Mechanistic Study of Homoleptic Trisamidolanthanide-Catalyzed Aldehyde and Ketone Hydroboration. Chemically Non-Innocent Ligand Participation

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Table of Contents

1. Experimental

1.1. Materials and Methods

Due to the air- and moisture sensitivity of the lanthanide-organic complexes used in this study, all manipulations of air-sensitive materials for this mechanistically-oriented study were carried out with rigorous exclusion of O_2 and moisture in flame- or oven-dried Schlenk-type glassware on either a dual-manifold Schlenk line, interfaced to a high- vacuum manifold (10^{-6} Torr), or in a N_2-filled mBraun glovebox with a high-capacity recirculator (<1 ppm O_2). Argon (Airgas) was purified by passage through a MnO column to remove O_2 and a column of Davison 4A molecular sieves to remove water, immediately before use. Toluene-d_8 (Cambridge Isotope Laboratories, 99+ atom % D) for NMR reactions and kinetic measurements was stored over Na/K alloy *in vacuo* and vacuum or filter transferred before use. $La[N(SiMe_3)_2]_3$ (La^{NTMS}) was purchased from Sigma-Aldrich or Strem and stored under inert atmosphere in a glovebox. Liquid substrates and substrate solutions were degassed by freeze-pump-thaw methods, dried over CaH_2 overnight, and distilled before use. Solid substrates were purified by sublimation under high vacuum and were stored in a glovebox. Pinacolborane (HBpin) was purchased from TCI America, distilled, and stored at -35 °C in a glovebox. The hexamethylbenzene and mesitylene internal integration standard for kinetic NMR studies was purchased from Strem and Sigma-Aldrich, sublimed under high- vacuum or dried over CaH_2, and stored in the glove box. All glassware used was oven-dried overnight. Elemental analysis was performed by Midwest Microlab.

1.2. Physical and Analytical Measurements

NMR spectra were recorded on Bruker Avance III HD (BBFO Smart Probe, FT, 400 MHz, ^{1}H; 400 MHz, ^{13}C; 101 MHz, ^{11}B; 128 MHz), Bruker Avance III 600 (BBFO Smart Probe, 600 MHz, ^{1}H; 600, ^{13}C; 151, ^{11}B; 193 MHz)), Bruker Avance III HD (TXO 5mm Prodigy Probe, 500MHz, ^{1}H; 1200, ^{13}C; 700) and Bruker Avance III (CryoProbe 5mm DCH, 500 MHz, ^{1}H; 1800; ^{13}C; 1400) instruments. Chemical shifts for ^{1}H and ^{13}C spectra were referenced using internal solvent resonances and are reported relative to tetramethylsilane (TMS). NMR experiments on air-sensitive samples were conducted in Teflon-valve-sealed sample tubes (J. Young).

1.3. Synthesis and Characterization of Complex 1

Synthesis of **1**: In a glovebox, La^{NTMS} (0.2 g, 0.323 mmol) was weighed into a 4 mL vial, 1 mL of anhydrous toluene was added, thoroughly mixed, and transferred to a flame-dried J-Young flask. Benzophenone (58.8 mg, 0.323 mmol) was weighed out and added to the solution. The resulting mixture was allowed to react for 1 h at room temperature and then concentrated, washed with cold toluene, and dried to afford a light-yellow powder. Single crystals suitable for X-ray crystallography were obtained from the concentrated solution. Isolated yield: 197 mg (76%).

(**1**) ^{1}H NMR (500 MHz, Toluene-d_8) δ 7.69 (d, J = 7.0 Hz, 4H, *o*-Ph), 7.14 – 7.11 (m, 2H, *p*-Ph), 7.07 – 7.04 (m, 4H, *m*-Ph), 0.33 (s, 58H, TMS) ppm. ^{13}C NMR (126 MHz, Toluene-d_8) δ 200.72, 137.09, 133.80, 131.36, 128.56, 4.43 ppm. Anal. Calcd. for $C_{31}H_{64}LaN_3OSi_6$: C, 46.41; H, 8.04; N, 5.24. Found: C, 45.61; H, 7.54: N, 5.16. The low percentage values and found CH ratio are consistent with incomplete combustion, although a combustion aid was utilized. This is common with rare-earth complexes.[1, 2]

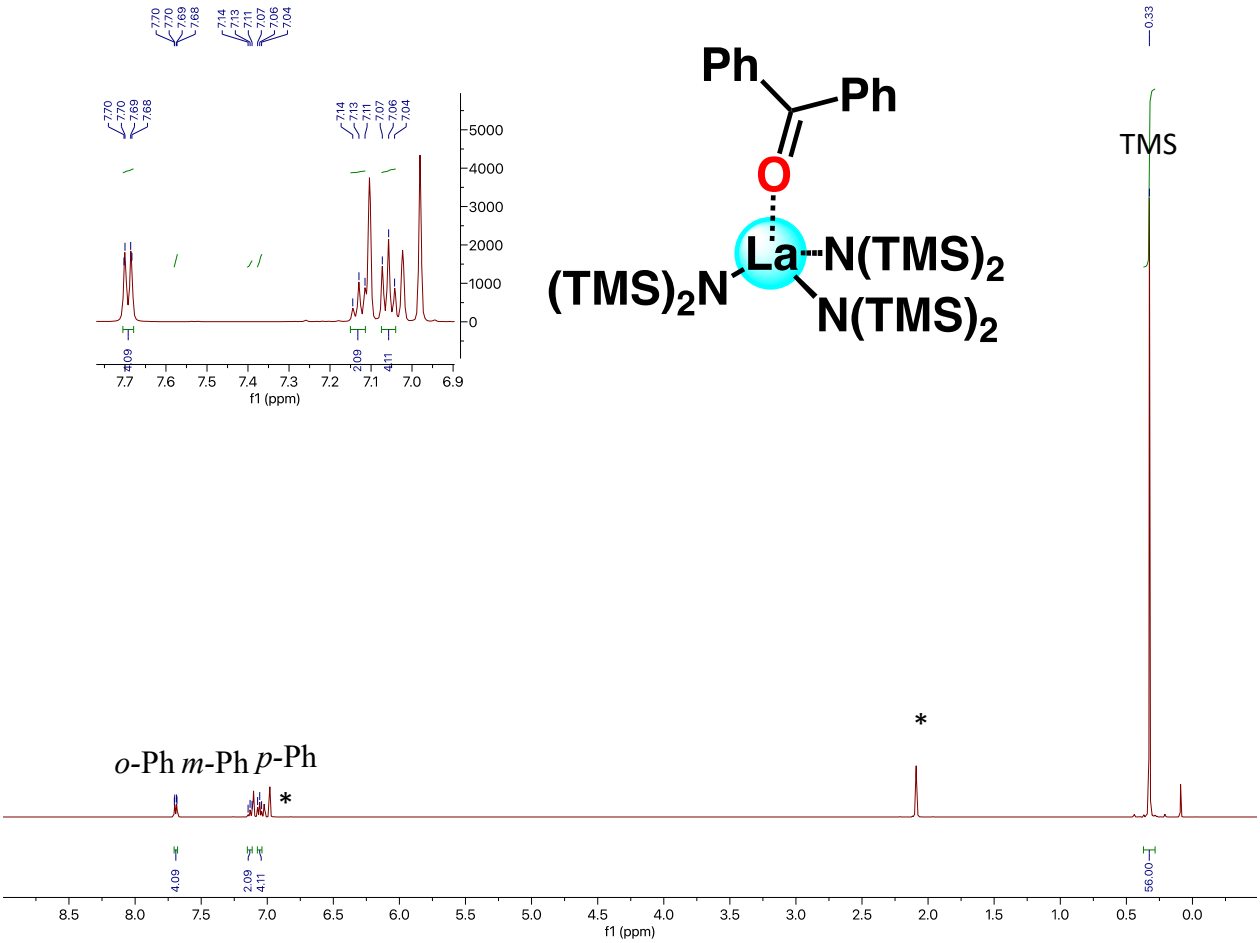


Figure S1. ^{1}H NMR spectrum of **1** in toluene-d_8. *o*-Ph = *ortho* phenyl protons, *p*-Ph = *para* phenyl protons, *m*-Ph = *meta* phenyl protons, TMS = trimethylsilyl, * = toluene-d_8. Close-up panel of the aromatic peaks.

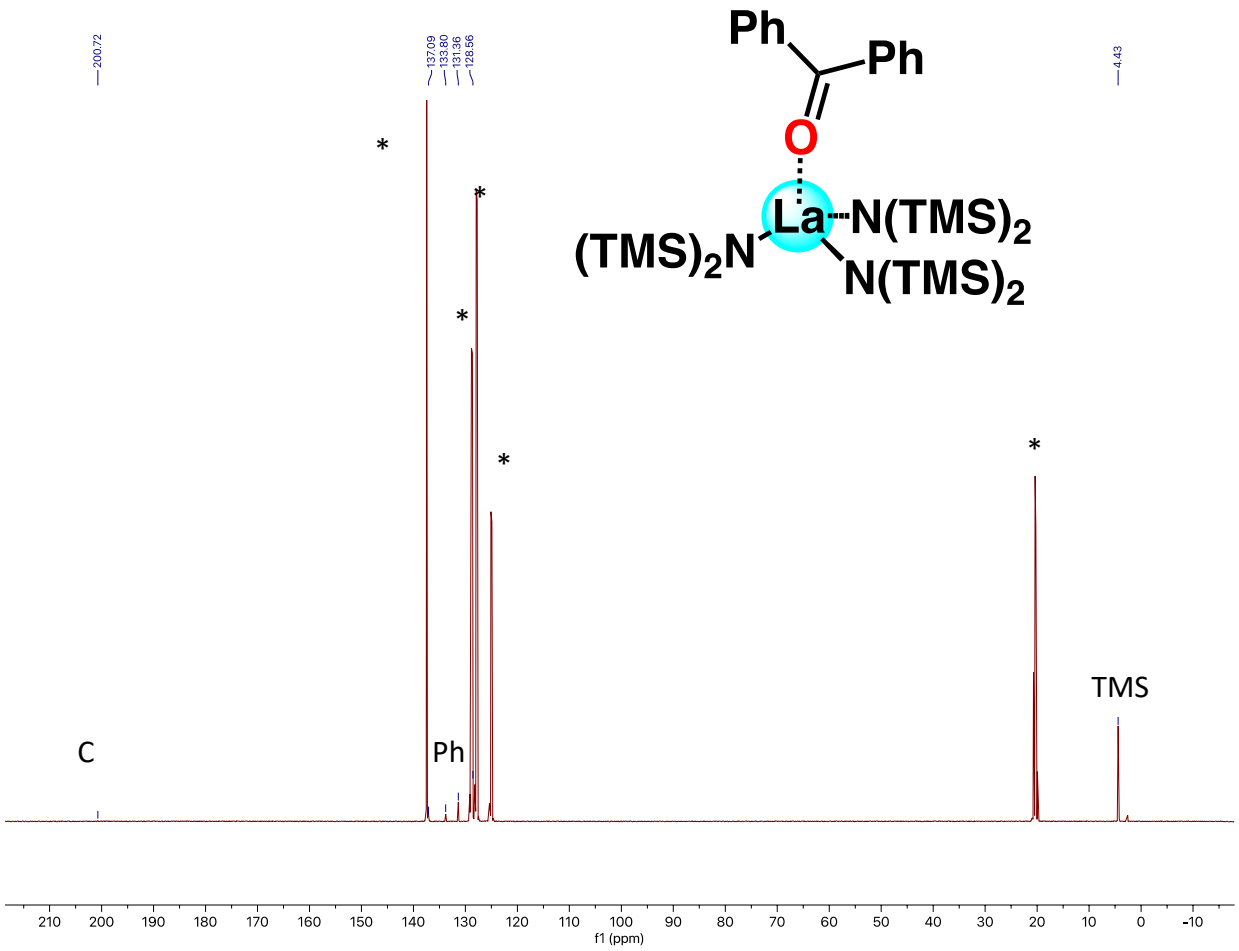


Figure S2. ^{13}C NMR spectrum of **1** in toluene-d_8. C = carbonyl carbon, Ph = phenyl carbons, TMS = trimethylsilyl, * = toluene-d_8.

