SUPPORTING INFORMATION

Sodium Diisopropylamide in Tetrahydrofuran: Selectivities, Rates, and Mechanisms of Arene Metalations

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. NMR Spectroscopy

III. Computations

I. Rate Studies

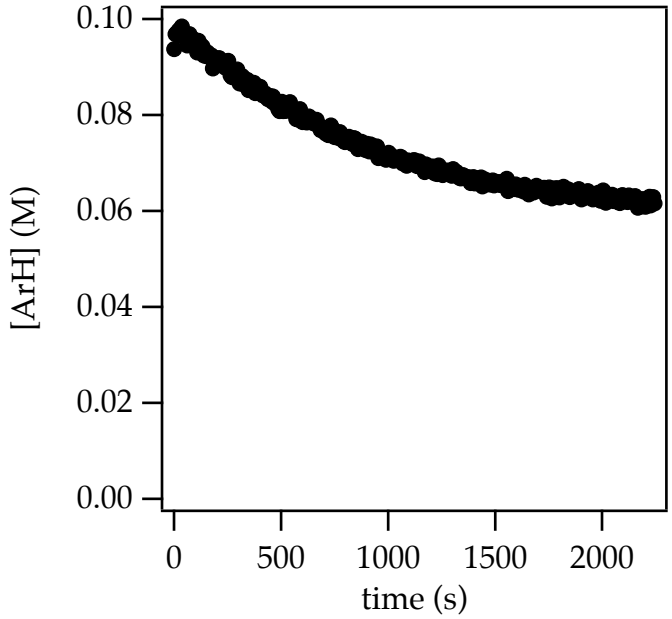


Figure S-1. Plot of 1,3-dimethoxybenzene (ArH) concentration versus time (ReactIR) for metalation with 0.10 M NaDA in 5.83 M THF/hexane at –78 °C. Incomplete metalation reflects near thermoneutrality.

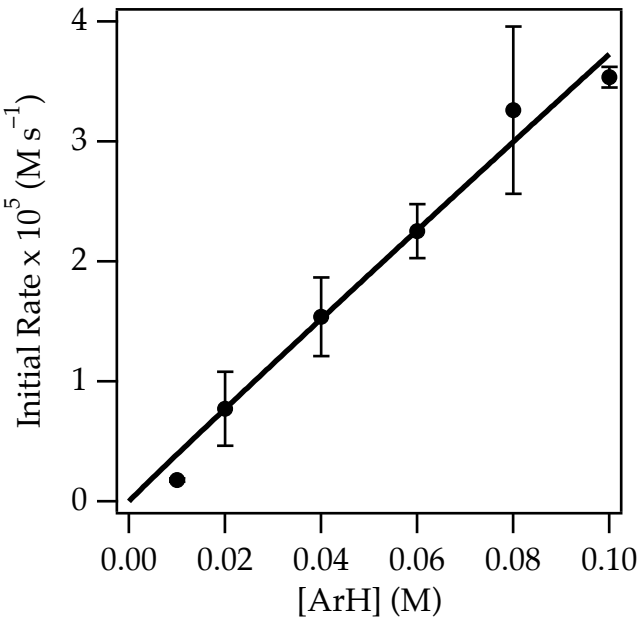


Figure S-2. Plot of initial rate versus 1,3-dimethoxybenzene concentration (ArH) for the metalation with 0.10 M NaDA in 6.02 M THF/hexane at –78 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax$: $a = 37 \pm 1$.

[ArH] (M)	Initial Rate × 10^5 (M s^{-1})	Standard deviation × 10^5 (M s^{-1})
0.010	0.18	0.01
0.020	0.8	0.3
0.040	1.5	0.3
0.060	2.3	0.2
0.080	3.3	0.7
0.100	3.54	0.08

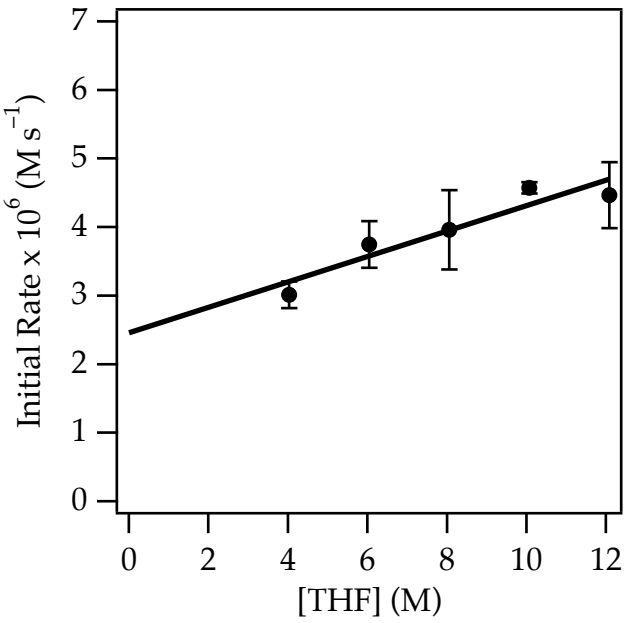


Figure S-3. Plot of initial rate versus THF concentration for the metalation of 0.010 M 1,3-dimethoxybenzene with 0.10 M NaDA in hexane cosolvent at –78 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax + b$: a = 0.19 ± 0.04; b = 2.5 ± 0.3.

[THF] (M)	Initial Rate × 10^6 (M s^{-1})	Standard deviation × 10^6 (M s^{-1})
4.03	3.0	0.2
6.04	3.7	0.3
8.05	4.0	0.6
10.1	4.58	0.08
12.1	4.5	0.5

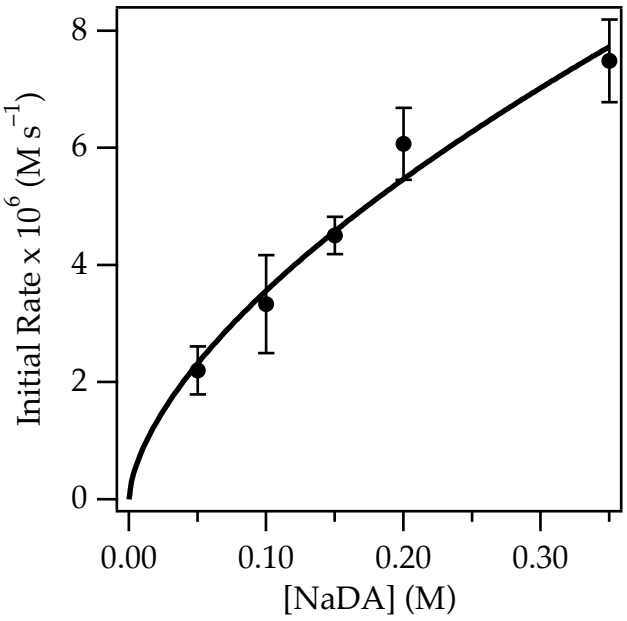


Figure S-4. Plot of initial rate versus NaDA concentration for the metalation of 0.010 M 1,3-dimethoxybenzene in 6.0 M THF/hexane at –78 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax^b$: $a = 15 \pm 2$; $b = 0.62 \pm 0.07$.

[NaDA] (M)	Initial Rate × 10^6 (M s^{-1})	Standard deviation × 10^6 (M s^{-1})
0.050	2.2	0.4
0.10	3.3	0.8
0.15	4.5	0.3
0.20	6.1	0.6
0.35	7.5	0.7

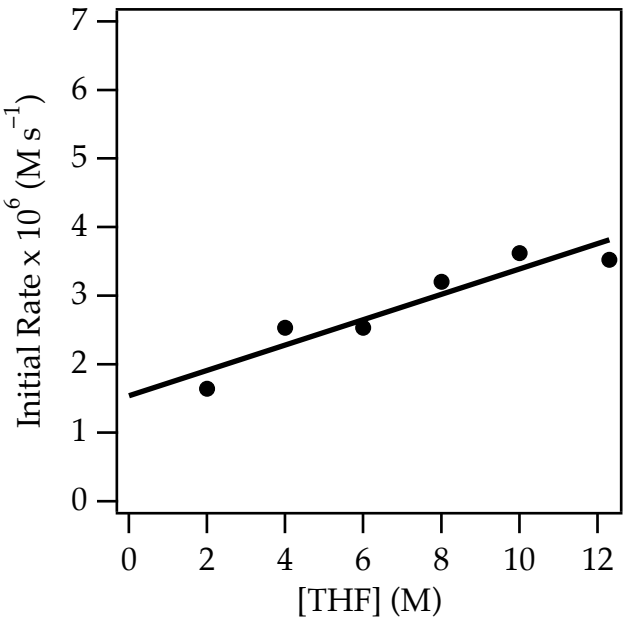


Figure S-5. Plot of initial rate versus THF concentration for the metalation of 0.010 M 1,3-dimethoxybenzene with 0.10 M NaDA in DMEA cosolvent at –78 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax + b$: a = 0.19 ± 0.03; b = 1.5 ± 0.3. That the rates or behavior are not significantly different from those collected in hexane cosolvent suggests that cosolvent is inconsequential.

[THF] (M)	Initial Rate × 10^6 (M s^{-1})
2.00	1.65
4.00	2.54
6.00	2.53
8.00	3.21
10.0	3.62
12.3	3.53

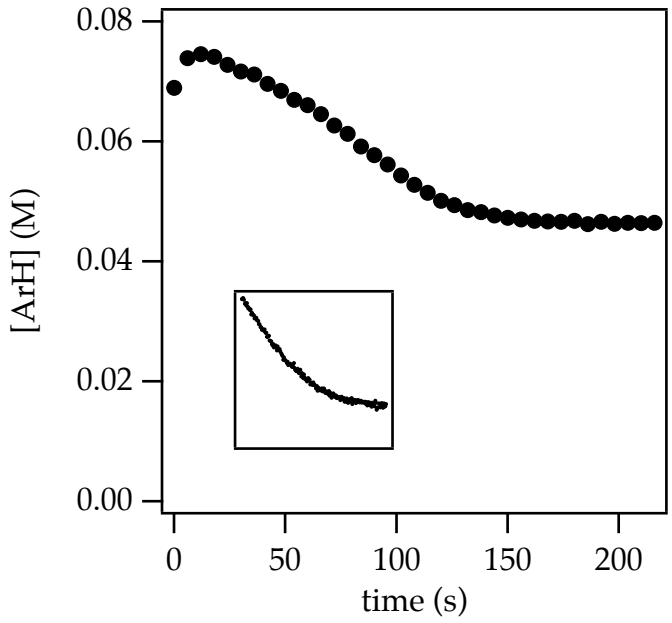


Figure S-6. Plot of 1,2,4-trimethoxybenzene (ArH) concentration versus time (ReactIR) for metalation of 0.080 M ArH with 0.10 M NaDA in neat THF at –78 °C. Inset: Plot of 1,2,4-trimethoxybenzene (ArH) concentration versus time (time to completion is ~1200 seconds) for metalation of 0.010 M ArH with 0.10 M NaDA in neat THF at –78 °C. The sigmoidal behavior at high concentration is indicative of autocatalysis.

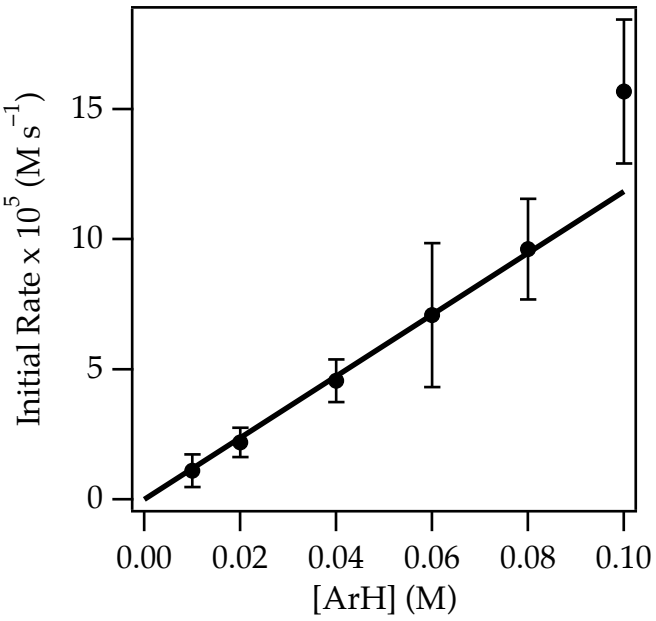


Figure S-7. Plot of initial rate versus 1,2,4-trimethoxybenzene concentration (ArH) for the metalation with 0.10 M NaDA in neat THF at –78 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax$: $a = 118 \pm 1$. The point corresponding to [ArH] = 0.10 M is omitted from the fit because of the early onset of autocatalytic acceleration.

[ArH] (M)	Initial Rate × 10^5 (M s^{-1})	Standard deviation × 10^5 (M s^{-1})
0.010	1.1	0.6
0.020	2.2	0.6
0.040	4.6	0.8
0.060	7	3
0.080	10	2
0.10	16	3

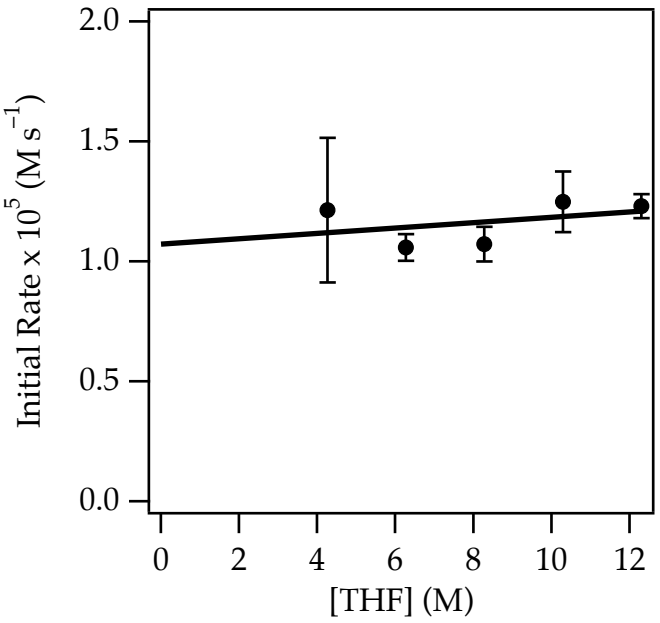


Figure S-8. Plot of initial rate versus THF concentration for the metalation of 0.010 M 1,2,4-trimethoxybenzene with 0.10 M NaDA in hexane cosolvent at –78 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax + b$: $a = 0.01 \pm 0.02$; $b = 1.1 \pm 0.1$.

[THF] (M)	Initial Rate × 10^5 (M s^{-1})	Standard deviation × 10^5 (M s^{-1})
4.26	1.2	0.3
6.27	1.06	0.06
8.28	1.07	0.07
10.3	1.2	0.1
12.3	1.23	0.05

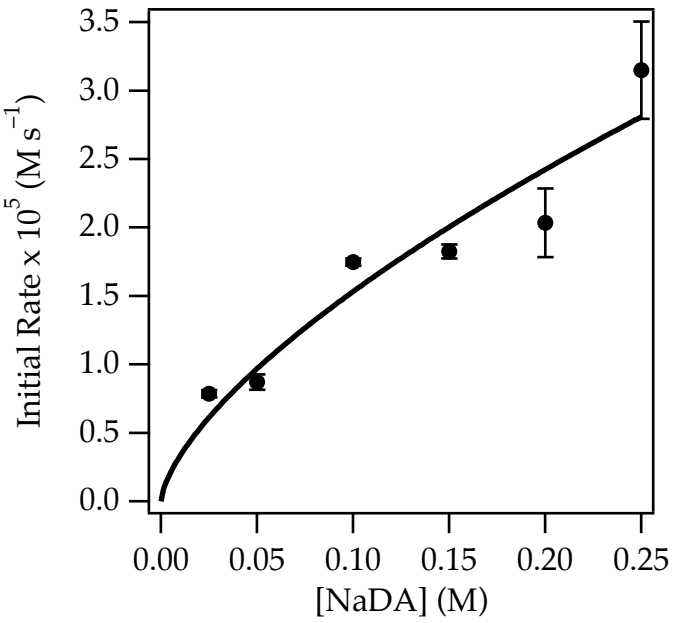


Figure S-9. Plot of initial rate versus NaDA concentration for the metalation of 0.010 M 1,3-dimethoxybenzene in 6.0 M THF/hexane at –78 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax^b$: $a = 7 \pm 2$; $b = 0.66 \pm 0.1$.

[NaDA] (M)	Initial Rate × 10^5 (M s^{-1})	Standard deviation × 10^5 (M s^{-1})
0.025	0.79	0.03
0.050	0.87	0.06
0.10	1.75	0.03
0.15	1.83	0.05
0.20	2.0	0.3
0.25	3.2	0.4

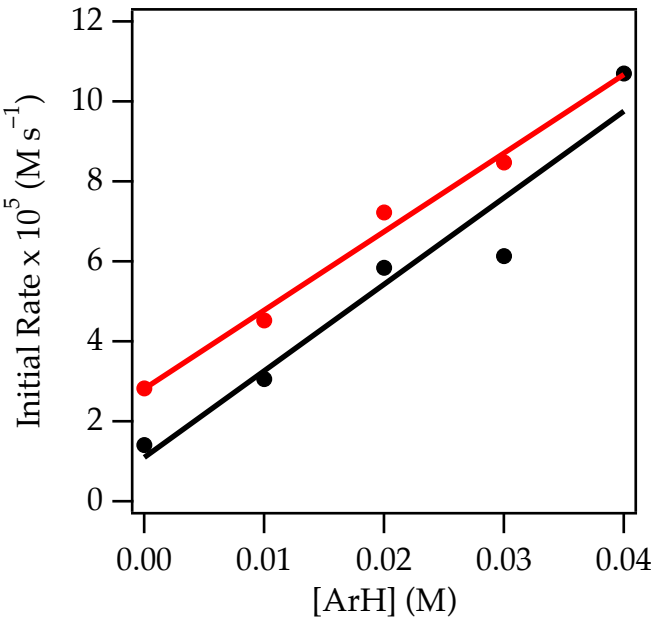


Figure S-10. Plot of initial rate versus previous cumulative concentration of added 1,2,4-trimethoxybenzene (ArH) for metalation in neat THF at –78 °C. The curves depict unweighted least-squares fits to the function $f(x) = ax + b$: (Black trace: [NaDA] = 0.10 M ; a = 220 ± 30; b = 1.1 ± 0.8) ; (Red trace: [NaDA] = 0.25 M ; a = 200 ± 20; b = 2.8 ± 0.4). In the event, a background spectrum was collected followed by addition of 0.010 M ArH. Upon completion, the collection was aborted and the process of serial injection was repeated. In the absence of autocatalysis, the initial rate should decrease reflecting the loss of NaDA titer. This experiment shows compensation for NaDA titer loss with autocatalysis, the expected positive NaDA dependence of initial rate in the absence of preformed arylsodium, and a surprising insensitivity of slope to initial NaDA titer.

[ArH] (M) (0.10 M NaDA)	Initial Rate × 10^5 (M s^{-1})	[ArH] (M) (0.25 M NaDA)	Initial Rate × 10^5 (M s^{-1})
0.000	1.41	0.000	2.83
0.010	3.06	0.010	4.52
0.020	5.84	0.020	7.22
0.030	6.13	0.030	8.48
0.040	10.7		

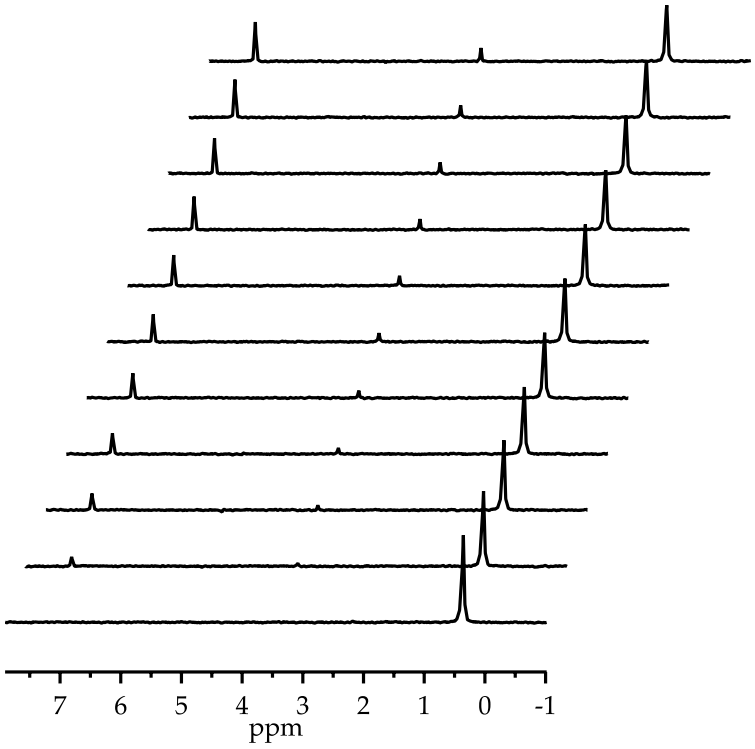


Figure S-11. Stacked ^{2}H NMR spectra for isotopic exchange of 0.23 M benzene (δ 7.15) with 0.10 M NaDA and 1.04 M *i*-Pr_2ND (δ 0.37) in 10.1 M THF (δ 3.42) at –78 °C. The concomitant emergence of benzene and THF resonances is consistent with competitive rates of exchange.

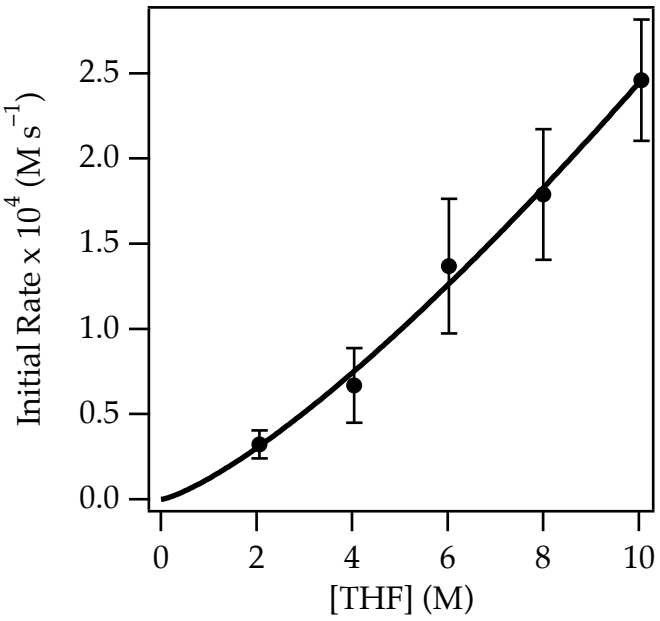


Figure S-12. Plot of initial rate versus THF concentration for the isotopic exchange of 0.23 M benzene with 0.10 M NaDA and 1.04 M *i*-Pr_2ND in hexane cosolvent at 25 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax^b$: a = 0.12 ± 0.02; b = 1.30 ± 0.09.

[THF] (M)	Initial Rate × 10^4 (M s^{-1})	Standard deviation × 10^4 (M s^{-1})
2.06	0.32	0.08
4.04	0.7	0.2
6.02	1.4	0.4
8.00	1.8	0.4
10.1	2.5	0.4

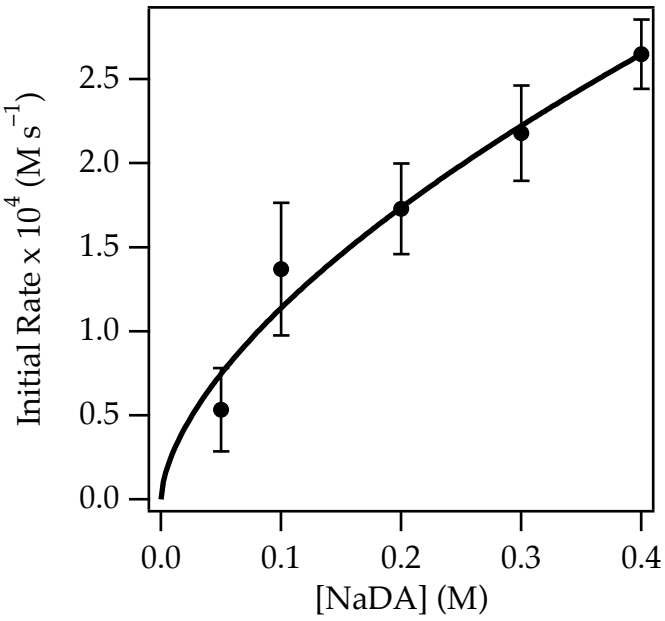


Figure S-13. Plot of initial rate versus NaDA concentration for the isotopic exchange of 0.23 M benzene and 1.04 M *i*-Pr_2ND in 6.02 M THF/hexane at 25 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax^b$: $a = 4.6 \pm 0.6$; $b = 0.61 \pm 0.09$.

[NaDA] (M)	Initial Rate × 10^4 (M s^{-1})	Standard deviation × 10^4 (M s^{-1})
0.050	0.5	0.2
0.10	1.4	0.4
0.20	1.7	0.3
0.30	2.2	0.3
0.40	2.7	0.2

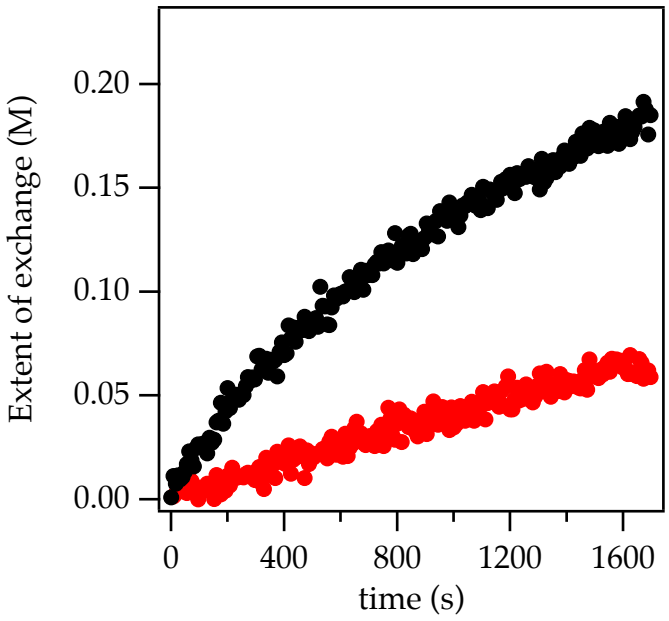


Figure S-14. Plot of benzene isotopologue concentration (black trace: benzene-h_6 and *i*-Pr_2ND; red trace: benzene-d_6 and *i*-Pr_2NH) versus time for the isotopic exchange of 0.23 M benzene with 0.10 M NaDA and 1.04 M diisopropylamine in 10.1 M THF at 25 °C. These plots collectively attest to an isotope effect of $k_H/k_D = 6.3$.

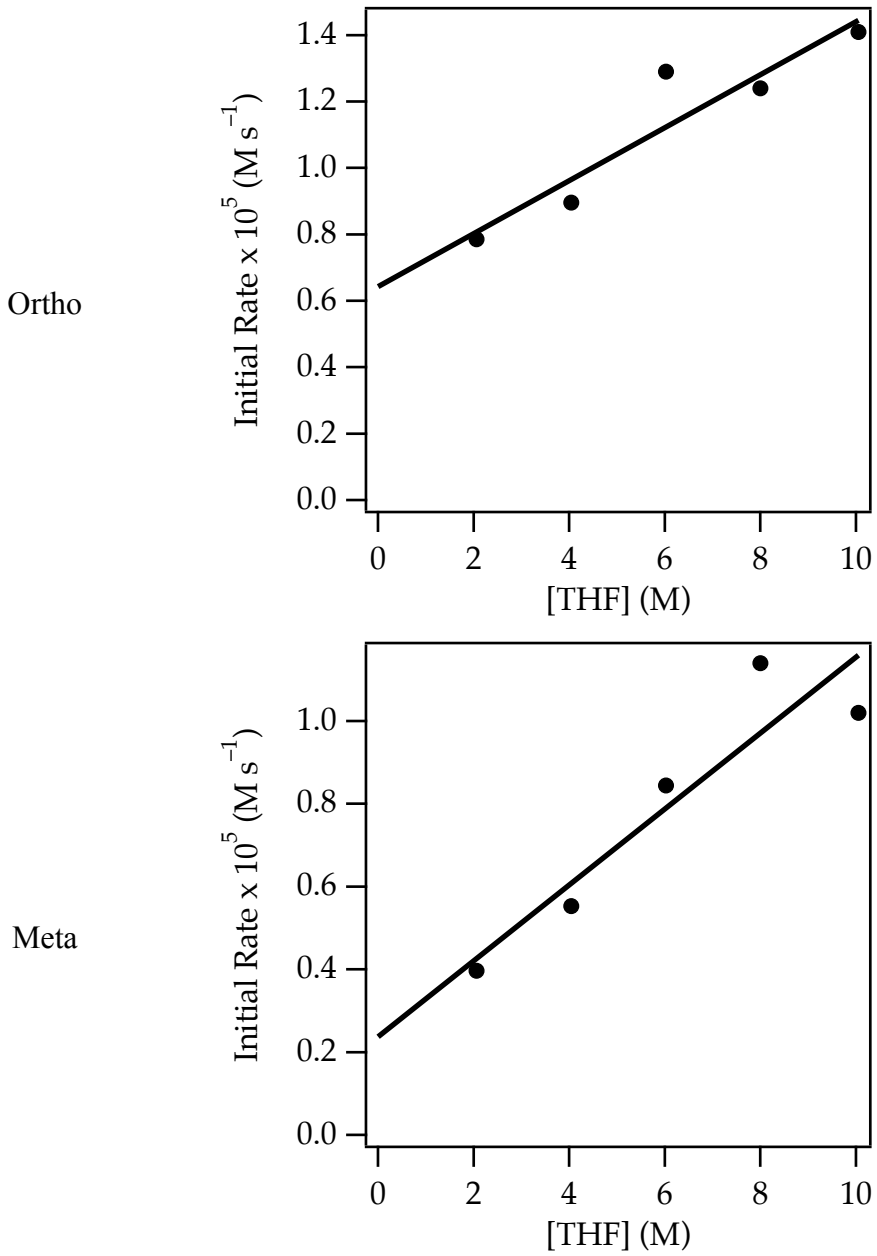
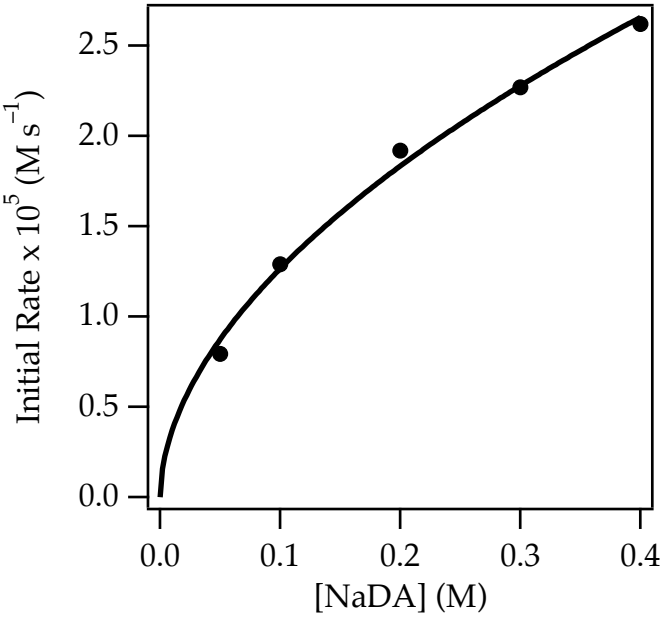


Figure S-15. Plot of initial rate versus THF concentration for the isotopic exchange of 0.44 M *N*,*N*-dimethylaniline with 0.10 M NaDA and 0.79 M *i*-Pr_2ND in hexane cosolvent at 25 °C. The curves depict unweighted least-squares fits to the function $f(x) = ax + b$: Ortho: ($a = 0.08 \pm 0.02$; $b = 0.6 \pm 0.1$); Meta: ($a = 0.09 \pm 0.02$; $b = 0.2 \pm 0.1$).

