

## SUPPORTING INFORMATION

### Aggregation and Solvation of Sodium Hexamethyldisilazide Across the Solvent Spectrum

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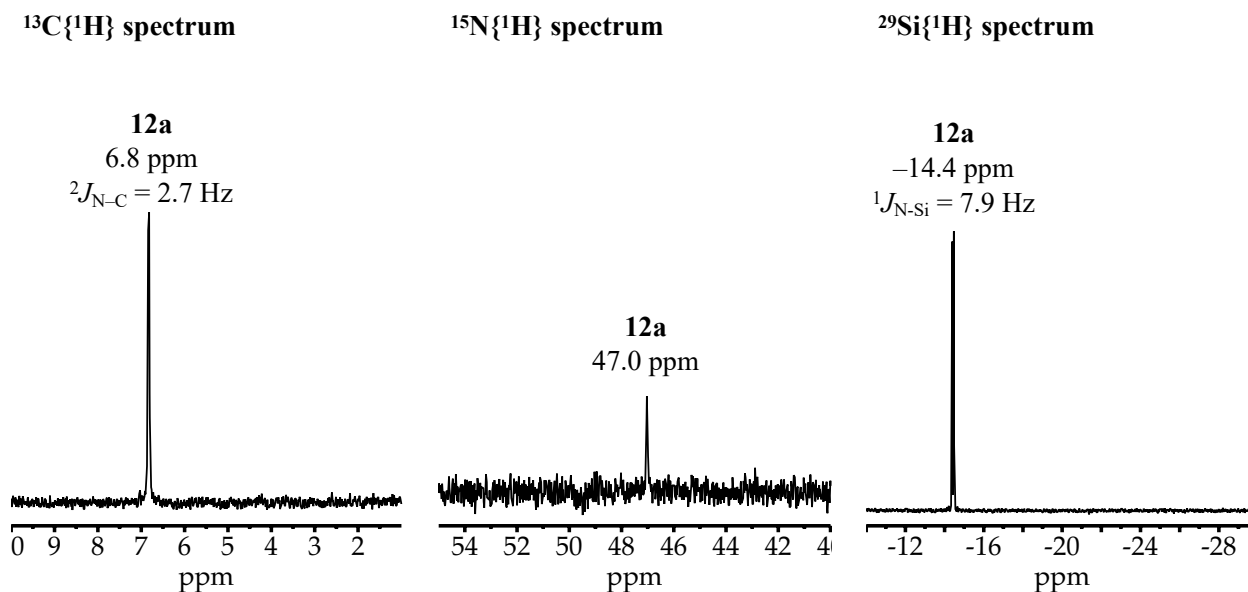
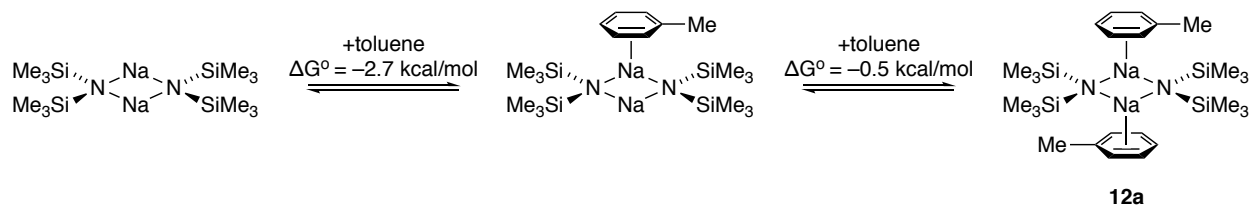
**Table S1.** Spectroscopic and computational data for NaHMDS dimers and monomers in different solvents.

Entry	Solvent	Structure ( $A_mS_n$ (#))	$^{13}\text{C}$ -Si shifts (ppm)	$^{15}\text{N}$ shifts (ppm)	$^{29}\text{Si}$ shifts (ppm ( $^1J_{\text{N-Si}}$ ))	Solvation Energy per S- Na (kcal/mol)
<b>a</b>	toluene	$A_2S_2$ ( <b>12a</b> )	6.8	47.0	-14.4 (7.9)	-1.6
<b>b</b>	benzene	$A_2S_2$ ( <b>12b</b> )	6.9	47.0	-14.2 (7.8)	-2.3
<b>c</b>	styrene	$A_2S_2$ ( <b>12c</b> )	6.8	47.5	-14.3 (7.8)	-1.5
<b>d</b>	DMEA	$A_2S_2$ ( <b>12d</b> )	6.5	46.2	-15.7 (8.7)	-5.9
<b>e</b>	Et <sub>3</sub> N	$A_2S_2$ ( <b>12e</b> )	6.5	46.6	-14.5 (7.6)	-4.1
<b>f</b>	<i>N</i> -Me-pyrrolidine	$A_2S_2$ ( <b>12f</b> )	-	-	-15.5 (8.7)	-6.7
<b>g</b>	pyridine	$A_2S_2$ ( <b>12g</b> )	6.6	44.4	-15.4 (8.8)	-7.3
		$AS_3$ ( <b>13g</b> )	6.8	47.6	-20.7 (13.0)	-5.5
<b>h</b>	pyrrolidine	$A_2S_2$ ( <b>12h</b> )	-	-	-15.5 (9.2)	-8.6
		$AS_4$ ( <b>13h</b> )	-	-	-19.7 (11.1)	-7.4
<b>i</b>	Et <sub>2</sub> O	$A_2S_2$ ( <b>12i</b> )	6.4	49.4	-15.5 (8.3)	-5.0
<b>j</b>	MTBE	$A_2S_2$ ( <b>12j</b> )	6.8	47.4	-15.6 (8.8)	-7.7
<b>k</b>	1,4-dioxane	$A_2S_2$ ( <b>12k</b> )	-	-	-	-6.5
		$AS_3$ ( <b>13k</b> )	-	-	-	-6.0
<b>l</b>	1,3-dioxolane	$A_2S_2$ ( <b>12l</b> )	-	-	-16.0 (8.6)	-
		$AS_4$ ( <b>13l</b> )	-	-	-21.1 (13.0)	-
<b>m</b>	THF	$A_2S_2$ ( <b>12m</b> )	6.3	45.3	-15.8 (8.7)	-6.7
		$AS_4$ ( <b>13m</b> )	6.5	49.0	-21.7 (13.3)	-5.5
<b>n</b>	HMPA	$A_2S_2$ ( <b>12n</b> )	-	-	-16.5 (9.8)	-13.6
		$AS_3$ ( <b>13n</b> )	-	-	-23.7 (13.4)	-11.46
<b>o</b>	DMPU	$A_2S_2$ ( <b>12o</b> )	-	-	-16.4	-10.9
		$AS_2$ ( <b>13o</b> )	-	-	-22.5 (13.6)	-13.1
<b>p</b>	DMF	$A_2S_4$ ( <b>12p</b> )	-	-	-	-8.2
		$AS_4$ ( <b>13p</b> )	-	-	-22.4 (13.7)	-9.3
<b>q</b>	DMSO	$A_2S_4$ ( <b>12q</b> )	-	-	-	-6.5
		$AS_3$ ( <b>13q</b> )	-	-	-20.0 (12.4)	-10.1
<b>r</b>	TMEDA	$A_2S_2$ ( <b>12r</b> )	8.7	-	-14.2 (5.8)	-7.4
		$AS_2$ ( <b>13r</b> )	8.1	-	-21.0 (11.3)	-9.5
<b>s</b>	( <i>R,R</i> )-TMCDA	$A_2SS'$ ( <b>15s</b> )	-	-	-15.7 (7.7)	-11.0
					-14.7 (7.1)	
<b>t</b>	(-)-sparteine ( <b>25</b> )	-	-	-	-	-

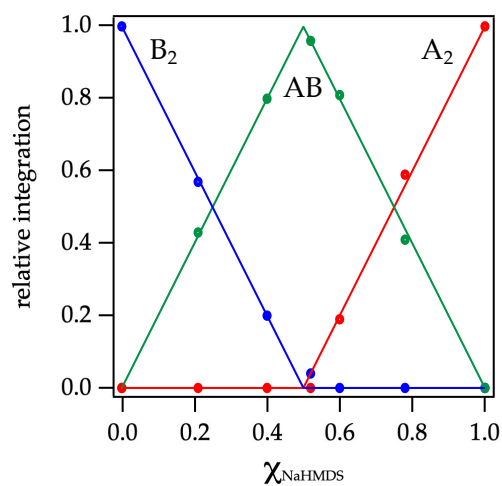
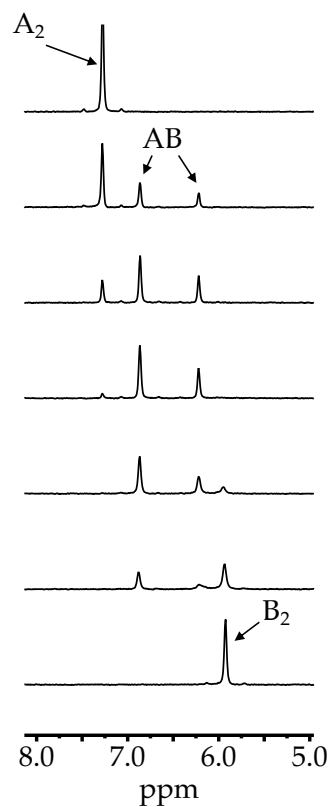
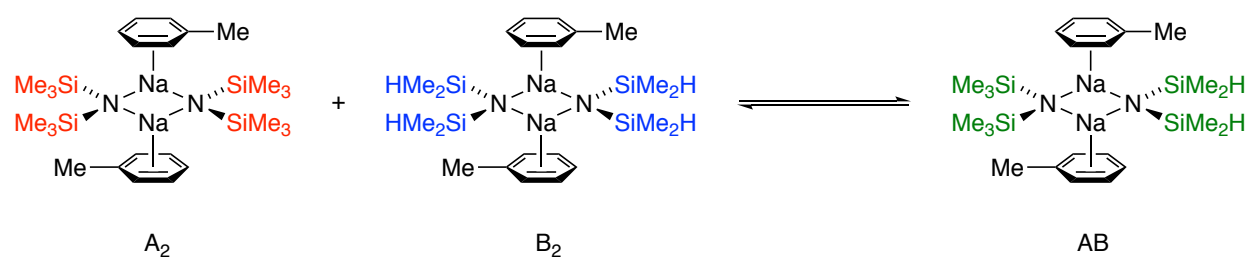
<b>u</b>	bipy	A <sub>2</sub> S ( <b>26u</b> )	–	–	–16.2 (8.8)	–
			–	–	–20.5 (12.5)	–
<b>v</b>	DME	A <sub>2</sub> S <sub>2</sub> ( <b>12u</b> )	–	–	–15.5 (7.8)	–13.2
		A <sub>2</sub> S <sub>2</sub> ( <b>12v</b> )	–	–	–14.8 (7.6)	–9.6
<b>w</b>	PMDTA	AS <sub>2</sub> ( <b>13v</b> )		46.5	–21.4 (13.7)	–11.7
		AS ( <b>13w</b> )	7.8	48.8	–22.7 (13.7)	–25.7
<b>x</b>	diglyme	AS ( <b>13x</b> )	6.5	49.7	–21.3 (12.7)	–23.4
<b>y</b>	12-crown-4	AS ( <b>13y</b> )	–	–	–22.4 (13.7)	–18.7
<b>z</b>	15-crown-5	AS ( <b>13z</b> )	–	–	–22.1 (13.0)	–29.4
<b>aa</b>	18-crown-6	A <sub>2</sub> S ( <b>16aa</b> )	–	–	–22.3 (13.6)	–
		AS ( <b>13aa</b> )	–	–	–21.6 (12.3)	–28.8
<b>bb</b>	TDA-1 ( <b>31</b> )	A <sub>2</sub> S ( <b>16bb</b> )	–	–	–20.5 (13.5)	–
		AS ( <b>13bb</b> )	–	–	–19.7 (12.8)	–23.8
<b>cc</b>	[2.2.2]crypt ( <b>32</b> )	A <sub>2</sub> S ( <b>16cc</b> )	–	–	–20.5 (13.5)	–
		AS ( <b>14cc</b> )	–	–	–27.2	–

## **I. NMR Spectroscopic Data and Computed Free Energies**

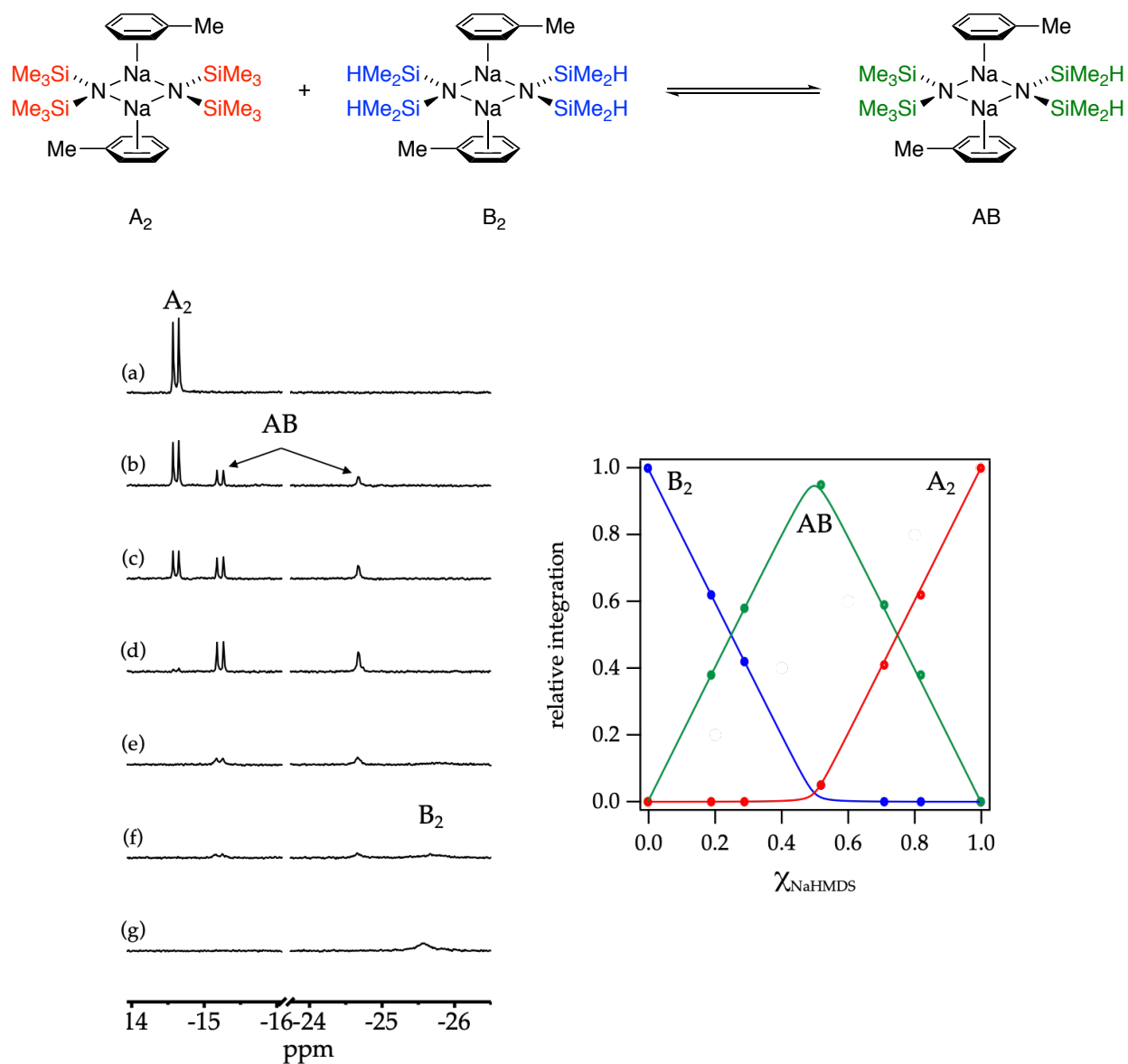
**Toluene (entry a):**



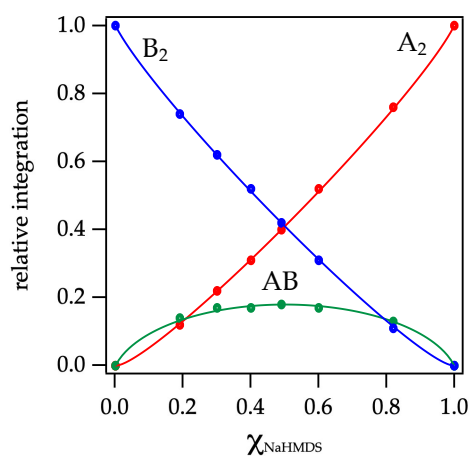
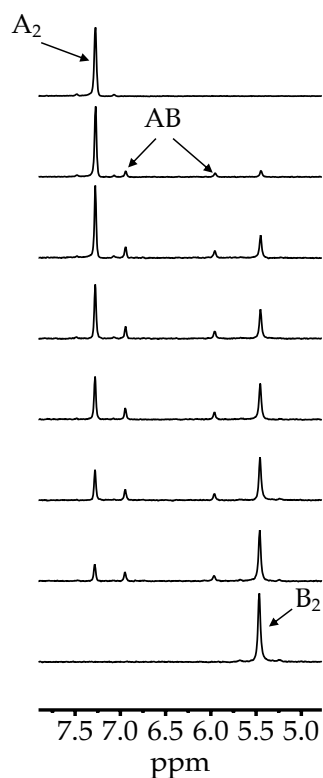
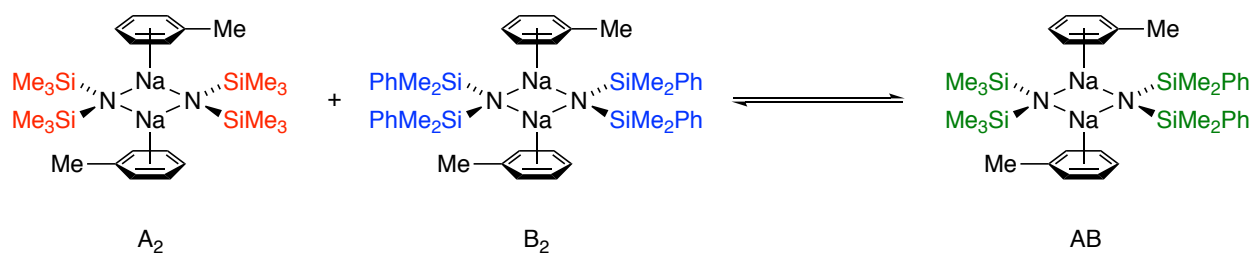
**Figure S1.** NMR spectra of 0.10 [<sup>15</sup>N]NaHMDS in 2:1 pentane/toluene-*d*<sub>8</sub> at 25 °C. <sup>13</sup>C and <sup>29</sup>Si spectra are referenced to a TMS internal standard (TMS chemical shift = 0.0 ppm for each).



**Figure S2.**  $^{13}\text{C}$  NMR spectra and affiliated Job plot showing relative integrations of NaHMDS-derived homodimer ( $\text{A}_2$ , red), NaTMDS-derived homodimer ( $\text{B}_2$ , blue), and heterodimer ( $\text{AB}$ , green) versus the measured mole fraction of NaHMDS ( $\chi_{\text{NaHMDS}}$ ) at 0.30 total molarity in neat toluene at  $-80^\circ\text{C}$ .

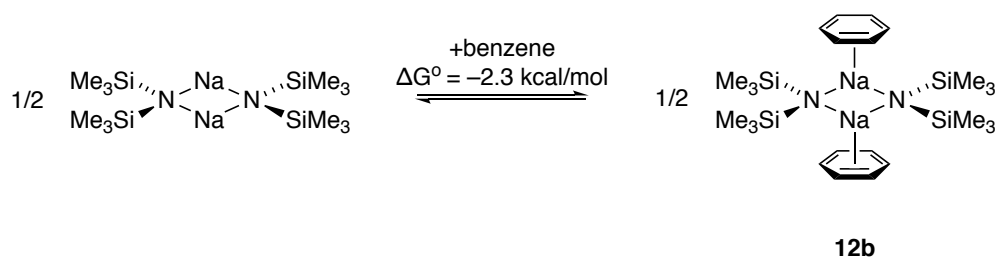


**Figure S3.** <sup>29</sup>Si{<sup>1</sup>H} NMR spectra and affiliated Job plot showing relative integrations of NaHMDS-derived homodimer (A<sub>2</sub>, red), NaTMDS-derived homodimer (B<sub>2</sub>, blue), and heterodimer (AB, green) versus the measured mole fraction of NaHMDS ( $X_{\text{NaHMDS}}$ ) at 0.20 total molarity in neat toluene at  $-80$  °C. The measured mole fractions,  $X_{\text{NaHMDS}}$ , in (a)–(g) are 1.00, 0.81, 0.71, 0.52, 0.29, 0.19, and 0.00, respectively.

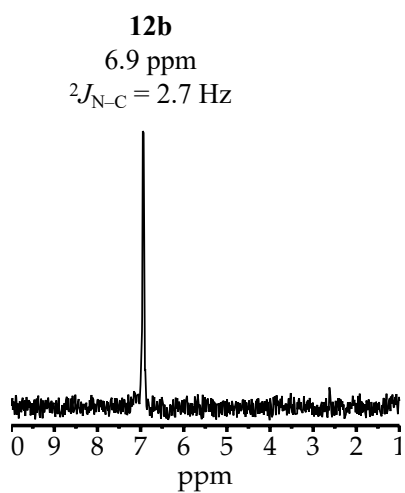


**Figure S4.** Job plot showing relative integrations of the  $^{13}\text{C}$  resonances of NaHMDS homodimer ( $A_2$ , red), NaDPTMDS-derived homodimer ( $B_2$ , blue), and heterodimer ( $AB$ , green) versus the measured mole fraction of NaHMDS ( $X_{\text{NaHMDS}}$ ) at 0.30 total molarity in neat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

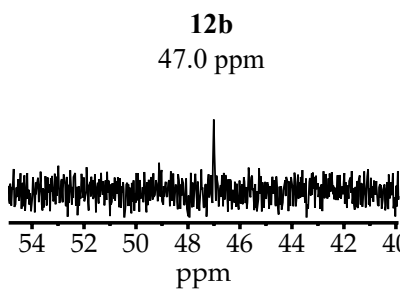
**Benzene (entry b):**



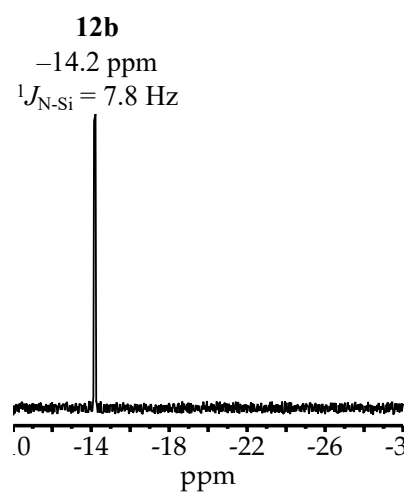
$^{13}\text{C}\{^1\text{H}\}$  spectrum



$^{15}\text{N}\{^1\text{H}\}$  spectrum



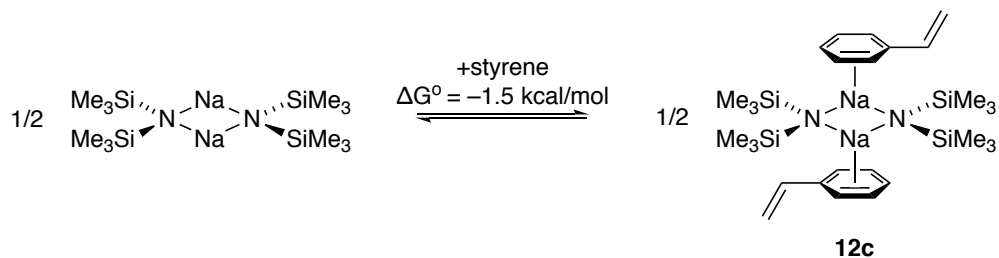
$^{29}\text{Si}\{^1\text{H}\}$  spectrum



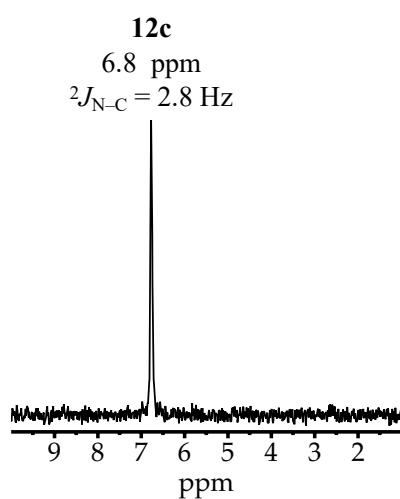
**Figure S5.** NMR spectra of 0.10  $[^{15}\text{N}]\text{NaHMDS}$  in benzene at 25 °C. (TMS chemical shift = 0.0 ppm for each).



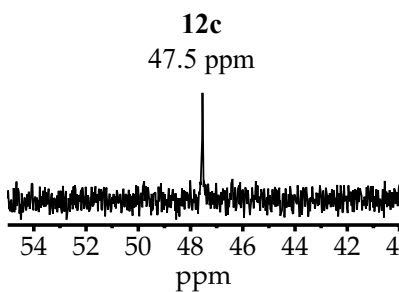
**Styrene (entry c):**



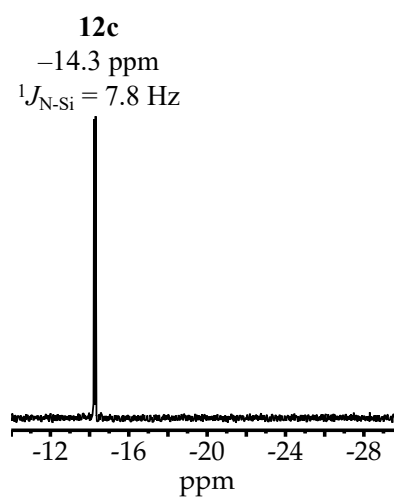
$^{13}\text{C}\{^1\text{H}\}$  spectrum



$^{15}\text{N}\{^1\text{H}\}$  spectrum

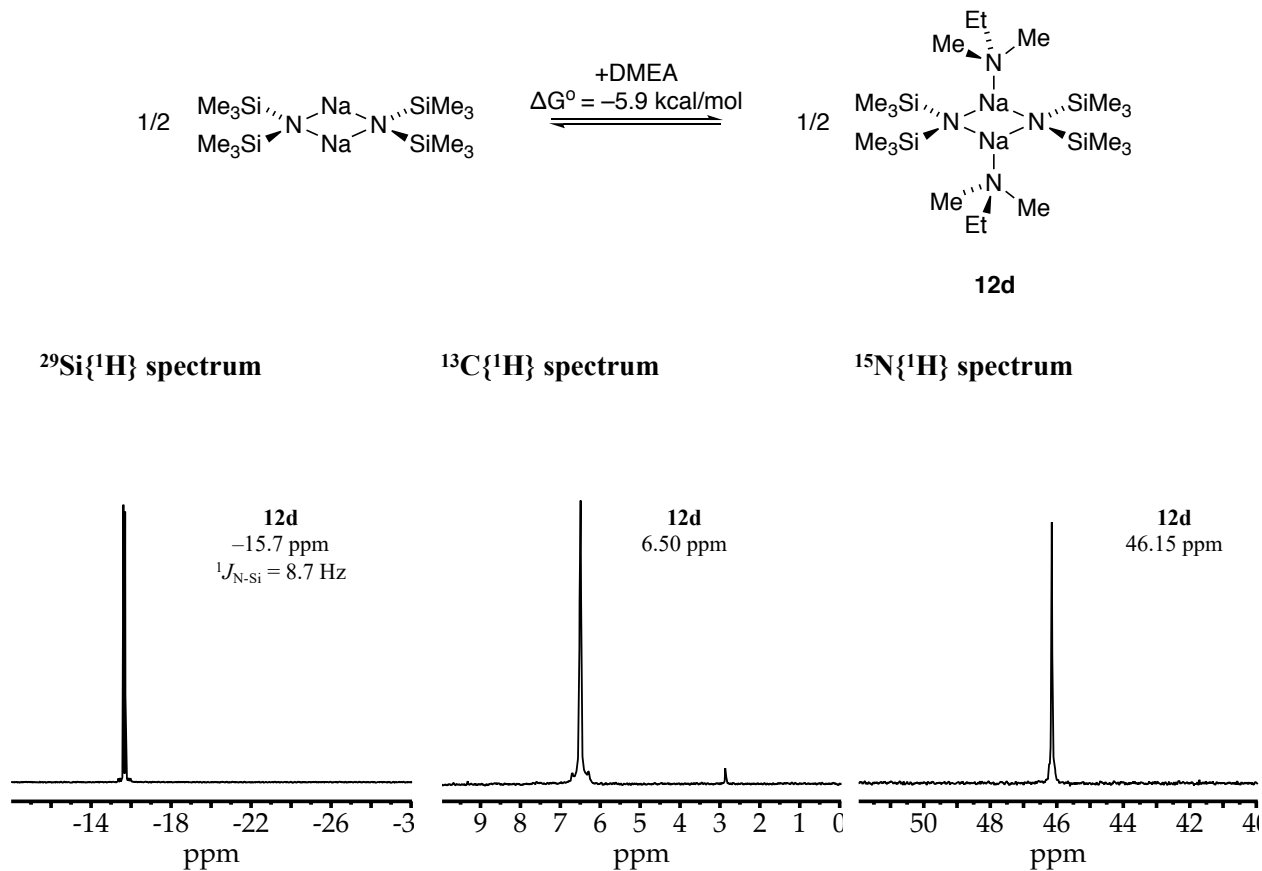


$^{29}\text{Si}\{^1\text{H}\}$  spectrum

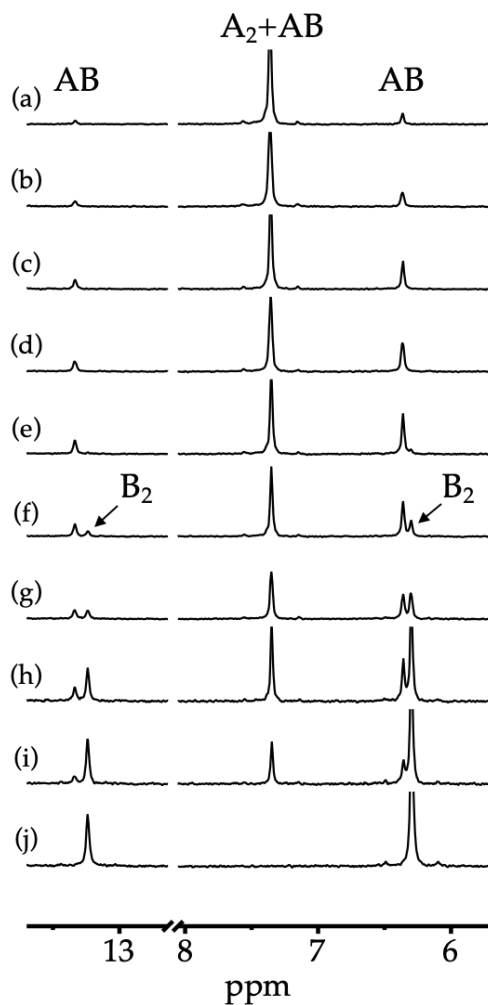
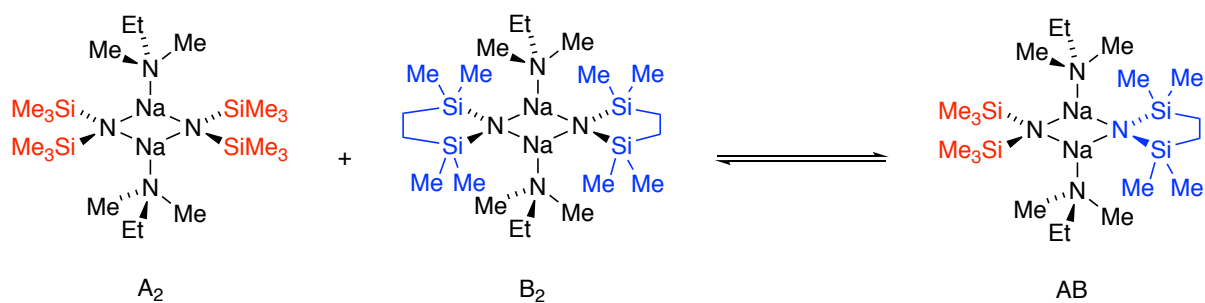


**Figure S6.** NMR spectra of 0.10 M  $^{15}\text{N}$ NaHMDS in styrene at 25 °C. (TMS chemical shift = 0.0 ppm for each).

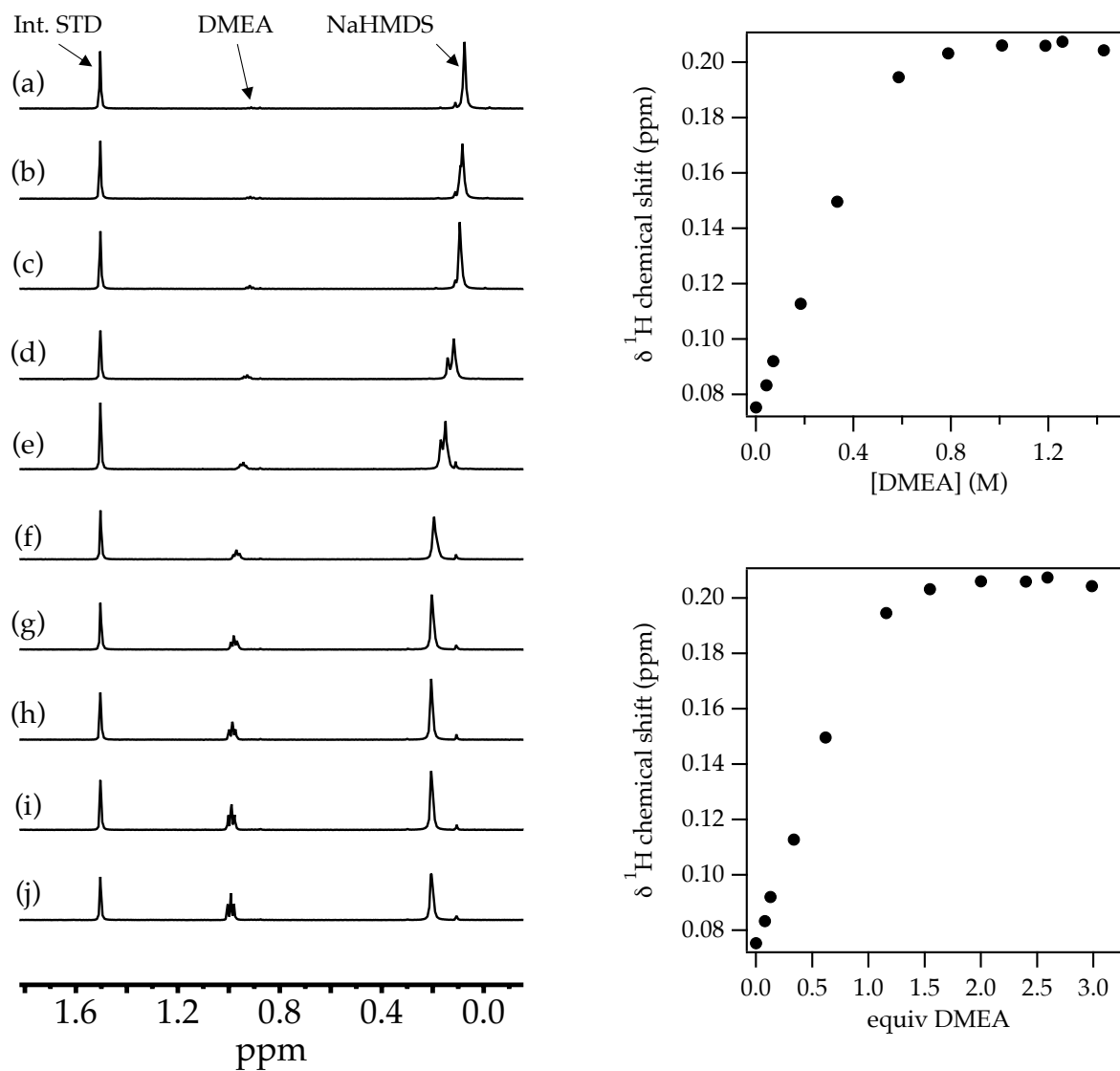
**DMEA (entry d):**



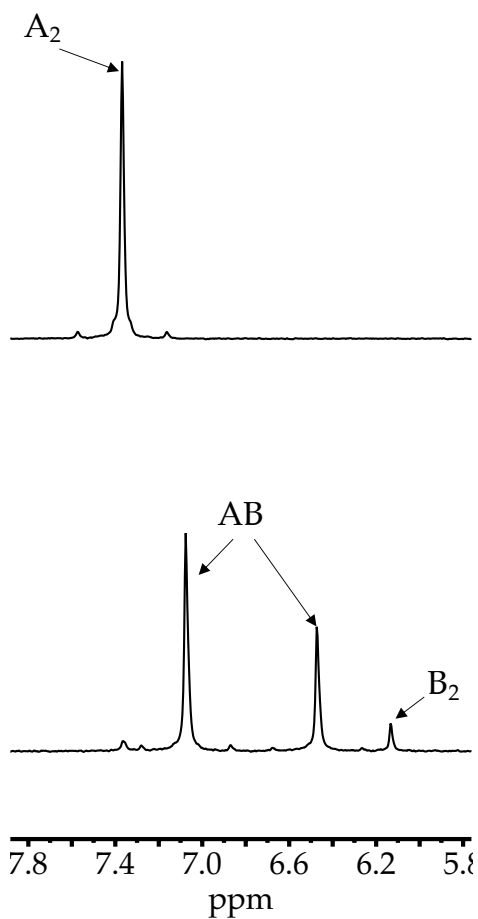
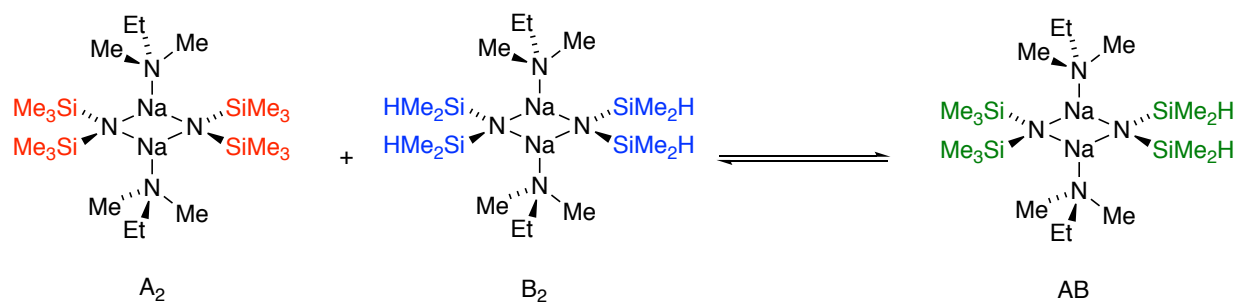
**Figure S7.** NMR spectra of  $^{15}\text{N}$ NaHMDS in neat DMEA at  $-120^\circ\text{C}$ . Concentrations vary from 0.20 M NaHMDS ( $^{15}\text{N}$  and  $^{29}\text{Si}$ ) to 0.30 M NaHMDS ( $^{13}\text{C}$ ).  $^{13}\text{C}$  spectrum is referenced to cyclopentane internal standard (26.05 ppm).  $^{15}\text{N}$  is referenced to DMEA (25.70 ppm).  $^{29}\text{Si}$  is referenced to TMS internal standard (0.00 ppm).



**Figure S8.**  $^{13}\text{C}$  NMR 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  $-80^\circ\text{C}$ . Addition of DMEA was necessary to dissolve **20** which is insoluble in neat toluene.  $^{13}\text{C}$  spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).

