

Spin-state crossover in photo-catalyzed nitrile dihydroboration via Mn-thiolate cooperation

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Electronic Supplementary Information:

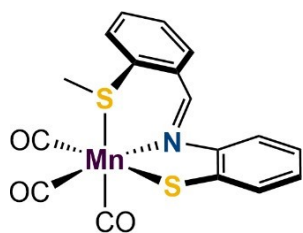
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I. General Considerations.

Unless otherwise stated, all reactions were carried out under an atmosphere of dry, oxygen-free dinitrogen by means of standard Schlenk or glovebox techniques. Benzene- d_6 and acetonitrile- d_3 were degassed by three freeze-pump-thaw cycles, and subsequently dried by running through a column of activated alumina. THF- d_8 was run through a small plug of activated alumina before use. Toluene, hexanes, diethyl ether, acetonitrile, and THF were dried on columns of activated alumina using a J. C. Meyer (formerly Glass Contour) solvent purification system and stored over activated 4 Å molecular sieves. Photolysis was performed with a High Intensity UVA/UVB Tekizoo Sun Lamp. ^1H , $^{13}\text{C}\{^1\text{H}\}$, and ^{11}B NMR spectra were recorded on Bruker AvanceII and AvanceIII spectrometers operating at 300 or 400, and 500 MHz respectively, with respect to proton nuclei. ^1H NMR spectra were referenced to residual protons (C_6D_6 , δ 7.15), (CD_3CN , δ 1.96), ($\text{C}_4\text{D}_8\text{O}$, δ 3.58) with respect to tetramethylsilane at δ 0.00. $^{13}\text{C}\{^1\text{H}\}$ NMR spectra were referenced to relative solvent resonances (C_6D_6 , δ 128.26, CD_3CN , δ 118.26). EPR spectra were recorded on a Bruker Elexsys E580 X-band spectrometer and were modelled using EasySpin (v 5.25), a package developed by Stoll and Schweiger based on Matlab.¹ Optimized values were searched for the following parameters: isotropic g value (g_{iso}), zero field splitting parameters (D and E), hyperfine coupling constants (a_{Mn} and a_{N}), and isotropic peak-to-peak line width (ΔB). FT-IR data were collected on a Thermo Scientific Nicolet 6700 spectrometer. All reagents were purchased from commercial suppliers. The $[\text{S}^{Me}\text{N}^H\text{S}]$ ligand (L^H) was synthesized according to a literature procedure.²

II. Synthetic Protocols



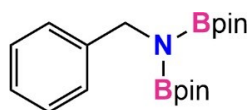
Synthesis of $[\text{Mn}(\kappa^3\text{-SNS}^{Me})(\text{CO})_3]$ (1**).** A vial equipped with a magnetic stir bar was charged with $\text{Mn}(\text{CO})_5\text{Br}$ (0.200 g, 0.730 mmol) and 5 mL of toluene. A solution of $\text{S}^{Me}\text{N}^H\text{S}$ (0.188 g, 0.730 mmol) and lithium[bis(trimethylsilyl)amide] (0.122 g, 0.730 mmol) in 2 mL of toluene was added dropwise to the suspension, giving an immediate color change from yellow-orange to reddish-brown. The solution was stirred for 16 h, filtered through Celite, and concentrated under vacuum. The residue was washed with Et_2O (3 x 2 mL), hexane (3 x 2 mL), and dried under vacuum to yield 0.253 g of a red-brown powder (92% yield). Crystals suitable for single crystal X-ray diffraction were obtained from a concentrated acetonitrile solution at -30 °C. ^1H NMR (CD_3CN , 22 °C, 300 MHz): δ 2.47 (br s, 3H, S- CH_3); 6.94 (ddd, 1H, Ar- H , $^4J_{\text{HH}} = 1.5$ Hz, $^3J_{\text{HH}} = 7$ Hz, $^3J_{\text{HH}} = 8.5$ Hz); 7.05 (ddd, 1H, Ar- H , $^4J_{\text{HH}} = 1.5$ Hz, $^3J_{\text{HH}} = 7$ Hz, $^3J_{\text{HH}} = 8$ Hz); 7.42 (dd, 1H, Ar- H , $^4J_{\text{HH}} = 1.5$ Hz, $^3J_{\text{HH}} = 8$

Hz); 7.49 (dd, 1H, Ar-H, $^4J_{HH} = 1.5$ Hz, $^3J_{HH} = 8$ Hz); 7.64 (multiplet, 2H, Ar-H); 7.81 (multiplet, 2H, Ar-H); 8.72 (s, 1H, imine-H). $^{13}\text{C}\{^1\text{H}\}$ NMR (CD_3CN , 22 °C, 75 MHz): δ 19.5 (s, S-CH₃); 110.5 (s, Ar-C); 120.6 (s, Ar-C); 122.4 (s, Ar-C); 126.1 (s, Ar-C); 127.6 (s, Ar-C); 129.1 (s, Ar-C); 131.6 (s, Ar-C); 133.5 (s, Ar-C); 134.9 (s, Ar-C); 151.5 (s, Ar-C); 15.0 (s, Ar-C); 164.3 (s, N=CH); 216.6 (s, Mn-CO); 220.1 (s, Mn-CO); 222.7 (s, Mn-CO). IR (ATM, cm^{-1}): 1898, 1922, 2009 (CO). HRMS (ESI-QTOF, $\text{C}_6\text{H}_5\text{Cl}$): Calcd for $\text{C}_{17}\text{H}_{12}\text{MnNO}_3\text{S}_2$ m/z 397.9717 ($[\text{M}^+]$). Found m/z 397.9736.

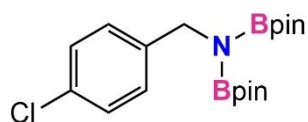
III. Catalysis Protocols

General Procedure 'A' for Dihydroboration of Nitriles.

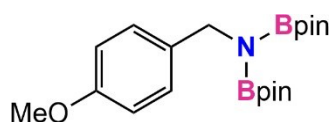
A catalyst stock solution was first prepared by dissolving **1** (10 mg) in C_6D_6 (1 mL). A vial containing **1** (0.001 g, 100 μL , 0.003 mmol, 1 mol%) in 0.6 g of THF was charged first with nitrile substrate (0.32 mmol), and subsequently with 2.2 equiv. pinacolborane (0.090 g, 102 μL , 0.70 mmol) to give a dark yellow-brown solution. The solution was charged to an NMR tube, removed from the glovebox, and placed 15 cm away from a UV light sun lamp for the appropriate reaction time. Yield was determined by ^1H NMR in reference to internal standard mesitylene. In the glovebox, volatile materials were removed under reduced pressure. Hexane was added to extract the product, the solution was filtered through Celite, and placed in the freezer at -35 °C overnight to afford white crystals.



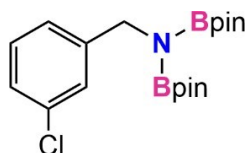
Dihydroboration of benzonitrile. Conducted according to *General Procedure A* using benzonitrile (0.032 g, 32 μL , 0.32 mmol), pinacolborane (0.090 g, 102 μL , 0.70 mmol), and catalytic **1**. The solution was placed under white light lamp with a cooling fan for 4 h (99% NMR yield). ^1H NMR shifts matched with literature values.³



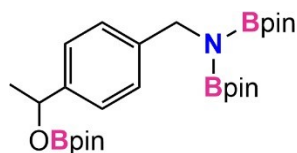
Dihydroboration of 4-chlorobenzonitrile. Conducted according to *General Procedure A* using 4-chlorobenzonitrile (0.044 g, 0.32 mmol), pinacolborane (0.090 g, 102 μL , 0.70 mmol), and catalytic **1**. The solution was placed under white light lamp with a cooling fan for 4h (99% NMR yield). ^1H NMR shifts matched with literature values.³

**Dihydroboration of 4-methoxybenzonnitrile.**

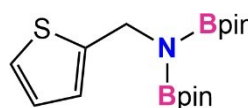
Conducted according to *General Procedure A* using 4-methoxybenzonnitrile (0.042 g, 0.32 mmol), pinacolborane (0.090 g, 102 μ L, 0.70 mmol), and catalytic **1**. The solution was placed under white light lamp with a cooling fan for 4 h (99% NMR yield). ^1H NMR shifts matched with literature values.³

**Dihydroboration of 3-chlorobenzonnitrile.**

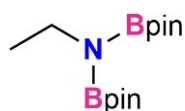
Conducted according to *General Procedure A* using 3-chlorobenzonnitrile (0.044 g, 0.32 mmol), pinacolborane (0.090 g, 102 μ L, 0.70 mmol), and catalytic **1**. The solution was placed under white light lamp with a cooling fan for 6 h (92% NMR yield). ^1H NMR shifts matched with literature values.³

**Trihydroboration of 4-acetyl-benzonnitrile.**

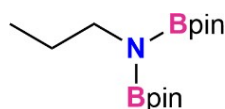
Conducted according to *General Procedure A* using 4-acetyl-benzonnitrile (0.022 g, 29 μ L, 0.32 mmol), pinacolborane (0.135 g, 153 μ L, 1.06 mmol, 3.3 equiv), and catalytic **1**. The solution was placed under white light lamp with a cooling fan for 5 h (95% NMR yield). ^1H NMR shifts matched with literature values.³

**Dihydroboration of 2-cyanyl-thiophene.**

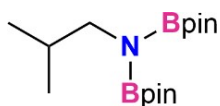
Conducted according to *General Procedure A* using 2-cyanyl-thiophene (0.035 g, 0.32 mmol), pinacolborane (0.090 g, 102 μ L, 0.70 mmol), and catalytic **1**. The solution was placed under white light lamp with a cooling fan for 5 h (96% NMR yield). ^1H NMR shifts matched with literature values.³

**Dihydroboration of acetonitrile.**

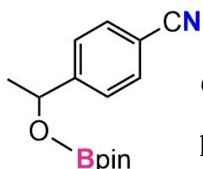
Conducted according to *General Procedure A* using acetonitrile (0.013 g, 17 μ L, 0.32 mmol), pinacolborane (0.090 g, 102 μ L, 0.70 mmol), and catalytic **1**. The solution was placed under white light lamp with a cooling fan for 8 h (95% NMR yield). ^1H NMR shifts matched with literature values.³

**Dihydroboration of propionitrile.**

Conducted according to *General Procedure A* using propionitrile (0.017 g, 22 μ L, 0.32 mmol), pinacolborane (0.090 g, 102 μ L, 0.70 mmol), and catalytic **1**. The solution was placed under white light lamp with a cooling fan for 8 h (92% NMR yield). ^1H NMR shifts matched with literature values.³



Dihydroboration of isobutylnitrile. Conducted according to *General Procedure A* using isobutylnitrile (0.022 g, 29 μ L, 0.32 mmol), pinacolborane (0.090 g, 102 μ L, 0.70 mmol), and catalytic **1**. The solution was placed under white light lamp with a cooling fan for 8 h (85% NMR yield). ^1H NMR shifts matched with literature values.³



Hydroboration of 4-acetyl-benzonitrile. Conducted according to a modified *General Procedure A* using 4-acetyl-benzonitrile (0.022 g, 29 μ L, 0.32 mmol), pinacolborane (0.090 g, 102 μ L, 0.70 mmol), and catalytic **1**. Reactants were mixed in a vial and subsequently charged to an NMR tube. After approx. 5 minutes at room temperature the crude ^{11}B NMR showed full conversion to the carbonyl-reduced products (99% NMR yield). ^1H NMR shifts matched with literature values.⁴

Hydroboration of 4-methoxystyrene. Conducted according to *General Procedure A* using 4-methoxystyrene (0.042 g, 42 μ L, 0.32 mmol), pinacolborane (0.041 g, 45 μ L, 0.32 mmol), and catalytic **1**. The solution was placed under white light lamp with a cooling fan for 16 h (85% NMR yield). ^{11}B NMR showed incomplete conversion to the reduced product, featuring a mixture of unreacted pinacolborane and hydroborated product (23% yield by NMR). Increasing catalyst loading to 5% gave a slight increase in product conversion (48%), but not appreciable enough to pursue further substrates. See Figure S23.

Larger Scale Dihydroboration of benzonitrile. Conducted according to *General Procedure A* in a 10 mL scintillation vial using: benzonitrile (0.250 g, 250 μ L, 2.42 mmol), pinacolborane (0.683 g, 775 μ L, 5.32 mmol) and catalytic **1** (0.048 g, 0.121 mmol). The solution was irradiated with a UV light sun lamp for 10 hours. Workup according to *General Procedure A* yielded 0.75 g of diborylamine product (86% yield).

Control Studies

Attempted dihydroboration with HL1 and/or MnCO_5Br . A solution of catalytic MnCO_5Br (0.01 g, 0.025 mmol) in THF was charged with benzonitrile (0.032 g, 32 μ L, 0.32 mmol) and pinacolborane (0.090 g, 102 μ L, 0.70 mmol). Another solution of catalytic MnCO_5Br (0.01 g, 0.025 mmol) and $\text{S}^{\text{Me}}\text{N}^{\text{H}}\text{S}$ (0.009 g, 0.025 mmol) in THF was charged with benzonitrile (0.032 g, 32 μ L, 0.32 mmol) and pinacolborane (0.090 g, 102 μ L, 0.70 mmol). Both reactions were irradiated with a UV light sun lamp for 16 h. Analysis of the crude ^{11}B NMR spectra showed less than 10% conversion to the reduced diborylamine product.

Hydroboration of 4-acetyl-benzonitrile in absence of light. Conducted according to a modified *General Procedure A* using 4-acetyl-benzonitrile (0.022 g, 29 μ L, 0.32 mmol), pinacolborane (0.135 g, 153 μ L, 1.06 mmol, 3.3 equiv), and catalytic **1**. A solution of 4-acetyl benzonitrile and **1** was added to an NMR tube wrapped in aluminum foil to protect from light. Pinacolborane was charged to the light-protected reaction mixture. The NMR tube was enclosed in a box to avoid possible light exposure and kept overnight. Analysis of the crude NMR the next day showed conversion to exclusively the carbonyl reduced product with ca. 2 equiv. of unreacted HBpin.

IV. Mechanistic Studies

Stoichiometric Studies

Stoichiometric reaction of **1 and HBpin.** A dark yellow-brown solution of **1** (0.01 g, 0.025 mmol) and HBpin (0.003 g, 3.5 μ L, 0.025 mmol) in 0.5 mL of THF- d_8 was prepared and charged to an NMR tube. The solution was irradiated for 30 minutes which initiated a color change to a dark red-orange. Analysis of the resultant crude ^1H NMR showed the disappearance of the characteristic imine C–H resonance at δ 8.81, accompanied by the growth of a new singlet at δ 4.85 indicative of a C– H_2 group. See **Figure S24**.

Attempted stoichiometric dihydroboration. A dark yellow-brown solution of **1** (0.01 g, 0.025 mmol) and HBpin (0.003 g, 3. μ L, 0.025 mmol) in 0.5 mL of THF was prepared and charged to an NMR tube. The solution was irradiated for 30 minutes which initiated a color change to a dark red-orange and analysis of the ^1H NMR confirmed borylation of the imine. Benzonitrile (0.003 g, 3 μ L, 0.025 mmol) and an additional equivalent of HBpin (0.003 g, 3.5 μ L, 0.025 mmol) were then added to the reaction mixture, which was subsequently irradiated for an additional 4 h. No color change was seen and formation of nitrile dihydroboration product was not observed.

Analysis of crude catalysis mixture. The dihydroboration of benzonitrile was conducted according to *General Procedure A* except with a larger catalyst loading of **1** (0.015 g). After catalysis completion, the sample was worked up according to *General Procedure A*. After hexanes product extraction, the remaining crude residue was dried under reduced pressure, redissolved in CD_3CN , and analyzed by ^1H NMR. Analysis of the crude ^1H NMR showed the retention of the imine C–H resonance.

Stoichiometric reaction of 1 and benzonitrile. A dark yellow-brown solution of **1** (0.01 g, 0.025 mmol) and benzonitrile (0.003 g, 3 μ L, 0.025 mmol) in 0.5 mL of acetonitrile- d_3 was prepared and charged to an NMR tube. The reaction mixture was irradiated for 2 h and no color change was observed and no change in the ^1H NMR spectrum was observed.

^{13}C -labelling Studies

General Preparation of ^{13}C -labelled $[\text{Mn}(\kappa^3\text{-SNS}^{Me})(\text{CO})_3]$ (1***).** A solution of **1** (0.020 g, 0.05 mmol) in 0.6 mL THF was charged to an NMR tube equipped with a rubber septum. The NMR tube was charged with ca. 2 mL of ^{13}CO and exposed to a white-light lamp for 30 minutes. $^{13}\text{C}\{^1\text{H}\}$ NMR confirmed successful transfer of the ^{13}CO to the Mn complex as indicated by observed signals at 216, 220, and 222 ppm (**Figure S2**).

Dihydroboration of benzonitrile catalyzed by ^{13}C -1. A sample of ^{13}C -**1** was prepared (0.01 g, 0.025 mmol, 10 mol%) in 0.6 mL THF. Benzonitrile (0.015 g, 12 μ L, 0.143 mmol) and HBpin (0.041 g, 46 μ L, 0.32 mmol, 2.2 equiv) were added to the solution. The NMR tube was exposed to white-light and monitored by $^{13}\text{C}\{^1\text{H}\}$ NMR every hour until reaction completion. The resulting $^{13}\text{C}\{^1\text{H}\}$ NMR spectra are shown in **Figure S24**.

EPR Studies

Observation of paramagnetic intermediate. A catalytic reaction mixture of benzonitrile, HBpin, and 10% **1** was prepared according to *General Procedure A*. An initial EPR spectrum of the mixture afforded no signal. The reaction mixture in the EPR tube was irradiated for 45 min and an EPR spectrum was recorded with continuous irradiation in the cavity. The resulting EPR spectrum is shown in **Figure S25**. The spectrum was modelled with the Easyspintool in MATLAB as a fit for hyperfine coupling to ^{55}Mn and ^{14}N with the following parameters:

```
%%
clc
Sys.g = 1.995;
Sys.Nucs = '55Mn,14N'; %nuclei
Sys.A = [42.5 41.2]; %MHz
Sys.lwpp = 0.5; %mT for random distribution
Exp.mwFreq = 9.8; %GHz
Exp.Range = [280 420]; %sweepwidth
[C,spp] = garlic(Sys,Exp);
%%
plot(B,spc,'black',C,spp,'r');
xlabel 'Magnetic Field (mT)';
```

V. NMR Spectra

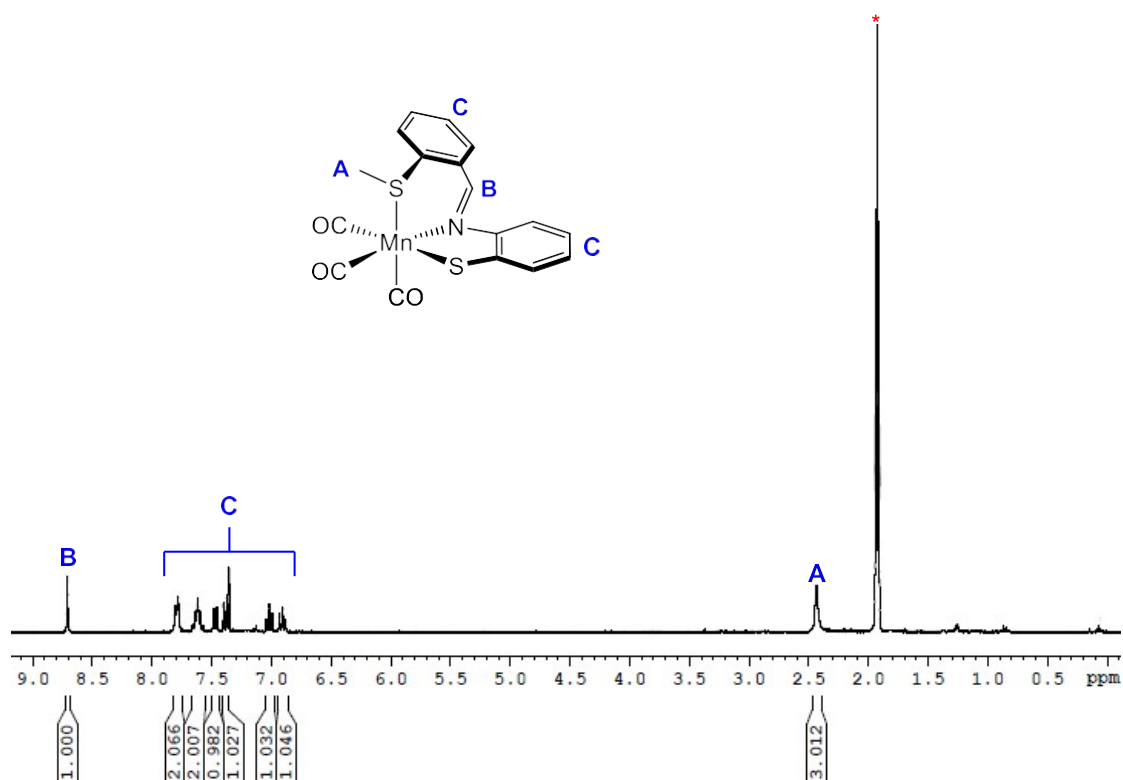


Figure S1. ^1H spectrum of $[\text{Mn}(\kappa^3\text{-SNS}^{\text{Me}})(\text{CO})_3]$ (1). * is protic impurity in acetonitrile- d_3 .

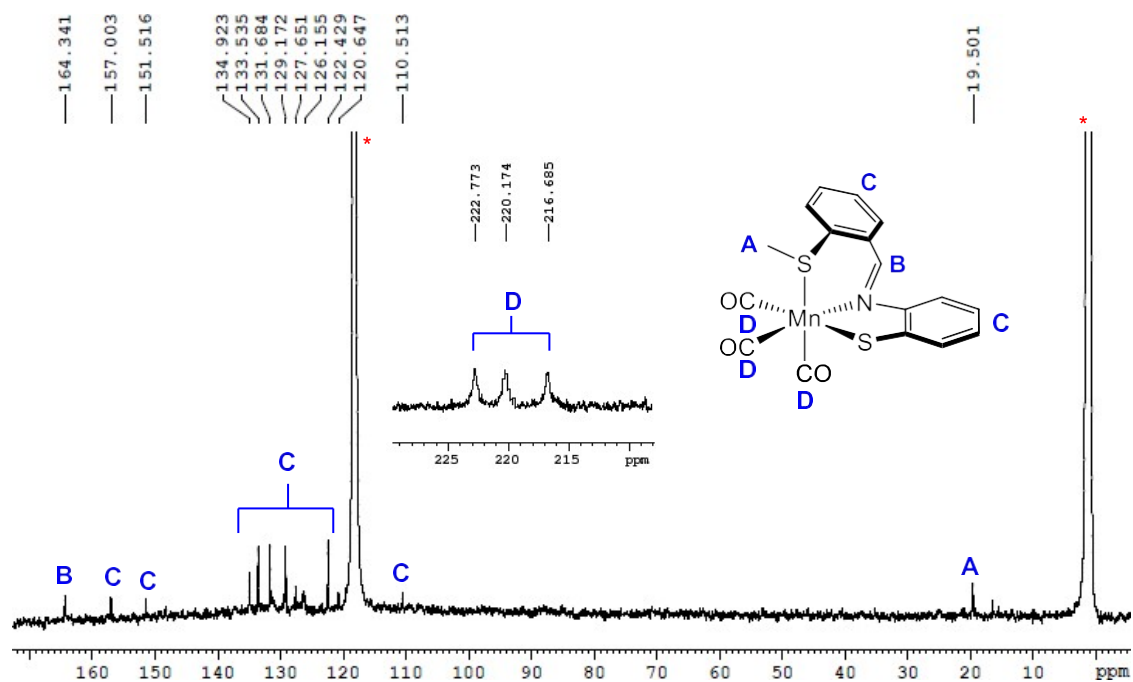


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ spectrum of $[\text{Mn}(\kappa^3\text{-SNS}^{\text{Me}})(\text{CO})_3]$ (1). * is acetonitrile- d_3 .

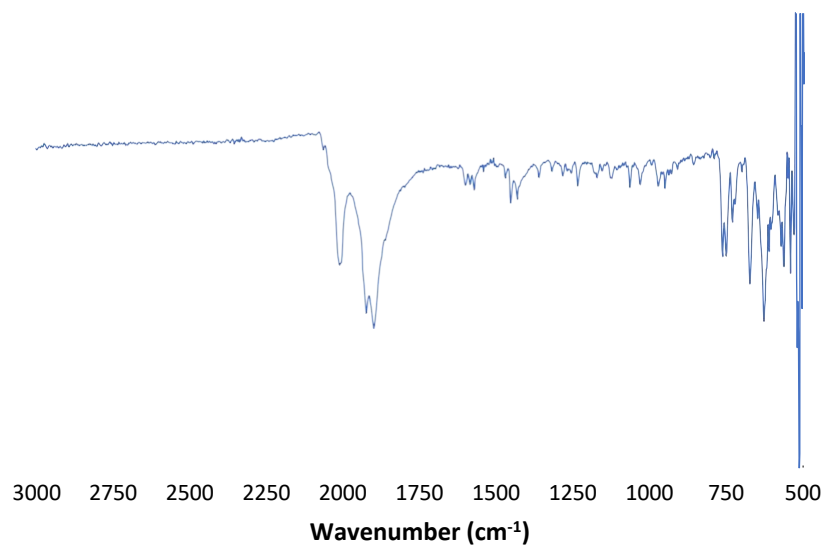


Figure S3. FT-IR (solid) spectrum of **1**.

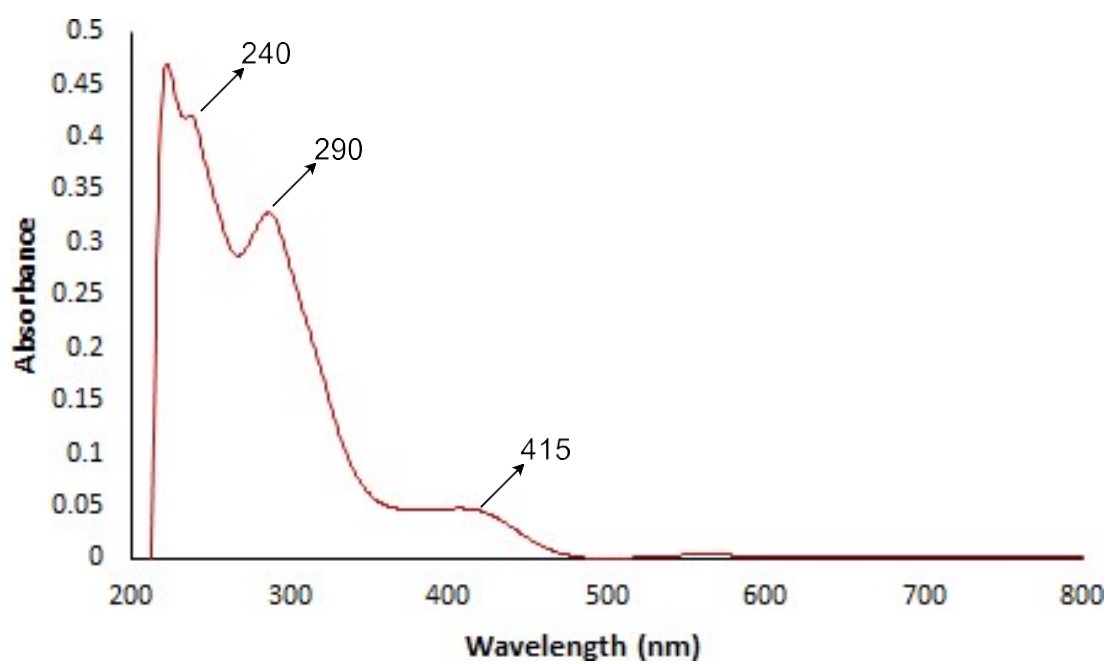


Figure S4. UV-vis spectrum of **1**.

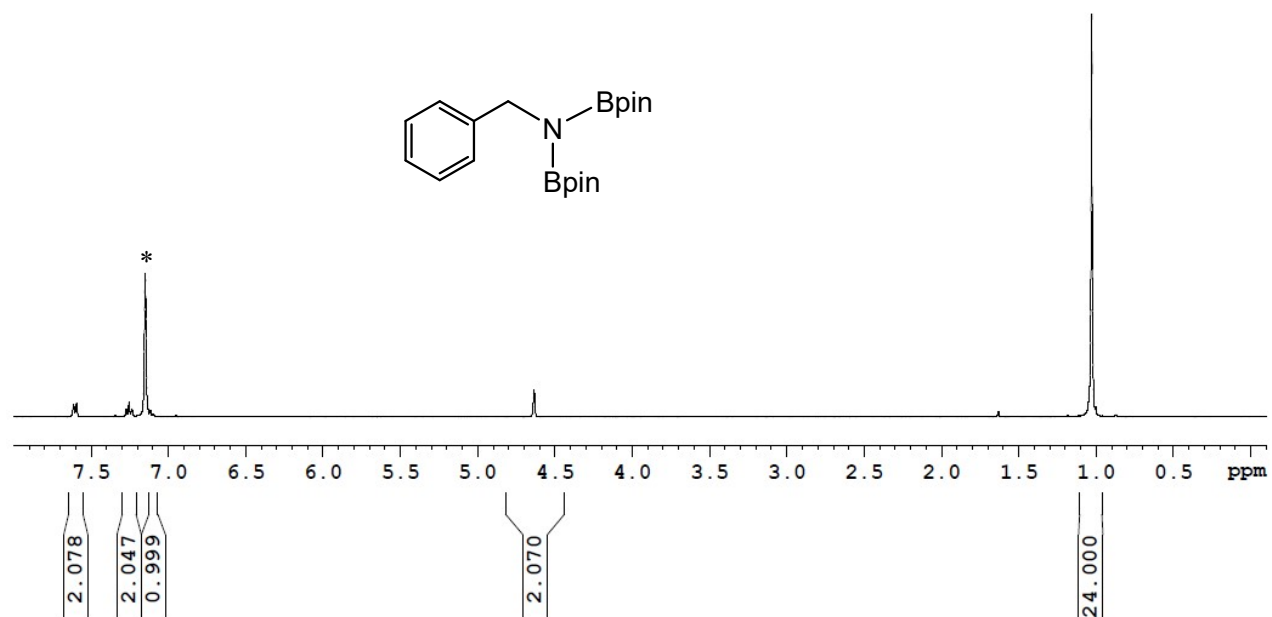


Figure S5. ^1H spectrum of benzonitrile dihydroboration product. * is protic impurity in benzene- d_6 .