[THF] (M)	Ortho Initial Rate × 10^5 (M s^{-1})	Meta Initial Rate × 10^5 (M s^{-1})
2.06	0.786	0.397
4.04	0.896	0.553
6.02	1.29	0.844
8.00	1.24	1.14
10.1	1.41	1.02

Ortho



Meta

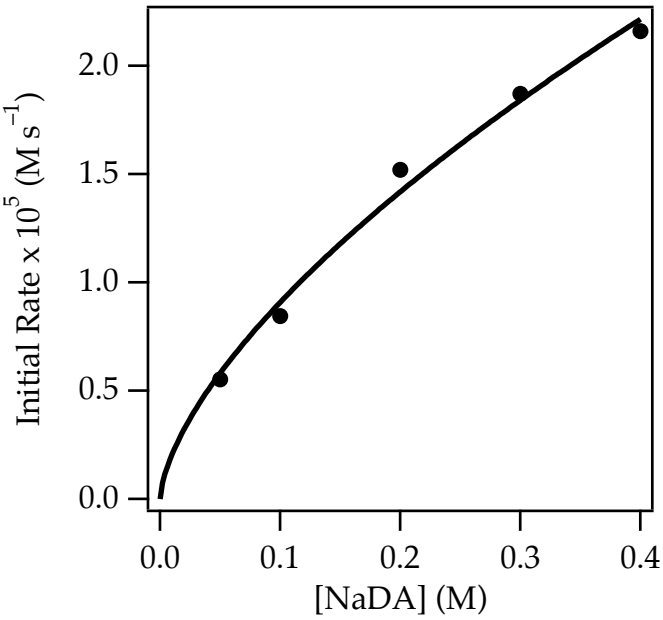
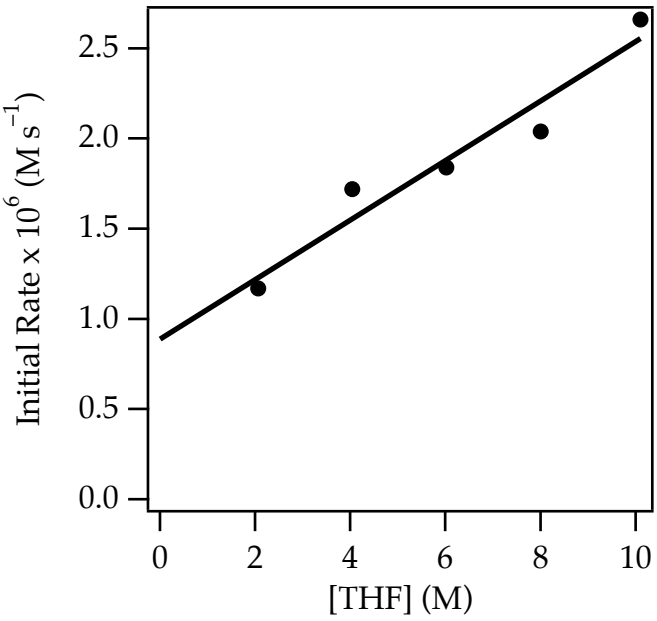


Figure S-16. Plot of initial rate versus NaDA concentration for the isotopic exchange of 0.44 M *N*,*N*-dimethylaniline with 0.79 M *i*-Pr_2ND in 6.02 M THF/hexane at 25 °C. The curves depict unweighted least-squares fits to the function $f(x) = ax^b$: Ortho: ($a = 4.3 \pm 0.2$; $b = 0.53 \pm 0.03$); Meta: ($a = 4.0 \pm 0.3$; $b = 0.65 \pm 0.05$).

[NaDA] (M)	Ortho Initial Rate × 10^5 (M s^{-1})	Meta Initial Rate × 10^5 (M s^{-1})
0.050	0.793	0.553
0.10	1.29	0.844
0.20	1.92	1.52
0.30	2.27	1.87
0.40	2.62	2.16

Ortho



Meta

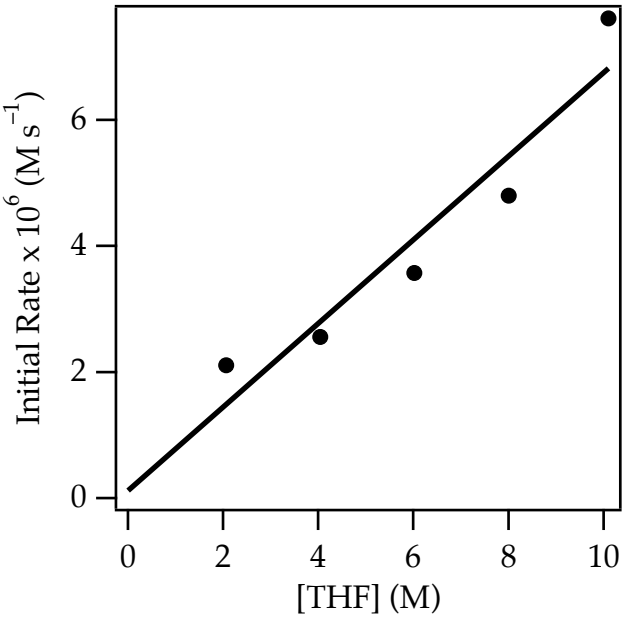


Figure S-17. Plot of initial rate versus THF concentration for the isotopic exchange of 0.35 M *N*,*N*-diethylaniline with 0.10 M NaDA and 0.79 M *i*-Pr_2ND in hexane cosolvent at 25 °C. The curves depict unweighted least-squares fits to the function $f(x) = ax + b$: Ortho: ($a = 0.16 \pm 0.02$; $b = 0.9 \pm 0.2$); Meta: ($a = 0.6 \pm 0.1$; $b = 0.1 \pm 0.8$).

[THF] (M)	Ortho Initial Rate × 10^6 (M s^{-1})	Meta Initial Rate × 10^6 (M s^{-1})
2.06	1.17	2.11
4.04	1.72	2.56
6.02	1.84	3.57
8.00	2.04	4.8
10.1	2.66	7.61

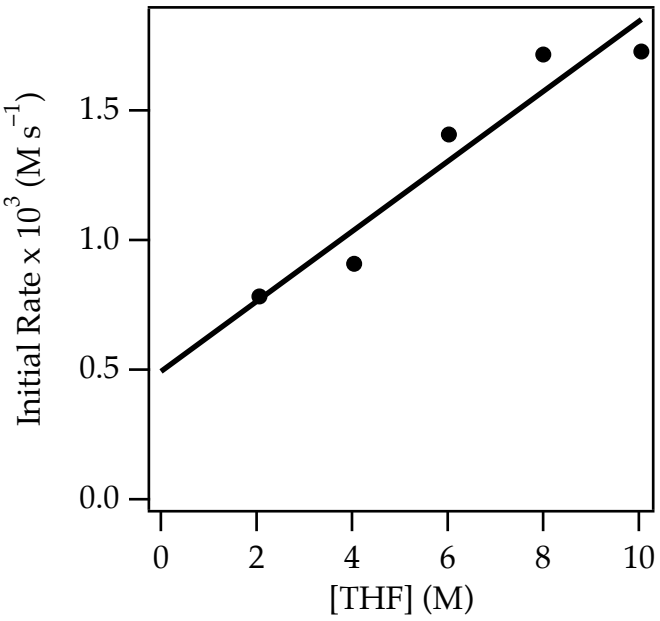


Figure S-18. Plot of initial rate versus THF concentration for the ortho selective isotopic exchange of 0.51 M anisole with 0.10 M NaDA and 0.79 M *i*-Pr_2ND in hexane cosolvent at –20 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax + b$: $a = 0.12 \pm 0.02$; $b = 0.5 \pm 0.2$.

[THF] (M)	Initial Rate × 10^3 (M s^{-1})
2.06	0.782
4.04	0.908
6.02	1.41
8.00	1.72
10.1	1.73

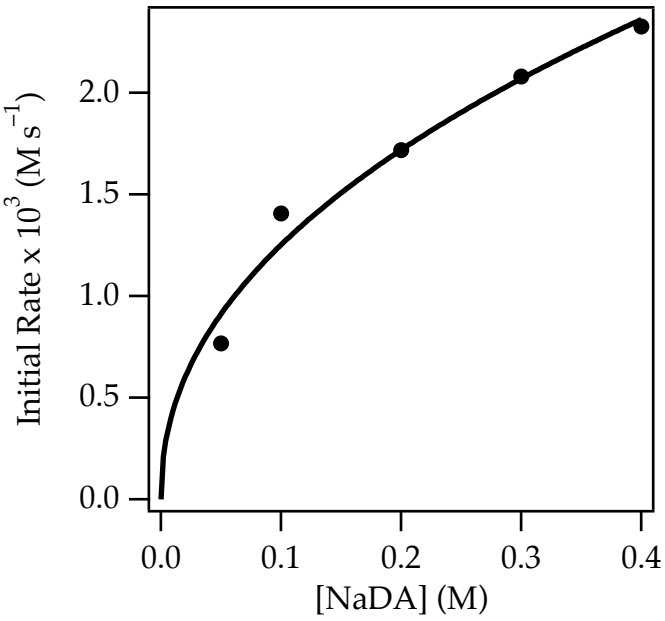
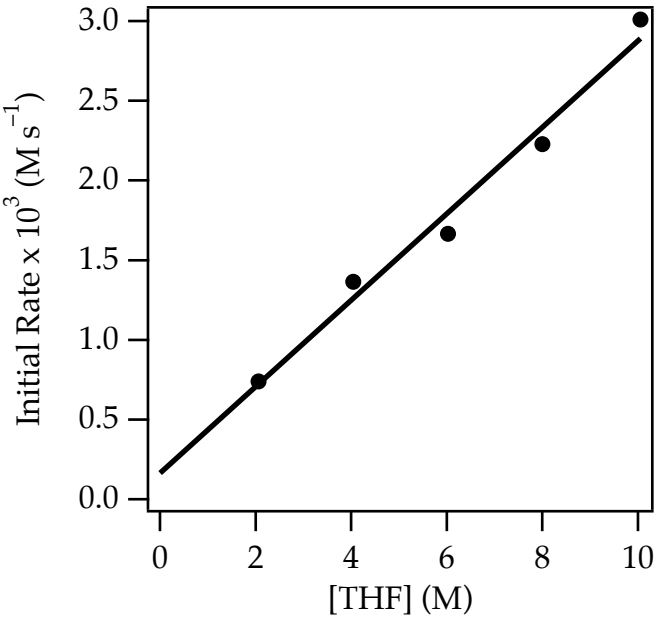


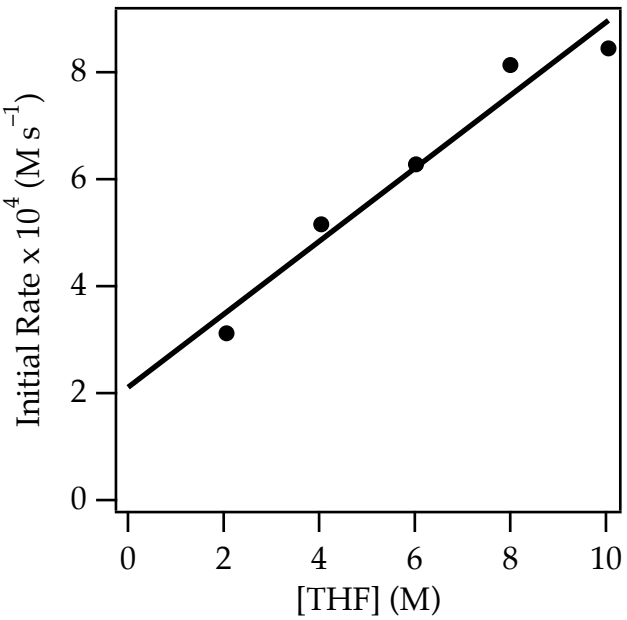
Figure S-19. Plot of initial rate versus NaDA concentration for the ortho selective isotopic exchange of 0.51 M anisole and 0.79 M *i*-Pr_2ND in 6.02 M THF/hexane at –20 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax^b$: $a = 3.6 \pm 0.3$; $b = 0.46 \pm 0.06$.

[NaDA] (M)	Initial Rate × 10^3 (M s^{-1})
0.050	0.768
0.10	1.41
0.20	1.72
0.30	2.08
0.40	2.33

Ortho


Initial Rate x 10^3 (M s^-1)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
2
4
6
8
10
[THF] (M)

Meta


Initial Rate x 10^4 (M s^-1)
8
6
4
2
0
0
2
4
6
8
10
[THF] (M)

Para

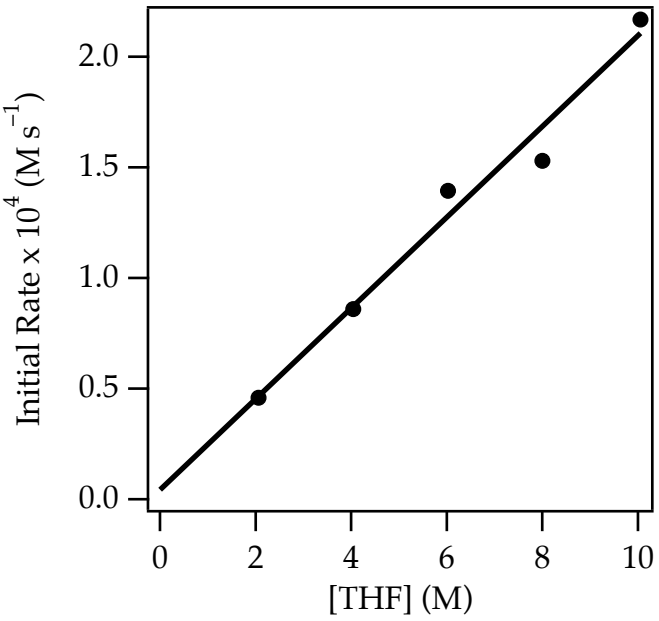
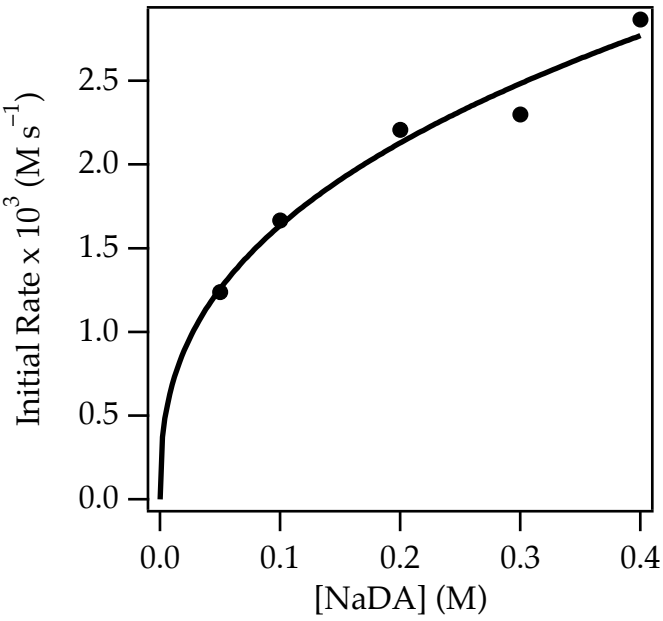


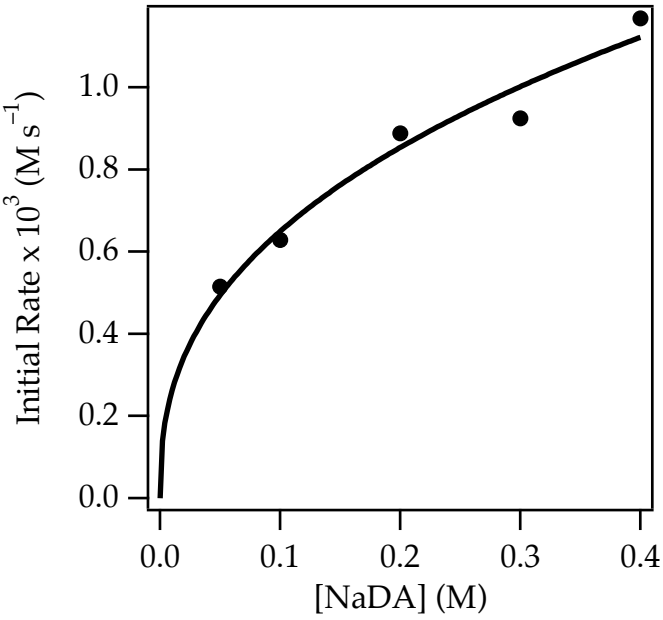
Figure S-20. Plot of initial rate versus THF concentration for the isotopic exchange of 0.45 M benzotrifluoride with 0.10 M NaDA and 0.79 M *i*-Pr_2ND in hexane cosolvent at –20 °C. The curves depict unweighted least-squares fits to the function $f(x) = ax + b$: Ortho: (a = 0.27 ± 0.02; b = 0.2 ± 0.1); Meta: (a = 0.68 ± 0.08; b = 2.1 ± 0.6); Para: (a = 0.21 ± 0.02; b = 0.04 ± 0.1).

[THF] (M)	Ortho × 10^3 (M s^{-1})	Meta × 10^4 (M s^{-1})	Para × 10^4 (M s^{-1})
2.06	0.740	3.12	0.459
4.04	1.37	5.16	0.859
6.02	1.67	6.28	1.39
8.00	2.23	8.14	1.53
10.1	3.01	8.45	2.17

Ortho


Initial Rate x 10^3 (M s^-1)
2.5
2.0
1.5
1.0
0.5
0.0
0.0
0.1
0.2
0.3
0.4
[NaDA] (M)

Meta


Initial Rate x 10^3 (M s^-1)
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.1
0.2
0.3
0.4
[NaDA] (M)

Para

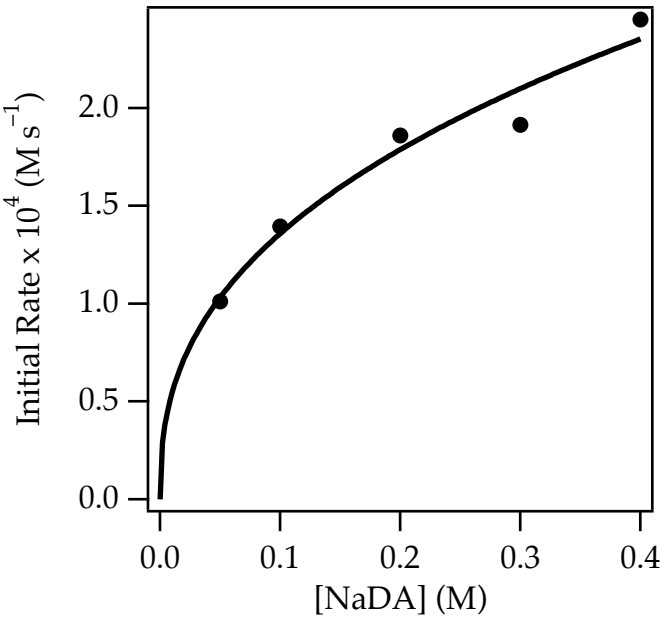
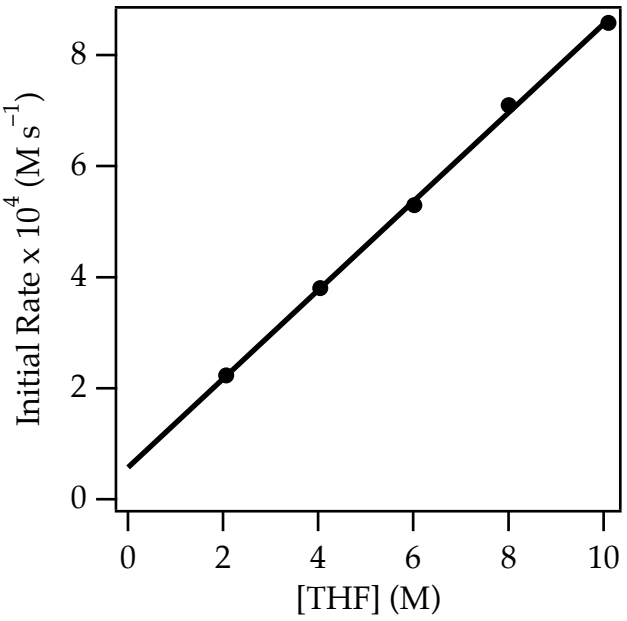


Figure S-21. Plot of initial rate versus NaDA concentration for the isotopic exchange of 0.45 M benzotrifluoride with 0.79 M *i*-Pr_2ND in 6.02 M THF/hexane at –20 °C. The curves depict unweighted least-squares fits to the function $f(x) = ax^b$: Ortho: (a = 3.9 ± 0.3; b = 0.38 ± 0.04); Meta: (a = 1.6 ± 0.1; b = 0.40 ± 0.05); Para: (a = 3.4 ± 0.3; b = 0.40 ± 0.05).

[NaDA] (M)	Ortho × 10^3 (M s^{-1})	Meta × 10^3 (M s^{-1})	Para × 10^4 (M s^{-1})
0.050	1.24	0.515	1.01
0.10	1.67	0.628	1.39
0.20	2.21	0.888	1.86
0.30	2.30	0.925	1.91
0.40	2.87	1.17	2.45

Ortho



Meta

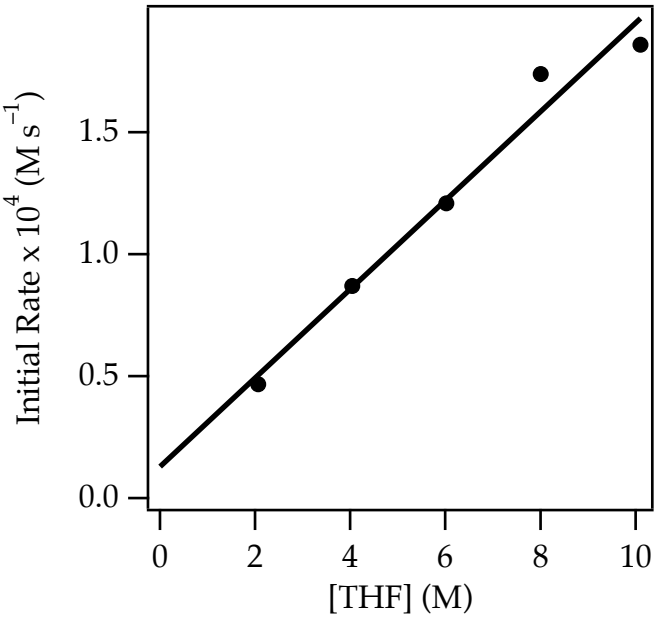


Figure S-22. Plot of initial rate versus THF concentration for the isotopic exchange of 0.45 M benzotrifluoride with 0.10 M NaDA and 0.79 M *i*-Pr_2ND in hexane cosolvent at –40 °C. The curves depict unweighted least-squares fits to the function $f(x) = ax + b$: Ortho: (a = 0.80 ± 0.02; b = 0.6 ± 0.1); Meta: (a = 0.18 ± 0.02; b = 0.1 ± 0.1).

[THF] (M)	Ortho × 10^4 (M s^{-1})	Meta × 10^4 (M s^{-1})
2.06	2.23	0.468
4.04	3.81	0.870
6.02	5.30	1.21
8.00	7.10	1.74
10.1	8.59	1.86

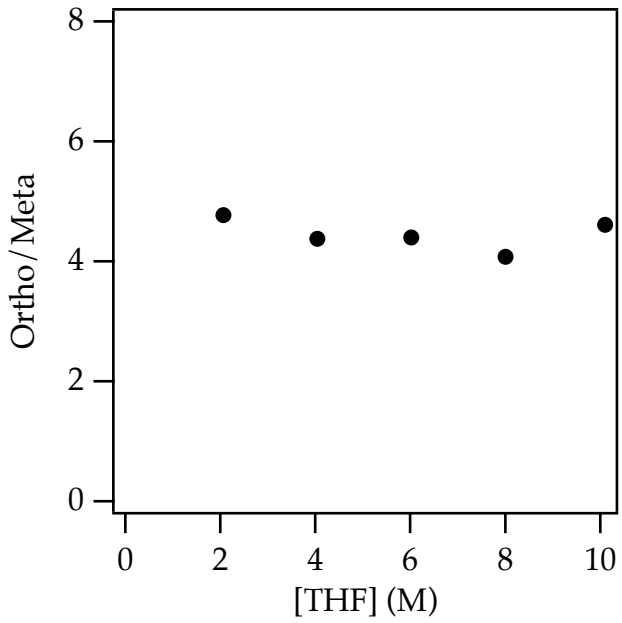


Figure S-23. Plot of initial proportions (ratio of initial rates) of ortho and meta deuteration versus THF concentration for the isotopic exchange of 0.45 M benzotrifluoride with 0.10 M NaDA and 0.79 M *i*-Pr_2ND in hexane cosolvent at –40 °C. The invariance demonstrated argues for a common solvate eliciting the exchanges.

[THF] (M)	Ortho:Meta
2.06	4.77
4.04	4.38
6.02	4.40
8.00	4.08
10.1	4.61

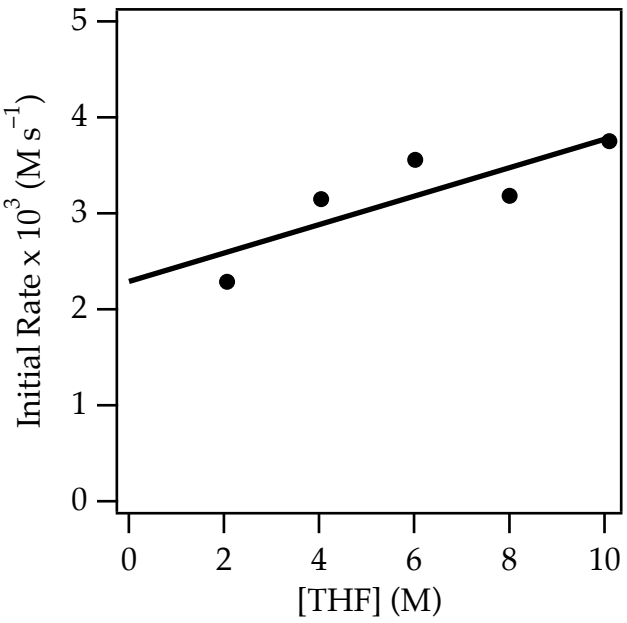


Figure S-24. Plot of initial rate versus THF concentration for the ortho selective isotopic exchange of 0.32 M 4,4-dimethyl-2-phenyl-2-oxazoline with 0.10 M NaDA and 0.79 M *i*-Pr_2ND in hexane cosolvent at –20 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax + b$: $a = 0.15 \pm 0.06$; $b = 2.3 \pm 0.4$.

[THF] (M)	Initial Rate × 10^3 (M s^{-1})
2.06	2.29
4.04	3.15
6.02	3.56
8.00	3.18
10.1	3.75

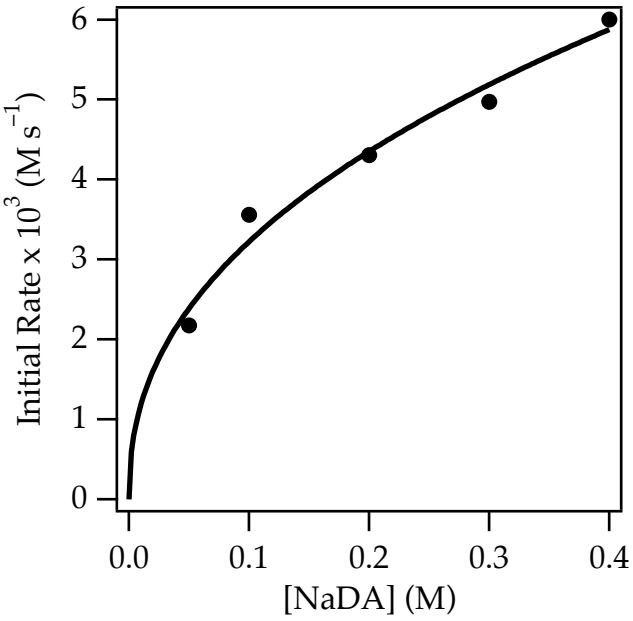


Figure S-25. Plot of initial rate versus NaDA concentration for the ortho selective isotopic exchange of 0.32 M 4,4-dimethyl-2-phenyl-2-oxazoline and 0.79 M *i*-Pr_2ND in 6.02 M THF/hexane at –20 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax^b$: $a = 8.7 \pm 0.6$; $b = 0.43 \pm 0.05$.

