Supporting Information

Sodium Isopropyl(trimethylsilyl)amide (NaPTA): A Stable and Highly Soluble Lithium Diisopropylamide Mimic

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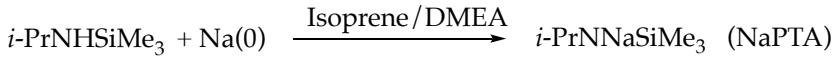


Sodium isopropyl(trimethylsilyl)amide: Method A Purified NaPTA can be prepared as a white crystalline solid as illustrated for NaPTA. Sodium dispersion in toluene (9.0 mL, 100 mmol) was added to a 100 mL Schlenk flask. The toluene was removed *in vacuo* and *N,N*-dimethylethylamine (30.0 mL) and isopropy(trimethylsilyl)amine (5.9 g, 45.0 mmol) were added to the flask. While stirring, isoprene (750 μL, 7.5 mmol) was added over the course of 10 min. Stirring was halted after 30 min, and the mixture was filtered through a fine frit and evaporated to dryness to give a yellowish solid. Recrystallization from hexane gave NaPTA as a white solid (5.5 g, 80% yield.)

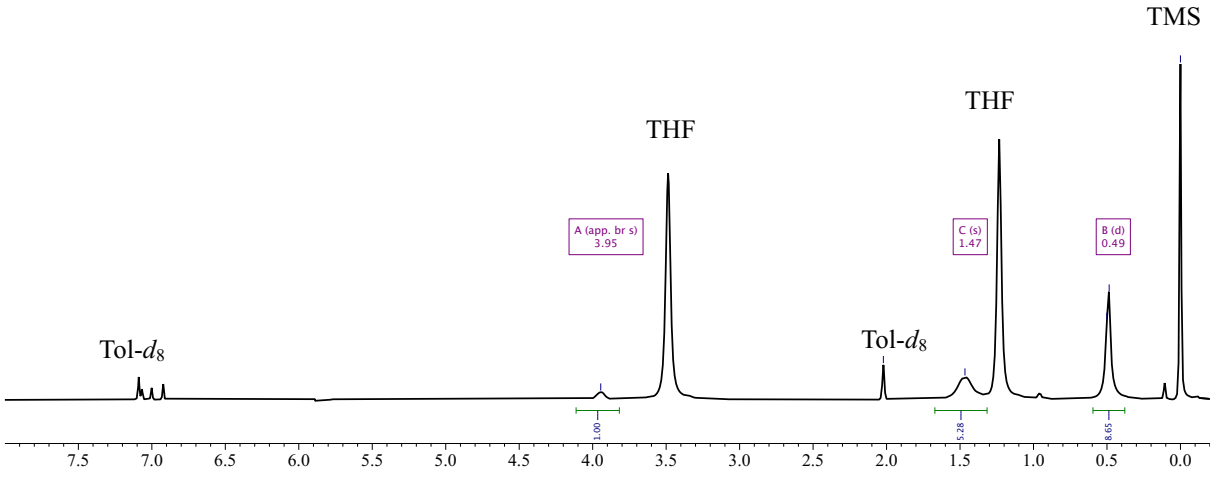


Figure S1. ^{1}H NMR spectrum (10% THF/toluene-d_8, 500 MHz) of NaPTA at –110 ^{o}C. δ 3.95 (app,br s 1H), 1.47 (br s, 6H), 0.49 (s, 9H).

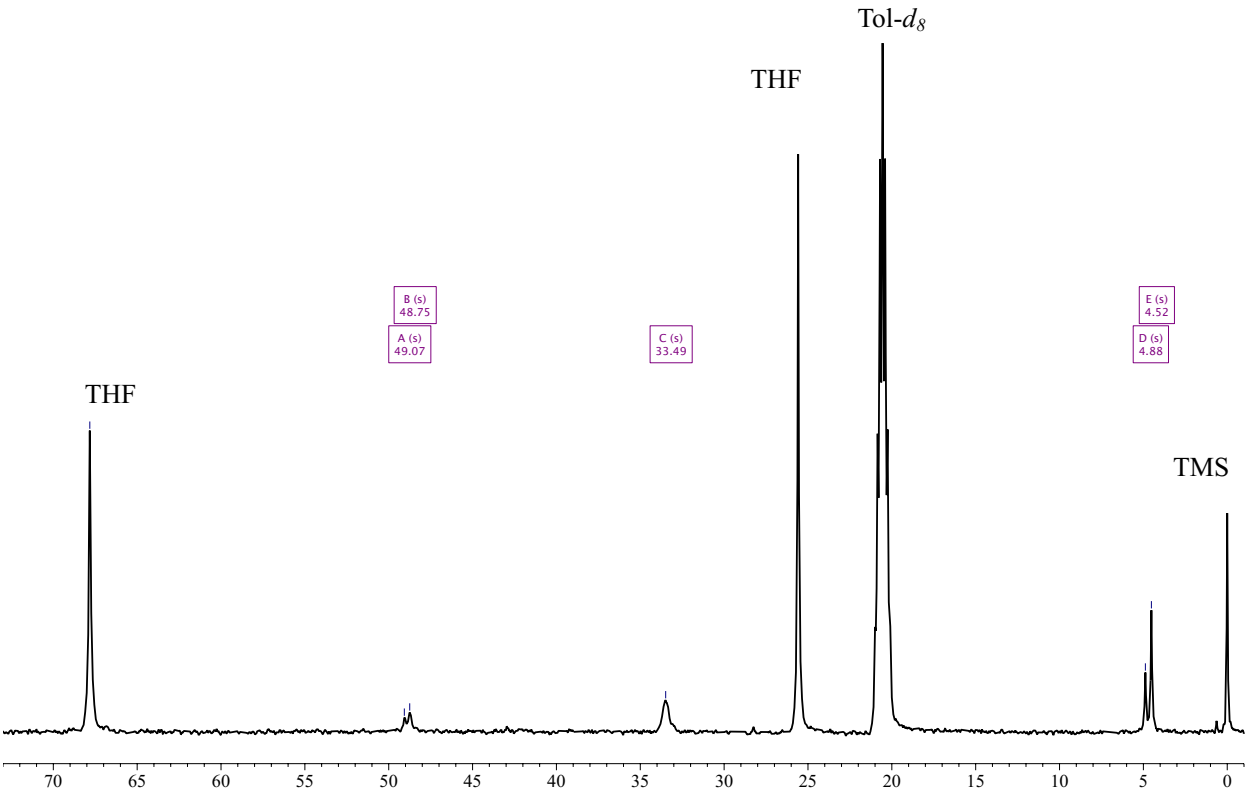


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum (10% THF/ toluene-d_8, 125.8 MHz) of NaPTA at –110: δ 49.1, 48.8, 33.5, 4.9, 4.5.

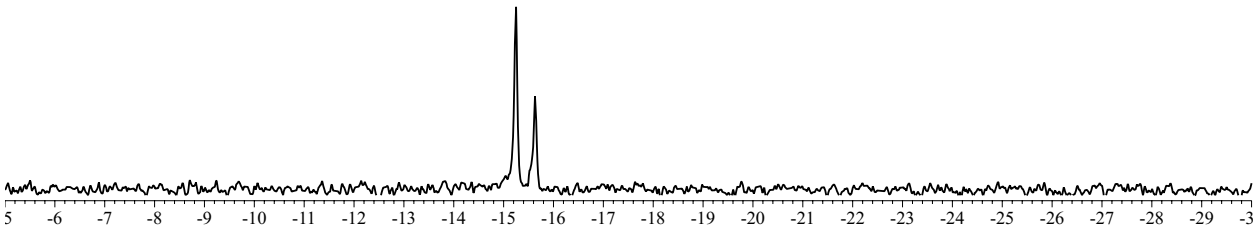


Figure S3. ^{29}Si NMR spectrum (10% THF/ toluene-d_8, 99.36MHz) of 0.30 M NaPTA at –110 ºC: δ –15.3, –15.6.

Method B. A 2.0–2.5 M solution of NaPTA in neat THF to be used without any purification was prepared as follows. Sodium slices (1.2 g) cut from sodium cubes were placed in a 50.0 mL pear-shaped flask. Dry THF (15.0 mL) and isopropyl(trimethylsilyl)amine (5.24 mL, 40.0 mmol) were added to the flask under positive argon pressure and the mixture was maintained at 20 °C. Isoprene (1.85 mL, 20.0 mmol) was added at 0 °C all at once. Stirring for 2 min yielded a brown-yellow solution. Darkening of the sodium surface appears to correlate with the completion of the reaction. The solution is readily decanted by canula from unreacted sodium slices. Titration routinely affords 80–90% of the anticipated normality (1.7–1.9 M). The spent sodium is quenched by sequentially adding hexane followed by isopropanol.

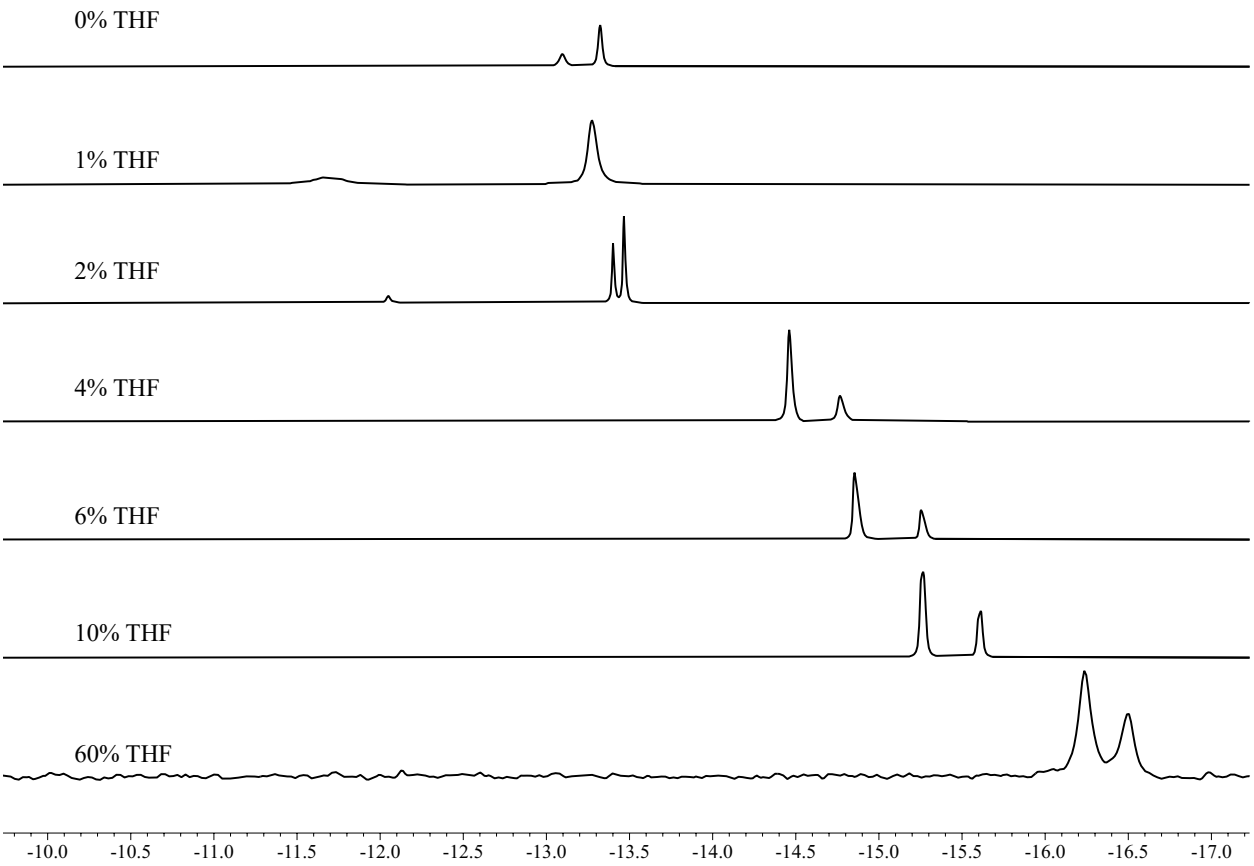
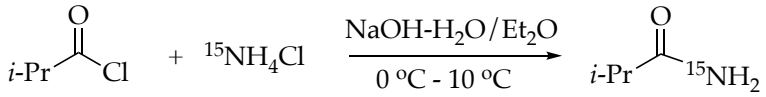


Figure S4. ^{29}Si NMR spectra (99.36 MHz) of 0.30 M NaPTA in toluene-d_8 at varying THF concentrations at –110 ºC. Migration shows possibly toluene effect or possibly higher solvates intervening.

Synthesis of [^{15}N]NaPTA



[^{15}N]isobutyramide. Isobutyryl chloride (15.0 mL, 120.0 mmol) in the Et_2O (50 mL) was layered onto a solution of [^{15}N]NH_4Cl (5.0 g, 91.5 mmol) in H_2O (20.0 mL) in 250.0 mL flask. The flask was cooled 0 °C, and NaOH (22.0 g, 550 mmol) in H_2O (30 mL) was slowly added by pipette to the aqueous layer with slow stirring to avoid mixing of layers. A white precipitate formed during the addition. The flask was warmed to room temperature with stirring for 15 mins followed by vigorous stirring for an additional 10 min. The white solid was collected by filtration and washed with Et_2O. After drying under vacuum, the resulting white solid was purified by flash chromatography (15% EtOAc/hexane) to give [^{15}N]isobutyramide (9.5 g, 90% yield). HRMS (DART-Orbitrap) m/z $[M+H]^+$ calcd for $C_4H_{10}NO$ 89.0727, found 89.0726

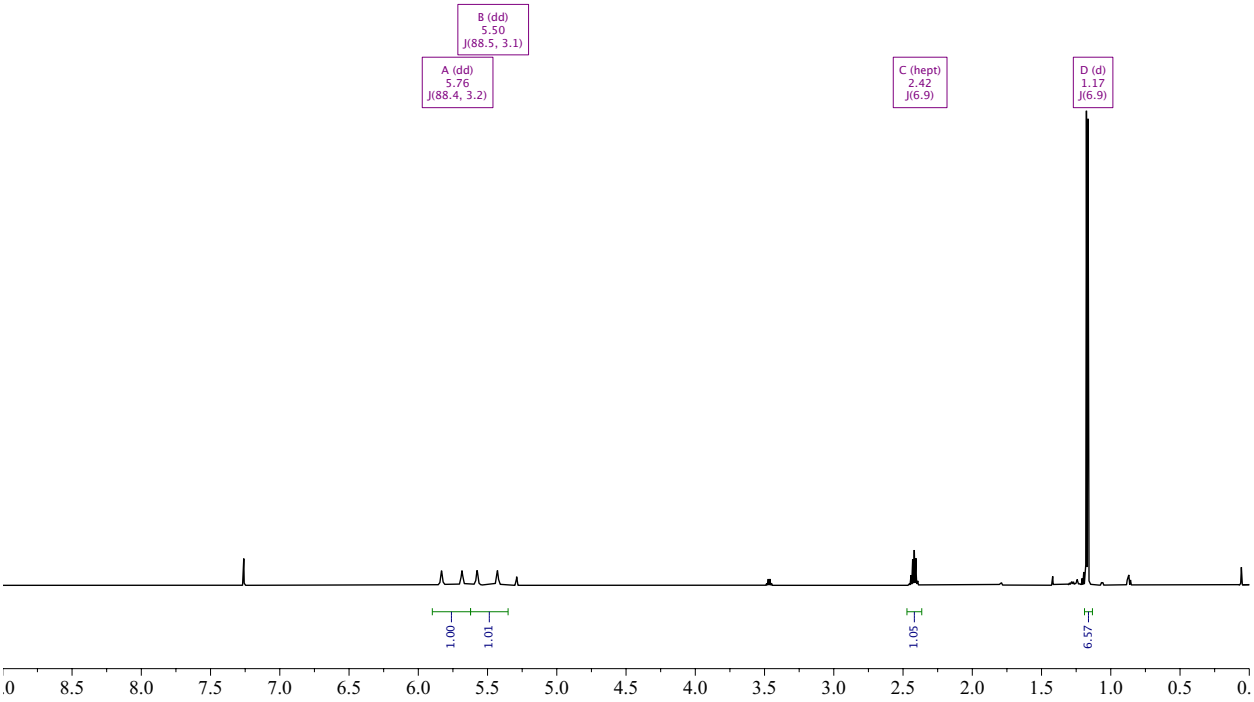


Figure S5. ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of [^{15}N]isobutyramide at room temperature. δ 5.76 (dd, $J_{H\text{-}N}$ = 88.4, $J_{H\text{-}H}$ = 3.1 Hz), 5.56 (dd, $J_{H\text{-}N}$ = 88.4, $J_{H\text{-}H}$ = 3.2 Hz, 1H), 2.42 (hept, J = 6.9 Hz, 1H), 1.17 (d, $J_{H\text{-}H}$ = 6.9 Hz, 6H).

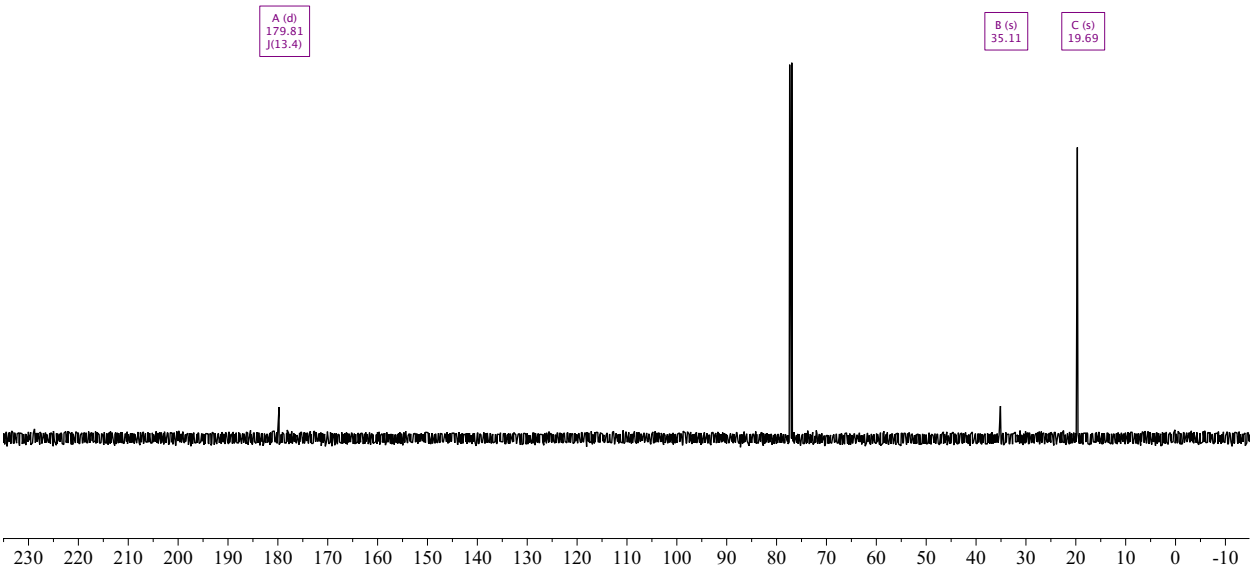
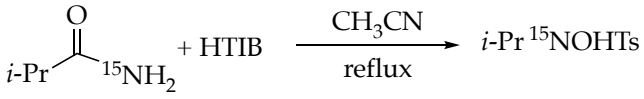


Figure S6. $^{13}C\{^{1}H\}$ NMR (D_2O, 125.8 MHz) of [^{15}N]isobutyramide in at room temperature. δ 179.8 ($J_{C\text{-}N}$ = 13.4 Hz), 35.1, 19.7.



[^{15}N]Isopropyl ammonium tosylate. To a 250 mL flask containing [^{15}N]isobutyramide (8.8 g, 100.0 mmol) in CH_3CN (150 mL) was added [hydryoxy(tosyloxy)]iodobenzene (HTIB) at room temperature. The solution was refluxed for 3.0 hr, then cooled to –20 °C overnight. The resulting white solid was collected by filtration and washed with cold acetonitrile to give [^{15}N]isopropyl ammonium tosylate (9.5 g, 90% yield.)

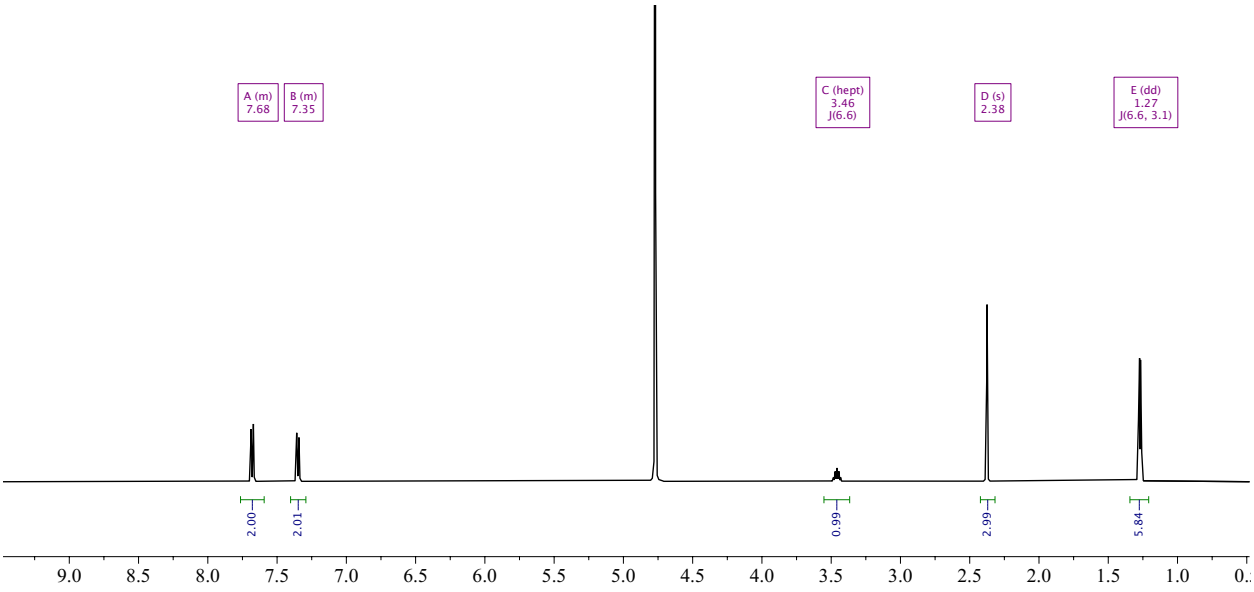


Figure SS7. ^{1}H NMR spectrum (25°C, D_2O, δ = 4.77 ppm, 500 MHz) of [^{15}N]isopropyl ammonium tosylate at room temperature. δ 7.68 (m, 2H), 7.35 (m, 1H), 3.46 (hept, $J_{H\text{-}H}$ = 6.6 Hz, 1H), 2.38 (s, 3H), 1.27 (dd, $J_{H\text{-}H}$ = 6.6 Hz, $J_{H\text{-}N}$ = 3.1 Hz, 6H).

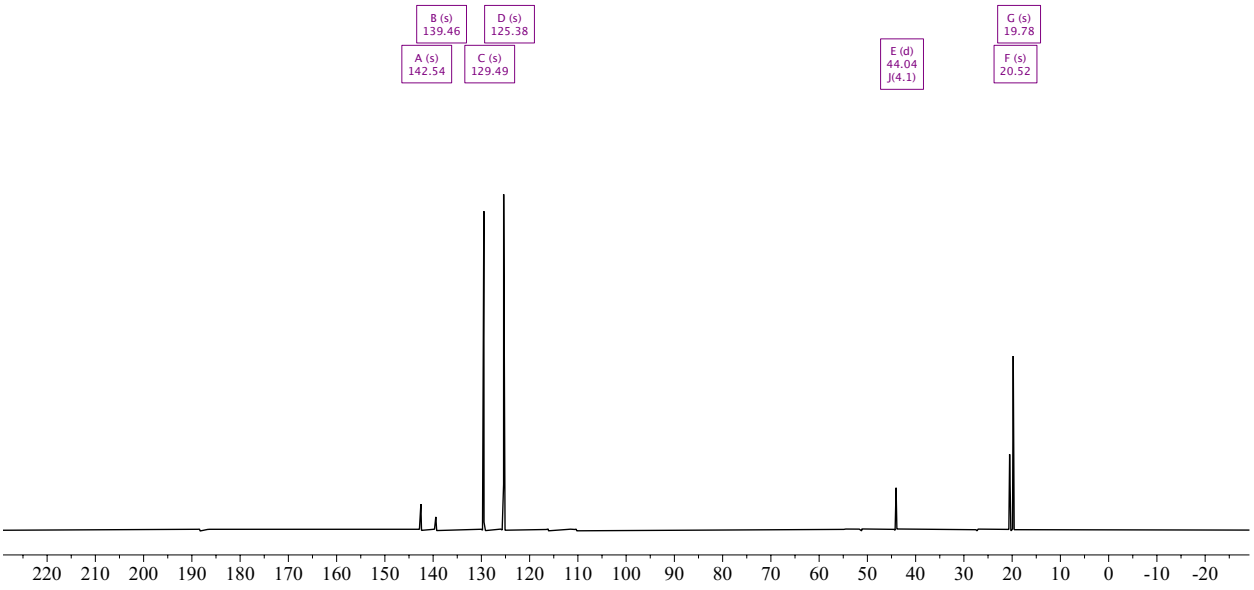
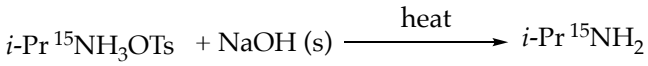


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum (25°C, D_2O, δ = 4.77 ppm, 500 MHz) of [^{15}N]isopropyl ammonium tosylate at room temperature. δ 142.5, 139.5, 129.5, 125.4, 44.0 (d, $J_{C\text{-}N}$ = 4.3 Hz), 20.5, 19.8.



[^{15}N]isopropylamine. [^{15}N]isopropyl ammonium tosylate (11.6 g, 0.050 mol) with granular NaOH (6.0 g, 0.15 mol) were added to a 50 mL one-neck round-bottom flask equipped with an NaOH-filled drying tube used to transfer the amine gas to an empty 15 mL pear flask cooled to –78 °C. The mixture was heated with a heat gun for approximately 30 min. After the transfer of the amine was complete, it was distilled at atmospheric pressure (BP = 99 °C) to afford [^{15}N]isopropylamine (1.30 g, 48% yield).

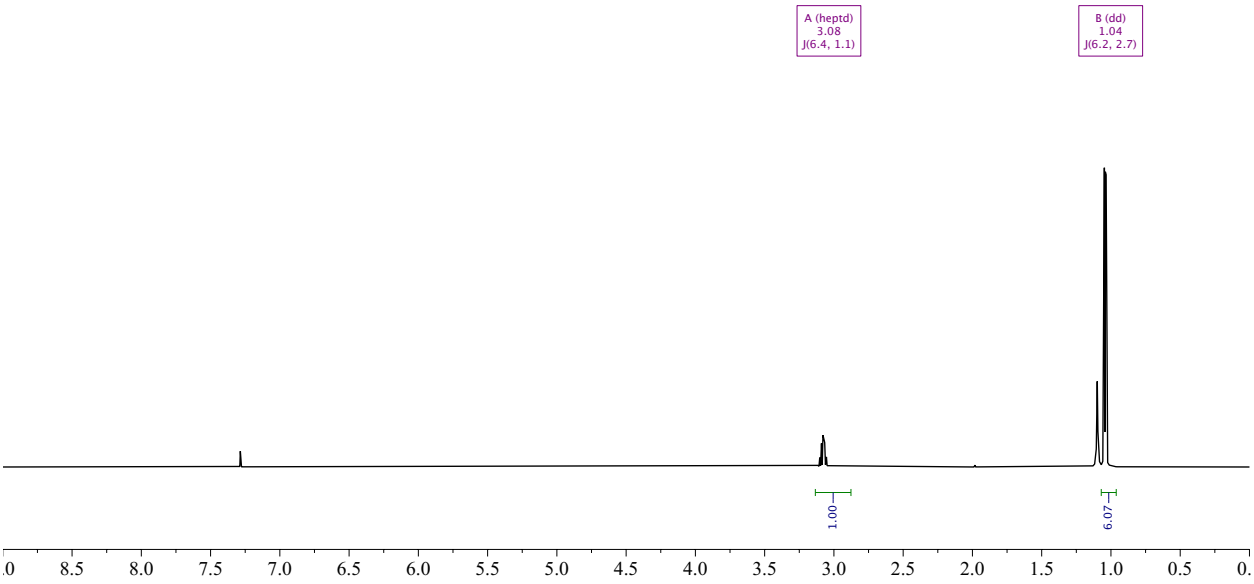


Figure S9. ^{1}H NMR spectra of [^{15}N]isopropylamine ($CDCl_3$, 500 MHz) at room temperature. δ 3.08 (heptd, $J_{H\text{-}H}$ = 6.4, $J_{H\text{-}N}$ = 1.1, Hz, 1H), 1.10 (s, 1H), 1.04 (dd, $J_{H\text{-}H}$ = 6.2, $J_{H\text{-}N}$ = 2.7 Hz, 6H).

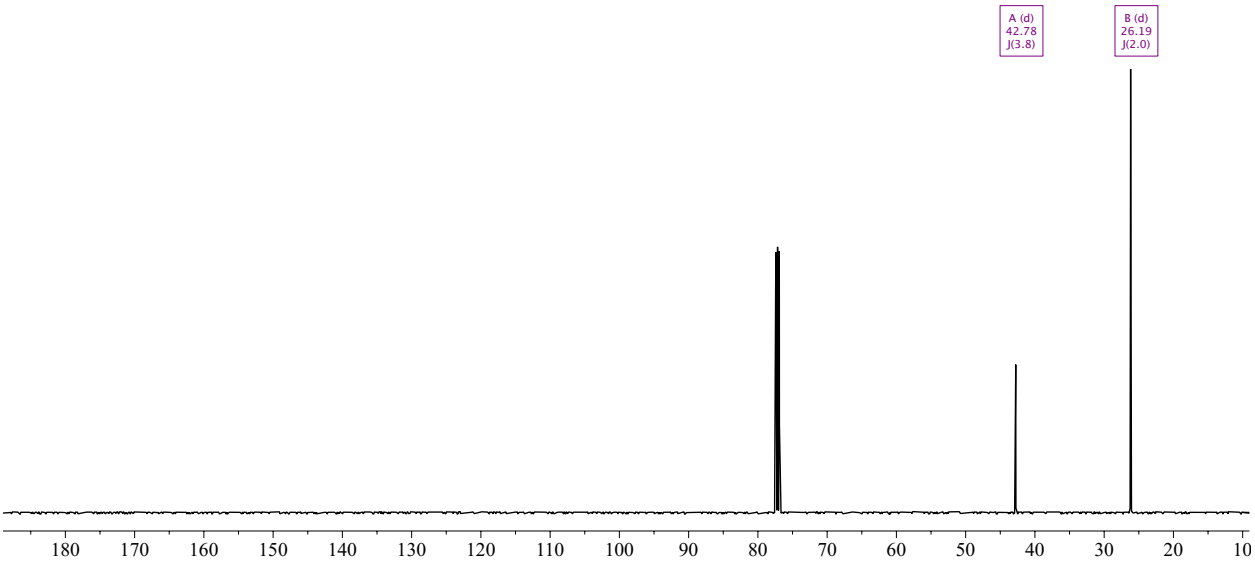


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 125.8 MHz) of [^{15}N]isopropylamine at room temperature. δ 42.7 (d, $J_{C\text{-}N}$ = 3.9 Hz), 26.2 (d, $J_{C\text{-}N}$ = 2.4 Hz).

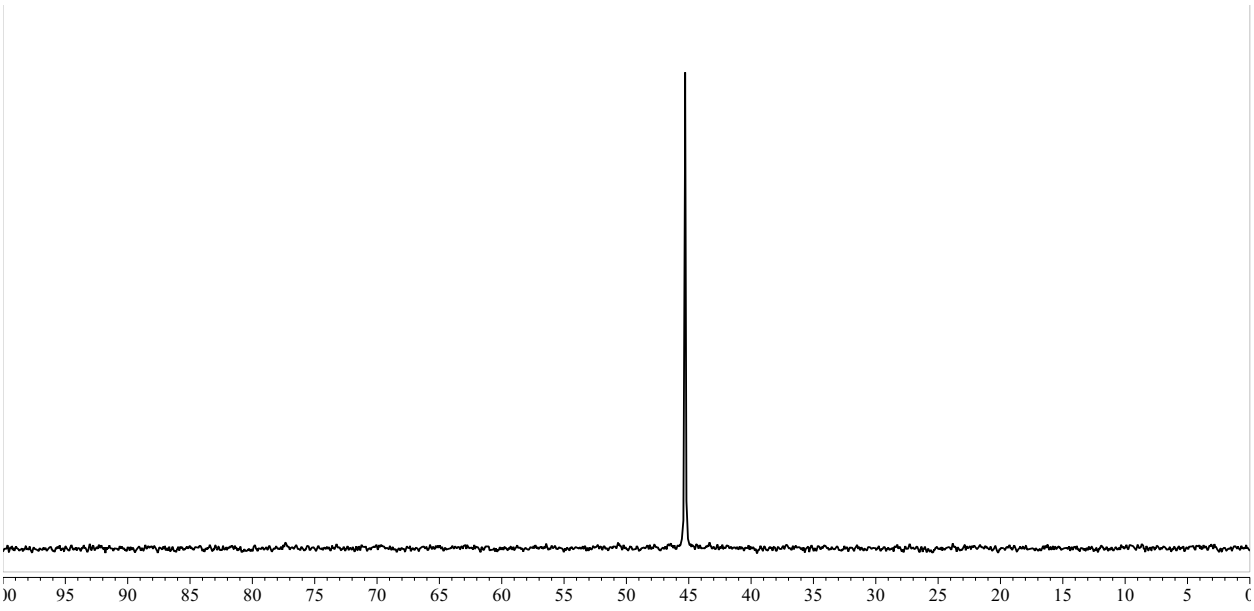


Figure S11. $^{15}N\{^{1}H\}$ NMR spectrum ($CDCl_3$, 50.66 MHz) of [^{15}N]isopropylamine at room temperature. δ 45.3.

