SUPPORTING INFORMATION

Sodium Diisopropylamide: Aggregation, Solvation, and Stability

Russell F. Algera, Yun Ma, and David B. Collum*

Department of Chemistry and Chemical Biology
Baker Laboratory, Cornell University
Ithaca, New York 14853–1301
E-mail: dbc6@cornell.edu

I. NMR spectroscopic studies

II. Rate studies

III. Computations

I. NMR spectroscopic studies

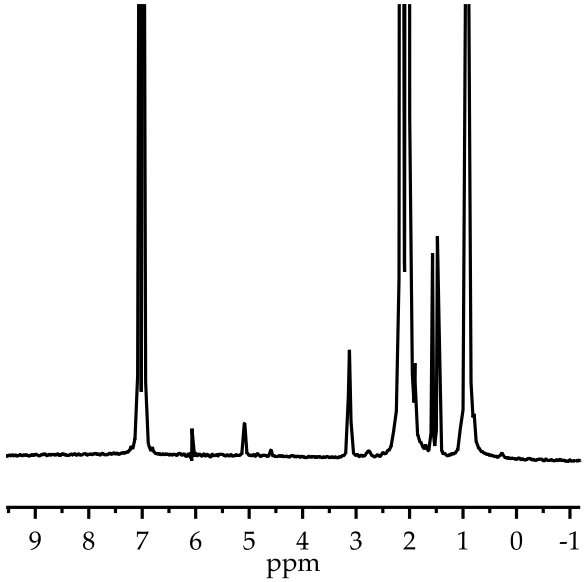


Figure S-1. ^{1}H NMR spectrum of 600 uL extract of 0.50 M NaDA in DMEA prepared from 4.0 mL DMEA, 0.50 mL diisopropylamine (1 equiv), 3.0 mL sodium dispersion (30% w/w) in toluene, and 175 uL isoprene (0.50 equiv). Aside from the solvent resonances the only remaining signals are affiliated with 2-methyl-2-butene (δ 5.08, δ 1.57, δ 1.48, δ 1.45) and NaDA (δ 3.12, δ 0.90).

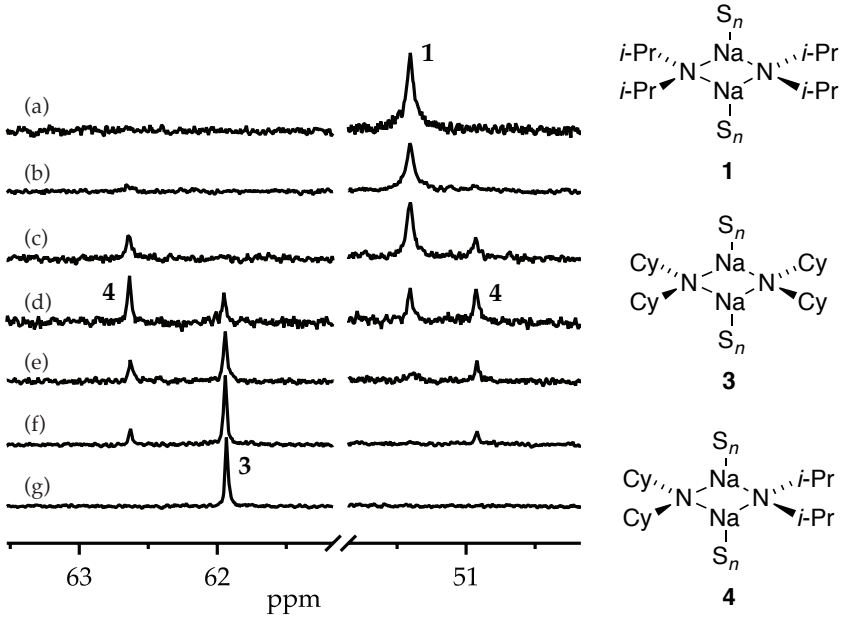


Figure S-2. ^{13}C NMR spectra for 0.20 M solutions of NaDA and NaDCA in DMEA with varying χ_{NaDA} at –80 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.97, 0.82, 0.56, 0.34, 0.14, and 0.00, respectively.

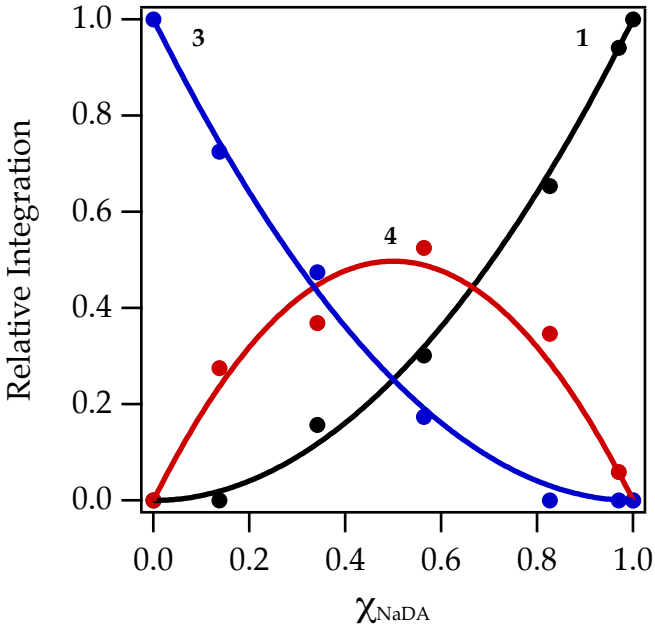


Figure S-3. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.20 M solutions of NaDA and NaDCA in DMEA with varying χ_{NaDA} at –80 °C. Fitting the data to an aggregating dimer ensemble affords $K_{eq} = 4 \pm 1$.

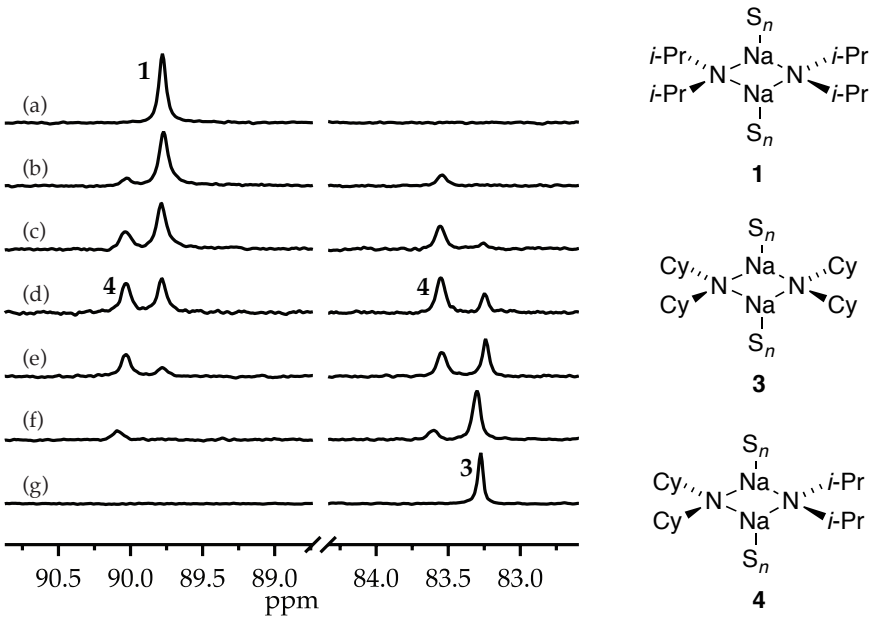


Figure S-4. ^{15}N NMR spectra for 0.10 M solutions of NaDA and NaDCA in DMEA with varying χ_{NaDA} at –100 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.86, 0.71, 0.58, 0.40, 0.17, and 0.00, respectively.

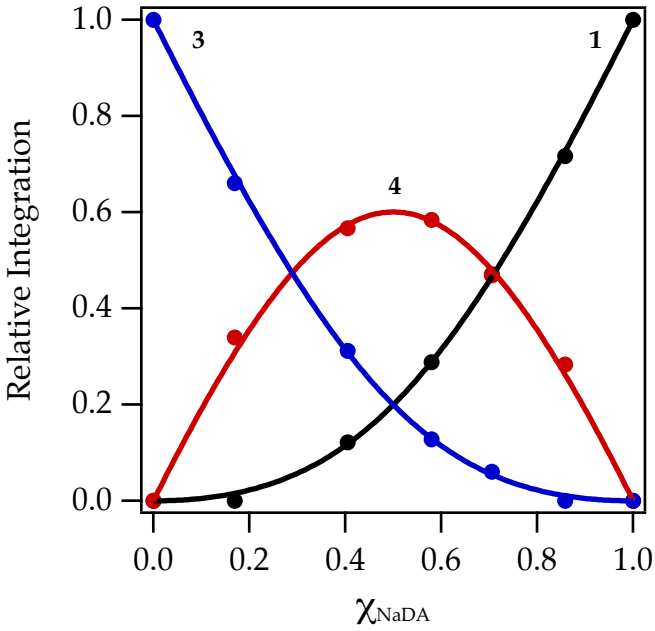


Figure S-5. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.10 M solutions of NaDA and NaDCA in DMEA with varying χ_{NaDA} at –100 °C. Fitting the data to an aggregating dimer ensemble affords K_{eq} = 9.0 ± 0.9.

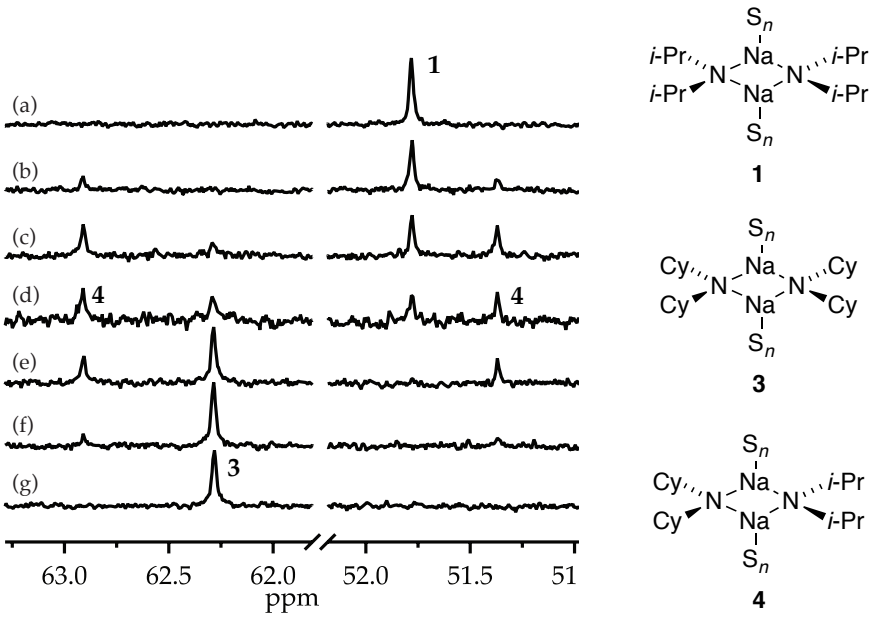


Figure S-6. ^{13}C NMR spectra for 0.10 M solutions of NaDA and NaDCA in DMBA with varying χ_{NaDA} at –80 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.97, 0.82, 0.56, 0.34, 0.14, and 0.00, respectively.

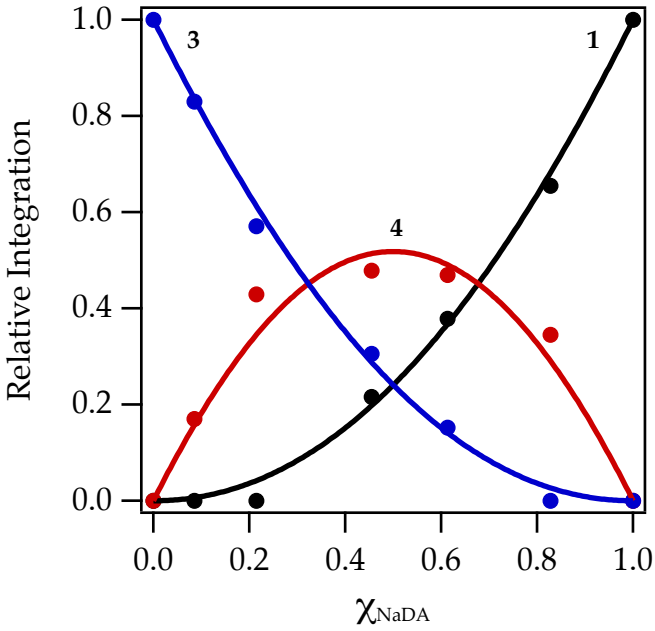


Figure S-7. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.10 M solutions of NaDA and NaDCA in DMBA with varying χ_{NaDA} at –80 °C. Fitting the data to an aggregating dimer ensemble affords $K_{eq} = 5 \pm 1$.

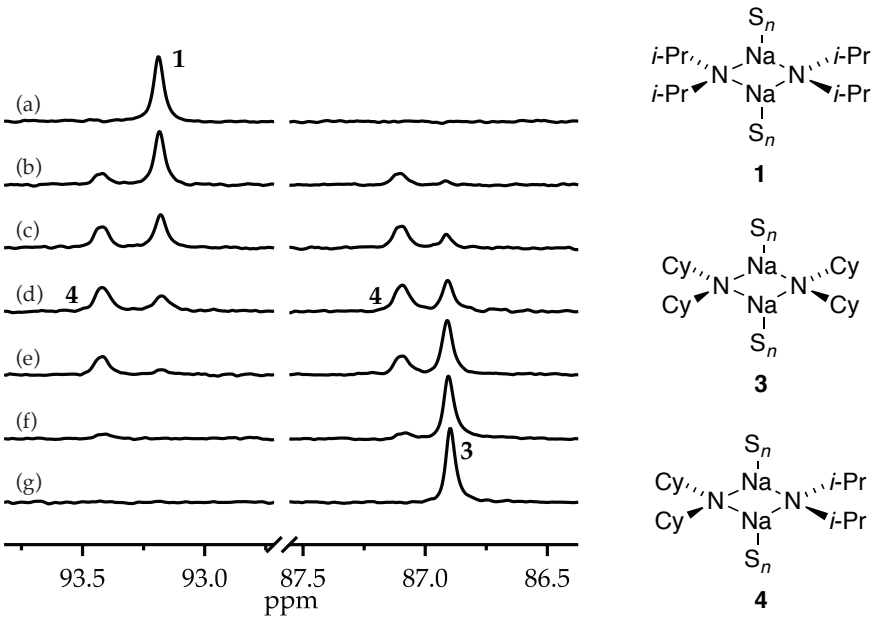


Figure S-8. ^{15}N NMR spectra for 0.10 M solutions of NaDA and NaDCA in DMBA with varying χ_{NaDA} at –80 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.78, 0.60, 0.47, 0.30, 0.11, and 0.00, respectively.

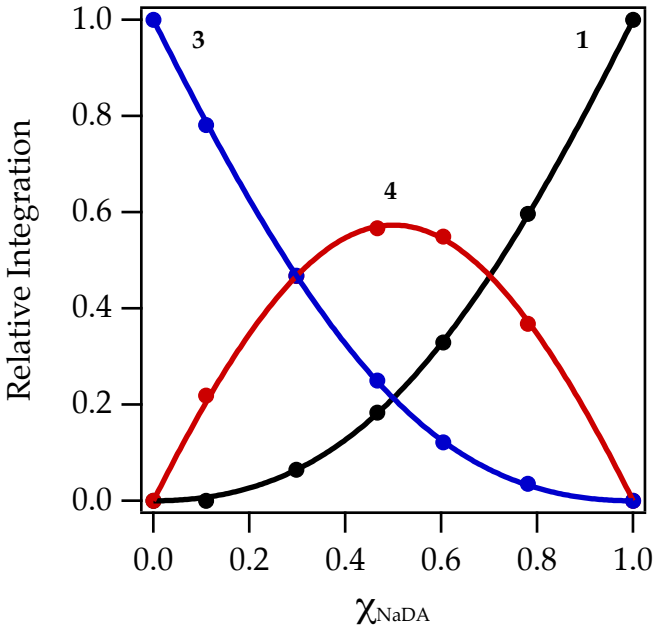


Figure S-9. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.10 M solutions of NaDA and NaDCA in DMBA with varying χ_{NaDA} at –80 °C. Fitting the data to an aggregating dimer ensemble affords K_{eq} = 7.2 ± 0.3.

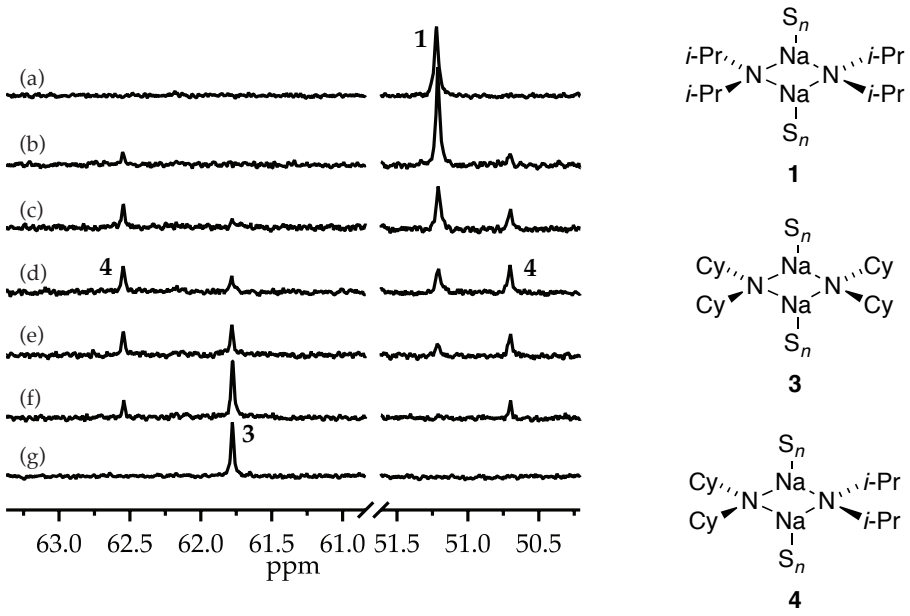


Figure S-10. ^{13}C NMR spectra for 0.10 M solutions of NaDA and NaDCA in *N*-methylpyrrolidine with varying χ_{NaDA} at –80 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.94, 0.72, 0.59, 0.36, 0.17, and 0.00, respectively.

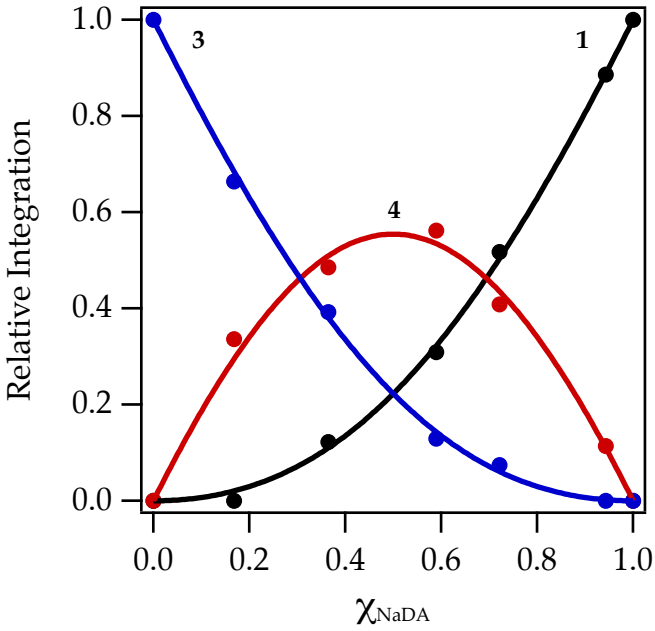


Figure S-11. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.10 M solutions of NaDA and NaDCA in *N*-methylpyrrolidine with varying χ_{NaDA} at –80 °C. Fitting the data to an aggregating dimer ensemble affords $K_{eq} = 6.2 \pm 0.9$.

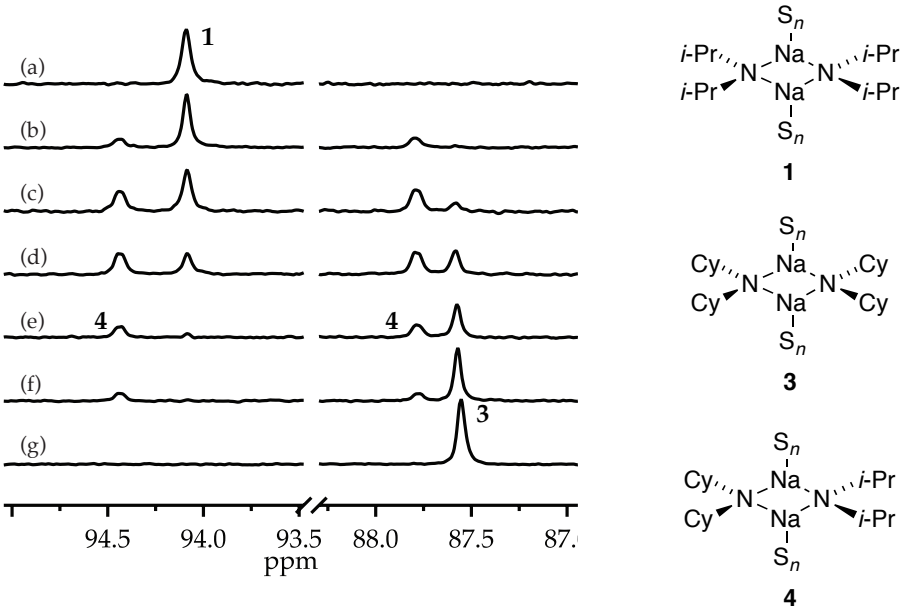


Figure S-12. ^{15}N NMR spectra for 0.10 M solutions of NaDA and NaDCA in *N*-methylpyrrolidine with varying χ_{NaDA} at –85 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.83, 0.65, 0.54, 0.28, 0.15, and 0.00, respectively.

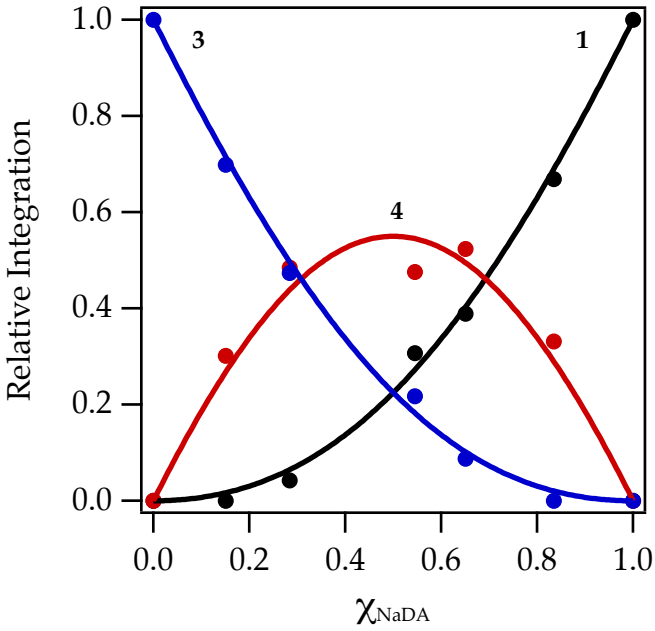


Figure S-13. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.10 M solutions of NaDA and NaDCA in *N*-methylpyrrolidine with varying χ_{NaDA} at –85 °C. Fitting the data to an aggregating dimer ensemble affords $K_{eq} = 6 \pm 1$.

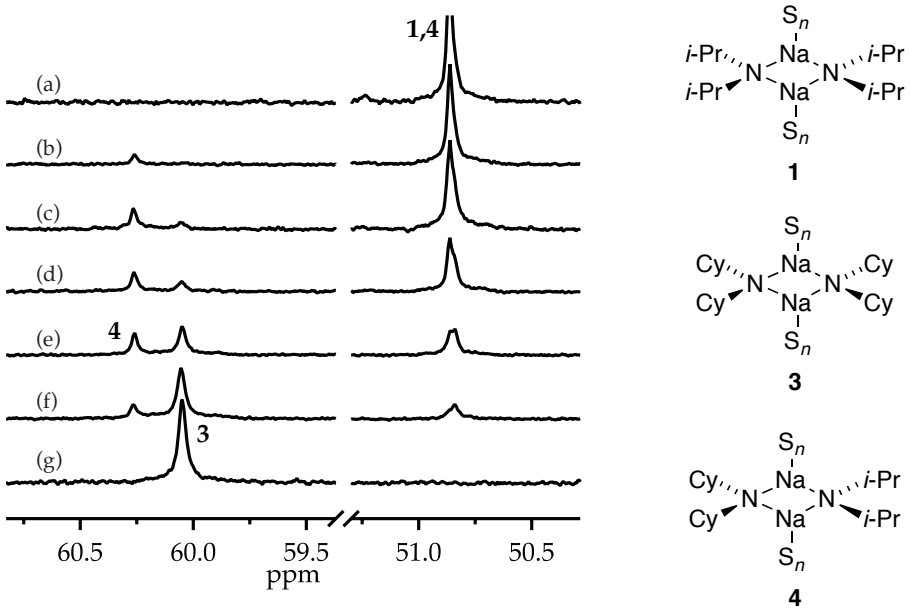


Figure S-14. ^{13}C NMR spectra for 0.30 M solutions of NaDA and NaDCA in 6.15 M THF/hexane with varying χ_{NaDA} at −100 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.91, 0.83, 0.66, 0.31, 0.16, and 0.00, respectively.

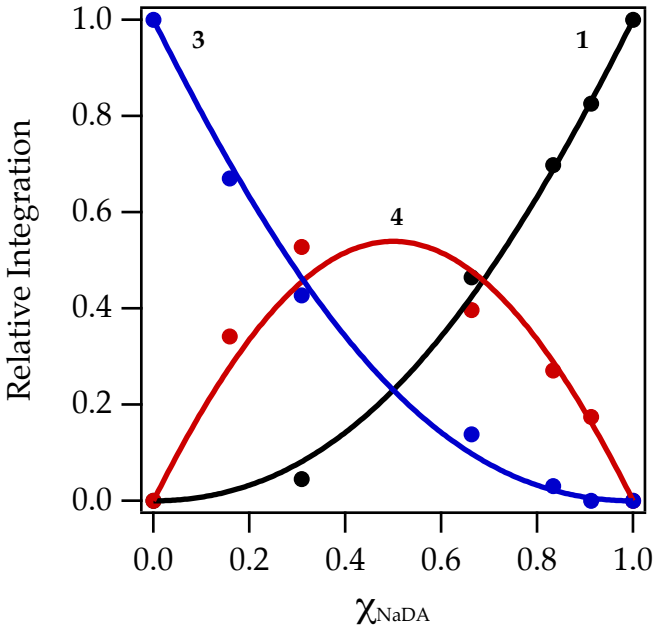


Figure S-15. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.30 M solutions of NaDA and NaDCA in 6.15 M THF/hexane with varying χ_{NaDA} at −100 °C. Fitting the data to an aggregating dimer ensemble affords $K_{eq} = 6 \pm 2$.

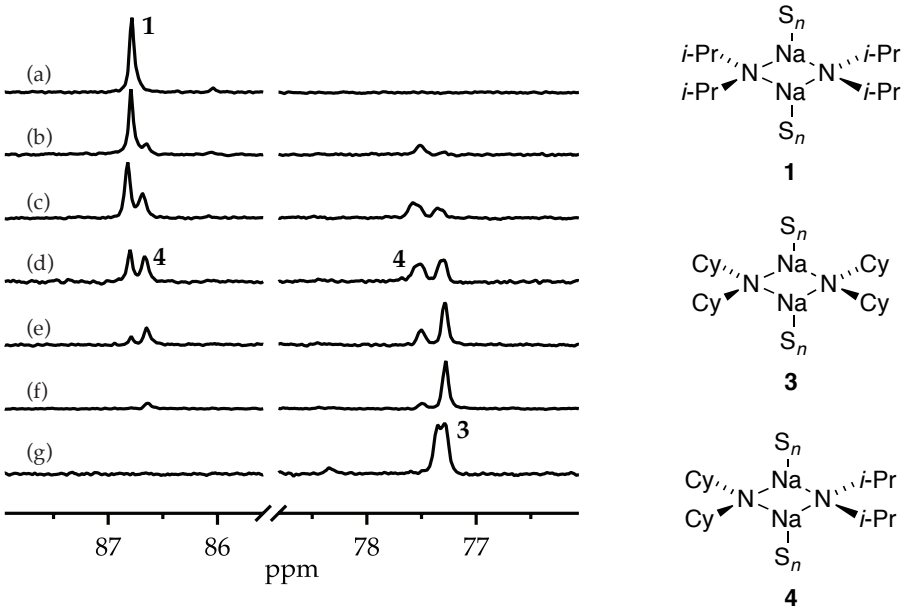


Figure S-16. ^{15}N NMR spectra for 0.086 M solutions of NaDA and NaDCA in 1.76 M THF/DMEA with varying χ_{NaDA} at −100 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.81, 0.64, 0.52, 0.27, 0.11, and 0.00, respectively. Apparent duplication in spectrum (g) is an irreproducible artifact.

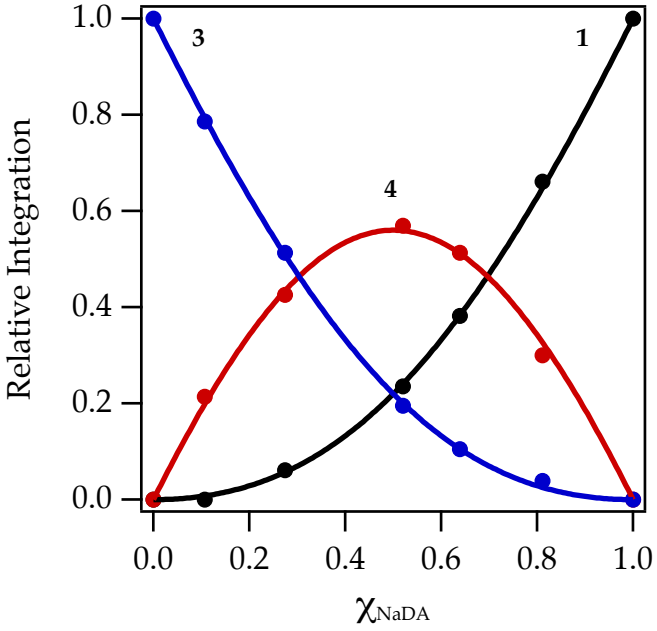


Figure S-17. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.086 M solutions of NaDA and NaDCA in 1.76 M THF/DMEA with varying χ_{NaDA} at −100 °C. Fitting the data to an aggregating dimer ensemble affords $K_{eq} = 6.5 \pm 0.5$.

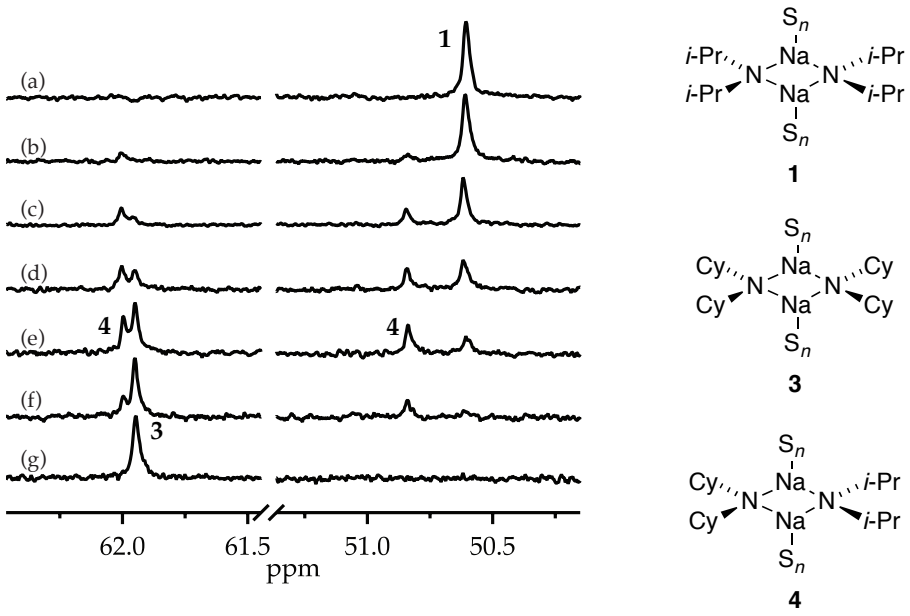


Figure S-18. ^{13}C NMR spectra for 0.17 M solutions of NaDA and NaDCA in 1.37 M 1,2-dimethoxyethane/DMEA with varying χ_{NaDA} at –80 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.94, 0.76, 0.59, 0.33, 0.23, and 0.00, respectively.

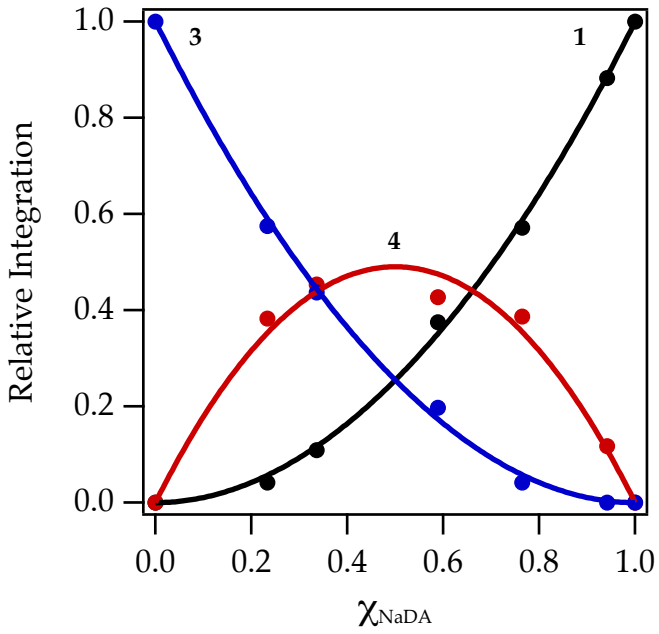


Figure S-19. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.17 M solutions of NaDA and NaDCA in 1.37 M 1,2-dimethoxyethane/DMEA with varying χ_{NaDA} at –80 °C. Fitting the data to an aggregating dimer ensemble affords $K_{eq} = 3.7 \pm 0.6$.

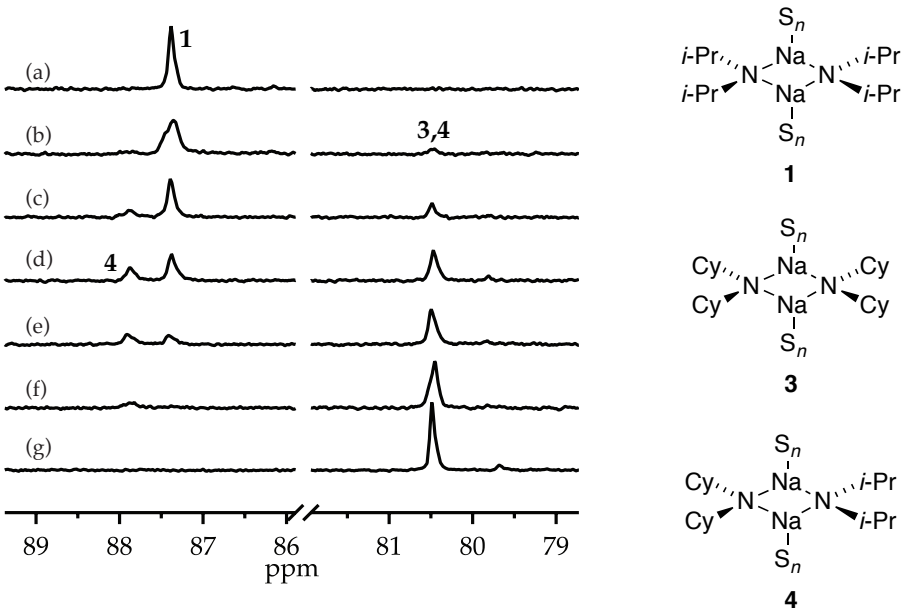


Figure S-20. ^{15}N NMR spectra for 0.086 M solutions of NaDA and NaDCA in 1.37 M 1,2-dimethoxyethane/DMEA with varying χ_{NaDA} at −100 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.94, 0.76, 0.59, 0.33, 0.23, and 0.00, respectively.

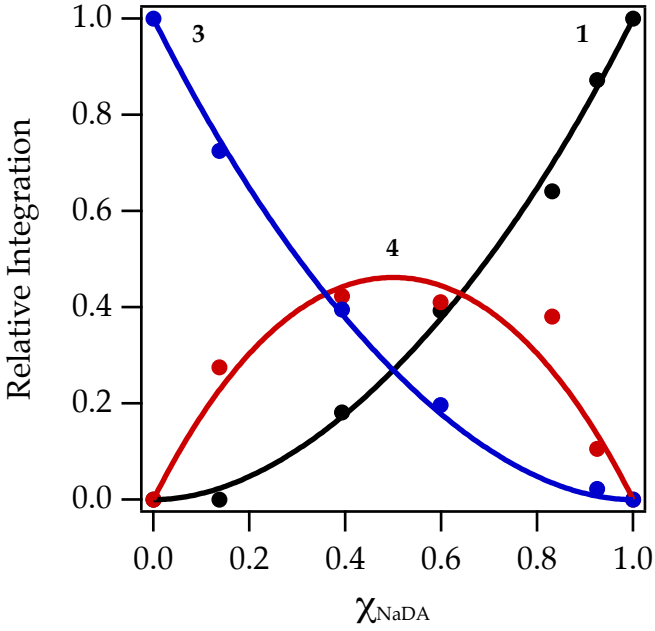


Figure S-21. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.086 M solutions of NaDA and NaDCA in 1.37 M 1,2-dimethoxyethane/DMEA with varying χ_{NaDA} at −100 °C. Fitting the data to an aggregating dimer ensemble affords $K_{eq} = 2.9 \pm 0.9$.

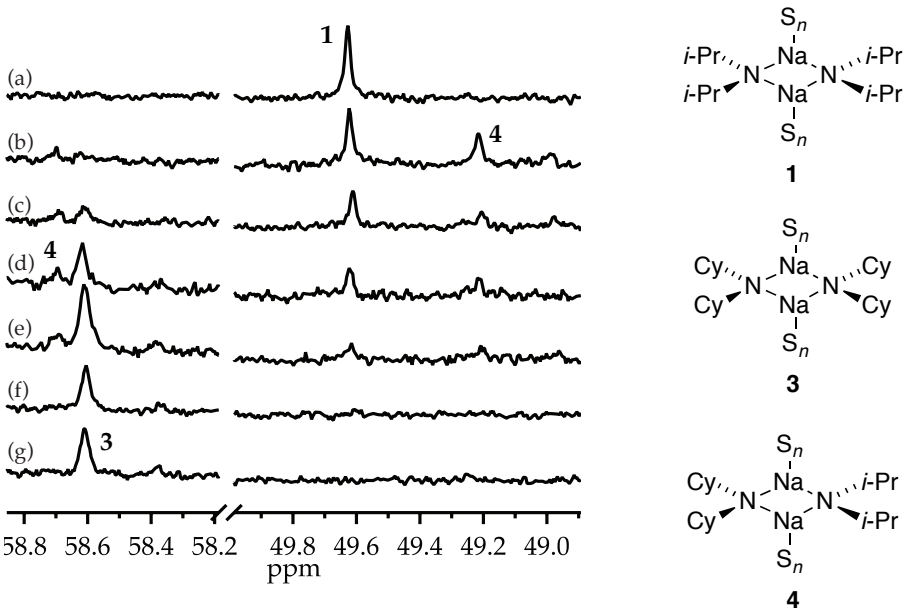


Figure S-22. ^{13}C NMR spectra for 0.086 M solutions of NaDA and NaDCA in 0.95 M TMEDA/DMBA with varying χ_{NaDA} at –80 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.68, 0.69, 0.47, 0.14, 0.06, and 0.00, respectively.

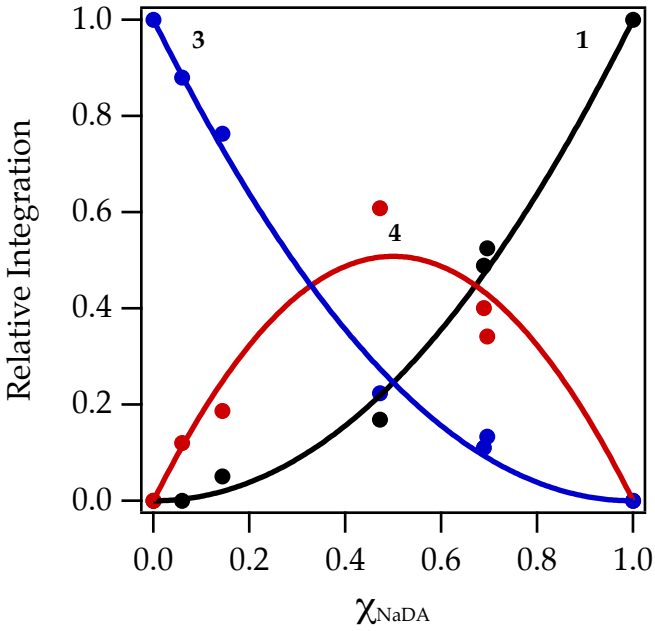


Figure S-23. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.086 M solutions of NaDA and NaDCA in 0.95 M TMEDA/DMBA with varying χ_{NaDA} at –80 °C. Fitting the data to an aggregating dimer ensemble affords $K_{eq} = 4 \pm 1$.

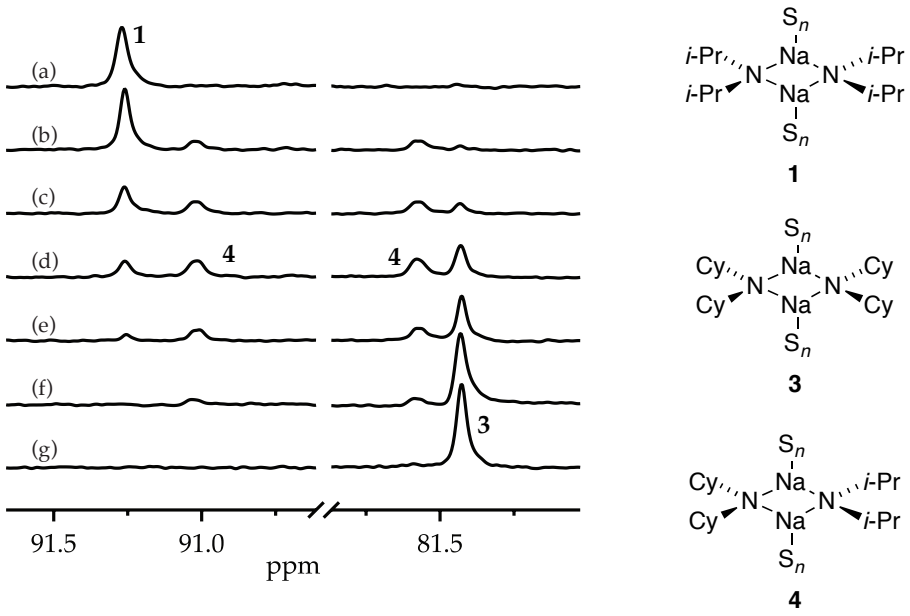


Figure S-24. ^{15}N NMR spectra for 0.086 M solutions of NaDA and NaDCA in 0.95 M TMEDA/DMBA with varying χ_{NaDA} at –80 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.81, 0.62, 0.42, 0.27, 0.08, and 0.00, respectively.

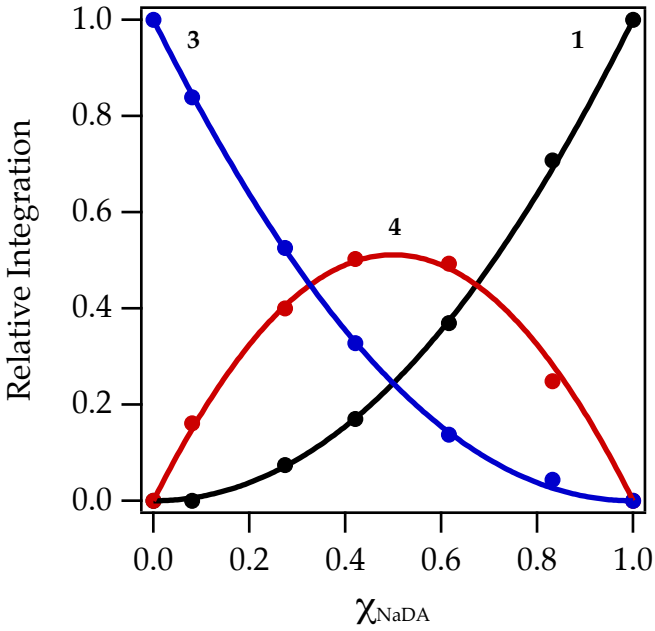


Figure S-25. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.086 M solutions of NaDA and NaDCA in 0.95 M TMEDA/DMBA with varying χ_{NaDA} at –80 °C. Fitting the data to an aggregating dimer ensemble affords $K_{eq} = 4.4 \pm 0.4$.

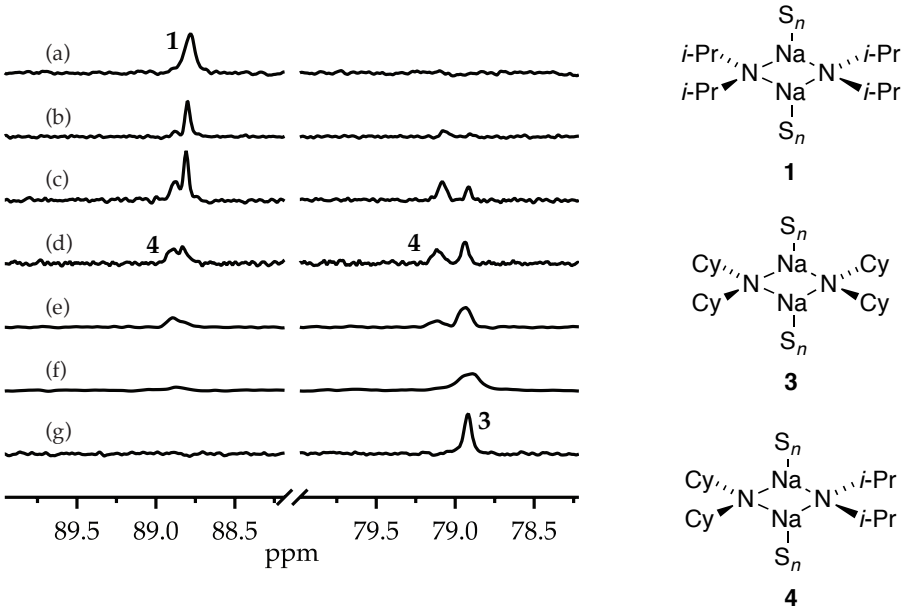


Figure S-26. ^{15}N NMR spectra for 0.086 M solutions of NaDA and NaDCA in 0.68 M PMDTA/DMEA with varying χ_{NaDA} at –80 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.79, 0.63, 0.50, 0.31, 0.13, and 0.00, respectively.

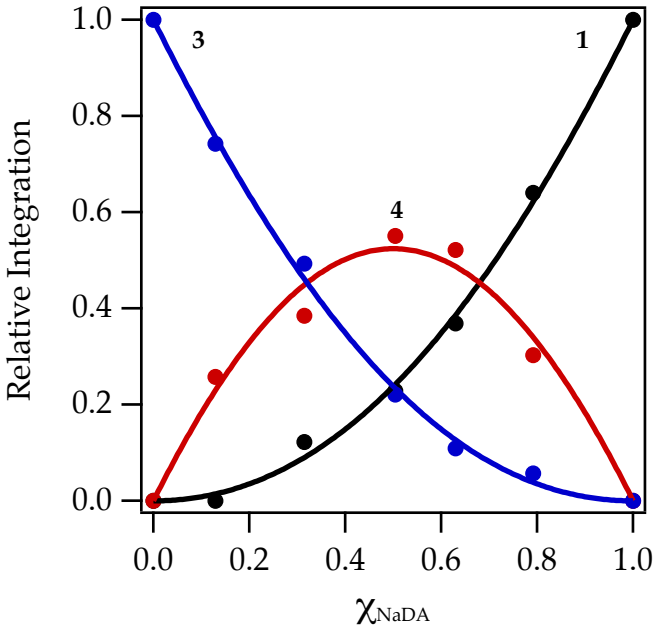


Figure S-27. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.086 M solutions of NaDA and NaDCA in 0.68 M PMDTA/DMEA with varying χ_{NaDA} at –80 °C. Fitting the data to an aggregating dimer ensemble affords $K_{eq} = 4.9 \pm 0.9$.

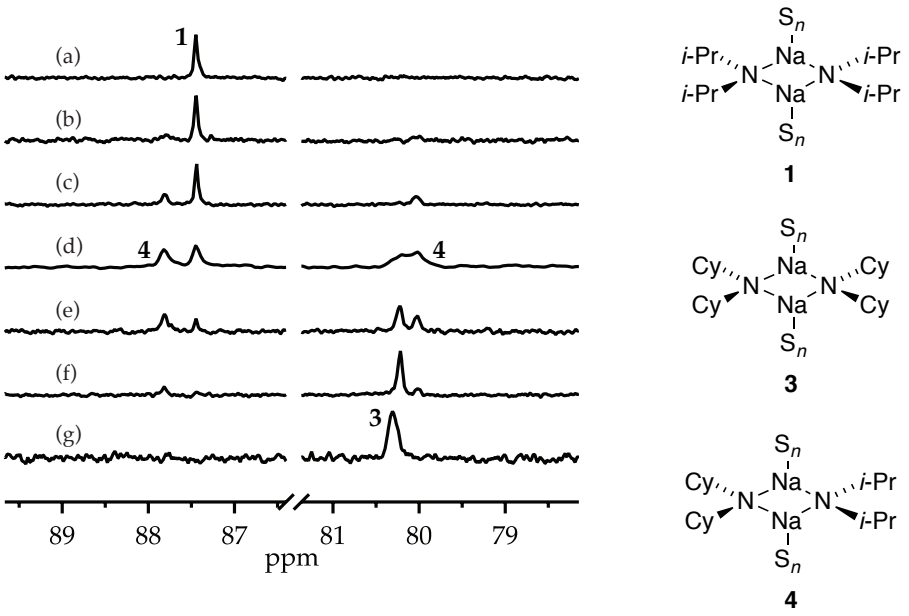


Figure S-28. ^{15}N NMR spectra for 0.086 M solutions of NaDA and NaDCA in 1.00 M diglyme/DMEA with varying χ_{NaDA} at –80 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.88, 0.76, 0.44, 0.35, 0.14, and 0.00, respectively.