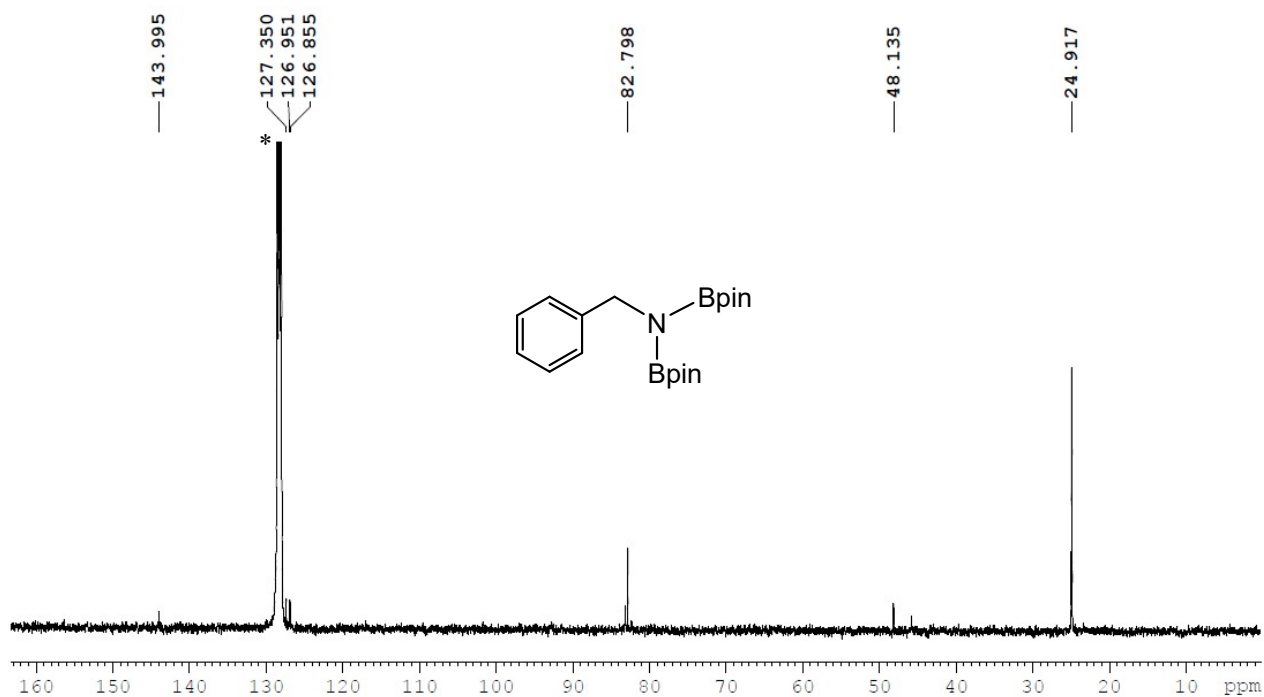


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ spectrum of benzonitrile dihydroboration product. * is benzene- d_6 .

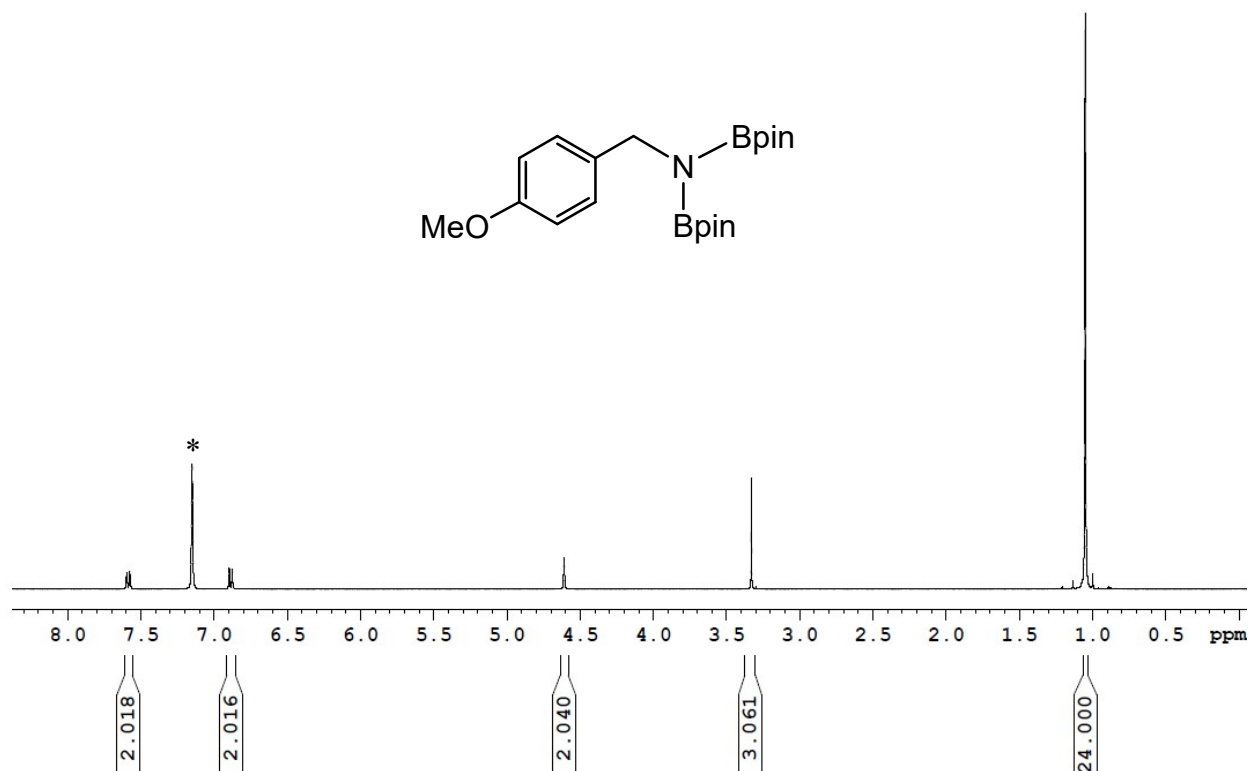


Figure S7. ^1H spectrum of 4-methoxy benzonitrile dihydroboration product. * is protic impurity in benzene- d_6 .

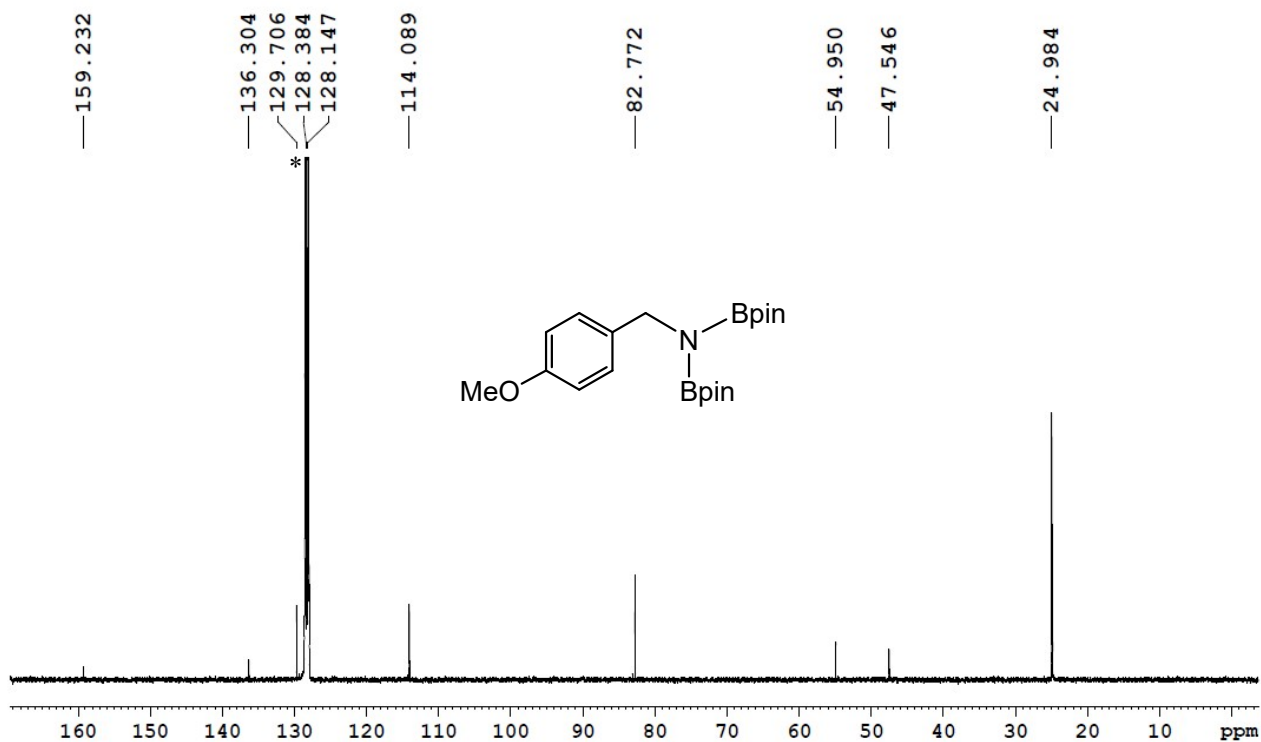


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ spectrum of 4-methoxy benzonitrile dihydroboration product. * is benzene- d_6 .

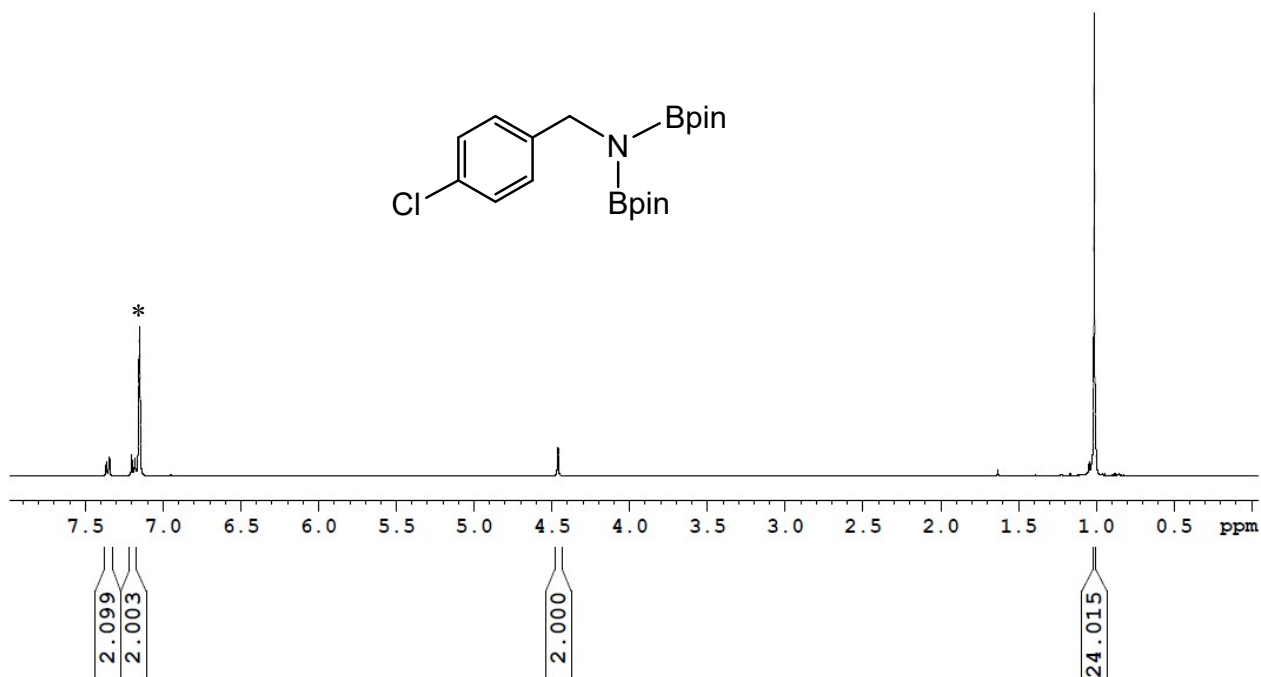


Figure S9. ¹H spectrum of 4-chloro benzonitrile dihydroboration product. * is protic impurity in benzene-*d*₆.

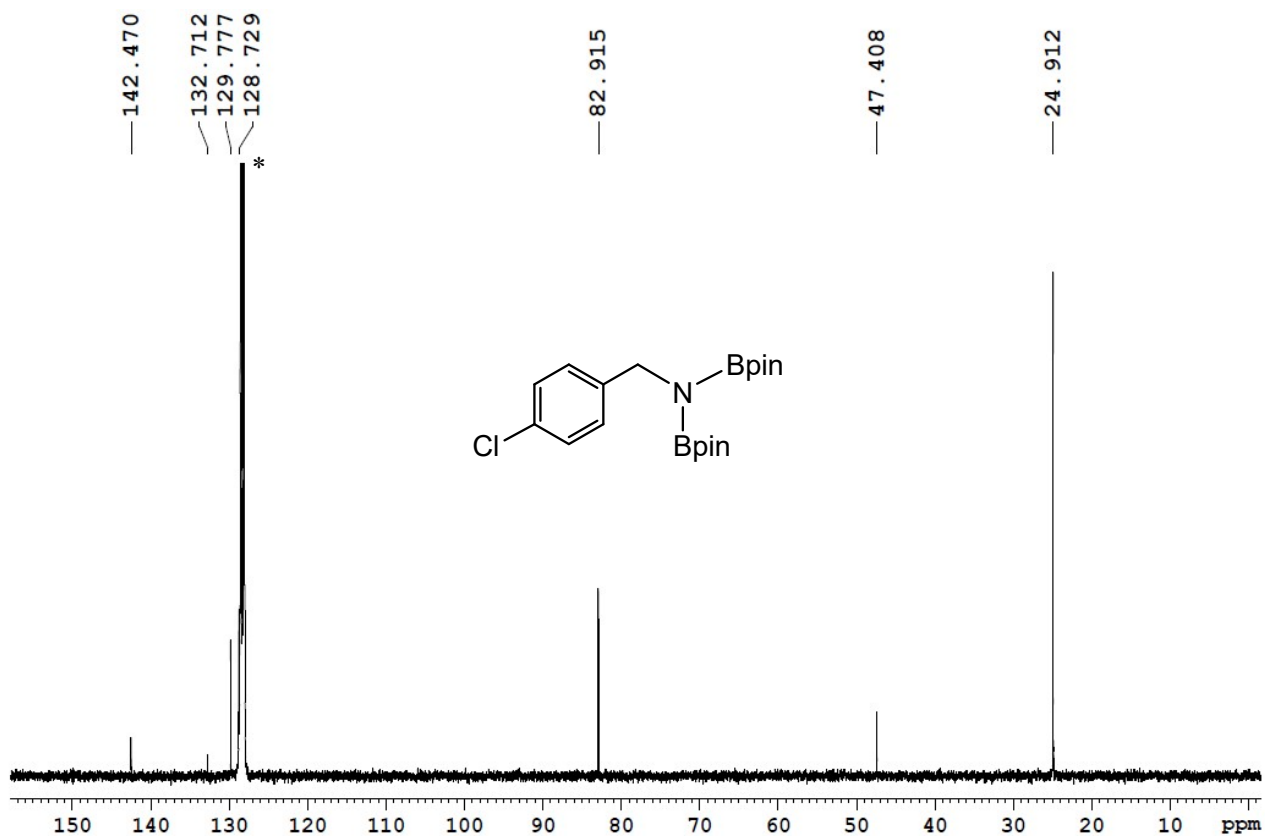


Figure S10. ¹³C{¹H} spectrum of 4-chloro benzonitrile dihydroboration product. * is benzene-*d*₆.

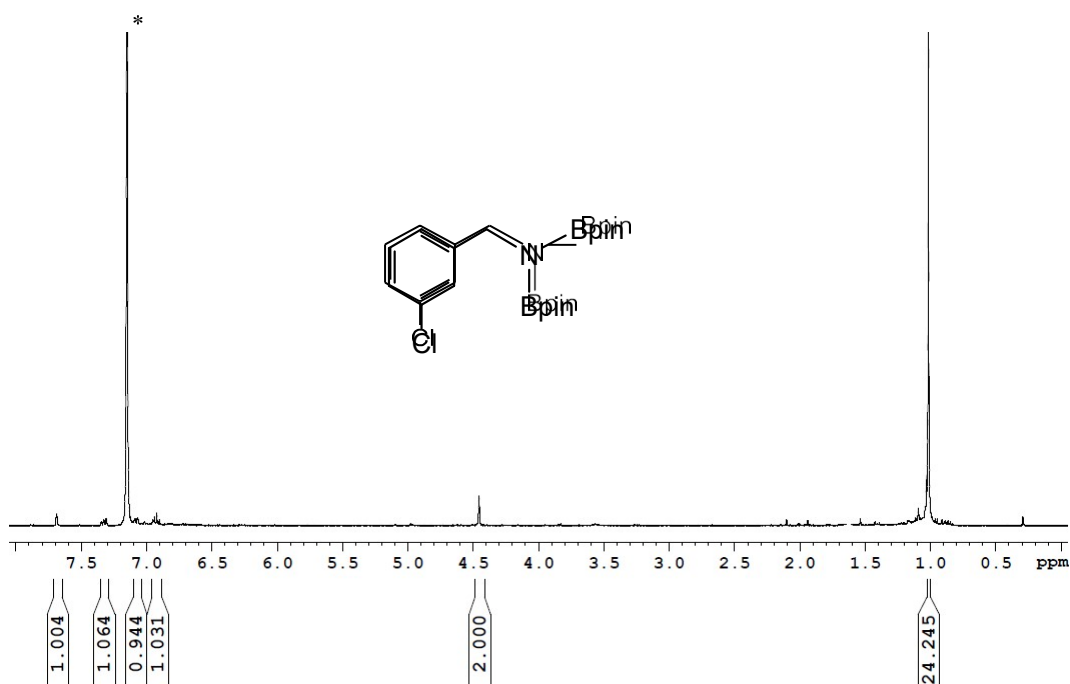


Figure S11. ^1H spectrum of 3-chloro benzonitrile dihydroboration product. * is protic impurity in benzene- d_6 .

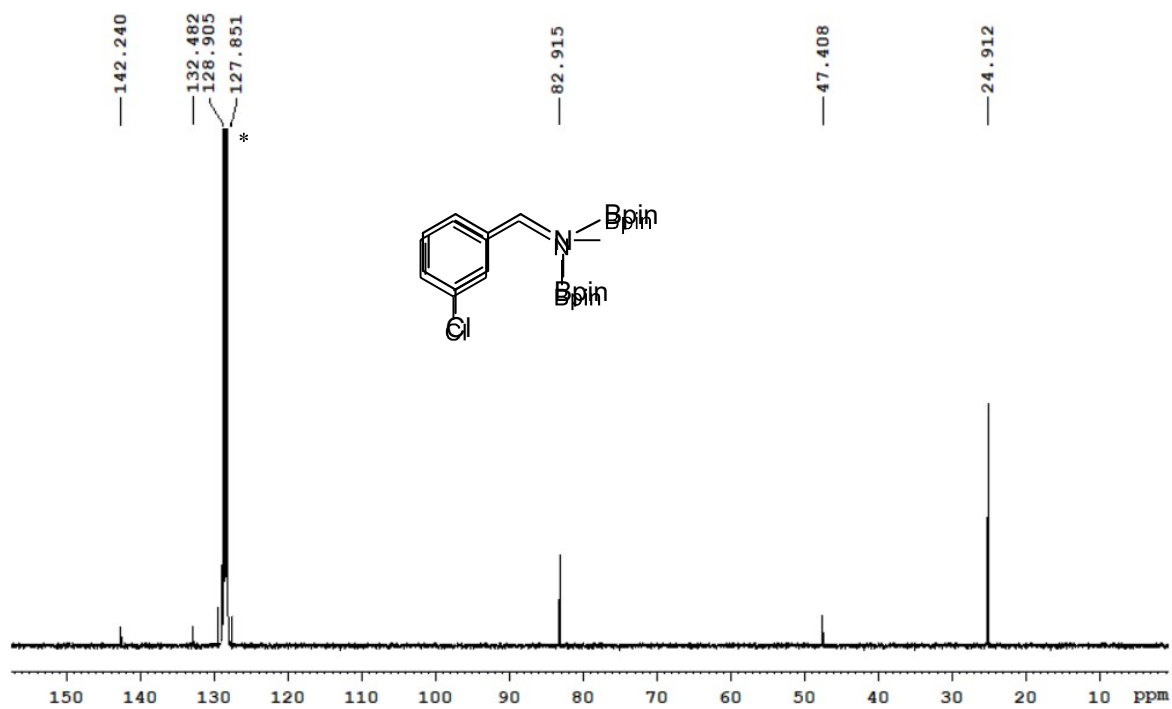


Figure S12. $^{13}\text{C}\{^1\text{H}\}$ spectrum of 3-chloro benzonitrile dihydroboration product. * is benzene- d_6 .

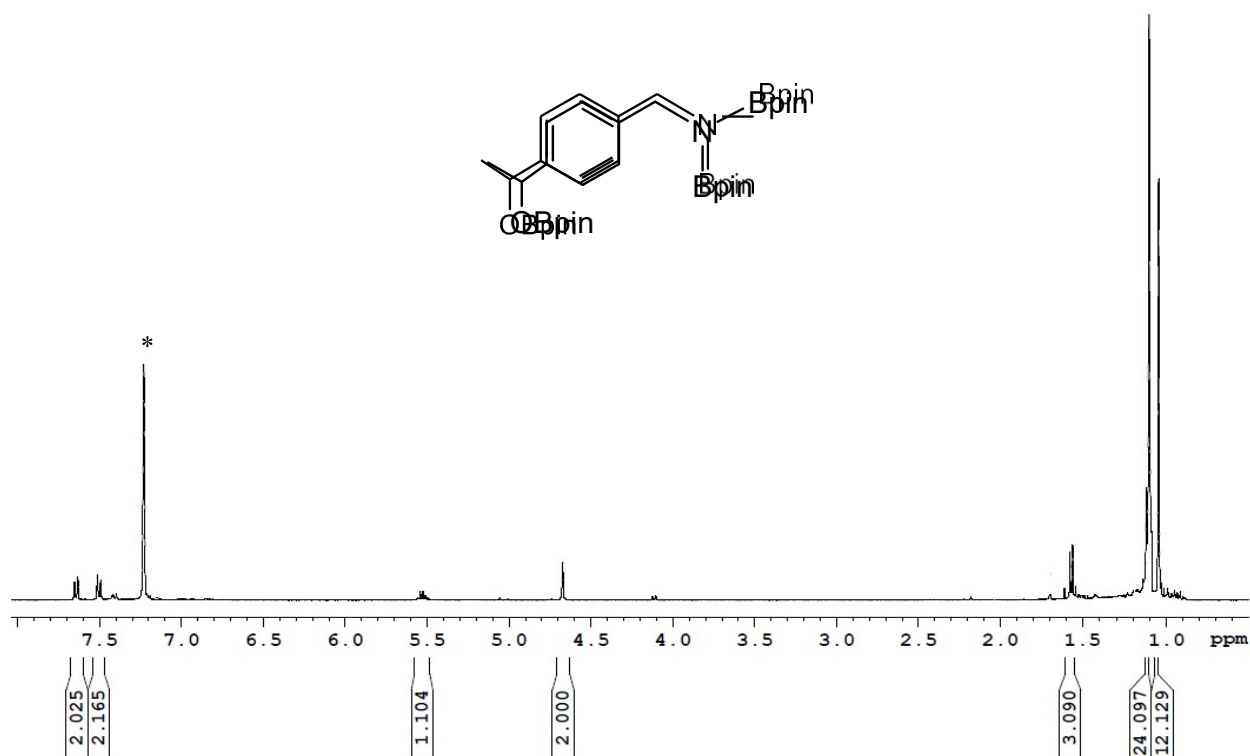


Figure S13. ^1H spectrum of 4-acetyl benzonitrile trihydroboration product. * is protic impurity in benzene- d_6 .

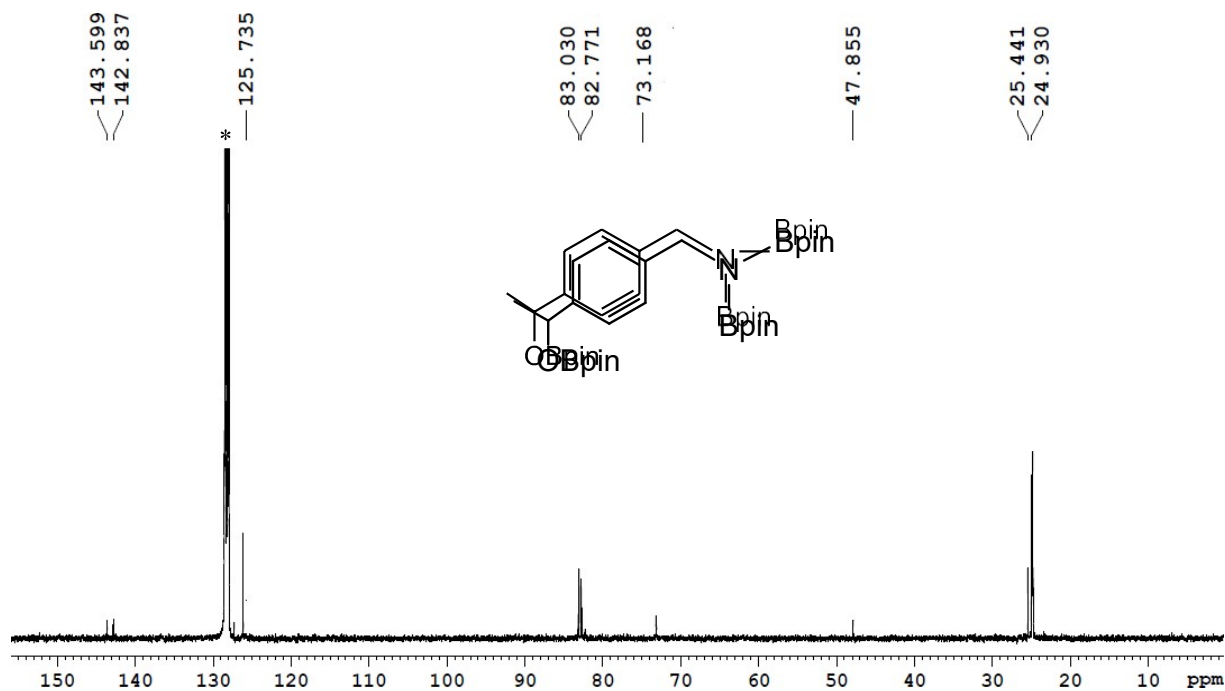


Figure S14. $^{13}\text{C}\{^1\text{H}\}$ spectrum of 4-acetyl benzonitrile trihydroboration product. * is benzene- d_6 .

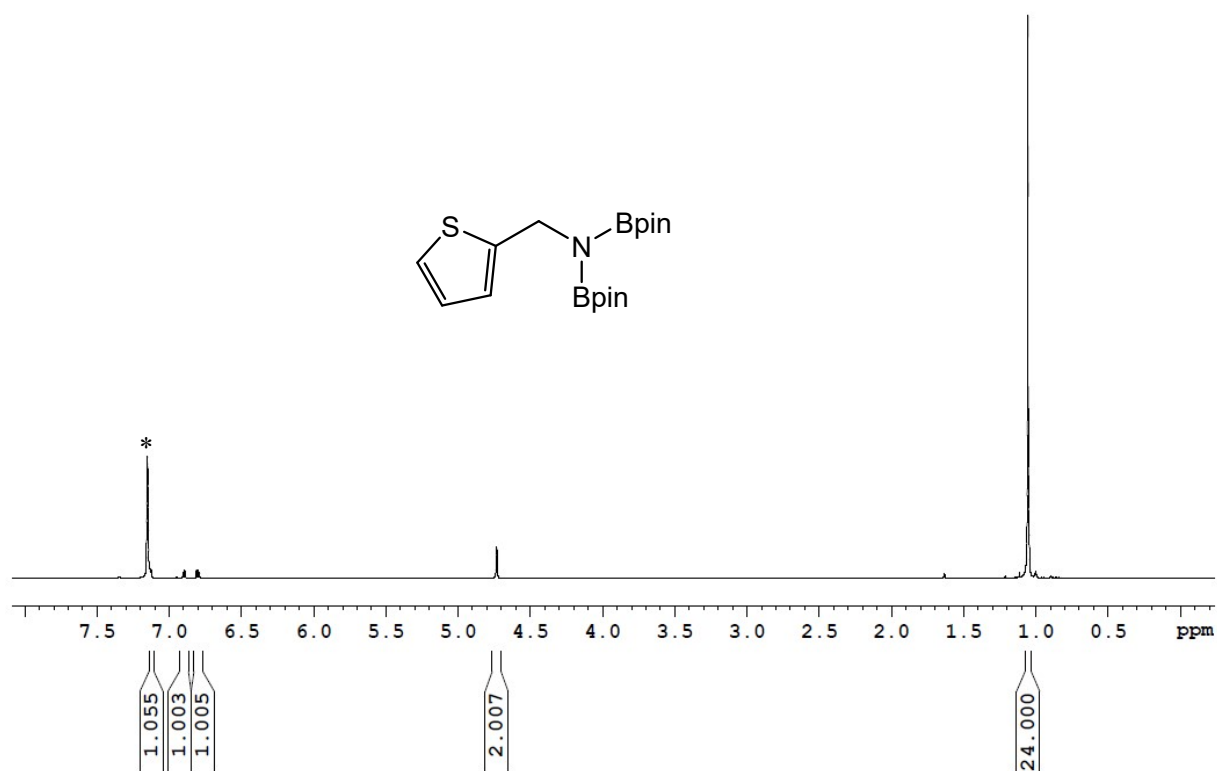


Figure S15. ¹H spectrum of 2-cyanyl-thiophene dihydroboration product. * is protic impurity in benzene-*d*₆.