[^{15}N]isopropyl(trimethylsilyl)amine. To a stirred solution of [^{15}N]isopropylamine (1.8 g, 30.0 mmol) in THF (30 mL), *n*-BuLi (2.50 M, 30.0 mmol) was added dropwise at ambient temperature and stirred for 6.0 hrs. To the resulting solution Me_3SiCl (3.6 g, 33.00 mmol) in THF (40.0 mL) was added dropwise at 0 °C. The colorless suspension was warmed to ambient temperature and stirred for 1.0 hr. The solvent was removed in vacuo, and the colorless residue was extracted with hexane (30 mL) and filtered. Removal of solvent in vacuo afforded [^{15}N]isopropyl(trimethylsilyl)amine as a colorless liquid (3.10 g, 84% yield). HRMS (DART-Orbitrap)) m/z[M+H]$^+$ calcd for $C_6H_{18}{}^{15}NSi$ 133.1173, found 133.1165.

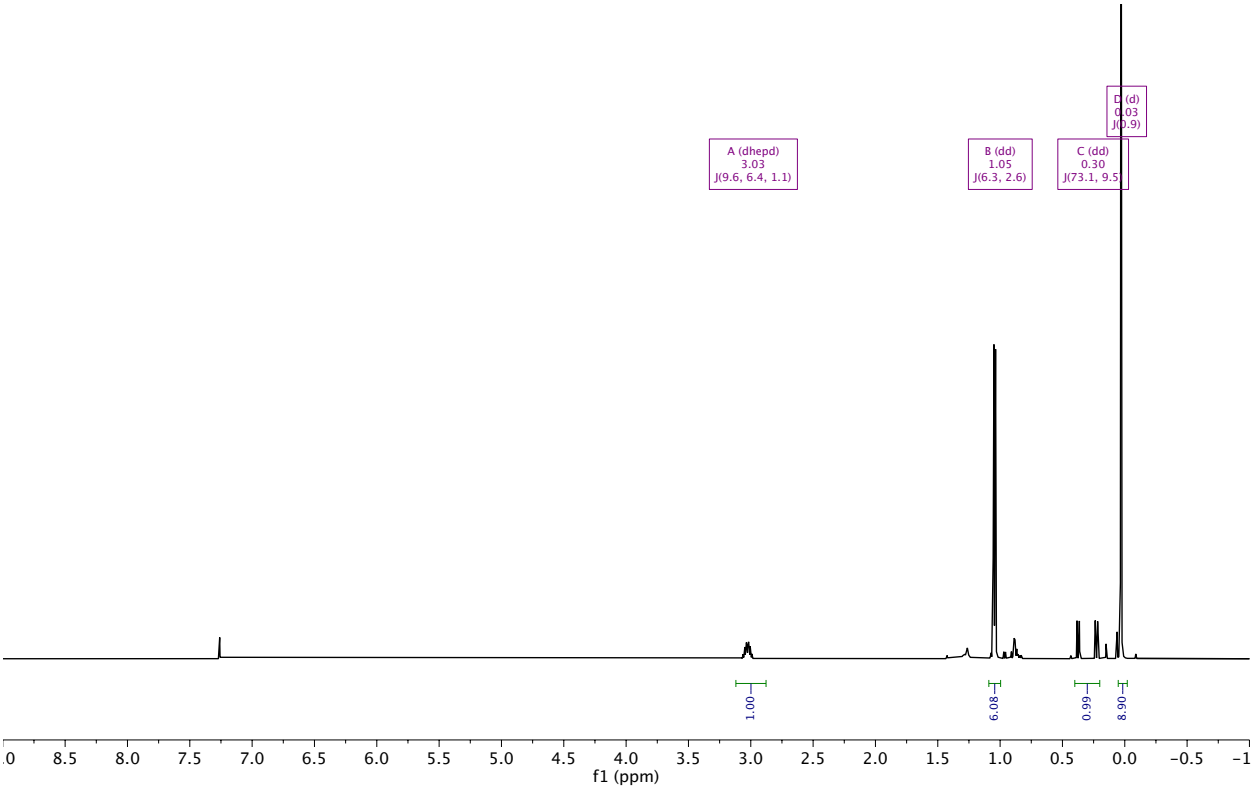


Figure S12. ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of [^{15}N]isopropyl(trimethylsilyl)amine at room temperature. δ 3.03 (dhepd, $J_{H\text{-}H}$ = 9.6, 6.4 Hz, $J_{H\text{-}N}$ = 1.1 Hz 1H), 1.05 (dd, $J_{H\text{-}H}$ = 6.3, $J_{H\text{-}N}$ = 2.6 Hz, 6H), 0.30 (dd, $J_{H\text{-}H}$ = 9.5, $J_{H\text{-}N}$ = 73.1 Hz, 1H), 0.03 (d, $J_{H\text{-}N}$ = 1.0 Hz, 9H).

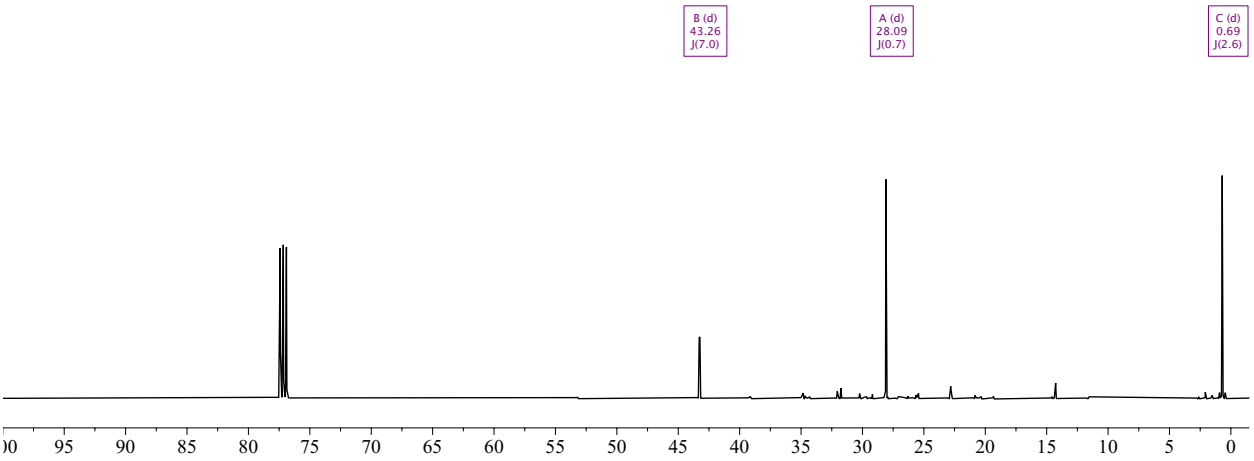


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Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 125.8 MHz) of [^{15}N]isopropyl(trimethylsilyl)amine at room temperature. δ 43.1 (d, $J_{C\text{-}N}$ = 7.1 Hz), 27.9 (d, $J_{C\text{-}N}$ = 0.9 Hz), 0.5 (d, $J_{C\text{-}N}$ = 2.7 Hz).

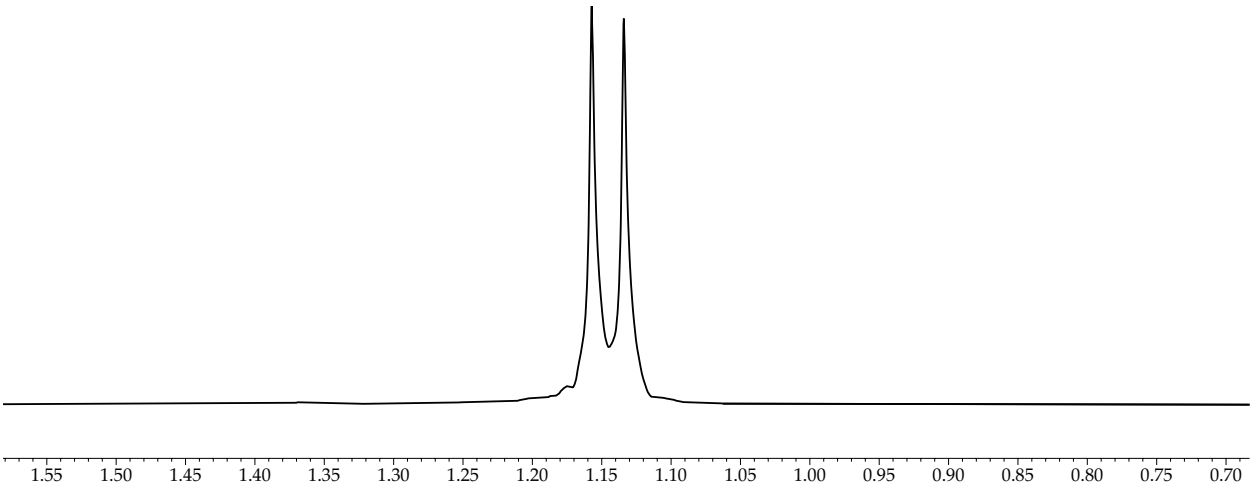


Figure S14. ^{29}Si NMR ($CDCl_3$, 99.36 MHz) spectrum of [^{15}N]isopropyl(trimethylsilyl)amine in at room temperature. δ 1.2 (d, $J_{Si\text{-}N}$ = 16.9 Hz).

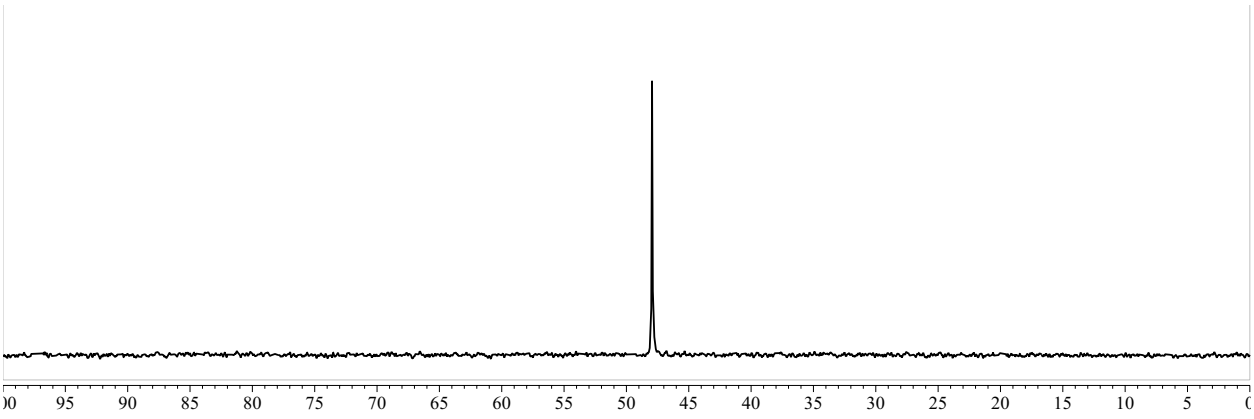
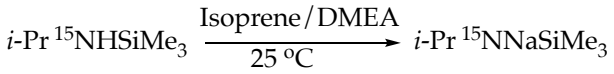


Figure S15. $^{15}N\{^{1}H\}$ NMR spectrum ($CDCl_3$, 50.66 MHz) of [^{15}N]isopropyl(trimethylsilyl)amine at room temperature. δ 47.9.



[^{15}N]Sodium isopropyl(trimethylsilyl)amide: Purified [^{15}N]NaPTA can be prepared as a white crystalline solid as illustrated for [^{15}N]NaPTA. Sodium dispersion in toluene (1.8 mL, 14 mmol) was added to a 50 mL Schlenk flask. The toluene was removed *in vacuo* and *N,N*-dimethylethylamine (20.0 mL) and [^{15}N]isopropy(trimethylsilyl)amine (1.5 g, 11.5 mmol) were added to the flask. While stirring, isoprene (375 µL, 5.5 mmol) was added over the course of 10 min at 0 °C. Stirring was halted after 30 min, and the mixture was filtered through a fine frit and evaporated to dryness to give a yellowish solid. Recrystallization from hexane gave [^{15}N]NaPTA as a white solid (1.4 g, 80% yield.)

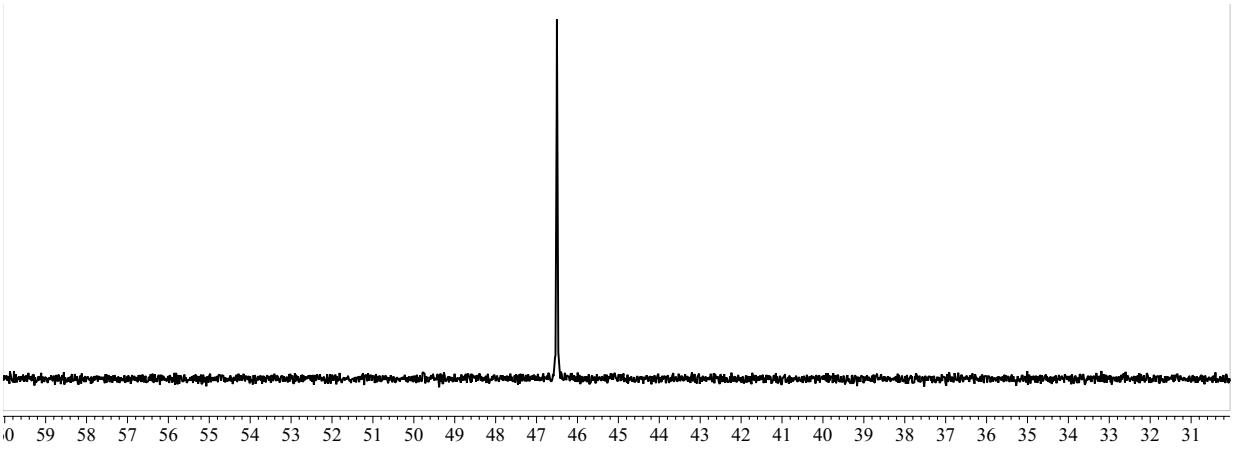


Figure S16. ^{15}N{^{1}H} NMR spectrum (10% THF/toluene-d_8, 50.66 MHz) of [^{15}N]NaPTA at –110 °C: δ 47.9.

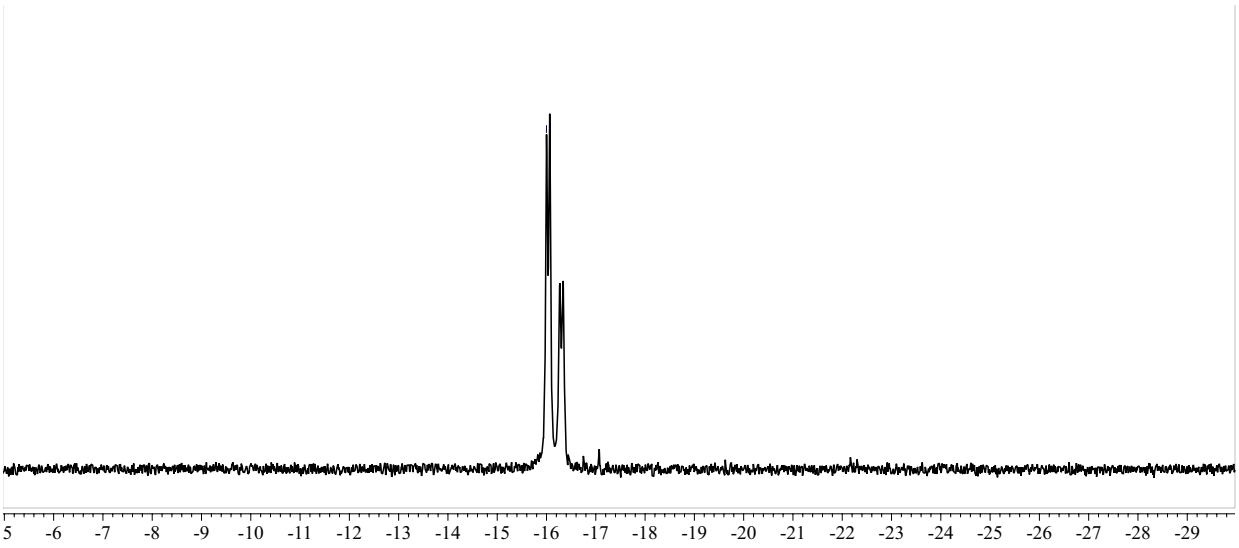


Figure S17. ^{29}Si NMR spectrum (10% THF/toluene-d_8, 99.36 MHz) of [^{15}N]NaPTA at –110 °C. δ –14.9 (d, J_{Si-N} = 6.5 Hz**)**, –15.3 (d, J_{Si-N} = 6.5 Hz).

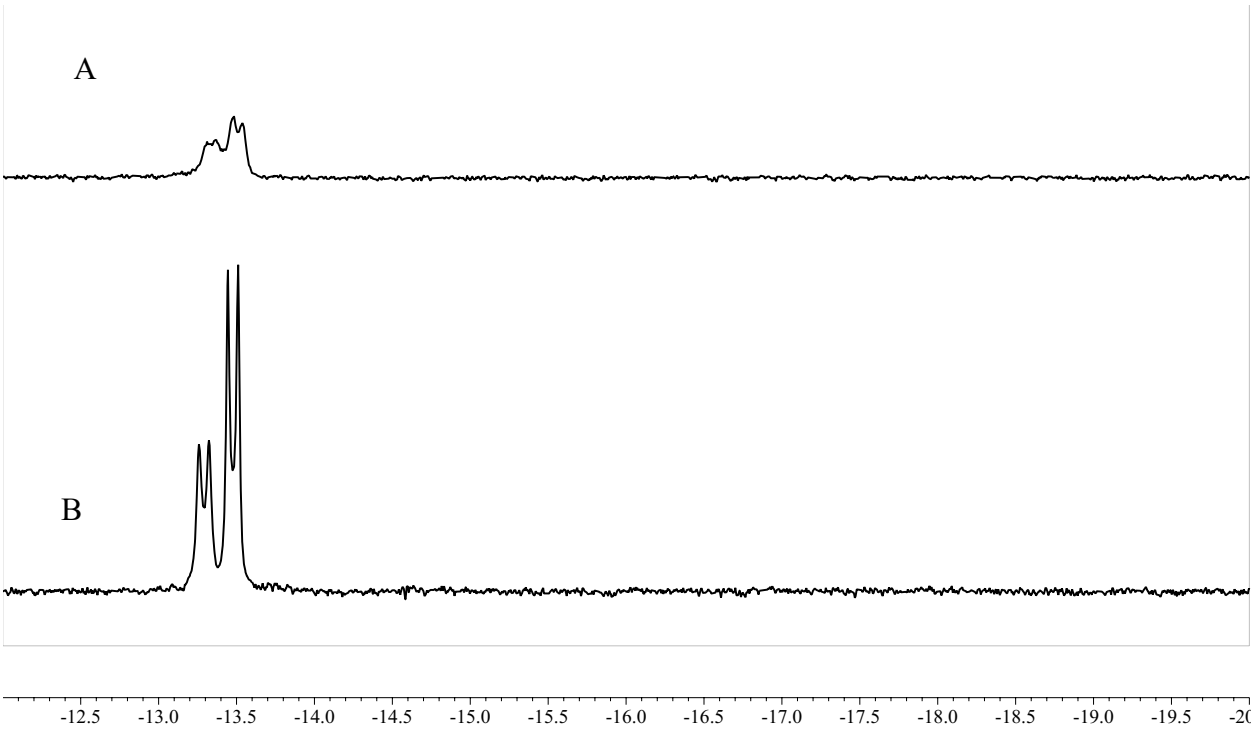


Figure S18. ^{29}Si NMR spectra (toluene-d_8, 99.36 MHz) of [^{15}N]NaPTA at varying temperature. (A) –80 °C: δ –13.0 (d, $J_{Si\text{-}N}$ = 6.3 Hz), –13.2 (d, $J_{Si\text{-}N}$ = 6.5 Hz); (B) –90 °C: δ –13.0 (d, $J_{Si\text{-}N}$ = 6.4 Hz), –13.2 (d, $J_{Si\text{-}N}$ = 6.5 Hz).

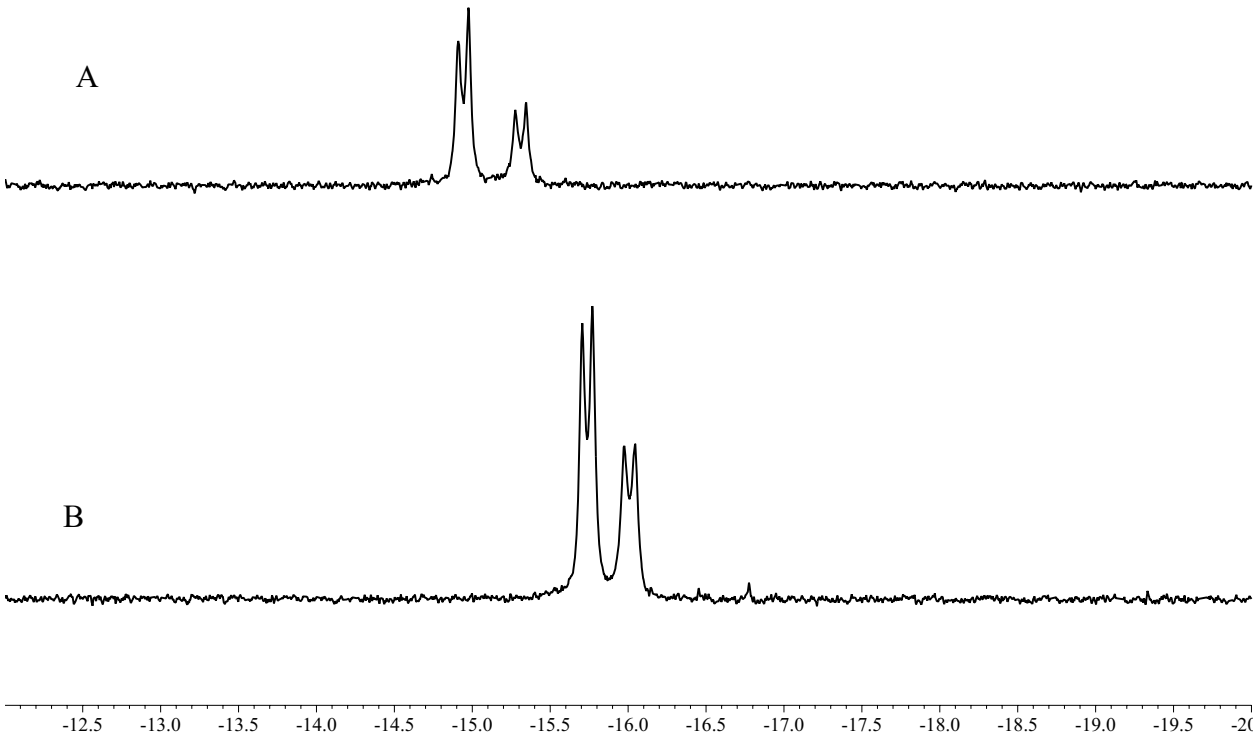


Figure S19. ^{29}Si NMR spectrum (99.36 MHz) of [^{15}N]NaPTA in THF/ toluene-d_8 varying THF at –110 ºC. (A) 1.2 M THF: δ –14.9 (d, $J_{Si\text{-}N}$ = 6.5 Hz**)**, –15.3 (d, $J_{Si\text{-}N}$ = 6.5 Hz); (B) 3.0 M THF: δ –15.7 (d, $J_{Si\text{-}N}$ = 6.5 Hz**)**, –16.0 (d, $J_{Si\text{-}N}$ = 6.6 Hz).

Table 1. Reactions of NaPTA in THF.

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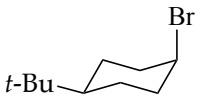
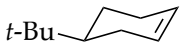
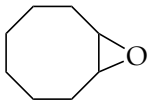
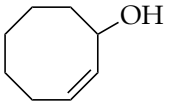
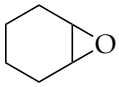
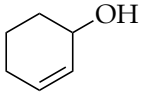
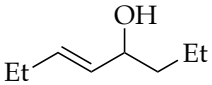
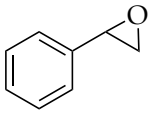
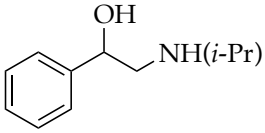
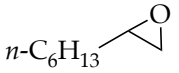
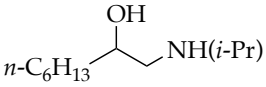
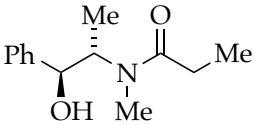
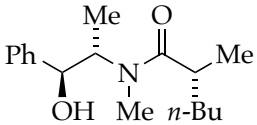
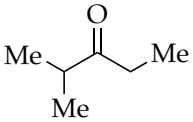
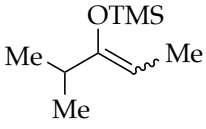
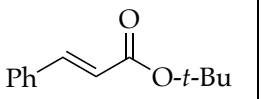
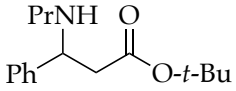
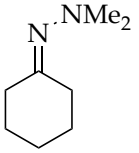
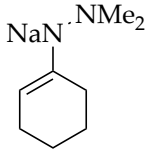
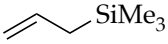
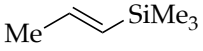
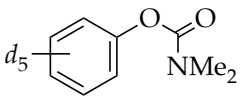
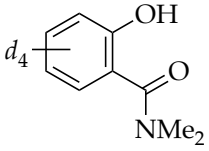
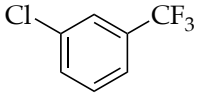
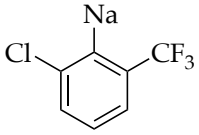
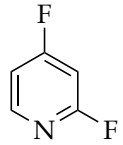
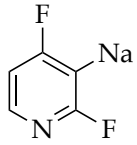
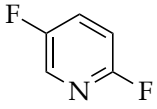
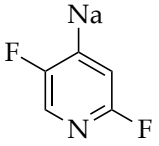
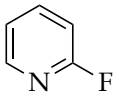
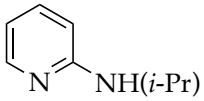
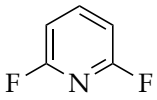
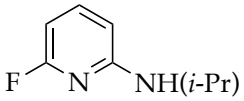
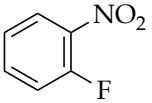
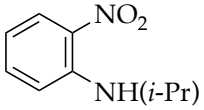
1		25 °C, 1 hr		11	91%
2	*n*-$C_8H_{17}Br$	25 °C, 3 hr	*n*-$C_6H_{13}CH{=}CH_2$ + 8% substitution	4	81%
3		66 °C, 8 hr		4	88%
4		66 °C, 8 hr		1	80%
5		66 °C, 8 hr	 (99:1 *trans:cis*)	3	80%
6		66 °C, 8 hr		--	70%
7		66 °C, 8 hr		--	74%
8		–40 °C, 2 hr (w/ *n*-BuBr)		--	82%
9		–78 °C, 1 hr (w/ TMSCl)	 (*Z*:*E* = 2:1)	--	80%

10		–78 °C		--	82%
11		–30 °C, 1 hr		8	(50%)[a]
12		25 °C, 2 hr	 (40:1 *trans:cis*)	12	95%
13		25 °C, 2 hr	 (>50:1 *cis:trans*)	30	86%
14		–40 °C, 1 hr		1	90%
15		–60 °C, 1 hr		2	(35%)[b]
16		–78 °C, 10 min		--	(92%)[b]
17		–78 °C, 30 min		--	(90%)[b]
18		–25 °C, 3 hr		--	82%
19		25 °C, 3 hr		--	70%
20		66 °C, 2 hr		--	78%

a a [a]Shown by *in situ* IR spectroscopy. *b* Shown by deuteration.

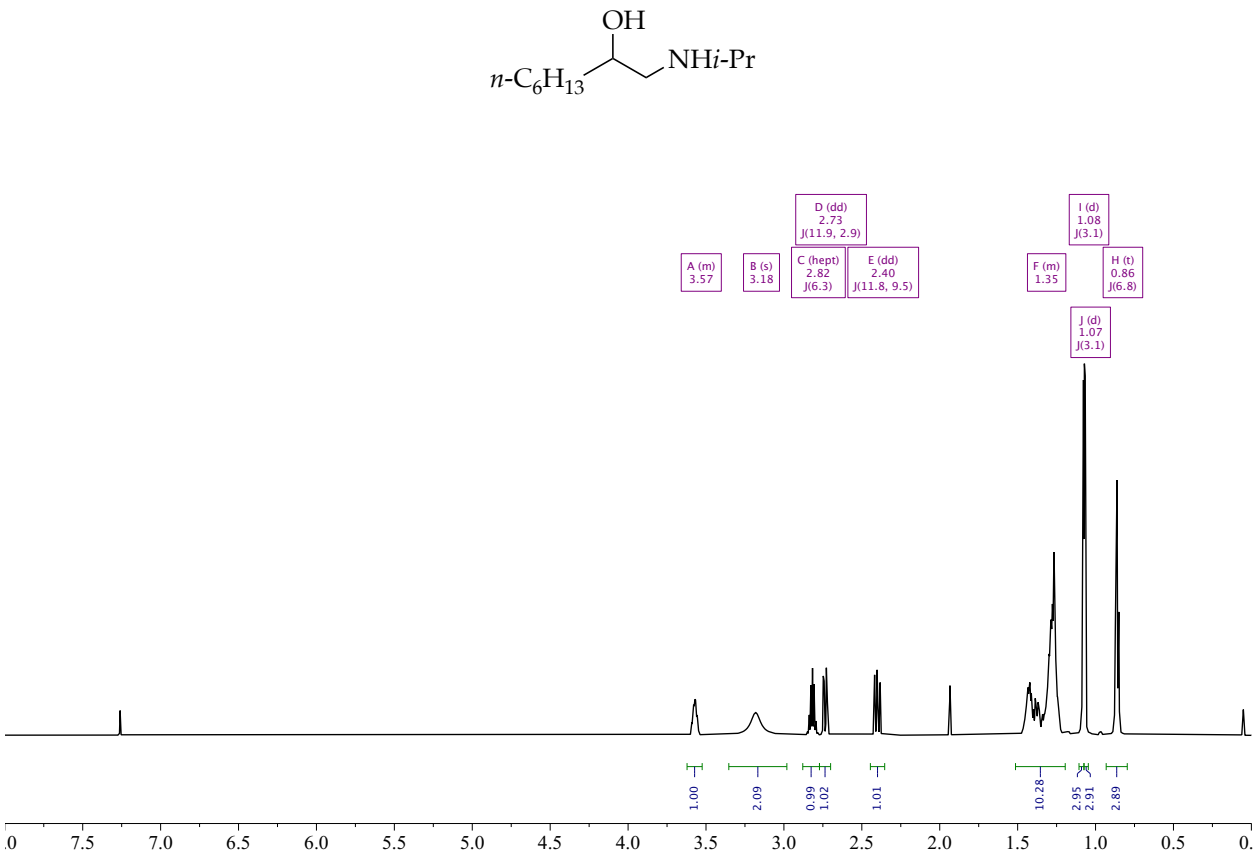


Figure S20. ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of 1-(isopropylamino)octan-2-ol at room temperature. δ 3.63–3.51 (m, 1H), 3.18 (br. s, 2H), 2.82 (hept, J = 6.3 Hz, 1H), 2.73 (dd, J = 11.9, 2.9 Hz, 1H), 2.40 (dd, J = 11.8, 9.5 Hz, 1H), 1.49–1.20 (m, 10H), 1.08 (d, J = 3.1 Hz, 3H), 1.07 (d, J = 3.1 Hz, 3H), 0.86 (t, J = 6.8 Hz, 2H).