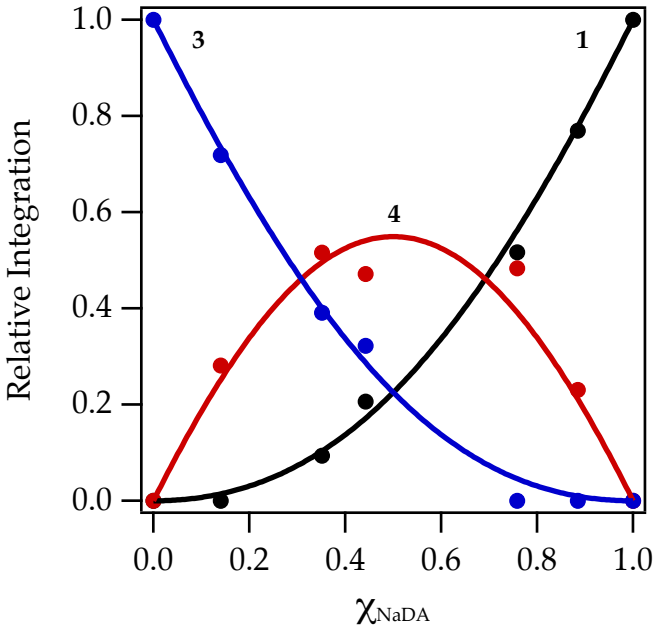


Figure S-29. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.086 M solutions of NaDA and NaDCA in 1.00 M diglyme/DMEA with varying χ_{NaDA} at –80 °C. Fitting the data to an aggregating dimer ensemble affords $K_{eq} = 6 \pm 2$.

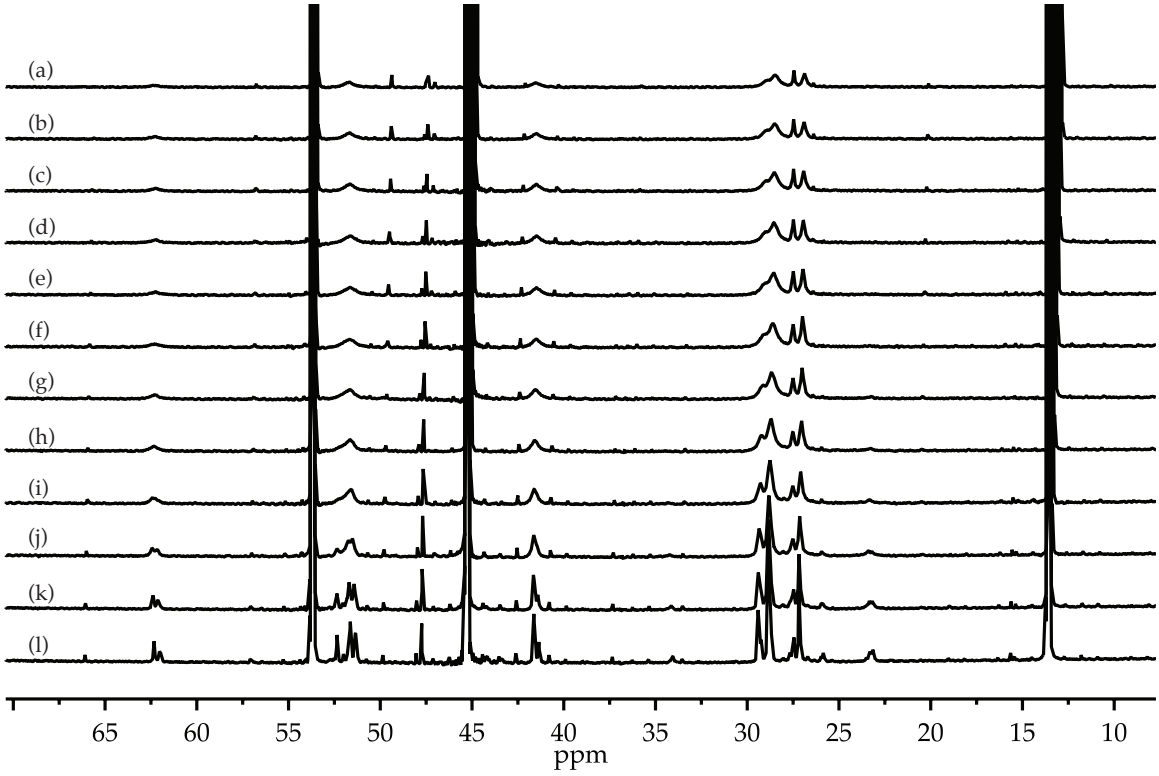


Figure S-30. Variable temperature ^{13}C NMR spectra for a mixture of 0.35 M NaDA and 0.35 M NaICA in DMEA with 10% v/v benzene-d_6 as an internal standard. The temperatures are (a) +10 °C, (b) 0 °C, (c) –10 °C, (d) –20 °C, (e) –30 °C, (f) –40 °C, (g) –50 °C, (h) –60 °C, (i) –70 °C, (j) –80 °C, (k) –90 °C, and (l) –99 °C respectively. These spectra demonstrate highly fluxional aggregate subunit exchange.

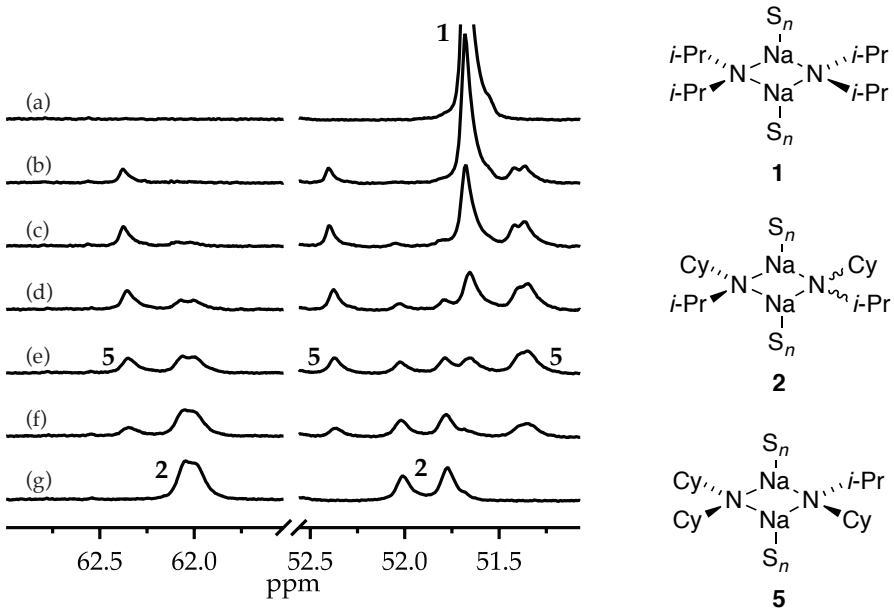


Figure S-31. ^{13}C NMR spectra for 0.50 M solutions of NaDA and NaICA in DMEA with varying χ_{NaDA} at –98 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.87, 0.72, 0.55, 0.36, 0.15, and 0.00, respectively.

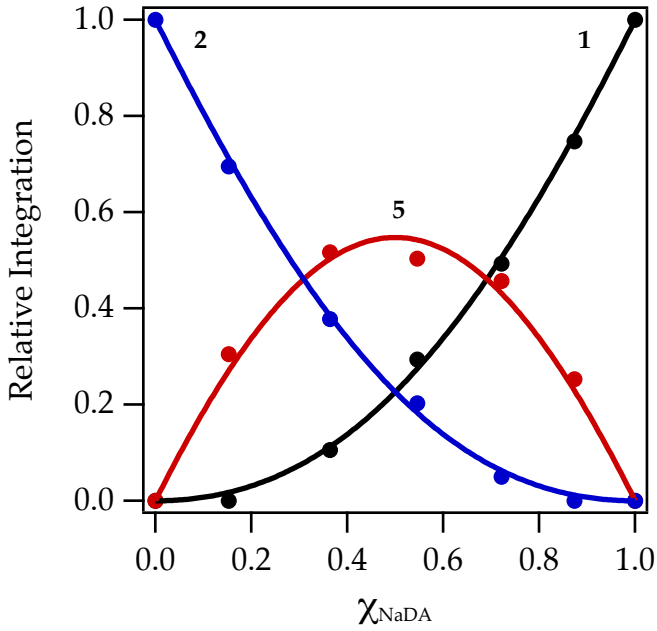


Figure S-32. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.50 M solutions of NaDA and NaICA in DMEA with varying χ_{NaDA} at –98 °C. Fitting the data to an aggregating dimer ensemble affords K_{eq} = 5.9 ± 0.9.

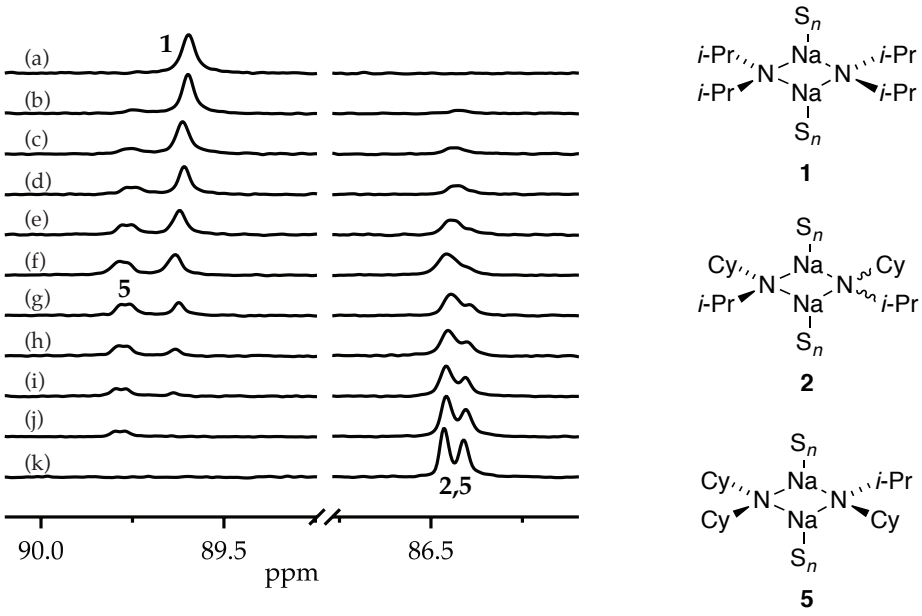


Figure S-33. ^{15}N NMR spectra for 0.30 M solutions of NaDA and NaICA in DMEA with varying χ_{NaDA} at –109 °C. The measured mole fractions, χ_{NaDA}, in (a)–(k) are 1.00, 0.91, 0.82, 0.72, 0.67, 0.56, 0.44, 0.28, 0.27, 0.12, and 0.00, respectively.

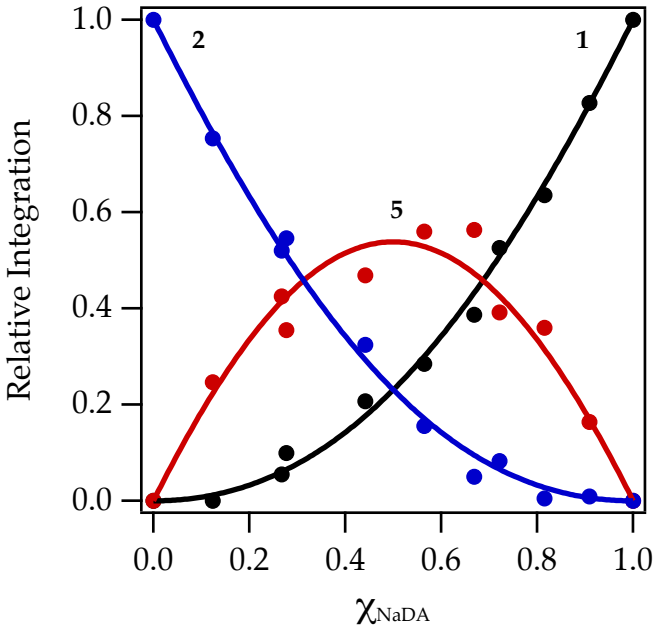


Figure S-34. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.30 M solutions of NaDA and NaICA in DMEA with varying χ_{NaDA} at –109 °C. Fitting the data to an aggregating dimer ensemble affords $K_{eq} = 5 \pm 1$.

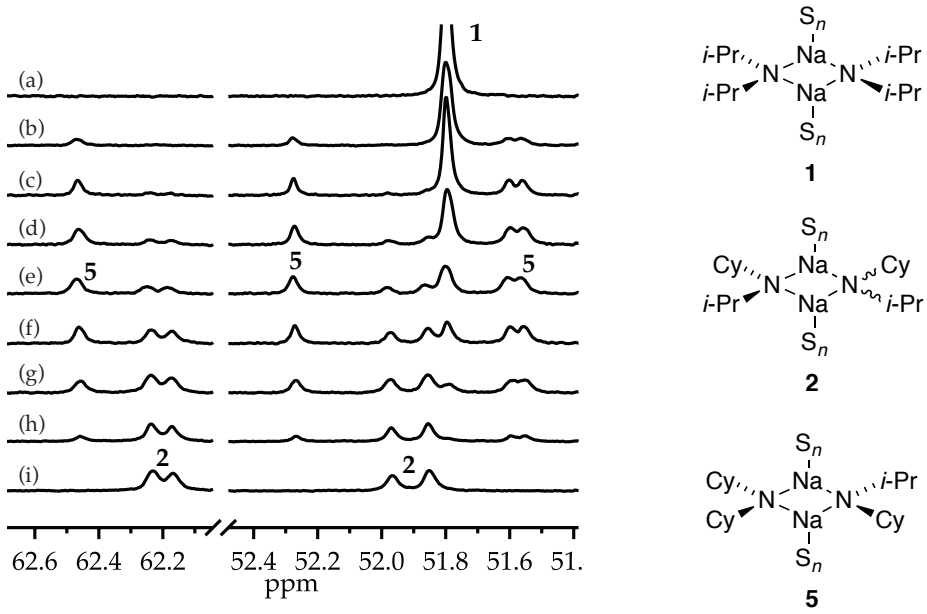


Figure S-35. ^{13}C NMR spectra for 0.31 M solutions of NaDA and NaICA in DMBA with varying χ_{NaDA} at –100 °C. The measured mole fractions, χ_{NaDA}, in (a)–(i) are 1.00, 0.88, 0.77, 0.62, 0.52, 0.36, 0.27, 0.11, and 0.00, respectively.

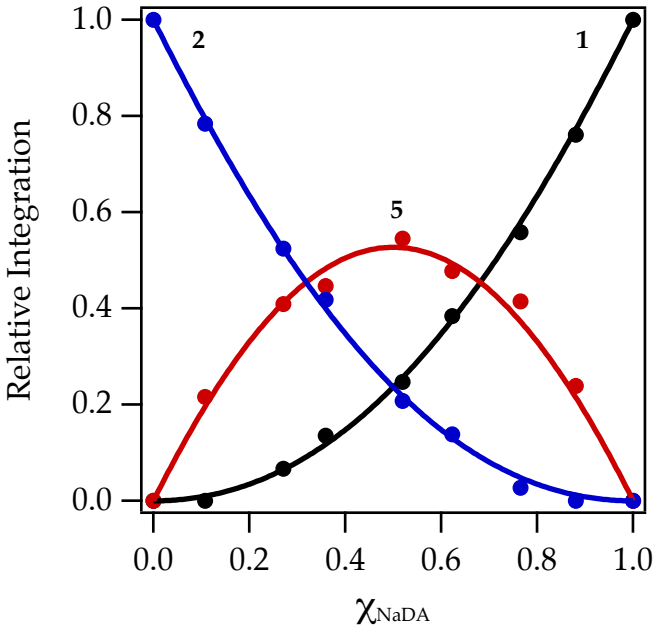


Figure S-36. Job plot showing the relative integrations versus the measured mole fraction of NaDA for 0.31 M solutions of NaDA and NaICA in DMBA with varying χ_{NaDA} at –100 °C. Fitting the data to an aggregating dimer ensemble affords K_{eq} = 5.0 ± 0.5.

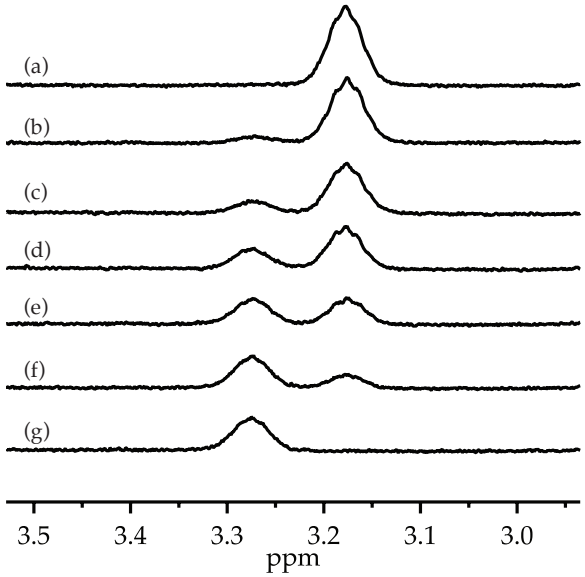


Figure S-37. ^{1}H NMR spectra for 0.10 M solutions of NaDA and NaICA in TMCDA/DMEA with varying χ_{NaDA} at 21 °C. The measured mole fractions, χ_{NaDA}, in (a)–(g) are 1.00, 0.82, 0.67, 0.50, 0.33, 0.16, and 0.00, respectively. The absence of time-averaged resonance perturbation is taken to imply monomeric NaDA.

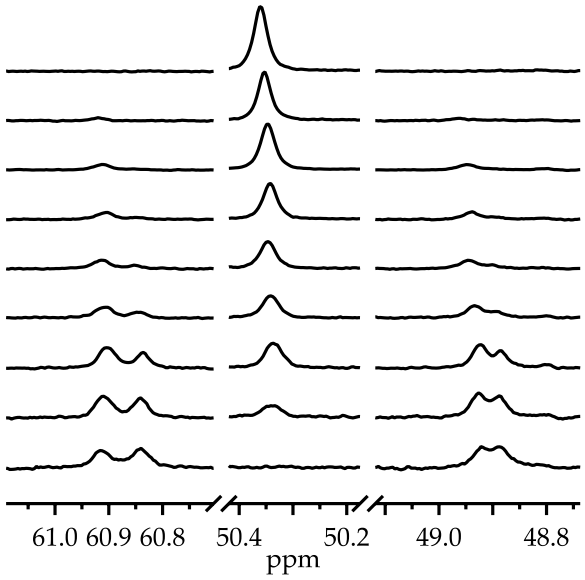


Figure S-38. ^{13}C NMR spectra for 0.40 M solutions of NaDA and NaICA in 0.40 M TMEDA/DMEA with varying χ_{NaDA} at −80 °C. Due to poor resolution of homo- from heteroaggregates a Job plot was not extracted from this data.

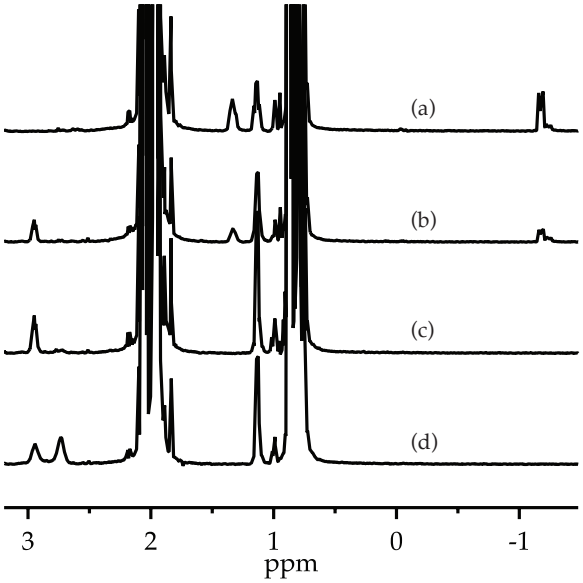


Figure S-39. [1]H NMR spectra for 0.40 M solutions of *n*-BuNa in DMEA with 10% v/v benzene-d_6 varying diisopropylamine at –80 °C. The equivalents of diisopropylamine in (a)–(d) are 0.00, 0.50, 1.0, and 2.0, respectively. The spectra show quantitative conversion of *n*-BuNa into NaDA up to 1.0 equiv diisopropylamine with concomitant appearance of *n*-butane resonances.

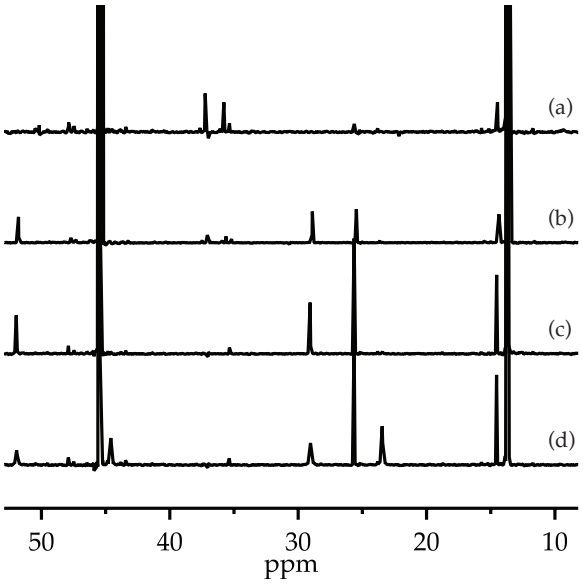


Figure S-40. [13]C NMR spectra for 0.40 M solutions of *n*-BuNa in DMEA with 10% v/v benzene-d_6 varying diisopropylamine at –80 °C. The equivalents of diisopropylamine in (a)–(d) are 0.00, 0.50, 1.0, and 2.0, respectively. The spectra show quantitative conversion of *n*-BuNa into NaDA up to 1.0 equiv diisopropylamine with concomitant appearance of *n*-butane resonances.

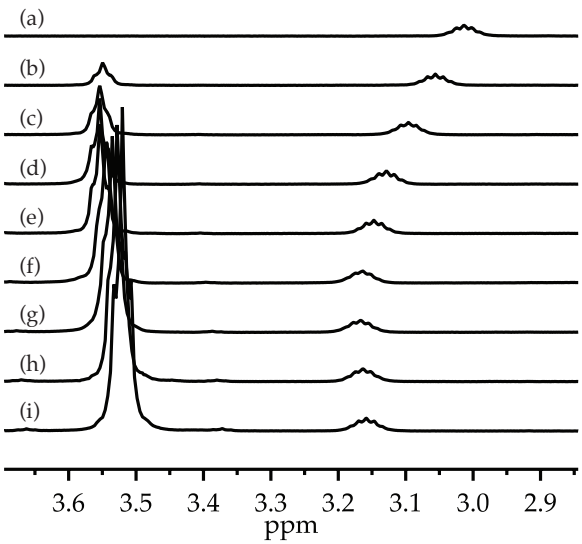


Figure S-41. ^{1}H NMR spectra for 0.30 M solutions of NaDA in DMBA with 10% v/v benzene-d_6 varying THF at –80 °C. The equivalents of THF in (a)–(i) are 0.00, 0.63, 1.19, 1.885, 2.44, 3.77, 5.025, 5.975, and 7.325, respectively.

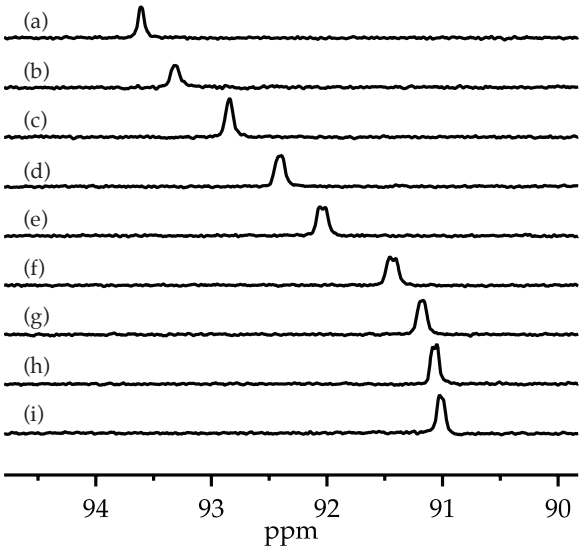


Figure S-42. ^{15}N NMR spectra for 0.30 M solutions of NaDA in DMBA with 10% v/v benzene-d_6 varying THF at –80 °C. The equivalents of THF in (a)–(i) are 0.00, 0.63, 1.19, 1.885, 2.44, 3.77, 5.025, 5.975, and 7.325, respectively.

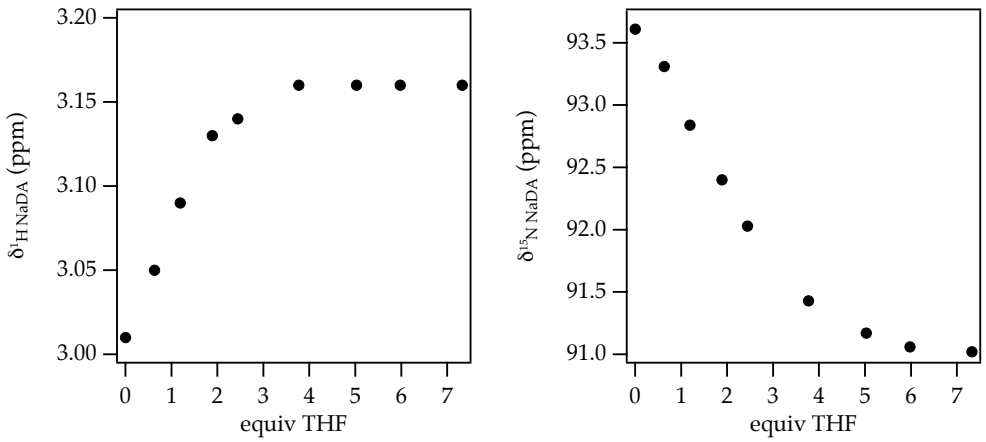


Figure S-43. Plots of chemical shift affiliated with NaDA for 0.30 M solutions of NaDA in DMBA with 10% v/v benzene-d_6 varying THF at –80 °C. Non-quantitative substitution is evidenced by chemical shift saturation at >3.0 equiv THF/Na.

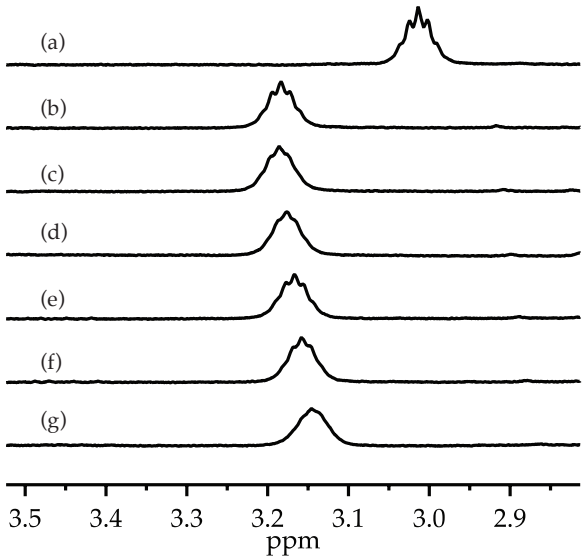


Figure S-44. ^{1}H NMR spectra for 0.25 M solutions of NaDA in DMBA with 10% v/v benzene-d_6 varying TMEDA at –80 °C. The equivalents of TMEDA in (a)–(g) are 0.00, 0.50, 1.0, 2.0, 3.0, 4.0, and 5.0, respectively.

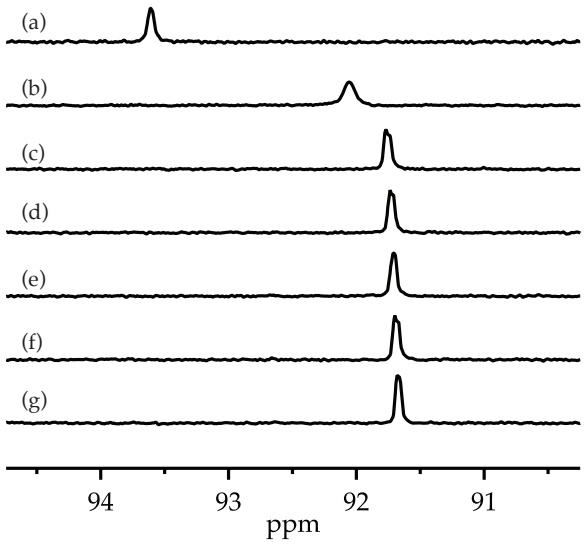


Figure S-45. ^{15}N NMR spectra for 0.25 M solutions of NaDA in DMBA with 10% v/v benzene-d_6 varying TMEDA at –80 °C. The equivalents of TMEDA in (a)–(g) are 0.00, 0.50, 1.0, 2.0, 3.0, 4.0, and 5.0, respectively.

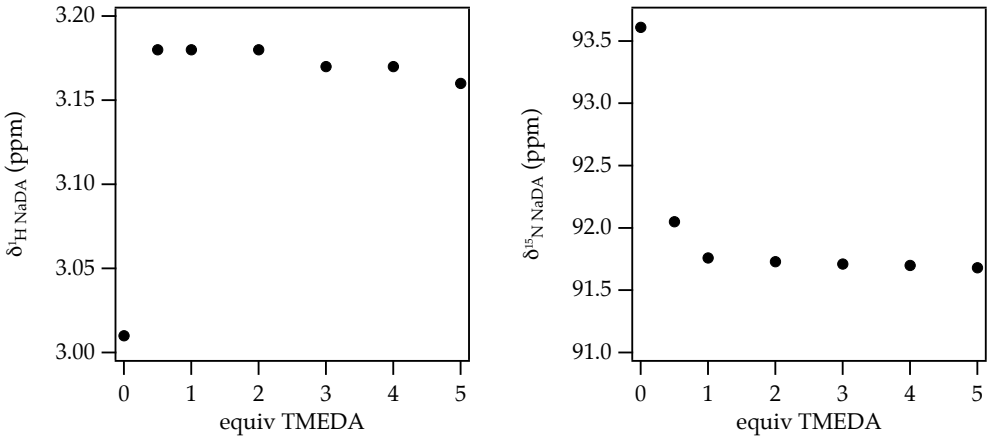


Figure S-46. Plots of chemical shift affiliated with NaDA for 0.30 M solutions of NaDA in DMBA with 10% v/v benzene-d_6 varying THF at –80 °C.

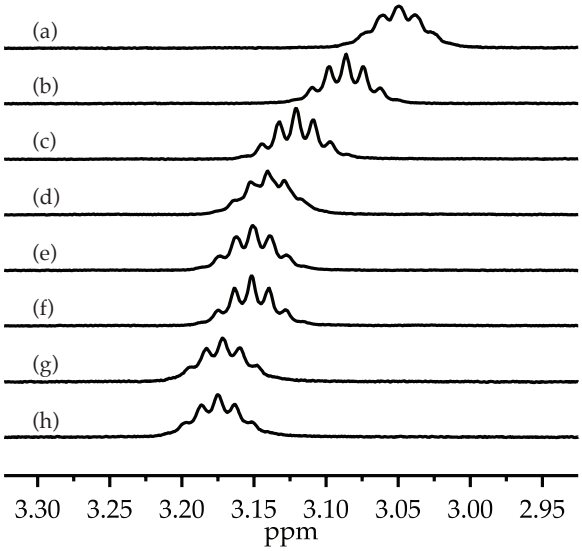


Figure S-47. ^{1}H NMR spectra for 0.30 M solutions of NaDA in DMBA with 10% v/v benzene-d_6 varying TMCDA at –30 °C. The equivalents of TMCDA in (a)–(h) are 0.00, 0.55, 1.08, 1.58, 2.15, 2.09, 5.99, and 7.72, respectively.

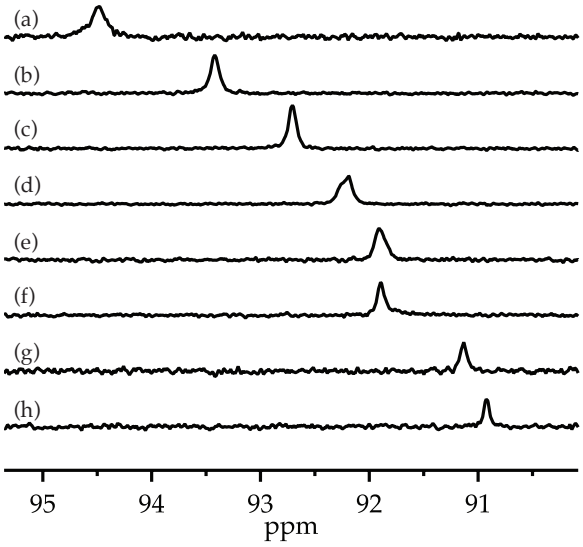


Figure S-48. ^{15}N NMR spectra for 0.30 M solutions of NaDA in DMBA with 10% v/v benzene-d_6 varying TMCDA at –30 °C. The equivalents of TMCDA in (a)–(h) are 0.00, 0.55, 1.08, 1.58, 2.15, 2.09, 5.99, and 7.72, respectively.

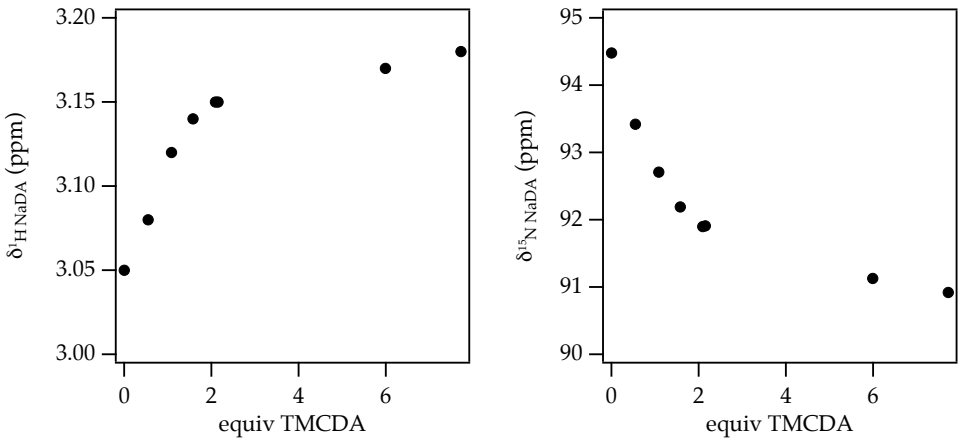


Figure S-49. Plots of chemical shift affiliated with NaDA for 0.30 M solutions of NaDA in DMBA with 10% v/v benzene-d_6 varying TMCDA at –30 °C. Non-quantitative substitution is evidenced by chemical shift saturation at >3.0 equiv TMCDA/Na.

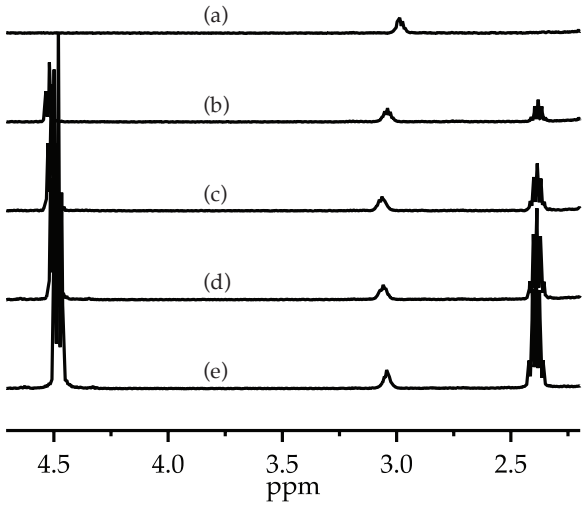


Figure S-50. ^{1}H NMR spectra for 0.30 M solutions of NaDA in DMEA with 10% v/v benzene-d_6 varying oxetane at –80 °C. The equivalents of oxetane in (a)–(e) are 0.00, 0.79, 2.09, 3.09, and 5.10, respectively.

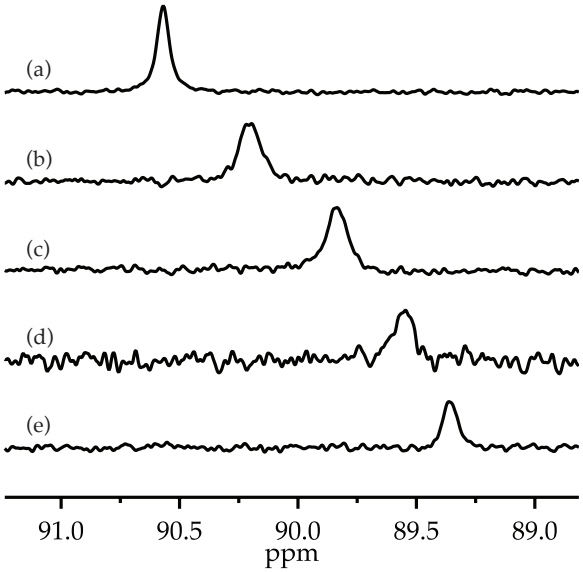


Figure S-51. ^{15}N NMR spectra for 0.30 M solutions of NaDA in DMEA with 10% v/v benzene-d_6 varying oxetane at –80 °C. The equivalents of oxetane in (a)–(e) are 0.00, 0.79, 2.09, 3.09, and 5.10, respectively.

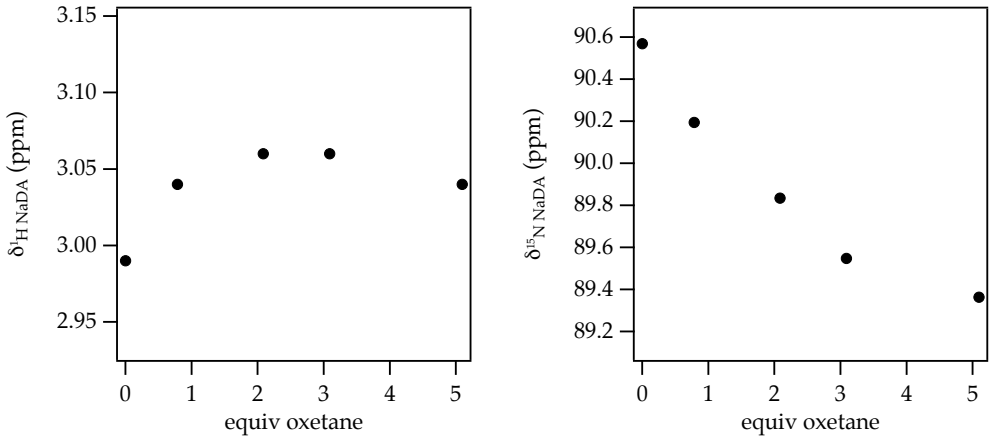


Figure S-52. Plots of chemical shift affiliated with NaDA for 0.30 M solutions of NaDA in DMEA with 10% v/v benzene-d_6 varying oxetane at –80 °C. Non-quantitative substitution is evidenced by chemical shift saturation at >3.0 equiv oxetane/Na.

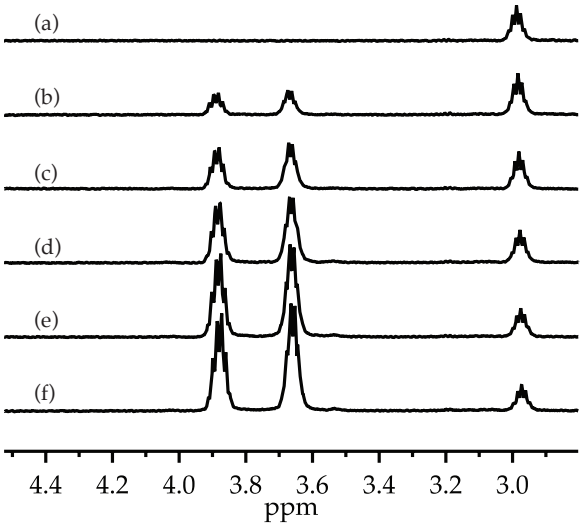


Figure S-53. ^{1}H NMR spectra for 0.30 M solutions of NaDA in DMEA with 10% v/v benzene-d_6 varying 2,5-dimethyltetrahydrofuran at –80 °C. The equivalents of 2,5-dimethyltetrahydrofuran in (a)–(f) are 0.00, 1.20, 2.74, 4.36, 7.30, and 9.03, respectively.

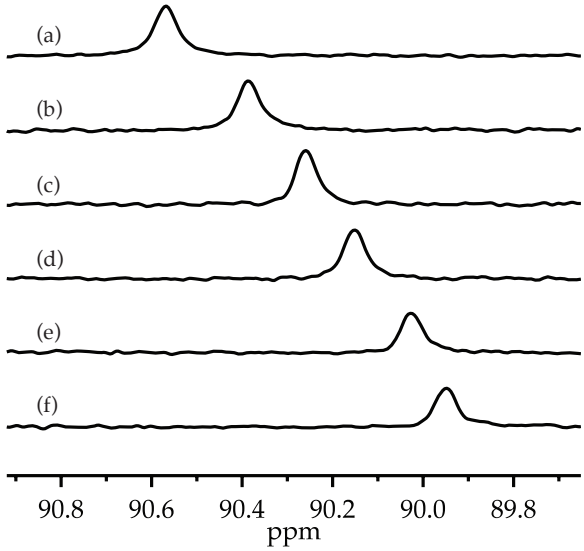


Figure S-54. ^{15}N NMR spectra for 0.30 M solutions of NaDA in DMEA with 10% v/v benzene-d_6 varying 2,5-dimethyltetrahydrofuran at –80 °C. The equivalents of 2,5-dimethyltetrahydrofuran in (a)–(f) are 0.00, 1.20, 2.74, 4.36, 7.30, and 9.03, respectively.

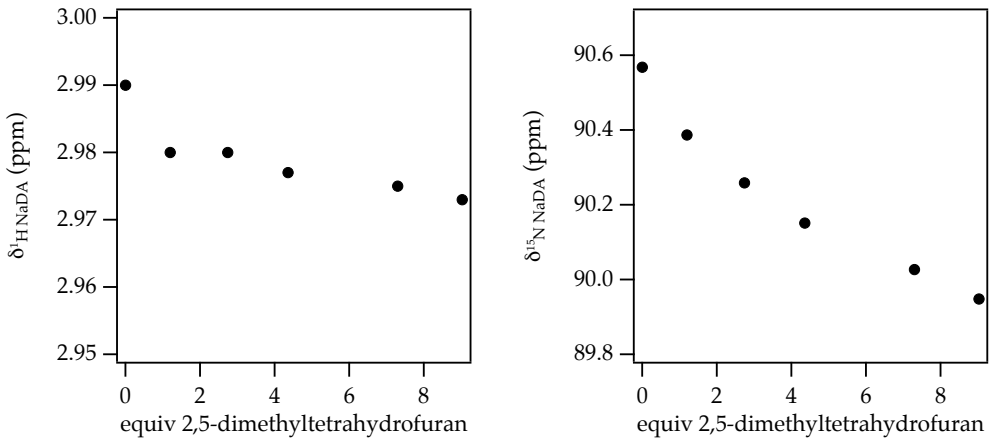


Figure S-55. Plots of chemical shift affiliated with NaDA for 0.30 M solutions of NaDA in DMEA with 10% v/v benzene-d_6 varying 2,5-dimethyltetrahydrofuran at –80 °C.

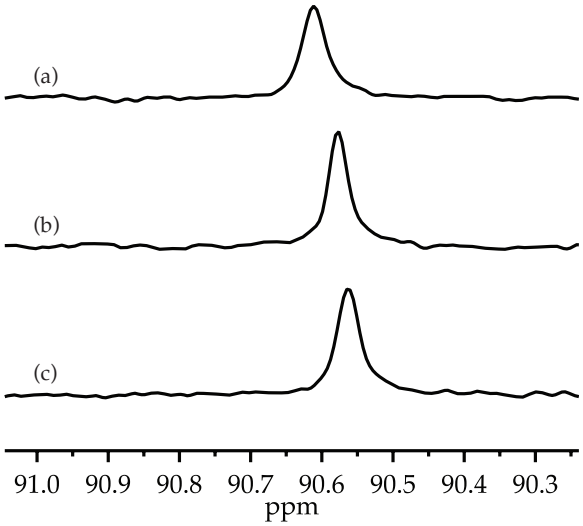


Figure S-56. ^{15}N NMR spectra for 0.30 M solutions of NaDA in DMEA with 10% v/v cyclohexane-d_{12} varying anisole at –80 °C. The equivalents of anisole in (a)–(c) are 0.00, 1.35, and 2.55, respectively.

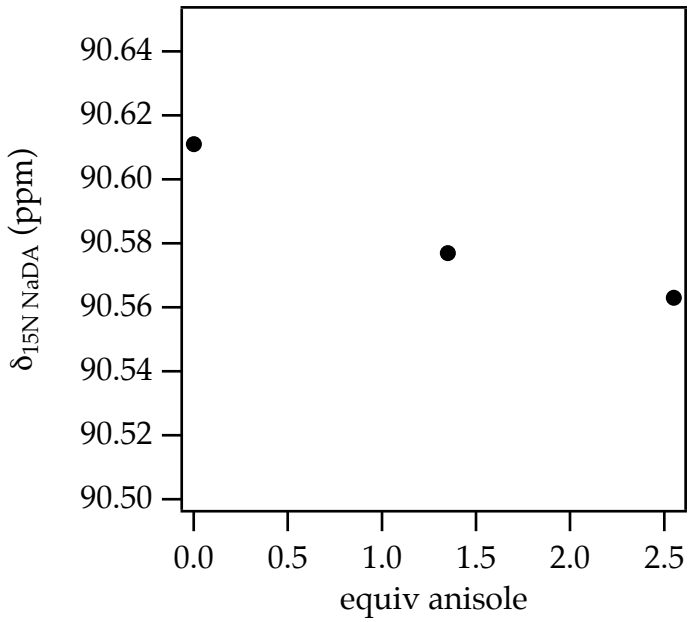


Figure S-57. Plots of chemical shift affiliated with NaDA for 0.30 M solutions of NaDA in DMEA with 10% v/v cyclohexane-d_{12} varying anisole at –80 °C.

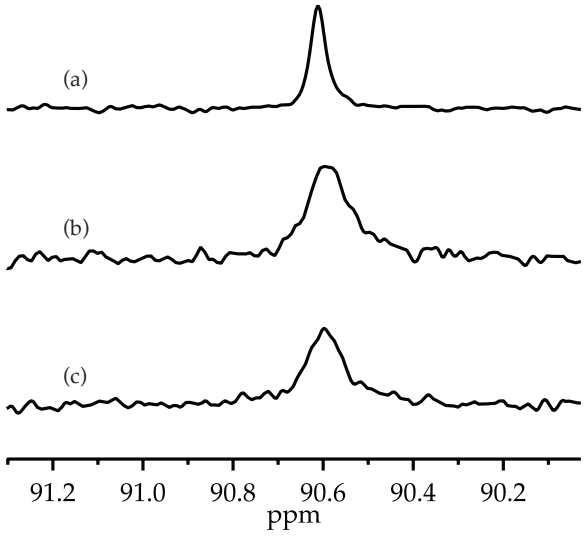


Figure S-58. ^{15}N NMR spectra for 0.30 M solutions of NaDA in DMEA with 10% v/v cyclohexane-d_{12} varying anisole at –80 °C. The equivalents of benzotrifluoride in (a)–(c) are 0.00, 1.30, and 2.92, respectively.

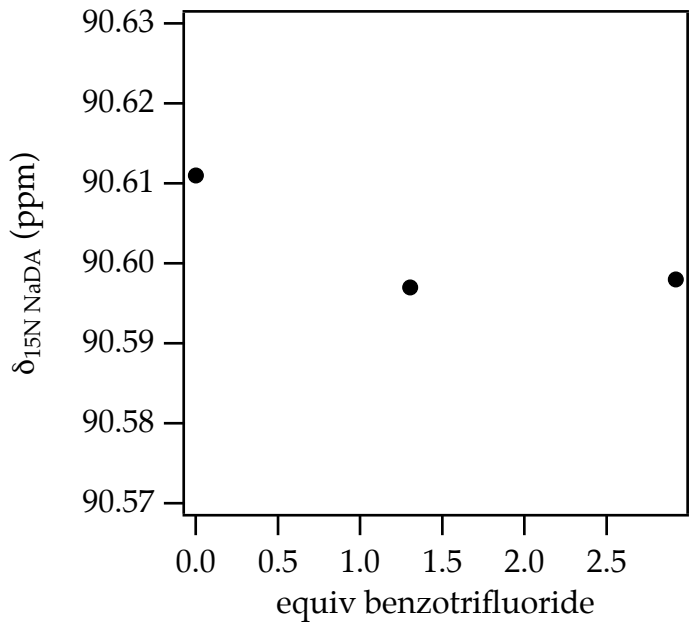


Figure S-59. Plots of chemical shift affiliated with NaDA for 0.30 M solutions of NaDA in DMEA with 10% v/v cyclohexane-d_{12} varying benzotrifluoride at –80 °C.

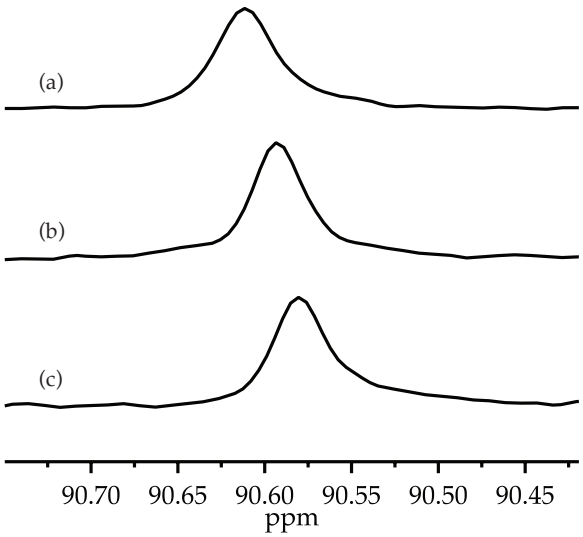


Figure S-60. ^{15}N NMR spectra for 0.30 M solutions of NaDA in DMEA with 10% v/v cyclohexane-d_{12} varying anisole at –80 °C. The equivalents of chlorobutane in (a)–(c) are 0.00, 1.30, and 2.92, respectively.

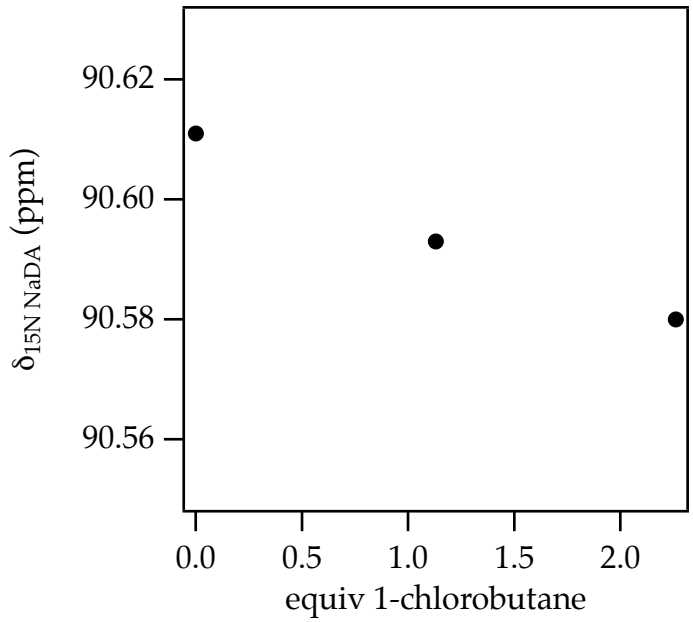


Figure S-61. Plots of chemical shift affiliated with NaDA for 0.30 M solutions of NaDA in DMEA with 10% v/v cyclohexane-d_{12} varying chlorobutane at –80 °C.