[NaDA] (M)	Initial Rate × 10^3 (M s^{-1})
0.050	2.18
0.10	3.56
0.20	4.31
0.30	4.97
0.40	6.00

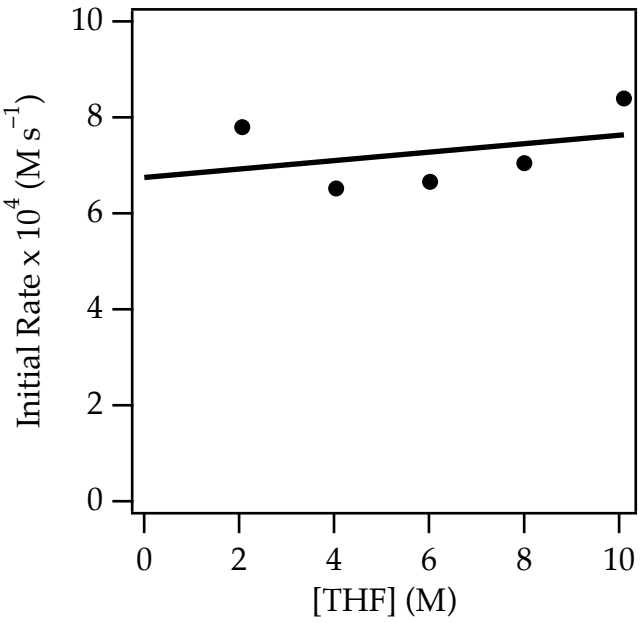


Figure S-26. Plot of initial rate versus THF concentration for the ortho selective isotopic exchange of 0.32 M 4,4-dimethyl-2-phenyl-2-oxazoline with 0.10 M NaDA and 0.79 M *i*-Pr_2ND in hexane cosolvent at –40 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax + b$: $a = 0.09 \pm 0.1$; $b = 6.8 \pm 0.9$.

[THF] (M)	Initial Rate × 10^4 (M s^{-1})
2.06	7.80
4.04	6.52
6.02	6.66
8.00	7.05
10.1	8.39

III. NMR Spectroscopy

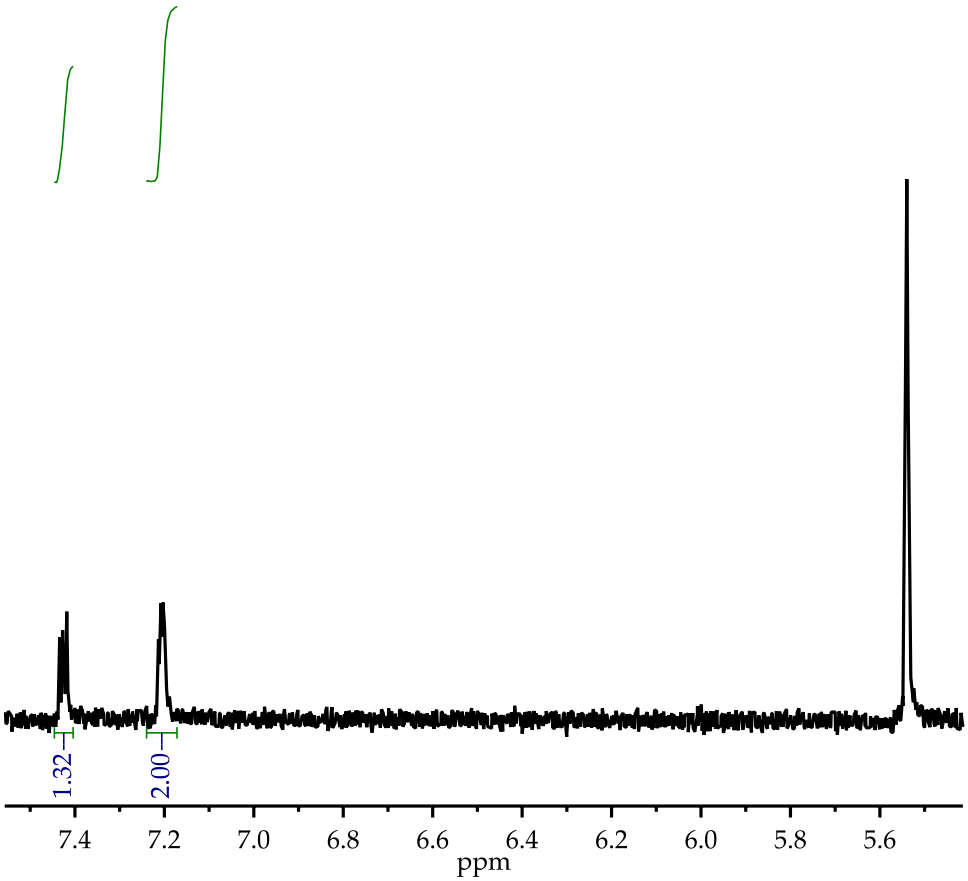


Figure S-27. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 1,2-dichlorobenzene with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). Loss of the resonance at δ 7.42 ppm indicates ortho selective metalation.

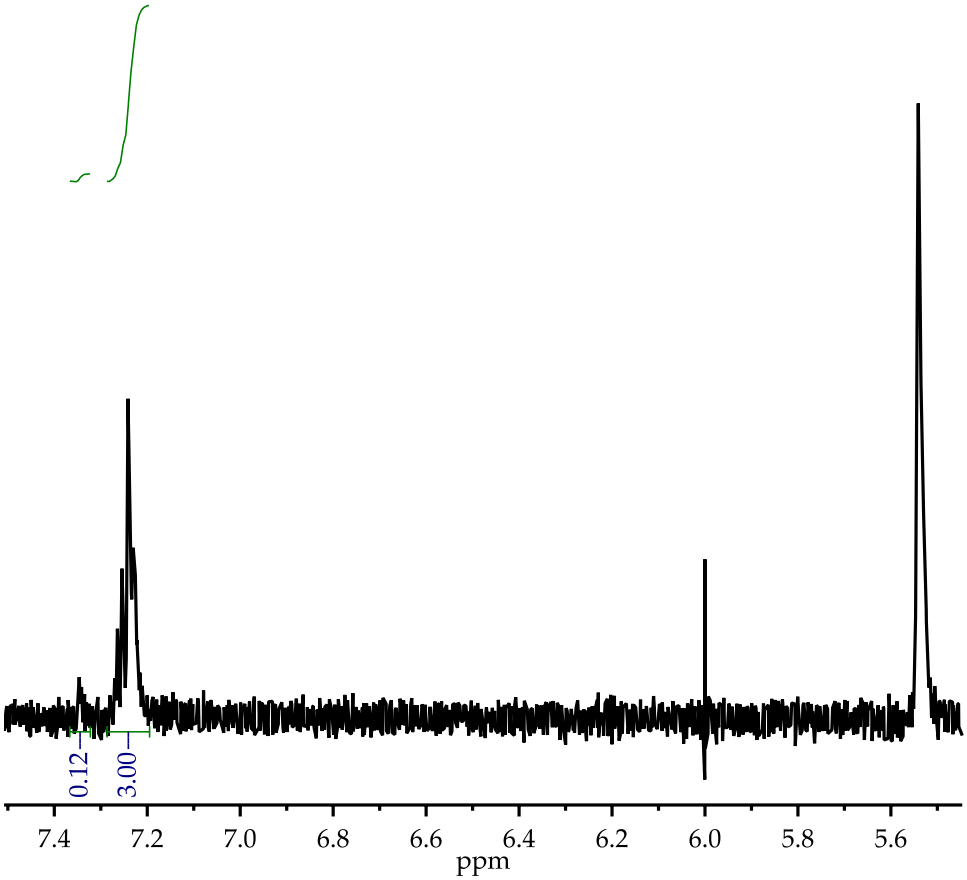


Figure S-28. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 1,3-dichlorobenzene with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). Loss of the resonance at δ 7.35 ppm indicates doubly ortho selective metalation.

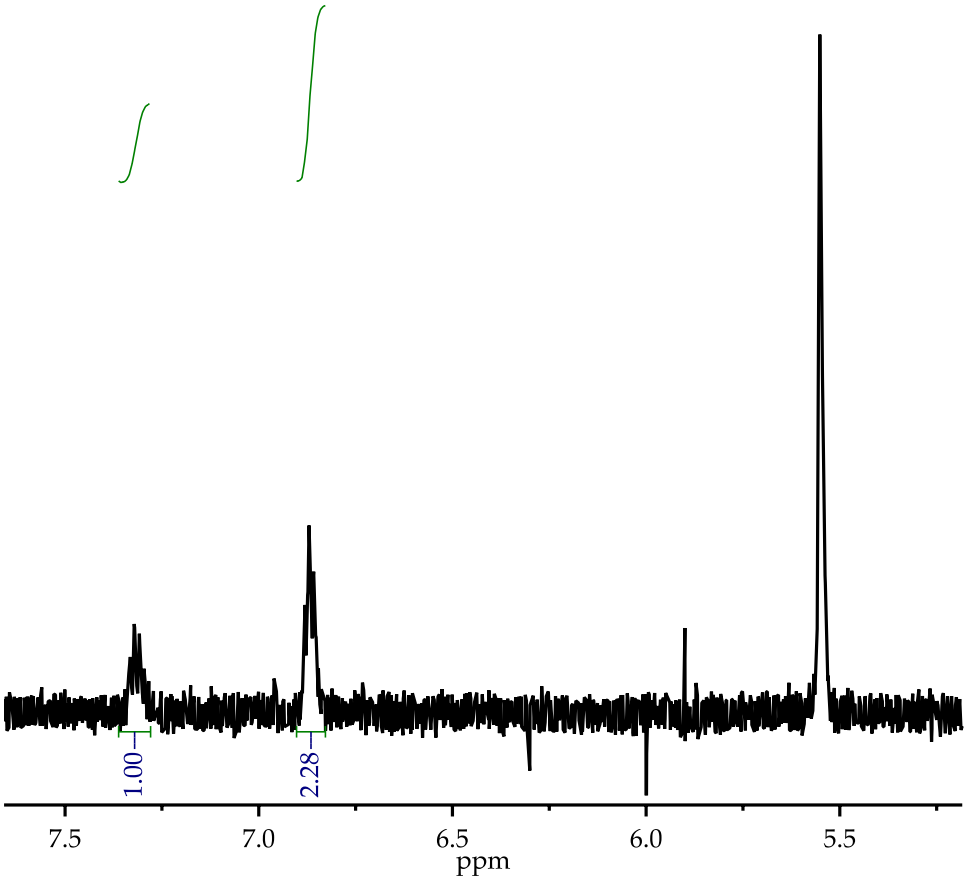


Figure S-29. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 1,3-difluorobenzene with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). Loss of the resonance at δ 6.87 ppm is consistent with doubly ortho selective metalation.

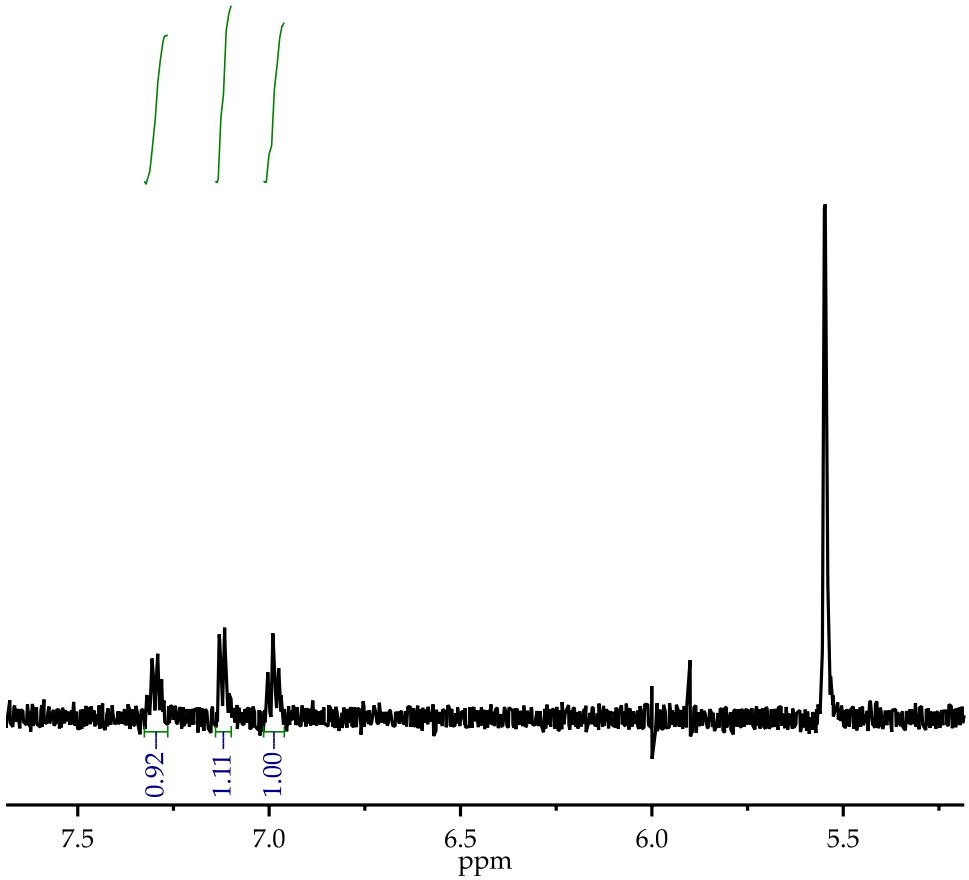


Figure S-30. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 1-chloro-3-fluorobenzene with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). Loss of the resonance at δ 7.11 ppm is consistent with doubly ortho selective metalation.

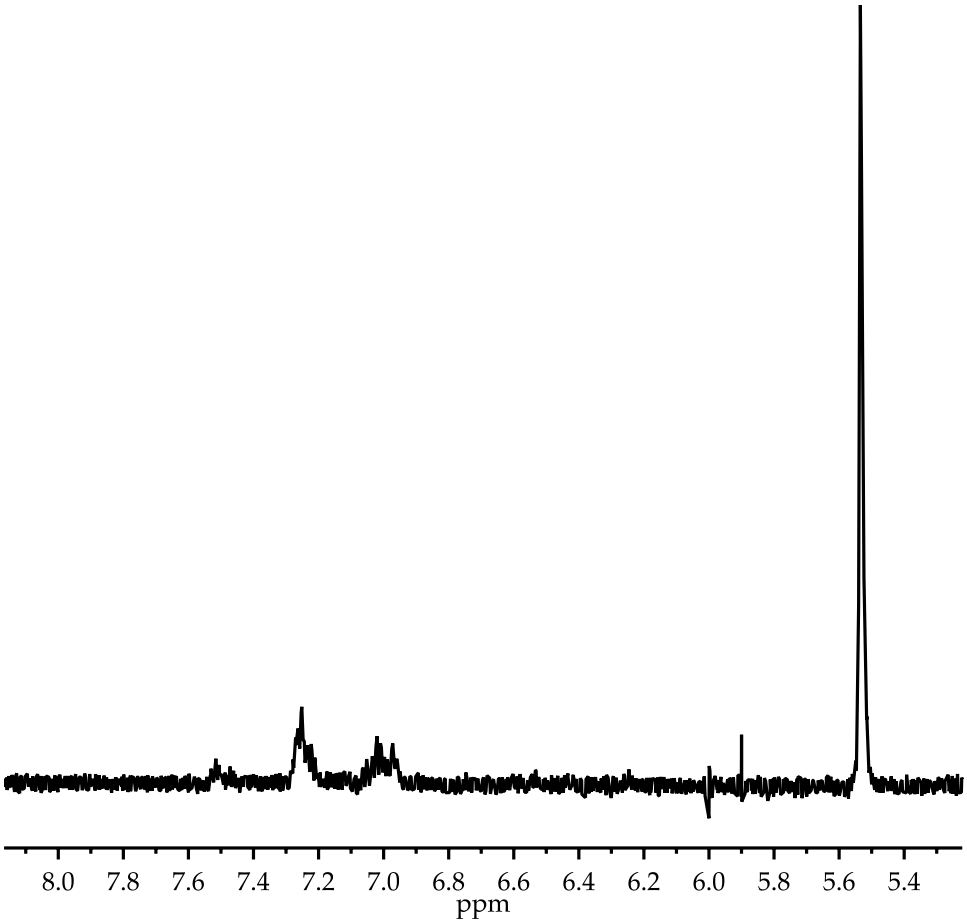


Figure S-31. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 1-bromo-2-fluorobenzene with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). The appearance of extraneous resonances is consistent with decomposition.

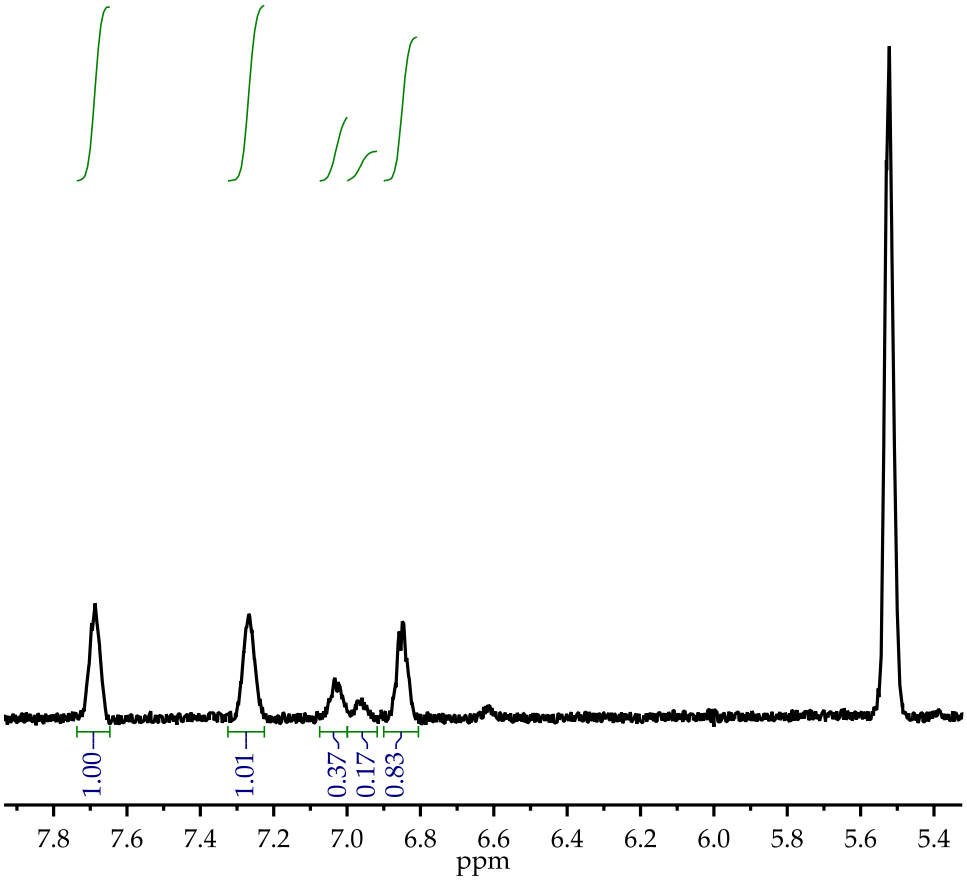


Figure S-32. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 1-fluoro-2-iodobenzene with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 µL MeOD (100 µL cyclohexene internal standard added at δ 5.54 ppm).

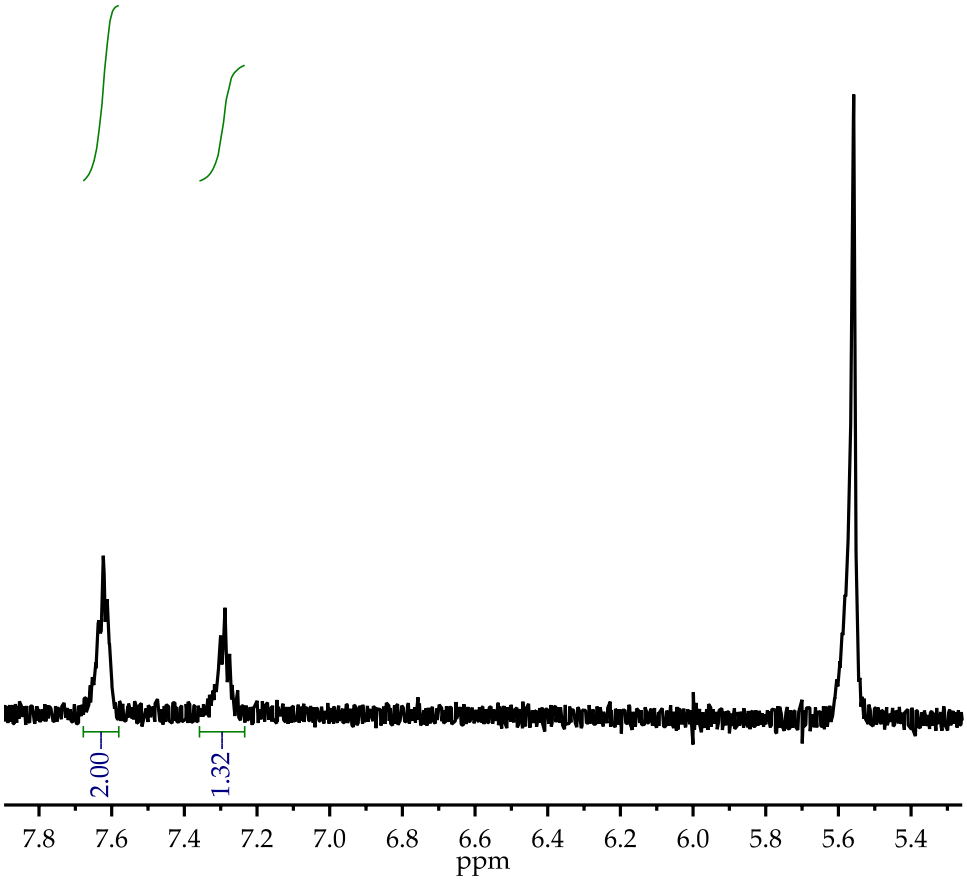


Figure S-33. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 2-fluorobenzotrifluoride with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). Loss of the resonance at δ 7.28 ppm is consistent with selective metalation ortho to fluorine.

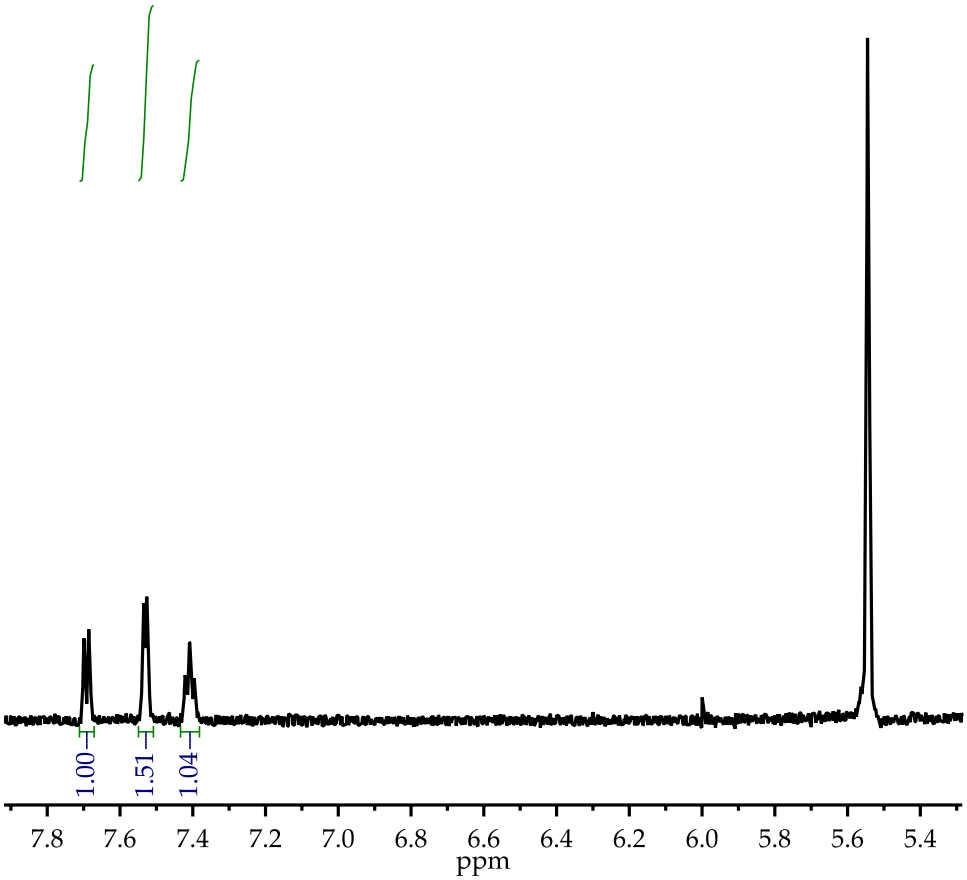


Figure S-34. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 2-chlorobenzotrifluoride with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). Loss of the resonance at δ 7.53 ppm is consistent with selective metalation ortho to chlorine.

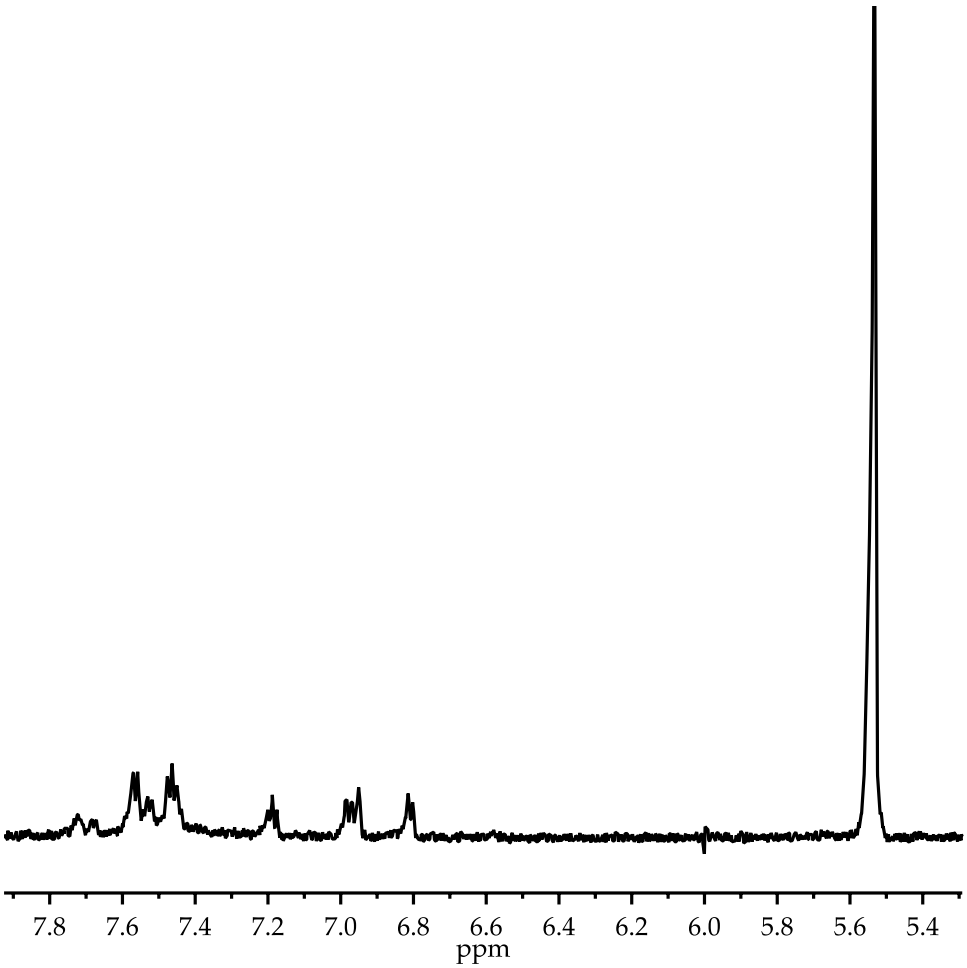


Figure S-35. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 2-bromobenzotrifluoride with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). The appearance of extraneous resonances is consistent with decomposition.