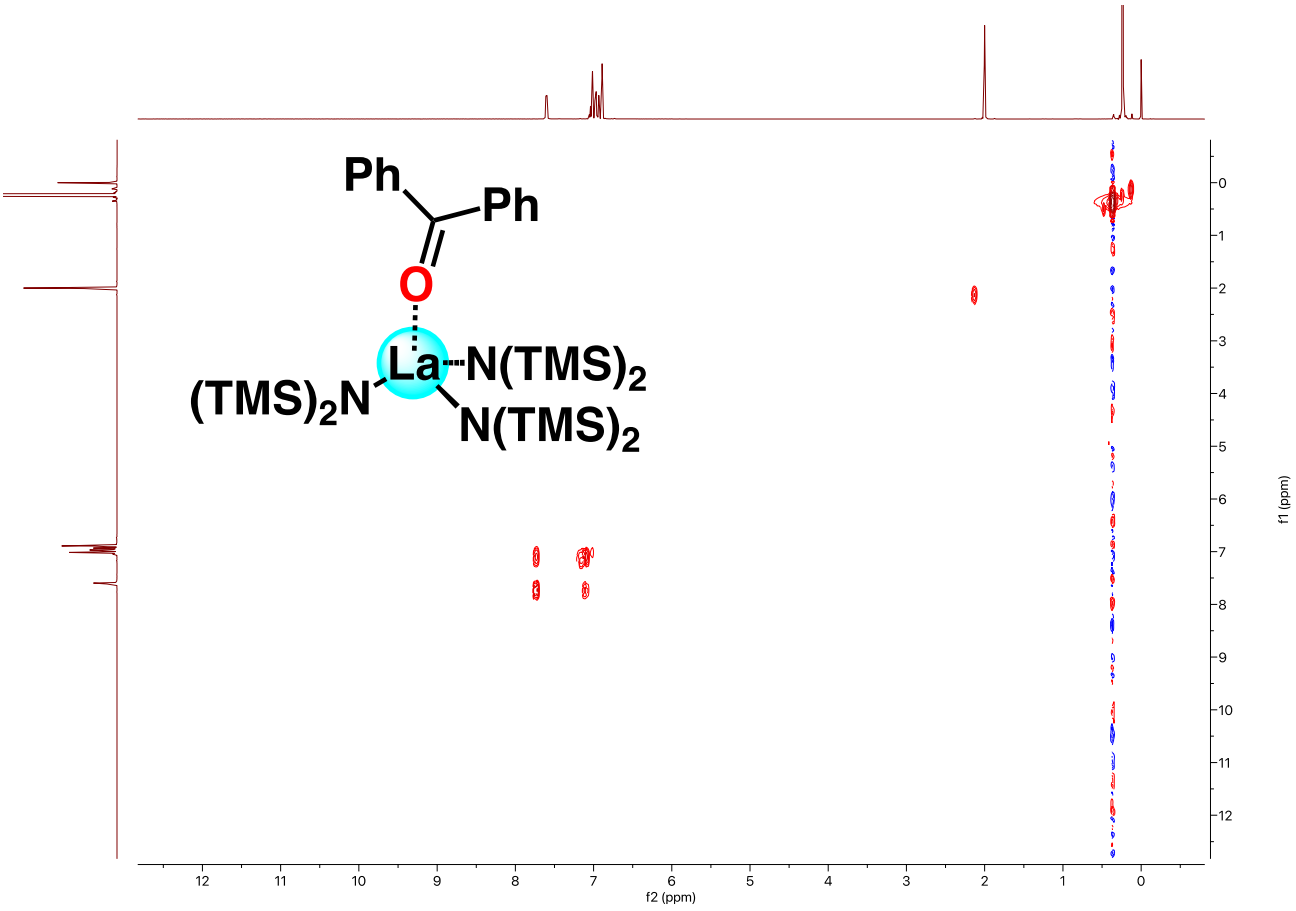


Figure S3. $^{1}H - {}^{1}H$ COSY NMR spectrum of **1** in toluene-d_8.

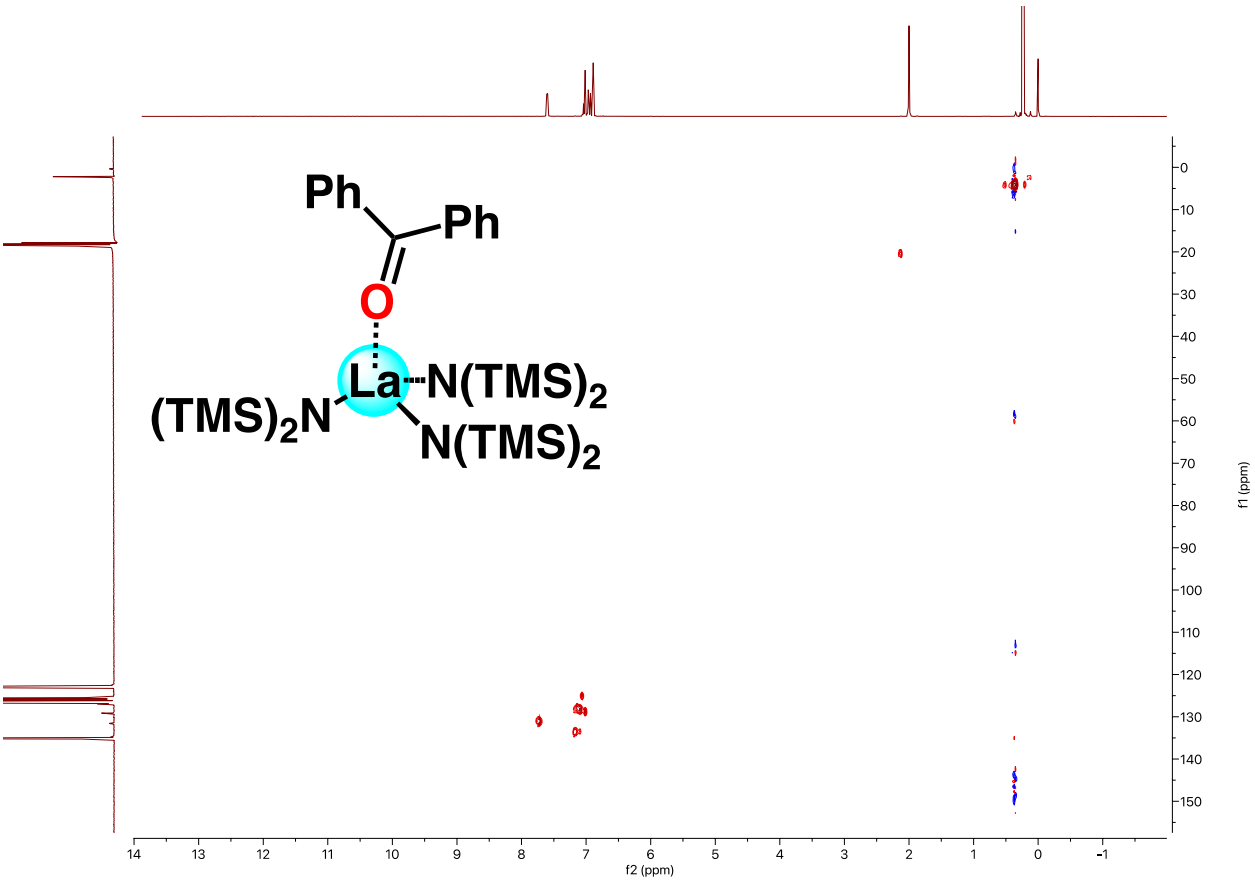


Figure S4. ^{1}H – ^{13}C HSQC NMR spectrum of **1** in toluene-d_8.

1.4. Synthesis and Characterization of Complex 4

Synthesis of **4**: In a glovebox, La^{NTMS} (0.2 g, 0.323 mmol) was weighed into a 4 mL vial, 1 mL of anhydrous toluene was added, thoroughly mixed, and transferred to a flame-dried J-Young flask. Benzaldehyde (32.8 μg, 0.323 mmol) was syringed into the solution. The resulting mixture was allowed to react for 1 h at room temperature and then concentrated, washed with cold toluene, and dried to afford a white powder. Single crystals suitable for X-ray crystallography were obtained from a concentrated solution of toluene at room temperature. Isolated yield: 117 mg (56%).

(**4**) ^{1}H NMR (500 MHz, Toluene-d_8) δ 7.63 – 7.61 (m, 2H, *o*-Ph), 7.57 – 7.47 (m, 2H, *o*-Ph), 7.30 – 7.21 (m, 2H, *p*-Ph), 7.09 – 7.04 (m, 4H, *m*-Ph), 0.27 (s, 18H, TMS), 0.26 (s, 72H, N*) ppm. ^{13}C NMR (126 MHz, Toluene-d_8) δ 157.65, 140.89, 130.10, 126.60, 125.60 ppm. Anal. Calcd. for $C_{44}H_{100}La_2N_6O_2Si_{10}$ · 0.25 equiv. Toluene: C, 41.41; H, 7.75; N, 6.33. Found: C, 41.76; H, 7.73: N, 6.26.