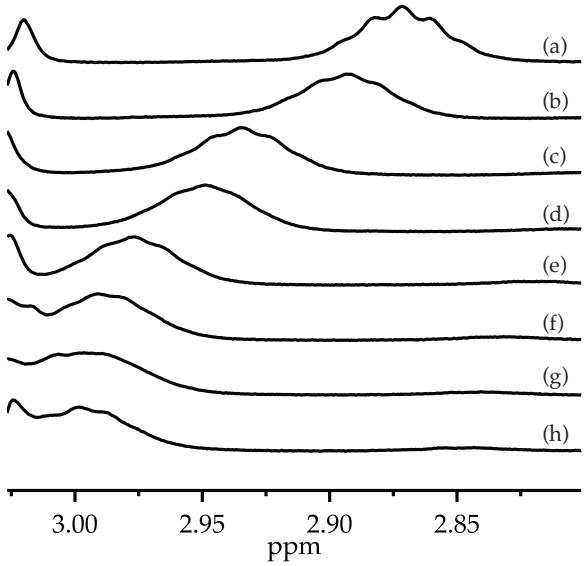


Figure S-62. ^{1}H NMR spectra for 0.10 M solutions of NaDA in *N,N*-diethylmethylamine with 10% v/v cyclohexane-d_{12} varying THF at –80 °C. The equivalents of THF in (a)–(h) are 0.00, 0.63, 0.78, 1.35, 1.83, 2.11, 2.78, and 3.56, respectively.

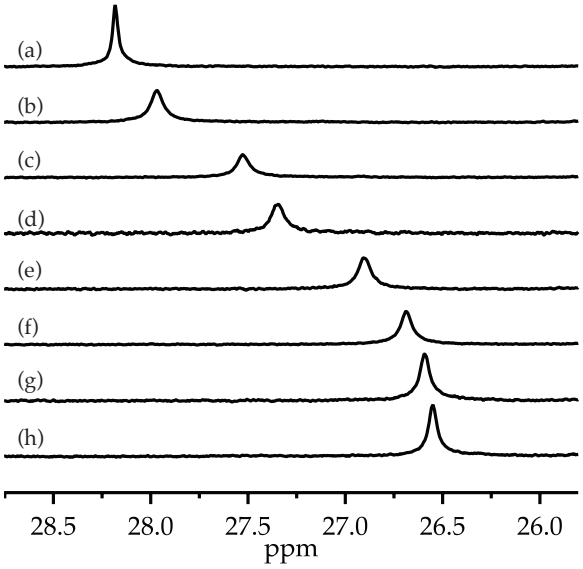


Figure S-63. ^{13}C NMR spectra for 0.10 M solutions of NaDA in *N,N*-diethylmethylamine with 10% v/v cyclohexane-d_{12} varying THF at –80 °C. The equivalents of THF in (a)–(h) are 0.00, 0.63, 0.78, 1.35, 1.83, 2.11, 2.78, and 3.56, respectively.

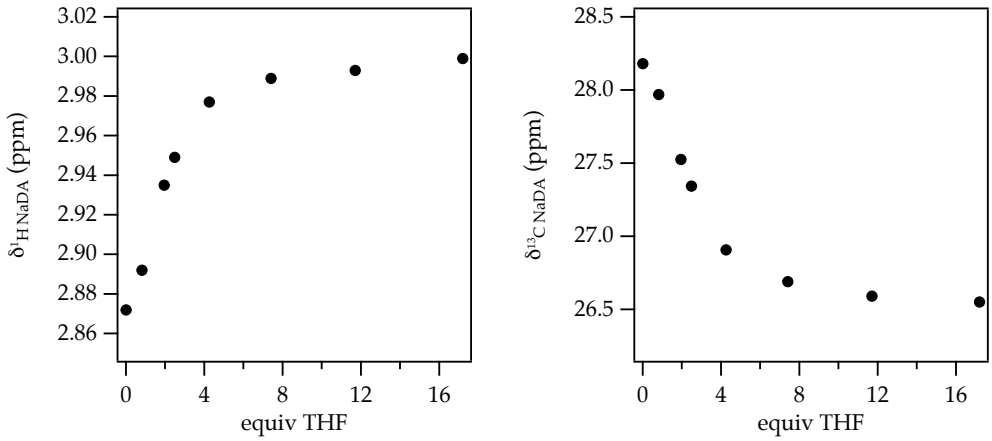


Figure S-64. Plots of chemical shift affiliated with NaDA for 0.10 M solutions of NaDA in *N,N*-diethylmethylamine with 10% v/v cyclohexane-d_{12} varying THF at –80 °C. Non-quantitative substitution is evidenced by chemical shift saturation at >3.0 equiv THF/Na despite the weaker binding affinity of *N,N*-diethylmethylamine relative to *N,N*-dimethylethylamine.

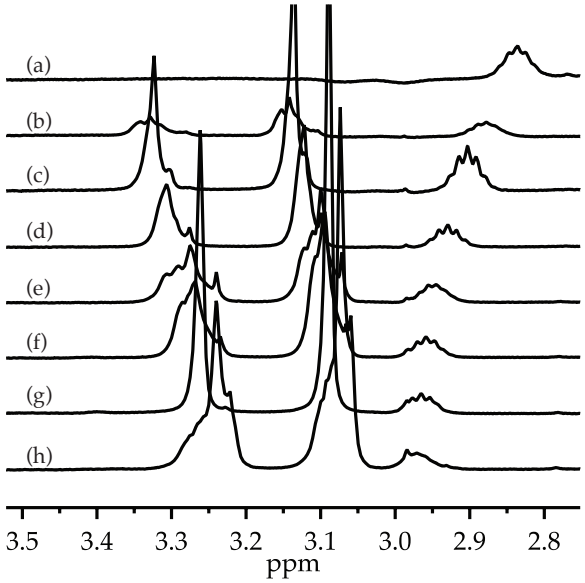


Figure S-65. ^{1}H NMR spectra for 0.10 M solutions of NaDA in DMEA with 10% v/v cyclohexane-d_{12} varying 1,2-dimethoxyethane at –80 °C. The equivalents of DME in (a)–(h) are 0.00, 0.63, 0.78, 1.35, 1.83, 2.11, 2.78, and 3.56, respectively.

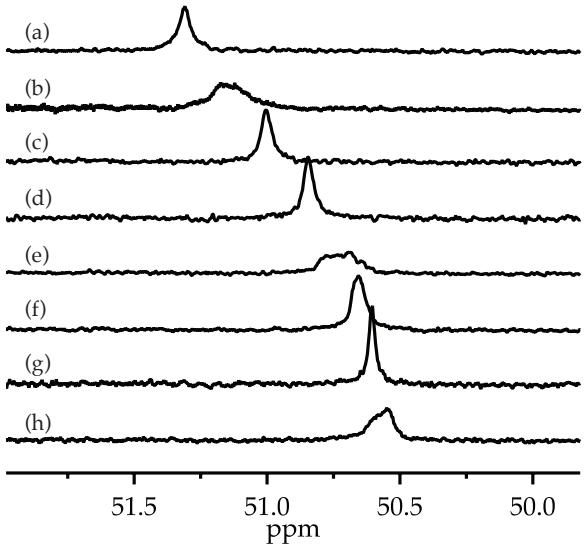


Figure S-66. ^{13}C NMR spectra for 0.10 M solutions of NaDA in DMEA with 10% v/v cyclohexane-d_{12} varying 1,2-dimethoxyethane at –80 °C. The equivalents of DME in (a)–(h) are 0.00, 0.63, 0.78, 1.35, 1.83, 2.11, 2.78, and 3.56, respectively.

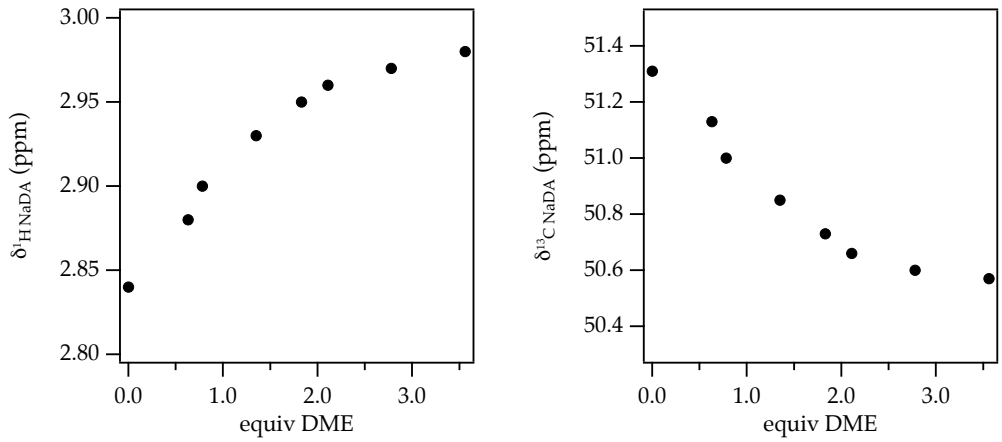


Figure S-67. Plots of chemical shift affiliated with NaDA for 0.10 M solutions of NaDA in DMEA with 10% v/v cyclohexane-d_{12} varying DME at –80 °C. Non-quantitative substitution is evidenced by chemical shift saturation at >3.0 equiv DME/Na.

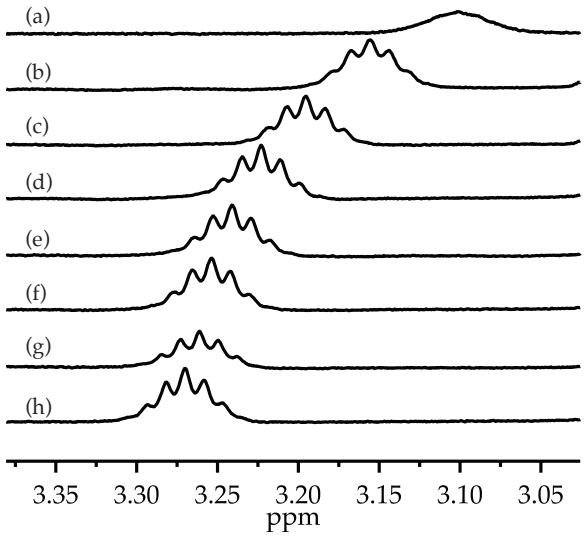


Figure S-68. ^{1}H NMR spectra for 0.10 M solutions of NaDA in DMEA with 10% v/v cyclohexane-d_{12} varying TMEDA at –40 °C. The equivalents of TMEDA in (a)–(h) are 0.00, 0.37, 0.83, 1.43, 1.87, 3.04, 4.61, and 4.99, respectively.

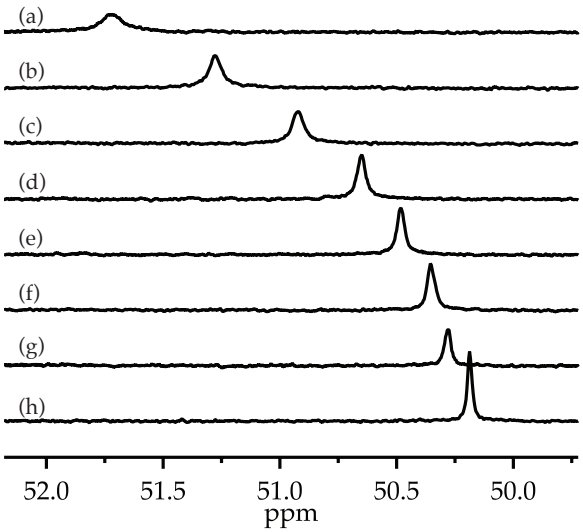


Figure S-69. ^{13}C NMR spectra for 0.10 M solutions of NaDA in DMEA with 10% v/v cyclohexane-d_{12} varying TMEDA at –40 °C. The equivalents of TMEDA in (a)–(h) are 0.00, 0.37, 0.83, 1.43, 1.87, 3.04, 4.61, and 4.99, respectively.

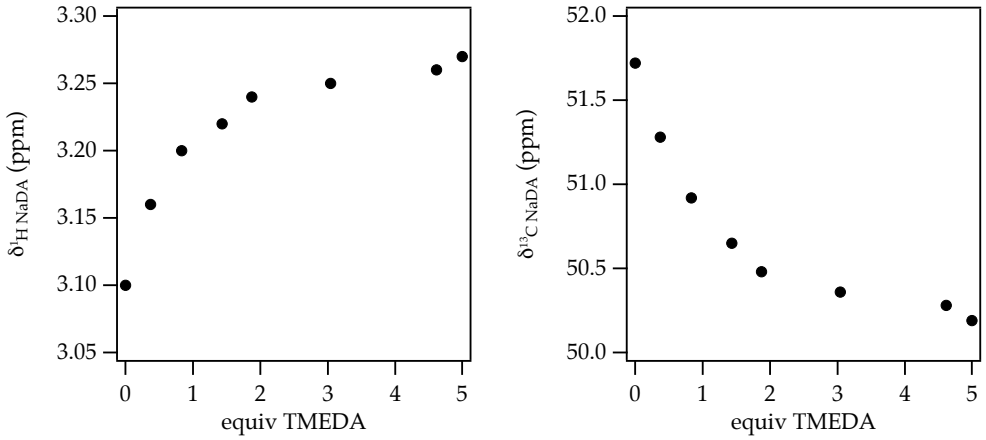


Figure S-70. Plots of chemical shift affiliated with NaDA for 0.10 M solutions of NaDA in DMEA with 10% v/v cyclohexane-d_{12} varying TMEDA at –40 °C.

Figures 71 and 72 describe a solvent swap between TMEDA and DME and are fit to the following equilibrium (with the somewhat restrictive but simplifying assumption to exclude a mixed solvate):

$$A_2(TMEDA)_2 + 2\,DME \underset{}{\overset{K_{eq}}{\rightleftharpoons}} A_2(DME)_2 + 2\,TMEDA$$

Assuming that the resonances affiliated with $A_2(TMEDA)_2$ and $A_2(DME)_2$ are time-averaged:

$$\begin{aligned}\delta_{obs} &= \delta_{A_2(TMEDA)_2}\chi_{A_2(TMEDA)_2} + \delta_{A_2(DME)_2}\chi_{A_2(DME)_2} \\ &= \delta_{A_2(TMEDA)_2}\left(1-\chi_{A_2(DME)_2}\right) + \delta_{A_2(DME)_2}\chi_{A_2(DME)_2} \\ &= \delta_{A_2(TMEDA)_2} + \left(\delta_{A_2(DME)_2} - \delta_{A_2(TMEDA)_2}\right)\chi_{A_2(DME)_2} \\ &= \delta_{A_2(TMEDA)_2} + \Delta\delta\chi_{A_2(DME)_2}\end{aligned}$$

What remains is to calculate $\chi_{A_2(DME)_2}$ as a function of χ_{DME}:

$$\begin{aligned}K_{eq} &= \frac{\left[A_2(DME)_2\right]\left[TMEDA\right]^2}{\left[A_2(TMEDA)_2\right]\left[DME\right]^2} \\ &= \frac{\chi_{A_2(DME)_2}\left(2(1-\chi_{DME}) - (1-\chi_{A_2(DME)_2})\right)^2}{\left(1-\chi_{A_2(DME)_2}\right)\left(2\chi_{DME} - \chi_{A_2(DME)_2}\right)^2}\end{aligned}$$

The factor of 2 appearing in the numerator and denominator represents the relative stoichiometry of solvent to NaDA. The fitting expression as input into Igor Pro is:

```
f(xd) = a+b*((1/(6*(1+keq)))*(2*(-2+keq+4*xd+4*keq*xd)+(2*2^(1/3)*((1-
2*xd)^2+keq^2*(1-2*xd)^2+keq*(-7-8*xd+8*xd^2)))/(2-12*xd+24*xd^2-
16*xd^3-2*keq^3*(-1+2*xd)^3+keq*(33-36*xd+72*xd^2-48*xd^3)-
3*keq^2*(7+12*xd-24*xd^2+16*xd^3)+3*Sqrt(3)*Sqrt(keq*(1+keq)^2*(8*(-
1+xd)*(-1+2*xd)^3+8*keq^2*xd*(-1+2*xd)^3+keq*(-1+80*xd+48*xd^2-
256*xd^3+128*xd^4))))^(1/3)+2^(2/3)*(2-12*xd+24*xd^2-16*xd^3-2*keq^3*(-
1+2*xd)^3+keq*(33-36*xd+72*xd^2-48*xd^3)-3*keq^2*(7+12*xd-
24*xd^2+16*xd^3)+3*Sqrt(3)*Sqrt(keq*(1+keq)^2*(8*(-1+xd)*(-
1+2*xd)^3+8*keq^2*xd*(-1+2*xd)^3+keq*(-1+80*xd+48*xd^2-
256*xd^3+128*xd^4))))^(1/3)))
```

(a)

where xd represents χ_{DME}, keq represents K_{eq}, a represents $\delta_{A_2(TMEDA)_2}$, and b represents $\Delta\delta$.

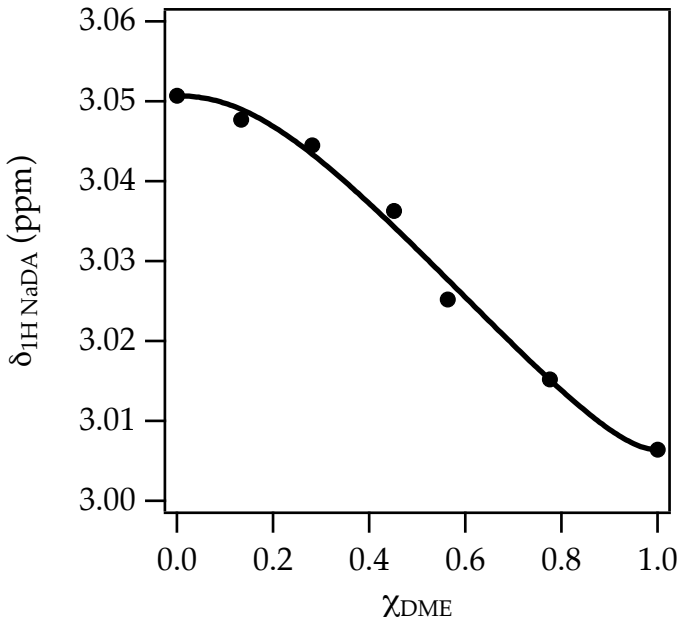


Figure S-71. Plot of ^{1}H NMR chemical shift affiliated with NaDA for 0.10 M solutions of NaDA in DMEA with 2 equiv added ligand varying the mole fraction of DME with TMEDA at –80 °C. A best-fit to equation (a) gives K_{eq} = 0.5 ± 0.1; a = 3.0507; b = –0.0443.

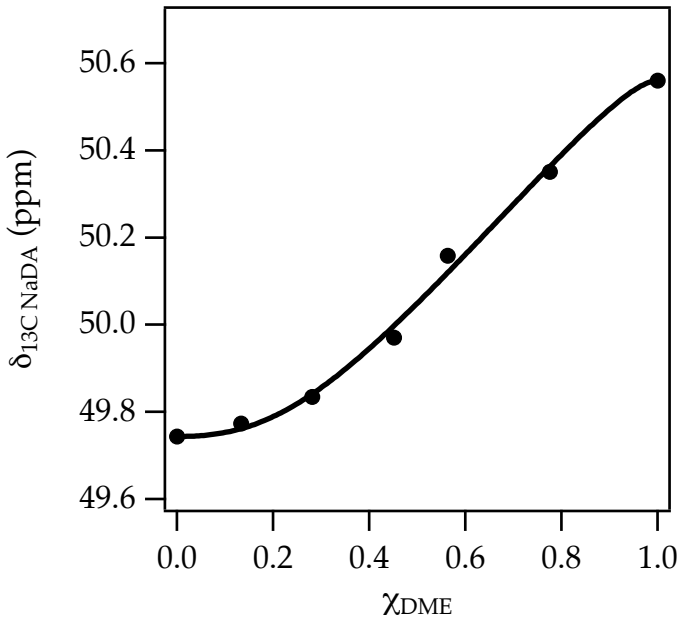


Figure S-72. Plot of ^{13}C NMR chemical shift affiliated with NaDA for 0.10 M solutions of NaDA in DMEA with 2 equiv added ligand varying the mole fraction of DME with TMEDA at –80 °C. A best-fit to equation (a) gives K_{eq} = 0.21 ± 0.04; a = 49.744; b = 0.8166.

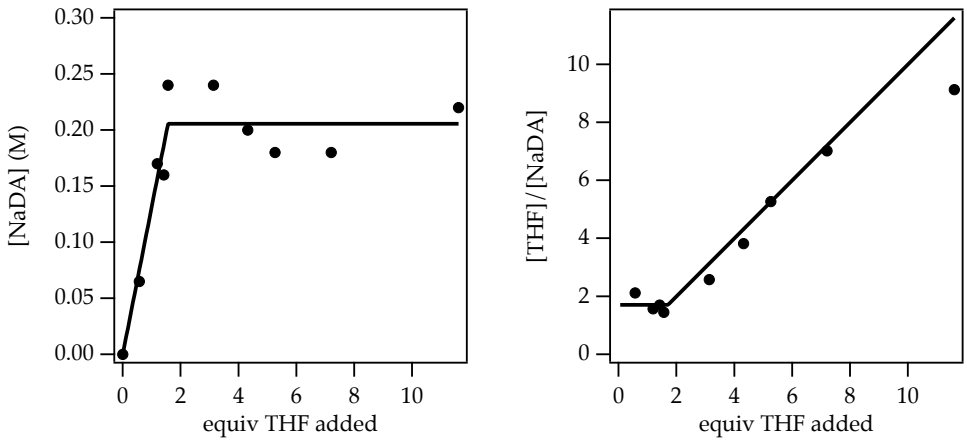


Figure S-73. Plots of (a) NaDA solubility vs THF concentration and (b) [THF]/[NaDA] vs THF concentration with solid NaDA suspended in cyclohexane-d_{12} internally standardized with benzene.

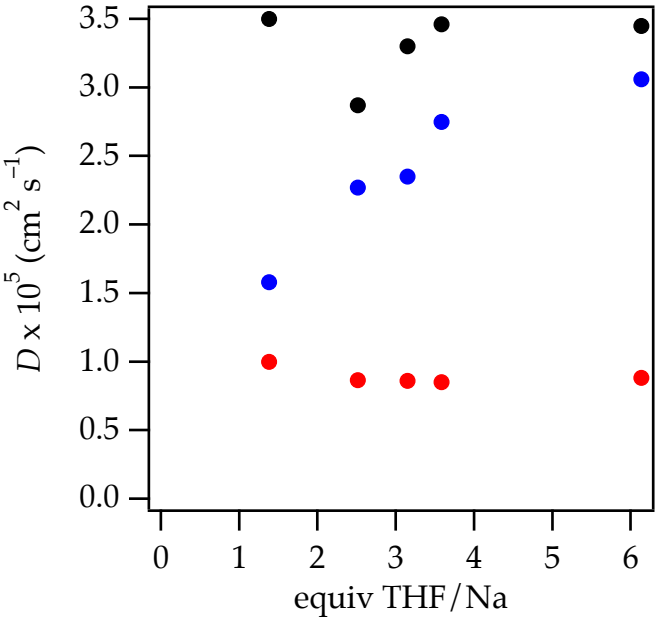


Figure S-74. Plot of diffusion constant (NaDA = red points, THF = blue, and benzene = black points) vs equivalents of THF per unit normality of NaDA at 25 °C. THF was titrated into a suspension of NaDA/cyclohexane-d_{12} containing benzene as an internal standard. These data show that below 2 equiv THF/Na the diffusion coefficient of THF approximates that of NaDA implying that all THF is bound. Above 2 equiv THF/Na, the diffusion coefficient of THF rises to that of free, consistent with time-averaging. Furthermore, the diffusion coefficient of NaDA remains invariant.

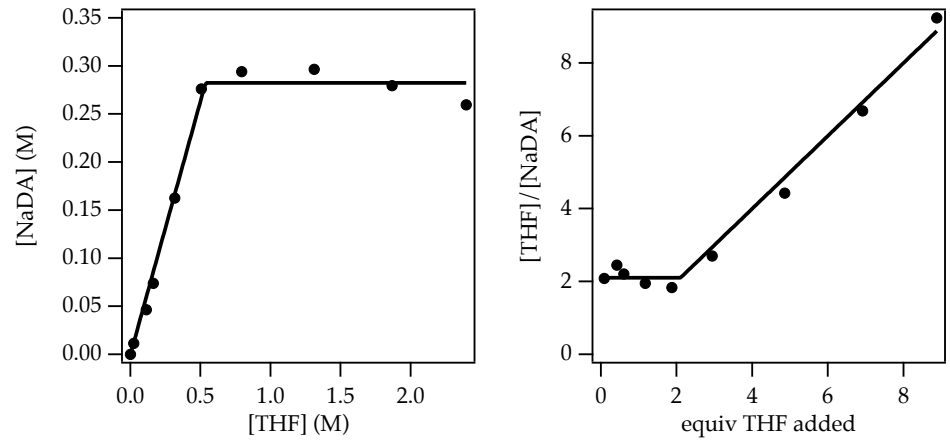


Figure S-75. Plots of (a) NaDA solubility vs THF concentration and (b) [THF]/[NaDA] vs THF concentration with solid NaDA suspended in toluene-d_8 internally standardized with benzene. Both plots support a 2:1 THF:NaDA stoichiometry.

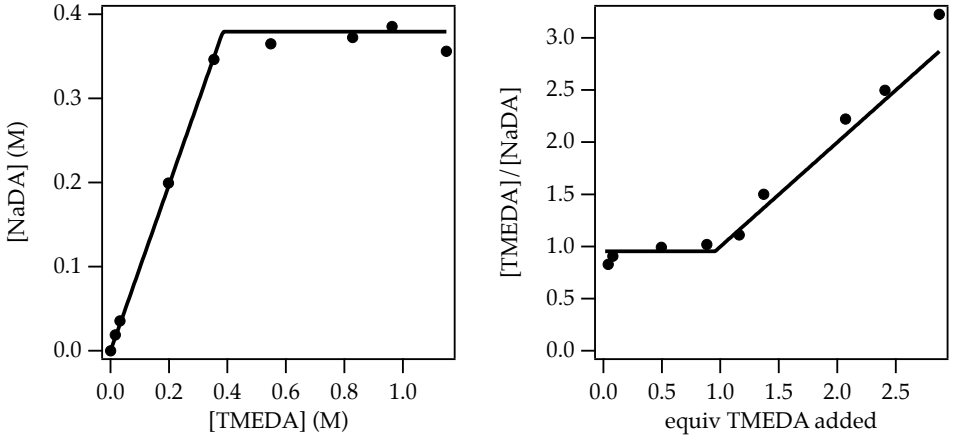


Figure S-76. Plots of (a) NaDA solubility vs TMEDA concentration and (b) [TMEDA]/[NaDA] vs THF concentration with solid NaDA suspended in toluene-d_8 internally standardized with benzene. Both plots support a 1:1 TMEDA:NaDA stoichiometry.

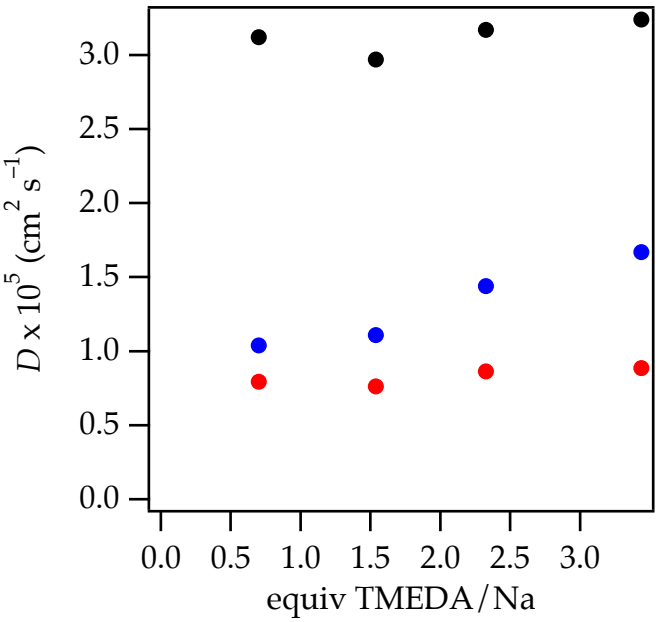


Figure S-77. Plot of diffusion constant (NaDA = red points, TMEDA = blue, and benzene = black points) vs equivalents of TMEDA per unit normality of NaDA at 25 °C. TMEDA was titrated into a suspension of NaDA/cyclohexane-d_{12} containing benzene as an internal standard. These data show that below 1 equiv TMEDA/Na the diffusion coefficient of TMEDA approximates that of NaDA implying that all TMEDA is bound. Above 1 equiv TMEDA/Na, the diffusion coefficient of TMEDA rises to that of free, consistent with time-averaging. Furthermore, the diffusion coefficient of NaDA remains invariant.

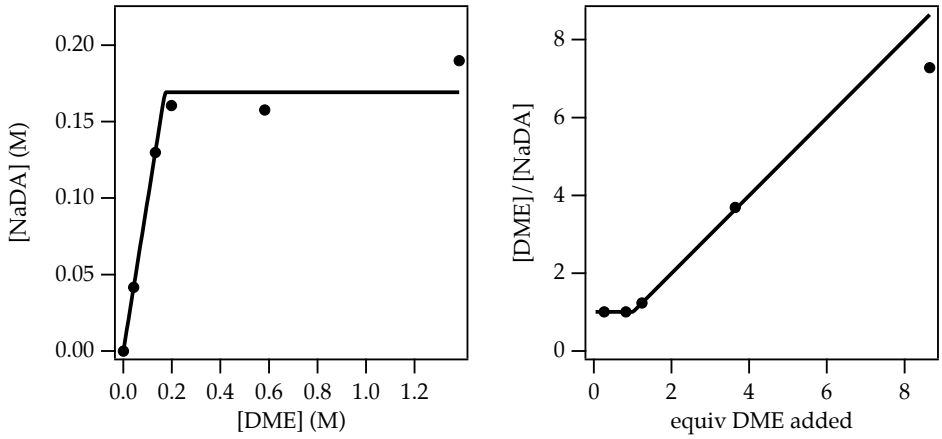


Figure S-78. Plots of (a) NaDA solubility vs DME concentration and (b) [DME]/[NaDA] vs DME concentration with solid NaDA suspended in toluene-d_8 internally standardized with benzene. Both plots support a 1:1 DME:NaDA stoichiometry.

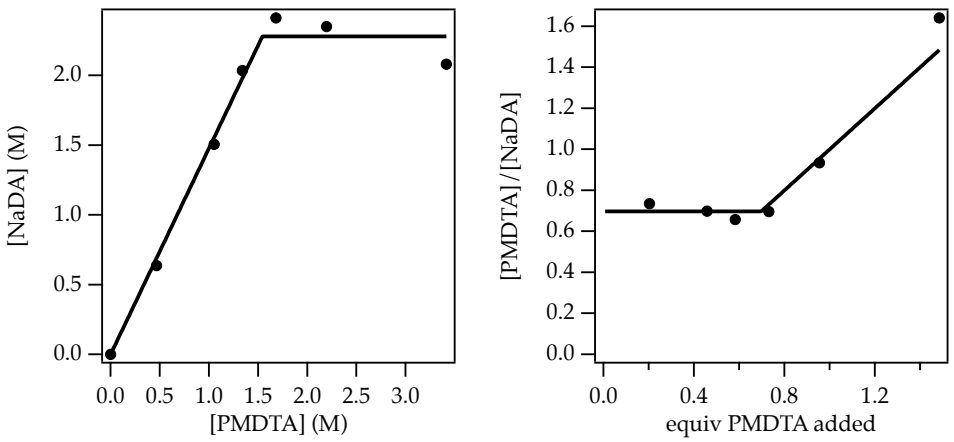


Figure S-79. Plots of (a) NaDA solubility vs PMDTA concentration and (b) [PMDTA]/[NaDA] vs PMDTA concentration with solid NaDA suspended in toluene-d_8 internally standardized with benzene. Both plots support substoichiometric binding of PMDTA to NaDA consistent with measurable solubility of both $A_2(PMDTA)_1$ and $A_2(PMDTA)_2$.

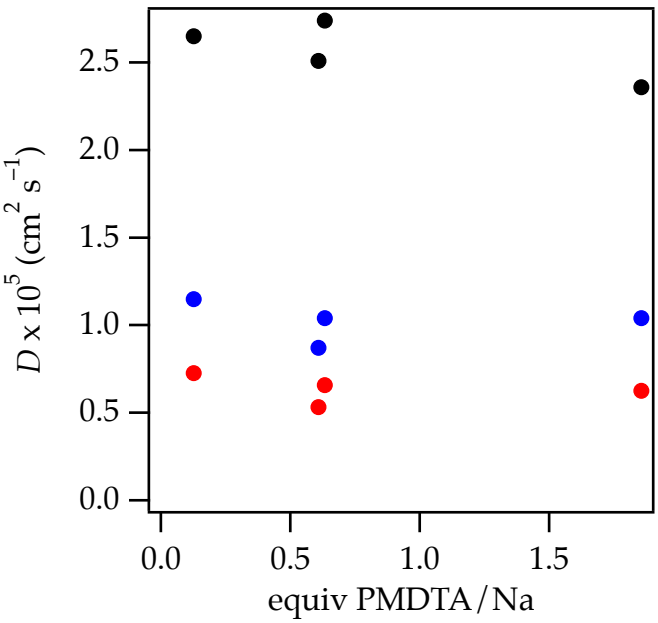


Figure S-80. Plot of diffusion constant (NaDA = red points, PMDTA = blue, and benzene = black points) vs equivalents of PMDTA at 25 °C. PMDTA was titrated into a suspension of NaDA/cyclohexane-d_{12} containing benzene as an internal standard.

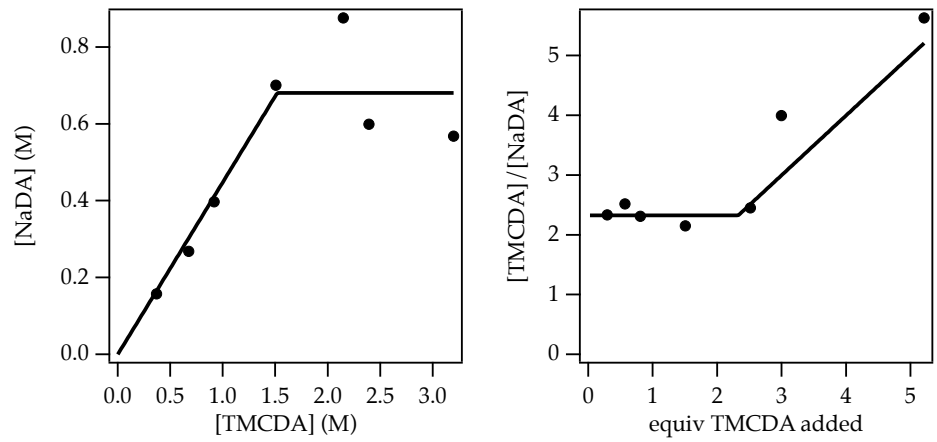


Figure S-81. Plots of (a) NaDA solubility vs TMCDA concentration and (b) [TMCDA]/[NaDA] vs TMCDA concentration with solid NaDA suspended in toluene-d_8 internally standardized with benzene. Both plots support a 2:1 TMCDA:NaDA stoichiometry.

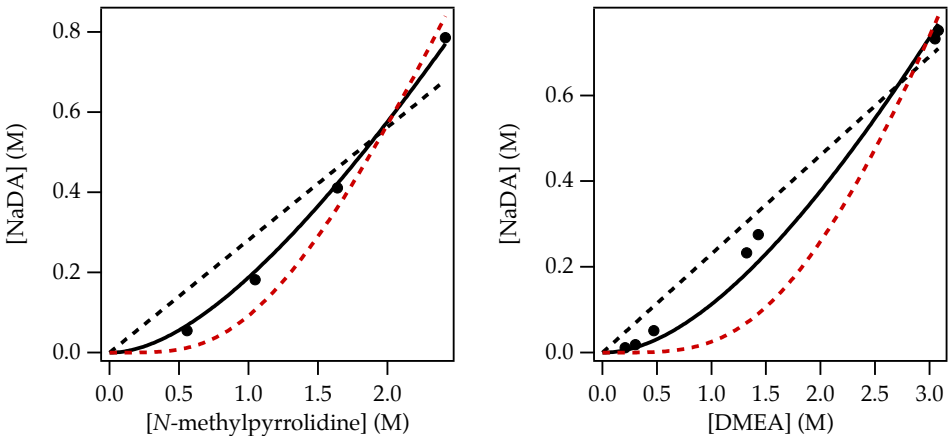


Figure S-82. Plots of NaDA solubility vs trialkylamine concentration with solid NaDA suspended in toluene-d_8 internally standardized with benzene. See equation 7 in manuscript. (Solid black line: best fit to disolvated dimer, Black dashed line: best fit to monosolvated dimer, red dashed line: best fit to tetrasolvated dimer). Both plots suggest a stoichiometry of 2 trialkylamine/NaDA dimer.

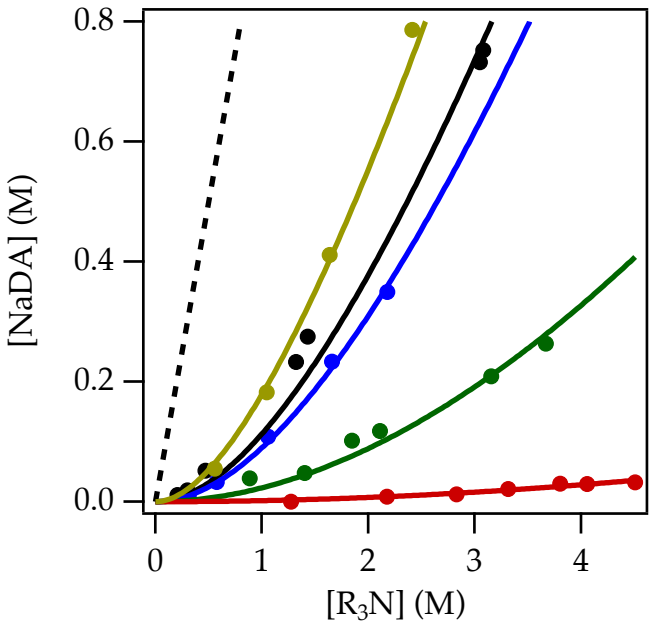


Figure S-83. Plot of NaDA solubility vs trialkylamine concentration with solid NaDA suspended in toluene-d_8 internally standardized with benzene. The dashed line represents quantitative solubilization to disolvated dimer. All traces represent unweighted least-squares fits to [NaDA]=(1/K_{solv}+4[R_3N]–Sqrt(1+8K_{solv}[R_3N])/K_{solv})/4 according to to disolvated dimer in equilibrium with solid NaDA. The trialkylamines and corresponding equilibrium constants are: *N*-methylpyrrolidine (yellow trace, K_{solv} = 0.132 ± 0.005); DMEA (black trace, K_{solv} = 0.102 ± 0.003); DMBA (blue trace, K_{solv} = 0.054 ± 0.001); *N,N*-diethylmethylamine (green trace, K_{solv} = 0.0121 ± 0.0007); and triethylamine (red trace, K_{solv} = 0.00089 ± 0.00004).

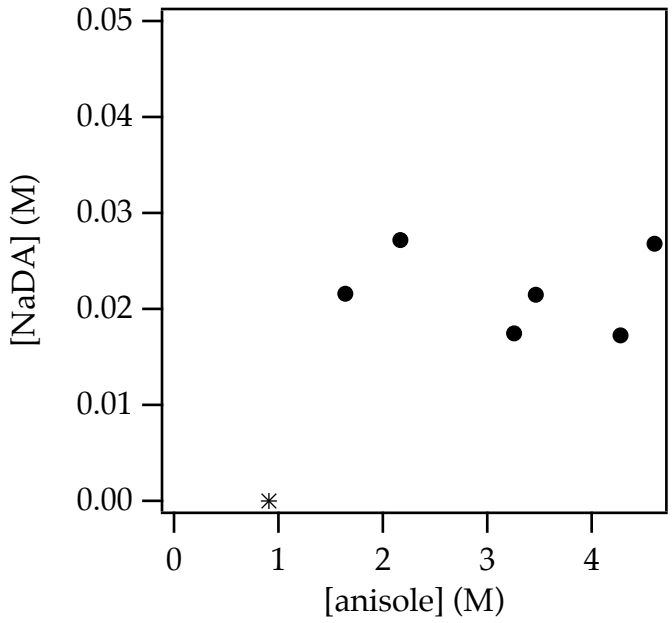


Figure S-84. Plot of NaDA solubility vs anisole concentration with solid NaDA suspended in toluene-d_8 internally standardized with benzene. Anisole does not appreciably solubilize NaDA.

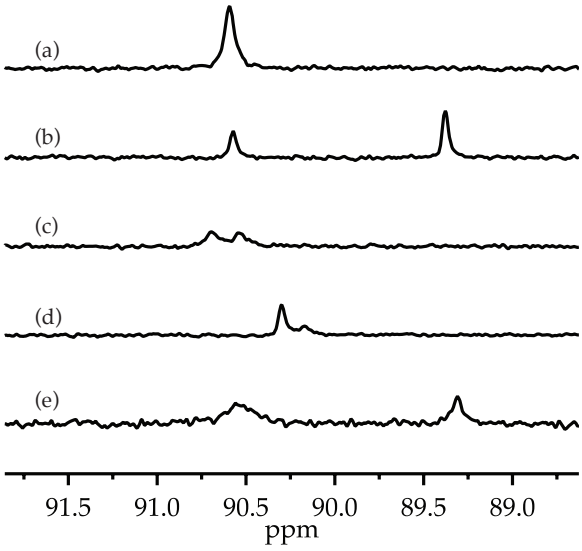


Figure S-85. ^{15}N NMR spectra for total titer of 0.30 M solutions of NaDA in DMEA with 10% v/v benzene-d_6 or cyclohexane-d_{12} recorded at –80 °C for (a) NaDA, and with (b) equimolar (b) NaTMP, (c) sodium *cis*-2,6-dimethylpiperidide, (d) sodium diisobutylamide, and (e) sodium hexamethyldisilazide. Heteroaggregation within the class of sodium amides is notable.

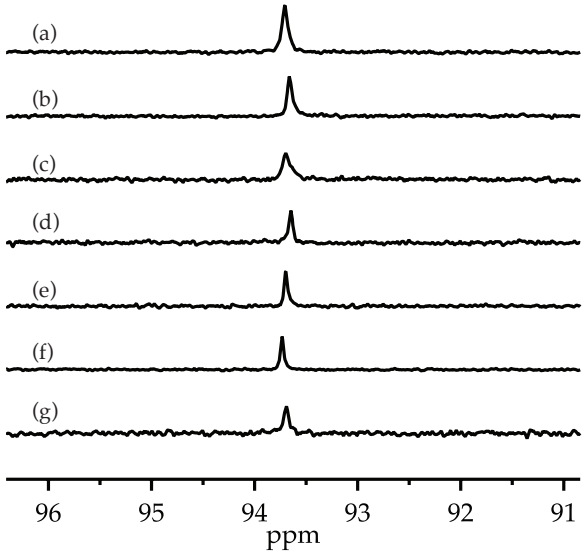


Figure S-86. ^{15}N NMR spectra for 0.30 M solutions of NaDA in DMEA with 10% v/v benzene-d_6 or cyclohexane-d_{12} recorded at –80 °C with equimolar (b) *n*-BuNa, (c) 2,6-dimethoxyphenylsodium, (d) sodium cycloheptenolate, (e) sodium *iso*-butoxide, (f) sodium *tert*-butoxide, and (g) sodium phenolate. Absence of resolved heteroaggregation is notable.

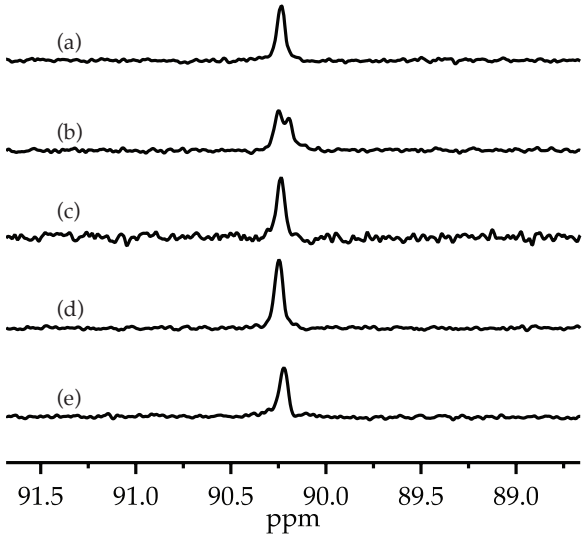


Figure S-87. ^{15}N NMR spectra for 0.40 M total base titer of NaDA in THF with 10% v/v cyclohexane-d_{12} with varying equimolar sodium salts at –80 °C. The salts in are (b) sodium isopropylcyclohexylamide, (c) sodium hexamethyldisilazide, (d) sodium *tert*-butoxide, and (e) sodium *iso*-butoxide. The absence of apparent mixed aggregation for NaHMDS is notable.

II. Rate Studies

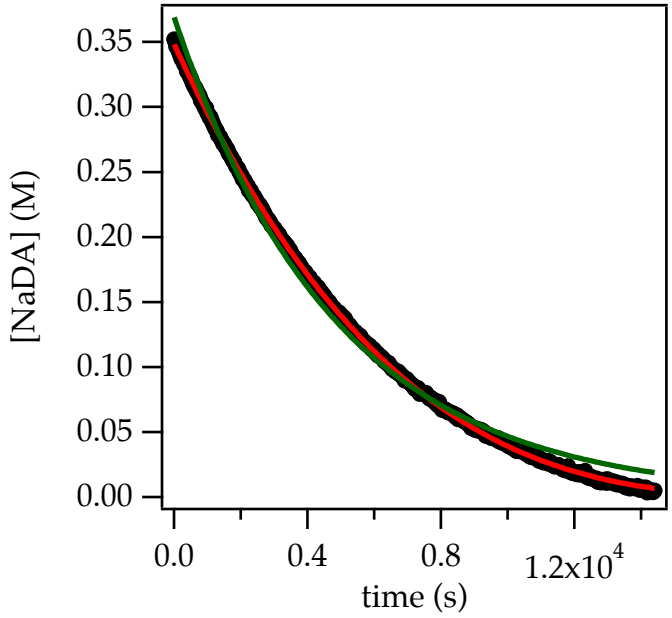


Figure S-88. Plot of NaDA concentration vs time in neat THF at 25 ºC followed with ^{1}H NMR. The green curve depicts an unweighted least-squares fit to the function $f(t) = ae^{-kt}$: $a = 0.369 \pm 0.004$; $k = (2.07 \pm 0.01) \times 10^{-4}$. The red curve depicts an unweighted least-squares fit to the function $f(t) = ([A]_0^{(1-n)} - kt(1-n))^{1/(1-n)}$: $[A]_0 = 0.3484 \pm 0.0002$; $n = 0.698 \pm 0.002$, $k = (1.061 \pm 0.009) \times 10^{-5}$.

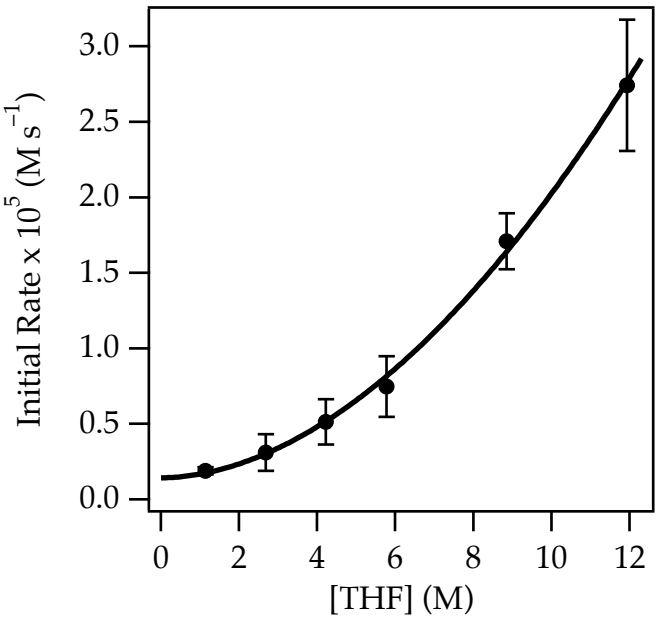


Figure S-89. Plot of initial rates vs THF concentration for the decomposition of THF with 0.20 M NaDA at 25 ºC. The curve depicts an unweighted least-squares fit to the function $f(x) = ax^b + c$: $a = (2.5 \pm 0.8) \times 10^{-2}$; $b = 1.9 \pm 0.1$; $c = (1.4 \pm 0.5) \times 10^{-1}$.

[THF] (M)	Initial rate × 10^5 (M s^{-1})	Standard deviation × 10^5 (M s^{-1})
1.1	0.19	0.02
2.7	0.3	0.1
4.2	0.5	0.1
5.8	0.7	0.2
8.9	1.7	0.2
11.9	2.7	0.4

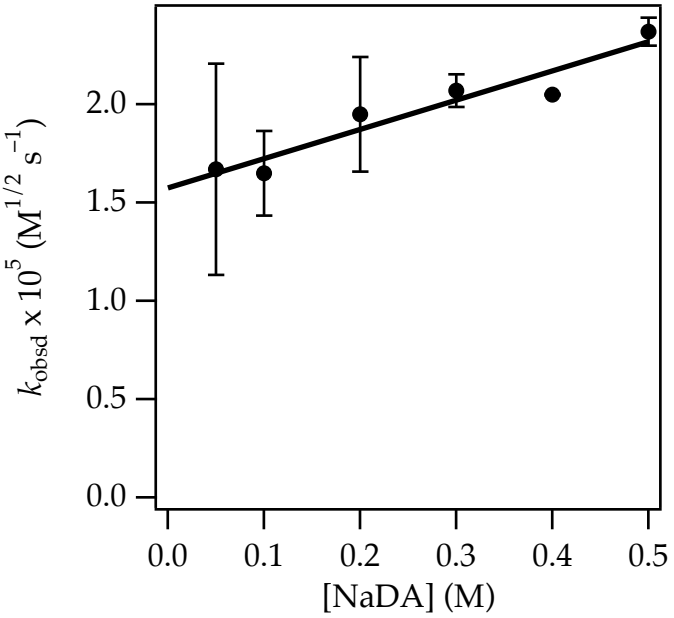


Figure S-90. Plot of half-order rate constants vs NaDA concentration for the decomposition of THF in neat THF at 25 ºC. The curve depicts an unweighted least-squares fit to the function $f(x) = ax + b$: $a = 1.5 \pm 0.2$; $b = 1.58 \pm 0.07$.