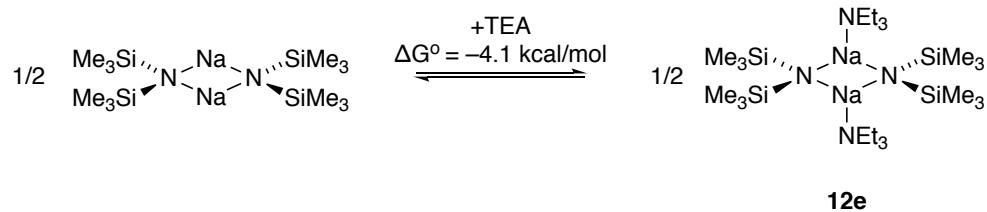


**Figure S9.**  $^1\text{H}$  NMR spectra for 0.56 M solutions of NaHMDS in toluene with cyclopentane internal standard varying DMEA at 25 °C. The equivalents of THF in (a)–(j) are 0.00, 0.08, 0.13, 0.34, 0.61, 1.15, 1.54, 2.00, 2.40, 2.59, and 2.98, respectively. Plots of chemical shift affiliated with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



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

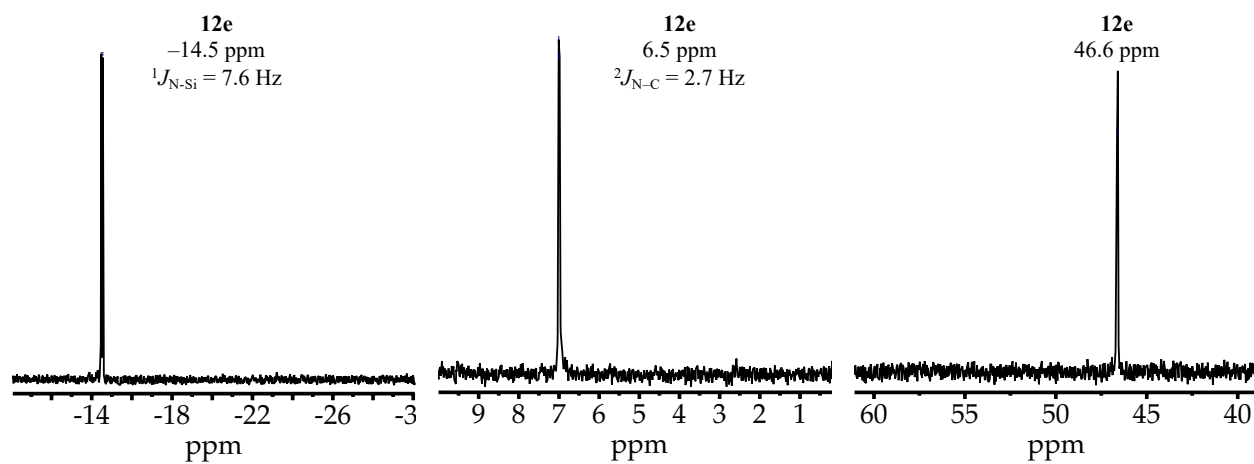
**Triethylamine (entry e):**



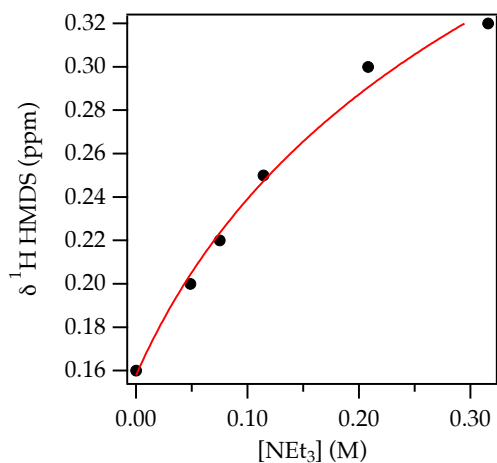
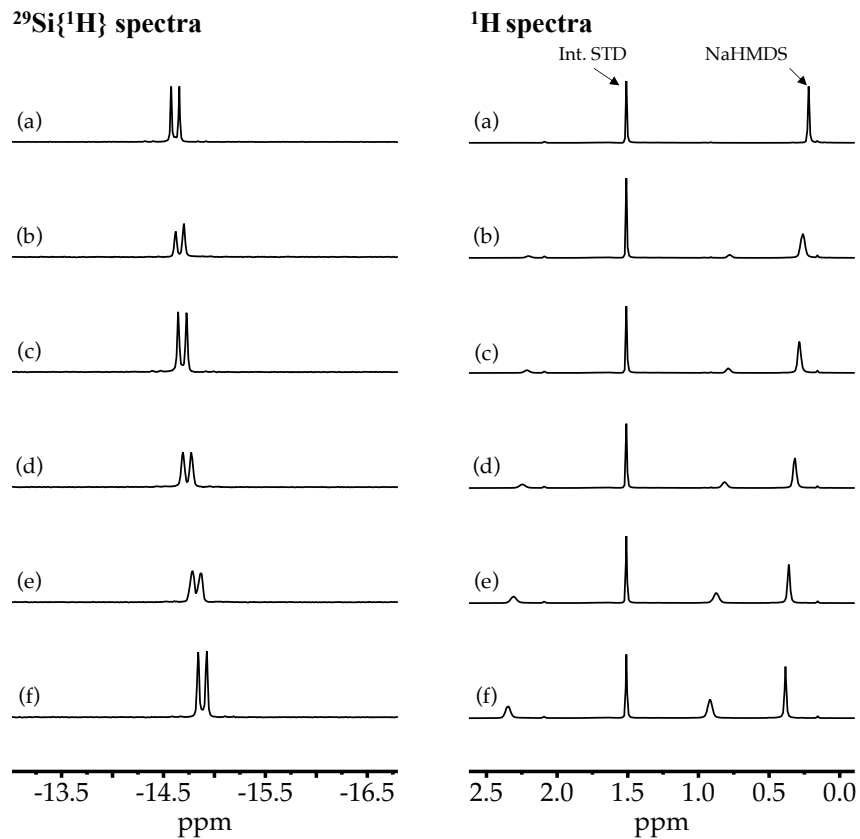
**$^{29}\text{Si}\{^1\text{H}\}$  spectrum**

**$^{13}\text{C}\{^1\text{H}\}$  spectrum**

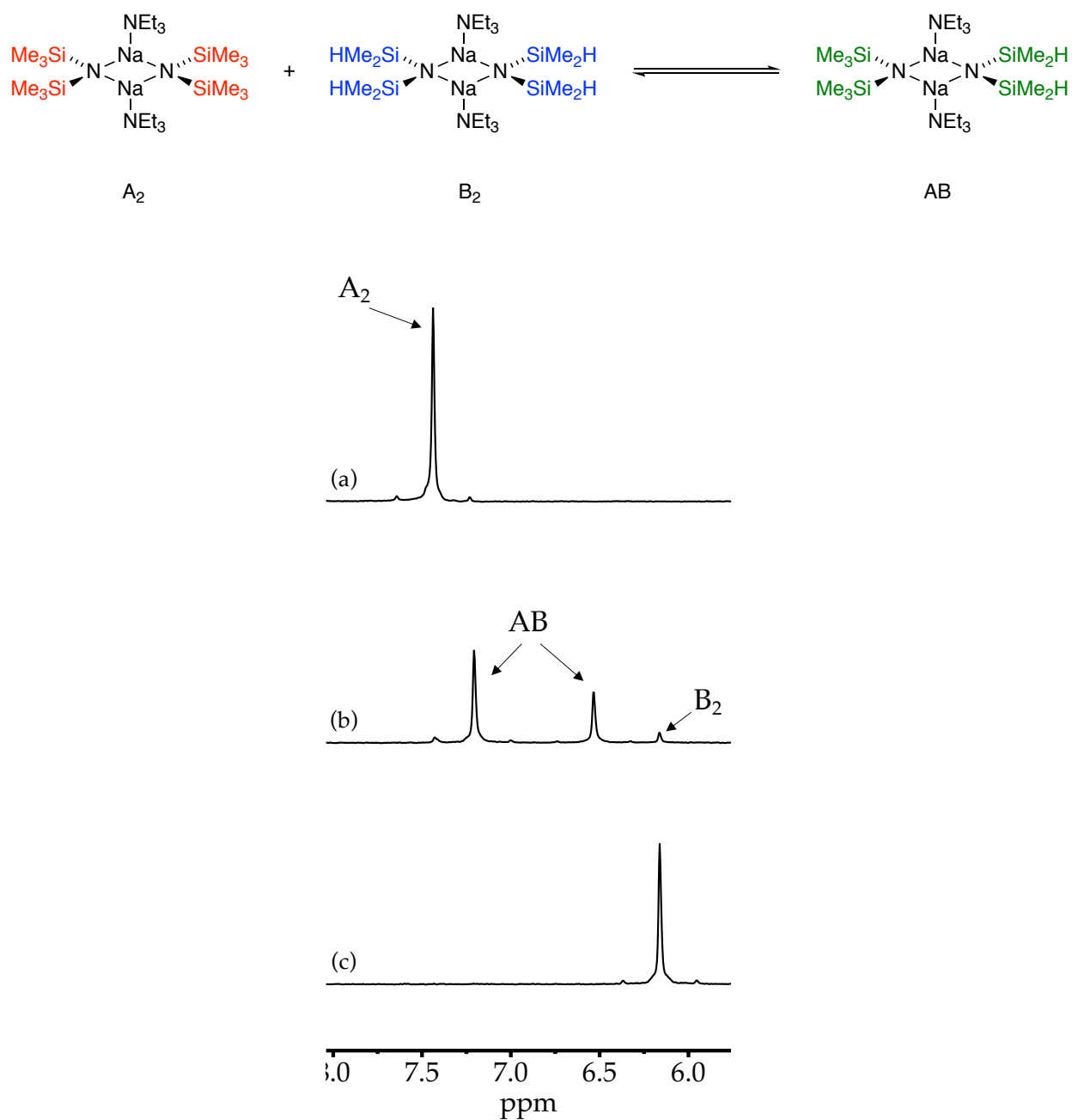
**$^{15}\text{N}\{^1\text{H}\}$  spectrum**



**Figure S11.** NMR spectra of 0.10 M  $^{15}\text{N}$ NaHMDS in neat triethylamine at 25 °C.  $^{13}\text{C}$  and  $^{29}\text{Si}$  spectra are referenced to TMS internal standard (0.00 ppm).

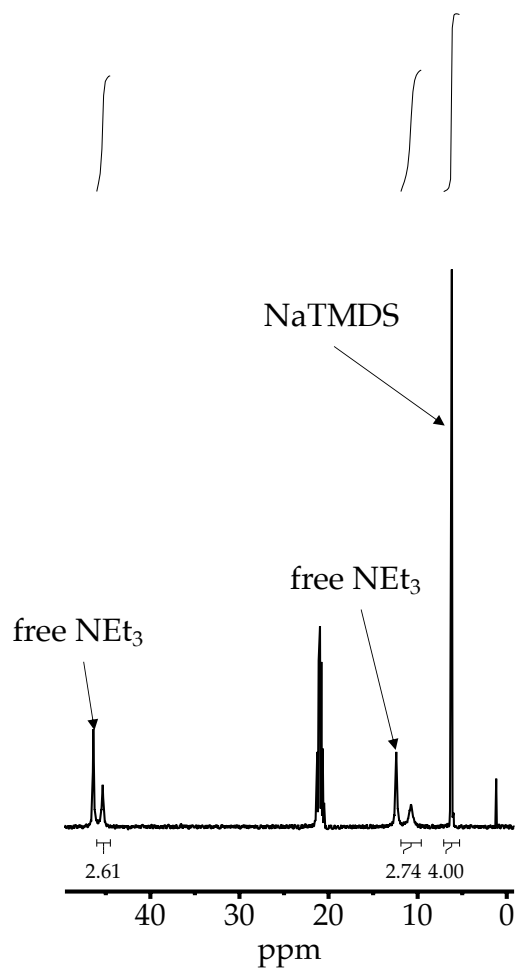


**Figure S12.**  $^1\text{H}$  and  $^{29}\text{Si}$  NMR spectra for 0.19 M solutions of NaHMDS in toluene with cyclopentane internal standard (1.51 ppm) varying triethylamine concentration at  $-80\text{ }^\circ\text{C}$ . The concentration of triethylamine in (a)–(f) are 0.00, 0.05, 0.08, 0.11, 0.21,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

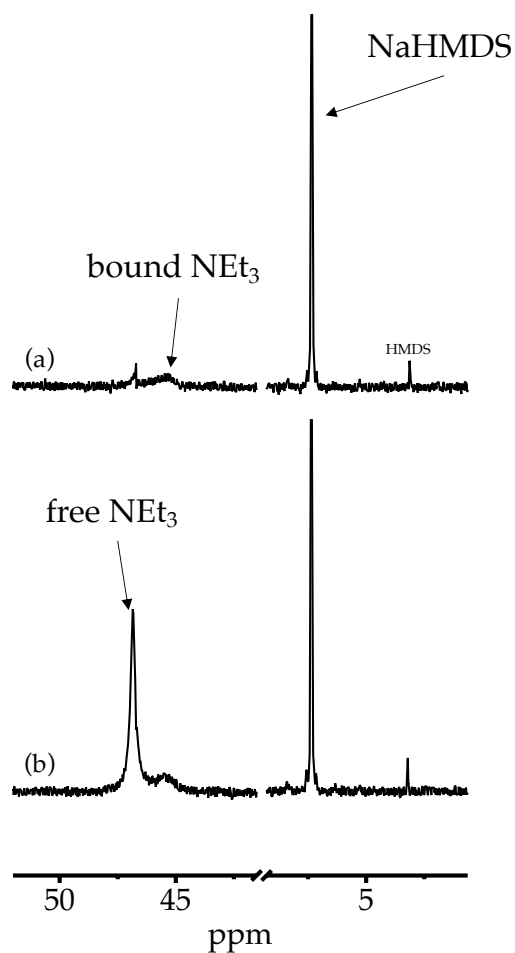


**Figure S13.**  $^{13}\text{C}$  NMR spectra of with mixing NaHMDS and NaTMDS at 0.20 total molarity in 0.50 M triethylamine in toluene- $d_8$  cosolvent at  $-80^\circ\text{C}$ . The measured mole fractions,  $X_{\text{NaHMDS}}$ , in (a)–(c) are 1.00, 0.50, and 0.00, respectively.  $^{13}\text{C}$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



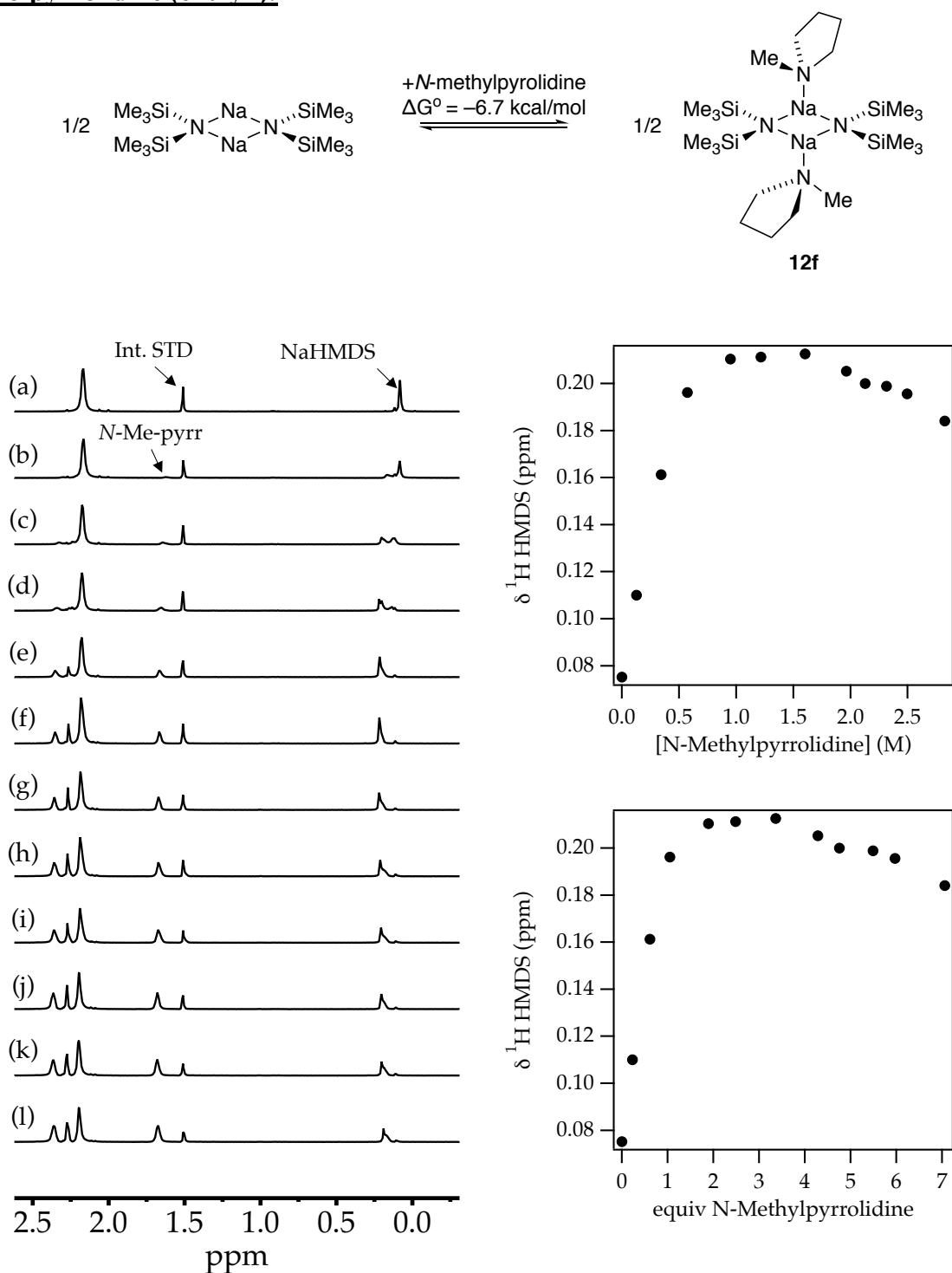


**Figure S14.**  $^{13}\text{C}$  NMR spectra of NaTMDS at 0.20 total molarity in 0.50 M triethylamine in toluene- $d_8$  cosolvent at  $-100\text{ }^\circ\text{C}$ . Free and bound triethylamine are observed at this temperature. Relative integrations so a 1:1 stoichiometry of triethylamine to NaTMDS.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

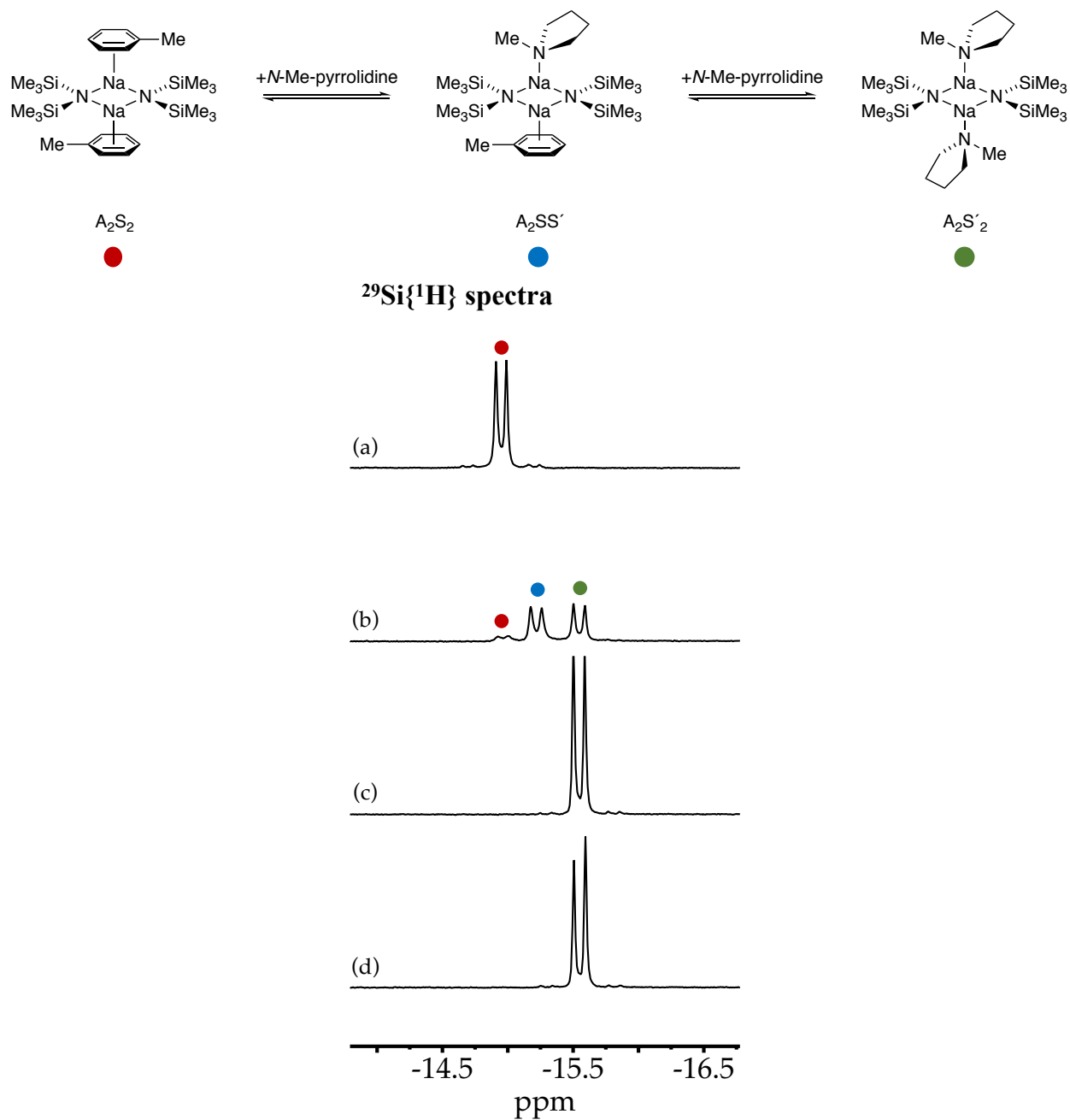


**Figure S15.**  $^{13}\text{C}$  NMR spectra of  $^{15}\text{N}$ NaHMDS at 0.10 M in 2:1 pentane/toluene- $d_8$  cosolvent with varying amounts of triethylamine added at  $-120^\circ\text{C}$ . The concentration of triethylamine in (a) and (b) are 0.15 M and 0.44 M, respectively. Free and bound triethylamine 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.  $^{13}\text{C}$  spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).

**N-Me-pyrrolidine (entry f):**

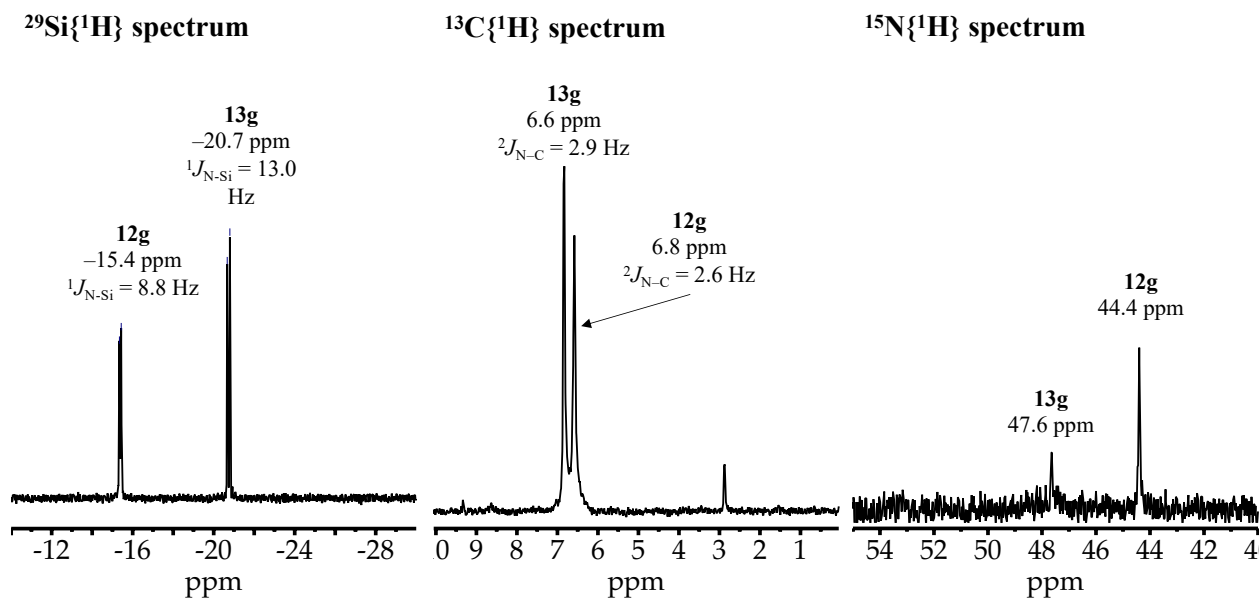
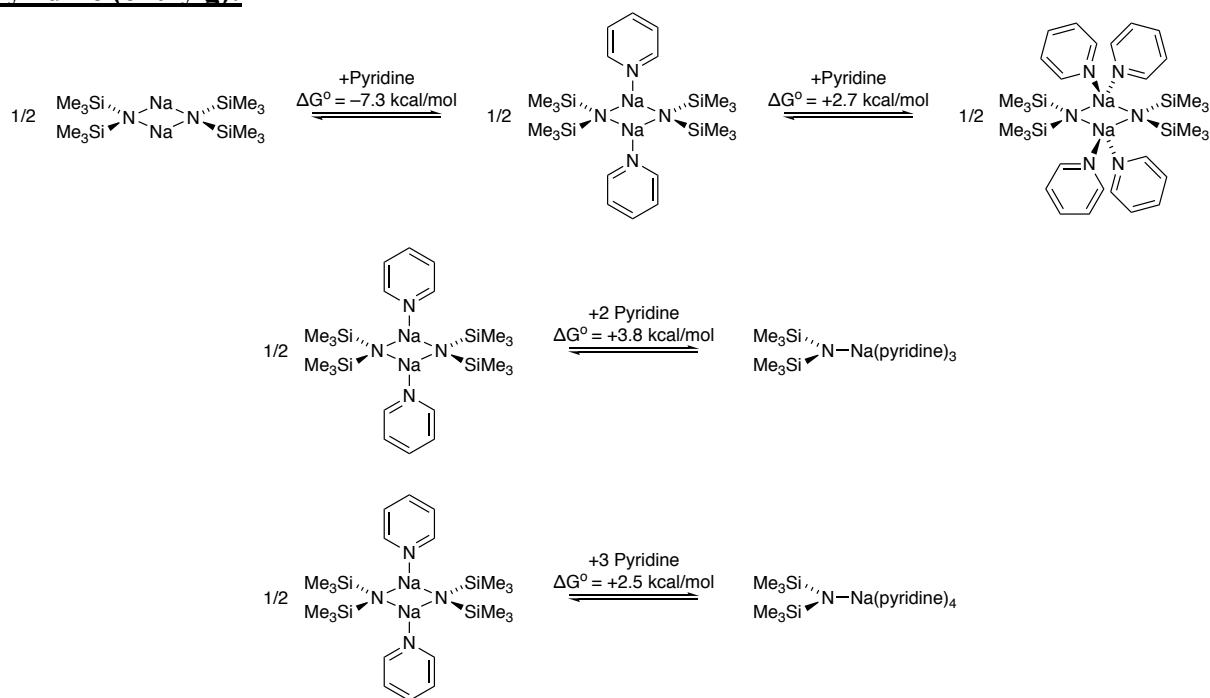


**Figure S16.**  $^1\text{H}$  NMR spectra for 0.55 M solutions of NaHMDS in toluene with cyclopentane internal standard (1.51 ppm) varying *N*-Me-pyrrolidine concentration at 25 °C. The concentrations of *N*-Me-pyrrolidine in (a)–(l) are 0.00, 0.13, 0.34, 0.57, 0.95, 1.21, 1.60, 1.96, 2.12, 2.31, 2.50,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



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

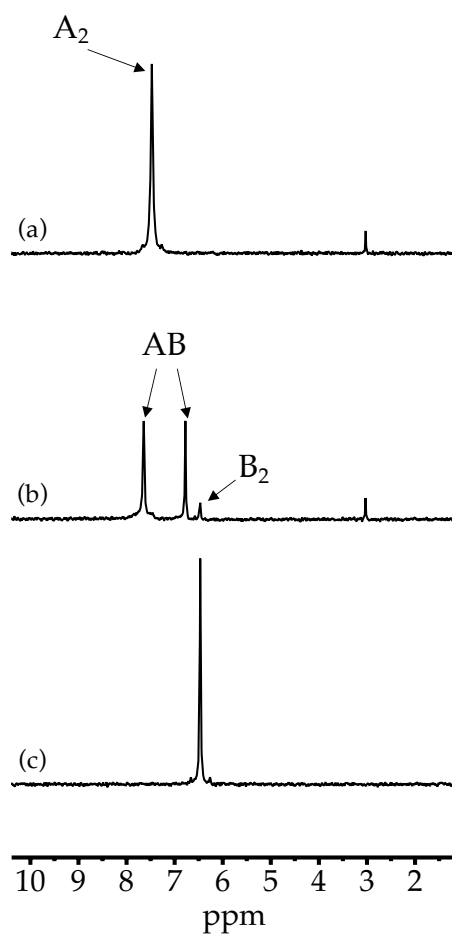
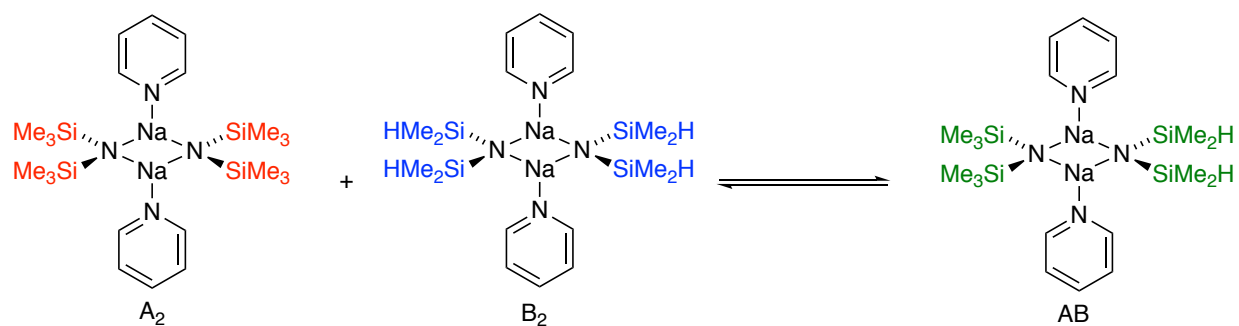
**Pyridine (entry g):**



**Figure S18.** NMR spectra of  $[\text{}^{15}\text{N}]\text{NaHMDS}$  at intermediate concentrations of pyridine. Conditions vary on a per spectrum basis. Conditions in which each spectra were taken are delineated below.

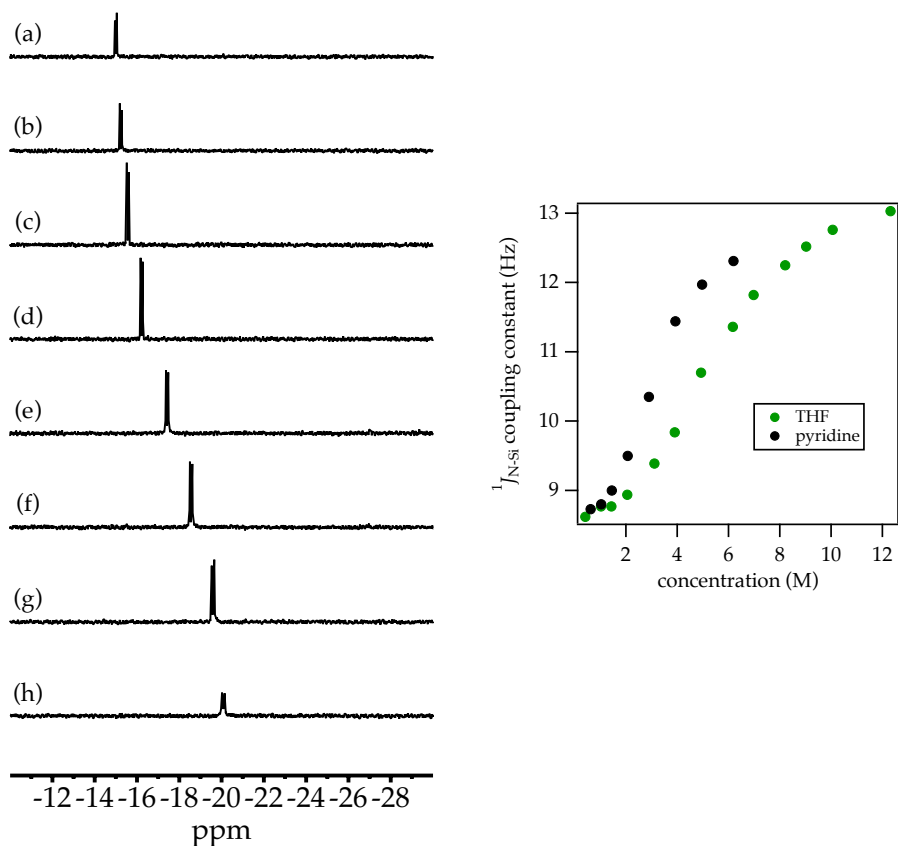
$^{29}\text{Si}$  and  $^{13}\text{C}$  spectra: 0.15 M  $[\text{}^{15}\text{N}]\text{NaHMDS}$  with 0.45 M pyridine in DMEA cosolvent at  $-120^\circ\text{C}$ . The  $^{13}\text{C}$  spectrum is referenced to cyclopentane (26.05 ppm).

$^{15}\text{N}$  spectrum: 0.10 M  $[\text{}^{15}\text{N}]\text{NaHMDS}$  with 0.3 M pyridine in MTBE cosolvent at  $-110^\circ\text{C}$ .



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

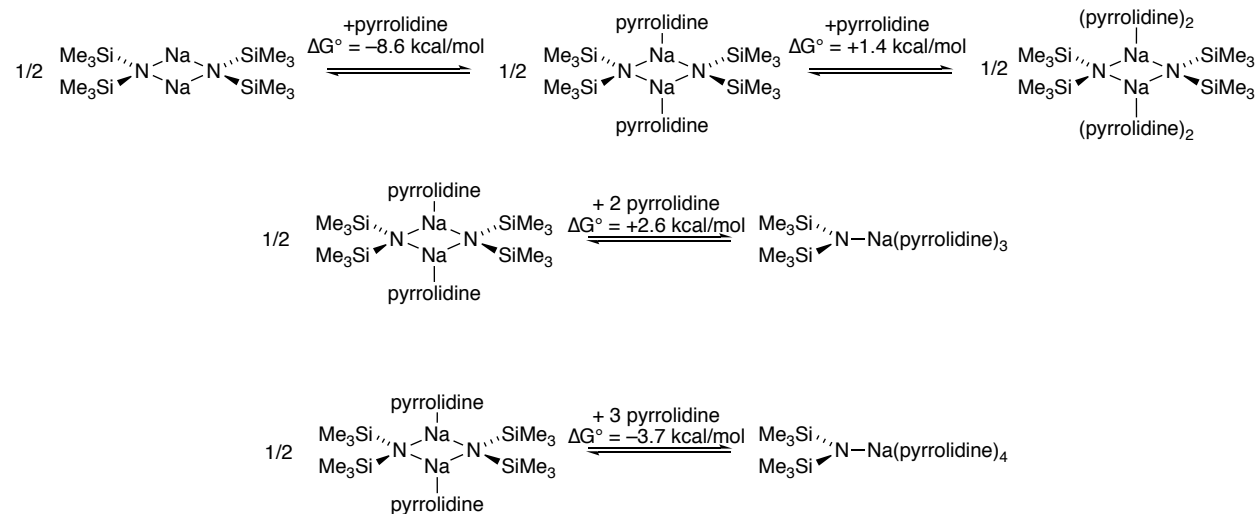
### $^{29}\text{Si}\{^1\text{H}\}$ spectra



**Figure S20.**  $^{29}\text{Si}\{^1\text{H}\}$  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.

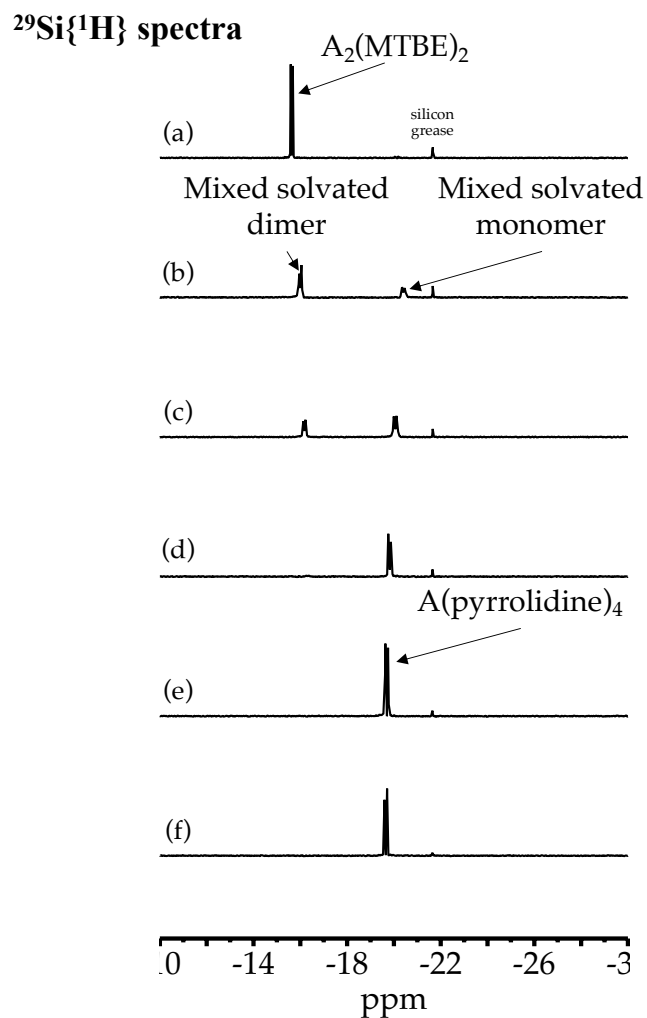
[THF] (M)	$^1J_{\text{N-Si}}$ coupling constant (Hz)	[pyridine] (M)	$^1J_{\text{N-Si}}$ coupling constant (Hz)
0.41	8.62	0.62	8.73
1.02	8.77	1.03	8.80
1.43	8.77	1.44	9.00
2.05	8.94	2.06	9.50
3.10	9.39	2.89	10.35
3.90	9.84	3.92	11.44
4.92	10.7	4.96	11.97
6.16	11.36	6.19	12.31
6.97	11.82		
8.20	12.25	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

### Pyrrolidine (entry h):



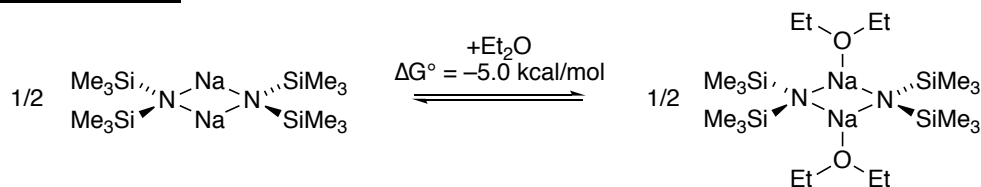
**Figure S21.** DFT computed energies of various NaHMDS pyrrolidine solvation states.





**Figure S22.**  $^{29}\text{Si}$  NMR spectra of 0.20 M  $[\text{}^{15}\text{N}]\text{NaHMDS}$  in MTBE cosolvent with varying amounts of pyrrolidine added at  $-110\text{ }^\circ\text{C}$ . 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.  $^{29}\text{Si}$  spectra are referenced to a TMS internal standard (TMS chemical shift = 0.0 ppm for each).

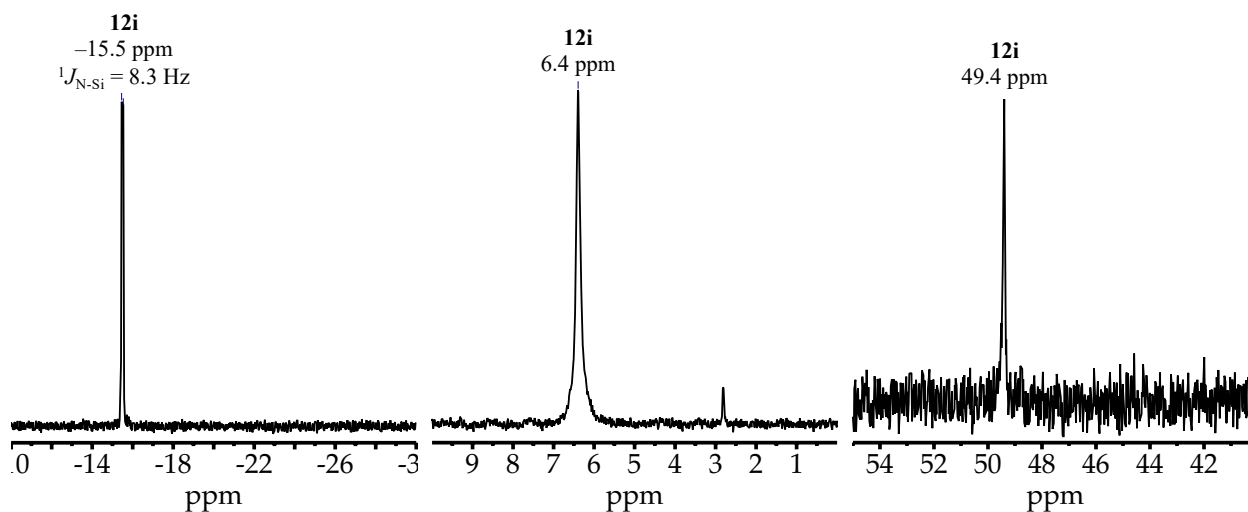
### Diethyl ether (entry i):



$^{29}\text{Si}\{^1\text{H}\}$  spectrum

$^{13}\text{C}\{^1\text{H}\}$  spectrum

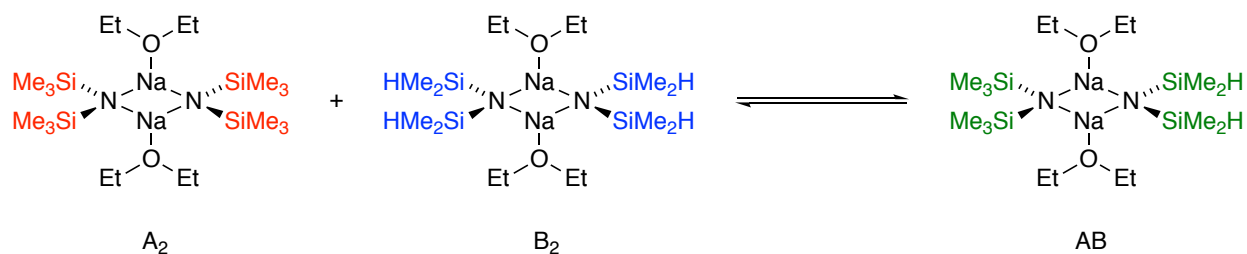
$^{15}\text{N}\{^1\text{H}\}$  spectrum



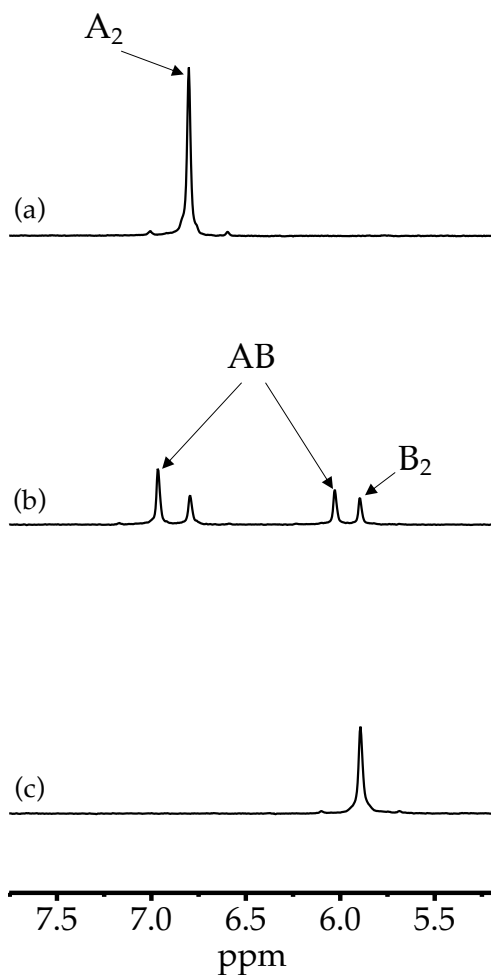
**Figure S23.** NMR spectra of  $^{15}\text{N}$ NaHMDS in various cosolvents with added diethyl ether. Conditions vary on a per spectrum basis. Conditions in which each spectra were taken are delineated below.

$^{29}\text{Si}$  and  $^{13}\text{C}$  spectra: 0.15 M  $^{15}\text{N}$ NaHMDS with 4.5 M diethyl ether in DMEA cosolvent at  $-120^\circ\text{C}$ . Cyclopentane internal standard was used.

$^{15}\text{N}$  spectrum: 0.10 M  $^{15}\text{N}$ NaHMDS in neat diethyl ether (9.60 M) at  $25^\circ\text{C}$ . TMS internal standard was used.