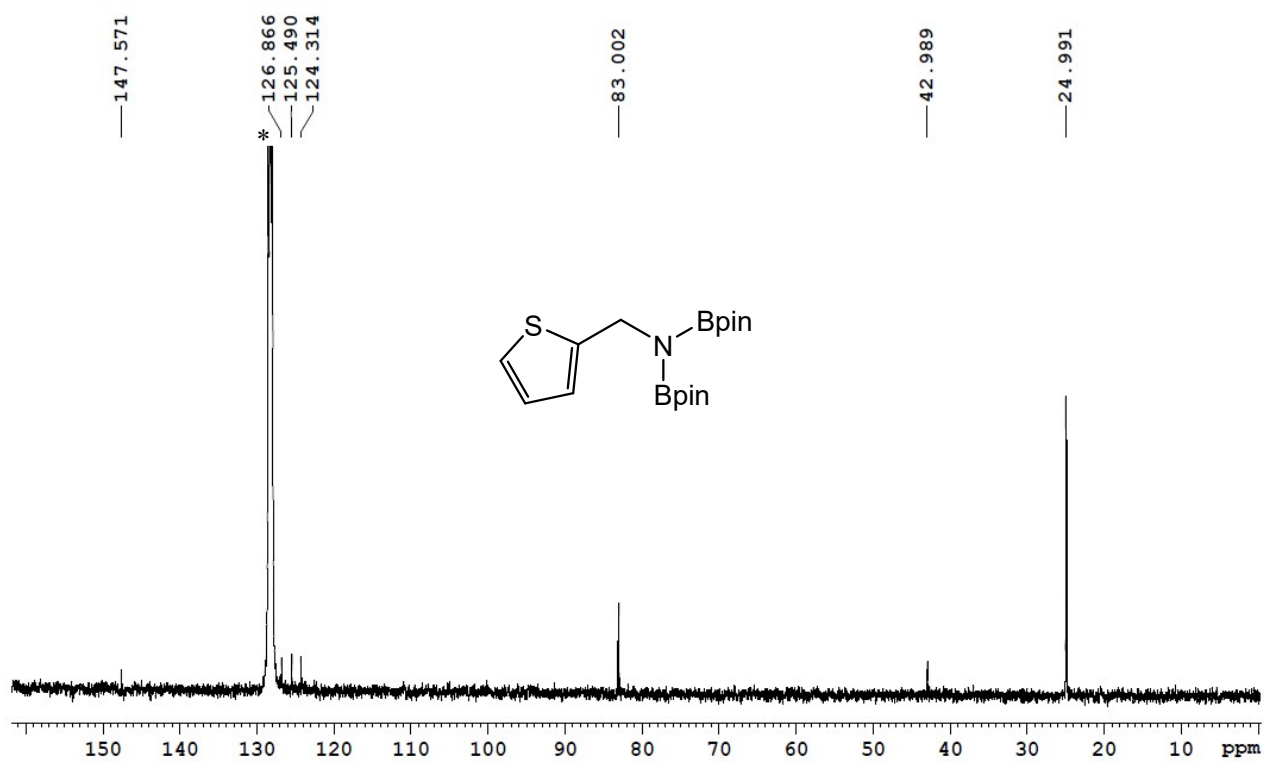


Figure S16. ¹³C{¹H} spectrum of 2-cyanyl-thiophene benzonitrile dihydroboration product. * is benzene-*d*₆.

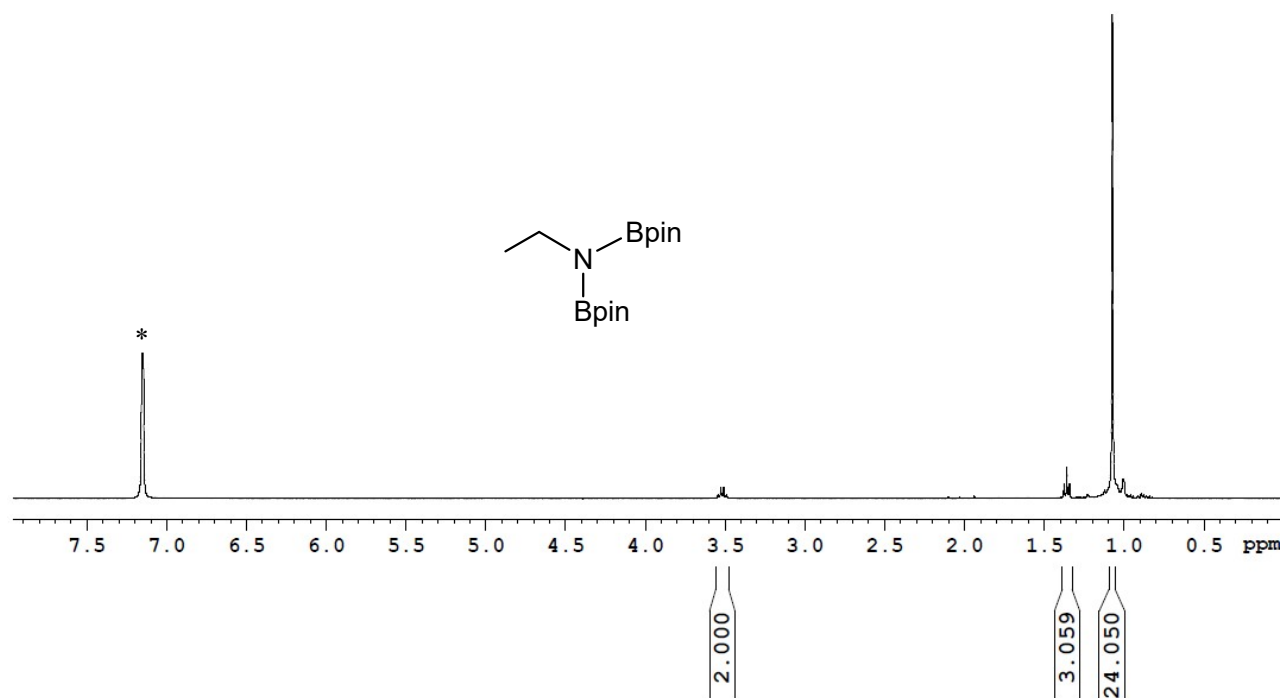


Figure S17. ^1H spectrum of acetonitrile dihydroboration product. * is protic impurity in benzene- d_6 .

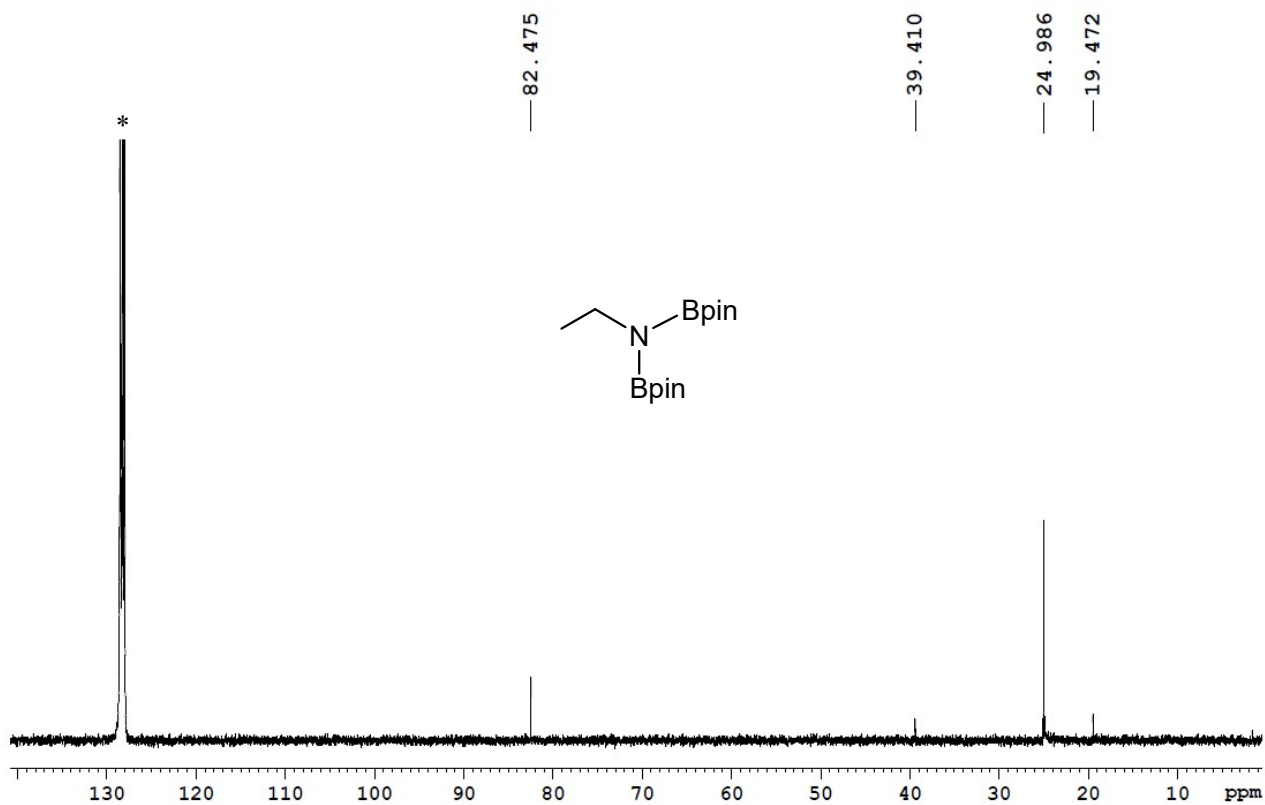


Figure S18. $^{13}\text{C}\{^1\text{H}\}$ spectrum of acetonitrile dihydroboration product. * is benzene- d_6 .

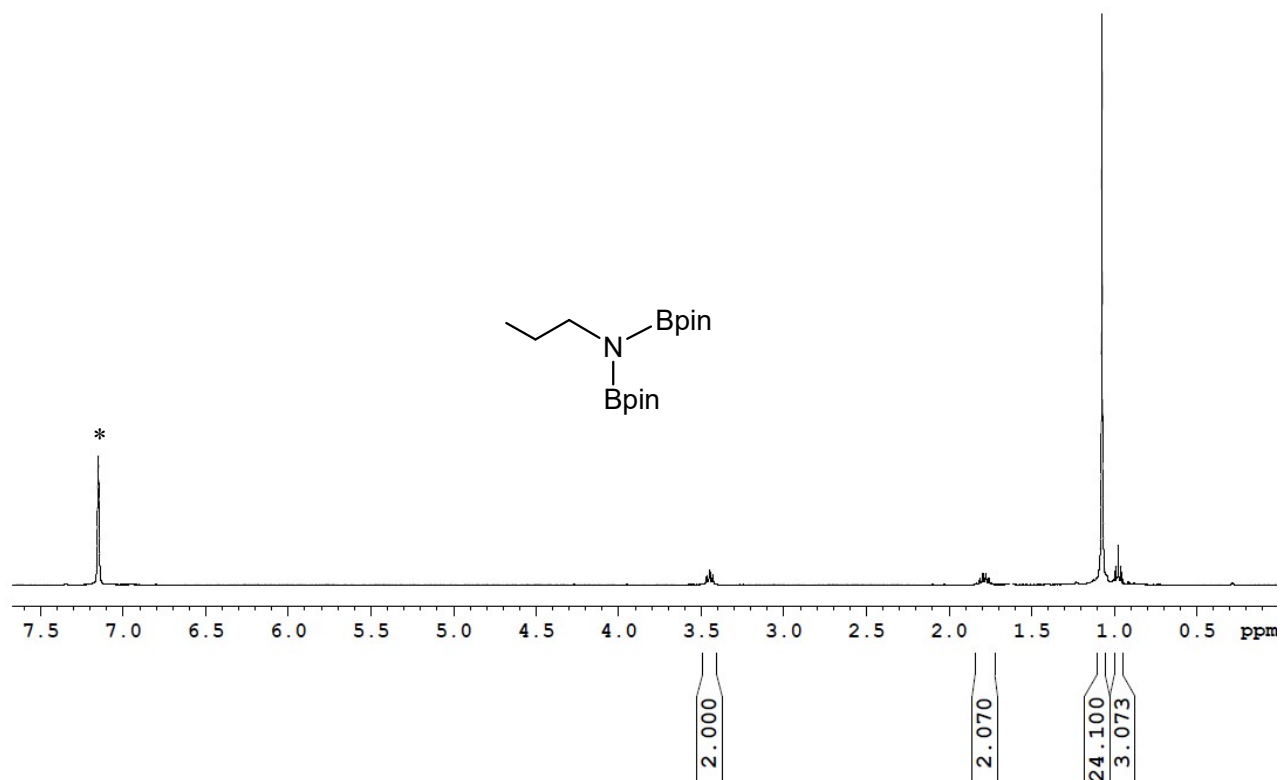


Figure S19. ^1H spectrum of propionitrile dihydroboration product. * is protic impurity in benzene- d_6 .

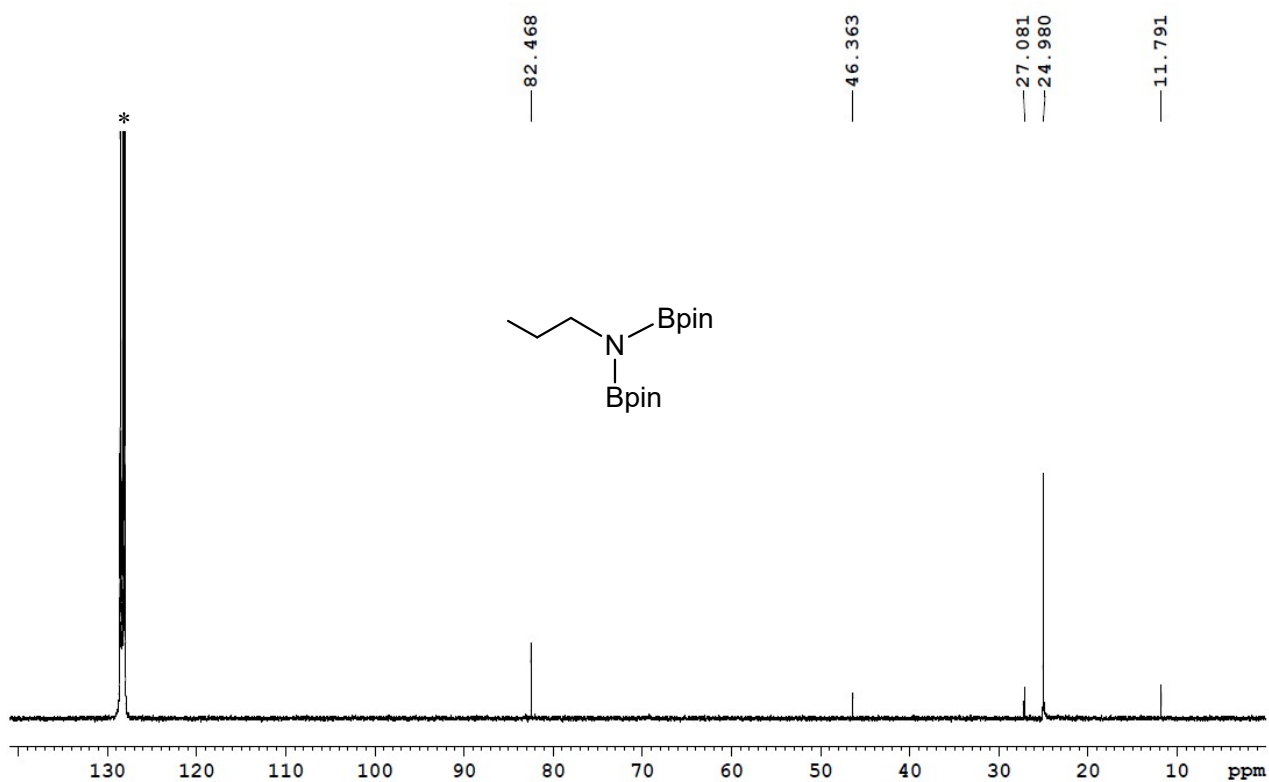


Figure S20. $^{13}\text{C}\{^1\text{H}\}$ spectrum of propionitrile dihydroboration product. * is benzene- d_6 .

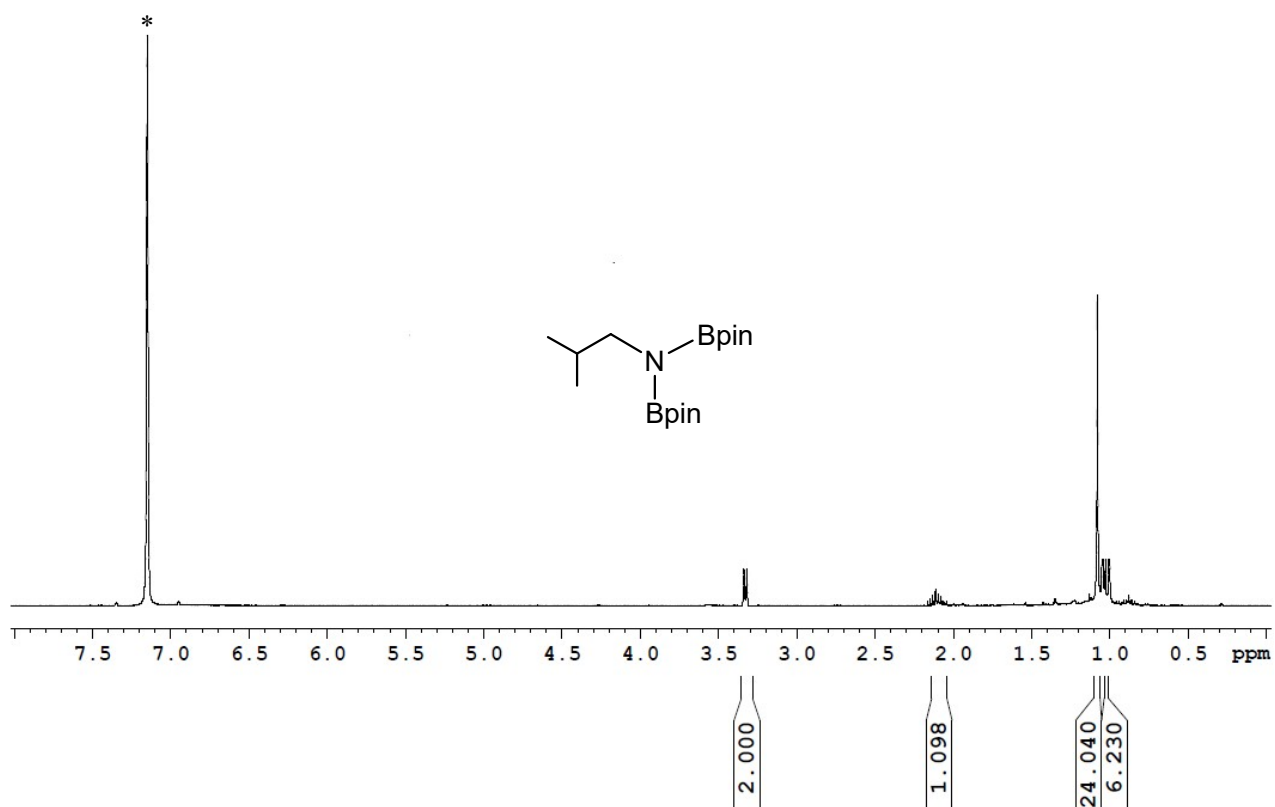


Figure S21. ^1H spectrum of isobutylnitrile dihydroboration product. * is protic impurity in benzene- d_6 .

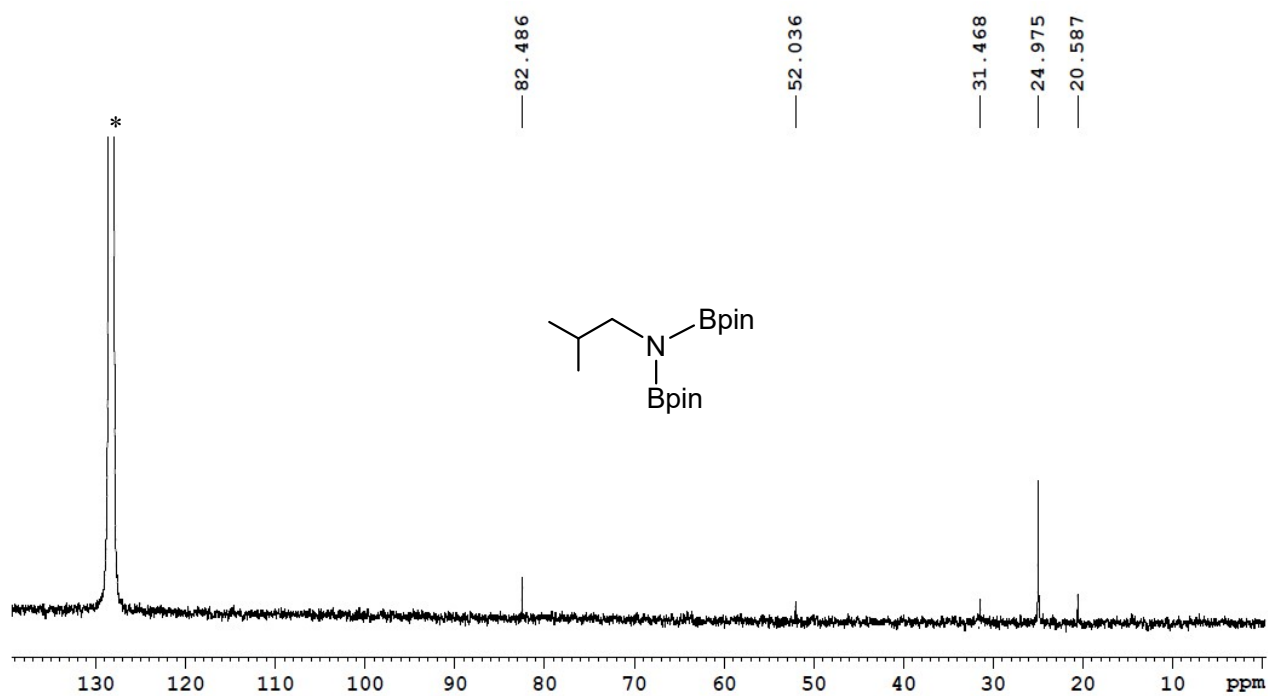


Figure S22. $^{13}\text{C}\{^1\text{H}\}$ spectrum of isobutylnitrile dihydroboration product. * is benzene- d_6 .

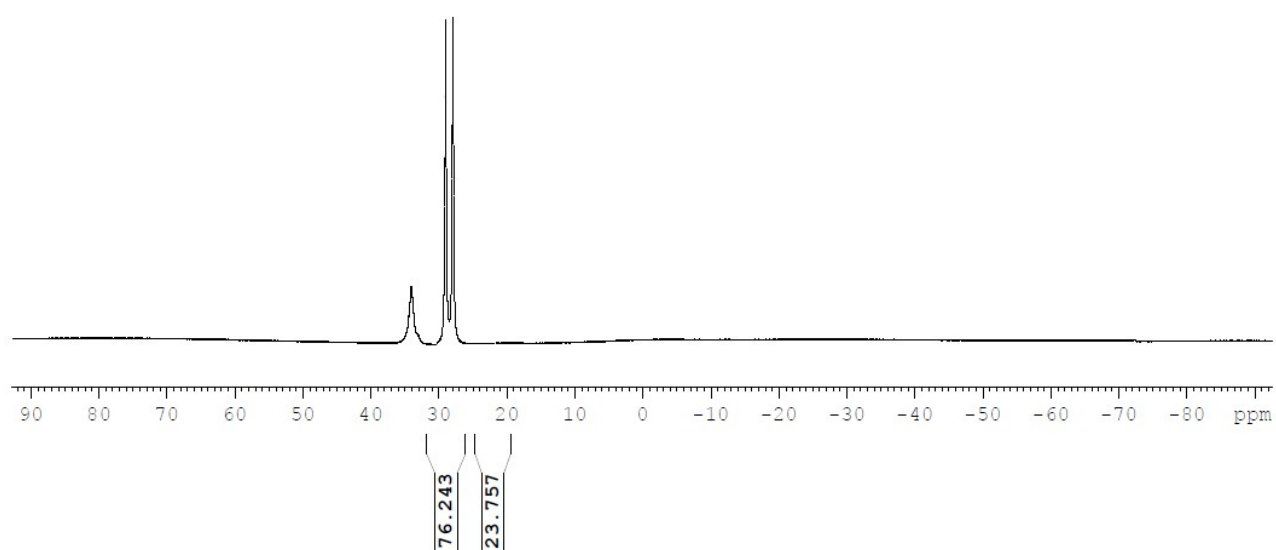


Figure S23. Crude ^{11}B NMR spectrum (96 MHz, THF) of 4-methoxystyrene hydroboration product.

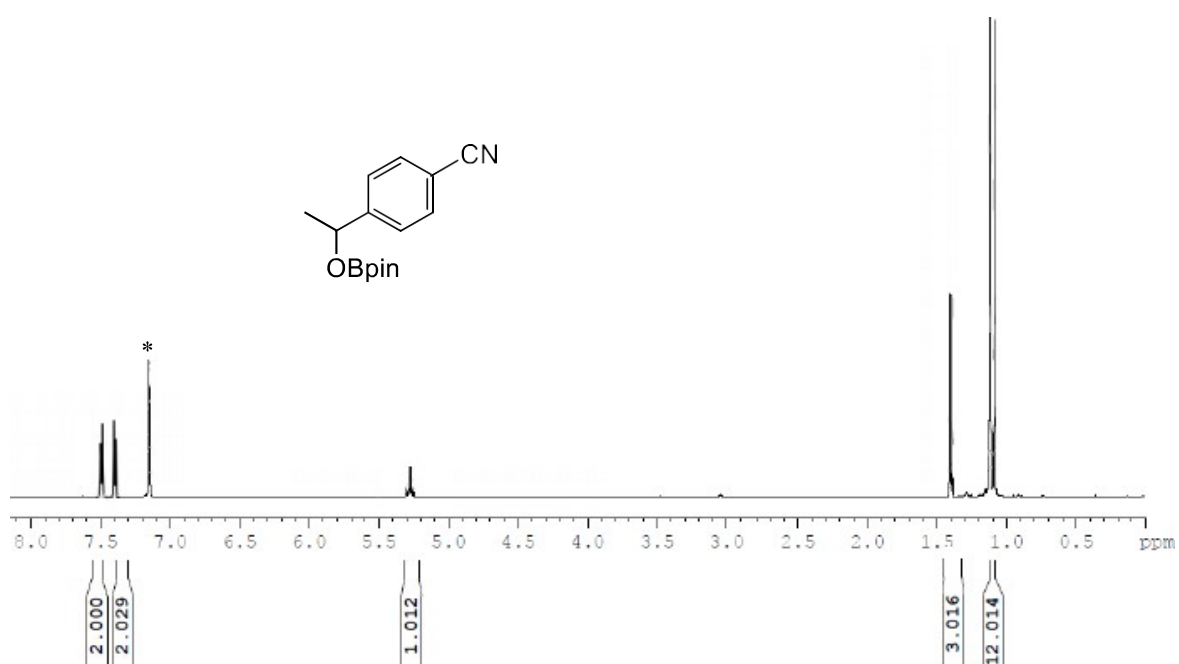


Figure S24. ^1H spectrum of 4-acetyl benzonitrile hydroboration product. * is protic impurity in benzene- d_6 .

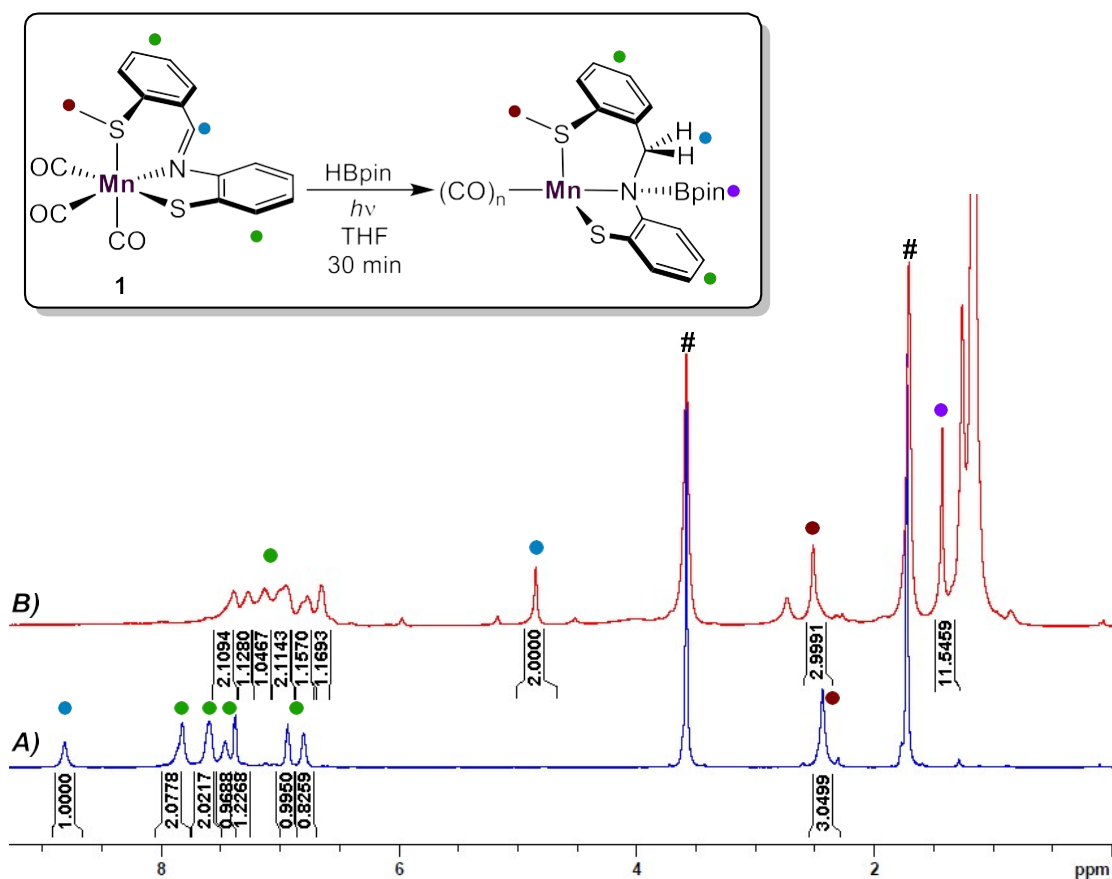


Figure S25. Stacked plot of ^1H NMR spectra showing A) complex **1** in THF- d_8 , and B) reaction of **1** and 1.2 equiv. of HBpin – irradiated for 30 min. # is THF.