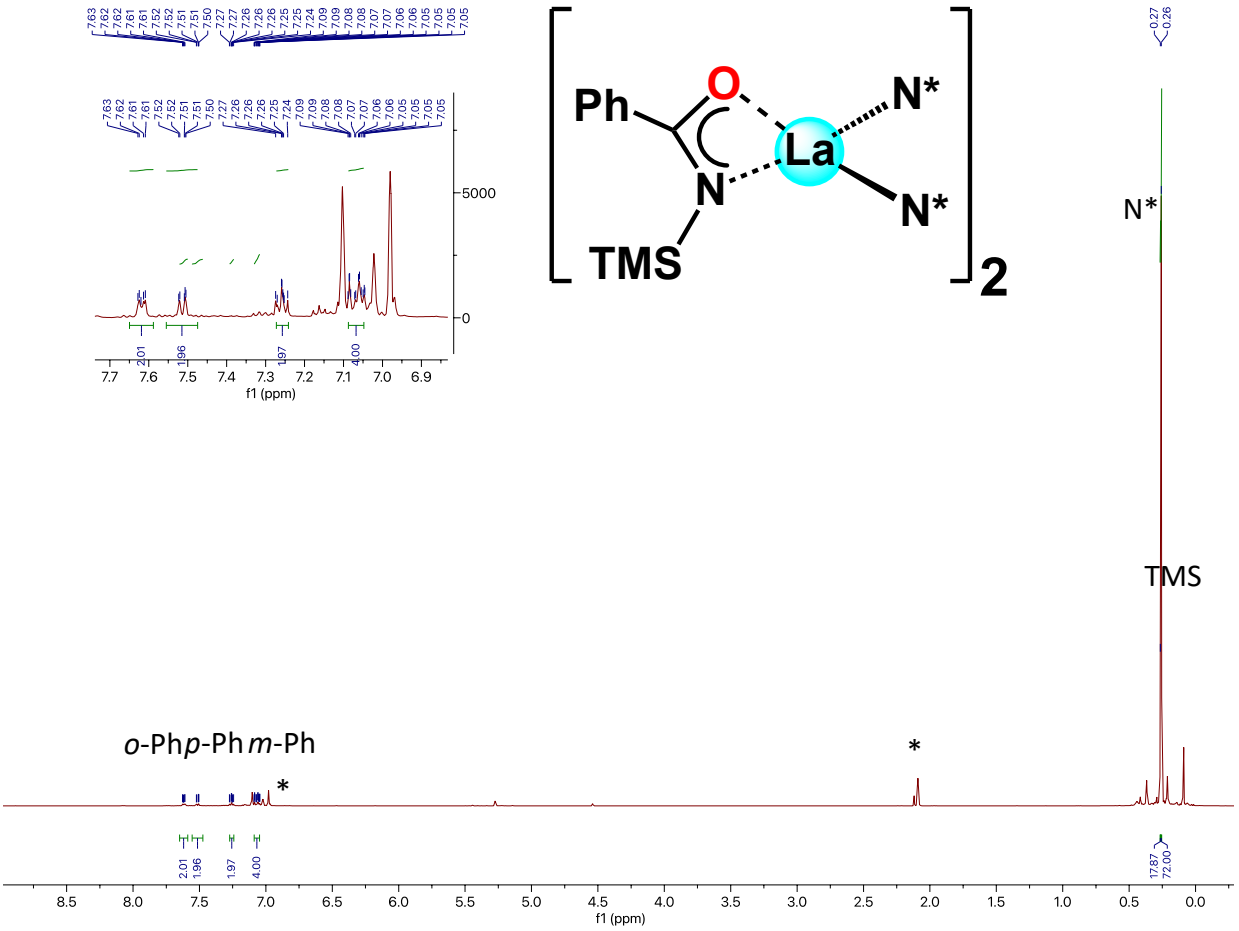


Figure S5. ^{1}H NMR spectrum of **4** in toluene-d_8. *o*-Ph = *ortho* phenyl protons, *p*-Ph = *para* phenyl protons, *m*-Ph = *meta* phenyl protons, TMS = trimethylsilyl, N* = N(TMS)$_2$, * = toluene-d_8. Close-up panel of the aromatic peaks.

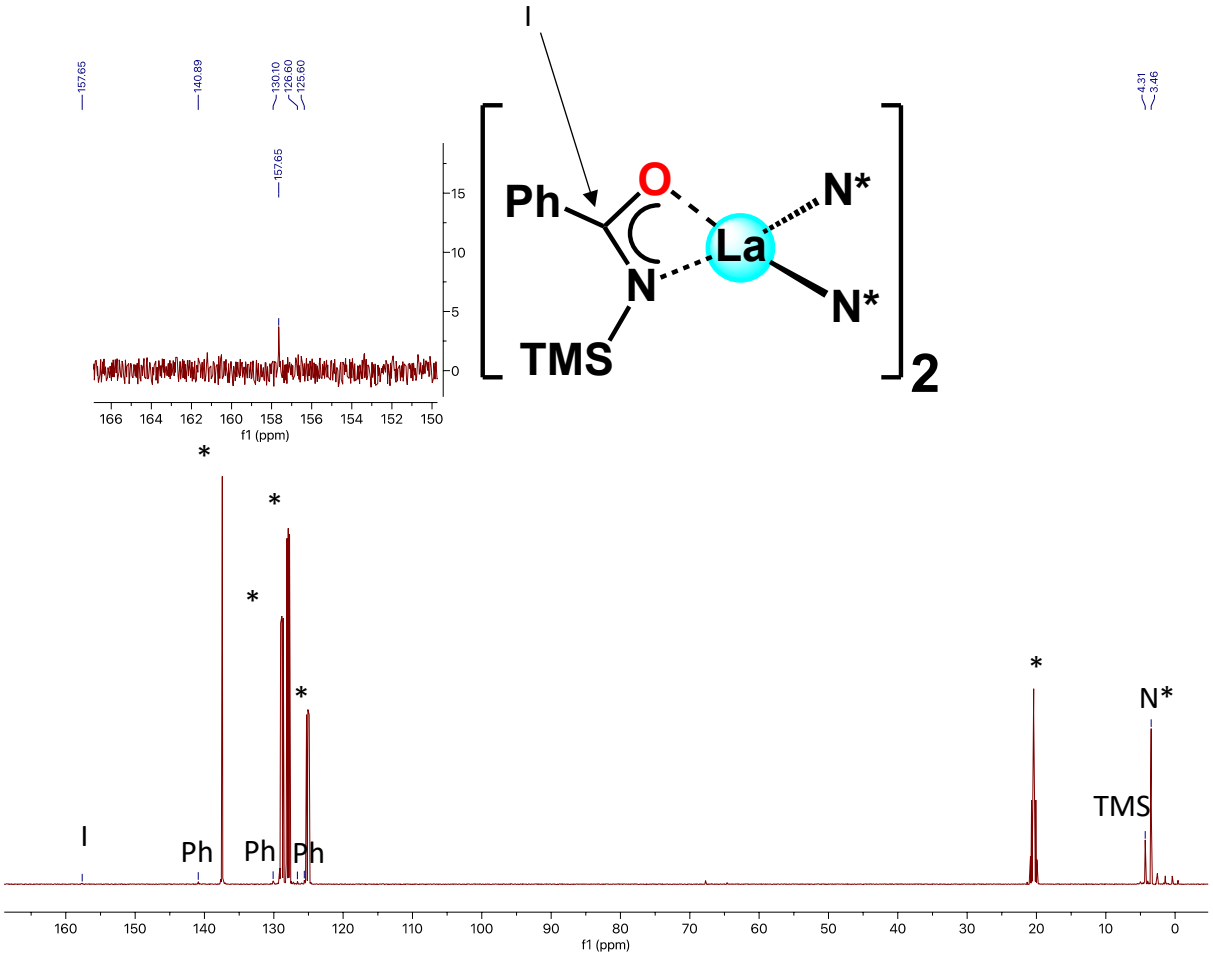


Figure S6. ^{13}C NMR spectrum of **4** in toluene-d_8. I = imino carbon, Ph = phenyl carbons, TMS = trimethylsilyl, N* = N(TMS)$_2$, * = toluene-d_8. Close-up panel of the imino peak.

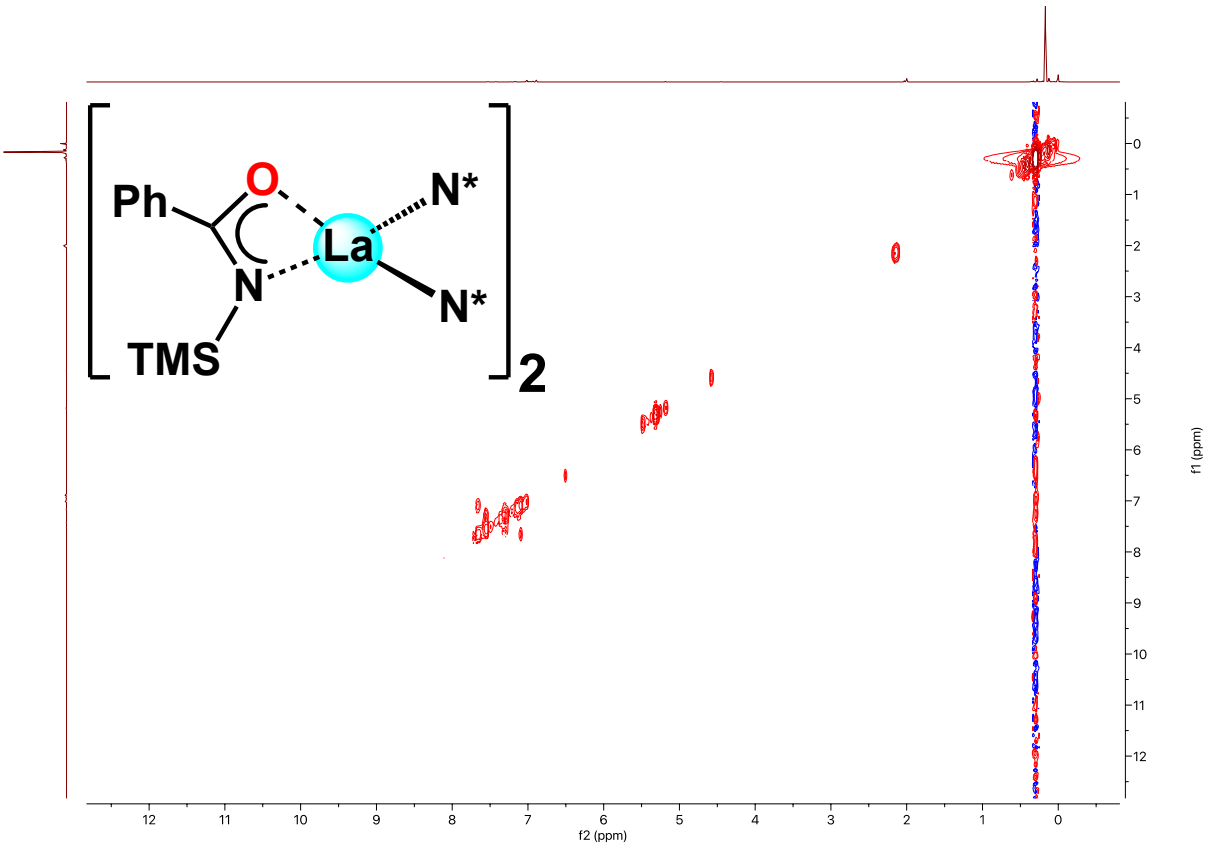


Figure S7. $^{1}H - {}^{1}H$ COSY NMR spectrum of **4** in toluene-d_8.

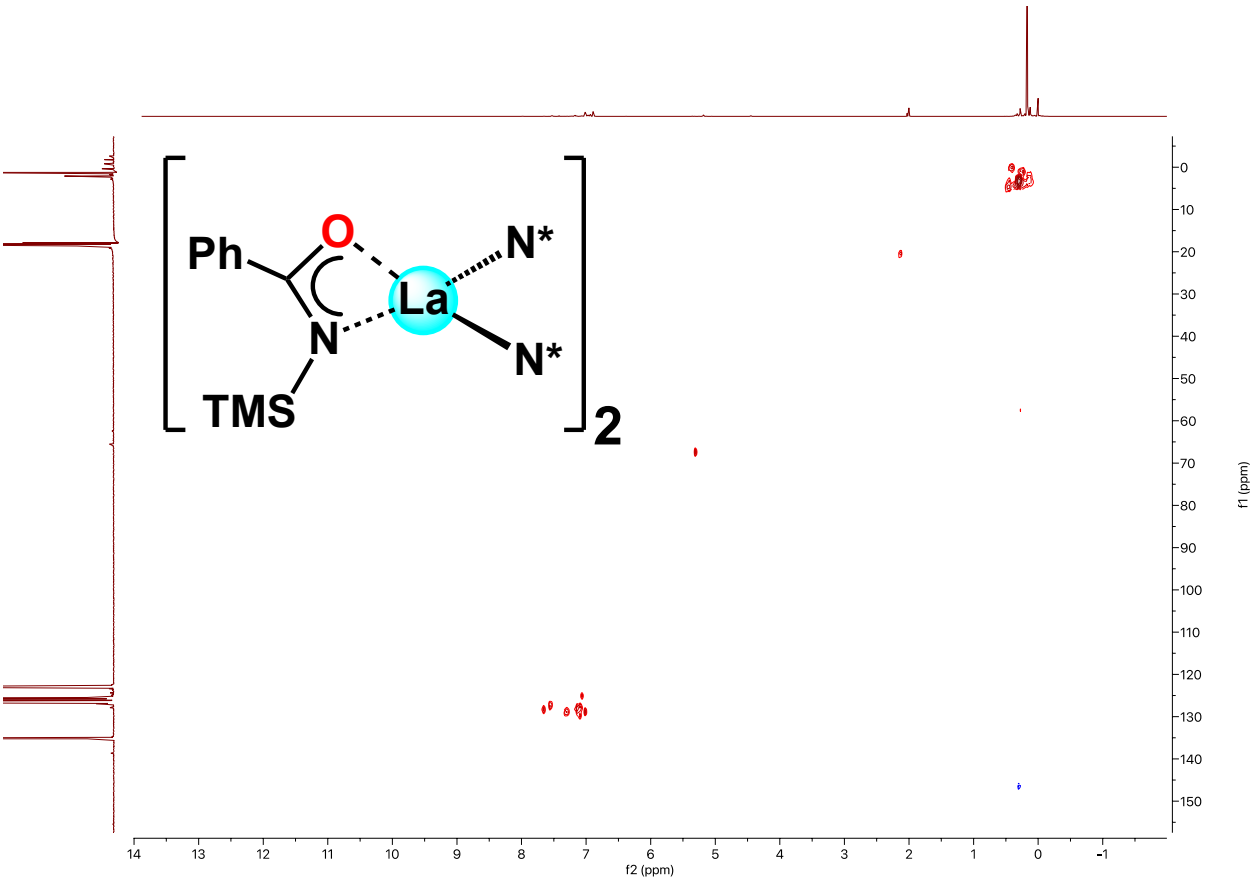


Figure S8. $^{1}H - {}^{13}C$ HSQC NMR spectrum of **4** in toluene-d_8.