[NaDA] (M)	$k_{obsd} \times 10^5$ ($M^{1/2}$ s^{-1})	Standard deviation × 10^5 ($M^{1/2}$ s^{-1})
0.05	1.7	0.5
0.10	1.7	0.2
0.20	2.0	0.3
0.30	2.07	0.08
0.40	2.05	0.003
0.50	2.37	0.07

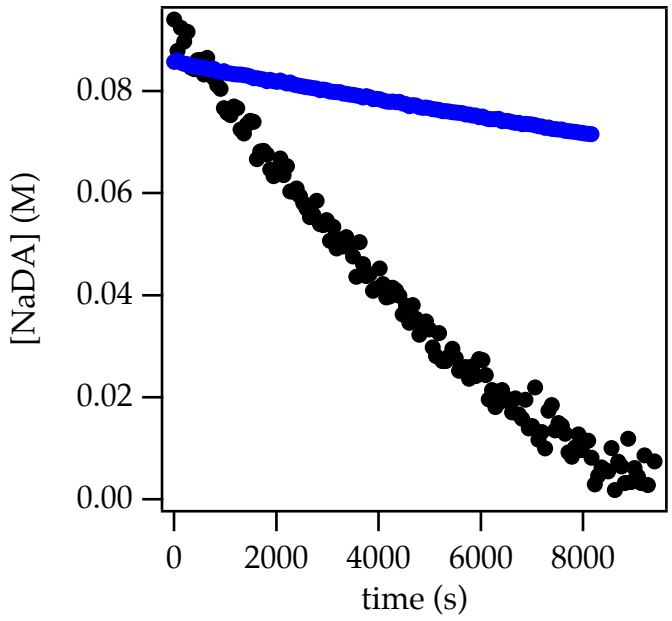


Figure S-91. Plot of NaDA concentration versus time in neat THF (black trace) and in neat THF-d_8 (blue trace) at 25 °C followed by ^{1}H NMR. This corresponds to an isotope effect of k_H/k_D = 7.2.

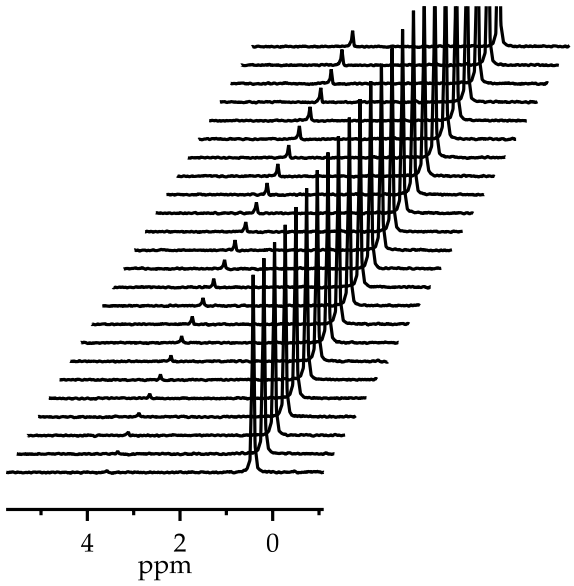


Figure S-92. ^{2}H NMR spectra of 0.20 M NaDA in 6.15 M THF and 3.57 M *N*-deuteriodiisopropylamine at 25 °C over the course of 1.3 hours. Appearance of a deuterium resonance at 3.58 ppm represents selective isotopic exchange into the alpha position of THF.

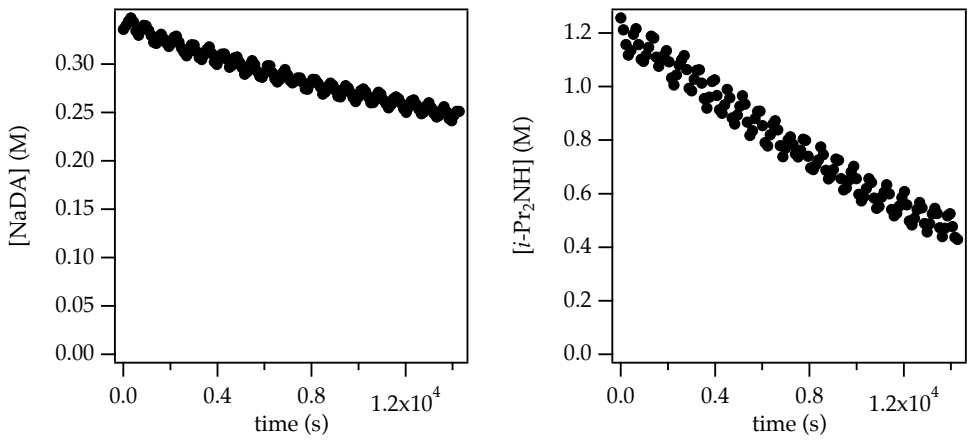


Figure S-93. Plots of NaDA and *N*-protiodiisopropylamine isotopologue concentration versus time in 10.3 M THF-d_8 at 25 °C. These demonstrate competitive NaDA decomposition and NaDA-mediated isotopic exchange of THF and diisopropylamine.

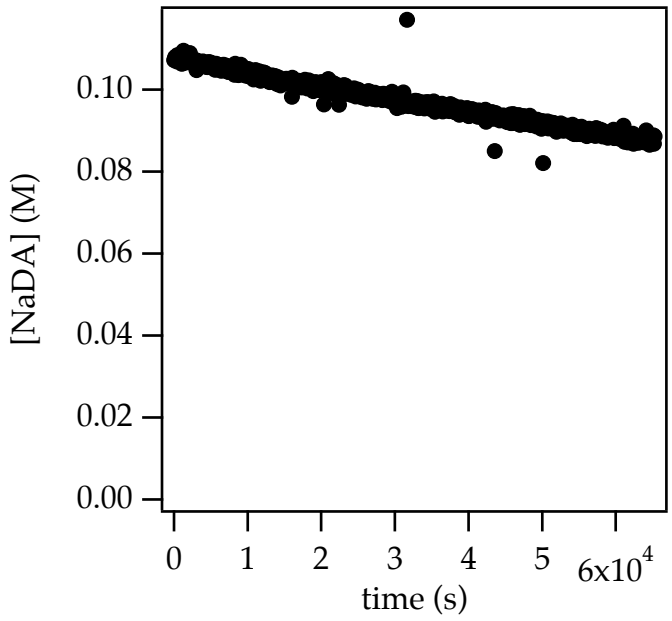


Figure S-94. Plot of NaDA concentration versus time in 2.3 M 3,3,4,4-tetradeuteriotetrahydrofuran/hexane at 25 °C. This rate of decomposition corresponds to an isotope effect of $k_H/k_D = 6$.

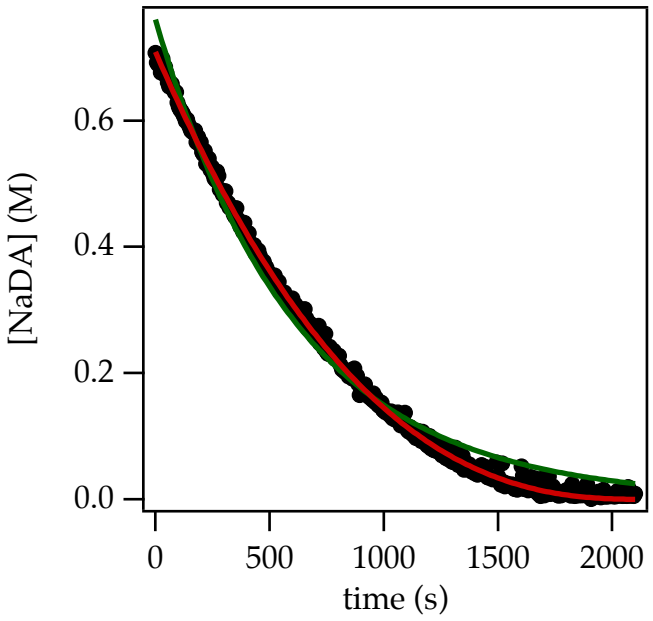


Figure S-95. Plot of NaDA concentration vs time in 4.41 M 1,2-dimethoxyethane at –10 ºC. The green curve depicts an unweighted least-squares fit to the function $f(t) = ae^{-kt}$: $a = 0.76 \pm 0.005$; $k = (1.63 \pm 0.01) \times 10^{-3}$. The red curve depicts an unweighted least-squares fit to the function $f(t) = ([A]_0^{(1-n)} - kt(1-n))^{1/(1-n)}$: $[A]_0 = (1.63 \pm 0.01) \times 10^{-3}$; $n = 0.605 \pm 0.007$, $k = (1.00 \pm 0.009) \times 10^{-3}$.

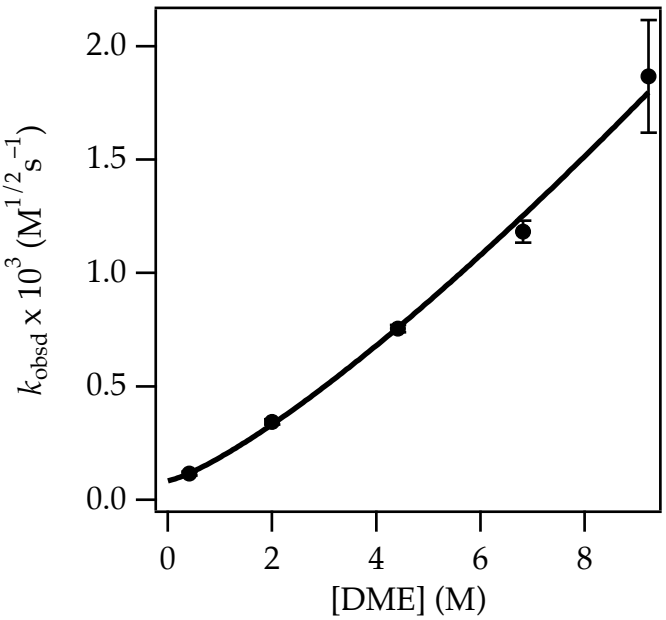


Figure S-96. Plot of k_{obsd} vs DME concentration for the decomposition of DME with 0.40 M NaDA at –10 ºC. The curve depicts an unweighted least-squares fit to the function $f(x) = ax^b + c$: $a = 0.10$; $b = 1.3$; $c = 0.08$.

[DME] (M)	$k_{obsd} \times 10^3$ ($M^{1/2}$ s^{-1})	Standard deviation × 10^3 ($M^{1/2}$ s^{-1})
0.41	0.116	0.009
2.00	0.34	0.01
4.41	0.75	0.02
6.81	1.18	0.05
9.22	1.9	0.2

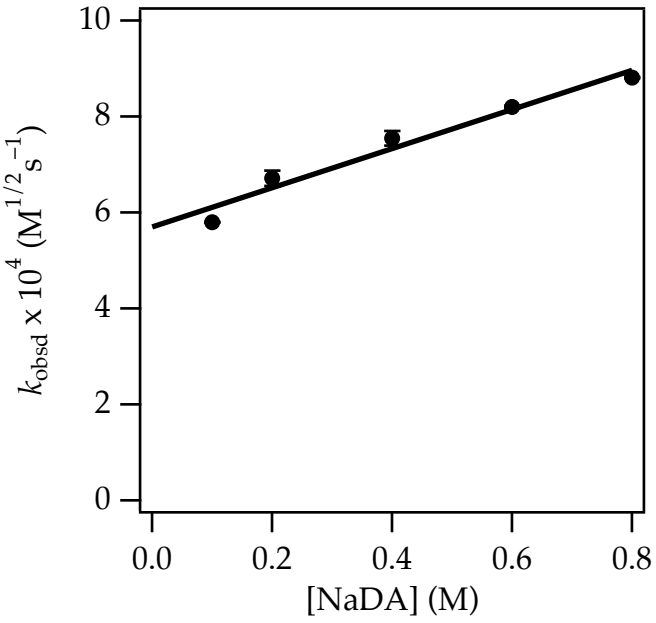


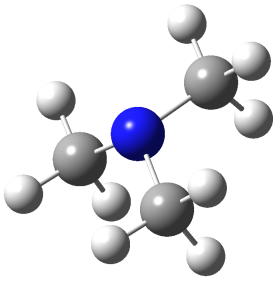
Figure S-97. Plot of k_{obsd} vs NaDA concentration in 4.41 M 1,2-dimethoxyethane at –10 ºC. The green curve depicts an unweighted least-squares fit to the function $f(x) = ax + b$: $a = 4.1 \pm 0.5$; $k = 5.7 \pm 0.2$.

[NaDA] (M)	$k_{obsd} \times 10^3$ ($M^{1/2}$ s^{-1})	Standard deviation × 10^3 ($M^{1/2}$ s^{-1})
0.10	5.801	0.006
0.20	6.7	0.2
0.40	7.5	0.2
0.60	8.20	0.02
0.80	8.81	0.02

III. Computations

Geometries are optimized at the B3LYP level of theory using the 6–31G(d) basis set. Energies are defined as follows: G is the sum of electronic and thermal free energies calculated at the B3LYP level of theory (T = 195 K). G_{MP2} is derived from a MP2 single point calculation corresponding to the DFT-optimized geometry and includes a thermal correction from the DFT calculation.

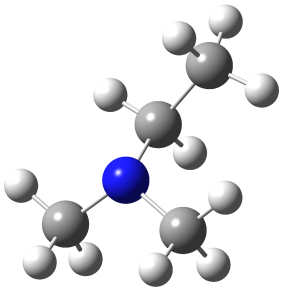
Table S-1. Geometric coordinates and thermally corrected MP2 energies for trimethylamine.



G = –174.368911 Hartree
G_{MP2} = –173.7228423 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	0.00000000	–1.38888500	0.43318300
C	1.20281000	–2.08332800	0.00000000
H	2.08800400	–1.57037600	0.39236800
H	1.20117800	–3.10640400	0.39236800
H	1.30265200	–2.14097200	–1.10331300
C	–1.20281000	–2.08332800	0.00000000
H	–1.20117800	–3.10640400	0.39236800
H	–2.08800400	–1.57037600	0.39236800
H	–1.30265200	–2.14097200	–1.10331300
H	–0.88682600	0.51012500	0.39236800
H	0.88682600	0.51012500	0.39236800
H	0.00000000	0.11528900	–1.10331300

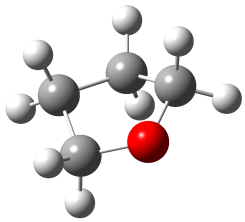
Table S-2. Geometric coordinates and thermally corrected MP2 energies for *N,N*-dimethylethylamine (DMEA).



G = –213.656332 Hartree
G_{MP2} = –212.8628209 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
H	–0.84676100	0.44583500	–0.53371500
H	–0.27139700	–0.06375300	1.07346700
H	0.13787400	–1.02031100	–0.37462200
N	1.20269200	0.78314300	–0.24717900
C	1.00866600	2.16698900	0.16431700
H	0.84396600	2.27724500	1.25587800
H	1.87500200	2.77507100	–0.11085400
H	0.13554500	2.58116700	–0.35151900
C	2.37332900	0.16457200	0.37736600
H	2.31290700	0.20916500	1.48530500
H	2.35523600	–0.89917900	0.10985500
C	3.70218400	0.76094500	–0.08912300
H	3.83862600	1.79375200	0.24849100
H	4.53671100	0.17463800	0.31175700
H	3.76275200	0.74783200	–1.18254400

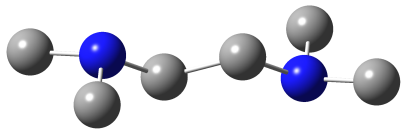
Table S-3. Geometric coordinates and thermally corrected MP2 energies for tetrahydrofuran (THF).



G = –232.349410 Hartree
G_{MP2} = –231.5699006 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
H	–0.78342300	0.39255100	–0.65898600
H	–0.37024600	0.05270400	1.03571900
C	0.43180600	–1.42749800	–0.35852800
H	–0.17836300	–2.19189500	0.13257700
H	0.36797200	–1.58612700	–1.44174200
C	1.89932000	–1.42749800	0.09488700
H	2.50948900	–2.19189500	–0.39621800
H	1.96315400	–1.58612700	1.17810100
C	2.33112600	0.00000000	–0.26363900
H	3.11454900	0.39255100	0.39534600
H	2.70137200	0.05270400	–1.29935800
O	1.16556300	0.82060000	–0.13182000

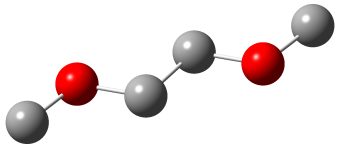
Table S-4. Geometric coordinates and thermally corrected MP2 energies for *N,N,N',N'*-tetramethylethylenediamine (TMEDA).



G = –347.542183 Hartree
G_{MP2} = –346.2912902 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
H	–0.11054600	–0.13667800	1.09344600
H	1.07059200	0.12471400	–0.19503400
C	–0.49784800	–1.26597800	–0.71159800
H	–1.56844000	–1.39069200	–0.51656400
H	–0.38730200	–1.12930000	–1.80504400
N	0.16864400	–2.47827900	–0.23211000
C	–0.58572400	–3.67542600	–0.57979000
H	–0.67988000	–3.83535000	–1.67277100
H	–0.09308900	–4.55672000	–0.15383400
H	–1.59483800	–3.61521800	–0.15795200
C	1.54493400	–2.58929400	–0.69943500
H	2.00030900	–3.49287300	–0.27966300
H	1.62408000	–2.64728900	–1.80390800
H	2.13884100	–1.73494000	–0.36256900
N	–0.66649200	1.21230100	–0.47948800
C	0.08787600	2.40944800	–0.13180800
H	–0.40475900	3.29074200	–0.55776400
H	0.18203200	2.56937200	0.96117300
H	1.09699000	2.34924000	–0.55364600
C	–2.04278200	1.32331600	–0.01216300
H	–2.12192800	1.38131100	1.09231000
H	–2.49815700	2.22689500	–0.43193500
H	–2.63668900	0.46896200	–0.34902900

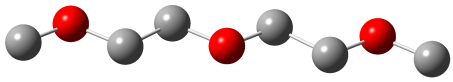
Table S-5. Geometric coordinates and thermally corrected MP2 energies for 1,2-dimethoxyethane (DME).



G = –308.732430 Hartree
G_{MP2} = –307.7282485 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
H	0.03334800	–0.65127400	–0.88899700
H	0.03341400	–0.65119500	0.88905100
C	–1.29324400	0.80127400	0.00000000
H	–1.32659200	1.45254800	–0.88899700
H	–1.32665800	1.45246900	0.88905100
O	–2.36656800	–0.11839900	–0.00007900
C	–3.62755000	0.51427300	0.00018800
H	–3.76824000	1.14522100	–0.89254200
H	–4.38477100	–0.27428400	0.00010300
H	–3.76804200	1.14484900	0.89321000
O	1.07332400	0.91967300	–0.00007900
C	2.33430600	0.28700100	0.00018800
H	3.09152700	1.07555800	0.00010400
H	2.47479700	–0.34357600	0.89321000
H	2.47499600	–0.34394600	–0.89254200

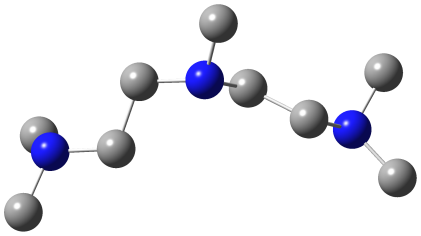
Table S-6. Geometric coordinates and thermally corrected MP2 energies for diglyme.



G = –462.505071 Hartree
G_{MP2} = –461.0185898462 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
H	0.84888300	0.68886300	0.00086100
H	0.06140700	-0.64244500	-0.89341000
H	0.06063800	-0.64374300	0.89252600
O	-1.17301000	0.78407800	0.00007400
C	-2.35185200	0.00495100	-0.00077900
H	-2.39994500	-0.64592000	0.88788800
H	-2.39934900	-0.64481900	-0.89027700
C	-3.53466800	0.96210400	-0.00046500
H	-3.48774800	1.61098300	0.88878600
H	-3.48779500	1.61173300	-0.88916400
O	-4.71540900	0.18325300	-0.00078800
C	-5.89616100	0.96210600	-0.00045900
H	-5.94292900	1.61114900	0.88866400
H	-5.94319600	1.61150900	-0.88930700
C	-7.07898000	0.00492500	-0.00048500
H	-7.03123900	-0.64526600	-0.88965100
H	-7.03114300	-0.64544600	0.88854300
O	-8.25781900	0.78409000	-0.00034200
C	-9.43082300	-0.00000500	0.00007700
H	-10.2796770	0.68889200	0.00018700
H	-9.49209900	-0.64322600	-0.89278200
H	-9.49163200	-0.64295300	0.89316400

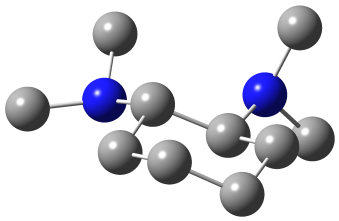
Table S-7. Geometric coordinates and thermally corrected MP2 energies for *N*,*N*,*N*',*N*'',*N*''-pentamethyldiethylenetriamine (PMDTA).



G = –521.015934672 Hartree
G_{MP2} = –518.85875533274 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
H	-0.03384800	0.37685800	-1.02775600
H	-0.36886000	-1.04550800	-0.00532200
H	1.04762500	-0.01665100	0.32128100
N	-0.76467800	0.87893700	0.87507100
C	-0.65267800	0.44208700	2.26136800
H	0.40231400	0.42795500	2.55667500
H	-1.17454700	1.13534600	2.92699600
H	-1.06844800	-0.57216800	2.42997000
C	-2.15509800	1.00163000	0.43276200
H	-2.16354500	1.07321200	-0.66004700
H	-2.74431100	0.09913700	0.69146300
C	-2.83490800	2.26869200	0.97037600
H	-2.80394400	2.30218700	2.07544200
H	-2.24947400	3.12474300	0.61906500
N	-4.20546500	2.40665200	0.46759800
C	-4.62140100	3.80443700	0.42424500
H	-5.62814400	3.88496100	0.00303500
H	-4.63369700	4.28661400	1.42221700
H	-3.94399500	4.37359900	-0.22107400
C	-5.16631800	1.57939300	1.20690400
H	-5.51623300	2.10246800	2.11673100
H	-4.66792000	0.66728200	1.54706300
C	-6.34754700	1.14940500	0.32579600
H	-6.85180100	2.03305100	-0.11338800
H	-5.93241900	0.58169400	-0.51360200
N	-7.29673700	0.29020500	1.03656100
C	-8.09910000	-0.50037200	0.11241900
H	-8.75249500	-1.17436300	0.67792200
H	-8.74041000	0.11430000	-0.55106100
H	-7.44560100	-1.11155300	-0.51917200
C	-8.15541800	1.03633000	1.94820900
H	-8.80627700	1.76752000	1.42669000
H	-8.80047100	0.34046300	2.49598500
H	-7.55576500	1.58175700	2.68229800

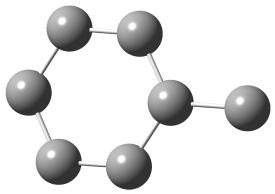
Table S-8. Geometric coordinates and thermally corrected MP2 energies for trans-*N*,*N*,*N*',*N*'-tetramethylcyclohexane-1,2-diamine (TMCDA).



G = –503.506161 Hartree
G_{MP2} = –501.71092144347 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
C	0.58407200	-1.33858000	-0.46811100
C	-0.31093600	-2.55965400	-0.14869700
C	-1.73646700	-2.29717100	-0.73415200
C	-2.30246500	-0.92843500	-0.28176700
C	-1.37740500	0.24303700	-0.61787100
H	-1.27840500	0.34049400	-1.70906500
H	-1.80719800	1.18601200	-0.25592300
H	-3.28935600	-0.78096600	-0.73863000
H	-2.46330000	-0.94192300	0.80504000
H	-1.58524200	-2.26161200	-1.82091400
N	-2.69011300	-3.40294700	-0.51089700
C	-3.70451400	-3.51635200	-1.54687600
H	-4.27597300	-4.43974800	-1.39368300
H	-4.43042400	-2.67966400	-1.56741000
H	-3.22557100	-3.57667500	-2.52964700
C	-3.27577500	-3.47407800	0.82131300
H	-2.49407700	-3.40260700	1.58438900
H	-4.02883200	-2.69188000	1.02988500
H	-3.76994300	-4.44576300	0.94328000
H	-0.38363700	-2.62268300	0.95675000
N	0.26542000	-3.81721100	-0.68623400
C	1.71914800	-3.85915500	-0.81929400
H	1.99045900	-4.82497100	-1.25948000
H	2.08630000	-3.08303000	-1.49352800
H	2.26578600	-3.77294000	0.14177700
C	-0.16796700	-4.99824300	0.05847300
H	0.21433200	-5.00967200	1.10046700
H	-1.25482100	-5.04324900	0.07240700
H	0.20858500	-5.89788800	-0.44216400
H	0.74158100	-1.29307000	-1.55550400
H	1.56930400	-1.47537000	-0.01147400
H	-0.08718700	0.00203500	1.09651800
H	0.69414800	0.80969100	-0.25905900

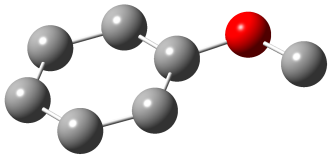
Table S-9. Geometric coordinates and thermally corrected MP2 energies for toluene.



G = –271.456720 Hartree
G_{MP2} = –270.51845425408 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
C	-1.51153900	0.00011200	-0.02049600
C	-2.23126200	1.20232700	-0.01826500
C	-3.62678000	1.20521300	-0.00714200
C	-4.33045400	-0.00022800	-0.00080300
C	-3.62642000	-1.20559200	-0.00714300
C	-2.23102200	-1.20239600	-0.01826100
H	-1.69069000	-2.14681100	-0.02716300
H	-4.16374100	-2.15065800	-0.00790300
H	-5.41721800	-0.00039600	0.00457200
H	-4.16426900	2.15018200	-0.00789800
H	-1.69115600	2.14685500	-0.02715200
H	0.38463400	-0.01284400	1.02881700
H	0.40855600	-0.87980400	-0.50885200
H	0.40829300	0.89211200	-0.48701000

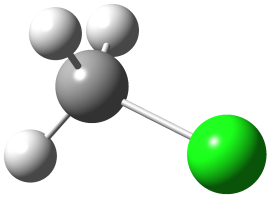
Table S-10. Geometric coordinates and thermally corrected MP2 energies for anisole.



G = –346.656107 Hartree
G_{MP2} = –345.53029645492 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
O	-1.00742000	-0.99726700	0.00026100
C	-2.31417500	-0.59621800	0.00015800
C	-3.26420100	-1.62867200	0.00011700
C	-4.62082000	-1.32550500	0.00008000
C	-5.05242100	0.00576300	0.00007900
C	-4.10508600	1.02657500	0.00013800
C	-2.73608600	0.73838800	0.00018200
H	-2.01850900	1.55108900	0.00025300
H	-4.42444200	2.06569300	0.00015400
H	-6.11298900	0.23985600	0.00004300
H	-5.34726400	-2.13406300	0.00004000
H	-2.91175700	-2.65555100	0.00011100
H	-0.05775100	0.63475600	0.89449000
H	0.95169700	-0.53489100	-0.00018600
H	-0.05816200	0.63468100	-0.89451300

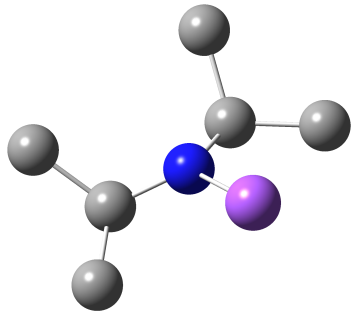
Table S-11. Geometric coordinates and thermally corrected MP2 energies for chloromethane.



G = –500.084149 Hartree
G_{MP2} = –499.32993145919 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
H	0.00000000	1.03379600	-0.34631800
H	-0.89529300	-0.51689800	-0.34631800
H	0.89529300	-0.51689800	-0.34631800
Cl	0.00000000	0.00000000	1.80340400

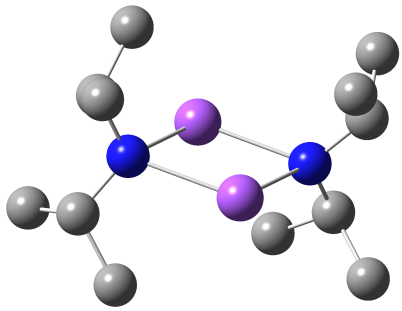
Table S-12. Geometric coordinates and thermally corrected MP2 energies for monomeric sodium diisopropylamide (A).



G = –453.929223 Hartree
G_{MP2} = –452.4226915 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	–0.49364100	0.57106100	–1.23076500
C	0.00000000	0.00000000	–2.46153000
H	1.05813000	–0.32092100	–2.34002200
C	0.00000000	1.07421300	–3.56842400
H	0.63239400	1.92406100	–3.28028100
H	0.35726800	0.68953000	–4.53177700
H	–1.02826300	1.44104300	–3.73875000
C	–0.77662400	–1.23521400	–2.98792000
H	–0.74423300	–2.06276600	–2.27364400
H	–1.83236800	–0.97368600	–3.14357800
H	–0.36670100	–1.60169400	–3.94048500
Na	–1.53148000	2.42658800	–1.23076500
H	1.05813000	–0.32092100	–0.12150800
C	0.00000000	1.07421300	1.10689400
H	–1.02826300	1.44104300	1.27722000
H	0.35726800	0.68953000	2.07024700
H	0.63239400	1.92406100	0.81875100
C	–0.77662400	–1.23521400	0.52639000
H	–0.74423300	–2.06276600	–0.18788600
H	–0.36670100	–1.60169400	1.47895500
H	–1.83236800	–0.97368600	0.68204800

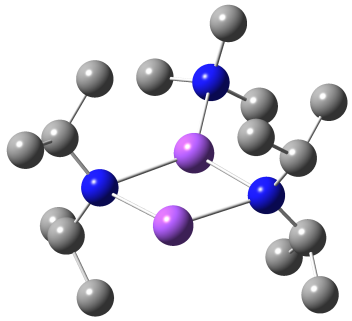
Table S-13. Geometric coordinates and thermally corrected MP2 energies for dimeric sodium diisopropylamide (A_2).



G = –907.924828 Hartree
G_{MP2} = –904.9165246 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	–1.86413800	–0.00055200	1.40661100
Na	–1.86422600	–0.00009500	–1.40644000
N	–3.72835100	–0.00009000	0.00006000
C	–4.55517700	–1.18500500	0.22778400
C	–5.01821700	–1.86247200	–1.08379500
H	–5.51404500	–1.13634500	–1.73832800
H	–5.72172000	–2.68793700	–0.90490600
H	–4.15210500	–2.26879000	–1.62751500
C	–3.81939800	–2.21719200	1.09889700
H	–4.39379200	–3.14392100	1.21756600
H	–3.63365000	–1.82075400	2.10914200
H	–2.85380000	–2.49329500	0.64883800
H	–5.47786800	–0.92302900	0.78272900
C	–4.55518500	1.18484100	–0.22755700
C	–5.01785300	1.86243400	1.08408200
H	–5.72134000	2.68793900	0.90531100
H	–4.15157900	2.26872400	1.62755900
H	–5.51357800	1.13638300	1.73878200
C	–3.81955900	2.21688800	–1.09896900
H	–4.39394200	3.14362500	–1.21764900
H	–3.63402200	1.82027600	–2.10918000
H	–2.85386000	2.49300400	–0.64914300
H	–5.47802600	0.92284700	–0.78222900
C	0.82709500	–1.18469400	–0.22782000
C	1.29062000	–1.86197900	1.08368300
H	1.99434500	–2.68722000	0.90465100
H	0.42474800	–2.26856300	1.62758700
H	1.78635900	–1.13570000	1.73811300
C	0.09135200	–2.21710300	–1.09869200
H	0.66592100	–3.14371600	–1.21742300
H	–0.09471800	–1.82077400	–2.10891900
H	–0.87409200	–2.49335300	–0.64840500
H	1.74959400	–0.92252600	–0.78300700
C	0.82653000	1.18511600	0.22775200
C	1.28925300	1.86284300	–1.08380000
H	1.99257800	2.68845500	–0.90489400
H	0.42298400	2.26902400	–1.62737100
H	1.78518400	1.13691600	–1.73847900
C	0.09051900	2.21698900	1.09904300
H	0.66462400	3.14389500	1.21773700
H	–0.09500000	1.82038000	2.10926000
H	–0.87522100	2.49280300	0.64912000
H	1.74934600	0.92335100	0.78258100

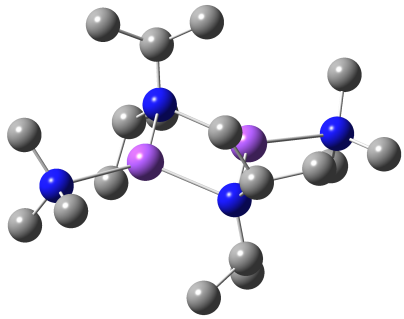
Table S-14. Geometric coordinates and thermally corrected MP2 energies for trimethylamine-solvated dimeric sodium diisopropylamide, A_2(trimethylamine).



G = –1082.299639 Hartree
G_{MP2} = –1078.653955 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	–1.86413800	–0.00055200	1.40661100
Na	–1.86422600	–0.00009500	–1.40644000
N	–3.72835100	–0.00009000	0.00006000
C	–4.55517700	–1.18500500	0.22778400
C	–5.01821700	–1.86247200	–1.08379500
H	–5.51404500	–1.13634500	–1.73832800
H	–5.72172000	–2.68793700	–0.90490600
H	–4.15210500	–2.26879000	–1.62751500
C	–3.81939800	–2.21719200	1.09889700
H	–4.39379200	–3.14392100	1.21756600
H	–3.63365000	–1.82075400	2.10914200
H	–2.85380000	–2.49329500	0.64883800
H	–5.47786800	–0.92302900	0.78272900
C	–4.55518500	1.18484100	–0.22755700
C	–5.01785300	1.86243400	1.08408200
H	–5.72134000	2.68793900	0.90531100
H	–4.15157900	2.26872400	1.62755900
H	–5.51357800	1.13638300	1.73878200
C	–3.81955900	2.21688800	–1.09896900
H	–4.39394200	3.14362500	–1.21764900
H	–3.63402200	1.82027600	–2.10918000
H	–2.85386000	2.49300400	–0.64914300
H	–5.47802600	0.92284700	–0.78222900
C	0.82709500	–1.18469400	–0.22782000
C	1.29062000	–1.86197900	1.08368300
H	1.99434500	–2.68722000	0.90465100
H	0.42474800	–2.26856300	1.62758700
H	1.78635900	–1.13570000	1.73811300
C	0.09135200	–2.21710300	–1.09869200
H	0.66592100	–3.14371600	–1.21742300
H	–0.09471800	–1.82077400	–2.10891900
H	–0.87409200	–2.49335300	–0.64840500
H	1.74959400	–0.92252600	–0.78300700
C	0.82653000	1.18511600	0.22775200
C	1.28925300	1.86284300	–1.08380000
H	1.99257800	2.68845500	–0.90489400
H	0.42298400	2.26902400	–1.62737100
H	1.78518400	1.13691600	–1.73847900
C	0.09051900	2.21698900	1.09904300
H	0.66462400	3.14389500	1.21773700
H	–0.09500000	1.82038000	2.10926000
H	–0.87522100	2.49280300	0.64912000
H	1.74934600	0.92335100	0.78258100

Table S-15. Geometric coordinates and thermally corrected MP2 energies for A_2(trimethylamine)$_2$.

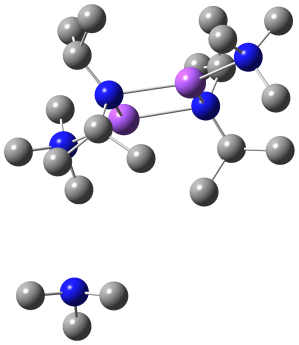


G = –1256.672802 Hartree
G_{MP2} = –1252.389985 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	–1.52538400	–1.84418200	–0.02794400
Na	1.38853700	–1.94263100	0.00468600
N	–0.13093200	–3.78140600	0.00511000
C	–0.29165000	–4.59764500	1.20716900
C	1.04899700	–5.13118500	1.77125100
H	1.62375700	–5.64227100	0.99025100
H	0.90433200	–5.84045000	2.59923300
H	1.65908100	–4.29578500	2.14639100
C	–1.02333200	–3.82769500	2.31747000
H	–1.09381800	–4.41063800	3.24459400
H	–2.04673600	–3.56971200	2.01212600
H	–0.49338300	–2.89573600	2.55875900
H	–0.91221000	–5.49465100	1.00241800
C	–0.01602300	–4.63308600	–1.17646100
C	–1.38334600	–5.11362600	–1.72458300
H	–1.27739300	–5.84930600	–2.53523100
H	–1.95307500	–4.25846700	–2.11812800
H	–1.97817900	–5.57760400	–0.92914700
C	0.74860300	–3.92592600	–2.30611300
H	0.77879900	–4.52794700	–3.22323100
H	1.78761900	–3.72184500	–2.01215100
H	0.27044800	–2.96902700	–2.55928500
H	0.56039900	–5.55468400	–0.95210700
C	0.09490800	0.81227400	1.21244300
C	–1.27664700	1.32710900	1.71595600
H	–1.17874100	2.03616200	2.55093700
H	–1.89414100	0.48486100	2.06155900
H	–1.82059400	1.83454100	0.91041200
C	0.78683100	0.04653500	2.35065700
H	0.80589400	0.62464400	3.28340800
H	1.82675700	–0.19329900	2.09014900
H	0.26111800	–0.89498100	2.56284800
H	0.71242300	1.71740600	1.04006800
C	–0.06257100	0.85810000	–1.18114300
C	1.31951600	1.39626600	–1.63036800
H	1.23713600	2.14156800	–2.43478600
H	1.94261200	0.56893800	–2.00044400
H	1.84780000	1.86755300	–0.79358100
C	–0.71376100	0.13165000	–2.36725800
H	–0.70908000	0.74516100	–3.27716000
H	–1.75913800	–0.12702000	–2.15059400
H	–0.17418100	–0.79806400	–2.59733000
H	–0.68942600	1.75509400	–0.99316000
N	–4.07836500	–1.88196900	–0.18967600
C	–4.44457300	–1.56924600	–1.57598300
H	–4.06695600	–0.57793200	–1.84512400
H	–3.99830500	–2.30593500	–2.25203500
H	–5.53923200	–1.57669400	–1.72903400
C	–4.56567900	–3.21991000	0.16844500

H –4.10774100 –3.96710100 –0.48591300
H –4.28625800 –3.45162600 1.20076100
H –5.66474500 –3.29770200 0.08073800
C –4.63516200 –0.87513200 0.72167700
H –4.34307700 –1.10681300 1.75104200
H –4.24073800 0.11342200 0.46818400
H –5.73883800 –0.83636600 0.67526100
N 3.93326200 –2.03633200 –0.15188900
C 4.33115600 –1.67381700 –1.51735900
H 3.89372800 –2.38006300 –2.23032200
H 3.96450900 –0.67051400 –1.75445900
H 5.42871200 –1.68474400 –1.64756500
C 4.48748000 –1.07361500 0.80718500
H 4.11415100 –0.07017300 0.58049500
H 4.17323800 –1.33860700 1.82196300
H 5.59233500 –1.05025900 0.78264000
C 4.38938500 –3.39465800 0.16674300
H 4.06352700 –3.66904600 1.17455200
H 3.94974800 –4.10664400 –0.53828600
H 5.48979900 –3.48577600 0.11681600

Table S-16. Geometric coordinates and thermally corrected MP2 energies for A_2(trimethylamine)$_3$. Third trimethylamine does not coordinate to Na.

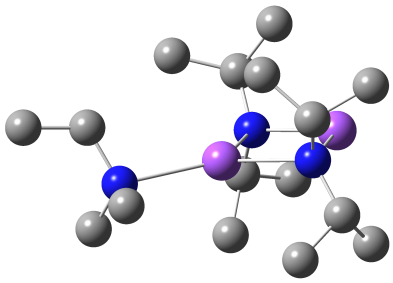


G = –1431.035378 Hartree
G_{MP2} = –1426.111795 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	1.14408300	–2.01194900	0.55251800
Na	–1.52252300	–1.18299400	1.43628800
N	–0.34111100	–3.18088200	2.00661500
C	–0.76939500	–4.47150200	1.47392300
C	–2.26688700	–4.77835700	1.73069200
H	–2.51078600	–4.66712300	2.79351800
H	–2.54390400	–5.79950700	1.42939000
H	–2.89697000	–4.07414900	1.16730800
C	–0.49782200	–4.57317000	–0.03514800
H	–0.87151500	–5.51433400	–0.45868900
H	0.57918000	–4.52256500	–0.24671100
H	–0.99032300	–3.75217100	–0.57577100
H	–0.20510600	–5.30673400	1.93935900
C	–0.04887600	–3.29010700	3.43447100
C	1.37066700	–3.83476000	3.73233400
H	1.52902300	–4.03235000	4.80259700
H	2.13053800	–3.10761400	3.40868700
H	1.54919400	–4.77063400	3.19013400
C	–0.22193000	–1.94090600	4.14964400
H	0.05697400	–1.99843700	5.20953100
H	–1.26509300	–1.59971700	4.10149700
H	0.41113300	–1.17025300	3.68760800
H	–0.75153900	–3.98816600	3.93546300
C	–0.54417300	0.23257600	–1.33560500
C	0.50950700	0.10799100	–2.46526400
H	0.10911700	0.40511800	–3.44559800
H	0.85479100	–0.93338400	–2.54342200
H	1.38271100	0.73768100	–2.25864500
C	–1.70538300	–0.72626800	–1.63882700
H	–2.07675800	–0.60773700	–2.66501300
H	–2.55269400	–0.55445000	–0.96134000
H	–1.38413000	–1.77165700	–1.52672300
H	–0.96527800	1.25622100	–1.42611100
C	0.67739000	1.19950200	0.48978900
C	–0.28574600	2.23859200	1.11566400
H	0.21870400	3.18448600	1.36135100
H	–0.72107800	1.83867700	2.04295700
H	–1.10823600	2.46784400	0.42795000
C	1.76600500	0.85034000	1.51716500
H	2.23169800	1.74739200	1.94511500
H	2.56537500	0.25253500	1.05850400
H	1.34250900	0.27484900	2.35259700
H	1.19947900	1.72924600	–0.33336700
N	3.37598800	–2.87038900	–0.35129100
C	4.37691000	–1.80346400	–0.23637100
H	4.04193400	–0.92081100	–0.78989300
H	4.50306000	–1.52566000	0.81506000
H	5.36157100	–2.11161600	–0.63314000
C	3.79459400	–4.04590500	0.42168400

H	3.90863000	–3.77513600	1.47556800
H	3.03006800	–4.82546700	0.35234100
H	4.75277300	–4.46118200	0.05946800
C	3.18200100	–3.22970500	–1.76109900
H	2.41763400	–4.00915800	–1.84274600
H	2.84357100	–2.35315000	–2.32208600
H	4.11122800	–3.60568700	–2.22695700
N	–3.76869400	–0.43451300	2.37214400
C	–3.53259400	0.72267600	3.24266500
H	–2.85652200	0.44439300	4.05811500
H	–3.06699600	1.52894700	2.66798900
H	–4.46999900	1.10622500	3.68612000
C	–4.64300100	–0.05780800	1.25263800
H	–4.15790700	0.72054300	0.65406700
H	–4.83462500	–0.92970800	0.61771100
H	–5.61485400	0.33486200	1.60578000
C	–4.37543100	–1.52979000	3.13808100
H	–4.53361900	–2.39267300	2.48533200
H	–3.70646300	–1.83087400	3.95031700
H	–5.34759600	–1.23814200	3.57679900
N	–5.80247200	–2.91964800	–0.84984900
C	–6.89220300	–2.17381700	–1.46774800
H	–7.57252600	–1.80257600	–0.69351900
H	–6.48919800	–1.31244000	–2.01120000
H	–7.48361600	–2.78256100	–2.18031700
C	–4.84045400	–3.37108000	–1.84958600
H	–4.43202000	–2.50845500	–2.38636500
H	–4.01164300	–3.88938300	–1.35653400
H	–5.28470400	–4.06179000	–2.59361200
C	–6.31011700	–4.03937600	–0.06489100
H	–5.47797800	–4.55331000	0.42777700
H	–6.99180500	–3.66911000	0.70871900
H	–6.85858500	–4.78213600	–0.67747500

Table S-17. Geometric coordinates and thermally corrected MP2 energies for A_2(DMEA).

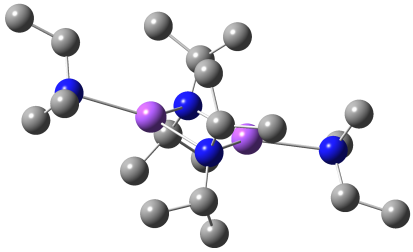


G = –1121.583807 Hartree
G_{MP2} = –1117.790684 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	1.64333500	–1.61536200	0.27072200
Na	–1.13257800	–2.11634500	–0.24262100
N	0.66391900	–3.69895800	0.04677200
C	1.20613300	–4.43048200	–1.09808800
C	0.11093000	–5.09084200	–1.97047800
H	–0.55030000	–5.70957000	–1.35276900
H	0.53051600	–5.73098600	–2.75987900
H	–0.50448900	–4.31822800	–2.45570500
C	2.07660700	–3.52446500	–1.98542700
H	2.42827200	–4.04180600	–2.88667600
H	2.96822000	–3.17772700	–1.44127200
H	1.50954500	–2.64366800	–2.32107800
H	1.86935700	–5.25364900	–0.76632100
C	0.45778500	–4.59327100	1.18401600
C	1.75187000	–4.87293900	1.98690800
H	1.60467600	–5.63108700	2.76955500
H	2.10047400	–3.94913500	2.47267500
H	2.55239600	–5.22620700	1.32691500
C	–0.61025000	–4.04043200	2.14043000
H	–0.72305600	–4.66541800	3.03502300
H	–1.59265300	–3.98760700	1.65089100
H	–0.34246200	–3.02981800	2.48124700
H	0.08361200	–5.58308000	0.84891200
N	–3.60651600	–2.63237700	–0.59280500
C	–4.28147300	–2.17007800	0.64093500
H	–3.81125700	–2.69929500	1.47961400
H	–4.03548900	–1.10794500	0.76034100
C	–5.80490900	–2.34902300	0.72545100
H	–6.10236200	–3.40130500	0.66682900
H	–6.16029700	–1.96013300	1.68620800
H	–6.32963800	–1.80123600	–0.06430100
C	–4.04929200	–1.89482000	–1.78207600
H	–3.93485600	–0.81914600	–1.61283600
H	–3.42589700	–2.17668400	–2.63769700
H	–5.09925400	–2.09536300	–2.05254000
C	–3.74314300	–4.07927100	–0.80302200
H	–3.10154700	–4.38739200	–1.63465700
H	–3.41475400	–4.61492400	0.09328200
H	–4.77578900	–4.38827800	–1.03546800
C	–0.04847300	0.83437800	–1.19936300
C	1.29109200	1.54930300	–1.50350300
H	1.20812200	2.25814500	–2.33991300
H	2.06295300	0.80938200	–1.76452900
H	1.64434000	2.10702200	–0.62847900
C	–0.46751900	0.01528000	–2.42973700
H	–0.44093600	0.61251800	–3.34974900
H	–1.48927600	–0.37165700	–2.31811900
H	0.20919700	–0.83880500	–2.57760300
H	–0.80743900	1.63697400	–1.09427300

C	–0.17400100	0.81261300	1.20360300
C	–1.65968500	1.06400600	1.55848100
H	–1.77948700	1.77080300	2.39220100
H	–2.14525800	0.11965600	1.84481700
H	–2.19788000	1.47146500	0.69450800
C	0.53193900	0.18074400	2.41481400
H	0.34945000	0.74152700	3.33995700
H	1.62187900	0.14926100	2.26431000
H	0.17566000	–0.84604100	2.58385800
H	0.28296600	1.81415100	1.07713300

Table S-18. Geometric coordinates and thermally corrected MP2 energies for $A_2(DMEA)_2$.

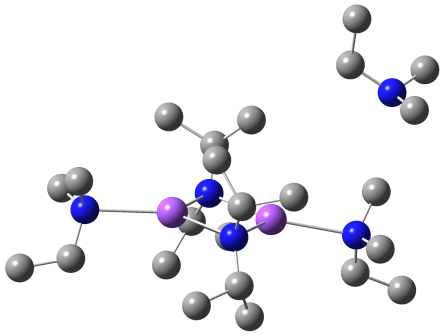


G = –1335.242772 Hartree
G_{MP2} = –1330.66575 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	–1.52538400	–1.84418200	–0.02794400
Na	1.38853700	–1.94263100	0.00468600
N	–0.13093200	–3.78140600	0.00511000
C	–0.29165000	–4.59764500	1.20716900
C	1.04899700	–5.13118500	1.77125100
H	1.62375700	–5.64227100	0.99025100
H	0.90433200	–5.84045000	2.59923300
H	1.65908100	–4.29578500	2.14639100
C	–1.02333200	–3.82769500	2.31747000
H	–1.09381800	–4.41063800	3.24459400
H	–2.04673600	–3.56971200	2.01212600
H	–0.49338300	–2.89573600	2.55875900
H	–0.91221000	–5.49465100	1.00241800
C	–0.01602300	–4.63308600	–1.17646100
C	–1.38334600	–5.11362600	–1.72458300
H	–1.27739300	–5.84930600	–2.53523100
H	–1.95307500	–4.25846700	–2.11812800
H	–1.97817900	–5.57760400	–0.92914700
C	0.74860300	–3.92592600	–2.30611300
H	0.77879900	–4.52794700	–3.22323100
H	1.78761900	–3.72184500	–2.01215100
H	0.27044800	–2.96902700	–2.55928500
H	0.56039900	–5.55468400	–0.95210700
C	0.09490800	0.81227400	1.21244300
C	–1.27664700	1.32710900	1.71595600
H	–1.17874100	2.03616200	2.55093700
H	–1.89414100	0.48486100	2.06155900
H	–1.82059400	1.83454100	0.91041200
C	0.78683100	0.04653500	2.35065700
H	0.80589400	0.62464400	3.28340800
H	1.82675700	–0.19329900	2.09014900
H	0.26111800	–0.89498100	2.56284800
H	0.71242300	1.71740600	1.04006800
C	–0.06257100	0.85810000	–1.18114300
C	1.31951600	1.39626600	–1.63036800
H	1.23713600	2.14156800	–2.43478600
H	1.94261200	0.56893800	–2.00044400
H	1.84780000	1.86755300	–0.79358100
C	–0.71376100	0.13165000	–2.36725800
H	–0.70908000	0.74516100	–3.27716000
H	–1.75913800	–0.12702000	–2.15059400
H	–0.17418100	–0.79806400	–2.59733000
H	–0.68942600	1.75509400	–0.99316000
N	–4.07836500	–1.88196900	–0.18967600
C	–4.44457300	–1.56924600	–1.57598300
H	–4.06695600	–0.57793200	–1.84512400
H	–3.99830500	–2.30593500	–2.25203500
H	–5.53923200	–1.57669400	–1.72903400
C	–4.56567900	–3.21991000	0.16844500

H –4.10774100 –3.96710100 –0.48591300
H –4.28625800 –3.45162600 1.20076100
H –5.66474500 –3.29770200 0.08073800
C –4.63516200 –0.87513200 0.72167700
H –4.34307700 –1.10681300 1.75104200
H –4.24073800 0.11342200 0.46818400
H –5.73883800 –0.83636600 0.67526100
N 3.93326200 –2.03633200 –0.15188900
C 4.33115600 –1.67381700 –1.51735900
H 3.89372800 –2.38006300 –2.23032200
H 3.96450900 –0.67051400 –1.75445900
H 5.42871200 –1.68474400 –1.64756500
C 4.48748000 –1.07361500 0.80718500
H 4.11415100 –0.07017300 0.58049500
H 4.17323800 –1.33860700 1.82196300
H 5.59233500 –1.05025900 0.78264000
C 4.38938500 –3.39465800 0.16674300
H 4.06352700 –3.66904600 1.17455200
H 3.94974800 –4.10664400 –0.53828600
H 5.48979900 –3.48577600 0.11681600

Table S-19. Geometric coordinates and thermally corrected MP2 energies for $A_2(DMEA)_3$.

