869460
N	-0.0565070	-1.7753170	-0.9180740	H	1.8626760	3.5748790	1.3579640
Si	-0.6212030	-2.1379630	-2.4880110	H	2.0081590	2.8132600	2.9624820
C	-0.7276990	-3.9838710	-2.9367280	C	-0.5006830	0.8550640	3.1182550
H	-1.1142680	-4.0984070	-3.9620900	H	-1.5822180	0.6680120	3.2100140
H	0.2576580	-4.4744320	-2.8955020	H	-0.0143620	-0.0905580	2.8345920
H	-1.4027570	-4.5355140	-2.2631350	H	-0.1148030	1.1462150	4.1078130
C	-2.3883760	-1.4725450	-2.6815540	C	-1.0947480	3.7411130	2.5266960
H	-3.0754260	-2.0472390	-2.0374620	H	-0.7125810	3.9899210	3.5295570
H	-2.4308330	-0.4188080	-2.3686840	H	-0.9646950	4.6292130	1.8888570
H	-2.7607360	-1.5367030	-3.7158980	H	-2.1772580	3.5556590	2.6208600
C	0.4542950	-1.3738190	-3.8579130	C	-1.3269470	2.0648470	-2.6258300
H	0.5971910	-0.2928270	-3.7054010	H	-0.6400850	1.2232520	-2.8057830

H	1.4529570	-1.8392420	-3.8446210	H	-1.1899860	2.7967760	-3.4375420
H	0.0216540	-1.5181960	-4.8603870	H	-2.3503790	1.6677090	-2.7101070
Si	1.0710020	-2.7591800	-0.0920950	C	0.1458330	4.2908000	-1.0962030
C	1.4807820	-1.9695210	1.5888990	H	0.1542260	4.9156380	-0.1883430
H	1.7004300	-0.8892900	1.5309290	H	1.1675190	3.9124930	-1.2402190
H	0.5893470	-2.0919140	2.2230660	H	-0.1015180	4.9474770	-1.9462860
H	2.3250500	-2.4591210	2.1006600	H	-3.6220830	3.1621740	-0.9091210
C	0.5600560	-4.5346210	0.3551030	H	-2.7917570	4.6588660	-1.3774710
H	0.1871910	-5.0992320	-0.5121230	H	-2.8854800	4.2081170	0.3393440
H	1.4354560	-5.0735550	0.7526270	C	-4.0907510	1.3203750	0.8740970
H	-0.2145700	-4.5338040	1.1354940	C	-4.4918550	0.3173730	1.9338110
C	2.6737320	-2.9728740	-1.1075570	H	-4.7201000	0.8367100	2.8831850
H	3.4747840	-3.4863120	-0.5512910	H	-5.3928750	-0.2517940	1.6326250
H	2.4522350	-3.5806370	-2.0005010	O	-3.4022540	-0.5531570	2.0854850
H	3.0581070	-2.0024280	-1.4624990	C	-3.6202500	-1.6599770	2.9162790
O	2.2163130	1.6848150	-2.3182400	C	-2.3333410	-2.4698530	2.9096030
C	3.2542630	2.2766610	-1.5641790	H	-2.5051400	-3.4520390	3.3881150
C	4.1694360	1.2059500	-1.0273240	H	-1.5595440	-1.9334250	3.4772940
H	4.9803920	1.6922090	-0.4547600	O	-1.8245820	-2.6189720	1.6120040
H	4.6239220	0.6389430	-1.8605760	C	-2.6214750	-3.3810200	0.7387520
O	3.4364090	0.3291360	-0.2024470	H	-2.0293550	-3.5318140	-0.1724400
C	4.2711880	-0.5113540	0.5781480	H	-2.8725100	-4.3611890	1.1821730
C	4.5416440	0.1034060	1.9483320	H	-3.5577820	-2.8535000	0.4769140
H	4.8923200	1.1492400	1.8412610	H	-3.8628170	-1.3484060	3.9490410
H	3.6022510	0.1320790	2.5199920	H	-4.4755350	-2.2525190	2.5379250
O	5.4577920	-0.6706810	2.6712910	H	-4.8751960	2.0854120	0.7418210
C	6.7979080	-0.3599360	2.4213860	H	-3.1623210	1.8239330	1.1835320
H	7.0372680	0.6737060	2.7322740	O	-3.8022490	0.6744570	-0.3462350
H	7.4170110	-1.0535630	3.0035040	C	-4.9222360	0.4946130	-1.1765310
H	7.0675260	-0.4686410	1.3546900	H	-5.3510560	1.4699370	-1.4669970
H	5.2162660	-0.7013670	0.0398080	H	-4.5886960	-0.0347920	-2.0763940

H	3.7673730	-1.4752260	0.7004780	H	-5.7089240	-0.1043170	-0.6844210
H	3.8442890	2.9653680	-2.1916430	C	1.9320830	2.3369290	-3.5371450
H	2.8289940	2.8517490	-0.7243910	H	1.1836140	1.7403740	-4.0699210

Table S127. Geometric coordinates and single point energies for NaHMDS diglyme monosolavted monomer.



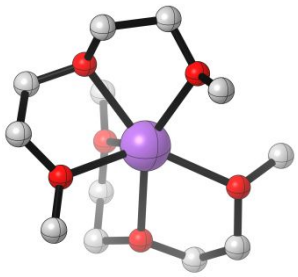
G = -1496.760861 Hartrees

G_{SP} = -1497.89186 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	-2.2425320	0.5847510	-1.2769620	C	1.3565430	3.2822750	0.5438790
N	-1.3870850	0.0202350	0.0641940	H	0.3500730	3.2759190	0.1077510
Si	-1.7620900	-0.5669460	1.5996000	H	1.2693530	3.2789700	1.6433600
C	-2.7942470	0.6006230	2.6829670	H	1.8909050	4.1927090	0.2247870
H	-3.7967870	0.7415320	2.2487880	H	3.9164420	0.6732620	-0.9870560
H	-2.9214130	0.2154340	3.7071400	H	4.8792450	0.4835000	0.5121670
H	-2.3192410	1.5926150	2.7424800	H	3.0011550	-3.0176590	-1.5438930
C	-2.6613990	-2.2413570	1.6095560	H	3.3485820	-1.3364330	-2.0015130
H	-2.0807190	-3.0028140	1.0644330	C	0.5455350	-2.6985410	-1.1011060
H	-2.8355640	-2.6130550	2.6319140	H	0.7791040	-3.1894170	-0.1403460
H	-3.6392510	-2.1552860	1.1099380	H	-0.4537770	-2.2477390	-1.0256950
C	-0.1180740	-0.8532310	2.5349350	H	0.5747080	-3.4490030	-1.9080090
H	0.4499690	0.0884210	2.6369210	C	-3.2725740	2.1497320	-0.9643070
H	-0.2716150	-1.2530830	3.5492560	H	-4.0665640	1.9501830	-0.2275480
H	0.5203990	-1.5753230	1.9947140	H	-2.6415110	2.9550920	-0.5554520
Na	0.7989960	0.2225360	-0.1968220	H	-3.7502010	2.5218500	-1.8846620
O	1.4492020	-1.6426660	-1.3747500	C	-0.9786400	1.0397800	-2.6342870
C	2.8138390	-1.9641030	-1.2718630	H	-0.3599070	0.1643020	-2.8964420
C	3.3173220	-1.6913490	0.1403950	H	-1.4607110	1.3938080	-3.5587040
H	2.8206680	-2.3621980	0.8566440	H	-0.3038020	1.8458200	-2.2942070

H	4.4057440	-1.8679070	0.2076180	C	-3.4237940	-0.6844600	-2.0530900
O	2.9939190	-0.3797090	0.5527570	H	-2.8868370	-1.6094490	-2.3176410
C	3.8597490	0.6408430	0.1167150	H	-4.2175310	-0.9568980	-1.3394330
C	3.3097460	1.9522770	0.6284670	H	-3.9073580	-0.2980900	-2.9643530
H	3.2607910	1.9273550	1.7326930	H	3.9760470	2.7807230	0.3264500
				O	2.0232420	2.1247650	0.0911280

Table S128 Geometric coordinates and single point energies for sodium cation solvated by 2 equivalents of diglyme.



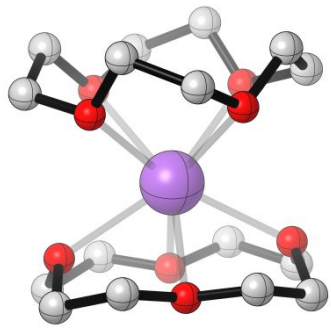
G = -1086.045878 Hartrees

G_{SP} = -1087.154175 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.0001490	0.2279490	-0.0000940	O	-0.6926860	-1.3369500	1.5407340
O	0.6920520	-1.3378920	-1.5404950	C	-1.9639070	-1.9117670	1.3492880
C	1.9629960	-1.9132290	-1.3488000	C	-2.2685200	-1.8833630	-0.1379550
C	2.2675550	-1.8843820	0.1384450	H	-3.2850190	-2.2687090	-0.3266400
H	3.2838960	-2.2700320	0.3273450	H	-1.5441250	-2.5214850	-0.6632050
H	1.5428640	-2.5219630	0.6639370	O	-2.1052920	-0.5933940	-0.6881340
O	2.1048720	-0.5940810	0.6880600	C	-3.1449080	0.3268640	-0.4344770
C	3.1450260	0.3255110	0.4341300	C	-2.6614680	1.6697840	-0.9421500
C	2.6623820	1.6688250	0.9414850	H	-2.4368830	1.5888280	-2.0158560
H	2.4378610	1.5883210	2.0152480	H	-3.4382790	2.4399960	-0.8090420
H	3.4395950	2.4385680	0.8080800	O	-1.4627390	2.0407760	-0.2903310
O	1.4638320	2.0401540	0.2895040	C	-1.6325990	2.8697310	0.8427320
C	1.6338690	2.8705980	-0.8424490	H	-2.2560480	2.3839560	1.6128320
H	2.2580940	2.3861250	-1.6127310	H	-0.6328040	3.0567430	1.2529720
H	0.6342060	3.0574940	-1.2530570	H	-2.0976560	3.8274900	0.5597980
H	2.0981480	3.8283030	-0.5580650	H	-3.3648690	0.3841680	0.6472240
H	3.3648990	0.3824730	-0.6476090	H	-4.0704090	0.0260320	-0.9560400
H	4.0703730	0.0242160	0.9556980	H	-2.7218980	-1.3626180	1.9388960
H	2.7212630	-1.3646440	-1.9385700	H	-1.9760810	-2.9603800	1.6972710

H	1.9746990	-2.9619810	-1.6963770	C	-0.2038690	-1.4495260	2.8599810
C	0.2031710	-1.4508040	-2.8596820	H	-0.1454200	-2.5071180	3.1665500
H	0.1442380	-2.5085000	-3.1658030	H	0.8028580	-1.0145320	2.8680890
H	-0.8033610	-1.0153620	-2.8679640	H	-0.8510160	-0.9096620	3.5714780
H	0.8505470	-0.9115320	-3.5714190				

Table S129. Geometric coordinates and single point energies for sodium cation solvated by 2 equivalents of 12-crown-4.