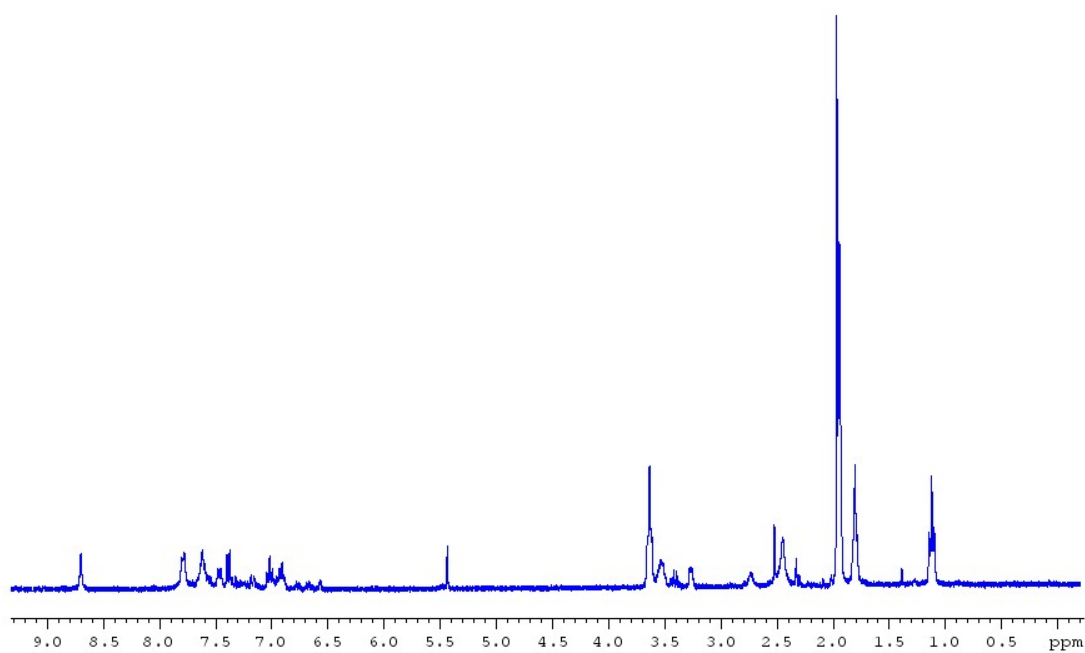


Figure S26. Crude ^1H NMR spectrum of crude catalyst residue after reaction workup showing retention of imine C–H resonance.

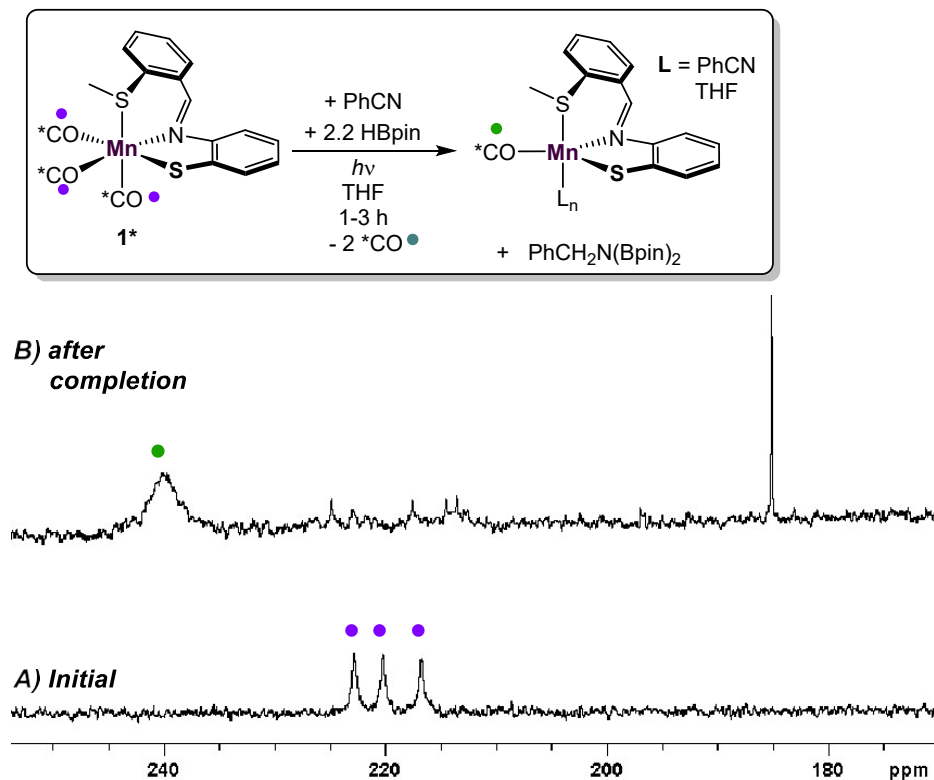


Figure S27. Stacked plot of $^{13}\text{C}\{^1\text{H}\}$ spectra showing reaction of 10 mol% ^{13}C -labelled **1*** with benzonitrile and 2.2 equiv. of HBpin. (A) (Blue trace) Initial $^{13}\text{C}\{^1\text{H}\}$ spectrum of reaction mixture prior to light exposure showing unreacted **1***. (B) $^{13}\text{C}\{^1\text{H}\}$ spectrum of reaction mixture after completion, showing disappearance of **1*** and growth of a new species at 240 ppm.

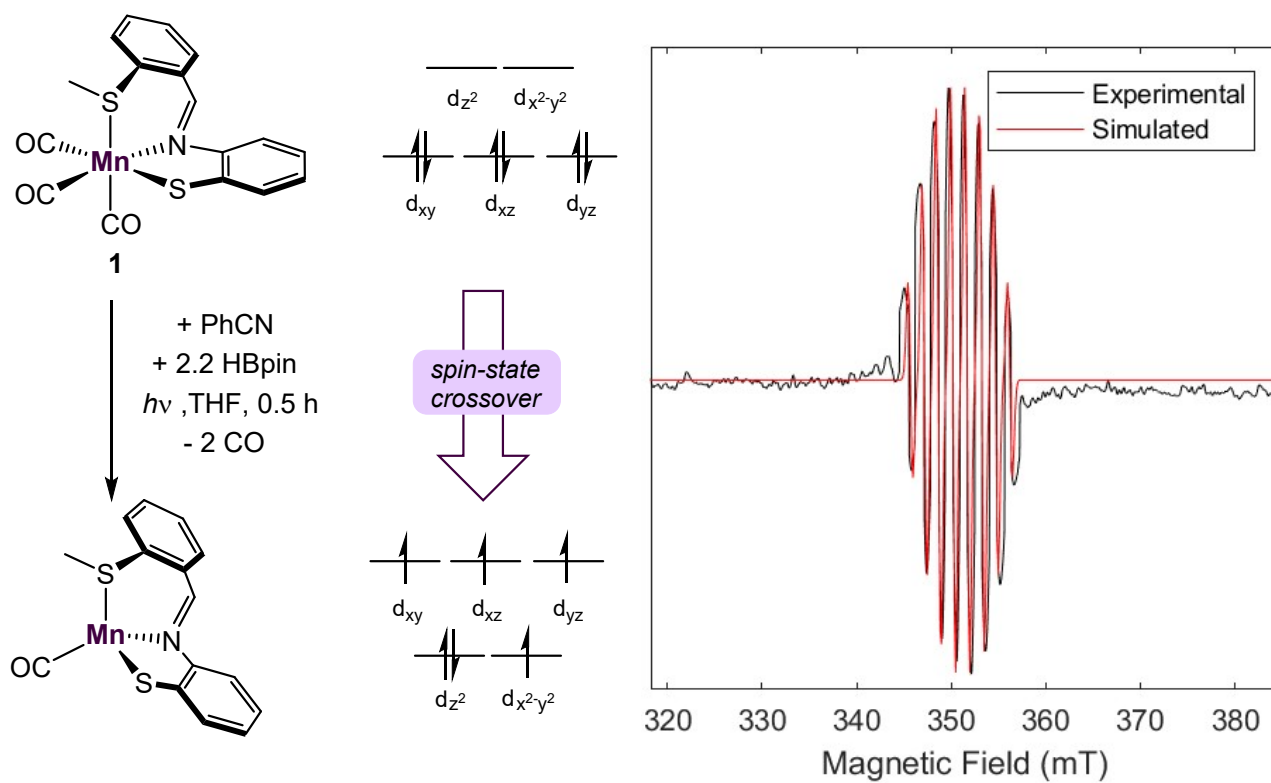


Figure S28. 298 K isotropic EPR spectrum of catalytic reaction mixture in THF after irradiation for 45 min.

VI. Crystallographic Details

Crystals of **1** were mounted on thin glass fibers using cyanoacrylate glue and cooled to 200 ± 2 K during data collection. The data were collected on a Bruker single-crystal diffractometer equipped with a sealed Mo tube source (wavelength 0.71073 Å) and APEX II CCD detector. The raw data collection and processing were performed with the Bruker APEX II software package.⁵ Semi-empirical absorption correction based on equivalent reflections was applied.⁶ Systematic absences and unit cell parameters were consistent with monoclinic $P2_1/n$ (#14) for **1**. The structure was solved by intrinsic phasing and refined with a full-matrix least-squares procedure based on F^2 , using SHELXL.⁷ All non-hydrogen atoms were refined anisotropically. The hydrogen atoms bonded to carbon atoms were placed in idealized positions.

Refinement details for $\text{Mn}(\kappa^3\text{-S}^{\text{Me}}\text{NS})(\text{CO})_3$ (1**).**

The structure was refined without additional restraints / constraints. No disorder was present.

Table S1. Crystal data and structure refinement for $\text{Mn}(\kappa^3\text{-S}^{\text{Me}}\text{NS})(\text{CO})_3$ (1**).**

| | |
|---|---|
| Identification code | tb271_fin |
| Empirical formula | $\text{C}_{17}\text{H}_{12}\text{MnNO}_3\text{S}_2$ |
| Formula weight | 397.34 |
| Temperature/K | 200(2) |
| Crystal system | monoclinic |
| Space group | $P2_1/n$ |
| a/Å | 9.0462(6) |
| b/Å | 18.5124(13) |
| c/Å | 9.7604(7) |
| $\alpha/^\circ$ | 90 |
| $\beta/^\circ$ | 93.8678(19) |
| $\gamma/^\circ$ | 90 |
| Volume/Å ³ | 1630.8(2) |
| Z | 4 |
| $\rho_{\text{calc}}/\text{cm}^3$ | 1.618 |
| μ/mm^{-1} | 1.080 |
| F(000) | 808.0 |
| Crystal size/mm ³ | $0.390 \times 0.180 \times 0.100$ |
| Radiation | MoK α ($\lambda = 0.71073$) |
| 2Θ range for data collection/ $^\circ$ | 4.4 to 56.604 |
| Index ranges | $-12 \leq h \leq 11, -24 \leq k \leq 24, -13 \leq l \leq 12$ |
| Reflections collected | 19706 |
| Independent reflections | 4034 [$R_{\text{int}} = 0.0407$, $R_{\text{sigma}} = 0.0347$] |
| Data/restraints/parameters | 4034/0/218 |

| | |
|--|----------------------------------|
| Goodness-of-fit on F^2 | 1.025 |
| Final R indexes [$I \geq 2\sigma(I)$] | $R_1 = 0.0326$, $wR_2 = 0.0732$ |
| Final R indexes [all data] | $R_1 = 0.0525$, $wR_2 = 0.0835$ |
| Largest diff. peak/hole / $e \text{ \AA}^{-3}$ | 0.42/-0.30 |

Table S2. Bond Lengths for $\text{Mn}(\kappa^3\text{-S}^{\text{Me}}\text{NS})(\text{CO})_3$ (1).

| Atom | Atom | Length/ \AA | Atom | Atom | Length/ \AA |
|------|------|----------------------|------|------|----------------------|
| C1 | C2 | 1.395(3) | C11 | C12 | 1.386(3) |
| C1 | C6 | 1.402(3) | C12 | C13 | 1.382(3) |
| C1 | S1 | 1.754(2) | C13 | S2 | 1.784(2) |
| C2 | C3 | 1.386(3) | C14 | S2 | 1.794(2) |
| C3 | C4 | 1.379(3) | C15 | O1 | 1.146(3) |
| C4 | C5 | 1.386(3) | C15 | Mn1 | 1.797(2) |
| C5 | C6 | 1.390(3) | C16 | O2 | 1.149(3) |
| C6 | N1 | 1.440(2) | C16 | Mn1 | 1.805(2) |
| C7 | N1 | 1.285(3) | C17 | O3 | 1.143(3) |
| C7 | C8 | 1.461(3) | C17 | Mn1 | 1.802(2) |
| C8 | C9 | 1.390(3) | N1 | Mn1 | 2.0587(16) |
| C8 | C13 | 1.409(3) | S1 | Mn1 | 2.3898(6) |
| C9 | C10 | 1.383(3) | S2 | Mn1 | 2.3592(6) |
| C10 | C11 | 1.376(3) | | | |

VII. DFT Calculations

All calculations were carried out using DFT⁸ as implemented in the Jaguar 9.1 suite⁹ of *ab initio* quantum chemistry programs. Geometry optimizations were performed with the B3LYP functional including Grimme's D3 dispersion correction.¹⁰⁻¹⁵ The 6-31G** basis set was used for main group atoms and Mn was represented using the Los Alamos LACVP basis set that includes relativistic effective core potentials. The energies of optimized structures were reevaluated by additional single-point calculations on each optimized geometry using Dunning's correlation consistent triple- ζ basis set cc-pVTZ(-f)¹⁶ which includes a double set of polarization functions. For Mn, we used a modified version of LACVP, designated as LACV3P, in which the exponents were decontracted to match the effective core potential with the triple- ζ quality. For boron, the 6-311G** basis set was used. Solvation energies were evaluated by a self-consistent reaction field (SCRF)¹⁷⁻²⁰ approach based on accurate numerical solutions of the Poisson-Boltzmann equation. In the results reported, solvation calculations were carried out at the same level of theory as the geometry optimization, employing a dielectric constant of $\epsilon = 2.284$ for benzene. As is the case for all continuum models, the

solvation energies are subject to empirical parameterization of the atomic radii that are used to generate the solute surface. We employed the standard set of Van der Waals radii in Jaguar for H (1.150 Å), B(2.042 Å), C(1.900 Å), N(1.600 Å), O (1.600 Å), S(1.900 Å) and Mn (1.480 Å). Analytical vibrational frequencies within the harmonic approximation were computed with the 6-31G**/LACVP basis set to confirm proper convergence to well-defined minima or saddle points on the potential energy surface. The intermediates were confirmed with no vibrational frequency, while transition states showed a single imaginary frequency.

The energy components have been computed with the following protocol. The free energy in solution-phase, $G(\text{sol})$, has been calculated as follows, with $T = 298$ K to match the experimental room temperature conditions:

$$G(\text{sol}) = G(\text{gas}) + G_{\text{solv}}$$

$$G(\text{gas}) = H(\text{gas}) - TS(\text{gas})$$

$$H(\text{gas}) = E(\text{SCF}) + \text{ZPE}$$

$$\Delta E(\text{SCF}) = \sum E(\text{SCF}) \text{ for products} - \sum E(\text{SCF}) \text{ for reactants}$$

$$\Delta G(\text{sol}) = \sum G(\text{sol}) \text{ for products} - \sum G(\text{sol}) \text{ for reactants}$$

Time dependent-density functional theory (TD-DFT) calculations were used to model dissociation of carbonyls upon UV light irradiation. Calculations were carried out with the Q-Chem 5.0 software. Using geometry obtained from the above method, TD-DFT calculations were carried out with the B3LYP-D3 functional and 6-31G**/LACVP basis set.

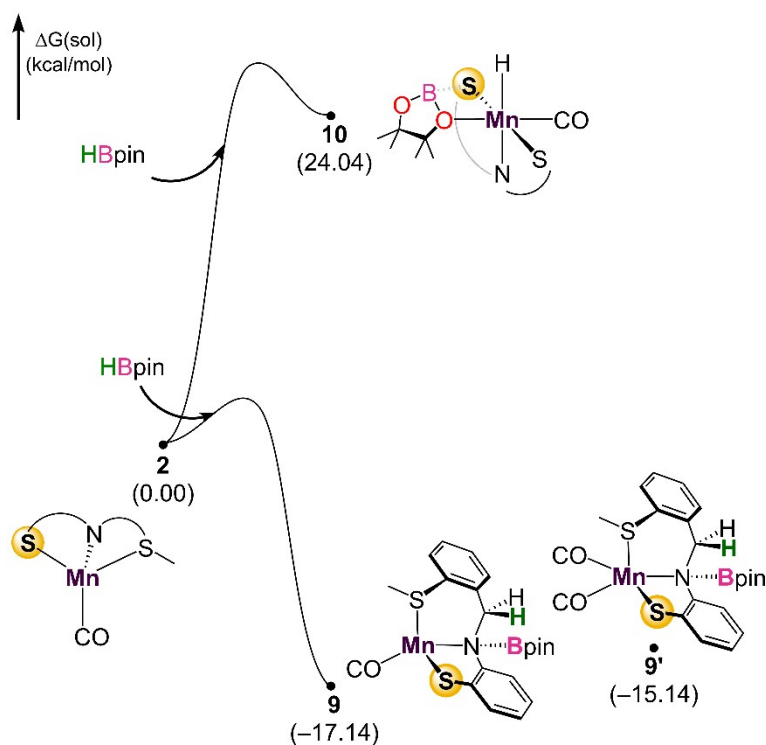


Figure S29. Thermodynamics of the off-cycle intermediate **9** and a proposed Mn–H species.

Two undesirable intermediates **9** and **10** are depicted in **Figure S29**. In accordance with the catalytic incapability of the off-cycle intermediate **9**, HBpin insertion to imine gives rise to a highly exergonic pathway. The intermediate **9** will be a thermodynamic sink considering further hydride transfer steps. Additional CO can bind to **9** resulting in **9'**, while the two energetically close intermediates are unable to participate in the catalytic cycle. Manganese hydride species, **10** is 23.8 kcal/mol higher in energy than **2**. Coordination of nitrile followed by a Bpin moiety transfer step will furnish a more unreasonable pathway than the proposed mechanism in terms of energy. We envision that the instability of the Manganese hydride species is attributed to the SNS ligand scaffold generating a weak ligand field. The catalytic pathway initiates with removing two COs which are strong field ligands. Regarding the Mn(I) center supported by the soft SNS ligand, the hydride moiety which contains dense electrons is placed in a deleterious environment.

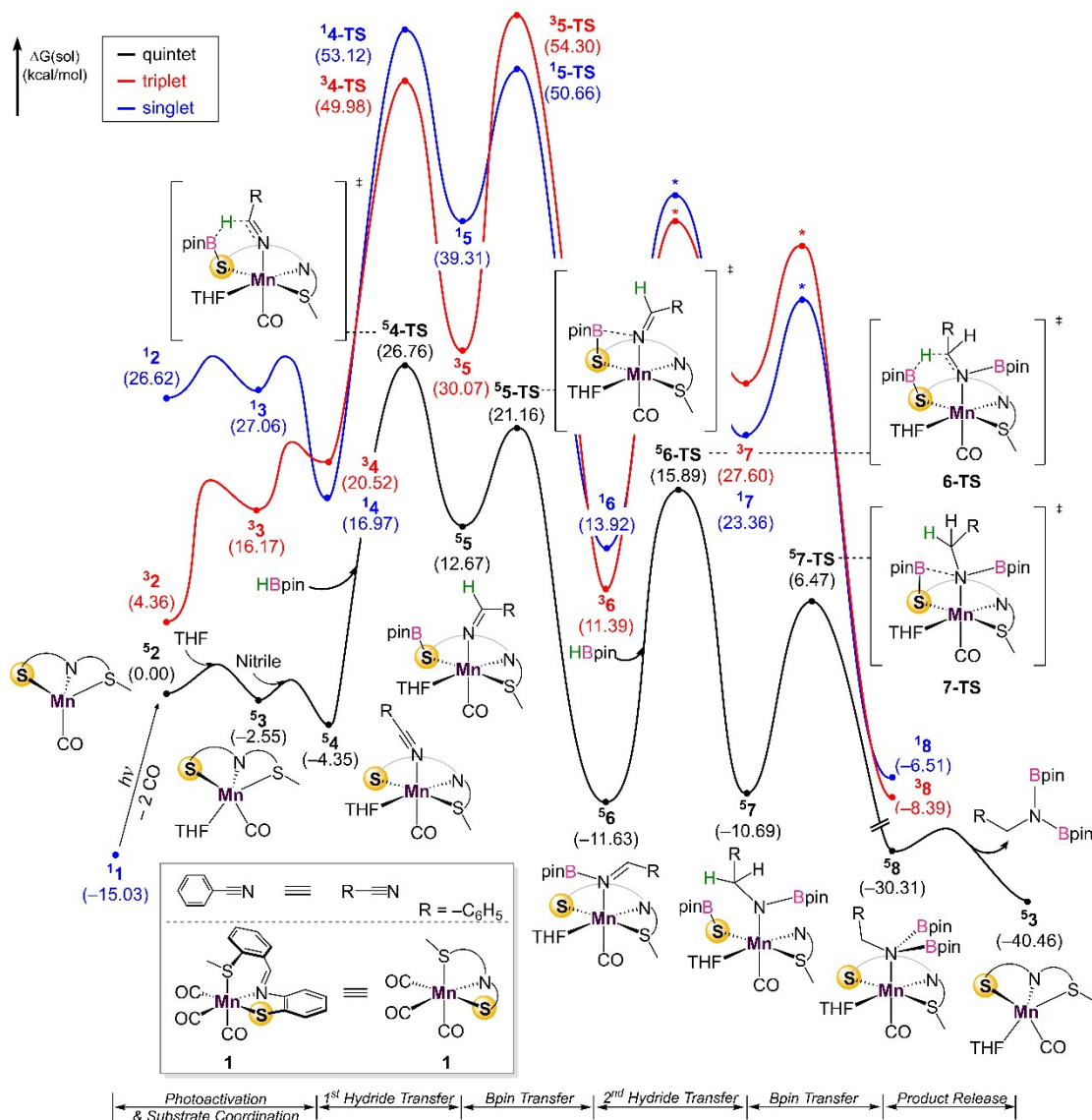


Figure S30. Energy profile including all spin states.

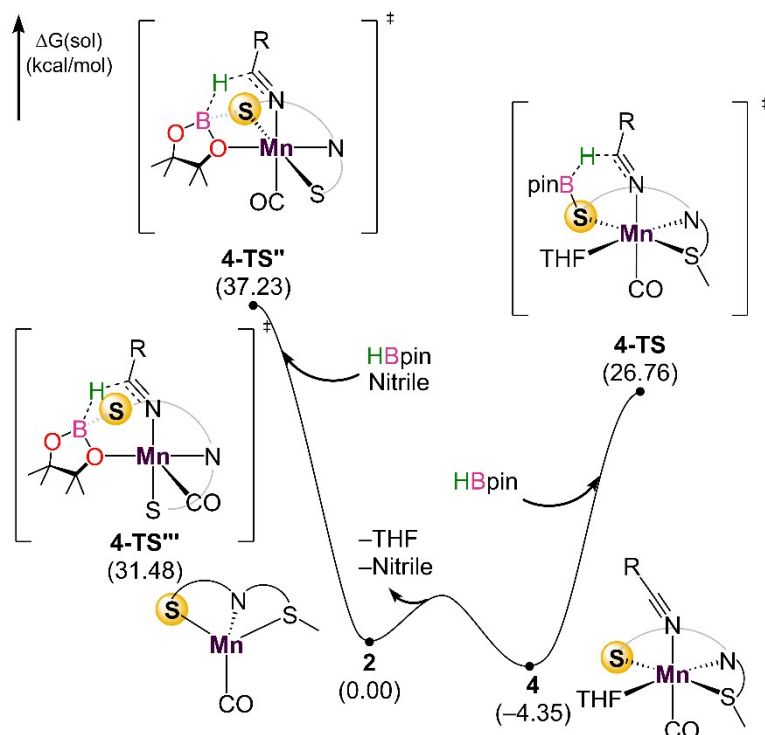


Figure S31. Energy profile for the hydride transfer in the presence and absence of coordinating THF.

The oxygen atom of HBpin can bind to the Mn center in lieu of THF as depicted in **4-TS''**. In the outer sphere mechanism traversing **4-TS**, the π -accepting CO ligand should be in the trans position to the transient amido moiety. In compliance with the formation of a sterically hindered Mn–S–B–O metallacycle in **4-TS''**, a conformer featuring a distinct position of the CO ligand trans to the thiolate moiety, **4-TS'''** is favored by 5.8 kcal/mol. Due to the strong trans effect of the CO ligand, the thiolate moiety departs from the Mn center resulting in 3.6 Å of Mn–S distance. Relieved structural hindrance is reflected in the lower barrier of 35.8 kcal/mol, while the proposed pathway traversing **4-TS** having barrier of 31.1 kcal/mol is still favored. The amido species generated during hydride transfer in **4-TS'''** is not stabilized by an electron-withdrawing ligand. Moreover, the Mn(I) species adopts a trigonal bipyramidal geometry giving rise to the 16-electron species as Mn–S bond cleaves, while **4-TS** affords 18-electron species comprising the stabilized amido moiety.

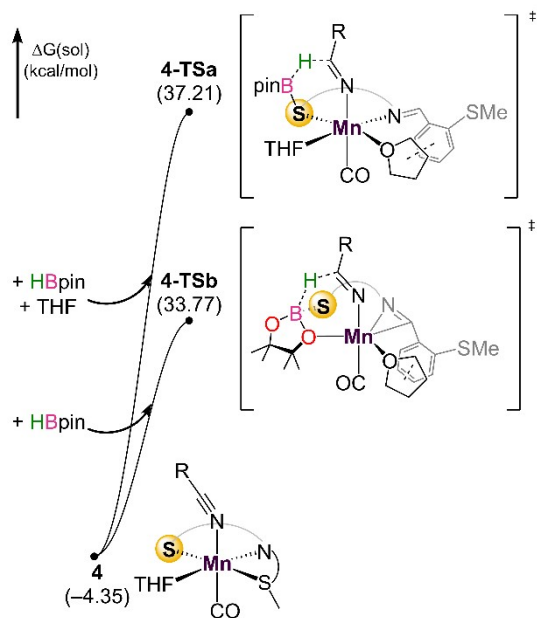


Figure S32. Possible pathways incorporating the cleavage of the thioether group.

| | B3LYP-D3 | M06 |
|---------------|----------|-------|
| 4-TS | 26.76 | 30.04 |
| 4-TS' | 33.92 | 38.10 |
| 4-TS'' | 34.89 | 33.66 |

B3LYP-D3 & M06/cc-pVTZ(-f)//B3LYP-D3 & M06/LACVP**PCM ($\epsilon = 7.6$ for THF)
 Energies in kcal·mol⁻¹
 Referenced to [SNS]Mn(CO)(THF)

Figure S33. Comparison between the B3LYP-D3 functional and M06 functional.

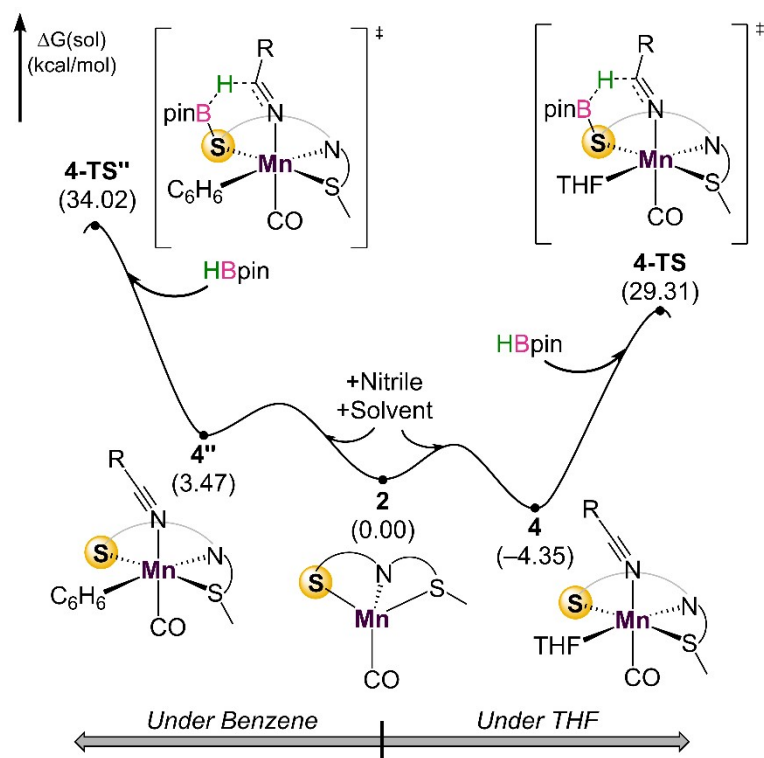


Figure S34. Comparison of the energy profiles for the reaction under THF and benzene as the solvent.