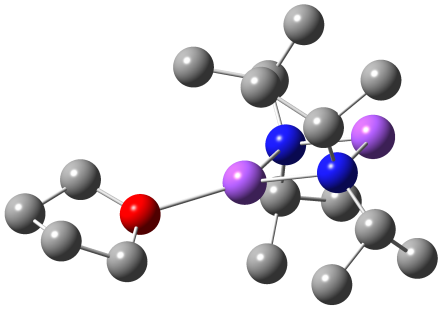


G = –1548.889846 Hartree
G_{MP2} = –1543.524643 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	–1.23734300	1.19589400	–1.67456800
Na	1.41999500	–0.02790100	–1.91529600
N	0.18076200	1.12667500	–3.60178400
C	–0.41904800	0.40380200	–4.72186600
C	0.57427100	–0.53136600	–5.45611000
H	1.47416700	0.01607500	–5.75973400
H	0.13769500	–0.98114900	–6.35992000
H	0.88494400	–1.34971500	–4.78910000
C	–1.63484100	–0.42062000	–4.27158900
H	–2.05418900	–1.01427100	–5.09424900
H	–2.43617200	0.22716200	–3.89194600
H	–1.35542500	–1.12350100	–3.47408300
H	–0.80038200	1.10474300	–5.49320800
C	0.89021000	2.31043700	–4.08167300
C	–0.03676500	3.52166400	–4.35212600
H	0.49682900	4.36057500	–4.82238400
H	–0.46824800	3.88189200	–3.40736800
H	–0.86396400	3.24044600	–5.01410600
C	1.98766400	2.74302500	–3.09628600
H	2.48185700	3.67032900	–3.41264500
H	2.76561500	1.97204100	–3.00517500
H	1.56491900	2.92279600	–2.09760200
H	1.41011900	2.10624100	–5.04124000
N	3.80315300	–0.98314000	–2.13458100
C	4.63898200	–0.17061500	–1.22355800
H	4.52991900	0.87550700	–1.53720200
H	4.19091100	–0.24876900	–0.22559100
C	6.13371300	–0.51565500	–1.13646900
H	6.64131300	–0.40224100	–2.10028600
H	6.61982900	0.16262900	–0.42633300
H	6.30108700	–1.53790100	–0.78115000
C	3.74561000	–2.39276200	–1.73265500
H	3.42920700	–2.46525000	–0.68699800
H	3.00949500	–2.91699700	–2.35187900
H	4.70968100	–2.91758800	–1.84217900
C	4.21469900	–0.86221200	–3.53816000
H	3.47282300	–1.35132100	–4.17724800
H	4.25801700	0.19459000	–3.81994900
H	5.19770000	–1.31848400	–3.74318600
C	–0.46536000	–1.32548700	0.40249700
C	–1.96628200	–1.36430200	0.78760200
H	–2.26709600	–2.33992900	1.19749700
H	–2.59037500	–1.16163100	–0.09567800
H	–2.19557400	–0.60271400	1.54186900
C	–0.20982200	–2.36636300	–0.69883500
H	–0.61519000	–3.35196600	–0.43585700
H	0.86579300	–2.49114400	–0.88143800
H	–0.68368200	–2.06004800	–1.64214900
H	0.08309700	–1.69149200	1.29459600

C	0.31023700	0.81282600	1.17342500
C	1.68340800	0.48632700	1.81373000
H	1.84025000	1.02317000	2.76063100
H	2.49441100	0.76854600	1.12686800
H	1.77656400	–0.58584900	2.02171100
C	0.27405100	2.31174400	0.83810300
H	0.56526500	2.93057700	1.69627500
H	–0.73245700	2.62888100	0.53217600
H	0.96767500	2.54244200	0.01726800
H	–0.44135000	0.66403400	1.97770800
N	–3.44487500	2.45457500	–1.30757000
C	–3.10026500	3.88558300	–1.45369000
H	–2.30025800	4.09897000	–0.73268000
H	–2.66540900	4.00882700	–2.45282300
C	–4.22901300	4.91121500	–1.26350000
H	–3.82561900	5.92095700	–1.39961300
H	–5.03526700	4.77842400	–1.99250600
H	–4.66505400	4.86314300	–0.26009300
C	–4.40049900	2.00016100	–2.32707000
H	–4.00245000	2.21765100	–3.32438800
H	–4.55256600	0.91862200	–2.23604200
H	–5.38764300	2.48539600	–2.23709700
C	–3.93512200	2.12926800	0.03716200
H	–4.03402700	1.04402000	0.13261000
H	–3.21478500	2.47294200	0.78686700
H	–4.91521800	2.58274900	0.26232900
N	–5.67047900	–1.51590500	–2.10577000
C	–4.77592800	–2.54950000	–2.64086100
H	–4.41280100	–2.19154600	–3.61273200
H	–3.90193600	–2.59400000	–1.97899500
C	–5.35310200	–3.96632400	–2.80814100
H	–4.58324900	–4.63383700	–3.21221500
H	–5.68699800	–4.38756300	–1.85342300
H	–6.20200700	–3.98426100	–3.50074000
C	–6.08847100	–1.75796500	–0.73089100
H	–5.20773300	–1.93790100	–0.10481800
H	–6.60255600	–0.86898800	–0.34679200
H	–6.77639900	–2.61584500	–0.61168400
C	–6.80255100	–1.21676500	–2.97247300
H	–7.31601600	–0.32137100	–2.60294200
H	–6.44432500	–1.00786100	–3.98669600
H	–7.55188200	–2.02801800	–3.03367600

Table S-20. Geometric coordinates and thermally corrected MP2 energies for A_2(THF).

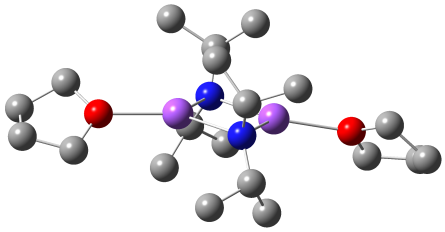


G = –1140.283547 Hartree
G_{MP2} = –1136.500101 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	–0.60417900	2.22714100	0.24108300
Na	2.03359200	1.24318100	–0.12545200
N	1.32071300	3.51466200	0.13361700
C	1.26956900	4.45915500	–0.98018500
C	2.58852200	4.51758900	–1.78910100
H	3.43862200	4.71555900	–1.12511600
H	2.57654800	5.30343900	–2.55802100
H	2.76756700	3.55523400	–2.29057100
C	0.10972200	4.13208300	–1.93607500
H	0.10168900	4.78451800	–2.81804700
H	–0.86234500	4.25561700	–1.43428800
H	0.18412400	3.09690800	–2.30149600
H	1.08351600	5.49165500	–0.62161800
C	1.92784200	4.12739200	1.31314900
C	0.93415600	4.97747700	2.14152400
H	1.42584500	5.51851000	2.96294400
H	0.15825100	4.33144800	2.57913300
H	0.43418500	5.71819800	1.50673200
C	2.56436100	3.06501800	2.22527700
H	2.96419900	3.50252500	3.14876500
H	3.39181800	2.55000700	1.71746700
H	1.82016600	2.31063700	2.52171100
H	2.75156700	4.81286700	1.02581200
C	–0.21334000	–0.76836300	–1.22498800
C	–1.67980400	–0.73541200	–1.71941100
H	–1.84952700	–1.40420600	–2.57557900
H	–1.95138300	0.28510300	–2.02823800
H	–2.36596600	–1.03657100	–0.91934500
C	0.71035400	–0.28202400	–2.35424200
H	0.50576500	–0.79491700	–3.30233800
H	1.76736200	–0.45854500	–2.10863700
H	0.57171900	0.79475400	–2.53371000
H	0.03458200	–1.83858700	–1.07028600
C	–0.36805000	–0.78061700	1.17900000
C	0.76802500	–1.71123200	1.66968600
H	0.44676100	–2.37455900	2.48581800
H	1.61626000	–1.11306100	2.03422300
H	1.12916000	–2.34204300	0.84888700
C	–0.80602700	0.13131900	2.33780000
H	–1.00928600	–0.43297700	3.25640300
H	–1.72639400	0.67891900	2.08313200
H	–0.01958600	0.86297800	2.57703000
H	–1.23461400	–1.43896400	0.96846000
C	5.28897000	1.32327100	–0.91989000
H	5.01938500	2.38104700	–0.85429900
H	5.34378700	1.03868700	–1.97970600
C	6.57336500	0.95697800	–0.17760400
H	7.46810600	1.10863600	–0.78838100
H	6.67334700	1.55969500	0.73280300

C 6.31952400 –0.51703300 0.17579800
H 6.92460000 –0.87290200 1.01465000
H 6.52896800 –1.15727800 –0.68908000
C 4.82109200 –0.52060300 0.49707000
H 4.31796900 –1.45364400 0.22609500
H 4.63425000 –0.31899500 1.55969600
O 4.24371700 0.55658700 –0.27969800

Table S-21. Geometric coordinates and thermally corrected MP2 energies for $A_2(THF)_2$.

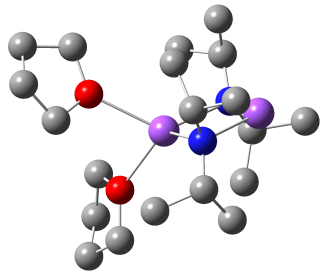


G = –1372.641355 Hartree
G_{MP2} = –1368.082109 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	1.20626700	2.05338800	–0.00334200
Na	–1.65209100	1.69480200	–0.02245300
N	–0.44700600	3.74759500	0.00024000
C	–0.33185500	4.57865000	1.19581300
C	–1.69646700	4.88111600	1.86353600
H	–2.39680600	5.30371700	1.13288900
H	–1.61068100	5.59593800	2.69517300
H	–2.13773000	3.95397500	2.25806900
C	0.60287000	3.93556700	2.23435300
H	0.63768300	4.50875800	3.16962800
H	1.63145500	3.86794900	1.85223600
H	0.26082200	2.92146000	2.48958100
H	0.11599700	5.56553500	0.95804200
C	–0.76469800	4.55945400	–1.17007400
C	0.47386400	5.24904800	–1.79561300
H	0.20425300	5.94379400	–2.60473200
H	1.15500600	4.49201400	–2.21141000
H	1.02616900	5.81791800	–1.03849700
C	–1.46654100	3.72290400	–2.25331600
H	–1.64860600	4.30324600	–3.16692100
H	–2.43755800	3.34887100	–1.89992700
H	–0.84780100	2.85809100	–2.53637900
H	–1.47197600	5.37706200	–0.91437600
C	–0.12810100	–0.83006600	1.19491300
C	1.22913000	–1.13049900	1.87840100
H	1.13449000	–1.84369400	2.71047100
H	1.66515300	–0.20216700	2.27602100
H	1.93803400	–1.55395900	1.15653300
C	–1.07510000	–0.18687900	2.22221600
H	–1.12047800	–0.75964400	3.15729700
H	–2.09914100	–0.11958000	1.82813100
H	–0.73646000	0.82749500	2.48093900
H	–0.57221700	–1.81764400	0.95301800
C	0.33218900	–0.81238400	–1.16585600
C	–0.89830200	–1.50333400	–1.80554600
H	–0.61871800	–2.19775400	–2.61156100
H	–1.57536000	–0.74687200	–2.22900900
H	–1.45865400	–2.07297000	–1.05493400
C	1.04609700	0.02418700	–2.24116700
H	1.23951000	–0.55642700	–3.15229200
H	2.01237900	0.39928300	–1.87617900
H	0.42993300	0.88830400	–2.53182000
H	1.03712600	–1.62914500	–0.90108500
C	–4.87320000	2.53687600	0.34223500
H	–4.35895000	3.50181200	0.35464400
H	–5.11463200	2.25350300	1.37590300
C	–6.11408300	2.50200900	–0.54974500
H	–7.01405800	2.84240700	–0.02924800
H	–5.96797000	3.13618900	–1.43217000

C	–6.16639900	1.02042900	–0.95456500
H	–6.73870800	0.83982000	–1.86916400
H	–6.61172200	0.42150000	–0.15144900
C	–4.68191800	0.67945500	–1.11940500
H	–4.43820700	–0.35593200	–0.86338100
H	–4.33361400	0.87766200	–2.14157700
O	–3.96946700	1.55588700	–0.21491600
C	4.22492800	3.04112000	–1.13130100
H	3.98648400	4.08378300	–0.90156700
H	3.86134100	2.81397000	–2.14213500
C	5.71097300	2.70185400	–0.97873300
H	6.27057900	2.85762900	–1.90566900
H	6.16834900	3.32035300	–0.19754100
C	5.66177700	1.23126300	–0.53528900
H	6.56859300	0.90224500	–0.01936400
H	5.50174900	0.57515700	–1.39904600
C	4.43396600	1.22184600	0.37536200
H	3.91724000	0.25902700	0.41784200
H	4.69123700	1.52871400	1.39840200
O	3.52501400	2.19271700	–0.19103200

Table S-22. Geometric coordinates and thermally corrected MP2 energies for $A_2(THF)_2$.

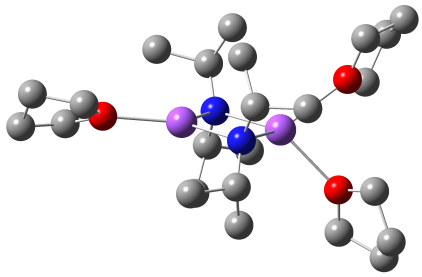


G = –1372.62809295 Hartree
G_{MP2} = –1368.0759101783 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	-1.58521600	1.53530000	-1.15644700
Na	-2.87713800	0.00424900	-0.00033300
N	-1.59018300	-1.53064100	1.15610900
C	-1.78768300	-2.90992200	0.71262000
C	-3.24211300	-3.41765400	0.88711000
H	-3.59686900	-3.26447400	1.91232900
H	-3.33995600	-4.48835200	0.65636900
H	-3.91888000	-2.86825200	0.21345800
C	-1.37758300	-3.09012200	-0.75491300
H	-1.51553000	-4.12682400	-1.08842300
H	-0.32734900	-2.81427700	-0.90403700
H	-1.98683700	-2.45537100	-1.41431100
H	-1.15326900	-3.61188300	1.29368000
C	-1.49742900	-1.47010700	2.61350100
C	-0.09785500	-1.85961700	3.15436000
H	-0.07315500	-1.90343900	4.25289400
H	0.65383300	-1.12802900	2.82566800
H	0.20661500	-2.84324500	2.77785900
C	-1.86350300	-0.07544000	3.13979700
H	-1.76412000	-0.01030300	4.23094500
H	-2.90180300	0.18159800	2.88572000
H	-1.21059500	0.69292200	2.70392700
H	-2.20984700	-2.17099900	3.09412900
C	-1.49234900	1.47441500	-2.61383200
C	-0.09150300	1.85976200	-3.15441500
H	-0.06643100	1.90345200	-4.25294500
H	0.65795900	1.12597600	-2.82553600
H	0.21582300	2.84252000	-2.77793400
C	-1.86243700	0.08082200	-3.14015400
H	-1.76296300	0.01534800	-4.23127100
H	-2.90156200	-0.17311800	-2.88634900
H	-1.21192600	-0.68945400	-2.70408800
H	-2.20258300	2.17740100	-3.09462900
C	-1.77849400	2.91519300	-0.71305200
C	-3.23132500	3.42740200	-0.88765300
H	-3.32586500	4.49841300	-0.65698700
H	-3.90980200	2.88011600	-0.21400000
H	-3.58651300	3.27523700	-1.91287100
C	-1.36792000	3.09418800	0.75450000
H	-1.50253700	4.13135300	1.08793100
H	-0.31857400	2.81500200	0.90369800
H	-1.97923900	2.46145000	1.41391500
H	-1.14184900	3.61515800	-1.29408000
O	1.80851800	1.19172800	1.06568700
C	2.05827200	1.62476400	2.42124900
H	2.20325300	0.73931100	3.04733100
H	1.17534500	2.16670200	2.78389300
C	3.28810700	2.53534200	2.35453000
H	3.29168900	3.28902800	3.14747200
H	4.20895500	1.94623700	2.44214600
C	3.16650800	3.13245700	0.94402300
H	4.11380500	3.51131000	0.54862000
H	2.44037800	3.95352000	0.93785100
C	2.63162000	1.94309100	0.14538500
H	2.01113200	2.22739800	-0.70919000
H	3.44585400	1.29763000	-0.21147100
O	1.80484800	-1.19745100	-1.06557300
C	2.62565600	-1.95119000	-0.14516100
H	2.00422600	-2.23374500	0.70931000
H	3.44167700	-1.30807400	0.21185000

C	3.15725600	-3.14207300	-0.94374000
H	4.10340700	-3.52364300	-0.54820500
H	2.42877600	-3.96104800	-0.93768700
C	3.28076300	-2.54528200	-2.35421400
H	3.28232400	-3.29896500	-3.14716700
H	4.20328700	-1.95878600	-2.44167500
C	2.05352900	-1.63121600	-2.42109600
H	2.20110700	-0.74618300	-3.04716700
H	1.16910800	-2.17064500	-2.78384000

Table S-23. Geometric coordinates and thermally corrected MP2 energies for $A_2(THF)_3$.

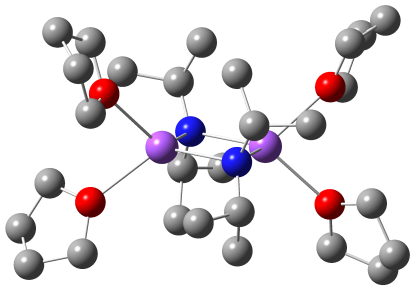


G = –1604.985211 Hartree
G_{MP2} = –1599.656902 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	–1.37221100	1.61422400	–1.05216600
Na	1.53994100	1.61379600	–1.05228800
N	0.00020100	3.22833300	–2.10452100
C	0.08877000	3.28401800	–3.56025400
C	1.48585700	3.71302600	–4.08009100
H	1.79565000	4.66290700	–3.62888000
H	1.50368300	3.84389000	–5.17217800
H	2.23697700	2.95583700	–3.81455000
C	–0.28101300	1.93496200	–4.19370900
H	–0.19112800	1.95836400	–5.28778900
H	–1.31555500	1.65514000	–3.95002100
H	0.37640700	1.13546800	–3.82622700
H	–0.62493100	4.02076200	–3.98500300
C	–0.16966600	4.56833900	–1.54917500
C	–1.60919500	5.13013000	–1.69305900
H	–1.68075200	6.17721000	–1.36389500
H	–2.30792600	4.53653800	–1.08453900
H	–1.95138100	5.08686100	–2.73337900
C	0.21883800	4.60805800	–0.06455500
H	0.10520600	5.61520300	0.35787900
H	1.25810400	4.28938600	0.07653300
H	–0.41973400	3.93512700	0.52524200
H	0.49055800	5.30598200	–2.05452500
C	–0.17016200	–1.34002400	–0.55523300
C	–1.60993800	–1.90126300	–0.41160800
H	–1.68175900	–2.94845800	–0.74035400
H	–2.30821200	–1.30768000	–1.02066800
H	–1.95247900	–1.85740600	0.62856700
C	0.21863400	–1.38016700	–2.03976100
H	0.10458500	–2.38734400	–2.46200900
H	1.25805900	–1.06201000	–2.18078700
H	–0.41953500	–0.70705800	–2.62979500
H	0.48970100	–2.07778300	–0.04957800
C	0.08850600	–0.05575800	1.45573900
C	1.48577900	–0.48418000	1.97556400
H	1.50330800	–0.61634100	3.06750200
H	2.23626400	0.27409600	1.71132800
H	1.79658700	–1.43321500	1.52327600
C	–0.28183700	1.29305300	2.08938900
H	–0.19196000	1.26952200	3.18347000
H	–1.31648000	1.57253500	1.84572900
H	0.37532200	2.09283300	1.72205200
H	–0.62490800	–0.79285900	1.88032900
C	4.17570600	3.53681100	–0.78151000
H	3.52948000	3.88925700	–1.59038600
H	4.97908800	2.92569500	–1.21484000
C	4.73293500	4.65837200	0.09685700
H	5.67012800	5.06897800	–0.29106900
H	4.00785600	5.47658600	0.17591200

C	4.88957800	3.95028500	1.45144000
H	4.91469300	4.63794900	2.30205400
H	5.81108000	3.35583000	1.46814300
C	3.65967400	3.03754700	1.47468900
H	3.81506600	2.10701900	2.02873500
H	2.78606500	3.55177200	1.89606300
O	3.38213800	2.70816600	0.09675700
C	–4.52515100	2.21862300	–2.07414000
H	–4.12564400	1.93427900	–3.05268000
H	–4.46336100	3.30989900	–1.97738200
C	–5.94369300	1.70526000	–1.81711400
H	–6.70987800	2.40018600	–2.17330800
H	–6.09957800	0.74056100	–2.31445400
C	–5.94379400	1.52584200	–0.29097200
H	–6.71174500	0.83293500	0.06535600
H	–6.09686000	2.49093900	0.20647800
C	–4.52659300	1.00877800	–0.03455800
H	–4.12656400	1.29003800	0.94463600
H	–4.46739700	–0.08246900	–0.13368300
O	–3.69850600	1.61405200	–1.05348900
C	3.65634000	0.18912400	–3.58137100
H	3.80751500	1.11964100	–4.13655800
H	2.78359600	–0.32840500	–4.00054600
C	4.88909300	–0.71969200	–3.55952300
H	4.91551800	–1.40721500	–4.41021400
H	5.80869400	–0.12232100	–3.57702800
C	4.73582200	–1.42834700	–2.20484800
H	5.67455100	–1.83632800	–1.81786800
H	4.01305200	–2.24865400	–2.28336300
C	4.17623000	–0.30851100	–1.32568800
H	3.53102700	–0.66298000	–0.51685300
H	4.97824600	0.30420000	–0.89215100
O	3.38065000	0.51904000	–2.20322700

Table S-24. Geometric coordinates and thermally corrected MP2 energies for $A_2(THF)_4$.

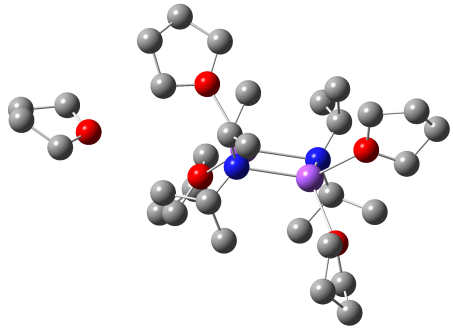


G = –1837.332143 Hartree
G_{MP2} = –1831.236629 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	–1.48782200	–0.00229500	1.93850100
Na	1.48627700	–0.00141900	1.93984900
N	–0.00163300	–0.00349500	3.87816600
C	0.13437100	1.18897300	4.70889200
C	1.53098600	1.34612100	5.36809700
H	1.80641800	0.45078600	5.93751200
H	1.56750300	2.19981300	6.06105900
H	2.29781100	1.50118200	4.59626500
C	–0.17005500	2.46071100	3.90433700
H	–0.06293000	3.36432000	4.51966700
H	–1.19109900	2.43565900	3.50593700
H	0.51659400	2.55967200	3.05253600
H	–0.58942000	1.18923600	5.55306900
C	–0.13652400	–1.19695000	4.70762600
C	–1.53217700	–1.35484100	5.36865100
H	–1.56774700	–2.20941900	6.06056200
H	–2.30018700	–1.50879100	4.59776700
H	–1.80669900	–0.46022200	5.93962700
C	0.16684300	–2.46771800	3.90113400
H	0.06068300	–3.37204300	4.51558200
H	1.18734900	–2.44213700	3.50136400
H	–0.52106400	–2.56577700	3.05023700
H	0.58844000	–1.19820200	5.55080800
C	–0.13581300	1.19354900	–0.82915400
C	–1.53158400	1.35075000	–1.49014200
H	–1.56779500	2.20594600	–2.18124800
H	–2.29986700	1.50327200	–0.71924900
H	–1.80526100	0.45646800	–2.06204100
C	0.16660300	2.46433800	–0.02235500
H	0.05993200	3.36869100	–0.63666700
H	1.18707400	2.43939700	0.37753100
H	–0.52147800	2.56181200	0.82846500
H	0.58911000	1.19565200	–1.67238100
C	0.13539100	–1.19241300	–0.83088500
C	1.53104000	–1.34902400	–1.49225200
H	1.56668100	–2.20253200	–2.18547500
H	2.29914100	–1.50412300	–0.72168600
H	1.80540000	–0.45349200	–2.06186000
C	–0.16734200	–2.46424900	–0.02584200
H	–0.06070800	–3.36781300	–0.64132700
H	–1.18787700	–2.43968900	0.37391400
H	0.52058200	–2.56294400	0.82496400
H	–0.58963800	–1.19308100	–1.67400500
C	4.12582800	–1.29238800	3.40166400
H	3.46195300	–0.84814200	4.14827000
H	4.90709300	–0.56269400	3.14884700
C	4.72534800	–2.63403600	3.82735300
H	5.65829700	–2.51729100	4.38729000
H	4.01704800	–3.18686200	4.45540300

C	4.90703100	–3.34061000	2.47535200
H	4.96996600	–4.42993100	2.55689900
H	5.81708300	–2.98378700	1.97799400
C	3.66199900	–2.88198900	1.71047300
H	3.81334700	–2.80921900	0.62940700
H	2.80812800	–3.54659300	1.89744200
O	3.34661400	–1.56785600	2.21676600
C	–3.66251300	–2.88379200	2.16263700
H	–3.81438900	–2.81331800	3.24377600
H	–2.80812400	–3.54746000	1.97469900
C	–4.90687700	–3.34166600	1.39623000
H	–4.96913500	–4.43086700	1.31257300
H	–5.81739900	–2.98630500	1.89377300
C	–4.72484500	–2.63241000	0.04567800
H	–5.65754800	–2.51513500	–0.51456000
H	–4.01588200	–3.18363700	–0.58303000
C	–4.12634300	–1.29121600	0.47423800
H	–3.46219400	–0.84527800	–0.27112100
H	–4.90816300	–0.56239300	0.72785100
O	–3.34780900	–1.56840300	1.65919000
C	3.65859200	2.88203700	2.16666000
H	3.81582500	2.81214600	3.24711300
H	2.80055900	3.54202000	1.98278500
C	4.89794700	3.34538900	1.39510000
H	4.95337200	4.43473800	1.30866700
H	5.81214700	2.99686400	1.89072200
C	4.71645900	2.63181800	0.04674500
H	5.64837800	2.51857900	–0.51563300
H	4.00249500	3.17713000	–0.58145000
C	4.12695900	1.28847300	0.48051700
H	3.46560600	0.83507700	–0.26278500
H	4.91390400	0.56600900	0.73676600
O	3.34653800	1.56555900	1.66407900
C	–4.12621500	1.28783100	3.40165300
H	–3.46237500	0.83948900	4.14583400
H	–4.91006900	0.56118300	3.14800600
C	–4.72113900	2.62991700	3.83225000
H	–5.65320800	2.51422300	4.39387200
H	–4.00995800	3.17907700	4.46025600
C	–4.90383500	3.34057500	2.48253100
H	–4.96339000	4.42985400	2.56712300
H	–5.81610800	2.98778200	1.98636700
C	–3.66191000	2.88044500	1.71341700
H	–3.81643500	2.81012200	0.63262800
H	–2.80592900	3.54261500	1.89925300
O	–3.34809600	1.56461700	2.21637900

Table S-25. Geometric coordinates and thermally corrected MP2 energies for $A_2(THF)_5$.

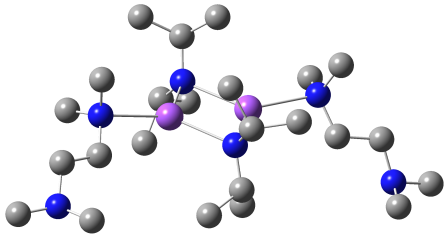


G = –2069.674813 Hartree
G_{MP2} = –2062.804851 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	–1.78822200	0.27070200	1.65397800
Na	–2.93724200	–0.32817500	–0.41245400
N	–1.17278000	–0.58943900	–2.07622200
C	–1.28075400	0.36336700	–3.17544500
C	–2.56471500	0.19633800	–4.03211600
H	–2.65995000	–0.82755400	–4.41251000
H	–2.57516100	0.87127500	–4.90108200
H	–3.45376400	0.41109300	–3.42263300
C	–1.22264200	1.80803500	–2.65933800
H	–1.31008200	2.53537300	–3.47793100
H	–0.27999000	1.99410600	–2.13212200
H	–2.04196700	2.00517300	–1.95471700
H	–0.43566700	0.26783000	–3.89203700
C	–0.79164400	–1.90827400	–2.56980600
C	0.70567400	–2.02701700	–2.96295000
H	0.94227000	–3.00881700	–3.39988200
H	1.34007400	–1.88415600	–2.07697200
H	0.98515800	–1.26513200	–3.70019100
C	–1.11322500	–2.99704400	–1.53627000
H	–0.82914500	–3.99516400	–1.89660400
H	–2.18467500	–3.00678500	–1.30439800
H	–0.57153800	–2.81991700	–0.59733300
H	–1.35833200	–2.18804600	–3.48479000
O	–4.61542700	–2.11609300	–0.56124300
C	–5.22537700	–2.21698300	–1.86609100
H	–4.52249100	–1.81464800	–2.60045700
H	–6.13791300	–1.60471500	–1.88090300
C	–5.54224000	–3.70038000	–2.06178200
H	–6.37132200	–3.86498700	–2.75687600
H	–4.66260100	–4.22938500	–2.44649000
C	–5.85066400	–4.14824900	–0.62479400
H	–5.73527600	–5.22523500	–0.46971600
H	–6.87696300	–3.87457600	–0.35126000
C	–4.84055300	–3.33015400	0.18657700
H	–5.19705300	–3.06250300	1.18586300
H	–3.88486500	–3.85983100	0.29100300
O	–4.93608100	1.04310900	–0.77519900
C	–5.23195100	2.19712500	–1.58882200
H	–5.19417500	1.89836800	–2.64057200
H	–4.45992100	2.95888000	–1.41698800
C	–6.61069800	2.68822500	–1.13799400
H	–6.74630300	3.76152500	–1.30223800
H	–7.40417200	2.15859400	–1.67924300
C	–6.61663400	2.29048300	0.34594500
H	–7.62165200	2.20592100	0.77070800
H	–6.05580900	3.02217200	0.93909200
C	–5.87798300	0.95057300	0.31661100
H	–5.31848300	0.73629900	1.23135600
H	–6.56268500	0.11440400	0.12088200

C	–1.86260700	1.62480900	2.19205100
C	–0.58916500	2.06820200	2.96123800
H	–0.71179500	3.05457800	3.43324700
H	0.26700400	2.12260600	2.27446100
H	–0.33539800	1.35467300	3.75366600
C	–2.14277900	2.64573400	1.07988300
H	–2.18627700	3.67132800	1.47118900
H	–3.09424900	2.42698600	0.58123100
H	–1.35403100	2.61724800	0.31598800
H	–2.69718000	1.73595300	2.91868500
C	–1.97169700	–0.71414300	2.71511200
C	–3.44457600	–0.87311500	3.17898000
H	–3.53689800	–1.54679400	4.04405600
H	–4.05647300	–1.28150700	2.36244300
H	–3.87633000	0.09229800	3.46815500
C	–1.43913000	–2.08994100	2.29003200
H	–1.58685900	–2.84288100	3.07623100
H	–0.36883400	–2.03742000	2.05980400
H	–1.95653200	–2.44861400	1.38967900
H	–1.40329900	–0.44426300	3.63156200
O	1.87446100	–1.25867900	0.89978700
C	2.35697800	–2.61313500	0.76976600
H	2.65213600	–2.78124700	–0.27057700
H	1.53353200	–3.29773500	1.01207000
C	3.52184300	–2.74922200	1.75758400
H	3.62739600	–3.76974900	2.13899600
H	4.45850900	–2.45254100	1.27417800
C	3.14454100	–1.72649400	2.84008200
H	3.99875600	–1.39162300	3.43707200
H	2.39079700	–2.14043900	3.52059300
C	2.54298800	–0.60185800	1.99827900
H	1.80159100	0.00300200	2.52751200
H	3.32447700	0.05672700	1.59864100
O	1.73941100	1.68764700	–0.40652100
C	2.72400300	1.26619700	–1.38244400
H	2.22198100	0.62789700	–2.11573300
H	3.49647300	0.67883900	–0.87192500
C	3.29450600	2.55369000	–1.98653700
H	4.32813000	2.43182500	–2.32545400
H	2.69233700	2.87922000	–2.84298400
C	3.14680000	3.54778400	–0.82443200
H	3.14094100	4.59469800	–1.14330300
H	3.96049400	3.41560700	–0.10082700
C	1.81314200	3.11317400	–0.21379300
H	1.73010100	3.31993800	0.85694100
H	0.96645800	3.59064200	–0.72616400
C	5.70403000	–1.53748800	–1.65744200
H	4.79981400	–1.35290300	–2.24644800
H	5.77168200	–2.61780100	–1.46083000
C	6.98428200	–1.01565900	–2.31603800
H	7.42975900	–1.73816400	–3.00654800
H	6.78032800	–0.09373300	–2.87381500
C	7.86164100	–0.71814500	–1.09032400
H	8.65953800	0.00394800	–1.28873400
H	8.32472800	–1.64101500	–0.72139400
C	6.82901200	–0.19549700	–0.08380900
H	7.08323100	–0.43004900	0.95606700
H	6.70532200	0.89399800	–0.16742200
O	5.58299000	–0.83304300	–0.41016300

Table S-26. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_1\text{-TMEDA})_2$.

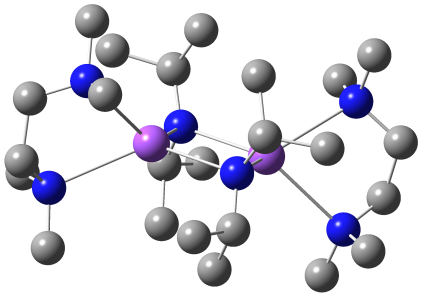


G = –1603.013461 Hartree
G_{MP2} = –1597.523737 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	1.42691500	–1.81857700	0.60446700
Na	–1.48487200	–1.79704200	0.49807000
N	–0.05599700	–3.63705700	1.06709000
C	0.07081200	–4.76894300	0.14968200
C	–1.28640000	–5.41429200	–0.22757800
H	–1.85862900	–5.67286000	0.67136200
H	–1.16166900	–6.33306600	–0.81876600
H	–1.88914000	–4.71137400	–0.82087100
C	0.80159700	–4.36828200	–1.14046300
H	0.85533700	–5.19875200	–1.85569500
H	1.83126900	–4.04766500	–0.93110000
H	0.28136100	–3.54060600	–1.64180600
H	0.67697800	–5.58293200	0.59923600
C	–0.20431800	–4.11221900	2.44108100
C	1.13698100	–4.50643800	3.10964300
H	0.99242800	–4.97613100	4.09342700
H	1.76271100	–3.61326900	3.25129600
H	1.69409800	–5.21230500	2.48282800
C	–0.90291800	–3.06631300	3.32201800
H	–0.97116600	–3.38898600	4.36872800
H	–1.92484100	–2.87287500	2.96900700
H	–0.35210200	–2.11513000	3.30866000
H	–0.84147600	–5.01998700	2.48623000
N	–4.03772500	–1.60202900	0.58981800
C	–4.39361200	–1.23522800	1.96578600
H	–4.09186700	–2.03342500	2.65163300
H	–3.86105100	–0.31964300	2.24581600
H	–5.47253600	–1.05230900	2.10126300
C	–4.44538000	–0.54827100	–0.34708300
H	–3.90303000	0.37273000	–0.11041800
H	–4.18778800	–0.84484300	–1.36874900
H	–5.52556500	–0.32614200	–0.31323100
C	–4.52448600	–2.94316900	0.20611600
H	–4.19300200	–3.13735500	–0.82092900
H	–4.01006400	–3.66389800	0.85139600
C	–6.04842900	–3.17153900	0.26105800
H	–6.55429200	–2.33250700	–0.23032500
H	–6.39606400	–3.18163700	1.31430000
N	–6.44689100	–4.38820700	–0.44608000
C	–7.89171900	–4.43709700	–0.63377300
H	–8.15489600	–5.32191100	–1.22338200
H	–8.45611200	–4.48216500	0.31900300
H	–8.22503100	–3.55079900	–1.18452700
C	–5.97038200	–5.60327500	0.20706200
H	–6.35563800	–5.71730300	1.24066700
H	–6.29339100	–6.47470200	–0.37177500
H	–4.87783000	–5.62027000	0.24452100
N	3.97358400	–1.71912700	0.92709400
C	4.25327500	–1.71751200	2.36791500

H	3.73262100	–0.87583300	2.83810300
H	3.88206400	–2.64446500	2.81611900
H	5.32643700	–1.62176400	2.60306500
C	4.43644100	–2.94857600	0.25261400
H	3.87202400	–3.77930800	0.69126600
H	4.14684500	–2.87994600	–0.80317700
C	5.94827300	–3.24855100	0.30385900
H	6.25392400	–3.50985300	1.33726400
H	6.50173800	–2.34347700	0.02909000
N	6.33110700	–4.29271500	–0.64667900
C	5.80180900	–5.60446900	–0.28751200
H	6.11479400	–6.33824000	–1.03741300
H	6.15393700	–5.95574300	0.70350700
H	4.70861600	–5.59198600	–0.27643500
C	7.77891200	–4.35046400	–0.80937200
H	8.31407100	–4.62581700	0.12125100
H	8.03215700	–5.09163300	–1.57512200
H	8.15468200	–3.37695500	–1.14234800
C	4.46918800	–0.49029300	0.29699300
H	4.25056300	–0.51060400	–0.77492500
H	3.95134300	0.37094600	0.73154600
H	5.55325700	–0.33582100	0.43115900
C	–0.05168300	0.44249600	–1.39287600
C	1.34242700	0.74451200	–1.99692800
H	1.27641900	1.19010100	–3.00013200
H	1.92862500	–0.18307500	–2.07954500
H	1.90141900	1.43973500	–1.36003100
C	–0.76323500	–0.58727700	–2.28350300
H	–0.75838100	–0.29025200	–3.33993500
H	–1.81194800	–0.71324700	–1.98185200
H	–0.26787600	–1.56587700	–2.21891700
H	–0.63409600	1.38151500	–1.49340200
C	0.11017800	1.14885400	0.89582800
C	–1.24143400	1.85779000	1.16511100
H	–1.11950300	2.78700000	1.74054700
H	–1.90865400	1.19386900	1.73458800
H	–1.74347300	2.11307100	0.22462700
C	0.73155900	0.75054600	2.24298800
H	0.76449300	1.59312900	2.94530700
H	1.76136800	0.38959900	2.11347200
H	0.14738800	–0.04949200	2.71921600
H	0.77973600	1.92672700	0.47237300

Table S-27. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_2\text{-TMEDA})_2$.

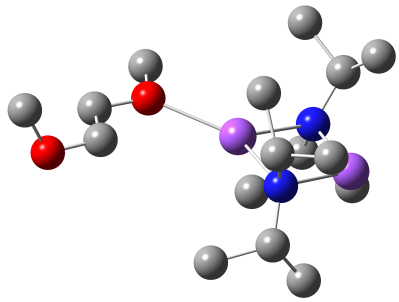


G = –1603.019019 Hartree
G_{MP2} = –1597.547374 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
Na	3.05721500	–0.00011800	–0.00031400
N	1.52818100	–1.92051300	–0.00165300
C	1.37796100	–2.74104600	–1.19936200
C	0.04645900	–3.53419800	–1.28550800
H	0.01751900	–4.18331300	–2.17222800
H	–0.80450200	–2.83982600	–1.34527800
H	–0.10699600	–4.17212000	–0.40849500
C	1.49765900	–1.88234000	–2.46530000
H	1.41558700	–2.49107200	–3.37530500
H	2.45672500	–1.35301900	–2.49669300
H	0.70505200	–1.12383400	–2.50505100
H	2.17843100	–3.50846800	–1.28437500
C	1.67918700	–2.74345800	1.19428200
C	3.01109200	–3.53615000	1.27860900
H	3.04044800	–4.18693200	2.16408800
H	3.86177200	–2.84153500	1.33958200
H	3.16469300	–4.17235700	0.40037900
C	1.55929000	–1.88742000	2.46200900
H	1.64163300	–2.49799800	3.37074900
H	0.60004800	–1.35850500	2.49451100
H	2.35163800	–1.12872200	2.50323900
H	0.87914700	–3.51151000	1.27787900
N	1.52844100	1.92048300	0.00154900
C	1.67930200	2.74344700	–1.19438100
C	3.01110200	3.53631700	–1.27872000
H	3.16462100	4.17254400	–0.40049100
H	3.04039500	4.18710400	–2.16420000
H	3.86187100	2.84180100	–1.33966700
C	1.55955400	1.88736900	–2.46209600
H	1.64187400	2.49793700	–3.37084300
H	0.60037700	1.35833800	–2.49462500
H	2.35200100	1.12876100	–2.50328500
H	0.87912400	3.51135700	–1.27802900
C	1.37795100	2.74095400	1.19927200
C	0.04634100	3.53391800	1.28535500
H	0.01726000	4.18291200	2.17216000
H	–0.80455600	2.83946200	1.34497100
H	–0.10710300	4.17194700	0.40841800
C	1.49765700	1.88220700	2.46517600
H	1.41551600	2.49089200	3.37520800
H	2.45676100	1.35296400	2.49653900
H	0.70510400	1.12364000	2.50488700
H	2.17829300	3.50849000	1.28440900
N	5.27016700	–0.43275500	–1.49561500
C	5.38410100	–1.89352600	–1.58920900
H	4.54313000	–2.28878700	–2.16416300
H	5.34019300	–2.35007800	–0.59827500
H	6.32533600	–2.20382200	–2.08153700
C	5.22320700	0.14395700	–2.84377700

H	5.08006900	1.22677500	–2.78041500
H	4.37991500	–0.28000600	–3.39646500
H	6.14721400	–0.05522600	–3.41828000
C	6.39718100	0.14812200	–0.75051000
C	6.39706900	–0.14855000	0.75091500
N	5.27014900	0.43264300	1.49589600
C	5.22301300	–0.14384800	2.84414000
H	6.14697000	0.05537400	3.41871800
H	5.07982800	–1.22666700	2.78094600
H	4.37968400	0.28024400	3.39666900
C	5.38435800	1.89340600	1.58922000
H	5.34036300	2.34978600	0.59820500
H	6.32571900	2.20362800	2.08135000
H	4.54353600	2.28889700	2.16423800
H	7.36164800	0.20894800	1.16241000
H	6.37784400	–1.23132500	0.91153000
H	7.36169200	–0.20964400	–1.16192300
H	6.37827200	1.23090300	–0.91111700
N	–2.21322400	–0.43692200	1.49480700
C	–2.32798100	–1.89779000	1.58514300
H	–2.28553500	–2.35206500	0.59309300
H	–3.26888200	–2.20864100	2.07779800
H	–1.48660800	–2.29491700	2.15821800
C	–2.16548900	0.13677400	2.84420700
H	–2.02168500	1.21963900	2.78321400
H	–1.32230800	–0.28895200	3.39570100
H	–3.08943400	–0.06309000	3.41858300
C	–3.33991400	0.14637800	0.75117200
C	–3.33983100	–0.14641800	–0.75114600
N	–2.21308400	0.43689900	–1.49468500
C	–2.16528800	–0.13678600	–2.84409200
H	–2.02143000	–1.21964600	–2.78310700
H	–1.32212300	0.28899400	–3.39556500
H	–3.08923400	0.06303700	–3.41847700
C	–2.32786100	1.89777500	–1.58505400
H	–2.28558800	2.35205200	–0.59300600
H	–3.26867200	2.20858900	–2.07787300
H	–1.48638200	2.29491000	–2.15798300
H	–3.32032900	–1.22877000	–0.91452600
H	–4.30454500	0.21182500	–1.16166800
H	–3.32047100	1.22872800	0.91458000
H	–4.30465600	–0.21191400	1.16158300

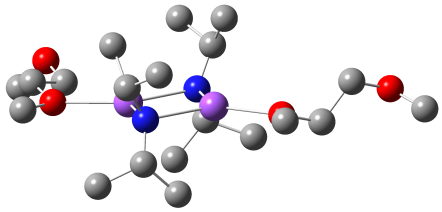
Table S-28. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_1$-DME).



G = –1216.65947528 Hartree
G_{MP2} = –1212.6531545446 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	-2.24436400	-0.54704800	0.02356700
Na	-0.07075700	-2.39893300	-0.05191500
N	-2.42886800	-2.86504200	-0.04166800
C	-3.19299600	-3.34025600	1.11163600
C	-2.61466200	-4.62910700	1.74342800
H	-2.50122400	-5.41267700	0.98458900
H	-3.25786400	-5.03066000	2.53941700
H	-1.62460300	-4.42836900	2.17760200
C	-3.29703200	-2.25684200	2.19832100
H	-3.79240600	-2.62603700	3.10467100
H	-3.88085600	-1.39277700	1.84428100
H	-2.29826300	-1.90466000	2.49521500
H	-4.23631600	-3.58290700	0.82676600
C	-2.83730300	-3.56005000	-1.26183400
C	-4.13336300	-2.99108500	-1.88975300
H	-4.48996900	-3.59655700	-2.73531000
H	-3.95805100	-1.96908000	-2.25840900
H	-4.93971800	-2.94660300	-1.14866300
C	-1.71907700	-3.53070200	-2.31660200
H	-2.03450200	-3.98861000	-3.26225000
H	-0.82857700	-4.07386000	-1.97096200
H	-1.42430900	-2.49516600	-2.54293400
H	-3.03959500	-4.63289700	-1.06180100
O	1.53508200	-4.15986400	0.00642500
C	2.93126200	-4.21705300	-0.28470700
C	3.50678200	-2.80139900	-0.29847500
O	4.88128200	-2.81979400	-0.63681700
C	5.75220700	-2.99945400	0.46548700
H	6.77055800	-2.95766700	0.07109500
H	5.61039800	-3.96933600	0.96577600
H	5.62531800	-2.19972900	1.21139300
H	3.34309400	-2.31479100	0.67534500
H	2.99942200	-2.20289000	-1.06162800
H	3.43669300	-4.83346400	0.47354900
H	3.09236300	-4.68837400	-1.26541200
C	0.95875000	-5.46072700	0.11356500
H	1.42587700	-6.02453500	0.93290800
H	1.08281400	-6.02065900	-0.82388100
H	-0.10419400	-5.33018700	0.32314000
C	0.69860400	0.49138600	1.18590400
C	0.03042100	1.73352700	1.82536400
H	0.62929600	2.15398100	2.64580800
H	-0.95655000	1.46422700	2.23077400
H	-0.11835300	2.52559600	1.08276900
C	0.81580600	-0.60873200	2.25284900
H	1.27694700	-0.23663600	3.17604800
H	1.42863700	-1.44961000	1.89864300
H	-0.17755800	-0.99812800	2.52057400
H	1.73852900	0.79326300	0.94079400
C	0.31922900	0.81390500	-1.17328500
C	1.61127600	0.36509200	-1.89620800
H	1.89857500	1.04972900	-2.70695800
H	1.47379500	-0.63484600	-2.33400600
H	2.44971900	0.31344300	-1.19208900
C	-0.84137600	0.82344000	-2.18359100
H	-0.58681900	1.36898100	-3.10070300
H	-1.73391600	1.30788300	-1.75808500
H	-1.10928200	-0.20063300	-2.48377900
H	0.47962900	1.87296400	-0.89100200

Table S-29. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_1\text{-DME})_2$.

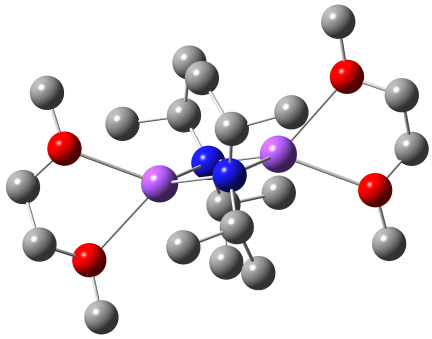


G = –1525.39470430 Hartree
G_{MP2} = –1520.3880625878 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	-1.42929000	1.88197900	-0.01952600
Na	1.44889400	1.88190100	-0.05501500
N	0.00096600	3.78087600	-0.05863900
C	-0.24086900	4.60620100	-1.24086300
C	1.04646300	5.21274200	-1.85223900
H	1.61916200	5.75965700	-1.09361200
H	0.82900600	5.91522700	-2.66967700
H	1.68773700	4.41506600	-2.25434000
C	-0.97697300	3.81244000	-2.33285200
H	-1.09891200	4.39808400	-3.25275200
H	-1.98055000	3.50987200	-2.00259800
H	-0.41614100	2.90459800	-2.59749200
H	-0.89582500	5.47044500	-1.00264400
C	0.16667300	4.60940200	1.13366200
C	-1.17149900	5.11668900	1.72855100
H	-1.02031400	5.83033300	2.55133600
H	-1.75567100	4.27059900	2.11998800
H	-1.77376200	5.61989500	0.96273600
C	0.93401900	3.85440300	2.23116000
H	1.00741900	4.43929000	3.15657400
H	1.95801400	3.61478700	1.91363000
H	0.42528900	2.91261300	2.48166600
H	0.76428900	5.51982000	0.91534300
O	3.82644500	2.22645600	-0.08918600
C	4.89639300	1.35610800	0.27638600
C	4.50477900	-0.08538100	-0.04885700
O	5.51221500	-0.99175200	0.36103300
C	6.54363600	-1.18842300	-0.58855500
H	7.21713500	-1.94052600	-0.16995800
H	7.12168500	-0.27276700	-0.78562300
H	6.14310100	-1.56045800	-1.54440300
H	4.29578600	-0.18421300	-1.12553700
H	3.59534800	-0.35467200	0.49736300
H	5.80374900	1.64296600	-0.27525200
H	5.11081600	1.44899200	1.35146500
C	4.19972000	3.60104400	-0.01107300
H	5.01889400	3.81848000	-0.71050900
H	4.51827300	3.86399400	1.00755000
H	3.32288400	4.19083400	-0.28274300
O	-3.76643400	2.01519700	-0.13017500
C	-4.58680100	0.92799400	-0.57020800
C	-5.36020400	0.27844600	0.58553900
O	-6.12225500	-0.82559300	0.13157000
C	-7.40894900	-0.48783100	-0.35235300
H	-7.37394400	0.17281400	-1.23167200
H	-8.01525300	0.00083300	0.42668000
H	-7.89221300	-1.42442400	-0.64131300
H	-4.64484300	-0.10902800	1.31866300
H	-6.00264700	1.01311500	1.09627100
H	-3.91043500	0.18775300	-1.00646700
H	-5.26782500	1.27671800	-1.35954700
C	-4.45371000	3.25746700	0.00888800
H	-5.23049700	3.20898300	0.78193200
H	-4.91135300	3.55459200	-0.94498100
H	-3.70802900	4.00006700	0.29974100
C	0.16368600	-0.84811300	-1.17887900
C	-1.17873100	-1.35109500	-1.76676400
H	-1.03596700	-2.08527600	-2.57297700

H	-1.74874500	-0.50522200	-2.17984800
H	-1.79168700	-1.82450700	-0.99102300
C	0.94310200	-0.11951900	-2.28541600
H	1.00899000	-0.71729000	-3.20320600
H	1.97085100	0.10669900	-1.96891800
H	0.44855500	0.82654300	-2.54974300
H	0.75268800	-1.75834100	-0.94053200
C	-0.21719000	-0.81254200	1.19687900
C	1.09425400	-1.32630100	1.83836300
H	0.91080100	-2.02076600	2.67095900
H	1.68247300	-0.48213200	2.22801400
H	1.70801000	-1.85260700	1.09804400
C	-1.02462800	-0.04545300	2.25747700
H	-1.12789700	-0.61680500	3.18854200
H	-2.03928500	0.18061600	1.89905600
H	-0.53073000	0.90320900	2.51334300
H	-0.81418700	-1.71720300	0.96194600

Table S-30. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_2\text{-DME})_2$.