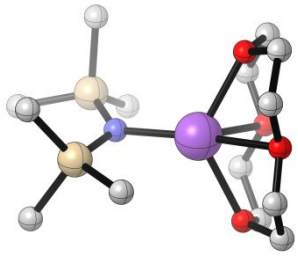
G = -1390.901291 Hartrees

G_{SP} = -1392.347785 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.1617200	-0.0003450	0.0000630	C	-1.9426210	0.4378040	2.5184860
O	1.3990120	-2.1242230	0.1130100	C	-2.4558700	-0.8475550	1.9011890
C	2.1798230	-2.3487360	-1.0465480	O	-1.3737450	-1.4506560	1.2324280
C	1.8214300	-1.3210180	-2.1034110	C	-1.7001250	-2.5659990	0.4283070
H	2.4793660	-1.4532230	-2.9812460	C	-2.3019370	-2.1334100	-0.8942180
H	0.7724950	-1.4507900	-2.4248750	H	-3.2670070	-1.6189970	-0.7361250
O	2.0081350	-0.0653950	-1.5013830	H	-2.5008540	-3.0200190	-1.5213470
C	1.7246120	1.0861480	-2.2526650	H	-0.7521450	-3.0866140	0.2424650
C	2.0625000	2.2663690	-1.3570720	H	-2.3911570	-3.2449770	0.9566200
O	1.4058910	2.1216900	-0.1115140	H	-2.8566080	-1.5150140	2.6849980
C	2.1856330	2.3434990	1.0492720	H	-3.2804880	-0.6253850	1.1981490
C	1.8218500	1.3170500	2.1054690	H	-2.7474240	0.9524760	3.0691130
O	2.0060970	0.0608130	1.5038720	H	-1.1407840	0.2067560	3.2358840
C	1.7179130	-1.0897930	2.2547840	H	-3.2642310	1.6268970	0.7313200
C	2.0531280	-2.2711210	1.3596170	H	-2.4958350	3.0258850	1.5179830
H	1.7534100	-3.2127480	1.8489750	H	-0.7437130	3.0879320	-0.2427090
H	3.1432740	-2.2949230	1.2046280	H	-2.3810370	3.2505020	-0.9597730
H	2.3267100	-1.1417200	3.1754830	H	-3.2765890	0.6330500	-1.2030150

H	0.6502710	-1.1155760	2.5381970	H	-2.8477190	1.5216250	-2.6890830
H	2.4782790	1.4472870	2.9847200	H	-2.7437760	-0.9460630	-3.0732080
H	0.7725780	1.4499360	2.4246000	H	-1.1348860	-0.2043320	-3.2364870
H	3.2535480	2.2264770	0.8055530	O	-1.3832240	-1.2700070	-1.5294910
H	2.0267840	3.3622720	1.4406970	C	-1.9388500	-0.4334470	-2.5208450
H	1.7667090	3.2089720	-1.8469320	C	-2.4501230	0.8531770	-1.9045240
H	3.1524760	2.2865170	-1.2003790	O	-1.3677350	1.4535860	-1.2337380
H	2.3346730	1.1360270	-3.1726330	C	-1.6927130	2.5697650	-0.4301930
H	0.6573640	1.1156020	-2.5372540	C	-2.2980970	2.1387480	0.8912270
H	2.0179190	-3.3668990	-1.4383120	O	-1.3828800	1.2728950	1.5282010
H	3.2477490	-2.2356580	-0.8010310				

Table S130. Geometric coordinates and single point energies for NaHMDS 12-crown-4 monosolvated monomer.



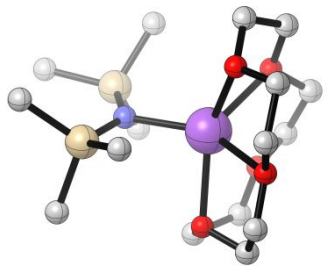
G = -1649.17557 Hartrees

G_{SP} = -1650.476357 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Si	1.8750590	1.7945020	0.2939630	H	-3.9017760	0.7202320	-1.9266750
N	1.5217860	0.1741580	-0.0658560	H	-4.2991440	2.2334690	-0.0398650
Si	2.6919430	-1.0611770	-0.0812830	H	-2.5496120	2.5966110	0.0915120
C	4.4860620	-0.4759390	-0.3162600	H	-4.0143170	1.0793960	2.3351570
H	5.1848570	-1.3243310	-0.2422990	H	-2.2504230	1.3671460	2.2779430
H	4.6174510	-0.0168690	-1.3087690	H	-3.6936080	-1.3372500	2.0873760
H	4.7830920	0.2688330	0.4386350	H	-2.7367360	-0.7627130	3.4875750
C	2.4541200	-2.3095270	-1.5065620	H	-1.2313210	-3.2359300	1.9656340
H	2.4328540	-1.7802420	-2.4731520	H	-2.7282170	-2.8344280	1.0629790
H	3.3050830	-3.0090400	-1.5288870	H	-0.8758700	-3.5945900	-0.4405520
H	1.5388220	-2.9173490	-1.4362580	H	0.1128870	-2.2091830	0.1073280
C	2.6874800	-2.0831720	1.5253390	H	-1.2639830	0.1266950	-3.6892720
H	2.9520230	-1.4313600	2.3732350	H	-2.7419330	-0.6034710	-2.9876090
H	1.6906320	-2.5011620	1.7421150	C	2.9156150	2.7237490	-0.9910480
H	3.4069370	-2.9169000	1.4955940	H	2.4641030	2.6296480	-1.9909030
Na	-0.7377870	0.2179310	0.1436190	H	2.9997570	3.7948410	-0.7474830
O	-1.8463000	0.8607270	-1.8365470	H	3.9334940	2.3089550	-1.0442010
C	-1.7376760	-0.2125690	-2.7538790	C	0.2301310	2.7804390	0.3835120
C	-0.9103110	-1.3171590	-2.1240600	H	0.4263570	3.8502770	0.5509160

H	-0.8083690	-2.1601970	-2.8313940	H	-0.3344020	2.6923310	-0.5602900
H	0.1020640	-0.9430770	-1.8766000	H	-0.4086590	2.4518160	1.2251630
O	-1.5971340	-1.7057940	-0.9514110	C	2.6920120	2.0920970	1.9845110
C	-0.9213540	-2.5585580	-0.0575170	H	2.0712890	1.6609690	2.7863110
C	-1.6853170	-2.5289450	1.2512480	H	3.6803350	1.6097300	2.0408240
O	-1.6590620	-1.2123290	1.7683890	H	2.8305390	3.1648320	2.1942410
C	-2.8259910	-0.7273440	2.3888920	C	-3.2846980	1.8255750	-0.2034080
C	-3.0611890	0.6998640	1.9237060	C	-3.1146560	1.4471320	-1.6643200
O	-3.0826070	0.6406510	0.5229740	H	-3.2336240	2.3395050	-2.3028140

Table S131. Geometric coordinates and single point energies for NaHMDS 15-crown-5 monosolvated monomer.



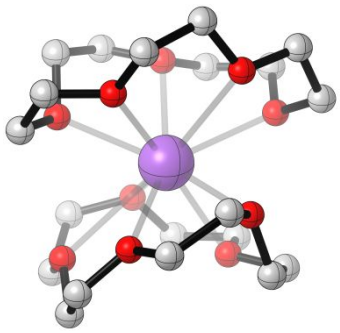
G = -1802.792272 Hartrees

G_{SP} = -1804.266908 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.5972540	-0.0698330	-0.1100940	H	-0.3612660	1.2939380	-2.8415300
O	-1.6597600	-0.1018050	-2.2211750	N	1.6639230	-0.1245940	-0.2454870
C	-1.4525960	1.1754120	-2.7783610	Si	2.0790870	-1.7318470	-0.5579930
C	-2.0212990	2.2800670	-1.9008150	C	2.6050420	-2.7105660	0.9888720
O	-1.4852230	2.1129080	-0.6152890	H	1.7637210	-2.7642800	1.6989810
C	-2.1696410	2.7675410	0.4196290	H	2.9134660	-3.7410790	0.7498740
C	-1.3974330	2.5417410	1.7027400	H	3.4469690	-2.2120570	1.4962500
O	-1.1551220	1.1644920	1.8083360	C	0.5434680	-2.6575900	-1.2177020
C	-0.6686530	0.6993100	3.0440550	H	-0.2440710	-2.6473160	-0.4452190
C	0.0139730	-0.6409260	2.7830760	H	0.7618070	-3.7107050	-1.4543590
O	-0.7009810	-1.4351080	1.8626710	H	0.1530620	-2.1673630	-2.1243290
C	-2.0141570	-1.7901800	2.2000020	C	3.4456620	-2.0076860	-1.8490960
C	-2.6505000	-2.3702640	0.9564920	H	3.5488820	-3.0762900	-2.0973010
O	-2.6534250	-1.3637150	-0.0281110	H	3.2193980	-1.4590460	-2.7770990
C	-3.0213010	-1.7962200	-1.3149670	H	4.4195900	-1.6516950	-1.4798810
C	-2.9762960	-0.5906030	-2.2263150	Si	2.5817220	1.2807750	-0.0838410
H	-3.6850890	0.1661530	-1.8451770	C	1.9250670	2.6956690	-1.1779830
H	-3.2867840	-0.8746750	-3.2481680	H	0.8586350	2.8752240	-0.9645020
H	-4.0419960	-2.2215300	-1.3123150	H	2.4749070	3.6378210	-1.0229350