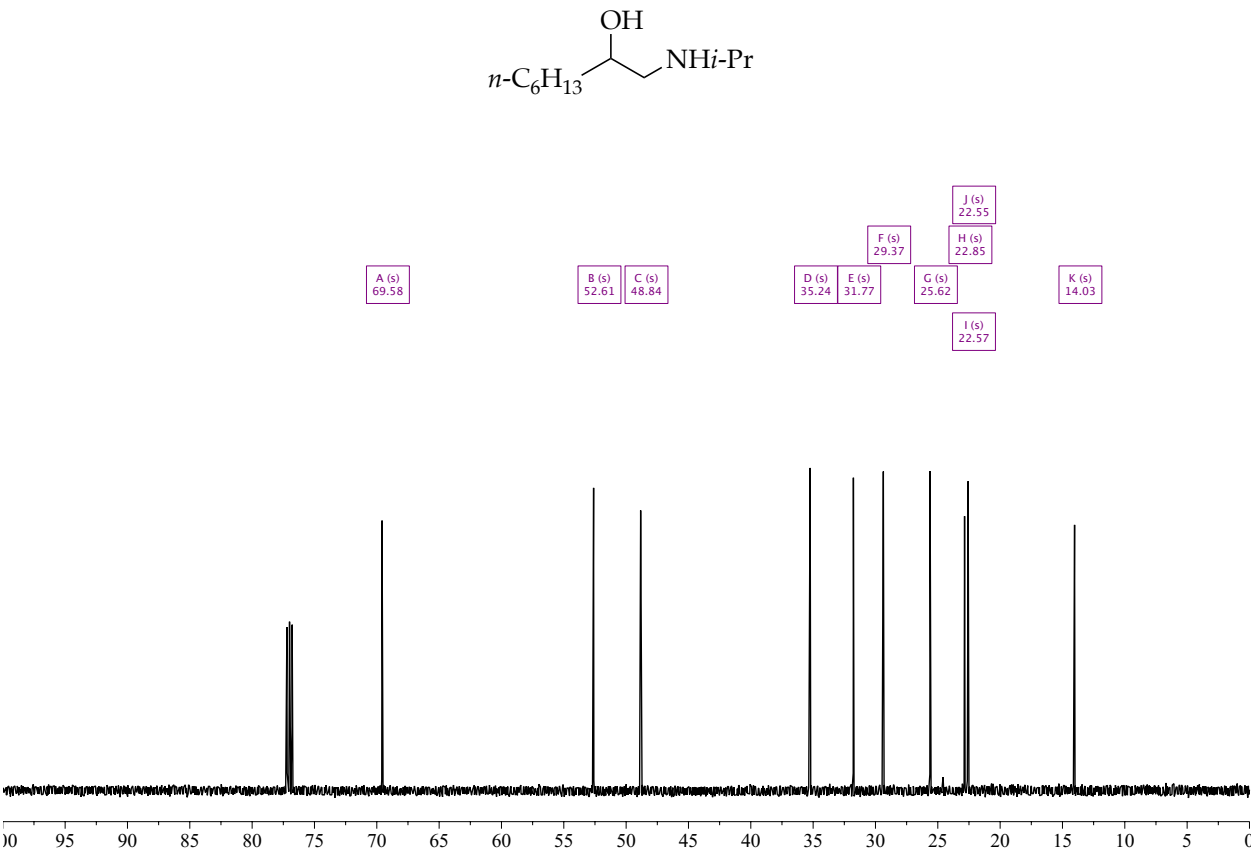


Figure S21. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 125.8 MHz) of 1-(isopropylamino)octan-2-ol at room temperature. δ 69.6, 52.6, 48.8, 35.2, 31.8, 29.4, 25.6, 22.9, 22.6, 14.0.

HRMS (DART-Orbitrap) m/z$[M+H]^+$ calcd for $C_{11}H_{23}ON$ 188.2005, found 188.2009.

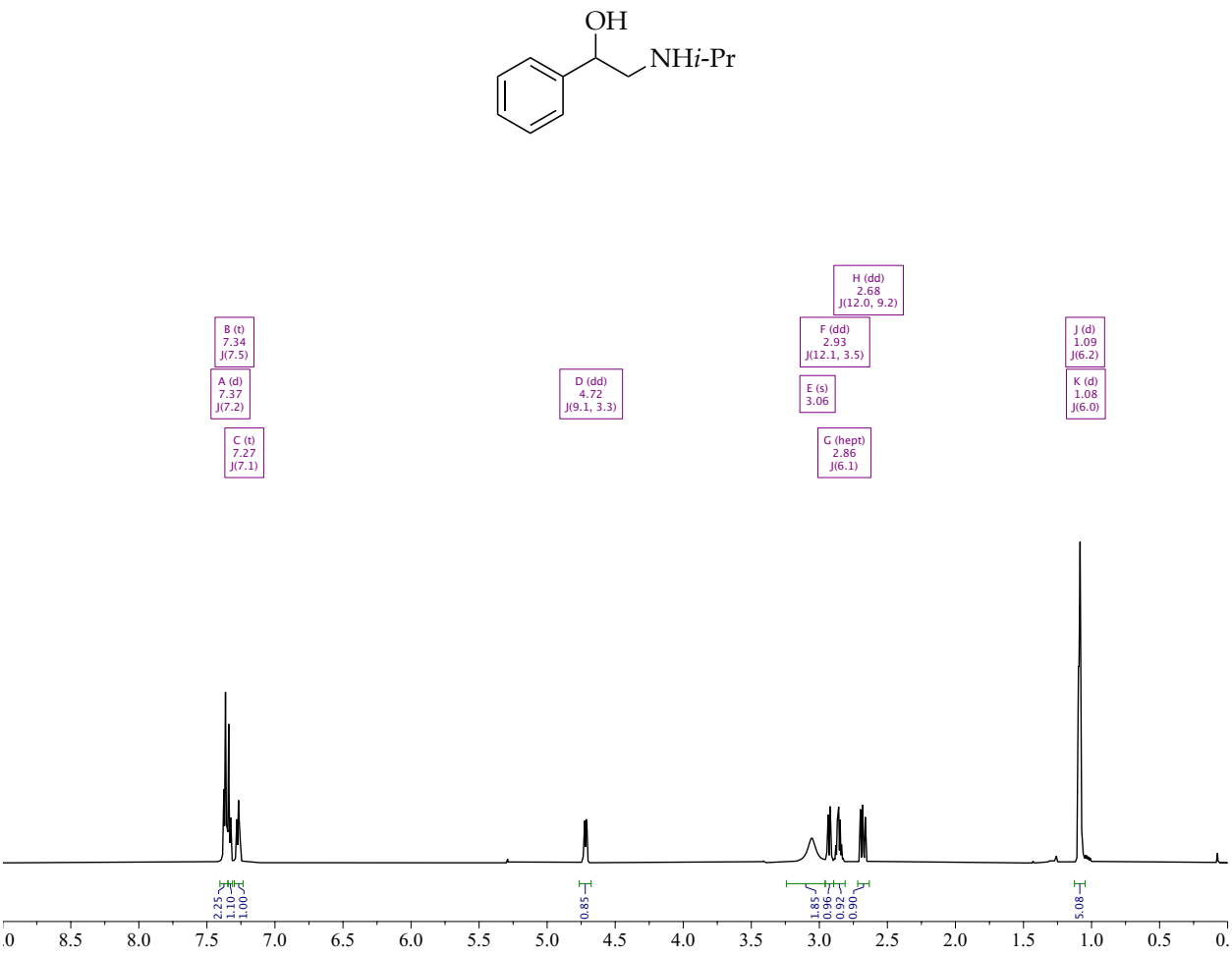


Figure S22. ^{1}H NMR spectra ($CDCl_3$, 500 MHz) of 2-(isopropylamino)-1-phenylethan-1-ol at room temperature. δ 7.37 (d, J = 7.2 Hz, 2H), 7.34 (t, J = 7.5 Hz, 2H), 7.27 (t, J = 7.1 Hz, 1H), 4.72 (dd, J = 9.1, 3.3 Hz, 1H), 3.06 (br. s, 1H), 2.93 (dd, J = 12.1, 3.5 Hz, 1H), 2.86 (hept, J = 6.1 Hz, 1H), 2.68 (dd, J = 12.0, 9.2 Hz, 1H), 1.09 (d, J = 6.2 Hz, 3H), 1.08 (d, J = 6.0 Hz, 3H).

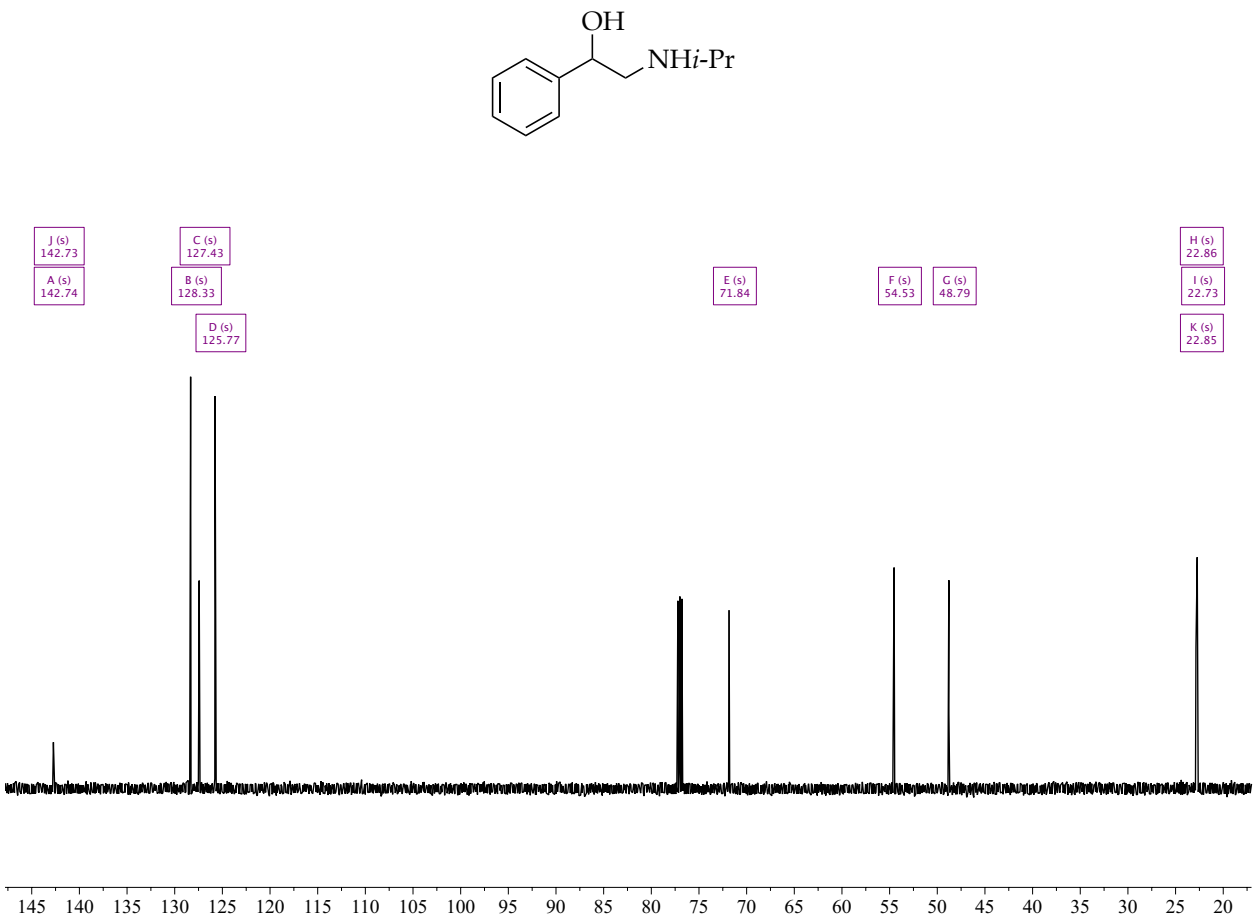


Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 125.8 MHz) of 2-(isopropylamino)-1-phenylethan-1-ol at room temperature. δ 142.7, 142.7, 128.3, 127.4, 125.8, 71.8, 54.5, 48.8, 22.9, 22.9, 22.7.

HRMS (DART-Orbitrap) m/z$[M+H]^+$ calcd for $C_{11}H_{17}ON$ 180.1377, found 188.1382.

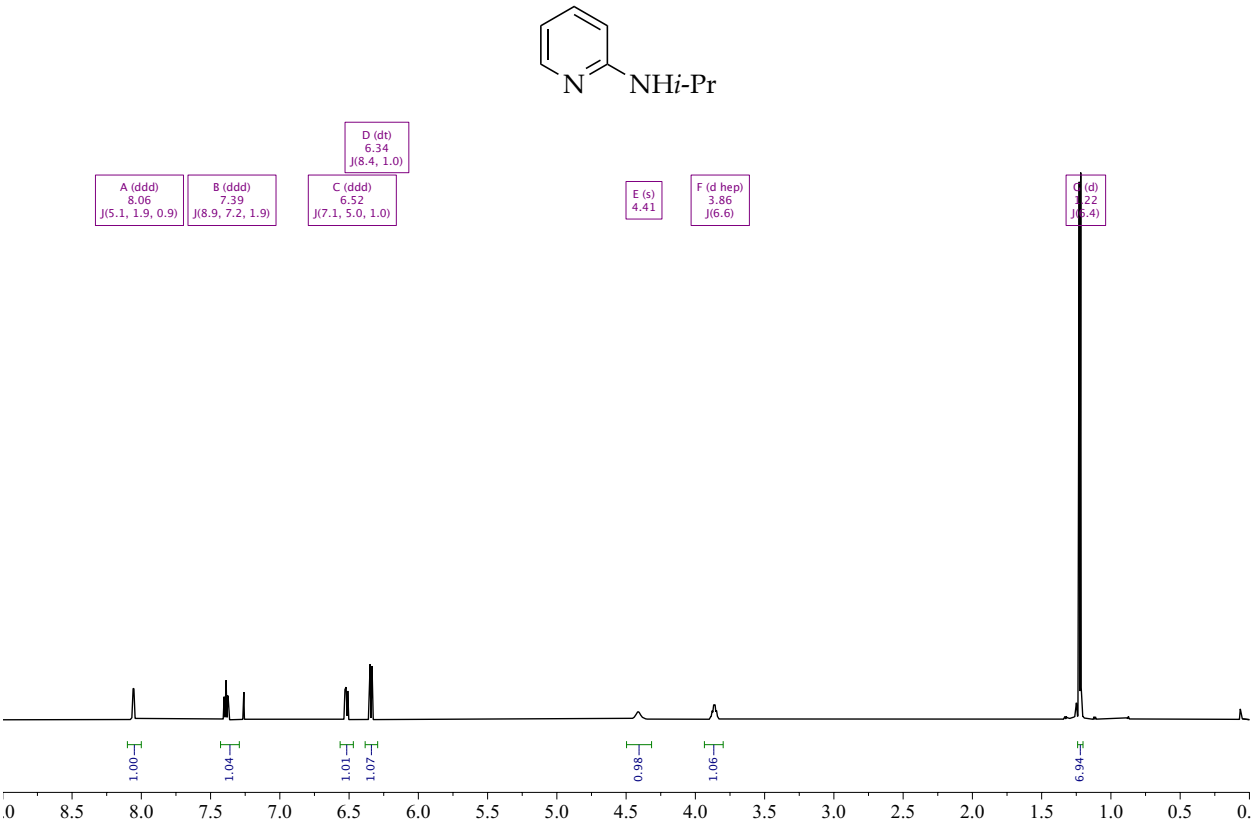


Figure S24. ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of *N*-isopropylpyridin-2-amine at room temperature. δ 8.06 (ddd, *J* = 5.1, 1.9, 0.9 Hz, 1H), 7.39 (ddd, *J* = 8.9, 7.2, 1.9 Hz, 1H), 6.52 (ddd, *J* = 7.1, 5.0, 1.0 Hz, 1H), 6.34 (dt, *J* = 8.4, 1.0 Hz, 2H), 4.41 (br s, 1H), 3.86 (dhept, *J* = 6.6 Hz, 1H), 1.22 (d, *J* = 6.4 Hz, 6H).

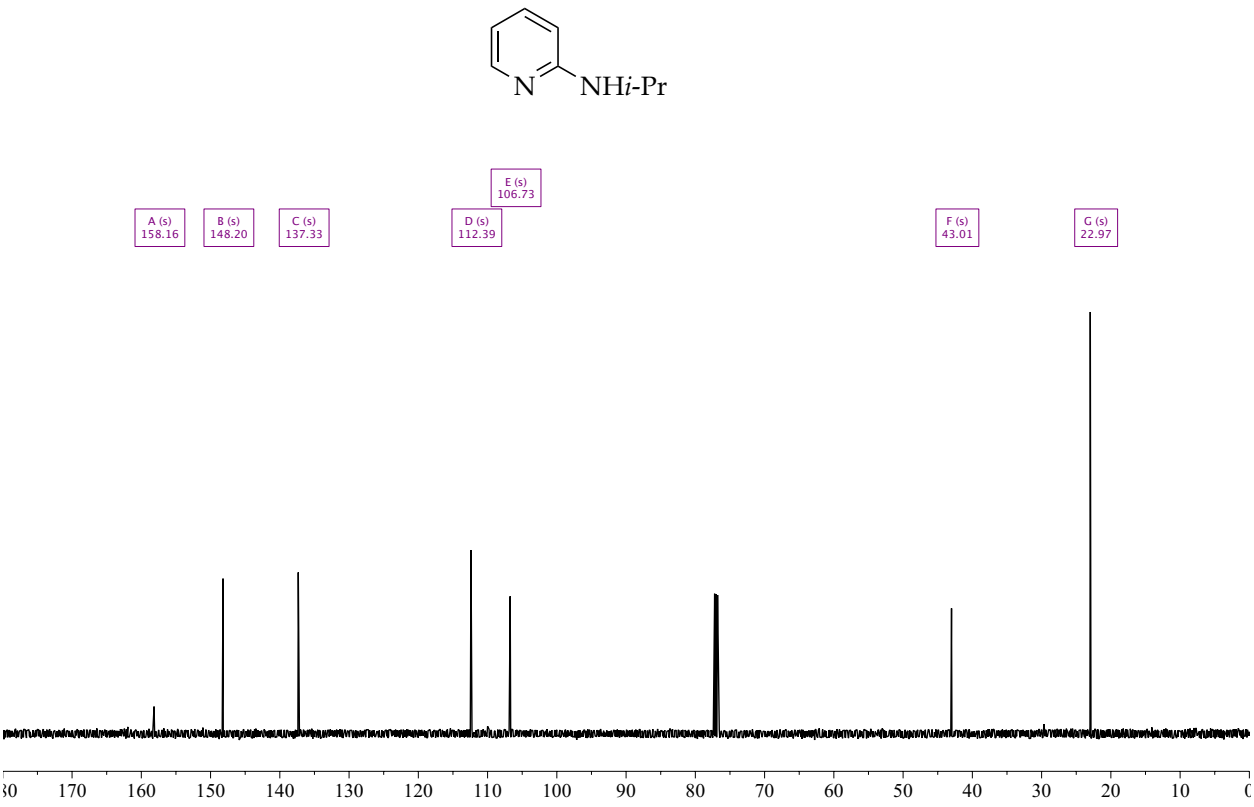


Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 125.8 MHz) of *N*-isopropylpyridin-2-amine at room temperature. δ 158.2, 148.2, 137.3, 112.4, 106.7, 43.0, 23.0.

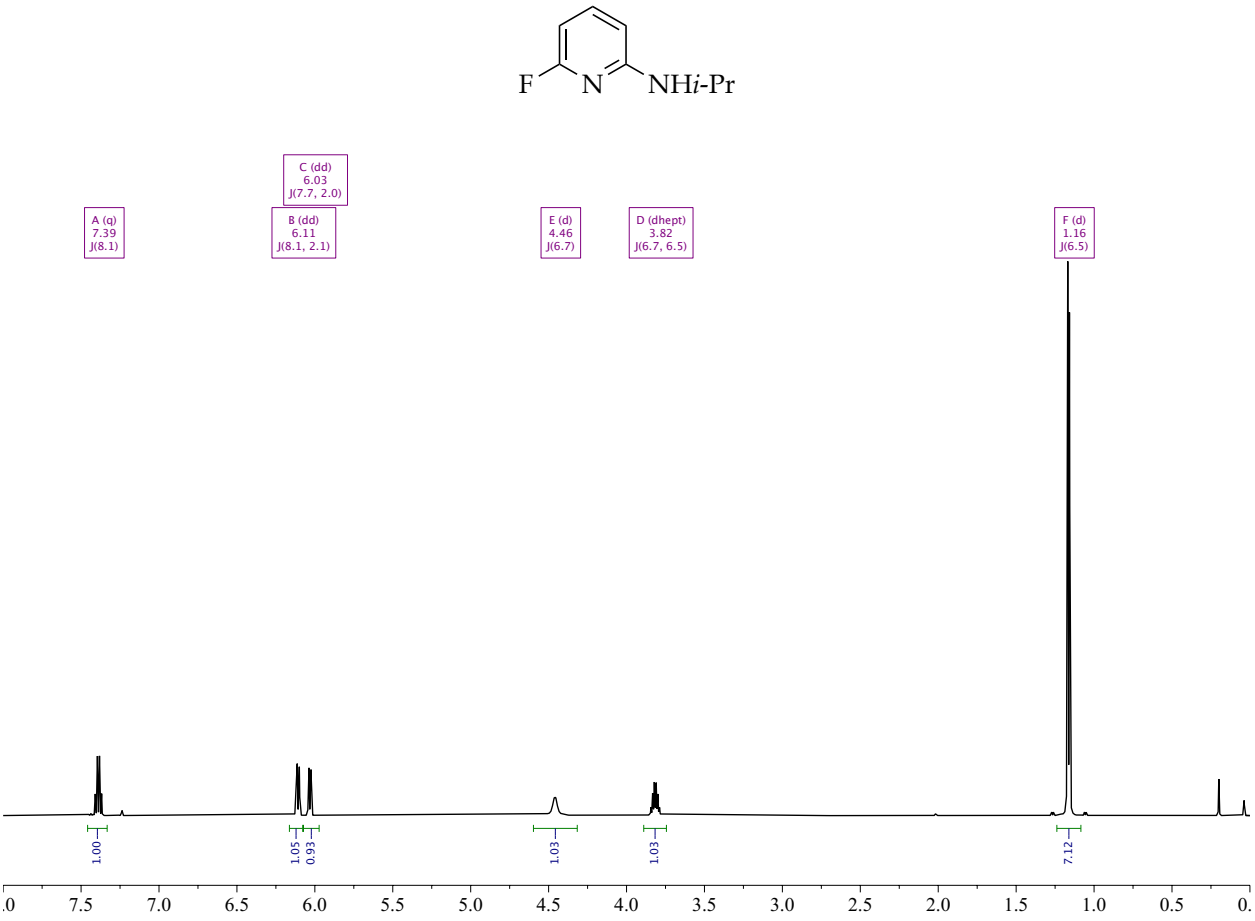


Figure S26. ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of 6-fluoro-*N*-isopropylpyridin-2-amine at room temperature. δ 7.39 (q, $J_{H\text{-}F}$ = 8.1 Hz, 1H), 6.11 (dd, J = 8.1, $J_{H\text{-}F}$ = 2.0 Hz, 1H), 6.03 (dd, J = 7.7, $J_{H\text{-}F}$ = 2.0 Hz, 1H), 4.46 (d, J = 6.7 Hz, 1H), 3.82 (dhept, J = 6.7, 6.5 Hz, 1H), 1.16 (d, J = 6.5 Hz, 6H).

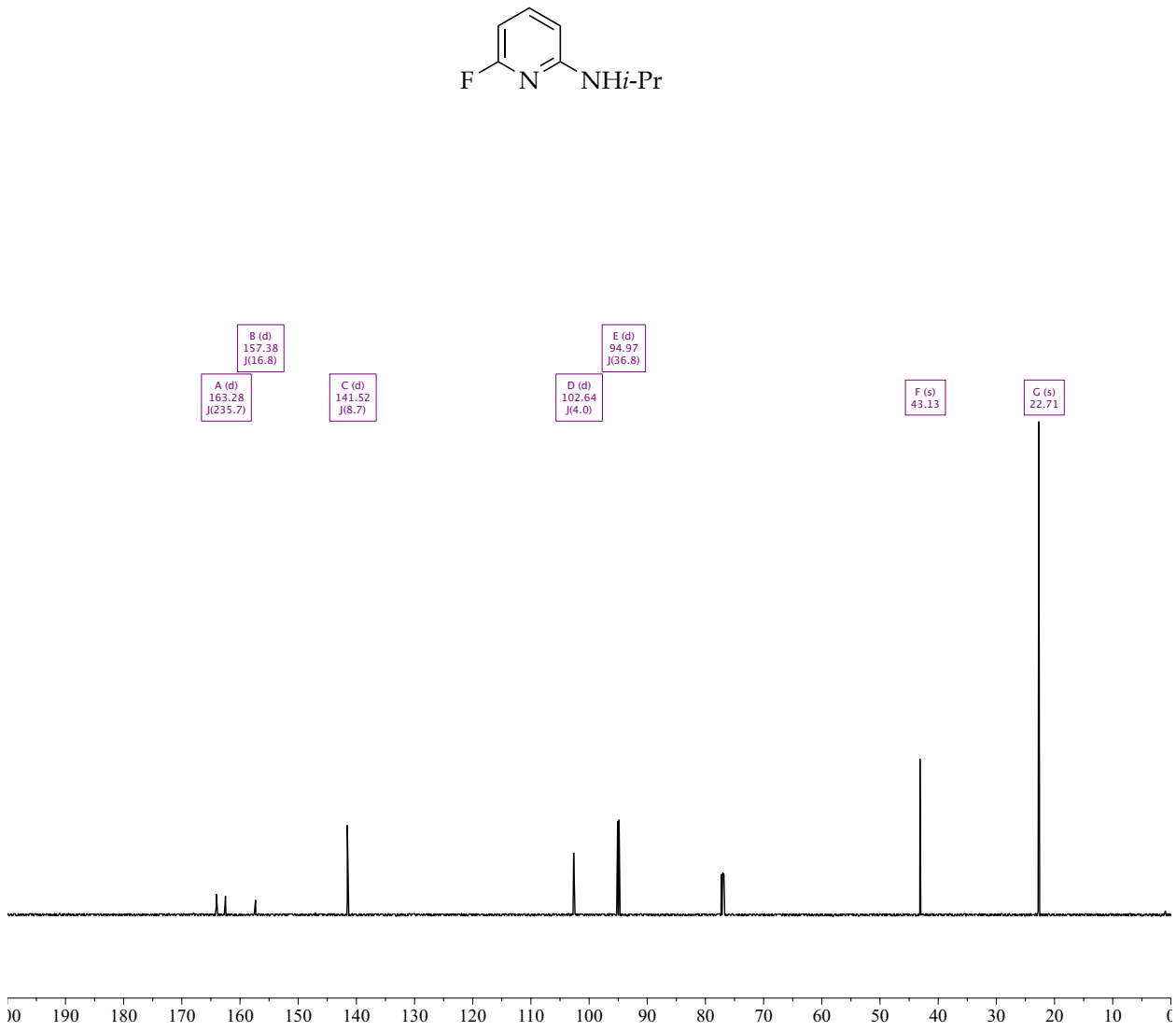


Figure S27. ^{13}C NMR spectrum ($CDCl_3$, 125.8 MHz) of 6-fluoro-*N*-isopropylpyridin-2-amine at room temperature. δ 163.3 (d, $J_{C\text{-}F}$ = 235.7 Hz), 157.4 (d, $J_{C\text{-}F}$ = 16.8 Hz), 141.5 (d, $J_{C\text{-}F}$ = 8.7 Hz), 102.6 (d, $J_{C\text{-}F}$ = 4.0 Hz), 95.0 (d, $J_{C\text{-}F}$ = 36.8 Hz), 43.1, 22.7.

HRMS (DART-Orbitrap) m/z[M+H]$^+$ calcd for $C_{11}H_{19}NF$ 198.1488, found 198.1568.

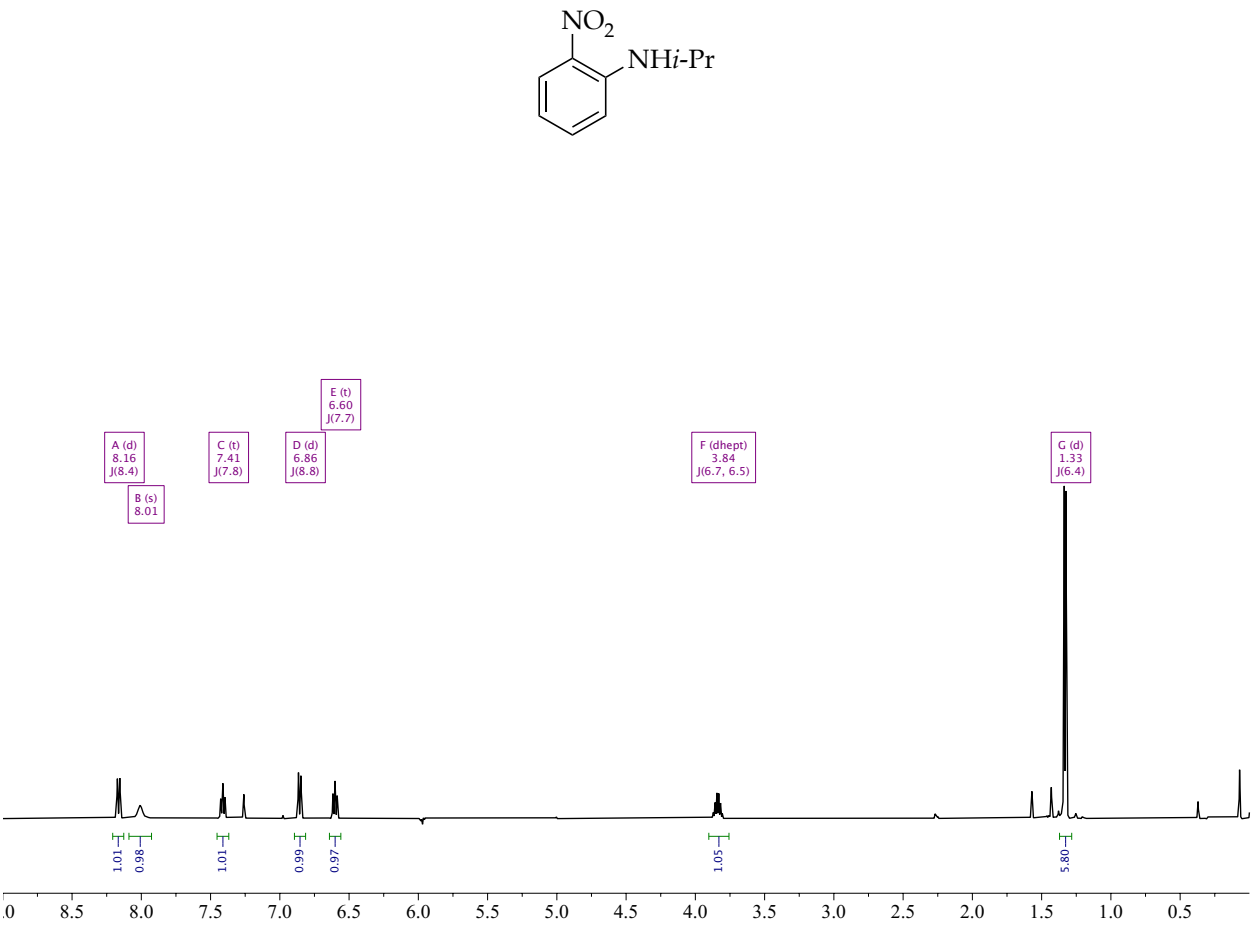


Figure S28. ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of *N*-isopropyl-2-nitroaniline at room temperature. δ 8.16 (d, J = 8.4 Hz, 1H), 8.01(s,b 1H), 7.41 (t, J = 7.8 Hz, 1H), 6.86 (d, J = 8.8, 1H), 6.60 (t, J=7.7 Hz, 1H), 3.84 (dhept, J = 6.7, 6.5 Hz, 1H), 1.33 (d, J = 6.4 Hz, 6H).

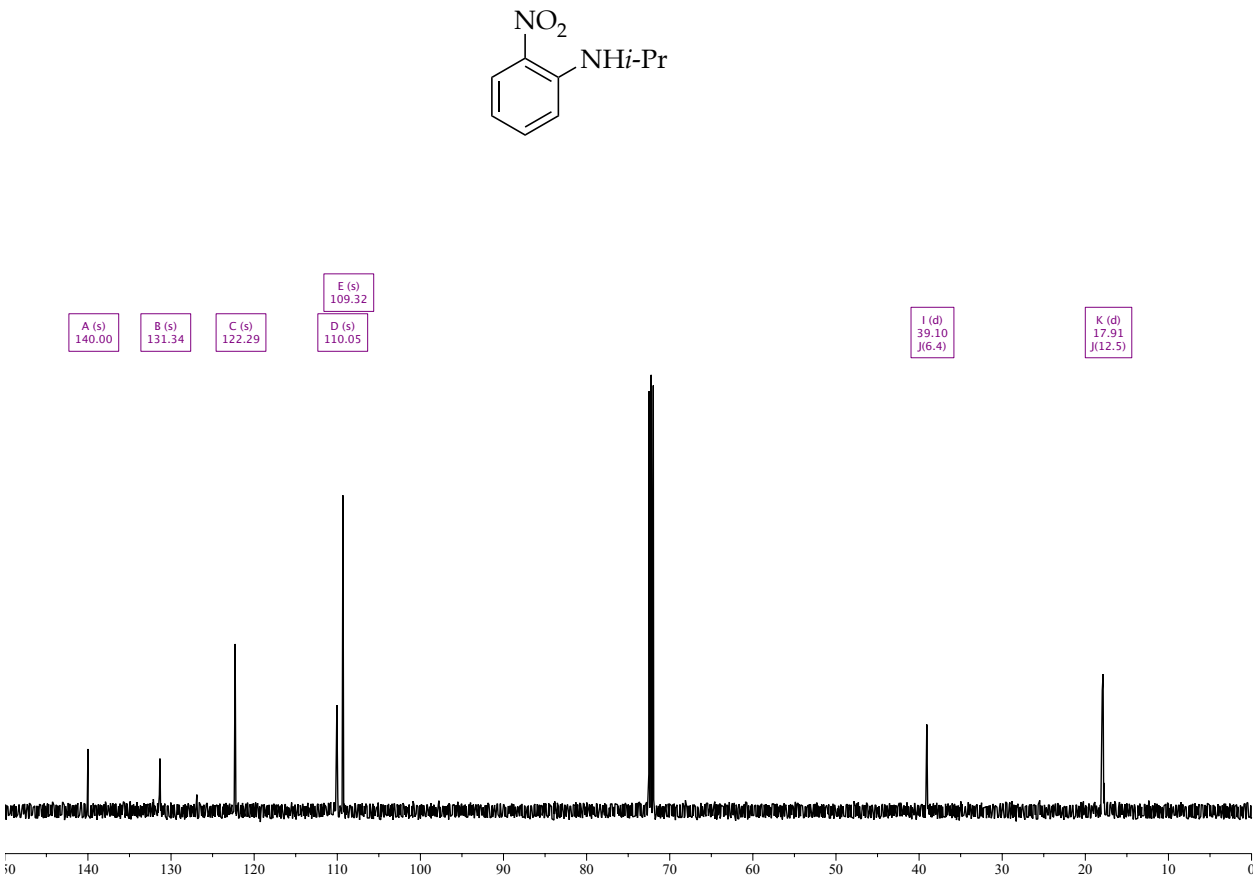


Figure S29. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 125.8 MHz) of *N*-isopropyl-2-nitroaniline at room temperature. δ 140.0, 131.3, 122.3, 110.1, 109.3, , 39.1, 17.9.