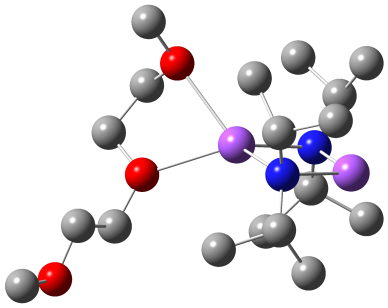


G = –1525.40916130 Hartree
G_{MP2} = –1520.3982444128 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	-1.49338400	-1.91330300	-0.00120700
Na	-2.98435800	0.00208500	-0.00038100
N	-1.49115300	1.91515700	-0.00051800
C	-1.70789100	2.75492700	1.17422800
C	-3.15270800	3.31173300	1.27461900
H	-3.43425900	3.83893500	0.35597000
H	-3.27441400	4.01353500	2.11337800
H	-3.86537400	2.48644300	1.41214800
C	-1.36839200	2.00570000	2.46994300
H	-1.56046700	2.61907300	3.36042400
H	-0.31037700	1.71681200	2.47756700
H	-1.96752900	1.08955600	2.56541800
H	-1.04603400	3.64652300	1.16513200
C	-1.27388400	2.75470100	-1.17530700
C	0.17101100	3.31139300	-1.27528200
H	0.29304100	4.01305300	-2.11410700
H	0.88359000	2.48597600	-1.41248100
H	0.45235400	3.83870300	-0.35663500
C	-1.61272200	2.00526000	-2.47106000
H	-1.42054100	2.61865000	-3.36150100
H	-2.67064400	1.71601200	-2.47910400
H	-1.01328600	1.08929800	-2.56627700
H	-1.93571800	3.64633700	-1.16664500
O	-5.06510500	0.14310600	-1.40493900
C	-6.21126600	-0.30099200	-0.69236000
C	-6.21171300	0.30011400	0.69753500
H	-7.12675200	-0.02683100	1.21647000
H	-6.22207100	1.39927300	0.63804700
O	-5.06278700	-0.13899000	1.40870200
C	-5.12856400	0.17881100	2.79444200
H	-4.20555600	-0.18247200	3.25026900
H	-5.21039900	1.26296000	2.95151400
H	-5.98668200	-0.32116200	3.26612400
H	-7.12833600	0.02208200	-1.21011100
H	-6.21685100	-1.40018300	-0.63297600
C	-5.13261200	-0.17196800	-2.79122600
H	-5.99295600	0.32667600	-3.26024200
H	-4.21143100	0.19279900	-3.24798000
H	-5.21177900	-1.25599300	-2.95048400
C	-1.27736800	-2.75341600	1.17341300
C	0.16737100	-3.31030200	1.27455400
H	0.28852000	-4.01236200	2.11317600
H	0.87995200	-2.48505900	1.41280800
H	0.44951000	-3.83723200	0.35593000
C	-1.61760700	-2.00452800	2.46912600
H	-1.42610800	-2.61815800	3.35955400
H	-2.67560800	-1.71558800	2.47618300
H	-1.01845000	-1.08845600	2.56520100
H	-1.93925000	-3.64499300	1.16367000
C	-1.70964500	-2.75247400	-1.17644300
C	-3.15437200	-3.30935400	-1.27768100
H	-3.27565400	-4.01084300	-2.11675700
H	-3.86693200	-2.48398500	-1.41528000
H	-3.43637100	-3.83689800	-0.35937000
C	-1.37000200	-2.00251000	-2.47167500
H	-1.56144200	-2.61560900	-3.36247700
H	-0.31212100	-1.71308700	-2.47886100
H	-1.96955500	-1.08662900	-2.56697300

H	-1.04767100	-3.64400600	-1.16762400
O	2.08075300	-0.14060700	-1.40466100
C	3.22757000	0.30110500	-0.69165000
C	3.22671700	-0.30083500	0.69788300
H	4.14223500	0.02417900	1.21717800
H	3.23512500	-1.39997300	0.63776600
O	2.07842800	0.13991800	1.40908900
C	2.14383300	-0.17776800	2.79487300
H	1.22116600	0.18450700	3.25061000
H	2.22456400	-1.26197400	2.95211500
H	3.00243200	0.32141000	3.26652100
H	4.14416000	-0.02321500	-1.20947200
H	3.23501100	1.40025000	-0.63158100
C	2.14859300	0.17595500	-2.79058200
H	3.00826300	-0.32326400	-3.26022800
H	1.22691200	-0.18708100	-3.24771000
H	2.22915900	1.26006000	-2.94860000

Table S-31. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_2$-diglyme).

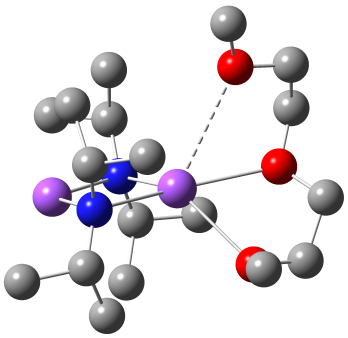


G = –1370.435942 Hartree
G_{MP2} = –1365.9498254213 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	-0.05457500	2.45799800	0.11836700
Na	-2.02479800	1.83451200	-0.92418700
N	-2.11914400	-0.46053000	-1.15997900
C	-2.01413700	-1.04641700	-2.49426800
C	-2.99272800	-0.42328500	-3.52156700
H	-4.02231400	-0.44233000	-3.14592700
H	-2.98033100	-0.95069800	-4.48642300
H	-2.72257900	0.62725500	-3.71068000
C	-0.58265400	-0.93120100	-3.03907700
H	-0.50191300	-1.32115800	-4.06193300
H	0.12693600	-1.48171300	-2.40939800
H	-0.26372300	0.12124900	-3.06651400
H	-2.24667200	-2.13167600	-2.47390000
C	-3.25823700	-1.02199700	-0.43342100
C	-2.95793600	-2.39154000	0.22385400
H	-3.85761800	-2.84593900	0.66384400
H	-2.20779500	-2.27526900	1.01675800
H	-2.56351100	-3.09622400	-0.51831400
C	-3.75982900	-0.05200600	0.64940400
H	-4.55440200	-0.49452600	1.26295100
H	-4.17253900	0.86714300	0.20458400
H	-2.94258500	0.23129000	1.32854700
H	-4.12193500	-1.19142900	-1.10855600
C	0.69587900	3.35666800	-0.75762700
C	2.21803900	3.07717600	-0.75811800
H	2.78466200	3.83420300	-1.31957600
H	2.42033400	2.09702100	-1.21156900
H	2.60499700	3.06033800	0.26755800
C	0.17896500	3.29994100	-2.20506700
H	0.79323000	3.90077100	-2.88711000
H	-0.84975200	3.68666800	-2.27766000
H	0.18949100	2.26760700	-2.58331000
H	0.57950000	4.41248800	-0.43835800
C	-0.02934100	2.95237200	1.49369300
C	-1.11960800	4.01326300	1.78289300
H	-1.02241100	4.45674900	2.78464200
H	-2.11894100	3.55765300	1.71259000
H	-1.06931600	4.82821500	1.05121400
C	-0.16143100	1.80164600	2.50247400
H	-0.21021000	2.16418400	3.53755700
H	0.69703700	1.12178100	2.42440400
H	-1.07838800	1.22278600	2.31675200
H	0.93999800	3.44129600	1.72135500
O	0.33550100	-1.81339200	1.70079700
C	0.80145800	-1.84902000	3.04375800
H	1.89174900	-1.72648400	3.10881900
H	0.51905900	-2.79552900	3.52581700
H	0.32099300	-1.02043800	3.56619200
C	0.83215400	-2.86436400	0.87667200
C	2.18925800	-2.53345100	0.27466000
H	2.94932800	-2.40638900	1.05826800
H	2.50887600	-3.36442600	-0.37355000
O	2.04589400	-1.34047000	-0.49024000
C	3.15449100	-1.02293200	-1.33154600
H	2.77926300	-0.31695500	-2.07678400
H	3.50238200	-1.92296900	-1.85726900

C	4.31214300	-0.38341000	-0.56626500
H	4.69997000	-1.06478100	0.21108500
H	3.96023200	0.53197300	-0.06480600
O	5.31379700	-0.09590300	-1.51832800
C	6.42847700	0.57217300	-0.96313500
H	6.92094000	-0.03570600	-0.18695300
H	7.13517700	0.74825100	-1.77792400
H	6.14243900	1.53868700	-0.52019800
H	0.09643700	-2.98802100	0.07641700
H	0.89258200	-3.80513000	1.44341600

Table S-32. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_{>2}$-diglyme).

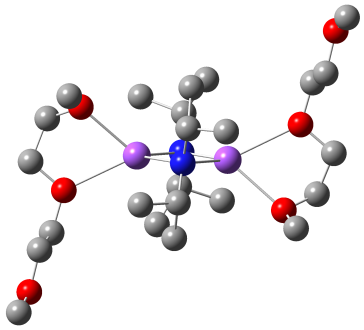


G = –1370.43597530 Hartree
G_{MP2} = –1365.9545961612 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	-2.41730200	-0.22824500	0.68195100
Na	-1.95927700	2.02869500	0.67971900
N	0.22224700	2.49924700	0.09876800
C	0.95021500	3.19051300	1.16112800
C	0.43366600	4.62223600	1.46039100
H	0.39339200	5.23825900	0.55579900
H	1.07096800	5.14427500	2.18825700
H	-0.58441000	4.57773900	1.87867300
C	0.91672400	2.38972500	2.47002300
H	1.48451800	2.89537100	3.26194100
H	1.33053400	1.38292300	2.34236000
H	-0.11437100	2.28078400	2.83836100
H	2.02554200	3.30854800	0.90608400
C	0.54417000	3.05982800	-1.21399800
C	1.93497800	2.63936000	-1.75383500
H	2.16745900	3.13384400	-2.70784800
H	1.97587400	1.55316600	-1.90658100
H	2.73051500	2.90302300	-1.04725200
C	-0.52297500	2.68133800	-2.24977000
H	-0.27894800	3.07289300	-3.24552900
H	-1.50688500	3.08277900	-1.96869700
H	-0.62161200	1.59069700	-2.34171800
H	0.55729300	4.16835500	-1.19199200
C	-2.55419800	-0.97500700	1.93124400
C	-1.91755600	-2.38744500	1.87631800
H	-2.09638300	-2.95986100	2.79839900
H	-0.83096600	-2.31190000	1.72683700
H	-2.33174400	-2.97021800	1.04545900
C	-1.95027100	-0.19869700	3.11009500
H	-2.00562400	-0.76865700	4.04725500
H	-2.48263200	0.74960300	3.26920100
H	-0.89388000	0.03658300	2.92506500
H	-3.61798000	-1.13890600	2.19289300
C	-3.44078900	-0.62668900	-0.28225700
C	-4.86379000	-0.11147200	0.05623200
H	-5.62018700	-0.51305400	-0.63294600
H	-4.89260300	0.98675700	-0.01553200
H	-5.16561200	-0.38434000	1.07311000
C	-3.08701400	-0.15262800	-1.69893500
H	-3.85105700	-0.45933700	-2.42480400
H	-2.12134700	-0.54855900	-2.03134000
H	-3.02930600	0.94506900	-1.74137400
H	-3.53068200	-1.73475500	-0.34260500
O	0.08605600	-1.77307600	-1.90983100
C	-0.49761100	-3.05195300	-1.68210100
H	0.09105300	-3.65506500	-0.97675600
H	-0.59901300	-3.60349800	-2.62756900
H	-1.48460500	-2.87242300	-1.25543900
C	1.39565000	-1.81755900	-2.46319200
C	2.46193800	-1.90502200	-1.38098700
H	2.35722900	-2.83230700	-0.79856200
H	3.46121800	-1.90594600	-1.84500800
O	2.29930300	-0.75979900	-0.55683800
C	3.30675200	-0.54735600	0.42528300
H	3.19978400	0.49906500	0.72262000
H	4.30569200	-0.68689000	-0.01558800

C	3.15751800	-1.44331100	1.64576900
H	3.95861500	-1.19265300	2.36182400
H	3.27760100	-2.50772800	1.38193900
O	1.88346600	-1.21921000	2.21680200
C	1.70149000	-1.91144800	3.44162800
H	2.44065300	-1.59094400	4.19115200
H	0.69850700	-1.67382800	3.79799500
H	1.78767300	-2.99996300	3.30302200
H	1.52609300	-0.88346400	-3.01823200
H	1.49590400	-2.65857000	-3.16499100

Table S-33. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_2$-diglyme$)_2$.

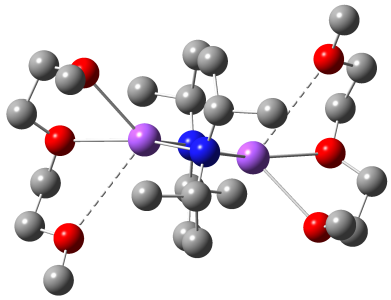


G = –1832.944252 Hartree
G_{MP2} = –1826.9718314106 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	1.30053300	1.91850100	0.68995000
Na	2.60017400	-0.00192700	1.37628600
N	1.29976800	-1.91448500	0.68591900
C	0.72848800	-2.76146400	1.73262600
C	1.77535800	-3.24166000	2.77075700
H	2.63703100	-3.69791100	2.26855500
H	1.36399000	-3.98335300	3.47190600
H	2.13684600	-2.38663300	3.36042000
C	-0.42002600	-2.06239800	2.47317300
H	-0.81414800	-2.68040900	3.29089900
H	-1.24677500	-1.84792500	1.78447700
H	-0.08197100	-1.11453500	2.91252600
H	0.28761700	-3.68369600	1.29992700
C	1.87107100	-2.75892800	-0.36284800
C	0.82418200	-3.23655000	-1.40215100
H	1.23559900	-3.97640800	-2.10521200
H	0.46254000	-2.38007200	-1.98961000
H	-0.03741600	-3.69419400	-0.90108700
C	3.01964300	-2.05811900	-1.10166800
H	3.41357600	-2.67408900	-1.92101700
H	3.84653800	-1.84553900	-0.41253700
H	2.68170000	-1.10907600	-1.53854200
H	2.31182900	-3.68224500	0.06763200
O	5.21610900	-0.11319200	1.35148300
C	5.79369300	-0.10014600	2.65138100
C	4.72504600	-0.51454300	3.65353400
O	3.55964100	0.30097300	3.60040800
C	3.70831500	1.58739200	4.19285500
H	4.43370900	2.20935300	3.65241200
H	4.02123600	1.49420400	5.24278200
H	2.73111500	2.06943600	4.14517300
H	4.38246500	-1.52791800	3.42486700
H	5.15243200	-0.50926500	4.66841800
H	6.19568800	0.89434500	2.89102400
H	6.62707900	-0.81839600	2.70803900
C	6.15476700	-0.03127900	0.27963700
H	5.62008500	-0.35003500	-0.61803100
H	6.98614600	-0.73043500	0.44892200
C	6.70044000	1.38064000	0.06769600
H	7.23237400	1.74171600	0.96513700
H	5.86874000	2.07554100	-0.12781400
O	7.58174000	1.30994500	-1.03384900
C	8.13455400	2.56322300	-1.37891800
H	8.72555800	2.98845500	-0.55149100
H	8.79158300	2.39921300	-2.23684000
H	7.35449700	3.28896300	-1.65728400
C	0.64218200	2.72765000	1.70872200
C	-0.45900200	3.68116600	1.17761000
H	-0.94174700	4.23456400	1.99505700
H	-1.22992200	3.10361000	0.64698600
H	-0.06059700	4.42108500	0.47470600
C	0.01614100	1.82634800	2.78302200
H	-0.40728700	2.41579600	3.60664700
H	0.75394700	1.13536900	3.20937900
H	-0.79967000	1.21944900	2.36534500
H	1.35738400	3.38491600	2.25388100

C	1.95877400	2.72987100	-0.32713300
C	3.05954800	3.68270600	0.20602400
H	3.54241100	4.23764400	-0.61030400
H	3.83043100	3.10443000	0.73590800
H	2.66072800	4.42129800	0.91008100
C	2.58519300	1.83086300	-1.40313000
H	3.00886000	2.42205700	-2.22538600
H	1.84758000	1.14073200	-1.83120300
H	3.40087700	1.22309500	-0.98646100
H	1.24344700	3.38797400	-0.87112600
O	-2.61540400	-0.11011600	0.02666100
C	-3.19388900	-0.09261600	-1.27281100
C	-2.12661700	-0.50577800	-2.27691900
O	-0.96016500	0.30817100	-2.22283300
C	-1.10801400	1.59654300	-2.81126200
H	-1.83011700	2.21859800	-2.26655200
H	-1.42477000	1.50692100	-3.86034900
H	-0.12957000	2.07627800	-2.76570400
H	-1.78506500	-1.52014800	-2.05113900
H	-2.55489800	-0.49735600	-3.29141000
H	-3.59449800	0.90316300	-1.50940500
H	-4.02840900	-0.80943200	-1.33082700
C	-3.55330800	-0.03163900	1.09941900
H	-3.01771500	-0.35242400	1.99581500
H	-4.38432700	-0.73093600	0.92890600
C	-4.09975200	1.37932900	1.31566000
H	-4.63338400	1.74223000	0.41996800
H	-3.26826500	2.07436800	1.51161400
O	-4.97927100	1.30518700	2.41840500
C	-5.53271200	2.55711900	2.76732800
H	-6.12538200	2.98378700	1.94183500
H	-6.18826600	2.39044200	3.62586300
H	-4.75289400	3.28291100	3.04623500

Table S-34. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_{>2}$-diglyme$)_2$.

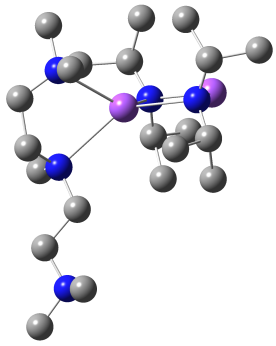


G = –1832.945987 Hartree
G_{MP2} = –1826.9743127492 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	-1.44703300	1.92552600	-0.39074700
Na	-2.89387400	-0.00027600	-0.78037200
N	-1.44688700	-1.92034500	-0.38955500
C	-1.31634800	-2.73651200	-1.59256300
C	-2.52070800	-3.66749900	-1.89344700
H	-2.69383900	-4.38900300	-1.08710900
H	-2.35939200	-4.24349000	-2.81548100
H	-3.43676300	-3.07266100	-2.00995600
C	-1.07621700	-1.85212900	-2.82477200
H	-0.94208900	-2.46045700	-3.72941400
H	-0.18234600	-1.22951100	-2.70554900
H	-1.92773900	-1.18137400	-3.01055500
H	-0.43261900	-3.41541100	-1.54680000
C	-1.57765300	-2.73562700	0.81403700
C	-0.37355700	-3.66672800	1.11558900
H	-0.53507000	-4.24207500	2.03799200
H	0.54263300	-3.07203600	1.23178700
H	-0.20055600	-4.38881100	0.30974400
C	-1.81750800	-1.85029500	2.04561500
H	-1.95174700	-2.45793500	2.95070200
H	-2.71123400	-1.22754800	1.92599800
H	-0.96580000	-1.17963100	2.23086600
H	-2.46157800	-3.41429800	0.76875300
C	-1.02711600	2.75333500	-1.51781800
C	0.36317600	3.41951300	-1.33177800
H	0.60230600	4.10904000	-2.15523300
H	1.14734800	2.64949200	-1.29319300
H	0.41139900	3.99627900	-0.40113100
C	-0.99798000	1.94195100	-2.82118900
H	-0.67224800	2.55920500	-3.67014000
H	-1.98403600	1.53045100	-3.06340800
H	-0.29941400	1.10006700	-2.73614000
H	-1.73329900	3.59440800	-1.69818800
C	-1.86716300	2.75404600	0.73572800
C	-3.25769500	3.41958400	0.54925100
H	-3.49711300	4.10952000	1.37228000
H	-4.04156900	2.64924000	0.51110000
H	-3.30609000	3.99578000	-0.38173600
C	-1.89590700	1.94369800	2.03974800
H	-2.22162400	2.56156500	2.88825700
H	-0.90970300	1.53263300	2.28209300
H	-2.59428500	1.10158000	1.95550600
H	-1.16128600	3.59551900	0.91537800
O	1.52634800	0.81386200	2.01846200
C	2.02627300	2.14423400	1.94519000
H	2.74670500	2.27221100	1.12557300
H	2.50592900	2.42940200	2.89304300
H	1.16738500	2.79003600	1.76021200
C	2.51687100	-0.17208700	2.27680700
C	3.20935600	-0.63929600	1.00384000
H	3.74920900	0.18889700	0.52224900
H	3.94233500	-1.42405600	1.25247400
O	2.19901000	-1.15438100	0.15127500
C	2.64763200	-1.87094600	-0.99278000
H	1.75545800	-2.36723700	-1.38207900
H	3.37785100	-2.64058300	-0.69630600

C	3.26060800	-0.98639700	-2.06906200
H	3.53935000	-1.62553600	-2.92497800
H	4.18624300	-0.50253600	-1.71219800
O	2.31376300	-0.01117200	-2.45172400
C	2.76915900	0.81302200	-3.50949400
H	2.97535900	0.22269200	-4.41574700
H	1.97517300	1.53129500	-3.71908600
H	3.68497800	1.35686800	-3.22902400
H	1.99102600	-1.01939800	2.72739700
H	3.26174000	0.20178600	2.99594100
O	-4.42002100	0.81250500	-2.79930900
C	-4.92096700	2.14255100	-2.72719600
H	-5.64094400	2.27088400	-1.90723800
H	-5.40150200	2.42624200	-3.67505000
H	-4.06249800	2.78931500	-2.54360400
C	-5.40973100	-0.17433700	-3.05736300
C	-6.10284400	-0.64084000	-1.78448000
H	-6.64337800	0.18749300	-1.30389400
H	-6.83531400	-1.42611700	-2.03297900
O	-5.09284100	-1.15483700	-0.93085200
C	-5.54191100	-1.87047100	0.21360700
H	-4.64993600	-2.36660400	0.60356900
H	-6.27215600	-2.64022200	-0.08250000
C	-6.15504200	-0.98500000	1.28903100
H	-6.43442500	-1.62348200	2.14523100
H	-7.08032400	-0.50101100	0.93142500
O	-5.20799000	-0.00990500	1.67150600
C	-5.66361400	0.81524600	2.72842800
H	-5.87055100	0.22566100	3.63499900
H	-4.86944600	1.53334500	2.93792400
H	-6.57905200	1.35927600	2.44707000
H	-4.88301800	-1.02172200	-3.50679200
H	-6.15433300	0.19838400	-3.77737400

Table S-35. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_2$-PMDTA).

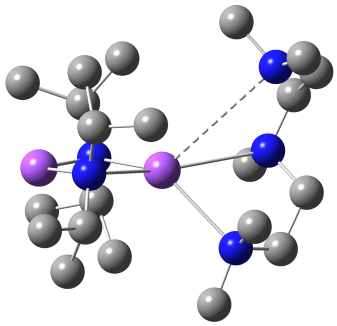


G = –1428.642611 Hartree
G_{MP2} = –1423.7985040308 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	-1.04777900	-1.85798300	-0.87568900
Na	0.97859500	-1.98001700	1.23201600
N	-0.32373700	-3.82123500	0.09109000
C	-1.13252800	-4.59356700	1.03179900
C	-0.29852300	-5.30605900	2.12668900
H	0.48960100	-5.92453100	1.68251100
H	-0.91667700	-5.95861600	2.75963100
H	0.18598800	-4.56385300	2.77759900
C	-2.19071400	-3.71113600	1.70714200
H	-2.77891900	-4.27135700	2.44538900
H	-2.89013600	-3.29980100	0.96642800
H	-1.72381200	-2.86573000	2.23094800
H	-1.69579900	-5.39828900	0.51901600
C	0.29992600	-4.69174000	-0.90379700
C	-0.68365300	-5.25570400	-1.96207300
H	-0.19412400	-5.97317000	-2.63555100
H	-1.08555200	-4.43654800	-2.57890400
H	-1.53337700	-5.76671800	-1.49740000
C	1.42547500	-3.96077500	-1.64694900
H	1.92475800	-4.61601100	-2.37145900
H	2.18302800	-3.58319900	-0.95078200
H	1.03763700	-3.09851000	-2.20921500
H	0.77277500	-5.57904700	-0.42988100
C	-0.97807100	0.89338000	0.61840700
C	-1.97818900	1.52892800	-0.38256300
H	-2.63171100	2.26799500	0.10213600
H	-2.62216200	0.75019800	-0.82139700
H	-1.46173300	2.03357100	-1.20578800
C	-1.78650000	0.16609700	1.70060500
H	-2.50774500	0.83549100	2.18595300
H	-1.12952900	-0.24743600	2.47423100
H	-2.36009300	-0.67027500	1.27526100
H	-0.48288500	1.74646800	1.13007700
C	1.01347600	0.76306500	-0.72604900
C	2.10059400	1.37458800	0.19374700
H	2.80004900	2.01671100	-0.36048300
H	2.68181000	0.57558800	0.67596400
H	1.65094500	1.98252700	0.98706800
C	1.69218700	-0.09520200	-1.80136000
H	2.47329600	0.46110700	-2.33521600
H	0.96159700	-0.44124900	-2.54533500
H	2.16556400	-0.98296200	-1.36021700
H	0.56590800	1.62177300	-1.26529200
N	1.42391300	-1.53108100	3.78502700
C	1.62586900	-0.08247200	3.92556500
H	0.69135500	0.43871800	3.70428600
H	2.37395000	0.27587100	3.21525300
H	1.94747900	0.19092400	4.94782900
C	0.32922300	-1.95810000	4.66630100
H	0.14535300	-3.02903800	4.54090700
H	-0.58673300	-1.42121600	4.40336900
H	0.54997000	-1.76324600	5.73190100
C	2.64618600	-2.27777500	4.12443200
C	3.80147900	-2.12165100	3.12984000
N	3.52751100	-2.66640400	1.79117000
C	4.43040400	-2.11157000	0.76191800

H	4.28456400	-1.02675000	0.76181900
H	4.09488600	-2.47579300	-0.21522100
C	5.92999000	-2.44447600	0.89663900
H	6.33126500	-2.05874600	1.85585300
H	6.04871400	-3.53325400	0.92128500
N	6.69843400	-1.94927200	-0.24566000
C	7.99572400	-2.60766600	-0.34237200
H	7.85811400	-3.69111700	-0.42396000
H	8.51439700	-2.26327400	-1.24365300
H	8.65492100	-2.40827500	0.52603300
C	6.86034100	-0.49932700	-0.23266300
H	7.41595300	-0.13558800	0.65547800
H	7.41082400	-0.18782800	-1.12644900
H	5.88865300	0.00125400	-0.25539400
C	3.51643800	-4.13558400	1.79231700
H	4.43862400	-4.57434300	2.21100900
H	2.66967700	-4.50909000	2.37306000
H	3.39083600	-4.49917600	0.76925600
H	4.68509700	-2.60109100	3.58861200
H	4.05137600	-1.06157400	3.01638100
H	3.02049500	-1.97396500	5.12152700
H	2.37564200	-3.33574000	4.20587400

Table S-36. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_{>2}$-PMDTA).

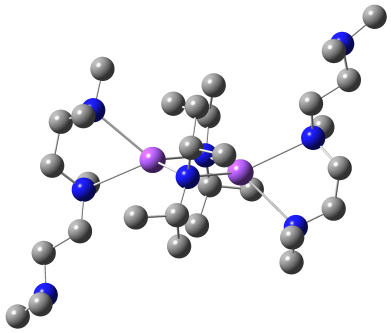


G = –1428.636406 Hartree
G_{MP2} = –1423.7976291129 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
Na	-2.79224200	0.42637800	-0.93188400
N	-1.33275800	2.15085200	-0.61722400
C	-0.72979400	2.88196000	-1.72693600
C	0.70736000	3.38715000	-1.44888000
H	1.09733900	3.98815500	-2.28294400
H	1.38883300	2.54038300	-1.28806000
H	0.73967900	4.01488500	-0.55024000
C	-0.72195400	2.01732700	-2.99385100
H	-0.27873800	2.54911500	-3.84553600
H	-1.74329000	1.72850500	-3.27920300
H	-0.14305100	1.09732000	-2.84028500
H	-1.31832700	3.78081800	-1.99174600
C	-1.65679500	2.99869600	0.52603200
C	-2.37865500	4.33163100	0.21081000
H	-2.67415100	4.83916900	1.13819300
H	-3.28569700	4.14386000	-0.38157600
H	-1.75018500	5.02778200	-0.35352300
C	-2.54099000	2.21562000	1.51044600
H	-2.68647900	2.75828500	2.45325100
H	-2.10805400	1.23842900	1.75242200
H	-3.54199400	2.04876000	1.07981100
H	-0.74777900	3.29487600	1.10524500
N	-1.81535700	-1.64401900	-0.59750800
C	-1.81587800	-2.36063200	-1.87582000
C	-3.01732700	-2.01569300	-2.79803000
H	-3.96935400	-2.14997500	-2.27392500
H	-3.03926000	-2.63370100	-3.70738000
H	-2.95569100	-0.96764100	-3.13651100
C	-0.52113500	-2.11899000	-2.67509200
H	-0.52706200	-2.63655200	-3.64429800
H	0.35095500	-2.46627900	-2.11037400
H	-0.38978600	-1.04800000	-2.87649300
H	-1.86900000	-3.45309000	-1.70273300
C	-2.24063500	-2.51068700	0.49524800
C	-2.08392800	-1.80379800	1.84828000
H	-2.33416000	-2.47323500	2.68076000
H	-2.75117000	-0.93366300	1.91407400
H	-1.05720500	-1.44875600	2.00360500
C	-3.69273600	-3.04736400	0.40858900
H	-3.92649200	-3.71303400	1.25154600
H	-3.85986600	-3.61617100	-0.51180700
H	-4.41067700	-2.21324800	0.42384600
H	-1.59907000	-3.42228700	0.54240600
N	1.26967400	0.57188900	2.25975700
C	2.07936900	1.70284700	1.78569200
H	2.60371100	1.43880300	0.86400100
H	2.81878500	2.03052900	2.54127600
H	1.41758500	2.54323300	1.56154000
C	0.43255300	1.00209100	3.38563500
H	-0.21327900	0.17848800	3.70587800
H	-0.20022300	1.83658700	3.07530000
H	1.03716400	1.32652900	4.25304800
C	2.10439500	-0.55862100	2.69078400
C	3.01359200	-1.14372200	1.60817000
N	2.31940000	-1.64399400	0.41429800
C	3.26801300	-1.96507700	-0.66938100

H	2.67693700	-2.35215700	-1.50594600
H	3.93946800	-2.79129900	-0.35987300
C	4.17751800	-0.83215100	-1.16199500
H	4.84816800	-0.51708800	-0.35605700
H	4.83533100	-1.27524600	-1.93814100
N	3.49315400	0.35873200	-1.66382400
C	4.42143100	1.48164000	-1.77941400
H	5.24176600	1.29278600	-2.49918300
H	3.87741500	2.37223300	-2.10872700
H	4.86874300	1.69862000	-0.80333100
C	2.84496900	0.11001600	-2.94975200
H	2.33200500	1.01660300	-3.28220700
H	3.56817600	-0.18733600	-3.73495600
H	2.09661100	-0.68078700	-2.85806800
C	1.56130200	-2.86124000	0.73298900
H	0.81526400	-2.66101200	1.50372200
H	2.22071000	-3.67633800	1.08839500
H	1.02302700	-3.20575400	-0.15245800
H	3.71843300	-0.37081700	1.29973500
H	3.61536000	-1.94588900	2.08072500
H	1.43569200	-1.32957400	3.08866200
H	2.76258000	-0.25543700	3.52972200

Table S-37. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_2\text{-PMDTA})_2$.

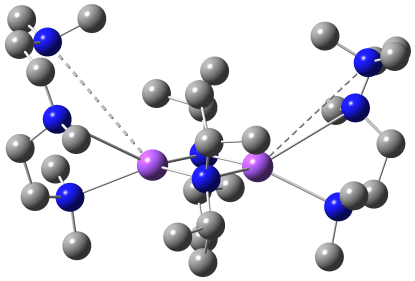


G = –1949.360434 Hartree
G_{MP2} = –1942.682454404 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	-1.28555700	-0.83563300	1.91947100
Na	1.28649900	0.83349100	1.91973600
N	0.00072100	-0.00178000	3.83661400
C	-0.51921300	1.08348900	4.66441300
C	0.56636600	1.90482100	5.41109100
H	1.21761600	1.26335200	6.01446800
H	0.12151600	2.65040500	6.08562300
H	1.20064100	2.43835900	4.68822900
C	-1.35939800	2.05939300	3.83059700
H	-1.76472500	2.87180500	4.44792000
H	-2.20181300	1.54995600	3.34925900
H	-0.75851400	2.51922600	3.03552200
H	-1.19913200	0.71039400	5.46091000
C	0.52115800	-1.08782600	4.66309600
C	-0.56400200	-1.90985900	5.40960500
H	-0.11879200	-2.65605700	6.08322200
H	-1.19866100	-2.44274200	4.68660200
H	-1.21493600	-1.26894100	6.01390500
C	1.36086400	-2.06295400	3.82789400
H	1.76639100	-2.87603900	4.44420000
H	2.20312400	-1.55312000	3.34670900
H	0.75957700	-2.52192000	3.03262700
H	1.20153900	-0.71549100	5.45955700
C	-0.74924000	0.94842700	-0.81850600
C	-1.87990700	0.32567900	-1.67959800
H	-2.38191600	1.08478600	-2.29570100
H	-2.63540800	-0.14176800	-1.03090500
H	-1.50339300	-0.44763900	-2.35753400
C	-1.37186700	2.04358900	0.05715300
H	-1.91261800	2.78429600	-0.54639400
H	-0.60653500	2.57388000	0.63463900
H	-2.08630700	1.62155100	0.77572400
H	-0.09615400	1.48498100	-1.54221900
C	0.74903900	-0.94759000	-0.81966400
C	1.87996100	-0.32404200	-1.67983000
H	2.38150800	-1.08238300	-2.29725900
H	2.63580200	0.14193100	-1.03047800
H	1.50374400	0.45059800	-2.35641800
C	1.37112100	-2.04415400	0.05460500
H	1.91169300	-2.78424500	-0.54986500
H	0.60538800	-2.57489900	0.63114700
H	2.08558400	-1.62342300	0.77391500
H	0.09583400	-1.48294500	-1.54412200
N	2.27789200	3.29855200	1.47795000
C	2.33978800	3.41542800	0.01555100
H	1.32704600	3.40065800	-0.39414700
H	2.87653800	2.56931400	-0.41853100
H	2.83672800	4.35132200	-0.30338200
C	1.46632700	4.39370400	2.02178200
H	1.37222800	4.28507900	3.10616000
H	0.46351700	4.36239600	1.58681400
H	1.90467700	5.38607400	1.80592700
C	3.61853400	3.34478300	2.07987500
C	4.51034000	2.13404400	1.78801700
N	4.01893400	0.86522300	2.34322700
C	4.63689300	-0.30595700	1.69211000

H	4.37907400	-0.25149600	0.62920400
H	4.15686700	-1.20670600	2.08954700
C	6.16047900	-0.47273200	1.86299900
H	6.70018500	0.37928100	1.40155900
H	6.39989800	-0.45423800	2.93215700
N	6.63334600	-1.75335000	1.33610700
C	7.96611700	-2.07110800	1.83355700
H	7.95805500	-2.09490600	2.92858200
H	8.26486900	-3.06230300	1.47512900
H	8.74005700	-1.34588300	1.51103500
C	6.60252500	-1.81085500	-0.12137700
H	7.24972400	-1.04622900	-0.59737900
H	6.94522400	-2.79674100	-0.45263900
H	5.58381200	-1.67501500	-0.49388400
C	4.13471700	0.82414700	3.80602700
H	5.15378500	1.04896000	4.16750500
H	3.44649600	1.54020600	4.26175600
H	3.84973500	-0.16791200	4.16507100
H	5.51668800	2.38149900	2.17330000
H	4.61850900	2.00695200	0.70569400
H	4.16427600	4.24791400	1.74112400
H	3.49162800	3.45048400	3.16259500
N	-2.27606500	-3.30108700	1.47630400
C	-2.33969400	-3.41704000	0.01391200
H	-2.87619900	-2.57020800	-0.41908000
H	-2.83778000	-4.35232500	-0.30503100
H	-1.32743600	-3.40297400	-0.39703000
C	-1.46366900	-4.39643000	2.01852100
H	-1.36857100	-4.28858700	3.10289000
H	-0.46127100	-4.36453900	1.58264200
H	-1.90197900	-5.38875200	1.80236800
C	-3.61600300	-3.34807200	2.07976900
C	-4.50890100	-2.13789900	1.78892200
N	-4.01791400	-0.86882700	2.34398200
C	-4.63652800	0.30206300	1.69298300
H	-4.37860100	0.24792800	0.63008400
H	-4.15712800	1.20308100	2.09056300
C	-6.16024700	0.46788100	1.86373700
H	-6.69936200	-0.38450900	1.40230300
H	-6.39976600	0.44931600	2.93287000
N	-6.63385600	1.74815800	1.33668400
C	-7.96678200	2.06525900	1.83413700
H	-8.26608400	3.05624300	1.47558200
H	-8.74034000	1.33957100	1.51174300
H	-7.95869400	2.08921600	2.92915900
C	-6.60311500	1.80548400	-0.12081000
H	-7.24987300	1.04040700	-0.59668600
H	-6.94641700	2.79111800	-0.45219700
H	-5.58433500	1.67020700	-0.49333800
C	-4.13349900	-0.82779700	3.80680400
H	-3.44529300	-1.54395300	4.26239300
H	-5.15253700	-1.05256800	4.16839000
H	-3.84839400	0.16422000	4.16588100
H	-4.61810300	-2.01070100	0.70672100
H	-5.51474500	-2.38610400	2.17502200
H	-3.48779700	-3.45371100	3.16234500
H	-4.16158100	-4.25153200	1.74161000

Table S-38. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_{>2}$-PMDTA)$_2$.

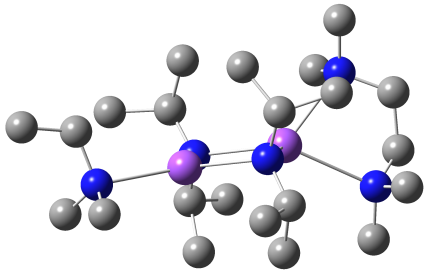


G = –1949.349829 Hartree
G_{MP2} = –1942.6762392766 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	-1.48433700	0.02688500	1.99322100
C	-0.05603100	1.21435000	-0.81102000
C	-1.39934500	1.45189400	-1.54601500
H	-1.36334300	2.35999600	-2.16458100
H	-2.21928300	1.56235100	-0.82352000
H	-1.65202900	0.61722300	-2.20972000
C	0.25018600	2.45021500	0.04462000
H	0.25916000	3.36512600	-0.56257800
H	1.23271400	2.36732700	0.52850400
H	-0.50053900	2.58570400	0.83286100
H	0.71672100	1.21233300	-1.60844800
C	-0.15878400	-1.20804100	-0.80829500
C	0.78677800	-1.34345800	-2.02812900
H	0.61472600	-2.29373400	-2.55092800
H	1.83575300	-1.32171300	-1.70020400
H	0.65011100	-0.54118900	-2.76026000
C	0.03517900	-2.45858900	0.05876400
H	-0.18506700	-3.37576900	-0.50292400
H	-0.60796800	-2.44651600	0.94434900
H	1.07509700	-2.52855500	0.40934900
H	-1.18715100	-1.29538500	-1.23370700
Na	1.54045600	0.02493700	1.85209600
N	0.05713600	0.00855000	3.84549600
C	0.11438200	1.22565200	4.65224800
C	1.45767100	1.46404200	5.38700000
H	1.42270500	2.37455900	6.00205800
H	2.27809000	1.57049200	4.66445700
H	1.70879900	0.63155900	6.05403000
C	-0.18999400	2.45884100	3.79212400
H	-0.19763200	3.37599100	4.39594500
H	-1.17265000	2.37552000	3.30857300
H	0.56088500	2.59029000	3.00334300
H	-0.65870400	1.22747700	5.44936800
C	0.21365900	-1.19684100	4.65818800
C	-0.73410500	-1.32751000	5.87684000
H	-0.56309100	-2.27583700	6.40349900
H	-1.78253400	-1.30683400	5.54712100
H	-0.59858600	-0.52251900	6.60619600
C	0.02028100	-2.45017700	3.79504400
H	0.23692200	-3.36570700	4.36080500
H	0.66638300	-2.44269500	2.91154000
H	-1.01859900	-2.51940200	3.44125900
H	1.24119200	-1.28354500	5.08568500
N	-3.83659600	-1.03414200	1.64133600
C	-4.26345300	-0.46193500	0.35600200
H	-4.33170600	0.62660000	0.42815900
H	-5.24039400	-0.86583500	0.02709600
H	-3.51840500	-0.70544000	-0.40684400
C	-3.60580700	-2.47596000	1.48863000
H	-3.24705600	-2.89927700	2.43279600
H	-2.84873800	-2.65139200	0.72007700
H	-4.52666600	-3.01517000	1.19707600
C	-4.84648700	-0.83535500	2.69551300
C	-5.30734200	0.60548600	2.93314100
N	-4.26522100	1.55552500	3.32203600
C	-4.77298000	2.93391900	3.35990200

H	-3.93643900	3.57368200	3.66159400
H	-5.54525800	3.05054000	4.14870100
C	-5.39556600	3.48084200	2.06837400
H	-6.35391800	2.98483000	1.87582500
H	-5.64378600	4.54424900	2.27251100
N	-4.58086900	3.34415900	0.86425300
C	-5.33259700	3.76024100	-0.31481100
H	-5.62706700	4.82836900	-0.28877000
H	-4.72687400	3.59677200	-1.21194700
H	-6.24491500	3.16026700	-0.40514000
C	-3.32203500	4.07539600	0.95864100
H	-2.75953900	3.94968700	0.02942200
H	-3.46985700	5.16066400	1.13043000
H	-2.71135200	3.67643900	1.77222400
C	-3.70740000	1.22450900	4.63452400
H	-3.19506800	0.26077500	4.60893300
H	-4.48383000	1.19225100	5.42489800
H	-2.96392200	1.97418100	4.91730400
H	-5.77930400	0.97028700	2.01951000
H	-6.10664700	0.55574200	3.70263900
H	-4.44755300	-1.26959700	3.61877500
H	-5.76176100	-1.41127300	2.45158800
N	3.89344500	-1.03462900	2.20486600
C	4.32162700	-0.45846000	3.48798300
H	4.39060800	0.62978500	3.41219200
H	5.29851800	-0.86193200	3.81757100
H	3.57694600	-0.69893600	4.25215800
C	3.66220500	-2.47584300	2.36247000
H	3.30245400	-2.90210300	1.42001300
H	2.90577400	-2.64848000	3.13229000
H	4.58310300	-3.01446600	2.65498200
C	4.90254200	-0.83979500	1.14915300
C	5.36473000	0.59985000	0.90691900
N	4.32342200	1.54978600	0.51575200
C	4.83269900	2.92747200	0.47295500
H	3.99650400	3.56722300	0.17027800
H	5.60418800	3.04080000	-0.31709300
C	5.45735400	3.47768400	1.76207000
H	6.41564800	2.98162300	1.95477500
H	5.70597000	4.54034700	1.55456500
N	4.64415900	3.34491700	2.96764700
C	5.39738100	3.76473500	4.14441700
H	5.69166300	4.83282100	4.11470500
H	4.79287000	3.60393200	5.04285500
H	6.30991900	3.16518800	4.23538000
C	3.38514400	4.07572100	2.87250600
H	2.82394700	3.95313100	3.80292500
H	3.53260000	5.16040700	2.69679100
H	2.77342300	3.67383900	2.06115000
C	3.76404700	1.21506000	-0.79514100
H	3.24946700	0.25262500	-0.76558600
H	4.53989900	1.17816500	-1.58587800
H	3.02210800	1.96536700	-1.08025700
H	5.83766700	0.96694000	1.81913000
H	6.16349800	0.54684200	0.13706200
H	4.50228600	-1.27628500	0.22751600
H	5.81746100	-1.41593300	1.39388400

Table S-39. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_2$-TMEDA)(DMEA).

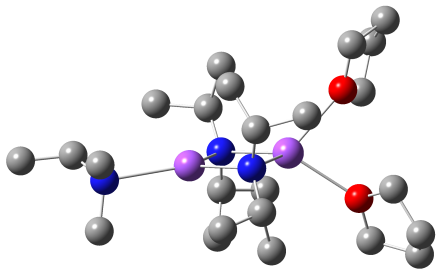


G = –1469.132936 Hartree
G_{MP2} = –1464.1083699377 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	1.44209100	-1.81992000	-0.44295400
Na	-1.52586400	-1.97126100	-0.26139400
N	0.13895200	-3.78065100	-0.71459700
C	-0.02064700	-4.35658500	-2.04782500
C	-1.42307400	-4.96387900	-2.31190200
H	-1.68736900	-5.70267900	-1.54680400
H	-1.47854900	-5.46559800	-3.28863100
H	-2.18842000	-4.17411400	-2.29405900
C	0.27659500	-3.31585600	-3.13622700
H	0.14433100	-3.73223200	-4.14322500
H	1.31068800	-2.95204200	-3.06091500
H	-0.39095900	-2.44891800	-3.04761600
H	0.69484500	-5.18410600	-2.22803400
C	0.28346900	-4.81864400	0.30138500
C	1.58658700	-5.65597900	0.20920200
H	1.60460100	-6.45675300	0.96159800
H	2.46107000	-5.01154500	0.37930500
H	1.70663100	-6.12756400	-0.77146900
C	0.22599700	-4.21068400	1.70906600
H	0.27760100	-4.98395900	2.48630100
H	-0.69719600	-3.63965300	1.86127400
H	1.06798300	-3.52393300	1.87629700
H	-0.54519100	-5.56168100	0.25777700
N	3.98981700	-1.82619900	-0.58265000
C	4.46656100	-0.51157300	-1.02384500
H	4.00578100	-0.26408600	-1.98610600
H	4.16757200	0.25180500	-0.29871300
H	5.56119200	-0.46449500	-1.15282700
C	4.40967200	-2.14922800	0.79785700
H	3.98816300	-1.37281800	1.44970100
H	3.91873900	-3.09232300	1.06917400
C	5.91724300	-2.27029000	1.06966000
H	6.44995500	-1.33683000	0.85979400
H	6.07668000	-2.51050200	2.12683900
H	6.37898900	-3.06748000	0.47774500
C	4.36205500	-2.86824400	-1.54633000
H	3.97033600	-3.83437900	-1.21423700
H	3.91334800	-2.63682700	-2.51860200
H	5.45181800	-2.95859300	-1.69172000
C	-0.07578900	1.04276000	-1.01929500
C	1.13642500	2.00988400	-1.06720900
H	0.98881700	2.80088300	-1.81580100
H	2.04927900	1.45798900	-1.33100900
H	1.31196200	2.50262700	-0.10545000
C	-0.22500600	0.42428200	-2.41580600
H	-0.33569900	1.19482700	-3.18949500
H	-1.09686900	-0.23796500	-2.47146800
H	0.65935800	-0.17444300	-2.67728900
H	-0.96794700	1.69528200	-0.88002000
C	-0.05457800	0.56384500	1.34688600
C	-1.46771300	1.03200100	1.78073900
H	-1.45517600	1.53210600	2.75979200
H	-2.14799100	0.17068800	1.85029800
H	-1.89212900	1.73622100	1.05628000
C	0.47200200	-0.43712300	2.38408900
H	0.42409600	-0.03065300	3.40262800

H 1.51968400 -0.69919900 2.18039700
H -0.11367900 -1.36540000 2.37107500
H 0.59255300 1.45810100 1.44597500
N -3.80800100 -1.30407800 -1.47529100
C -3.95496300 0.13274500 -1.20701600
H -3.16348700 0.68218500 -1.72212300
H -3.85228700 0.34063200 -0.13998600
H -4.93354900 0.51799200 -1.55032300
C -3.85027000 -1.53689700 -2.92419000
H -3.69952300 -2.59953800 -3.13600000
H -3.04926500 -0.97402800 -3.41157900
H -4.81257700 -1.22418900 -3.37021200
C -4.87068800 -2.08428500 -0.82165000
C -4.77669600 -2.14908800 0.70457100
N -3.58210300 -2.83404300 1.22339200
C -3.47255800 -2.59915800 2.66845500
H -4.34757700 -2.98632200 3.22274300
H -3.38397500 -1.52698600 2.86627100
H -2.57731000 -3.09365900 3.05591600
C -3.63851600 -4.27939500 0.96682200
H -3.64573500 -4.48329800 -0.10599700
H -4.53375400 -4.74398400 1.42138200
H -2.74855300 -4.75803400 1.38250500
H -5.69795400 -2.64009500 1.07472600
H -4.78237500 -1.13498800 1.11699200
H -5.86739600 -1.67399300 -1.07678800
H -4.84058400 -3.09717400 -1.23616300

Table S-40. Geometric coordinates and thermally corrected MP2 energies for $A_2(THF)_2(DMEA)$.