H	-2.3148230	-2.5672710	-1.6722350	H	2.0174010	2.4201220	-2.2416360
H	-3.6810030	-2.7050420	1.1764230	C	2.5134660	1.9708860	1.6957690
H	-2.0659740	-3.2416240	0.6095870	H	1.4645410	2.1621760	1.9743630
H	-2.0327610	-2.5345510	3.0173390	H	2.9232250	1.2396740	2.4122530
H	-2.5978900	-0.9063180	2.5134430	H	3.0713860	2.9135850	1.8114640
H	0.1706250	-1.1766710	3.7369510	C	4.4309560	1.1221580	-0.4916610
H	0.9831540	-0.4633630	2.2925600	H	4.9074650	0.3509260	0.1353070
H	-1.5038640	0.6199150	3.7659100	H	4.9602980	2.0729800	-0.3191050
H	0.0772020	1.3929640	3.4691950	H	4.5806220	0.8351540	-1.5441600
H	-1.9943840	2.9115390	2.5565180	H	-3.1259630	2.2352190	-1.8595000
H	-0.4411770	3.0944580	1.6771770	H	-1.7449050	3.2633050	-2.3238360
H	-3.1905840	2.3503170	0.5130380	H	-1.8791430	1.2421180	-3.7953450
H	-2.2521300	3.8519580	0.2232550				

Table S132. Geometric coordinates and single point energies for sodium cation solvated by 2 equivalents of 15-crown-5.



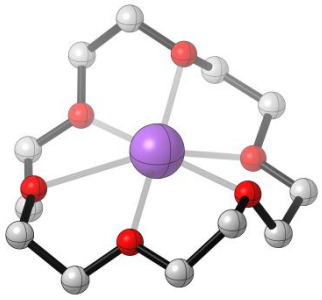
G = -1698.099228 Hartrees

G_{SP} = -1699.900099 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.0001370	0.0521820	0.0005990	C	0.7924550	-1.9761210	-2.3743950
O	1.7741890	1.8961410	-0.7874750	C	-0.4679110	-2.7791860	-2.0817980
C	2.8243280	1.4058280	-1.5963100	O	-1.1899300	-2.1039720	-1.0849200
C	3.6826950	0.4008210	-0.8563490	C	-2.4885610	-2.5939090	-0.8566760
O	2.8735800	-0.6779590	-0.4700020	C	-3.4071510	-1.4266170	-0.5832430
C	3.4055930	-1.4291640	0.5855780	O	-2.8745270	-0.6733220	0.4705630
C	2.4849640	-2.5938180	0.8632420	C	-3.6820900	0.4079170	0.8533030
O	1.1876050	-2.1005600	1.0913650	C	-2.8227390	1.4130070	1.5919750
C	0.4640830	-2.7739150	2.0883950	O	-1.7713460	1.9001950	0.7828340
C	-0.7953640	-1.9687520	2.3795530	C	-2.1866780	2.8496350	-0.1733640
O	-0.5526280	-0.5834560	2.3546230	C	-1.2589540	2.8093480	-1.3641640
C	0.3389130	-0.1038560	3.3298560	O	-1.1910090	1.4810520	-1.8174790
C	0.5567310	1.3635690	3.0618880	C	-0.5553080	1.3563260	-3.0648470
O	1.1927990	1.4838530	1.8142570	C	-0.3398260	-0.1121630	-3.3287750
C	1.2633300	2.8108400	1.3575120	H	0.0715580	-0.2627060	-4.3437770
C	2.1915830	2.8463930	0.1670200	H	-1.3131370	-0.6301490	-3.2633130
H	3.2116760	2.6202610	0.5174100	H	-1.1772250	1.7956560	-3.8662640
H	2.2050380	3.8612640	-0.2712230	H	0.4150310	1.8847840	-3.0484930

H	1.6699760	3.4776550	2.1402470	H	-1.6646920	3.4748760	-2.1484680
H	0.2505700	3.1667580	1.1011870	H	-0.2454420	3.1640560	-1.1091660
H	1.1792390	1.8041430	3.8621610	H	-3.2075290	2.6254670	-0.5228110
H	-0.4127720	1.8935200	3.0439160	H	-2.1973380	3.8654090	0.2628590
H	-0.0731200	-0.2509320	4.3450970	H	-3.4493100	2.2430910	1.9637390
H	1.3114170	-0.6235760	3.2661770	H	-2.3509520	0.9090560	2.4433160
H	-1.2135900	-2.2820560	3.3538210	H	-4.1438020	0.8658180	-0.0406800
H	-1.5540930	-2.1315840	1.6080960	H	-4.5073080	0.0749110	1.5102340
H	1.0895790	-2.8739790	2.9952340	H	-3.4854450	-0.7972550	-1.4904340
H	0.1814400	-3.7957820	1.7742840	H	-4.4171970	-1.8051210	-0.3374170
H	2.8608070	-3.1353740	1.7486430	H	-2.8646370	-3.1373740	-1.7407860
H	2.4847170	-3.3039860	0.0164170	H	-2.4905680	-3.3015250	-0.0077460
H	3.4857840	-0.7973230	1.4908790	H	-1.0939950	-2.8791690	-2.9882340
H	4.4146990	-1.8103840	0.3400910	H	-0.1865010	-3.8011940	-1.7670260
H	4.1464730	0.8599330	0.0359340	H	1.2104870	-2.2920490	-3.3479090
H	4.5064410	0.0647350	-1.5135560	H	1.5508800	-2.1382350	-1.6024680
H	3.4519520	2.2342440	-1.9700420				
H	2.3512000	0.9010680	-2.4464130				
O	0.5513480	-0.5904780	-2.3525800				

Table S133. Geometric coordinates and single point energies for sodium cation solvated by 1 equivalent of 18-crown-6.



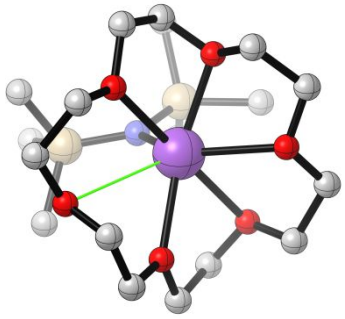
G = -1083.697944 Hartrees

G_{SP} = -1084.800035 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.3980640	-0.5188200	0.3049100	H	-1.7360760	-1.8436290	-1.4749280
O	-2.4353790	0.5087880	0.2649620	H	-0.0526890	-3.6281810	-1.9033980
C	-2.8816100	1.7005360	-0.3468610	H	0.0659130	-3.9279170	-0.1399430
C	-2.0568750	2.8344240	0.2259530	H	2.5267210	-3.0677170	-1.3954740
O	-0.6800440	2.5599140	0.1538030	H	2.1105220	-3.2404390	0.3398290
C	-0.0711920	2.7634000	-1.0964430	H	2.9520360	-0.6512940	-1.0556640
C	1.4172540	2.7795940	-0.8466450	H	3.9829090	-1.6433970	0.0262040
O	1.7376560	1.5825340	-0.1765190	H	4.1032420	0.1696900	1.6579870
C	3.0450040	1.5334700	0.3475140	H	2.5444110	0.7553800	2.2976970
C	3.0635490	0.4240080	1.3880970	H	3.7747510	1.3581630	-0.4629510
O	2.3641550	-0.7123740	0.9346050	H	3.3106940	2.4893990	0.8303390
C	2.9444870	-1.3368510	-0.1898240	H	1.9740920	2.8688330	-1.7955950
C	2.1099180	-2.5446860	-0.5174120	H	1.6674220	3.6429720	-0.2064820
O	0.7938280	-2.1032670	-0.7692540	H	-0.3311490	1.9557510	-1.8097530
C	-0.1296320	-3.1592830	-0.9073330	H	-0.3851040	3.7222470	-1.5450820
C	-1.5075030	-2.5906320	-0.6913550	H	-2.2904090	2.9433460	1.2935500
O	-1.5109930	-1.9971140	0.5883860	H	-2.3019480	3.7828490	-0.2832780
C	-2.7879770	-1.6654890	1.0836630	H	-2.7815720	1.6250190	-1.4455500
H	-3.4585720	-2.5419300	1.0641140	H	-3.9466590	1.8813720	-0.1224840

H	-2.6414910	-1.3649230	2.1298380	H	-4.3172150	-0.1775640	0.8125830
Na	0.0483890	-0.0831060	0.3789820	H	-3.6796380	-0.8241630	-0.7198720
H	-2.2604120	-3.3955940	-0.7539370				

Table S134. Geometric coordinates and single point energies for NaHMDS 18-crown-6 monosolvated monomer. The green bond indicates a longer than average N–Na contact.