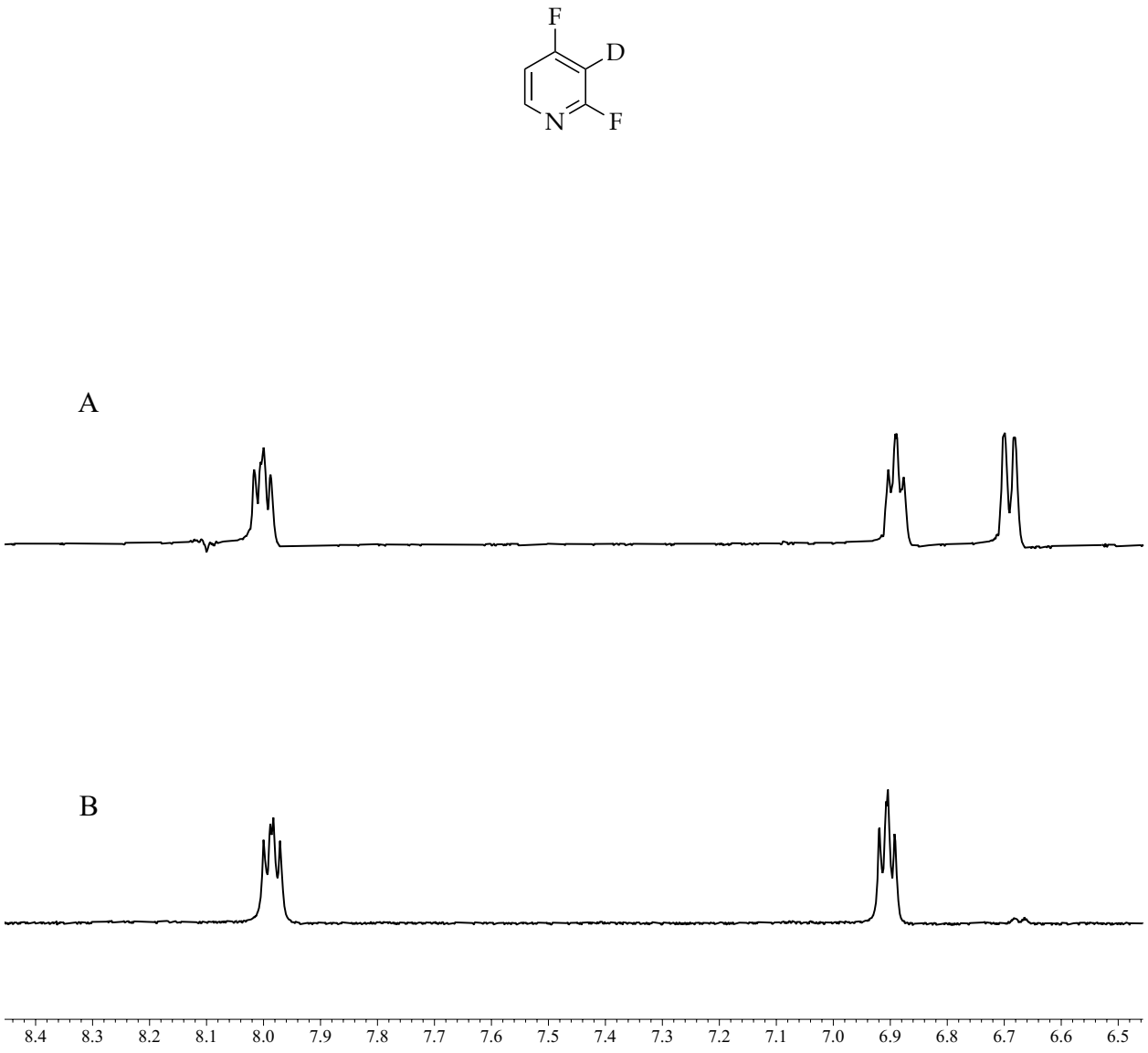


Figure S30. ^{1}H NMR spectra (THF, 500 MHz) of 2,4-difluoropyridine and 2,4-difluoropyridine-3-*d* in THF at room temperature. (A) 2,4-difluoropyridine; (B) 2,4-difluoro-3-*d*.

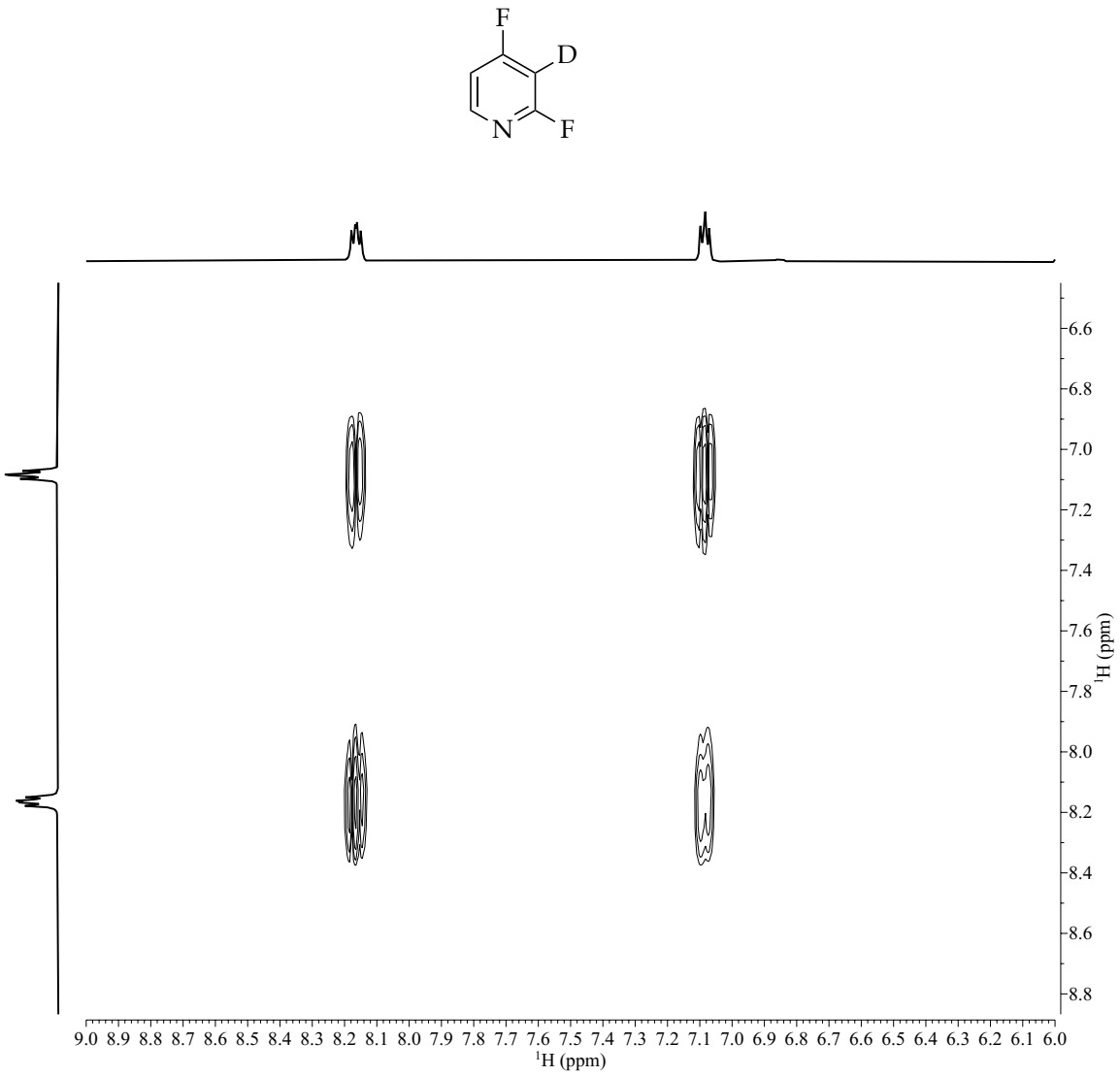


Figure S31. Expansion of the aromatic region of a gradient COSY spectrum of 2,4-difluoro-3-*d* at 25 °C showing coupling between H-5 and H-6.

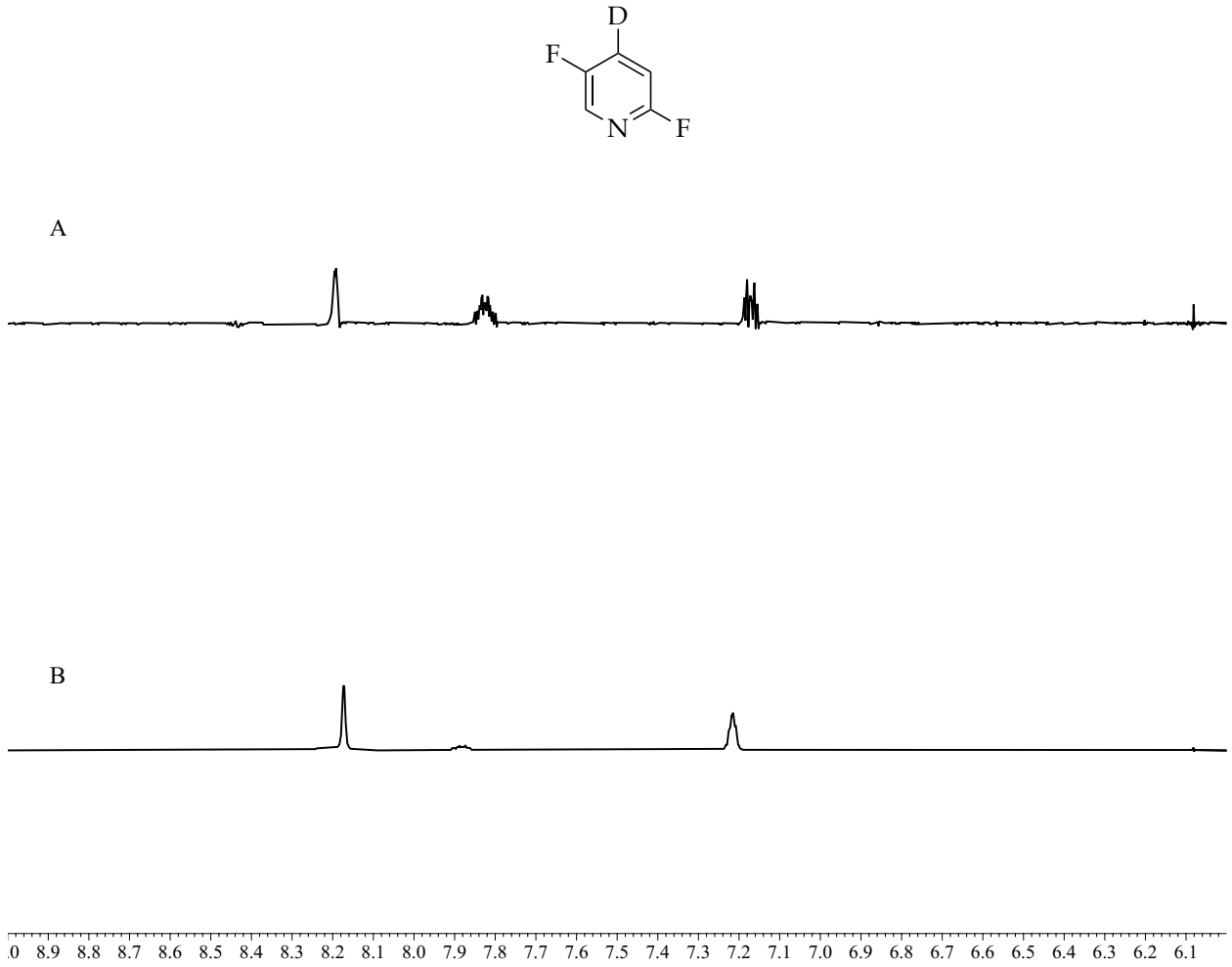


Figure S32. ^{1}H NMR spectra ($CDCl_3$, 500 MHz) of 2,5-difluoropyridine and 2,5-difluoropyridine-4-*d* in THF at room temperature. (A) 2,4-difluoropyridine; (B) 2,5-difluoropyridine-4-d_1.

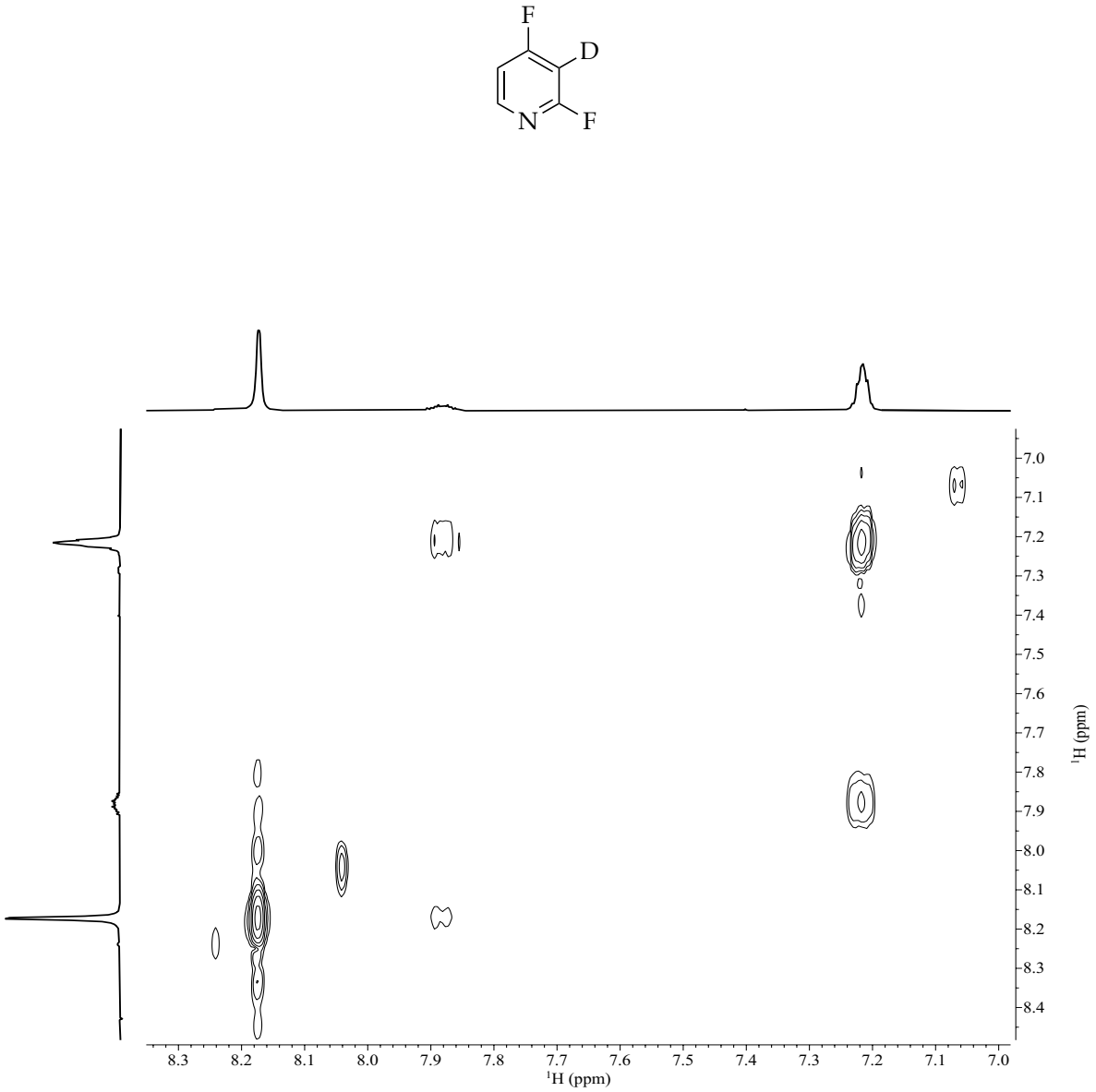


Figure S33. Expansion of the aromatic region of a gradient COSY spectrum of 2,5-difluoropyridine-4-*d* at 25 °C showing no coupling between H-3 and H-6.

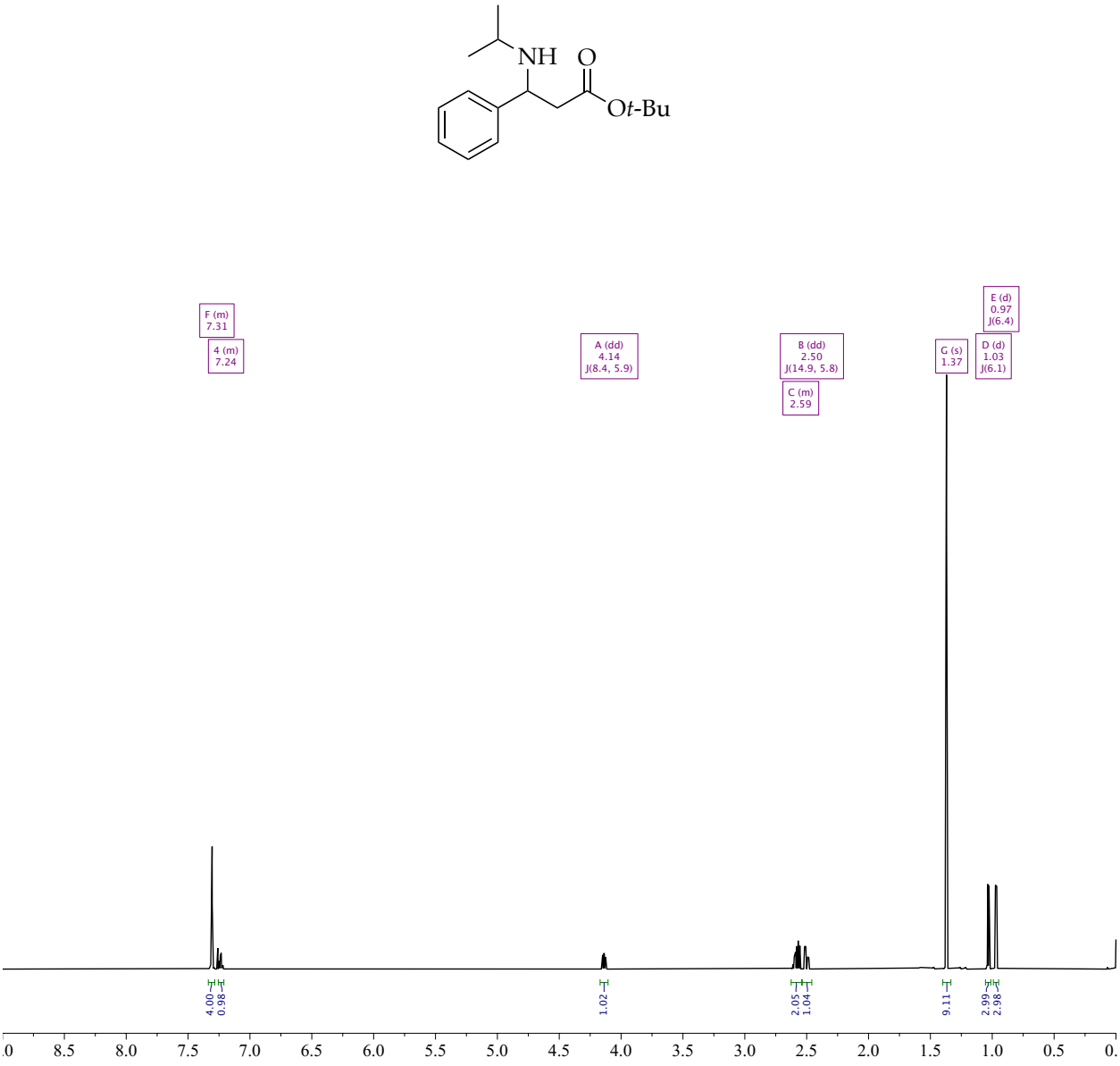


Figure S34. ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of *tert*-butyl 3-(isopropylamino)-3-phenylpropanoate at room temperature. δ 7.33-7.29 (m, 4H), 7.26 -7.21 (m, 1H), 4.14 (dd, J = 8.4, 5.9 Hz, 1H), 2.64-6.54 (m, 2H), 2.50 (dd, J = 14.9, 5.9 Hz, 1H), 1.37 (s, 9H) 1.04 (d, J = 6.4 Hz, 3H), 0.97 (d, J = 6.4 Hz, 3H).

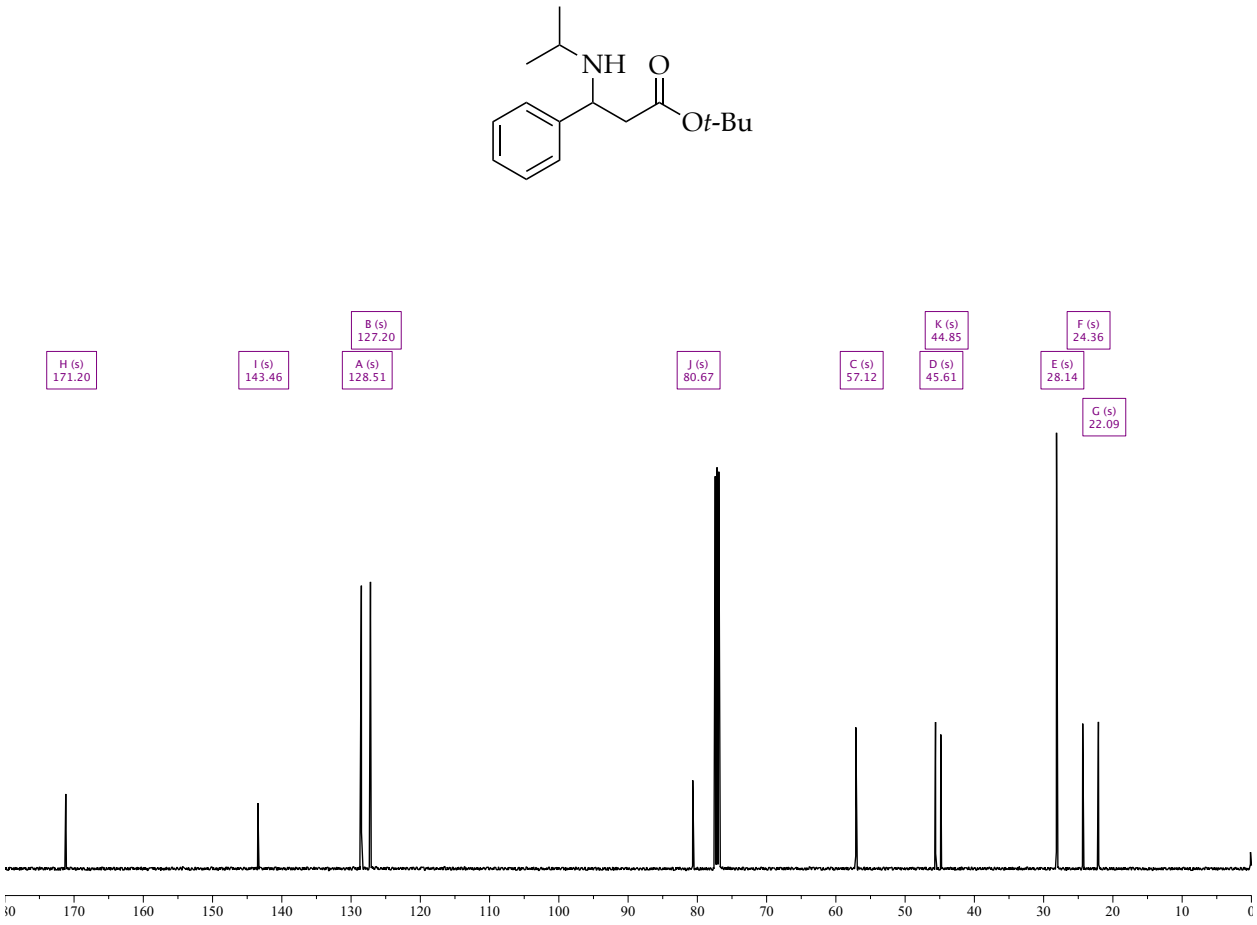
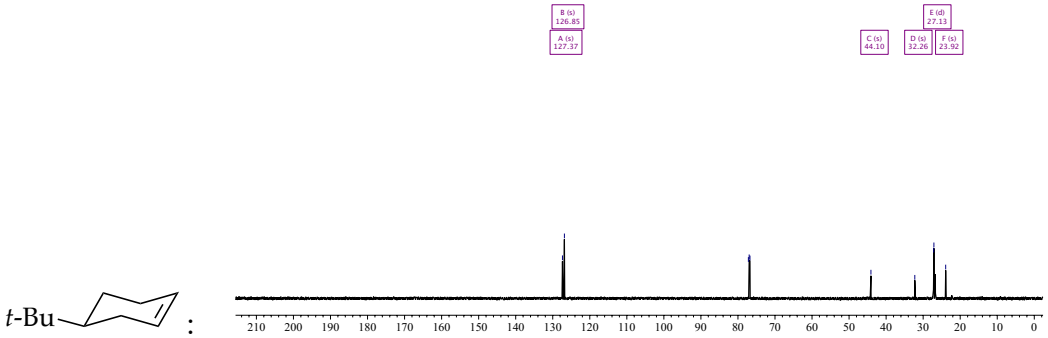
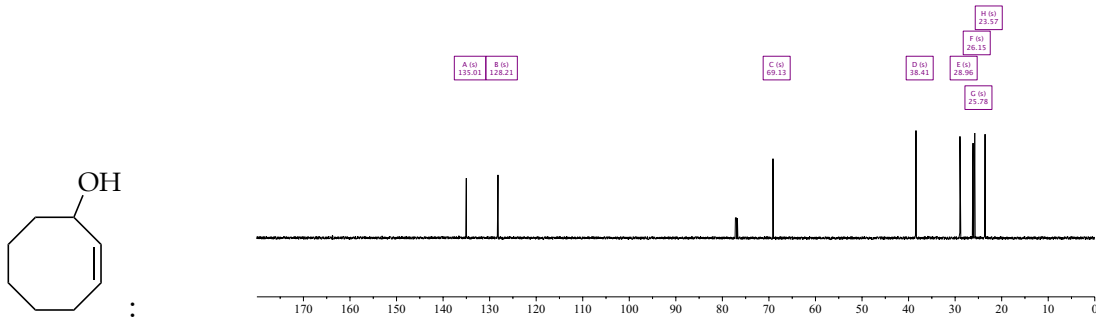


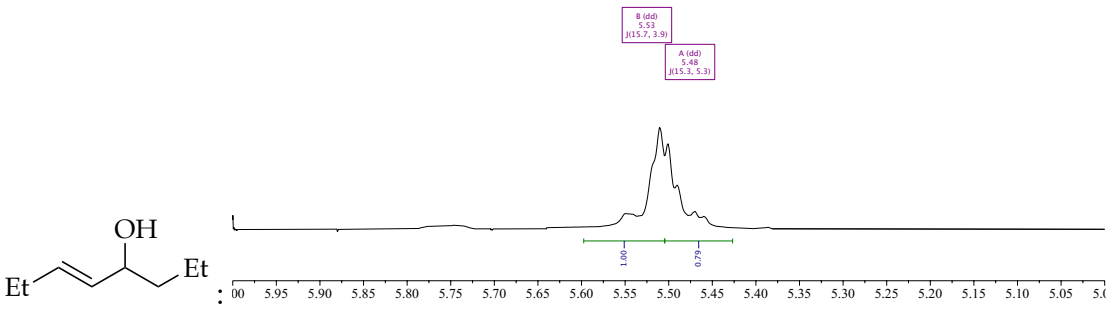
Figure S35. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 125.8 MHz) of *tert*-butyl 3-(isopropylamino)-3-phenylpropanoate at room temperature. δ 171.2, 143.5, 128.5, 127.2, 80.7, 57.1, 45.9, 44.9, 28.1, 24.4, 22.1.

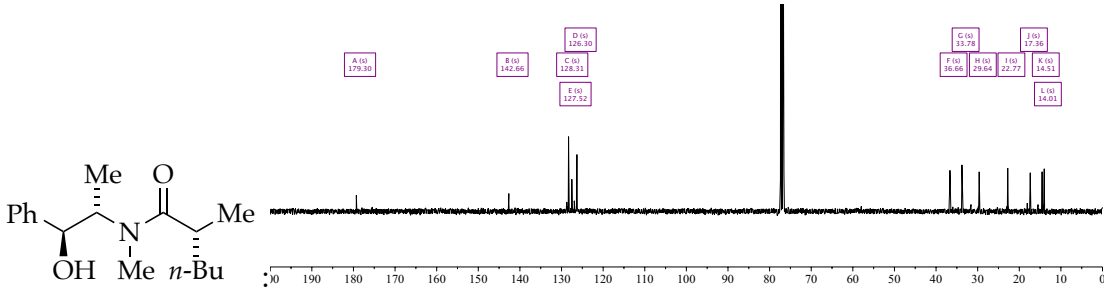
HRMS (DART-Orbitrap) m/z$[M+H]^+$ calcd for $C_{16}H_{26}NO_2$ 264.1958, found 264.1931.

Literature compound:

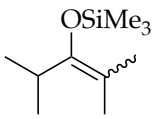




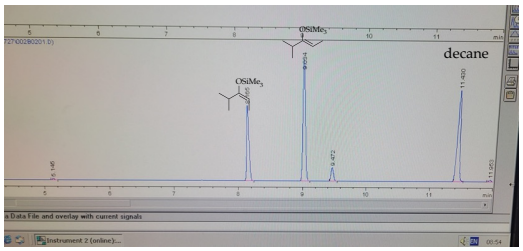


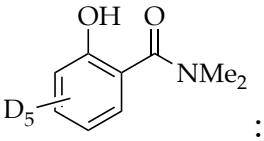


* Minor peaks are carboxamide rotamers

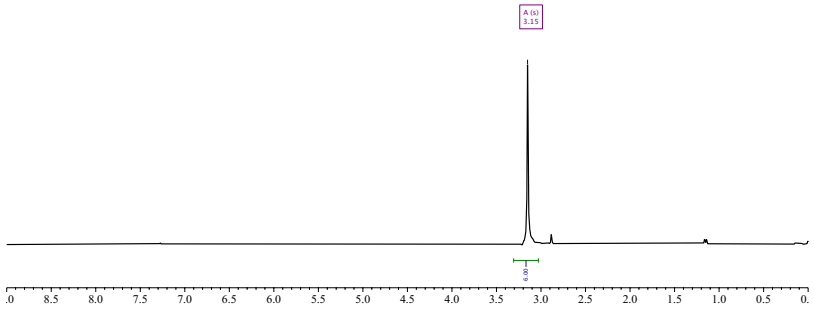

OSiMe3

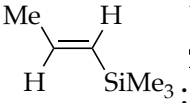
Z:*E* =2:1 :


OSiMe3
OSiMe3
decane
11.420

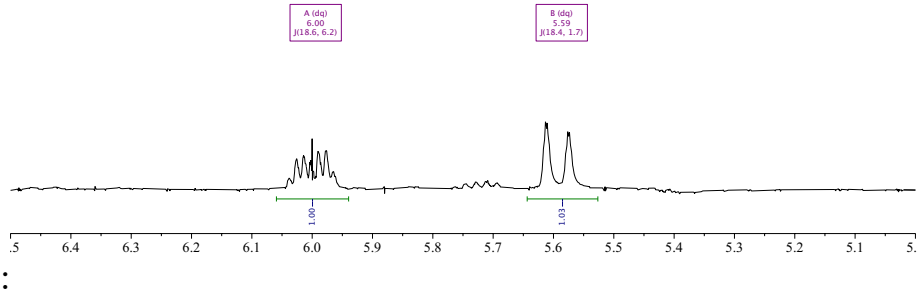

OH
O
NMe2
D5

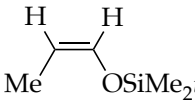
:


A (s)
3.15
6.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5

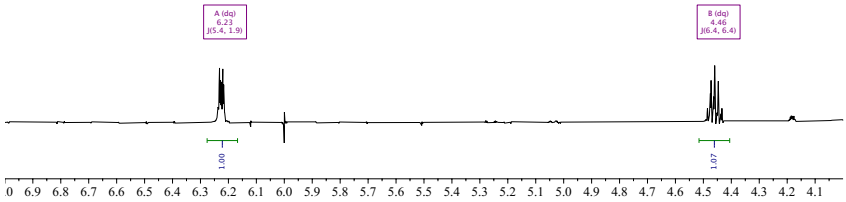

Me
H
H
SiMe3

:


A (dq)
6.00
J(18.6, 6.2)
B (dq)
5.59
J(18.4, 1.7)
1.00
1.03
6.4
6.3
6.2
6.1
6.0
5.9
5.8
5.7
5.6
5.5
5.4
5.3
5.2
5.1


H
H
Me
OSiMe2t-Bu

:


A (dq)
6.23
J(5.4, 1.9)
B (dq)
4.46
J(6.4, 6.4)
1.00
1.07
6.9
6.8
6.7
6.6
6.5
6.4
6.3
6.2
6.1
6.0
5.9
5.8
5.7
5.6
5.5
5.4
5.3
5.2
5.1
5.0
4.9
4.8
4.7
4.6
4.5
4.4
4.3
4.2
4.1

DFT Calculations

General computational methods

All density functional theory (DFT) calculations were performed using Gaussian 16.[S1] Geometries were optimized at the M06-2X[S2] level of theory using Grimme's zero-dampened D3 dispersion correction[S3] (M06-2X-D3(0)) with the double-ζ polarization-consistent segment-contracted basis set pcseg-1 from Jensen and co-workers.[S4]

For improved accuracy single point energies were calculated with the same dispersion corrected M06-2X-D3(0) functional[S2, S3] using the slightly larger (triple-ζ) basis sets of the same family; pcseg-2.[S4]

A pruned (99, 590) integration grid (equivalent to Gaussian's "UltraFine" option) was used for all calculations. Solvation effects were accounted for by the Self Consistent Reaction Field method using the SMD model of Truhlar and coworkers (Solvent = THF).[S5]

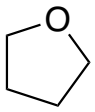
Jensen's segment-contracted polarization-consistent basis sets were obtained from the Basis Set Exchange[S6] and included in Gaussian using the "gen" keyword. CYLview[S7] was used to render all ball-and-stick models.