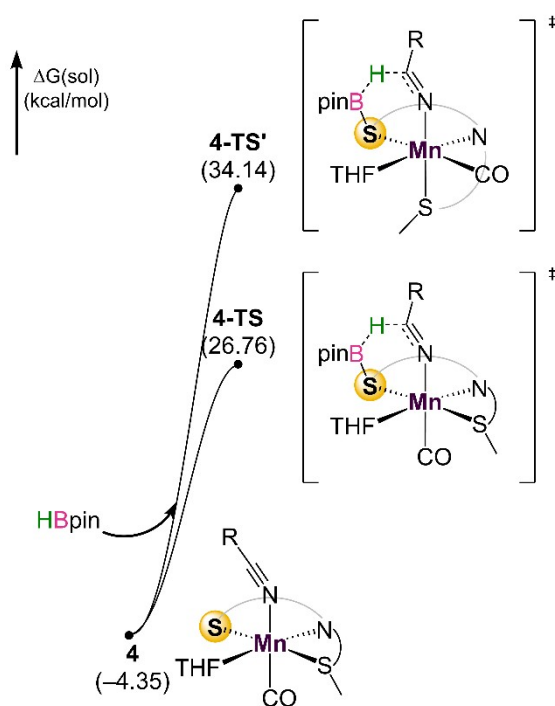


Figure S35. Comparison between *fac*- and *mer*-conformations in the turnover-limiting transition state.

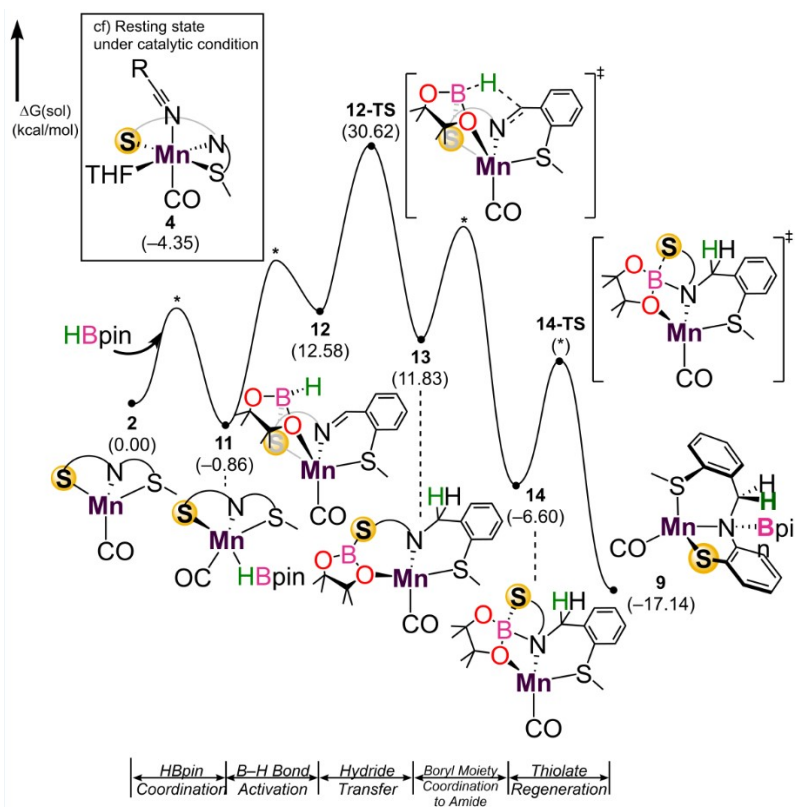


Figure S36. Off-cycle pathway in the absence of benzonitrile.

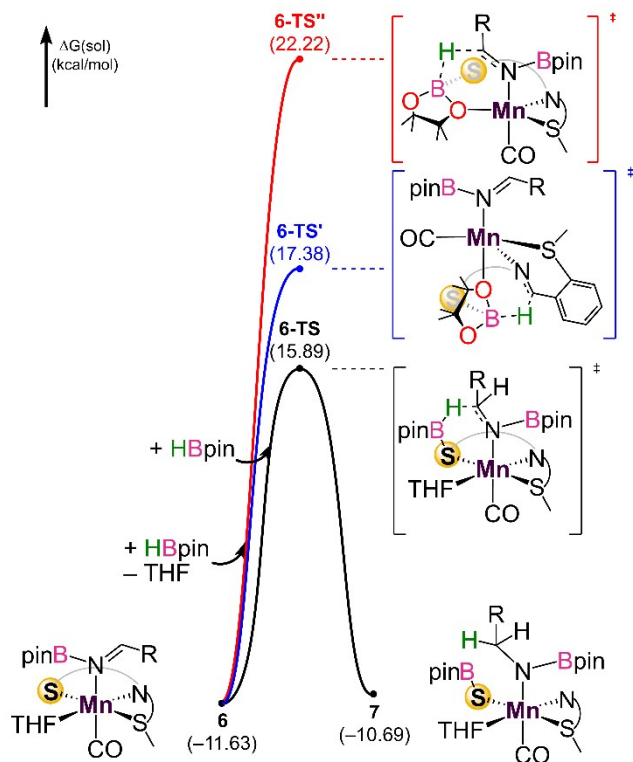


Figure S37. Comparison of transition states related to THF dissociation in intermediate 6.

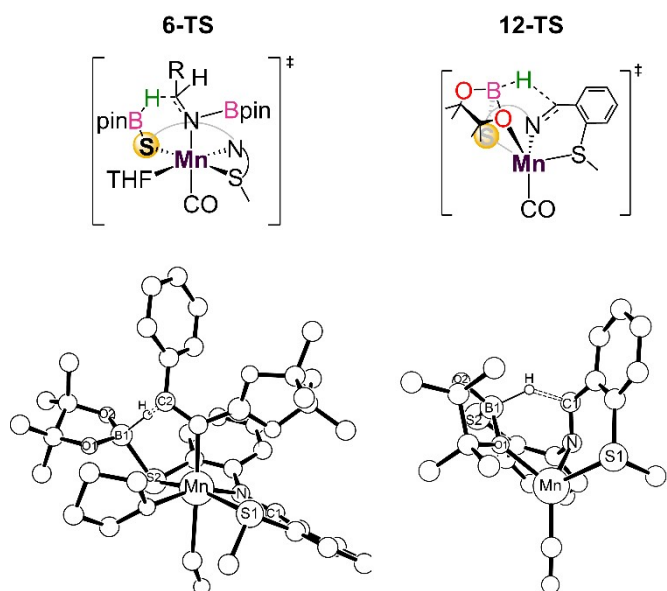


Figure S38. Comparison of 3D structures of **6-TS** and **12-TS**.

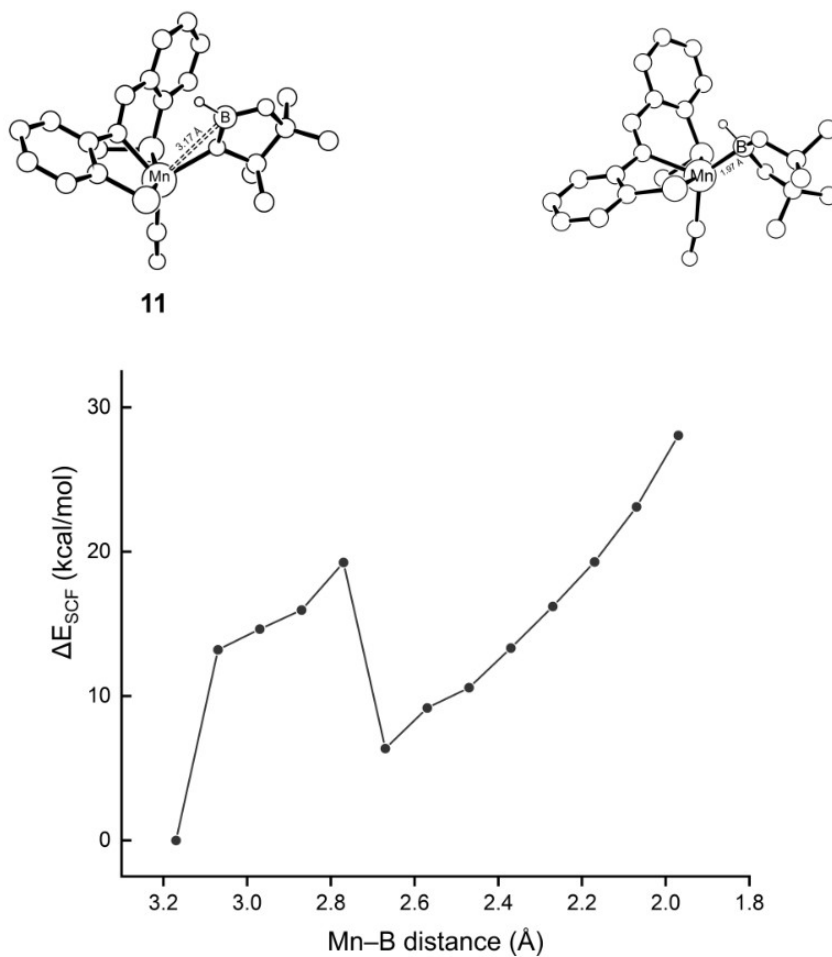


Figure S39. Scanning the potential energy surface of the Mn–B in **11**. Forced geometries are unstable and an adduct could not be optimized.

Table S3 Computed energy components for DFT optimized structures

| | E_{SCF} (eV) | ZPE (kcal/mol) | S_{gas} (cal/mol·K) | G_{solv} (kcal/mol) |
|-------------------------------|----------------------------------|-----------------------------|------------------------------------|------------------------------------|
| Label | B3LYP-D3/ cc-pVTZ(-f), LACV3P | B3LYP-D3/ 6-31G**, LACVP | B3LYP-D3/ 6-31G**, LACVP | B3LYP-D3/ 6-31G**, LACVP |
| Benzene | -6322.006 | 63.16 | 64.09 | -2.30 |
| Benzonitrile | -8832.844 | 62.36 | 77.13 | -6.64 |
| CO | -3084.527 | 3.15 | 47.24 | 0.00 |
| Diborylamine (product) | -31259.999 | 308.87 | 175.52 | -8.57 |
| HBpin | -11211.936 | 120.07 | 90.99 | -4.11 |
| Off-cycle intermediate, 9 | -55009.910 | 268.56 | 196.53 | -13.45 |
| Off-cycle intermediate, 9' | -58094.859 | 272.97 | 212.01 | -12.46 |
| Mn–H species, 10 | -55007.832 | 261.43 | 199.82 | -12.08 |
| THF | -6327.710 | 73.37 | 72.17 | -3.00 |
| 1 | -49967.473 | 157.97 | 158.41 | -12.77 |
| 2 | -43796.262 | 144.76 | 152.64 | -13.91 |
| ³ 2 | -43796.222 | 146.54 | 143.33 | -15.03 |
| ¹ 2 | -43795.191 | 146.38 | 140.66 | -17.18 |
| 3 | -50124.836 | 219.11 | 181.93 | -10.96 |
| ³ 3 | -50124.270 | 220.76 | 171.66 | -12.35 |
| ¹ 3 | -50123.898 | 221.55 | 165.65 | -12.62 |
| 4 | -58958.301 | 281.25 | 229.29 | -13.74 |
| ³ 4 | -58957.422 | 281.90 | 226.35 | -13.01 |
| ¹ 4 | -58957.827 | 285.05 | 206.11 | -16.40 |
| 4'' | -58952.280 | 270.71 | 227.52 | -12.64 |
| 4-TS | -70170.020 | 401.65 | 260.80 | -9.74 |
| ³ 4-TS | -63840.801 | 327.80 | 223.89 | -9.73 |
| ¹ 4-TS | -63840.674 | 330.01 | 212.40 | -15.16 |

| | | | | |
|-------------------|------------|--------|--------|--------|
| 4-TS' | -70169.685 | 401.79 | 256.36 | -11.63 |
| 4-TS'' | -70163.979 | 391.06 | 259.77 | -9.51 |
| 4-TS''' | -63841.398 | 327.03 | 228.67 | -12.06 |
| 4-TSa | -76497.964 | 476.08 | 291.76 | -10.11 |
| 4-TSb | -70169.490 | 401.30 | 259.59 | -14.83 |
| 5 | -70170.604 | 403.47 | 271.63 | -9.02 |
| ³ 5 | -70170.281 | 405.70 | 251.88 | -9.54 |
| ¹ 5 | -70169.978 | 406.46 | 244.90 | -10.12 |
| 5-TS | -70170.458 | 403.60 | 255.16 | -8.94 |
| ³ 5-TS | -70169.428 | 406.29 | 241.56 | -8.64 |
| ¹ 5-TS | -70169.560 | 406.28 | 240.76 | -9.46 |
| 6 | -70171.500 | 404.85 | 263.68 | -16.42 |
| ³ 6 | -70170.759 | 405.50 | 264.45 | -13.24 |
| ¹ 6 | -70170.895 | 408.61 | 243.93 | -16.81 |
| 6-TS | -81383.325 | 525.13 | 302.74 | -11.26 |
| 6-TS' | -75054.799 | 449.65 | 273.71 | -12.96 |
| 6-TS'' | -75054.763 | 450.32 | 264.63 | -12.32 |
| 7 | -81384.497 | 527.19 | 309.92 | -10.73 |
| ³ 7 | -81383.115 | 527.29 | 298.63 | -10.12 |
| ¹ 7 | -81383.593 | 531.77 | 284.36 | -12.07 |
| 7-TS | -81383.854 | 527.17 | 300.66 | -11.14 |
| 8 | -81385.333 | 529.09 | 306.50 | -14.09 |
| ³ 8 | -81384.562 | 529.90 | 303.23 | -13.97 |
| ¹ 8 | -81384.644 | 532.29 | 290.02 | -16.54 |
| 11 | -55008.981 | 265.15 | 202.88 | -13.51 |
| 12 | -55008.567 | 265.26 | 198.82 | -10.93 |

| | | | | |
|-------|------------|--------|--------|--------|
| 12-TS | -55007.865 | 264.64 | 190.96 | -10.60 |
| 13 | -55008.701 | 267.43 | 196.90 | -11.13 |
| 14 | -55009.578 | 268.29 | 190.56 | -12.08 |

Table S4 Coordinates and vibrational frequencies for optimized structure

Coordinates

=====
Benzene
=====

C1 2.850831 0.621417 2.515819
 C2 1.541382 0.520834 2.990118
 C3 3.355939 1.860838 2.117780
 H4 1.148406 -0.443438 3.299794
 H5 4.374694 1.939092 1.748774
 C6 0.737040 1.659674 3.066378
 C7 2.551596 2.999677 2.194039
 H8 -0.281715 1.581419 3.435384
 H9 2.944572 3.963950 1.884363
 C10 1.242147 2.899094 2.668338
 H11 0.616368 3.785113 2.727668
 H12 3.476610 -0.264602 2.456489

=====
Benzonitrile
=====

C1 -1.356772 -0.000004 -3.530825
 C2 -2.514299 -0.355166 -2.834338
 C3 -0.199246 0.355152 -2.834328
 H4 -3.413275 -0.631047 -3.376948
 H5 0.699736 0.631035 -3.376931
 C6 -2.521015 -0.357164 -1.441759
 C7 -0.192562 0.357137 -1.441754
 H8 -3.414855 -0.631366 -0.891723
 H9 0.701272 0.631334 -0.891703
 C10 -1.356802 -0.000016 -0.741197
 H11 -1.356768 0.000004 -4.616845
 C12 -1.356735 0.000006 0.693504
 N13 -1.356608 0.000049 1.856712

=====
CO
=====

C1 -0.293499 0.001892 -2.165194
 O2 -0.830929 0.125413 -3.161392

=====
Diborylamine
=====

C1 -5.331882 0.197436 -2.942489
 C2 -5.378927 1.307495 -1.827688
 O3 -3.977584 1.658762 -1.686571
 C4 -6.108842 2.578547 -2.281694
 C5 -5.905872 0.845054 -0.473550
 O6 -4.183976 0.608677 -3.727321
 C7 -6.553298 0.143099 -3.855053
 C8 -5.017514 -1.196470 -2.384712
 B9 -3.383559 1.366610 -2.892335
 H10 -2.012096 0.410873 -4.883020
 H11 -5.746888 2.906529 -3.260625
 H12 -7.190572 2.425322 -2.341968
 H13 -5.907392 3.375066 -1.560511
 H14 -6.423249 -0.649871 -4.597280
 H15 -7.458137 -0.073498 -3.277249

H16 -6.692971 1.083820 -4.389763
 H17 -5.890820 1.681178 0.231333
 H18 -6.937875 0.489088 -0.562191
 H19 -5.291444 0.044089 -0.059362
 H20 -4.150529 -1.162818 -1.718725
 H21 -5.866311 -1.612892 -1.833851
 H22 -4.781355 -1.864220 -3.217775
 C23 -3.163293 4.437554 -6.485276
 C24 -2.921726 4.100146 -7.819427
 C25 -2.280319 2.892947 -8.115683
 H26 -3.232086 4.765479 -8.620485
 H27 -3.665476 5.370767 -6.240303
 C28 -2.765256 3.580690 -5.455264
 H29 -2.972505 3.848629 -4.421999
 C30 -2.124811 2.371093 -5.741823
 H31 -2.090186 2.613870 -9.151199
 C32 -1.888209 2.039549 -7.085419
 H33 -1.392659 1.099672 -7.325395
 C34 -1.648312 1.417480 -4.653602
 N35 -2.078862 1.785781 -3.298245
 C36 -0.448725 4.066184 -0.952034
 C37 0.354409 4.276680 -2.288241
 O38 -1.621453 3.343421 -1.409054
 C39 -0.904894 5.349882 -0.265002
 C40 0.280816 3.157062 0.044506
 O41 -0.027174 3.105566 -3.055660
 C42 -0.116495 5.501753 -3.084219
 C43 1.871473 4.291791 -2.135950
 B44 -1.265321 2.714798 -2.581280
 H45 -1.206253 5.510933 -3.178073
 H46 0.202838 6.437463 -2.615031
 H47 0.305478 5.451285 -4.091504
 H48 2.338420 4.431002 -3.115333
 H49 2.185413 5.115960 -1.486526
 H50 2.239476 3.353972 -1.716377
 H51 -1.458781 5.102744 0.645208
 H52 -0.043434 5.966014 0.013909
 H53 -1.561504 5.935333 -0.910763
 H54 0.632974 2.245170 -0.446234
 H55 1.137745 3.662349 0.500564
 H56 -0.417687 2.869875 0.834955
 H57 -0.554033 1.384387 -4.676394

=====
HBpin
=====

C1 1.732851 3.125565 2.270194
 C2 1.678059 3.555808 3.786512
 B3 1.521066 5.383667 2.441474
 H4 1.417159 6.521531 2.113864
 O5 1.304723 4.339117 1.585048
 O6 1.866451 4.999959 3.708139
 C7 3.153034 2.824263 1.775798
 H8 3.840873 3.631171 2.042615
 H9 3.533496 1.887314 2.192981
 H10 3.137358 2.739934 0.685998
 C11 2.780080 2.970677 4.665079

H12 2.667749 3.338863 5.688617
H13 2.716251 1.877657 4.685592
H14 3.771397 3.257599 4.311313
C15 0.787884 1.990831 1.885264
H16 0.885061 1.779129 0.816856
H17 1.034739 1.078713 2.438507
H18 -0.253111 2.250311 2.083459
C19 0.305220 3.330532 4.433076
H20 -0.493724 3.750811 3.816160
H21 0.104906 2.266684 4.589758
H22 0.283572 3.834958 5.402530

=====
Off-cycle intermediate, 9'
=====

Mn1 -1.038075 -0.275055 -0.493579
C2 -2.886073 0.103722 -0.065677
O3 -4.004996 0.306791 0.191284
N4 0.310911 -1.346103 0.988567
C5 1.618770 -0.685438 0.992607
C6 1.983102 0.228719 -0.017674
C7 3.286398 0.764706 0.041190
C8 4.176402 0.419298 1.051185
C9 3.794828 -0.475836 2.055588
C10 2.514609 -1.019176 2.014362
H11 2.196621 -1.722970 2.781033
H12 4.479031 -0.741328 2.855577
H13 5.170989 0.857649 1.059606
H14 3.584554 1.470254 -0.728182
S15 0.906392 0.749833 -1.331910
C16 0.409230 -2.800323 0.605015
C17 1.123090 -3.024705 -0.709904
C18 0.481661 -2.901834 -1.957191
C19 1.190980 -3.114265 -3.142341
C20 2.551903 -3.413845 -3.100195
C21 3.205455 -3.520247 -1.874650
C22 2.486834 -3.334910 -0.695622
H23 2.994128 -3.399565 0.262421
H24 4.267261 -3.743192 -1.834966
H25 3.096052 -3.561604 -4.028637
H26 0.694665 -3.036373 -4.102824
S27 -1.264931 -2.455148 -1.990064
C28 -1.400718 -1.517566 -3.559083
H29 -2.350300 -0.981244 -3.503824
H30 -0.574383 -0.805650 -3.617488
H31 -1.409865 -2.188841 -4.419246
H32 0.943543 -3.341257 1.393858
C33 -1.154200 -0.142602 4.131200
C34 -1.949532 -1.488835 3.886975
O35 -1.182562 -2.115532 2.813629
C36 -1.967785 -2.446088 5.074201
C37 -3.368353 -1.275368 3.353606
O38 -0.513592 0.089742 2.846157
C39 -0.020298 -0.278287 5.153889
C40 -2.027491 1.063937 4.457517
B41 -0.470224 -1.116125 2.204455
H42 -0.609376 -3.195682 0.590878
H43 -0.959301 -2.742824 5.366831
H44 -2.460935 -1.981405 5.934063
H45 -2.524004 -3.349562 4.808917

H46 0.596117 0.623567 5.114946
H47 -0.404609 -0.397750 6.170960
H48 0.621453 -1.132417 4.918779
H49 -3.769132 -2.237901 3.023121
H50 -4.027736 -0.874848 4.129051
H51 -3.379122 -0.594419 2.501316
H52 -2.732105 1.273857 3.651350
H53 -2.588064 0.894829 5.382851
H54 -1.396494 1.946408 4.594602

=====
Off-cycle intermediate, 9'
=====

Mn -0.875688358 -0.041342832 -0.643521367
C -1.474169940 1.355516870 0.670474165
O -1.716776656 2.260125491 1.336145510
N 0.748396042 -1.541970602 1.289364314
C 1.921937625 -0.698144251 1.349989643
C 2.265839628 0.205161556 0.319944309
C 3.440036136 0.967762990 0.490786765
C 4.240782610 0.844596016 1.620303974
C 3.892976024 -0.053155297 2.632856093
C 2.738358121 -0.814686021 2.483268244
H 2.442961535 -1.517133979 3.259232645
H 4.506370062 -0.154709966 3.523226790
H 5.135356103 1.455206042 1.711942493
H 3.710752257 1.670932834 -0.290865991
S 1.358316260 0.433890585 -1.191880937
C 0.999660949 -2.919047198 0.794272286
C 1.195952669 -3.008657783 -0.702650200
C 0.118200741 -2.891784174 -1.603174074
C 0.332826412 -2.936564964 -2.981294620
C 1.627127294 -3.099397351 -3.477389298
C 2.703303833 -3.213727969 -2.602682514
C 2.478701803 -3.170789244 -1.227307240
H 3.315888272 -3.240450297 -0.538230380
H 3.712635194 -3.325392789 -2.986727128
H 1.786585752 -3.124225011 -4.551491265
H -0.487818795 -2.827313965 -3.679917951
S -1.511463862 -2.578199956 -0.893844259
C -2.631908471 -2.664373580 -2.330688126
H -3.634887203 -2.496486321 -1.932658553
H -2.402062917 -1.890574525 -3.064609487
H -2.582781483 -3.655477613 -2.786018482
H 1.890549153 -3.317163741 1.296089011
C -1.403747803 -0.508576513 4.049833620
C -2.184750938 -1.730216787 3.434822111
O -1.163980226 -2.361144569 2.615154267
C -2.692187697 -2.747223466 4.450465779
C -3.316537508 -1.310187110 2.488219338
O -0.438328114 -0.207919630 3.006683086
C -0.596083136 -0.881462443 5.298984350
C -2.249376019 0.732262855 4.316617888
B -0.253216603 -1.371894039 2.294119063
H 0.151016099 -3.536360677 1.101319159
H -1.870625649 -3.180789276 5.023136779
H -3.396972456 -2.278619207 5.145243113
H -3.210233196 -3.559617383 3.932638695
H 0.089871056 -0.062105388 5.529753922
H -1.243420395 -1.050576123 6.164594175

H -0.001525332 -1.783351666 5.125379971
H -3.668223470 -2.193056866 1.947104638
H -4.159117716 -0.873043196 3.031356336
H -2.961054852 -0.582597436 1.752664650
H -2.712727231 1.110837210 3.405628601
H -3.033555130 0.509526426 5.048033812
H -1.616886825 1.526557899 4.722849123
O -2.303558261 1.061502329 -3.251119758
C -1.860544582 0.638963582 -2.275199127

Mn-H species, 10

Mn1 -1.452986 -0.822408 -0.987755
C2 -1.424118 -3.383376 -0.844131
O3 -1.643035 -4.492815 -0.732747
N4 0.589123 -0.865196 -0.499679
C5 1.208622 0.054397 0.347620
C6 0.503375 0.763689 1.354168
C7 1.151063 1.706755 2.155769
C8 2.508261 1.981525 1.992937
C9 3.219079 1.299120 1.004049
C10 2.583205 0.361815 0.199170
H11 3.135554 -0.129099 -0.596135
H12 4.274318 1.507690 0.846918
H13 2.996535 2.717023 2.624646
H14 0.578675 2.220491 2.922351
S15 -1.243524 0.439728 1.711234
C16 1.361522 -1.901706 -0.931475
C17 1.185346 -2.699258 -2.096744
C18 0.362569 -2.417845 -3.244693
C19 0.237251 -3.349047 -4.281444
C20 0.908146 -4.569450 -4.250608
C21 1.765359 -4.843983 -3.169498
C22 1.904930 -3.936077 -2.140803
H23 2.557460 -4.170783 -1.303079
H24 2.319438 -5.778287 -3.138099
H25 0.786985 -5.281664 -5.060345
H26 -0.391568 -3.097693 -5.130968
S27 -0.527373 -0.875028 -3.471312
C28 0.838944 0.355387 -3.475715
H29 0.350300 1.347078 -3.793134
H30 1.291476 0.432550 -2.425869
H31 1.618029 0.022599 -4.263683
H32 2.191067 -2.198789 -0.286089
C33 -3.500274 2.887267 -0.591190
C34 -2.259670 2.635077 -1.533589
O35 -1.538531 1.572460 -0.814425
C36 -2.619988 2.116091 -2.920185
C37 -1.286018 3.811326 -1.615347
O38 -3.002552 2.456516 0.721705
C39 -4.700486 1.991396 -0.909910
C40 -3.920337 4.348188 -0.484076
B41 -1.980089 1.600668 0.496928
H42 -3.169962 -0.948457 -0.920250
H43 -3.112077 1.143507 -2.859574
H44 -3.283761 2.821547 -3.429964
H45 -1.717747 2.007422 -3.526625
H46 -5.438139 2.097312 -0.109659
H47 -5.171219 2.283568 -1.853452

H48 -4.401252 0.940141 -0.966369
H49 -0.371644 3.478714 -2.114477
H50 -1.713388 4.641289 -2.185141
H51 -1.015166 4.170283 -0.618774
H52 -3.113471 4.976740 -0.102679
H53 -4.226988 4.726357 -1.465113
H54 -4.771500 4.434936 0.196133

THF

H1 -0.970467 -0.001838 -3.396327
O2 0.386955 0.367352 -1.865922
C3 0.145626 -0.323432 -0.636131
C4 -1.327212 -0.756304 -0.663309
C5 -1.958525 0.378171 -1.484006
C6 -0.855536 0.651458 -2.516544
H7 0.840807 -1.168195 -0.560065
H8 0.340907 0.352010 0.212195
H9 -1.757754 -0.868401 0.335593
H10 -1.435846 -1.711810 -1.189407
H11 -2.119036 1.259854 -0.852778
H12 -2.914854 0.110269 -1.941598
H13 -0.843669 1.690071 -2.868432

I

Mn1 -0.009895 -0.007277 -0.021713
C2 1.284727 0.179190 1.234747
O3 2.105600 0.307977 2.031955
C4 -0.245064 1.783746 -0.104581
O5 -0.396920 2.924648 -0.206327
C6 -1.279145 -0.220139 1.245823
O7 -2.072422 -0.328572 2.081037
N8 0.391661 -2.032683 -0.307678
C9 1.784801 -2.324656 -0.428184
C10 2.562018 -1.351757 -1.097389
C11 3.921867 -1.641902 -1.310214
C12 4.483275 -2.827093 -0.846066
C13 3.708513 -3.761046 -0.145662
C14 2.355230 -3.508939 0.056005
H15 1.747561 -4.207205 0.625032
H16 4.159510 -4.664233 0.252934
H17 5.541623 -3.014907 -1.005790
H18 4.534816 -0.910009 -1.827131
S19 1.819020 0.154641 -1.627502
C20 -0.454420 -2.996707 -0.453718
C21 -1.914914 -2.856066 -0.468366
C22 -2.588609 -1.745118 -1.033076
C23 -3.983880 -1.714370 -1.032310
C24 -4.717147 -2.763298 -0.472611
C25 -4.065460 -3.872557 0.063406
C26 -2.674470 -3.918962 0.043336
H27 -2.153779 -4.782100 0.450146
H28 -4.633080 -4.695184 0.485956
H29 -5.801788 -2.711034 -0.470220
H30 -4.516849 -0.877848 -1.467478
S31 -1.590463 -0.460387 -1.808055
C32 -2.762248 0.932104 -1.927157
H33 -2.159415 1.793014 -2.221198