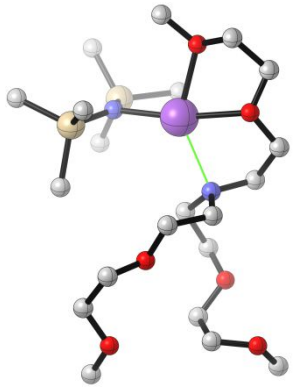
G = -1956.382789 Hartrees

G_{SP} = -1958.034129 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.1021370	-0.9121900	-3.1293960	H	0.8769430	-0.4887930	-2.3887680
C	-2.8134350	-1.9367570	-1.8560050	H	-1.1615970	2.2705770	-3.6994680
O	-1.6695000	-1.1185430	-1.8589230	H	-2.2619320	1.4015330	-2.5781760
Na	-0.4722300	0.4037310	0.0127110	H	-2.1667720	3.8350140	-2.0433060
O	-0.0691840	1.9905340	1.7483200	H	-0.3888480	3.7086210	-1.8386310
C	0.1765980	1.1388320	2.8409160	H	-1.9141510	4.4745000	0.5976850
C	-1.0764080	0.3811430	3.2528290	H	-0.1785200	4.1035340	0.3090770
O	-1.7298370	-0.0382570	2.0800330	H	-2.0454470	2.4964030	2.1225610
C	-2.9124710	-0.7531090	2.3197460	H	-0.8224330	3.6880560	2.6796730
H	-3.6729820	-0.0995460	2.7881660	N	1.6569640	-0.4202900	0.1605270
H	-2.7135930	-1.6035630	2.9969060	Si	2.9236970	0.6418650	-0.2167070
C	-3.4166640	-1.2827660	1.0009050	C	3.7727790	0.2752140	-1.8870120
O	-2.4666210	-2.1969290	0.5418580	H	3.0768400	0.4313380	-2.7274660
C	-2.7665580	-2.8613310	-0.6497860	H	4.6469240	0.9251560	-2.0539640
H	-1.9623750	-3.5964020	-0.7883670	H	4.1166370	-0.7710980	-1.9295350
H	-3.7297410	-3.4040940	-0.5745240	C	2.3226930	2.4431500	-0.3505530
H	-3.5449770	-0.4365300	0.2974690	H	1.4641760	2.4985770	-1.0387730
H	-4.4038110	-1.7644900	1.1430710	H	3.1226470	3.0964960	-0.7340420

H	-1.7622320	1.0129330	3.8512500	H	2.0020790	2.8148520	0.6339160
H	-0.7921990	-0.4880830	3.8729720	C	4.3312570	0.6894600	1.0647930
H	0.5733370	1.7000470	3.7067540	H	5.0536800	1.4903270	0.8383220
H	0.9411710	0.4376900	2.4708260	H	3.9247110	0.8729380	2.0728320
C	-1.0697260	2.9590200	1.8851640	H	4.8810070	-0.2634550	1.0956320
C	-1.1626630	3.6647460	0.5523830	Si	1.7397850	-2.0818640	0.4775010
O	-1.5079590	2.7100020	-0.4239170	C	0.6641910	-2.5553110	1.9764380
C	-1.3431470	3.1598350	-1.7458970	H	-0.3782660	-2.2350260	1.8199220
C	-1.3033550	1.9494050	-2.6503850	H	0.6644200	-3.6421680	2.1581480
O	-0.2368140	1.1569530	-2.2082330	H	1.0554740	-2.0641210	2.8838690
C	0.0855460	0.0145060	-2.9657080	C	1.0839620	-3.1138940	-0.9890870
H	0.4758800	0.2967550	-3.9608860	H	0.0856530	-2.7429010	-1.2705940
H	-3.7227680	-1.3068660	-1.8554160	H	1.7484770	-2.9938210	-1.8614790
H	-2.8547360	-2.5636980	-2.7636560	H	1.0100000	-4.1897490	-0.7615580
H	-0.7528880	-1.8677820	-3.5618430	C	3.4679620	-2.7817840	0.8561540
H	-1.8574020	-0.4870950	-3.8188660	H	4.1796070	-2.5595810	0.0445710
H	3.8740840	-2.3486780	1.7836960	H	3.4297350	-3.8759330	0.9812900

Table S135. Geometric coordinates and single point energies for NaHMDS TDA-1 monosolvated monomer. The green bond indicates a longer than average N–Na contact.



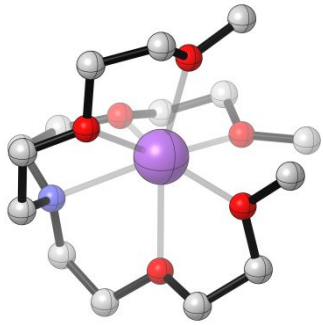
G = -2130.496217 Hartrees

G_{SP} = -2132.352323 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-4.8880460	-1.0029350	-1.3026870	H	5.5328780	4.1404870	-0.3068200
O	-3.8592920	-1.8799810	-0.8963590	H	6.2436580	2.6672430	0.4209410
C	-3.7182930	-3.0316350	-1.6805470	H	4.7146760	3.3396720	1.0703190
C	-2.6549150	-3.8991860	-1.0396690	H	2.7509170	3.1131640	-0.2994830
O	-1.5282680	-3.0894180	-0.8089870	H	3.5544180	3.7882050	-1.7479530
C	-0.3995610	-3.7282610	-0.2539670	H	1.7774420	2.3144050	-2.4537180
C	0.3300620	-2.7501460	0.6600020	H	3.3415510	1.5306910	-2.8544780
N	0.5013890	-1.4220300	0.0817560	H	0.5028610	0.3102720	-2.0572250
C	0.8435710	-0.4212320	1.1051620	H	1.9099840	-0.4179400	-2.8726860
C	1.9691450	-0.8286560	2.0538690	H	0.9076260	-2.1850200	-1.8016150
O	3.1131350	-1.2500250	1.3569840	H	2.3769280	-1.8311260	-0.8553630
C	4.0880210	-0.2551680	1.1524600	H	1.2978350	-3.2065440	0.9505500
C	4.9859280	-0.6679810	-0.0045530	H	-0.2680760	-2.6342770	1.5796410
O	5.3640350	-2.0165470	0.0164620	H	0.2512150	-4.1041020	-1.0622910
C	6.0070260	-2.4168890	1.1889890	H	-0.7086460	-4.5989900	0.3495390
H	5.3170170	-2.4321520	2.0508870	Na	-1.8679910	-0.8944330	-0.2796990
H	6.3890100	-3.4337700	1.0302020	N	-2.5607000	1.1301010	0.3112240

H	6.8632460	-1.7577390	1.4328730	Si	-3.0910260	1.1064410	1.9133780
H	5.8716770	-0.0018400	-0.0124050	C	-4.8757840	1.7047660	2.1611460
H	4.4425420	-0.5042110	-0.9436890	H	-5.5765900	1.1000100	1.5637820
H	3.6333170	0.7114800	0.8800810	H	-5.1903500	1.6485580	3.2153740
H	4.6701280	-0.1147230	2.0853090	H	-4.9772590	2.7506270	1.8310220
H	2.1949840	0.0129950	2.7338700	C	-3.0567320	-0.7057050	2.5244460
H	1.6482610	-1.6694660	2.6890380	H	-3.4687810	-0.8149990	3.5395340
H	1.1006050	0.5130690	0.5935420	H	-3.6524550	-1.3460630	1.8508350
H	-0.0596920	-0.2079290	1.7042960	H	-2.0257470	-1.1021460	2.5545490
C	1.3630780	-1.4657650	-1.1026640	C	-2.0236860	2.1101470	3.1249180
C	1.4880210	-0.1686740	-1.8800080	H	-0.9682110	1.7977500	3.0735350
O	2.3368040	0.7426850	-1.2296470	H	-2.0608950	3.1803340	2.8634810
C	2.6826160	1.8472650	-2.0232060	H	-2.3626750	2.0068120	4.1679650
C	3.3955890	2.8601940	-1.1645480	Si	-2.1761150	2.3548630	-0.7808140
O	4.6183710	2.3265190	-0.7393200	C	-3.3186710	3.8691190	-0.7398760
C	5.3014630	3.1605460	0.1499240	H	-3.0606730	4.6077410	-1.5152980
H	-2.4116070	-4.7453540	-1.7067260	H	-4.3672220	3.5663010	-0.8882700
H	-3.0246200	-4.3042680	-0.0800730	H	-3.2546880	4.3719920	0.2387890
H	-3.4182210	-2.7573320	-2.7103640	C	-2.2753050	1.6608610	-2.5570700
H	-4.6667120	-3.5966500	-1.7411750	H	-3.3252220	1.4482620	-2.8151560
H	-4.8024700	-0.7751550	-2.3793160	H	-1.8811470	2.3607710	-3.3110130
H	-4.7541550	-0.0756880	-0.7287420	H	-1.7143610	0.7149760	-2.6641580
H	-5.8790950	-1.4458420	-1.1057810	C	-0.4036140	3.0233970	-0.5658430
H	0.3272440	2.2014090	-0.6414360	H	-0.2910080	3.4672800	0.4368420
H	-0.1441570	3.7926000	-1.3123680				

Table S136. Geometric coordinates and single point energies for sodium cation solvated by 1 equivalent of TDA-1.



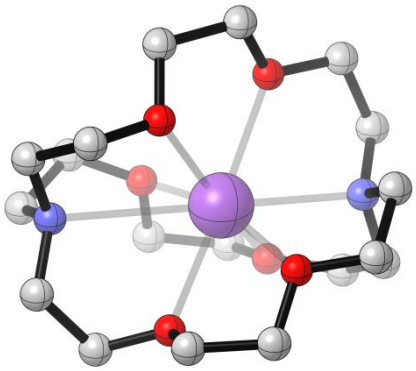
G = -1257.851318 Hartrees

G_{SP} = -1259.147573 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.8895110	1.1531010	-1.7745950	H	-2.9568960	-0.1130920	1.8347390
O	-1.6307010	0.5260590	-1.8254570	H	-3.6954200	1.4327330	1.3145260
C	-1.4112620	-0.2123280	-3.0066650	H	-1.8225680	-1.9103430	2.5213640
C	0.0724640	-0.2781450	-3.2739620	H	-1.9005150	-3.4935070	1.6948180
O	0.7180580	-0.7524720	-2.1186320	H	0.4543970	-3.4220870	1.1178080
C	2.1040510	-0.9368320	-2.2842740	H	0.2688440	-3.1237680	2.8737230
C	2.7407860	-1.0763630	-0.9130420	H	2.5332790	-2.4311520	1.4909280
N	2.3614320	-0.0061320	-0.0022550	H	2.3159770	-1.5734350	3.0275370
C	2.7453630	-0.2620430	1.3782930	H	3.8458960	-0.3320760	1.5083070
C	2.1080370	-1.5183770	1.9444310	H	2.3980660	0.5810690	1.9915330
O	0.7212350	-1.4656300	1.7061940	H	3.8409610	-1.1593380	-1.0381620
C	0.0765980	-2.7043560	1.8700300	H	2.3884810	-2.0270020	-0.4892830
C	-1.4081640	-2.5059460	1.6870700	H	2.5316760	-0.0893130	-2.8486810
O	-1.6331390	-1.8454330	0.4619330	H	2.3089430	-1.8482810	-2.8730970
C	-2.9002760	-2.1004920	-0.0944620	H	0.4533710	0.7295180	-3.5254440
H	-2.9867310	-1.4925450	-1.0017600	H	0.2598890	-0.9426150	-4.1363340
H	-3.0093790	-3.1654930	-0.3583540	H	-1.9043940	0.2712770	-3.8672050
H	-3.7129320	-1.8258440	0.6004490	H	-1.8284490	-1.2306790	-2.9003530