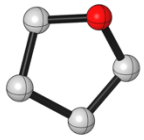
A vibrational frequency analysis was conducted at the same level of theory as the geometry optimizations (M06-2X-D3(0)/pcseg-1/SMD(THF)). The optimized geometries characterized as local minima on the potential energy surface have no imaginary frequencies, while each transition state possesses exactly one.

The energies in this section are defined as follows: G is the sum of electronic and thermal free energies calculated at the M06-2X-D3(0)/pcseg-1 level of theory (T = 295.15 K) and G_{SP} is a thermally corrected single point energy at the M06-2X-D3(0)/pcseg-2 level of theory. The uncorrected SCF energy at final convergence (M06-2X-D3(0)/pcseg-2) is given in the comment line as E(M062X). All energies are reported in Hartree atomic units (Eh). Atomic coordinates are given in the standard cartesian (.xyz) file format (atom count and comment lines are included).

Table S2. Geometric coordinates and thermal corrected single point energies for tetrahydrofuran (THF)

G: –232.197829 Eh G(sp): – 232.341142 Eh

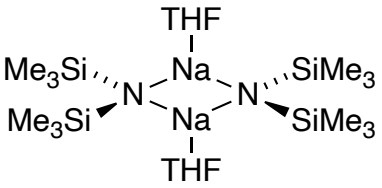


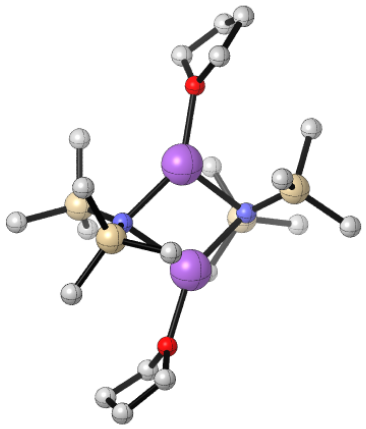


13
THF_THF: optimized structure // E(RM062X) = -232.441249027 A.U. after 10 cycles

C	0.000193531183	-0.001120142042	-0.002218343448
O	-0.003348689250	0.001831686221	1.416587492296
C	1.365118788039	-0.001121684663	1.791131543289
C	2.047552984932	-0.981357489864	0.827081194122
H	3.066742585831	-0.664428870106	0.584974417430
H	2.103795309919	-1.980554397200	1.270795269330
H	1.783097557965	1.012859761982	1.678218028126
H	1.429104810742	-0.291947522954	2.843390856502
C	1.112187907216	-0.980272993237	-0.403542169761
H	1.618244867414	-0.661088421721	-1.319971282967
H	0.700282953596	-1.979292745326	-0.578797908991
H	-0.996733824418	-0.292894433246	-0.344172528780
H	0.219324265658	1.013088007676	-0.374971594194

Table S3. Geometric coordinates and thermal corrected single point energies for the di-THF solvated sodium bis(trimethylsilyl)amide (NaHMDS) dimer.
G: –2534.771554 Eh G(sp): –2535.567351 Eh



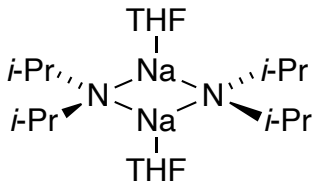


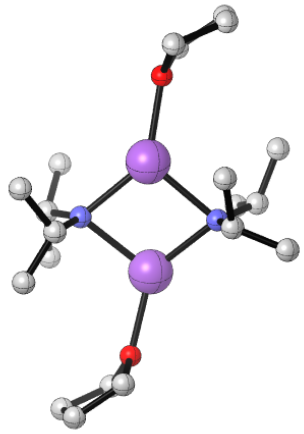
82
Na2HMDS2THF2: optimized structure // E(RM062X) = -2536.21961146 A.U. after 11 cycles

Na	-0.083915782750	0.190253214326	-0.230245059876
Na	0.310154212628	0.276312873037	2.723526939932
N	1.929439892861	0.257943996747	1.033600740448
N	-1.660313130361	-0.137502162104	1.500947416456
Si	-2.516908305491	1.268580153027	1.938456981023
Si	-2.422168063480	-1.600941947121	1.073095349058
Si	2.494128662670	-1.341409287920	1.185701198774
Si	2.822910324890	1.502291730866	0.291564071609
C	4.368949890684	-1.565681658532	1.288307858266
H	4.779157433052	-1.056932016812	2.172066382261
H	4.625561116457	-2.632207034043	1.371509568280
H	4.886372617479	-1.170556647551	0.402975029879
C	1.910713305380	-2.432371426829	-0.252898729214
H	2.197277725684	-3.486861929844	-0.123869651773
H	0.816114906630	-2.412099345683	-0.374480866218
H	2.358031336143	-2.080115277847	-1.195152325740
C	1.825678860930	-2.119996713198	2.783418239507
H	2.145144626363	-3.168756300379	2.872917180763
H	2.214835689989	-1.592186058561	3.668928358186
H	0.727324400129	-2.134123735086	2.838119497941
C	-1.550881762151	-3.140491679477	1.740687179365
H	-0.523534203848	-3.241159136118	1.364317620183
H	-1.507559208337	-3.135606125763	2.839683022797
H	-2.099768804382	-4.045021687561	1.437947793455
C	-4.220001851038	-1.782476843072	1.641441938794
H	-4.861924050264	-0.962353066428	1.290237424569
H	-4.647027400317	-2.721854039078	1.260193974527
H	-4.286068709340	-1.813100045314	2.738563307179
C	-2.439755544314	-1.833101954279	-0.813878771947
H	-2.996050902263	-2.736129609091	-1.106358161983

H	-2.909768807103	-0.975838744670	-1.319250619541
H	-1.424777398014	-1.949612179989	-1.225491571800
C	-3.547102238521	1.115483326216	3.519392742562
H	-3.835011047080	2.101951759247	3.912763667674
H	-4.470338501885	0.543633507929	3.353609359152
H	-2.965503326779	0.593588393108	4.291641795265
C	-1.303775458626	2.700899089530	2.234866553706
H	-0.547761024920	2.541391526366	3.019464296629
H	-0.770245431169	2.958603987576	1.309100833057
H	-1.861539603250	3.600259781578	2.536193990961
C	-3.672268349089	1.928277667220	0.589616004967
H	-4.450822235202	1.197495272025	0.328481150248
H	-4.178849130665	2.853776363921	0.901330832863
H	-3.109336183314	2.151607411891	-0.329338791647
C	1.750217991067	3.046307111734	0.059025371376
H	0.792877262810	2.850821191249	-0.447656052565
H	1.515316434139	3.506192857562	1.029878531706
H	2.280576689379	3.801617972024	-0.539859652699
C	3.457133929405	1.031960504288	-1.435140243843
H	3.896800638102	1.889554098604	-1.966582021615
H	4.228151526788	0.249169995226	-1.379034987051
H	2.633199232352	0.635216278936	-2.044280990538
C	4.331097593775	2.098632051068	1.265129803330
H	5.100356477246	1.318131221334	1.342773280291
H	4.794139034972	2.974502543008	0.786964726689
H	4.046713958565	2.387432433430	2.287344956244
O	0.178654097250	0.197543546065	-2.461077897275
C	0.195252923397	-0.937736679425	-3.331111201562
C	0.385170379761	1.355206282498	-3.282686325864
C	1.326997779467	-0.640074442734	-4.303898900096
H	0.353357500925	-1.831268511693	-2.720654827403
H	-0.775209382262	-1.015627200536	-3.844972148618
C	1.253753977088	0.890237544419	-4.466331389080
H	-0.591324430132	1.728561288973	-3.620158893110
H	0.863926172008	2.118986770302	-2.661675388748
H	1.207350106028	-1.175545432400	-5.250553337163
H	2.283814583713	-0.938779081532	-3.860658389857
H	0.785939565480	1.170499392704	-5.415355357907
H	2.248958412586	1.344389854676	-4.437391551354
O	-0.313869990559	0.362879837585	4.888355546995
C	-0.369024536159	-0.860958811145	5.626817491949
C	-0.762111580892	1.409912248369	5.759650519455
C	-1.652573585092	-0.750431310120	6.434089000519
H	-0.358851618840	-1.689036325032	4.911440057859
H	0.515308707549	-0.935912095984	6.278346290137
C	-1.710531951140	0.748690642931	6.778131914824
H	0.109547960136	1.861318985692	6.252279570055
H	-1.250087725167	2.167008234054	5.138218500252
H	-1.639462827374	-1.390370594858	7.321588687858
H	-2.506393134626	-1.044538563926	5.813000978810
H	-1.360806195589	0.933008585555	7.799001357301
H	-2.728174472325	1.143497665156	6.697977315281

Table S4. Geometric coordinates and thermal corrected single point energies for the di-THF solvated sodium diisopropylamide (NaDA) dimer.
G: –1371.867915 Eh G(sp): –1372.519151 Eh



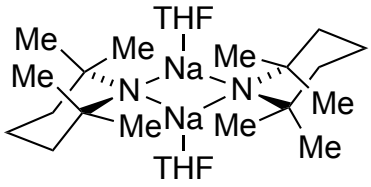


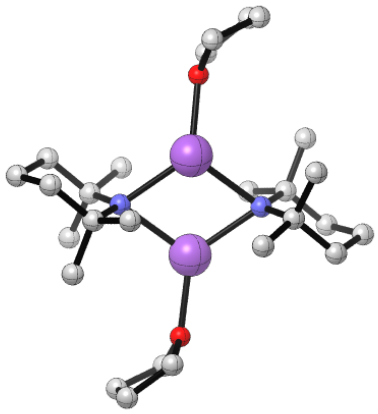
70
Na2DA2THF2: optimized structure // E(RM062X) = -1373.10334360 A.U. after 11 cycles

Na	-0.223695336169	-0.610740580865	-0.354245363079
Na	0.039364531645	-0.243156912178	2.528601831856
N	1.702732476245	-0.327645717139	0.937807896598
N	-1.895164481676	-0.166543765780	1.166265568097
C	2.650978761022	-2.266325299799	-0.304069529677
H	3.438017944683	-3.036997163090	-0.318603933931
H	1.678538053366	-2.784559532032	-0.335515816496
H	2.742999717106	-1.666600361609	-1.218904192256
C	2.562972858137	-2.245112129697	2.192831371366
H	3.275854567203	-3.082645004329	2.214990361057
H	2.705202412080	-1.646659658487	3.103064131236
H	1.548519416177	-2.674484067435	2.221822180552
C	-2.201140954470	-2.541777632644	1.465748519821
H	-1.941785468413	-2.720653937230	0.412899825196
H	-1.276992628426	-2.627596158176	2.060186208798
H	-2.874235705503	-3.348425340933	1.786724147839
C	-3.274472393992	-1.014365143457	3.115446590666
H	-3.866685762972	-0.104579702831	3.273259356651
H	-3.887839297215	-1.867692266167	3.445263766788
H	-2.388524572500	-0.949913383223	3.765391601830
C	-2.150796283318	2.055037008493	2.346954231880
H	-2.481852700780	3.096510960907	2.209088016306
H	-2.675473662975	1.646659560440	3.220676460678
H	-1.076587850186	2.095170533255	2.583215787229
C	-3.852856507751	1.351450617994	0.633006230818
H	-4.556208180799	0.992546323322	1.396595211399
H	-4.094132178428	2.403904976342	0.430839705699
H	-4.035777844775	0.779282560549	-0.286427059323
C	2.895797153527	1.065340245359	-0.804679709451
H	3.134399706990	2.102301867592	-1.085407203439

H	3.838318105136	0.498213782922	-0.803848676406
H	2.248260738733	0.634966020687	-1.579370306013
C	3.107425084543	1.632470673175	1.634598433549
H	4.016008588707	1.033481095644	1.789685322556
H	3.424347126530	2.648579411318	1.355624452707
H	2.579234096473	1.690689082222	2.596484712111
O	0.107324720678	-0.377124699845	-2.578269786232
C	0.644207291664	-1.316946007902	-3.509263733246
C	0.123832773868	0.902352166502	-3.221216469776
C	1.814448951317	-0.580717243440	-4.146799567020
H	0.922310206016	-2.219123483926	-2.956590966659
H	-0.125640654022	-1.572503490984	-4.253652680074
C	1.325602043949	0.880742238664	-4.185235085089
H	-0.822953737497	1.041407216604	-3.760839436111
H	0.197918438896	1.664810160598	-2.438571654835
H	2.058559449886	-0.973785499814	-5.138486994799
H	2.703642418448	-0.676466649474	-3.512990120404
H	1.011132551257	1.171826501735	-5.192557312274
H	2.110252478990	1.574273102837	-3.867535282734
O	-0.138270218329	-0.266756435704	4.783327329258
C	-0.386477552387	-1.455341870306	5.540834840512
C	-0.471368458976	0.831793170713	5.632828828258
C	-1.585199169412	-1.133989335110	6.452140678659
H	-0.572493557799	-2.269522034269	4.832709518387
H	0.511544315227	-1.695849949935	6.126775908127
C	-1.756788866382	0.393864947451	6.324234031826
H	0.343299523486	0.988676994699	6.356243344644
H	-0.573552097081	1.724410039665	5.008881583957
H	-1.373093704236	-1.433983204924	7.483189004299
H	-2.487208383178	-1.663262817251	6.129649082298
H	-1.892241013766	0.889571441681	7.290329872320
H	-2.619703200786	0.634634933814	5.693268218450
C	-2.832861368370	-1.159669536254	1.643308137613
C	-2.391239695515	1.200825203252	1.080469461427
C	2.199133711299	0.987315022382	0.568711808905
C	2.713740018556	-1.366303753269	0.945689373967
H	1.310097872902	1.645363252453	0.494677343058
H	3.740105446064	-0.947949978227	0.979577581882
H	-3.774153841490	-1.176929707158	1.049272172981
H	-1.793483420392	1.704883381570	0.295000036683

Table S5. Geometric coordinates and thermal corrected single point energies for the di-THF solvated sodium 2,2',6,6'-tetramethylpiperidide (NaTMP) dimer.
G: –1605.082461 Eh G(sp): –1605.864647 Eh





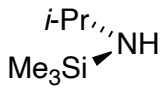
84
Na2TMP2THF2: optimized structure // E(RM062X) = -1606.58097536 A.U. after 11 cycles

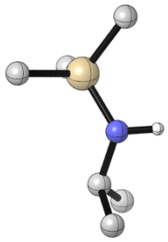
Na	-0.149692075958	0.104511445788	-0.285250920450
Na	0.222458552660	-0.082539316470	2.468925005354
O	0.170559209093	-0.135710937113	-2.504299989057
C	-0.896085899200	-0.321177357440	-3.436710464795
C	1.367896899419	-0.586812221962	-3.148031138150
C	-0.603693941903	-1.675376914217	-4.066189567120
H	-1.840619431323	-0.268872347498	-2.886669081583
H	-0.870617892616	0.486831248222	-4.183782707308
C	0.936181986609	-1.702670286981	-4.119676841519
H	1.824484087246	0.258988415518	-3.680017317498
H	2.056431453690	-0.925771789995	-2.366912543273
H	-1.066411450627	-1.782600157424	-5.051998960732
H	-0.984522994098	-2.474116766096	-3.419280808597
H	1.304868660342	-1.492394711361	-5.128708878645
H	1.330870449019	-2.677168876754	-3.815946439751
O	-0.278319656596	0.121917069391	4.660537486472
C	-1.501059066898	0.587549103797	5.242841891309
C	0.728154418866	0.238580284915	5.667985510582
C	-1.100967049404	1.664226416228	6.270125883306
H	-2.132415242269	0.965360767103	4.431998684937
H	-2.009565713070	-0.259931214195	5.722806935188
C	0.437030853357	1.579124235444	6.327532001686
H	0.627634295959	-0.594394402815	6.380350037062
H	1.705652754539	0.174952900542	5.180067358342
H	-1.551432585687	1.447540374226	7.243921247018
H	-1.435135141018	2.659358314017	5.961057462682
H	0.829117027616	1.631902350649	7.347778068711
H	0.892736781659	2.386431479143	5.742939830783
C	1.718881580742	2.507223623440	0.948839123495
C	-0.659485601170	2.844507223629	1.541979927769
C	1.672136692716	3.755506277820	0.036863881688
C	-0.722297075992	4.089022451523	0.628257471840

C	0.633700614833	4.771184524289	0.496615785532
H	1.409121861360	3.420121550386	-0.979714954693
H	2.668282540318	4.220830558250	-0.025106812007
H	-1.479199676127	4.797608329692	0.999530651435
H	-1.049517767417	3.759773665329	-0.371602258720
H	0.575407019540	5.608098583672	-0.213022259138
H	0.932765359423	5.208905066044	1.460465279897
C	0.748326838641	-2.825188495564	0.645674779514
C	-1.631130595550	-2.487276122840	1.226249270560
C	0.811468161766	-4.061877625066	1.570037240558
C	-1.587105739963	-3.726561913337	2.150382215116
C	-0.544078311395	-4.744500804960	1.705813989461
H	1.137732155186	-3.723773949297	2.567300007787
H	1.569110003817	-4.773230197205	1.205446914916
H	-2.582410494070	-4.193918780748	2.211392162315
H	-1.330583139937	-3.380248357104	3.164971963264
H	-0.486237678967	-5.573344666978	2.424924172013
H	-0.839236830549	-5.193854035045	0.746108073072
N	0.397823277479	1.909202575325	1.149811525525
N	-0.309762330334	-1.888253750898	1.030738253001
C	2.602422809405	1.472501624905	0.246923792502
H	3.591259370547	1.886768217238	0.004015846629
H	2.759182788869	0.597922387949	0.891091860892
H	2.145715240721	1.139982034582	-0.698020090479
C	2.085631441304	-2.091693250326	0.772167053140
H	2.147556310759	-1.267532730159	0.048380308842
H	2.218177409263	-1.678420866550	1.783312973961
H	2.934271806209	-2.761909430850	0.574825560378
C	0.686046113852	-3.312521713456	-0.828849480623
H	-0.067774084518	-4.089304593124	-0.995325422901
H	0.440605314756	-2.463367132267	-1.480156169335
H	1.652867790486	-3.729706748503	-1.151625517644
C	2.471667997748	2.873999143955	2.255546922423
H	2.051371530487	3.747751629453	2.763275258059
H	2.428163962373	2.027165255541	2.956469997098
H	3.531868981966	3.093928848667	2.057128554264
C	-0.597855249639	3.319370409910	3.020300532934
H	0.172940722531	4.076720240590	3.197788417549
H	-1.557236125099	3.757393606437	3.337702620422
H	-0.379144615931	2.460825101820	3.669273203980
C	-1.996526014267	2.112133322790	1.407389176597
H	-2.133543297189	1.720114731648	0.388338824420
H	-2.051819515857	1.272484092175	2.113307561358
H	-2.845774571891	2.775813733910	1.623534149778
C	-2.372523977386	-2.867460977582	-0.083306588626
H	-1.949037061881	-3.746488557320	-0.579025842966
H	-3.434661043722	-3.084197969814	0.108318477332
H	-2.321732443694	-2.027057757305	-0.791450555206
C	-2.523132552617	-1.448424677236	1.911156318936
H	-2.072329904617	-1.101884542500	2.853630707772
H	-2.681615481299	-0.582642844261	1.255225693598
H	-3.511075349593	-1.864896671894	2.153964073881

Table S6. Geometric coordinates and thermal corrected single point energies for *N*-isopropyltrimethylsilazane.

G: –582.741383 Eh G(sp): –582.956834 Eh





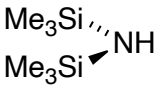
25

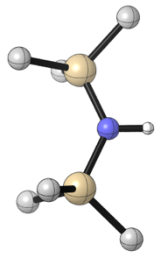
PTA(H): optimized structure // E(RM062X) = -583.156373722 A.U. after 10 cycles

N	0.282511120189	0.162243823190	0.125768012855
H	0.137743527510	-0.144761379592	1.086051106710
C	1.690733341591	0.100913889636	-0.263455920137
H	1.762508644294	0.530469360306	-1.274381964684
C	-1.099919257906	0.982053176566	-2.339385438021
H	-1.800740962392	1.704287595965	-2.780332746961
H	-0.157005304893	1.057088381189	-2.898340375507
H	-1.504785635789	-0.025990168730	-2.499672390327
C	-0.283967695993	3.104591411376	-0.331278092645
H	-1.033822072299	3.791666995064	-0.749375878053
H	-0.133074349697	3.374817010238	0.722625270843
H	0.658993825058	3.285669106648	-0.865729599892
C	2.580174048851	0.920087625236	0.670135786339
H	2.256684705582	1.967516175774	0.702000929155
H	2.524540868938	0.515800883909	1.690768827455
H	3.630347972639	0.892368933313	0.351782892135
C	2.158513621940	-1.349052017775	-0.334460454821
H	1.542628274927	-1.917797963345	-1.040587372651
H	3.207379126602	-1.417062162906	-0.649410883520
H	2.068390249798	-1.821550923390	0.653724668902
Si	-0.851033169762	1.319653097888	-0.511587256244
C	-2.449345008587	1.072549601073	0.430384817747
H	-3.226616965347	1.757443563928	0.065814126171
H	-2.824235267928	0.047075563455	0.314313675869
H	-2.315146023253	1.265093213143	1.503551324456

Table S7. Geometric coordinates and thermal corrected single point energies for hexamethyldilizane.

G: –873.458277 Eh G(sp): –873.709478Eh





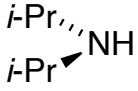
28

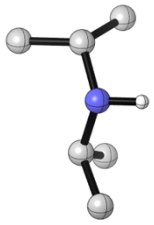
HMDS: optimized structure // E(RM062X) = -873.923091460 A.U. after 10 cycles

N	0.189363189864	0.334406679674	-0.213461991147
H	-0.207988796989	-0.356194441469	0.421481072813
Si	1.818033885833	-0.003022324971	-0.745801884406
Si	-0.840519577950	1.700676387648	-0.561372757754
C	2.519898490780	-1.325047131040	0.380239040293
H	3.540805110821	-1.595632421729	0.078753095207
H	2.556818036307	-0.981706806615	1.422646700023
H	1.911259771172	-2.239140883773	0.345811466315
C	2.855882597198	1.556763618293	-0.644018147842
H	2.457244235733	2.359115363389	-1.280083540757
H	2.904969055670	1.933859334904	0.386325093623
H	3.883578810382	1.356434042473	-0.978705742858
C	1.853997585709	-0.622155400046	-2.517918847981
H	2.877747856707	-0.877910098144	-2.825709759655
H	1.233741463903	-1.521631335246	-2.631505659233
H	1.475075594088	0.134970028910	-3.217341522760
C	-0.677755307257	2.160404397758	-2.372624937470
H	0.350620161373	2.443862979076	-2.635870855047
H	-0.977533118417	1.327789486254	-3.022972426839
H	-1.321820915528	3.019732278506	-2.607223005418
C	-0.383887593972	3.199692192776	0.473455755132
H	-0.440983379881	2.968011855767	1.545785658635
H	0.638804874792	3.538292230396	0.259719888066
H	-1.062971295527	4.040746485751	0.274384988495
C	-2.603420355645	1.203401470412	-0.169830200608
H	-3.295566078999	2.037277937725	-0.348718497106
H	-2.925947102618	0.358110434167	-0.792065357077
H	-2.707102016697	0.907589995098	0.883285593350

Table S8. Geometric coordinates and thermal corrected single point energies for diisopropylamine.

G: –292.025728 Eh G(sp): –292.206067 Eh





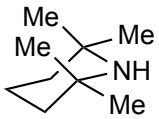
22

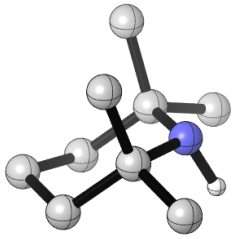
DIPA: optimized structure // E(RM062X) = -292.393150646 A.U. after 10 cycles

N	0.032896733244	-0.176952172808	-0.004143532351
H	0.066838194471	-0.205797583646	1.015330706817
C	1.400422907591	-0.017838979554	-0.519357585727
H	1.669371469260	1.023505321803	-0.289607677802
C	-0.812385990781	-1.275812964366	-0.477543837517
H	-0.942309114112	-1.139037836893	-1.559878755008
C	1.436582232837	-0.163919468678	-2.034766525207
H	2.420858867393	0.134297140622	-2.414866382117
H	1.258480194621	-1.200619230597	-2.347752775782
H	0.680086566540	0.474934134164	-2.506813248693
C	2.459366983530	-0.895908720635	0.155783314920
H	3.465236546676	-0.561405244595	-0.131518103933
H	2.385273837071	-0.817896154485	1.248563554058
H	2.367169069729	-1.952424320811	-0.118802751406
C	-0.273384881585	-2.688767345348	-0.236413307993
H	0.629246384563	-2.890560404474	-0.822811317100
H	-0.032884280547	-2.832730734039	0.826505820909
H	-1.024720440898	-3.438416328865	-0.518807511312
C	-2.178631057302	-1.110889356330	0.178787435959
H	-2.576277209732	-0.107484349316	-0.010384577759
H	-2.892310196091	-1.850502586461	-0.202369267501
H	-2.099304374685	-1.248125113160	1.266739588979

Table S9. Geometric coordinates and thermal corrected single point energies for 2,2,6,6-tetramethyl-piperidine.

G: –408.636953 Eh G(sp): –408.882356 Eh



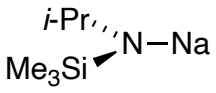


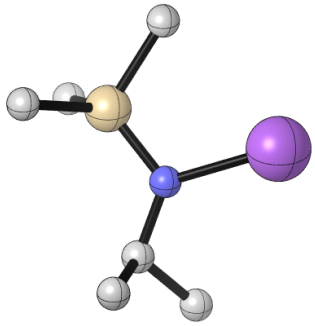
29
TMP(H): optimized structure // E(RM062X) = -409.133374300 A.U. after 11 cycles

C	-0.011782243190	0.026301642593	0.021919052005
C	-0.023764754695	0.091319055866	1.560649213710
C	2.529713859969	0.100238407975	1.538467780475
C	2.491042020656	0.036901531757	0.000052556033
C	1.231696495886	0.678976453514	-0.577211388700
H	-0.033487650648	-1.032908745558	-0.280325996063
H	-0.926387191273	0.490339248901	-0.373802032349
H	3.394566704882	0.509134528132	-0.411105707455
H	2.516580980861	-1.021765611112	-0.303799696159
H	1.228688169642	1.760137536256	-0.379062287803
H	1.222829602175	0.568363609682	-1.668981816447
N	1.259707124753	-0.369561121919	2.140156872510
H	1.262520450335	-1.387210186293	2.057128785337
C	2.867181995722	1.518583684310	2.010509546242
H	2.735161041001	1.595754281683	3.096640641533
H	3.914433700800	1.746362512326	1.772571668562
H	2.251036417557	2.287595742869	1.535250398490
C	3.613115784880	-0.841720768012	2.061276216792
H	4.592352743684	-0.572721274510	1.646861135347
H	3.669714124622	-0.789234008625	3.156029803932
H	3.396503600926	-1.880265138272	1.776269146952
C	-0.360983124228	1.508456959014	2.036053726576
H	-1.413691976210	1.729891402314	1.817041630365
H	-0.209158499977	1.588942103678	3.119368349860
H	0.242300324273	2.279235082111	1.547374203170
C	-1.091716037404	-0.856609277949	2.103833062579
H	-1.129557660186	-0.802712933710	3.199323630745
H	-2.079728475747	-0.594587205511	1.706122641996
H	-0.873459157844	-1.894236928974	1.816703700151

Table S10. Geometric coordinates and thermal corrected single point energies for the unsolvated NaPTA monomer.

G: –744.42927 Eh G(sp): –744.655258 Eh



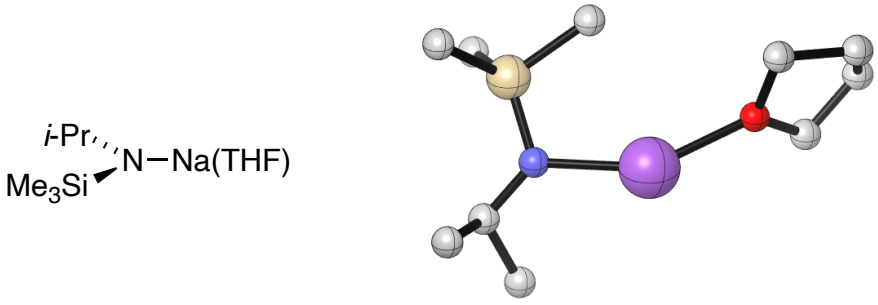


25
A1S0: optimized structure // E(RM062X) = -744.840816033 A.U. after 11 cycles

Na	-0.275863173558	0.018491002174	-0.072067826220
N	0.038444912317	0.050082153651	2.095165520106
C	2.491343925855	-0.032513340737	2.045430116676
H	2.475462666136	-1.124757198533	1.940084544835
H	2.512846937719	0.406431715508	1.034930434410
H	3.423256238789	0.253139038599	2.554035113078
C	1.325630407048	1.970439171897	2.985336636364
H	0.453128364656	2.335618095413	3.541850047383
H	2.232613577742	2.277909593653	3.527432536058
H	1.326189944407	2.467778402750	2.003802205718
C	-2.076212600378	0.892715503984	4.134529761571
H	-3.000175631127	0.532949113636	4.611943680657
H	-1.372977513116	1.151137775947	4.940059577391
H	-2.317099623134	1.820577282827	3.595946852642
C	-2.700499357251	-0.824946560308	1.710892852284
H	-2.978202458426	0.044710517813	1.094736554590
H	-2.409522082428	-1.650296253307	1.042071534585
H	-3.619017992942	-1.149126044824	2.221429362784
C	-1.126955946222	-1.954919071027	4.049912429016
H	-2.047325435014	-2.201308856626	4.599658325877
H	-0.855538531656	-2.828163810686	3.439484670417
H	-0.329268320522	-1.815680977696	4.794391971667
Si	-1.339354240382	-0.410992395863	2.964524979625
C	1.245453129186	0.450033173723	2.793367923877
H	1.304730504875	0.003032996168	3.809655760207

Table S11. Geometric coordinates and thermal corrected single point energies for the mono-THF solvated NaPTA monomer.

G: –976.64056 Eh G(sp): –977.004552 Eh



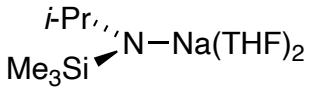
38
A1THF1_thf: optimized structure // E(RM062X) = -977.302595135 A.U. after 11 cycles

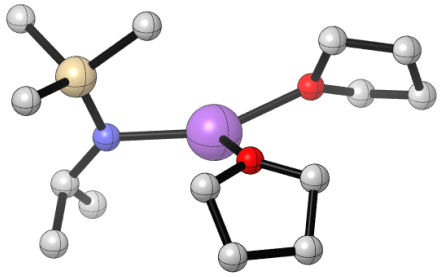
Na	-0.083319835181	0.009573637822	0.024468524193
N	-0.011589304756	-0.032822849409	2.236030075605
C	2.429219946491	-0.133923674254	2.438052797000
H	2.435872908333	-1.188994269148	2.135670918476
H	2.552118156764	0.481180936575	1.532505247980
H	3.298966676024	0.044758476426	3.086620504328
C	1.156762830091	1.676498142750	3.599244879487
H	0.227943454731	1.946498439943	4.117732953442
H	1.999018405617	1.866698953104	4.281677996645
H	1.258290356352	2.343366381741	2.730212669398
C	-2.395922686792	0.663486709891	4.032179440379
H	-3.399687505703	0.298302038097	4.297646087384
H	-1.834688452940	0.783953848253	4.970620563737
H	-2.509888171589	1.661593282779	3.585014958817
C	-2.677730086690	-0.752930682386	1.363983415468
H	-2.836704537449	0.190967723536	0.818916178458
H	-2.302650920590	-1.506550282487	0.653523128328
H	-3.669816806352	-1.096439304198	1.691608492199
C	-1.500044668670	-2.187053273137	3.770910850142
H	-2.498434653420	-2.452794224227	4.148763631748
H	-1.161296130108	-3.001170605156	3.114108343981
H	-0.820607553781	-2.160051961632	4.635565246703
Si	-1.510426241994	-0.528213661616	2.843587245091
C	1.105882183013	0.217605696923	3.123773183800
H	1.059141630165	-0.408648641977	4.042074727027
O	-1.036784910771	-0.650158187905	-1.871070744788
C	-0.481400679684	-1.626866434485	-2.777657327497
C	-2.354781714389	-0.258265593009	-2.308021864219
C	-1.630221293667	-2.028734165616	-3.690394099779
H	0.334267313369	-1.152750743688	-3.338250319431
H	-0.078085677094	-2.457166545963	-2.189225950910
C	-2.453118318788	-0.742577923364	-3.744871834291
H	-3.099076195823	-0.748127090535	-1.666606394617
H	-2.443413853089	0.827067759380	-2.197589667194

H	-2.216601199102	-2.835206929129	-3.233559478724
H	-1.279559768883	-2.367106942949	-4.669805420114
H	-3.489321635773	-0.899418508632	-4.058467692459
H	-1.987761728132	-0.018435224997	-4.424907117194

Table S12. Geometric coordinates and thermal corrected single point energies for the di-THF solvated NaPTA monomer.