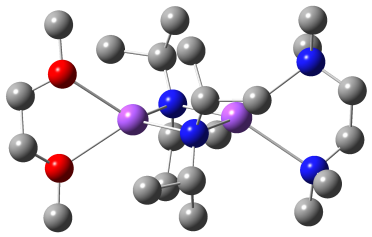


G = –1586.285283 Hartree
G_{MP2} = N/A (Internal consistency failure #1 in GetIJB)

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	-1.48162200	-1.65800800	1.07596800
Na	-2.93271000	-0.09120700	0.02157300
N	-1.59740800	1.54781800	-1.06594700
C	-1.69682600	2.91637600	-0.56392900
C	-3.08351100	3.57602100	-0.77882000
H	-3.40108400	3.51752300	-1.82580700
H	-3.08113700	4.63796400	-0.49340600
H	-3.84177000	3.06414800	-0.16984400
C	-1.36371000	2.98218500	0.93287100
H	-1.41846200	4.01061000	1.31343600
H	-0.35713800	2.59592700	1.13008000
H	-2.07508700	2.38166800	1.51762400
H	-0.96622700	3.58845200	-1.06485900
C	-1.52385000	1.53812300	-2.52484100
C	-0.12907400	1.92430000	-3.08372300
H	-0.12975900	2.00683100	-4.18044700
H	0.61730600	1.16895800	-2.80038200
H	0.20305100	2.88893700	-2.68227100
C	-1.91609700	0.16620000	-3.09144100
H	-1.84108900	0.13984900	-4.18639200
H	-2.95093500	-0.09024600	-2.82418000
H	-1.26225600	-0.62337000	-2.69762600
H	-2.23343200	2.26217900	-2.97614200
N	-5.48730700	-0.33238700	0.03972100
C	-6.11911100	1.00018500	-0.06161400
H	-5.75989300	1.58955800	0.79132400
H	-5.71647700	1.47863700	-0.96201400
C	-7.65448600	1.05247800	-0.09798500
H	-7.97899300	2.09665400	-0.16970900
H	-8.06537600	0.52066900	-0.96273400
H	-8.10333500	0.62910900	0.80687200
C	-5.82581500	-1.02576400	1.28851900
H	-5.19944100	-1.91720000	1.38886200
H	-5.62098400	-0.36744400	2.13963900
H	-6.88235300	-1.33925800	1.33946500
C	-5.77754100	-1.18050300	-1.12153900
H	-5.50684400	-0.65065400	-2.04145300
H	-5.17857900	-2.09550400	-1.06171900
H	-6.83750100	-1.47815300	-1.19178400
C	-1.41929200	-1.64381800	2.53549400
C	-0.00407100	-1.92654500	3.10472100
H	-0.00630400	-2.00594900	4.20169300
H	0.68719800	-1.11972200	2.82361000
H	0.40045900	-2.86583000	2.70941300
C	-1.91582200	-0.30442100	3.09840200
H	-1.84414500	-0.27016700	4.19325400
H	-2.96750800	-0.12899000	2.83108400
H	-1.32344300	0.53159800	2.70330300
H	-2.07713400	-2.41819800	2.98265900
C	-1.46604600	-3.02922100	0.57215200
C	-2.79490200	-3.80215900	0.77624200
H	-2.70172900	-4.86173000	0.49752600
H	-3.58672300	-3.36041800	0.15411300
H	-3.12845900	-3.76492900	1.81927800
C	-1.11742400	-3.06545900	-0.92186700
H	-1.09434000	-4.09369200	-1.30645800

H -0.13992500 -2.60679500 -1.10957200
H -1.86542800 -2.51471700 -1.50938000
H -0.68796300 -3.64084700 1.07889100
O 1.90448900 -1.05863900 -1.10111700
C 2.23360200 -1.40021700 -2.46539400
H 2.39683400 -0.47503500 -3.02642800
H 1.37992600 -1.92942000 -2.90803800
C 3.47440500 -2.29669700 -2.39222200
H 3.52529300 -3.00551900 -3.22404100
H 4.38886400 -1.69150100 -2.40638800
C 3.30090600 -2.97192300 -1.02290800
H 4.23639800 -3.35737400 -0.60613400
H 2.58923500 -3.80248600 -1.09354800
C 2.70982800 -1.83584500 -0.18766900
H 2.06414400 -2.17487100 0.62719000
H 3.49512100 -1.19182900 0.23132300
O 1.82377000 1.19234300 1.11396400
C 2.58389700 2.01460400 0.20089400
H 1.92054900 2.31762900 -0.61403100
H 3.40336900 1.41502300 -0.21825900
C 3.11152500 3.18269600 1.03517400
H 4.02961700 3.61208200 0.62271000
H 2.35943700 3.97765100 1.09667500
C 3.30835400 2.52415100 2.40950500
H 3.31806100 3.23915200 3.23755000
H 4.25116900 1.96440700 2.43383200
C 2.11278700 1.56883500 2.47768800
H 2.31158800 0.66023200 3.05395400
H 1.22791000 2.06228800 2.90032100

Table S-41. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_2\text{-DME})_2(\kappa_2\text{-TMEDA})$.

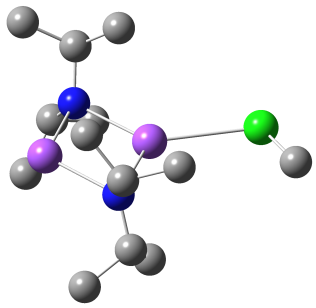


G = –1564.214966 Hartree
G_{MP2} = –1558.9742080149 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	-1.54737800	1.79994000	0.65734900
Na	1.47757200	1.79993600	0.65734300
N	0.00001800	3.59988100	1.31469500
C	0.19644200	4.76287400	0.45520000
C	1.59336500	5.42672400	0.59261900
H	1.80851800	5.70196100	1.63056200
H	1.67702600	6.33937100	-0.01547000
H	2.37583500	4.72548700	0.26937200
C	-0.01549800	4.39840300	-1.02031900
H	0.11657700	5.26816000	-1.67727600
H	-1.02098000	3.99560700	-1.18674000
H	0.69953100	3.63076300	-1.34451800
H	-0.53826100	5.56948000	0.67385100
C	-0.15635100	4.01231000	2.70690900
C	-1.56103000	4.57826000	3.04406000
H	-1.60972400	4.98314800	4.06554600
H	-2.32082400	3.78778500	2.95841700
H	-1.83908700	5.38436000	2.35557400
C	0.15429900	2.85543200	3.66552000
H	0.00572300	3.14355100	4.71471000
H	1.19521400	2.53045200	3.54756300
H	-0.49341800	1.99134400	3.46458300
H	0.55550000	4.81915500	2.97815000
C	-0.15638000	-0.41242800	-1.39221200
C	-1.56106800	-0.97836600	-1.72933900
H	-1.60979100	-1.38321800	-2.75083700
H	-2.32086400	-0.18789800	-1.64364500
H	-1.83909900	-1.78449200	-1.04087300
C	0.15425400	0.74445700	-2.35082000
H	0.00564500	0.45634600	-3.40000700
H	1.19517700	1.06942200	-2.23289000
H	-0.49344800	1.60855100	-2.14985800
H	0.55546600	-1.21927400	-1.66346400
C	0.19642400	-1.16299600	0.85949000
C	1.59334100	-1.82685200	0.72205400
H	1.67700500	-2.73949900	1.33014400
H	2.37581900	-1.12561800	1.04528900
H	1.80847900	-2.10209200	-0.31589100
C	-0.01549900	-0.79853100	2.33501200
H	0.11658100	-1.66829100	2.99196400
H	-1.02097800	-0.39573400	2.50144500
H	0.69953400	-0.03089400	2.65921000
H	-0.53828600	-1.96959600	0.64084000
C	3.65401800	2.95774800	-1.89676700
H	3.69518700	4.02857900	-1.65489300
H	2.75434400	2.75387800	-2.47902600
H	4.53889400	2.68664300	-2.49043800
O	3.57906200	2.16371900	-0.71811600
C	4.71604200	2.33026300	0.11742100
C	4.71604400	1.26959800	1.19725600
H	5.63905100	1.37718000	1.78883200
H	4.71025600	0.26600400	0.74483400
O	3.57906100	1.43613300	2.03278900
C	3.65402000	0.64210500	3.21144000
H	4.53889200	0.91321900	3.80511400
H	3.69519900	-0.42872600	2.96956800

H	2.75434300	0.84596800	3.79369700
H	5.63905100	2.22268700	-0.47415200
H	4.71024500	3.33385600	0.56984300
N	-3.76712400	0.84636600	1.89465700
C	-3.90725500	-0.55063800	1.46481700
H	-3.87614300	-0.62590800	0.37614200
H	-4.85259400	-0.99902600	1.82495900
H	-3.07262800	-1.13845900	1.85431000
C	-3.70889300	0.90441800	3.35962900
H	-3.55937100	1.93768800	3.68641700
H	-2.86518700	0.30788100	3.71830000
H	-4.63097300	0.51774600	3.83272000
C	-4.88662000	1.66912400	1.41148300
C	-4.88663600	1.93081300	-0.09673100
N	-3.76712300	2.75352200	-0.57995900
C	-3.70892700	2.69540400	-2.04492700
H	-3.55945100	1.66211300	-2.37166900
H	-2.86520500	3.29189300	-2.40364200
H	-4.63100300	3.08209000	-2.51801600
C	-3.90717800	4.15055800	-0.15019300
H	-3.87604200	4.22589400	0.93847400
H	-4.85250100	4.59897200	-0.51034500
H	-3.07253000	4.73831700	-0.53973400
H	-4.85504200	0.97803400	-0.63487900
H	-5.85551700	2.40156400	-0.35554000
H	-4.85498400	2.62189100	1.94964500
H	-5.85550500	1.19839300	1.67031300

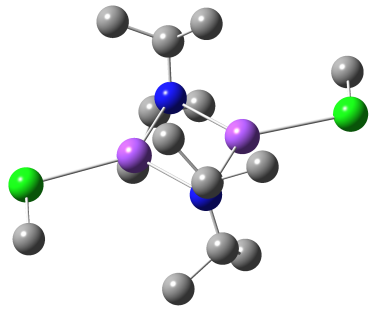
Table S-42. Geometric coordinates and thermally corrected MP2 energies for A_2(chloromethane).



G = –1408.007570 Hartree
G_{MP2} = –1404.2493505455 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
C	-0.89400900	-0.06094500	-1.15603700
H	-1.93773300	-0.25832400	-0.84003700
C	-0.51422100	-1.21888100	-2.09444000
H	-1.12891900	-1.23539600	-3.00286000
H	0.53418300	-1.13358100	-2.41769300
H	-0.64785700	-2.19159600	-1.59619500
C	-0.93048200	1.25767400	-1.96504700
H	-1.68287300	1.23828700	-2.76637500
H	-1.16220700	2.10533300	-1.30986800
H	0.04986400	1.44816500	-2.42643900
C	-0.67677000	0.58562000	1.15670200
H	-1.37200600	1.38982200	0.84286900
C	-1.52947500	-0.43734900	1.94495900
H	-0.87951800	-1.19930000	2.40142200
H	-2.11397400	0.03291500	2.74862600
H	-2.23153200	-0.95167400	1.27857000
C	0.32879000	1.24871700	2.11222100
H	0.83028300	2.10139700	1.63203100
H	-0.15445400	1.62676700	3.02152400
H	1.09725100	0.52877000	2.43232500
Na	1.30990900	-1.90900700	0.16199700
N	3.54080700	-1.22728600	0.01629200
C	4.33640600	-1.45976400	-1.18878300
H	5.40464800	-1.21628800	-1.01333000
C	3.87859200	-0.54925300	-2.33976500
H	4.41854700	-0.75972300	-3.27113600
H	2.80821500	-0.69325200	-2.54872900
H	4.04230400	0.51160600	-2.10060500
C	4.30661400	-2.93141000	-1.66784100
H	4.99523700	-3.11375200	-2.50510400
H	4.58365500	-3.61156000	-0.85422800
H	3.29292600	-3.20048000	-2.00085800
C	4.28405800	-1.60635200	1.21639100
H	4.93002300	-2.48593000	1.02419300
C	5.22713500	-0.48934000	1.72676300
H	4.63895500	0.37504100	2.06893000
H	5.85945900	-0.81961100	2.56325000
H	5.89284400	-0.15486900	0.92146700
C	3.33636500	-2.02133600	2.35431600
H	2.77964800	-2.93430900	2.09241800
H	3.87513500	-2.23053800	3.28663100
H	2.61223400	-1.22243500	2.57206500
Na	2.23347500	0.74267000	-0.15800400
Cl	3.43258100	3.40438400	-0.31321500
C	5.22485900	3.18396500	-0.12462000
H	5.67461600	3.24552600	-1.11485900
H	5.58804400	3.98456100	0.51852100
H	5.40231100	2.20850900	0.32665700

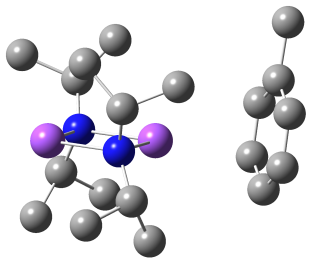
Table S-43. Geometric coordinates and thermally corrected MP2 energies for A_2(chloromethane)$_2$.



G = –1908.090904 Hartree
G_{MP2} = –1903.5829307761 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
C	0.49645800	0.67104200	1.20101200
H	1.40038800	1.27392900	0.97619500
C	0.92642600	-0.34679200	2.27020700
H	1.24555800	0.14136000	3.19946700
H	0.09407700	-1.01771400	2.52956000
H	1.76665700	-0.96290300	1.91826600
C	-0.52790900	1.65224800	1.82082000
H	-0.10486400	2.22913600	2.65574900
H	-0.88524600	2.36569500	1.06934900
H	-1.40009900	1.09984900	2.20109600
C	0.17278100	0.84679400	-1.17889900
H	0.01226000	1.91514600	-0.92942600
C	1.59409200	0.76124200	-1.78858400
H	1.77188400	-0.24918300	-2.18638600
H	1.74588900	1.47809600	-2.60834600
H	2.35347900	0.96722900	-1.02416400
C	-0.85826400	0.50924800	-2.26801500
H	-1.88106300	0.73327600	-1.93204300
H	-0.68801300	1.08247400	-3.18784600
H	-0.80727300	-0.55611300	-2.53612200
Na	0.44870600	-2.31363400	0.01730600
N	-1.66097300	-3.36764100	-0.00020600
C	-2.15891700	-4.03686900	1.20125500
H	-3.05831900	-4.64583300	0.97488700
C	-2.59944300	-3.01738600	2.26448100
H	-2.92174800	-3.50372300	3.19359600
H	-1.77167200	-2.34177600	2.52630800
H	-3.44017100	-2.40637700	1.90508300
C	-1.13184300	-5.00998000	1.82934800
H	-1.55525600	-5.58590000	2.66476000
H	-0.76736300	-5.72443600	1.08226700
H	-0.26432800	-4.45136900	2.21135900
C	-1.82508000	-4.21942700	-1.17687200
H	-1.65738500	-5.28584100	-0.92367200
C	-3.24538500	-4.14591300	-1.79016300
H	-3.43076000	-3.13734300	-2.18890000
H	-3.38909500	-4.86468700	-2.60970800
H	-4.00539200	-4.35797700	-1.02794000
C	-0.79393500	-3.87784300	-2.26460900
H	0.22970300	-4.09366600	-1.92578200
H	-0.95809600	-4.45510800	-3.18299800
H	-0.85167100	-2.81368300	-2.53598400
Na	-2.10906900	-1.05360700	0.00777000
Cl	-4.83357900	0.01667800	-0.11809900
C	-5.93184600	-1.41460100	-0.32125100
H	-6.39727100	-1.61711300	0.64261700
H	-6.68040700	-1.15125600	-1.06750500
H	-5.33058600	-2.26077600	-0.65168200
Cl	3.17168700	-3.38865400	-0.10678000
C	4.27985800	-1.96759200	-0.32735000
H	3.69958900	-1.14487800	-0.74337400
H	4.68541800	-1.70580800	0.64921200
H	5.07273800	-2.27290800	-1.00903000

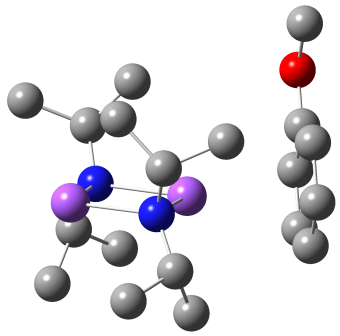
Table S-44. Geometric coordinates and thermally corrected MP2 energies for A_2(toluene).



G = –1179.379050 Hartree
G_{MP2} = –1175.4436453786 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	-1.22250500	-2.02740000	-0.42329400
Na	1.52929100	-1.70790900	0.31965000
N	0.43864800	-3.71767400	-0.05990700
C	0.09493800	-4.63786200	1.02309300
C	1.30632900	-5.02984000	1.90431800
H	2.13209100	-5.40753900	1.29056900
H	1.05435800	-5.80762800	2.63940900
H	1.67232100	-4.15059200	2.45556700
C	-1.00487200	-4.05319800	1.92273000
H	-1.22799700	-4.70865300	2.77394100
H	-1.94022500	-3.90862600	1.36484700
H	-0.69650200	-3.08136100	2.33459100
H	-0.31355700	-5.58863000	0.62149300
C	1.03076400	-4.44167300	-1.18527000
C	-0.02313400	-5.01479200	-2.16328700
H	0.42638000	-5.64987000	-2.94014300
H	-0.55994600	-4.19633600	-2.66522300
H	-0.76053800	-5.61912600	-1.62196600
C	2.01517100	-3.55695500	-1.96934000
H	2.41086300	-4.06471300	-2.85766700
H	2.87754800	-3.27661600	-1.34521700
H	1.52380100	-2.63653100	-2.31741100
H	1.62307200	-5.30858300	-0.83225400
C	-0.22645500	0.75909000	1.23039800
C	-1.72347200	1.03773600	1.50627800
H	-1.87473000	1.70269800	2.36883600
H	-2.25537200	0.09624300	1.70693400
H	-2.19319500	1.50726100	0.63418800
C	0.38871000	0.05110700	2.44915600
H	0.16961500	0.57595100	3.38736800
H	1.48418300	-0.00763000	2.35859300
H	-0.00684300	-0.97006700	2.55170500
H	0.26446200	1.75084900	1.18111600
C	0.05879400	0.89371300	-1.15599300
C	1.42701000	1.60007000	-1.31942700
H	1.41617100	2.34941900	-2.12383000
H	2.20709800	0.86118300	-1.55720000
H	1.71987500	2.11016900	-0.39471200
C	-0.26946000	0.14321800	-2.45540300
H	-0.16789800	0.78793100	-3.33738700
H	-1.29887000	-0.23939400	-2.44425600
H	0.41216300	-0.70820900	-2.59581900
H	-0.69677300	1.70227100	-1.07106000
C	-5.27537200	-2.53872100	1.65180500
C	-4.70101500	-2.39407200	0.26165300
C	-4.64661200	-1.14236400	-0.36982400
C	-4.15495600	-1.01155700	-1.67099200
C	-3.69815800	-2.13587400	-2.36659200
C	-3.73704200	-3.38948600	-1.74667500
C	-4.23388100	-3.51297600	-0.44556400
H	-4.26336500	-4.49289600	0.02498500
H	-3.38009500	-4.26998300	-2.27321900
H	-3.32055300	-2.03744800	-3.38069800
H	-4.12652800	-0.03198300	-2.14021900
H	-4.99512400	-0.26079400	0.16240700
H	-6.34994600	-2.76084500	1.61019400
H	-4.79577100	-3.35468300	2.20235200
H	-5.15487900	-1.61893100	2.23308200

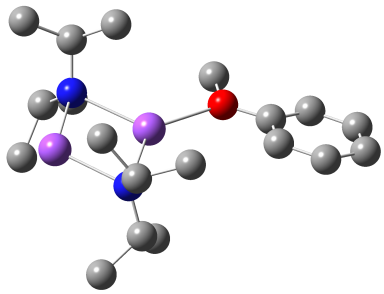
Table S-45. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_6$-anisole).



G = –1254.579897 Hartree
G_{MP2} = –1250.457202034 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	0.48396000	-2.30176200	-0.44643100
Na	-1.96779800	-1.13334900	0.46173200
N	-1.59427500	-3.39217300	0.09034300
C	-2.19449500	-4.09359600	-1.04375900
C	-3.73716600	-3.97077400	-1.09781100
H	-4.18879900	-4.26585700	-0.14390800
H	-4.17884600	-4.59899500	-1.88454000
H	-4.02587700	-2.92776100	-1.29758900
C	-1.61281100	-3.59617200	-2.37533800
H	-2.09735600	-4.07241900	-3.23678600
H	-0.53696900	-3.80604600	-2.44543400
H	-1.75696900	-2.51114800	-2.48065000
H	-1.97422300	-5.18093100	-1.00013600
C	-1.72177000	-4.18308300	1.31454900
C	-0.57136300	-5.20184300	1.50295400
H	-0.73404000	-5.86578200	2.36411800
H	0.38122500	-4.67395500	1.65850900
H	-0.46627100	-5.83075700	0.61101400
C	-1.80881900	-3.28428600	2.55968700
H	-1.83342200	-3.86556900	3.49000000
H	-2.72040500	-2.66818400	2.53750400
H	-0.93881100	-2.61428000	2.62096400
H	-2.65592700	-4.77807900	1.30799800
C	-0.16061000	0.95365000	-1.09837500
C	1.00937500	0.91459100	-2.10998700
H	0.93644600	1.70819400	-2.86760100
H	1.02692900	-0.05302700	-2.63263200
H	1.96863000	1.03066600	-1.59254600
C	-1.48394600	0.72901400	-1.84853600
H	-1.58502700	1.39256300	-2.71631100
H	-2.34750300	0.91899900	-1.19268600
H	-1.55187600	-0.30310700	-2.22251200
H	-0.20345400	1.99340600	-0.71759900
C	0.81859900	0.57311200	1.06797300
C	0.02000600	1.49462500	2.02200200
H	0.66636200	2.00329000	2.75167900
H	-0.72267600	0.90657200	2.58261800
H	-0.51889100	2.26593100	1.45970500
C	1.50786900	-0.52533200	1.89180400
H	2.04949400	-0.11224700	2.75214900
H	2.23483000	-1.07936100	1.28313100
H	0.76716000	-1.23670900	2.28581600
H	1.63514800	1.19686700	0.65063200
C	4.63299100	-3.24153400	2.01708900
O	4.69979900	-2.50484400	0.80233200
C	3.95443000	-2.92627400	-0.25501900
C	4.07742000	-2.16334000	-1.42902100
C	3.36066800	-2.51317900	-2.56732600
C	2.50811900	-3.62677500	-2.56022800
C	2.38487100	-4.38086000	-1.39243500
C	3.09681700	-4.03614600	-0.23366300
H	2.98716100	-4.64263500	0.65791600
H	1.73215800	-5.24926200	-1.36867700
H	1.95981900	-3.90573700	-3.45493200
H	3.46804800	-1.91608600	-3.46840600
H	4.74309500	-1.30617700	-1.42082200
H	4.95903600	-4.27965200	1.87399100
H	5.31397600	-2.73940800	2.70563400
H	3.61940500	-3.23000000	2.43742200

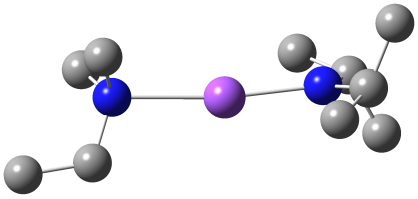
Table S-46. Geometric coordinates and thermally corrected MP2 energies for $A_2(\kappa_1$-anisole).



G = –1254.583358 Hartree
G_{MP2} = –1250.453962567 Hartree

Atom	X	Y	Z
N	0.00000000	0.00000000	0.00000000
Na	0.56241700	2.31674000	0.10594000
Na	-2.02089700	1.13316300	0.07416600
N	-1.55974700	3.41208800	0.19533100
C	-1.72032600	4.16148400	1.44069500
C	-3.11205300	3.98124500	2.09518000
H	-3.91342600	4.20465900	1.38171200
H	-3.25091200	4.63565900	2.96751900
H	-3.24038700	2.94103500	2.43057700
C	-0.63911000	3.77278800	2.46243300
H	-0.78533300	4.27758300	3.42518400
H	0.36682700	4.03597300	2.10636700
H	-0.66124900	2.69060800	2.65943200
H	-1.60170100	5.25219700	1.26987000
C	-2.19626700	4.10684900	-0.92342300
C	-1.29809900	5.19223900	-1.56293300
H	-1.82504400	5.77286700	-2.33344300
H	-0.41785500	4.72862800	-2.03118200
H	-0.94647600	5.89896700	-0.80153200
C	-2.63815600	3.11845000	-2.01654600
H	-3.04065300	3.63054700	-2.89910700
H	-3.42918200	2.44646200	-1.64837900
H	-1.79045700	2.50558200	-2.35754800
H	-3.11872800	4.62732500	-0.59764100
O	2.59287000	3.61464200	0.10250600
C	2.38784600	5.01235500	-0.12329700
H	2.76317800	5.31018900	-1.10906600
H	1.30951300	5.16871100	-0.08434700
H	2.87896900	5.60689000	0.65552900
C	3.89649300	3.15302200	0.14464500
C	4.06099600	1.80047500	0.46671200
C	5.34043400	1.25562300	0.52295900
C	6.46293000	2.04732400	0.26282000
C	6.28865400	3.39227500	-0.05376600
C	5.01008500	3.95602300	-0.11594600
H	4.90119000	5.00471500	-0.36537200
H	7.15098000	4.02133900	-0.25754900
H	7.45962300	1.61880300	0.30895800
H	5.45804000	0.20531500	0.77495500
H	3.19005800	1.18579800	0.67465300
C	0.06975100	-0.95082300	1.10921600
C	1.45186200	-0.98281800	1.80442500
H	1.51974600	-1.77329500	2.56550300
H	1.65253400	-0.02081800	2.29767700
H	2.24789900	-1.16034100	1.07149800
C	-1.01217600	-0.66101800	2.16396400
H	-0.91772100	-1.31090700	3.04241800
H	-2.02156200	-0.82261400	1.75376600
H	-0.94180000	0.37700600	2.52155500
H	-0.12031500	-1.98519700	0.75978300
C	0.52005200	-0.59268100	-1.23215100
C	-0.50337800	-1.49996000	-1.95762500
H	-0.06293100	-2.02252700	-2.81879900
H	-1.34877200	-0.89858300	-2.32480200
H	-0.90351900	-2.26052900	-1.27718800
C	1.00589500	0.49284000	-2.20645200
H	1.33036300	0.06880000	-3.16458700
H	1.85947900	1.04730100	-1.79200800
H	0.19836800	1.20714400	-2.42926800
H	1.40314600	-1.23124000	-1.02473500

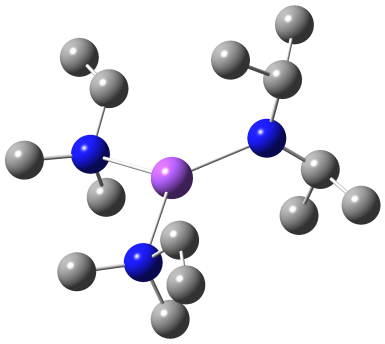
Table S-47. Geometric coordinates and thermally corrected MP2 energies for A(DMEA).



G = –667.600467 Hartree
G_{MP2} = –665.30224408634 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	-0.81435400	1.18542300	0.13670000
Na	-2.96028500	1.13153200	0.10013000
N	-5.38529300	1.12546500	-0.22784000
C	-6.02296100	1.26631500	1.10326900
H	-5.66044100	0.43426800	1.72073100
H	-5.62865700	2.18780500	1.55079000
C	-7.55715500	1.29856100	1.15116100
H	-8.00117000	0.37768800	0.75925600
H	-7.88259400	1.40376600	2.19178500
H	-7.96989400	2.14376500	0.59076600
C	-5.72491600	-0.14616100	-0.88431700
H	-5.11452900	-0.26391000	-1.78647800
H	-5.50667900	-0.98038300	-0.20902900
H	-6.78278800	-0.21026300	-1.18400600
C	-5.67778800	2.26026300	-1.11682100
H	-5.41716800	3.19899000	-0.61628200
H	-5.07218500	2.17531400	-2.02591200
H	-6.73515000	2.31123700	-1.42093800
C	-0.07199700	2.41313900	0.30776200
C	0.58310000	2.93310300	-0.99652100
H	1.20134300	3.82609700	-0.82384900
H	-0.19524500	3.18521000	-1.73033900
H	1.22551100	2.16739600	-1.44575700
C	-0.99329600	3.50638900	0.87324700
H	-0.47340200	4.46308200	1.00937800
H	-1.40809800	3.19713800	1.84148300
H	-1.82993400	3.69356400	0.17733800
H	0.75282200	2.30322400	1.04578600
C	0.62981700	-0.48364600	1.33043600
H	1.21494200	0.31443100	1.80113800
H	1.29867900	-1.34437700	1.18459300
H	-0.16241300	-0.77360500	2.03480300
C	-0.83580600	-1.14195300	-0.60040500
H	-0.25843100	-2.06820800	-0.71351500
H	-1.22699300	-0.85571200	-1.58536700
H	-1.68894600	-1.37584000	0.06045500
H	0.84718000	0.15517300	-0.70400900

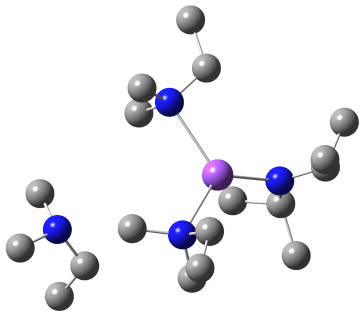
Table S-48. Geometric coordinates and thermally corrected MP2 energies for A(DMEA)$_2$.



G = –881.258599 Hartree
G_{MP2} = –878.17621582906 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	-0.14687300	-0.80480300	1.19288600
Na	-0.17507000	-3.00373000	1.11050300
N	1.90902000	-4.36420600	1.33937200
C	2.84252200	-3.43123500	0.66233100
H	2.56737800	-3.42627400	-0.40029200
H	2.61921700	-2.42691600	1.04262800
C	4.34420900	-3.72258100	0.79289900
H	4.61524300	-4.70454900	0.38948100
H	4.90565300	-2.96878900	0.23004500
H	4.68484100	-3.67467700	1.83257600
C	1.93346200	-5.71069100	0.76286400
H	1.13396500	-6.31233400	1.20982900
H	1.75732400	-5.65244600	-0.31672200
H	2.88520000	-6.24287400	0.92873800
C	2.11932000	-4.41346900	2.79159600
H	2.09111500	-3.39855600	3.20114600
H	1.31451800	-4.99580700	3.25583900
H	3.07636800	-4.87940000	3.07864900
C	-0.39987000	-0.02226300	2.38192700
C	-1.87160500	0.45018800	2.51480900
H	-2.02318500	1.12638300	3.36963000
H	-2.53388900	-0.41867200	2.64279400
H	-2.19227500	0.98002300	1.61045300
C	-0.01443700	-0.81819000	3.63931400
H	-0.22601300	-0.26707500	4.56505600
H	1.05320200	-1.06984800	3.62075900
H	-0.58644500	-1.76007000	3.68515900
H	0.21754300	0.90228500	2.41286000
C	1.37020300	0.71927700	-0.10875300
H	1.57180600	1.31597000	0.78798100
H	1.41871600	1.39537300	-0.97549500
H	2.17719900	-0.02079200	-0.20290600
C	-0.20347400	-0.86336500	-1.25661700
H	-0.06815600	-0.29000400	-2.18278000
H	-1.20992100	-1.30112300	-1.26919400
H	0.53185800	-1.68556700	-1.27796600
H	-0.76881700	0.80365700	-0.06212700
N	-2.31140600	-4.31895000	1.14370400
C	-3.13610000	-3.43075800	0.28909100
H	-2.95906400	-2.40506400	0.63501800
H	-2.71856300	-3.49233400	-0.72418700
C	-4.64430300	-3.71242900	0.23136300
H	-5.12382400	-3.59587700	1.20898200
H	-5.11664500	-2.99742500	-0.45127700
H	-4.86651900	-4.71880700	-0.14039200
C	-2.71566200	-4.27274100	2.55435300
H	-1.98677700	-4.82411000	3.16006800
H	-2.73395900	-3.23315200	2.89717200
H	-3.70749600	-4.71762700	2.73856300
C	-2.27485600	-5.70050000	0.65762200
H	-1.96304100	-5.71364700	-0.39234300
H	-1.54396800	-6.27240700	1.24057500
H	-3.24476900	-6.21961600	0.73639500

Table S-49. Geometric coordinates and thermally corrected MP2 energies for $A(DMEA)_3$.

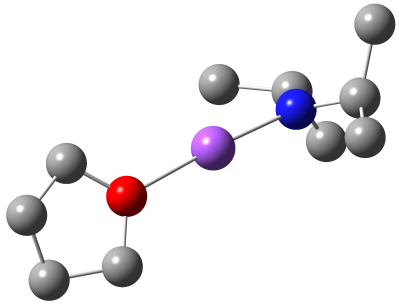


G = –1094.904275 Hartree
G_{MP2} = –1091.0333779922 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	-1.39938700	-0.29968700	0.20957800
Na	-2.83656000	-0.31031300	-1.46238700
C	-1.75269400	-0.41306600	1.60648300
C	-1.92663200	0.95313700	2.32113000
H	-2.10041000	0.84424800	3.40245400
H	-2.77883700	1.49586600	1.88788800
H	-1.03504500	1.57666700	2.18912500
C	-3.04645200	-1.22811000	1.76726400
H	-3.36813700	-1.29977200	2.81480900
H	-2.91211900	-2.24359700	1.37458800
H	-3.86811600	-0.75136900	1.20623600
H	-0.97946400	-0.96189300	2.18863400
C	0.93431200	-1.22603000	0.17605700
H	0.77847000	-1.69802700	1.15291300
H	1.99861400	-0.95587700	0.10385200
H	0.71611700	-1.97856400	-0.59439300
C	0.21814000	0.59112400	-1.40301000
H	1.27634900	0.79717400	-1.60980900
H	-0.34274500	1.52815200	-1.51824200
H	-0.12879800	-0.11677400	-2.17449800
H	0.37575400	0.77122900	0.70971200
N	-3.29464600	-2.46341300	-2.65367700
C	-1.97402900	-3.11778800	-2.48895300
H	-1.27326800	-2.57992600	-3.14039500
H	-1.64816700	-2.92189700	-1.46028900
C	-1.89435600	-4.62068500	-2.79313500
H	-2.18178700	-4.85341800	-3.82445200
H	-0.86239900	-4.96111800	-2.65345000
H	-2.52711000	-5.21064500	-2.12155700
C	-3.74241900	-2.43585900	-4.04776700
H	-4.65911200	-1.84087200	-4.12368400
H	-2.97377000	-1.96884200	-4.67343600
H	-3.95894600	-3.43676500	-4.45833400
C	-4.32700400	-3.04733200	-1.78754800
H	-3.95883500	-3.08524200	-0.75700000
H	-5.22395600	-2.41772100	-1.81040500
H	-4.62084700	-4.06713600	-2.08805400
N	-4.28604400	1.55095300	-2.29821700
C	-3.41618700	2.33470500	-3.20216800
H	-2.48640300	2.53580400	-2.65544600
H	-3.15362100	1.67883800	-4.04322400
C	-3.97420500	3.65602900	-3.75275300
H	-4.20707700	4.36817800	-2.95438500
H	-3.22453900	4.12304800	-4.40120500
H	-4.87932100	3.50514100	-4.35076400
C	-4.59163900	2.26724500	-1.05266800
H	-5.13113300	1.59729000	-0.37510800
H	-3.65995500	2.56311700	-0.56071900
H	-5.21523400	3.16321100	-1.20976700
C	-5.51509000	1.08723900	-2.95130600
H	-5.26027800	0.56925400	-3.88260200
H	-6.03725400	0.38137000	-2.29528700
H	-6.21343100	1.90567100	-3.19626000
N	-7.80951300	-1.20006200	-0.69947500
C	-7.56556200	-0.46803700	0.55141100
H	-6.63912800	-0.86666100	0.98441300
H	-7.36041700	0.57551900	0.27870700

C	-8.67331900	-0.49616800	1.61898900
H	-8.88427300	-1.51442300	1.96338800
H	-8.35877600	0.08771200	2.49141900
H	-9.60964100	-0.06236200	1.25070800
C	-7.94934600	-2.63913800	-0.50706000
H	-7.95406700	-3.13824100	-1.48301200
H	-7.09629700	-3.01915700	0.06560500
H	-8.87488400	-2.93338700	0.02095800
C	-8.91191100	-0.65683500	-1.48436400
H	-8.76347800	0.41842300	-1.63410200
H	-8.92781900	-1.13756000	-2.46940500
H	-9.90706500	-0.80472000	-1.02609900

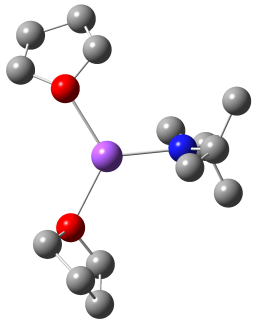
Table S-50. Geometric coordinates and thermally corrected MP2 energies for A(THF).



G = –686.298172 Hartree
G_{MP2} = –684.01022527908 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	0.82105000	1.17250700	-0.19343300
Na	2.96586900	1.08849700	-0.28816300
O	5.24066500	1.05289300	-0.24086500
C	6.01958300	0.93434200	0.97549000
C	7.41356500	1.44756500	0.61876600
C	7.54068800	1.01877400	-0.85176900
C	6.12091000	1.24327000	-1.37815600
H	5.82933000	0.53743500	-2.16233800
H	5.98381100	2.26479200	-1.75463800
H	7.81219900	-0.04089500	-0.91897300
H	8.28475000	1.59562800	-1.40805000
H	8.19057200	1.02416600	1.26139300
H	7.45384900	2.53932000	0.70671800
H	5.52010200	1.51556400	1.75676700
H	6.04284000	-0.12011900	1.28038700
C	0.08848300	2.40934200	-0.33568500
C	-0.48518100	2.95195900	0.99753800
H	-1.09713500	3.85390400	0.85037100
H	0.33620300	3.19686000	1.68535500
H	-1.11473700	2.20114200	1.48826200
C	0.99311400	3.48213800	-0.96380000
H	0.48281600	4.44704400	-1.07657700
H	1.34381000	3.15852600	-1.95249400
H	1.87373500	3.65884300	-0.32166200
H	-0.77816700	2.30508400	-1.02519500
C	-0.71002000	-0.48579400	-1.28877400
H	-1.31064100	0.31625200	-1.73251500
H	-1.38037000	-1.33668100	-1.09856700
H	0.03766700	-0.79119000	-2.03403800
C	0.85459200	-1.14757800	0.56216200
H	0.27361000	-2.06588000	0.71497700
H	1.30384900	-0.85829500	1.52105600
H	1.66670800	-1.39595100	-0.14319000
H	-0.80425300	0.17203600	0.74930000

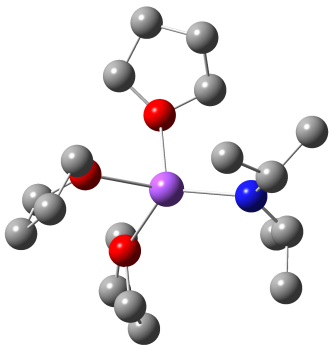
Table S-51. Geometric coordinates and thermally corrected MP2 energies for A(THF)$_2$.



G = –918.654819 Hartree
G_{MP2} = –915.5919319 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	0.32396800	-0.86040000	1.11636200
Na	0.40281600	-3.05892200	1.00595500
C	0.70607700	-0.14025900	2.31201100
C	-0.48582000	0.50198800	3.06907900
H	-0.15660400	1.12082700	3.91697400
H	-1.15435800	-0.28054400	3.45488900
H	-1.07411800	1.14221200	2.40192300
C	1.45586400	-1.07547400	3.27520100
H	1.74083000	-0.57255400	4.20835000
H	2.36706100	-1.46554900	2.80262600
H	0.81638800	-1.93068600	3.55055300
H	1.41025900	0.69432400	2.09561700
C	1.23546600	0.64200100	-0.68356000
H	1.85376400	1.17954000	0.04441400
H	0.95226700	1.35765200	-1.46964700
H	1.85986000	-0.13975200	-1.13912700
C	-0.79614600	-0.78335800	-1.05636000
H	-1.03925000	-0.17103600	-1.93431800
H	-1.73316200	-1.16432300	-0.63107300
H	-0.20798500	-1.64487500	-1.41441800
H	-0.65366800	0.84996200	0.29984100
O	-1.52643700	-4.16746600	1.54608100
C	-2.52651600	-3.20427100	1.95129400
C	-3.70959400	-3.41332400	0.98467200
C	-3.46648100	-4.82555000	0.38139200
C	-2.24528400	-5.34326300	1.15777800
H	-1.56931000	-5.97045900	0.57018400
H	-2.55059100	-5.89924300	2.05733100
H	-3.23613800	-4.75321500	-0.68596900
H	-4.32877300	-5.48983500	0.49146800
H	-3.70999000	-2.65107000	0.20047000
H	-4.66594400	-3.34660000	1.51157900
H	-2.81515300	-3.41362300	2.99136500
H	-2.05563200	-2.21798100	1.89155200
O	2.33972700	-4.23528300	0.57793600
C	3.03374800	-5.10950500	1.48503300
C	4.26861500	-4.32253200	1.91618500
C	4.66030600	-3.61616700	0.60604700
C	3.30501500	-3.36663400	-0.08222800
H	3.32512500	-3.61228000	-1.14992200
H	2.94487400	-2.33942800	0.04110000
H	5.28962600	-4.27202100	-0.00582900
H	5.21097300	-2.68653000	0.77457500
H	5.06220800	-4.96164100	2.31489600
H	3.99474100	-3.59020700	2.68368400
H	2.34788500	-5.35368700	2.30219200
H	3.30943300	-6.04089200	0.96819600

Table S-52. Geometric coordinates and thermally corrected MP2 energies for $A(THF)_3$.

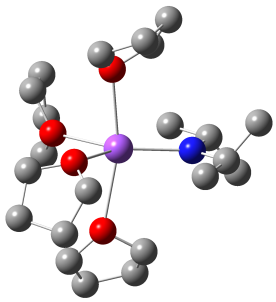


G = –1151.005014 Hartree
G_{MP2} = –1147.1675224913 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	0.03697800	-1.44769500	-0.00555400
Na	-1.62913700	-2.70746800	0.85508100
C	1.05418900	-1.96115700	-0.89916600
C	2.48591200	-1.91619600	-0.30268300
H	3.25448000	-2.21046100	-1.03345700
H	2.55699700	-2.59237100	0.56076800
H	2.73019800	-0.90638500	0.04644200
C	0.73512100	-3.40706800	-1.30983500
H	1.51509100	-3.84280100	-1.94846100
H	-0.21868900	-3.44686000	-1.85233900
H	0.65037600	-4.04219900	-0.41336600
H	1.10686100	-1.38614000	-1.85105200
C	-0.75476100	0.60992500	-1.21151900
H	-0.35147100	0.22475400	-2.15506400
H	-0.68803300	1.70842600	-1.24270500
H	-1.81822400	0.33089700	-1.17076100
C	-0.63176900	0.52392100	1.30021700
H	-0.71713900	1.61911600	1.30697400
H	-0.04016700	0.21747100	2.17076400
H	-1.64493700	0.11227700	1.42348400
H	1.02124700	0.44078600	-0.03503700
O	-3.77059200	-1.79013900	1.46984400
C	-4.00373900	-1.41627400	2.84917200
C	-5.13633300	-0.38599300	2.82062400
C	-4.93276400	0.27912200	1.45004400
C	-4.49715000	-0.90524400	0.58660300
H	-3.83258400	-0.62813700	-0.23682400
H	-5.36303500	-1.44539700	0.17774700
H	-4.13168500	1.02468200	1.50073500
H	-5.83318300	0.76793800	1.06628400
H	-5.07847900	0.31806700	3.65597300
H	-6.11251100	-0.88394600	2.86343500
H	-4.24965100	-2.32146300	3.41338600
H	-3.07768900	-0.99304000	3.25531600
O	-2.65478000	-4.81467400	0.29498800
C	-4.06730200	-5.00803400	0.46698200
C	-4.62377300	-5.29092600	-0.94503300
C	-3.37193900	-5.72640200	-1.75724200
C	-2.25459900	-5.76530100	-0.70273400
H	-1.27396000	-5.46340300	-1.07297100
H	-2.17496700	-6.76269500	-0.24292000
H	-3.13761700	-4.98831700	-2.53010300
H	-3.50133700	-6.69492100	-2.24926400
H	-5.07421400	-4.39254400	-1.37727200
H	-5.39506700	-6.06658300	-0.91911800
H	-4.23543200	-5.86635000	1.13535600
H	-4.45844000	-4.10429400	0.93689400
O	-0.95591000	-3.37334000	3.01517000
C	0.38681300	-2.88857100	3.25503100
C	1.23467600	-4.15408300	3.33801700
C	0.29272300	-5.12539200	4.07177600
C	-1.10583900	-4.68679500	3.59058100
H	-1.83093000	-4.64351700	4.41373200
H	-1.50897900	-5.34031100	2.80894800
H	0.38286000	-4.99457600	5.15618500
H	0.49733600	-6.17670600	3.84672400
H	2.18199700	-3.99762400	3.86287800

H 1.45955200 -4.51569600 2.32766500
H 0.63321600 -2.22801600 2.41552500
H 0.40917200 -2.32717800 4.20179800

Table S-53. Geometric coordinates and thermally corrected MP2 energies for A(THF)$_4$.

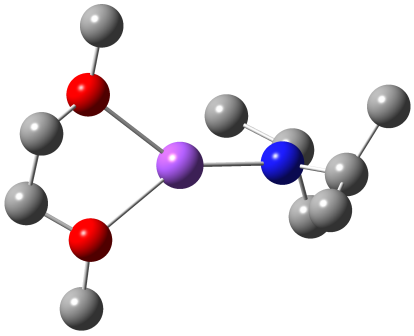


G = –1383.347523 Hartree
G_{MP2} = –1378.7491330234 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	-0.16303500	-1.15006300	-0.86721100
Na	-1.05524100	-3.18325600	-0.17901100
O	-2.09399200	-3.81745000	1.95806600
C	-1.37646200	-4.45772900	3.02433200
C	-1.29579500	-3.40460700	4.14070000
C	-2.54446600	-2.51333500	3.89726300
C	-3.13966900	-3.06077500	2.58247600
H	-3.44637000	-2.28943300	1.87397200
H	-3.99704500	-3.72248100	2.78335700
H	-2.25665800	-1.46470800	3.78793000
H	-3.26860000	-2.57784000	4.71528900
H	-0.38007700	-2.81488400	4.03906200
H	-1.28981100	-3.86363300	5.13403200
H	-1.93611000	-5.34640200	3.35780000
H	-0.41050000	-4.76092700	2.61945200
O	-1.41971100	-5.45124800	-1.19694800
C	-2.38432500	-6.29030200	-0.53253700
C	-3.53882900	-6.52704900	-1.54035700
C	-3.08645900	-5.75969700	-2.80363800
C	-1.57415400	-5.66963000	-2.60575600
H	-1.09682400	-4.83564900	-3.12288500
H	-1.07360800	-6.60733700	-2.89713600
H	-3.50540600	-4.74928700	-2.80769600
H	-3.36782100	-6.26170800	-3.73437800
H	-4.49678800	-6.15989000	-1.16120600
H	-3.65547700	-7.59577200	-1.74824000
H	-1.90467900	-7.23779800	-0.24865400
H	-2.68705700	-5.76497600	0.37568900
O	1.02997200	-4.26856100	0.74969100
C	2.06321800	-3.25798300	0.91140200
C	3.33798500	-3.81985800	0.24981200
C	2.81441400	-5.00336900	-0.58350100
C	1.62918800	-5.47420100	0.25694100
H	1.96843900	-6.10130100	1.09825500
H	0.86088700	-6.01062100	-0.30377200
H	3.56421800	-5.78514100	-0.74305700
H	2.46090600	-4.65738400	-1.56138700
H	4.04931300	-4.17222600	1.00585900
H	3.84522100	-3.06680500	-0.36053000
H	1.68112200	-2.35739100	0.41858200
H	2.20692700	-3.06503800	1.98242800
C	0.39597100	-0.96919200	-2.19224700
C	1.92202200	-0.69464500	-2.24679300
H	2.26679800	-0.53296200	-3.27806500
H	2.47910200	-1.54586500	-1.83060000
H	2.19464500	0.19464000	-1.66772000
C	0.09982500	-2.21181400	-3.04727500
H	0.46439400	-2.10037900	-4.07695200
H	-0.98019300	-2.40466000	-3.08864100
H	0.59024500	-3.09580000	-2.61172100
H	-0.06854500	-0.11753500	-2.74383600
C	-0.64588600	1.31756700	-0.50383800
H	-0.24705400	1.61918700	-1.47865600
H	-0.46508300	2.14692400	0.19461500
H	-1.73252500	1.19526400	-0.61427500
C	-0.58022800	-0.31788200	1.38744500
H	-0.43822000	0.51319800	2.09116900
H	-0.10629000	-1.21040100	1.81585300

H -1.65964400 -0.51364400 1.30756400
H 1.07183100 0.25651700 0.18121600
O -3.49022600 -2.66095700 -0.94885900
C -4.86268100 -2.98179800 -0.71634200
C -5.58650700 -1.63799100 -0.45546800
C -4.56465600 -0.57252200 -0.93695800
C -3.48783600 -1.39996400 -1.64804800
H -3.75289100 -1.57017200 -2.70448600
H -4.12457600 -0.04496500 -0.08425700
H -5.01342700 0.17717400 -1.59558500
H -5.82727200 -1.50994400 0.60468300
H -6.52847200 -1.58779400 -1.01079300
H -5.28263000 -3.48215900 -1.60341000
H -4.90355700 -3.68016500 0.12433700
H -2.46589800 -1.01035500 -1.56696200

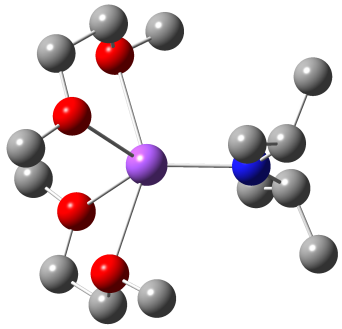
Table S-54. Geometric coordinates and thermally corrected MP2 energies for A(κ_2-DME).



G = –762.690778 Hartree
G_{MP2} = –760.16525617353 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	0.78311100	-0.40728500	1.14341600
Na	2.94885900	-0.40710500	1.14279900
O	4.86341000	0.78703600	1.84396400
C	6.03463200	0.35006300	1.16601000
C	6.03421200	-1.16538500	1.12140600
H	6.05386400	-1.57698700	2.14256500
H	6.93602400	-1.51012900	0.59291100
O	4.86332600	-1.60167500	0.44241900
C	4.81471500	-3.01377800	0.25186600
H	3.87000700	-3.23416200	-0.24867700
H	5.65051000	-3.34962300	-0.37689800
H	4.85016800	-3.54354800	1.21412200
H	6.05545800	0.76166500	0.14487300
H	6.93617600	0.69426100	1.69532000
C	4.81553200	2.19913800	2.03461900
H	4.85158900	2.72897100	1.07241700
H	3.87079500	2.42001000	2.53489100
H	5.65132000	2.53447100	2.66366900
C	-0.00038800	-0.81435300	2.28661900
C	-0.63585700	-2.22118900	2.14097600
H	-1.29049400	-2.47268900	2.98861600
H	0.15405300	-2.98264700	2.07435200
H	-1.23717600	-2.28756600	1.22719300
C	0.86867800	-0.79127200	3.55466100
H	0.31824100	-1.12172000	4.44486900
H	1.25425600	0.21918900	3.74116000
H	1.72847700	-1.47316000	3.43638000
H	-0.84419800	-0.11677500	2.48675400
C	-0.63511900	1.40700800	0.14546000
H	-1.23659400	1.47358800	1.05912300
H	-1.28952700	1.65865400	-0.70231600
H	0.15498500	2.16825600	0.21220100
C	0.86935200	-0.02329800	-1.26783800
H	0.31916600	0.30714900	-2.15820000
H	1.25484900	-1.03382100	-1.45417900
H	1.72919500	0.65854300	-1.14947700
H	-0.84393800	-0.69736400	-0.20034900

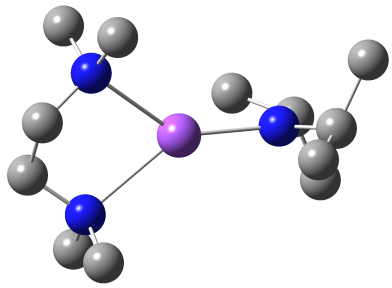
Table S-55. Geometric coordinates and thermally corrected MP2 energies for A(κ_2-DME)$_2$.