Na	-0.1705470	0.0017840	0.0023340	H	-2.9839910	1.9157110	-2.5653090
O	-1.6141060	1.3305020	1.3742710	H	-2.9742560	1.6359310	-0.7947830
C	-1.3921980	2.7219070	1.3182330	H	-3.7120200	0.4256140	-1.8882320
C	0.0923670	2.9828120	1.3901970	H	2.5466820	2.4991970	1.3487650
O	0.7338060	2.2136730	0.4035280	H	0.2829120	4.0607500	1.2416980
C	2.1219670	2.4376690	0.3311170	H	0.4741670	2.6991850	2.3889680
C	2.7524850	1.3146650	-0.4726840	H	-1.8110650	3.1358570	0.3825480
H	2.4048240	1.4252420	-1.5091280	H	-1.8819750	3.2303010	2.1663670
H	3.8538580	1.4557970	-0.4781820	C	-2.8733580	0.9776650	1.8940710
H	2.3365390	3.4015360	-0.1631600	H	-2.9694960	1.2929570	2.9462520

Table S137. Geometric coordinates and single point energies for sodium cation solvated by 1 equivalent of [2.2.2]cryptand.



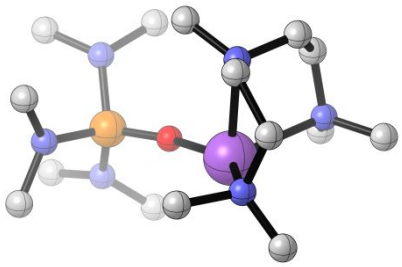
G = -1428.485745 Hartrees

G_{SP} = -1429.964928 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.2924790	-1.2929850	0.5449090	C	3.0932620	0.1208850	1.4033430
N	-2.9114100	0.0001320	-0.0015840	H	4.1923300	0.1740010	1.5554870
C	-3.2892740	0.1733900	-1.3955930	H	2.6595880	1.0534360	1.7916150
C	-2.2845240	1.0366380	-2.1440180	H	3.0662790	-1.9636170	2.0394620
O	-0.9950330	0.4667000	-2.1642950	H	2.6966290	-0.7859840	3.3151280
C	-0.8424770	-0.5982420	-3.0727850	H	1.1159330	-3.2086670	1.8423480
C	0.6302920	-0.8685280	-3.2429870	H	0.7620030	-2.5254050	3.4604830
O	1.1751870	-1.1221400	-1.9739500	H	-1.2925020	-3.3357250	2.3229970
C	2.5464480	-1.4376250	-1.9974400	H	-1.3465810	-1.5797990	2.6574880
C	3.0956300	-1.2740930	-0.5922560	H	-1.3426350	3.0942280	0.0368820
N	2.7236130	-0.0002880	0.0022460	H	-1.2898490	3.6814090	1.7252670
C	3.0963730	1.1520640	-0.8023810	H	1.1174510	3.1982730	1.8583890
C	2.5447710	2.4498800	-0.2418430	H	0.7671010	4.2595640	0.4578510
O	1.1732770	2.2701710	0.0171810	H	3.0682400	2.7450560	0.6848790
C	0.6258610	3.2436630	0.8683720	H	2.7030230	3.2615990	-0.9734230
C	-0.8469740	2.9605010	1.0152090	H	4.1958020	1.2558960	-0.9224620
O	-0.9994290	1.6422330	1.4858120	H	2.6644960	1.0226410	-1.8049230

C	-2.2896430	1.3399220	1.9675660	H	2.6614420	-2.0765840	0.0209690
C	-3.2921200	1.1207410	0.8442510	H	4.1948870	-1.4316260	-0.6199160
H	-4.3053910	0.9935750	1.2763130	H	2.7043190	-2.4773310	-2.3339320
H	-3.3403900	2.0319950	0.2287520	H	3.0718470	-0.7834540	-2.7157320
H	-2.1856470	0.4276650	2.5724000	H	0.7714850	-1.7307790	-3.9191030
H	-2.6426580	2.1425360	2.6394080	H	1.1237490	0.0118070	-3.6961930
Na	0.1601250	-0.0006770	-0.0012520	H	-1.3398990	-1.5125320	-2.7021810
O	-0.9999830	-2.1097490	0.6764830	H	-1.2835460	-0.3409710	-4.0522310
C	-2.2897890	-2.3750290	0.1726090	H	-2.6357010	1.2201340	-3.1751330
H	-2.6432290	-3.3586090	0.5302050	H	-2.1795530	2.0151810	-1.6538080
H	-2.1847330	-2.4411490	-0.9198180	H	-3.3372680	-0.8148120	-1.8779210
C	-0.8495270	-2.3603570	2.0538160	H	-4.3019780	0.6120160	-1.5034060
C	0.6227980	-2.3738460	2.3750380	H	-4.3054980	-1.6035700	0.2179020
O	1.1705280	-1.1500330	1.9577710	H	-3.3412630	-1.2163100	1.6418510
C	2.5411280	-1.0141490	2.2460600				

Table S138. Geometric coordinates and single point energies for sodium cation solvated by 1 equivalent PMDTA and 1 equivalent of HMPA.



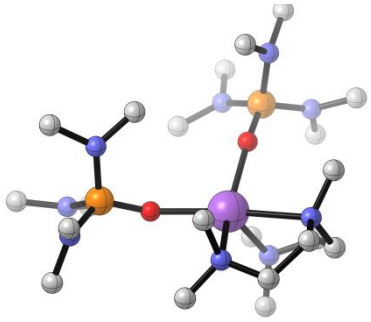
G -1501.622245 Hartrees

G_{SP} = -1502.946949 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
N	-2.1614640	0.0854770	1.4840440	H	3.7623100	-0.3856090	3.0876740
C	-2.7946910	-1.2298480	1.6083970	H	4.7134150	-1.0539380	1.7362330
C	-2.0516540	-2.3280640	0.8554300	C	2.1388690	-1.9526450	1.6206320
N	-2.0895280	-2.1758450	-0.6003240	H	2.8478560	-2.7543990	1.3478810
C	-1.0725130	-3.0193130	-1.2221440	H	1.9352420	-2.0323610	2.7000450
H	-1.1146120	-2.9081500	-2.3148710	H	1.2020990	-2.1094540	1.0731310
H	-0.0753950	-2.7047970	-0.8826210	N	3.2287430	-0.3401070	-1.4110870
H	-1.2182000	-4.0905560	-0.9811530	C	2.7750340	-1.2315330	-2.4657060
C	-3.4056950	-2.4883500	-1.1438640	H	3.1611040	-2.2562410	-2.3264270
H	-4.1729700	-1.8222610	-0.7267110	H	1.6805630	-1.2646600	-2.4781950
H	-3.3997530	-2.3519630	-2.2339700	H	3.1298370	-0.8644130	-3.4414830
H	-3.7032060	-3.5337100	-0.9283940	C	4.6713250	-0.1914530	-1.3140600
Na	-1.2805970	0.0728810	-0.7434500	H	5.1662420	-1.1405180	-1.0437780
N	-3.0579290	1.7138970	-0.8633140	H	5.0783570	0.1403680	-2.2821560
C	-3.9009310	1.4098260	0.2953180	H	4.9301640	0.5663280	-0.5629630
C	-3.1272460	1.1780450	1.5892410	N	2.5926550	1.6855980	0.1300200
H	-3.8546800	1.0041050	2.4065850	C	2.8416810	2.6067070	-0.9694000
H	-2.5832580	2.0930910	1.8645130	H	3.6497510	3.3024210	-0.6956030
H	-4.4872820	0.5102720	0.0488930	H	3.1405140	2.0575290	-1.8688350

H	-4.6366310	2.2230100	0.4666260	H	1.9435250	3.2041510	-1.2038630
C	-3.8684760	1.7333410	-2.0770630	C	2.1654060	2.3452520	1.3544890
H	-4.3591120	0.7597670	-2.2158650	H	1.9676760	1.6060840	2.1395020
H	-3.8265350	-1.1648750	1.2349230	H	2.9525460	3.0299550	1.7074640
H	-4.6531910	2.5137970	-2.0393050	H	1.2501920	2.9413370	1.1890920
H	-3.2332060	1.9299970	-2.9516840	H	-0.9947390	-2.3186180	1.1642420
C	-2.3539890	2.9818120	-0.7038870	H	-2.4604780	-3.3144390	1.1568200
H	-1.6416730	2.9332540	0.1325340	H	-2.8759140	-1.5209150	2.6743800
H	-1.7861260	3.2061990	-1.6176000	C	-1.0580910	0.2349380	2.4242500
H	-3.0489180	3.8243640	-0.5168640	H	-0.3000730	-0.5415180	2.2497310
O	0.8180210	-0.3008800	-0.4753890	H	-0.5680910	1.2065310	2.2698740
P	2.2416420	0.0798960	-0.1378970	H	-1.3936390	0.1737420	3.4782380
N	2.6684660	-0.6330480	1.3151850				
C	3.9182680	-0.3343670	1.9987370				
H	4.2636630	0.6761070	1.7495930				

Table S139. Geometric coordinates and single point energies for sodium cation solvated by 1 equivalent PMDTA and 2 equivalents of HMPA.