G: –1208.846862 Eh G(sp): –1209.348261 Eh





51

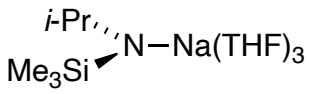
A1THF2_thf: optimized structure // E(RM062X) = -1209.76265866 A.U. after 11 cycles

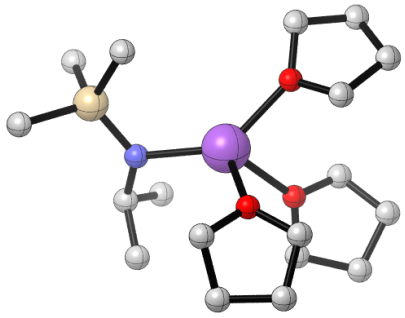
Na	0.762257277361	-0.549078483946	0.273648675570
N	0.496739163628	0.025689676437	2.423709098191
C	2.840434458265	0.167509799870	3.121368230904
H	2.886239997473	-0.917975451027	3.276130210927
H	3.153491759933	0.374864461158	2.086030311630
H	3.564288242358	0.645394006688	3.797481488194
C	1.396666454433	2.205504290418	3.182417052561
H	0.385733234767	2.599970622195	3.347940820944
H	2.079711995504	2.707172716764	3.885179823860
H	1.697583807875	2.475747478544	2.158728123374
C	-2.188511528723	1.185843672194	3.350470048296
H	-3.220770358846	0.872978260576	3.570316592786
H	-1.804541968811	1.691850986749	4.248872385471
H	-2.232129487711	1.932473827192	2.544256586516
C	-1.961757991918	-1.127615915202	1.401100780909
H	-1.984650206624	-0.472021002541	0.517018928724
H	-1.469437807002	-2.071680290564	1.117787641489
H	-3.004841799619	-1.377076768462	1.644989862511
C	-1.296167517187	-1.493609148140	4.344055685014
H	-2.352577385513	-1.660306249547	4.602201463453
H	-0.846836236644	-2.471327993311	4.117634600014
H	-0.797350201512	-1.105741926924	5.244693275563
Si	-1.097658065793	-0.302084741983	2.874960797908
C	1.412248056691	0.677015663976	3.335901152158
H	1.167805153904	0.469672789011	4.401797585184
O	-0.410860312247	0.866384483445	-1.016689585575
C	-0.354599913876	1.111863152084	-2.420255394388
C	-0.990234772440	2.036267338566	-0.435433750617
C	0.041575734985	2.588805774207	-2.553971848659
H	0.364480464684	0.408384682492	-2.850640168037
H	-1.348200018527	0.926423759790	-2.856127373622
C	-0.336288797760	3.199364519138	-1.183838276588
H	-2.079036345144	2.014775872496	-0.596317774635

H	-0.778636143938	2.008197138637	0.637869435197
H	-0.487424757466	3.063707322169	-3.385512125605
H	1.115153507344	2.686843978602	-2.741293470885
H	-1.014868822194	4.052746162939	-1.271840261603
H	0.558821721160	3.534627960492	-0.650330535396
O	0.698921423702	-1.895891919186	-1.514654338524
C	1.682836330201	-2.553301616953	-2.314282539748
C	-0.572349388310	-2.207747322304	-2.096959633534
C	1.213692203305	-2.314012464450	-3.743783461152
H	2.657474168096	-2.118256601881	-2.077295678385
H	1.695885884202	-3.625604089170	-2.067526430569
C	-0.323610544448	-2.316632320027	-3.612733341080
H	-0.928616628214	-3.160471321627	-1.681049566899
H	-1.266618193302	-1.412157839507	-1.810555900904
H	1.583787130295	-3.079324177704	-4.432574496322
H	1.572836542393	-1.340063770095	-4.094843457652
H	-0.761037145533	-3.239390458343	-4.006329202519
H	-0.772527980243	-1.479398528009	-4.156024716453

Table S13. Geometric coordinates and thermal corrected single point energies for the tri-THF solvated NaPTA monomer.

G: –1441.054135 Eh G(sp): –1441.692415 Eh





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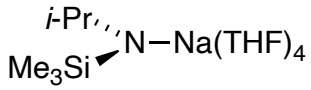
A1THF3_thf: optimized structure // E(RM062X) = -1442.22229169 A.U. after 11 cycles

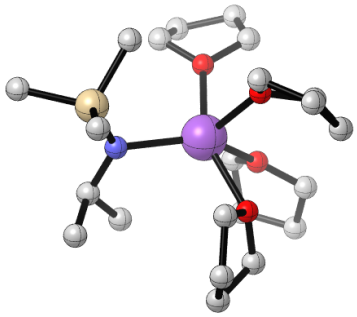
Na	-0.526401508372	-0.087815068418	0.333584062034
N	-0.207632946027	0.074178421300	2.567570004097
C	1.704357027994	-1.484080378553	2.614515523775
H	1.081940888490	-2.285425810312	3.034792571179
H	1.672829353586	-1.576749915368	1.517201052518
H	2.742093155771	-1.642471384181	2.946831397361
C	2.062852481223	0.985206315313	2.455984284706
H	1.738187034646	1.973305396161	2.808822150053
H	3.120451735974	0.848570723060	2.728908751942
H	1.984346125502	0.981318830645	1.357438558763
C	-1.560040429398	1.363002804173	4.958268286637
H	-2.425800870172	1.265543167628	5.630437441984
H	-0.654725258130	1.328816693425	5.583057176589
H	-1.601338444386	2.362158671200	4.500077061072
C	-3.103095433751	0.230286704463	2.598464427079
H	-3.087474992292	1.182411765759	2.047090318629
H	-3.224171453221	-0.579844853681	1.863695487113
H	-4.002253584531	0.232879082325	3.232003154479
C	-1.733695853111	-1.611940682834	4.592355828287
H	-2.613136947585	-1.591313379662	5.253854960853
H	-1.847950244384	-2.466833583473	3.909459340588
H	-0.854720951534	-1.813173111270	5.223532083839
Si	-1.522591996990	0.011562634695	3.617193492829
C	1.152606029393	-0.110153275933	3.024848191152
H	1.250018035999	-0.052518733704	4.132298703716
O	-0.099666647271	1.842506864379	-0.766086444114
C	0.354915914665	2.140729530655	-2.085600487063
C	0.089559650999	3.022480395043	0.016995022658
C	1.479016883898	3.185008949399	-1.926196311690
H	0.686405017081	1.200300287521	-2.537932948108
H	-0.483228671317	2.540540317443	-2.674367053337
C	1.451111826123	3.538484170990	-0.425879355679
H	-0.709121488105	3.745727145814	-0.211172033355

H	0.028099498971	2.732484621940	1.070990360537
H	1.275365660773	4.063112137259	-2.547375420165
H	2.452250965770	2.784890024097	-2.229806187558
H	1.572451424657	4.609708687314	-0.238303232113
H	2.241492671525	3.005880872438	0.116579571628
O	1.122747344858	-0.893359049853	-1.007073878643
C	2.410740514915	-0.298940865593	-1.164028833573
C	1.132182302318	-2.074380812853	-1.803859999843
C	2.825412970689	-0.582686963320	-2.621350382252
H	2.313205264166	0.763603855285	-0.920837352523
H	3.110356294661	-0.761732699200	-0.452390024812
C	1.798492301249	-1.630815344705	-3.101653798473
H	1.721891442742	-2.854575565182	-1.296927618831
H	0.098053611448	-2.416947106926	-1.904523645198
H	3.848658101551	-0.968830877838	-2.661363887788
H	2.790593946805	0.323491063911	-3.235097610836
H	2.259352030532	-2.465475427492	-3.638503478871
H	1.054708137564	-1.170851321628	-3.763798077816
O	-1.950458859232	-1.102159107864	-1.084407645830
C	-2.979573068201	-2.085959205000	-1.000036680020
C	-1.887753746145	-0.676614334470	-2.447471969564
C	-2.787498606436	-2.927337321607	-2.255649924592
H	-2.844854290986	-2.634507396853	-0.063969435561
H	-3.962347375301	-1.590128187162	-0.992234009075
C	-2.300238750693	-1.896713726512	-3.294074724643
H	-2.576673097629	0.167485558825	-2.593868713893
H	-0.864092341399	-0.335178381288	-2.630139048538
H	-3.708312745950	-3.434397759286	-2.559241512372
H	-2.023064456671	-3.691470030806	-2.075574913175
H	-3.096059972478	-1.625237184316	-3.994744931257
H	-1.461343828398	-2.284286698842	-3.881569229581

Table S14. Geometric coordinates and thermal corrected single point energies for the tetra-THF solvated NaPTA monomer.

G: –1673.254823 Eh G(sp): –1674.029722 Eh





77

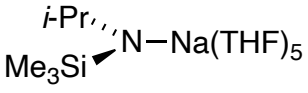
A1THF4_thf: optimized structure // E(RM062X) = -1674.67744436 A.U. after 11 cycles

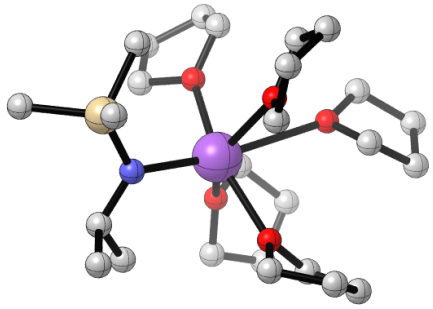
N	0.072881192656	-0.012713343071	0.016556075721
C	0.072654554618	0.020262080508	2.445473758163
H	1.169548389391	0.078100819256	2.467148167783
H	-0.320928717923	1.048672373858	2.422090689618
H	-0.264900678395	-0.460323711256	3.375845356594
C	-1.907532960121	-0.933785655061	1.240629847264
H	-2.241748788522	-1.572923102482	0.411969986477
H	-2.231860004493	-1.409260360320	2.179361732982
H	-2.425521229355	0.031838785282	1.142242992685
C	-1.909324805695	-0.240834562525	-2.320175655811
H	-1.963043418621	-0.605035174868	-3.358322641019
H	-2.702679184540	-0.749248169436	-1.752896282040
H	-2.159075798937	0.830854079353	-2.336432599583
C	1.035058323799	0.344829885889	-2.709429376138
H	1.277918453014	1.348777251755	-2.330278917004
H	1.978869650530	-0.217132936250	-2.770013085600
H	0.647846513862	0.446469114401	-3.734693142807
C	0.087720227641	-2.416832504607	-1.828552537385
H	0.008663000141	-2.689738009874	-2.891767889350
H	1.084754478910	-2.724330747371	-1.479464868519
H	-0.651750987433	-3.020191671629	-1.280910128658
Si	-0.180801571811	-0.549569487179	-1.559639942369
C	-0.384539744937	-0.724232092759	1.185663415514
H	0.057970979541	-1.745217615244	1.254909165506
O	-1.096089203833	3.340059354776	1.014685615455
C	-1.521697207976	3.508605523050	2.369620019161
C	-2.187230596425	2.858616421775	0.207754857138
C	-2.785813619976	2.673897943508	2.511658456812
H	-0.702296234984	3.186846372363	3.023255361695
H	-1.728808971747	4.574270751071	2.556623325791
C	-3.410055880166	2.818351284350	1.122905476386
H	-2.321479703731	3.534773201995	-0.645285736321
H	-1.910028954747	1.861063253228	-0.160942274307

H	-3.433452752293	3.034461421266	3.317146305707
H	-2.528910226572	1.627280176402	2.715168529214
H	-3.968967687150	3.760226488258	1.057832367239
H	-4.089808879407	1.999870891240	0.864163280445
O	2.976341189156	2.030558302418	-0.331905867193
C	3.782995031006	0.870913032274	-0.490111333301
C	3.814127854179	3.164936166542	-0.528682458732
C	5.080571882247	1.232232809966	0.222327478624
H	3.235979568083	0.024499447584	-0.063406088334
H	3.959842643888	0.682131312411	-1.561402702403
C	5.236145064088	2.727358900056	-0.112485108927
H	3.781557683848	3.460989788834	-1.587671282861
H	3.404602314442	3.977974390387	0.080003894251
H	5.928281519606	0.628470397073	-0.116577280026
H	4.964776903972	1.083309081984	1.302097780544
H	5.938251696689	2.873868987665	-0.940149606769
H	5.608956975615	3.301722928737	0.741454116935
O	0.524987985669	3.618817172851	-1.525533153965
C	0.772098141646	4.962682725205	-1.126726887784
C	-0.337950946805	3.645383818457	-2.664066262589
C	-0.562474894764	5.662933103584	-1.329706443745
H	1.115353700250	4.941513212291	-0.088022711193
H	1.558900842033	5.402280818211	-1.761883437546
C	-1.088065740127	4.993269778209	-2.610777565926
H	0.264573386166	3.556402129582	-3.578847042496
H	-0.995287474555	2.771854283635	-2.596283858243
H	-0.459589429292	6.748231279112	-1.428412043911
H	-1.212005953444	5.445727609693	-0.473548308657
H	-0.844818939417	5.597362234142	-3.491477057962
H	-2.174370423298	4.858615055733	-2.593349069585
O	1.751797073667	3.462144634182	1.861021751502
C	2.723116457614	2.784401563223	2.651308967102
C	1.531527402959	4.715342215838	2.500762537351
C	2.257419526506	3.026215915136	4.083566650874
H	2.738933393290	1.734764889902	2.345682617743
H	3.718332058931	3.226036387817	2.471148858934
C	1.640367364910	4.439798144793	4.013106576384
H	2.307430882166	5.425820750126	2.174026297561
H	0.554847234066	5.086572655016	2.177240008392
H	3.075235267161	2.950507505623	4.806577276774
H	1.496767983255	2.282715712782	4.349864986928
H	2.277014575420	5.187626185308	4.496320206833
H	0.660820076419	4.474725597189	4.500474311371
Na	0.774478339361	2.170833686590	0.220987147520

Table S15. Geometric coordinates and thermal corrected single point energies for the penta-THF solvated NaPTA monomer.

G: –1905.453502 Eh G(sp): –1906.364979 Eh





90

A1THF5_thf: optimized structure // E(RM062X) = -1907.12766212 A.U. after 11 cycles

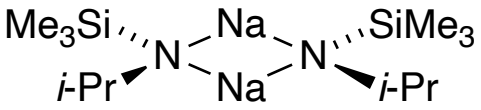
N	-0.501900796508	-0.532978588281	-0.105624275387
C	-1.365584721709	-0.378819389458	2.174645385231
H	-0.351429399274	-0.200297670957	2.556224904728
H	-1.810780700851	0.602043895617	1.951589101515
H	-1.956532409186	-0.865450642184	2.965890808023
C	-2.738065877072	-1.515470209036	0.423941415141
H	-2.729450828950	-2.172484676937	-0.456173114968
H	-3.339557720324	-2.007052975613	1.204901666676
H	-3.241682081701	-0.581077084457	0.135070490543
C	-1.051332122465	-1.640342562274	-2.932050579333
H	-0.537956720005	-2.167523565224	-3.751604504389
H	-1.944249216716	-2.228948952654	-2.674401744682
H	-1.404467142041	-0.677226050853	-3.330471029017
C	1.633274962948	-0.544524014244	-2.116908932543
H	1.496327471355	0.539870764245	-2.029253488583
H	2.526927501542	-0.807204609767	-1.532053621431
H	1.830992118112	-0.801769930710	-3.168522294395
C	0.621046267248	-3.193717268143	-1.003764514260
H	1.127203594831	-3.665204991298	-1.859898713551
H	1.319398342200	-3.215493507285	-0.153368257954
H	-0.236519709991	-3.831252970306	-0.741800633212
Si	0.099700647906	-1.406925056316	-1.419177428730
C	-1.305181908997	-1.209924298166	0.890867480489
H	-0.869688443115	-2.194324041112	1.181862942335
O	-1.793433803708	2.737523513070	0.731367742909
C	-3.047470196906	2.404361495347	0.147348638891
C	-2.054771014895	3.834709600507	1.598988407503
C	-3.659992140225	3.756381810193	-0.216325662190
H	-2.862262414398	1.736977706386	-0.697550449841
H	-3.667135836104	1.876447922867	0.890758746422
C	-3.100746950377	4.700468765701	0.871898456940
H	-2.466288481863	3.455336928719	2.546963330338

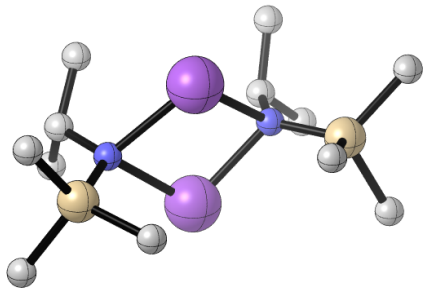
H	-1.097537697388	4.328559438460	1.797195891426
H	-4.753612535082	3.721190780903	-0.230951142050
H	-3.318865268943	4.066388483867	-1.210611355295
H	-3.877571193362	5.033470021331	1.567372089315
H	-2.648726060741	5.594041383886	0.428577310495
O	0.704869141262	2.267103193872	2.567617055196
C	-0.074979122973	2.332453050850	3.758043142435
C	1.846151262518	3.080719180752	2.809988899037
C	0.112644258863	3.760282816494	4.312608480543
H	-1.105943640707	2.083136387073	3.497224512411
H	0.296509519532	1.582326358637	4.473190638250
C	1.272544877778	4.328614697405	3.469167007640
H	2.536594202487	2.553223164014	3.492057004498
H	2.331646268329	3.251612420247	1.850061927872
H	0.365732328450	3.728993423615	5.377486271326
H	-0.796741458275	4.361008391718	4.207423248507
H	2.012655954760	4.871416512549	4.066484427279
H	0.895629033961	4.998161655917	2.685916192269
O	0.346733478295	2.569450700148	-1.856360418724
C	1.358772398819	3.069711977894	-2.735493082530
C	-0.835588191286	2.242169167639	-2.595160785567
C	0.660478623255	3.314666724860	-4.068065018704
H	1.797058391686	3.967947293303	-2.286079782841
H	2.148135412196	2.311141347229	-2.839836368856
C	-0.408584922870	2.221839852987	-4.055646951661
H	-1.210705134851	1.281910587560	-2.221750002168
H	-1.593755868442	3.021487622247	-2.413718001561
H	1.348724047608	3.249824492617	-4.916506086486
H	0.188624646658	4.306025138163	-4.078432510075
H	0.037608996668	1.250034473197	-4.305502885997
H	-1.241502530500	2.408754851584	-4.740657540027
O	1.200540472743	4.474824486344	0.118228372593
C	2.231293782762	5.441994085417	0.276767023789
C	0.129125069933	5.164834703569	-0.512986200970
C	1.526584838659	6.783120302180	0.569963094747
H	2.895096348722	5.108337805262	1.081306733187
H	2.818024428598	5.506194971476	-0.654523268905
C	0.048592919659	6.492446606751	0.236615030601
H	0.369380821527	5.338306683469	-1.576352234367
H	-0.757743828825	4.529540116237	-0.458950623273
H	1.936580569592	7.581230161809	-0.057201783451
H	1.652024390379	7.085964695935	1.614253869914
H	-0.419655651005	7.281275797246	-0.361017114936
H	-0.537816166551	6.371789154843	1.155923701923
Na	0.235344126969	1.696198505928	0.296276340718
O	2.504737681530	1.460524322825	0.313419291315
C	3.016075878430	0.433333379337	1.158124663290
C	3.601599884258	2.065681001808	-0.348725537820
C	4.437886249690	0.876782312649	1.562336937511
H	2.321942033666	0.335522667375	1.999396377512
H	3.035672645477	-0.517036572922	0.605695715094
C	4.696445400794	2.136983948085	0.713604227385
H	3.914786671211	1.441239374358	-1.202962675626

H	3.265450715267	3.040161732156	-0.716427089013
H	5.163652022519	0.088617294818	1.336557870114
H	4.508160224570	1.090892856189	2.633398974615
H	5.698981939552	2.157898048578	0.274720507383
H	4.573860998345	3.043911751142	1.317345916169

Table S16. Geometric coordinates and thermal corrected single point energies for the unsolvated *cis*-NaPTA dimer.

G: –1488.897652 Eh G(sp): –1489.345590Eh





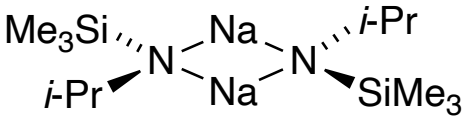
50
A2S0_cis_thf: optimized structure // E(RM062X) = -1489.73288359 A.U. after 10 cycles

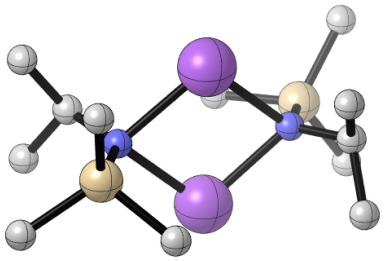
Na	-0.019301296434	-0.155335400732	0.064557257320
Na	0.117238280450	0.120845949278	2.940185646226
N	1.852751975450	-0.120860007372	1.427393584037
N	-1.725712759392	-0.377298436159	1.622313878505
C	3.482409308685	-1.474778642127	2.783420295385
H	3.192061258160	-0.927350669366	3.690350626314
H	3.748581313780	-2.501140356277	3.073269117390
H	4.386668034713	-0.997201675635	2.378375718428
C	2.782955601096	-2.241461918868	0.504854975023
H	3.073360631966	-3.273179179842	0.751618314896
H	1.968134251688	-2.290007097359	-0.231206283401
H	3.639071082517	-1.750592085076	0.022085766806
C	-1.420898476572	-2.681575394329	0.781376788330
H	-1.624202495326	-2.379359921520	-0.256333138514
H	-0.334254739820	-2.631937478727	0.961896872583
H	-1.719925828153	-3.734182470746	0.882679771604
C	-1.948325451738	-2.290338867488	3.192587305083
H	-2.457299172923	-1.643798788280	3.919045632865
H	-2.326828230897	-3.314752679990	3.321837682291
H	-0.873927034934	-2.311407251680	3.440670369162
C	-4.074022836220	0.802435810886	3.137022794467
H	-4.852922925452	1.576635481725	3.072453910396
H	-4.584714646943	-0.164167641959	3.259300506471
H	-3.495441317212	0.988700398654	4.053549183172
C	-2.157212085428	2.510944387780	1.498225914664
H	-1.494863804940	2.718299890831	2.352254322937
H	-1.568039044631	2.631496710299	0.577241150168
H	-2.924317655874	3.299094403730	1.492290362685
C	4.273186466348	0.982247115078	-0.116299340499
H	4.781996985355	1.938821214431	-0.309414076065
H	5.032331423010	0.279240558259	0.255176845174
H	3.908893576574	0.599697797182	-1.080495453354
C	3.663349464534	2.031231751713	2.636765199577

H	4.418826866311	1.382302951474	3.101059566305
H	4.162843450646	2.973371142645	2.364817993131
H	2.914008125285	2.268257737579	3.407062245960
C	-4.137998460285	0.663973059614	0.126814770898
H	-4.943826650175	1.411171345053	0.171115897517
H	-3.599286397409	0.810655837434	-0.820764077979
H	-4.613072020379	-0.327048869356	0.083697814884
Si	-2.956075281201	0.802525477399	1.604057992437
C	-2.157665788314	-1.767781417104	1.765664624632
H	-3.239286795340	-1.891736693851	1.548229916178
C	2.350618209108	-1.453230953968	1.748278175598
H	1.521272390824	-2.041092476241	2.197668457252
C	1.739616917224	2.570947479059	0.389515202055
H	1.312724951288	2.286888454953	-0.585441205041
H	0.908172835062	2.819367371861	1.065704484454
H	2.303268086948	3.500597204296	0.222991922505
Si	2.851446256638	1.222029497262	1.119109660542

Table S17. Geometric coordinates and thermal corrected single point energies for the unsolvated *trans*-NaPTA dimer.

G: –1488.896832Eh G(sp): –1489.344815 Eh





50

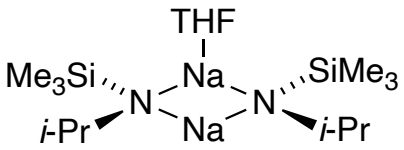
A2S0_trans_thf: optimized structure // E(RM062X) = -1489.73328092 A.U. after 10 cycles

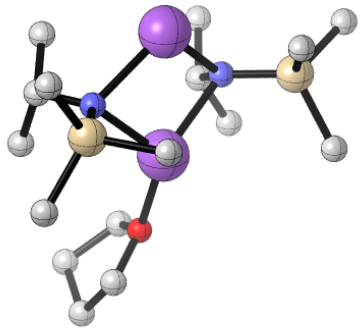
Na	0.120717376131	0.325996806235	-0.036405351388
Na	-0.068601418282	-0.090515839854	2.825000350241
N	1.827759712611	0.018828992497	1.511647295363
N	-1.767976932502	0.349403798793	1.298868184842
C	4.067583921940	-1.849971130346	2.514549327184
H	3.908836540732	-1.585410375814	3.569565611419
H	4.347582326820	-2.913580843178	2.477606393680
H	4.929706188403	-1.272648675003	2.151929243050
C	2.910200864426	-2.227326060228	-0.245283535303
H	3.247628905278	-3.273571334755	-0.196586387364
H	2.023157298515	-2.201471351471	-0.897435904165
H	3.701441859659	-1.649314621708	-0.743041658810
C	-2.300418229161	-1.544468007452	-0.192602112593
H	-2.220719475727	-0.911290221852	-1.087890748268
H	-1.320301117216	-2.011932922802	-0.002281618774
H	-3.008502841549	-2.353772415728	-0.419651287905
C	-2.931060173674	-1.632618387653	2.228110961167
H	-3.255863653279	-1.052941738080	3.102005661067
H	-3.679659639728	-2.416197760816	2.040153556293
H	-1.983912894353	-2.135471988984	2.481328049413
C	-3.632228249894	2.016116504090	3.016932167541
H	-4.012465373979	3.039504490846	3.151653967952
H	-4.501607588215	1.365374893101	2.841632731419
H	-3.172674595716	1.704093772604	3.966091873905
C	-0.950951676802	3.056312428836	2.006606489111
H	-0.399276782430	2.741577181184	2.906092702013
H	-0.226622447624	3.131677836982	1.181895802026
H	-1.313502245564	4.075841915569	2.203912076472
C	3.649428419492	1.236712314210	0.282100769651
H	4.146156039908	2.211730971090	0.176825970958
H	4.427374880428	0.485817045517	0.484629519673
H	3.186522846296	0.985395811412	-0.682411752638

C	3.272263901308	1.645252718582	2.725985244540
H	4.019875371555	0.894485504528	3.016586233410
H	3.775648292628	2.620622223055	2.656101859995
H	2.525425739068	1.704583614826	3.529157693816
C	1.189798172969	-2.722352617836	2.172159582522
H	0.226564000743	-2.622888582800	1.647238771765
H	1.501713257383	-3.770399247863	2.054691772781
H	1.014510828951	-2.573257935144	3.249958696266
C	2.602938687024	1.249176979803	1.404108501409
Si	2.506218030088	-1.542080352156	1.482080874036
H	1.909516089629	2.080553004648	1.162913207488
C	-3.281538448612	2.679709430486	0.096084322318
H	-3.705349920151	3.666504027281	0.333070302947
H	-2.590040053077	2.808114415752	-0.749507078428
H	-4.108590779019	2.043023399999	-0.250815118352
Si	-2.394194408339	1.908737297800	1.584163129125
C	-2.732542572320	-0.711861635115	1.018488693284
H	-3.736171484623	-0.308132731735	0.768101577115

Table S18. Geometric coordinates and thermal corrected single point energies for the mono-THF solvated *cis*-NaPTA dimer.

G: –1721.107594 Eh G(sp): –1721.693388 Eh





63

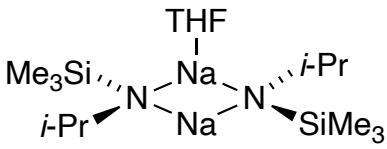
A2THF1_cis_thf: optimized structure // E(RM062X) = -1722.19571340 A.U. after 11 cycles

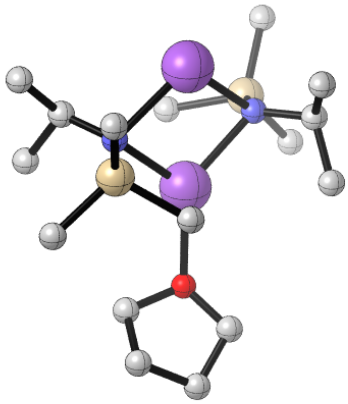
Na	-0.086245802911	-0.157197342873	0.125871991146
Na	0.130611678076	0.303898874443	2.993150924868
N	1.815447407519	-0.080012834227	1.408179783550
N	-1.770445150368	-0.221047009185	1.711975360071
C	3.247455537396	-0.993655880115	3.259008038790
H	2.813582384020	-0.271390092743	3.964729857872
H	3.495021551932	-1.909544213565	3.815054956453
H	4.189370462066	-0.567503331251	2.881949905689
C	2.913278204509	-2.298840195649	1.144235996427
H	3.181739868060	-3.231674564503	1.661512252747
H	2.214699354261	-2.544176144005	0.333387083404
H	3.823298068906	-1.884262679817	0.688802816483
C	-1.497553260828	-2.584183200764	1.061810817634
H	-1.665673055443	-2.365438474794	-0.002972271928
H	-0.415447368057	-2.535325698845	1.269463217571
H	-1.818587603382	-3.620116280055	1.238473476134
C	-2.083811197871	-2.000325471074	3.416426092981
H	-2.619209681093	-1.304531694499	4.075847365028
H	-2.463436200452	-3.015406155838	3.607304308951
H	-1.018820416162	-1.983063787498	3.697286091851
C	-3.924541880337	1.196176757918	3.329721166183
H	-4.630431820045	2.038712075194	3.278577033325
H	-4.514791531623	0.288418661957	3.524062445209
H	-3.273464466418	1.361375240433	4.200691734948
C	-2.001451946789	2.673368033126	1.489378327685
H	-1.236776927029	2.847851152712	2.262350074844
H	-1.503515771744	2.719534489515	0.509795556847
H	-2.697668290439	3.523549093927	1.534862516097
C	4.433971667889	0.818204313127	0.067467362184
H	4.939092965297	1.740184900827	-0.258144391482

H	5.134679763738	0.275136034711	0.717577067041
H	4.262194774401	0.200576064748	-0.825665561418
C	3.282282136745	2.429285333861	2.339918414075
H	3.945676871101	1.962243447692	3.081296987371
H	3.802096837714	3.315279777167	1.944934822006
H	2.389082909125	2.785508140958	2.876194629421
O	0.345601943468	-0.228340473689	5.169024565296
C	0.852873837112	-1.474204147433	5.680294787198
C	-0.659506957495	0.300110114525	6.058713092043
C	-0.170101488617	-1.925177584908	6.709991189780
H	0.976250761111	-2.167377103950	4.840339051835
H	1.834312663004	-1.295208254674	6.140540829237
C	-0.621650415591	-0.587692945466	7.295461998342
H	-0.422352418740	1.349021277397	6.265263403763
H	-1.632889633033	0.243509478049	5.552705039874
H	0.260550832015	-2.604190127608	7.452008810762
H	-1.009806276775	-2.431329156114	6.216654209965
H	0.123487854075	-0.216116031945	8.009435665657
H	-1.591153355413	-0.633977169434	7.800097698869
C	-4.215582767021	0.936687963629	0.348409718635
H	-4.947293255835	1.755369661851	0.412087361204
H	-3.740930505263	0.989368963074	-0.642190541736
H	-4.777493182768	-0.007768720070	0.392854573211
Si	-2.916492107365	1.036364929889	1.727964357462
C	-2.244230104152	-1.582247235739	1.948505760404
H	-3.321706864330	-1.699067170782	1.705610656230
C	2.285366818095	-1.272517897367	2.095256521766
H	1.407806522163	-1.792197794230	2.544540991486
C	1.797579138705	2.266813599365	-0.274557826402
H	1.588289888813	1.722247665626	-1.208892884916
H	0.840845329299	2.599544507017	0.156707611996
H	2.344603244318	3.177080585330	-0.560314788542
Si	2.801754688778	1.223377641070	0.948896774565

Table S19. Geometric coordinates and thermal corrected single point energies for the mono-THF *trans*-NaPTA dimer.