1.5. Synthesis and Characterization of Complex 8

Synthesis of **8**: In a glovebox, La^{NTMS} (0.2 g, 0.323 mmol) was weighed into a 4 mL vial, 1 mL of anhydrous toluene was added, thoroughly mixed, and transferred to a flame-dried J-Young flask. HBpin (140.4 μg, 0.968 mmol) was syringed into the solution. The resulting mixture was allowed to react for 1 h and then concentrated, washed with cold toluene, and dried to afford a white powder. Single crystals suitable for X-ray crystallography were obtained from the concentrated solution. Isolated yield: 220 mg (47%).

(**8**) ^{1}H NMR (500 MHz, Toluene-d_8) δ 1.57 (br, 12 H, $(BH_3)_4$), 1.02 (s, 48H, Me), 0.33 (s, 72, TMS) ppm. ^{13}C NMR (126 MHz, Toluene-d_8) δ 81.60, 24.56, 3.72 ppm. ^{11}B NMR (128 MHz, Toluene-d_8) δ 25.74, -5.94 ppm. Anal. Calcd. for $C_{48}H_{132}LaN_4O_8Si_8$: C, 39.46; H, 3.84; N, 9.11. Found: C, 39.40; H, 3.75: N, 8.82.

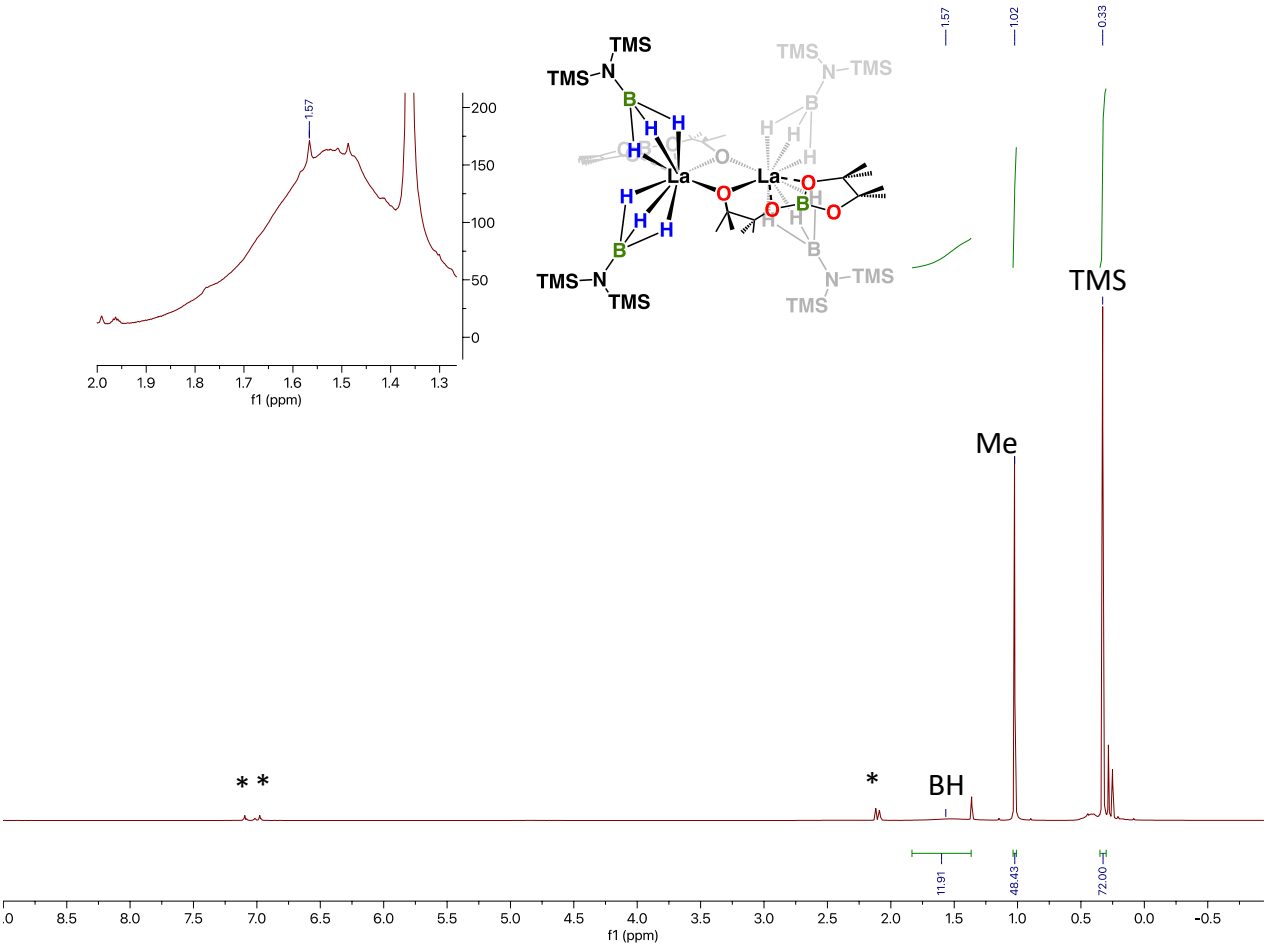


Figure S9. ^{1}H NMR spectrum of **8** in toluene-d_8. BH = borohydrides, Me = methyls from pinacol, TMS = trimethylsilyl, * = toluene-d_8.

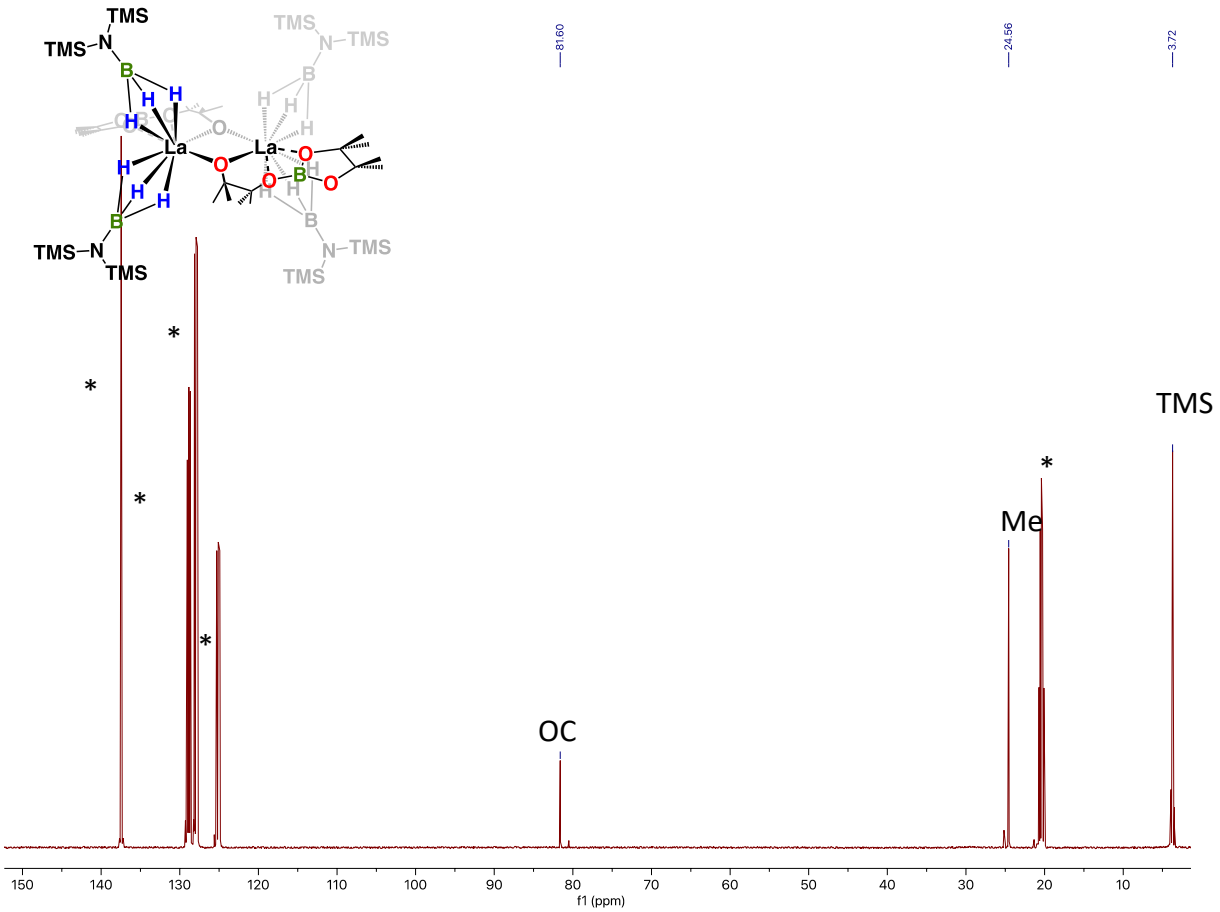


Figure S10. ^{13}C NMR spectrum of **8** in toluene-d_8. OC = methoxy carbons, Me = methyl carbons from pinacol, TMS = trimethylsilyl, * = toluene-d_8.