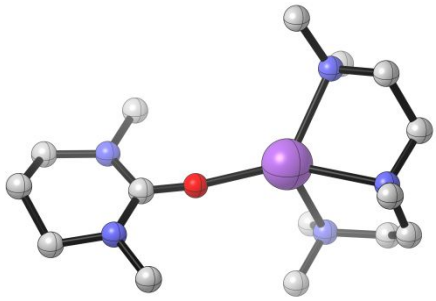
G = -2321.057699 Hartrees

G_{SP} = -2323.071221 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.0344970	1.1819260	0.1109100	C	-2.4418910	-2.2456260	2.4213540
N	1.4855140	2.9892840	-0.7649960	H	-2.0010160	-3.2495910	2.2866960
C	2.0648820	3.5117230	0.4725100	H	-1.6411700	-1.4983680	2.4222920
C	2.2723680	2.4435290	1.5426820	H	-2.9433220	-2.2260590	3.4021900
N	1.0268570	1.9396050	2.1150960	C	-4.5700770	-2.7919650	1.3520460
C	1.2609150	0.7250180	2.8800750	H	-4.3114880	-3.8355780	1.1014330
H	0.3085500	0.3517890	3.2829510	H	-5.0536140	-2.7919100	2.3422960
H	1.6827470	-0.0497000	2.2242090	H	-5.3017310	-2.4269720	0.6206290
H	1.9551290	0.8903190	3.7301280	N	-4.4397390	-0.1363420	-0.1898050
C	0.3380150	2.9278110	2.9299690	C	-5.2672070	0.3573700	0.9016440
H	0.0711590	3.8128420	2.3376080	H	-6.3131380	0.0391680	0.7608720
H	-0.5949240	2.4960000	3.3174850	H	-4.9087020	-0.0306960	1.8617410
H	0.9529910	3.2595850	3.7914560	H	-5.2499180	1.4597640	0.9400710
H	2.7943040	1.5837920	1.0897480	C	-4.8211630	0.3964110	-1.4875840
H	2.9341370	2.8510950	2.3373130	H	-4.1686060	0.0042620	-2.2754040
H	1.4115320	4.3023820	0.8674240	H	-5.8608850	0.1123980	-1.7188900
H	-2.4655430	3.5778310	0.9727870	H	-4.7611030	1.4986940	-1.4977620
C	-2.6775870	3.1191940	-0.0036520	O	1.5115510	-0.3020180	-0.3851970

N	-1.4414010	2.9362960	-0.7424710	P	2.6294860	-1.3015890	-0.2535380
C	-0.6994930	4.1809720	-0.8812380	N	2.1443530	-2.5189060	0.7814550
C	0.6930110	3.9894780	-1.4747900	C	2.9871600	-3.6643670	1.0722870
H	1.2036970	4.9733810	-1.5060150	H	4.0375500	-3.4400490	0.8464750
H	0.6028210	3.6690900	-2.5229170	H	2.9196980	-3.9186890	2.1426100
H	-0.6207790	4.6308990	0.1217430	H	2.6860550	-4.5540980	0.4924120
H	-1.2479340	4.9159840	-1.5089470	C	0.7561250	-2.6682110	1.1802640
C	-1.6848620	2.2677800	-2.0086360	H	0.2923700	-3.5499030	0.7018600
H	-0.7371710	2.0091190	-2.5046700	H	0.6941060	-2.8070170	2.2731100
H	-2.2245120	1.3285470	-1.8182330	H	0.1797550	-1.7748880	0.9060530
H	-2.2851770	2.8834620	-2.7106390	N	3.0727300	-1.8183250	-1.7795850
H	-3.4002880	3.7678280	-0.5415230	C	2.1299520	-1.7203870	-2.8811900
H	-3.1355800	2.1354670	0.1726220	H	1.5901230	-2.6696640	-3.0503560
H	3.0383830	4.0014370	0.2666080	H	1.4031880	-0.9270400	-2.6748370
C	2.5170300	2.4230600	-1.6200420	H	2.6719370	-1.4700620	-3.8064580
H	3.0719710	1.6534820	-1.0703620	C	4.1549690	-2.7624650	-1.9967820
H	2.0595480	1.9306190	-2.4900540	H	3.7912270	-3.8022720	-2.0746640
H	3.2295830	3.1930820	-1.9797840	H	4.6777130	-2.5157160	-2.9342720
O	-1.7821420	-0.1179840	0.4951580	H	4.8848820	-2.7070360	-1.1793650
P	-2.9971650	-0.9208210	0.1115180	N	4.0904420	-0.8182210	0.3960850
N	-2.6990120	-1.7051800	-1.3365090	C	5.0662760	-0.0696110	-0.3819580
C	-3.6726180	-2.6074950	-1.9261300	H	6.0661500	-0.5212830	-0.2742650
H	-4.6886010	-2.3491690	-1.6016760	H	4.7936670	-0.0707490	-1.4434110
H	-3.6386490	-2.5260370	-3.0243160	H	5.1292760	0.9762010	-0.0341200
H	-3.4754020	-3.6604240	-1.6574670	C	4.3763960	-0.8230440	1.8221800
C	-1.3417150	-1.8989980	-1.8168210	H	3.6250970	-1.4041170	2.3678910
H	-1.0059640	-2.9415560	-1.6676310	H	5.3669760	-1.2711240	2.0035950
H	-1.2932840	-1.6834430	-2.8973860	H	4.3883190	0.2028140	2.2299450
H	-0.6441860	-1.2345040	-1.2912420	N	-3.4005260	-1.9324550	1.3772850

Table S140 Geometric coordinates and single point energies for sodium cation solvated by 1 equivalent PMDTA and 1 equivalents of DMPU.



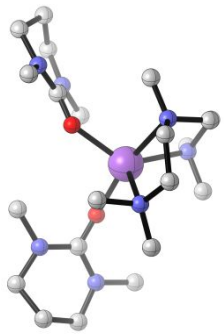
G = -1102.160998 Hartrees

G_{SP} = -1103.265272 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.7805410	0.1293820	-0.1738770	C	-2.9426230	-0.8693030	-2.4446980
N	-2.9543740	-0.6196230	-1.0060780	H	-2.6643000	0.0424090	-2.9902370
C	-3.8578120	0.4872550	-0.6772330	H	-2.2032880	-1.6457410	-2.6870990
C	-3.2675800	1.8669330	-0.9450520	H	-3.9310420	-1.2025340	-2.8162450
N	-2.0578660	2.1562640	-0.1736800	O	1.3546310	-0.0757460	-0.0994600
C	-1.4295110	3.3815250	-0.6566800	C	2.5989670	-0.0308480	-0.1166940
H	-0.4991600	3.5688510	-0.1031240	N	3.2695430	0.9140330	0.5984580
H	-1.1839830	3.2830280	-1.7227870	C	4.7168570	1.0947540	0.5751620
H	-2.0896230	4.2618190	-0.5320080	C	5.3249020	0.4467720	-0.6520730
C	-2.3355980	2.2603170	1.2548120	C	4.7809560	-0.9617760	-0.7882410
H	-2.7031700	1.3036390	1.6535670	N	3.3272500	-0.9231640	-0.8435470
H	-1.4111480	2.5137480	1.7931590	C	2.6677230	-2.0157790	-1.5285400
H	-3.0888470	3.0415790	1.4783200	H	2.8062110	-2.9675660	-0.9892170
H	-3.0138320	1.9623510	-2.0117770	H	1.5977350	-1.8062040	-1.6082420
H	-4.0515760	2.6257940	-0.7429030	H	3.0872270	-2.1263320	-2.5385760
H	-4.1376510	0.4113770	0.3824910	H	5.1226070	-1.5960670	0.0500390
H	-1.7724710	-0.5032540	3.1932740	H	5.1391990	-1.4287530	-1.7159850
C	-1.1707800	-1.3364130	2.8032490	H	5.0645630	1.0240000	-1.5518320
N	-1.4661250	-1.5508640	1.3922740	H	6.4189720	0.4322160	-0.5656760

C	-2.8895700	-1.8124710	1.1939040	H	5.1573830	0.6740710	1.4963330
C	-3.3123130	-1.8365320	-0.2722020	H	4.9249380	2.1752260	0.5809070
H	-4.4029410	-2.0276530	-0.3205290	C	2.5306610	1.8265870	1.4472950
H	-2.8370500	-2.6890060	-0.7786590	H	1.5679820	1.3851490	1.7234690
H	-3.4500810	-1.0346770	1.7366700	H	3.1093720	2.0098430	2.3633590
H	-3.1855630	-2.7785880	1.6535730	H	2.3543610	2.7943060	0.9489980
C	-0.6310380	-2.6224980	0.8606470	H	-1.3874840	-2.2337050	3.4155780
H	-0.7719140	-2.7272080	-0.2254440	H	-0.1079290	-1.0848400	2.9252610
H	0.4257720	-2.3795230	1.0340900	H	-4.8045340	0.3967450	-1.2462430
H	-0.8582730	-3.5994010	1.3319100				

Table S141. Geometric coordinates and single point energies for sodium cation solvated by 1 equivalent PMDTA and 2 equivalents of DMPU.