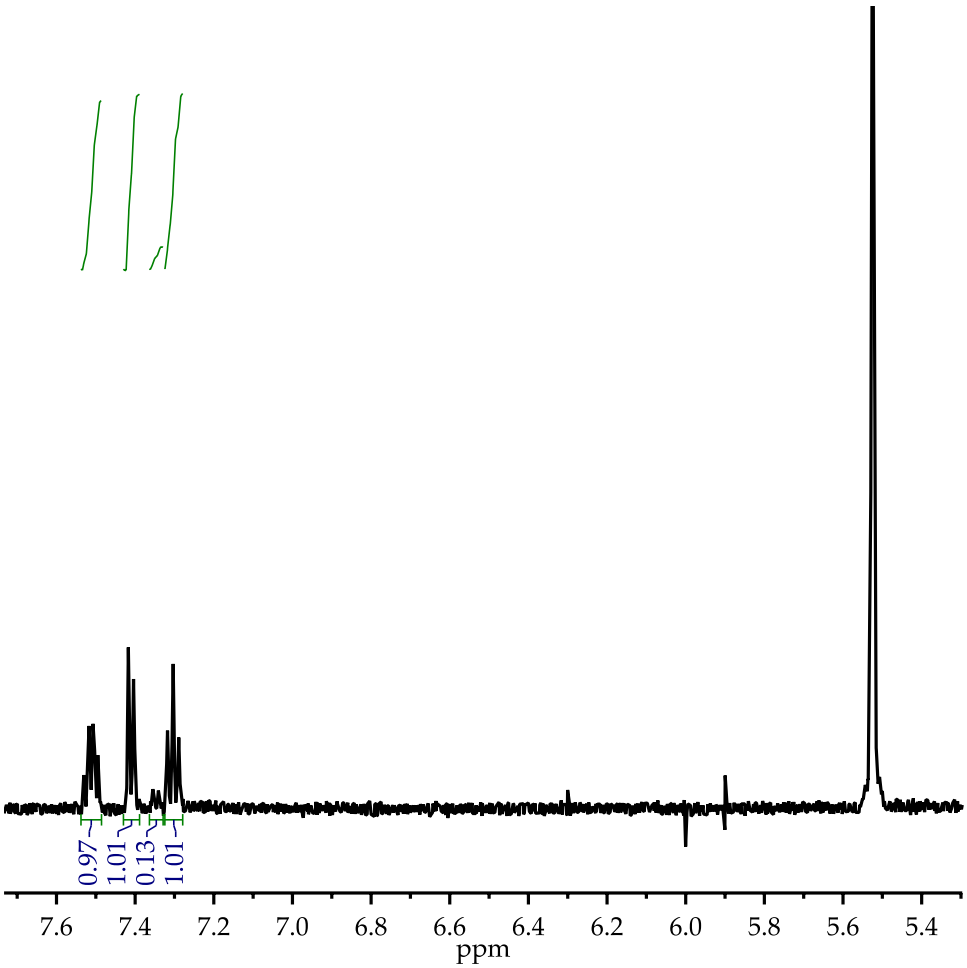


Figure S-36. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 3-fluorobenzotrifluoride with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). Loss of the resonance at δ 7.34 ppm indicates doubly ortho metalation.

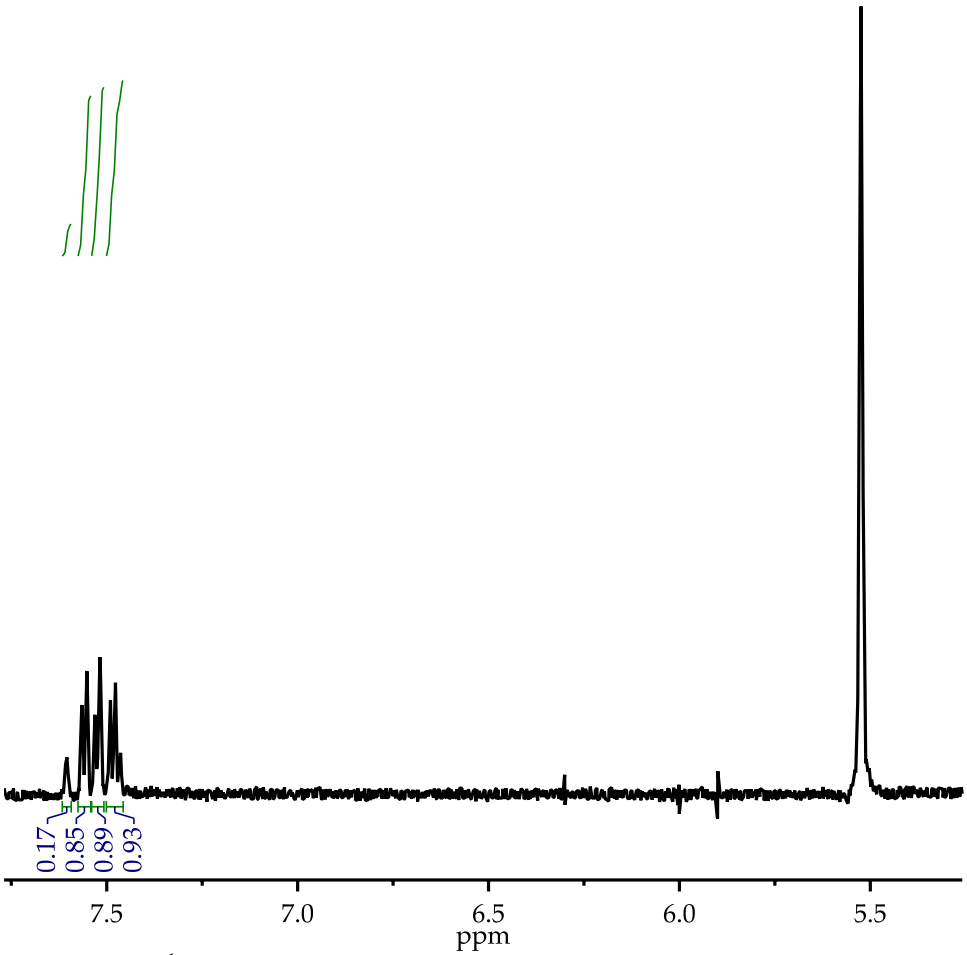


Figure S-37. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 3-chlorobenzotrifluoride with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 µL MeOD (100 µL cyclohexene internal standard added at δ 5.54 ppm). Loss of the resonance at δ 7.60 ppm indicates doubly ortho metalation.

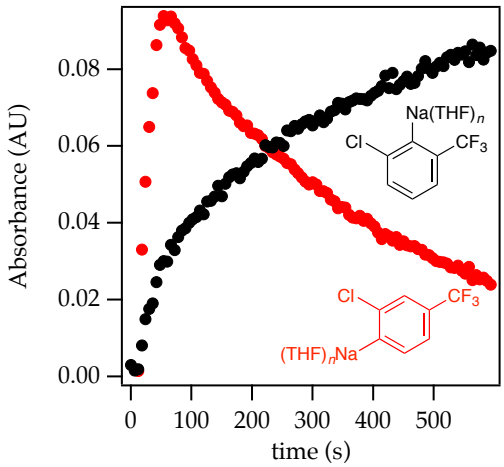


Figure S-38. In situ absorbance trace for the metalation of 0.040 M 3-chlorobenzotrifluoride with 0.10 M NaDA in neat THF at –116 °C. The rapid burst corresponds to the initial metalation event whereas the subsequent decay corresponds to equilibration of the arylsodiums.

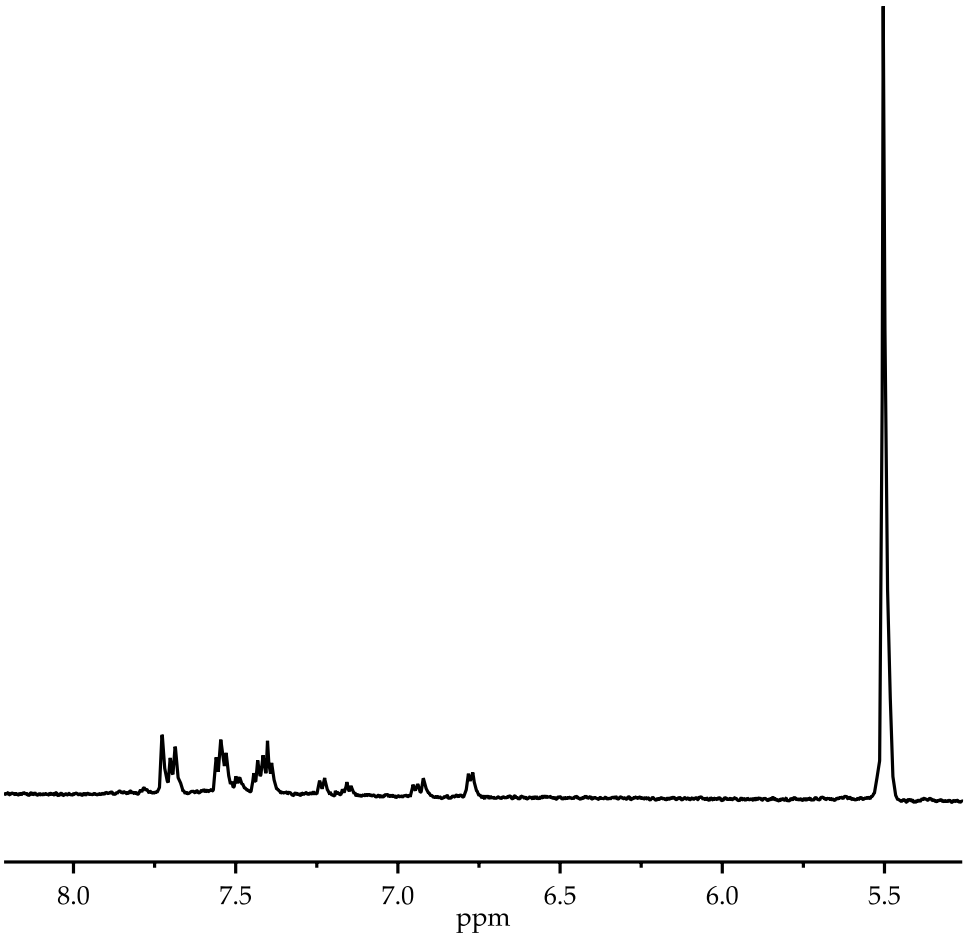


Figure S-39. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 3-bromobenzotrifluoride with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). The appearance of extraneous resonances is consistent with decomposition (possibly isomerization).

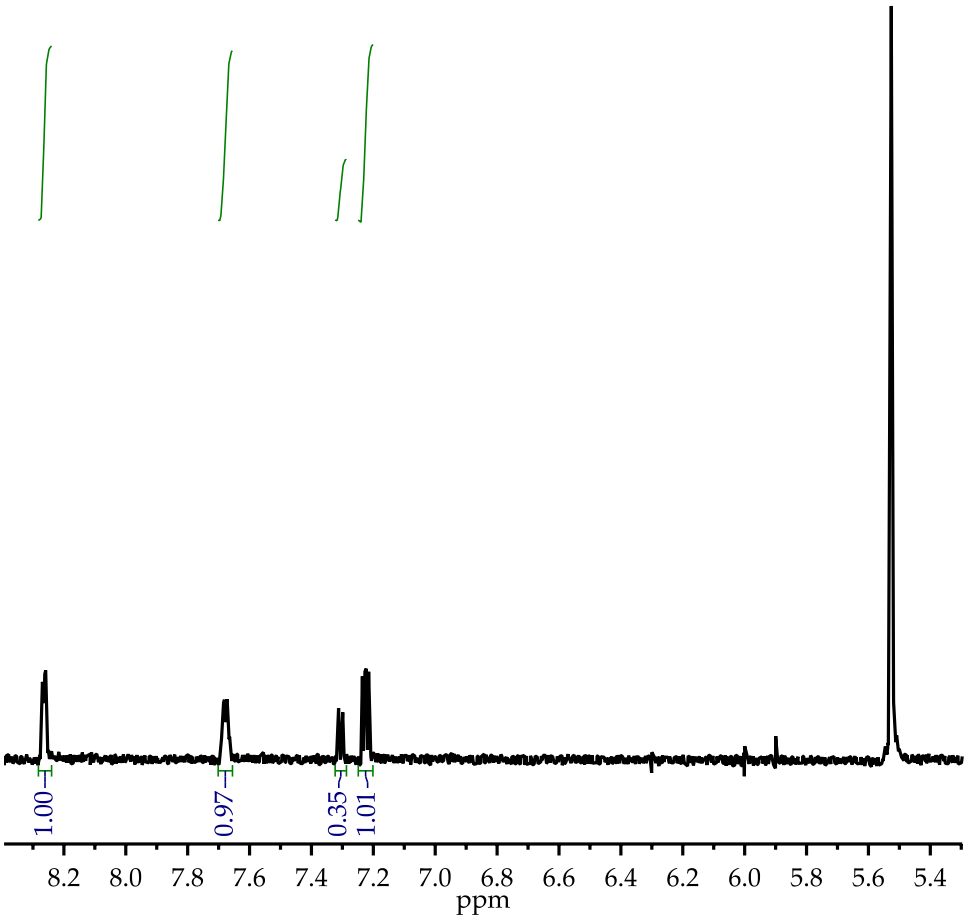


Figure S-40. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 2-chloropyridine with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). Loss of the resonance at δ 7.31 ppm indicates ortho metalation to chlorine.

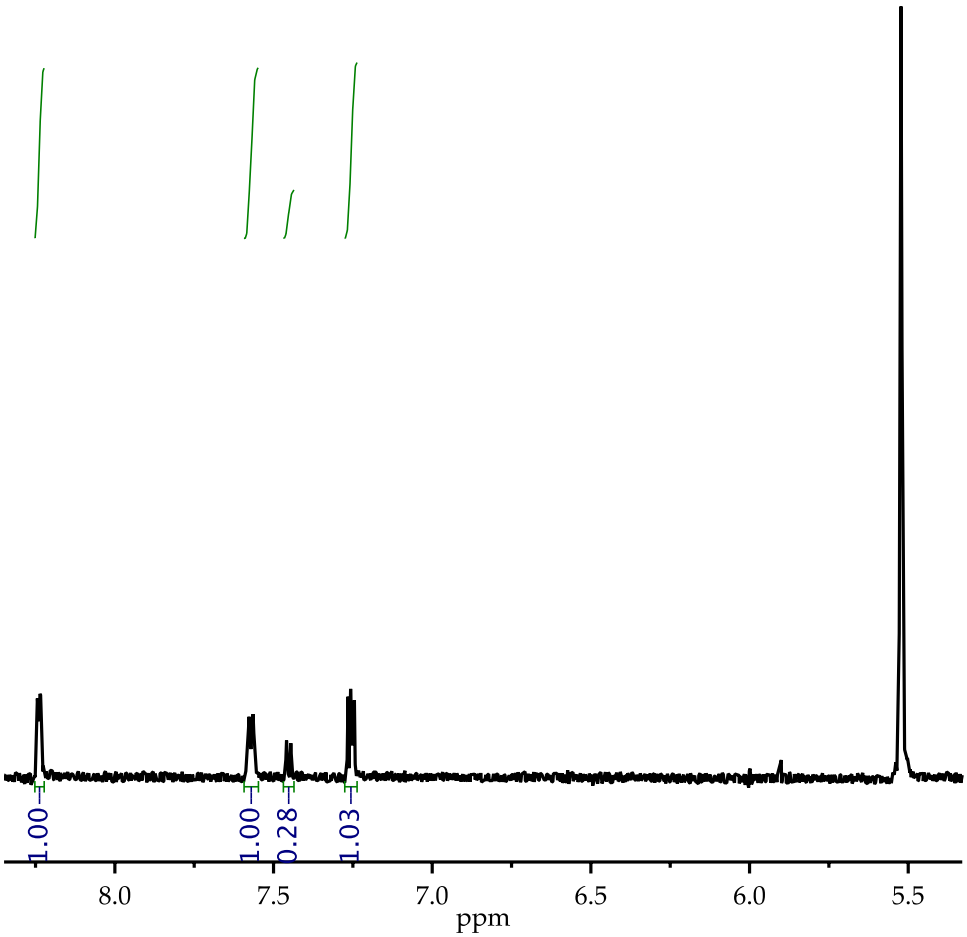


Figure S-41. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 2-bromopyridine with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). Loss of the resonance at δ 7.46 ppm indicates ortho metalation to bromine.

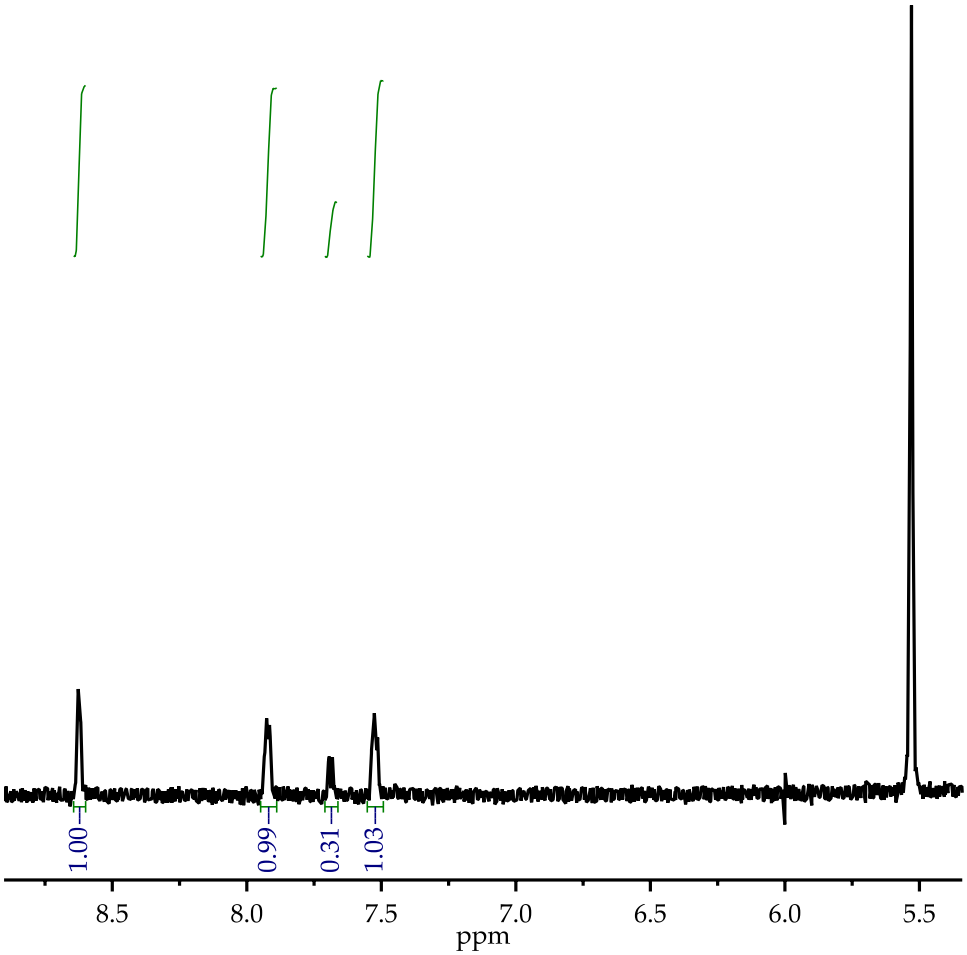


Figure S-42. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 2-(trifluoromethyl)pyridine with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). Loss of the resonance at δ 7.69 ppm indicates ortho metalation to CF_3.

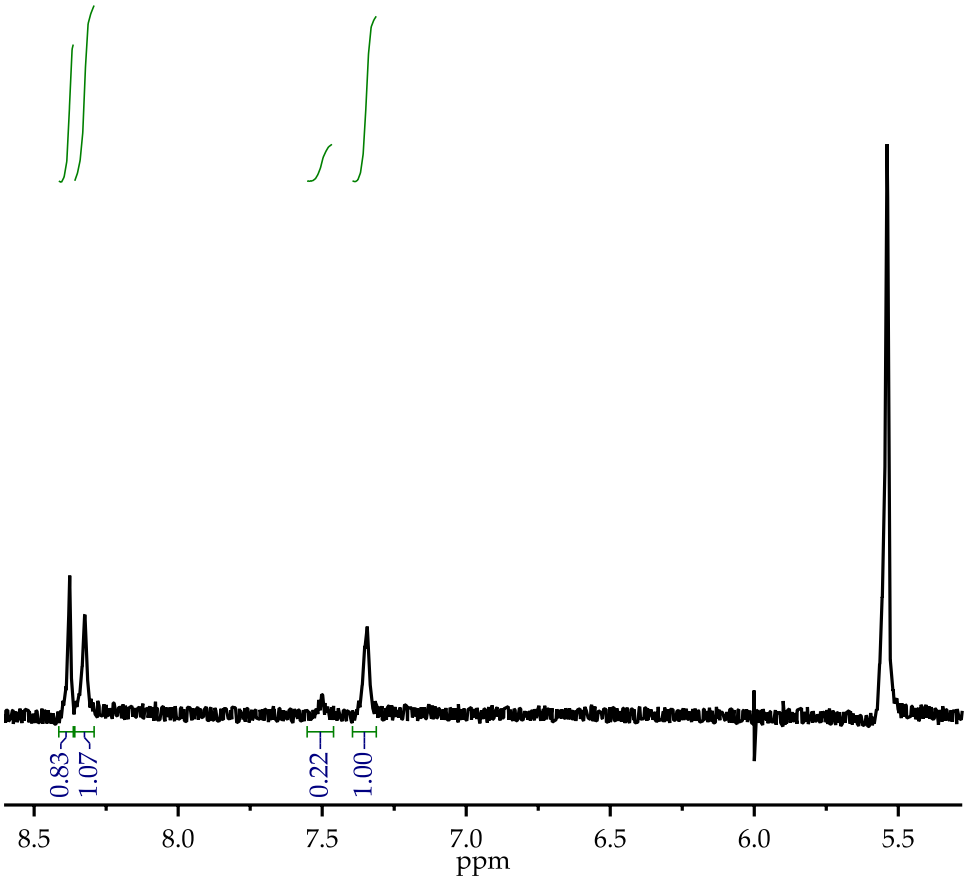


Figure S-43. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 3-fluoropyridine with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 µL MeOD (100 µL cyclohexene internal standard added at δ 5.54 ppm). Loss of the resonance at δ 7.5 ppm indicates metalation at the 4 position.

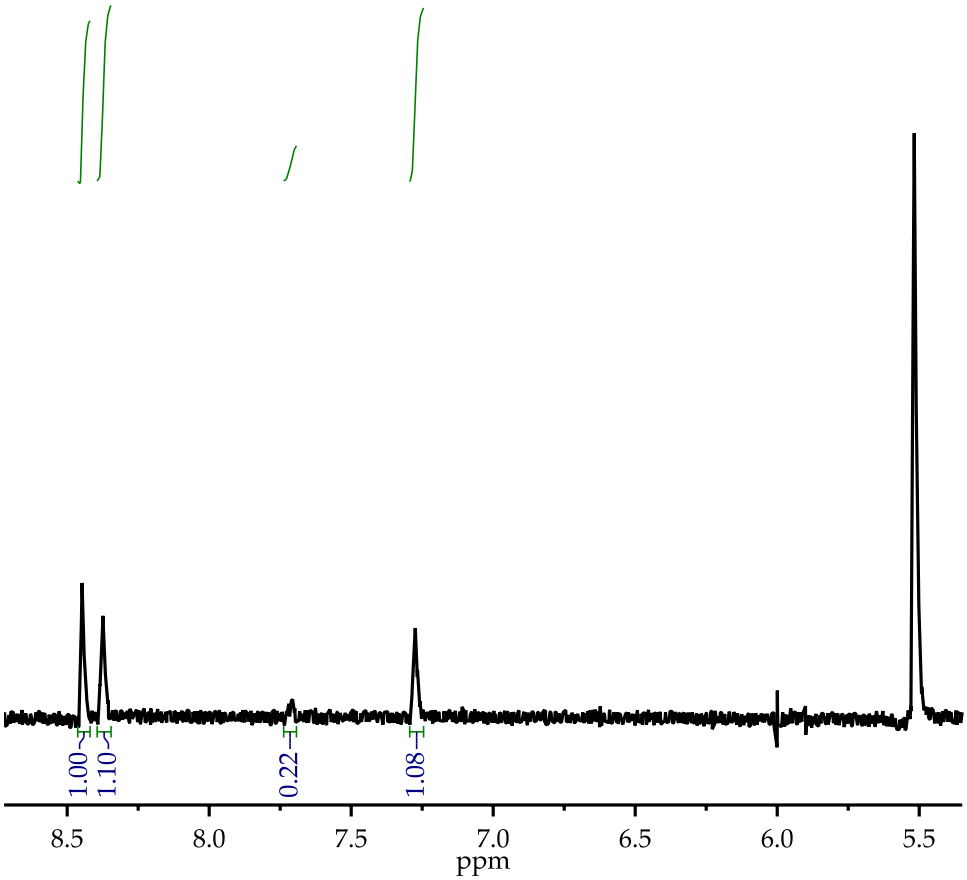


Figure S-44. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 3-chloropyridine with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 µL MeOD (100 µL cyclohexene internal standard added at δ 5.54 ppm). Loss of the resonance at δ 7.7 ppm indicates metalation at the 4 position.

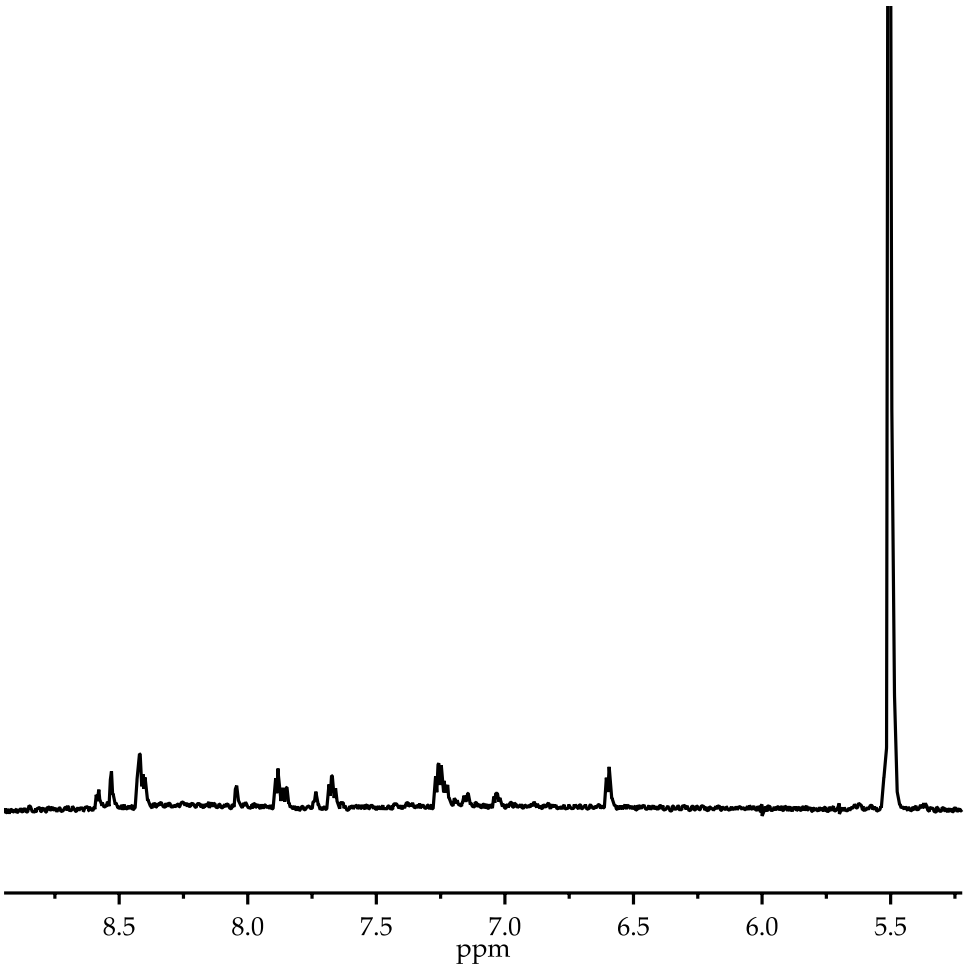


Figure S-45. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 3-bromopyridine with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). The appearance of extraneous resonances is consistent with decomposition (possibly isomerization).

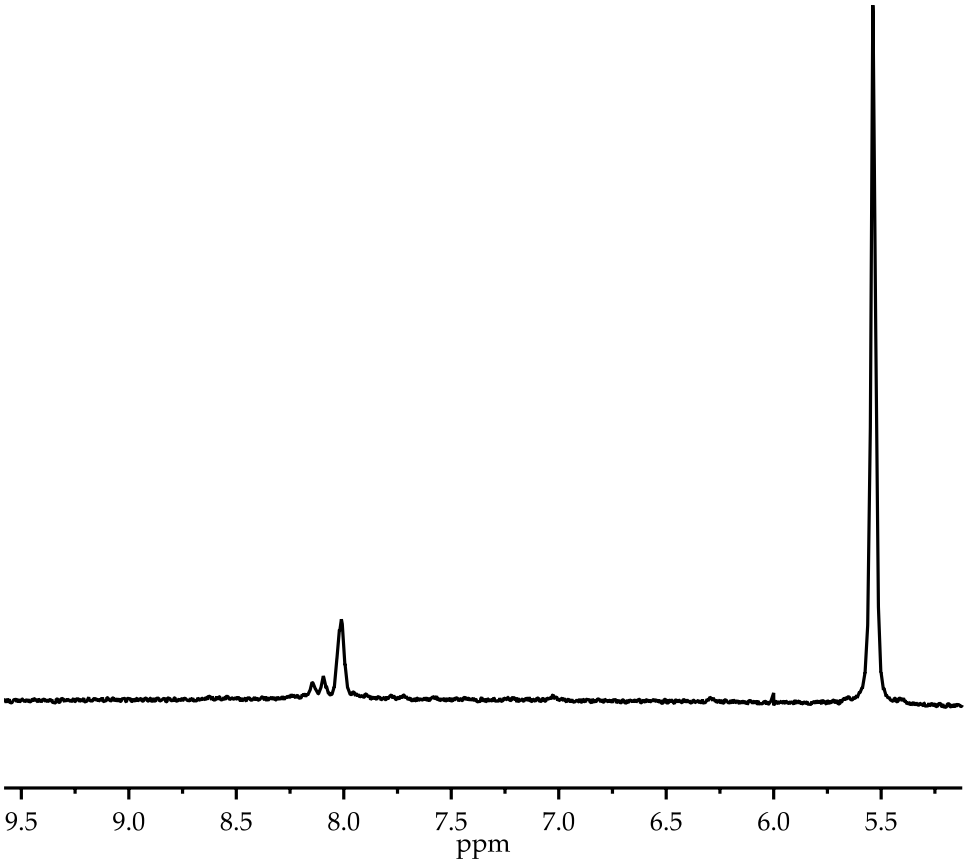


Figure S-46. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 2-fluoropyrazine with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). That there are no resonances corresponding to starting material is consistent with decomposition.