H34 -3.517651 0.743579 -2.691869
H35 -3.222850 1.128619 -0.956921
H36 -0.079233 -4.010728 -0.611155

2

Mn1 0.025025 -0.797409 0.603353
C2 -1.372434 -0.715737 1.962152
O3 -2.188727 -0.592090 2.779395
N4 0.586500 -2.275138 -0.837257
C5 1.964397 -2.367655 -1.124419
C6 2.834453 -1.423265 -0.509119
C7 4.210912 -1.525969 -0.795105
C8 4.706691 -2.491747 -1.659815
C9 3.837182 -3.393254 -2.289938
C10 2.478161 -3.322368 -2.023469
H11 1.799307 -3.987365 -2.548629
H12 4.216518 -4.126814 -2.994395
H13 5.773746 -2.533640 -1.860677
H14 4.885489 -0.818679 -0.323042
S15 2.289303 -0.141489 0.582522
C16 -0.254650 -3.238876 -1.062303
C17 -1.705013 -3.110250 -0.891747
C18 -2.444101 -1.894002 -0.992605
C19 -3.819527 -1.911925 -0.739902
C20 -4.477635 -3.096482 -0.407579
C21 -3.773618 -4.298952 -0.348409
C22 -2.407501 -4.295199 -0.599930
H23 -1.845957 -5.224207 -0.542829
H24 -4.282287 -5.226270 -0.106074
H25 -5.545433 -3.073791 -0.211740
H26 -4.400471 -1.001178 -0.810469
S27 -1.614791 -0.379366 -1.515239
C28 -2.813698 0.922732 -1.067616
H29 -2.272148 1.861265 -1.205480
H30 -3.690676 0.919105 -1.718246
H31 -3.100159 0.825174 -0.017939
H32 0.098969 -4.229610 -1.361774

3²

Mn 0.070054014 -0.456076579 0.140849883
C -0.296538606 1.053400254 1.064813320
O -0.585126749 2.027301997 1.638639762
N 0.482411247 -2.268661345 -0.698938143
C 1.862094105 -2.550461547 -0.954236142
C 2.815040230 -1.736017335 -0.306887436
C 4.175711869 -2.032327732 -0.489360600
C 4.577801052 -3.066255768 -1.329910330
C 3.627833725 -3.825210541 -2.023135256
C 2.274233807 -3.562538160 -1.836864442
H 1.538583591 -4.115481302 -2.413149555
H 3.939003848 -4.598583985 -2.718500002
H 5.637341033 -3.263847707 -1.468688765
H 4.913920572 -1.422642196 0.022640374
S 2.282246184 -0.368698921 0.672203003
C -0.339767466 -3.280041617 -0.791186017
C -1.796248376 -3.310736370 -0.775429667
C -2.687474011 -2.207459663 -0.803196307

C -4.067474998 -2.426252641 -0.868171498
C -4.592932443 -3.717149215 -0.859468443
C -3.733489381 -4.816098609 -0.818547462
C -2.362831470 -4.606085044 -0.792998178
H -1.692062741 -5.460977251 -0.779034301
H -4.129189711 -5.826820314 -0.815355436
H -5.669027396 -3.858841293 -0.889548553
H -4.747511936 -1.584040316 -0.920744264
S -2.052574169 -0.531894050 -0.826852677
C -3.327173367 0.380039788 0.124405335
H -2.867524116 1.332315568 0.389841895
H -4.213105004 0.556253951 -0.487099709
H -3.580828411 -0.172004452 1.030603632
H 0.100900403 -4.269663531 -0.915055692

1²

Mn 0.085546701 -0.329479090 0.033956827
C -0.677462913 -0.804581900 1.547009401
O -1.159740913 -1.137214797 2.556514660
N 0.508308852 -2.162205929 -0.617750073
C 1.881532003 -2.393090336 -0.908189547
C 2.812674484 -1.421350292 -0.464640891
C 4.175849831 -1.633777669 -0.743220957
C 4.600638497 -2.749578308 -1.452796834
C 3.669490649 -3.684198773 -1.927089344
C 2.319398131 -3.497429488 -1.663301727
H 1.595815368 -4.187986252 -2.084724927
H 3.993886558 -4.535035843 -2.518084447
H 5.659074878 -2.884746115 -1.658252904
H 4.894935488 -0.899613276 -0.393464176
S 2.280488299 0.009878331 0.419320191
C -0.326958704 -3.161973787 -0.635408979
C -1.783817860 -3.109629671 -0.608645071
C -2.600166800 -1.975786653 -0.866046126
C -3.988664101 -2.116873863 -0.914392279
C -4.597653255 -3.344637422 -0.652878167
C -3.813251005 -4.466369635 -0.383431324
C -2.430425555 -4.344590440 -0.386319413
H -1.814902552 -5.220718164 -0.199651302
H -4.274692607 -5.428163774 -0.183693099
H -5.680875209 -3.418832776 -0.664400952
H -4.612947529 -1.261246510 -1.144741326
S -1.842803063 -0.377129748 -1.209774364
C -3.066521777 0.779423815 -0.485126632
H -2.558571106 1.745382455 -0.442494487
H -3.955724103 0.872335779 -1.110916092
H -3.323925032 0.451561465 0.523283852
H 0.078384547 -4.173145163 -0.688318335

3

Mn1 -0.698809 -0.305275 0.595453
C2 -2.686290 -0.548225 0.948889
O3 -3.801989 -0.707985 1.215550
N4 0.695295 -1.919450 0.156151
C5 1.883587 -1.685317 0.899285
C6 2.248721 -0.336150 1.156308
C7 3.416101 -0.113116 1.908909

C8 4.186845 -1.167575 2.394468
C9 3.800070 -2.491650 2.159556
C10 2.650566 -2.741929 1.414642
H11 2.318626 -3.764183 1.254592
H12 4.378050 -3.317548 2.563132
H13 5.081212 -0.955527 2.974235
H14 3.708139 0.913292 2.109231
S15 1.293625 1.039452 0.555337
C16 0.680400 -2.881323 -0.721146
C17 -0.476148 -3.261468 -1.521098
C18 -1.455860 -2.373447 -2.041423
C19 -2.575064 -2.894348 -2.705960
C20 -2.734306 -4.266161 -2.883969
C21 -1.741002 -5.145211 -2.437908
C22 -0.626453 -4.640335 -1.782564
H23 0.140672 -5.320742 -1.420102
H24 -1.838095 -6.214227 -2.601175
H25 -3.610957 -4.644478 -3.401252
H26 -3.310775 -2.206191 -3.110443
S27 -1.300952 -0.581377 -2.029078
C28 0.322011 -0.317457 -2.841697
H29 0.388807 0.756671 -3.023798
H30 1.132547 -0.607903 -2.174060
H31 0.356909 -0.863308 -3.786310
H32 1.577577 -3.492020 -0.862652
H33 -0.630294 0.238156 4.480876
O34 -0.518452 -0.978944 2.795174
C35 -0.627822 -2.368218 3.192982
C36 0.064344 -2.474696 4.561171
C37 0.982335 -1.239666 4.578621
C38 0.136016 -0.212809 3.834399
H39 -1.687982 -2.641326 3.221969
H40 -0.129997 -2.964061 2.423072
H41 0.610394 -3.415880 4.669796
H42 -0.672140 -2.415265 5.370266
H43 1.902243 -1.433624 4.020173
H44 1.245093 -0.914822 5.589349
H45 0.703324 0.575104 3.335469

33

Mn -0.809991432 -0.587127150 0.661844291
C -2.356935233 -1.487816331 0.909335973
O -3.355438021 -2.069964203 1.096104465
N 0.702935693 -2.051421188 0.149578698
C 1.890447468 -1.808215844 0.884636079
C 2.203591615 -0.446599665 1.145692596
C 3.382540748 -0.187842254 1.869360244
C 4.192279962 -1.222554739 2.333898985
C 3.850486305 -2.559108064 2.095127465
C 2.700413854 -2.845968653 1.362487624
H 2.402658070 -3.876064845 1.183829417
H 4.466683103 -3.365044488 2.481732316
H 5.088832802 -0.985921476 2.901038293
H 3.646762090 0.845930345 2.071684136
S 1.149433871 0.847580990 0.565413594
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C -0.483728321 -3.198918123 -1.629799293
C -1.449926496 -2.233383721 -2.012817130

C -2.574178206 -2.627270968 -2.744416928
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C -1.780832570 -4.906805290 -2.797092941
C -0.656617310 -4.521609692 -2.075070492
H 0.095809995 -5.261102668 -1.811707522
H -1.899968072 -5.941421261 -3.104228683
H -3.635351156 -4.245683557 -3.683021604
H -3.306190168 -1.878186472 -3.028965462
S -1.288056492 -0.466035892 -1.673355692
C 0.226385313 -0.075748180 -2.631504215
H 0.400289952 0.993378020 -2.508301504
H 1.079842959 -0.612361898 -2.219949057
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H 1.142916470 -0.208773715 5.611867697
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13

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C 4.134140538 -1.218332977 2.323252772
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C 2.560460576 -2.802930754 1.416546826
H 2.214170958 -3.823588780 1.277363951
H 4.309925561 -3.365067017 2.541414478
H 5.046273100 -1.005450112 2.874765336
H 3.677777170 0.864265169 2.001755054
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C -1.492962571 -2.169245412 -2.052011264
C -2.559728631 -2.528529998 -2.875872696
C -2.724391122 -3.850862135 -3.292660111
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C -0.722531643 -4.464040331 -2.096133683
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H -0.734107405 0.747248325 4.206418511
O -0.399740814 -0.720635255 2.769659697
C -0.474618101 -2.014633212 3.425211042
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H -1.519380091 -2.337329035 3.442548032
H 0.102225772 -2.713602920 2.814636707
H 0.720662588 -2.685200557 5.135884332
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H 0.653005071 1.006456683 3.101943803

4"

Mn1 1.626446 1.096149 -0.003494
N2 0.790107 0.543544 -1.807433
C3 0.501123 1.672248 -2.609018
C4 0.240737 2.926164 -1.985018
C5 -0.029036 4.034375 -2.802277
C6 -0.043123 3.934340 -4.193480
C7 0.228109 2.707788 -4.801302
C8 0.498580 1.591793 -4.012559
H9 0.741684 0.642152 -4.480870
H10 0.238700 2.618488 -5.884298
H11 -0.261672 4.811499 -4.796790
H12 -0.249552 4.985365 -2.324881
S13 0.249654 3.105211 -0.208766
C14 0.292307 -0.641707 -2.201807
C15 0.484115 -1.913864 -1.585853
C16 1.456467 -2.292084 -0.595375
C17 1.415904 -3.563142 -0.005175
C18 0.458960 -4.506285 -0.364096
C19 -0.460459 -4.184401 -1.379612
C20 -0.436478 -2.938437 -1.969675
H21 -1.167935 -2.697767 -2.737791
H22 -1.198407 -4.915493 -1.699471
H23 0.442800 -5.481119 0.113101
H24 2.169726 -3.813449 0.736365
S25 2.837333 -1.258059 -0.103202
C26 3.722719 -1.026257 -1.693988
H27 4.585656 -0.392843 -1.481224
H28 4.042935 -1.997006 -2.076629
H29 3.064421 -0.520584 -2.400641
H30 -0.444623 -0.625097 -3.006607
N31 3.594639 2.110223 -0.550741
C32 3.843399 3.187425 -0.916791
C33 4.034168 4.528116 -1.359191
C34 2.914051 5.380151 -1.360323
C35 5.294537 4.979496 -1.785535
C36 3.071682 6.691481 -1.796890
C37 5.429783 6.294986 -2.216738
C38 4.321829 7.148547 -2.222813
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H40 6.144211 4.304879 -1.778107

H41 2.214004 7.357004 -1.806054
H42 6.398361 6.655577 -2.549000
H43 4.434869 8.173918 -2.562978
C44 -0.126356 0.040549 1.155312
O45 -1.158843 -0.346200 1.430704
C46 2.617455 0.054030 3.270884
C47 1.444162 0.005028 4.023504
C48 2.951941 1.223728 2.576655
H49 1.179183 -0.902521 4.558810
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C51 0.600925 1.120935 4.082469
C52 2.105366 2.337636 2.632111
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H56 0.260862 3.141136 3.406055
H57 3.265934 -0.814590 3.209590

4-TS"

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O -5.005527086 -3.657919388 -0.446624211
N -0.784077185 -2.364233241 -1.640685549
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C 2.577825285 -3.927729657 -1.300090702
C 2.616760849 -4.771747358 -2.409370632
C 1.542330103 -4.775855665 -3.296797854
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H -0.376537625 -3.962554045 -3.771572256
H 1.564538426 -5.398321259 -4.187539732
H 3.483005226 -5.403070405 -2.583463876
H 3.415918906 -3.896618745 -0.611633534
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C -4.202970492 0.498362789 -2.320374084
C -4.796598689 0.349043942 -3.574016209
C -4.475768207 -0.762121923 -4.353977149
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H -5.511184644 1.086175291 -3.927890238
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H -0.707635141 0.705864777 0.683111625
H -0.414447373 -0.137932186 -0.857751710
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C -1.311528620 -2.470770698 3.124732598
O -0.840812822 -2.423682771 1.741500433
C -1.742861318 -3.905258512 3.449347776
C -2.495952035 -1.520397952 3.257662053
O 1.039670995 -2.627268040 3.078692805
C 0.099462319 -2.565659060 5.301365929

C 0.203913537 -0.514973078 3.846463253
B 0.580693898 -2.794321879 1.755801340
H 0.564263071 -4.103932205 1.397370875
H -0.900286540 -4.597340389 3.398216974
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H -2.486909986 -4.232192665 2.717230394
H 1.028956712 -2.212090424 5.756261653
H -0.737969567 -2.210325189 5.911921807
H 0.109905566 -3.657013132 5.318429531
H -3.338758217 -1.894364798 2.666808773
H -2.815259149 -1.452418577 4.302617897
H -2.253901840 -0.519767053 2.897330730
H 0.102419356 -0.133915972 2.826290736
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C 1.515999840 -8.513749386 0.326360339
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C 0.633948794 -7.448594794 0.182059995
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C 1.918627832 -6.169447294 1.802954252
H -0.209502661 -7.499603731 -0.498866289
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4-TS"
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C5 -0.365916 4.000487 -2.033714
C6 -0.341840 4.092630 -3.426074
C7 -0.034089 2.965314 -4.189394
C8 0.259947 1.755869 -3.566222
H9 0.542074 0.889631 -4.157148
H10 -0.008101 3.028710 -5.274009
H11 -0.564463 5.040253 -3.908051
H12 -0.606313 4.866801 -1.426484
S13 -0.135886 2.659116 0.393338
B14 0.889473 4.272326 0.963933
O15 0.298301 5.528044 0.654013
C16 0.424882 6.358601 1.830220
C17 0.456884 5.293153 2.982551
O18 1.163973 4.201459 2.355840
C19 -0.947226 4.797009 3.360740
H20 -1.510996 4.505874 2.470743
H21 -0.854677 3.917135 4.004850
H22 -1.513419 5.559863 3.904440
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H24 1.187767 4.905362 4.975150
H25 2.275373 5.906748 4.006267
H26 0.785949 6.606453 4.682278
C27 1.741809 7.141853 1.726847
H28 1.862840 7.841477 2.559712

H29 2.599189 6.463695 1.710178
H30 1.745142 7.713550 0.794500
C31 -0.759784 7.319572 1.871677
H32 -1.706511 6.783292 1.787401
H33 -0.760616 7.895947 2.803450
H34 -0.694035 8.022727 1.035848
C35 0.194656 -0.709546 -2.052115
C36 0.562455 -2.030007 -1.659339
C37 1.696531 -2.436312 -0.876239
C38 1.846011 -3.773013 -0.481452
C39 0.925558 -4.749483 -0.848019
C40 -0.153779 -4.388641 -1.675227
C41 -0.316843 -3.077522 -2.071364
H42 -1.167899 -2.808395 -2.692743
H43 -0.867283 -5.141061 -2.000919
H44 1.058434 -5.777190 -0.524381
H45 2.718360 -4.045653 0.106301
S46 3.042289 -1.339974 -0.424913
C47 3.663257 -0.771361 -2.055552
H48 4.413946 -0.007409 -1.843727
H49 4.100895 -1.610899 -2.598870
H50 2.844975 -0.320832 -2.616565
H51 -0.605459 -0.645864 -2.791886
H52 1.963150 4.048265 0.237716
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C55 3.866269 4.552039 -0.957858
C56 3.222313 5.776283 -1.172771
C57 5.221583 4.389944 -1.294180
C58 3.940362 6.837678 -1.721315
C59 5.929120 5.459100 -1.832297
C60 5.289523 6.684069 -2.046232
H61 2.175817 5.883214 -0.907727
H62 5.696428 3.428762 -1.123841
H63 3.444630 7.788720 -1.892163
H64 6.978662 5.338610 -2.085188
H65 5.845455 7.517414 -2.466506
C66 0.275981 -0.508050 1.440332
O67 -0.647394 -1.089228 1.756683
C68 2.656046 1.535559 2.892523
C69 3.446447 0.422648 2.583465
C70 3.161764 -0.821687 3.159806
H71 4.273260 0.526934 1.886923
H72 2.861657 2.505108 2.454088
C73 1.581671 1.404863 3.781293
H74 3.764102 -1.687980 2.902391
C75 2.095707 -0.946072 4.051284
H76 0.967747 2.275535 3.981455
C77 1.306902 0.168151 4.363641
H78 1.870255 -1.911300 4.496621
H79 0.470322 0.062563 5.049081

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4-TS'
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C4 -0.670525 2.869063 -1.667955
C5 -0.677916 3.989239 -2.504179

C6 -0.335292 3.871372 -3.851944
C7 0.027794 2.625173 -4.366657
C8 0.034589 1.503498 -3.542036
H9 0.358806 0.545094 -3.935429
H10 0.319675 2.525724 -5.408740
H11 -0.342863 4.750646 -4.489652
H12 -0.949268 4.953815 -2.087397
S13 -1.022571 3.046164 0.090226
B14 0.083263 4.626716 0.529101
O15 -0.419300 5.885897 0.115791
C16 -0.128489 6.828469 1.169755
C17 -0.106359 5.906453 2.441887
O18 0.417880 4.669951 1.911942
C19 -1.510865 5.615440 2.989640
H20 -2.174491 5.275044 2.190092
H21 -1.441489 4.818207 3.736656
H22 -1.954230 6.494442 3.467921
C23 0.809964 6.389486 3.564019
H24 0.753413 5.703630 4.414750
H25 1.850241 6.434931 3.236095
H26 0.508029 7.383062 3.912462
C27 1.240326 7.465728 0.888170
H28 1.484041 8.241885 1.620362
H29 2.033711 6.713873 0.895207
H30 1.221721 7.924110 -0.104362
C31 -1.216155 7.899019 1.174098
H32 -2.210495 7.451255 1.215781
H33 -1.094331 8.573841 2.028814
H34 -1.151733 8.493750 0.258061
C35 -0.704284 -0.696520 -1.808228
C36 -0.812061 -1.960442 -1.148464
C37 -0.767738 -2.257310 0.254134
C38 -0.883584 -3.580973 0.700976
C39 -1.022575 -4.647666 -0.181560
C40 -1.099483 -4.382693 -1.558939
C41 -1.010607 -3.083295 -2.012657
H42 -1.064111 -2.888257 -3.081123
H43 -1.229395 -5.195216 -2.268422
H44 -1.093408 -5.662560 0.197556
H45 -0.878317 -3.784819 1.767218
S46 -0.707601 -0.965728 1.510279
C47 0.455877 -1.697434 2.731465
H48 -0.064671 -2.361358 3.423390
H49 1.237722 -2.248104 2.204253
H50 0.901636 -0.861774 3.271140
H51 -1.005887 -0.716976 -2.855534
H52 1.158454 4.270760 -0.188199
C53 1.233765 2.579827 4.601724
C54 2.511084 2.918419 3.814397
C55 2.647521 1.700547 2.908192
H56 3.387406 3.067231 4.451837
H57 2.342333 3.808678 3.203221
C58 0.350591 1.937481 3.529865
H59 1.453407 1.867525 5.406003
H60 0.756259 3.457637 5.044321
O61 1.278878 1.341821 2.570569
H62 -0.299858 1.141515 3.906085
H63 -0.236041 2.683295 2.992314
H64 3.109152 0.847320 3.424355

H65 3.170405 1.891203 1.970017
N66 2.280973 2.336774 -0.242200
C67 2.297759 3.493029 -0.572980
C68 3.114080 4.458374 -1.308076
C69 2.574129 5.660082 -1.779859
C70 4.455744 4.134790 -1.572036
C71 3.375602 6.536463 -2.509669
C72 5.250008 5.019025 -2.294766
C73 4.711384 6.221096 -2.765108
H74 1.535688 5.891748 -1.572234
H75 4.850351 3.191451 -1.207525
H76 2.955630 7.467387 -2.879724
H77 6.288695 4.771295 -2.495589
H78 5.333751 6.908383 -3.331555
C79 2.248223 -0.716466 0.001237
O80 2.663570 -1.544037 -0.671763

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4-TS
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Mn1 1.385144 0.869650 0.393029
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C5 -0.464850 3.965471 -2.152949
C6 -0.306289 4.023343 -3.538056
C7 0.073540 2.875348 -4.236093
C8 0.306454 1.683789 -3.556034
H9 0.644946 0.803936 -4.095051
H10 0.204526 2.909693 -5.314582
H11 -0.480792 4.957358 -4.064360
H12 -0.764403 4.845815 -1.593434
S13 -0.464935 2.703089 0.319385
B14 0.577125 4.282956 0.909950
O15 0.018292 5.550100 0.596619
C16 0.214948 6.396498 1.749104
C17 0.230441 5.353366 2.922832
O18 0.862669 4.211955 2.303051
C19 -1.181265 4.928923 3.353497
H20 -1.781680 4.643956 2.485408
H21 -1.103978 4.059787 4.014479
H22 -1.699632 5.726248 3.895410
C23 1.052986 5.770015 4.139259
H24 0.991654 4.999123 4.913430
H25 2.104666 5.905174 3.879894
H26 0.672292 6.704974 4.564374
C27 1.561567 7.119025 1.595189
H28 1.734022 7.831548 2.407791
H29 2.389206 6.405191 1.571567
H30 1.565337 7.668168 0.649729
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H32 -1.895892 6.916423 1.753837
H33 -0.874237 8.003570 2.723812
H34 -0.849369 8.094912 0.953103
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C36 0.390336 -2.061264 -1.550497
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C38 1.480315 -3.816798 -0.202479
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³4-TS
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¹4-TS
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4
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14

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4-TSa

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O 1.363118164 4.486636756 3.147285957
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H -2.870325837 3.812896753 2.363029449

4-TSb

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5-TS

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C7 -1.270904 3.027680 -3.889216
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H12 -2.562320 4.460966 -1.095017
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C17 -0.572592 5.467295 2.983275
O18 -0.410254 4.053443 2.654010
C19 -2.044716 5.654890 3.371119
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H21 -2.282319 4.976483 4.195101
H22 -2.248012 6.680210 3.694329
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H29 1.884915 5.528739 1.702691
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H32 -2.050475 7.261658 1.274158
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H34 -0.654209 7.855899 0.366519
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C36 0.822583 -1.652976 -1.637961
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C38 2.564238 -2.990022 -0.512668
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C40 0.895118 -4.110641 -1.839498
C41 0.335193 -2.892870 -2.161046
H42 -0.541305 -2.859710 -2.804470
H43 0.466863 -5.022399 -2.247972
H44 2.451022 -5.132212 -0.714562

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C69 3.627605 5.046247 -2.067173
C70 4.503161 3.514275 -0.418945
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C72 5.785465 3.693338 -0.928624
C73 5.992502 4.547186 -2.018460
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H77 6.626900 3.170439 -0.480555
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³⁵-TS
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15-TS

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5

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6-TS

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6-TS'
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36

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16
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| H | 0.405162549 | 4.341993725 | 2.626935112 | C36 | 1.960465 | -2.239643 | -1.183478 |
| H | -0.008316864 | 2.623744434 | 2.421454783 | C37 | 3.015810 | -2.156318 | -0.210911 |
| H | -2.756854543 | 5.720632240 | 0.008863140 | C38 | 4.039166 | -3.113840 | -0.173373 |
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| 7-TS | | | | C58 | 0.272661 | 1.987945 | 3.447675 |
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| C4 | -0.496350 | 2.039421 | -1.716950 | H63 | -0.170406 | 2.643123 | 2.698887 |
| C5 | -1.119902 | 2.880379 | -2.639149 | H64 | 2.495797 | 0.588495 | 4.447244 |
| C6 | -1.225499 | 2.515503 | -3.978508 | H65 | 3.449960 | 1.336821 | 3.137935 |
| C7 | -0.699194 | 1.287150 | -4.381514 | C66 | -0.550382 | -0.518273 | 1.263696 |
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7
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8

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C 1.694036872 0.308486175 0.060263147
C 0.972072441 1.065680246 1.012642214
C 1.674738867 1.992442043 1.792984719
C 3.048069139 2.177228066 1.635956319
C 3.751152282 1.428426854 0.691035751
C 3.073968156 0.495306484 -0.090646979
H 3.601291913 -0.077146649 -0.848895840
H 4.818976485 1.573601010 0.555509532
H 3.566337236 2.907502930 2.250713910
H 1.126758195 2.568139307 2.532206693
S -0.797756030 0.894922877 1.230761483
C 1.466032152 -1.845762362 -0.771420785
C 0.914816471 -3.024337670 -1.424691823
C -0.054535536 -3.089011153 -2.462493189
C -0.573326627 -4.326813478 -2.858133889
C -0.143534662 -5.514539926 -2.270035474
C 0.849110680 -5.474300578 -1.287913329
C 1.369705328 -4.252039750 -0.888530037
H 2.125038122 -4.224897676 -0.107632819
H 1.211358319 -6.391136919 -0.832906747
H -0.563983612 -6.461936721 -2.593322211
H -1.315788724 -4.351084639 -3.649770569
S -0.721994977 -1.668370062 -3.315194521
C 0.773026622 -0.894290281 -4.037891725
H 0.415288248 -0.041938119 -4.619563737
H 1.430975033 -0.537461652 -3.245583374
H 1.281027643 -1.606157516 -4.691453557
H 2.321476225 -2.059145639 -0.125226273
C -3.214677269 -2.324880763 1.700840670
C -3.137569748 -1.899716648 0.193670859
O -1.713951639 -1.628556650 0.050347882
C -3.509722679 -2.977525236 -0.819335465
C -3.917549381 -0.608146054 -0.089190750
O -2.217646695 -1.498562099 2.315863960
C -2.808909182 -3.794112791 1.907339088
C -4.559796672 -2.050682181 2.370837912
B -1.175449690 -1.283570914 1.393678364
H -0.060833719 -1.666033057 1.612896309
H -2.838098698 -3.834686703 -0.749671946
H -4.539806437 -3.314335517 -0.663718467
H -3.435058781 -2.573882870 -1.833744089

H -2.665998138 -3.965671962 2.977741777
H -3.573452530 -4.486808714 1.541553085
H -1.865134999 -4.012001763 1.398817134
H -3.699376478 -0.255364488 -1.105877495
H -4.997210231 -0.770806085 -0.027926306
H -3.642066515 0.179559229 0.616456618
H -4.784901697 -0.983102186 2.382952279
H -5.369893045 -2.580760785 1.857849124
H -4.527068889 -2.397819870 3.407584056

12-TS

Mn -0.847402469 -0.063001645 -1.606553426
C -1.411997722 1.391740391 -2.736334152
O -1.781597096 2.274562072 -3.399572421
N 0.918249700 -0.709665830 -0.731884716
C 1.418804084 0.409079105 -0.008657039
C 1.062846611 0.744054238 1.323682490
C 1.685937820 1.863280145 1.912704835
C 2.575237271 2.664612745 1.209812546
C 2.871043536 2.372810021 -0.126787067
C 2.294352391 1.257695464 -0.716011423
H 2.521026733 0.988649892 -1.744227762
H 3.551536658 3.000402178 -0.694063741
H 3.021790348 3.526500848 1.697035166
H 1.429681501 2.116336467 2.938085276
S -0.170764589 -0.040865220 2.360682175
C 0.932180765 -1.904032496 -0.118775141
C 0.705794056 -3.200997008 -0.832071449
C 0.064074638 -3.407746890 -2.075168617
C -0.125151191 -4.711520590 -2.555448376
C 0.311274905 -5.820486740 -1.835112982
C 0.953605933 -5.629739223 -0.612006798
C 1.140903123 -4.339507524 -0.129334105
H 1.624459830 -4.195989891 0.833421578
H 1.303286793 -6.479448569 -0.033617366
H 0.149754861 -6.820026341 -2.227378894
H -0.626581873 -4.846017141 -3.509046833
S -0.595310969 -2.102730374 -3.135949883
C 0.947634753 -1.522414960 -3.946995837
H 0.659176293 -0.719332052 -4.628739784
H 1.622851992 -1.140599433 -3.179534713
H 1.401659772 -2.345187338 -4.502134442
H 1.634930528 -2.008477952 0.714635007
C -3.239499575 -2.263752989 1.211303797
C -3.264342707 -1.030692376 0.246612426
O -1.834624705 -0.784953744 0.074837173
C -3.878533544 -1.288983822 -1.125173660
C -3.858991648 0.227169393 0.884907874
O -2.110647913 -1.974413676 2.055949236
C -2.963460997 -3.581941169 0.471099915
C -4.481157985 -2.395636864 2.088806380
B -1.156345928 -1.270914913 1.299538332
H -0.192060631 -2.050264530 0.804062510
H -3.342458892 -2.073888976 -1.662553149
H -4.927284905 -1.586118455 -1.026344005
H -3.844725402 -0.376416041 -1.730814483
H -2.732111650 -4.353765619 1.209752419
H -3.828716972 -3.908699613 -0.114205969