G: –1721.107735 Eh G(sp): –1721.693632 Eh





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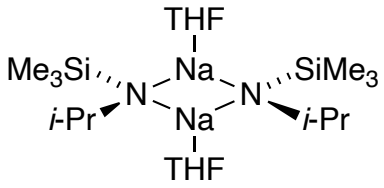
A2THF1_trans_thf: optimized structure // E(RM062X) = -1722.19603113 A.U. after 11 cycles

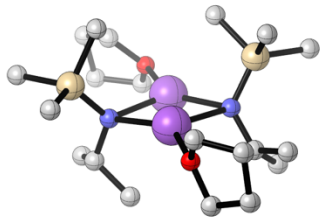
Na	-0.000369260522	0.151280732020	-0.031672847969
Na	-0.076229419376	0.372345860570	2.850645323118
N	1.787698956068	0.162778620721	1.437327960910
N	-1.841947756921	0.483281719912	1.315188224449
C	4.019306072210	-1.376064267783	2.924645119793
H	3.841210521298	-0.882138738521	3.889846270714
H	4.311583178161	-2.416311126556	3.134878241392
H	4.886495295948	-0.885238404054	2.459641356346
C	3.025640511684	-2.382100910838	0.282381810433
H	3.340119372473	-3.393471376155	0.581518824555
H	2.193803577444	-2.494743913142	-0.429852139572
H	3.864386419408	-1.924790291268	-0.261174273818
C	-2.435565443378	-1.645559819919	0.216845278316
H	-2.415518830156	-1.181034720493	-0.779286642218
H	-1.441346572907	-2.072807376615	0.428540494710
H	-3.146430571443	-2.482893148073	0.179727989559
C	-2.899607249966	-1.309519102245	2.650656880945
H	-3.174790835248	-0.588779318078	3.431927119078
H	-3.639838369342	-2.123569797776	2.658078818976
H	-1.922537985313	-1.744647321555	2.914798124597
C	-3.755038600533	2.306556979791	2.801534274382
H	-4.120793025134	3.343688223096	2.829597605807
H	-4.627742434571	1.657356966086	2.637533034904
H	-3.348822985410	2.070761084737	3.795936940798
C	-0.993011152553	3.204316792372	1.900895238332
H	-0.664670840131	3.066139382415	2.943333913938
H	-0.121367778992	3.046351582393	1.247176790195
H	-1.275907960967	4.262732492592	1.804290026978
C	3.678824836550	1.108390779985	0.073543329733
H	4.159221352274	2.047114263290	-0.237278734953

H	4.454937852070	0.466918565357	0.516291004453
H	3.300518269298	0.604554020077	-0.826148630328
C	3.088757830615	2.095524161571	2.302385924836
H	3.803106754016	1.457644184235	2.842267420093
H	3.600664565212	3.030330348618	2.029418428696
H	2.271875119326	2.346941450098	2.993025389316
C	1.166483269643	-2.389316978577	2.643139805542
H	0.282793608151	-2.522465560489	1.999583969995
H	1.543073060391	-3.395406197941	2.879670692136
H	0.830592794065	-1.942902952967	3.591151723877
C	2.543136810502	1.355024877839	1.075007331863
Si	2.496406306317	-1.343468158841	1.786039902826
H	1.857284754649	2.072560863018	0.577589782381
C	-3.216755914334	2.764941208721	-0.132864843673
H	-3.636868658851	3.771175863043	0.010887651058
H	-2.470043104323	2.826177513845	-0.938109954237
H	-4.030090805557	2.115909275115	-0.489956291322
Si	-2.442390384135	2.069810208943	1.453161790915
C	-2.804007980520	-0.613163565384	1.287168964010
H	-3.829523849179	-0.267839869308	1.037380099713
O	0.141999867550	-0.006499204288	5.055011044409
C	1.506341509935	0.144196504080	5.487648522351
C	-0.535963669216	-0.976301062433	5.877871016436
C	1.805526219157	-1.110942245274	6.288253425181
H	2.131121936265	0.268746085607	4.595028305292
H	1.586817455573	1.047803227174	6.108144970228
C	0.458707432863	-1.360461286037	6.969094622736
H	-1.454880446191	-0.523478232760	6.264729245449
H	-0.801506079434	-1.836757493879	5.249146019183
H	2.629894542680	-0.968196667491	6.993594442552
H	2.061984318046	-1.940288572669	5.615826898336
H	0.348500442190	-0.698615438279	7.836527650619
H	0.323046898967	-2.392848824870	7.304434128040

Table S20. Geometric coordinates and thermal corrected single point energies for the di-THF solvated *cis*-NaPTA dimer.

G: –1953.315747 Eh G(sp): –1954.039624 Eh





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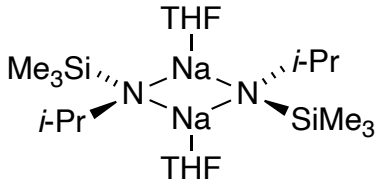
cis-NaTMiPS_dimer: optimized structure // E(RM062X) = -1954.65601022 A.U. after 11 cycles

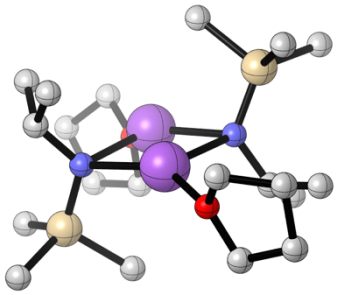
Na	0.010601900972	-0.362821240315	0.008763279480
Na	0.003261807673	-0.270299134725	2.910649675864
N	1.825553668993	-0.163037017435	1.468123909807
N	-1.830911393476	-0.263748601367	1.454968910328
Si	-2.849174466246	-1.570552298059	1.077476053279
C	4.397011471349	-1.302492915393	2.720105579359
H	4.278631635706	-0.724100589518	3.647552644026
H	4.841761075521	-2.272798661218	2.988491603768
H	5.124596059372	-0.773508032303	2.088295208665
C	3.102981872841	-2.722271773857	0.397709885065
H	3.581160685736	-3.653145770545	0.738534266630
H	2.177041399674	-3.003182586780	-0.127483113661
H	3.773250395817	-2.259331142330	-0.340467683482
C	-1.887718197042	-3.183272482374	1.288004157020
H	-0.946075234513	-3.183734625388	0.717115229546
H	-1.636603785632	-3.369494701320	2.341883015686
H	-2.477242586647	-4.042028775321	0.934669440582
C	-4.436559507983	-1.728632669521	2.108505447130
H	-5.072091803723	-0.837052841195	2.002773987830
H	-5.032939051271	-2.593475148203	1.781230574062
H	-4.224358001324	-1.860199408360	3.179286565538
C	-3.457716342300	-1.549683116513	-0.725115244449
H	-4.148185292119	-2.376965653028	-0.947133399006
H	-3.984734224766	-0.611723741045	-0.955448526896
H	-2.612301134655	-1.626866489725	-1.426227714242
C	-2.832576448426	1.413076860234	2.982472699625
H	-3.305921805422	2.403530197781	3.059997925912
H	-3.533915553696	0.665270250223	3.374807461221
H	-1.944713281764	1.411871970871	3.635175660252
C	-1.478135291373	2.134182675853	1.005197002674
H	-0.526169827819	2.113533769085	1.561234324386
H	-1.256499572659	1.964813470638	-0.059225850769
H	-1.892788933369	3.147980909000	1.096001502813
C	3.332314378195	0.744954346944	-0.327260106257

H	3.652460759955	1.671696380322	-0.826673985231
H	4.237350793897	0.228346175114	0.026502958393
H	2.844509205833	0.100096813996	-1.071050365061
C	3.067091000574	1.958666415214	1.851408355865
H	3.941285802645	1.459896600535	2.292375483165
H	3.404618814696	2.896045287076	1.385032623133
H	2.377088402599	2.209813294010	2.667852599350
O	0.450634986697	-0.023136192219	-2.156860836941
C	0.621954920509	-1.046332284067	-3.139848146791
C	0.900816803008	1.201314297911	-2.749236867747
C	1.972164303071	-0.730429495192	-3.766702150717
H	0.572219893004	-2.015153334552	-2.634017303573
H	-0.192794772524	-0.982223947800	-3.876883380971
C	2.013515013087	0.810231399291	-3.739875762838
H	0.054057887055	1.677910107648	-3.261730022607
H	1.238120245046	1.854695126441	-1.938192609180
H	2.065375340683	-1.141447310621	-4.776475953189
H	2.773930400586	-1.152640320590	-3.150507642477
H	1.809032828396	1.233241131643	-4.728508646983
H	2.991237139148	1.178856658490	-3.415226729392
O	-0.609536998565	-0.525231443462	5.061096784124
C	-1.645745198129	-1.527063768497	5.106689852805
C	-0.799062226859	0.435029772829	6.113079681198
C	-2.422799106183	-1.260090609778	6.390474315821
H	-2.274802900815	-1.403085216523	4.214206546307
H	-1.173712777541	-2.515771611865	5.082210368924
C	-2.235932497601	0.246311184507	6.572757734472
H	-0.086090493369	0.219637548716	6.920686548963
H	-0.587472720168	1.431904511182	5.711342745534
H	-1.971087539670	-1.802504889975	7.229976824868
H	-3.470906680424	-1.563704745859	6.307978666924
H	-2.389168483471	0.581780929510	7.603062686135
H	-2.921502984385	0.800624011369	5.919935106997
C	1.682595129930	-2.583444693726	3.052526351414
H	0.691998220642	-2.833767329279	2.640975755909
H	2.177071644263	-3.541692607845	3.268765280905
H	1.541529695692	-2.078254234867	4.021356686722
C	-2.433457791891	1.062624564776	1.541816528926
C	2.380579113743	1.027258369893	0.844098321193
Si	2.727326834018	-1.550085766428	1.849461591634
H	-3.359916836107	1.148158964435	0.933806464922
H	1.546868103955	1.626430453128	0.415022414214

Table S21. Geometric coordinates and thermal corrected single point energies for the di-THF solvated *trans*-NaPTA dimer.

G: –1953.317697 Eh G(sp): –1954.041226 Eh





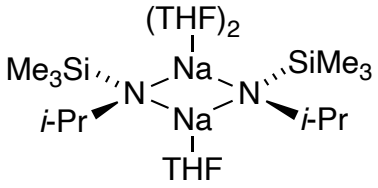
76
trans-NaTMiPS_dimer: optimized structure // E(RM062X) = -1954.65683633 A.U. after 11 cycles

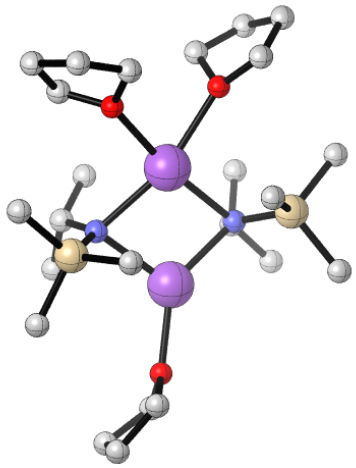
Na	-0.220220586882	-0.510036790557	-0.121308493589
Na	-0.304790746207	-0.724287633791	2.792007230270
N	1.554385746432	-0.535893389334	1.411615018104
N	-2.089775842768	-0.584979204668	1.249865891611
C	3.984901264350	-1.972879571043	2.638342307190
H	3.754013112841	-1.624640071795	3.655442888457
H	4.409754690289	-2.984837002491	2.721754647024
H	4.772370912224	-1.320620178843	2.234565608824
C	2.983349192579	-2.784927295350	-0.084127600654
H	3.398497771402	-3.791483714185	0.077767123798
H	2.135417206117	-2.886903654380	-0.778866122838
H	3.756366334854	-2.188850999416	-0.589491370131
C	-2.530322402425	-2.710475326947	0.095481436258
H	-2.577785141140	-2.208730227646	-0.880772181369
H	-1.492902965980	-3.041061245467	0.265142497948
H	-3.161319769470	-3.609464113011	0.046757214979
C	-2.970575658969	-2.502846160563	2.550567913025
H	-3.267828374118	-1.828702106163	3.365069377971
H	-3.659813445111	-3.360577846394	2.547384110228
H	-1.964171868395	-2.891711884685	2.775351362622
C	-3.673843134160	1.081109082549	3.233761765845
H	-3.974152681588	2.115871721267	3.458831782881
H	-4.586414204024	0.465603587834	3.246880667140
H	-3.025922959623	0.724157561808	4.045634527841
C	-1.385849167402	2.213654076002	1.541221058348
H	-0.526280674335	1.935266124978	2.170447101284
H	-1.005675729686	2.361998431073	0.518345029587
H	-1.737637142587	3.194734163350	1.893029595625
C	3.236456025190	0.713351041944	0.025446830195
H	3.580657928487	1.721543293327	-0.249922935639
H	4.112588968011	0.146184425548	0.374953688213
H	2.851099792984	0.216967898103	-0.875225736702
C	2.695732462310	1.454335961285	2.361879966147
H	3.522988527609	0.870866790636	2.790248190439

H	3.064933226760	2.467975403851	2.145256488559
H	1.910879449431	1.531094990780	3.127068911255
O	0.498292883882	0.064791797795	-2.169097940080
C	0.817936766187	-0.854540755194	-3.215279208079
C	0.995135424254	1.347588329452	-2.571472829555
C	2.228271803072	-0.462357443308	-3.627035822788
H	0.725883908847	-1.869020983705	-2.816280619520
H	0.104293275577	-0.727216086795	-4.043660750120
C	2.211439277121	1.070568991506	-3.476454327848
H	0.202407639499	1.880429988105	-3.113818380645
H	1.238473586317	1.905274723178	-1.661369596996
H	2.470470669819	-0.787743399187	-4.643339245365
H	2.952140938691	-0.915439569768	-2.939739871815
H	2.083590258442	1.562429994868	-4.446100112882
H	3.140066926242	1.443273272316	-3.033594164867
O	-0.740968249386	-0.087981339494	4.902102849958
C	-1.112639432993	-0.939386276266	5.987252624401
C	-0.778032137176	1.258224148320	5.391763811114
C	-2.255337489856	-0.196671996366	6.664242921250
H	-1.387868930491	-1.913987436523	5.573083903966
H	-0.253545947727	-1.063865421087	6.664172249760
C	-1.855289385264	1.281751166983	6.493456442046
H	0.212001562957	1.519238251146	5.789831114526
H	-1.003174937179	1.911071577768	4.541962839895
H	-2.373716706202	-0.487286248702	7.712550696101
H	-3.195705963582	-0.407952533310	6.142669178644
H	-1.443133355054	1.693587807305	7.420143730420
H	-2.712402957999	1.898493199069	6.206042801955
C	1.263807268624	-3.252529398751	2.349692315764
H	0.315174830888	-3.347205849259	1.798832991686
H	1.721352117703	-4.252498108146	2.365011295151
H	1.032186061332	-3.002443609078	3.397848451080
C	2.151074168728	0.754619905128	1.109655923210
Si	2.426755779671	-1.982681321196	1.550780594910
H	1.361018198954	1.429602279192	0.715568753736
C	-4.055045163812	1.523205586131	0.282213279862
H	-4.470819155868	2.507482660577	0.543895622408
H	-3.599514127500	1.604944374978	-0.715243790062
H	-4.899240358857	0.822900218745	0.202333229113
Si	-2.783354495108	0.934253906747	1.560382213259
C	-2.959045976575	-1.752421829068	1.210608306068
H	-4.015868052810	-1.484050629683	0.996771900837

Table S22. Geometric coordinates and thermal corrected single point energies for the tri-THF solvated *cis*-NaPTA dimer.

G: –2185.516842 Eh G(sp): –2186.377122 Eh





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A2THF3_cis_thf: optimized structure // E(RM062X) = -2187.11132641 A.U. after 11 cycles

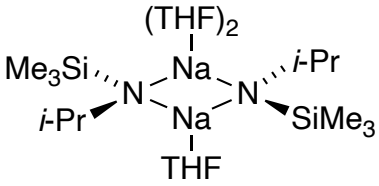
Na	0.126457936668	-0.123077660907	-0.001704546648
Na	0.279784410083	-0.252974454269	2.981517382598
N	2.018550865874	-0.254310781540	1.479756150178
N	-1.524469509790	-0.777897186653	1.600476661868
C	3.668960710937	-1.612816215506	2.801422904250
H	3.381781935470	-1.076217940126	3.716270396341
H	3.943972620690	-2.641378570107	3.077227622540
H	4.566827014832	-1.123672488205	2.395676363978
C	2.963167184137	-2.353146252967	0.517092516050
H	3.221285601186	-3.398965989151	0.742899592654
H	2.156024995691	-2.352572096268	-0.227478614575
H	3.841280165341	-1.875252739954	0.061092443132
C	-0.985304751444	-2.904067999785	0.508935334415
H	-1.061373640597	-2.460253450067	-0.493709733836
H	0.058952350216	-2.818376060169	0.847746468616
H	-1.225310774405	-3.973483334526	0.419517110562
C	-1.842682957253	-2.902683835440	2.850830311621
H	-2.482714759589	-2.402485005776	3.588851896548
H	-2.160068211340	-3.953972314100	2.777179753759
H	-0.809635929161	-2.892694942908	3.234509701903
C	-3.510947151197	0.246651951437	3.669740775816
H	-4.069090798380	1.153631312366	3.949875209955
H	-4.226765404440	-0.589817700211	3.674030720253
H	-2.765250812045	0.044715186387	4.451103417076
C	-1.775901068451	2.083507059870	1.943489138781
H	-0.886120941298	2.125775262157	2.590159529923
H	-1.447715343871	2.324904253407	0.920540505752
H	-2.440969871359	2.897956643583	2.267336664489
C	4.320710892979	0.808825974279	-0.232509822594

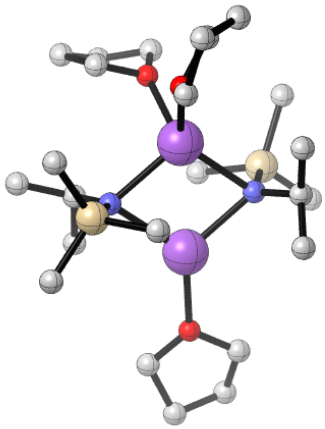
H	4.741013949124	1.760282326147	-0.594049409445
H	5.157565333788	0.218245417708	0.170160650877
H	3.911159131434	0.260770069022	-1.091126269720
C	3.931081818372	1.899017329965	2.531973383083
H	4.720834973993	1.249089170946	2.934435700092
H	4.409664870673	2.838251357848	2.213695524697
H	3.249069959095	2.141104112062	3.361249154379
O	1.348015823568	0.251577616078	-2.018803611844
C	1.259385224837	-0.963713465673	-2.754681425992
C	2.077046654931	1.171216903534	-2.831667950770
C	2.648556230430	-1.129976381801	-3.354607873066
H	0.967320207069	-1.767072157227	-2.069167348103
H	0.490599124366	-0.871995502412	-3.540052299208
C	3.043746352270	0.322029862611	-3.682872104343
H	1.372335154312	1.727755290651	-3.468002303279
H	2.580688518140	1.875797133859	-2.163520629503
H	2.651864825279	-1.784808987473	-4.231455728140
H	3.322177540799	-1.557203220591	-2.602187684295
H	2.908219975216	0.539466324738	-4.747459548084
H	4.089800710334	0.524668812409	-3.432390962858
O	-0.208286042738	0.288025743504	5.115269457084
C	-0.078553513725	-0.653817906700	6.182275946827
C	-0.810308968056	1.467383903969	5.664812327592
C	-1.379800810293	-0.512569922274	6.956621694085
H	0.081926919149	-1.643502084409	5.743580965185
C	-1.679003896107	0.994108106033	6.846452619883
H	-0.015793792385	2.150290376491	5.994890150700
H	-1.382418859901	1.947675992087	4.865129690083
H	-1.286307144673	-0.854010136804	7.992034649329
H	-2.164728562746	-1.102832085787	6.470219095391
H	-1.396390240303	1.522638554626	7.762580757531
H	-2.742055754456	1.182067300620	6.666691195439
C	-4.118483306845	0.615892655399	0.755406022388
H	-4.845096642413	1.352818858906	1.130162649889
H	-3.747907372282	0.970438825982	-0.215563984910
H	-4.663644936518	-0.325366434489	0.590658143083
Si	-2.670800011845	0.411695129332	1.966716934363
C	-1.901165408061	-2.174959880033	1.498657750502
H	-2.939634120017	-2.306368000857	1.119329879977
O	-1.476355687900	0.154313704340	-1.634532645657
C	-1.438181186610	1.166639371000	-2.633004887626
C	-2.542185325197	-0.738949581659	-1.959099941080
C	-2.905328396615	1.465599391604	-2.909136948077
H	-0.869517748617	2.013054536756	-2.235934715788
H	-0.931183429828	0.788379065455	-3.536045432527
C	-3.557562286579	0.077329387067	-2.785591257686
H	-2.143232572088	-1.581918977586	-2.543432013975
H	-2.939502002132	-1.118310319106	-1.012184167372
H	-3.062357067436	1.925888710475	-3.889709307788
H	-3.292150813295	2.149310381404	-2.144489569780
H	-3.700750531866	-0.377789691308	-3.771354817189
H	-4.535638564469	0.126498015439	-2.296511204818
H	0.792239206401	-0.388055163272	6.800991608851

C	2.529971784259	-1.580682993742	1.771923762201
H	1.709847339805	-2.188979964768	2.216625249251
C	1.834836593809	2.469190455276	0.493960270172
H	1.188689495636	2.177495414560	-0.347035546408
H	1.186639311013	2.810033895943	1.314927764704
H	2.414334826110	3.344177326733	0.162880261777
Si	2.982800591383	1.082078131455	1.093571898066

Table S23. Geometric coordinates and thermal corrected single point energies for the tri-THF *trans*-NaPTA dimer.

G: –2185.523893 Eh G(sp): –2186.384785 Eh





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A2THF3_trans_thf: optimized structure // E(RM062X) = -2187.11925526 A.U. after 11 cycles

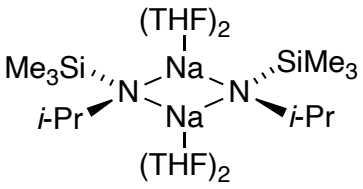
Na	0.001729760959	0.032919974170	0.003998602795
Na	0.287153850538	-0.221821672426	2.853490262958
N	2.008947389582	-0.047715892356	1.254505882632
N	-1.704584652711	0.056892151738	1.684780625592
C	3.977037022317	-2.242773732022	2.162157940122
H	3.613484545798	-2.190327174280	3.199342742482
H	4.216542379121	-3.295933567555	1.948396612874
H	4.918525536320	-1.677593818670	2.113585546909
C	3.416454336245	-1.870858322922	-0.770394080845
H	3.559449481379	-2.944148334072	-0.969663553087
H	2.763329166535	-1.463470130797	-1.556295395366
H	4.399772658723	-1.389315394819	-0.870708289145
C	-2.824698322570	-1.546239033979	0.161538355551
H	-3.068738481185	-0.745859336013	-0.550454684311
H	-1.858779655081	-1.981769442032	-0.137190902879
H	-3.592666755777	-2.329790036030	0.072345942241
C	-2.436763085247	-2.120383835693	2.568165770959
H	-2.410976848923	-1.736752655662	3.596963809288
H	-3.193630871692	-2.916766675028	2.518552111756
H	-1.458352772449	-2.571356770709	2.344312594969
C	-3.469373897541	2.170533457153	2.989733226918
H	-3.777208769454	3.221550167978	2.884463504641
H	-4.381785028994	1.558309254292	2.944802441384
H	-3.039021540088	2.048397194861	3.993936937068
C	-0.697931595310	2.764044638778	1.912790836142
H	-0.350572867530	2.676594066952	2.954579351583
H	0.138396930241	2.482655905828	1.254381634362
H	-0.914817014863	3.828806090548	1.740597602240
C	4.156966528957	1.172106129192	0.715918166959

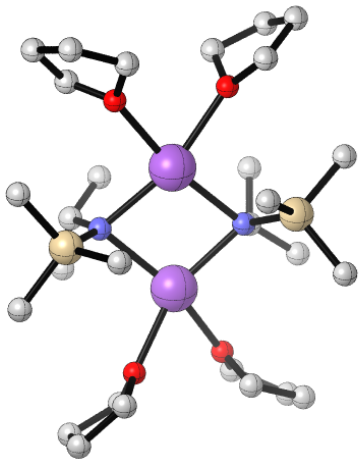
H	4.644949779691	2.155122617529	0.786222434521
H	4.801475082632	0.444883097234	1.231868684279
H	4.116234068642	0.889765667653	-0.343687098109
C	2.878299459414	1.672512958071	2.796977646503
H	3.449284881204	0.935497076958	3.381754183746
H	3.384565924281	2.646568721811	2.877504944775
H	1.887183569141	1.779255916899	3.259712185477
O	0.377072676465	1.852672317260	-1.284733043725
C	1.663265619277	1.653265855070	-1.887249004660
C	0.025455563827	3.221065473817	-1.472209650774
C	2.371607443481	3.022443560921	-1.857688693956
H	2.172032792775	0.878221472829	-1.303475140157
H	1.525681362598	1.294430963711	-2.917289333576
C	1.328651851047	3.969040319168	-1.239149188532
H	-0.346554871828	3.367641368154	-2.499463667312
H	-0.769605353302	3.467186712966	-0.763776811462
H	2.632880542337	3.337944475989	-2.873485101356
H	3.294757856919	2.991263211782	-1.270897130188
H	1.329263996803	4.963660485611	-1.695950368248
H	1.495622611789	4.084238605049	-0.161077579892
C	1.224888278316	-2.809708976302	1.129084929015
H	0.309536723279	-2.488741691778	0.609498063876
H	1.489978598191	-3.800348773435	0.730326062225
H	0.966422551015	-2.958866810211	2.189618189955
C	2.756473259220	1.194838201499	1.343427616243
Si	2.662617994377	-1.580871013907	0.954044202204
H	2.198233901398	1.989490287295	0.804308033952
C	-3.078263711832	2.187957308117	0.024655215549
H	-3.289812206527	3.267345630563	-0.019748221540
H	-2.480828122842	1.922202399799	-0.859852488368
H	-4.044082789533	1.666690072728	-0.065877091456
Si	-2.222819031157	1.674379400659	1.646699183166
C	-2.721888246166	-0.981737874481	1.585559388817
H	-3.734950832254	-0.602792871441	1.841660065069
O	-0.052315223462	-1.215093469332	-1.891769336024
C	-0.943123547153	-0.585083414738	-2.832556478355
C	0.052225253075	-2.620291335933	-2.177521862486
C	-1.615603109452	-1.725284853992	-3.582994418133
H	-1.644325526309	0.051893906106	-2.281006297211
H	-0.348912251895	0.048906811675	-3.504483388915
C	-0.517548612764	-2.787800479943	-3.577334629692
H	1.102499329689	-2.912804472362	-2.082009991733
H	-0.541202205824	-3.181773102342	-1.441616398882
H	-1.938499911954	-1.428330594043	-4.585418061045
H	-2.491682656965	-2.083373852765	-3.026632304918
H	0.245009114299	-2.553495961049	-4.330656717593
H	-0.885556206038	-3.802290766395	-3.757598797097
O	0.442057750939	-0.022252606731	5.082982554012
C	1.601595744113	0.216086203224	5.902828921542
C	-0.747902485989	-0.035064762028	5.894347129603
C	1.117283829174	0.064940985999	7.337599939950
H	2.378939295083	-0.501547518063	5.621140887320
H	1.966331987744	1.233200395079	5.708301655498

C	-0.325576899959	0.556291210780	7.230028843810
H	-1.523141662249	0.540835438987	5.378328203144
H	-1.087515003998	-1.073300410603	6.006536287487
H	1.725764650457	0.639223045157	8.042541110566
H	1.137745811493	-0.989611548975	7.639170185849
H	-0.353127874147	1.652223623350	7.187154498433
H	-0.965893054157	0.223919015155	8.052469105794

Table S24. Geometric coordinates and thermal corrected single point energies for the tetra-THF solvated *cis*-NaPTA dimer.

G: –2417.71695 Eh G(sp): –2418.712883 Eh





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A2THF4_cis: optimized structure // E(RM062X) = -2419.56552207 A.U. after 11 cycles

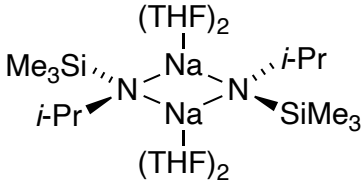
Na	0.046231300794	0.170016150259	-0.058700126259
Na	-0.140974132800	0.092447001256	3.023570306452
N	1.752509130707	-0.065176427855	1.611812261079
N	-1.836601655247	-0.205979773025	1.373406262722
C	3.297044197666	-1.580065358360	2.898629697094
H	3.158002006814	-0.939863989366	3.774915056721
H	3.432828684142	-2.619572286473	3.234517236861
H	4.223844642815	-1.272313981364	2.390912023594
C	2.327458804225	-2.321231874554	0.723505176537
H	2.494392047577	-3.374818789902	0.996943754045
H	1.464533703614	-2.283241252098	0.046686116164
H	3.207543923626	-1.966936462686	0.168405327636
C	-1.497832032974	-2.501092034449	0.578707893949
H	-1.333682084703	-2.158332471668	-0.453072780154
H	-0.522190449519	-2.545566534585	1.085664767490
H	-1.904020039578	-3.522245089145	0.532359614712
C	-2.664366809373	-2.105859372202	2.742243640924
H	-3.300460124669	-1.428978383297	3.327103361533
H	-3.143657861740	-3.096690001483	2.717307328879
H	-1.704480492585	-2.212866221271	3.273698965130
C	-4.121129133237	1.207679758310	2.844750158535
H	-4.616788853305	2.189030736749	2.908832521831
H	-4.909951709604	0.455753841155	2.685861491212
H	-3.643944432845	0.993563104068	3.806554764335
C	-1.738760362932	2.681395846891	1.568991635575
H	-1.005298079046	2.612750307413	2.386487586521
H	-1.176892762813	2.832339634202	0.634166238533
H	-2.327263261652	3.595875831205	1.736201949035
C	4.293514109025	0.592093401339	0.029200805642
H	4.855071843473	1.460847260143	-0.349213859177

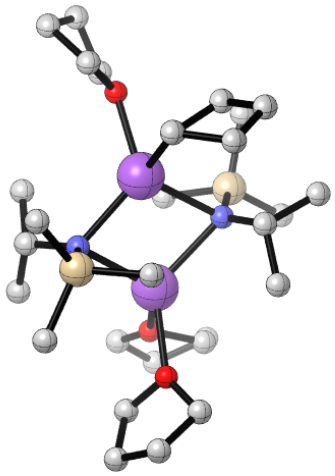
H	5.019249420270	-0.067325835791	0.529051697080
H	3.882178806193	0.044164565974	-0.827212368529
C	3.884694141993	1.885667132881	2.677477955598
H	4.520542136664	1.147231191175	3.186566947883
H	4.544644931875	2.691659690888	2.318842907864
H	3.212294965682	2.324856679247	3.429464030031
O	1.551255119127	0.284346826666	-1.967134740595
C	1.426968684263	-0.943997961021	-2.674879568686
C	2.423624136423	1.113645463344	-2.734621975086
C	2.841889505262	-1.242097955361	-3.152882571955
H	1.014989712350	-1.696984867146	-1.995279866573
H	0.737560594522	-0.820587951714	-3.526405678289
C	3.389769158571	0.162215282690	-3.470378278576
H	1.828492201640	1.702774418665	-3.448485228991
H	2.921867866638	1.798715371647	-2.042919420984
H	2.858123705015	-1.914483262733	-4.016337075541
H	3.413169494246	-1.710135733934	-2.342726045372
H	3.376804429516	0.360693599711	-4.547183228312
H	4.420391956127	0.282898149955	-3.121925618520
O	-1.405859679083	0.967671074580	4.836549738846
C	-1.727421120980	0.015884206495	5.847565046481
C	-1.858453015229	2.245565767882	5.285415022544
C	-3.091807119098	0.449346998555	6.368882790460
H	-1.712970536313	-0.979436292520	5.393735389220
H	-0.972006742108	0.051120453648	6.648708355413
C	-3.037117271161	1.983571316105	6.244470838121
H	-1.032315557141	2.762279899631	5.796352535697
H	-2.140197717414	2.823546367157	4.399485341185
H	-3.262550744178	0.112388690165	7.396196385844
H	-3.886446323109	0.032929154380	5.740014730665
H	-2.852755494797	2.454967972049	7.215342436713
H	-3.974473966960	2.389211976825	5.850846840067
C	-3.936182546375	1.478287762976	-0.095854549184
H	-4.575474359028	2.360799831288	0.062041442039
H	-3.309334754525	1.663415227068	-0.976286334947
H	-4.601765152981	0.630666466256	-0.318583153206
Si	-2.848818366806	1.150861720978	1.430453189265
C	-2.414856694120	-1.535984188512	1.336370453618
H	-3.397826861405	-1.560430111138	0.811890497798
O	-1.281037128195	0.470203795478	-1.946933546661
C	-1.019246539782	1.389097552794	-3.000861511663
C	-2.336114227544	-0.391928307442	-2.371075057288
C	-2.395855884153	1.729087165485	-3.559560203522
H	-0.478907415355	2.242081640538	-2.578638556936
H	-0.388561996833	0.913426771037	-3.768733702678
C	-3.168215878846	0.406664482250	-3.395371255590
H	-1.904333686124	-1.294792261275	-2.829245940218
H	-2.894015406644	-0.680065808054	-1.474214043039
H	-2.346853826204	2.066785260712	-4.599637751097
H	-2.855240240729	2.526719141807	-2.965483690480
H	-3.230021010157	-0.136511231953	-4.344123249849
H	-4.190005934121	0.577108203765	-3.041946405626
O	1.028242863030	-0.503651349560	4.944115355221

C	1.529451997908	0.670417994939	5.574122644550
C	1.388257117856	-1.615827978721	5.756706683371
C	2.885881135493	0.264531526065	6.145109091880
H	1.582581457130	1.461684099325	4.818695140023
H	0.841023573124	0.988967430858	6.373065029479
C	2.715323558223	-1.240242655346	6.442310140776
H	0.595320819825	-1.795207440103	6.499075887994
H	1.460304491917	-2.490246829900	5.101749075951
H	3.138433340092	0.846062537473	7.037266925316
H	3.673530271074	0.429828011249	5.402378482943
H	2.662311381666	-1.438196779372	7.517625663901
H	3.551610488175	-1.820221358091	6.039681931724
C	2.094405136785	-1.433197589205	1.956273566377
H	1.237407004838	-1.894580702101	2.498629462466
C	2.002780348776	2.602366900002	0.484323210076
H	1.387307610884	2.354645024929	-0.393173151603
H	1.344388787979	3.060421618612	1.237346483884
H	2.714924578278	3.379366537059	0.167757865076
Si	2.907257459910	1.110437730405	1.232119782851

Table S25. Geometric coordinates and thermal corrected single point energies for the tetra-THF *trans*-NaPTA dimer.