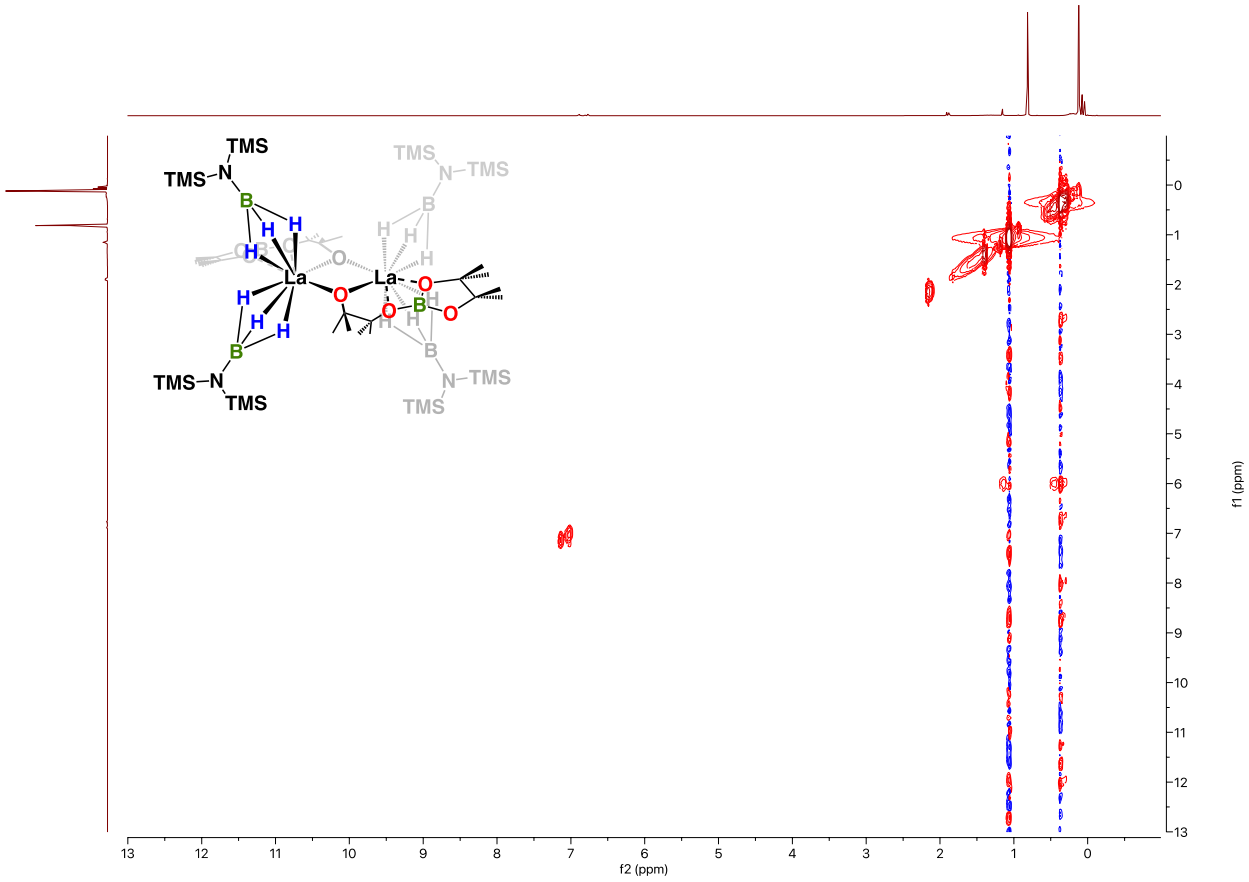


Figure S11. ^{1}H – ^{1}H COSY NMR spectrum of **8** in toluene-d_8.

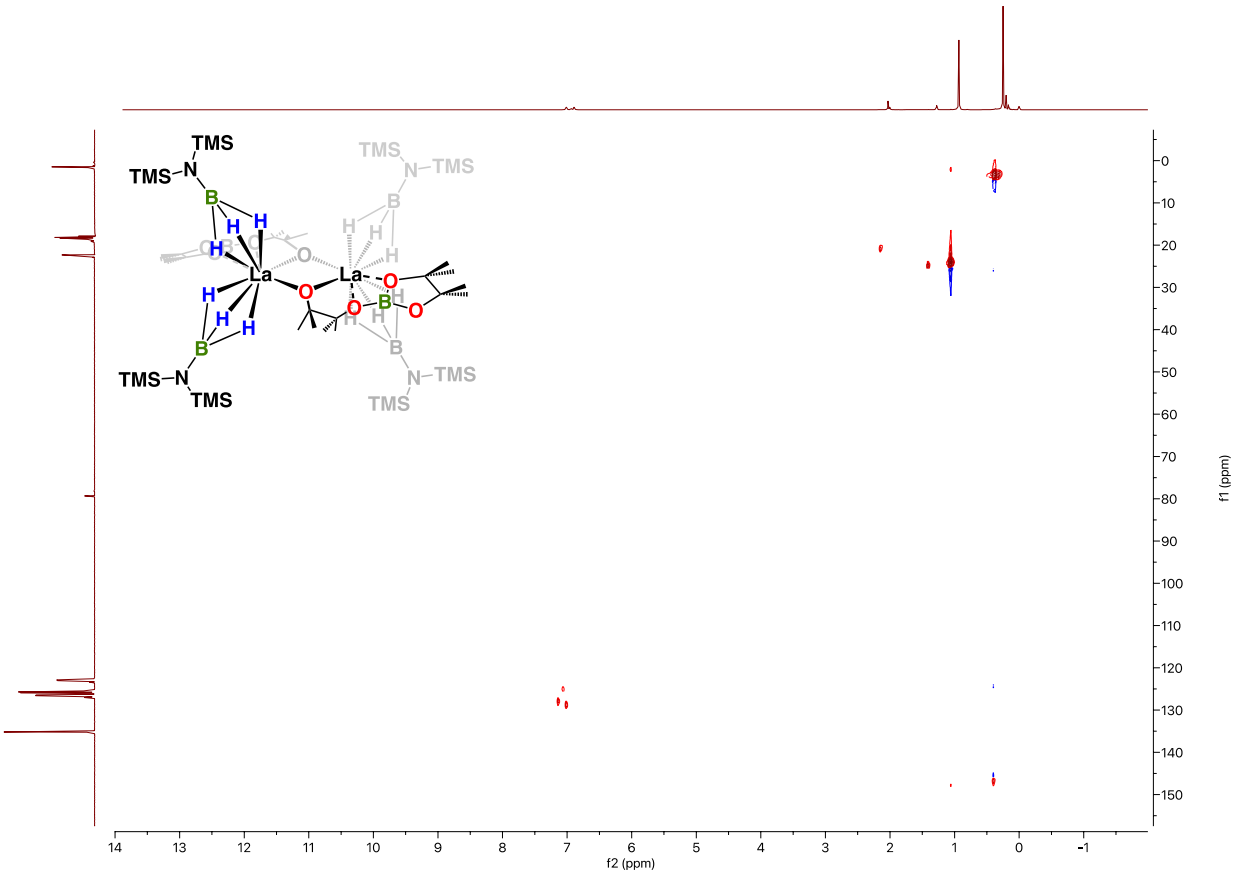


Figure S12. ^{1}H – ^{13}C HSQC NMR spectrum of **8** in toluene-d_8.

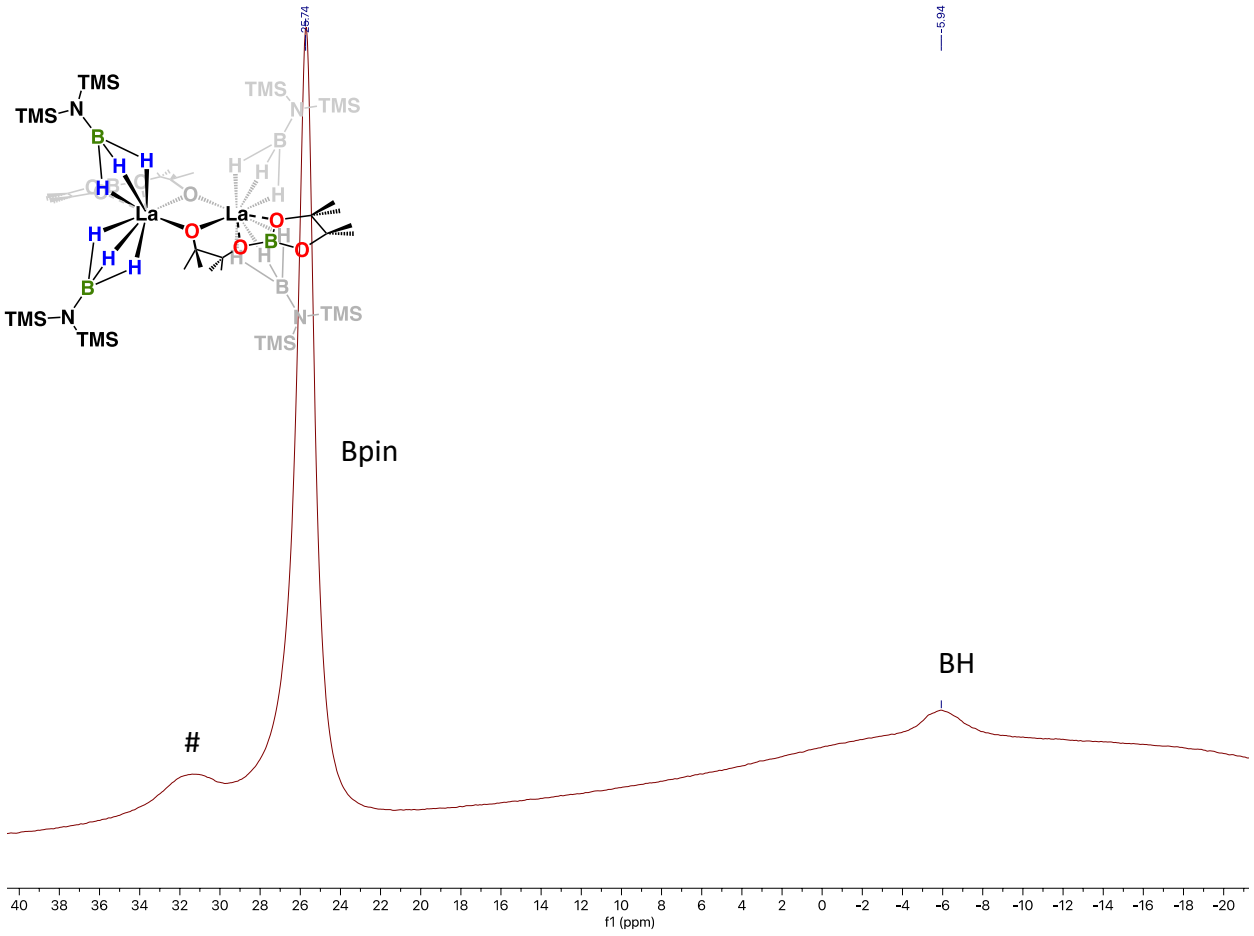
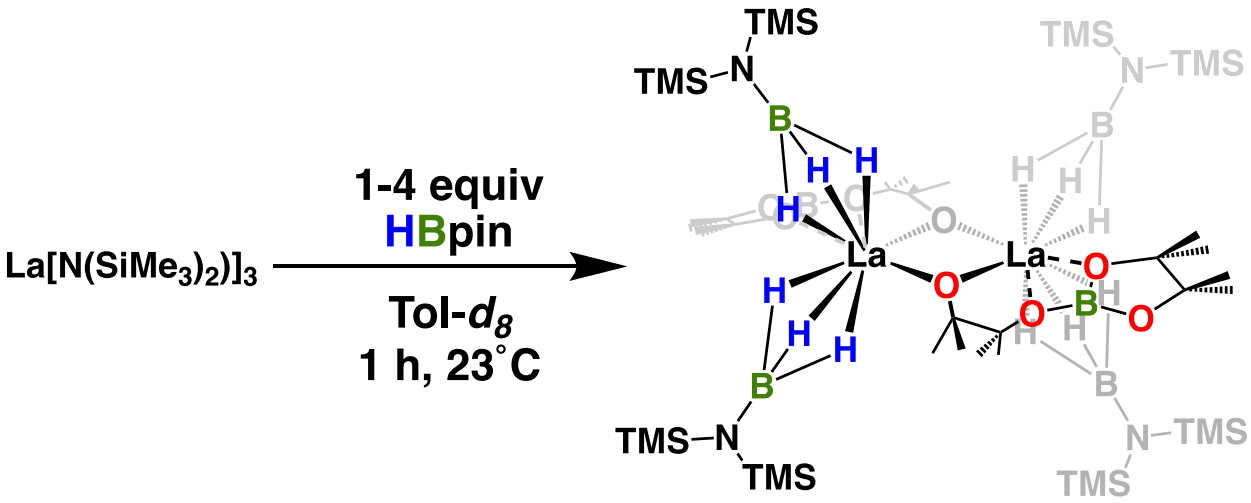


Figure S13. ^{11}B NMR spectrum of **8** in toluene-d_8. Bpin = boron pinacol, BH = borohydride, # = unidentified side product. Refer to Figure S16 to more clearly observe the quartet at -5.94 ppm.