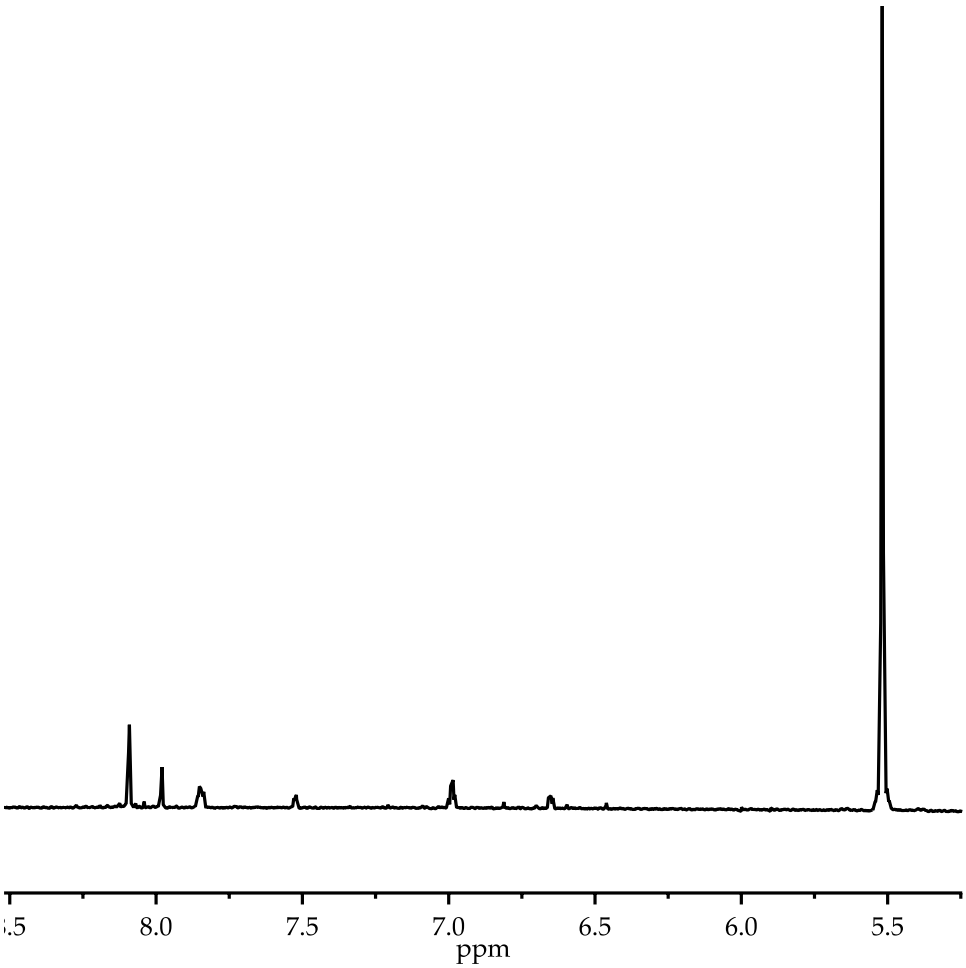


Figure S-47. Isolated ^{1}H NMR spectrum for metalation of 0.38 M 5-chloro-2-fluoropyridine with 0.40 M NaDA in 1.00 mL THF at –78 °C after quenching with 500 μL MeOD (100 μL cyclohexene internal standard added at δ 5.54 ppm). That there are no resonances corresponding to starting material is consistent with decomposition (possibly isomerization).

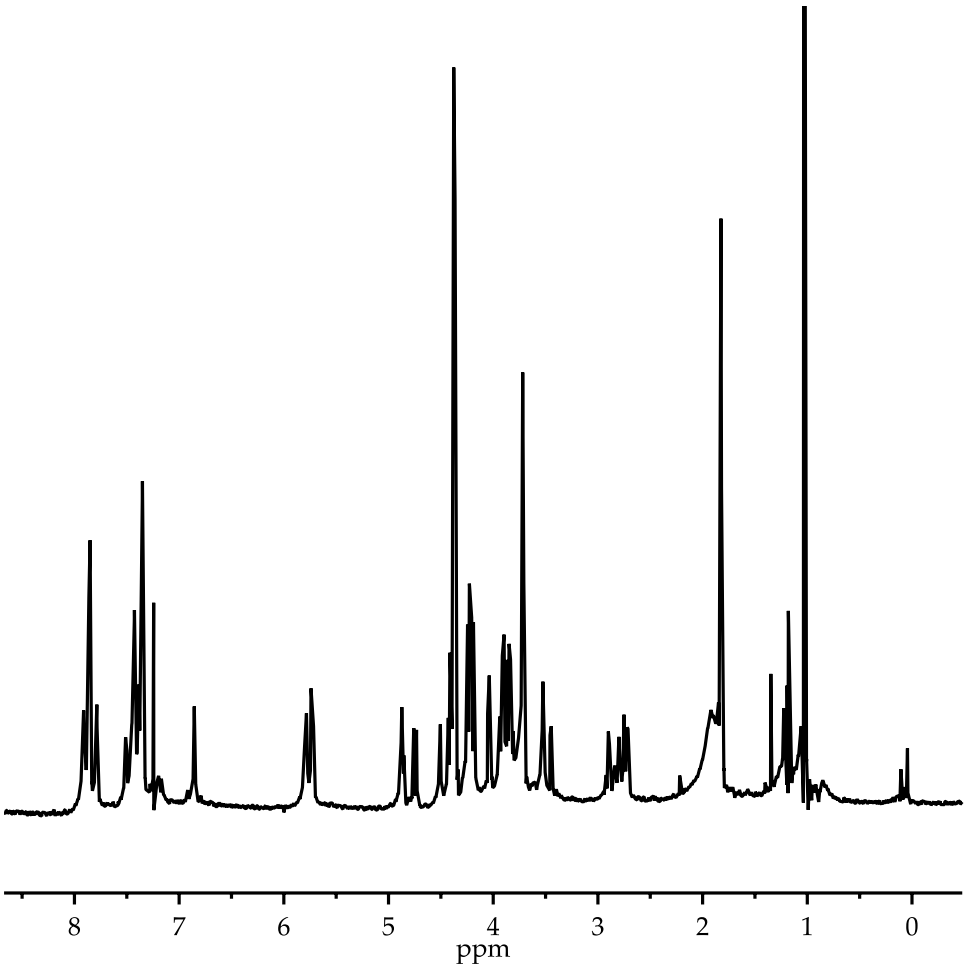


Figure S-48. Isolated ^{1}H NMR spectrum for metalation of 0.20 M 2-phenyl-2-oxazoline with 0.22 M NaDA in 1.00 mL THF at –78 °C after quenching with 200 μL MeOD. That there are no resonances corresponding to starting material is consistent with decomposition (likely due to heterocycle metalation).

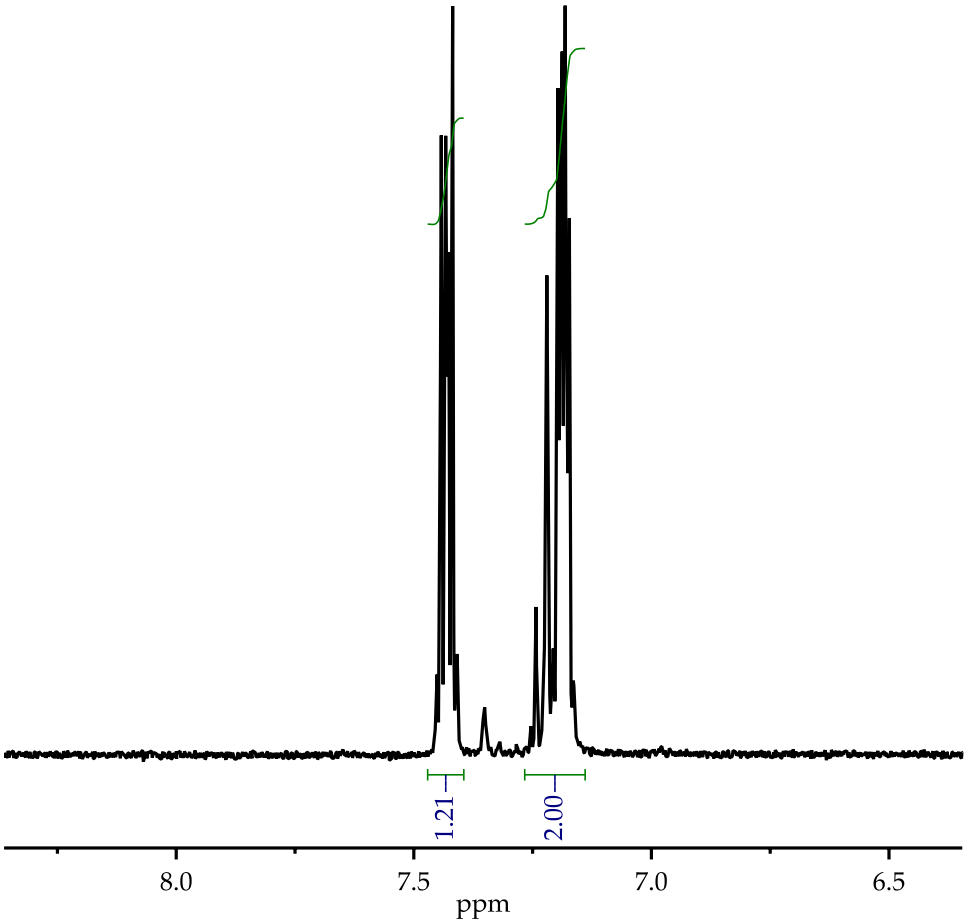


Figure S-49. Isolated ^{1}H NMR spectrum for metalation (preparative scale) of 0.43 M 1,2-dichlorobenzene with 0.55 M NaDA in 8.00 mL THF/DMEA at –78 °C after quenching with 1.00 mL MeOD.

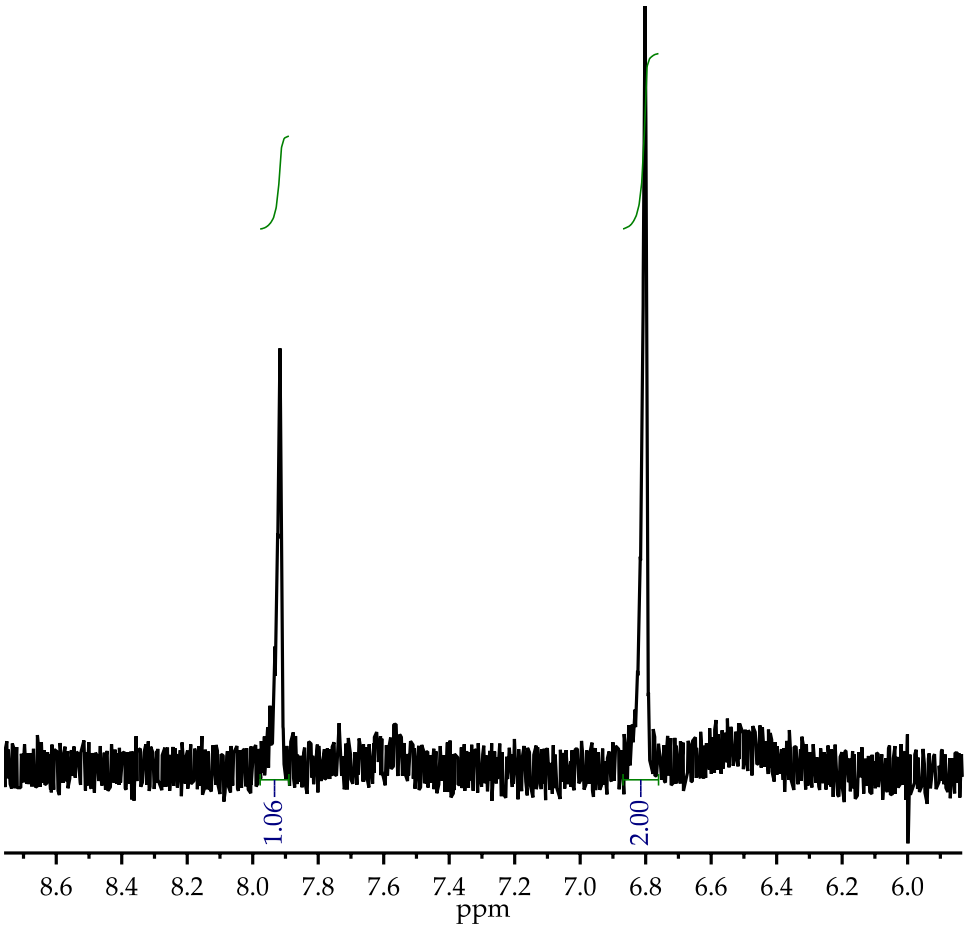
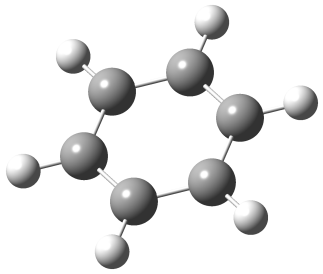


Figure S-50. Isolated ^{1}H NMR spectrum for metalation of 0.33 M furan with 0.50 M NaDA in 3.00 mL THF/DMEA at –78 °C after quenching with 1.00 mL MeOD. Loss of the resonance at δ 7.9 ppm indicates metalation at the ortho position.

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. 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.

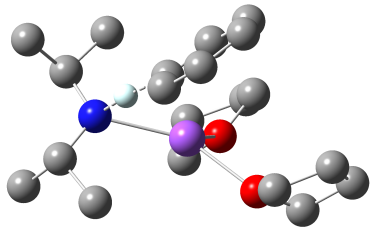
Table S-1. Geometric coordinates and thermally corrected MP2 energies for benzene.



G = –232.175329 Hartree
G_{MP2} = –231.384408 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
C	-1.31606100	-0.46743600	-0.00008800
C	-2.37885200	0.43829200	0.00007500
C	-2.12569900	1.81175800	-0.00000800
C	-0.80983000	2.27912400	-0.00007100
C	0.25311600	1.37327300	0.00008000
H	1.27700800	1.73720900	0.00009300
H	-0.61278400	3.34777000	-0.00003700
H	-2.95276200	2.51656500	0.00001500
H	-3.40282600	0.07461100	0.00019900
H	-1.51286400	-1.53613500	-0.00006500
H	0.82689200	-0.70501800	0.00007500

Table S-2. Geometric coordinates and thermally corrected MP2 energies for $[A(THF)_2(benzene)]^{‡}$.

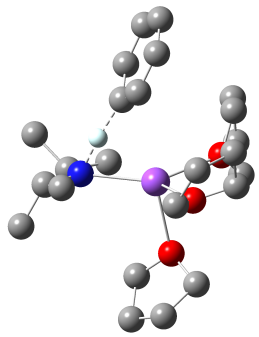


G = –1150.818289 Hartree
G_{MP2} = –1146.981102 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	-0.07521700	0.69649400	-1.28704100
Na	-1.32079800	2.68866900	-1.29831200
O	-0.06676300	4.59724200	-1.86091400
C	1.25636500	4.67242300	-1.27189500
H	1.52139000	3.67398400	-0.91148600
H	1.21923200	5.36354400	-0.41924000
C	2.17424400	5.19230400	-2.37950400
H	3.04122700	5.72982800	-1.98456100
H	2.53774400	4.36101400	-2.99394100
C	1.22309000	6.08490400	-3.19189700
H	1.55775200	6.25237300	-4.21973300
H	1.10706200	7.06195700	-2.70813800
C	-0.08632900	5.29499900	-3.12771900
H	-0.98046800	5.92606000	-3.15875800
H	-0.15017500	4.55503400	-3.93613100
O	-3.03147000	3.87635400	-0.30291700
C	-3.13151600	5.30493700	-0.23080000
H	-2.19437600	5.71405300	-0.61501500
H	-3.24738300	5.60736200	0.82092000
C	-4.38211500	5.67430000	-1.05583800
H	-4.93701600	6.49331000	-0.58830500
H	-4.10542000	5.99818100	-2.06390400
C	-5.19818100	4.35170800	-1.10643900
H	-5.25772700	3.96884100	-2.12849600
H	-6.21900600	4.47195600	-0.73202900
C	-4.38336000	3.38368000	-0.23402800
H	-4.71712100	3.40589800	0.81427300
H	-4.37918600	2.35325500	-0.59301000
C	0.90458100	0.25095500	-2.28502300
C	0.76065800	-1.23199200	-2.69440500
H	1.50881000	-1.50900700	-3.44874200
H	-0.23560700	-1.41795400	-3.11307100
H	0.89453200	-1.90360800	-1.83911700
C	0.80273400	1.13920800	-3.53453000
H	1.56746600	0.87049800	-4.27385300
H	0.94290200	2.19564000	-3.27040500
H	-0.17723800	1.03191900	-4.01345700
H	1.92996100	0.37974600	-1.89539200
C	1.36841900	0.12147800	0.69685900
H	1.34665500	-0.35624100	1.68496000
H	1.63052100	1.18005600	0.83285400
H	2.17174200	-0.35204900	0.12305700
C	-1.08874100	0.54614900	0.93811600
H	-1.12395400	-0.02287200	1.87509400
H	-2.08018600	0.49235100	0.47612700
H	-0.88449900	1.59541400	1.20289800
H	-0.20173000	-1.08438400	-0.11128100
C	-2.98907500	1.49040100	-3.46371500
C	-4.27204300	1.50864300	-4.03045100
C	-5.27191700	0.69152100	-3.50042700
C	-4.97155700	-0.13451700	-2.41221900
C	-3.68605500	-0.12260000	-1.85977200
C	-2.64232200	0.68741000	-2.35641900
H	-3.49145600	-0.78311100	-1.01144300
H	-5.74141700	-0.78663800	-2.00099200

H -6.26883500 0.68781400 -3.93596000
H -4.48785200 2.14462700 -4.88885500
H -1.27657600 0.58224300 -1.80066800
H -2.22793300 2.12440600 -3.93459200

Table S-3. Geometric coordinates and thermally corrected MP2 energies for $[A(THF)_3(benzene)]^{‡}$.

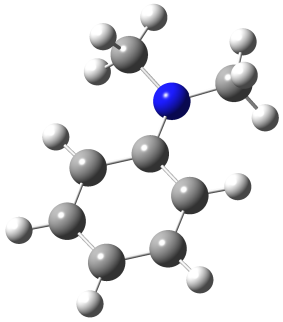


G = –1383.16906 Hartree
G_{MP2} = –1378.565616 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	0.44578400	2.19724800	-0.92002000
C	0.98423600	2.44241800	-2.26173900
C	2.46474200	2.86871800	-2.28428200
H	2.81561800	2.99335500	-3.31688100
H	3.09052900	2.10416500	-1.80326600
H	2.63580500	3.81788100	-1.76572000
C	0.81668400	1.17768800	-3.11498500
H	1.15220800	1.34863800	-4.14564100
H	-0.23049000	0.86257500	-3.14928900
H	1.41912300	0.35693600	-2.69828600
H	0.42097200	3.24238200	-2.78265300
C	0.55120600	3.34807700	-0.01228300
C	-0.19557200	4.61673600	-0.48333000
H	-0.08348100	5.43181900	0.24377100
H	-1.26537600	4.41361100	-0.60969500
H	0.18733700	4.98066000	-1.44300700
C	0.05776400	2.94703900	1.38743500
H	0.14835600	3.78303800	2.09220500
H	0.64633700	2.11036300	1.78508600
H	-0.99443200	2.64224300	1.36283900
H	1.61137400	3.63580600	0.10999300
O	-1.26792300	-0.80520900	1.87405500
C	-0.74336000	-0.78533100	3.20939800
H	0.32289600	-0.56245600	3.13507600
H	-0.87085100	-1.78030000	3.66509900
C	-1.57565700	0.27359600	3.95194900
H	-1.70281600	0.01888800	5.00860800
H	-1.08450100	1.24947400	3.89989500
C	-2.92005700	0.29667500	3.17136800
H	-3.12808200	1.29542800	2.77921800
H	-3.76979700	-0.00137700	3.79300900
C	-2.69798500	-0.69400000	2.01300000
H	-3.10810100	-1.68658800	2.25489800
H	-3.09599700	-0.35649000	1.05604600
O	0.05646700	-2.26209100	-0.95842000
C	-0.75632600	-3.28174300	-0.35371100
H	-1.13455000	-2.87519300	0.58492500
H	-0.13603500	-4.16861000	-0.14407400
C	-1.82613100	-3.58765600	-1.40501500
H	-2.24526900	-4.59242600	-1.29477600
H	-2.64095200	-2.86280100	-1.32061300
C	-1.06611400	-3.39381100	-2.74274200
H	-1.65451000	-2.80350900	-3.45038000
H	-0.83425900	-4.34978000	-3.22252500
C	0.23249000	-2.65877400	-2.33023800
H	1.10474600	-3.32478900	-2.40250800
H	0.43366600	-1.75511500	-2.90799200
O	2.07643900	-0.49510800	1.15402600
C	2.72197800	-1.77444700	1.11304200
H	1.98593000	-2.49828900	0.75910300
H	3.06080500	-2.05935100	2.12207800
C	3.90494700	-1.56990400	0.16815600
H	4.68865900	-2.32323500	0.29506100
H	3.55519500	-1.60996800	-0.86934300
C	4.37224500	-0.14449500	0.53208800
H	4.75628000	0.39858000	-0.33616300

H	5.17110800	-0.17757200	1.28036600
C	3.10384200	0.52341000	1.11674500
H	3.27716100	0.89686700	2.13462300
H	2.71126300	1.33318600	0.49848000
C	-2.66437500	0.24976900	-1.85262100
C	-4.01771600	-0.10617900	-1.94584500
C	-4.97808400	0.62699000	-1.24597400
C	-4.56642200	1.71416800	-0.46968900
C	-3.20762300	2.04095900	-0.39138200
C	-2.19608600	1.32610600	-1.06883200
H	-2.93375600	2.90246500	0.22233200
H	-5.30699400	2.30584500	0.06786000
H	-6.03177400	0.36514400	-1.31566700
H	-4.32590100	-0.94423800	-2.57135300
H	-0.80687600	1.84219000	-1.03040700
H	-1.95312900	-0.34489600	-2.43331200

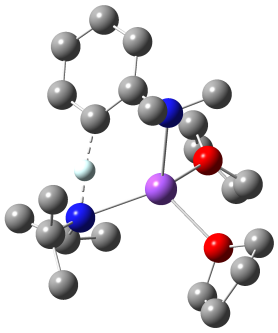
Table S-4. Geometric coordinates and thermally corrected MP2 energies for *N*,*N*-dimethylaniline.



G = –366.074355 Hartree
G_{MP2} = –364.8242641 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	0.72012000	-1.24344700	-0.21151800
C	2.11168500	-1.24343500	-0.12852700
C	2.84535500	-2.45103800	-0.09125700
C	4.23729500	-2.44166400	-0.04358300
C	4.95132500	-1.24331800	-0.02116700
C	4.23718200	-0.04502800	-0.04304200
C	2.84524100	-0.03576900	-0.09070800
H	2.33087100	0.91782900	-0.09814900
H	4.76644500	0.90462400	-0.01759100
H	6.03658400	-1.24327200	0.01855300
H	4.76664100	-3.39128200	-0.01857800
H	2.33109200	-3.40468900	-0.09920300
C	-0.00012200	-2.48667000	0.00099000
H	-1.07047000	-2.30304200	-0.11472300
H	0.28596200	-3.23783800	-0.74460400
H	0.16977700	-2.91944100	1.00092900
H	-1.07033500	-0.18354200	-0.11594000
H	0.16967000	0.43341600	0.99970900
H	0.28648400	0.75060600	-0.74601500

Table S-5. Geometric coordinates and thermally corrected MP2 energies for ortho [A(THF)$_2$(*N*,*N*-dimethylaniline)]‡.

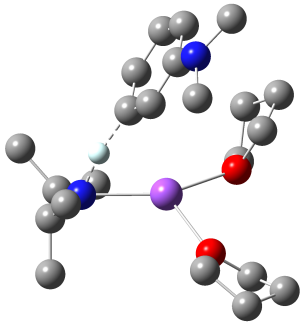


G = –1284.681788 Hartree
G_{MP2} = –1280.394604 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	-0.61472500	-1.27376400	0.38936200
Na	-0.63280500	-3.40404000	-0.70873500
O	1.49151200	-4.44814600	-0.80867000
C	2.09063100	-5.11921100	-1.92455700
H	1.30249000	-5.31866900	-2.65499700
H	2.52062500	-6.07838200	-1.59568800
C	3.17847900	-4.15656400	-2.40607800
H	3.96924200	-4.66264000	-2.96779200
H	2.73660500	-3.39365600	-3.05542200
C	3.68450600	-3.52206500	-1.08622300
H	3.83412100	-2.44416800	-1.19161300
H	4.63726000	-3.95859600	-0.77130300
C	2.56941600	-3.84512500	-0.06142500
H	2.91916700	-4.55714600	0.69885700
H	2.15643900	-2.96472900	0.43513000
O	-1.70531200	-5.44244700	-0.06415100
C	-1.04887900	-6.63101000	0.39141400
H	0.02179700	-6.41795600	0.42257000
H	-1.22889600	-7.44594600	-0.32733800
C	-1.67933200	-6.95528100	1.76030100
H	-1.78394300	-8.03483600	1.90512100
H	-1.05971900	-6.57098000	2.57582000
C	-3.04993900	-6.22228600	1.71787100
H	-3.09849600	-5.45285800	2.49343300
H	-3.89473200	-6.90067400	1.86969400
C	-3.08532900	-5.58170900	0.31863500
H	-3.59574500	-6.23441200	-0.40525400
H	-3.53894500	-4.59032100	0.27759100
N	-1.85811700	-3.29561600	-2.84313000
C	-3.07333200	-2.84779400	-2.14241000
C	-4.33284300	-3.24121300	-2.62240800
C	-5.49482000	-2.81022400	-1.97999400
C	-5.39097600	-1.97082400	-0.87164500
C	-4.12367400	-1.59247400	-0.41557900
C	-2.92006400	-2.01637700	-1.00920400
H	-4.07436700	-0.93170900	0.45100300
H	-6.28924100	-1.61673900	-0.36813800
H	-6.46831200	-3.12096700	-2.35322900
H	-4.42378000	-3.87943000	-3.49817300
C	-1.94212100	-4.62595900	-3.45103700
H	-2.61865400	-4.67681200	-4.32158100
H	-0.94404600	-4.91605100	-3.80447100
H	-2.27088100	-5.35275900	-2.70427900
C	-1.44049900	-2.31410400	-3.85505600
H	-1.39257000	-1.32349100	-3.40474800
H	-0.44692300	-2.57719200	-4.24121400
H	-2.14259300	-2.27616200	-4.70698300
C	-0.76547300	-1.37250800	1.84936900
C	-1.91850700	-0.53037100	2.44343900
H	-1.86349200	-0.50102400	3.54021900
H	-2.89083800	-0.95288700	2.16724200
H	-1.88713000	0.50374100	2.08397200
C	-0.93704300	-2.83580000	2.28364700
H	-1.04661900	-2.91890900	3.37260000
H	-0.06977800	-3.44171400	1.98866600
H	-1.83466000	-3.27318400	1.82994000

H	0.15947400	-1.01272000	2.33343000
C	1.52661600	0.02863100	0.22993000
H	1.94313000	1.02453100	0.02548900
H	2.02059600	-0.68862800	-0.44011600
H	1.79118500	-0.23345900	1.26059200
C	-0.28660400	0.33366600	-1.46850200
H	0.14578000	1.30564300	-1.73595100
H	-1.36194900	0.36463600	-1.66787900
H	0.16198800	-0.42098400	-2.12792900
H	-0.41876400	0.83530600	0.59460400
H	-1.72571900	-1.54188900	-0.28941800

Table S-6. Geometric coordinates and thermally corrected MP2 energies for meta [A(THF)$_2$(*N*,*N*-dimethylaniline)]‡.

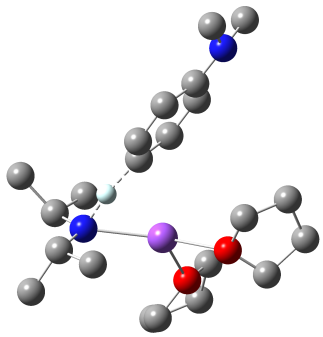


G = –1284.713867 Hartree
G_{MP2} = –1280.420192 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	0.71523500	-0.12254100	1.27107600
Na	1.81785200	1.67560100	2.32039000
O	1.21731500	3.89655000	1.97848600
C	1.03752700	4.80970200	3.07880400
H	1.69309700	4.47585800	3.88621600
H	-0.00617000	4.76857800	3.42529100
C	1.37114500	6.18416000	2.50526300
H	0.93828200	7.00326600	3.08733800
H	2.45774700	6.32548800	2.46655600
C	0.78562000	6.07272500	1.08771200
H	1.24437100	6.76325500	0.37421200
H	-0.29096200	6.27658400	1.10716300
C	1.04851800	4.60127700	0.72515800
H	0.22389300	4.14491400	0.16793700
H	1.97068000	4.47674900	0.14542800
O	3.00085200	2.27328200	4.28180700
C	2.90262000	1.59399400	5.54946900
H	2.04741500	0.91462400	5.49779300
H	2.72230400	2.32930300	6.34828500
C	4.24721900	0.89479500	5.72694200
H	4.45965500	0.64237400	6.77033400
H	4.27184900	-0.02138100	5.12794000
C	5.21642600	1.93564200	5.14214700
H	6.14685900	1.49219100	4.77862800
H	5.46741400	2.69033700	5.89672300
C	4.40151100	2.55664900	3.99662500
H	4.52872200	3.64342800	3.92847600
H	4.64168300	2.10351400	3.03076100
C	3.48818400	0.01669200	1.22386000
C	4.19578300	0.91177100	0.39921500
C	5.60913200	1.04279200	0.39922200
C	6.33318500	0.25181000	1.31721500
C	5.66053400	-0.64852400	2.14561500
C	4.26915500	-0.76392500	2.10109100
H	3.78964400	-1.49177700	2.75976200
H	6.24588500	-1.26508900	2.82844000
H	7.41410300	0.31327100	1.37466900
N	6.27139300	1.90499600	-0.48915900
C	7.66526300	2.22446100	-0.23968600
H	8.02630000	2.89311700	-1.02513200
H	7.83414100	2.71450300	0.73592600
H	8.28399600	1.32065000	-0.27035500
C	5.49486800	2.89779400	-1.20687100
H	6.15907900	3.46337300	-1.86536500
H	4.73598600	2.42072100	-1.83569200
H	4.97773400	3.61425100	-0.54122000
H	3.62845800	1.51804400	-0.30599000
C	0.22581400	-1.23692400	2.09166100
C	0.74660100	-2.61656400	1.62938500
H	0.29635500	-3.43283800	2.21036900
H	1.83563100	-2.67596100	1.73928300
H	0.51073200	-2.79265100	0.57401800
C	0.58475100	-1.00979000	3.56905000
H	0.24658300	-1.84122100	4.20054600
H	0.11412100	-0.09012400	3.94380500
H	1.67233200	-0.92385000	3.69517200

H -0.87648600 -1.27561400 2.04189500
C -1.35722400 0.71562200 0.15959900
H -1.98580400 0.22193200 0.90928800
H -1.91873600 0.73538000 -0.78483500
H -1.19945800 1.75193800 0.48959000
C 0.85675800 0.74028000 -1.03708100
H 0.31662000 0.84788800 -1.98575900
H 1.79476900 0.21125700 -1.22841900
H 1.10699700 1.75168500 -0.68453300
H -0.21580700 -0.99719100 -0.43101200
H 2.00997100 -0.16619700 1.15001300

Table S-7. Geometric coordinates and thermally corrected MP2 energies for para [A(THF)$_2$(*N*,*N*-dimethylaniline)]‡.