G = -1522.132993 Hartrees

G_{SP} = -1523.706012 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.0066320	-0.6711770	0.1610860	C	-2.4516610	1.4451960	-0.0424210
N	-1.4632240	-2.2626150	-1.0142490	N	-2.6897770	1.4866610	1.2994190
C	-1.3350280	-3.5551710	-0.3485440	C	-3.9224720	1.9816380	1.8991370
C	-1.3214000	-3.4565780	1.1736850	C	-5.0621930	1.9183700	0.9011730
N	-0.2792500	-2.5773250	1.6954340	C	-4.6249360	2.5624120	-0.4001160
C	-0.4110410	-2.4199650	3.1362400	N	-3.4116050	1.9247150	-0.8853550
H	0.3118870	-1.6744980	3.4977650	C	-3.1459330	2.0269740	-2.3059780
H	-1.4231020	-2.0729900	3.3874320	H	-3.0799180	3.0824690	-2.6162240
H	-0.2338140	-3.3711080	3.6769310	H	-2.1974600	1.5324420	-2.5341320
C	1.0559610	-3.0560380	1.3647210	H	-3.9545910	1.5481840	-2.8786280
H	1.2087220	-3.0610120	0.2760690	H	-4.4664970	3.6482490	-0.2652480
H	1.8017570	-2.3757370	1.7963160	H	-5.3993920	2.4418980	-1.1709400
H	1.2421870	-4.0787830	1.7512840	H	-5.3352520	0.8688630	0.7122090
H	-2.2904130	-3.0775640	1.5336460	H	-5.9457920	2.4291260	1.3053000
H	-1.2161400	-4.4834840	1.5839800	H	-3.7808330	3.0162670	2.2590970
H	-0.4099390	-4.0408230	-0.6869470	H	-4.1513580	1.3608870	2.7775900
H	2.8313040	-2.5724250	-1.2791050	C	-1.6344540	1.0298130	2.1859460
C	2.6648720	-1.6064880	-1.7780860	H	-0.6493580	1.3663390	1.8360910

N	1.2423010	-1.3149120	-1.8498780	H	-1.8101700	1.4451940	3.1857850
C	0.5214030	-2.3833310	-2.5333410	H	-1.6171430	-0.0711280	2.2680360
C	-0.9970620	-2.2940870	-2.3981570	O	1.6780800	0.4981490	0.9946290
H	-1.4462380	-3.1366050	-2.9637880	C	2.6966680	1.1147340	0.6482280
H	-1.3515830	-1.3738960	-2.8863690	N	2.6176270	2.3051040	-0.0204220
H	0.8797990	-3.3417940	-2.1257450	C	3.8029990	3.1087190	-0.2741140
H	0.7686860	-2.4033370	-3.6161240	C	4.9582750	2.1998110	-0.6458660
C	1.0250030	-0.0140980	-2.4711490	C	5.1929060	1.2135670	0.4805150
H	-0.0292280	0.2853270	-2.3951440	N	3.9382070	0.6135480	0.9178130
H	1.6186470	0.7431260	-1.9371780	C	4.0434000	-0.5875660	1.7221690
H	1.3282460	-0.0085410	-3.5381500	H	3.1910920	-0.6514460	2.4068770
H	3.1342530	-1.6552780	-2.7816610	H	4.0714380	-1.4985070	1.1000250
H	3.1742170	-0.8246710	-1.1943310	H	4.9693950	-0.5396760	2.3107830
H	-2.1602340	-4.2358970	-0.6433640	H	5.6824910	1.7122380	1.3357880
C	-2.8262370	-1.7602290	-0.9194880	H	5.8639360	0.4055120	0.1507530
H	-3.0933380	-1.5731280	0.1320170	H	4.7087410	1.6631200	-1.5743260
H	-2.9075230	-0.8041990	-1.4515410	H	5.8698250	2.7833450	-0.8289470
H	-3.5634250	-2.4711340	-1.3443230	H	4.0601760	3.7240740	0.6081590
O	-1.3910390	0.9671290	-0.4748560	H	3.5711480	3.7995750	-1.0960370
H	1.1224330	3.6114590	0.7273130	C	1.3279990	2.9599610	-0.1397250
H	1.3302240	3.5809790	-1.0458000	H	0.5263780	2.2176110	-0.2236330

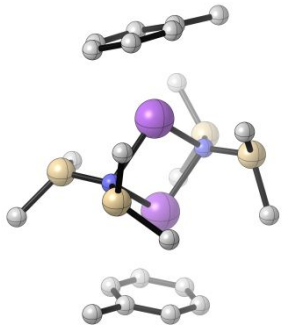
Table S142. Geometric coordinates and single point energies for unsolvated sodium cation.

G = -162.014812 Hartrees

G_{SP} = -162.0655113 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	0.0000000	0.0000000	0.0000000				

Table S143. Geometric coordinates and single point energies for NaTMDS toluene disolvated dimer.



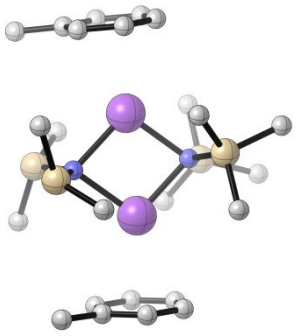
G = -2454.877614 Hartrees

G_{SP} = -2456.478908 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	1.3560690	0.5695680	-0.0151840	H	-3.1443990	-1.5272450	-2.7503130
N	0.4661130	-1.5899940	-0.1468950	H	-3.9641470	0.7089840	-2.0513070
Na	-1.5190960	-0.3320020	0.0906210	C	-4.7266550	1.5179740	0.4464030
N	-0.6305460	1.8131210	0.2825150	H	-5.2813270	2.0500950	-0.3382950
Si	-0.7919530	3.0782640	-0.8637890	H	-5.3476690	1.4814810	1.3510020
C	0.7552100	3.3023500	-1.9382900	H	-3.8268420	2.1137600	0.6775920
H	1.6224310	3.5909180	-1.3265160	H	-4.6352160	-0.7778600	1.9285190
H	1.0019940	2.3756830	-2.4824960	H	-3.8518550	-3.0201220	1.2253820
H	0.5947110	4.0924150	-2.6880680	Si	0.7206920	-2.6576970	1.1672420
C	-2.2086530	2.8534910	-2.1013510	C	1.5790380	-1.7789560	2.6079060
H	-2.0823840	1.9348280	-2.6967510	H	2.5728360	-1.4149160	2.3074490
H	-3.1839550	2.8117660	-1.5947800	H	0.9940580	-0.9135090	2.9589230
H	-2.2298620	3.7034580	-2.8010740	H	1.7150630	-2.4572510	3.4640930
H	-1.0321080	4.4108810	-0.2098290	C	-0.8727360	-3.4141790	1.8612990
Si	-0.7481150	2.1054390	1.9642800	H	-1.4168330	-3.9554560	1.0715470
C	-1.6183970	0.6544320	2.8348460	H	-0.6489460	-4.1259700	2.6709840
H	-2.6744010	0.5920150	2.5271640	H	-1.5449320	-2.6421930	2.2713210
H	-1.1378050	-0.3181120	2.6291180	H	1.5927550	-3.8359000	0.8198760

H	-1.6054080	0.7852510	3.9276070	Si	0.4316330	-2.0839990	-1.7842730
C	0.9458070	2.3045860	2.7965210	C	0.3372270	-0.5354840	-2.8814360
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	C	1.9002420	-3.1104830	-2.3910580
C	-3.8666550	-2.2024530	0.5039110	H	1.7351520	-3.4251460	-3.4331770
C	-4.3068280	-0.9367010	0.8989240	H	2.8419540	-2.5427720	-2.3526500
C	-4.3322230	0.1363200	-0.0029030	H	2.0295390	-4.0171350	-1.7807310
C	-3.9300850	-0.1055820	-1.3268540	H	-0.7781250	-2.9100280	-2.1493580
C	-3.4753160	-1.3653210	-1.7228380	C	4.0776370	1.7212330	1.0369480
C	-3.4329860	-2.4180270	-0.8045740	C	3.8160960	2.3050380	-0.2019660
H	-3.0621990	-3.3964460	-1.1116420	C	3.7470660	1.4969250	-1.3416210
H	5.0173430	-2.3558450	-0.6835770	C	3.9304510	0.1174070	-1.2351720
H	3.8816570	-0.5045010	-2.1320670	C	4.1913030	-0.4856950	0.0066110
H	3.5487370	1.9467290	-2.3160400	C	4.2644890	0.3402860	1.1360110
H	3.6777140	3.3838550	-0.2827140	H	4.4791330	-0.1045480	2.1100130
H	4.1373790	2.3412060	1.9325160	C	4.3657160	-1.9751970	0.1154570
H	3.3935180	-2.4834940	0.0164390	H	4.7987850	-2.2566840	1.0841130

Table S144. Geometric coordinates and single point energies for NaHMDS/NaTMDS heterodimer with 2 equivalents of toluene bound.



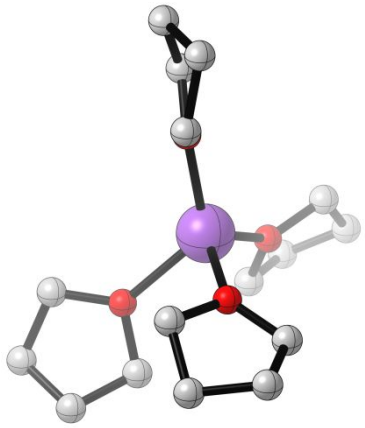
G = -2533.3757 Hartrees

G_{SP} = -2535.070267 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	1.5322680	0.0340290	-0.0905760	C	-4.1494050	1.0882110	0.9870230
N	-0.0004910	-1.7374800	0.0039500	H	-4.0772840	2.0667230	1.4644990
Na	-1.5290280	0.0381270	0.0925820	H	-3.6929610	-0.0164020	2.7900130
N	0.0039970	1.8006480	0.0012620	H	-3.8562880	-2.2333050	1.6953450
Si	-0.0715380	2.5358340	-1.5379280	C	-4.4074760	-2.7935530	-0.9066690
C	0.5494010	4.3228520	-1.6427400	H	-5.1080960	-3.4491740	-0.3701580
H	0.6578830	4.6318680	-2.6945250	H	-4.7362660	-2.7160120	-1.9510740
H	-0.1440310	5.0247230	-1.1563100	H	-3.4206230	-3.2823980	-0.8964300
H	1.5326000	4.4272300	-1.1554970	H	-4.7947940	-0.3265610	-2.0433070
C	0.9882380	1.5719780	-2.7982990	H	-4.6346840	1.8929810	-0.9570320
H	2.0440900	1.8723210	-2.7156230	Si	0.3558060	-2.5900140	1.4454290
H	0.9368480	0.4766390	-2.6701810	C	1.4435570	-1.5464800	2.5996470
H	0.6675980	1.7888110	-3.8294900	H	2.4288040	-1.3232020	2.1623480
C	-1.8398140	2.5505840	-2.2342610	H	0.9582480	-0.5890880	2.8495590
H	-2.2590480	1.5342660	-2.3307870	H	1.6254310	-2.0776370	3.5467380
H	-2.4970630	3.1247340	-1.5609930	C	-1.1670060	-3.0775380	2.4579180
H	-1.8815710	3.0180760	-3.2306730	H	-1.8624080	-3.6712580	1.8440160
Si	0.0788510	2.5299440	1.5432540	H	-0.8887010	-3.6787290	3.3371270