1.6. Stoichiometric addition of HBpin to La^{NTMS}

In a glovebox, La^{NTMS} (25 mg, 0.04 mmol) was weighed into a 4 mL vial, 500 µL of toluene-d_8 was added, thoroughly mixed, and transferred to a J-Young NMR tube. HBpin (5.85 µL, 0.04 mmol) and mesitylene (5 µL) as the internal standard were syringed into the NMR tube and mixed with the solution. The sealed NMR tube was removed from the glove box and left at room temperature for the indicated reaction times (Scheme S1). After 1 h, an additional equivalent of HBpin was added to the solution and spectra were recorded. This was done for 4 h and the resulting mixtures were analyzed *in situ*.

Scheme S1. Stoichiometric addition of HBpin to La^{NTMS}.



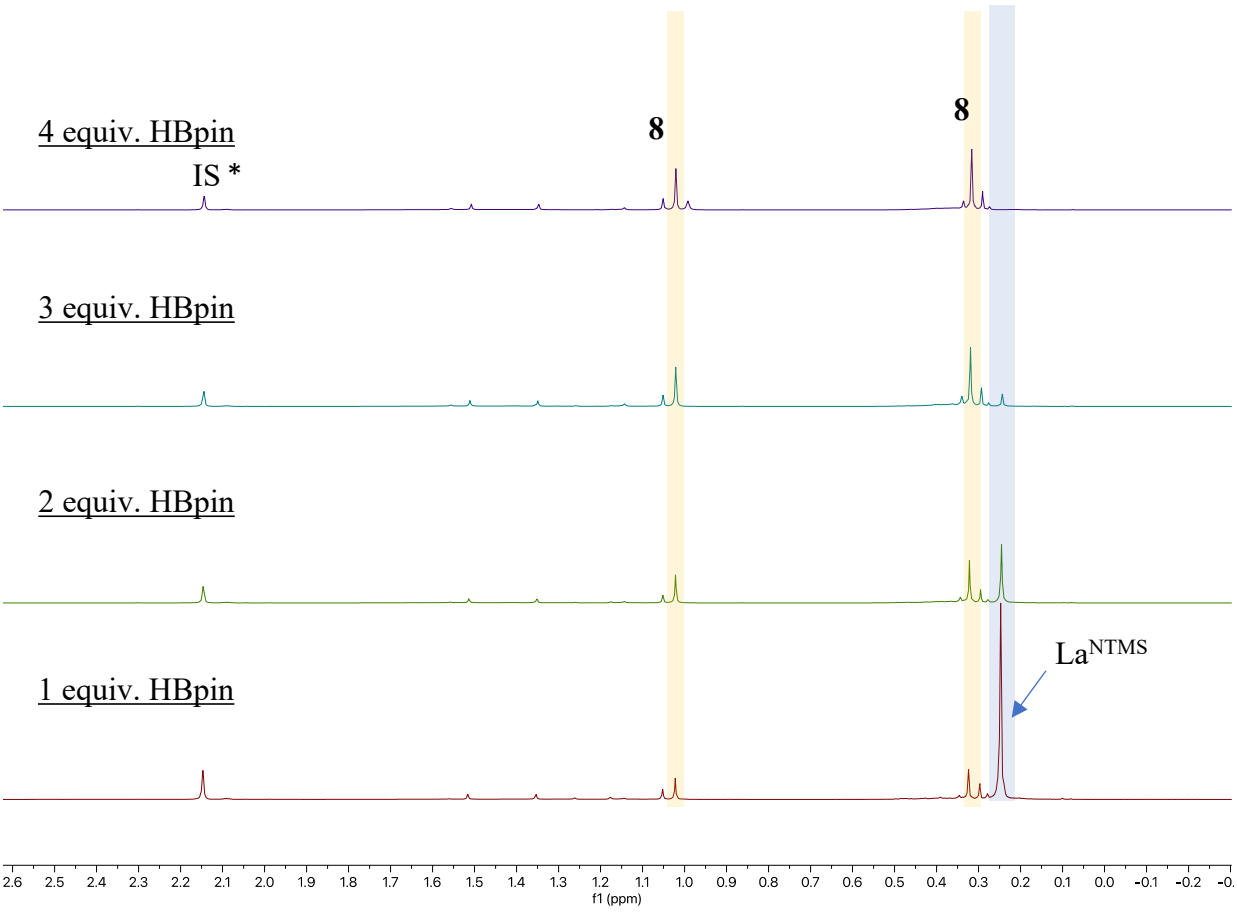


Figure S14. Close-up of stacked ^{1}H NMR spectra of the reaction from the addition of HBpin to La^{NTMS} represented in Scheme S1 after 1 h for each equivalent of HBpin. La^{NTMS} = La^{NTMS} (highlighted in blue), IS = internal standard (mesitylene), 8 = Complex **8** (highlighted in yellow), * = toluene-d_8.

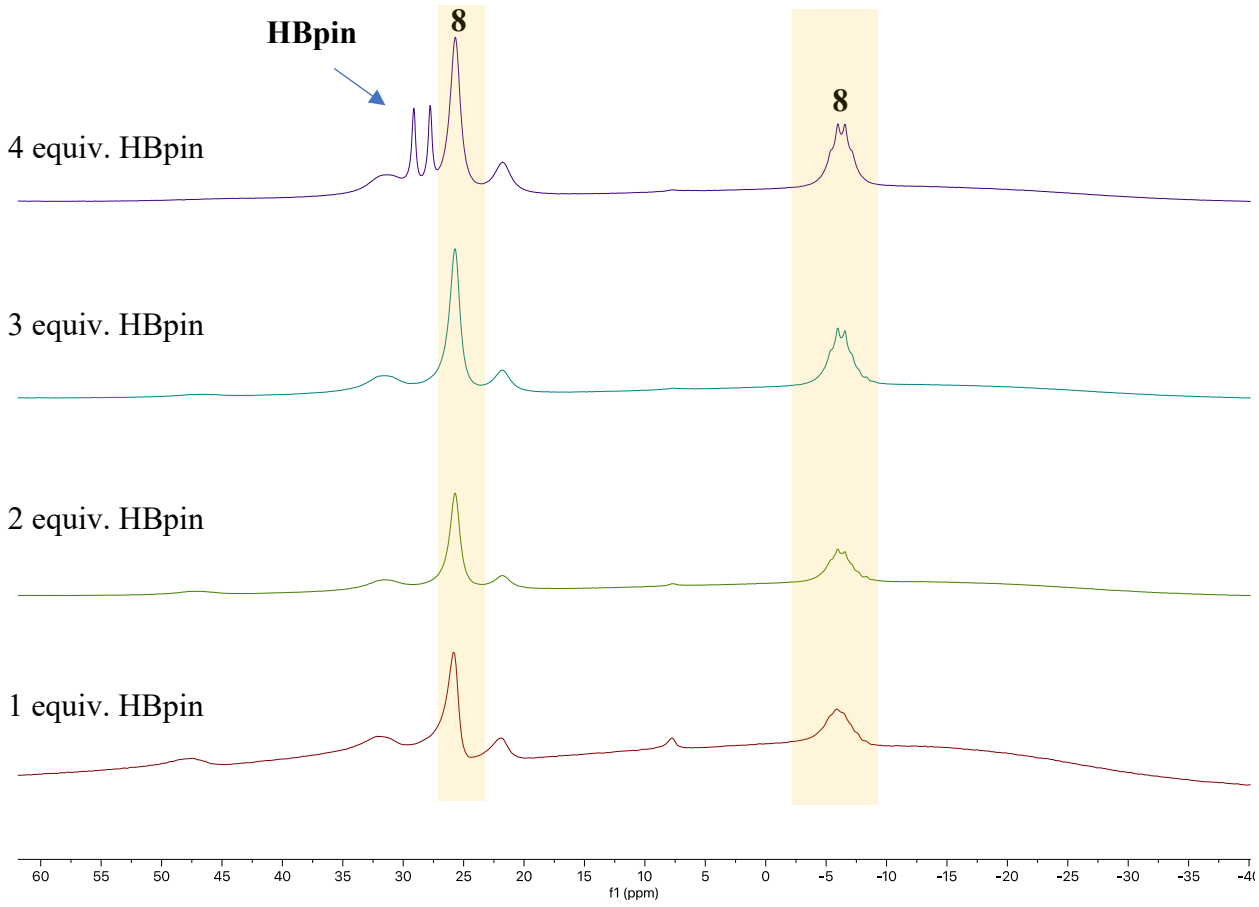


Figure S15. Stacked ^{11}B NMR spectra of the reaction from the addition of HBpin to La^{NTMS} represented in Scheme S1 after 1 h for each equivalent of HBpin. 8 = Complex **8** (highlighted in yellow), HBpin = HBpin.

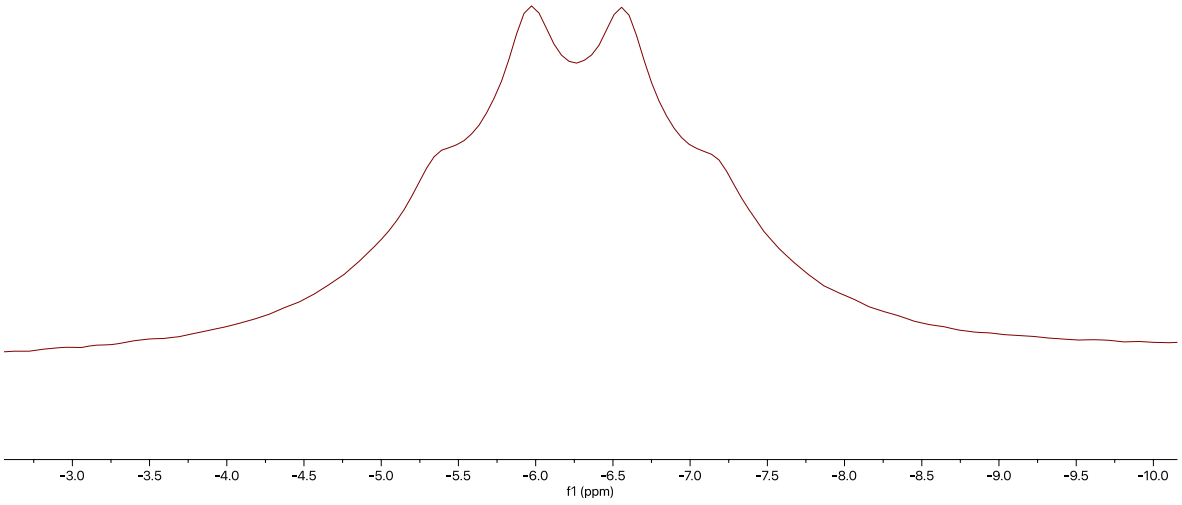


Figure S16. Close-up of the quartet in ^{11}B NMR spectrum of the reaction from the addition of HBpin to La^{NTMS} represented in Scheme S1 after 4 h and 4 equivalents equivalent of HBpin revealing a quartet (I = 3/2 for ^{11}B). This is the boron which is bound to three hydrides in complex **8**.