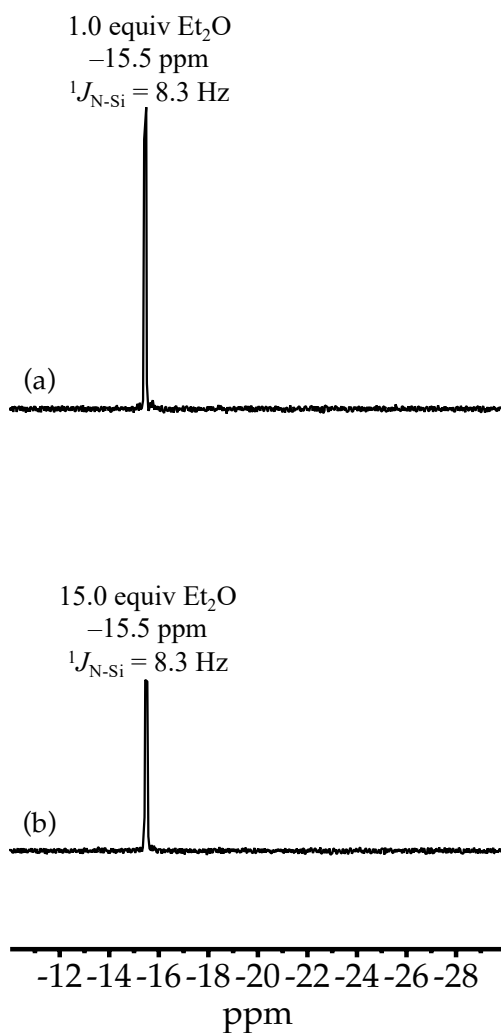


**<sup>13</sup>C{<sup>1</sup>H} spectra**



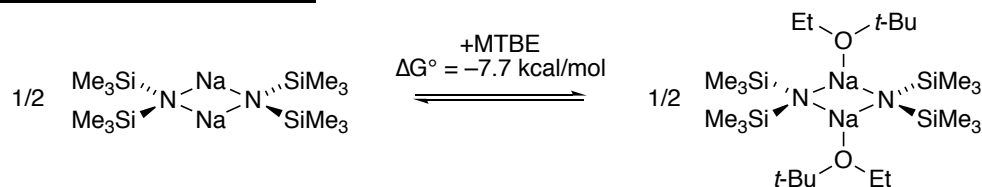
**Figure S24.** <sup>13</sup>C NMR spectra of with mixing NaHMDS and NaTMDS at 0.20 total molarity in 0.80 M diethyl ether in toluene-*d*<sub>8</sub> cosolvent at -80 °C. The measured mole fractions,  $X_{\text{NaHMDS}}$ , in (a)–(c) are 1.00, 0.50, and 0.00, respectively. <sup>13</sup>C spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).

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



**Figure S25.**  $^{29}\text{Si}$  NMR spectra of 0.15 M  $[^{15}\text{N}]\text{NaHMDS}$  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.

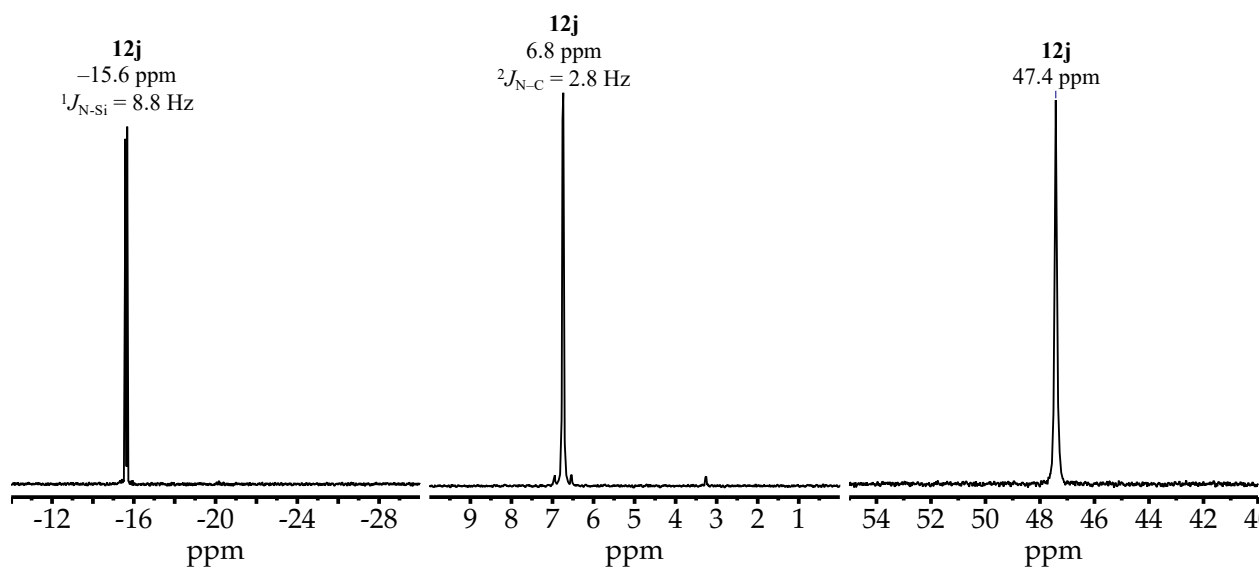
**Methyl *tert*-butyl ether (entry j):**



$^{29}\text{Si}\{^1\text{H}\}$  spectrum

$^{13}\text{C}\{^1\text{H}\}$  spectrum

$^{15}\text{N}\{^1\text{H}\}$  spectrum

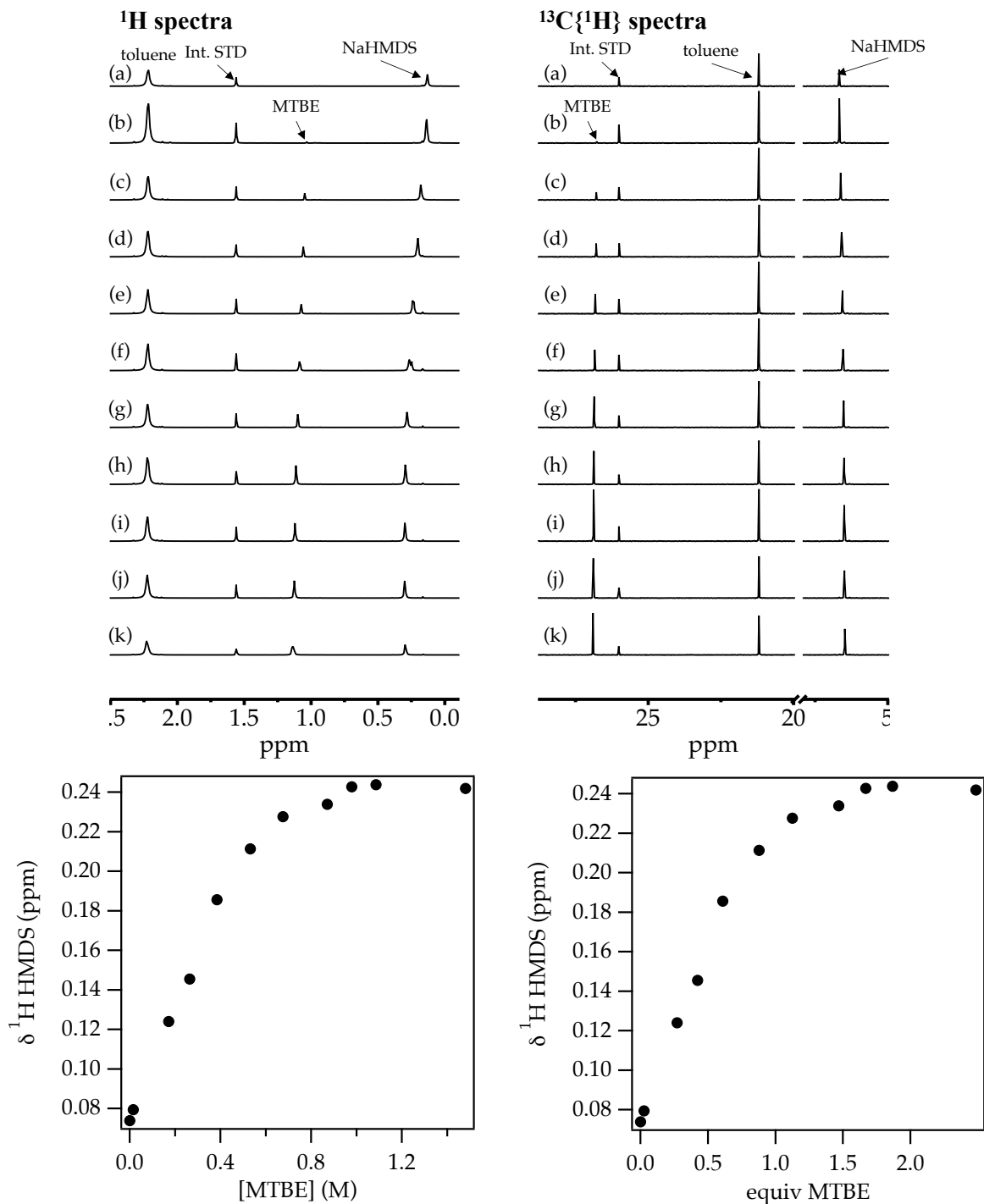


**Figure S26.** NMR spectra of  $^{15}\text{N}$ NaHMDS at intermediate concentrations of methyl *tert*-butyl ether. Conditions vary on a per spectrum basis. Conditions in which each spectra where taken are delineated below.

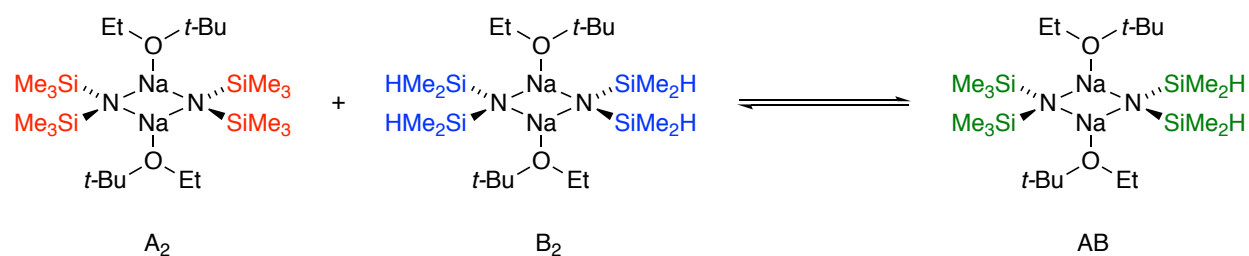
$^{29}\text{Si}$  spectrum: 0.20 M  $^{15}\text{N}$ NaHMDS in neat MTBE at  $-110^\circ\text{C}$ . TMS internal standard was used.

$^{13}\text{C}$  spectrum: 0.30 M  $^{15}\text{N}$ NaHMDS with 5.55 M MTBE in toluene cosolvent at  $-80^\circ\text{C}$ .  $^{13}\text{C}$  spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).

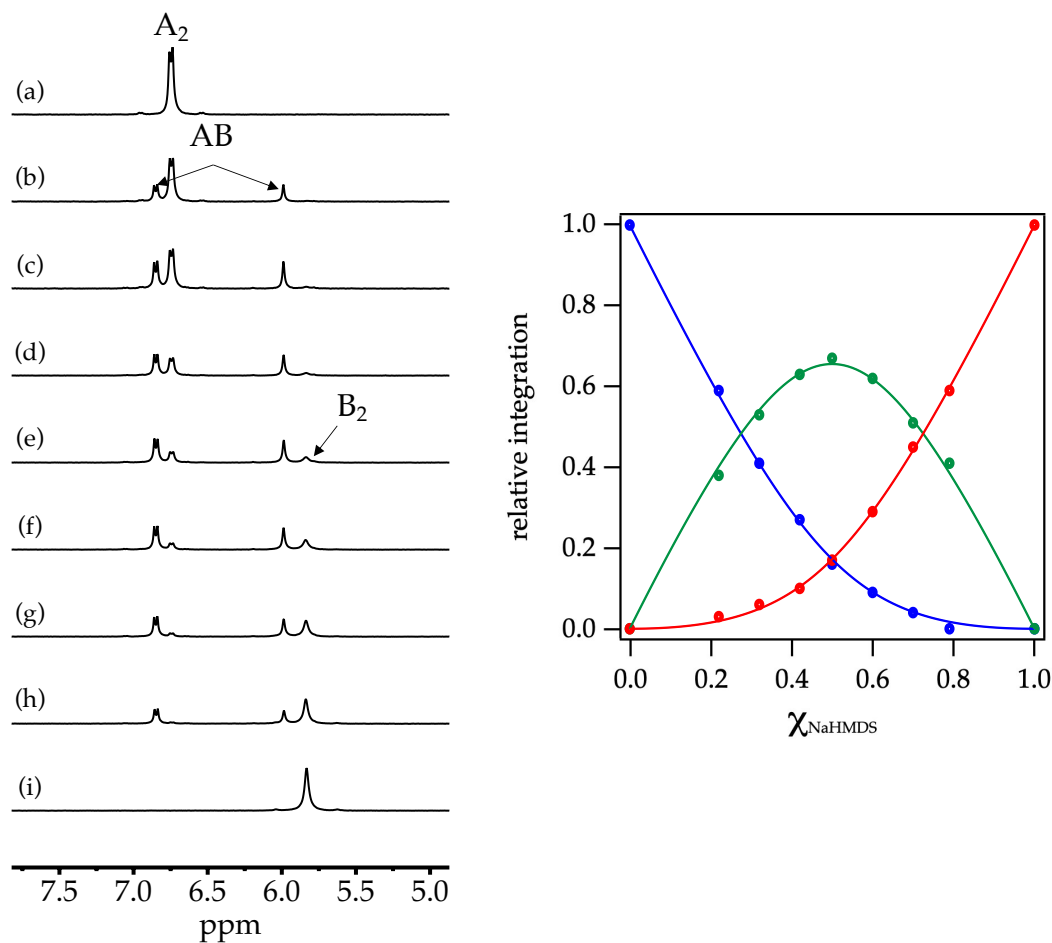
$^{15}\text{N}$  spectrum: 0.15 M  $^{15}\text{N}$ NaHMDS with 2.75 M MTBE in DMEA cosolvent at  $-110^\circ\text{C}$ .  $^{15}\text{N}$  spectra are referenced to DMEA (25.7 ppm).



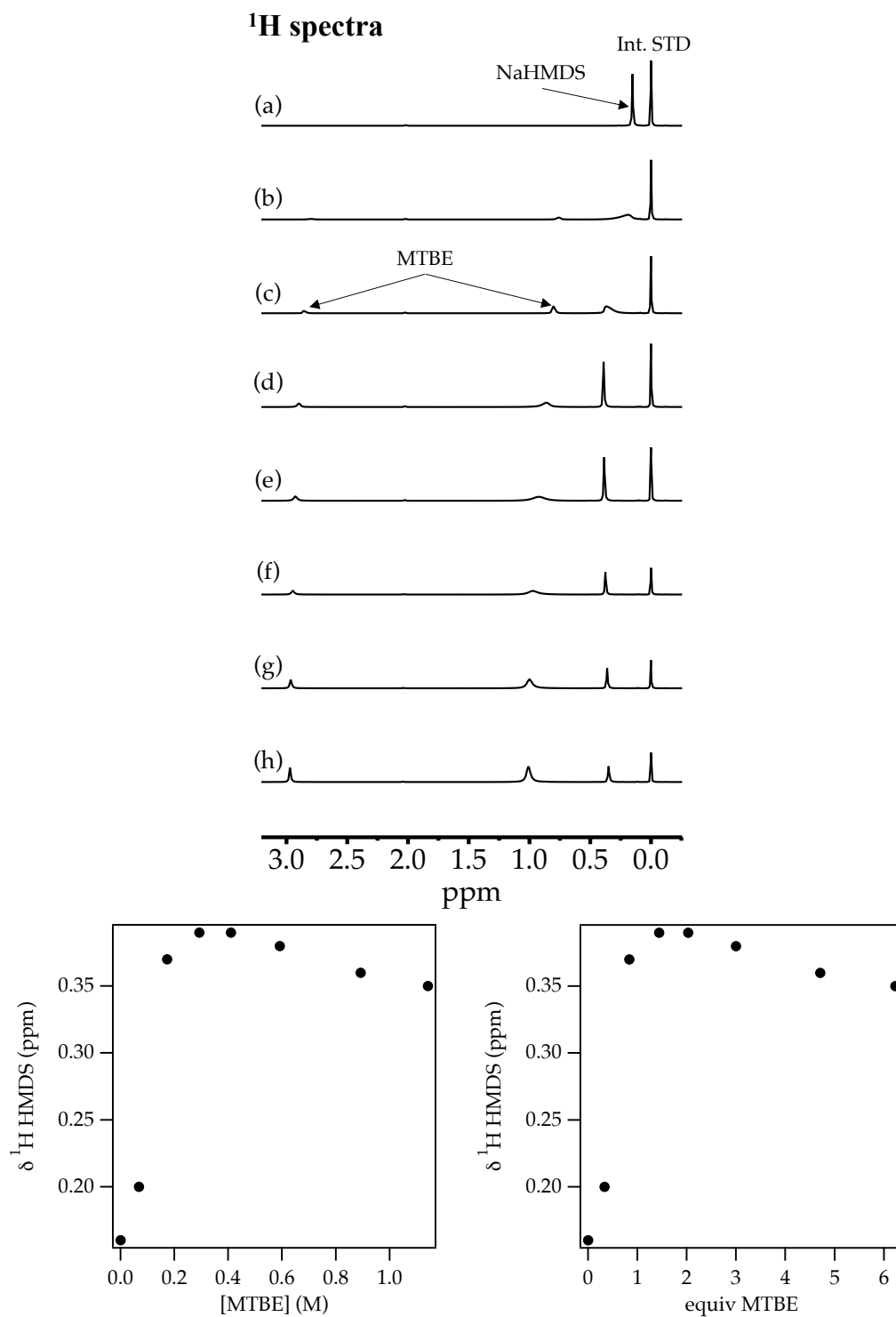
**Figure S27.**  $^1\text{H}$  and  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra for 0.60 M solutions of NaHMDS in toluene with cyclopentane internal standard varying methyl *tert*-butyl ether concentration at 25 °C. The concentrations of methyl *tert*-butyl ether in (a)–(k) are 0.00, 0.02, 0.17, 0.26,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



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



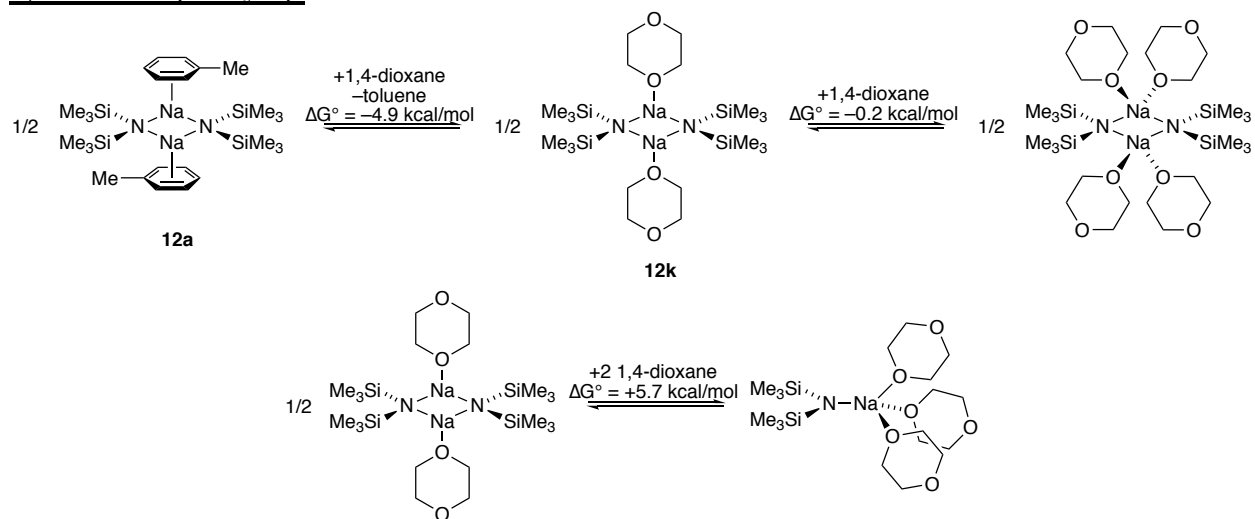
**Figure S28.**  $^{13}\text{C}$  NMR spectra and affiliated Job plot showing relative integrations of NaHMDS-derived homodimer (A<sub>2</sub>, red), NaTMDS-derived homodimer (B<sub>2</sub>, blue), and heterodimer (AB, green) versus the measured mole fraction of NaHMDS ( $\chi_{\text{NaHMDS}}$ ) at 0.30 total molarity in 5.50 M methyl tert-butyl ether in toluene cosolvent at  $-80\text{ }^\circ\text{C}$ . The measured mole fractions,  $\chi_{\text{NaHMDS}}$ , 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.**  $^1\text{H}$  NMR spectra for 0.20 M solutions of NaHMDS in toluene with TMS internal standard varying methyl *tert*-butyl ether concentration at  $-80\text{ }^\circ\text{C}$ . 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.

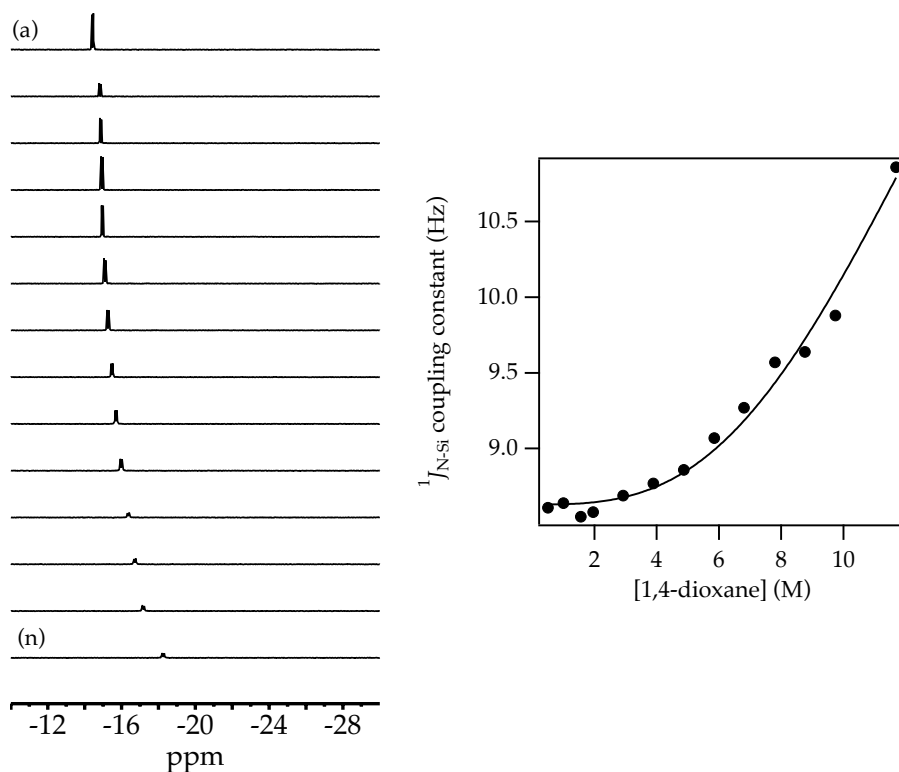


**1,4-dioxane (entry k):**



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

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

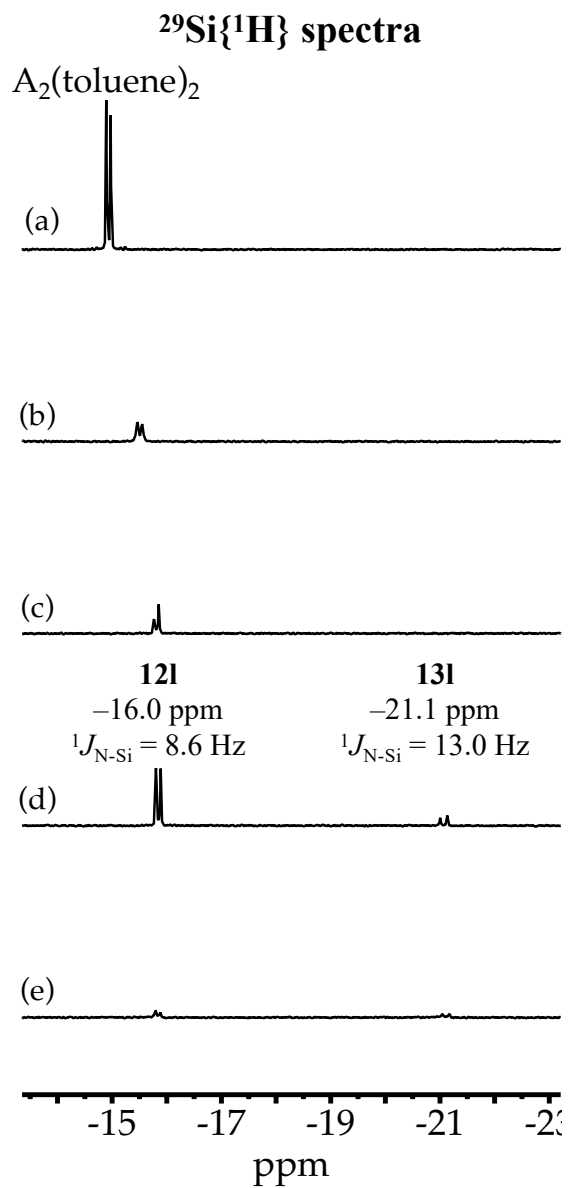


**Figure S31.**  $^{29}\text{Si}$  NMR spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of 1,4-dioxane at +20 °C. 1,4-Dioxane concentration for (a)–(n) are as follows: 0.50, 1.00, 1.56, 1.95, 2.92, 3.89, 4.87, 5.85, 6.80, 7.80, 8.76, 9.74, and 11.69, respectively. The curve is fit to the function described in the “Derivation” section of this Supporting Information on page S-117 with  $n = 3$ .

[1,4-dioxane] (M)	$^1J_{\text{N-Si}}$ 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

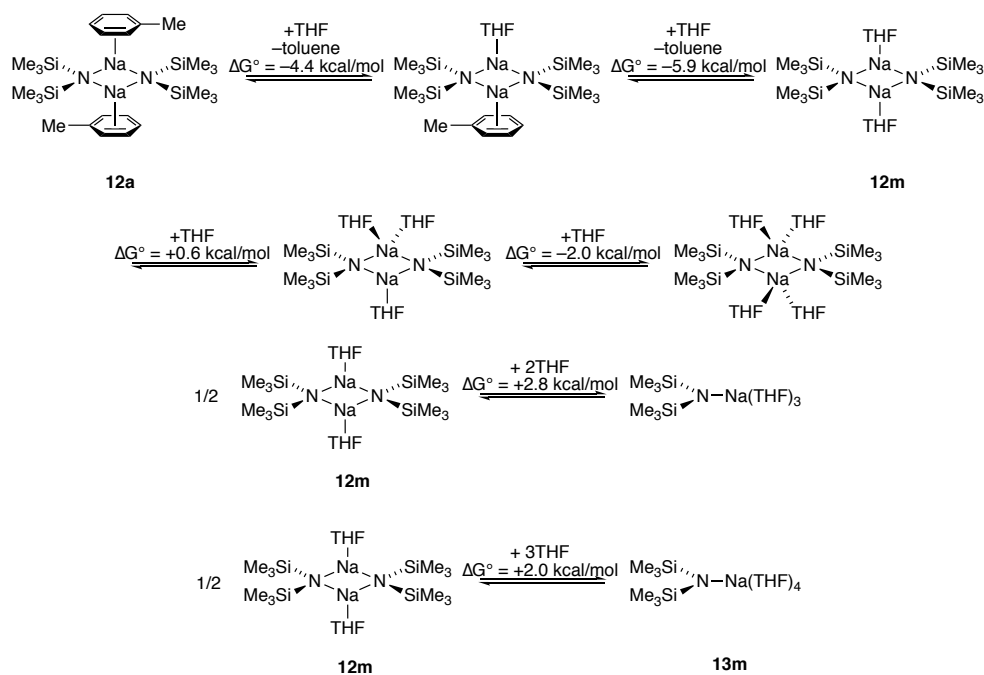
\* due to polymeric network at the bottom of the tube an accurate concentration was not obtained. 0.50 M and 1.00 M are idealized concentrations.

**1,3-dioxolane (entry I):**

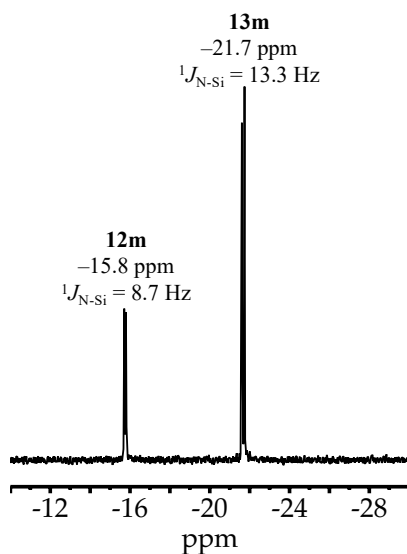


**Figure S32.**  $^{29}\text{Si}$  NMR spectra of 0.10 M  $[^{15}\text{N}]\text{NaHMDS}$  in 2:1 pentane/toluene cosolvent with varying amounts of 1,3-dioxolane added at  $-120^\circ\text{C}$ . The equivalents of dioxolane for (a)–(e) are as follows: 0.0, 0.5, 1.0, 3.0, and 5.0 equiv respectively. At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

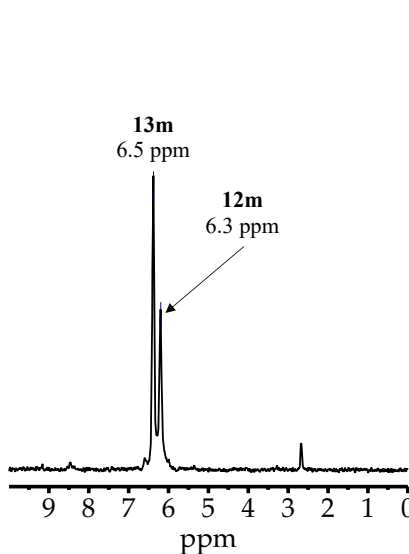
### Tetrahydrofuran (entry m):



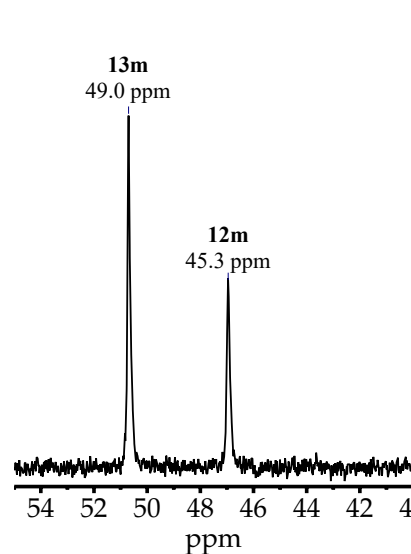
$^{29}\text{Si}\{^1\text{H}\}$  spectrum



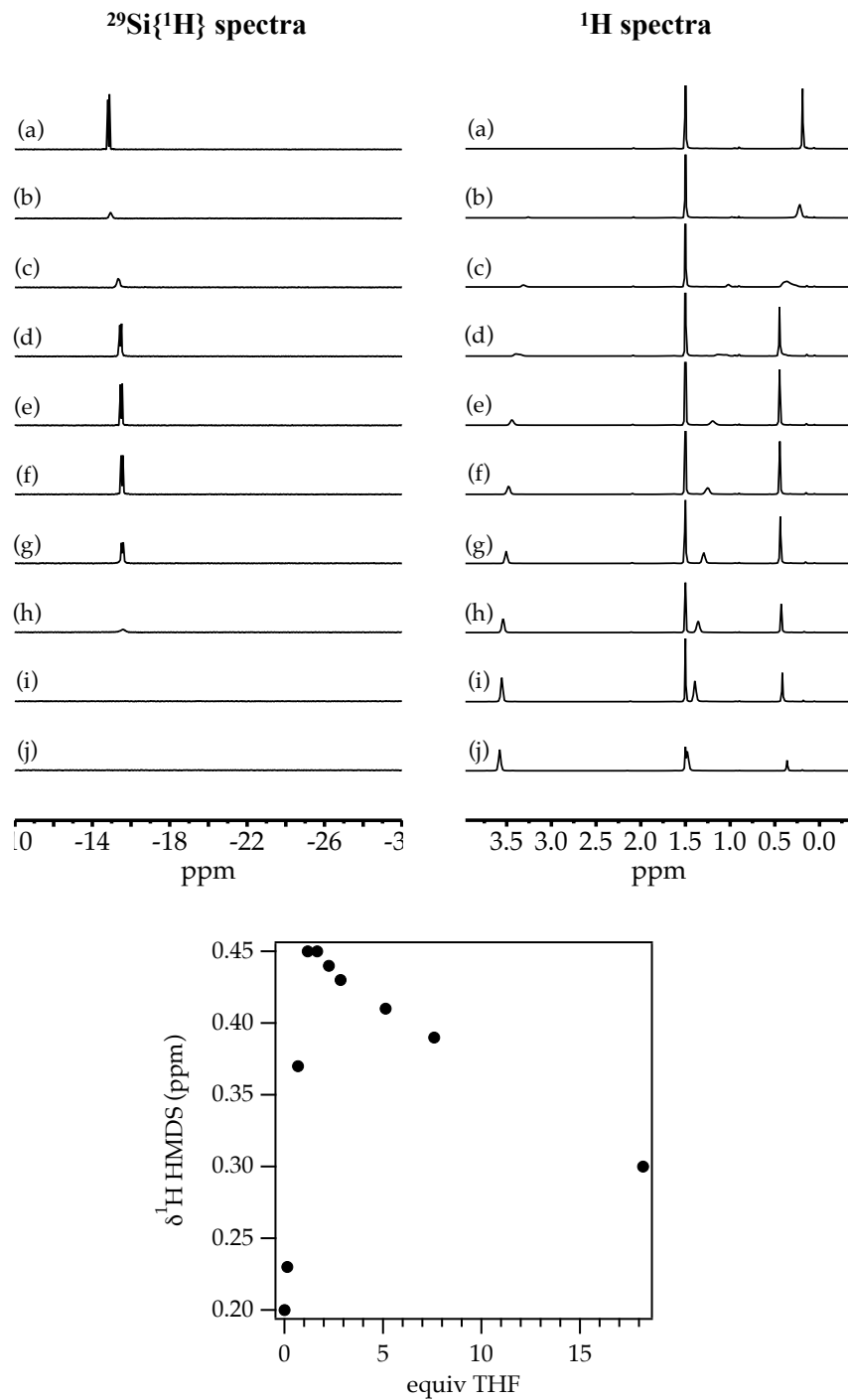
$^{13}\text{C}\{^1\text{H}\}$  spectrum



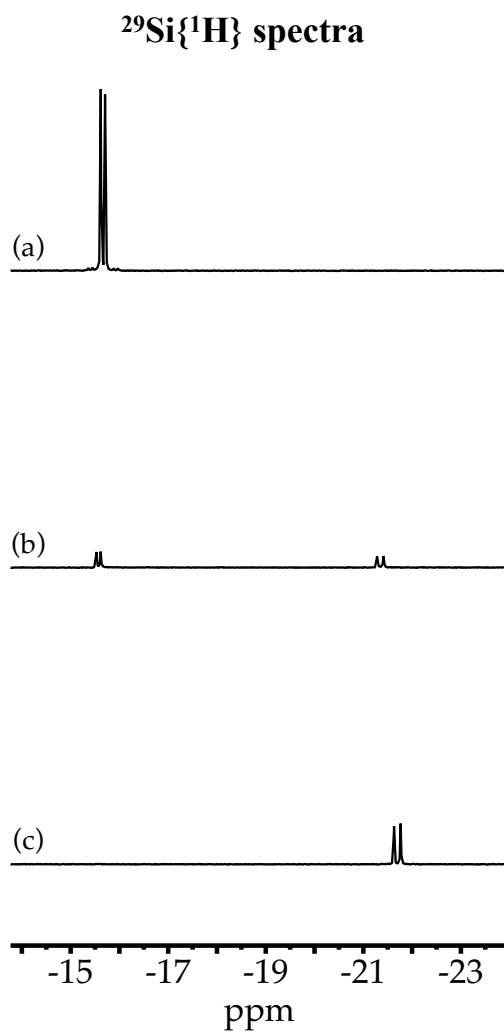
$^{15}\text{N}\{^1\text{H}\}$  spectrum



**Figure S33.** NMR spectra of 0.15 M  $^{15}\text{N}$ NaHMDS in 0.75 M THF with DMEA cosolvent at  $-120^\circ\text{C}$ .  $^{13}\text{C}$  spectra are referenced relative cyclopentane (26.05 ppm).  $^{15}\text{N}$  spectra are referenced to DMEA (25.7 ppm).

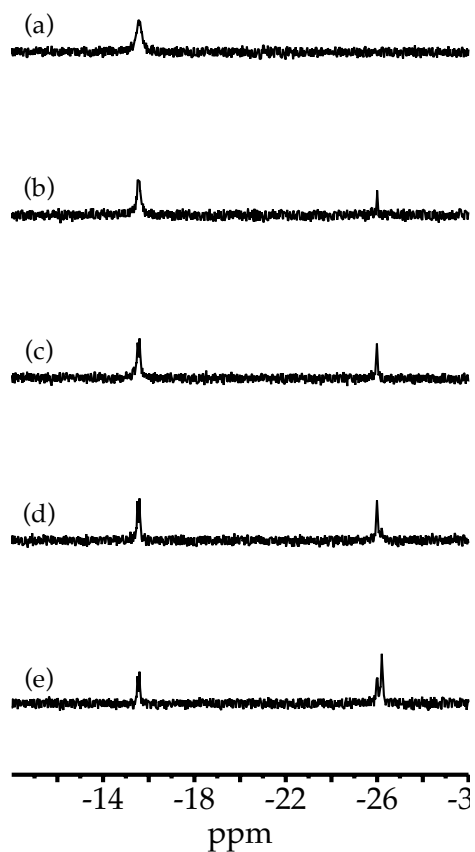


**Figure S34.**  $^1\text{H}$  and  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra for the titration of 0.23 M NaHMDS in toluene- $d_8$  with THF at  $-80\text{ }^\circ\text{C}$ . Equiv of THF for (a)–(j) are as follows: 0.0, 0.1, 0.7, 1.2, 1.7, 2.3, 2.8, 5.1, 7.6, and 18.2, respectively.  $^1\text{H}$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



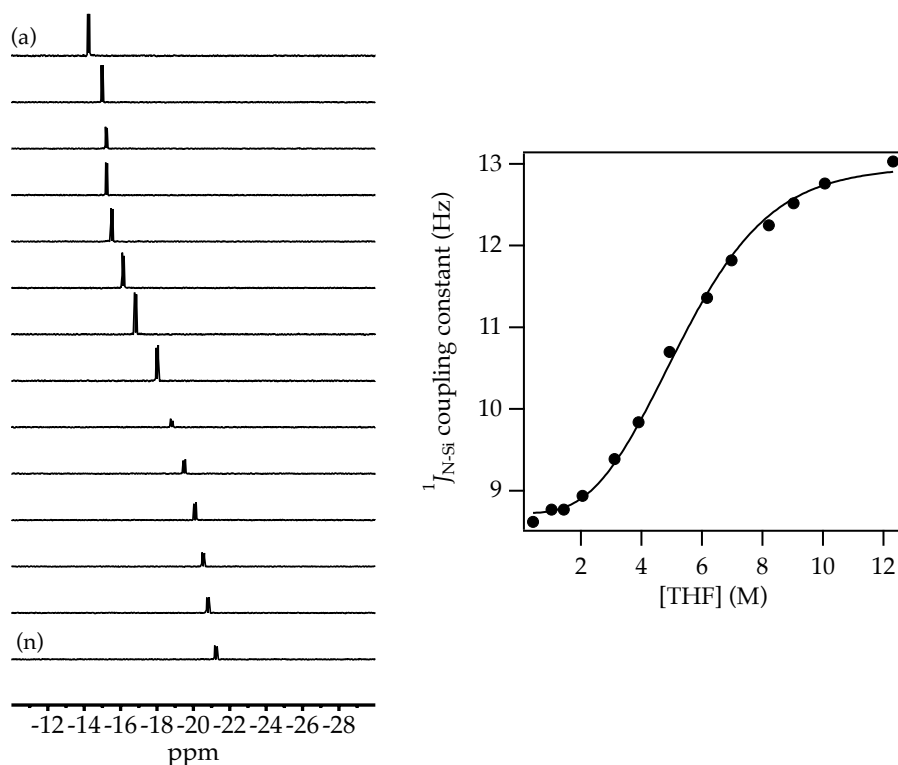
**Figure S35.**  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra for the titration of 0.15 M NaHMDS in DMEA with THF at  $-120\text{ }^\circ\text{C}$ . Equiv of THF for (a)–(c) are as follows: 0.0, 4.0, and 10.0, respectively.

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



**Figure S36.**  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra of NaHMDS-derived homodimer ( $A_2$ ), NaTMDS-derived homodimer ( $B_2$ ), and heterodimer ( $AB$ ) at 0.20 total molarity with 5.0 equiv THF in toluene cosolvent at  $-80\text{ }^\circ\text{C}$ . 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.

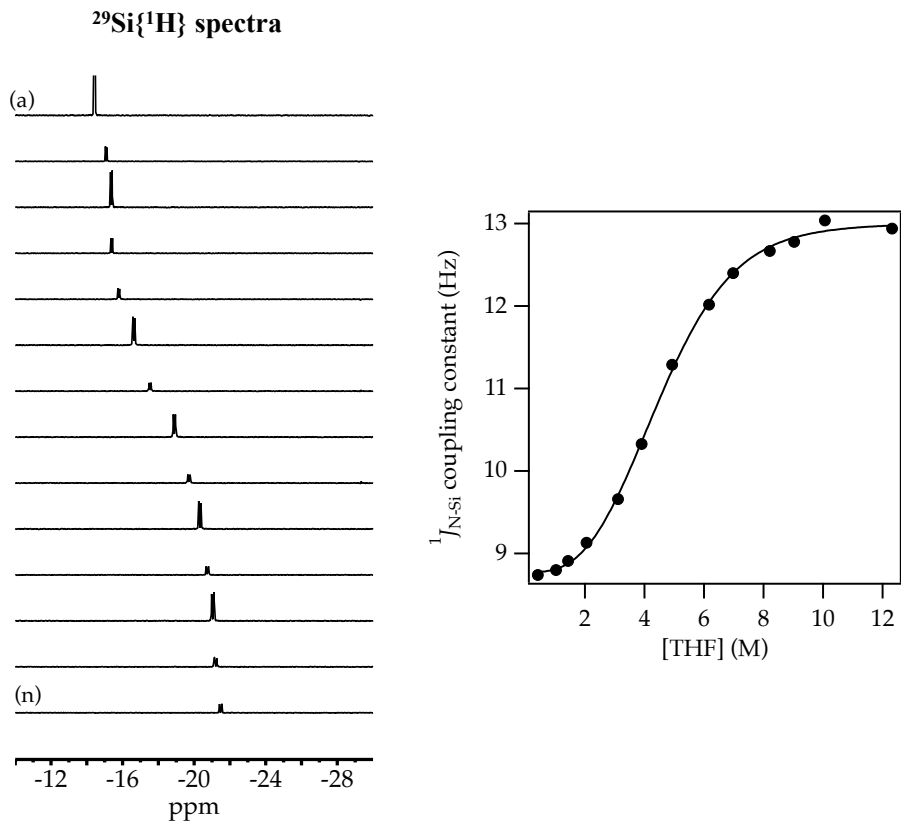
### $^{29}\text{Si}\{^1\text{H}\}$ spectra



**Figure S37.**  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of THF at +50 °C. THF concentration for (a)–(n) are as follows: 0.00, 0.41, 1.02, 1.43, 2.05, 3.10, 3.90, 4.92, 6.16, 6.97, 8.2, 9.02, 10.05, and 12.31, respectively. The curve is fit to the function described in the “Derivation” section of this Supporting Information on page S-117 with  $n = 3$ .