C	-0.9818480	1.5605740	2.7987620	H	-1.6979800	-2.1796800	2.8152560
H	-2.0378300	1.8605560	2.7162430	H	1.1102570	-3.8742310	1.2073150
H	-0.9293450	0.4657870	2.6663860	Si	-0.3613180	-2.5878610	-1.4376010
H	-0.6625420	1.7734330	3.8311880	C	-1.4412730	-1.5366040	-2.5923450
C	1.8463940	2.5419510	2.2414340	H	-2.4262360	-1.3075480	-2.1573800
H	2.5043720	3.1188270	1.5712130	H	-1.6242810	-2.0653230	-3.5405860
H	1.8868970	3.0054840	3.2397430	H	-0.9493550	-0.5819750	-2.8400330
H	2.2655910	1.5252990	2.3344580	C	1.1586900	-3.0835440	-2.4503070
C	-0.5421710	4.3164930	1.6549130	H	0.8776990	-3.6882320	-3.3262550
H	-0.6509230	4.6213550	2.7078820	H	1.6902310	-2.1881030	-2.8128040
H	0.1515060	5.0201810	1.1714650	H	1.8544560	-3.6754500	-1.8350540
H	-1.5251890	4.4229140	1.1677540	H	-1.1238900	-3.8673760	-1.2000830
C	-4.4635520	0.9911150	-0.3684030	C	4.4623900	0.9803180	0.3688090
C	-4.5534630	-0.2620620	-0.9797960	C	4.1530520	1.0876550	-0.9869350
C	-4.3355900	-1.4395150	-0.2535410	C	3.9393170	-0.0743800	-1.7364710
C	-4.0274340	-1.3274270	1.1110420	C	4.0253840	-1.3267130	-1.1281750
C	-3.9359650	-0.0795480	1.7277200	C	4.3277820	-1.4491520	0.2368450
H	5.0861840	-3.4651060	0.3376220	C	4.5465690	-0.2773110	0.9719230
H	3.8546350	-2.2281820	-1.7193720	H	4.7844440	-0.3497150	2.0357020
H	3.7004170	-0.0032530	-2.7991590	C	4.3926080	-2.8077890	0.8810970
H	4.0850720	2.0696320	-1.4578440	H	4.7260100	-2.7392240	1.9246700
H	4.6342360	1.8775990	0.9641910	H	3.4021750	-3.2894910	0.8720700

Table S145. Geometric coordinates and single point energy for sodium cation with 4 THF's bound.

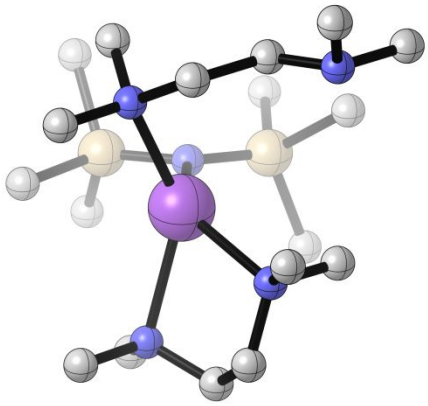


G = -1090.38512 Hartrees
G_{SP} = -1091.488096 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.1452940	0.4415110	-0.0249740	H	-4.4236740	1.2177090	-2.4032890
O	1.2782990	2.0434920	0.5767840	H	-4.8633140	2.6892970	-1.5060370
C	2.6516720	1.9692460	0.1701290	H	-4.6726770	1.4952190	0.6475660
H	3.1962950	1.3031650	0.8609890	H	-5.4766810	0.2843960	-0.3811210
H	2.6914050	1.5382320	-0.8401320	O	-0.5337580	-1.3408590	1.2924640
C	3.1711350	3.3967330	0.2610850	C	-0.2090360	-1.5663890	2.6730790
C	2.3921480	3.9224030	1.4669180	H	0.8609160	-1.3460560	2.8234660
C	1.0239520	3.2833730	1.2557060	H	-0.7976380	-0.8784800	3.2955010
H	0.4908980	3.0738810	2.1935240	C	-0.5213090	-3.0369710	2.9340590
H	0.3814820	3.9105960	0.6168390	C	-0.2884130	-3.6595230	1.5567950
H	2.8454980	3.5602040	2.4012150	C	-0.8489260	-2.5780550	0.6440810
H	2.3410900	5.0169650	1.5141420	H	-0.4031570	-2.5612770	-0.3619600
H	2.9043970	3.9594160	-0.6457520	H	-1.9435850	-2.6700470	0.5432190
H	4.2596420	3.4434130	0.3877140	H	0.7884910	-3.7994580	1.3724200
O	-2.2444210	0.9049640	-0.6064890	H	-0.7865400	-4.6276190	1.4231550
C	-3.3070380	0.0368760	-0.1882180	H	-1.5728050	-3.1594710	3.2318940
H	-3.3638820	-0.8210580	-0.8797430	H	0.1078980	-3.4665410	3.7229880

H	-3.0738220	-0.3365090	0.8188060
C	-4.5674980	0.8863970	-0.2625970
C	-4.2601790	1.7740130	-1.4687110
C	-2.7757310	2.0612340	-1.2723990
H	-2.2318170	2.2110760	-2.2153770
H	-2.6183660	2.9426980	-0.6299990
C	2.2165540	-1.5870580	-0.6259460
H	1.8450440	-1.8137730	0.3847630
H	3.1483220	-1.0034570	-0.5363950
H	1.6379340	-3.5631380	-1.3067950
H	3.3959210	-3.2865420	-1.3554910
H	3.1576760	-1.6860060	-3.2068320
H	1.9968050	-2.9494550	-3.6721290
O	1.2265170	-0.8017170	-1.2990570
C	1.1090150	-1.2110350	-2.6707000
H	0.1206080	-1.6781010	-2.8150250
H	1.1728220	-0.3235890	-3.3152280
C	2.2401120	-2.2090530	-2.9004820
C	2.4185320	-2.8120830	-1.5064320

Table S146. Geometric coordinates and single point energies for NaHMDS TMEDA disolvated monomer with κ^2-κ^1 connectivity.



G = -1729.014742 Hartrees
G_{SP} = -1730.400684 Hartrees

Atom	X	Y	Z	Atom	X	Y	Z
C	2.2882370	0.3808350	3.0377250	H	-4.0080720	-2.3805700	1.4740540
Si	1.7641340	1.5352550	1.6143780	C	-1.7990610	-0.9417160	2.1407170
N	1.5946190	0.7076200	0.1422500	H	-2.2656010	0.0285280	1.9184330
Si	2.8224100	0.5571370	-1.0183520	H	-2.2574360	-1.3427980	3.0687570
C	4.5046580	-0.0348450	-0.3464210	H	-0.7284080	-0.7734830	2.3336550
H	5.2434780	-0.1442270	-1.1568430	H	-1.9582440	-3.5632170	2.2282480
H	4.9097010	0.6927110	0.3746930	H	-1.8720630	-3.8435070	0.4850750
H	4.4257240	-1.0013890	0.1748920	H	0.3615490	-2.6471770	2.2216000
C	3.2330570	2.1542190	-1.9653330	H	0.2494280	-4.3319060	1.6952970
H	3.6616950	2.9041610	-1.2828170	C	2.1458400	-2.7842790	0.4793640
H	3.9669850	1.9692860	-2.7664500	H	2.5686050	-3.7325850	0.8711110
H	2.3338200	2.5983950	-2.4200580	H	2.6823900	-2.5140050	-0.4387170
C	2.3431040	-0.7221980	-2.3806350	H	2.3100790	-1.9771700	1.2071240
H	3.1235010	-1.4926390	-2.4916290	C	0.4904540	-3.8393110	-0.8981980
H	1.3977480	-1.2497820	-2.1663410	H	1.0860510	-3.5354250	-1.7700800
H	2.2345150	-0.2424400	-3.3668220	H	0.7769060	-4.8773500	-0.6273930
Na	-0.1292200	-0.6795330	-0.2973620	H	-0.5672720	-3.8402420	-1.1978470

N	0.7216880	-2.9081270	0.1939820	N	-1.2699000	0.2926900	-2.2095360
C	0.0015490	-3.2884200	1.4019720	C	-2.5864340	0.6917230	-1.7285490
C	-1.5117250	-3.1796190	1.2853300	C	-2.5259430	1.6652350	-0.5528290
N	-2.0024970	-1.8337340	1.0055820	N	-3.7246570	1.6173650	0.2684540
C	-3.4205420	-1.8858930	0.6727470	C	-3.6161140	2.5337890	1.3869890
H	-3.8026230	-0.8633580	0.5445550	H	-4.4834290	2.4177760	2.0521160
H	-3.5685130	-2.4520560	-0.2590310	H	-2.7028060	2.3259620	1.9610370
H	-3.5701220	3.5941780	1.0580890	H	-0.6472180	1.5655370	2.3504650
C	-4.9338010	1.8727350	-0.4887600	H	1.5633070	-0.4415080	3.1674620
H	-5.7991160	1.8562820	0.1883310	H	3.2652930	-0.0762600	2.8109490
H	-4.9144630	2.8618990	-0.9964920	H	2.3740310	0.9050640	4.0027290
H	-5.0932540	1.0982750	-1.2516360				
H	-2.3413560	2.6983960	-0.9244530				
H	-1.6591880	1.4164400	0.0860700				
H	-3.1192700	-0.2159570	-1.4051860				
H	-3.1748230	1.1372880	-2.5607190				
C	-1.4070390	-0.6527150	-3.3054970				
H	-1.9403910	-0.2111570	-4.1726520				
H	-0.4136850	-0.9805640	-3.6421520				
H	-1.9731180	-1.5351140	-2.9699020				
C	-0.4694380	1.4452340	-2.6086090				
H	0.4689130	1.0950650	-3.0564670				
H	-1.0045230	2.0749730	-3.3500950				
H	-0.1970370	2.0470370	-1.7309650				
C	3.0092410	2.9714530	1.6150270				
H	2.7039810	3.7463500	0.8941380				
H	3.0692990	3.4400920	2.6101670				
H	4.0228900	2.6409590	1.3392620				
C	0.1261870	2.3280390	2.1720130				
H	0.2511300	2.8971500	3.1067960				
H	-0.2473100	3.0191630	1.3988200				