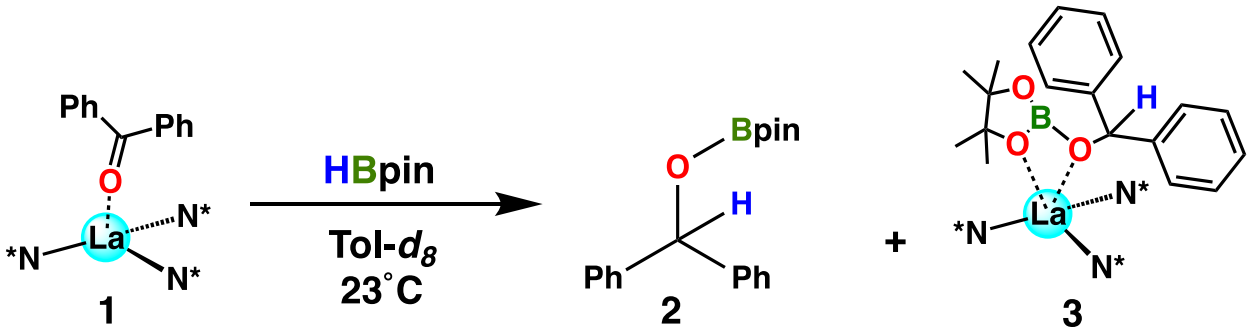
1.7. Stoichiometric Reaction Studies of Complex 1 with HBpin.

In a glovebox, complex **1** (40 mg, 0.05 mmol) was weighed into a 4 mL vial, 500 µL of toluene-d_8 was added, thoroughly mixed, and transferred to a J-Young NMR tube. HBpin (7.23 µL, 0.05 mmol) and mesitylene (5 µL) as the internal standard were syringed into the NMR tube and mixed with the solution. The sealed NMR tube was removed from the glove box and allowed to react at room temperature (Scheme S2). The TMS peaks are not reported due to the overlapped nature of the complex mixture.

(**2**) ^{1}H NMR (500 MHz, Toluene-d_8) δ 7.40 – 7.35 (m, 4H), 7.09 – 7.07 (m, 4H), 7.00 – 6.97 (m, 2H), 6.32 (s, 1H), 0.98 (s, 12H) ppm. ^{13}C NMR (126 MHz, Toluene-d_8) δ 143.88, 128.42, 127.31, 126.93, 82.69, 78.42, 24.49 ppm. ^{11}B NMR (128 MHz, Toluene-d_8) δ 22.88, -5.94 ppm.

(**3**) ^{1}H NMR (500 MHz, Toluene-d_8) δ 7.32 – 7.28 (m, 4H), 7.17 – 7.12 (m, 4H), 7.02 – 7.00 (m, 2H), 5.98 (s, 1H), 1.02 (s, 12H) ppm. ^{13}C NMR (126 MHz, Toluene-d_8) δ 144.00, 128.52, 127.41, 127.15, 83.91, 79.39, 24.49 ppm. ^{11}B NMR (128 MHz, Toluene-d_8) δ 25.74, -5.94 ppm.

Scheme S2. Stoichiometric reaction between complex **1** and HBpin as observed by NMR.



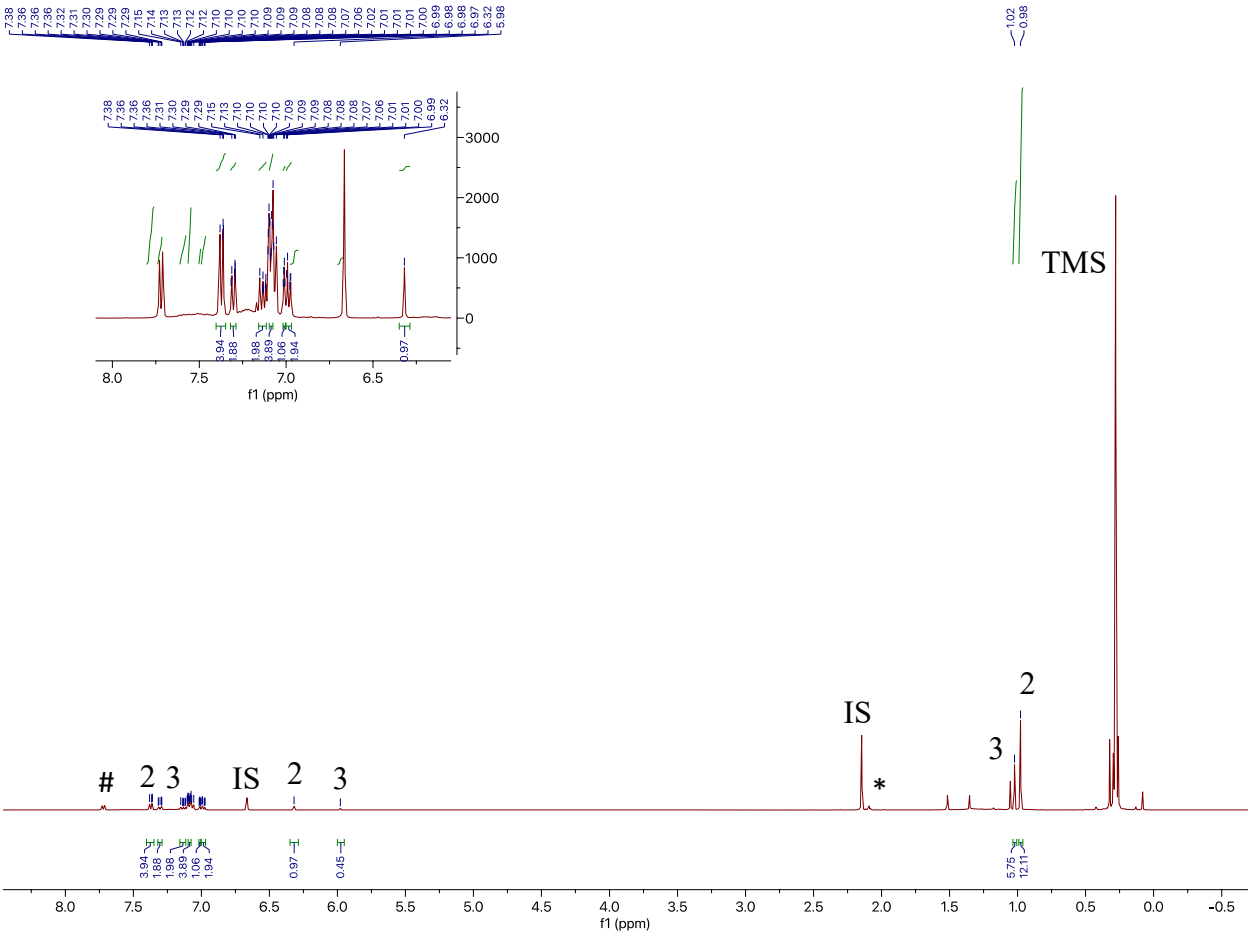


Figure S17. ^{1}H NMR spectrum of a **2** and **3** mixture in toluene-d_8. 2 = Complex **2**, 3 = Complex **3**, * = toluene-d_8, TMS = $SiMe_3$, IS = internal standard (mesitylene), # = unidentified side product.

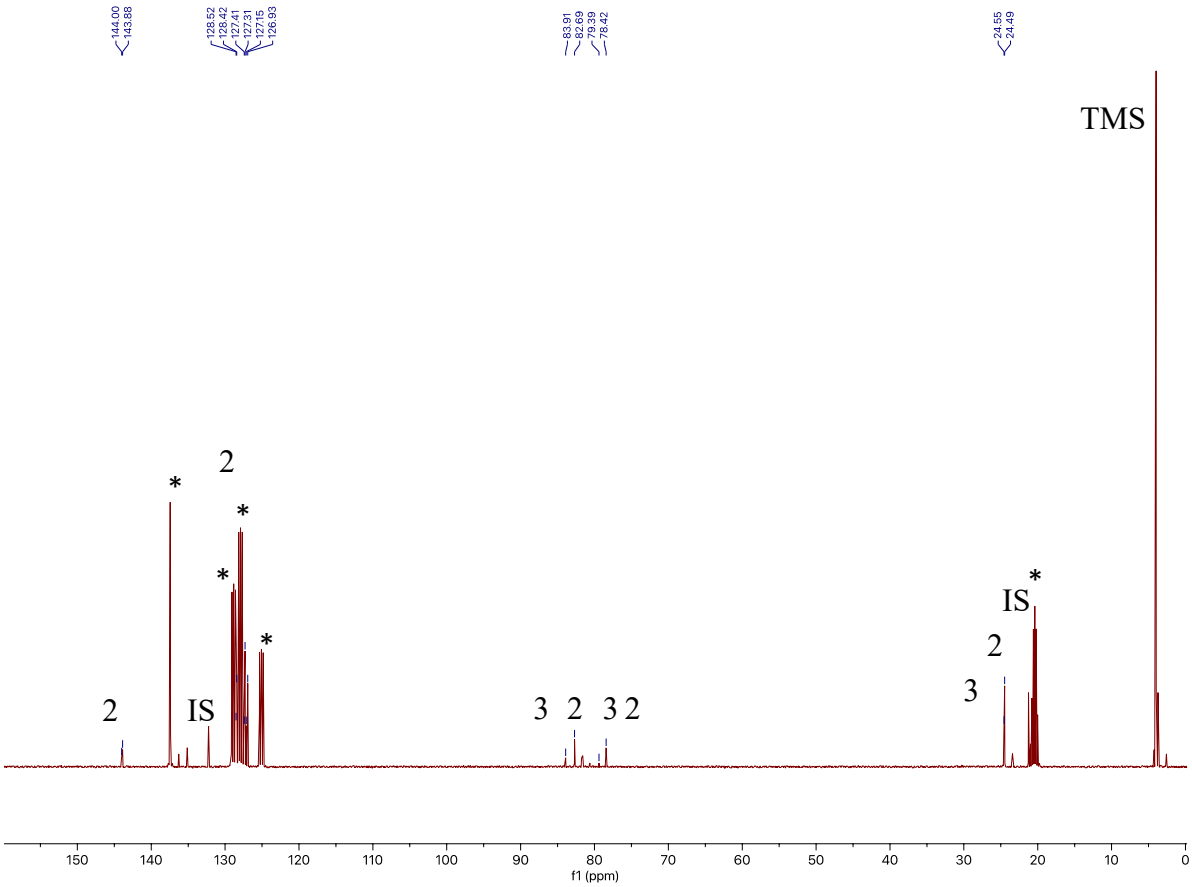


Figure S18. ^{13}C NMR spectrum of **2** and **3** mixture in toluene-d_8. 2 = Complex **2**, 3 = Complex **3**, * = toluene-d_8, TMS = $SiMe_3$, IS = internal standard (mesitylene).