G: –2417.729303 Eh G(sp): –2418.725433 Eh





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A2THF4_trans: optimized structure // E(RM062X) = -2419.57717084 A.U. after 11 cycles

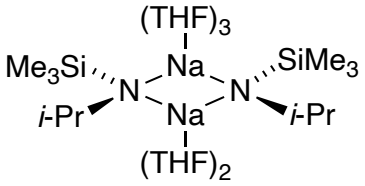
Na	-0.250330047299	-0.090751432336	0.038977190213
Na	0.073166584747	0.256250814039	2.876553695855
N	1.822342101370	-0.048524157327	1.233219351696
N	-1.923015812791	0.428839047057	1.604276884138
C	3.914239928485	-2.171909925942	2.097834105758
H	3.922203424638	-1.746763244424	3.111371158112
H	3.951510565664	-3.267977260517	2.195492470308
H	4.849290164129	-1.863380531298	1.608249257238
C	2.822086584037	-2.232269938474	-0.681598853858
H	2.969306661874	-3.323945270275	-0.704162900591
H	2.012357362369	-1.984982080250	-1.384513074838
H	3.746390145686	-1.773685684644	-1.062395383144
C	-2.907001553796	-1.696346325896	0.843441810862
H	-2.865186125294	-1.364709625215	-0.203439769101
H	-1.975033227642	-2.237012597675	1.066014889249
H	-3.742761331417	-2.403998355800	0.949221486450
C	-3.130442296867	-0.989079916673	3.229862405776
H	-3.293298700940	-0.144240909088	3.912367698458
H	-3.946257885856	-1.713090554584	3.378702960883
H	-2.182951870871	-1.473419641244	3.510884699667
C	-3.210822565967	2.774485332214	3.043773173386
H	-3.363147447560	3.862877271739	2.976804224900
H	-4.201593933452	2.311482127612	3.166377513238
H	-2.630219970224	2.569728630053	3.954592959566
C	-0.668417490506	3.047767770238	1.428708488095
H	-0.206144571958	3.092822545997	2.426449942592
H	0.052818950248	2.578659705933	0.742078057837
H	-0.823215852523	4.085620919174	1.097634326603
C	3.992845621402	0.963131538921	0.401914130338
H	4.502863207794	1.925382375760	0.248202421367

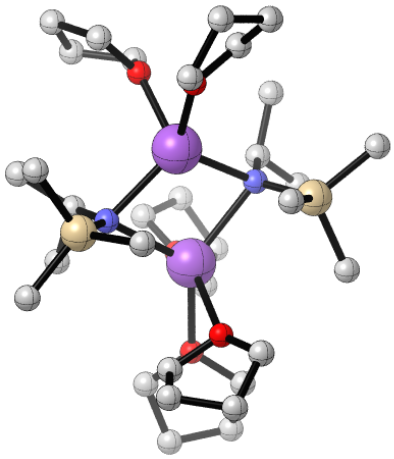
H	4.628666604271	0.353806886732	1.060585302473
H	3.931564634671	0.456114183000	-0.569496715399
C	2.775506711955	1.937590105883	2.338389377482
H	3.389753609082	1.357389769065	3.044065492813
H	3.255399269950	2.916835316613	2.185810669996
H	1.801817149980	2.113137459056	2.809289496171
O	0.211889531733	1.408376840103	-1.581633156937
C	1.461242707020	1.063161624127	-2.188601746450
C	-0.136436217732	2.710003557756	-2.040027191983
C	2.199163166923	2.393876242358	-2.438412431473
H	1.978391951756	0.390894515365	-1.495895515253
H	1.268276132569	0.528123449273	-3.130317917609
C	1.182050416988	3.469875025083	-2.015228737342
H	-0.545556400674	2.643506116605	-3.061830044891
H	-0.902957813663	3.111490520943	-1.371172510671
H	2.461579062703	2.492659015060	-3.497078377425
H	3.124796553645	2.459161309653	-1.858164474740
H	1.177525284562	4.339873068759	-2.679360392998
H	1.383814130100	3.816657939623	-0.994324089377
O	0.055491053742	1.739465037693	4.659230872649
C	-0.838806684029	1.287033938854	5.682644983973
C	0.615003221513	2.968253013195	5.117133386204
C	-1.358993784727	2.553285308070	6.393021466966
H	-1.620355602345	0.695215331040	5.196249771152
H	-0.289382574555	0.632848532737	6.375178643127
C	-0.563960065532	3.698780537108	5.741961900425
H	1.401486701992	2.759580906341	5.860953043235
H	1.062412035856	3.483273097130	4.262709924413
H	-1.159969779280	2.494616246448	7.468275393660
H	-2.438177032393	2.680812911455	6.262158257196
H	-0.250246764616	4.465005629668	6.457573563276
H	-1.152332336531	4.183181713287	4.953470279542
C	0.967172551861	-2.765338168669	1.620912866478
H	0.110385462983	-2.682894941300	0.935471661254
H	1.267481704119	-3.823888240662	1.626400462463
H	0.611041082169	-2.508462945251	2.629358221256
C	2.605161101703	1.159460411135	1.027956142591
Si	2.390013330473	-1.637505756838	1.079551466843
H	2.056602086755	1.838510551923	0.340485532991
C	-3.387196564113	2.574840946024	0.052496463459
H	-3.525281185416	3.664056810157	-0.022428780052
H	-2.966128239923	2.218746374211	-0.898740365104
H	-4.388177442497	2.127617693411	0.148857785952
Si	-2.293267596257	2.083365215511	1.529189999287
C	-3.035310539446	-0.494011772427	1.782310140538
H	-4.016261808317	-0.025041780751	1.547513164378
O	-0.579241744130	-1.569324587381	-1.655167529167
C	-1.414740416095	-0.978050500920	-2.669988864877
C	-0.683697840181	-3.000071822549	-1.704962973399
C	-2.191327749330	-2.133178576620	-3.291920264162
H	-2.057685192410	-0.221106042194	-2.204928019670
H	-0.764753682345	-0.480597212872	-3.401475236016
C	-1.234392077190	-3.306810713272	-3.087821234308

H	0.308194003897	-3.421000660002	-1.512552260178
H	-1.375439563626	-3.339971161391	-0.920253576895
H	-2.440724043576	-1.944590569843	-4.340549274006
H	-3.124250748678	-2.308378913436	-2.741508251664
H	-0.427897409553	-3.279883669649	-3.831368776063
H	-1.722207060300	-4.285009467826	-3.136291552587
O	0.300719457753	-1.194789777010	4.616515854190
C	1.683275773479	-1.054965891664	4.969246069410
C	-0.275923479466	-2.312917815759	5.306695897041
C	2.096620554078	-2.433771854236	5.452885481881
H	2.221707987865	-0.707327396590	4.079284705822
H	1.781989155418	-0.299508042394	5.765217275213
C	0.833884275248	-2.873982494370	6.195057020715
H	-1.150872306465	-1.968952468600	5.871897904090
H	-0.606723126222	-3.045047982147	4.557739896222
H	2.990897028796	-2.410893499090	6.083291443954
H	2.289193394563	-3.089874302552	4.593431601031
H	0.801417814171	-2.408826677964	7.187961115563
H	0.753063296391	-3.957688666802	6.320866398930

Table S26. Geometric coordinates and thermal corrected single point energies for the penta-THF solvated *cis*-NaPTA dimer.

G: –2649.921636 Eh G(sp): –2651.055345 Eh





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A2THF5_cis_thf: optimized structure // E(RM062X) = -2652.02470151 A.U. after 11 cycles

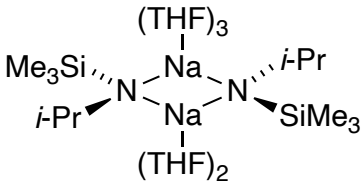
Na	0.012288682512	-0.027450617229	0.026385473801
Na	-0.011715213753	-0.003705013786	2.981499023519
N	1.901519231235	-0.017202312097	1.409138130486
N	-1.866078287500	0.184655325768	1.392038155507
C	4.423760757118	-1.654640554908	2.094212127919
H	4.140904739031	-1.812299680933	3.144668979962
H	4.964062545456	-2.552492154142	1.756087710160
H	5.141213793715	-0.820278389841	2.072960237656
C	3.732739353340	-1.217518720078	-0.768728451720
H	4.108121683730	-2.214622249201	-1.049455884236
H	2.995680619861	-0.920546595157	-1.530294653709
H	4.578133231355	-0.518814034159	-0.834942215481
C	-1.806393683610	-2.641364162629	0.794683002644
H	-1.677376914896	-2.514058218383	-0.291403316291
H	-0.806341479406	-2.660540341106	1.247129716549
H	-2.275333210075	-3.621884725001	0.966149518859
C	-3.272066885813	-1.719543113089	3.288510021613
H	-3.961107945831	-0.992609187971	3.744668810339
H	-3.753310579823	-2.708925179588	3.338377895118
H	-2.364136708595	-1.752409334701	3.908790208285
C	-3.422711007534	1.815023425997	2.487842942543
H	-3.753575588127	2.864957582024	2.495875487732
H	-4.317412383265	1.187177626394	2.354535851773
H	-2.989279084601	1.578769862087	3.467695041708
C	3.419942648722	1.797297765207	0.526911306813
H	3.638244883554	2.872807173898	0.603172979112
H	4.356092089790	1.254943346942	0.728809145414
H	3.118342551914	1.576950259082	-0.505350305663
C	2.777310764876	1.727953680684	2.938147052178

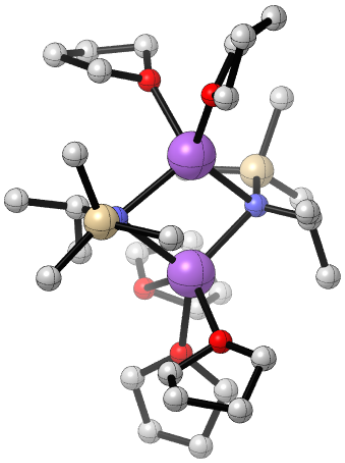
H	3.641024414690	1.105730170431	3.218707480784
H	3.071291384955	2.785449941484	3.029891387427
H	1.970977268363	1.542463565000	3.658595685543
O	0.186384517048	1.822735045562	-1.288070775894
C	1.073146222405	1.740651966825	-2.408397584273
C	-0.113073790193	3.197812078470	-1.067105269853
C	1.783821977015	3.106622347260	-2.502339605081
H	1.752446277346	0.901618018599	-2.226655866305
H	0.491354700289	1.525791294227	-3.316249636388
C	1.203615029700	3.910918301438	-1.327795972184
H	-0.893685823972	3.527033220806	-1.772454362848
H	-0.493092486649	3.298975868525	-0.045173430068
H	1.551079716223	3.591284931777	-3.456662017890
H	2.871991330618	3.007712653264	-2.436817641936
H	1.067551935643	4.971438667174	-1.561830038195
H	1.845735879106	3.830129131351	-0.443446870170
O	-0.355285438780	2.401291163817	3.746115056177
C	-1.065470486105	2.708022120241	4.942966883211
C	0.011596473026	3.653586688729	3.182110336681
C	-1.833053263135	4.016374691022	4.667577354949
H	-1.709382158872	1.858139160487	5.182047548956
H	-0.347982769831	2.847957913096	5.765795841729
C	-1.226941805660	4.528940194502	3.346529158888
H	0.868520965210	4.071802642632	3.737174874572
H	0.310670366947	3.488470762915	2.142764325202
H	-1.683117223036	4.728727581745	5.485636413522
H	-2.908761009362	3.839842155658	4.573589071417
H	-0.978635855362	5.594658309239	3.373070052303
H	-1.915547345188	4.358208799257	2.510714300699
C	1.884442867410	-2.860156337256	0.870450967994
H	1.234775735304	-2.825327333172	-0.017781387434
H	2.506410248317	-3.763506793689	0.782580558547
H	1.236554607965	-2.960892784571	1.748871904803
C	2.326441199818	1.368587874818	1.514684102181
Si	2.928707241020	-1.288587572530	0.965261432042
H	1.453904104232	2.018938937929	1.288562413013
C	-3.022010611604	1.916602214883	0.021396180876
H	-3.306347017776	2.980804463071	-0.016344555731
H	-2.309263732304	1.721620942750	-0.789906766349
H	-3.925132977407	1.319222302167	-0.170824852394
O	-0.273985858791	-1.097717545253	-1.946222903867
C	-1.558568457687	-0.679416630646	-2.443934073242
C	0.148878823084	-2.296093097064	-2.608997045103
C	-2.029016446827	-1.800663042427	-3.363126987102
H	-2.223315035568	-0.505713280452	-1.588300732260
H	-1.425419524643	0.268274039637	-2.984067681581
C	-0.704136715434	-2.374619838779	-3.865410614612
H	1.224204852877	-2.219632778765	-2.800732797482
H	-0.035460634502	-3.158497363726	-1.951470791548
H	-2.681385780460	-1.434146097393	-4.161450130409
H	-2.577419784639	-2.559993214258	-2.791024550505
H	-0.282757854554	-1.734206550152	-4.650609841005
H	-0.785909764615	-3.394514568389	-4.253196547924

O	0.159594507438	-2.399834361410	3.821486281353
C	1.476936210349	-2.378374161078	4.388711184329
C	-0.355822192223	-3.740436379368	3.851034624864
C	1.968891607407	-3.816433533586	4.345263701415
H	2.076626679068	-1.666543717780	3.808899490932
H	1.417754362950	-2.030921560684	5.430623808671
C	0.668375826413	-4.573273513734	4.618858134834
H	-1.345187623518	-3.731498314905	4.323024342196
H	-0.465213506178	-4.096285947142	2.817895232643
H	2.748897266919	-4.008534485990	5.089249501717
H	2.365617703569	-4.065206948648	3.353637255997
H	0.445461068915	-4.559554007010	5.693359638470
H	0.685170240603	-5.615487094910	4.285670117776
O	0.210779010922	0.070076060597	5.290940385807
C	-0.775252534374	-0.542906267948	6.125479432326
C	1.307314573226	0.548922519282	6.079326213262
C	-0.510438997967	0.008784922189	7.517761283421
H	-1.765593805977	-0.293210517636	5.727213330440
H	-0.652964928065	-1.637034523791	6.089684988827
C	1.014980525383	0.111292463970	7.513535146229
H	2.241145053460	0.129727268064	5.684534971137
H	1.351808248599	1.642097904421	5.980946127401
H	-0.903164487021	-0.639025752808	8.307506206146
H	-0.963270459815	1.002725045312	7.624915371659
H	1.458153917670	-0.873102690526	7.710147260881
H	1.410925912566	0.816700450851	8.250397379348
C	-4.474644937244	-1.272380421637	0.569374034189
H	-5.194864840072	-0.519595577950	0.920370503584
H	-4.335354581243	-1.120233529477	-0.511288132067
H	-4.944067967084	-2.259595229900	0.703314789419
C	-2.403841632898	1.532400955732	1.375238593894
H	-1.569710834957	2.238881455348	1.546892176937
Si	-2.815710589445	-1.211672896330	1.508757425174

Table S27. Geometric coordinates and thermal corrected single point energies for the penta-THF *trans*-NaPTA dimer.

G: –2649.923094 Eh G(sp): –2651.057688 Eh





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A2THF5_trans_thf: optimized structure // E(RM062X) = -2652.02632740 A.U. after 11 cycles

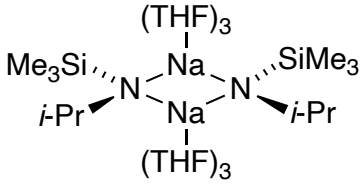
Na	-0.022936605178	-0.017908648842	0.003032802188
Na	-0.004198084013	0.003522411594	2.940755915062
N	1.885735172165	-0.011026434495	1.409542858605
N	-1.828062867053	0.429528493745	1.475360504232
C	4.144815551670	-1.952384978146	2.234056549674
H	3.958922653469	-1.691050343745	3.285897248735
H	4.337759492423	-3.035452738835	2.187497346233
H	5.073585818955	-1.446625093535	1.932379754380
C	3.409201185747	-1.756984931208	-0.650480225058
H	3.790695776104	-2.787507764108	-0.732476240225
H	2.636549079708	-1.624327875944	-1.421874581337
H	4.244052188942	-1.084029915584	-0.894990449883
C	-2.298650619614	-1.955136396623	1.133400906727
H	-2.042013749082	-1.891955476381	0.065011072428
H	-1.383080946912	-2.213356985244	1.686880108163
H	-3.019866270637	-2.775881660905	1.264302083408
C	-3.268797322589	-0.753942638454	3.102017481579
H	-3.684101333665	0.192904970028	3.472172206947
H	-4.024674891390	-1.541959442402	3.245320426640
H	-2.393480985577	-1.001051804099	3.721120076321
C	-3.802410679107	2.708721723687	1.985886707140
H	-4.080227448878	3.707236751385	1.614748768137
H	-4.695749090041	2.072076436609	1.890508354560
H	-3.575836547801	2.794850251165	3.057100199696
C	-0.892540355779	3.151149723988	1.079693691916
H	-0.580183250653	3.308385196600	2.121436101942
H	-0.030398091135	2.730547582181	0.540334610076
H	-1.117727077600	4.134006333932	0.638029269627
C	3.980915608811	1.377696504229	1.116477870903

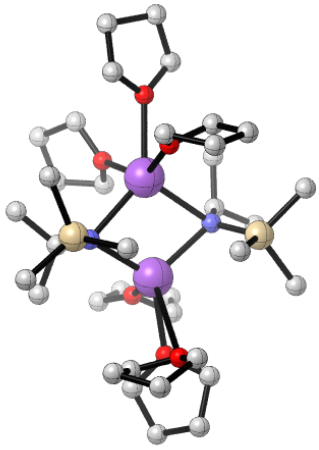
H	4.342497224392	2.415337213921	1.070006033730
H	4.535476516080	0.865919271744	1.916677768529
H	4.234402897016	0.891311312202	0.165052158857
C	2.200677599916	2.063145225041	2.706298070267
H	2.692042688889	1.530483507341	3.534276900768
H	2.584420378837	3.095149983175	2.685666370071
H	1.128829607743	2.139863499389	2.935287131022
O	0.555766020128	1.521943713831	-1.585616557135
C	1.901332510117	1.214369349141	-1.969464938304
C	0.238852156678	2.783764657291	-2.166412488925
C	2.617686126244	2.567750328323	-2.149996524839
H	2.327856091076	0.593129152264	-1.176351208936
H	1.883813350822	0.637878640126	-2.906829975317
C	1.500063835527	3.608205054118	-1.955410962015
H	0.018472367859	2.649277834630	-3.238623468034
H	-0.647725764015	3.178650174129	-1.664392269084
H	3.056022040457	2.638883402676	-3.151109188289
H	3.424802876173	2.697748495572	-1.422212300771
H	1.571942178538	4.450912953696	-2.650064618830
H	1.508767306380	4.002720747361	-0.931817604873
O	-0.092651000884	4.085005180021	4.325914028052
C	-1.331352574781	3.555896834711	4.807818801422
C	-0.301743452919	5.375248954560	3.743759380683
C	-2.317276116654	4.718639510286	4.788279548085
H	-1.648790427573	2.730774504201	4.151001964284
H	-1.169803955721	3.149703971578	5.811959843169
C	-1.811103655390	5.530875694344	3.597439148048
H	0.113224589957	6.142042164605	4.415177574611
H	0.238103019981	5.418162042760	2.790026697884
H	-2.229259537111	5.304805505061	5.712296689273
H	-3.356607813330	4.389735155431	4.686832966968
H	-2.127353191534	6.578925489954	3.613716313233
H	-2.154286480495	5.076690152915	2.659450537096
C	1.405735083589	-2.847630025179	1.270372465695
H	0.591784001703	-2.721224478796	0.543014957233
H	1.846219148228	-3.841788751028	1.100783369510
H	0.950063639162	-2.835137172109	2.266862195080
C	2.472688526024	1.321197096016	1.393302196779
Si	2.689221834099	-1.470298007983	1.096829003023
H	1.997764947691	1.933085778407	0.594722860883
C	-3.026703736279	2.004218734568	-0.794524586223
H	-3.363275114428	3.006369529736	-1.102376924021
H	-2.266974607470	1.668933060908	-1.514444089920
H	-3.889613294283	1.327356375724	-0.893330285033
Si	-2.360180371618	1.967552472662	0.991274384098
C	-2.833844109238	-0.611558647242	1.636926813920
H	-3.758721988584	-0.406575635835	1.053230001227
O	-0.091263509735	-1.469245284246	-1.770756088004
C	-0.885947471340	-0.881487051966	-2.820293420639
C	0.054525319962	-2.880266573068	-1.998760643152
C	-1.412987092430	-2.049901381470	-3.643311837468
H	-1.680968609384	-0.279938186865	-2.365161232146
H	-0.239958976645	-0.219889935652	-3.412118556419

C	-0.306085260960	-3.086194065102	-3.460751161309
H	1.081124446139	-3.164676971895	-1.748159109858
H	-0.636569431686	-3.425116108279	-1.338547886841
H	-1.592014331614	-1.772342336840	-4.686421755151
H	-2.352980023734	-2.423411292319	-3.218125656630
H	0.553236667506	-2.846767323424	-4.099831411313
H	-0.623132224603	-4.111889233004	-3.671804445132
O	-0.087890927166	-1.999364759594	4.135405706885
C	1.185817644382	-2.018140244201	4.801133662487
C	-0.738648759602	-3.272159015752	4.277289560194
C	1.513544722339	-3.489127987256	5.000644324390
H	1.904590641386	-1.476604926157	4.172801248956
H	1.092371760971	-1.496267629336	5.764227484594
C	0.121438819097	-4.070732268002	5.251861029012
H	-1.762673886972	-3.106064125929	4.632088887578
H	-0.782605347785	-3.754592071765	3.290606344560
H	2.210499247829	-3.650347191364	5.828923195875
H	1.952953275136	-3.912025401218	4.087961814193
H	-0.188328180051	-3.871604489734	6.285553455828
H	0.055113491072	-5.148125378631	5.073445941605
O	0.007204471036	0.777375953882	5.144134178020
C	-0.985742350105	0.286112752088	6.054677528398
C	1.053266892193	1.457650075466	5.860291744871
C	-0.348504789461	0.350914805198	7.437678804664
H	-1.877031909206	0.928256190509	5.990645792479
H	-1.256672530223	-0.728903492532	5.744573742132
C	0.579190404137	1.558860716761	7.307590893435
H	1.971138411720	0.856512822616	5.782980105232
H	1.216223139198	2.430928939263	5.385170502458
H	0.232106663072	-0.558775026133	7.635817443868
H	-1.094210428720	0.458126043869	8.231734861189
H	1.415490424064	1.540613223857	8.013405377889
H	0.021360682123	2.489028057587	7.469752309838

Table S28. Geometric coordinates and thermal corrected single point energies for the hexa-THF solvated *cis*-NaPTA dimer.

G: –2882.116768 Eh G(sp): –2883.386110 Eh





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A2THF6_cis_thf: optimized structure // E(RM062X) = -2884.47535342 A.U. after 11 cycles

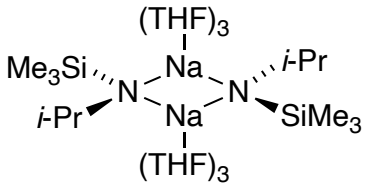
Na	0.084269171706	0.130791152001	0.044875008955
Na	-0.022859139446	0.038895007488	2.978137272230
N	2.016822492327	0.222629585772	1.462753215383
N	-1.849186034633	-0.115458213547	1.341774058974
C	4.300635057413	-1.657197395789	2.399305000197
H	3.915786802098	-1.783549163393	3.419436566425
H	4.767541891751	-2.609120644971	2.099775018247
H	5.108235444080	-0.911434416928	2.449551398651
C	4.063952732561	-1.050968202559	-0.468429223800
H	4.265964601452	-2.065961610171	-0.846144953566
H	3.577444178975	-0.490024168518	-1.277498453335
H	5.037274852777	-0.575962619701	-0.278989271858
C	-1.669824263956	-3.016322568065	1.275950071295
H	-1.262799511154	-2.980103609118	0.258322370182
H	-0.814592963560	-2.999490054683	1.958552910037
H	-2.203120013283	-3.970144476719	1.410366098489
C	-3.429772088296	-1.742355100515	3.382129586817
H	-4.207437023585	-1.000813582499	3.618050612062
H	-3.872738674999	-2.739335736148	3.536057300754
H	-2.619492246522	-1.617516249288	4.115449260149
C	-3.506941336253	1.570364058692	2.197299571437
H	-3.863500617859	2.604769929563	2.074006655737
H	-4.383154625592	0.907999640091	2.123330807311
H	-3.086001437886	1.466372715732	3.206280572865
C	3.963041082252	1.827880368075	1.130481967400
H	4.285353622836	2.855106949055	1.356427352228
H	4.739608915872	1.149835408656	1.514389024749
H	3.935116995788	1.714460755676	0.039291421083
C	2.731003020150	1.738375565986	3.290123513293

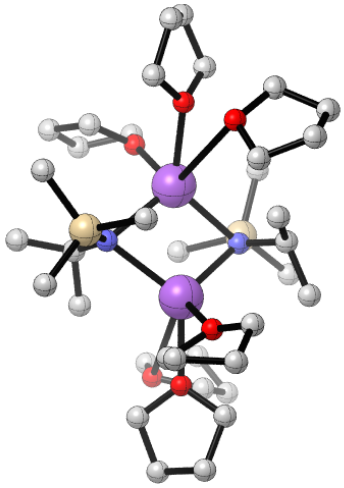
H	3.407652690566	0.979802621073	3.713525852023
H	3.136501900122	2.732626655925	3.538723026376
H	1.754061083571	1.642439184954	3.778478507252
O	0.144244333223	2.345789019789	-0.674619389688
C	1.406585879429	2.471249026054	-1.324670260290
C	-0.532998158797	3.577353213419	-0.897268233039
C	1.866915679011	3.900914015814	-1.024415188206
H	2.059863303312	1.687364143612	-0.927135763842
H	1.273326379812	2.317275906165	-2.408226079309
C	0.545810978579	4.661022679043	-0.763032555863
H	-0.969916307661	3.573839310938	-1.909275577994
H	-1.342402111142	3.655201168421	-0.165165126827
H	2.436990791357	4.320035632535	-1.859419851152
H	2.508631495900	3.918054125244	-0.137449915314
H	0.379266132167	5.474093232694	-1.476319680076
H	0.537092404751	5.094982120264	0.242922135278
O	-0.524028501322	2.354903722411	3.396440044283
C	-1.109930871201	2.880293315340	4.581204246331
C	-0.160937016602	3.479858181563	2.606738232067
C	-1.891621861261	4.132847347002	4.143622488762
H	-1.737690173981	2.102650034576	5.023485809822
H	-0.313282289631	3.142110132435	5.295408299472
C	-1.344649151374	4.437396623604	2.732630586055
H	0.760866438950	3.931995615918	3.012614983306
H	0.033010347303	3.123955457938	1.591385178735
H	-1.720167681712	4.960981788672	4.838864292383
H	-2.968404173808	3.938639411415	4.116808113185
H	-1.043428734493	5.482501469618	2.607789305291
H	-2.096431431179	4.204447298514	1.969225247238
C	1.829545482003	-2.599217018746	0.856027676113
H	1.160055585163	-2.461766993622	-0.009772796467
H	2.391983008765	-3.529783855798	0.682855386958
H	1.197691653177	-2.745542321743	1.741622414401
C	2.600197094391	1.522238518930	1.775062881613
Si	2.986432201899	-1.128254108054	1.112048748769
H	1.917171229303	2.308913606192	1.404895151967
C	-3.044932546782	1.379714157792	-0.260590273230
H	-3.439463025246	2.396812156756	-0.414651164505
H	-2.271931590294	1.200137431127	-1.020552169659
H	-3.864770570952	0.669478377317	-0.435506643190
O	-0.348380839438	-3.060407456203	-1.944040177885
C	-1.678190440436	-2.613678257439	-2.226031256915
C	-0.320275128497	-4.483655194381	-1.821389247131
C	-2.579559308991	-3.837876791941	-2.081781202203
H	-1.927682102063	-1.794990961554	-1.537367394051
H	-1.709254491406	-2.223044970363	-3.254882469957
C	-1.622385084603	-4.975741200771	-2.441311367567
H	0.576497515181	-4.855561259551	-2.329845236298
H	-0.256649109711	-4.755557559201	-0.755755245391
H	-3.458931753474	-3.783308589509	-2.731854206981
H	-2.924041238853	-3.943043694233	-1.045959652369
H	-1.516757778334	-5.055265992330	-3.530980241667
H	-1.933439387405	-5.950095107135	-2.051585960525

O	0.025392505982	-2.222576545268	4.031545880048
C	1.369470839333	-2.232985638629	4.507114485516
C	-0.513076676744	-3.482646139541	4.419567109135
C	1.879726670985	-3.668359538782	4.286086106675
H	1.922403717413	-1.463217626521	3.957753240128
H	1.372553687223	-1.974563251568	5.578471985522
C	0.585691877566	-4.482181743930	4.066264073307
H	-0.708324882585	-3.475017339139	5.505710240637
H	-1.455780490041	-3.636540799837	3.890412726647
H	2.445086231324	-4.016919891045	5.156618708365
H	2.539112343744	-3.727444998378	3.414456065225
H	0.535532018009	-5.385523583528	4.682124436988
H	0.489525880279	-4.779621604423	3.014926749274
O	0.217660488012	0.310724988589	5.349164708008
C	-0.871321448822	-0.214436089601	6.113432318143
C	1.249713190486	0.781558440115	6.226662436585
C	-0.737914234222	0.432300650778	7.482210642626
H	-1.805059555872	0.023268635323	5.590434237575
H	-0.780137391969	-1.308914803123	6.178904067077
C	0.781708732681	0.454353991486	7.643408635873
H	2.195652500537	0.293410911666	5.961720093743
H	1.365590301455	1.863656700351	6.076724161339
H	-1.255014381037	-0.130068503058	8.265760134286
H	-1.138369309311	1.454273544527	7.462360763269
H	1.140812289799	-0.537165178676	7.946643035873
H	1.138582220588	1.185105842132	8.375496414460
O	0.212721472475	-0.167548879738	-2.214493426708
C	1.322415277224	-0.766651147882	-2.887628351696
C	-0.658990879525	0.458298676827	-3.164182172257
C	0.806323545910	-1.080686679856	-4.280080422670
H	2.155424150038	-0.046329066981	-2.930699439076
H	1.619235488603	-1.648951592251	-2.314379018472
C	-0.091277764677	0.130243789520	-4.550037252272
H	-1.665805823540	0.048420793162	-3.020553927540
H	-0.696062323309	1.536949678965	-2.961952592145
H	0.227346080708	-2.011034276587	-4.251596222177
H	1.612660528818	-1.188763809162	-5.012630188473
H	-0.882130863738	-0.067587917782	-5.280458517594
H	0.511802865994	0.966998360334	-4.923315107432
C	-4.332654626971	-1.772299594580	0.539871248359
H	-5.103838231267	-1.017272773638	0.753945520433
H	-4.119717018398	-1.728690892779	-0.538092835688
H	-4.778945047789	-2.756818437591	0.752153457375
C	-2.453478644976	1.194086894128	1.146303306604
H	-1.659488234375	1.955440454676	1.237065285001
Si	-2.766399759770	-1.517573209232	1.603948745710

Table S29. Geometric coordinates and thermal corrected single point energies for the hexa-THF *trans*-NaPTA dimer.

G: –2882.117246 Eh G(sp): –2883.390276 Eh





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A2THF6_trans_thf: optimized structure // E(RM062X) = -2884.47315250 A.U. after 11 cycles

Na	0.098222599238	0.552477772457	0.164117427113
Na	0.053893160222	-0.136030510871	3.051983361229
N	1.974838164533	0.143932938070	1.554917263803
N	-1.688396250514	0.755347770066	1.728633538035
C	3.971309429882	-2.007506325162	2.513112011114
H	3.784659805781	-1.593108788703	3.513799865300
H	3.893830569258	-3.103786602528	2.586868579956
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H	0.671623450432	1.303313387957	-4.446393479176

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