H -2.104084025 -3.487287276 -0.197389147
H -3.625134624 1.088904395 0.252276573
H -4.946111449 0.149536233 0.979534583
H -3.424279766 0.401170471 1.871696443
H -4.596559580 -1.528495624 2.741077169
H -5.381768394 -2.500530200 1.473949091
H -4.392433322 -3.284654944 2.719394564

13

Mn -0.597989032 -0.469773098 -1.541360456
C -1.091371619 0.563404157 -3.090374164
O -1.430269235 1.204399238 -4.008271484
N 0.913858943 -1.015339320 -0.413570823
C 1.328177729 0.052779482 0.376730116
C 0.888368786 0.316231269 1.703578634
C 1.340620411 1.441707111 2.402293830
C 2.200828245 2.359255849 1.803528286
C 2.602193432 2.151633761 0.481218991
C 2.178795096 1.022373029 -0.208087060
H 2.505459379 0.832343729 -1.226592066
H 3.262893300 2.863670686 -0.007613231
H 2.536874740 3.231434866 2.356079577
H 0.986770913 1.608848434 3.415629939
S -0.286407679 -0.743235637 2.572150197
C 1.004478784 -2.381511408 0.098965367
C 1.470764342 -3.306820543 -1.012977837
C 0.632293935 -3.659261569 -2.087960784
C 1.093192871 -4.486841072 -3.117123173
C 2.404667889 -4.958678928 -3.099007656
C 3.250951693 -4.614053740 -2.047256724
C 2.777341367 -3.799894913 -1.018730102
H 3.437126559 -3.522283989 -0.201038629
H 4.274679189 -4.976332197 -2.026208968
H 2.755482215 -5.596699349 -3.905627736
H 0.440925549 -4.773663843 -3.934403428
S -1.061874262 -3.032118945 -2.092130442
C -1.508264464 -3.046906584 -3.865518825
H -2.416832258 -2.447515548 -3.948328787
H -0.714990381 -2.574921925 -4.447567437
H -1.705864793 -4.060406419 -4.220965065
H 1.715922623 -2.439997941 0.932719246
C -3.972058518 -1.274066953 1.139241469
C -3.481030761 -0.212163802 0.102966347
O -2.006775964 -0.333915755 0.249794981
C -3.872682200 -0.502264802 -1.338222832
C -3.826277930 1.229028860 0.477949522
O -2.943669211 -1.193599443 2.163921097
C -3.950111599 -2.703995337 0.590844178
C -5.318798532 -0.957339303 1.777526447
B -1.797181728 -0.737387873 1.577554788
H 0.052515725 -2.761145868 0.504140983
H -3.467036759 -1.454591749 -1.683740386
H -4.963169072 -0.542203438 -1.421844243
H -3.512518534 0.290009528 -1.998621040
H -4.084087208 -3.399184740 1.422350518
H -4.753589613 -2.869004860 -0.132572444
H -2.995449155 -2.929297606 0.109015756
H -3.252610357 1.906141957 -0.160146790

H -4.891675538 1.428406982 0.330502618
H -3.571567578 1.438066827 1.520254975
H -5.292477514 -0.008323374 2.314930545
H -6.103525897 -0.911505346 1.015427274
H -5.579353534 -1.744289993 2.490365902

14

Mn -1.097260732 -0.458628016 -1.525754678
C -0.958995905 0.407003361 -3.241848226
O -0.898807845 0.945827140 -4.271968092
N -0.226548270 -1.179411332 0.317198293
C 0.888456064 -0.274769968 0.481402869
C 0.767467887 0.663252854 1.529586896
C 1.786827596 1.599323611 1.732073015
C 2.907502974 1.604463587 0.900044737
C 3.016105769 0.690237782 -0.149407177
C 2.001984924 -0.246149153 -0.364877683
H 2.070908644 -0.947411002 -1.189249417
H 3.879021041 0.709245844 -0.808099834
H 3.692566210 2.336647858 1.065282341
H 1.695953640 2.323572256 2.536191785
S -0.714874084 0.534380206 2.475291243
C 0.073203114 -2.617227388 0.560489445
C 1.030849696 -3.229485764 -0.439320399
C 0.705021942 -3.415143858 -1.801195892
C 1.652100122 -3.935176135 -2.690404475
C 2.926197031 -4.281548444 -2.239609391
C 3.257911148 -4.118891128 -0.897204663
C 2.312300255 -3.596902884 -0.016718832
H 2.575120425 -3.439390133 1.024768979
H 4.247440661 -4.385268731 -0.538539488
H 3.650917510 -4.681133789 -2.943086534
H 1.409113242 -4.083573997 -3.735772679
S -0.954701706 -2.984541015 -2.357882061
C -0.780787805 -2.860304825 -4.171821810
H -1.719159091 -2.426714966 -4.521632088
H 0.040770933 -2.190048275 -4.431609653
H -0.643189464 -3.842864928 -4.627370730
H 0.481615538 -2.737266120 1.571904750
C -3.678563072 -1.566548654 1.088495899
C -3.710963176 -0.157261174 0.381500358
O -2.311891853 0.041193032 0.072402044
C -4.503948420 -0.103519536 -0.923165063
C -4.148504981 0.981692283 1.308697083
O -2.385170940 -1.611950035 1.705659660
C -3.777658895 -2.729494663 0.091470954
C -4.738679291 -1.737176498 2.176930940
B -1.494595322 -0.658093322 1.138915316
H -0.890396472 -3.133672367 0.549207043
H -4.100017367 -0.796823625 -1.667636185
H -5.554806747 -0.358633532 -0.752756128
H -4.460748357 0.906965748 -1.341892522
H -3.553074053 -3.661867969 0.616965359
H -4.775935556 -2.812999131 -0.350049375
H -3.051976856 -2.620523069 -0.716058086
H -3.934972795 1.935501498 0.819935881
H -5.220209782 0.927108992 1.520865781
H -3.599834654 0.961299191 2.251648503

H -4.595282583 -1.015144160 2.982035471
H -5.747687310 -1.617685478 1.766191333
H -4.660981617 -2.739958369 2.606908618

Frequencies

Benzene

414.09 414.12 620.41 620.45 693.76 717.37
864.13 864.13 975.64 975.68 1013.80 1015.93
1020.09 1067.75 1067.85 1189.33 1208.45 1208.57
1358.35 1378.11 1523.64 1523.80 1654.00 1654.01
3171.52 3181.53 3181.57 3198.10 3198.20 3209.20

Benzonitrile

148.48 167.06 391.82 410.78 465.11 562.93
572.21 637.02 703.78 774.07 778.23 860.92
942.85 982.86 1011.12 1015.62 1054.93 1113.23
1200.40 1212.02 1226.29 1336.89 1364.23 1486.12
1534.22 1631.88 1658.06 2347.81 3186.78 3197.78
3206.71 3216.91 3219.82

CO

2203.61

Diborylamine

20.69 27.27 29.34 31.16 53.56 58.12
88.06 111.03 114.57 120.82 157.32 193.16
203.16 225.46 228.66 239.92 243.28 252.89
284.03 292.76 294.82 305.45 322.52 323.83
326.82 329.44 337.19 337.83 366.63 370.49
379.70 379.93 403.03 410.86 419.19 440.60
454.90 473.52 494.49 511.32 525.71 528.04
568.64 585.60 587.16 631.05 639.90 657.98
661.54 677.02 690.36 710.49 713.57 751.06
807.83 840.85 863.02 867.86 869.12 869.95
893.66 913.98 939.65 940.71 946.27 947.25
955.08 976.02 977.81 983.67 991.07 997.23
1006.57 1013.56 1022.24 1022.34 1033.21 1033.54
1055.68 1078.51 1112.58 1146.79 1147.21 1151.94
1182.83 1192.28 1192.44 1193.88 1196.89 1215.89
1221.25 1249.86 1250.54 1270.26 1270.46 1293.90
1302.66 1308.20 1323.08 1341.53 1355.08 1364.08
1398.13 1414.82 1414.93 1416.97 1417.46 1427.30
1427.41 1436.76 1437.10 1461.26 1485.88 1486.17
1492.15 1493.05 1493.14 1496.51 1498.17 1499.59
1501.85 1502.11 1511.98 1517.36 1519.03 1520.64
1523.02 1523.64 1524.02 1539.43 1540.95 1541.66
1636.22 1662.53 3048.31 3048.39 3050.27 3050.45
3052.97 3053.24 3057.08 3057.14 3057.57 3099.95
3120.74 3121.04 3121.95 3122.29 3127.81 3127.85
3129.27 3129.96 3132.90 3134.48 3135.02 3135.35
3148.51 3150.16 3150.50 3151.59 3152.92 3164.41
3168.55 3183.25 3195.69

HBpin

95.08 231.19 246.71 285.05 292.10 296.30
321.41 332.14 361.37 372.42 398.72 449.58
512.93 523.12 583.09 667.74 748.51 806.37
867.91 905.22 937.33 946.66 964.64 977.77
1022.53 1031.00 1065.17 1144.70 1183.05 1190.97
1206.98 1244.25 1272.06 1301.97 1383.03 1415.48
1418.64 1428.49 1438.59 1484.91 1494.32 1497.09
1501.96 1518.11 1520.71 1522.99 1541.89 2714.12
3051.59 3054.41 3055.97 3060.55 3124.46 3125.12
3133.34 3133.99 3137.19 3137.85 3153.73 3154.06

Off-cycle intermediate, 9

20.06 24.65 36.95 42.78 48.98 53.92
68.73 73.43 89.66 100.65 109.48 115.05
131.14 143.16 155.70 158.12 182.00 185.67
212.15 234.90 237.39 244.69 258.69 271.01
292.53 296.19 301.96 302.48 308.03 320.91
333.04 341.54 356.75 371.94 380.94 395.21
405.45 412.35 432.31 439.61 445.51 448.96
473.25 490.26 514.41 521.35 534.93 560.56
580.77 591.31 593.27 651.08 669.91 678.90
691.18 699.47 707.00 739.91 751.27 764.41
780.94 795.58 842.70 854.18 869.14 872.85
880.50 938.30 941.39 944.33 947.40 954.74
971.33 983.92 986.93 990.91 991.85 999.81
1005.94 1024.63 1029.34 1050.25 1062.29 1065.63
1081.83 1091.07 1150.42 1156.76 1166.21 1181.52
1192.49 1196.42 1204.12 1206.26 1235.11 1244.82
1269.24 1274.62 1289.53 1295.09 1318.98 1329.95
1357.88 1365.76 1389.43 1400.94 1404.33 1417.15
1420.61 1429.85 1440.24 1469.75 1478.33 1484.55
1485.72 1489.75 1494.22 1496.51 1501.98 1508.05
1517.12 1518.81 1520.95 1522.21 1525.06 1543.42
1609.60 1630.31 1639.61 1651.14 2013.76 3051.76
3055.24 3056.32 3057.53 3060.14 3064.25 3113.62
3124.58 3126.43 3129.51 3133.70 3139.21 3151.87
3154.27 3160.29 3162.97 3166.29 3169.04 3177.73
3184.41 3193.56 3198.57 3206.21 3208.12 3219.17

Off-cycle intermediate, 9'

14.57 23.25 33.31 42.36 46.56 49.87
54.20 57.54 65.26 74.47 98.08 100.29
112.94 120.16 124.89 132.00 137.81 161.85
184.50 196.11 217.61 226.35 232.89 253.67
254.56 267.05 268.04 278.16 288.70 290.63
300.35 308.28 318.09 320.40 330.47 335.94
344.25 353.40 371.24 376.03 394.87 405.61
408.85 416.11 435.72 438.83 449.28 472.30
485.03 514.50 522.19 524.80 552.78 582.55
596.23 607.71 648.41 674.53 680.46 686.26
695.80 718.84 737.44 748.71 760.06 780.64
801.15 839.87 861.94 869.79 871.82 875.18
930.34 939.62 940.99 944.21 948.05 974.32
982.54 983.86 989.23 990.32 994.74 1013.86
1022.65 1033.20 1056.85 1064.74 1082.21 1087.39

1099.39 1147.14 1154.03 1165.28 1186.56 1192.39
1195.08 1206.28 1227.84 1236.83 1249.48 1270.64
1275.81 1289.92 1302.65 1322.28 1323.04 1355.77
1361.64 1368.64 1406.08 1414.72 1418.18 1428.67
1438.89 1466.64 1472.63 1477.15 1486.02 1488.74
1493.67 1495.39 1496.78 1499.99 1506.31 1511.06
1515.77 1519.66 1520.51 1523.68 1539.84 1609.42
1632.05 1638.79 1650.66 2038.88 2119.61 3035.05
3049.84 3051.13 3055.82 3059.40 3065.42 3107.67
3122.76 3124.51 3127.64 3128.57 3134.62 3137.01
3151.62 3162.57 3167.08 3167.51 3170.18 3177.31
3181.99 3190.51 3196.51 3204.67 3207.57 3225.10

Mn-H species, 10

19.83 31.10 33.98 39.81 50.08 52.43
59.32 72.45 98.99 103.22 114.62 116.68
120.27 131.86 144.37 159.41 168.89 179.03
197.18 209.87 235.64 238.58 247.85 254.34
280.74 283.84 300.03 301.26 317.88 321.60
326.25 337.27 342.42 351.02 357.08 367.97
370.72 393.38 419.00 429.04 450.15 455.29
460.28 480.77 498.62 521.73 528.00 529.31
553.24 575.76 580.51 604.77 620.68 644.17
659.71 672.02 673.39 684.22 706.35 714.17
744.48 750.73 768.40 802.27 815.62 831.02
853.72 858.11 865.04 875.54 913.85 944.08
945.66 949.32 953.94 970.66 976.26 982.09
985.12 1026.59 1037.18 1038.43 1046.99 1064.85
1080.97 1128.79 1133.83 1134.44 1151.07 1158.19
1169.96 1193.44 1195.15 1198.16 1205.60 1233.58
1242.72 1275.24 1279.20 1286.43 1298.15 1302.91
1320.32 1343.02 1376.65 1381.43 1411.50 1418.54
1423.89 1431.21 1435.84 1444.87 1448.89 1470.12
1485.96 1490.54 1495.31 1497.36 1502.76 1506.26
1510.19 1521.37 1522.48 1524.88 1529.97 1535.23
1546.88 1560.97 1601.53 1620.97 1636.59 2207.07
2548.00 2632.13 2692.75 3042.32 3054.05 3057.50
3061.91 3098.44 3125.35 3127.15 3130.49 3133.87
3136.43 3138.89 3151.03 3154.07 3168.07 3175.33
3184.38 3190.24 3190.61 3196.97 3208.76 3210.26

THF

50.37 263.18 583.02 673.58 852.73 891.26
911.25 922.43 931.06 977.19 1035.46 1112.85
1176.82 1190.73 1196.11 1262.02 1265.07 1321.31
1353.47 1375.72 1413.68 1500.75 1511.86 1537.67
1551.82 2987.21 2993.35 3051.90 3053.98 3067.95
3068.58 3113.89 3122.63

1

37.57 50.11 56.53 74.09 83.99 87.58
96.57 100.98 106.61 113.08 141.31 162.22
173.45 189.50 214.14 222.23 240.11 265.00
272.90 279.70 311.43 350.54 371.33 395.21
428.72 443.25 458.55 461.49 471.20 474.43
476.52 479.64 517.00 525.39 535.50 567.76

579.68 591.64 639.98 645.48 660.00 684.03
690.43 712.57 718.82 737.92 742.17 763.28
772.46 847.66 868.22 879.55 919.73 937.18
950.80 972.19 984.65 987.98 996.53 997.84
1062.31 1063.14 1082.76 1092.23 1154.36 1164.63
1195.15 1207.03 1207.80 1264.88 1289.57 1304.01
1337.12 1347.67 1369.59 1414.08 1473.94 1477.14
1479.85 1489.30 1492.91 1515.99 1602.25 1615.06
1629.50 1643.64 1666.18 2045.05 2067.10 2118.60
3065.78 3114.73 3165.79 3170.91 3178.03 3181.61
3184.22 3194.96 3201.87 3209.93 3214.19 3228.99

2

25.50 33.15 45.91 48.24 50.77 88.15
109.92 122.58 150.35 153.58 179.65 194.11
214.82 229.52 258.20 270.64 282.24 311.20
321.49 342.62 357.36 392.75 408.71 426.87
440.18 449.21 479.15 518.71 558.18 573.64
580.65 652.40 676.96 709.41 713.86 725.73
736.77 762.74 770.59 846.27 865.11 872.17
911.82 937.54 941.48 960.41 980.10 986.64
993.19 994.94 1057.12 1062.99 1079.54 1091.66
1152.27 1165.94 1197.68 1208.14 1210.38 1260.40
1291.02 1302.85 1327.89 1343.17 1367.56 1403.64
1471.87 1473.66 1481.51 1487.09 1492.54 1507.34
1579.80 1602.11 1618.84 1639.51 1644.71 2008.41
3057.48 3096.01 3155.91 3159.60 3179.69 3180.27
3187.83 3195.08 3202.99 3210.29 3214.21 3234.39

32

28.14 41.78 58.16 79.14 90.61 103.49
132.89 156.80 162.81 186.80 209.64 218.74
243.18 250.13 265.92 319.39 332.73 339.77
371.93 399.02 428.87 442.55 463.75 473.88
496.29 506.06 538.82 559.21 577.33 581.44
605.74 658.28 682.22 700.48 720.38 731.19
743.10 764.73 772.98 849.03 867.43 875.14
924.52 938.48 950.03 969.46 983.75 985.22
996.25 1002.99 1065.41 1066.72 1083.25 1093.37
1154.08 1169.77 1191.49 1202.50 1208.53 1253.15
1289.34 1301.77 1344.04 1357.40 1369.46 1434.17
1468.24 1474.12 1475.22 1490.29 1496.28 1515.52
1574.85 1610.62 1617.51 1635.28 1643.73 1989.49
3073.57 3128.60 3173.51 3178.77 3182.47 3186.65
3187.02 3195.34 3200.60 3208.78 3211.44 3223.32

12

31.36 47.32 57.10 72.03 85.18 101.24
128.05 149.52 185.00 190.62 205.96 221.07
239.98 262.24 267.80 317.19 333.62 349.51
377.56 400.66 426.02 443.93 457.26 472.22
497.11 515.34 530.60 551.72 566.11 579.98
608.23 656.15 678.02 698.04 717.86 731.54
739.88 764.42 772.37 847.25 865.77 873.52
919.18 935.01 944.32 960.50 976.66 985.55
988.29 993.86 1060.34 1064.46 1080.75 1090.44

1152.15 1167.17 1193.59 1205.95 1208.20 1260.11
1289.06 1302.88 1339.01 1354.19 1361.25 1424.78
1469.44 1473.28 1474.93 1485.95 1493.44 1514.33
1585.55 1606.58 1620.46 1638.83 1646.80 1993.94
3063.91 3127.08 3159.61 3174.71 3180.12 3180.84
3190.57 3194.04 3202.70 3210.17 3211.22 3220.89

3

26.09 29.82 42.62 51.86 59.20 66.26
79.56 89.64 92.30 106.80 112.85 118.70
129.71 139.61 140.93 147.71 158.17 170.19
185.86 203.99 211.08 245.07 271.34 289.79
302.09 316.30 323.88 333.22 340.56 358.11
366.43 412.91 446.60 465.28 480.31 522.09
558.75 569.80 585.85 588.36 649.21 677.14
690.00 691.16 706.54 735.30 744.72 764.86
774.24 842.13 845.38 869.13 879.90 883.09
901.83 906.89 923.61 925.16 931.35 944.86
963.50 979.58 981.84 986.48 992.01 998.71
1047.13 1055.84 1059.38 1072.92 1076.43 1081.41
1148.81 1160.00 1172.63 1194.11 1194.45 1200.29
1207.97 1218.27 1256.34 1259.60 1274.24 1285.89
1293.26 1327.28 1327.71 1348.69 1358.44 1363.93
1379.54 1397.26 1406.95 1463.50 1467.93 1468.95
1478.03 1490.93 1502.14 1502.77 1512.90 1532.62
1544.48 1556.62 1599.75 1605.35 1631.89 1636.83
2004.15 3019.52 3055.79 3063.99 3070.45 3083.00
3086.66 3104.59 3121.97 3133.89 3143.30 3169.14
3172.20 3174.70 3181.93 3185.81 3189.21 3197.69
3201.69 3205.93 3211.95

33

26.27 46.35 56.51 61.51 70.03 78.07
94.33 102.48 115.02 120.98 128.55 138.22
151.55 161.81 176.28 181.74 184.66 201.04
207.61 216.03 250.37 259.06 280.12 302.80
315.55 340.61 357.08 364.34 416.03 437.20
462.69 476.48 482.81 497.17 527.89 549.69
561.12 570.68 584.39 586.03 652.97 677.60
688.92 690.64 708.38 739.55 746.85 766.78
776.73 842.83 851.46 870.40 884.67 886.98
897.72 910.19 927.20 931.77 934.64 949.65
967.99 980.12 984.36 985.84 994.04 999.65
1048.91 1058.00 1058.48 1068.00 1079.15 1082.83
1147.54 1158.71 1172.78 1193.08 1195.04 1202.03
1207.87 1214.67 1257.85 1264.61 1272.78 1288.24
1294.47 1327.63 1331.51 1344.14 1358.97 1361.17
1383.11 1405.24 1408.51 1463.49 1470.69 1471.75
1473.06 1487.21 1501.58 1508.74 1511.90 1531.72
1544.01 1591.75 1602.45 1622.45 1640.34 1650.00
1966.88 3022.32 3060.12 3072.29 3073.12 3074.56
3076.07 3111.11 3126.03 3134.11 3154.11 3173.18
3175.44 3178.10 3179.20 3191.36 3192.63 3196.26
3203.67 3205.27 3213.52

13

32.52 47.97 61.31 64.36 72.08 86.01
97.31 104.89 121.56 125.72 135.21 151.22
163.75 176.60 186.30 192.47 200.66 214.34
218.70 257.49 266.42 278.22 278.42 304.50
335.19 347.02 364.82 399.58 426.85 459.09
476.24 486.97 503.22 529.16 540.79 572.19
575.85 586.11 588.60 627.76 656.37 677.62
689.79 691.70 712.89 740.10 747.36 766.38
776.72 841.54 847.85 870.02 883.66 886.93
900.03 902.45 926.80 928.26 932.83 944.13
962.95 979.59 984.26 985.33 992.07 997.78
1050.21 1058.54 1060.42 1071.39 1080.50 1083.06
1147.92 1158.14 1172.00 1192.42 1196.08 1201.03
1204.18 1218.35 1260.94 1264.00 1274.28 1286.48
1294.96 1327.78 1334.00 1345.12 1358.07 1358.51
1383.15 1405.62 1408.73 1464.42 1471.60 1473.28
1473.76 1488.11 1501.79 1510.70 1512.40 1531.34
1544.09 1589.50 1603.87 1620.94 1635.66 1643.57
1989.80 3011.96 3058.97 3070.23 3075.51 3077.16
3110.32 3124.73 3127.42 3134.79 3153.06 3174.51
3175.33 3175.62 3180.94 3186.59 3189.68 3197.26
3201.11 3206.22 3211.56

4"

12.79 15.80 18.32 30.58 38.90 43.75
45.91 54.33 61.37 64.31 69.44 80.87
86.18 89.30 94.15 102.25 109.29 114.53
131.83 137.32 143.46 155.12 163.16 173.00
179.49 192.30 207.75 212.47 234.48 244.17
252.53 259.76 286.76 319.42 330.16 357.97
380.02 395.71 409.64 413.93 421.10 425.10
449.05 463.38 475.53 476.52 528.18 557.52
567.18 569.01 575.96 601.82 617.92 619.86
636.09 649.47 673.78 687.94 701.14 709.76
710.77 714.22 716.23 744.23 745.97 765.29
774.95 780.77 813.79 849.24 859.46 866.19
870.06 870.46 886.44 917.40 938.70 943.16
951.88 966.35 974.37 985.98 986.43 993.39
993.65 998.69 1012.87 1014.72 1017.39 1020.41
1022.22 1041.02 1053.78 1060.88 1063.87 1067.00
1069.39 1078.36 1117.51 1148.68 1159.36 1192.64
1192.78 1195.25 1201.00 1207.06 1208.75 1210.74
1214.40 1230.31 1268.40 1279.30 1294.88 1322.97
1341.89 1343.20 1355.09 1358.15 1371.22 1380.71
1386.72 1449.86 1466.96 1468.37 1485.91 1486.68
1492.18 1497.06 1518.21 1521.78 1527.45 1531.48
1563.67 1605.24 1624.78 1625.15 1626.44 1642.28
1646.11 1651.44 2182.08 2304.97 3067.93 3110.61
3166.01 3167.91 3169.45 3177.71 3179.72 3180.23
3180.34 3182.06 3187.41 3187.72 3189.52 3192.51
3196.12 3198.60 3200.63 3206.48 3207.01 3209.49
3209.85 3217.19 3220.29

4-TS'''

-335.13 15.95 30.30 33.00 37.59 42.04
47.36 50.05 52.37 60.93 73.16 89.31
90.58 94.87 109.49 126.50 131.39 136.57

139.46 157.18 174.85 180.26 183.70 188.71
197.58 209.01 219.41 236.50 241.85 254.32
263.81 268.31 272.82 292.85 301.52 305.46
318.36 321.26 329.64 335.69 351.14 353.19
357.06 361.75 384.28 393.15 397.85 406.58
417.21 430.44 433.35 437.62 464.36 492.58
496.52 512.03 521.20 531.69 534.21 557.31
566.72 579.63 582.15 591.10 626.25 642.18
676.40 678.78 691.58 703.17 710.07 716.26
727.87 743.68 749.34 767.97 773.81 775.51
798.20 842.52 856.24 856.93 866.06 872.62
876.63 896.69 919.89 929.31 938.67 946.15
947.20 950.70 958.51 965.17 978.16 979.37
986.89 991.04 993.42 998.40 1001.68 1008.27
1010.34 1022.30 1033.29 1051.89 1058.84 1061.03
1077.75 1082.13 1084.37 1117.02 1144.52 1153.90
1157.94 1187.81 1192.13 1192.92 1197.11 1200.58
1202.96 1211.81 1218.29 1245.64 1246.17 1259.08
1266.73 1284.65 1293.78 1307.15 1315.31 1328.70
1336.05 1350.11 1353.10 1367.06 1412.89 1418.53
1427.35 1437.86 1451.38 1460.56 1469.43 1477.79
1485.88 1488.69 1491.05 1492.17 1493.76 1500.07
1501.24 1510.86 1513.52 1518.13 1522.55 1523.65
1539.19 1575.07 1609.99 1611.70 1633.17 1636.34
1642.51 1655.62 2047.42 2129.81 3048.71 3049.96
3053.93 3059.19 3066.27 3088.35 3115.17 3122.02
3128.78 3130.96 3138.54 3147.94 3151.81 3155.62
3165.20 3173.76 3175.80 3178.98 3187.48 3189.31
3193.59 3194.80 3196.94 3197.65 3206.55 3206.80
3209.95 3211.82 3214.05

4-TS"

-182.75 18.21 23.57 30.99 37.41 42.34
45.72 47.61 50.48 53.83 60.12 70.10
72.02 81.20 91.64 92.54 97.58 98.43
104.73 108.93 117.18 123.70 124.89 131.54
140.80 142.37 151.42 171.35 179.94 186.04
192.62 197.55 219.66 226.28 232.82 238.39
246.76 250.41 259.09 263.85 274.61 292.54
305.78 318.93 329.04 333.43 334.63 347.94
357.53 371.83 376.69 385.77 392.97 407.11
417.03 420.06 421.75 425.06 432.49 448.83
450.31 464.65 483.77 504.31 524.09 525.82
527.18 552.27 574.84 577.10 585.25 599.12
617.22 618.39 630.08 650.06 669.70 673.49
688.07 698.26 708.02 709.69 713.62 717.69
722.56 729.19 748.56 750.11 772.41 774.53
790.88 811.41 845.79 852.75 861.46 870.36
873.33 879.31 879.99 899.52 916.99 931.82
943.72 945.74 952.01 959.44 962.57 976.30
977.81 985.47 986.26 992.31 995.03 998.86
1000.51 1008.80 1009.76 1014.37 1016.79 1018.44
1020.75 1029.91 1040.35 1042.41 1054.87 1056.10
1061.08 1066.37 1068.33 1071.36 1084.86 1090.13
1120.47 1153.54 1160.08 1172.01 1184.66 1188.39
1196.59 1197.53 1199.17 1199.94 1203.33 1206.64
1212.37 1219.08 1220.46 1244.61 1257.47 1264.38
1278.20 1281.63 1304.89 1310.05 1327.97 1339.82

1347.97 1356.85 1359.50 1370.33 1372.59 1386.63
1411.66 1415.58 1425.21 1435.09 1451.32 1464.40
1473.23 1480.65 1484.40 1487.71 1492.85 1495.01
1498.65 1501.37 1509.11 1512.33 1516.66 1517.98
1518.66 1524.60 1526.74 1531.81 1540.15 1566.37
1609.77 1613.05 1625.04 1633.61 1640.67 1644.37
1655.44 1656.65 2100.36 2180.72 3046.00 3047.61
3050.36 3054.25 3068.25 3109.46 3113.09 3115.42
3121.74 3126.49 3134.94 3138.22 3147.11 3149.68
3167.08 3168.31 3174.75 3177.44 3180.42 3181.32
3183.84 3188.35 3188.95 3190.00 3192.34 3196.24
3200.05 3202.82 3206.18 3207.35 3211.21 3216.86
3221.34 3229.21 3239.40