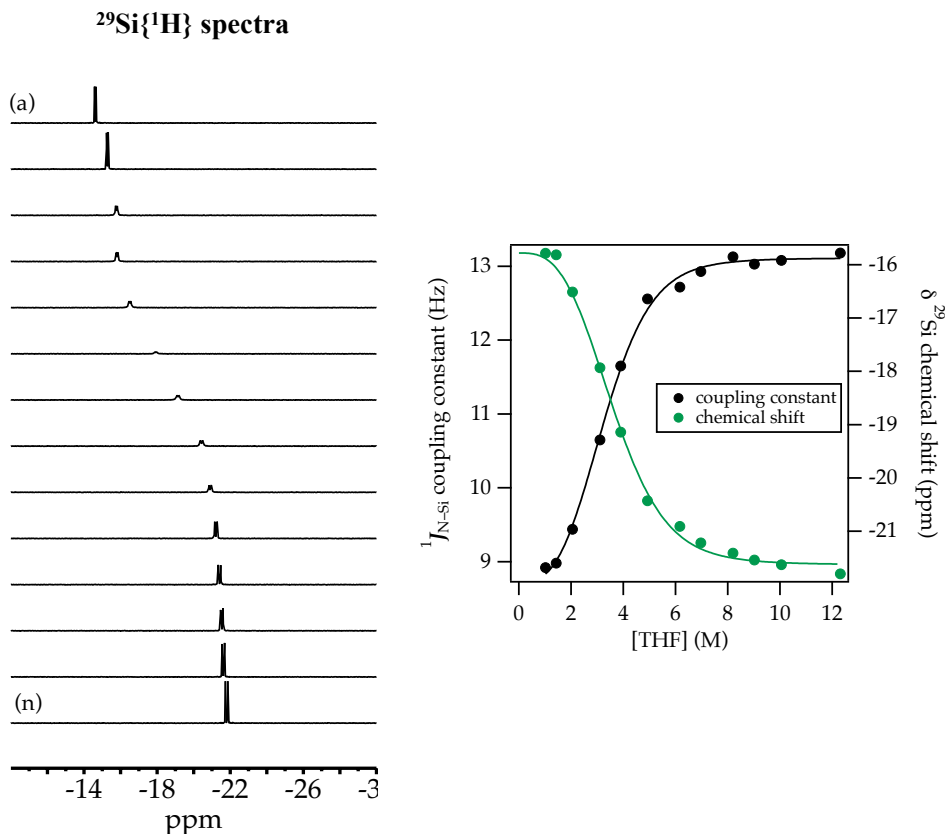
[THF] (M)	$^1J_{\text{N-Si}}$ coupling constant (Hz)
0.41	8.62
1.02	8.77
1.43	8.77
2.05	8.94
3.10	9.39
3.90	9.84
4.92	10.7
6.16	11.36
6.97	11.82
8.20	12.25
9.02	12.52
10.05	12.76
12.31	13.03





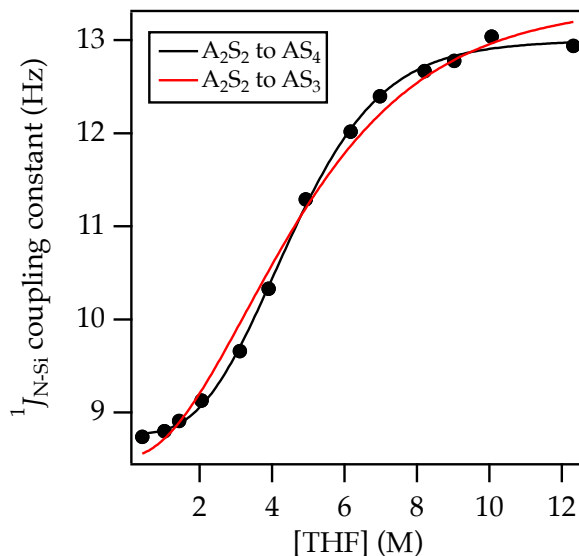
**Figure S38.**  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of THF at +20 °C. THF concentration for (a)–(n) are as follows: 0.00, 0.41, 1.02, 1.43, 2.05, 3.10, 3.90, 4.92, 6.16, 6.97, 8.2, 9.02, 10.05, and 12.31, respectively. The curve is fit to the function described in the “Derivation” section of this Supporting Information on page S-117 with  $n = 3$ .

[THF] (M)	$^1J_{\text{N-Si}}$ 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.**  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of THF at  $-20\text{ }^\circ\text{C}$ . 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  $n = 3$ .

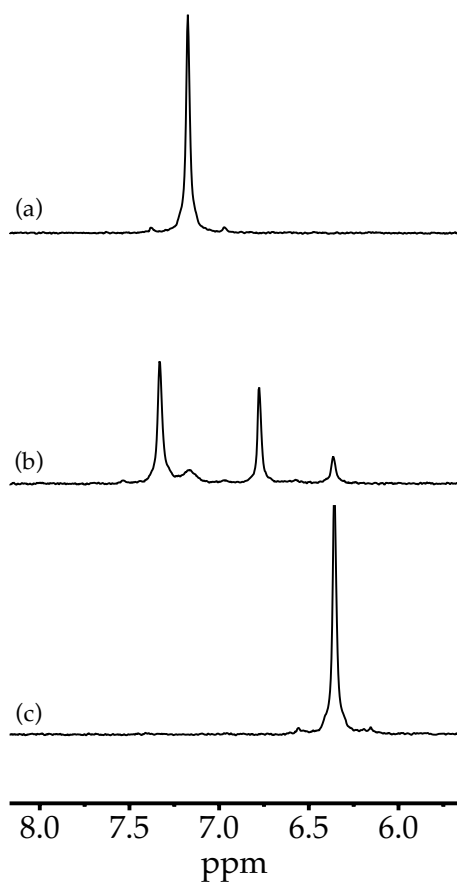
[THF] (M)	$^1J_{\text{N-Si}}$ coupling constant (Hz)	$^{29}\text{Si}$ chemical shift (ppm)
1.02	8.77	-15.78
1.43	8.91	-15.81
2.05	9.13	-16.51
3.10	9.66	-17.93
3.90	10.33	-19.14
4.92	11.29	-20.43
6.16	12.02	-20.91
6.97	12.4	-21.22
8.20	12.67	-21.41
9.02	12.78	-21.54
10.05	13.04	-21.63
12.31	12.94	-21.8



**Figure S40.**  $^{29}\text{Si}$  NMR spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of THF at +20 °C. THF concentration for (a)–(n) are as follows: 0.00, 0.41, 1.02, 1.43, 2.05, 3.10, 3.90, 4.92, 6.16, 6.97, 8.2, 9.02, 10.05, and 12.31, respectively. The difference in curvature for  $n = 2$  (red curve) versus  $n = 3$  (black curve) confirms monomer solvation with a superior fit to the data.

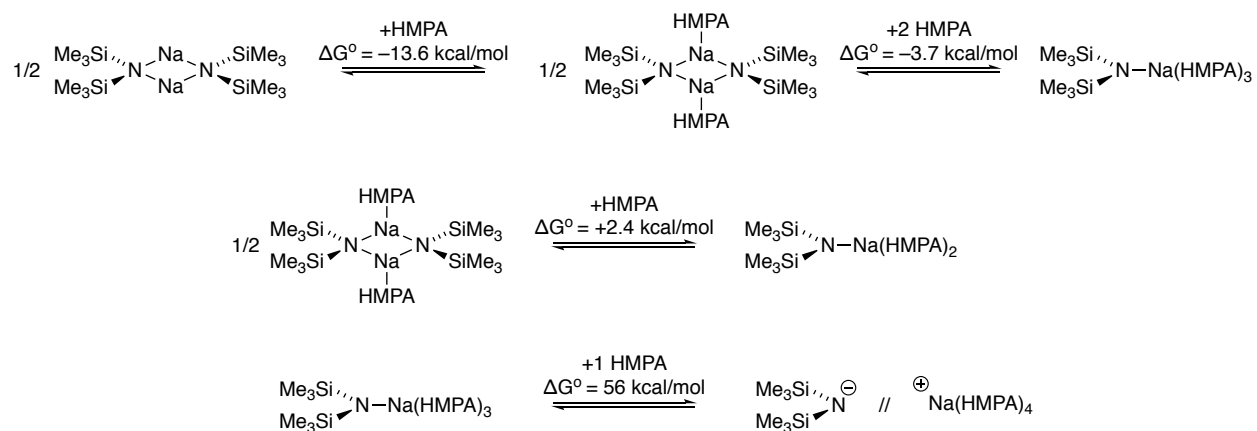
[THF] (M)	$^1J_{\text{N-Si}}$ coupling constant (Hz)
0.41	8.74
1.02	8.8
1.43	8.91
2.05	9.13
3.10	9.66
3.90	10.33
4.92	11.29
6.16	12.02
6.97	12.4
8.20	12.67
9.02	12.78
10.05	13.04
12.31	12.94

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

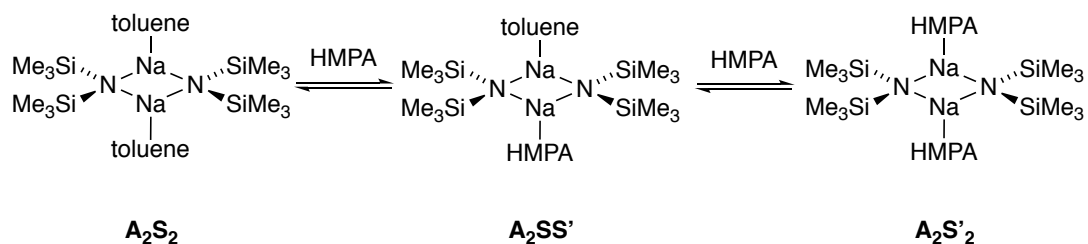


**Figure S41.**  $^{13}\text{C}$  NMR spectra of with mixing NaHMDS and NaTMDS at 0.20 total molarity in 0.85 M THF in toluene- $d_8$  cosolvent at  $-80\text{ }^\circ\text{C}$ . The measured mole fractions,  $X_{\text{NaHMDS}}$ , in (a)–(c) are 1.00, 0.50, and 0.00, respectively.  $^{13}\text{C}$  spectra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

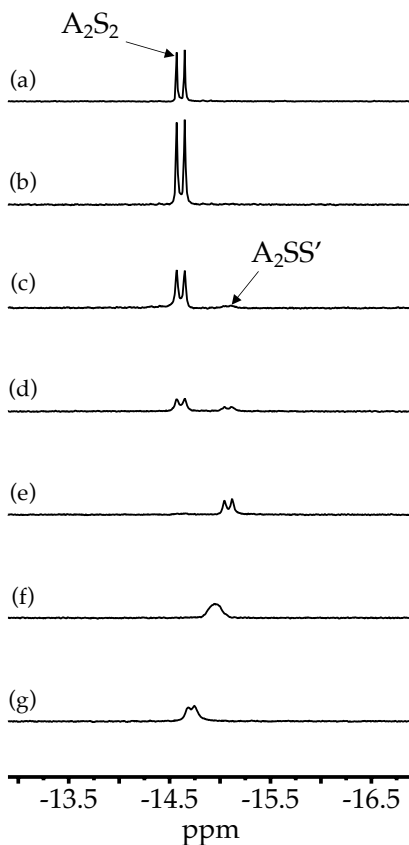
**HMPA (entry n):**



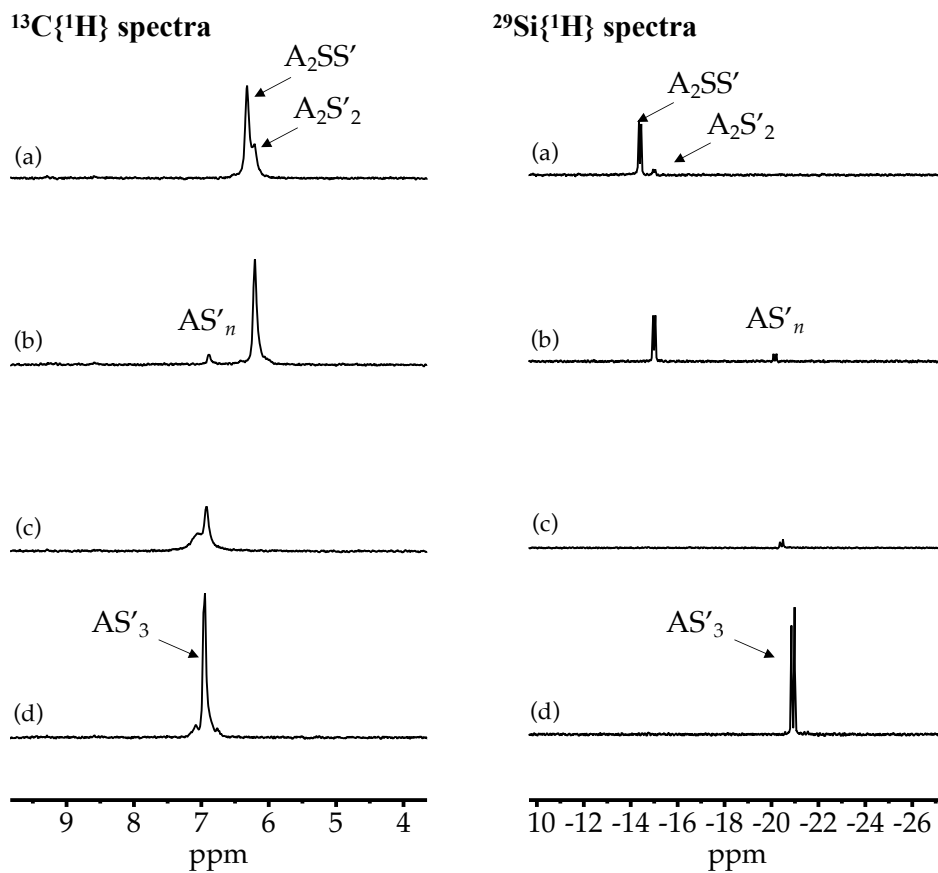
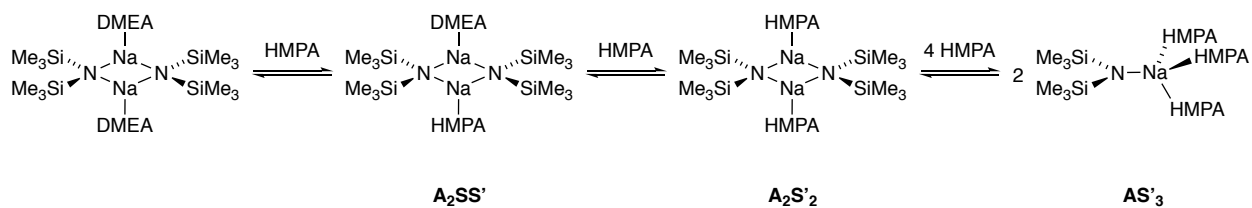
**Figure S42.** Computed free energies for the serial solvation of NaHMDS with HMPA.



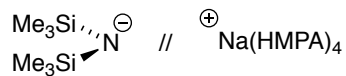
$^{29}\text{Si}\{^1\text{H}\}$  spectra



**Figure S43.**  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra for the titration of 0.10 M NaHMDS in toluene- $d_8$  with HMPA at  $-80^\circ\text{C}$ . 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).  $^{29}\text{Si}$  spectra are referenced to trace HMDS present in tube (2.00 ppm).

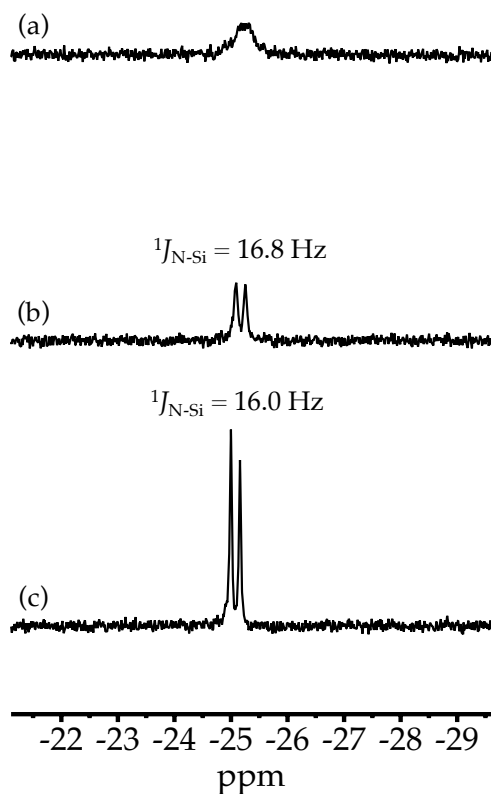


**Figure S44.**  $^{13}\text{C}\{^1\text{H}\}$  and  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra for the titration of 0.10 M NaHMDS in DMEA with HMPA at  $-120^\circ\text{C}$ . Equiv of HMPA for (a)–(d) are as follows: 0.6, 1.2, 3.0, and 5.0, respectively. The changing signal intensity from (c) to (d)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



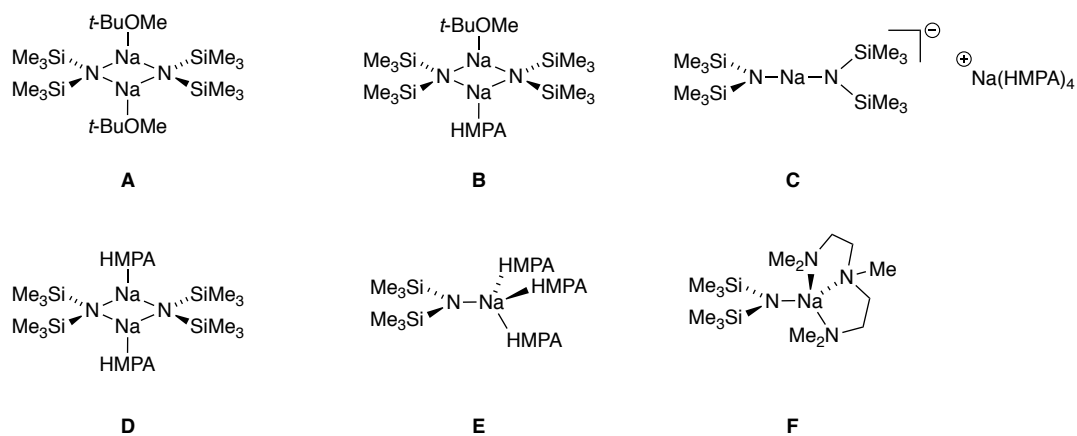
ion pair

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

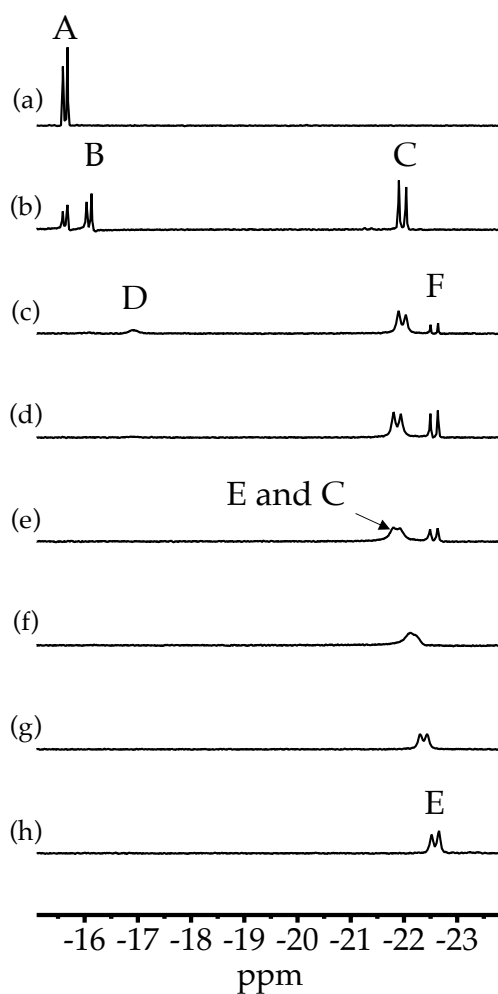


**Figure S45.**  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra of 0.10 M NaHMDS in 2:1 HMPA:MTBE at various temperatures. Temperatures for (a)–(c) are as follows: 0 °C, 25 °C, and 40 °C, respectively. The large coupling constants in (b) and (c) suggest an ion pair.  $^{29}\text{Si}$  spectra are referenced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

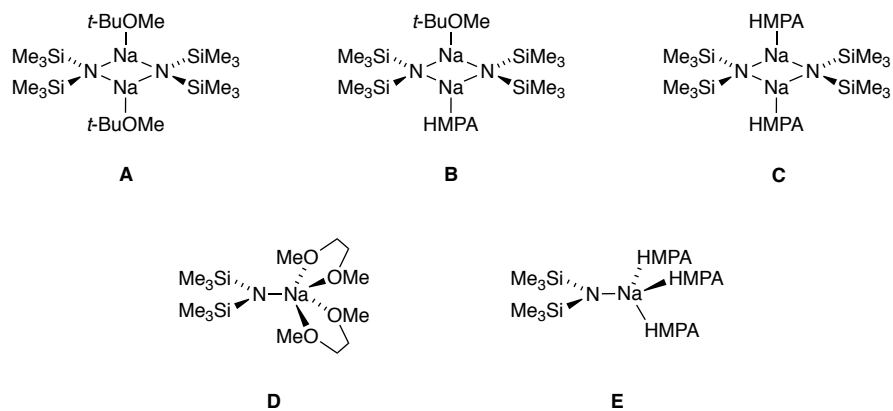




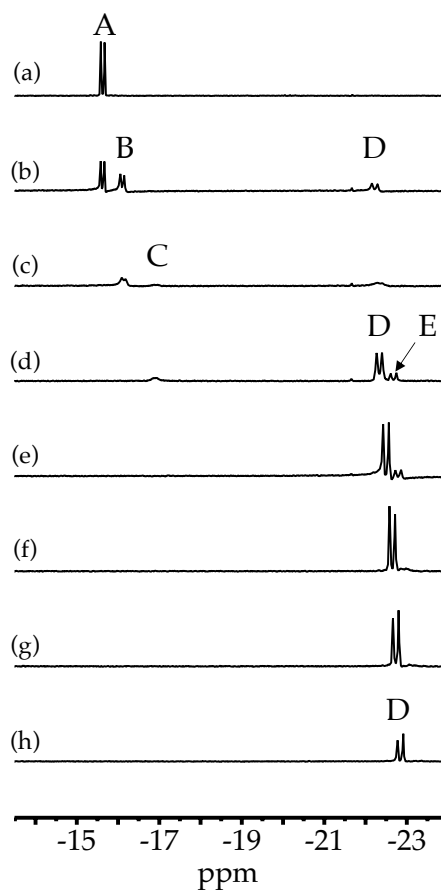
**$^{29}\text{Si}\{^1\text{H}\}$  spectra**



**Figure S46.**  $^{29}\text{Si}$  NMR spectra of 0.20 M  $[\text{}^{15}\text{N}]\text{NaHMDS}$  in MTBE at  $-110\text{ }^\circ\text{C}$  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.  $^{29}\text{Si}$  spectra are referenced to TMS internal standard (0.00 ppm).

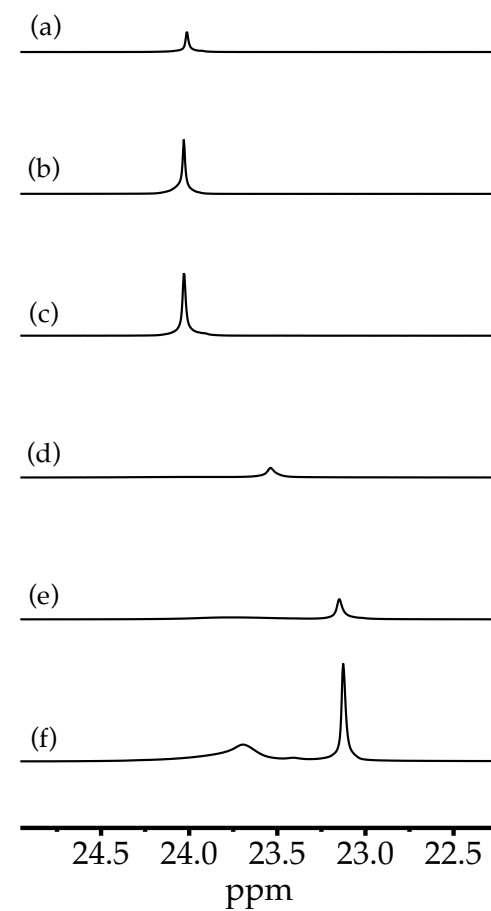


**$^{29}\text{Si}\{^1\text{H}\}$  spectra**



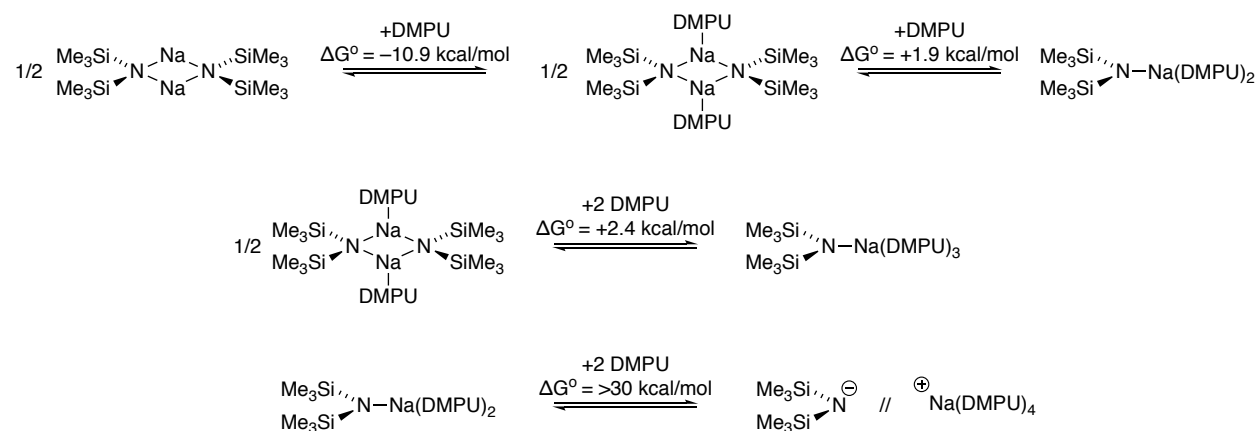
**Figure S47.**  $^{29}\text{Si}$  NMR spectra of 0.20 M  $[^{15}\text{N}]\text{NaHMDS}$  in MTBE at  $-110\text{ }^\circ\text{C}$  with incremental additions of 1:1 DME/HMPA. The equiv of total added ligand for (a) to (h) are as follows: 0.0, 0.5, 1.0, 2.0, 3.0, 4.0, 5.0, and 7.0, respectively.  $^{29}\text{Si}$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

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

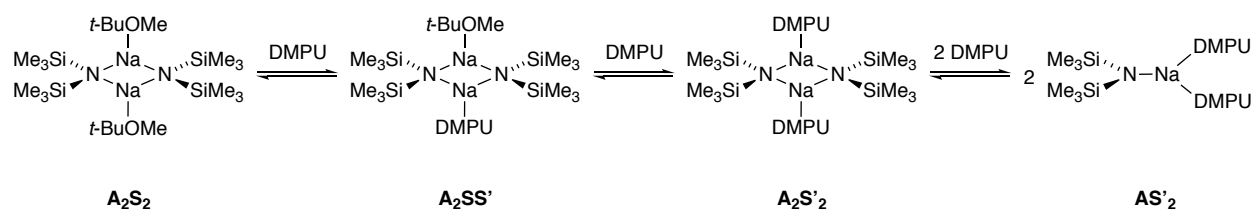


**Figure S48.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectra of 0.20 M  $[^{15}\text{N}]\text{NaHMDS}$  in 2:1 pentane/toluene with various quantities of HMPA at  $-80\text{ }^\circ\text{C}$ . The equiv of HMPA for (a) to (f) are as follows: 0.3, 0.5, 0.8, 1.0, 2.0, 3.0, and 5.0 respectively.

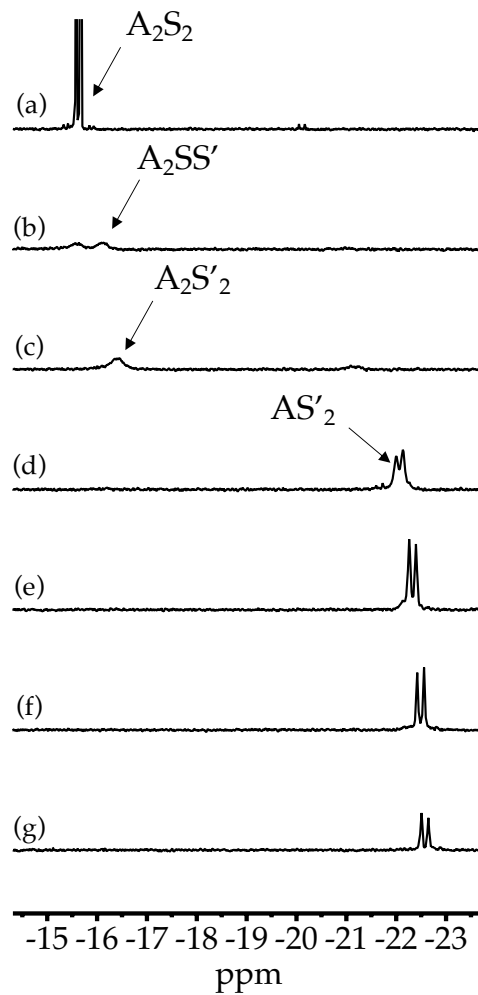
**DMPU (entry o):**



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

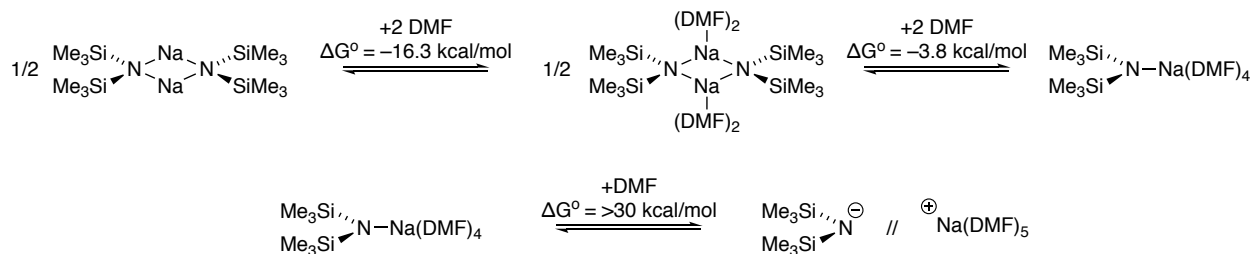


### $^{29}\text{Si}\{^1\text{H}\}$ spectra

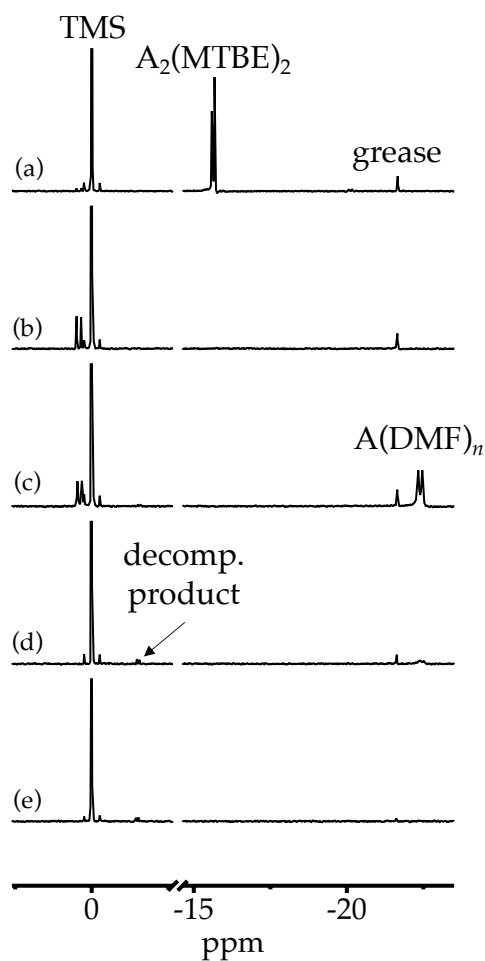


**Figure S50**  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra for the titration of 0.20 M NaHMDS in MTBE with DMPU at  $-110\text{ }^\circ\text{C}$ . Equiv of DMPU for (a)–(g) are as follows: 0.0, 0.5, 1.0, 2.0, 3.0, 5.0 and 7.0, respectively.  $^{29}\text{Si}$  spectra are referenced to TMS internal standard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

**DMF (entry p):**

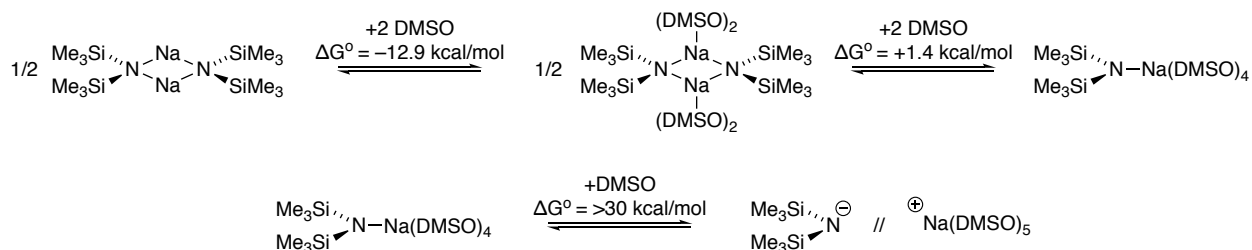


**$^{29}\text{Si}\{^1\text{H}\}$  spectra**

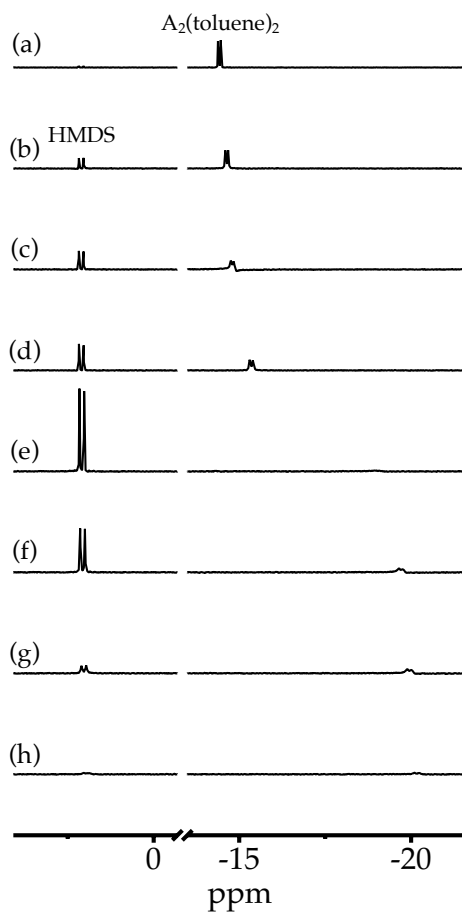


**Figure S51.**  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra for the titration of 0.20 M NaHMDS in MTBE with DMF at  $-110^\circ\text{C}$ . Equiv of DMF for (a)–(e) are as follows: 0.0, 1.0, 2.0, 4.0, and 7.0, respectively.  $^{29}\text{Si}$  spectra are referenced to TMS internal standard (0.00 ppm).

### DMSO (entry q):

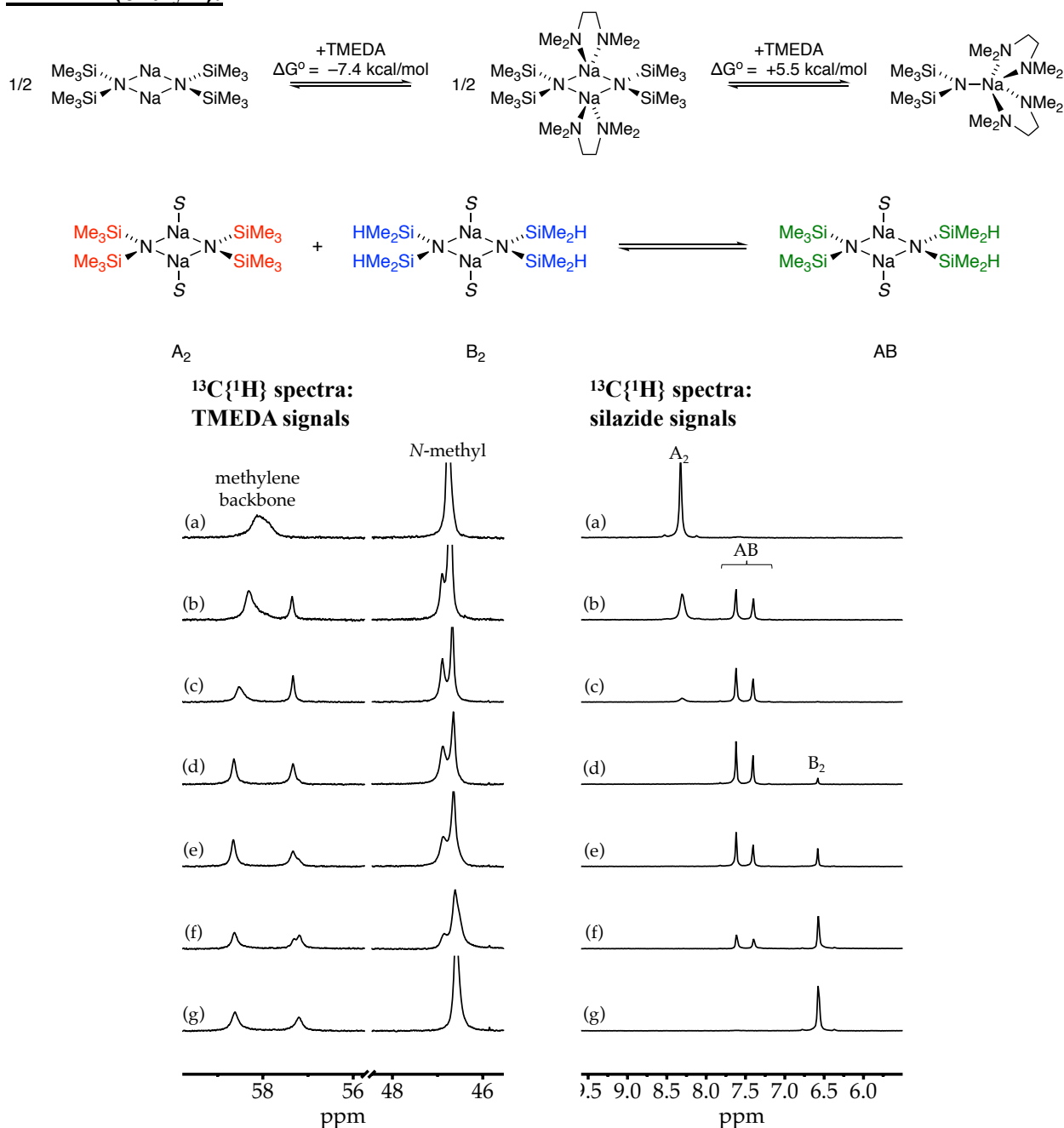


### $^{29}\text{Si}\{^1\text{H}\}$ spectra



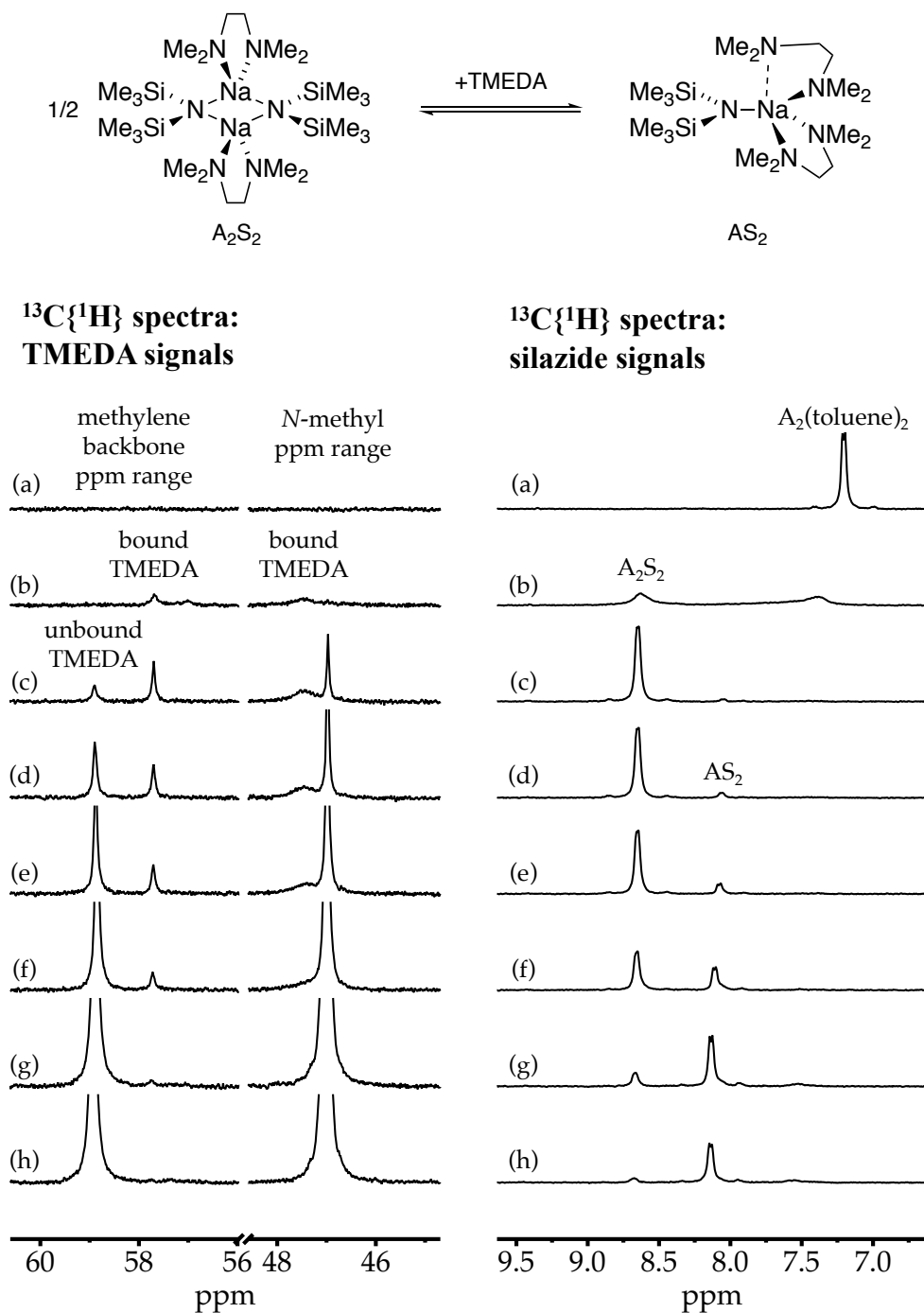
**Figure S52.**  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra for the titration of 0.10 M NaHMDS in toluene with DMSO at  $-80^\circ\text{C}$ . Equiv of DMSO for (a)–(h) are as follows: 0.0, 0.2, 0.4, 0.8, 0.9, 1.3, 2.0, and 3.0, respectively. The increasing intensity of the HMDS signal is most likely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

### TMEDA (entry r):



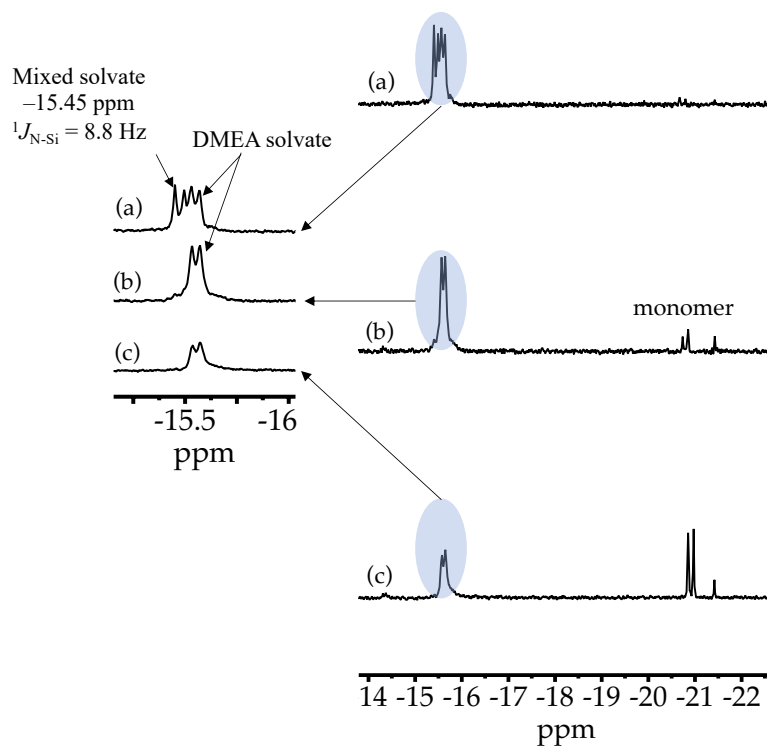
**Figure S53.**  $^{13}\text{C}$  NMR relative integrations of NaHMDS-derived homodimer ( $\text{A}_2$ ), NaTMS-derived homodimer ( $\text{B}_2$ ), and heterodimer ( $\text{AB}$ ) versus the measured mole fraction of NaHMDS ( $X_{\text{NaHMDS}}$ ) at 0.30 total molarity in 0.60 M TMEDA in toluene cosolvent at  $-100^\circ\text{C}$ . The measured mole fractions,  $X_{\text{NaHMDS}}$ , 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  $\text{AB}$  and NaTMS homodimer  $\text{B}_2$  as evident in the 2 methylene signals. Integration of the more upfield methylene signal results in a 1:1 ratio of for both heterodimer  $\text{AB}$  and NaTMS homodimer  $\text{B}_2$ .  $^{13}\text{C}$  spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).