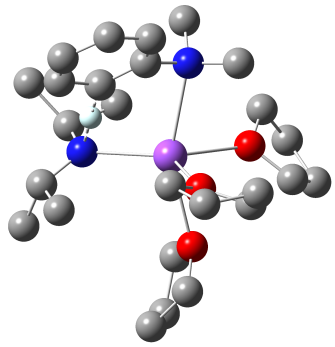


G = –1284.71471 Hartree
G_{MP2} = –1280.420866 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	-0.18750100	0.67695000	-1.28653600
Na	-0.79467600	2.95336600	-1.17122100
O	0.89246500	4.33612000	-2.07741400
C	2.23076400	3.90817000	-1.71589500
H	2.16512000	2.88073900	-1.34513800
H	2.59795800	4.55946100	-0.91151200
C	3.07055100	4.05167800	-2.98600000
H	4.12761000	4.23069000	-2.76864400
H	2.99593800	3.14468100	-3.59629200
C	2.38633300	5.23222400	-3.69333600
H	2.57742400	5.26295700	-4.76997600
H	2.71822600	6.18345900	-3.26076500
C	0.91116000	4.98204600	-3.37069500
H	0.31524400	5.89821300	-3.30529900
H	0.44703300	4.31290100	-4.10717100
O	-1.79579600	4.66428100	0.01632900
C	-1.39944000	6.04250000	-0.00586000
H	-0.46055200	6.09917600	-0.56113000
H	-1.22421000	6.38505300	1.02492200
C	-2.57656100	6.80731900	-0.65182600
H	-2.76663000	7.74995400	-0.12940700
H	-2.36566600	7.04958700	-1.69803000
C	-3.76926500	5.81681900	-0.54039700
H	-4.05792300	5.44000200	-1.52540500
H	-4.65310900	6.26854300	-0.08054100
C	-3.20745600	4.66522000	0.30442300
H	-3.35118400	4.84520600	1.38068600
H	-3.60054700	3.68161500	0.04285600
C	-2.83346200	1.44240600	-1.68487100
C	-3.24733700	2.22909100	-2.77867900
C	-4.57511700	2.59850900	-3.03164500
C	-5.61053500	2.18205600	-2.17038600
C	-5.23725800	1.37111100	-1.07551800
C	-3.89881000	1.03510700	-0.85604500
H	-3.69099000	0.40265400	0.01088800
H	-5.99214700	0.99252900	-0.39353200
N	-6.94718700	2.56626400	-2.38100700
C	-7.98818800	1.84002900	-1.67349700
H	-8.96038400	2.26352300	-1.93880100
H	-8.00503500	0.76074400	-1.90457400
H	-7.86976300	1.94884900	-0.58996500
C	-7.30963400	3.09040700	-3.68634300
H	-8.37344000	3.34182400	-3.68677600
H	-6.75698100	4.01155900	-3.90282600
H	-7.12014300	2.38202400	-4.51168500
H	-4.79776300	3.19508000	-3.91110800
H	-2.50796900	2.57181100	-3.51259100
C	0.30883500	-0.06758500	-2.45043100
C	-0.40506800	-1.41699200	-2.68804900
H	-0.00577400	-1.92519300	-3.57566300
H	-1.47981400	-1.25816300	-2.83553500
H	-0.28092700	-2.09737400	-1.83820500
C	0.18390900	0.80680700	-3.70748600
H	0.60325300	0.29999200	-4.58562100
H	0.72140900	1.75444000	-3.57299900
H	-0.86608300	1.03468700	-3.92339700

H	1.38433000	-0.28653400	-2.33068600
C	1.46898500	-0.33315200	0.32312400
H	1.55737600	-0.77361100	1.32472500
H	2.07973700	0.58018200	0.29520500
H	1.90029600	-1.04667000	-0.38668100
C	-0.57228900	0.87865700	1.12444900
H	-0.53370600	0.35912400	2.08968900
H	-1.61590600	1.14880600	0.93134000
H	0.01357000	1.80512900	1.23033700
H	-0.55618900	-0.95807500	0.04067800
H	-1.45176800	0.93042800	-1.47528900

Table S-8. Geometric coordinates and thermally corrected MP2 energies for ortho [A(THF)$_3$(*N*,*N*-dimethylaniline)]‡.

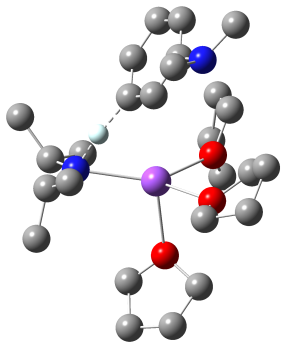


G = –1517.061097 Hartree
G_{MP2} = –1512.009277 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	-0.48006300	2.41085300	-0.11371100
C	-0.75740500	3.12662500	-1.36846300
C	0.37938300	4.05043600	-1.85307800
H	0.13016500	4.48101000	-2.83172600
H	1.31668700	3.48782400	-1.95653500
H	0.56584200	4.88674700	-1.17183100
C	-1.07529400	2.11213800	-2.47674900
H	-1.35054200	2.62187500	-3.40914600
H	-1.90537400	1.46315300	-2.18699200
H	-0.19845200	1.48250600	-2.68034600
H	-1.65298700	3.77488000	-1.27295400
C	-0.16055300	3.30736100	1.00801600
C	-1.37403600	4.10038700	1.54616300
H	-1.08105900	4.77568700	2.36145200
H	-2.14814000	3.42098600	1.92005400
H	-1.82776900	4.71359200	0.75929500
C	0.49963700	2.51233900	2.14339900
H	0.75904500	3.16298200	2.98891300
H	1.41967000	2.03134300	1.78721900
H	-0.17020100	1.73186400	2.51951200
H	0.59046900	4.05101500	0.69478100
O	1.68092800	-1.15302800	1.52238000
C	2.60272900	-2.15329500	1.06358300
H	2.74825800	-1.97708500	-0.00274100
H	2.16067400	-3.15082500	1.20953200
C	3.88617700	-1.99202900	1.91776700
H	4.19725400	-2.95348500	2.33807000
H	4.72246400	-1.60932900	1.32543900
C	3.47117700	-0.99022400	3.02539200
H	3.86765600	0.00792900	2.81293200
H	3.81857800	-1.28491200	4.02015600
C	1.94285800	-0.97472200	2.91821000
H	1.49604300	-1.80190300	3.49337200
H	1.47807900	-0.03697000	3.22631500
O	-0.69772000	-1.73777500	-1.63966200
C	-0.12638900	-3.04699900	-1.78816400
H	0.28252500	-3.35027700	-0.81939500
H	0.69726300	-3.01207900	-2.51722400
C	-1.26369100	-3.93935200	-2.28636200
H	-0.90334000	-4.82688800	-2.81577400
H	-1.88423800	-4.27077500	-1.44534100
C	-2.04636500	-2.96741100	-3.18272600
H	-3.09108800	-3.25819600	-3.32565400
H	-1.57643800	-2.90366400	-4.17153400
C	-1.91487000	-1.63726000	-2.42896000
H	-1.82409100	-0.77517900	-3.09585000
H	-2.74646700	-1.46041500	-1.74121800
O	2.13325700	-0.09262400	-1.40209600
C	2.22422500	-0.33451100	-2.81797000
H	1.21190200	-0.50786600	-3.19168800
H	2.82447900	-1.24063800	-2.99391800
C	2.90693100	0.89868600	-3.41060100
H	3.41923900	0.68364600	-4.35358100
H	2.17170200	1.69026200	-3.59113500
C	3.86256000	1.30195300	-2.27652400
H	4.15291700	2.35622800	-2.31182400

H	4.77703600	0.69779700	-2.31628500
C	3.04430500	0.96647800	-1.02308500
H	3.66114000	0.61208000	-0.18989300
H	2.44178100	1.81460400	-0.68006700
N	-1.83349600	-0.89298400	1.67035800
C	-2.95507300	-0.36036100	0.89119700
C	-4.14079000	-1.10231100	0.76241800
C	-5.21944300	-0.57314600	0.04848300
C	-5.11240300	0.70090500	-0.50906700
C	-3.91674900	1.41444600	-0.36411500
C	-2.79183300	0.91820400	0.32152700
H	-3.85618500	2.40261000	-0.82507000
H	-5.95126100	1.12886300	-1.05627200
H	-6.13681000	-1.14929100	-0.05443500
H	-4.24045000	-2.08627700	1.21573600
C	-1.71625000	-2.34974900	1.69641100
H	-0.74317000	-2.61681800	2.12568900
H	-2.49646500	-2.85073000	2.29777000
H	-1.76346100	-2.73555200	0.67511200
C	-1.87582400	-0.37535300	3.04378400
H	-0.94920300	-0.63025300	3.57217400
H	-1.98690200	0.70937100	3.01907700
H	-2.72475400	-0.79418400	3.61483600
H	-1.56578700	1.73563300	0.18551400

Table S-9. Geometric coordinates and thermally corrected MP2 energies for meta [A(THF)$_3$(*N*,*N*-dimethylaniline)]‡.

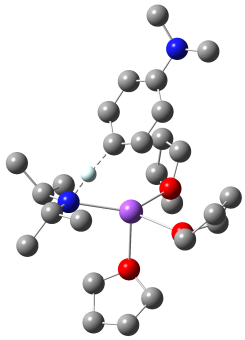


G = –1517.068011 Hartree
G_{MP2} = –1512.008325 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	-0.37279300	-1.29636500	-2.00537400
C	-0.46443500	-0.71647700	-3.34692100
C	-1.83618600	-0.06494700	-3.62152900
H	-1.91279400	0.29238000	-4.65779700
H	-1.98268300	0.79363600	-2.95186000
H	-2.66027100	-0.76835000	-3.45477400
C	0.64224600	0.32470500	-3.56473100
H	0.56495700	0.77520800	-4.56204400
H	1.63424000	-0.12312100	-3.46062500
H	0.55662900	1.13630300	-2.82781700
H	-0.32177600	-1.48760100	-4.12870700
C	-1.04531400	-2.59892800	-1.90511400
C	-0.28120800	-3.75593000	-2.59015400
H	-0.85882100	-4.68969100	-2.55714800
H	0.68169200	-3.93019100	-2.09684600
H	-0.07733000	-3.53335400	-3.64308900
C	-1.30034000	-2.95259800	-0.43092500
H	-1.78266100	-3.93367800	-0.33282300
H	-1.95153400	-2.20764700	0.04387900
H	-0.35764800	-2.98863900	0.12899600
H	-2.03727800	-2.54445100	-2.38979500
O	0.26287300	-0.58703500	2.30853400
C	-0.84539400	-0.82043600	3.18616300
H	-1.75349000	-0.58042000	2.63079000
H	-0.76978400	-0.14774300	4.05567800
C	-0.71553400	-2.29251600	3.61550400
H	-1.07760800	-2.44955000	4.63623800
H	-1.29827400	-2.93733100	2.95131100
C	0.80433200	-2.58316200	3.46426300
H	0.97587200	-3.40245500	2.76075800
H	1.27623800	-2.85509500	4.41328000
C	1.37961100	-1.26710200	2.90635700
H	1.78921100	-0.64040700	3.71379600
H	2.13560200	-1.40706900	2.13255700
O	0.98684000	2.19665500	0.36235200
C	1.99484500	2.24130500	1.40514300
H	2.40033500	1.23550200	1.53381400
H	1.50670700	2.55360400	2.33763600
C	3.04635200	3.25087800	0.93734000
H	3.53434600	3.75818200	1.77555000
H	3.81518300	2.73861100	0.34795300
C	2.21958200	4.19969100	0.05569900
H	2.82173000	4.75157700	-0.67244700
H	1.67618200	4.92762200	0.67066600
C	1.24445400	3.22937300	-0.61203500
H	0.28646500	3.68365400	-0.88640600
H	1.68557900	2.77655200	-1.50938700
O	-2.16375300	0.91379900	0.56551000
C	-2.34642300	2.23893500	1.07858800
H	-1.35276100	2.65074200	1.26431600
H	-2.90994900	2.20024200	2.02493900
C	-3.14377800	2.96119400	-0.01118600
H	-3.70675700	3.81584200	0.37642400
H	-2.46300300	3.32923200	-0.78623700
C	-4.05465400	1.84262300	-0.57506800
H	-4.10242800	1.87624700	-1.66692000

H	-5.07801600	1.93139400	-0.19713600
C	-3.39670100	0.53345700	-0.07323200
H	-4.03885200	0.02086200	0.65737300
H	-3.13611400	-0.16433400	-0.87044200
C	3.10770600	-0.37251800	-1.00141600
C	4.43190000	-0.44098400	-0.51594500
C	4.84313500	-1.62097100	0.12000200
C	3.94534200	-2.68862400	0.24084800
C	2.64870900	-2.58737900	-0.26446500
C	2.17631000	-1.41886000	-0.90484800
H	1.98777400	-3.45030200	-0.15405900
H	4.28081100	-3.60532900	0.72615500
H	5.85421000	-1.72855000	0.49929500
N	5.29178500	0.69649600	-0.66083600
C	6.53456500	0.67285700	0.09410100
H	7.26533200	-0.07057900	-0.27593200
H	7.00574200	1.66026100	0.03151600
H	6.32954600	0.45650000	1.14663400
C	5.52218800	1.12066400	-2.04272100
H	4.57889000	1.17634200	-2.58743300
H	5.98199000	2.11604900	-2.04651500
H	6.19127200	0.43053100	-2.58877400
H	2.80583000	0.56588500	-1.47236800
H	0.85076500	-1.39560100	-1.56811700

Table S-10. Geometric coordinates and thermally corrected MP2 energies for para [A(THF)$_3$(*N*,*N*-dimethylaniline)]‡.

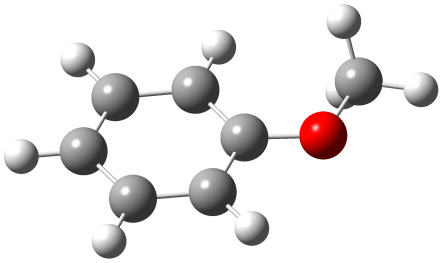


G = –1517.065405 Hartree
G_{MP2} = –1512.006045 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	0.30317600	2.18353400	-1.01385600
C	0.61274300	2.39443100	-2.43117800
C	2.06732100	2.82002400	-2.70855900
H	2.24038800	2.92631100	-3.78737100
H	2.76720700	2.06436500	-2.32587100
H	2.31932100	3.77844100	-2.24251300
C	0.31141000	1.10689100	-3.21076300
H	0.47404700	1.24833700	-4.28661600
H	-0.72702800	0.79546500	-3.06395700
H	0.97473500	0.29601600	-2.87489000
H	-0.03251200	3.18001400	-2.87295100
C	0.54824500	3.35500400	-0.16155000
C	-0.26387200	4.61451900	-0.53980300
H	-0.03676400	5.44731100	0.13886100
H	-1.34023100	4.41296900	-0.48819300
H	-0.03848100	4.95154200	-1.55743900
C	0.28014800	2.98864900	1.30740300
H	0.48297100	3.84039200	1.96867100
H	0.92177100	2.15783600	1.62766200
H	-0.76321200	2.68914500	1.45657900
H	1.61441800	3.64258200	-0.21274300
O	-0.90656900	-0.75280900	2.08898200
C	-0.14307500	-0.77216200	3.30367600
H	0.89881100	-0.59082100	3.03266300
H	-0.22462300	-1.76821600	3.76699100
C	-0.77731000	0.30670800	4.20118000
H	-0.75177700	0.01528500	5.25572500
H	-0.23901700	1.25395800	4.10462300
C	-2.22548300	0.43999500	3.65024300
H	-2.40797900	1.45045600	3.27524300
H	-2.98517800	0.22253700	4.40700900
C	-2.27799400	-0.57071300	2.49168200
H	-2.68116400	-1.53914800	2.82620000
H	-2.83464900	-0.22239900	1.62143100
O	-0.14072600	-2.28879100	-0.91080600
C	-0.82843300	-3.27889200	-0.12756200
H	-1.00485900	-2.84241800	0.85632700
H	-0.19256800	-4.17328600	-0.02344000
C	-2.09040900	-3.58524100	-0.93538900
H	-2.51405500	-4.56592100	-0.69800900
H	-2.84729900	-2.82141600	-0.73374700
C	-1.59376800	-3.48106200	-2.39891600
H	-2.31483800	-2.95457700	-3.03000900
H	-1.42865200	-4.46930900	-2.83969900
C	-0.25750100	-2.70528000	-2.28438500
H	0.59755600	-3.34764400	-2.53939600
H	-0.21429400	-1.80552300	-2.90078900
O	2.26012600	-0.50090800	0.76663500
C	2.90931200	-1.74957500	0.48330900
H	2.13932100	-2.43927400	0.13261000
H	3.37189100	-2.15092900	1.39901200
C	3.96638300	-1.40373700	-0.56298400
H	4.76222800	-2.15209300	-0.63065000
H	3.49587500	-1.31138900	-1.54854200
C	4.46570400	-0.03317600	-0.06794100
H	4.82742600	0.60241000	-0.88143000

H	5.28851100	-0.16162900	0.64407200
C	3.22790200	0.57042900	0.63093300
H	3.47001800	0.96299400	1.62651900
H	2.74079900	1.35386700	0.04558200
C	-2.92297400	0.22142300	-1.36740700
C	-4.28034300	-0.12283000	-1.25381100
C	-5.14107700	0.63521600	-0.44428600
C	-4.58009200	1.73956300	0.22793400
C	-3.22935900	2.05484800	0.08061900
C	-2.32526100	1.31461600	-0.71447200
H	-2.87042200	2.93138600	0.62584700
H	-5.20638400	2.34184300	0.88319300
N	-6.51247800	0.30886300	-0.25733100
C	-7.47446500	1.38612900	-0.46808800
H	-7.63268100	1.61107800	-1.53921800
H	-8.43984600	1.10145200	-0.03358400
H	-7.14258500	2.30232800	0.02154800
C	-6.97579700	-0.94714200	-0.81614400
H	-6.32671900	-1.76573100	-0.49061800
H	-7.98726100	-1.14658000	-0.44514900
H	-7.01567800	-0.95734900	-1.92214900
H	-4.66428100	-0.96803100	-1.81919800
H	-2.32039000	-0.41062100	-2.02680100
H	-0.94465300	1.82957700	-0.91221300

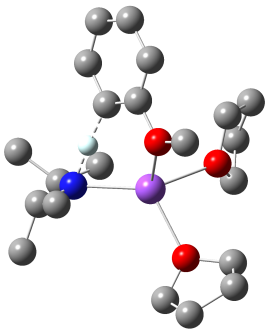
Table S-11. Geometric coordinates and thermally corrected MP2 energies for anisole.



G = –346.656107 Hartree
G_{MP2} = –345.5302965Hartree

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-12. Geometric coordinates and thermally corrected MP2 energies for $[A(THF)_2(anisole)]^{‡}$.

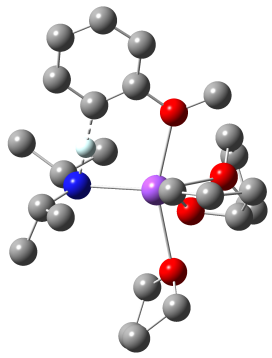


G = –1265.304445 Hartree
G_{MP2} = –1261.132571 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	0.22119900	1.24558300	0.73839300
Na	-0.89865300	3.22579900	0.16981100
O	-3.24074000	3.32202000	0.11767200
C	-3.99697000	4.50320500	-0.17682600
H	-3.28472100	5.30553600	-0.37898000
H	-4.60201600	4.77830200	0.70111700
C	-4.89173300	4.11188100	-1.36370100
H	-5.83781000	4.66119200	-1.35998400
H	-4.38614300	4.32840800	-2.31002100
C	-5.08274100	2.57924700	-1.18374200
H	-4.77864400	2.04001500	-2.08530200
H	-6.12248100	2.31157400	-0.97433100
C	-4.16600100	2.22948200	0.00863700
H	-4.74150300	2.14982300	0.94257500
H	-3.58157200	1.31687300	-0.12245300
O	-0.09100500	3.78548500	-1.95575400
C	1.31487700	3.76989400	-1.81373700
C	2.13649100	4.50789300	-2.67150200
C	3.51971900	4.48351200	-2.45666700
C	4.04591400	3.73939600	-1.40388800
C	3.17801300	3.01464300	-0.57475300
C	1.78620700	2.99591600	-0.74313900
H	3.61703300	2.42775600	0.23458100
H	5.12093800	3.71687800	-1.23530500
H	4.17307900	5.04856300	-3.11759600
H	1.73680100	5.09756500	-3.49158200
C	-0.64753800	4.37946500	-3.11374400
H	-0.23446300	3.93529700	-4.02848500
H	-1.72291400	4.18605100	-3.07412800
H	-0.47973000	5.46544500	-3.14015800
C	0.73290300	1.05949400	2.10037700
C	2.09186700	0.32919500	2.19593200
H	2.40387200	0.21469900	3.24247600
H	2.87448200	0.88560700	1.66611000
H	2.04406300	-0.67336100	1.75771700
C	0.83456400	2.42664900	2.79530800
H	1.21900400	2.32580700	3.81789200
H	-0.15356600	2.90304300	2.85871600
H	1.50629000	3.09625700	2.24455100
H	0.01894700	0.46259500	2.69616800
C	-0.99465700	-0.96218100	0.67966900
H	-1.16960000	-1.84778300	0.05479600
H	-1.95857000	-0.45970900	0.84250100
H	-0.63711200	-1.31494700	1.65292700
C	-0.49427000	0.32066100	-1.41892100
H	-0.58845800	-0.59560500	-2.01515500
H	0.19158700	0.99786000	-1.93505500
H	-1.48481300	0.79933200	-1.38846200
H	0.94367100	-0.56782300	-0.12853300
O	-0.84684800	5.44812100	1.01811800
C	-1.27264400	5.82136000	2.34096100
H	-1.63856600	4.92058300	2.84241900
H	-2.09852900	6.54594400	2.27436900
C	-0.04169300	6.44293000	2.99612600
H	-0.29274700	7.09387600	3.83911400
H	0.62897600	5.65418500	3.35433000

C	0.58819100	7.19518200	1.81244700
H	1.66146700	7.36604100	1.93449000
H	0.10500100	8.17078600	1.68337900
C	0.28278700	6.27408500	0.62035400
H	0.01047500	6.82813100	-0.28463500
H	1.11392900	5.60468300	0.38080800
H	1.02016500	2.05939100	0.03679700

Table S-13. Geometric coordinates and thermally corrected MP2 energies for $[A(THF)_3(anisole)]^{‡}$.

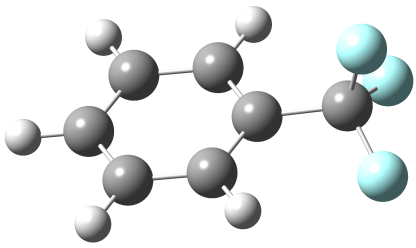


G = –1497.649036 Hartree
G_{MP2} = –1492.712932 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	-0.62823200	2.32616000	-0.27544100
C	-0.70079000	2.95874100	-1.59887300
C	0.48586400	3.87953900	-1.93811000
H	0.38072500	4.28712900	-2.95214700
H	1.43222900	3.32527600	-1.89203800
H	0.56283600	4.72929500	-1.25117500
C	-0.82996600	1.86102900	-2.66490700
H	-0.97111500	2.29237200	-3.66427900
H	-1.68832100	1.21802500	-2.44557500
H	0.07578200	1.23779400	-2.69042500
H	-1.61055400	3.58474200	-1.69302600
C	-0.50382900	3.27046700	0.84469600
C	-1.64028100	4.31313700	0.95027100
H	-1.47800200	4.98163800	1.80606600
H	-2.60915500	3.81797300	1.07994900
H	-1.70083200	4.93993800	0.05370200
C	-0.42138200	2.47295400	2.15500700
H	-0.31599300	3.13874500	3.02098800
H	0.44170700	1.79449400	2.14498800
H	-1.32960300	1.87435500	2.29440600
H	0.44033300	3.84068700	0.76134500
O	0.85311000	-1.14344900	2.04187200
C	2.20325900	-1.55534500	2.29043500
H	2.77345000	-1.34059400	1.38600600
H	2.22378500	-2.63905400	2.48958400
C	2.64644300	-0.76250400	3.53307000
H	3.34361700	-1.33550100	4.15192300
H	3.14953900	0.16352300	3.23829400
C	1.31055700	-0.44890500	4.26381400
H	1.17284700	0.62986900	4.37580600
H	1.26453000	-0.89504600	5.26179700
C	0.23420400	-1.04288700	3.33389600
H	-0.06554900	-2.04732200	3.67053100
H	-0.65892000	-0.42739000	3.22075300
O	0.02468700	-1.79655600	-1.65442600
C	0.56922500	-3.09259100	-1.33301600
H	0.73427200	-3.13860100	-0.25170400
H	1.54023100	-3.20285600	-1.83600100
C	-0.44363900	-4.12171300	-1.84464600
H	0.02705300	-5.07110800	-2.11762500
H	-1.20226400	-4.32578800	-1.08048800
C	-1.07273900	-3.38477800	-3.03723600
H	-2.06216200	-3.76481100	-3.30794200
H	-0.42532300	-3.46234300	-3.91893700
C	-1.12109000	-1.94257300	-2.52942300
H	-1.03794500	-1.19439000	-3.32210600
H	-2.03063400	-1.74024100	-1.95186100
O	2.47502500	0.11930400	-0.53772300
C	3.04460500	-0.29065300	-1.79339900
H	2.25704300	-0.79688100	-2.35586500
H	3.86904100	-0.99851600	-1.61274000
C	3.55652900	0.99298700	-2.44392200
H	4.33723900	0.80793600	-3.18840900
H	2.73117600	1.52116900	-2.93321700
C	4.05786300	1.78427500	-1.22417900
H	4.06058200	2.86581300	-1.38821800

H	5.07977700	1.48090900	-0.96820800
C	3.07347700	1.37032300	-0.11681200
H	3.57133800	1.21805800	0.84865900
H	2.25820400	2.08858700	0.01174800
O	-2.08047000	-1.02628400	0.77413800
C	-3.25760400	-0.30855800	0.45324300
C	-4.52108300	-0.89340600	0.59207600
C	-5.64916700	-0.13725500	0.24917700
C	-5.49572900	1.16529000	-0.21650600
C	-4.20543400	1.70354100	-0.33325100
C	-3.03980100	0.99524700	-0.00622700
H	-4.11185400	2.72953900	-0.69605100
H	-6.37024300	1.75608400	-0.48393500
H	-6.63854800	-0.57755400	0.35258200
H	-4.65808200	-1.90697500	0.95771500
C	-2.22134900	-2.35119900	1.24824900
H	-2.71968100	-2.99758600	0.51138200
H	-1.21029000	-2.71975100	1.43254800
H	-2.79614900	-2.38893800	2.18416300
H	-1.75084000	1.69377200	-0.12854800

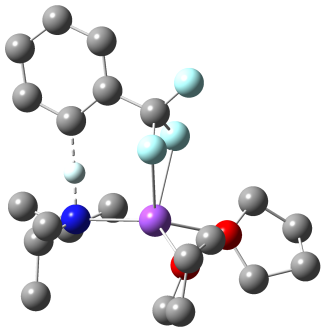
Table S-14. Geometric coordinates and thermally corrected MP2 energies for benzotrifluoride.



G = –569.208662 Hartree
G_{MP2} = –567.6372619 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
C	-1.50426100	0.00038700	-0.03310000
C	-2.20040600	1.21208400	-0.02091300
C	-3.59453900	1.20884800	0.00408400
C	-4.29185900	-0.00074400	0.01754000
C	-3.59353900	-1.20988900	0.00410600
C	-2.19952800	-1.21198800	-0.02098000
H	-1.65143000	-2.14836500	-0.03876200
H	-4.13387700	-2.15226700	0.00980200
H	-5.37829600	-0.00119900	0.03568900
H	-4.13556200	2.15083300	0.00974500
H	-1.65302100	2.14881900	-0.03854100
F	0.51822500	-1.08409000	-0.62017400
F	0.51893000	1.09607700	-0.59788500
F	0.47288700	-0.01343300	1.26904000

Table S-15. Geometric coordinates and thermally corrected MP2 energies for ortho [A(THF)$_2$(benzotrifluoride)]‡.