4-TS'

-253.20 21.88 26.08 35.89 36.97 43.50
46.11 48.44 54.86 57.92 70.28 74.88
76.50 80.52 90.74 92.54 101.83 104.64
112.73 121.15 134.13 139.02 139.56 148.78
155.19 159.10 169.96 176.89 188.48 192.92
198.48 209.90 220.39 231.84 234.39 240.42
246.27 247.59 258.91 265.97 273.38 280.89
289.22 298.97 300.75 309.12 322.18 335.73
338.45 347.67 356.77 365.24 379.81 382.31
392.00 405.45 418.50 425.35 431.44 444.87
452.69 457.73 483.42 506.18 519.24 522.51
523.96 550.03 573.97 578.62 581.98 586.43
594.76 630.71 650.28 669.66 674.86 681.31
691.99 704.54 707.28 711.81 714.18 729.57
739.64 747.46 770.84 774.59 794.58 795.35
849.28 853.53 855.67 856.44 869.14 874.37
875.91 881.46 888.34 919.49 928.67 931.10
931.14 934.34 943.11 948.90 960.37 965.46
970.92 978.10 981.56 983.58 985.48 990.20
998.30 1008.34 1014.66 1017.95 1022.61 1029.86
1041.68 1047.59 1051.88 1055.23 1055.76 1073.07
1076.84 1082.86 1092.84 1118.05 1151.00 1160.40
1163.75 1176.74 1187.16 1196.61 1197.56 1197.99
1198.98 1200.17 1209.94 1214.14 1216.83 1222.74
1246.93 1264.30 1267.30 1272.13 1277.41 1281.99
1285.91 1303.07 1307.65 1326.14 1331.53 1332.21
1340.11 1362.29 1368.01 1372.51 1392.09 1392.85
1411.80 1414.21 1420.79 1424.74 1434.69 1451.23
1456.94 1474.17 1480.87 1487.29 1491.14 1492.26
1496.44 1500.22 1501.63 1502.06 1507.27 1509.19
1512.31 1518.42 1520.57 1524.30 1525.89 1531.13
1537.85 1540.90 1556.07 1570.35 1608.72 1623.87
1632.19 1639.61 1655.74 2065.10 2088.42 3023.06
3045.03 3047.75 3050.98 3052.37 3055.16 3068.57
3070.87 3081.91 3113.85 3116.27 3120.08 3122.24
3124.36 3127.41 3134.34 3137.10 3139.44 3145.64
3148.14 3150.14 3155.99 3159.21 3168.19 3175.46
3178.06 3182.95 3184.64 3189.17 3191.02 3193.68
3200.71 3201.47 3207.77 3209.73 3211.88 3226.19

4-TS

-200.09 19.96 26.30 27.36 34.73 38.12

42.54 47.53 49.20 50.73 56.10 65.16
72.42 77.45 92.49 95.92 103.59 107.95
108.99 121.60 128.70 129.67 133.17 141.49
144.03 156.23 168.33 171.65 176.75 183.23
185.50 193.43 195.33 207.23 220.49 232.78
233.55 243.47 250.90 254.92 262.43 274.65
291.18 298.64 306.24 317.43 328.52 331.32
336.81 347.20 356.11 369.88 376.89 384.49
390.01 405.73 418.89 423.46 432.52 446.78
450.43 463.58 482.44 505.47 519.75 524.67
527.09 551.59 574.52 578.06 583.34 587.31
598.61 630.57 649.04 669.48 672.77 685.04
686.00 704.60 709.40 710.93 715.12 727.66
743.94 749.66 771.09 774.24 792.30 806.98
849.83 852.17 853.60 856.26 868.78 873.61
877.47 884.33 893.78 915.53 929.81 932.07
933.44 943.25 943.36 949.61 959.99 964.66
972.29 977.99 982.66 987.27 987.93 989.64
1001.52 1010.14 1015.31 1016.21 1021.18 1030.02
1037.53 1049.88 1053.10 1055.56 1061.43 1065.57
1071.97 1082.99 1089.75 1119.60 1152.11 1158.90
1167.86 1174.61 1187.47 1193.84 1196.42 1197.12
1198.90 1200.31 1208.79 1218.14 1218.89 1219.57
1246.59 1262.70 1264.60 1275.03 1277.07 1279.63
1282.07 1304.00 1308.49 1327.52 1331.43 1337.18
1345.31 1358.34 1369.45 1370.01 1389.81 1391.14
1411.73 1413.82 1417.09 1424.48 1434.38 1448.40
1462.72 1472.29 1477.09 1484.65 1487.19 1491.69
1494.00 1496.40 1500.00 1501.39 1507.45 1509.57
1518.06 1518.47 1521.71 1523.89 1526.60 1537.46
1540.21 1541.31 1559.76 1591.00 1608.42 1622.60
1633.83 1645.36 1655.61 2086.34 2209.27 3029.77
3045.26 3047.82 3051.02 3055.00 3056.25 3067.82
3069.08 3080.58 3106.58 3113.75 3115.79 3119.85
3121.96 3128.08 3134.92 3135.26 3136.28 3143.32
3146.49 3148.12 3149.72 3165.58 3169.65 3173.29
3179.63 3179.77 3181.46 3187.99 3189.42 3190.87
3198.79 3201.75 3206.52 3210.92 3212.59 3221.92

³4-TS

-368.08 23.95 33.72 34.77 36.36 39.93
42.57 55.31 59.82 63.85 76.57 83.84
105.80 112.14 117.45 127.22 134.27 146.23
152.48 168.88 176.62 177.92 198.58 211.66
218.12 226.60 240.12 255.09 264.39 266.88
274.82 280.73 283.78 294.25 303.97 309.45
313.47 324.34 331.14 339.17 348.60 354.61
365.81 376.42 381.20 387.74 393.58 406.46
417.75 426.09 437.53 441.88 456.69 462.54
485.42 510.21 518.81 534.55 538.54 556.94
581.53 581.90 585.04 619.39 629.07 648.89
665.91 674.91 681.24 686.70 705.71 720.97
723.41 724.85 748.08 748.39 768.57 772.75
783.71 793.01 853.57 854.55 863.86 868.33
871.28 873.54 921.64 936.84 940.54 943.09
947.89 950.88 957.39 976.27 977.18 979.53
986.50 989.71 999.63 1007.22 1011.50 1015.42
1022.02 1029.91 1042.97 1054.02 1060.86 1070.90

1075.84 1084.56 1114.20 1126.49 1146.45 1155.63
1159.68 1184.54 1193.26 1195.64 1197.27 1198.51
1209.56 1211.81 1235.29 1240.37 1257.32 1265.13
1275.53 1280.72 1294.83 1299.54 1327.34 1338.12
1348.00 1357.16 1366.33 1373.57 1411.77 1416.20
1424.92 1436.13 1453.73 1468.39 1473.51 1482.04
1484.26 1486.30 1490.30 1495.54 1499.09 1503.88
1508.03 1515.76 1520.40 1521.22 1524.08 1528.04
1544.67 1575.29 1611.84 1621.04 1621.49 1631.64
1653.49 1669.01 2079.05 2095.53 3048.14 3050.45
3054.38 3061.59 3071.03 3114.60 3118.61 3127.12
3129.63 3137.04 3143.30 3148.77 3149.98 3170.75
3175.85 3181.40 3184.00 3185.26 3185.71 3190.87
3191.71 3195.20 3196.36 3204.06 3208.71 3209.68
3213.58 3213.69 3216.21

¹4-TS

-209.33 25.63 31.31 39.86 49.20 58.84
61.44 66.56 74.57 84.85 89.93 95.95
111.31 113.83 126.73 128.09 143.87 158.24
173.90 179.16 182.95 185.38 191.08 203.65
229.74 244.73 251.94 257.28 262.05 281.56
288.46 298.61 304.17 309.73 328.22 346.50
347.92 356.34 362.61 369.38 373.33 383.14
399.67 404.94 415.83 419.69 423.41 440.82
450.47 463.35 476.46 496.84 509.60 519.45
524.53 533.62 540.31 553.84 560.96 568.78
574.07 582.77 589.42 606.94 630.23 651.95
666.24 675.93 686.87 697.47 710.02 717.10
737.99 744.44 754.35 769.86 778.02 778.99
845.93 847.58 852.75 867.42 867.67 874.75
879.77 916.94 921.53 938.67 942.71 946.58
956.40 964.51 966.26 974.55 975.79 981.31
987.71 989.20 995.77 999.97 1010.99 1018.26
1022.14 1028.25 1036.98 1053.40 1057.71 1063.22
1079.19 1083.86 1111.15 1131.40 1156.36 1160.92
1188.35 1190.07 1194.08 1199.10 1201.37 1202.78
1212.49 1222.52 1239.78 1264.30 1269.35 1276.16
1289.97 1293.81 1299.82 1314.20 1341.15 1349.09
1352.91 1363.86 1404.17 1413.81 1418.53 1419.18
1426.59 1439.03 1470.83 1471.91 1475.40 1483.81
1486.95 1490.12 1495.40 1499.51 1500.20 1505.01
1511.71 1513.49 1519.43 1522.50 1525.37 1541.53
1545.47 1572.72 1614.52 1619.67 1635.56 1638.59
1641.24 1654.30 1916.97 2005.96 3052.75 3058.22
3061.44 3065.55 3068.80 3119.21 3122.81 3129.48
3132.59 3136.62 3151.40 3156.45 3162.86 3164.55
3170.32 3171.93 3175.06 3180.02 3183.26 3187.50
3189.07 3190.35 3195.03 3200.09 3200.60 3205.01
3210.62 3212.25 3213.41

4

11.15 21.70 23.62 25.73 30.24 41.43
43.98 46.95 50.81 62.26 67.49 74.08
86.87 96.64 102.14 106.58 121.64 130.24
139.97 145.83 150.68 156.15 159.75 167.89
181.99 189.70 192.90 200.20 206.05 213.46

229.80 257.14 262.65 281.89 285.78 318.21
326.94 357.49 380.16 396.74 414.31 424.26
448.23 463.11 475.01 475.61 527.52 557.02
567.23 569.49 576.47 584.13 602.52 634.65
648.45 675.51 686.86 687.49 702.74 710.17
713.68 741.24 743.66 764.04 774.51 780.77
808.54 848.92 849.62 854.32 866.05 869.50
886.06 892.44 916.48 926.27 930.36 938.17
939.54 951.92 963.77 971.21 982.11 986.47
993.79 999.12 1012.98 1017.49 1040.97 1046.95
1053.46 1059.99 1065.32 1066.56 1078.04 1116.80
1147.49 1158.82 1171.20 1191.25 1192.62 1193.73
1201.00 1205.76 1214.20 1216.87 1231.15 1263.83
1268.97 1277.24 1279.05 1294.51 1322.00 1328.75
1340.87 1341.78 1354.20 1357.25 1369.79 1384.11
1390.31 1412.98 1448.39 1466.23 1468.45 1485.72
1488.96 1494.61 1496.41 1499.02 1510.89 1527.74
1531.36 1538.37 1541.96 1558.58 1603.00 1623.86
1625.12 1625.67 1651.01 2200.33 2312.02 3035.41
3058.98 3064.71 3065.89 3066.03 3107.48 3110.00
3121.51 3130.09 3141.62 3164.45 3165.76 3167.90
3176.07 3176.85 3178.34 3183.50 3185.79 3186.17
3193.81 3196.82 3198.31 3205.56 3207.06 3213.28

34

11.63 12.08 23.62 30.43 34.44 39.32
43.80 51.56 58.24 68.26 73.32 81.75
90.75 94.52 101.39 104.36 119.35 123.52
141.92 151.77 153.81 163.92 166.81 180.97
184.37 189.06 199.68 204.12 215.21 220.67
247.05 270.48 271.59 312.27 318.25 329.80
347.22 373.75 389.53 394.81 407.20 435.64
451.07 467.85 471.35 477.05 531.33 559.68
564.81 571.92 580.45 585.73 610.51 637.21
651.97 678.37 688.95 698.92 699.83 715.09
718.82 738.99 746.15 764.11 777.07 779.93
795.31 851.70 853.71 860.91 864.67 866.81
883.23 899.68 922.15 925.67 933.36 934.80
937.85 944.69 961.26 971.90 980.89 986.30
987.43 996.20 1012.94 1016.41 1041.87 1050.61
1051.87 1062.64 1064.21 1075.43 1078.84 1116.73
1148.63 1158.17 1171.19 1189.25 1193.27 1194.41
1198.59 1201.26 1204.19 1213.19 1229.48 1263.33
1270.84 1274.05 1280.31 1294.14 1328.63 1331.95
1339.37 1345.30 1351.33 1358.65 1365.55 1382.58
1386.07 1407.95 1450.73 1468.27 1471.78 1485.38
1486.17 1495.60 1496.54 1500.38 1509.78 1530.98
1531.39 1543.21 1545.94 1560.53 1602.49 1615.75
1623.82 1628.70 1655.44 2170.50 2332.82 3058.21
3059.56 3064.42 3067.95 3073.25 3117.68 3122.54
3131.61 3134.59 3137.64 3166.18 3169.49 3176.04
3179.14 3181.29 3186.62 3186.79 3187.22 3191.14
3198.51 3199.99 3207.44 3208.78 3214.76 3255.47

14

19.77 29.81 30.76 34.54 41.10 47.23
62.51 66.47 70.10 79.47 90.91 100.02

104.25 111.06 114.75 121.76 138.24 156.74
164.25 173.24 182.62 199.14 205.83 222.90
237.11 252.05 256.60 270.63 277.16 286.16
324.93 329.19 338.04 373.90 392.19 406.27
410.31 417.73 435.04 467.89 477.81 482.87
496.77 507.32 537.99 541.57 551.75 569.12
577.62 585.25 587.04 605.85 610.23 635.08
657.75 676.53 690.93 701.52 722.72 738.07
743.96 750.10 765.14 771.79 774.12 790.71
848.79 860.89 864.74 872.35 878.04 890.86
919.45 921.69 922.79 933.45 941.11 944.27
960.04 973.19 975.78 981.12 982.17 983.74
987.45 993.24 1010.17 1013.27 1052.40 1054.07
1060.57 1063.65 1083.10 1087.70 1091.98 1115.43
1148.77 1159.19 1175.33 1190.46 1195.07 1199.04
1199.79 1202.48 1204.90 1214.45 1236.42 1258.67
1259.95 1269.61 1283.22 1295.05 1326.13 1335.19
1336.85 1350.21 1351.08 1356.56 1366.60 1380.20
1408.04 1419.14 1466.58 1470.76 1472.30 1482.97
1484.59 1484.86 1500.01 1510.45 1511.27 1532.07
1536.50 1547.47 1572.38 1595.92 1614.98 1625.12
1631.39 1641.73 1652.54 2008.47 2312.22 3041.47
3054.05 3056.42 3061.11 3066.41 3102.01 3115.88
3122.16 3123.30 3131.81 3168.61 3169.89 3172.12
3174.98 3179.44 3186.38 3187.91 3193.80 3197.06
3197.92 3203.31 3205.81 3209.95 3213.67 3220.92

4-TSa

-221.21 14.17 18.39 26.79 31.64 35.36
38.65 42.95 46.47 49.13 53.21 61.69
68.29 70.20 76.15 80.55 88.34 91.77
93.05 96.91 101.82 104.49 108.07 111.05
118.20 126.27 129.08 133.84 138.30 141.25
143.99 148.20 150.19 165.78 174.88 180.28
187.32 188.60 197.76 204.34 219.66 223.91
236.88 239.30 248.60 257.49 261.28 273.53
278.28 281.32 288.74 294.40 303.54 308.25
318.55 322.87 335.44 345.28 367.33 373.31
376.66 382.05 387.39 405.22 419.93 421.14
434.60 445.01 448.60 463.08 484.88 506.86
520.28 525.92 535.58 557.51 575.78 578.74
584.90 584.98 589.14 612.41 626.68 641.03
673.00 674.03 684.21 693.28 695.89 700.65
708.35 713.10 721.34 729.66 741.40 747.21
765.20 771.02 785.05 792.16 851.66 854.16
856.09 856.84 863.11 866.33 866.87 875.85
883.57 885.16 896.24 896.31 899.61 924.39
925.92 930.94 933.46 934.70 943.41 944.85
945.68 947.79 964.44 968.28 969.68 972.49
978.87 984.53 988.57 990.81 991.65 1006.23
1009.74 1015.91 1021.42 1030.61 1042.30 1047.84
1048.40 1051.95 1053.50 1069.75 1070.86 1072.55
1076.13 1085.28 1092.40 1118.42 1149.65 1154.31
1166.39 1175.74 1177.28 1187.66 1189.60 1195.38
1197.01 1197.36 1198.01 1200.81 1201.89 1203.20
1209.38 1219.09 1221.21 1246.07 1260.94 1264.20
1266.01 1267.70 1270.77 1271.61 1275.31 1284.92
1302.36 1304.65 1324.40 1327.85 1328.97 1335.45

1340.90 1358.15 1359.19 1361.44 1369.47 1379.82
1381.48 1384.14 1407.33 1409.49 1411.73 1414.07
1424.45 1434.38 1447.12 1469.07 1473.25 1475.62
1486.34 1487.42 1490.72 1492.87 1498.65 1500.76
1502.31 1505.61 1511.41 1512.50 1513.73 1518.03
1519.93 1521.06 1523.69 1525.05 1525.53 1530.85
1540.52 1542.30 1549.54 1563.74 1584.42 1604.46
1617.91 1635.03 1644.64 1655.85 2087.16 2193.64
3019.47 3044.69 3046.93 3049.59 3050.33 3051.66
3052.57 3054.09 3059.76 3065.05 3065.83 3066.03
3081.78 3081.85 3106.39 3110.46 3113.03 3115.01
3120.50 3120.69 3123.32 3127.88 3135.65 3136.75
3138.39 3144.40 3147.57 3147.64 3151.68 3152.44
3154.73 3158.26 3169.62 3176.94 3178.42 3183.55
3189.53 3191.43 3199.10 3200.18 3201.84 3202.71
3208.24 3217.49 3222.86

4-TSb

-369.02 21.87 25.00 26.75 31.02 35.81
41.40 44.37 47.28 53.39 60.04 66.20
71.53 75.41 78.56 93.47 96.89 111.71
115.35 120.61 124.47 133.78 137.62 146.21
152.64 159.08 173.70 179.97 187.71 189.98
203.95 210.18 215.66 218.00 223.79 236.68
247.64 253.06 264.03 270.99 274.64 279.90
283.03 296.98 305.76 314.94 321.87 331.16
341.71 344.72 368.14 368.91 386.83 395.17
397.03 411.91 413.83 425.32 429.10 438.53
452.57 467.49 497.06 500.95 519.44 525.15
549.09 559.35 565.66 581.03 585.22 587.95
592.15 630.93 634.13 673.38 676.24 694.78
696.84 703.18 704.81 708.56 731.50 733.63
744.21 756.71 765.43 777.21 794.48 804.98
841.83 853.88 861.39 863.39 866.11 868.12
873.16 883.40 884.01 887.70 924.90 930.00
933.65 936.70 939.86 946.18 946.90 948.46
966.79 968.90 972.55 973.90 978.37 980.94
981.80 982.54 1005.28 1009.32 1017.45 1023.72
1032.17 1048.70 1051.41 1054.96 1055.70 1060.09
1077.18 1087.08 1106.90 1117.98 1143.87 1152.80
1156.91 1170.67 1186.89 1187.95 1189.88 1194.66
1196.88 1198.44 1201.22 1212.35 1212.60 1221.37
1243.26 1251.16 1260.12 1261.91 1266.67 1272.97
1285.15 1291.81 1296.34 1314.46 1328.03 1334.06
1336.81 1356.42 1358.01 1366.70 1366.80 1381.13
1407.21 1411.93 1415.80 1425.21 1435.93 1446.93
1469.54 1478.60 1482.82 1485.03 1487.95 1492.40
1495.52 1496.99 1500.33 1501.22 1504.69 1507.13
1510.70 1517.36 1521.38 1522.29 1524.81 1530.87
1541.99 1546.02 1567.28 1593.91 1605.24 1625.11
1633.85 1642.05 1656.78 2033.96 2221.85 3044.32
3049.51 3051.73 3054.94 3056.16 3059.19 3060.27
3064.57 3075.30 3079.80 3119.51 3120.11 3122.37
3128.96 3129.56 3131.10 3131.45 3142.15 3146.13
3147.16 3148.39 3150.75 3152.07 3158.15 3162.42
3172.18 3177.93 3179.87 3189.11 3189.41 3195.72
3198.73 3199.56 3207.26 3208.36 3211.96 3225.32

5-TS

-116.34 20.60 24.33 29.43 37.52 39.84
47.30 51.68 55.09 64.85 71.07 74.20
78.25 83.96 91.17 94.88 96.52 106.64
113.69 119.47 125.40 132.33 146.20 148.46
154.14 159.62 165.02 168.78 174.45 187.45
190.05 196.03 210.70 223.71 240.12 242.49
255.27 263.81 265.79 276.26 296.10 302.36
306.66 311.28 313.60 317.94 322.80 329.17
334.48 338.34 358.41 364.81 374.73 382.95
394.66 407.78 420.52 421.91 442.32 456.20
466.81 475.42 480.96 514.59 524.28 528.17
530.08 551.59 571.07 574.17 586.74 591.39
595.97 629.17 642.47 658.33 668.27 674.51
685.03 686.19 705.37 708.01 714.57 741.93
748.59 761.94 764.62 798.28 805.28 830.13
832.08 841.22 848.64 854.09 866.62 870.15
872.80 884.85 900.01 911.03 923.71 926.68
939.04 939.54 942.21 943.03 948.23 970.33
972.04 974.19 977.10 977.95 981.22 989.99
990.84 999.92 1004.35 1013.16 1022.30 1032.28
1032.61 1049.64 1051.54 1051.57 1063.76 1065.76
1079.74 1105.18 1136.82 1151.88 1158.47 1167.94
1169.86 1187.87 1190.75 1193.50 1196.54 1197.63
1201.65 1206.81 1219.74 1221.83 1235.16 1245.15
1262.48 1270.66 1275.42 1283.25 1284.31 1300.14
1305.64 1324.61 1326.84 1326.91 1331.96 1345.63
1351.60 1360.82 1362.56 1379.98 1387.92 1407.21
1416.47 1416.62 1419.64 1429.19 1439.54 1448.86
1471.35 1473.68 1485.63 1490.27 1492.37 1493.45
1493.77 1495.81 1500.05 1501.86 1505.83 1507.80
1516.08 1519.49 1522.47 1525.39 1530.23 1539.10
1543.35 1544.91 1559.36 1605.39 1622.84 1634.15
1636.44 1652.35 1711.37 2116.43 2913.59 3022.05
3050.93 3053.26 3053.99 3057.09 3063.00 3066.44
3070.96 3081.25 3104.35 3119.74 3123.23 3126.73
3132.27 3133.76 3135.26 3140.99 3150.40 3151.99
3155.08 3160.09 3162.24 3163.91 3165.82 3171.91
3173.42 3173.70 3179.04 3182.99 3184.85 3185.92
3192.11 3196.67 3199.63 3203.36 3206.01 3215.80

³⁵TS

-263.58 27.20 35.48 37.83 47.89 49.62
55.10 61.25 65.00 74.13 76.25 81.66
89.00 92.90 97.85 108.32 111.20 118.46
124.41 134.17 147.64 150.77 155.42 166.33
181.22 185.20 190.82 198.55 207.80 228.27
233.71 240.51 241.74 264.67 265.33 271.55
275.04 280.70 287.87 298.71 304.41 310.17
319.84 333.49 335.00 339.96 352.33 356.18
375.84 380.85 393.69 400.69 401.58 416.02
424.12 427.05 443.73 455.95 464.73 472.03
476.70 514.16 520.21 525.24 531.53 533.85
545.16 552.87 575.14 582.03 586.63 592.27
606.55 628.13 648.13 669.18 674.77 677.11
691.17 709.08 710.45 716.79 741.89 748.67
761.64 762.15 770.56 784.37 804.44 844.61

852.29 855.21 856.87 867.41 869.62 872.64
878.95 886.97 918.82 926.01 928.76 934.08
935.88 940.36 942.79 947.47 973.04 973.27
974.80 982.66 984.74 986.23 986.91 989.81
991.06 1011.48 1014.35 1016.28 1021.10 1032.52
1038.42 1050.78 1054.50 1063.69 1070.81 1075.33
1077.62 1106.93 1120.55 1133.60 1153.63 1159.40
1177.27 1190.24 1191.12 1191.66 1197.04 1197.55
1198.46 1202.28 1206.11 1213.70 1228.55 1245.97
1258.97 1268.91 1275.60 1277.71 1283.02 1291.69
1304.52 1306.95 1328.17 1330.75 1331.33 1348.60
1351.59 1359.28 1365.48 1382.19 1384.35 1413.94
1415.27 1417.19 1426.34 1427.86 1437.00 1451.61
1475.95 1476.85 1485.89 1489.86 1492.49 1494.19
1494.95 1497.31 1499.76 1501.61 1507.51 1510.52
1519.37 1522.21 1522.82 1529.91 1530.61 1536.10
1544.18 1547.37 1559.39 1604.94 1618.30 1625.46
1635.63 1649.15 1671.27 2049.55 2958.46 3048.75
3048.82 3050.73 3054.28 3058.54 3062.19 3067.75
3076.62 3085.24 3112.92 3116.13 3120.20 3122.90
3129.17 3129.54 3134.99 3136.29 3144.08 3148.85
3149.29 3159.83 3167.30 3167.85 3170.50 3174.44
3174.85 3175.75 3181.49 3185.33 3189.48 3194.18
3195.88 3202.13 3202.95 3205.08 3208.55 3212.99

15-TS

-260.27 14.13 30.52 38.78 44.58 48.48
55.88 57.76 66.18 72.84 77.26 83.99
90.42 98.25 103.36 106.75 117.48 119.60
126.64 133.61 142.25 152.11 155.54 162.49
173.29 181.38 185.70 200.95 203.63 213.11
225.13 242.92 247.86 259.96 262.31 272.41
276.26 283.66 285.10 299.99 306.90 321.43
326.82 333.62 334.99 345.93 362.50 368.64
373.77 383.90 396.97 403.09 405.68 420.97
427.78 429.17 449.05 465.39 472.66 478.68
491.13 510.36 517.45 521.56 534.43 541.44
564.23 568.66 573.47 583.38 587.96 589.89
607.21 628.45 648.87 652.89 671.34 673.44
687.77 711.67 713.36 728.09 748.71 753.35
754.26 760.30 768.50 796.25 815.95 817.57
847.85 851.25 862.41 869.68 872.80 876.06
877.38 892.68 916.71 923.52 926.03 935.04
940.54 944.35 945.29 948.85 968.43 969.76
975.94 979.31 981.01 982.24 983.00 990.71
992.20 994.36 1009.99 1012.73 1022.41 1031.51
1045.26 1049.96 1055.37 1058.33 1071.70 1078.12
1085.25 1105.54 1137.20 1153.06 1157.03 1164.01
1175.83 1183.98 1188.89 1193.01 1193.44 1194.08
1196.53 1208.41 1209.32 1214.33 1216.89 1241.37
1253.13 1270.03 1274.84 1279.06 1281.32 1296.76
1301.26 1312.53 1320.97 1325.46 1327.76 1345.04
1355.31 1355.99 1360.49 1362.69 1379.37 1412.51
1414.64 1418.63 1421.31 1427.39 1438.57 1449.54
1468.28 1474.62 1478.04 1484.56 1487.51 1492.31
1494.50 1496.70 1498.42 1502.80 1508.14 1509.27
1514.74 1519.17 1521.54 1522.16 1528.13 1530.83
1543.76 1545.31 1582.99 1616.60 1623.06 1632.66

1636.91 1650.52 1723.73 2009.44 2857.44 3050.17
3051.04 3053.54 3055.93 3056.17 3060.02 3063.29
3081.20 3081.51 3113.37 3120.30 3122.50 3128.38
3130.86 3131.70 3132.19 3134.60 3137.27 3150.83
3151.61 3160.18 3164.63 3168.79 3172.20 3175.14
3178.75 3181.96 3183.70 3184.06 3190.94 3196.18
3197.83 3204.99 3207.68 3208.76 3214.22 3216.33

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15.61 19.50 22.99 25.74 28.50 31.59
39.24 43.10 45.31 50.26 54.04 64.26
67.92 76.55 82.60 87.30 93.59 103.31
106.88 115.78 121.74 130.02 134.54 142.37
144.41 151.20 154.21 162.22 170.90 173.98
179.45 186.00 193.36 197.02 218.65 225.94
231.47 239.22 242.91 252.40 262.17 268.02
291.24 301.05 307.14 312.10 321.69 325.97
332.02 334.68 345.75 359.76 373.30 382.09
389.98 413.75 422.27 428.36 441.70 458.17
470.00 478.96 484.17 516.46 525.89 529.23
536.12 550.27 572.95 584.53 593.52 595.79
606.57 627.24 642.56 669.03 677.26 679.03
684.57 692.31 703.80 708.67 714.87 742.09
746.25 761.35 764.78 800.20 821.60 824.12
828.88 834.55 848.84 854.35 869.70 869.90
871.05 882.27 904.99 909.48 920.13 925.22
940.00 941.50 943.82 945.53 951.12 970.28
971.68 975.31 977.64 982.11 982.60 984.43
989.45 1002.34 1004.42 1007.04 1023.65 1032.13
1033.18 1046.81 1048.93 1054.47 1065.17 1065.49
1082.50 1103.52 1140.33 1151.90 1158.24 1167.55
1172.90 1186.24 1192.40 1194.49 1194.89 1199.70
1204.47 1206.32 1219.57 1239.16 1245.37 1251.29
1257.74 1275.54 1276.31 1285.63 1292.25 1302.70
1308.60 1326.40 1327.70 1330.31 1345.43 1345.78
1356.17 1363.37 1371.30 1378.24 1391.77 1413.24
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