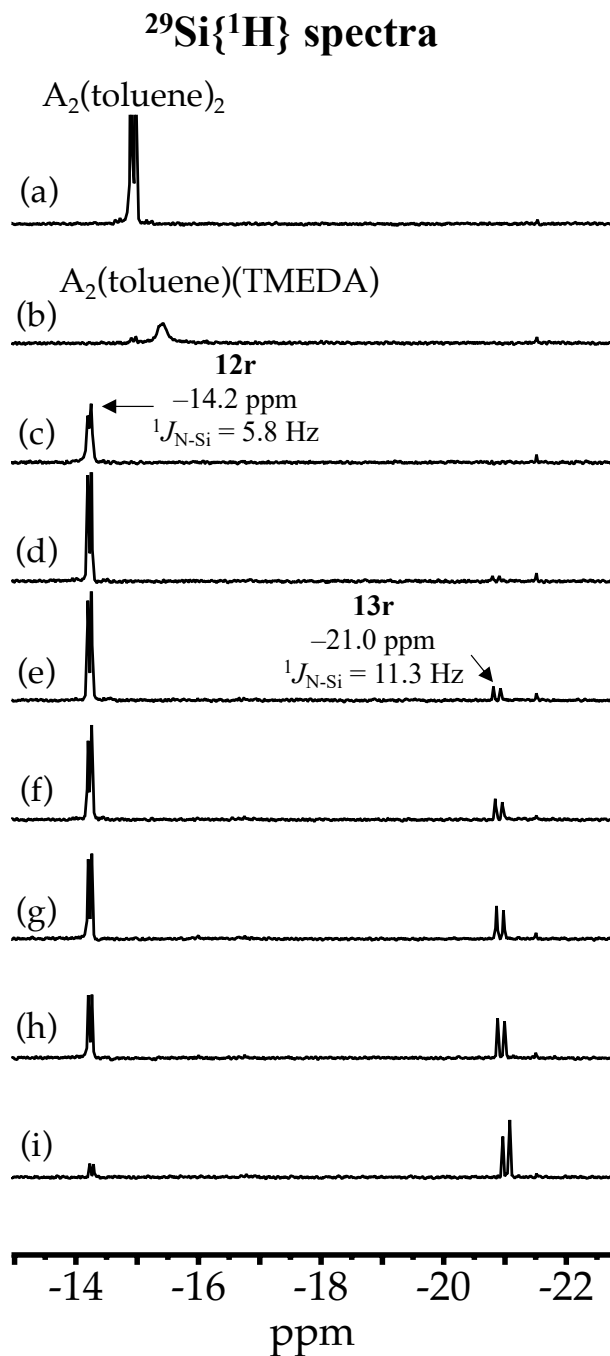


**Figure S54.** <sup>13</sup>C{<sup>1</sup>H} NMR spectra of 0.12 M [<sup>15</sup>N]NaHMDS in 2:1 pentane/toluene-*d*<sub>8</sub> cosolvent with varying amounts of TMEDA added at -120 °C. The equivalents of TMEDA for (a)–(h) are as follows: 0.00, 0.68, 0.89, 1.26, 2.04, 4.00, 7.18, 8.76, and 14.59 equiv, respectively. <sup>13</sup>C spectra are referenced relative the toluene ipso-carbon chemical shift (137.86 ppm).

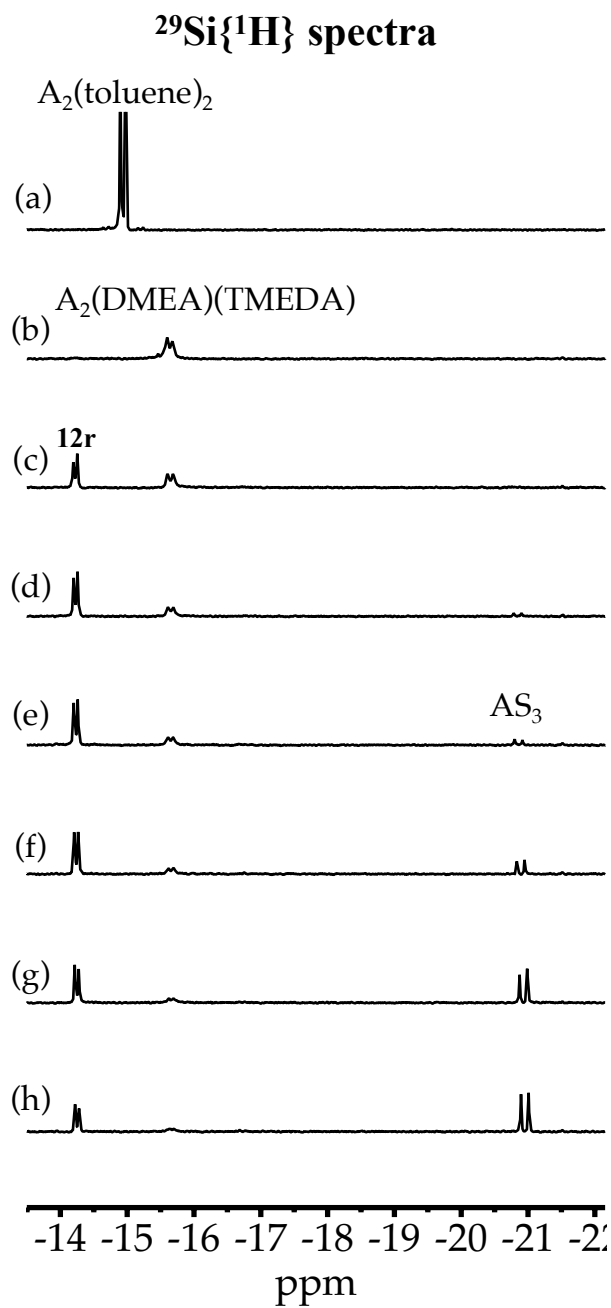
### $^{29}\text{Si}\{^1\text{H}\}$ spectra



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

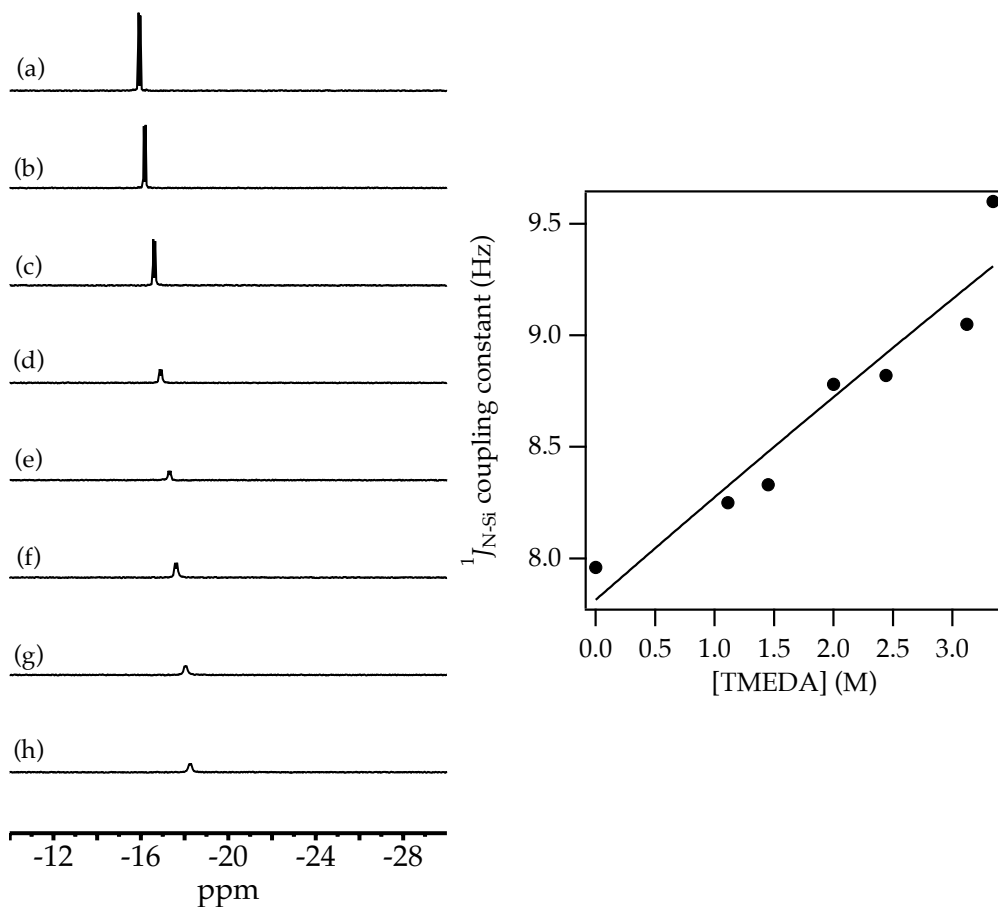


**Figure S56.**  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra of 0.10 M  $[\text{}^{15}\text{N}]\text{NaHMDS}$  in 2:1 pentane/toluene- $d_8$  cosolvent with varying amounts of TMEDA added at  $-120^\circ\text{C}$ . The equivalents of TMEDA for (a)–(i) are as follows: 0.00, 0.5, 1.0, 1.5, 2.0, 3.0, 4.0,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



**Figure S57**  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra of 0.10 M  $[^{15}\text{N}]\text{NaHMDS}$  in 2:1 pentane/toluene at  $-120\text{ }^\circ\text{C}$  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.

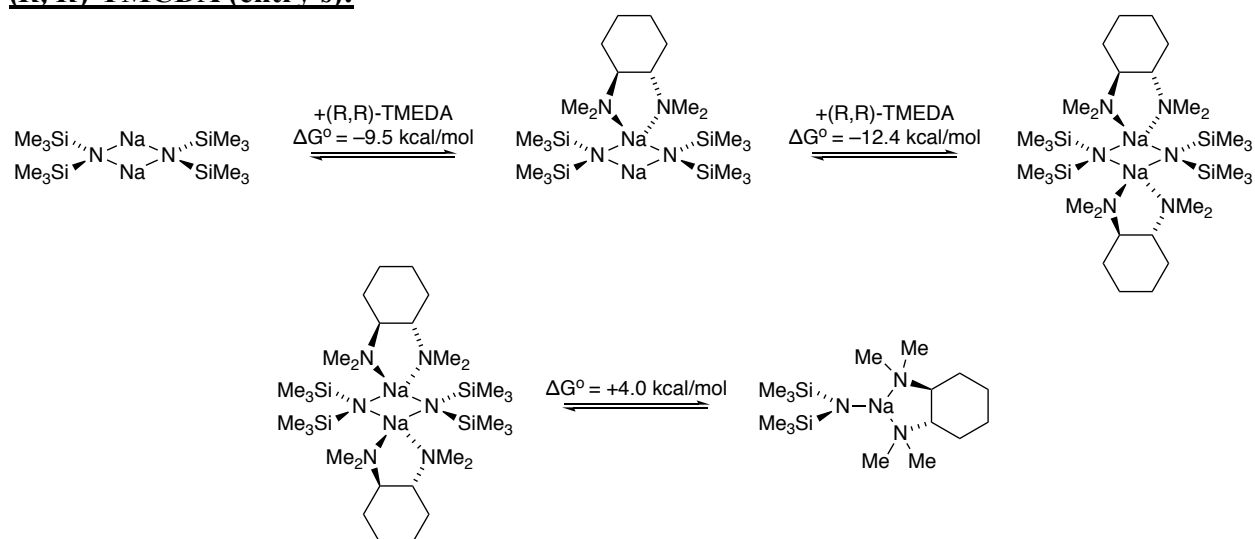
### $^{29}\text{Si}\{^1\text{H}\}$ spectra



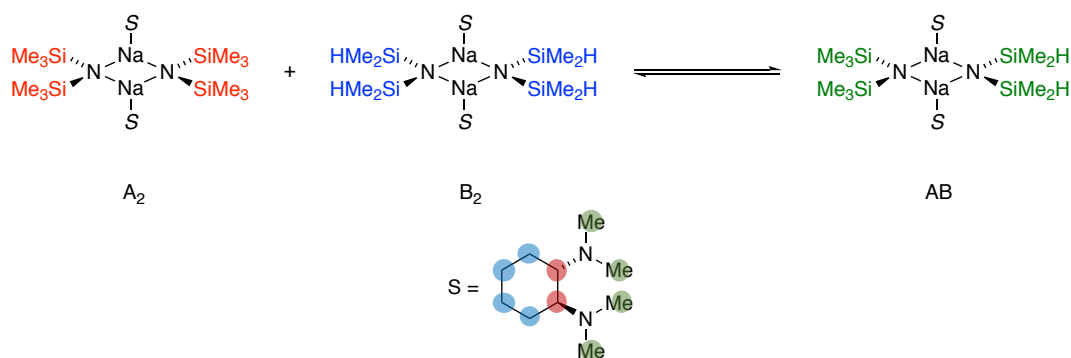
**Figure S58.**  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of TMEDA at  $-20\text{ }^\circ\text{C}$ . TMEDA concentration for (a)–(h) are as follows: 0.00, 1.11, 1.45, 2.00, 2.44, 3.12, and 3.34, respectively. The curve is fit to the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

[TMEDA] (M)	$^1J_{\text{N-Si}}$ 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):**

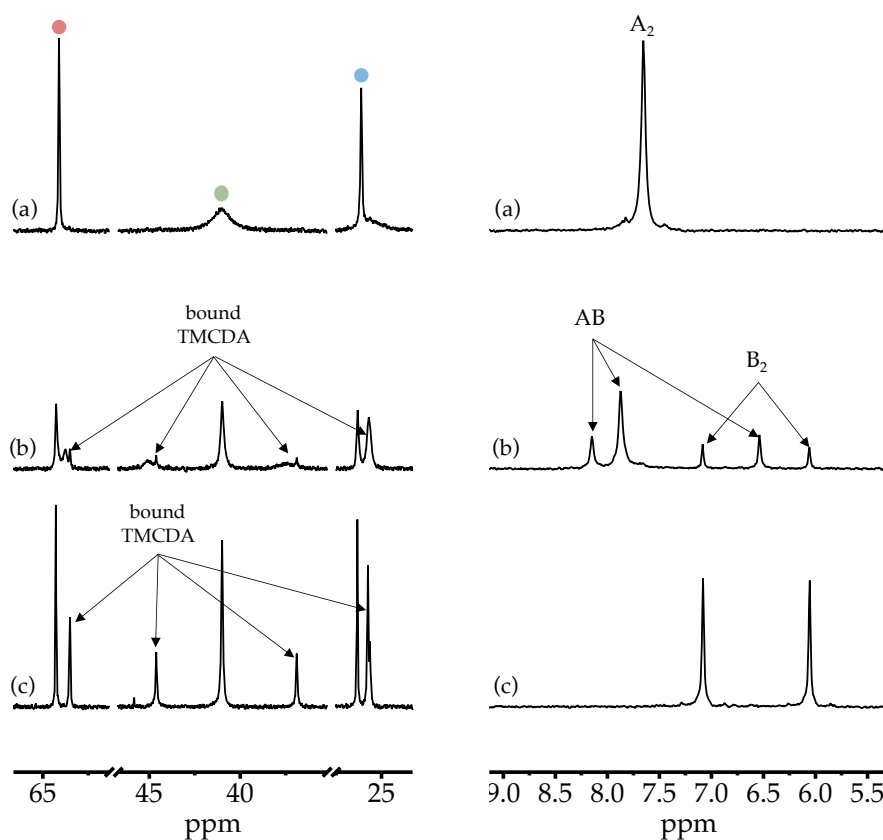


**Figure S59.** Computed free energies for the serial solvation of NaHMDS with TMCDA.



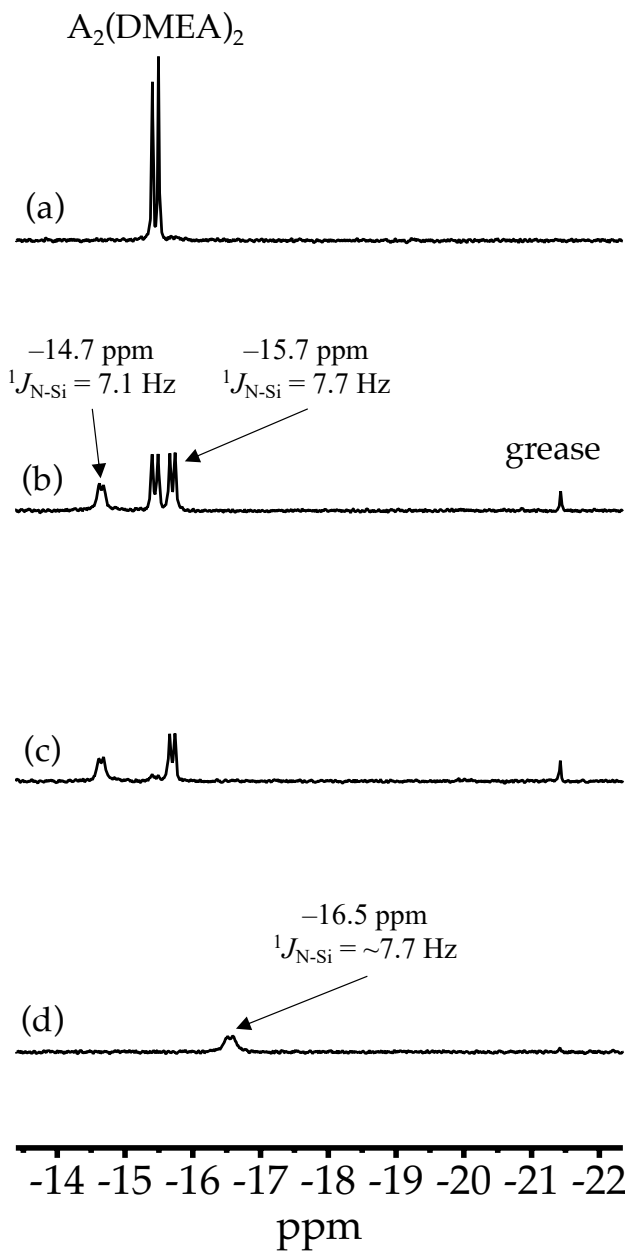
$^{13}\text{C}\{^1\text{H}\}$  spectra:  
TMCDA signals

$^{13}\text{C}\{^1\text{H}\}$  spectra:  
silazide signals



**Figure S60.**  $^{13}\text{C}$  NMR relative integrations of NaHMDS-derived homodimer ( $\text{A}_2$ ), NaTMS-derived homodimer ( $\text{B}_2$ ), and heterodimer ( $\text{AB}$ ) versus the measured mole fraction of NaHMDS ( $X_{\text{NaHMDS}}$ ) at 0.20 total molarity in 0.40 M (*R,R*)-TMCDA in toluene- $d_8$  cosolvent at  $-80^\circ\text{C}$ . The measured mole fractions,  $X_{\text{NaHMDS}}$ , in (a)–(c) are 1.00, 0.50, and 0.00, respectively. Free and bound TMCDA is observable for both heterodimer  $\text{AB}$  and NaTMS homodimer  $\text{B}_2$  as evident in the methylene and methyl signals noted above (methylene = red and blue; methyl = green). Integration of these signals for the NaTMS homodimer shows a 1:1 ratio of silazide to TMCDA.

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

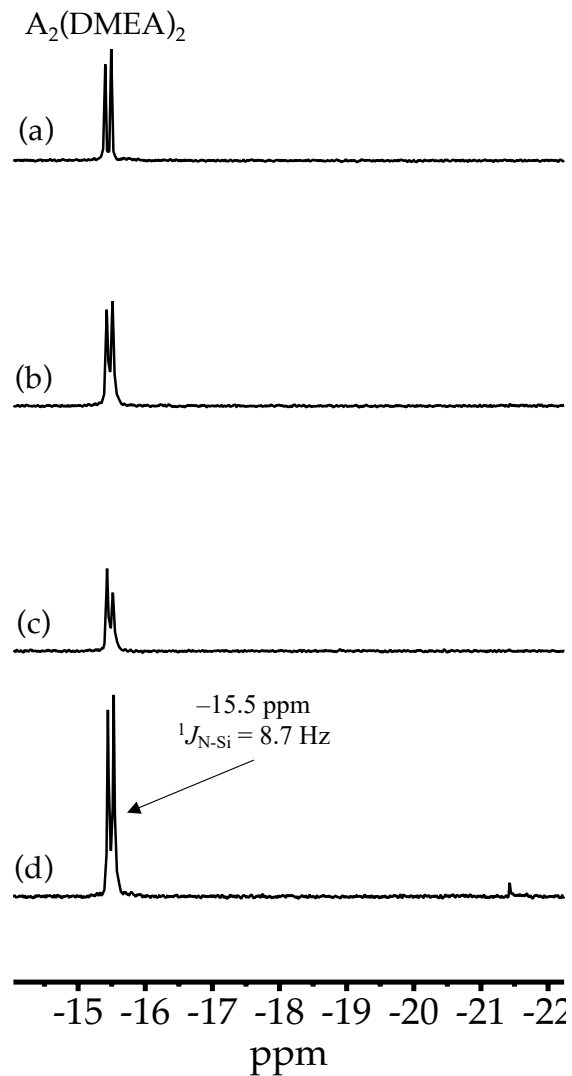


**Figure S61.**  $^{29}\text{Si}$  NMR spectra of 0.15 M  $^{15}\text{N}$ NaHMDS in DMEA cosolvent with varying amounts of TMCDA added at  $-120^\circ\text{C}$ . The equivalents of TMCDA for (a)–(c) are as follows: 0.0, 0.5, and 3.0 equiv, respectively. Spectrum (d) consists of 0.15 M  $^{15}\text{N}$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



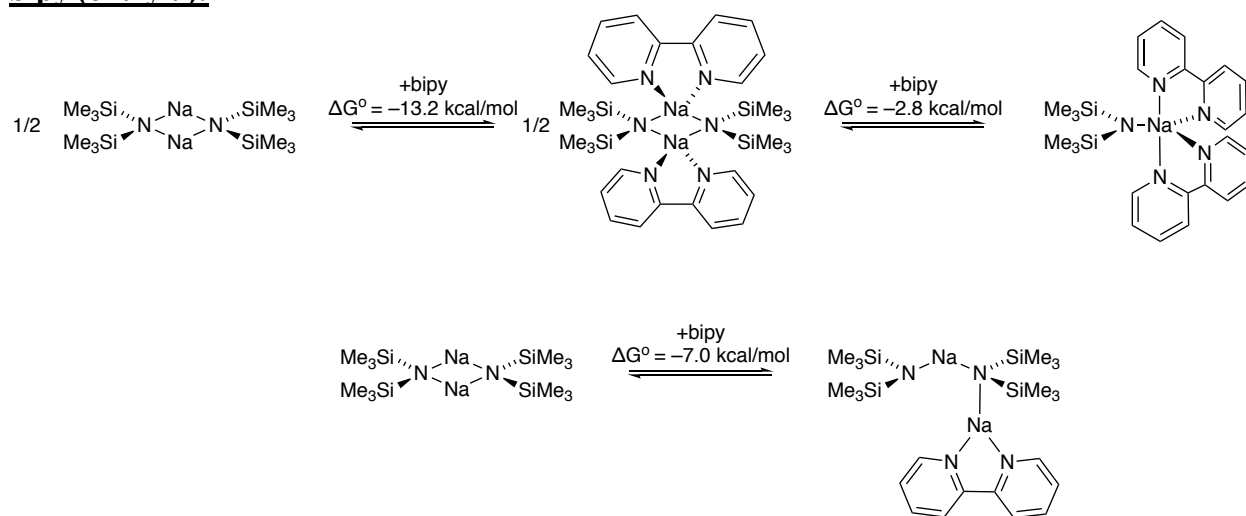
**(-)-sparteine (26):**

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



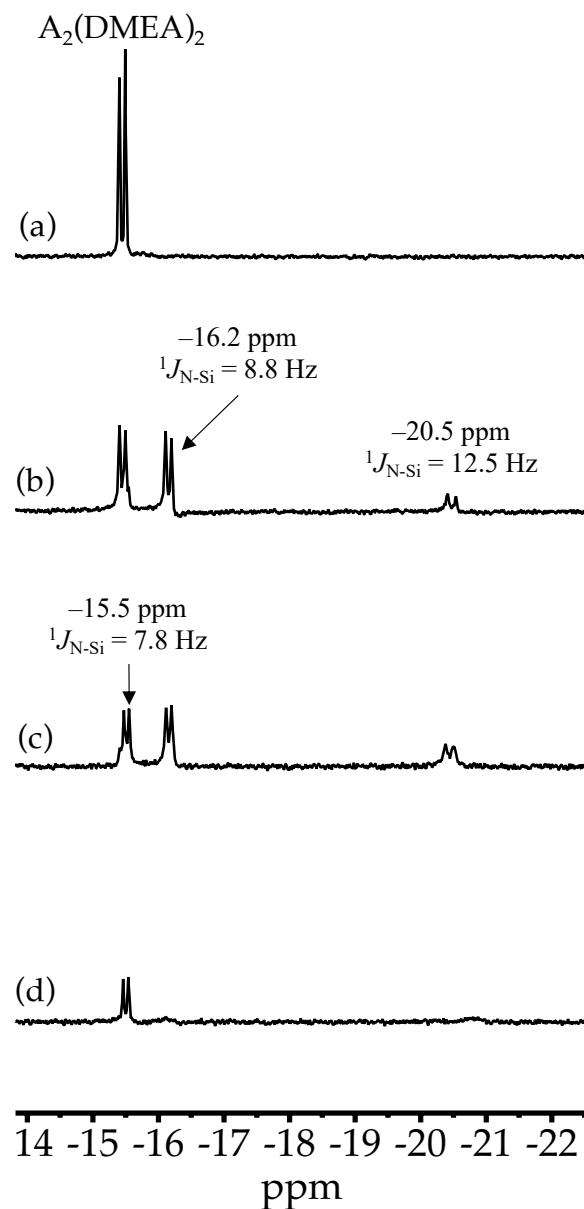
**Figure S62.**  $^{29}\text{Si}$  NMR spectra of 0.15 M  $[^{15}\text{N}]\text{NaHMDS}$  in DMEA cosolvent with varying amounts of sparteine added at  $-120^\circ\text{C}$ . The equivalents of sparteine for (a)–(d) are as follows: 0.0, 0.5, 1.0, and 3.0 equiv, respectively. The shift and coupling constant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

**bipy (entry u):**



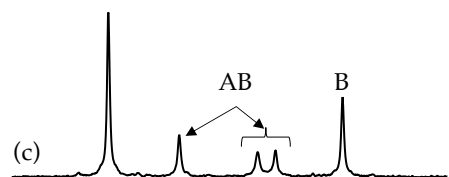
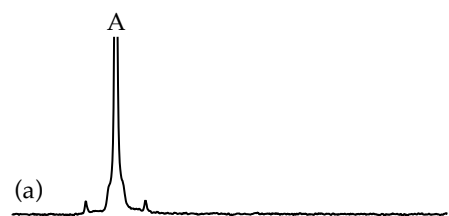
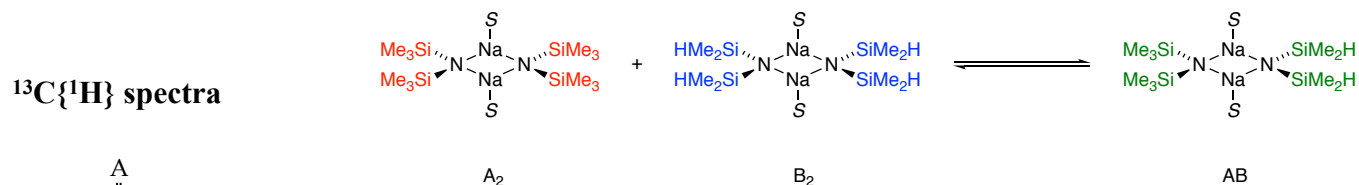
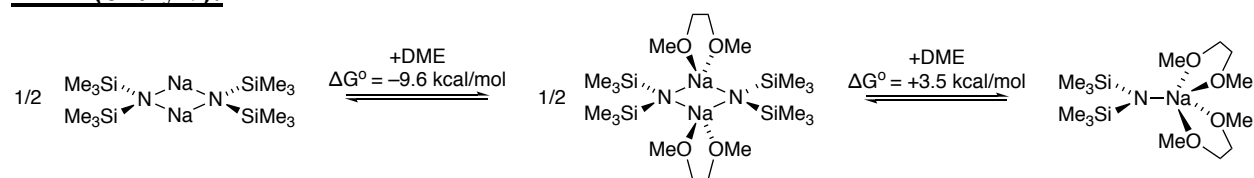
**Figure S63.** Computed free energies for the serial solvation of NaHMDS with bipy.

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



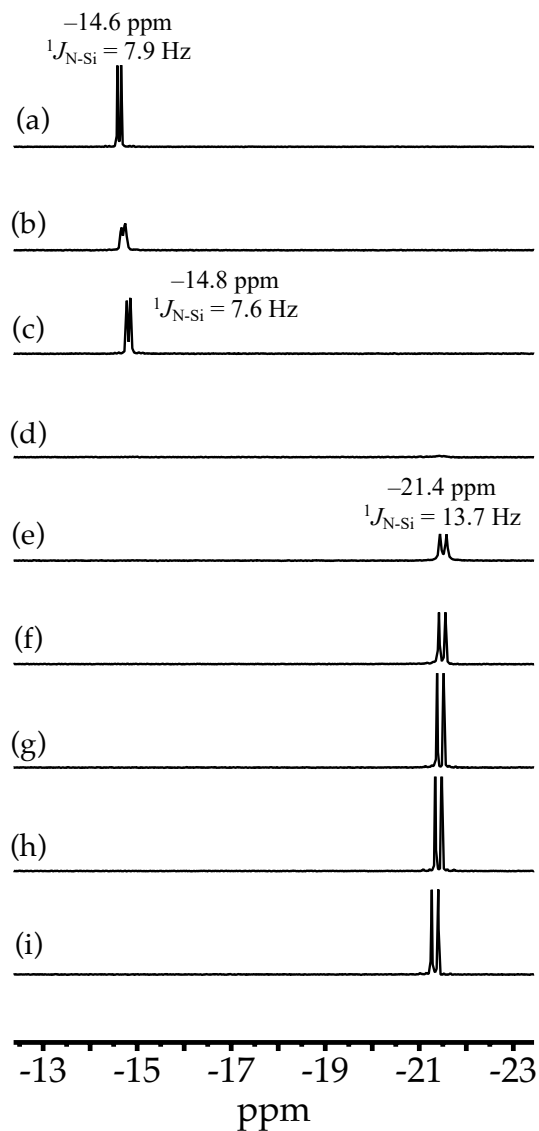
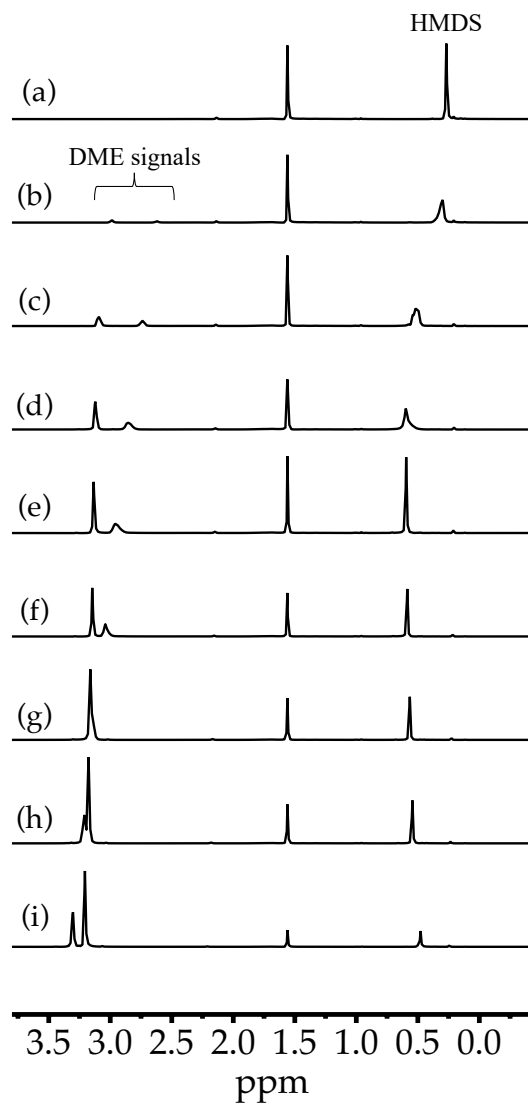
**Figure S64.**  $^{29}\text{Si}$  NMR spectra of 0.10 M  $[^{15}\text{N}]\text{NaHMDS}$  in DMEA cosolvent with varying amounts of bipy added at  $-120^\circ\text{C}$ . The equivalents of bipy for (a)–(d) are as follows: 0.0, 0.5, 1.0, and 3.0 equiv, respectively. Spectra (b) and (c) show DMEA disolvated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

### DME (entry v):



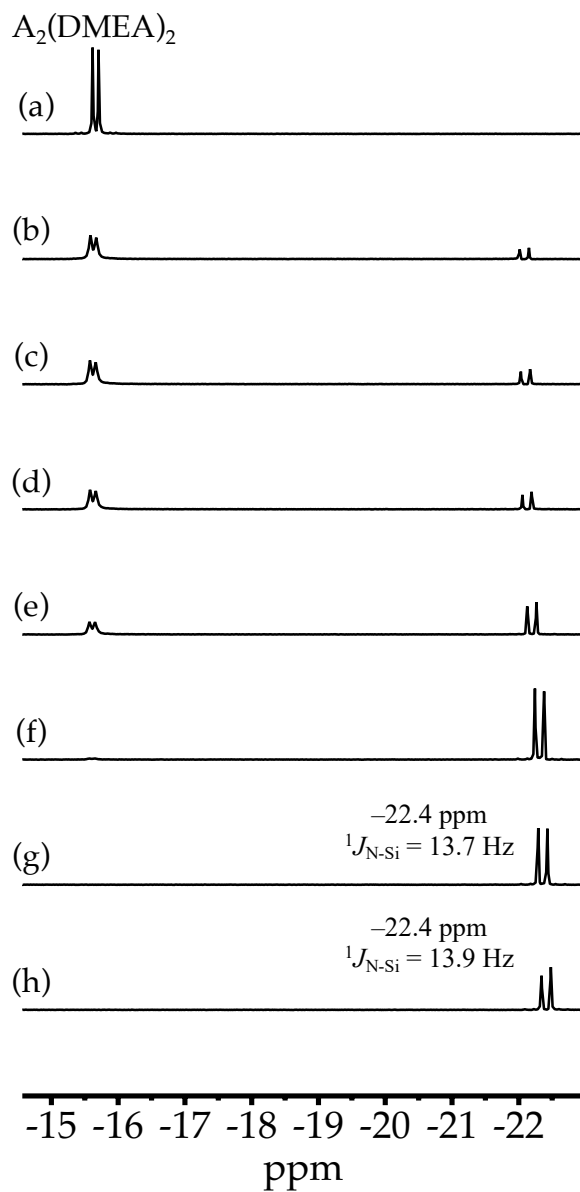
8.0 7.5 7.0 6.5 6.0  
ppm

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

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

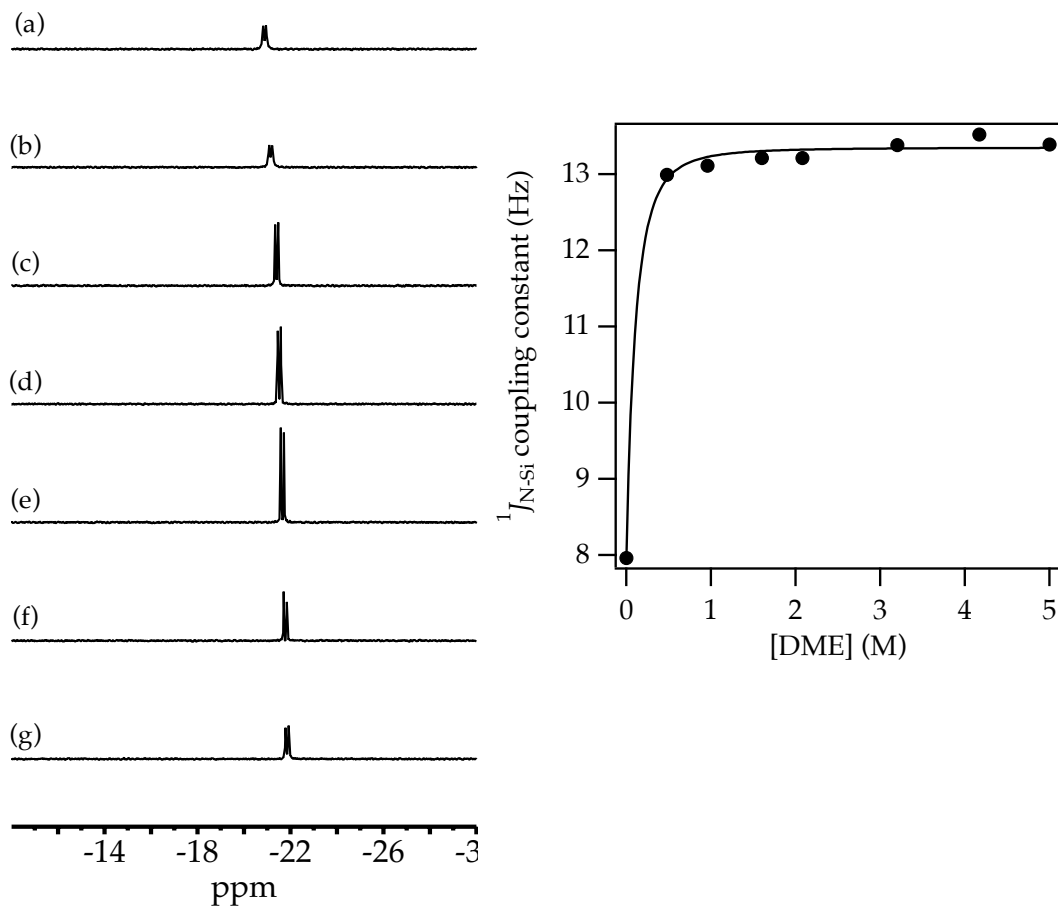
**Figure S66.**  $^1\text{H}$  and  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra for the titration of 0.20 M  $^{15}\text{N}$ NaHMDS in toluene- $d_8$  with DME at  $-80^\circ\text{C}$ . Equiv of DME for (a)–(i) are as follows: 0.0, 0.2, 0.9, 1.9, 2.8, 3.6, 5.4, 7.4, and 14.0, respectively.

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



**Figure S67.**  $^{29}\text{Si}$  NMR spectra of 0.20 M  $[^{15}\text{N}]\text{NaHMDS}$  in DMEA cosolvent with varying amounts of DME added at  $-120^\circ\text{C}$ . 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.