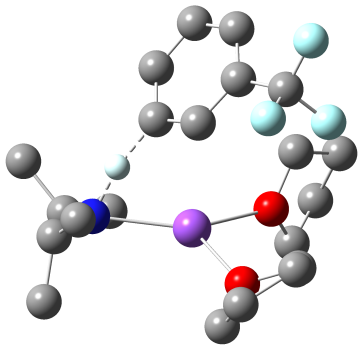


G = –1487.85847 Hartree
G_{MP2} = –1483.23883 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	-1.73284100	0.87952800	1.30232000
C	-1.92710400	2.33536500	1.28821700
C	-0.96138900	3.10414200	2.20993300
H	-1.10395100	4.18820800	2.10914700
H	0.08175200	2.86988500	1.95189600
H	-1.10431400	2.85253800	3.26607900
C	-1.78843700	2.85019700	-0.15324700
H	-2.00810700	3.92377000	-0.20886700
H	-2.47118200	2.32229200	-0.82509700
H	-0.76437800	2.70108700	-0.52585700
H	-2.95077000	2.60715500	1.61282400
C	-1.93824000	0.25213900	2.61961100
C	-3.36765600	0.39314400	3.18992100
H	-3.43358800	-0.05642300	4.18933100
H	-4.09647700	-0.10702200	2.54261700
H	-3.66622500	1.44317200	3.28468700
C	-1.56935000	-1.23763800	2.53136100
H	-1.74312900	-1.74580100	3.48816200
H	-0.50917200	-1.36841800	2.27649000
H	-2.17179100	-1.74011200	1.76568200
H	-1.25675900	0.70179400	3.36294100
O	1.52173500	-1.72019000	0.47247600
C	2.90693500	-1.48235200	0.79162800
H	2.99863900	-1.24999300	1.86271400
H	3.23420300	-0.61481800	0.21270900
C	3.63253200	-2.78198700	0.44565000
H	3.85695000	-2.81998700	-0.62709000
H	4.57048400	-2.90105400	0.99618700
C	2.57202200	-3.83213300	0.81248300
H	2.57832600	-4.01546500	1.89321500
H	2.71776800	-4.79118100	0.30696500
C	1.26815300	-3.14483600	0.39046200
H	0.99306900	-3.38293700	-0.64317600
H	0.42064900	-3.38468000	1.03904900
O	1.75085400	1.21850300	-1.06984200
C	1.95143700	1.05144500	-2.48956900
H	1.10072900	0.48833500	-2.87862600
H	2.87288200	0.47653900	-2.66570100
C	2.07044300	2.47047900	-3.03757200
H	2.57630500	2.50923700	-4.00686300
H	1.07482200	2.91425600	-3.14919100
C	2.85695600	3.16821100	-1.91524300
H	2.70389100	4.25080800	-1.89116400
H	3.93082300	2.98388700	-2.03408300
C	2.32637200	2.47986900	-0.64574400
H	3.11470700	2.28133200	0.08947000
H	1.53525700	3.05965900	-0.15964800
C	-1.94326700	-1.22143500	-1.98314600
C	-3.36045800	-0.89928000	-1.65297400
C	-4.36546700	-1.34843500	-2.52336800
C	-5.69309500	-1.04306300	-2.23532500
C	-5.98747600	-0.29641200	-1.09112400
C	-4.95848400	0.13220500	-0.24694000
C	-3.60046400	-0.14952100	-0.48185900
H	-5.23156900	0.71415000	0.63511300
H	-7.02349200	-0.05024600	-0.86182700

H -6.48687700 -1.38235600 -2.89597100
H -4.11773500 -1.92621700 -3.40978200
F -1.15939700 -0.08650600 -2.16007700
F -1.75807500 -1.96227600 -3.09045800
F -1.28834300 -1.88908200 -0.96633600
H -2.59864100 0.36972000 0.46477500

Table S-16. Geometric coordinates and thermally corrected MP2 energies for meta [A(THF)$_2$(benzotrifluoride)]‡.

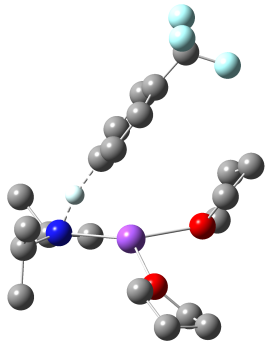


G = –1487.849176 Hartree
G_{MP2} = –1483.233186 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	0.53833500	-1.25360700	0.53323600
Na	2.41666100	-1.35135000	1.93539900
O	3.65376800	-2.94156400	3.09053000
C	3.34327100	-3.49963200	4.38232100
H	2.26750000	-3.38821000	4.55312800
H	3.88103500	-2.93828300	5.15985000
C	3.80959400	-4.95377300	4.32234000
H	4.02239700	-5.36822200	5.31225900
H	3.04501800	-5.57814100	3.84561200
C	5.05227800	-4.84310500	3.42508700
H	5.32262900	-5.78728600	2.94364900
H	5.91489000	-4.50380200	4.01072300
C	4.63328100	-3.77552700	2.40944800
H	5.45673600	-3.13883400	2.07678300
H	4.15347000	-4.20773100	1.52526700
O	3.47553500	0.46579400	2.92099100
C	4.89795700	0.48699000	3.15047100
H	5.32230200	-0.40314900	2.68525600
H	5.08418100	0.44937900	4.23350400
C	5.40412000	1.80906700	2.53429600
H	6.13104000	2.29442800	3.19224700
H	5.89241000	1.62595700	1.57458700
C	4.11570300	2.65869600	2.35591300
H	3.87094500	2.76779200	1.29503000
H	4.20344100	3.66146800	2.78420900
C	3.03769000	1.82642300	3.06260400
H	2.97195100	2.07751600	4.13236300
H	2.04282300	1.90348800	2.61882400
C	-0.47156000	-2.31307600	0.65106900
C	-0.86757500	-2.95256100	-0.69948000
H	-1.69333600	-3.66619200	-0.57793700
H	-0.01855300	-3.48772400	-1.14131400
H	-1.19127000	-2.19356500	-1.41989300
C	0.02017000	-3.40357000	1.61669400
H	-0.70671300	-4.22064400	1.70715300
H	0.18127200	-2.98858200	2.62165400
H	0.96450400	-3.83961800	1.26491100
H	-1.39680600	-1.90051900	1.08967100
C	-0.81120500	0.79218600	1.04544100
H	-1.24985600	1.70053700	0.61052300
H	-0.16323100	1.09005700	1.88182100
H	-1.63100100	0.19564500	1.46059900
C	1.13463200	0.87772700	-0.54890900
H	0.74327200	1.82454800	-0.94022600
H	1.67946100	0.37065200	-1.35059600
H	1.85691300	1.12247200	0.24384600
H	-0.68345800	-0.18991000	-0.85060000
C	4.05065000	-1.40942200	-0.44310500
C	5.32550900	-1.87166100	-0.81131600
C	5.46688500	-3.11805000	-1.42367800
C	4.32320800	-3.88903000	-1.64629900
C	3.07132900	-3.42516800	-1.22914200
C	2.87999500	-2.16824200	-0.61781100
H	2.20886200	-4.07300200	-1.39848600
H	4.41862500	-4.85506600	-2.13919300
H	6.44734700	-3.47418300	-1.72409400

C 6.53327500 -1.06783500 -0.44594500
F 6.33545200 0.26861000 -0.58474900
F 6.87619300 -1.24878300 0.87278400
F 7.63028500 -1.38552400 -1.16372400
H 3.98937500 -0.40563800 -0.01420400
H 1.58150600 -1.69258000 -0.14351100

Table S-17. Geometric coordinates and thermally corrected MP2 energies for para [A(THF)$_2$(benzotrifluoride)]‡.

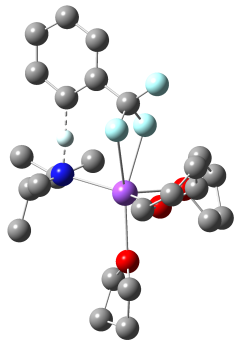


G = –1487.846339 Hartree
G_{MP2} = –1483.229946 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
N	0.88930300	0.35391800	1.10793700
Na	1.59641500	2.55622400	1.50479100
O	2.87430000	3.92784900	2.92867400
C	3.27066800	3.61143300	4.27788300
H	2.71351400	2.72222400	4.58486200
H	3.00505900	4.44455800	4.94611500
C	4.78147000	3.41336800	4.20218300
H	5.27148200	3.51495400	5.17523600
H	5.00572400	2.42133900	3.79745100
C	5.19549000	4.50606000	3.19996600
H	6.10279500	4.25191200	2.64722400
H	5.36522500	5.45639600	3.71840600
C	3.97559200	4.60843100	2.26426500
H	3.68247800	5.64719800	2.07047000
H	4.14391700	4.10265300	1.30938600
O	0.47976700	4.42099700	0.68769900
C	0.08550400	5.49683300	1.56506800
H	0.84483300	5.57569300	2.34713900
H	-0.88099500	5.25265000	2.02972600
C	-0.03182100	6.72377400	0.66338300
H	-0.68064900	7.49711500	1.08501600
H	0.95698600	7.16351100	0.48697100
C	-0.58793500	6.10278900	-0.62843400
H	-0.39027700	6.70579300	-1.51924800
H	-1.67243400	5.96737200	-0.54712200
C	0.12235100	4.74273600	-0.67847100
H	-0.50904600	3.94193600	-1.07578400
H	1.04584200	4.78481400	-1.26881700
C	0.76029200	-0.55604000	2.25207900
C	1.49441400	-1.90155000	2.05694300
H	1.30404700	-2.58990500	2.89127300
H	2.57727600	-1.74551300	1.98255400
H	1.16811000	-2.39848400	1.13682500
C	1.25536400	0.12685800	3.53763600
H	1.17858500	-0.53923200	4.40620100
H	0.66092600	1.02604000	3.75278000
H	2.31025300	0.41909800	3.44315000
H	-0.30508500	-0.79366400	2.41845600
C	-1.44557300	0.48771100	0.23049000
H	-2.11914900	0.15365000	-0.57083300
H	-1.47064800	1.58591600	0.26693600
H	-1.84862800	0.11558700	1.17920900
C	0.53157300	0.56525500	-1.32493400
H	-0.14301800	0.32090400	-2.15438100
H	1.52421200	0.16857700	-1.55780800
H	0.60988100	1.66141900	-1.27765400
H	-0.05247800	-1.09847200	-0.13034000
C	3.88122100	1.82003500	-0.56652900
C	5.18578100	2.28799200	-0.76393900
C	6.19268100	1.91303000	0.12999600
C	5.88514500	1.05792600	1.19529900
C	4.57100900	0.61892900	1.36883400
C	3.51363000	0.98491300	0.50937800
H	4.37015200	-0.04487800	2.21257900
H	6.67325600	0.74394100	1.87580900
C	7.57041900	2.48602800	0.00600800

F 7.71666400 3.61945700 0.75920600
F 7.87668600 2.83909800 -1.26258800
F 8.52893900 1.63179700 0.43083900
H 5.42635000 2.93336300 -1.60528000
H 3.12658800 2.11805500 -1.29877500
H 2.15322700 0.51702600 0.75550500

Table S-18. Geometric coordinates and thermally corrected MP2 energies for ortho [A(THF)$_3$(benzotrifluoride)]‡.

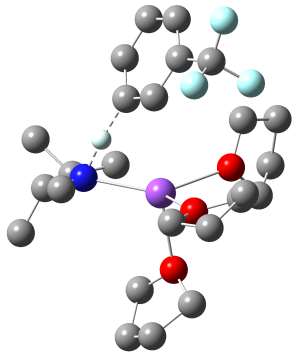


G = –1720.205921 Hartree
G_{MP2} = –1714.818508 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	1.31298700	-1.98633500	-0.33263100
C	1.35919400	-2.52257800	-1.70073600
C	0.11653400	-3.33480900	-2.10959800
H	0.19422400	-3.66211700	-3.15466800
H	-0.78665500	-2.71644500	-2.01251500
H	-0.01939400	-4.23138100	-1.49520900
C	1.55390800	-1.36430500	-2.68966800
H	1.71944100	-1.74020800	-3.70744800
H	2.40826500	-0.74519300	-2.40569000
H	0.65888100	-0.72386400	-2.71671100
H	2.23193500	-3.19195900	-1.83588000
C	1.10925200	-3.00764300	0.70828500
C	2.15122500	-4.14952400	0.73779200
H	1.89021300	-4.88935000	1.50598400
H	3.14952900	-3.76199200	0.96696800
H	2.20720000	-4.67870200	-0.21970000
C	1.07638900	-2.32165000	2.08345800
H	0.95224700	-3.05683500	2.88880000
H	0.24534800	-1.60848000	2.15472800
H	2.01094200	-1.77663400	2.25934200
H	0.12545200	-3.49669900	0.57340200
O	-0.79578900	0.89681600	2.12247400
C	-2.16212300	1.22639200	2.39947500
H	-2.76823800	0.75890700	1.62219500
H	-2.29103600	2.31906100	2.34675800
C	-2.42944300	0.71036000	3.82739100
H	-3.09354100	1.38345900	4.37806700
H	-2.90457400	-0.27502500	3.80423500
C	-1.01095400	0.62192100	4.45821000
H	-0.76499900	-0.41339000	4.71093100
H	-0.91672700	1.21849800	5.37035300
C	-0.08198200	1.13687000	3.34469500
H	0.10658500	2.21645600	3.44848000
H	0.87389200	0.61750300	3.27652000
O	-0.64208800	2.05125600	-1.14700200
C	-0.49152600	3.26254000	-0.37360300
H	-0.03645200	2.99241000	0.58162000
H	-1.48604900	3.69301800	-0.18374600
C	0.36409900	4.19393600	-1.22997400
H	0.21408700	5.24888700	-0.98073400
H	1.42254500	3.95125200	-1.10064600
C	-0.10693500	3.83174300	-2.64700600
H	0.62324700	4.08129800	-3.42231400
H	-1.04290400	4.35203200	-2.88337200
C	-0.34073600	2.31945000	-2.53799700
H	-1.17978700	1.96950300	-3.14965700
H	0.55379600	1.75053100	-2.81034800
F	2.39945900	1.48376900	-1.08900000
C	2.99298000	1.46422100	0.14600600
C	4.12722100	0.49778000	0.23653200
C	5.41705500	1.00422000	0.45690800
C	6.49289200	0.12076700	0.49458800
C	6.25875600	-1.24355500	0.30440900
C	4.95794500	-1.71025200	0.09029200
C	3.83070900	-0.86909700	0.05086500
H	4.82349800	-2.78336000	-0.05691400

H	7.09551700	-1.94093700	0.32337600
H	7.49992700	0.49303200	0.66574300
H	5.58096600	2.06967700	0.59440600
F	3.31505600	2.75172100	0.41718800
F	1.95322500	1.16151300	1.00801500
H	2.48029800	-1.44211800	-0.13817900
O	-2.30573300	-0.73594400	-0.35553500
C	-3.08972800	-0.28464700	-1.47882800
H	-2.55499400	-0.52009700	-2.41001500
H	-3.19103500	0.80089000	-1.40174800
C	-4.40900100	-1.05224200	-1.39353700
H	-5.09795700	-0.55555500	-0.69950800
H	-4.90755900	-1.14103600	-2.36344000
C	-3.94509000	-2.40083400	-0.82051700
H	-3.52592300	-3.02760300	-1.61595100
H	-4.74493200	-2.96452600	-0.33117100
C	-2.84552700	-1.97551600	0.15908700
H	-3.25065300	-1.78447100	1.16225000
H	-2.03102900	-2.69990100	0.24232800

Table S-19. Geometric coordinates and thermally corrected MP2 energies for meta [A(THF)$_3$(benzotrifluoride)]‡.

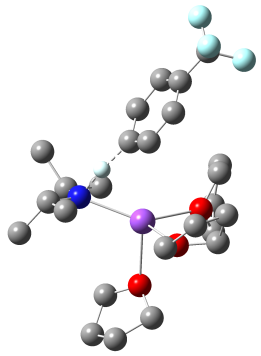


G = –1720.199407 Hartree
G_{MP2} = –1714.815785 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	0.82927000	1.88074100	-1.23603600
C	1.17150800	1.80600200	-2.66015200
C	2.67450400	1.61705800	-2.93931500
H	2.86258500	1.53675000	-4.01779800
H	3.03786800	0.69661800	-2.46135400
H	3.27670600	2.45117600	-2.56351600
C	0.38899700	0.65533900	-3.30800600
H	0.56295300	0.62031800	-4.39080000
H	-0.68691000	0.76706100	-3.14125300
H	0.70959600	-0.30914400	-2.88824300
H	0.86615900	2.72686500	-3.19546400
C	1.49449300	2.97046500	-0.50813900
C	1.24035100	4.38625700	-1.07401800
H	1.75705400	5.14618100	-0.47348800
H	0.16929000	4.62139100	-1.07388800
H	1.59990800	4.48421900	-2.10393600
C	1.07744100	2.92790800	0.97137100
H	1.57974000	3.71710300	1.54443900
H	1.34240600	1.96625300	1.43038300
H	-0.00398500	3.06985900	1.07890100
H	2.59101700	2.82435100	-0.52421800
O	-1.09551500	-0.17189600	2.09552600
C	-0.40885500	-0.60083100	3.28306100
H	0.65371700	-0.66828500	3.03816100
H	-0.76767900	-1.59835600	3.58316400
C	-0.76386400	0.44472100	4.33686500
H	-0.61134600	0.08793600	5.36024600
H	-0.15709600	1.34588300	4.19055700
C	-2.23985600	0.72195900	4.00293100
H	-2.57567600	1.70991600	4.33087600
H	-2.88194100	-0.02493000	4.48405200
C	-2.28696100	0.57390700	2.47114500
H	-3.16998300	0.03044700	2.12134700
H	-2.24833700	1.53306300	1.94901900
O	-0.87357000	-2.14747500	-0.74471800
C	-1.84938900	-2.83292700	0.08259300
H	-2.45227500	-2.08208400	0.59466800
H	-1.30867300	-3.42706600	0.83228400
C	-2.65806700	-3.71814600	-0.86735000
H	-3.05556300	-4.60745300	-0.36891200
H	-3.49708000	-3.15231600	-1.28244900
C	-1.63007900	-4.04225600	-1.96143100
H	-2.08517200	-4.33927100	-2.91090200
H	-0.96092300	-4.84869500	-1.63705000
C	-0.86587500	-2.72197600	-2.07231200
H	0.17615000	-2.84090100	-2.38617500
H	-1.36073100	-2.02782000	-2.76263300
O	1.99664000	-1.07192400	0.84553600
C	2.23802800	-2.47531700	0.66560400
H	1.29974600	-2.92054500	0.32795000
H	2.53517500	-2.93356100	1.62226600
C	3.37337300	-2.53977200	-0.35340600
H	3.90258100	-3.49767400	-0.34455500
H	2.97702700	-2.37444200	-1.36179600
C	4.25844400	-1.35610500	0.08287700
H	4.80978400	-0.91368900	-0.75162400

H	4.99086800	-1.68218700	0.82938900
C	3.25227000	-0.36185300	0.70445500
H	3.57923000	-0.01130300	1.69136900
H	3.05308000	0.50299200	0.06767100
C	-2.77284500	0.95961100	-1.09734700
C	-4.14891300	1.00197500	-0.81531600
C	-4.73752300	2.18587800	-0.36651300
C	-3.92988300	3.31289900	-0.20188900
C	-2.55740900	3.23510300	-0.46061100
C	-1.91956800	2.06270100	-0.91886200
H	-1.96227100	4.13647000	-0.29803600
H	-4.37797700	4.24721100	0.13252900
H	-5.80207800	2.22568300	-0.15814500
C	-4.95929500	-0.25099300	-0.91098600
F	-4.62281900	-1.01111300	-1.98851700
F	-4.76949200	-1.06574200	0.17757100
F	-6.28915400	-0.03033900	-0.98438800
H	-2.37172500	0.01453800	-1.46975500
H	-0.46230100	2.02839900	-1.13904500

Table S-20. Geometric coordinates and thermally corrected MP2 energies for para [A(THF)$_3$(benzotrifluoride)]‡.

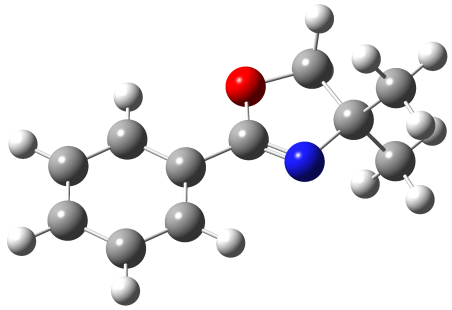


G = –1720.196051 Hartree
G_{MP2} = –1714.810885 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	0.24197200	2.19081600	-0.96051900
C	0.59175200	2.43135500	-2.36413600
C	2.06282200	2.82777100	-2.59561100
H	2.26494900	2.95687100	-3.66670800
H	2.73398700	2.04503400	-2.21583000
H	2.32716800	3.76746400	-2.09948600
C	0.28171600	1.17404900	-3.18821900
H	0.47649400	1.34202900	-4.25466600
H	-0.76682900	0.88116300	-3.08034800
H	0.91708400	0.33803300	-2.85969600
H	-0.02289000	3.24447400	-2.79948300
C	0.50414800	3.33158000	-0.07209600
C	-0.25891200	4.62620600	-0.43342000
H	-0.01789300	5.43378300	0.27021600
H	-1.34256000	4.46108300	-0.40689100
H	-0.00314500	4.98075200	-1.43771200
C	0.19314300	2.93742100	1.38093700
H	0.40765800	3.76569600	2.06755600
H	0.80219600	2.07949300	1.69425700
H	-0.86194600	2.66717100	1.50228100
H	1.57938500	3.58755700	-0.09227800
O	-0.92402700	-0.73953100	2.07566400
C	-0.12372100	-0.90629600	3.25571000
H	0.91864100	-0.77184400	2.96087900
H	-0.25872500	-1.92774600	3.64571100
C	-0.65757900	0.13931900	4.24638000
H	-0.54892900	-0.19064000	5.28397600
H	-0.11060200	1.08010800	4.13491500
C	-2.14199400	0.31905100	3.82246200
H	-2.36481400	1.36957700	3.61750500
H	-2.83895200	-0.02274600	4.59335000
C	-2.27214100	-0.52904400	2.54058300
H	-2.73005200	-1.50573600	2.75632600
H	-2.82361700	-0.04138200	1.73651000
O	-0.23934700	-2.23512800	-0.96408700
C	-0.91807100	-3.24200200	-0.19301700
H	-1.11553200	-2.81366200	0.79047000
H	-0.26596200	-4.12362100	-0.08400100
C	-2.16366300	-3.56967700	-1.01737500
H	-2.56878500	-4.56045300	-0.79099800
H	-2.94075400	-2.82597500	-0.81799300
C	-1.65402400	-3.44518200	-2.47488800
H	-2.37811700	-2.92732900	-3.10966200
H	-1.46736300	-4.42673200	-2.92152200
C	-0.33288500	-2.64728500	-2.34156100
H	0.53616200	-3.27340100	-2.58893500
H	-0.29717400	-1.74404000	-2.95332100
O	2.23999800	-0.55613900	0.74841900
C	2.87808400	-1.78521000	0.36177400
H	2.10856600	-2.41936800	-0.08315900
H	3.29554300	-2.28691100	1.24883000
C	3.98275500	-1.36018900	-0.60252400
H	4.76623300	-2.11608100	-0.71454100
H	3.55649100	-1.15622900	-1.59156700
C	4.48492000	-0.06017600	0.05107100
H	4.92338800	0.63577200	-0.66988600

H 5.24832000 -0.28464700 0.80437800
C 3.21745200 0.51615000 0.71421900
H 3.40623500 0.86036300 1.73828700
H 2.76848800 1.33144300 0.14133900
C -2.98484800 0.30332400 -1.43281800
C -4.33547800 -0.04682400 -1.33798600
C -5.18798000 0.71004600 -0.52927700
C -4.67533000 1.81271500 0.16273000
C -3.31977600 2.13050300 0.04751300
C -2.41289900 1.39247800 -0.74248500
H -2.96422900 3.00386100 0.59767200
H -5.33901400 2.41620400 0.77704300
C -6.61919900 0.30305000 -0.35566000
F -7.42376200 1.35215100 -0.06468300
F -6.77656100 -0.59058600 0.65986900
F -7.12345500 -0.29370300 -1.46273900
H -4.73431500 -0.89101500 -1.89603900
H -2.36079100 -0.30802700 -2.08888600
H -1.03418200 1.86432800 -0.89079100

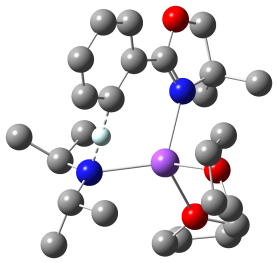
Table S-21. Geometric coordinates and thermally corrected MP2 energies for 4,4-dimethyl-2-phenyl-2-oxazoline.



G = –556.791586 Hartree
G_{MP2} = –554.9931048 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
C	-0.27684100	-1.53807700	0.00215100
N	1.07622900	-2.12991900	0.00175400
C	1.91870600	-1.17019800	0.00215400
C	3.38494600	-1.30775500	0.00216700
C	4.21631500	-0.17923100	0.00217500
C	5.60226000	-0.33440000	0.00224000
C	6.16554500	-1.61155800	0.00226100
C	5.33804000	-2.73883600	0.00223800
C	3.95445300	-2.59028200	0.00220900
H	3.29586200	-3.45250500	0.00222600
H	5.77379400	-3.73428800	0.00226400
H	7.24594700	-1.72975500	0.00230100
H	6.24252800	0.54360000	0.00226100
H	3.77235100	0.81025500	0.00214100
O	1.43926100	0.11310400	0.00259500
C	-1.02453600	-1.98577900	1.26669400
H	-2.03302800	-1.55493800	1.29749800
H	-1.11339600	-3.07649900	1.28888500
H	-0.48643000	-1.67075600	2.16732700
C	-1.02724600	-1.98895000	-1.25958000
H	-1.11702400	-3.07966100	-1.27835400
H	-2.03547000	-1.55744100	-1.28978000
H	-0.49060400	-1.67706300	-2.16216800
H	-0.38005600	0.50715500	-0.89310000
H	-0.38351200	0.51049800	0.88966200

Table S-22. Geometric coordinates and thermally corrected MP2 energies for N-bound [A(THF)$_2$(4,4-dimethyl-2-phenyl-2-oxazoline)]‡.

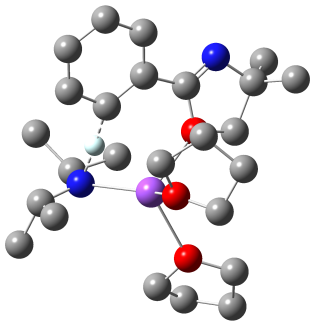


G = –1475.435071 Hartree
G_{MP2} = –1470.593339 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	0.48495200	1.67805300	-1.61754100
C	0.61172600	3.05883700	-1.13748500
C	-0.54556200	3.99134500	-1.54877400
H	-0.42002200	4.98384600	-1.09660000
H	-1.50690700	3.58223200	-1.20986800
H	-0.60363500	4.13303800	-2.63272700
C	0.71793900	3.05173300	0.39559700
H	0.92666900	4.05719600	0.78287400
H	1.51818000	2.38626400	0.73529600
H	-0.22876400	2.71379600	0.84247700
H	1.53880600	3.53922100	-1.51270100
C	0.33713800	1.56162800	-3.07419200
C	1.54515100	2.08594500	-3.88438700
H	1.37378200	1.97701400	-4.96351600
H	2.45512000	1.53329900	-3.62313100
H	1.73374000	3.14764400	-3.68930600
C	0.06161000	0.09842000	-3.44872400
H	-0.08444100	-0.01000700	-4.53099500
H	-0.84183100	-0.26847200	-2.94515100
H	0.89460500	-0.54757600	-3.15157300
H	-0.54381300	2.13574700	-3.41474100
O	-2.35749000	-0.09165100	0.20114500
C	-3.10987400	0.73728400	-0.70006000
H	-2.39158400	1.21820900	-1.36665200
H	-3.64682400	1.51023300	-0.12773200
C	-4.08488100	-0.23208500	-1.37429700
H	-4.98292300	0.27023000	-1.74570300
H	-3.59598100	-0.71976700	-2.22369800
C	-4.38968700	-1.26090700	-0.25360400
H	-4.33852800	-2.28694700	-0.62925800
H	-5.38857800	-1.11686900	0.16949400
C	-3.29839200	-0.98508400	0.81156100
H	-3.72866900	-0.50917000	1.70467100
H	-2.74797400	-1.87564700	1.12544300
O	0.42179200	-0.16508900	2.33349200
C	-0.10680600	0.65462200	3.38363800
H	-0.55047600	0.01086700	4.15861000
H	-0.89528600	1.27469900	2.95035000
C	1.09203100	1.44997100	3.94151200
H	1.11839800	2.45977100	3.52337500
H	1.03383500	1.54177100	5.03039000
C	2.32820400	0.62950800	3.47818700
H	2.98077300	0.34329300	4.30841200
H	2.92672600	1.19988600	2.76268000
C	1.71468300	-0.59883000	2.78774200
H	2.27121500	-0.94311800	1.91512100
H	1.58764600	-1.43483900	3.49286700
N	0.99920700	-2.07148800	-0.66358600
C	0.45792000	-3.44124200	-0.79742600
C	1.64940400	-4.22317500	-1.41794700
O	2.76349100	-3.31836300	-1.31918700
C	2.25722900	-2.10373300	-0.94291100
C	3.23058800	-0.99799800	-0.86112500
C	4.59325600	-1.35565200	-0.77789800
C	5.56650700	-0.37326500	-0.63420600
C	5.17917100	0.96860000	-0.59143700

C	3.82734400	1.30377600	-0.70181600
C	2.79592800	0.35350100	-0.83540300
H	3.56332400	2.36196900	-0.70128100
H	5.93260500	1.74761500	-0.48432700
H	6.61517700	-0.65076000	-0.56098300
H	4.88177800	-2.40184600	-0.81615300
H	1.90330000	-5.14214400	-0.88107400
H	1.49428600	-4.46052500	-2.47711600
C	-0.77472500	-3.44726600	-1.70995500
H	-1.16505600	-4.46520800	-1.83367800
H	-1.56917800	-2.82556100	-1.28254200
H	-0.52839000	-3.04622400	-2.69814000
C	0.10033400	-3.97412800	0.60089300
H	-0.63883900	-3.32366000	1.08118300
H	-0.31672700	-4.98712500	0.54023700
H	0.98806200	-4.00471000	1.24237200
H	1.58116600	0.98422000	-1.23878600

Table S-23. Geometric coordinates and thermally corrected MP2 energies for O-bound [A(THF)$_2$(4,4-dimethyl-2-phenyl-2-oxazoline)]‡.