G = –1071.431407 Hartree
G_{MP2} = –1067.9090046592 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	-0.81548700	-0.68332400	-0.98284900
Na	-3.06869200	-0.66927500	-0.97956000
O	-3.83735500	-2.77027800	0.33262300
C	-3.92798500	-3.69895200	-0.73838200
C	-5.00588300	-3.23696300	-1.69722900
O	-4.62549800	-1.98566400	-2.24954400
C	-5.57028700	-1.46440700	-3.17171300
H	-6.56745800	-1.38434900	-2.71314600
H	-5.22253300	-0.46826400	-3.44941100
H	-5.64157600	-2.10006600	-4.06620800
H	-5.96680000	-3.13793900	-1.16791000
H	-5.12792500	-3.98746400	-2.49433600
H	-2.96325100	-3.77279900	-1.26233000
H	-4.18972900	-4.69974900	-0.35774300
C	-2.81093600	-3.11795200	1.26493300
H	-2.89420700	-2.41879400	2.09953700
H	-2.95602600	-4.14362900	1.63506100
H	-1.82176500	-3.01027000	0.80381600
O	-3.77611300	1.44963200	-2.29122900
C	-3.86320600	2.37227800	-1.21510300
C	-4.96803100	1.92887700	-0.27828100
H	-5.92176900	1.85649900	-0.82461100
H	-5.08617800	2.67588200	0.52270100
O	-4.62648000	0.66472500	0.27023800
C	-5.59950800	0.15773000	1.17054200
H	-5.27888500	-0.84795500	1.44646700
H	-5.67360000	0.78803100	2.06862900
H	-6.58954800	0.10332800	0.69303300
H	-2.90624100	2.41984200	-0.67397400
H	-4.09463000	3.38183200	-1.59232900
C	-2.71936300	1.77480000	-3.19847500
H	-1.74445500	1.62013100	-2.72030100
H	-2.81305700	1.09375200	-4.04686800
H	-2.81977400	2.81128300	-3.55293800
C	-0.01462200	-1.41499600	-1.94284700
C	0.51120000	-2.77648400	-1.41247300
H	1.21214400	-3.25861500	-2.11102800
H	-0.32959800	-3.46546200	-1.24511200
H	1.03149400	-2.64834900	-0.45621500
C	-0.80322000	-1.66368600	-3.23945400
H	-0.23673900	-2.27272700	-3.95685500
H	-1.06320100	-0.71568600	-3.72431600
H	-1.74140600	-2.19722600	-3.02253600
H	0.89296600	-0.84741000	-2.24902300
C	0.63051200	1.32106900	-0.51748000
H	1.18417900	1.15223100	-1.44835200
H	1.32835900	1.76686000	0.20774200
H	-0.15854600	2.05739000	-0.72881400
C	-0.81244600	0.30695500	1.26901000
H	-0.22901400	0.87573700	2.00546300
H	-1.15512200	-0.61947000	1.74456000
H	-1.70295800	0.90485600	1.02141900
H	0.85814200	-0.62405500	0.33908200

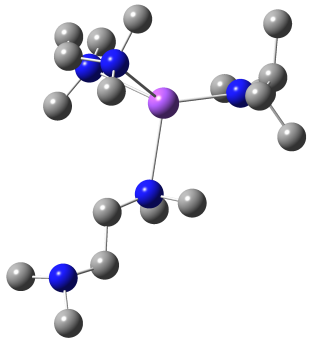
Table S-56. Geometric coordinates and thermally corrected MP2 energies for A(κ_2-TMEDA).



G = –801.500769 Hartree
G_{MP2} = –798.75006710089 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
Na	-2.07512000	-1.39054400	-2.05391900
N	-4.25115400	-1.39065200	-2.05449700
C	-5.03538600	-2.11317700	-1.08052400
C	-5.67218400	-3.41662400	-1.62843200
H	-6.27601500	-3.21347700	-2.52011800
H	-6.32511600	-3.90471500	-0.88958600
H	-4.88321500	-4.12548200	-1.91710600
C	-4.16747900	-2.46120500	0.14042100
H	-4.72073900	-3.03093000	0.89817100
H	-3.77823700	-1.54814300	0.60914800
H	-3.31104100	-3.08447500	-0.16951100
H	-5.87915100	-1.50474800	-0.68498300
C	-5.03502300	-0.66634900	-3.02740300
C	-5.66823200	0.63851900	-2.47871000
H	-6.32099700	1.12806200	-3.21674200
H	-4.87735300	1.34565500	-2.19100000
H	-6.27139900	0.43671500	-1.58627000
C	-4.16798300	-0.32036800	-4.24954700
H	-4.72103400	0.25042400	-5.00664800
H	-3.78126700	-1.23433000	-4.71855800
H	-3.30977700	0.30113600	-3.94090900
H	-5.88069900	-1.27287100	-3.42180800
N	-0.10362200	0.01802600	-1.46502000
C	1.05549700	-0.62455400	-2.10740800
C	1.05599000	-2.15515900	-2.00135200
H	1.05427600	-2.44921300	-0.94633500
H	2.00605700	-2.52995700	-2.42586500
N	-0.10328400	-2.79837100	-2.64276100
C	-0.26122600	-4.18143800	-2.17404900
H	-0.38737100	-4.19404000	-1.08675300
H	-1.15692700	-4.61855000	-2.62551200
H	0.60503800	-4.81640300	-2.43228500
C	-0.00093400	-2.78044200	-4.10785700
H	0.88215800	-3.33718600	-4.47011600
H	-0.89821900	-3.23371300	-4.53976700
H	0.06612900	-1.75367400	-4.47858900
H	1.05273100	-0.33049100	-3.16242500
H	2.00568800	-0.24919000	-1.68368400
C	-0.26236300	1.40111000	-1.93344500
H	-1.15764400	1.83801200	-1.48095900
H	0.60407200	2.03621000	-1.67611800
H	-0.38973400	1.41377300	-3.02059800
H	0.88323000	0.55700300	0.36152500
H	-0.89703900	0.45295600	0.43274900
H	0.06774200	-1.02676900	0.37060200

Table S-57. Geometric coordinates and thermally corrected MP2 energies for A(κ_1-TMEDA)(κ_2-TMEDA).

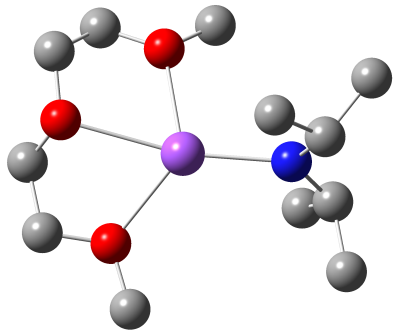


G = –1149.034569 Hartree
G_{MP2} = –1145.0459365636 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	-0.38474100	1.02366700	-0.98445000
C	-1.65664000	1.69282600	-0.67001300
C	-2.92123500	0.81254600	-0.59814700
H	-2.75061600	0.01742900	0.13519800
H	-3.11019100	0.31476100	-1.56904100
N	-4.08684000	1.57944100	-0.15038100
C	-5.13184000	0.71002200	0.37791000
H	-4.73517500	0.11280800	1.20562500
H	-5.95522700	1.32074100	0.76470300
H	-5.55033000	0.01612400	-0.37785700
C	-4.62480400	2.44599900	-1.19275000
H	-4.99641700	1.88419200	-2.07331100
H	-5.45850900	3.02958400	-0.78774300
H	-3.86548900	3.15308100	-1.53933100
H	-1.54858200	2.18567700	0.30366100
H	-1.79659900	2.48324000	-1.41723700
C	-0.34753400	0.46810900	-2.34111700
H	0.66565000	0.11465800	-2.55517900
H	-1.03628500	-0.38180600	-2.48505600
H	-0.60763100	1.24594700	-3.06832100
H	-0.61049900	-0.91692400	-0.06752500
H	1.05588800	-0.25371700	-0.15544400
H	-0.10635200	0.41079600	1.01017300
Na	1.88649400	2.35470700	-0.72896300
N	3.51439600	0.80042600	-0.54350800
C	4.20920800	0.48988500	0.69018300
C	5.46258400	1.37273200	0.93640400
H	6.13885400	1.33564300	0.07447300
H	6.03445300	1.05717300	1.82276100
H	5.16287900	2.42127200	1.07545700
C	3.27083300	0.60347200	1.90277800
H	3.80286100	0.45265300	2.85160900
H	2.46049000	-0.13114400	1.84141200
H	2.81236600	1.60399200	1.93984900
H	4.57818900	-0.55975500	0.70005300
C	4.16381400	0.18617800	-1.68484900
C	3.78434600	-1.30518000	-1.88414600
H	4.36644200	-1.78466000	-2.68589700
H	2.71784200	-1.39621800	-2.13443400
H	3.95603300	-1.87336800	-0.96267200
C	3.85961800	0.95939200	-2.97744700
H	4.29746900	0.47953900	-3.86310600
H	4.24800800	1.98245400	-2.90990900
H	2.77169000	1.01755900	-3.14386200
H	5.27191400	0.20191100	-1.58794300
C	0.29664700	4.46295900	-2.86203000
N	1.61440300	4.49353400	-2.22055100
C	1.73402900	5.63228900	-1.29484300
C	0.98935700	5.44809800	0.03109000
H	-0.06644600	5.23187600	-0.16616500
H	1.01352400	6.41383300	0.57204200
N	1.51582500	4.36295800	0.87378800
C	0.58195400	4.07525900	1.96876100
H	-0.39404100	3.79280600	1.56171400
H	0.96250200	3.23937000	2.56343800
H	0.43897200	4.94146900	2.64052000

C	2.83256200	4.70192600	1.43132000
H	2.79882100	5.62800500	2.03470000
H	3.17964500	3.88348500	2.06624900
H	3.57026600	4.82914800	0.63551600
H	2.79888500	5.78681400	-1.09657100
H	1.36891300	6.56367700	-1.76773600
C	2.66002200	4.56520500	-3.24949700
H	2.57476600	3.70596400	-3.92023000
H	2.59153600	5.48879600	-3.85296500
H	3.64614300	4.52658500	-2.77800000
H	0.10389500	5.37042300	-3.46427100
H	0.23290900	3.59284600	-3.52240800
H	-0.49427000	4.37459900	-2.11265100

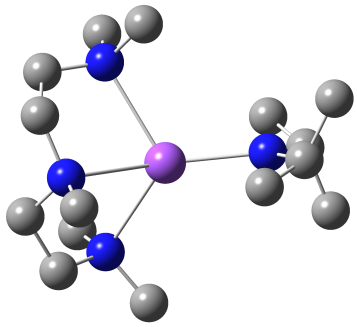
Table S-58. Geometric coordinates and thermally corrected MP2 energies for A(κ_3-diglyme).



G = –916.469894 Hartree
G_{MP2} = –913.4595743456 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	-0.77694500	0.60785300	1.05989100
Na	-2.98280600	0.67597000	0.82248600
O	-4.30273800	2.65510800	1.11377200
C	-3.73531800	3.93463000	0.84483700
H	-4.21087600	4.70817800	1.46395600
H	-3.84985400	4.20008000	-0.21572300
H	-2.67403600	3.86736000	1.08908100
C	-5.68233900	2.57635100	0.79058700
C	-6.18549200	1.19792300	1.16843200
H	-6.01128200	1.02717500	2.24080200
H	-7.26822800	1.13483600	0.97907500
O	-5.48806000	0.24403900	0.37608000
C	-5.80189100	-1.12119400	0.65105300
H	-5.46817800	-1.67461800	-0.23113800
H	-6.88850600	-1.25559200	0.75834400
C	-5.07876700	-1.65740200	1.88238800
H	-5.26176900	-2.74164600	1.95710700
H	-5.45267300	-1.19653900	2.81176000
O	-3.70498600	-1.37908200	1.71309900
C	-2.84612700	-1.93465800	2.70896500
H	-2.84826900	-3.03220000	2.65206300
H	-1.85281800	-1.53337000	2.48936000
H	-3.16307800	-1.62349500	3.71529700
H	-5.83215300	2.75187900	-0.28600400
H	-6.25300900	3.33639500	1.34695900
C	0.02206400	1.35539100	2.00400000
C	0.52147800	2.72497700	1.47161600
H	1.19735400	3.22779800	2.17953400
H	-0.33414600	3.39004500	1.28312000
H	1.06050000	2.60730100	0.52483200
C	-0.77041700	1.58671300	3.30089800
H	-0.20643900	2.18162400	4.03147600
H	-1.03960200	0.63148400	3.76695100
H	-1.70392100	2.13067100	3.08412900
H	0.94069000	0.80289700	2.30596000
C	0.76893000	-1.27413000	0.43855600
H	1.39806400	-1.07037100	1.31250600
H	1.42273400	-1.66155000	-0.35706000
H	0.05897900	-2.06588000	0.71576100
C	-0.91203200	-0.36227400	-1.18517900
H	-0.36274500	-0.84922900	-2.00138000
H	-1.39588500	0.53716300	-1.59179200
H	-1.69640000	-1.06442100	-0.85870700
H	0.76998800	0.68979900	-0.41330300

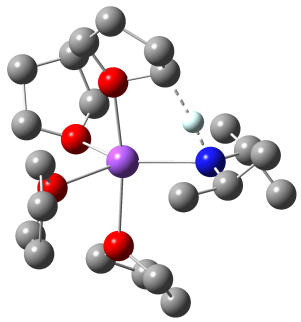
Table S-59. Geometric coordinates and thermally corrected MP2 energies for A(κ_3-PMDTA).



G = –974.680259 Hartree
G_{MP2} = –971.33304414171 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	0.62872200	0.42201700	-1.23079100
Na	2.84233800	0.53489600	-1.43116800
C	-0.31438700	0.93642300	-2.19713200
C	-0.78142300	2.38867100	-1.90948800
H	-1.57604700	2.71960700	-2.59546300
H	0.06660900	3.08207900	-2.00639200
H	-1.16596900	2.47830100	-0.88708600
C	0.28129600	0.87784800	-3.61293400
H	-0.39333700	1.30241500	-4.36834700
H	0.50629600	-0.15899400	-3.89085600
H	1.22151400	1.45260700	-3.65398100
H	-1.24477400	0.32646800	-2.24020300
C	-0.71409500	-1.37441100	-0.09950800
H	-1.25630400	-1.63354600	0.82250900
H	0.02147100	-2.16537700	-0.30258700
H	-1.43908000	-1.37831300	-0.92131600
C	1.03525000	-0.06647400	1.13497000
H	0.59584200	-0.40380600	2.08293500
H	1.49349000	0.91840100	1.29694900
H	1.83479600	-0.78014500	0.87531300
H	-0.77714400	0.71904800	0.34682600
N	4.18385300	2.68809500	-1.62439300
C	4.59882000	2.88475400	-3.01634500
H	5.18693900	2.03204500	-3.36817500
H	5.20479900	3.80022700	-3.14884600
H	3.71146500	2.96445400	-3.65199300
C	3.33475500	3.80679300	-1.19428100
H	2.97046100	3.62528000	-0.17901100
H	2.46379200	3.87709100	-1.85134400
H	3.87139900	4.77292900	-1.21326300
C	5.33675300	2.53151900	-0.72457400
C	6.00687200	1.15435900	-0.80508200
N	5.14785500	0.04782300	-0.34910600
C	5.60076800	-1.25396300	-0.87075900
H	5.09574300	-2.02955200	-0.28664100
H	6.68442700	-1.40103900	-0.70205600
C	5.31845500	-1.47914900	-2.36239200
H	5.87770300	-0.75014600	-2.96000900
H	5.72600500	-2.47252900	-2.63343900
N	3.90415500	-1.35680400	-2.73199100
C	3.75106600	-1.24440300	-4.18539400
H	4.11250100	-2.14203100	-4.72021700
H	2.69449700	-1.10006600	-4.42749800
H	4.30935000	-0.37685900	-4.55407000
C	3.09216100	-2.47578100	-2.23449800
H	2.03748200	-2.27034100	-2.43681200
H	3.38089200	-3.43616200	-2.70053100
H	3.19563500	-2.57295500	-1.15066900
C	5.08102200	0.00477800	1.11692300
H	4.70867000	0.95446800	1.50921000
H	6.06591800	-0.19698200	1.57683600
H	4.38155000	-0.77481200	1.43142200
H	6.30263100	0.95971100	-1.83935600
H	6.94423800	1.18926200	-0.21829400
H	4.98349100	2.70518200	0.29693100
H	6.10551900	3.30286500	-0.92195800

Table S-60. Geometric coordinates and thermally corrected MP2 energies for alpha proton metalation of THF by $A(THF)_4$.

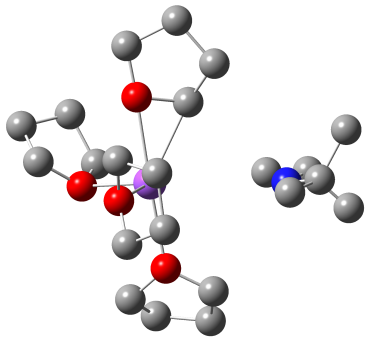


G = –1383.356806 Hartree
G_{MP2} = –1378.7606320539 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	-0.24182900	-1.04264800	-1.00897900
Na	-1.16418800	-3.27173800	-0.41059700
O	-2.06151000	-4.00404200	1.72995000
C	-1.35889600	-4.63243800	2.80870300
C	-1.42134200	-3.62410800	3.96767900
C	-2.72216600	-2.82239900	3.68408700
C	-3.20296500	-3.36391400	2.32078900
H	-3.53800800	-2.59995800	1.61901400
H	-4.00526200	-4.10626800	2.45241800
H	-2.51338900	-1.75066800	3.62802200
H	-3.48042300	-2.97251100	4.45866600
H	-0.55038200	-2.96208500	3.94316800
H	-1.43366300	-4.12253300	4.94180100
H	-1.86457900	-5.57397400	3.07713300
H	-0.35278300	-4.85150200	2.44923400
O	-1.45096700	-5.44336300	-1.59421000
C	-2.53937300	-6.20428200	-1.02700000
C	-3.67024300	-6.22613000	-2.08578400
C	-3.09493700	-5.39898100	-3.25676000
C	-1.59000100	-5.50669300	-3.02161700
H	-1.00639600	-4.68710000	-3.44532100
H	-1.18889500	-6.46329800	-3.39408900
H	-3.39675500	-4.35206700	-3.16676200
H	-3.40155700	-5.77469900	-4.23780600
H	-4.59813900	-5.79451300	-1.70157500
H	-3.88533100	-7.25396400	-2.39689100
H	-2.18595300	-7.21954200	-0.79803500
H	-2.81659700	-5.71017900	-0.09332800
O	0.95020200	-4.31345600	0.40807100
C	2.04784100	-3.42744200	0.72130300
C	3.30046500	-4.00064500	0.01563600
C	2.74448500	-5.16735400	-0.82641500
C	1.49468200	-5.56196500	-0.04151500
H	1.75410300	-6.19512100	0.82318400
H	0.71977300	-6.05374600	-0.63151600
H	3.45627000	-5.99110100	-0.93982200
H	2.45828100	-4.82102300	-1.82578000
H	4.02483000	-4.36633700	0.75145300
H	3.80505200	-3.24898800	-0.59824600
H	1.75773900	-2.43852200	0.35998100
H	2.18229800	-3.38775500	1.81097500
C	0.41840800	-0.81230100	-2.30184300
C	1.93686800	-0.58396100	-2.21498500
H	2.36503300	-0.47325300	-3.21958400
H	2.43049600	-1.43654000	-1.72996100
H	2.19346300	0.31842000	-1.65015500
C	0.13155000	-2.00984400	-3.21903700
H	0.51827200	-1.83703000	-4.23156300
H	-0.94638800	-2.18785700	-3.29217300
H	0.61278600	-2.91624100	-2.82371100
H	-0.00520100	0.07685400	-2.81019600
C	-0.45195000	1.41731900	-0.41722800
H	0.07112100	1.76219900	-1.31592000
H	-0.25009400	2.14460500	0.38001900
H	-1.52660200	1.43023800	-0.63095700
C	-0.69699600	-0.40070300	1.30874800

H -0.52462000 0.34637200 2.09379200
H -0.32423000 -1.36629800 1.67291000
H -1.77960700 -0.48780800 1.15809700
H 1.07916400 0.05872800 0.22540500
O -3.31132300 -2.59009800 -1.04353700
C -4.73749600 -2.72488900 -1.05014400
C -5.31969800 -1.29862700 -0.88613400
C -4.05595400 -0.39154600 -0.93489300
C -2.97307500 -1.24519000 -1.58776000
H -3.19963300 -1.29675600 -2.67471200
H -3.77558000 -0.10835400 0.09227200
H -4.23856400 0.53986100 -1.48447100
H -5.88404600 -1.19156100 0.04893700
H -6.00659600 -1.06746300 -1.70785100
H -5.06499000 -3.16965700 -2.00409500
H -5.02841300 -3.40869200 -0.24145100
H -1.44223300 -1.04073700 -1.26331700

Table S-61. Geometric coordinates and thermally corrected MP2 energies for optimized IRC of alpha proton metalation of THF by $A(THF)_4$.

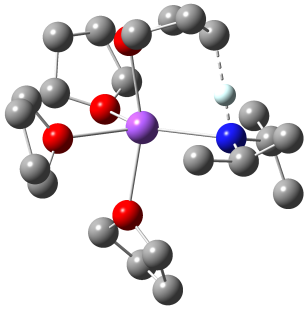


G = –1383.326809 Hartree
G_{MP2} = –1378.7226410519 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	0.77366500	1.03437700	-0.70710700
Na	4.41252000	1.41833600	0.18378300
O	5.25738200	0.51297200	2.17714500
C	4.81614200	0.79259500	3.50961200
C	3.99277700	-0.43838500	3.92977600
C	4.56417300	-1.58282600	3.04548500
C	5.60936400	-0.88076100	2.15497600
H	5.59810000	-1.18611200	1.10754800
H	6.62401700	-1.00207200	2.56438400
H	3.77411900	-2.03167200	2.43668200
H	5.01863900	-2.38187300	3.63915400
H	2.93207600	-0.28083800	3.71348500
H	4.08785000	-0.64297400	5.00061300
H	5.69097900	0.92725100	4.16500800
H	4.24984800	1.72535600	3.47178500
O	6.07875000	2.92165100	-0.69343400
C	7.41503100	2.36371800	-0.62237800
C	8.01657300	2.51205800	-2.02443100
C	6.76525900	2.47484000	-2.91513300
C	5.75900700	3.24728300	-2.06486700
H	4.72048500	2.95606700	-2.24878900
H	5.85607100	4.33381100	-2.20638700
H	6.42065100	1.44428400	-3.04185000
H	6.91846500	2.92453000	-3.90103700
H	8.73229300	1.71668200	-2.25281500
H	8.53348800	3.47410400	-2.12680200
H	7.97312800	2.90419300	0.14982800
H	7.32628000	1.31065100	-0.33623100
O	3.42250000	3.23639900	1.38119500
C	2.01224700	3.51354100	1.52409800
C	1.81163300	4.98543700	1.08418100
C	3.24946100	5.50619600	0.83927200
C	4.11538900	4.47699500	1.56926000
H	4.18552600	4.70656800	2.64511900
H	5.11793700	4.35652100	1.15498400
H	3.40481200	6.52515300	1.20744700
H	3.48697500	5.49280900	-0.22969500
H	1.30658100	5.56014000	1.86722600
H	1.19998400	5.05574100	0.18002100
H	1.47873500	2.78709300	0.90389300
H	1.72812200	3.37656000	2.57790700
C	0.19688000	1.57521300	-1.94658200
C	-1.13625400	2.28748500	-1.68643200
H	-1.50924500	2.74462000	-2.61043600
H	-1.00696800	3.07866300	-0.93744200
H	-1.91038200	1.60246000	-1.32398200
C	1.21157700	2.53807200	-2.57463900
H	0.84971700	2.90661200	-3.54187900
H	2.17217900	2.03503000	-2.72987000
H	1.38000700	3.40102600	-1.91793300
H	0.00596700	0.77797100	-2.68919300
C	-0.36734200	-1.23778200	-0.84239800
H	-0.97100200	-0.97342900	-1.71740700
H	-0.94961000	-1.95141800	-0.24591100
H	0.53587700	-1.74811700	-1.19634400
C	0.78523600	-0.41951500	1.24919600

H	0.22860600	-1.16310900	1.83168000
H	0.98389100	0.44613500	1.89061400
H	1.74792400	-0.86149400	0.96288300
H	-0.93703700	0.46404200	0.33817900
O	5.32511800	-0.30168600	-1.15562800
C	5.93036100	-1.38049800	-1.88106700
C	4.78486000	-2.33408400	-2.30195900
C	3.51409500	-1.62477700	-1.75188600
C	3.89937500	-0.15259000	-1.61421900
H	3.98307200	0.23676100	-2.65642800
H	3.25028200	-2.06605400	-0.77728900
H	2.65143300	-1.76970000	-2.41493300
H	4.92250900	-3.34551200	-1.89897700
H	4.73918500	-2.42175100	-3.39348000
H	6.45925400	-0.98815100	-2.76611500
H	6.67560400	-1.86253000	-1.23306700
H	1.71595100	0.66759200	-0.91535200

Table S-62. Geometric coordinates and thermally corrected MP2 energies for beta proton metalation of THF by $A(THF)_4$.

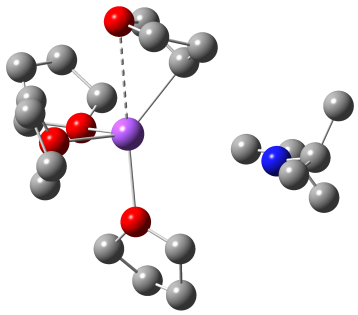


G = –1383.342987 Hartree
G_{MP2} = –1378.7505892499 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	0.63847200	0.49647100	-1.23218300
C	-0.31194200	0.80900200	-2.31346400
C	-1.38694000	1.84189200	-1.93740100
H	-2.03341400	2.04957400	-2.79961800
H	-0.92014600	2.78724000	-1.63123800
H	-2.03419600	1.50311600	-1.12157000
C	0.46490800	1.31343400	-3.53593600
H	-0.20801200	1.48530500	-4.38550600
H	1.21975500	0.58414700	-3.84137300
H	0.96464700	2.26495300	-3.30463400
H	-0.84697800	-0.10294900	-2.64101900
C	-0.79624400	-1.31231000	-0.17315400
H	-1.61829200	-1.19833400	-0.88805000
H	-1.23340000	-1.63510200	0.78078200
H	-0.14231300	-2.11050700	-0.54191600
C	1.06088400	-0.18317800	1.09497000
H	0.59943100	-0.49898200	2.03902900
H	1.59908200	0.75523500	1.28317300
H	1.79008700	-0.94753500	0.80799600
H	-0.70626400	0.75869500	0.37799000
Na	2.92864600	1.53652900	-1.10192800
O	4.76547300	1.87274400	0.61467400
C	4.53398200	2.45148600	1.90463100
C	4.84408200	1.32393700	2.90082900
C	5.91074900	0.47243400	2.15665300
C	5.97764500	1.11403600	0.75359500
H	6.01142100	0.40681100	-0.07468500
H	6.83836200	1.79729900	0.67892300
H	5.60235500	-0.57480800	2.09548700
H	6.88605200	0.50163800	2.65193500
H	3.94432800	0.73133000	3.09209300
H	5.20114300	1.71027800	3.86030100
H	5.21486300	3.30579600	2.05096600
H	3.50624700	2.81487600	1.91991700
O	4.13052000	2.97024300	-2.79021000
C	5.53844700	3.08669000	-2.52602600
C	6.18324100	2.10816300	-3.50840900
C	5.28208900	2.24377700	-4.76199400
C	4.00185900	2.93168900	-4.22411300
H	3.07941400	2.39574400	-4.45374700
H	3.91422200	3.96004000	-4.60348700
H	5.06290400	1.26736000	-5.20198100
H	5.75362300	2.85846300	-5.53539200
H	6.11961200	1.09582600	-3.09949500
H	7.23297300	2.34228300	-3.71122200
H	5.86377700	4.12277400	-2.71657900
H	5.68859500	2.85155100	-1.47191600
O	2.17186500	3.65762100	-0.09055400
C	0.93067900	3.80369800	0.62721600
C	0.27828500	5.11802500	0.13092000
C	1.26376100	5.63817000	-0.93894700
C	2.57315500	4.95841700	-0.53860800
H	3.07100700	5.50380400	0.28007300
H	3.27647700	4.81226700	-1.35961300
H	1.33853800	6.72992500	-0.95678200
H	0.96406900	5.29942000	-1.93656200

H 0.17916400 5.83402600 0.95347700
H -0.72093400 4.94778500 -0.27966600
H 0.33941300 2.91222600 0.41423600
H 1.13702300 3.84521900 1.70656100
O 4.33010400 -0.39602300 -1.74727900
C 4.18094700 -1.48550300 -0.79996400
C 3.07390800 -2.40971900 -1.35124800
C 2.35345600 -1.48814900 -2.34422900
C 3.55721400 -0.79027800 -2.92980800
H 4.23681300 -1.40776100 -3.56175100
H 3.35564000 0.13407200 -3.49003300
H 1.80774200 -2.06618700 -3.10537600
H 2.43523000 -2.79003600 -0.54074200
H 3.55326400 -3.29766900 -1.81104600
H 5.14812600 -1.99752200 -0.69340300
H 3.92017000 -1.04519100 0.17017600
H 1.33707400 -0.37908400 -1.66345700

Table S-63. Geometric coordinates and thermally corrected MP2 energies for IRC of beta proton metalation of THF by $A(THF)_4$.

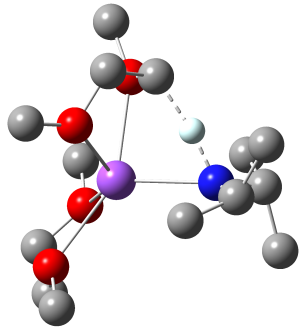


G = –1383.355071 Hartree
G_{MP2} = –1378.7487796731 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	0.79528400	-1.11621300	0.54467700
C	0.21607300	-1.85531700	1.67841000
C	-1.00430900	-2.67523000	1.23966100
H	-1.39370600	-3.25883900	2.08212500
H	-0.72490200	-3.36746700	0.43608700
H	-1.82139600	-2.04465500	0.87357200
C	1.29374900	-2.77213100	2.26629700
H	0.91318700	-3.30198100	3.14724000
H	2.17636100	-2.19476100	2.56259900
H	1.60859600	-3.51688300	1.52468700
H	-0.11074100	-1.17459200	2.48620500
C	-0.19010300	1.18016700	0.97215400
H	-0.68212500	0.86910800	1.90015200
H	-0.80954800	1.96388200	0.51872900
H	0.77761400	1.62312600	1.23621000
C	0.64061500	0.47070500	-1.31123400
H	0.06475100	1.29002900	-1.75731900
H	0.69192000	-0.35041100	-2.03372100
H	1.66037900	0.83522400	-1.13613200
H	-0.99124200	-0.40253100	-0.24492100
Na	4.89897800	-1.58675600	0.41248200
O	6.93999800	-1.42278800	-0.83087200
C	6.99004800	-1.65750500	-2.24307000
C	7.20278000	-0.26825500	-2.84707500
C	8.13354500	0.41206200	-1.81412700
C	7.94960300	-0.43077000	-0.52693100
H	7.58310800	0.13889300	0.33040400
H	8.88218700	-0.94701300	-0.25747800
H	7.86171500	1.45858500	-1.65314200
H	9.17640100	0.38937400	-2.14690100
H	6.24398900	0.25815400	-2.90650800
H	7.63282000	-0.30491300	-3.85284900
H	7.83102100	-2.32872100	-2.48311100
H	6.05263600	-2.14277400	-2.52360200
O	5.80012900	-3.32384300	1.82390700
C	7.19951000	-3.64861100	1.82338200
C	7.72741800	-3.05095900	3.12563700
C	6.56773100	-3.33656700	4.10158200
C	5.31996300	-3.37201700	3.18754300
H	4.66264500	-2.50883700	3.32177700
H	4.73307000	-4.28788700	3.33160000
H	6.48271500	-2.57553400	4.88207700
H	6.70991700	-4.30417000	4.59500400
H	7.87543100	-1.97239600	3.00519600
H	8.67453500	-3.49586500	3.44614100
H	7.33109600	-4.74236700	1.80475500
H	7.62669500	-3.21958700	0.91457500
O	4.01514500	-3.12061800	-1.20301300
C	2.73112300	-2.96075800	-1.86874000
C	2.21148100	-4.37984300	-2.15563300
C	2.99332100	-5.24150000	-1.15020800
C	4.33810100	-4.51968600	-1.10648400
H	4.97280100	-4.81434700	-1.95686700
H	4.89587000	-4.66312300	-0.17793400
H	3.08320000	-6.28896900	-1.45491600
H	2.51803800	-5.20937700	-0.16299100

H	2.44976900	-4.68622700	-3.18105300
H	1.12719300	-4.45012100	-2.02805200
H	2.07173800	-2.40678300	-1.19229700
H	2.88287400	-2.37657500	-2.78432700
O	6.17398000	1.20540600	1.69085800
C	5.33247600	1.94433200	0.78560900
C	3.88404700	1.64739400	1.20253500
C	4.01505200	0.24455200	1.82657200
C	5.30231900	0.49542500	2.61077400
H	5.18493200	1.13962400	3.51274900
H	5.85782900	-0.39871600	2.93363600
H	3.18687600	0.07503500	2.53563000
H	3.20438500	1.71850400	0.34304000
H	3.56576300	2.43081100	1.92266600
H	5.59332600	3.01074300	0.84403300
H	5.53718000	1.60160400	-0.24159600
H	1.71448500	-0.75755300	0.82263100

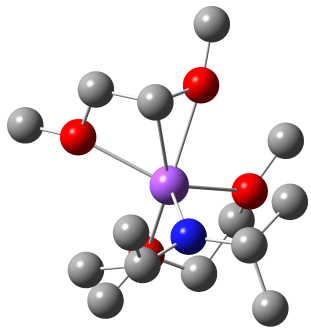
Table S-64. Geometric coordinates and thermally corrected MP2 energies for metalation of DME by A(κ_2-DME)$_2$.



G = –1071.424887 Hartree
G_{MP2} = –1067.9189017883 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	-2.10077900	1.07888100	-0.41282100
C	-3.12400800	1.39846100	0.59497000
C	-4.44398200	0.61746600	0.39323200
H	-4.82104100	0.74135300	-0.62835500
H	-5.22606400	0.96435600	1.08220500
H	-4.29562400	-0.45546300	0.56479400
C	-2.58216400	1.16612300	2.01313400
H	-3.34950800	1.35913900	2.77503300
H	-1.73382100	1.83412100	2.20618300
H	-2.23459700	0.13340800	2.13110600
H	-3.38320700	2.46844200	0.53250400
C	-2.29642500	1.82941400	-1.65683900
C	-1.88572200	3.31142800	-1.52797300
H	-2.08885100	3.86448300	-2.45548400
H	-0.81062400	3.38259900	-1.31350300
H	-2.42186100	3.81891700	-0.71856500
C	-1.50234800	1.19476600	-2.80809100
H	-1.69055000	1.72904000	-3.74779100
H	-1.75728200	0.14098200	-2.94621600
H	-0.42357700	1.25339300	-2.60576900
H	-3.36257100	1.82100400	-1.96479800
O	1.73183100	0.93985300	1.48746500
C	2.70641900	1.63126400	0.71813900
C	3.14758200	0.74045300	-0.42497400
O	2.01942300	0.44779000	-1.23153700
C	2.33038200	-0.33597800	-2.37746700
H	2.79863300	-1.28789000	-2.08789400
H	1.38540300	-0.53602200	-2.88277800
H	3.00896000	0.20905100	-3.04913000
H	3.58699000	-0.19053300	-0.03244900
H	3.91912600	1.26346000	-1.01213100
H	2.28325400	2.56916900	0.32618500
H	3.58082100	1.88011300	1.34005100
C	1.32994600	1.66480800	2.64400800
H	0.56871500	1.06704900	3.14776700
H	2.18199600	1.82176400	3.32114000
H	0.90079400	2.63932600	2.37223700
O	-0.75397900	-1.78103500	1.36514800
C	-1.71708600	-2.46242400	0.51428400
C	-1.87889400	-1.67577600	-0.75808700
O	-0.65640300	-1.77137000	-1.56200100
C	-0.47076600	-2.99560400	-2.24444200
H	-1.29789200	-3.18369100	-2.94696600
H	0.46424900	-2.93033900	-2.81378800
H	-0.39905700	-3.85635700	-1.56232700
H	-2.71868300	-2.09100700	-1.33816000
H	-1.34686900	-3.50067100	0.39914000
H	-2.68424700	-2.51720200	1.03966700
C	-0.44690700	-2.49421700	2.54417100
H	0.30262200	-1.91712900	3.09395800
H	-1.33625300	-2.62356000	3.18036900
H	-0.03508300	-3.49054700	2.31911900
H	-2.11028600	-0.21387200	-0.59524700

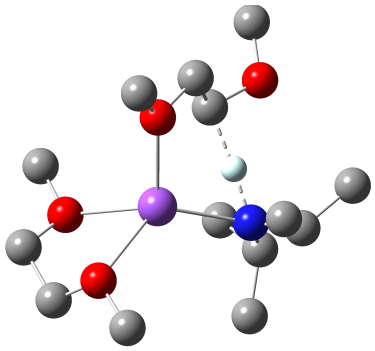
Table S-65. Geometric coordinates and thermally corrected MP2 energies for IRC of metalation of DME by A(κ_2-DME)$_2$.



G = –1071.412446 Hartree
G_{MP2} = –1067.9051265497 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	2.48177000	-0.71868000	-0.33393800
C	3.54653700	-0.52498700	0.67658600
C	4.61304300	0.49687200	0.23968100
H	5.07590300	0.21662200	-0.71305700
H	5.41320900	0.57696100	0.98621800
H	4.15914700	1.48704600	0.11494000
C	2.91354200	-0.11187000	2.01139200
H	3.68294600	0.08511000	2.76859900
H	2.26160400	-0.90890900	2.38698900
H	2.30889900	0.79411900	1.89028100
H	4.04208300	-1.49220900	0.82929100
C	2.87102400	-1.50829200	-1.51757800
C	3.03181300	-2.99581500	-1.17504100
H	3.29408800	-3.56894300	-2.07261400
H	2.09104200	-3.39324100	-0.77372400
H	3.81731400	-3.17357700	-0.43270600
C	1.80909300	-1.33123100	-2.60983400
H	2.12579900	-1.82439800	-3.53649700
H	1.62328600	-0.27312400	-2.82067000
H	0.85962400	-1.78233600	-2.29417000
H	3.83405700	-1.15518000	-1.93020900
O	-1.23474100	-1.41232600	1.61831900
C	-1.80996400	-2.53411100	0.96325900
C	-2.53805900	-2.05048900	-0.27422400
O	-1.60619900	-1.40740200	-1.12531100
C	-2.18372100	-0.92836000	-2.33629900
H	-3.02534800	-0.25290300	-2.12702700
H	-1.40047700	-0.37491300	-2.85336600
H	-2.53829600	-1.76590700	-2.95420500
H	-3.33896300	-1.34956700	0.01004100
H	-3.00065700	-2.91224300	-0.78189000
H	-1.02496800	-3.25542200	0.68716300
H	-2.52664900	-3.04164700	1.62809300
C	-0.64918600	-1.74261700	2.87036300
H	-0.22412500	-0.82273200	3.27570500
H	-1.40645200	-2.13358000	3.56544100
H	0.14917900	-2.48921500	2.75254000
O	-0.04028200	2.01698300	1.20299100
C	0.47322400	2.89036300	0.12564000
C	0.96397600	2.05131600	-1.00375000
O	-0.17693500	1.61861600	-1.84608700
C	-0.70010800	2.61385900	-2.70263400
H	0.06362800	2.95876400	-3.41918600
H	-1.53890400	2.18508000	-3.26761500
H	-1.06981200	3.49372300	-2.15358400
H	1.64243500	2.64707800	-1.63440900
H	-0.36401300	3.58911300	-0.08774800
H	1.30448700	3.48057400	0.54303100
C	-0.66216000	2.73138500	2.24835100
H	-1.02541000	2.00421000	2.98198400
H	0.04280000	3.41557200	2.74787900
H	-1.51623900	3.32711500	1.88734600
H	2.18247200	0.23384500	-0.64478400

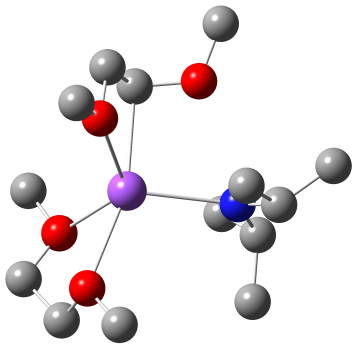
Table S-66. Geometric coordinates and thermally corrected MP2 energies for metalation of DME by A(κ_1-DME)(κ_2-DME).



G = –1071.394150 Hartree
G_{MP2} = –1067.8853881725 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	1.71726400	1.54583800	0.30000500
C	2.41197800	2.14714500	-0.84567400
C	3.94762600	1.98739700	-0.79026500
H	4.35823400	2.43530000	0.12124900
H	4.43033400	2.47865000	-1.64628400
H	4.22650600	0.92843900	-0.78276600
C	1.87177500	1.55678500	-2.15830800
H	2.39451200	1.96957200	-3.03035100
H	0.80177300	1.77903500	-2.27242600
H	1.99746400	0.46728100	-2.17907300
H	2.19917800	3.23102900	-0.87740900
C	1.83795200	2.33630800	1.52708700
C	0.81532400	3.48969800	1.57416500
H	0.96502700	4.12965900	2.45487200
H	-0.20628900	3.08544100	1.61511800
H	0.88816900	4.12481800	0.68367400
C	1.68010400	1.44365800	2.76731900
H	1.74220300	2.04066000	3.68567000
H	2.45927300	0.67641500	2.79471600
H	0.70102900	0.94152700	2.76684500
H	2.84055900	2.79745100	1.60323100
O	-2.23988300	0.56309300	-0.71892000
C	-3.12536000	0.51828000	0.39368900
C	-2.89795700	-0.77272700	1.15304400
O	-1.56141600	-0.79325700	1.63044900
C	-1.27125500	-1.92938900	2.43843700
H	-1.42909000	-2.86252000	1.87925500
H	-0.22169600	-1.85300300	2.72653800
H	-1.90133200	-1.93656900	3.33884600
H	-3.08054900	-1.63792100	0.49623300
H	-3.60771100	-0.82339800	1.99358100
H	-2.94690700	1.38148000	1.05319000
H	-4.17104900	0.55573700	0.05079400
C	-2.42984300	1.72406100	-1.52330500
H	-1.70655200	1.67046600	-2.33897600
H	-3.44704600	1.74664500	-1.93900900
H	-2.25370400	2.63999300	-0.94290000
O	0.87691200	-1.84369500	-1.05814400
C	2.22467300	-2.04175100	-0.54879500
C	2.41041600	-1.13303400	0.65820500
O	3.80612500	-0.96643100	0.96914900
C	4.46660600	-2.11925700	1.44156500
H	4.56833900	-2.90283200	0.67178200
H	5.47252800	-1.81918400	1.75820600
H	3.94122100	-2.56187500	2.30618800
H	2.33073800	-3.13054100	-0.37587500
H	2.94794600	-1.76337300	-1.33259100
C	0.56478900	-2.69282800	-2.14477100
H	-0.46023000	-2.46952800	-2.45649200
H	1.24296100	-2.52159500	-2.99446400
H	0.63022100	-3.75344900	-1.85796300
H	2.07974100	0.32175900	0.46335400
H	1.92354900	-1.60631300	1.53976100

Table S-67. Geometric coordinates and thermally corrected MP2 energies for IRC of metalation of DME by A(κ_1-DME)(κ_2-DME).



G = –1071.414510 Hartree
G_{MP2} = –1067.8956687304 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	1.72903400	-1.88740600	-0.11665200
C	2.55789000	-2.25498400	1.05569600
C	4.04993400	-2.42762600	0.71642200
H	4.20899400	-3.17548500	-0.06812400
H	4.61780300	-2.74835800	1.59825900
H	4.47036800	-1.47621600	0.36893200
C	2.37697800	-1.19407400	2.14757400
H	3.01402700	-1.40713100	3.01449300
H	1.33616600	-1.16078200	2.49081300
H	2.63515700	-0.20185800	1.76197100
H	2.17897600	-3.21084300	1.44068600
C	1.52527800	-2.95925100	-1.11293700
C	0.49611200	-3.98364600	-0.61903500
H	0.35646300	-4.77858100	-1.36125200
H	-0.47169300	-3.49410400	-0.45188000
H	0.80183000	-4.45906600	0.31940700
C	1.07420800	-2.33409000	-2.43788500
H	1.00394700	-3.10014400	-3.21892100
H	1.77760600	-1.56249700	-2.76815500
H	0.08886600	-1.86411000	-2.33222600
H	2.46845000	-3.50052000	-1.30631000
O	-2.01319100	-0.90698100	1.23213500
C	-3.02274000	-1.30741100	0.31462300
C	-3.18175800	-0.23111900	-0.74019400
O	-1.94538600	-0.07427000	-1.40935500
C	-1.96007300	0.92896700	-2.42249300
H	-2.36613300	1.87252100	-2.03061100
H	-0.91837700	1.08331200	-2.71020300
H	-2.56483500	0.60381600	-3.28134600
H	-3.48163400	0.71802100	-0.26799100
H	-3.97676900	-0.53005400	-1.44270600
H	-2.74657100	-2.26345800	-0.15701200
H	-3.98215900	-1.44632000	0.83772000
C	-1.87918900	-1.80474300	2.32491200
H	-1.08725700	-1.41319100	2.96646300
H	-2.81426500	-1.86498800	2.90079600
H	-1.60316000	-2.81244900	1.98299000
O	0.70456000	1.94252800	1.07049300
C	1.48114000	2.51130600	-0.06445900
C	1.56506400	1.52307400	-1.17342100
O	2.77811000	0.69712100	-1.05589500
C	3.96203900	1.31878100	-1.50761400
H	4.19167600	2.23977500	-0.94746800
H	4.79613200	0.61648000	-1.37649600
H	3.89200100	1.58399100	-2.57647000
H	0.93971200	3.41601200	-0.38679100
H	2.44346400	2.82516000	0.38832600
C	0.63565600	2.80745700	2.18153300
H	0.05944000	2.30503900	2.96539600
H	1.63639500	3.04740900	2.57630000
H	0.13491800	3.75747000	1.92979200
H	2.20450700	-1.09894300	-0.57893000
H	1.61737100	2.05298400	-2.13715500

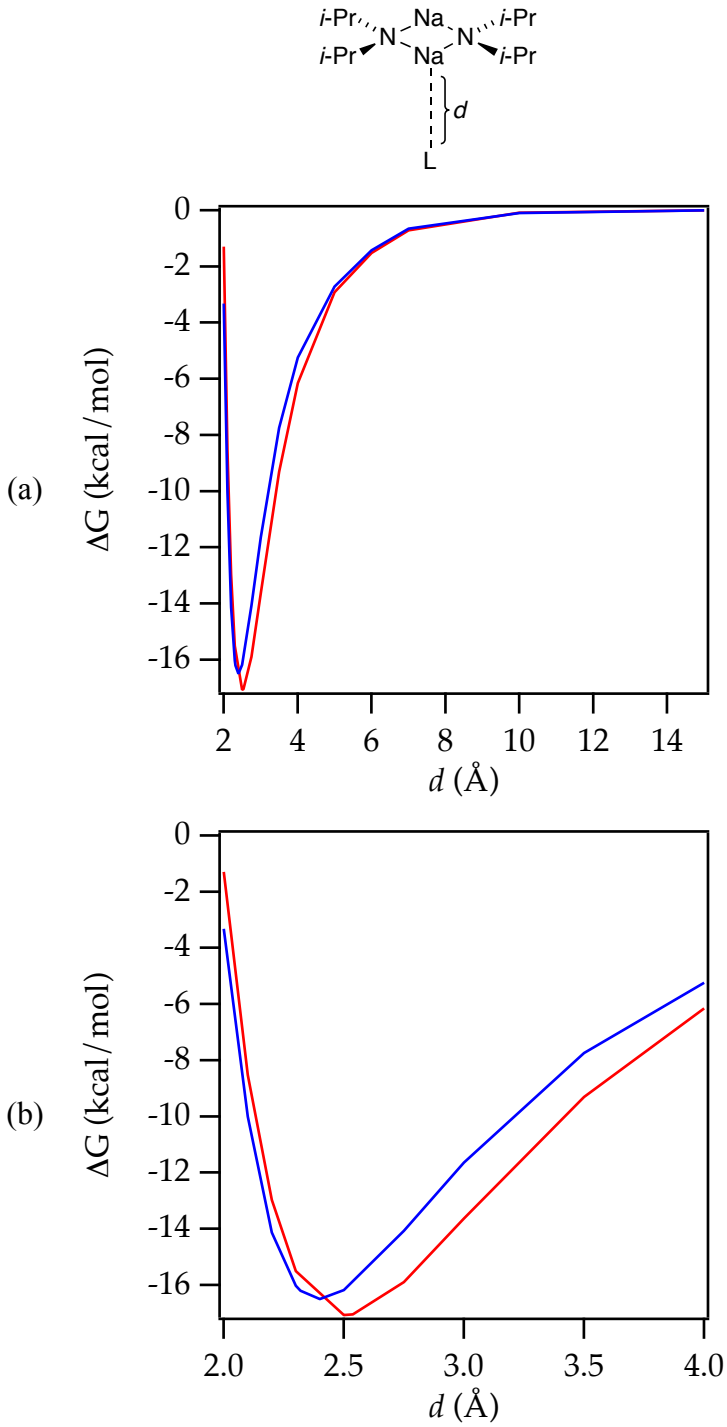


Figure S-98.Plots of binding energy affiliated with $(NaDA)_2\cdots L$ depicted above where L = THF (blue trace); trimethylamine (red trace) by single-point calculation at the MP2 level of theory. (b) is an expansion of (a). That trimethylamine is a stronger ligand (stronger Lewis base) for sodium than THF is evident in the higher stabilization at long Na···L distances. That THF is sterically less demanding than trimethylamine is evident by examining the potential energies at shorter Na···L distances.

IV. Full reference 12 (Gaussian):

Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.