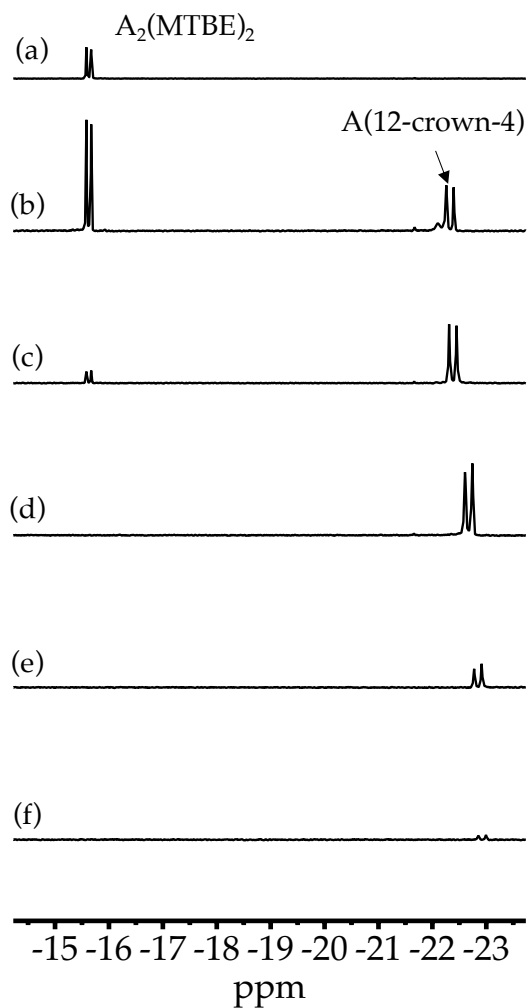
## $^{29}\text{Si}\{^1\text{H}\}$ spectra



**Figure S68.**  $^{29}\text{Si}\{^1\text{H}\}$  NMR spectra of 0.10 M NaHMDS in 2:1 pentane/toluene varying the concentration of DME at  $-20\text{ }^\circ\text{C}$ . 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)	$^1J_{\text{N-Si}}$ 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

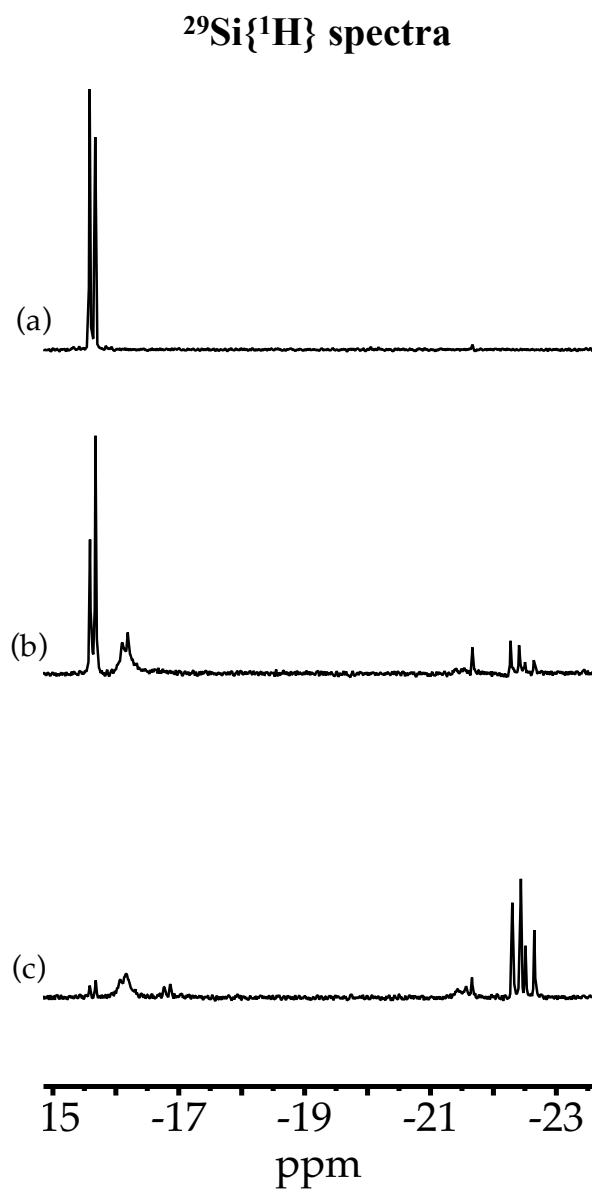
## $^{29}\text{Si}\{^1\text{H}\}$ spectra



**Figure S69.**  $^{29}\text{Si}$  NMR spectra of 0.20 M  $[^{15}\text{N}]\text{NaHMDS}$  in MTBE at  $-110\text{ }^\circ\text{C}$  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.

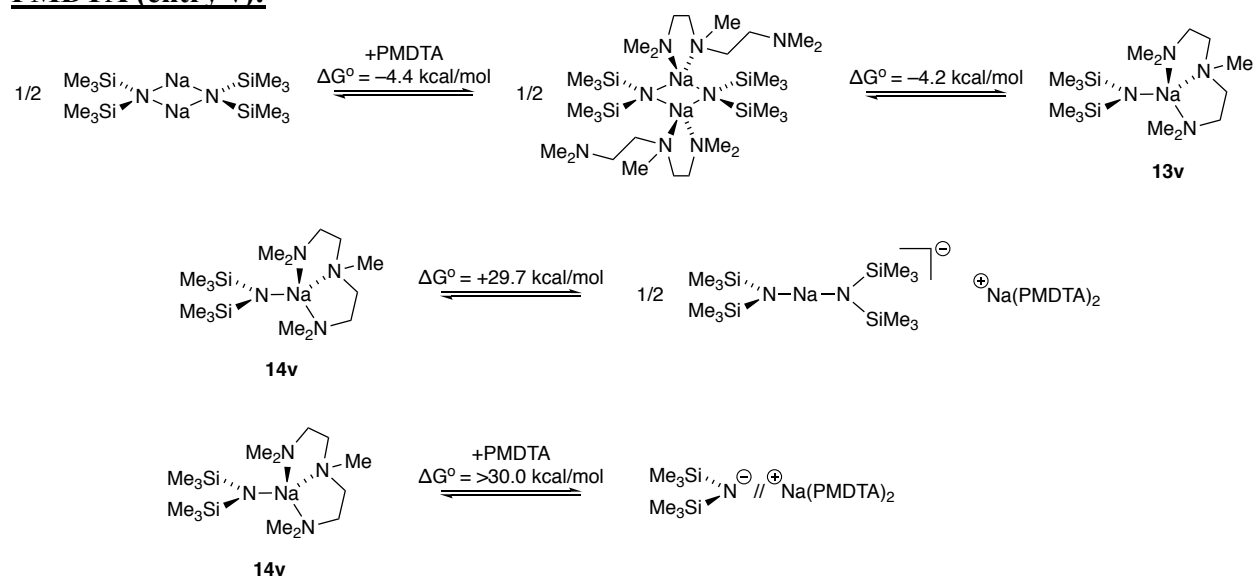


**NIPA (26):**



**Figure S70.**  $^{29}\text{Si}$  NMR spectra of 0.20 M  $[^{15}\text{N}]\text{NaHMDS}$  in MTBE at  $-110\text{ }^\circ\text{C}$  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.

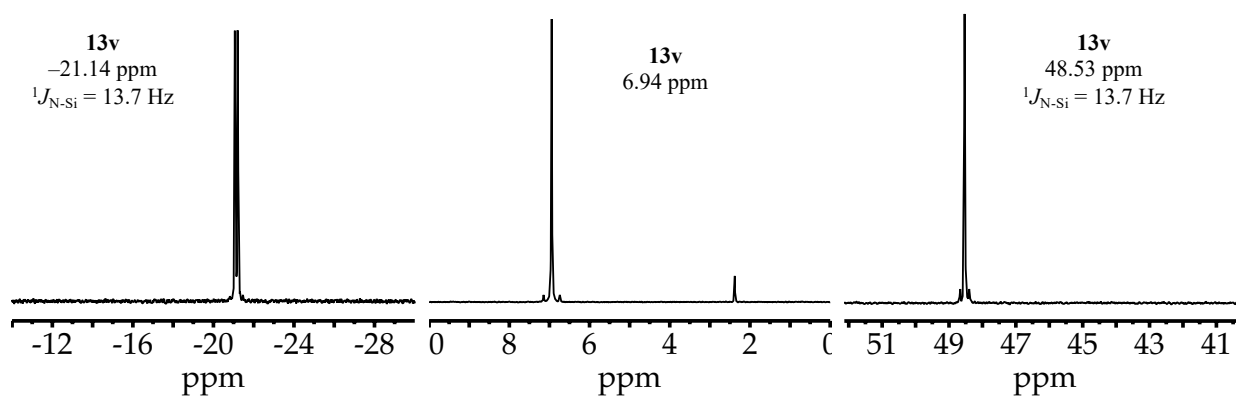
**PMDTA (entry v):**



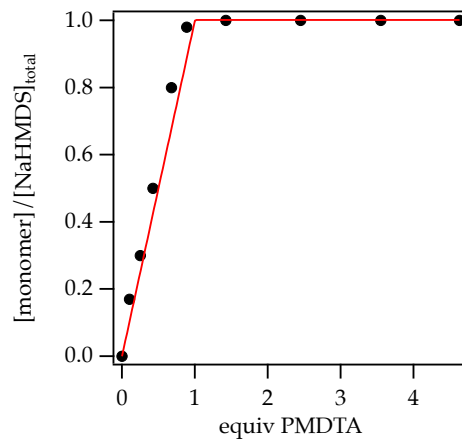
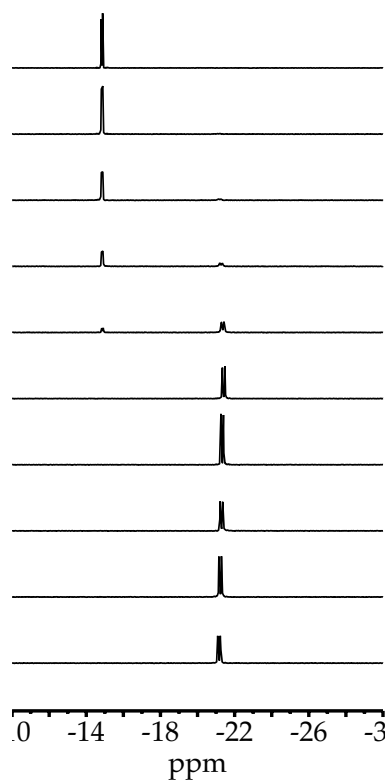
$^{29}\text{Si}\{^1\text{H}\}$  spectrum

$^{13}\text{C}\{^1\text{H}\}$  spectrum

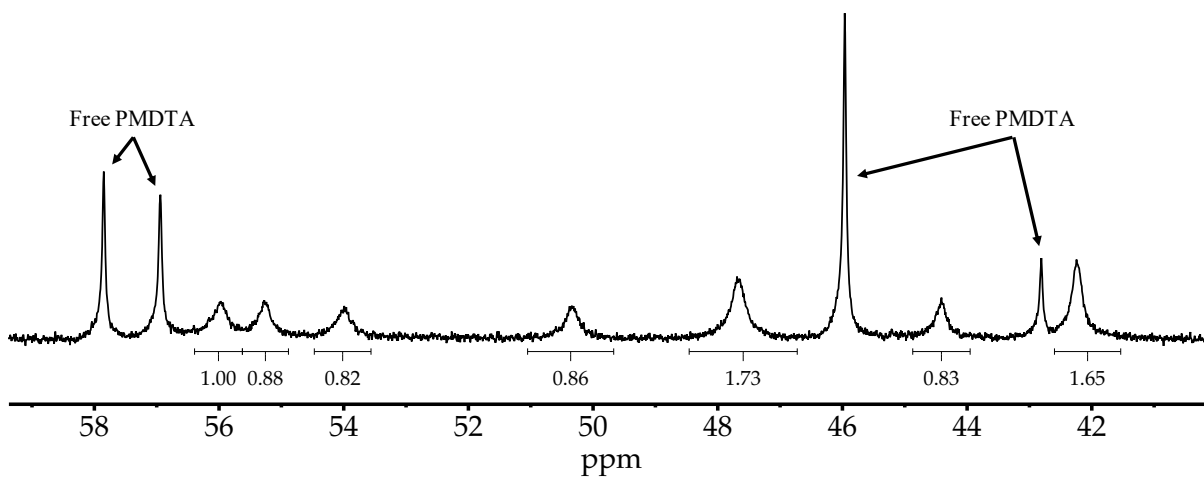
$^{15}\text{N}\{^1\text{H}\}$  spectrum



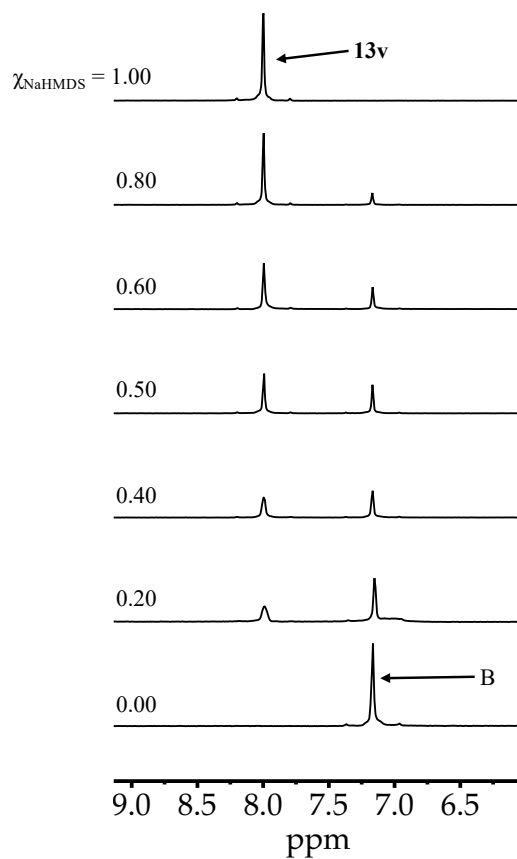
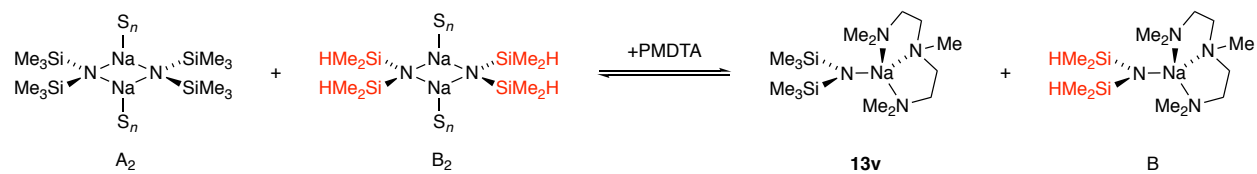
**Figure S71.** NMR spectra of  $[\text{}^{15}\text{N}]\text{NaHMDS}$  ( $^{29}\text{Si}$  and  $^{15}\text{N}$ ) and  $\text{NaHMDS}$  ( $^{13}\text{C}$ ) with at least 2 equiv PMDTA per sodium in toluene- $d_8$  cosolvent at  $-80^\circ\text{C}$ . Concentrations vary from 0.20 M  $\text{NaHMDS}$  ( $^{15}\text{N}$ ) to 0.30 M  $\text{NaHMDS}$  ( $^{29}\text{Si}$  and  $^{13}\text{C}$ ).



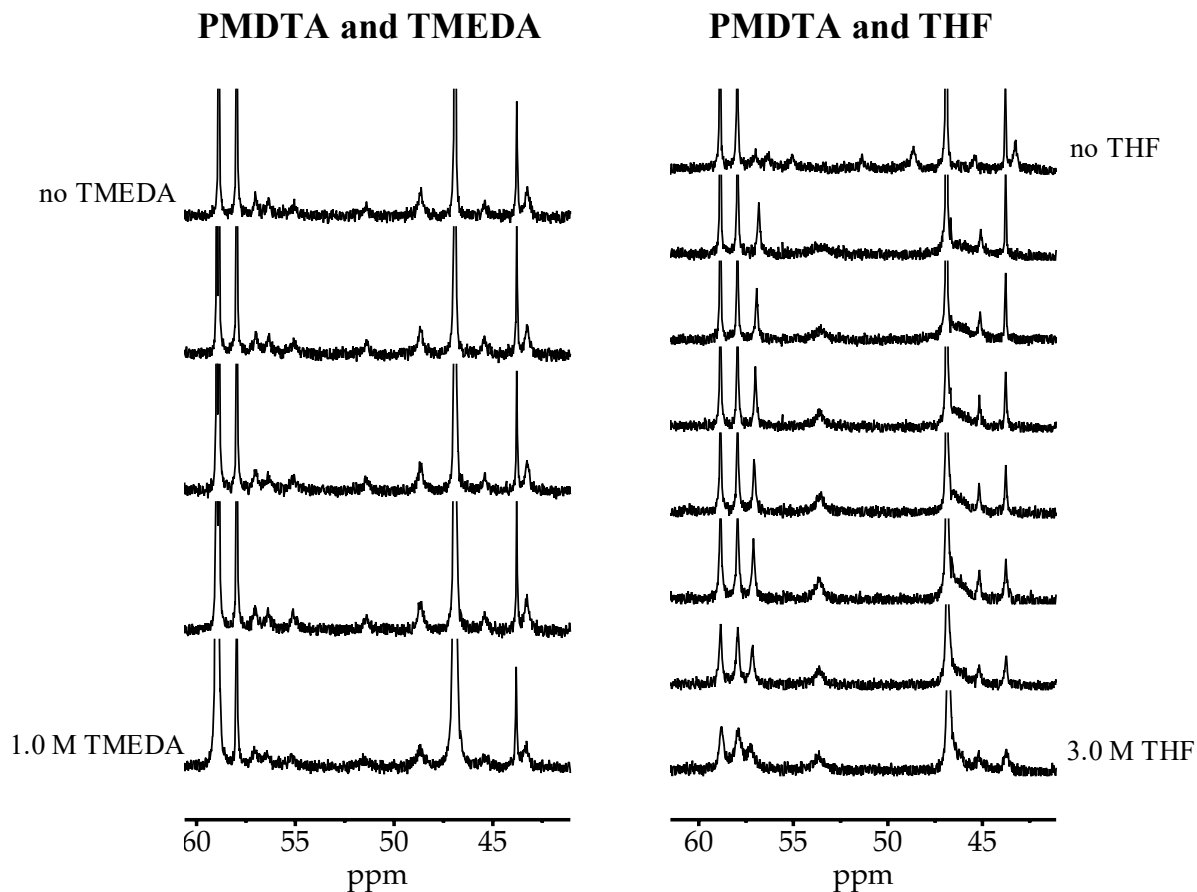
**Figure S72.**  $^{29}\text{Si}$  NMR spectra for 0.30 M solution of NaHMDS in toluene- $d_8$  with varying [PMDTA] at  $-80^\circ\text{C}$  and cyclopentane as an internal standard. The plot corresponds to the monomer concentration as a function equivalents of PMDTA added.



**Figure S73.**  $^{13}\text{C}$  NMR 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  $-120\text{ }^\circ\text{C}$ .

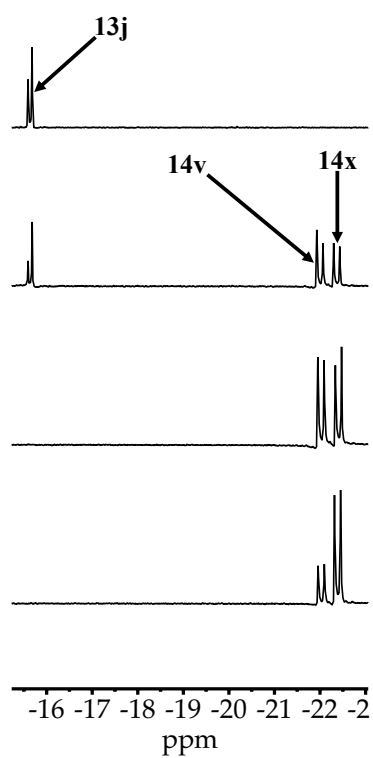


**Figure S74.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra for 0.30 M solutions of NaHMDS and NaTMDs in toluene- $d_8$  with at the indicated mole fractions ( $\chi_{\text{NaHMDS}}$ ) at  $-80\text{ }^\circ\text{C}$ .

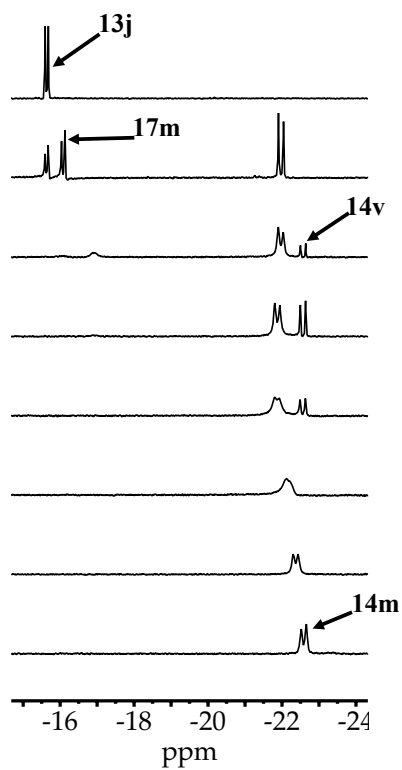


**Figure S75.**  $^{13}\text{C}$  NMR spectra showing free and bound PMDTA resonances as TMEDA and THF were titrated into solutions. Both titrations were run under the following starting conditions: 0.10 M NaHMDS in 2:1 pentane/toluene- $d_8$  and 2.0 equiv of PMDTA at  $-120\text{ }^\circ\text{C}$ .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

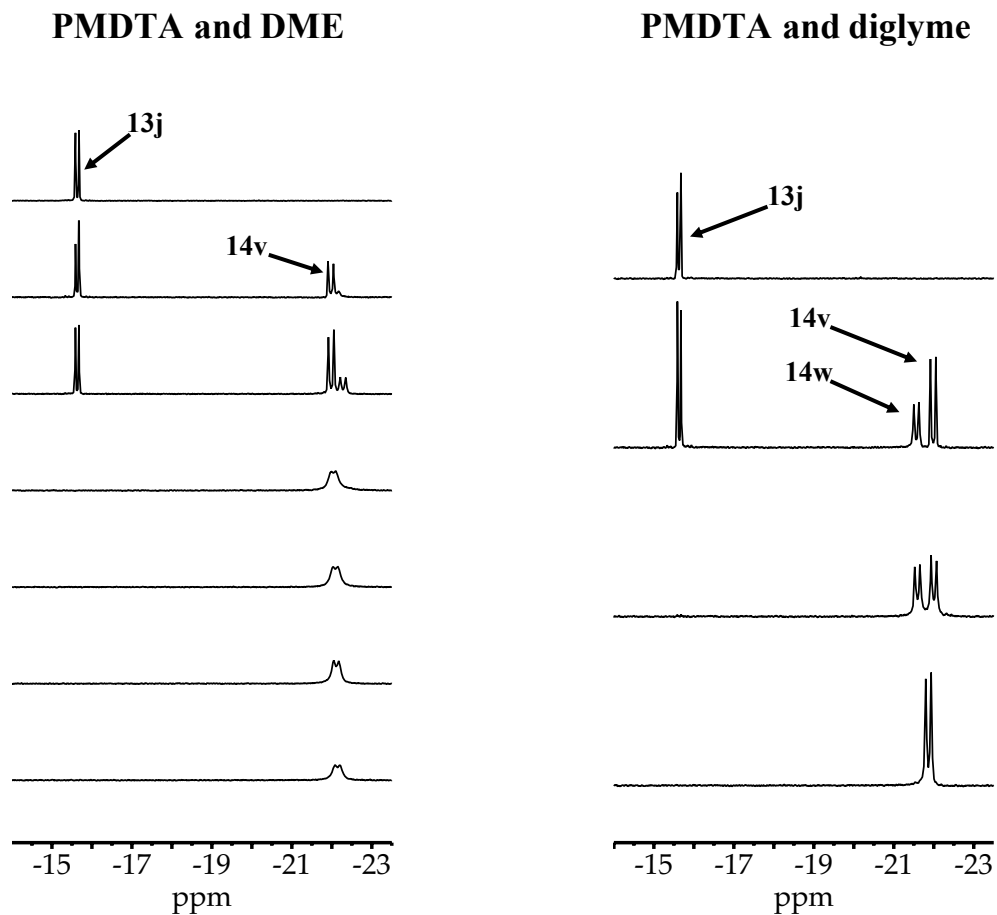
### PMDTA and 12-crown-4



### PMDTA and HMPA



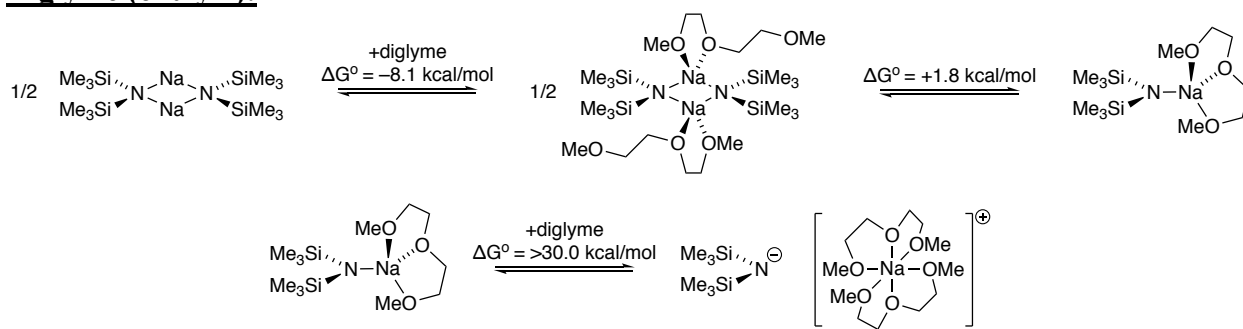
**Figure S76.**  $^{29}\text{Si}$  NMR spectra of 0.20 M  $^{15}\text{N}$ NaHMDS in MTBE at  $-110\text{ }^\circ\text{C}$  with incremental additions of 1:1 PMDTA/HMPA and 1:1 PMDTA/12-crown-4. The equiv of total added ligand from top to bottom are (A) PMDTA/12-crown-4: 0.0, 0.50, 1.0, and 1.5; and (B)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



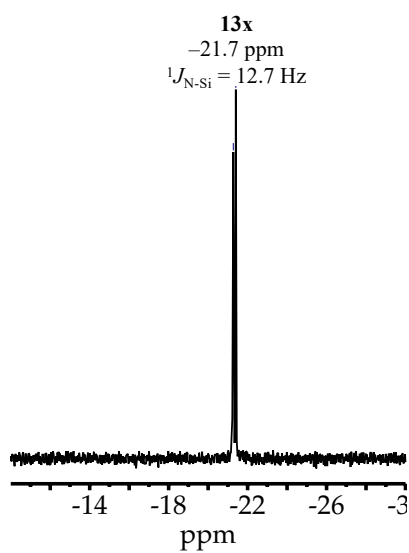
**Figure S77.**  $^{29}\text{Si}$  NMR spectra of 0.20 M  $^{15}\text{N}$ NaHMDS in MTBE at  $-110\text{ }^\circ\text{C}$  with incremental additions of 1:1 PMDTA/DME and 1:1 PMDTA/diglyme. The equiv of total added ligand are from top to bottom are (A) PMDTA/DME: 0.0, 0.50, 1.0, 2.0, 3.0, 4.0, and 6.0;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



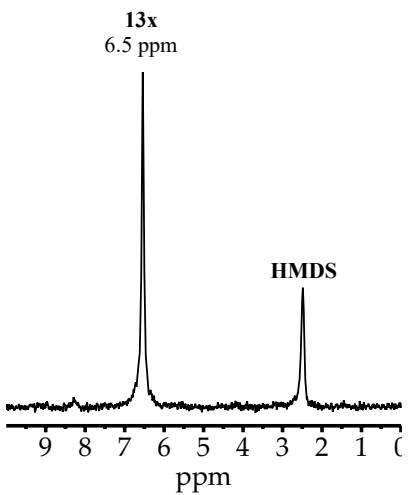
### Diglyme (entry x):



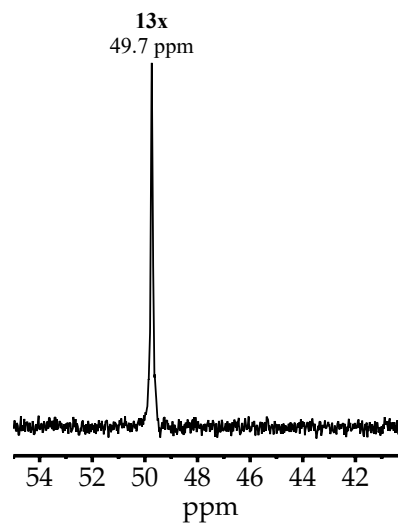
$^{29}\text{Si}\{^1\text{H}\}$  spectrum



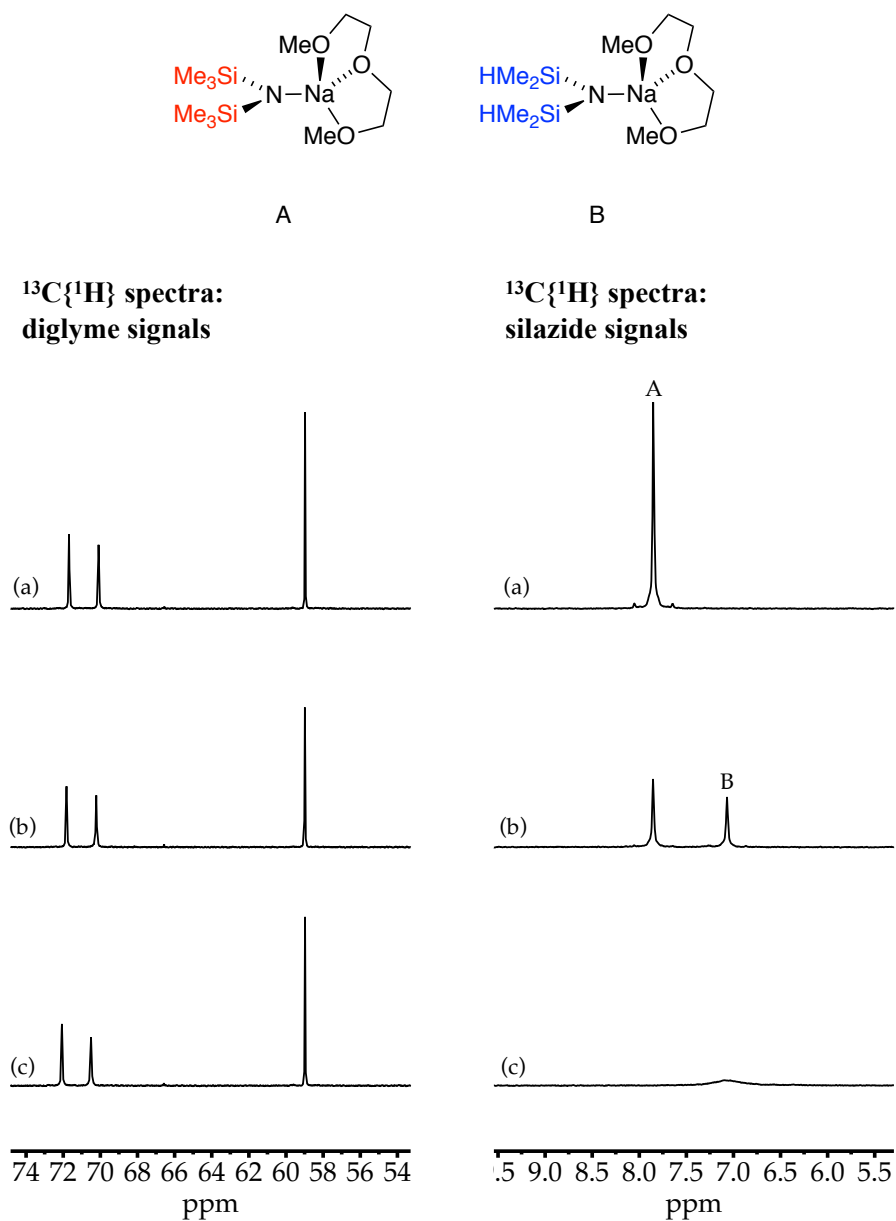
$^{13}\text{C}\{^1\text{H}\}$  spectrum



$^{15}\text{N}\{^1\text{H}\}$  spectrum

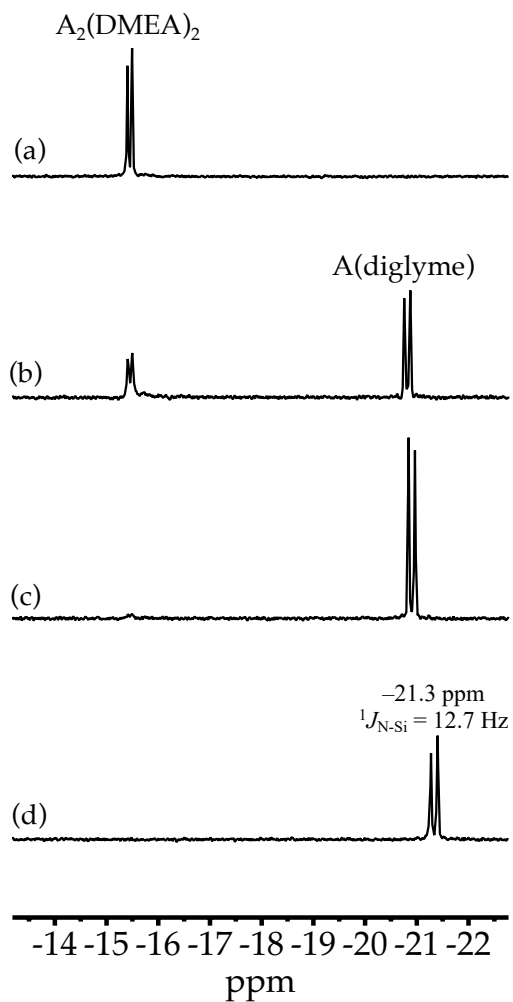


**Figure S78.** NMR spectra of 0.15 M  $^{15}\text{N}$ NaHMDS in 0.45 M diglyme with DMEA cosolvent at  $-120^\circ\text{C}$ .



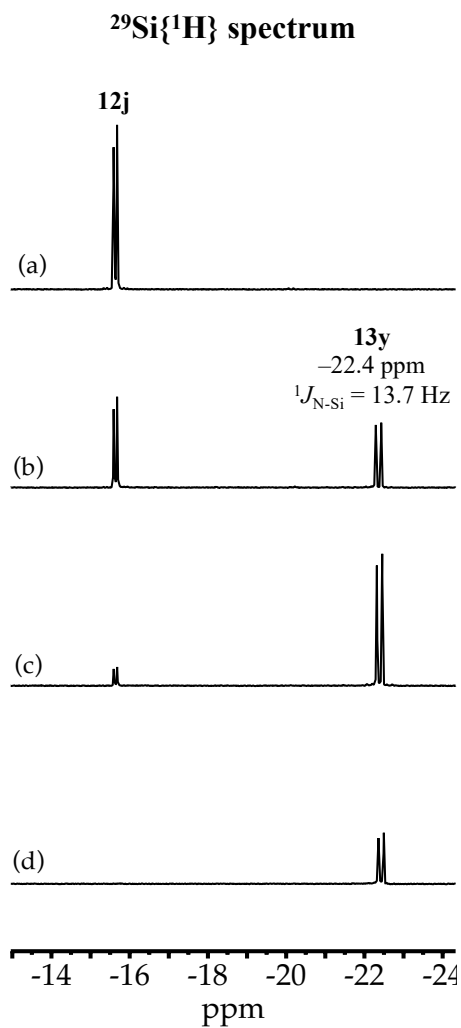
**Figure S79.**  $^{13}\text{C}$  NMR relative integrations of NaHMDS-derived homodimer ( $\text{A}_2$ ), NaTMDS-derived homodimer ( $\text{B}_2$ ), and heterodimer ( $\text{AB}$ ) versus the measured mole fraction of NaHMDS ( $X_{\text{NaHMDS}}$ ) at 0.20 total molarity in 0.40 M diglyme in toluene- $d_8$  cosolvent at  $-80^\circ\text{C}$ . The measured mole fractions,  $X_{\text{NaHMDS}}$ , in (a)–(c) are 1.00, 0.50, and 0.00, respectively.

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



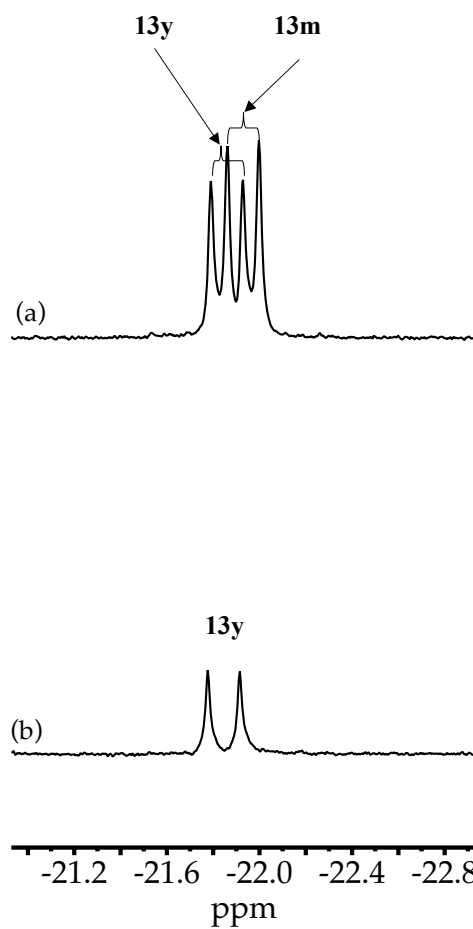
**Figure S80.**  $^{29}\text{Si}$  NMR spectra of 0.15 M  $[^{15}\text{N}]\text{NaHMDS}$  in DMEA cosolvent with varying amounts of diglyme added at  $-120^\circ\text{C}$ . The equivalents of diglyme for (a)–(d) are as follows: 0.0, 0.7, 1.0, and 3.0 equiv, respectively.

**12-crown-4 (entry v):**



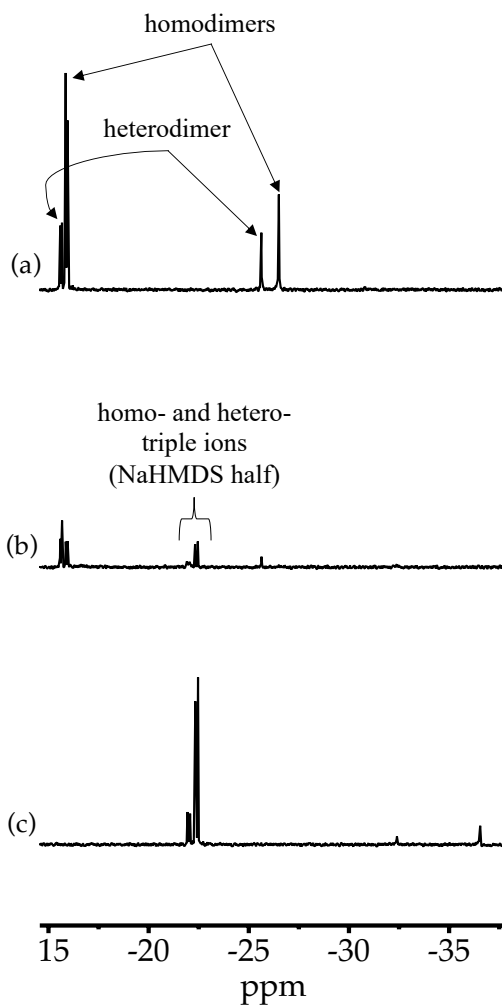
**Figure S81.**  $^{29}\text{Si}$  NMR spectra of 0.20 M  $[^{15}\text{N}]\text{NaHMDS}$  in MTBE cosolvent with varying amounts of 12-crown-4 added at  $-110\text{ }^\circ\text{C}$ . The equivalents of crown for (a)–(d) are as follows: 0.0, 0.3, 0.7, and 1.5 equiv, respectively.

$^{29}\text{Si}\{^1\text{H}\}$  spectrum



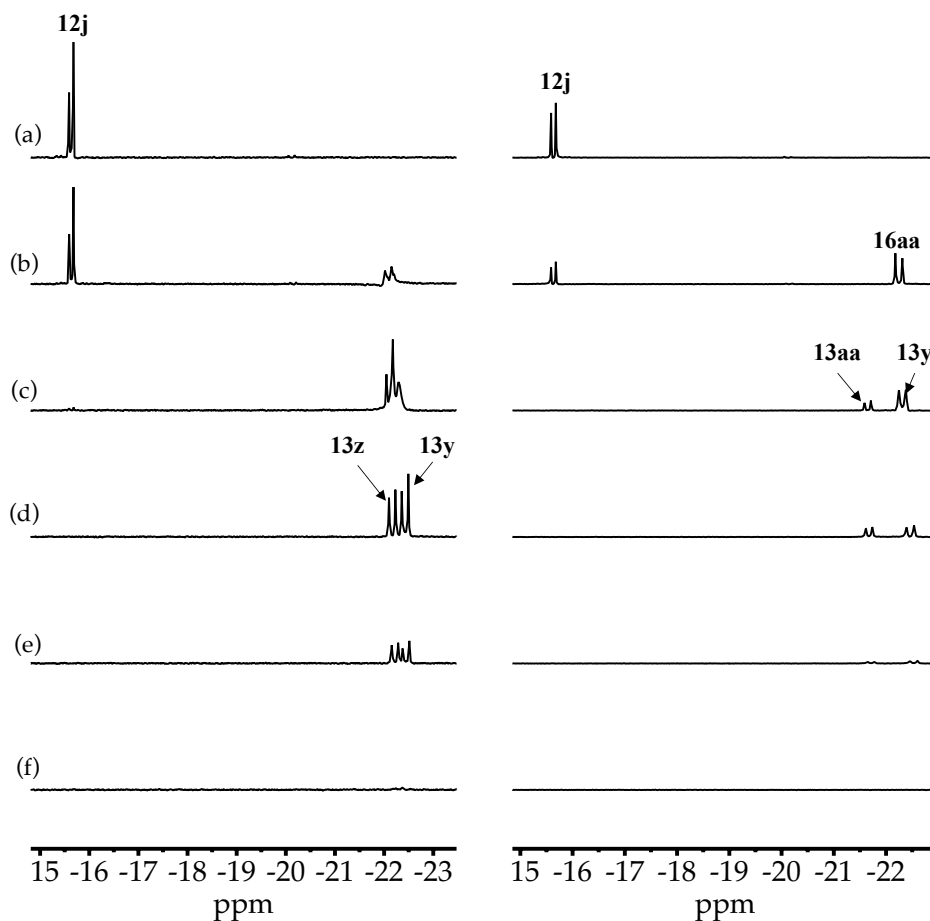
**Figure S82.**  $^{29}\text{Si}$  NMR spectra of 0.15 M  $[^{15}\text{N}]\text{NaHMDS}$  in THF cosolvent with varying amounts of 12-crown-4 added at  $-105\text{ }^\circ\text{C}$ . The equivalents of crown for (a) and (b) are as follows: 0.5 and 2.0 equiv, respectively.