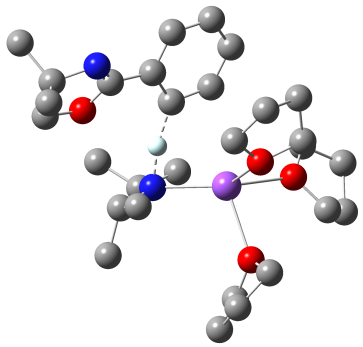


G = –1475.428268 Hartree
G_{MP2} = –1470.582911 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	-0.75341800	1.92260400	-1.15417500
C	-1.29609700	2.99501800	-0.30955000
C	-2.81192400	3.23182200	-0.46712000
H	-3.15633200	3.99795400	0.23942200
H	-3.37061000	2.30815200	-0.26394100
H	-3.07981800	3.57193100	-1.47250700
C	-0.99910200	2.67961600	1.16569700
H	-1.31114900	3.50474200	1.81798300
H	0.06991400	2.51217000	1.33375200
H	-1.54618200	1.78111000	1.48784500
H	-0.81129900	3.96915500	-0.52546900
C	-1.04122600	2.08338700	-2.58528600
C	-0.42126100	3.34874500	-3.22110700
H	-0.67074400	3.41824100	-4.28811500
H	0.67065500	3.33440400	-3.12385000
H	-0.78599200	4.26323400	-2.73996700
C	-0.57114100	0.83980700	-3.35341000
H	-0.82880300	0.91489700	-4.41732200
H	-1.04432100	-0.06569500	-2.95125200
H	0.51446000	0.71770200	-3.27662700
H	-2.13189400	2.14929800	-2.74746300
O	-1.74404700	-1.60247300	0.03509800
C	-3.01055000	-1.01583500	-0.33762500
H	-2.79360900	-0.02528500	-0.74477700
H	-3.64512200	-0.91144500	0.55535700
C	-3.61024300	-2.00581000	-1.33082800
H	-4.69327600	-1.89541900	-1.43897500
H	-3.15057800	-1.87195900	-2.31688100
C	-3.20100800	-3.35389800	-0.71171900
H	-3.12993200	-4.16137100	-1.44628500
H	-3.92925200	-3.65875900	0.04801500
C	-1.84021000	-3.03843500	-0.05725900
H	-1.75061000	-3.47582300	0.94503300
H	-0.99695200	-3.39003500	-0.66299400
O	0.95733500	-0.47240100	2.09945400
C	1.06329800	-1.75865300	2.71883600
H	0.45502800	-2.45755100	2.13909600
H	0.65818400	-1.70628700	3.74108800
C	2.56903900	-2.08147600	2.73329700
H	2.84862600	-2.65621900	3.62143100
H	2.84560600	-2.67344500	1.85524900
C	3.24302400	-0.68097600	2.68427100
H	3.86642500	-0.57862300	1.79216100
H	3.87399600	-0.48879300	3.55694600
C	2.05615500	0.29825500	2.62142100
H	1.78723500	0.66932100	3.62151800
H	2.21249600	1.14327800	1.94975800
C	1.58364700	-2.13198600	-2.19344000
C	3.04969000	-2.30934600	-2.67981300
N	3.65297100	-0.99434600	-2.40411100
C	2.83508200	-0.30543900	-1.70563400
C	3.06379700	1.03936000	-1.14521600
C	4.41612600	1.43234400	-1.05220500
C	4.74865800	2.68136300	-0.54340300
C	3.72694300	3.54598400	-0.13758600
C	2.39449800	3.14402400	-0.24922300

C	1.99667300	1.88435500	-0.74469500
H	1.62221600	3.85220400	0.05313100
H	3.97349200	4.53071200	0.25655600
H	5.79116500	2.98053900	-0.46689200
H	5.18963900	0.74552700	-1.38392800
O	1.61203500	-0.91280800	-1.41998200
C	3.79775100	-3.37844500	-1.86477200
H	3.39234700	-4.37914200	-2.06068500
H	4.86031200	-3.37663300	-2.12677900
H	3.71515300	-3.17550700	-0.79034900
C	3.12711400	-2.61990600	-4.17919000
H	4.17200300	-2.66811500	-4.50148500
H	2.65082600	-3.58172000	-4.40764300
H	2.62948200	-1.83785700	-4.76204000
H	0.87695500	-1.99604300	-3.02031300
H	1.23361600	-2.94098500	-1.54538700
H	0.58915900	1.86543300	-0.99317900

Table S-24. Geometric coordinates and thermally corrected MP2 energies for uncomplexed [A(THF)$_3$(4,4-dimethyl-2-phenyl-2-oxazoline)]‡.

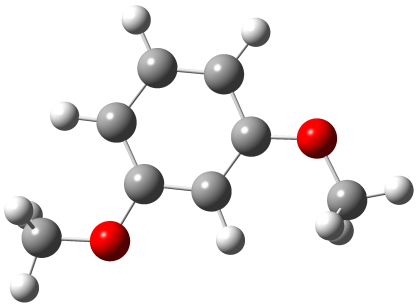


G = –1707.768871 Hartree
G_{MP2} = –1702.161605 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	1.46190900	-1.30882200	1.36391700
C	2.23818700	-2.34419800	0.66678300
C	1.66555300	-3.77000100	0.78595900
H	2.24777600	-4.47020300	0.17223800
H	0.62305100	-3.80084200	0.44149400
H	1.68708000	-4.14545300	1.81419300
C	2.35086700	-1.96999200	-0.81839900
H	3.01185100	-2.66432100	-1.35348200
H	2.75630800	-0.96114700	-0.93812400
H	1.36538800	-2.01108100	-1.30565000
H	3.27210800	-2.38921700	1.05256400
C	1.25200100	-1.59180500	2.79184100
C	2.55282600	-1.63936800	3.62516400
H	2.33738400	-1.84079000	4.68311300
H	3.08871000	-0.68675600	3.55326600
H	3.22994700	-2.42492800	3.27230600
C	0.29044700	-0.55989300	3.39849900
H	0.05369900	-0.80884100	4.44073900
H	-0.65237700	-0.53242000	2.83522000
H	0.73097800	0.44342700	3.38796500
H	0.75530100	-2.57041800	2.91123900
O	-1.54148500	-1.44001800	-1.18968600
C	-1.73385600	-1.41762200	-2.61153800
H	-1.12494700	-0.60060500	-3.00217500
H	-2.79462600	-1.22160700	-2.83728000
C	-1.31817300	-2.81722700	-3.08000800
H	-1.82815800	-3.11277800	-4.00183100
H	-0.24052000	-2.84405600	-3.26828500
C	-1.68194900	-3.72292100	-1.87290500
H	-0.84673600	-4.37535100	-1.60496100
H	-2.54536100	-4.36083700	-2.08505600
C	-2.00129100	-2.72388000	-0.73639700
H	-3.08384700	-2.67383900	-0.54547300
H	-1.48562100	-2.93569900	0.20237800
O	-1.94276000	1.31780400	0.75265400
C	-3.25436300	1.06780600	0.21505000
H	-3.24122800	0.06525100	-0.21502600
H	-3.47302700	1.79358600	-0.58412300
C	-4.20399400	1.25416800	1.39474500
H	-5.23621400	1.44344500	1.08459300
H	-4.19330000	0.36292400	2.03308000
C	-3.55898000	2.44925800	2.11626200
H	-3.80576300	2.49520600	3.18076300
H	-3.88612100	3.38873600	1.65641800
C	-2.05431400	2.22423000	1.87843400
H	-1.52130400	3.15216700	1.64401100
H	-1.56434500	1.74894800	2.73331900
O	0.30635400	1.24304200	-2.04224600
C	-0.41741300	2.48530600	-2.19108300
H	-0.92634900	2.69220300	-1.24580600
H	-1.17433700	2.36304100	-2.98034300
C	0.62663100	3.53227100	-2.57745600
H	0.19403500	4.37108600	-3.13180800
H	1.12146300	3.91927900	-1.68058400
C	1.61510700	2.69740300	-3.40561600
H	2.61223500	3.14254800	-3.46281300

H	1.24099400	2.55949300	-4.42757900
C	1.62472200	1.36989000	-2.64434300
H	1.79032300	0.49864100	-3.28602700
H	2.36949300	1.37246400	-1.84268600
H	2.12384400	-0.17640500	1.25610100
N	5.92632100	0.93387300	-0.59683100
C	6.83912900	-0.22398700	-0.53767000
C	6.06358600	-1.24282900	0.35026700
O	4.94829900	-0.49413600	0.86974900
C	4.95648000	0.70807000	0.21144100
C	3.86260200	1.64942100	0.53750800
C	4.14163900	3.01151600	0.31161600
C	3.19223400	3.98483300	0.61156100
C	1.96329100	3.58947100	1.14664900
C	1.70675200	2.22848500	1.35022200
C	2.62189400	1.19790300	1.05616500
H	0.74048300	1.96491400	1.78794900
H	1.21890900	4.34059000	1.41265300
H	3.41678000	5.03702800	0.45207700
H	5.11272100	3.29087100	-0.08783500
H	5.67193600	-2.09361000	-0.22069900
H	6.64419700	-1.62224600	1.19693900
C	8.15900600	0.21709500	0.11687100
H	8.87157100	-0.61627300	0.16723900
H	8.61430300	1.02939100	-0.45909400
H	7.98105800	0.58173400	1.13454400
C	7.09336900	-0.76365800	-1.95109900
H	7.56419700	0.00539600	-2.57237900
H	7.75388800	-1.63981800	-1.92695100
H	6.15114900	-1.05453700	-2.42839200

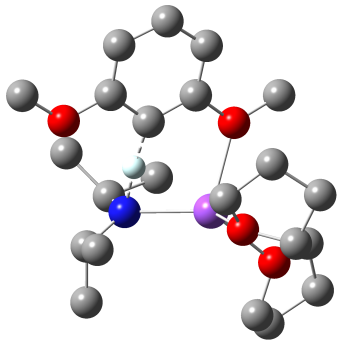
Table S-25. Geometric coordinates and thermally corrected MP2 energies for 1,3-dimethoxybenzene.



G = –461.148072 Hartree
G_{MP2} = –459.6873481 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
O	0.34788700	1.37448000	-0.00004400
C	1.67286500	1.70508400	-0.00003300
C	2.71107500	0.77532700	-0.00003600
C	4.04320700	1.22126200	-0.00002700
C	4.33791200	2.58624000	-0.00001700
C	3.27661000	3.50153700	-0.00001500
C	1.95515300	3.08237400	-0.00002300
H	1.13024800	3.78680900	-0.00002000
H	3.49820300	4.56560400	-0.00000700
H	5.36029600	2.94419900	-0.00001100
O	4.97946200	0.22475000	-0.00003100
C	6.34786400	0.59505200	-0.00001700
H	6.60952100	1.17606000	0.89437600
H	6.91149700	-0.33995600	-0.00001700
H	6.60953700	1.17606900	-0.89439900
H	2.53540800	-0.29321000	-0.00004700
H	-1.09119200	-0.03321200	0.00002300
H	0.37874100	-0.51272500	-0.89421100
H	0.37877900	-0.51267600	0.89422200

Table S-26. Geometric coordinates and thermally corrected MP2 energies for [A(THF)$_2$(1,3-dimethoxybenzene)]‡.

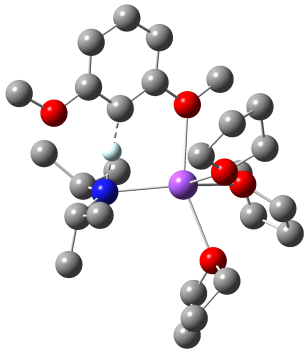


G = –1379.782638 Hartree
G_{MP2} = –1375.278621 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	-1.00529800	-2.08863900	0.14066700
C	-1.29173300	-2.67826900	1.45072500
C	-0.08776200	-3.43779800	2.04990000
H	-0.35603400	-3.92737600	2.99634600
H	0.73507700	-2.73737300	2.25345600
H	0.29127100	-4.21274700	1.37465500
C	-1.73824500	-1.59239000	2.44105900
H	-1.93959400	-2.02725800	3.42853500
H	-2.64733400	-1.09592900	2.09356300
H	-0.95015100	-0.83583900	2.57323400
H	-2.12480200	-3.40648800	1.39043800
C	-0.91840100	-3.08853100	-0.93158000
C	-2.29442600	-3.60759600	-1.41012800
H	-2.18266300	-4.42049800	-2.14085400
H	-2.86972000	-2.80079000	-1.87775400
H	-2.88629000	-3.99175000	-0.57235900
C	-0.13751800	-2.51577100	-2.12579100
H	-0.07691400	-3.23716400	-2.95136300
H	0.88711800	-2.25672100	-1.82558800
H	-0.62067000	-1.60796900	-2.50670600
H	-0.35062000	-3.97014600	-0.58448100
O	2.34906100	0.16816300	-0.28594500
C	3.00942200	0.29998200	-1.56565700
H	3.08708500	1.36536300	-1.80811500
H	2.39122800	-0.19120400	-2.32811400
C	4.37056400	-0.38845400	-1.41815200
H	4.72800900	-0.80801000	-2.36304700
H	5.12367100	0.32075400	-1.05504200
C	4.07785400	-1.45403100	-0.35040400
H	4.97366800	-1.80076600	0.17304600
H	3.58467800	-2.32329000	-0.80010000
C	3.10995100	-0.71569200	0.57317700
H	2.40480700	-1.37524500	1.08710500
H	3.64391800	-0.11121600	1.31898400
O	-0.13640300	1.76156600	1.53058700
C	0.79277800	2.84980700	1.59939200
H	1.68355500	2.55081100	1.04179100
H	1.07208500	3.02306800	2.64983400
C	0.04737700	4.06831900	1.01675100
H	0.30265200	4.98582600	1.55573200
H	0.30979500	4.22139200	-0.03473300
C	-1.45345400	3.68724000	1.16152600
H	-1.92885200	3.59275400	0.18127900
H	-2.02042200	4.42374600	1.73860700
C	-1.42040000	2.31956600	1.86429100
H	-1.49198100	2.42424100	2.95705100
H	-2.18128400	1.61967400	1.51513300
O	-1.05772900	0.96660600	-1.85438600
C	-2.44111600	0.87371000	-1.58141900
C	-2.79319100	-0.12828000	-0.67889900
C	-4.16389900	-0.21583700	-0.39277600
C	-5.12292300	0.64349200	-0.95458000
C	-4.69886700	1.62713000	-1.84794300
C	-3.35036100	1.76213200	-2.17648500
H	-3.04237000	2.53404600	-2.87415700
H	-5.42932700	2.29755200	-2.29452400

H -6.17827500 0.55846500 -0.71891000
O -4.50744500 -1.22157300 0.48994900
C -5.87402300 -1.42860800 0.78393600
H -6.45568800 -1.66190000 -0.11907300
H -5.91117800 -2.28297700 1.46382800
H -6.32692200 -0.55751500 1.27964100
C -0.63972700 1.77539900 -2.94016900
H 0.43253500 1.60084400 -3.06158600
H -1.15825800 1.49730400 -3.86619600
H -0.80696900 2.84397100 -2.74627900
H -1.94194600 -1.15257100 -0.22705000

Table S-27. Geometric coordinates and thermally corrected MP2 energies for [A(THF)$_3$(1,3-dimethoxybenzene)]‡.

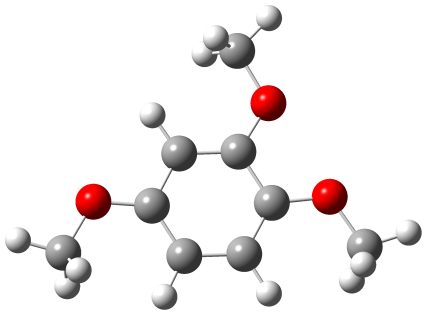


G = –1612.124014 Hartree
G_{MP2} = –1606.856626 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	1.22318300	1.93350300	-0.74527100
C	1.58510700	3.06159100	0.12155600
C	0.57499300	4.22796500	0.10223600
H	0.90933700	5.04191800	0.75983000
H	-0.40854600	3.88955700	0.45376400
H	0.44317600	4.65337300	-0.89829200
C	1.75490300	2.56676400	1.56469400
H	2.01741300	3.39533800	2.23543300
H	2.54693300	1.81739300	1.62526400
H	0.81956500	2.12065600	1.93289800
H	2.56329300	3.49093200	-0.16891400
C	1.22270400	2.28076200	-2.17495900
C	2.62688800	2.51803900	-2.77969900
H	2.55339500	2.85587300	-3.82254500
H	3.22099800	1.59826600	-2.75617600
H	3.17929200	3.28103000	-2.22154200
C	0.49872300	1.18313100	-2.96847600
H	0.50728600	1.39217000	-4.04632600
H	-0.54913300	1.11173400	-2.64641900
H	0.97752500	0.20927400	-2.80804700
H	0.64784900	3.20818800	-2.34276700
O	-2.07520700	0.84253300	1.08312000
C	-2.26682600	0.96828400	2.50151600
H	-1.41855200	0.47676000	2.98134400
H	-3.19458900	0.45373000	2.80134200
C	-2.37242100	2.47131100	2.74604100
H	-2.86468500	2.71552800	3.69264300
H	-1.37377400	2.92001000	2.74835700
C	-3.17223500	2.93494500	1.51402500
H	-2.94945600	3.96763200	1.23101500
H	-4.24846100	2.86693900	1.70907500
C	-2.75399700	1.93124600	0.41750300
H	-3.61992200	1.53669800	-0.13006700
H	-2.04691400	2.35715200	-0.30018500
O	-1.82045500	-1.42009500	-1.20638300
C	-3.00737500	-1.84433300	-0.51408100
H	-3.03573900	-1.29047400	0.42442200
H	-2.93802600	-2.92124100	-0.30005400
C	-4.20093200	-1.54378700	-1.45731100
H	-4.80856700	-2.44106200	-1.61171400
H	-4.85849800	-0.77101000	-1.04876000
C	-3.52690000	-1.08269100	-2.77302000
H	-3.53378800	0.00946800	-2.85041300
H	-4.01104900	-1.48803200	-3.66658400
C	-2.08911000	-1.57834200	-2.60548900
H	-2.00256800	-2.64082600	-2.88693300
H	-1.34153400	-1.00439800	-3.15464800
O	0.35296500	-1.15337400	2.15052600
C	0.05441100	-2.56201300	2.15018200
H	-0.32666700	-2.82744500	1.15944300
H	-0.73010800	-2.76810300	2.89427200
C	1.36195100	-3.26311400	2.51721200
H	1.20190900	-4.25718200	2.94653200
H	2.00141400	-3.36052900	1.63331800
C	1.97988500	-2.26111400	3.50408900
H	3.06430900	-2.36594100	3.60004400

H	1.53568300	-2.38132400	4.49983000
C	1.58480600	-0.91537000	2.88674100
H	1.39375500	-0.13648900	3.63200300
H	2.33560600	-0.55548300	2.17698200
O	1.49240300	-1.71599600	-0.95895500
C	1.17548500	-2.99257000	-1.48574200
H	1.45311900	-3.80224200	-0.79639000
H	0.09387500	-2.99930000	-1.62341400
H	1.67594800	-3.16555200	-2.44777300
C	2.85116000	-1.40817600	-0.74133100
C	3.83904900	-2.40317600	-0.82246000
C	5.15850100	-2.03304300	-0.56155900
C	5.48069400	-0.71679800	-0.23148300
C	4.44746900	0.23440100	-0.17799000
C	3.10322600	-0.07550300	-0.42544900
O	4.68913600	1.56268900	0.12872300
C	6.02490900	1.98001000	0.31776300
H	6.49703700	1.48269100	1.17804300
H	6.64159900	1.79790900	-0.57403900
H	5.98316400	3.05504000	0.50935500
H	6.51494400	-0.45601400	-0.03299300
H	5.94625700	-2.78084800	-0.61768200
H	3.61444300	-3.43228500	-1.08306500
H	2.15538400	0.96987600	-0.56745200

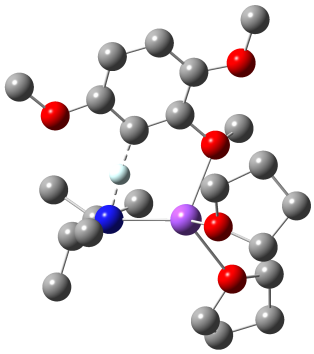
Table S-28. Geometric coordinates and thermally corrected MP2 energies for 1,2,4-trimethoxybenzene.



G = –575.631702 Hartree
G_{MP2} = –573.8372683 Hartree

Atom	X	Y	Z
C	0.00000000	0.00000000	0.00000000
O	-1.01121600	0.99094300	-0.00019200
C	-2.31601000	0.56997200	-0.00011600
C	-3.27033900	1.60366900	-0.00007300
C	-4.62789400	1.31213000	-0.00002400
C	-5.05945200	-0.04157000	0.00000000
C	-4.10471800	-1.04918600	-0.00000800
C	-2.72887300	-0.75678200	-0.00007300
H	-2.01710800	-1.57351100	-0.00006200
H	-4.41268300	-2.08856800	0.00002700
O	-6.41433300	-0.22975000	0.00004000
C	-6.88981200	-1.56191500	-0.00017900
H	-6.56298100	-2.11090600	0.89424100
H	-7.97944400	-1.49178200	-0.00072800
H	-6.56211700	-2.11087800	-0.89432000
O	-5.62092500	2.24483900	-0.00000900
C	-5.24640700	3.61138200	-0.00010300
H	-4.66401900	3.87101100	-0.89444600
H	-6.18039000	4.17652600	-0.00013900
H	-4.66404000	3.87112100	0.89422900
H	-2.90906200	2.62458400	-0.00004700
H	-0.05550800	-0.63615500	-0.89414100
H	0.95016500	0.53809400	0.00011700
H	-0.05577300	-0.63610000	0.89416300

Table S-29. Geometric coordinates and thermally corrected MP2 energies for [A(THF)$_2$(1,2,4-trimethoxybenzene)]‡.

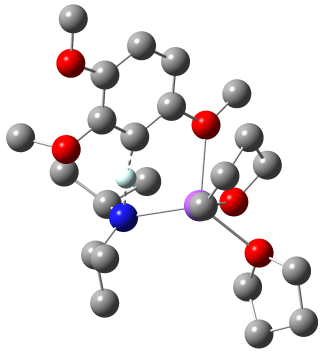


G = –1494.268476 Hartree
G_{MP2} = –1489.434081 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	0.30142200	2.31236400	-0.11815100
C	0.46085100	3.06402600	1.13143100
C	-0.82532100	3.76467400	1.61173000
H	-0.65609400	4.27944700	2.56680400
H	-1.62805000	3.02829900	1.76096400
H	-1.18588700	4.51253500	0.89718600
C	0.96032500	2.11841700	2.23472200
H	1.15408800	2.66806100	3.16457200
H	1.89091900	1.62566100	1.93652000
H	0.21178600	1.34412500	2.45970100
H	1.23415700	3.84914100	1.03092900
C	-0.13060900	3.12656700	-1.25983800
C	0.82844900	4.28337000	-1.62432600
H	0.47196900	4.82609800	-2.51012800
H	1.83432800	3.90047200	-1.82914400
H	0.91316500	5.00850100	-0.80775700
C	-0.31918500	2.21762000	-2.48452900
H	-0.68866200	2.78410000	-3.34876400
H	-1.04170300	1.41810900	-2.27118700
H	0.63078600	1.75080700	-2.76782500
H	-1.11724200	3.58623600	-1.05921800
O	-2.22139200	-0.67386200	-0.48261500
C	-2.71804000	-1.35727500	-1.65449500
H	-2.59381100	-2.43554300	-1.50805000
H	-2.11552900	-1.05013200	-2.51946800
C	-4.18120300	-0.92906000	-1.81064900
H	-4.50781700	-0.93776700	-2.85468300
H	-4.83977700	-1.59713000	-1.24321500
C	-4.17384100	0.47441800	-1.18463100
H	-5.16209700	0.80530100	-0.85199700
H	-3.78739800	1.21156100	-1.89755000
C	-3.19575800	0.29658000	-0.02399900
H	-2.65464400	1.20838700	0.24498700
H	-3.69681300	-0.10224500	0.86867800
O	0.35102900	-1.55603000	1.71475600
C	-0.42002600	-2.75796800	1.84060300
H	-1.33874600	-2.61310800	1.26744600
H	-0.68158000	-2.91068300	2.89869100
C	0.48859200	-3.89346500	1.32382000
H	0.37348900	-4.79829500	1.92861100
H	0.24225900	-4.15368400	0.28994100
C	1.92068500	-3.29380100	1.41193600
H	2.35118400	-3.17269700	0.41484000
H	2.59964900	-3.91449900	2.00476900
C	1.69902400	-1.91784600	2.06121400
H	1.78673700	-1.96624700	3.15709300
H	2.35856400	-1.13464900	1.68294800
O	1.55882200	-0.93752700	-1.46374500
C	2.76876000	-0.27117900	-1.14391200
C	2.69555500	1.02868100	-0.67460200
C	3.92166100	1.63164000	-0.33225600
C	5.14210200	0.96770300	-0.45918600
C	5.16357900	-0.36044700	-0.91547100
C	3.97652000	-1.00207900	-1.25043300
O	3.88535300	-2.32044700	-1.65862400
C	5.09309500	-3.04471600	-1.80504300

H 5.63428600 -3.12998800 -0.85250200
H 4.80945500 -4.04268600 -2.14711700
H 5.75624900 -2.58128700 -2.54852100
H 6.11581400 -0.87338000 -0.99294300
H 6.08535600 1.44195900 -0.20790800
O 3.81805200 2.92981500 0.13420400
C 5.00462000 3.60934900 0.48489000
H 5.68695000 3.71225100 -0.37174200
H 4.69950700 4.60374400 0.81905000
H 5.54165500 3.10520200 1.30214200
C 1.39057900 -1.23985800 -2.85187700
H 0.39921400 -1.69155700 -2.95585400
H 1.43789400 -0.32569600 -3.45601100
H 2.14997300 -1.94915700 -3.19094600
H 1.50375000 1.74067400 -0.43716800

Table S-30. Geometric coordinates and thermally corrected MP2 energies for [A(THF)$_2$(1,2,4-trimethoxybenzene)]‡ (methoxy away).



G = –1494.265437 Hartree
G_{MP2} = –1489.432843 Hartree

Atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	-0.57520900	-2.23638500	0.40903300
C	-0.43356100	-2.76202200	1.76975800
C	0.99682700	-3.25450000	2.08391800
H	1.05088400	-3.70778700	3.08335900
H	1.69875700	-2.40863000	2.05659000
H	1.34679000	-4.00277400	1.36456300
C	-0.82710000	-1.69732400	2.80260500
H	-0.70339800	-2.08049000	3.82358900
H	-1.86630800	-1.38565700	2.67343400
H	-0.17624000	-0.81332100	2.71046100
H	-1.10726800	-3.62669000	1.94018500
C	-0.55553500	-3.30072200	-0.60558800
C	-1.90486900	-4.04229300	-0.74766000
H	-1.82578000	-4.89173600	-1.43993300
H	-2.68007000	-3.36524900	-1.12472300
H	-2.24171900	-4.43351400	0.21917700
C	-0.12195100	-2.74789300	-1.97179700
H	-0.11461900	-3.53504300	-2.73719500
H	0.88862500	-2.32195800	-1.91459300
H	-0.80266800	-1.95727300	-2.30458400
H	0.19189500	-4.06575800	-0.33197300
O	2.25710300	0.51216900	-0.33998400
C	3.21978000	-0.55982000	-0.32797400
H	3.77376900	-0.57237700	-1.27863300
H	2.66414700	-1.49484600	-0.22377400
C	4.13703300	-0.23697200	0.84816800
H	3.65679700	-0.53503700	1.78721500
H	5.10552300	-0.74183200	0.78314200
C	4.24656800	1.29532600	0.74993600
H	5.04930600	1.57458400	0.05845900
H	4.45764200	1.77026600	1.71249200
C	2.87431100	1.71288000	0.18224700
H	2.19914100	2.11453600	0.94378000
H	2.96774700	2.44878600	-0.62578600
O	-0.44945900	2.07294900	1.12900300
C	-0.82463700	3.19581000	0.30072000
H	-0.86164800	2.85374800	-0.73751800
H	-0.05522300	3.97626300	0.39059700
C	-2.17604800	3.67581700	0.83113400
H	-2.35522400	4.73479900	0.62034200
H	-2.98562400	3.08871000	0.38469100
C	-2.05147600	3.36489000	2.33036200
H	-3.01830500	3.27663000	2.83415700
H	-1.47078100	4.14469300	2.83807900
C	-1.28649700	2.03967200	2.31733800
H	-0.63687700	1.90046500	3.18716200
H	-1.96377900	1.18354800	2.23590400
O	-1.45504100	0.42142300	-1.80303800
C	-2.72217600	0.27717700	-1.19681400
C	-2.74835100	-0.56378200	-0.07247400
C	-3.97148400	-0.65203300	0.58568800
C	-5.12633400	0.05107800	0.15854000
C	-5.05061000	0.84452700	-0.98387900
C	-3.83342500	0.96872800	-1.67131000
H	-3.79150700	1.60552200	-2.54988800
H	-5.91852500	1.38248300	-1.34851100

O	-6.25905800	-0.09791100	0.92452500
C	-7.42055600	0.60488200	0.52962400
H	-8.18809100	0.36020000	1.26735300
H	-7.25672700	1.69192200	0.52679900
H	-7.76721800	0.29682700	-0.46712000
O	-4.05025700	-1.39646500	1.75657500
C	-4.80426200	-2.60361700	1.67572600
H	-4.39721900	-3.27006600	0.90478200
H	-4.71126400	-3.08764300	2.65190400
H	-5.86155500	-2.40496900	1.46909500
C	-1.39597600	0.92994100	-3.12534600
H	-0.36573900	0.79394000	-3.46356800
H	-2.07441700	0.38030700	-3.78968400
H	-1.64762500	1.99917100	-3.16671400
H	-1.70367900	-1.45531300	0.23828500

IV. Full reference 38 (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.