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



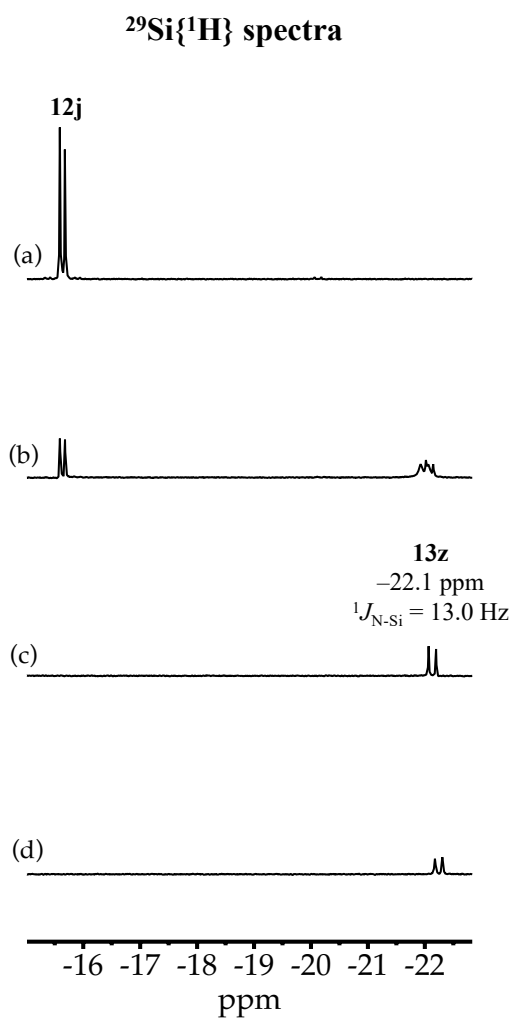
**Figure S83.** Titration of 12-crown-4 to a tube containing a 1:1 mix of NaHMDS and NaTMDS in MTBE cosolvent at  $-110\text{ }^{\circ}\text{C}$ . The equivalents of crown for (a)–(c) are as follows: 0.0, 0.4, and 1.5 equiv, respectively.

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



**Figure S84.**  $^{29}\text{Si}$  NMR spectra of 0.20 M  $[^{15}\text{N}]\text{NaHMDS}$  in MTBE at  $-110\text{ }^\circ\text{C}$  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.

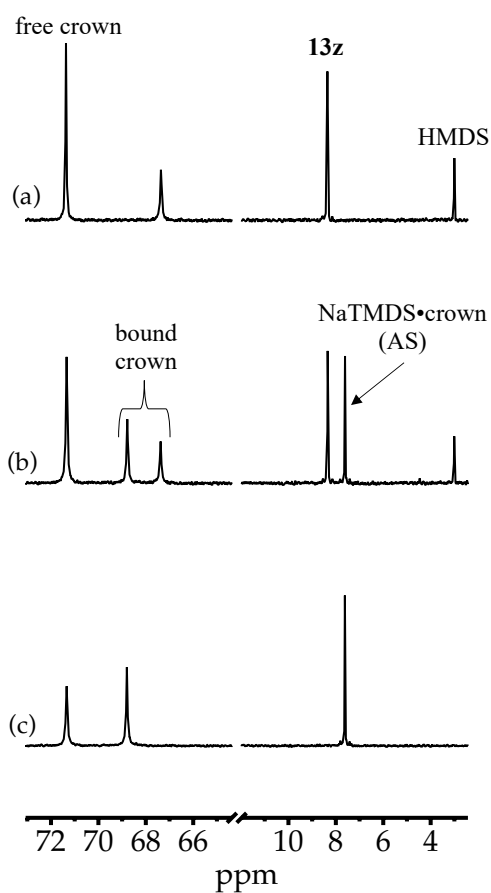
15-crown-5 (entry z):



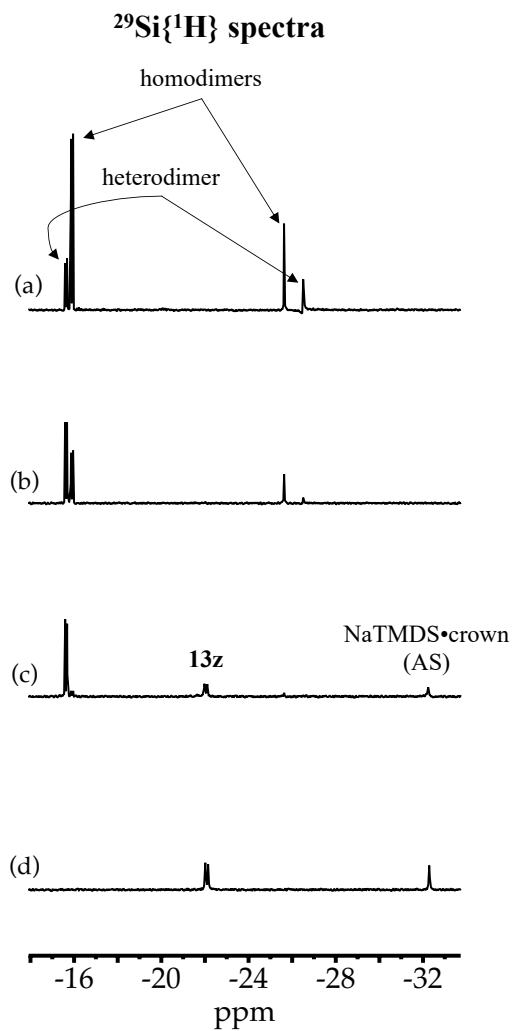
**Figure S85.**  $^{29}\text{Si}$  NMR spectra of 0.20 M  $[^{15}\text{N}]\text{NaHMDS}$  in MTBE cosolvent with varying amounts of 15-crown-5 added at  $-110\text{ }^\circ\text{C}$ . The equivalents of crown for (a)–(d) are as follows: 0.0, 0.3, 1.0, and 1.5 equiv, respectively.



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

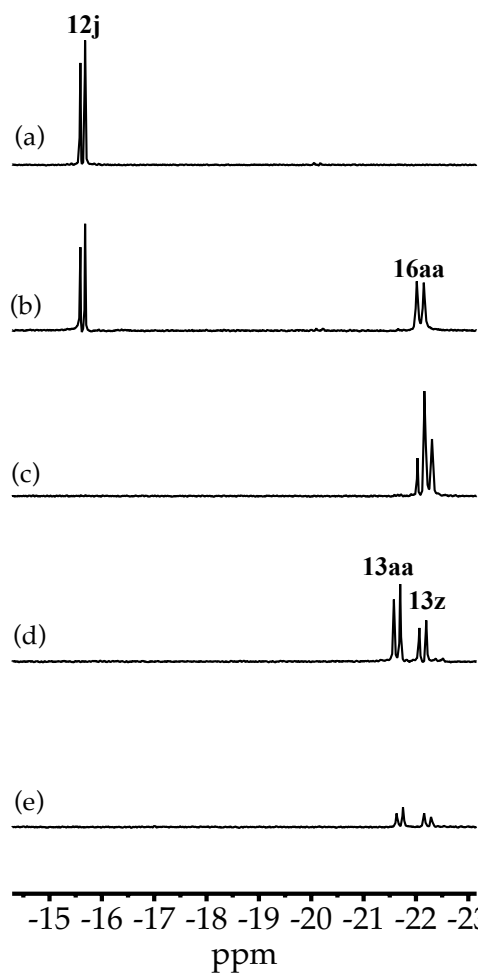


**Figure S86**  $^{13}\text{C}$  NMR spectra of with mixing NaHMDS and NaTMDS at 0.20 total molarity with 0.35 M 15-crown-5 in toluene- $d_8$  cosolvent at  $-80^\circ\text{C}$ . The measured mole fractions,  $X_{\text{NaHMDS}}$ , in (a)–(c) are 1.00, 0.50, and 0.00, respectively. Show are the crown carbon signals which appear to be in the slow exchange limit.



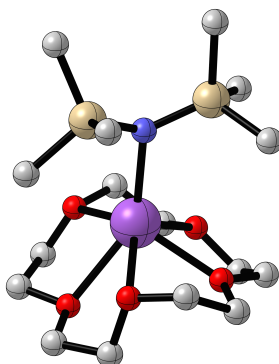
**Figure S87.** Titration of 15-crown-5 to a tube containing a 1:1 mix of NaHMDS and NaTMDS in MTBE cosolvent at  $-110\text{ }^{\circ}\text{C}$ . The equivalents of crown for (a)–(d) are as follows: 0.0, 0.3, 0.5 and 1.5 equiv, respectively.

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



**Figure S88.**  $^{29}\text{Si}$  NMR spectra of 0.20 M  $[^{15}\text{N}]\text{NaHMDS}$  in MTBE at  $-110\text{ }^\circ\text{C}$  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.

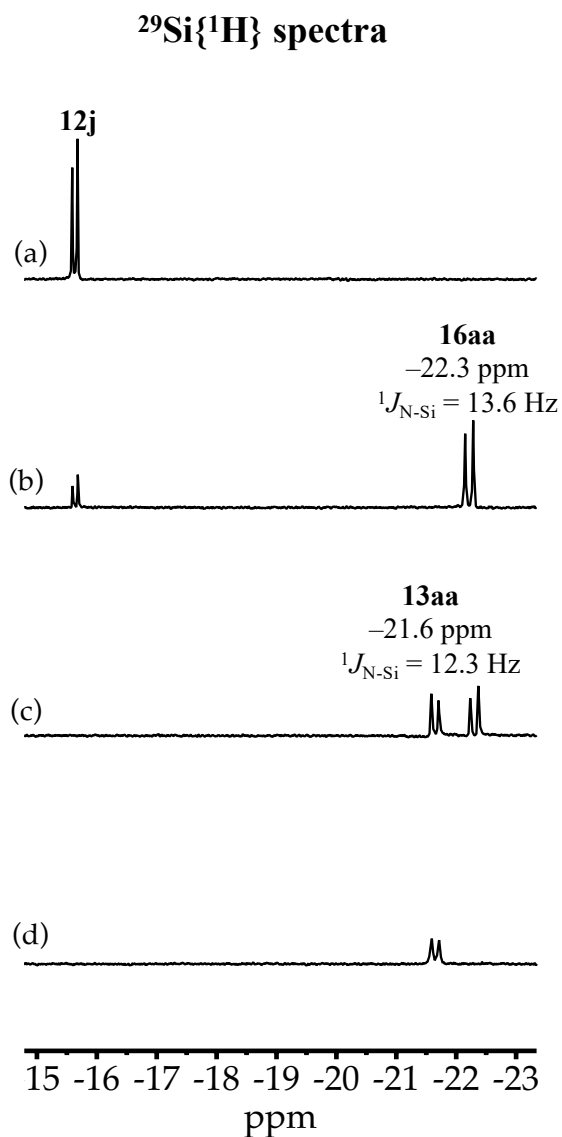
**Table S2.** Crystal structure for NaHMDS•15-crown5.  
Owing to the low resolution of the crystal, only coordinates (xyz) are presented.



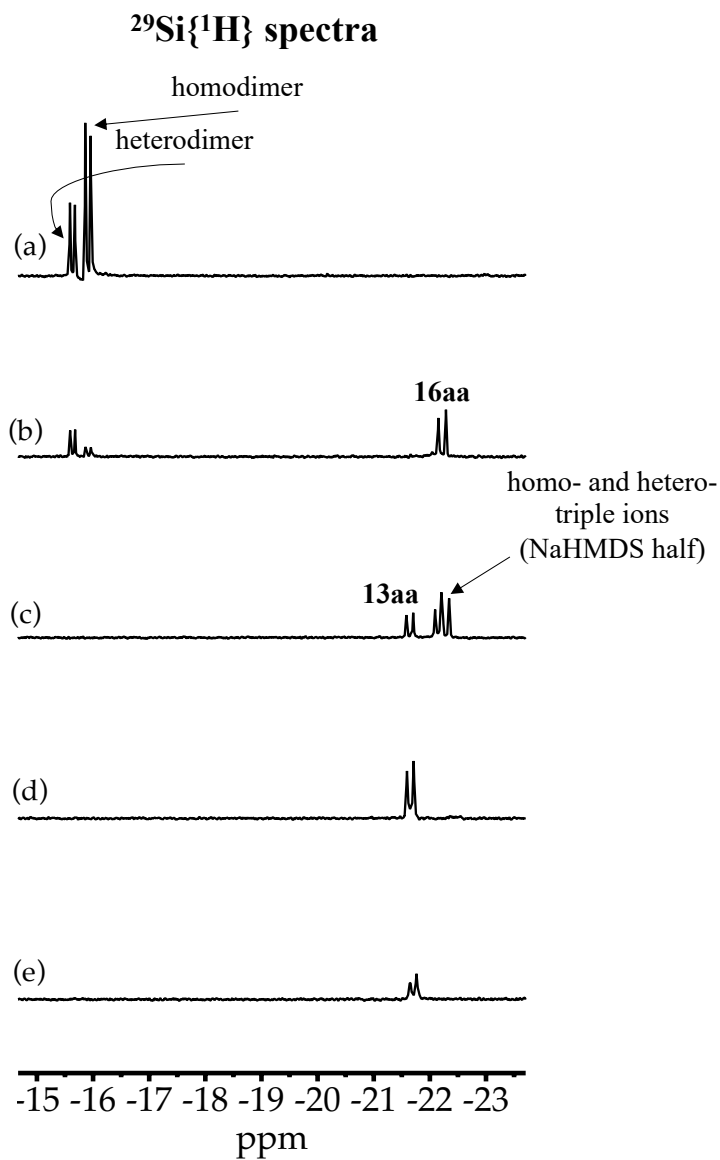
**13z**  
crystal  
structure

	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

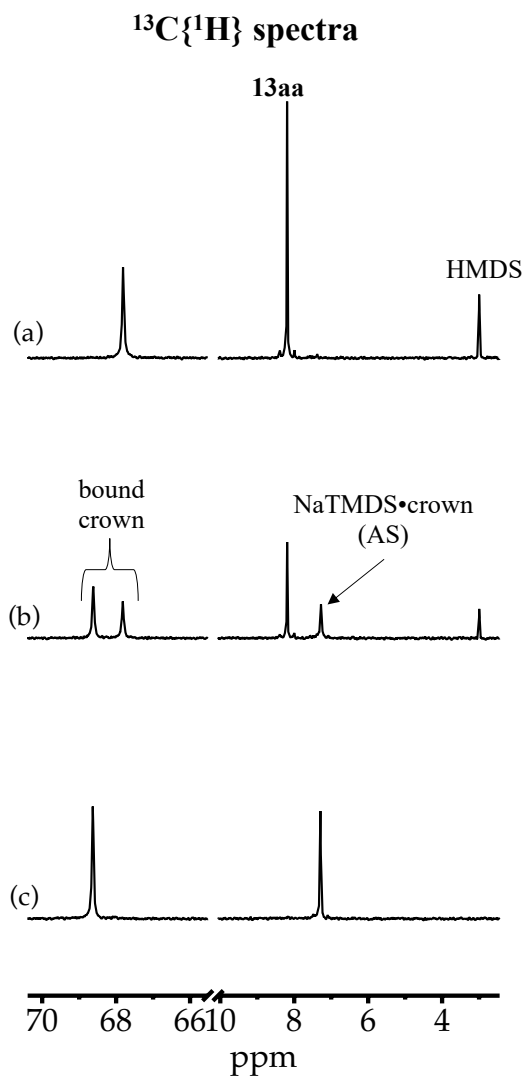
18-crown-6 (entry aa):



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



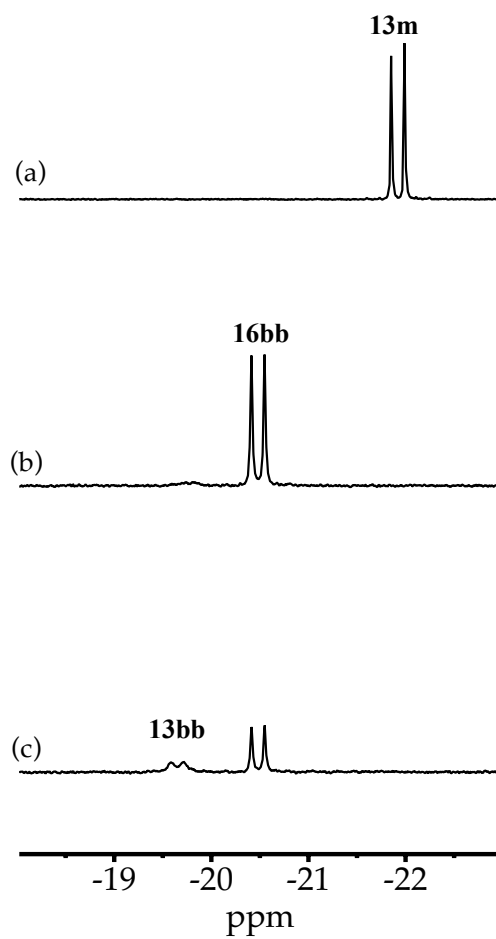
**Figure S90.** Titration of 18-crown-6 to a tube containing a 1:1 mix of NaHMDS and NaTMDS in MTBE cosolvent at  $-110\text{ }^{\circ}\text{C}$ . The equivalents of crown for (a)–(e) are as follows: 0.0, 0.5, 1.0, 1.5, and 2.0 equiv, respectively.



**Figure S91.**  $^{13}\text{C}$  NMR 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  $-80\text{ }^\circ\text{C}$ . The measured mole fractions,  $X_{\text{NaHMDS}}$ , 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):

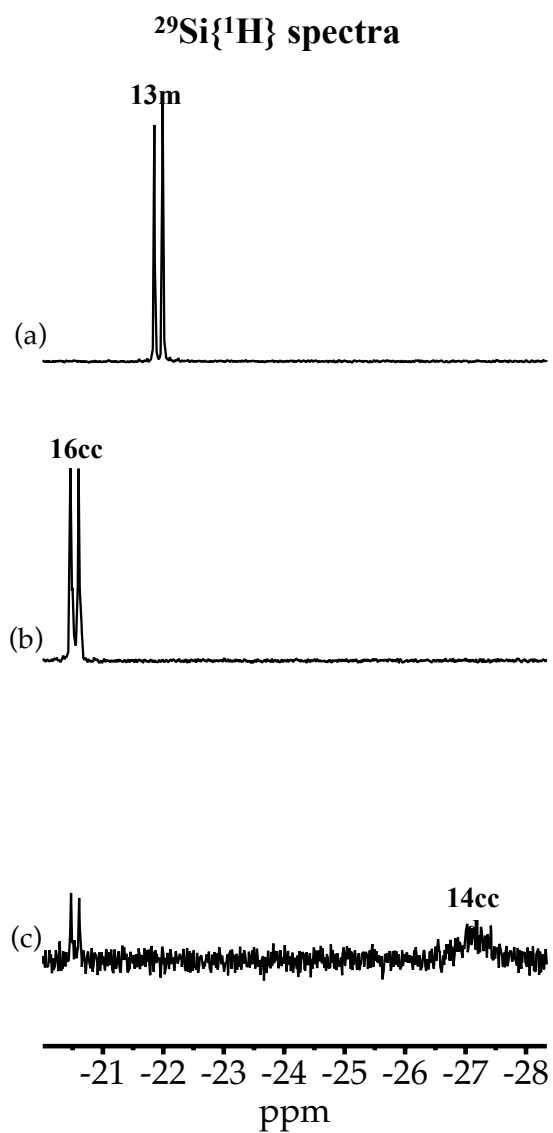
$^{29}\text{Si}\{^1\text{H}\}$  spectra



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



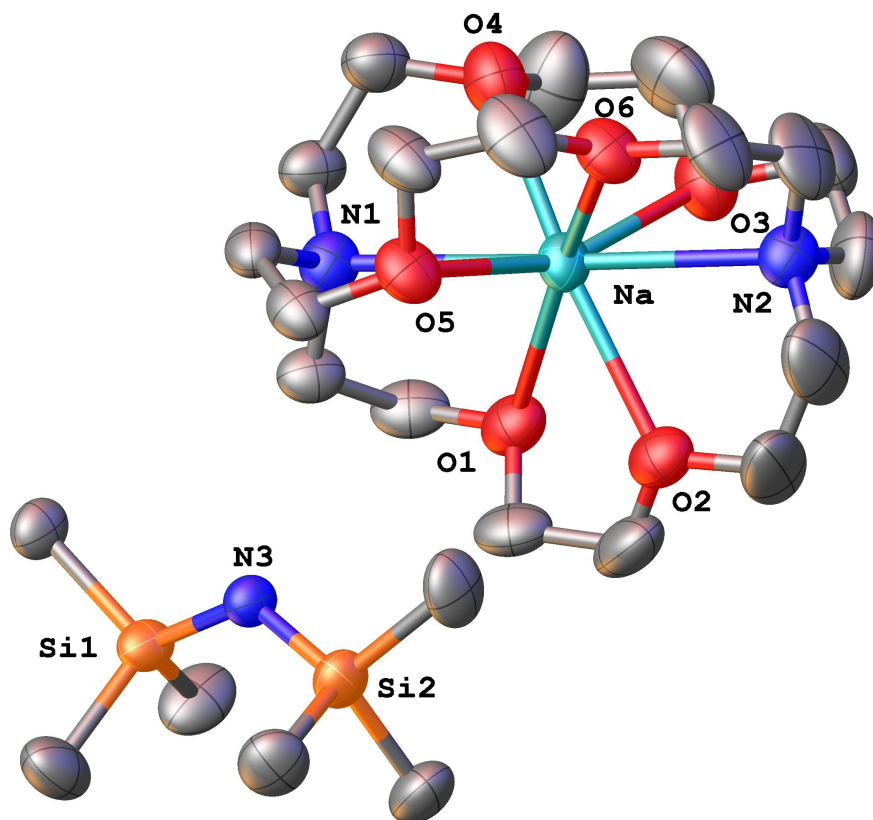
[2.2.2]cryptand (entry cc):



**Figure S93.**  $^{29}\text{Si}$  NMR spectra of 0.20 M  $[^{15}\text{N}]\text{NaHMDS}$  in THF cosolvent with varying amounts of [2.2.2]cryptand added at  $-105\text{ }^\circ\text{C}$ . 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.

Identification code	rrow4_abs7	
Empirical formula	C <sub>24</sub> H <sub>54</sub> N <sub>3</sub> Na O <sub>6</sub> Si <sub>2</sub>	
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 <sup>3</sup>	
Z	4	
Density (calculated)	1.164 Mg/m <sup>3</sup>	
Absorption coefficient	1.455 mm <sup>-1</sup>	
F(000)	1224	
Crystal size	0.231 x 0.14 x 0.073 mm <sup>3</sup>	
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 <sup>2</sup>	
Data / restraints / parameters	6804 / 1329 / 374	
Goodness-of-fit on F <sup>2</sup>	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 <sup>-3</sup>	



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

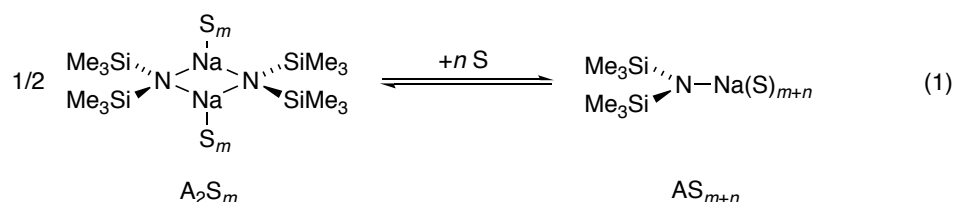
	x	y	z	$U(\text{eq})$
Si(1)	7796(1)	5762(1)	3660(1)	44(1)
Si(2)	7016(1)	6752(1)	4848(1)	47(1)
N(3)	6945(2)	6042(1)	4109(2)	40(1)
C(19)	7685(4)	6238(2)	2358(4)	74(1)
C(20)	7600(3)	4816(2)	3231(3)	50(1)
C(21)	9263(3)	5840(2)	4709(4)	77(1)
C(22)	5777(3)	6885(2)	5024(3)	69(1)
C(23)	7208(3)	7592(2)	4229(4)	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)

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### 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],  $J_{\text{obsd}}$  = 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.



Given:

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

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

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

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

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  $[AS_{m+n}]$ :

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

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

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

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

Rearranging affords the equation used as the fitting function:

$$J_{\text{obsd}} = \frac{4[A]_T J_{A_2 S_m} + J_{A_2 S_m} K_{\text{eq}}^2 [S]^{2n} - 2J_{AS_{m+n}} K_{\text{eq}}^2 [S]^{2n} - J_{A_2 S_m} \sqrt{8[A]_T K_{\text{eq}}^2 [S]^{2n} + K_{\text{eq}}^4 [S]^{4n}} + 2J_{AS_{m+n}} \sqrt{8[A]_T K_{\text{eq}}^2 [S]^{2n} + K_{\text{eq}}^4 [S]^{4n}}}{4[A]_T - K_{\text{eq}}^2 [S]^{2n} + \sqrt{8[A]_T K_{\text{eq}}^2 [S]^{2n} + K_{\text{eq}}^4 [S]^{4n}}}$$

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.

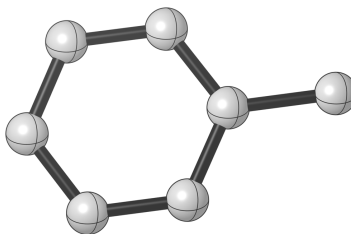
$$\begin{aligned} f(x) &= J_{\text{obs}} \\ x &= [S] \\ a &= [A]_T \\ b &= J_{A_2 S_m} \\ c &= J_{AS_{m+n}} \\ d &= K_{\text{eq}} \end{aligned}$$

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

## 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.

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



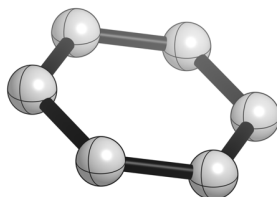
**G** = -271.12497 Hartrees

**G<sub>SP</sub>** = -271.4240179 Hartrees

<b>Atom</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
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.

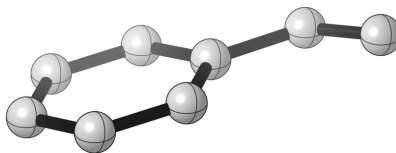


**G** = -231.883978 Hartrees

**G<sub>SP</sub>** = -232.1392645 Hartrees

<b>Atom</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
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.

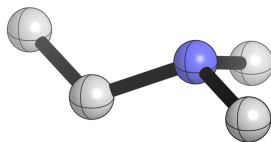


G = -309.15983 Hartrees

G<sub>SP</sub> = -309.5005756 Hartrees

<b>Atom</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
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.

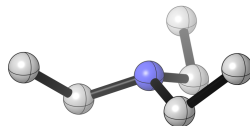


G = -213.373821 Hartrees

G<sub>SP</sub> = -213.6201404 Hartrees

<b>Atom</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
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.

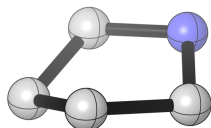


G = -291.846611 Hartrees

G<sub>SP</sub> = -292.1796866 Hartrees

<b>Atom</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
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.

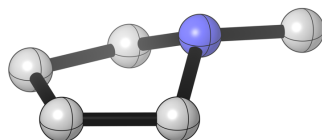


G = -212.198736 Hartrees

G<sub>SP</sub> = -212.4417845 Hartrees

<b>Atom</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
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.

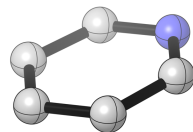


G = -251.434505 Hartrees

G<sub>SP</sub> = -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.

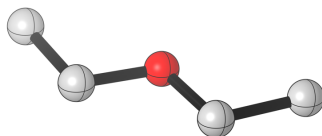


G = -247.915535 Hartrees

G<sub>SP</sub> = -248.192147 Hartrees

<b>Atom</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
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.



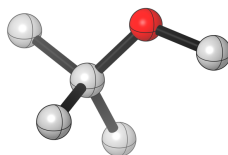
G = -233.241254 Hartrees

G<sub>SP</sub> = -233.5145333 Hartrees

<b>Atom</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
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.

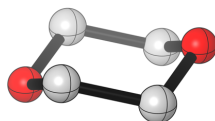


G = -272.479744 Hartrees

G<sub>SP</sub> = -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.

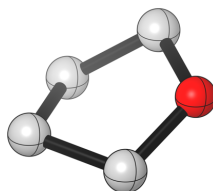


G = -307.183426 Hartrees

G<sub>SP</sub> = -307.5433292 Hartrees

<b>Atom</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
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

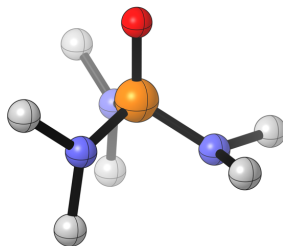
**Table S15.** Geometric coordinates and single point energies for THF.



**G** = -232.060313 Hartrees

**G<sub>SP</sub>** = -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				

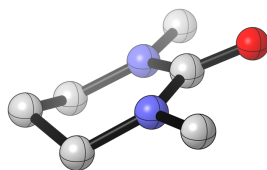
**Table S16.** Geometric coordinates and single point energies for HMPA.

G = -819.403088 Hartrees

G<sub>SP</sub> = -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.

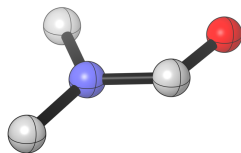


G = -419.945815 Hartrees

G<sub>SP</sub> = -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.

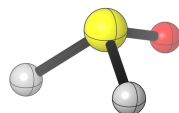


G = -248.116542 Hartrees

G<sub>SP</sub> = -248.4052246 Hartrees

<b>Atom</b>	<b>X</b>	<b>Y</b>	<b>Z</b>	<b>Atom</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
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.

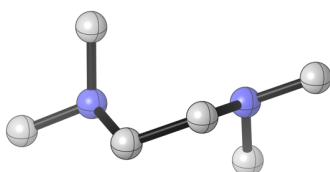


G = -552.775442 Hartrees

G<sub>SP</sub> = -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).



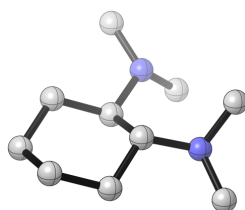
G = -347.098997 Hartrees

G<sub>SP</sub> = -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).

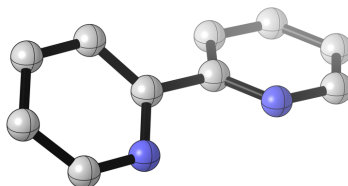


G = -502.865558 Hartrees

G<sub>SP</sub> = -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).

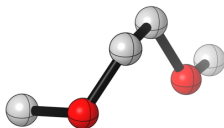


G = -494.662501 Hartrees

G<sub>SP</sub> = -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).

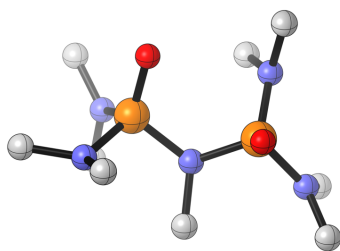


G = -308.347018 Hartrees

G<sub>SP</sub> = -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'''*-nonamethylimidodiphosphoramidate (NIPA).



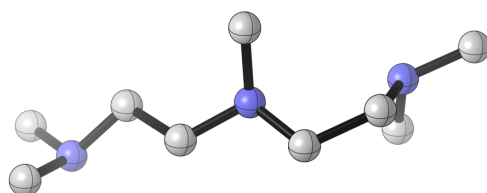
G = -1464.665262 Hartrees

G<sub>SP</sub> = -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'''*-pentamethyldiethylenetriamine (PMDTA).

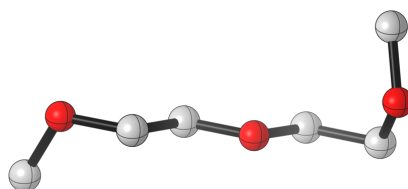


G = -520.058617 Hartrees

G<sub>SP</sub> = -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).

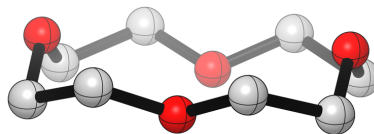


G = -461.935402 Hartrees

G<sub>SP</sub> = -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.

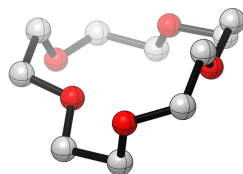


G = -614.356638 Hartrees

G<sub>SP</sub> = -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				

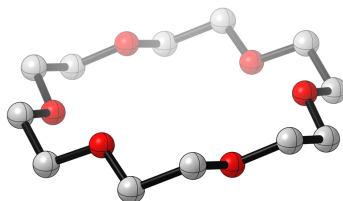


**Table S28.** Geometric coordinates and single point energies for 15-crown-5.

G = -767.952198 Hartrees

G<sub>SP</sub> = -768.844353 Hartrees

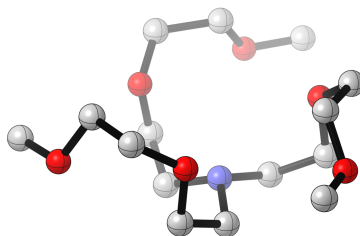
Atom	X	Y	Z	Atom	X	Y	Z
C	0.4305190	-0.6200380	-2.4999700	C	0.9068120	-2.5208980	-1.2221400
H	0.3717800	-1.1171900	-3.4885590	O	0.0000000	-1.4898330	-1.4924220
H	1.4817020	-0.3153580	-2.3382540	H	1.1287510	-3.0989190	-2.1431310
C	-0.4305190	0.6200380	-2.4999700	H	1.8596800	-2.1044590	-0.8434060
H	-0.3717800	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<sub>SP</sub> = -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

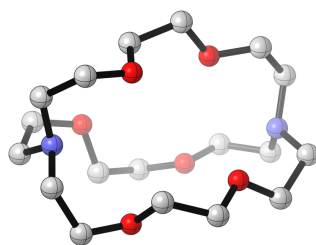
**Table S30.** Geometric coordinates and single point energies for TDA-1.

G = -1095.676597 Hartrees

G<sub>SP</sub> = -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.

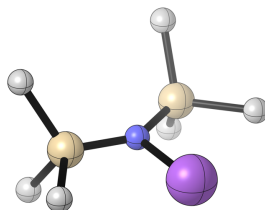
G = -1266.283094 Hartrees

G<sub>SP</sub> = -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.

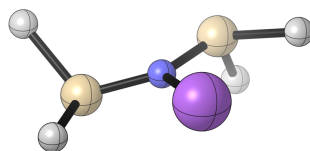


G = -1034.7736 Hartrees

G<sub>SP</sub> = -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.



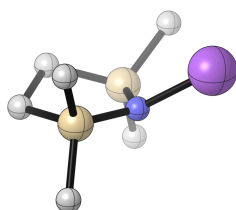
G = -956.273505 Hartrees

G<sub>SP</sub> = -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.

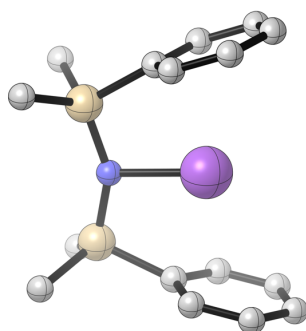


G = -1033.579549 Hartrees

G<sub>SP</sub> = -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.

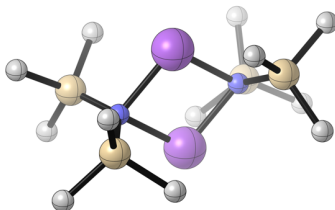


G = -1417.731619 Hartrees

G<sub>SP</sub> = -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

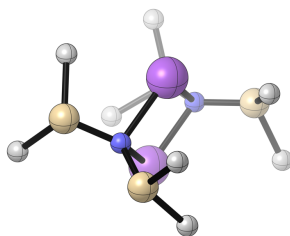
**Table S36.** Geometric coordinates and single point energies for NaHMDS unsolvated dimer.

G = -2069.611626 Hartrees

G<sub>SP</sub> = -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

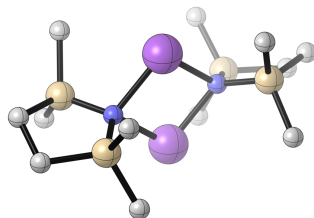
**Table S37.** Geometric coordinates and single point energies for NaTMDS unsolvated dimer.

G = -1912.612565 Hartrees

G<sub>SP</sub> = -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

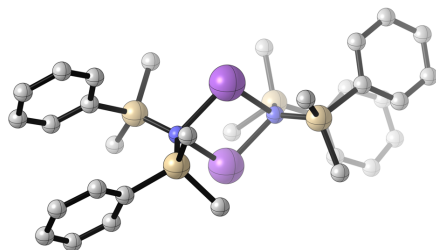
G<sub>SP</sub> = -2068.420947 Hartrees

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.



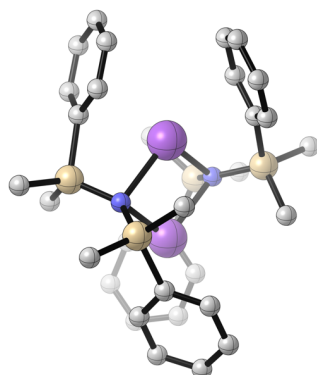
G = -2835.522747 Hartrees

G<sub>SP</sub> = -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.

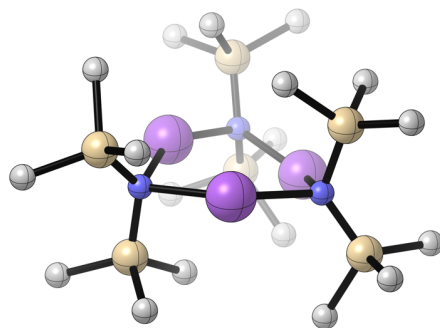


G = -2835.500531 Hartrees

G<sub>SP</sub> = -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.

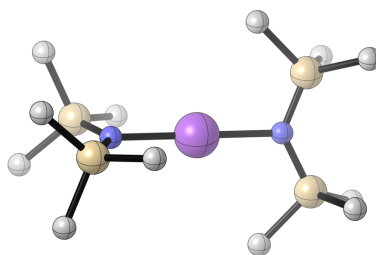
G = -3104.42812 Hartrees

G<sub>SP</sub> = -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  $(\text{SiMe}_3)_2\text{-N-Na-N}(\text{SiMe}_3)_2$  anion piece of triple ion.



G = -1907.397903 Hartrees

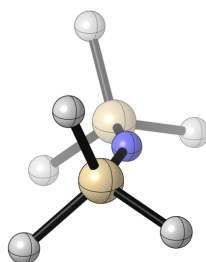
G<sub>SP</sub> = -1908.549853 Hartrees

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<sub>3</sub>)<sub>2</sub>N anion piece of separated ion pair.

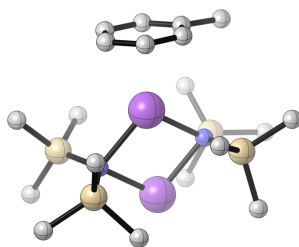


G = -872.551192 Hartrees

G<sub>SP</sub> = -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.



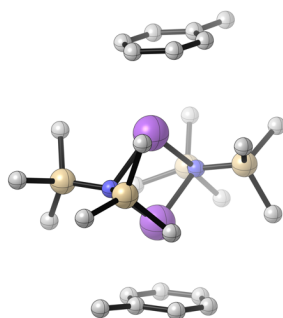
G = -2340.744069 Hartrees

G<sub>SP</sub> = -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.



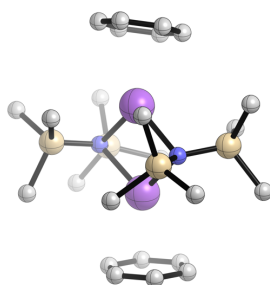
G = -2611.872211 Hartrees

G<sub>SP</sub> = -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

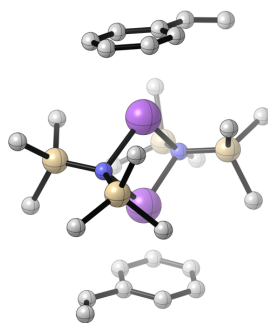
G<sub>SP</sub> = -2535.091764 Hartrees

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.



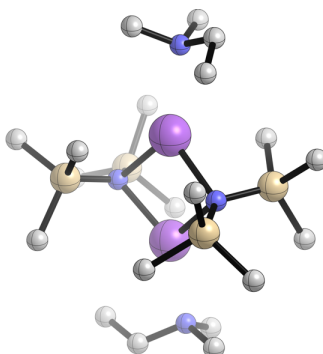
G = -2687.942165 Hartrees

G<sub>SP</sub> = -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.



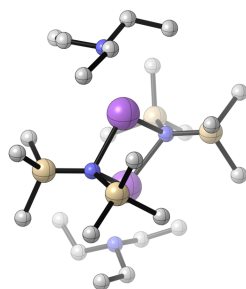
G = -2496.387851 Hartrees

G<sub>SP</sub> = -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.



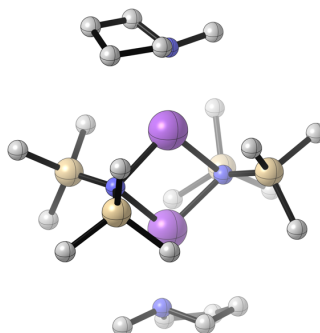
G = -2653.325993 Hartrees

G<sub>SP</sub> = -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

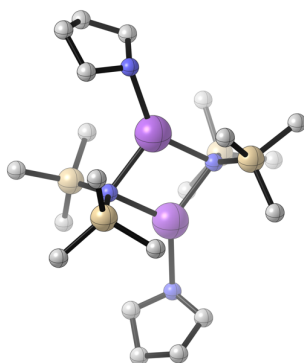
G<sub>SP</sub> = -2574.267725 Hartrees

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.



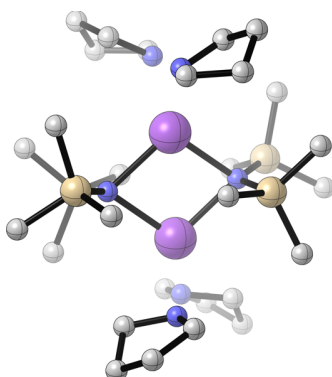
G = -2494.048679 Hartrees

G<sub>SP</sub> = -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

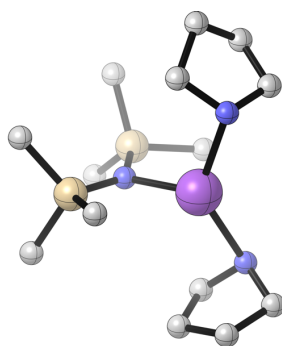
G<sub>SP</sub> = -2920.596227 Hartrees

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.



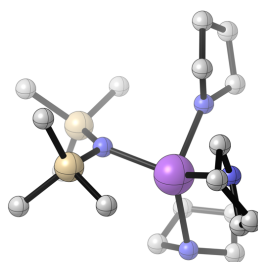
G = -1459.214564 Hartrees

G<sub>SP</sub> = -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

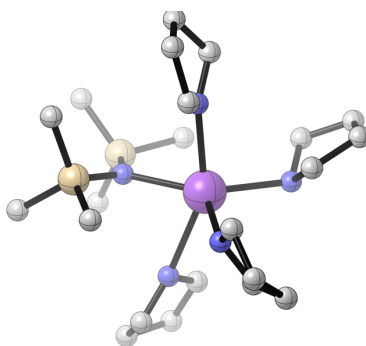
G<sub>SP</sub> = -1672.737941 Hartrees

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.



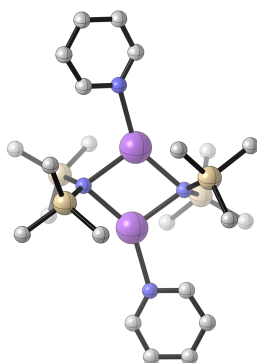
G = -1883.637203 Hartrees

G<sub>SP</sub> = -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.



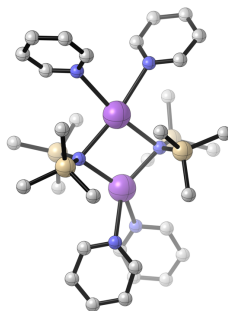
G = -2565.477035 Hartrees

G<sub>SP</sub> = -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.



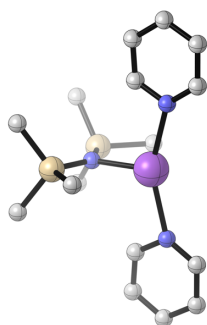
G = -3061.307522 Hartrees

G<sub>SP</sub> = -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

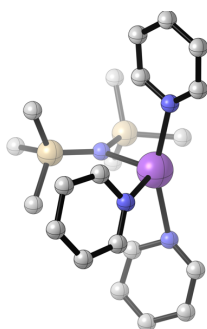
G<sub>SP</sub> = -1531.790063 Hartrees

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.



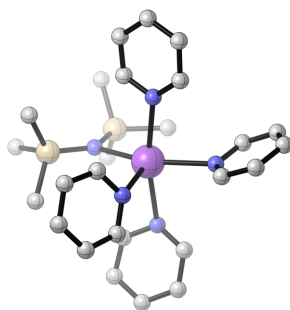
G = -1778.568232 Hartrees

G<sub>SP</sub> = -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.

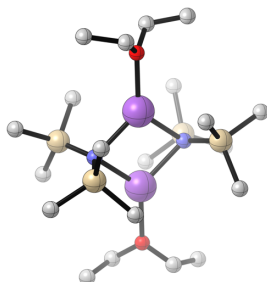


G = -2026.490481 Hartrees

G<sub>SP</sub> = -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<sub>2</sub>O dimer.

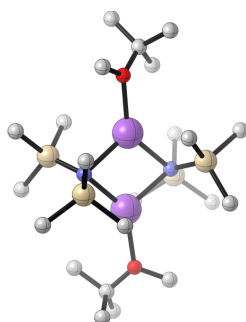
G = -2536.125652 Hartrees

G<sub>SP</sub> = -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

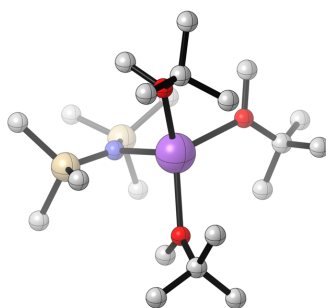
G<sub>SP</sub> = -2616.424086 Hartrees

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.



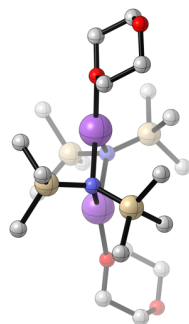
G = -1852.25893 Hartrees

G<sub>SP</sub> = -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.



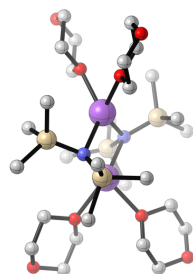
G = -2684.014117 Hartrees

G<sub>SP</sub> = -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<sub>SP</sub> = -3301.000578 Hartrees

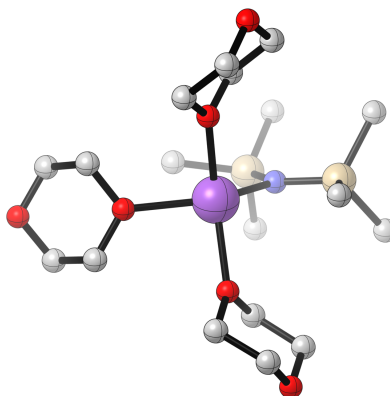
Atom	X	Y	Z	Atom	X	Y	Z
Si	0.7553370	-2.7621160	1.2851670	H	-0.2809900	-5.0577840	1.1252730
N	-0.0005390	-1.9158720	0.0000310	H	0.4598260	-4.7888990	2.7164770
Na	-1.4480080	0.0002580	0.0000410	C	4.3077290	-0.1642070	1.7281560
Na	1.4476780	-0.0001920	-0.0001530	O	3.2200890	0.6445490	1.3126900
N	0.0005870	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.



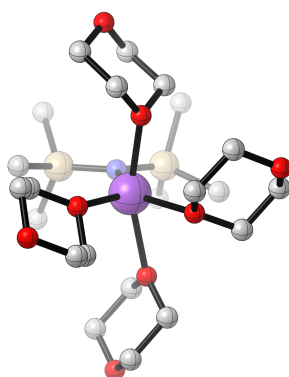
**G** = -1956.372468 Hartrees

**G<sub>SP</sub>** = -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.



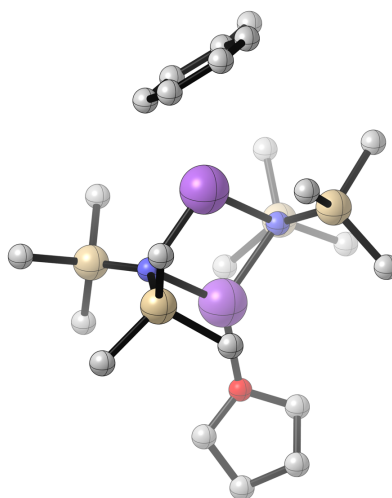
**G** = -2263.560388 Hartrees

**G<sub>SP</sub>** = -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.



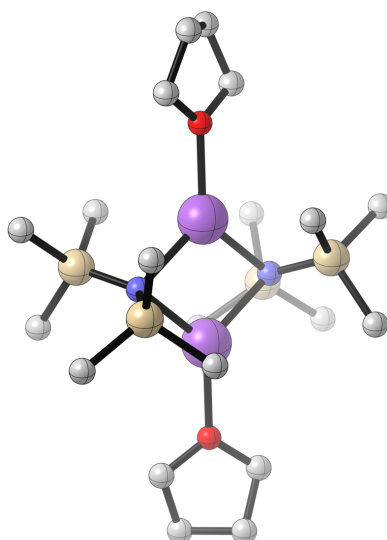
**G** = -2572.819764 Hartrees

**G<sub>SP</sub>** = -2572.158453 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

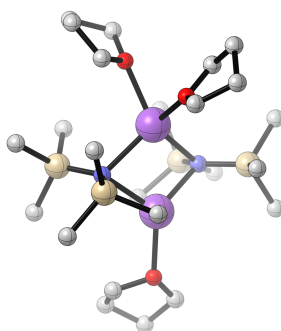
**G<sub>SP</sub>** = -2533.120241 Hartrees

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.



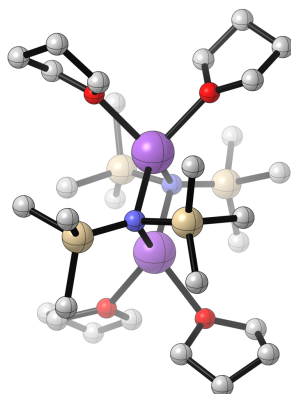
**G** = -2765.831427 Hartrees

**G<sub>SP</sub>** = -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

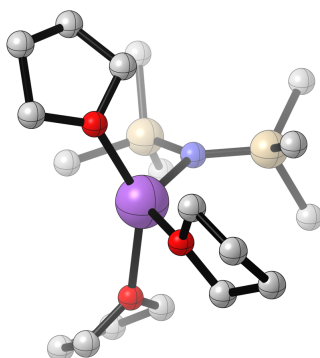
**G<sub>SP</sub>** = -2997.013147 Hartrees

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.



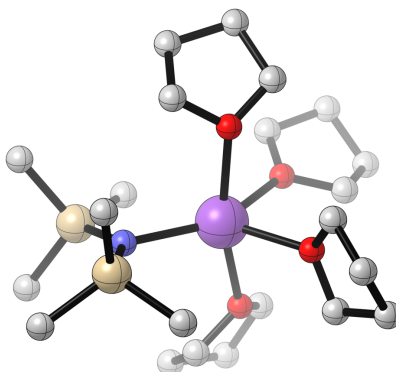
$G = -1731.006704$  Hartrees

$G_{SP} = -1732.396722$  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

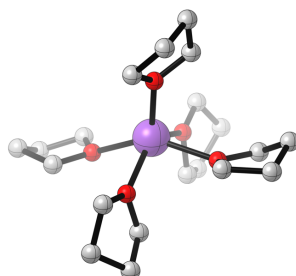
$G_{SP} = -1964.727222$  Hartrees

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.



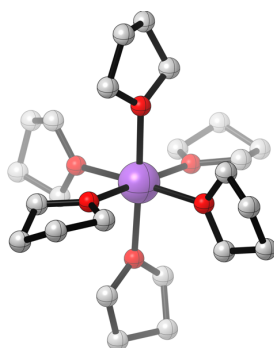
G = -1322.459668 Hartrees

G<sub>SP</sub> = -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.



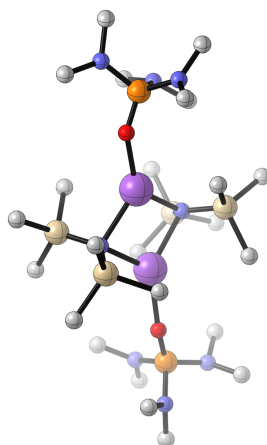
G = -1554.536592 Hartrees

G<sub>SP</sub> = -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<sub>SP</sub> = -3711.050065 Hartrees

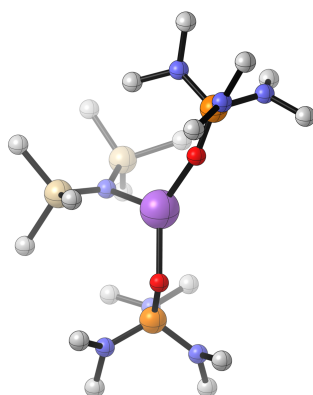
Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.5664420	0.4046260	-0.0754600	H	1.9687200	3.7063750	2.0476130
N	0.0794330	2.0635710	-0.0229720	H	0.9515430	3.6187890	3.5104620
Na	1.3683670	0.1372210	-0.1452490	H	1.6986510	2.1427120	2.8544820
N	-0.2803510	-1.5687600	0.0969770	Si	0.5672310	2.8924880	-1.4341090
Si	-0.5191320	-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.



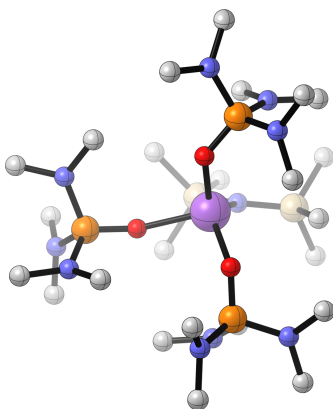
G = -2673.639552 Hartrees

G<sub>SP</sub> = -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

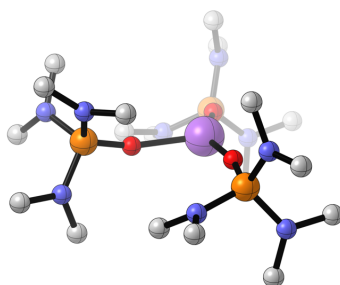
G<sub>SP</sub> = -3495.731653 Hartrees

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.



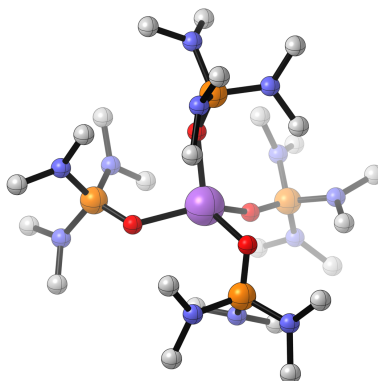
G = -2620.387829 Hartrees

G<sub>SP</sub> = -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<sub>SP</sub> = -3442.626722 Hartrees

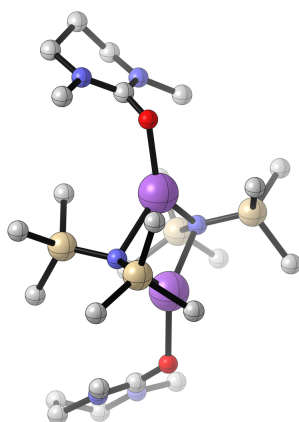
Atom	X	Y	Z	Atom	X	Y	Z
Na	-0.0631850	-0.3487530	0.0856390	H	0.5678010	-3.0268830	-0.8068320
O	1.6354010	0.5101470	-0.9815750	H	1.5855720	-1.9005610	-1.7470920
P	2.6520390	1.5418740	-1.3833220	C	3.7726720	-2.0884680	-0.3148200
N	1.9368440	2.8222380	-2.1747480	H	4.3630210	-1.8960630	0.5884790
C	2.5819180	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

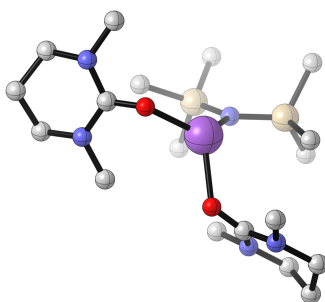
G<sub>SP</sub> = -2911.682836 Hartrees

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.



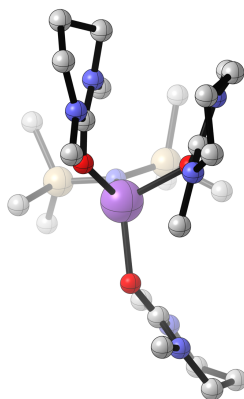
G = -1874.71751 Hartrees

G<sub>SP</sub> = -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

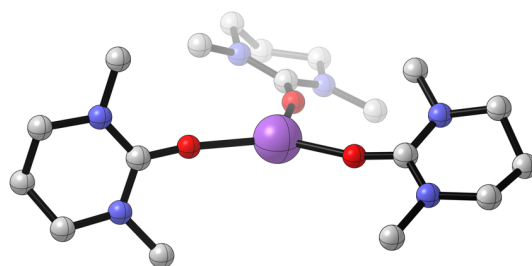
G<sub>SP</sub> = -2296.679577 Hartrees

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.



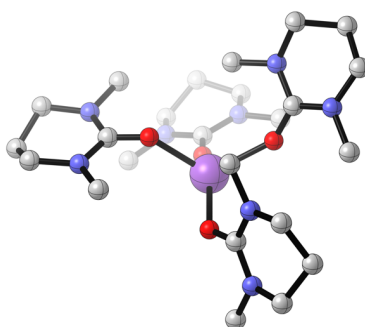
G = -1422.00152 Hartrees

G<sub>SP</sub> = -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.



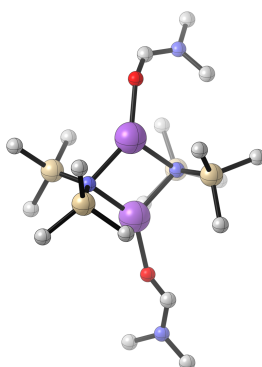
G = -1841.966869 Hartrees

G<sub>SP</sub> = -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.



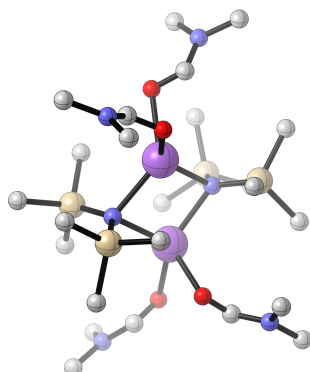
G = -2565.894022 Hartrees

G<sub>SP</sub> = -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<sub>SP</sub> = -3064.478895 Hartrees

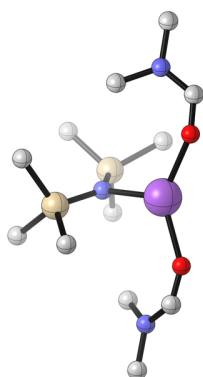
Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.3746360	0.3435970	0.0620200	H	4.2236260	0.5481030	-0.1043360
N	-0.4873010	-1.8623790	0.2998600	Si	-0.9685370	-2.7380420	-1.0838020
Na	1.4204690	-0.4857560	0.2253580	C	-1.1277210	-1.5858370	-2.5782120
N	0.5256380	1.7428580	0.2361890	H	-1.8897920	-0.8011410	-2.4391030
Si	0.5176280	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.



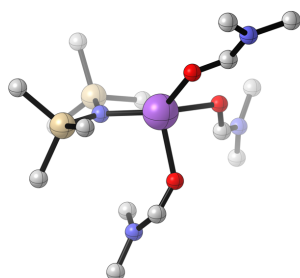
G = -1531.066646 Hartrees

G<sub>SP</sub> = -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.



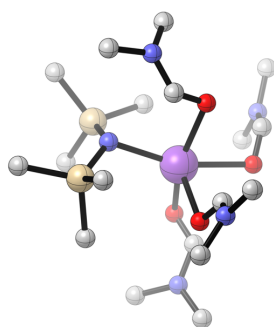
G = -1779.193206 Hartrees

G<sub>SP</sub> = -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

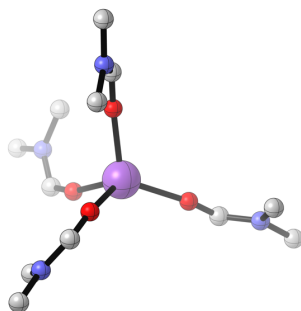
G<sub>SP</sub> = -2029.056022 Hartrees

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.



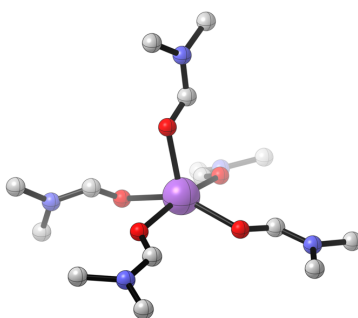
G = -1154.656055 Hartrees

G<sub>SP</sub> = -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.



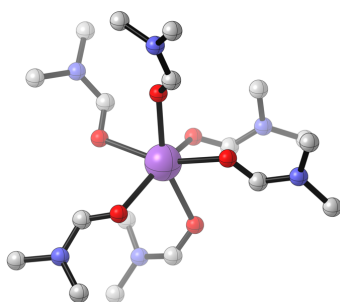
G = -1402.789499 Hartrees

G<sub>SP</sub> = -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.



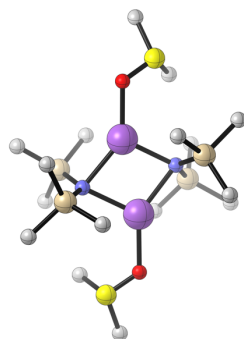
G = -1650.920751 Hartrees

G<sub>SP</sub> = -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

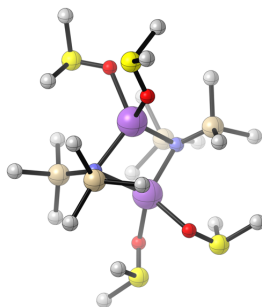
G<sub>SP</sub> = -3177.089036 Hartrees

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.



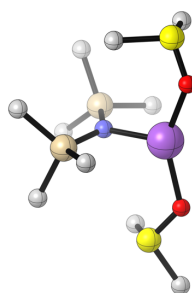
G = -4280.807505 Hartrees

G<sub>SP</sub> = -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.



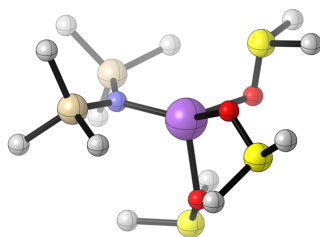
G = -2140.395238 Hartrees

G<sub>SP</sub> = -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.



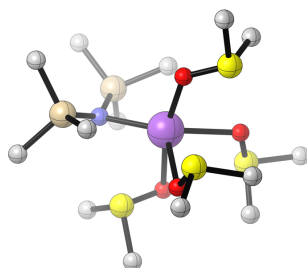
G = -2693.187629 Hartrees

G<sub>SP</sub> = -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

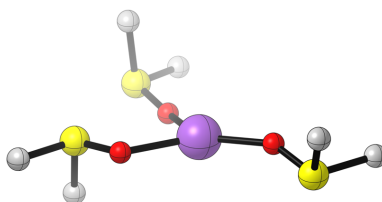
G<sub>SP</sub> = -3247.927531 Hartrees

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.

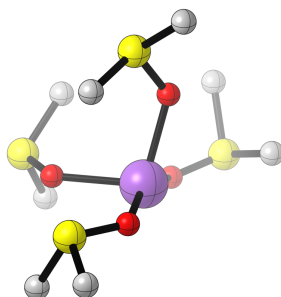


G = -1820.502293 Hartrees

G<sub>SP</sub> = -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.



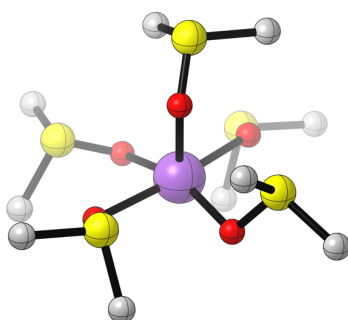
G = -2373.308057 Hartrees

G<sub>SP</sub> = -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.



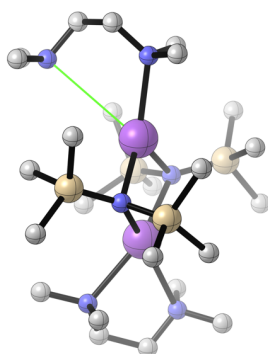
G = -2926.111957 Hartrees

G<sub>SP</sub> = -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<sub>SP</sub> = -2765.821037 Hartrees

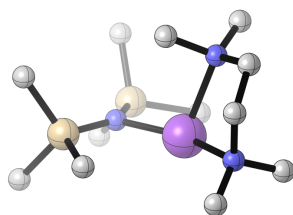
Atom	X	Y	Z	Atom	X	Y	Z
N	0.2894380	1.8569280	0.0388730	H	-0.6427280	5.0783660	0.1551780
Na	1.7377060	-0.0981030	-0.1733730	H	-1.9749690	4.1378710	0.8462750
Na	-1.3054120	0.1157010	0.4197330	H	-0.9459960	5.1337020	1.9018090
N	0.1844440	-1.7404070	0.6075800	N	-3.6728600	0.4986390	1.2226660
Si	0.7675580	-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.



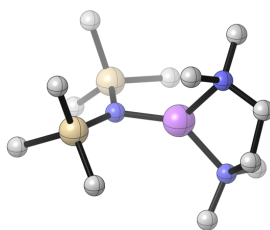
G = -1381.908281 Hartrees

G<sub>SP</sub> = -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.



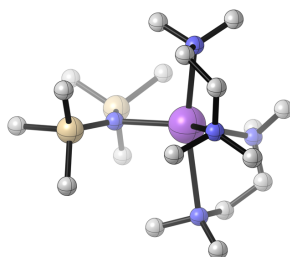
G = -1227.22675 Hartrees

G<sub>SP</sub> = -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.



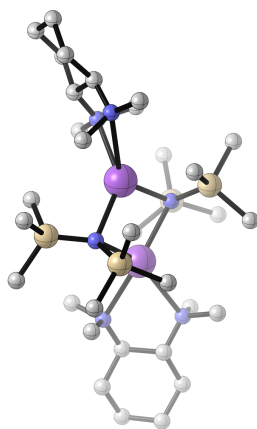
G = -1729.011139 Hartrees

G<sub>SP</sub> = -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<sub>SP</sub> = -3077.699253 Hartrees

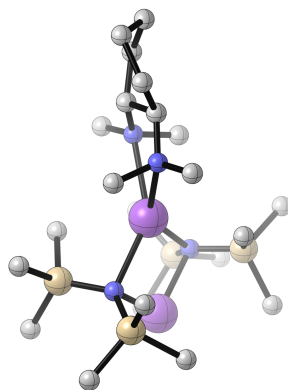
Atom	X	Y	Z	Atom	X	Y	Z
Na	1.5988980	-0.1281490	-0.0283950	H	5.3039760	-3.0361640	0.2825190
N	-0.0101300	-1.9520580	-0.2816790	H	4.5983840	-2.1100120	1.6384630
Na	-1.5205070	-0.0276390	-0.1702010	H	3.5555580	-3.0911840	0.6042160
N	-0.0234350	1.8474340	-0.3993980	H	5.0025660	-2.2593210	-2.0057870
Si	0.4836080	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.



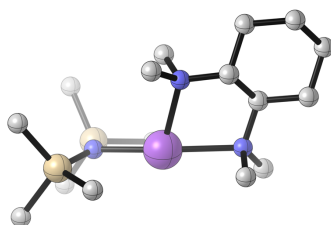
G = -2572.497021 Hartrees

G<sub>SP</sub> = -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.



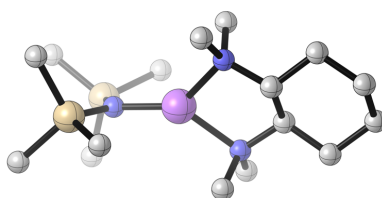
G = -1537.683691 Hartrees

G<sub>SP</sub> = -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.



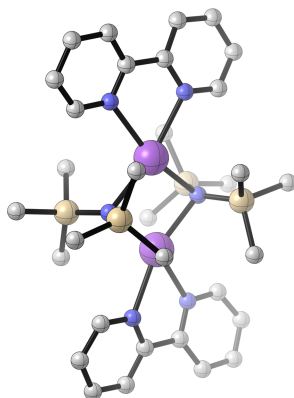
G = -1383.003398 Hartrees

G<sub>SP</sub> = -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

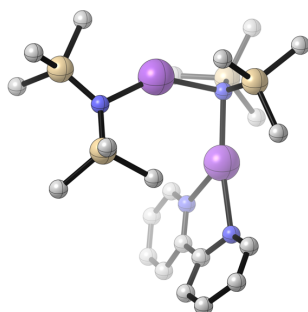
G<sub>SP</sub> = -3061.263951 Hartrees

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.



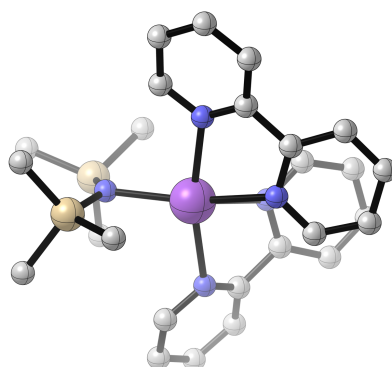
G = -2564.291623 Hartrees

G<sub>SP</sub> = -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.



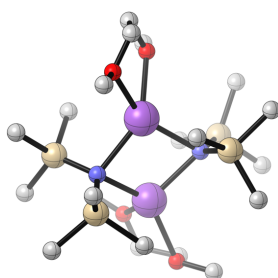
G = -2024.16868 Hartrees

G<sub>SP</sub> = -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.



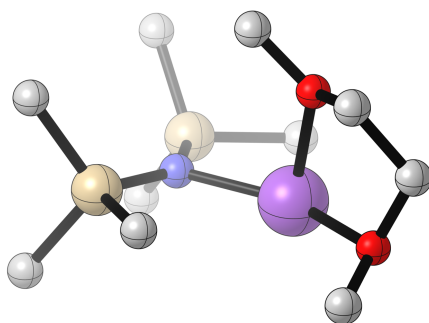
G = -2686.355084 Hartrees

G<sub>SP</sub> = -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

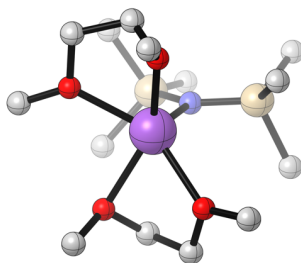
G<sub>SP</sub> = -1344.114079 Hartrees

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.



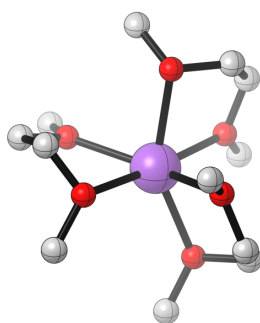
G = -1651.524745 Hartrees

G<sub>SP</sub> = -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.

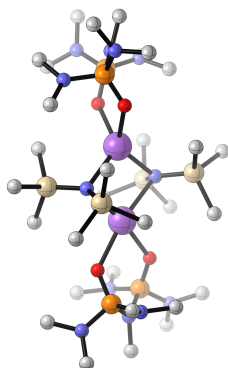


G -1087.214075 Hartrees

G<sub>SP</sub> = -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<sub>SP</sub> = -5002.574597 Hartrees

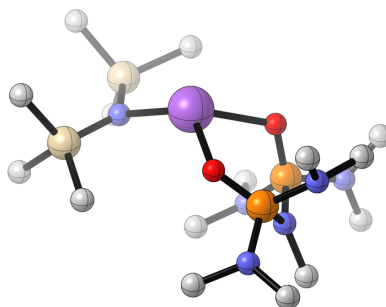
Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.5880630	-0.0268000	0.2337810	H	1.1265980	-4.9592130	-0.1443490
N	-0.0970000	-1.7896990	-0.3336780	H	2.4462270	-3.7546660	-0.1079700
Na	1.4831100	-0.0052670	0.0843710	H	2.0202690	-4.6834670	1.3676200
N	-0.1006490	1.7086550	0.8316110	Si	-0.2924760	-2.2444210	-1.9598850
Si	-0.1446230	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.



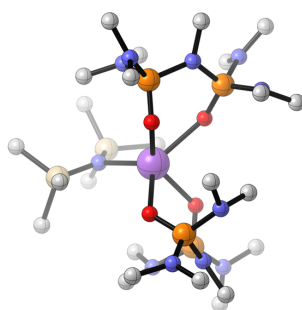
G = -2499.495146 Hartrees

G<sub>SP</sub> = -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

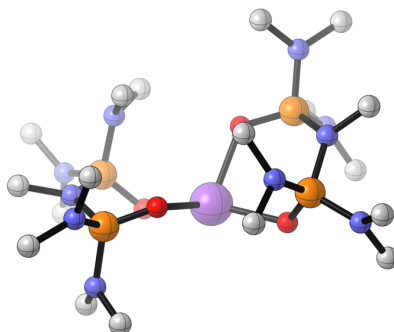
G<sub>SP</sub> = -3967.14406 Hartrees

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.



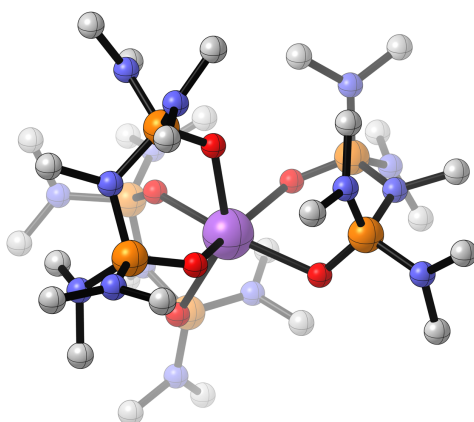
G = -3091.536447 Hartrees

G<sub>SP</sub> = -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<sub>SP</sub> = -4559.81512 Hartrees

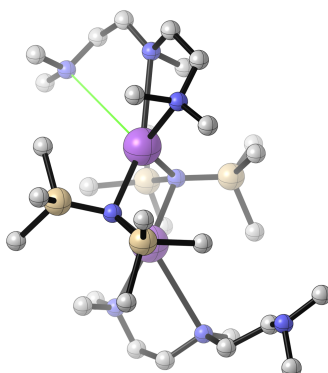
Atom	X	Y	Z	Atom	X	Y	Z
Na	0.0816630	-0.0709330	-0.6016480	H	-4.6406690	0.7003170	2.7558480
P	-0.9148330	-2.7284660	1.4172570	H	-5.5304980	3.2397260	1.0119870
N	-1.4922720	-2.4571970	2.9572900	H	-4.4958710	2.6956840	-0.3416460
C	-2.0607750	-3.4646540	3.8290580	C	-3.4983900	-3.3063900	0.8443970
H	-1.4609590	-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

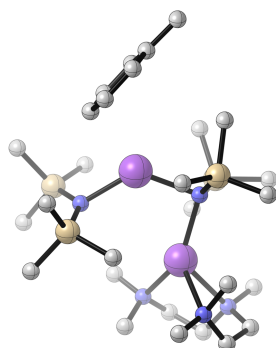
G<sub>SP</sub> = -3112.122829 Hartrees

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<sub>SP</sub> = -2862.894435 Hartrees

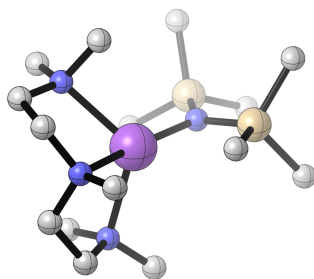
Atom	X	Y	Z	Atom	X	Y	Z
Na	-1.9847120	-0.2245020	0.0750880	C	-0.5469580	-4.3153440	1.3253130
Na	1.4742940	0.0906500	-0.1416620	H	-1.3249790	-4.0876530	2.0676090
N	1.1065740	2.3068110	0.0996460	H	-1.0406420	-4.7047750	0.4211980
Si	0.6538180	2.6288470	1.6981830	H	0.0705360	-5.1269530	1.7416230
C	-0.6030870	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.



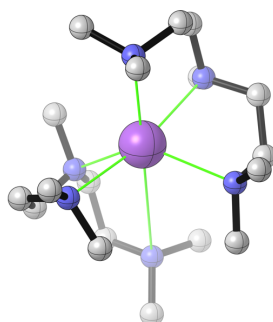
G = -1554.884204 Hartrees

G<sub>SP</sub> = -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.



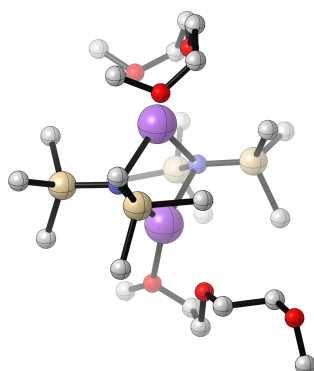
G = -1202.270772 Hartrees

G<sub>SP</sub> = -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 disolvated dimer.



G = -2993.531565 Hartrees

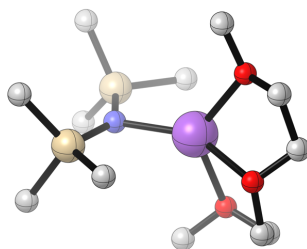
G<sub>SP</sub> = -2995.78937 Hartrees

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 monosolvated monomer.



G = -1496.760861 Hartrees

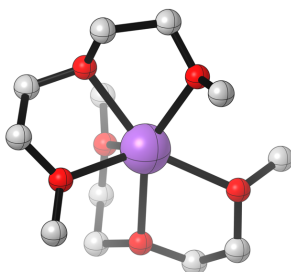
G<sub>SP</sub> = -1497.89186 Hartrees

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.



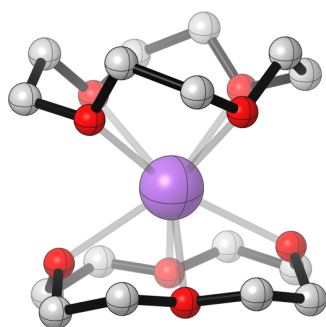
G = -1086.045878 Hartrees

G<sub>SP</sub> = -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.



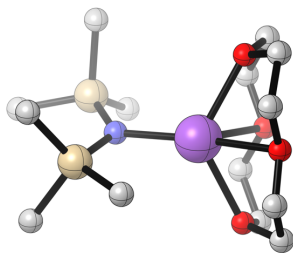
G = -1390.901291 Hartrees

G<sub>SP</sub> = -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.



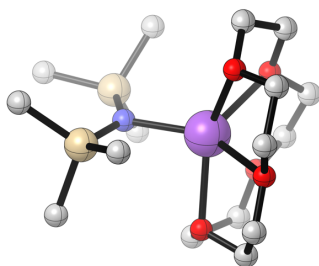
G = -1649.17557 Hartrees

G<sub>SP</sub> = -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

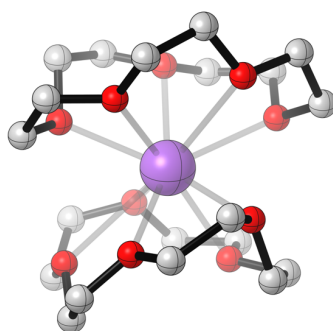
G<sub>SP</sub> = -1804.266908 Hartrees

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.



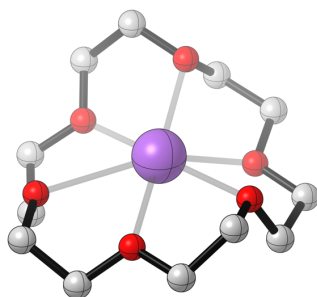
G = -1698.099228 Hartrees

G<sub>SP</sub> = -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.



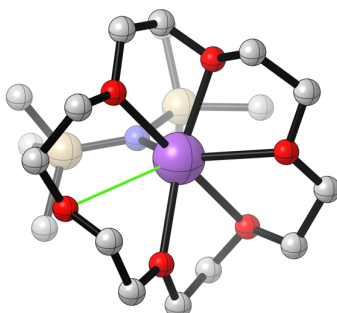
G = -1083.697944 Hartrees

G<sub>SP</sub> = -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.



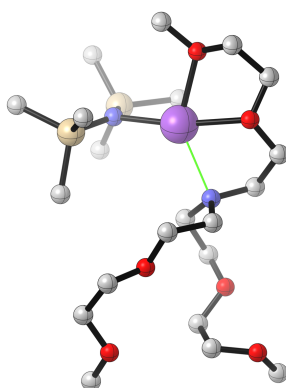
G = -1956.382789 Hartrees

G<sub>SP</sub> = -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

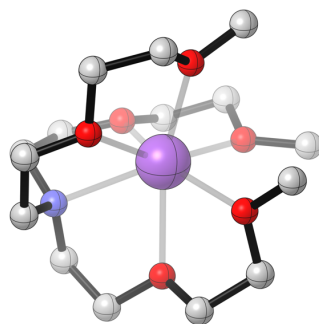
G<sub>SP</sub> = -2132.352323 Hartrees

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.



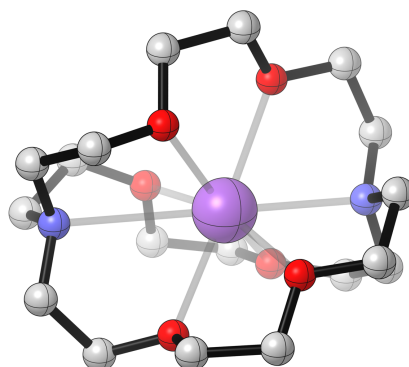
G = -1257.851318 Hartrees

G<sub>SP</sub> = -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.



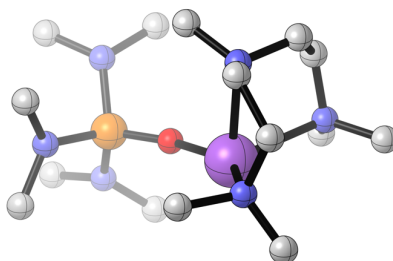
G = -1428.485745 Hartrees

G<sub>SP</sub> = -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.



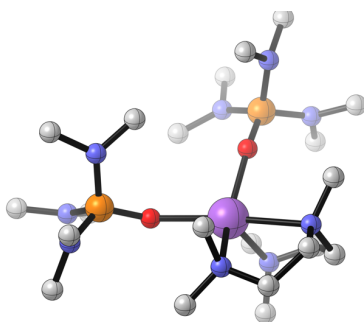
G -1501.622245 Hartrees

G<sub>SP</sub> = -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

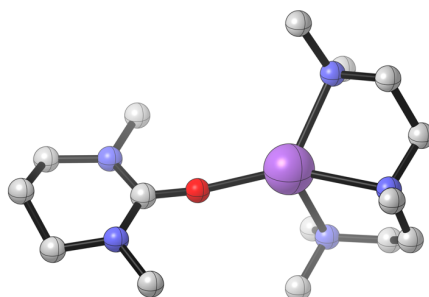
G<sub>SP</sub> = -2323.071221 Hartrees

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.



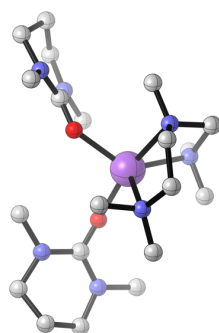
G = -1102.160998 Hartrees

G<sub>SP</sub> = -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<sub>SP</sub> = -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

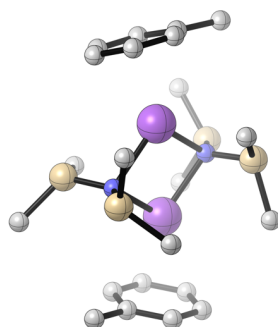
**Table S142.** Geometric coordinates and single point energies for unsolvated sodium cation.

G = -162.014812 Hartrees

G<sub>SP</sub> = -162.0655113 Hartrees

<b>Atom</b>	<b>X</b>	<b>Y</b>	<b>Z</b>	<b>Atom</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
Na	0.0000000	0.0000000	0.0000000				

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



G = -2454.877614 Hartrees

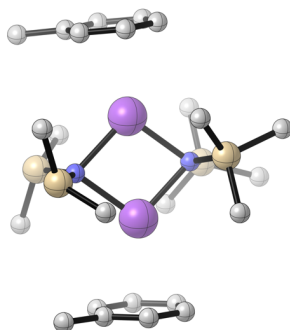
G<sub>SP</sub> = -2456.478908 Hartrees

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.



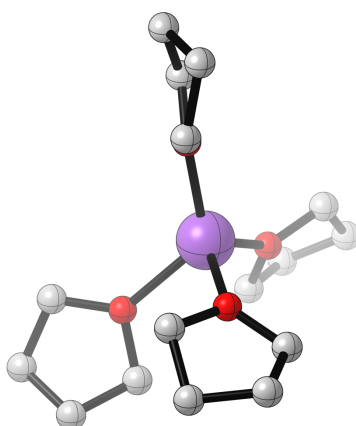
G = -2533.3757 Hartrees

G<sub>SP</sub> = -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.



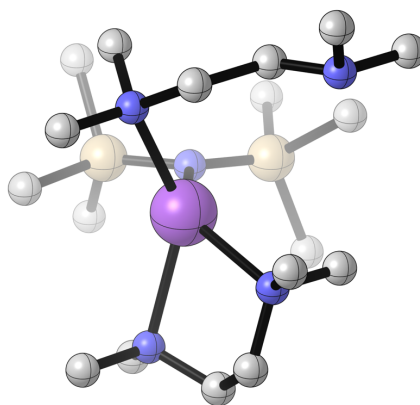
G = -1090.38512 Hartrees

G<sub>SP</sub> = -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  $\kappa^2$ - $\kappa^1$  connectivity.



G = -1729.014742 Hartrees

G<sub>SP</sub> = -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				