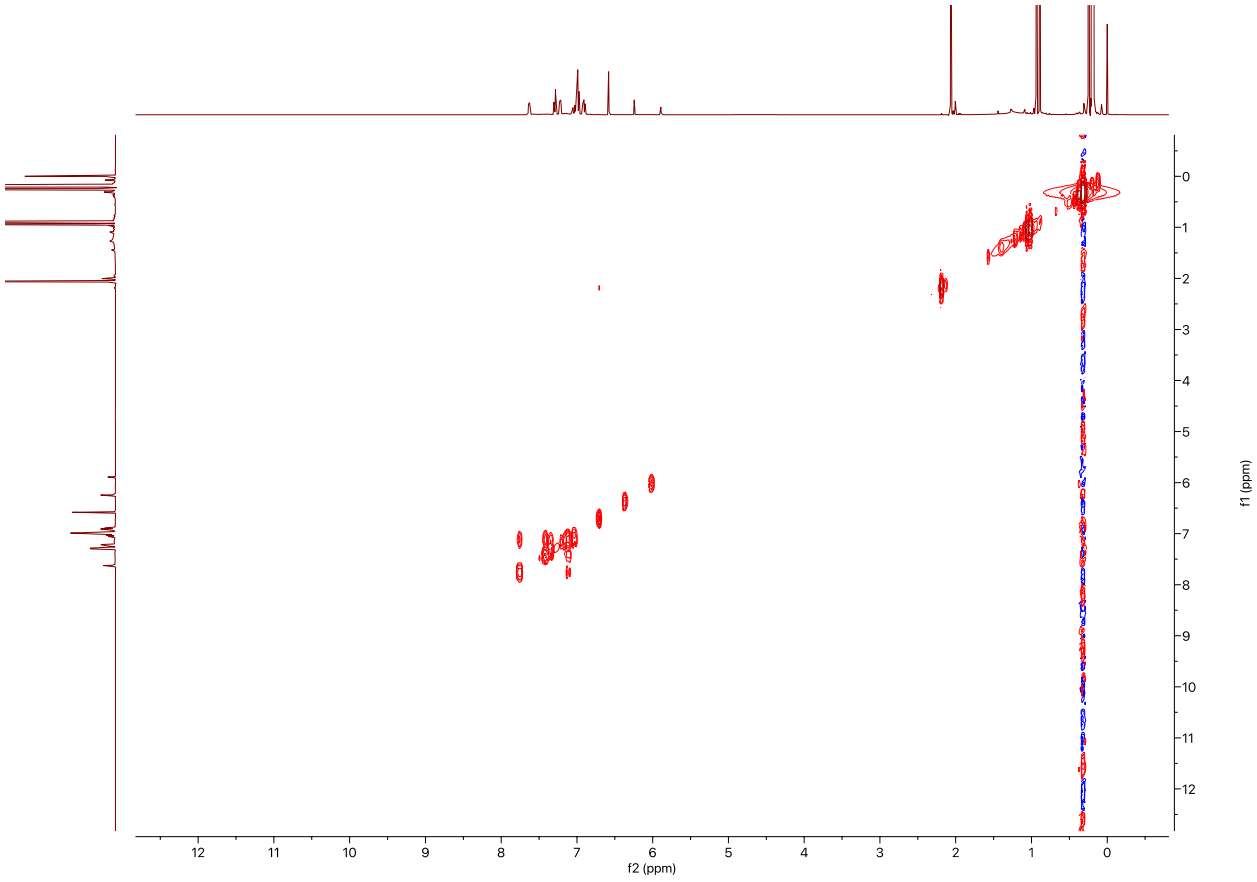


Figure S19. ^{1}H – ^{1}H COSY NMR spectrum of a **2** and **3** mixture in toluene-d_8.

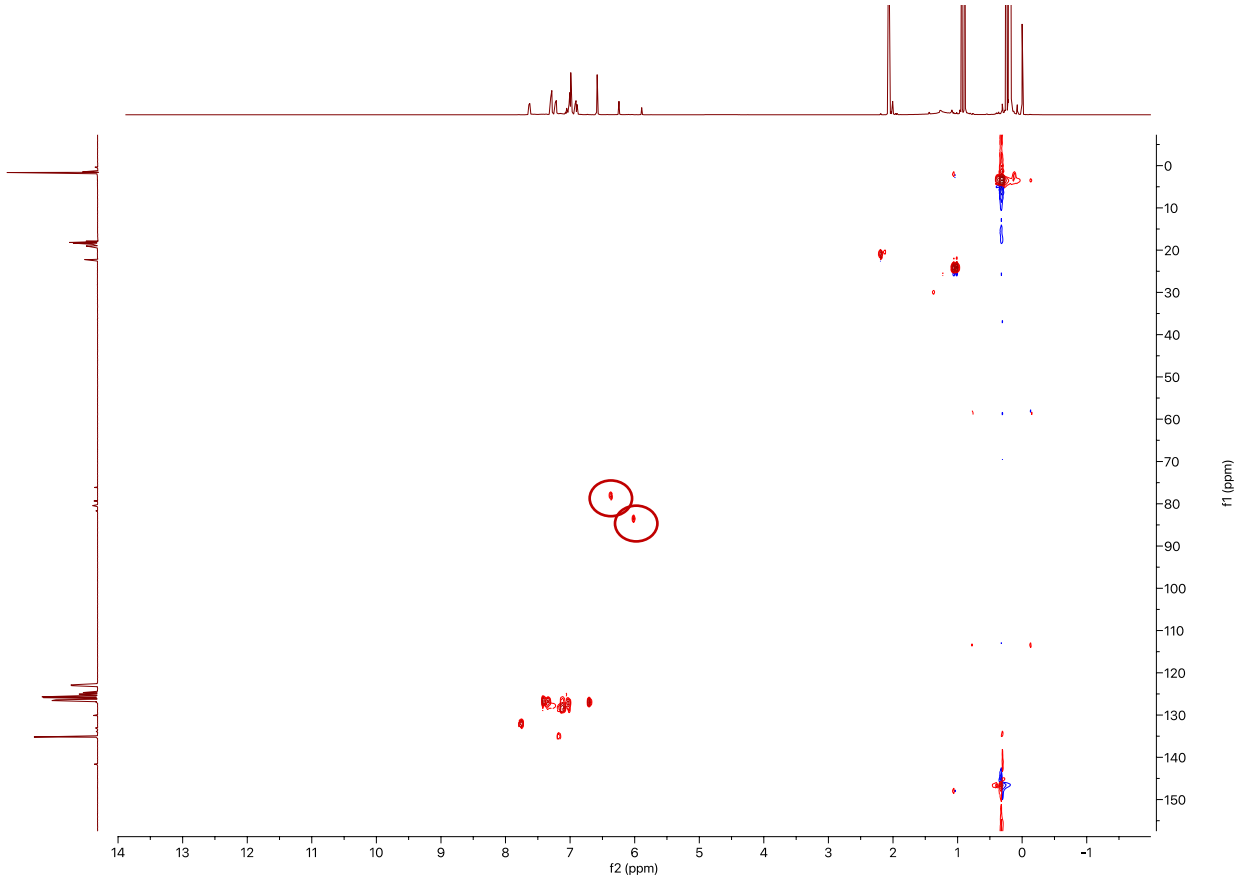


Figure S20. ^{1}H – ^{13}C HSQC NMR spectrum of a **2** and **3** mixture in toluene-d_8.

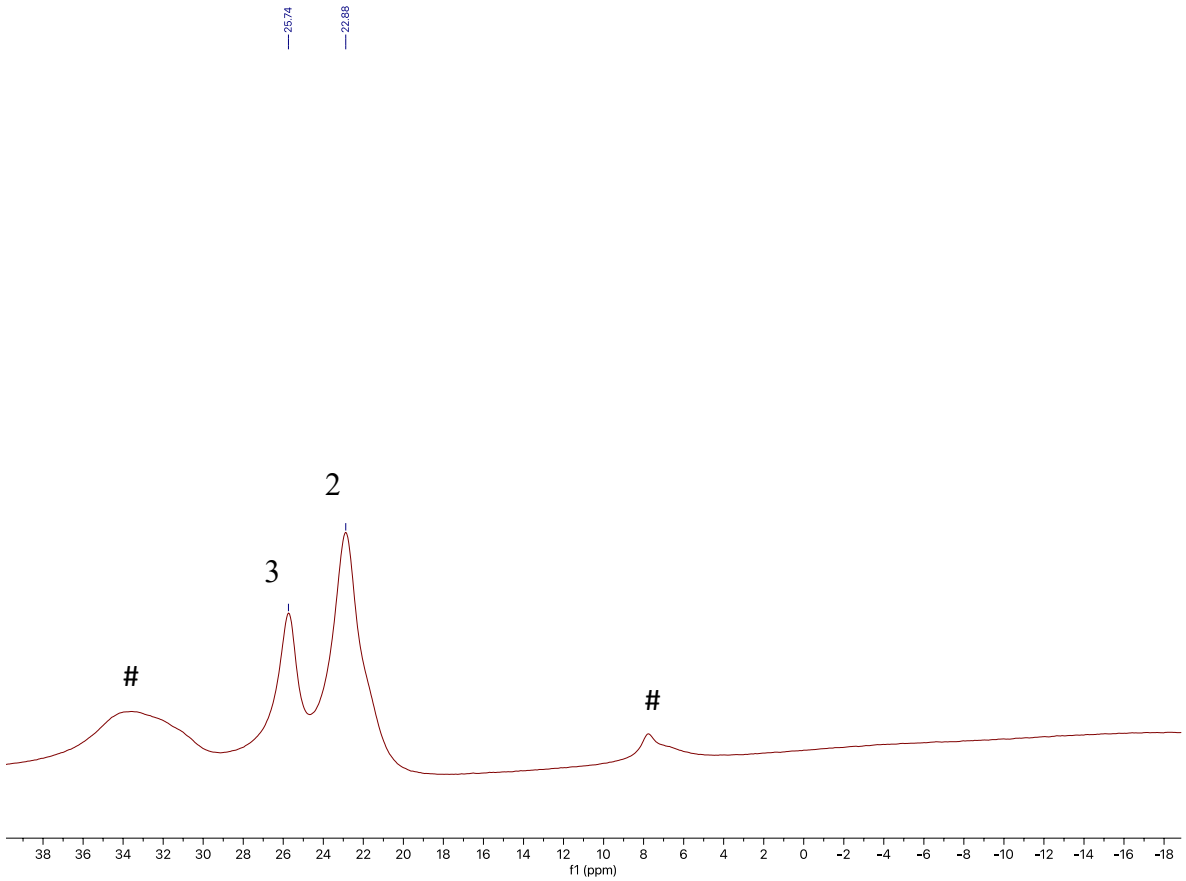
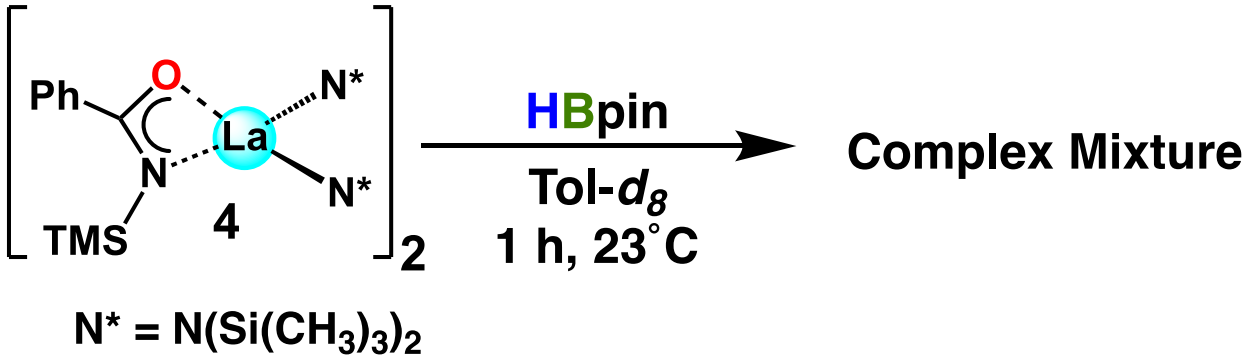


Figure S21. ^{11}B NMR spectrum of a **2** and **3** mixture in toluene-d_8. 2 = Complex **2**, 3 = Complex **3**, # = unidentified side product.

1.8. Stoichiometric Reaction Studies of 4 with HBpin.

In a glovebox, complex **4** (20 mg, 0.031 mmol) was weighed into a 4 mL vial, 500 µL of toluene-d_8 was added, thoroughly mixed, and transferred to a J-Young NMR tube. HBpin (4.45 µL, 0.031 mmol) and mesitylene (5 µL) as the internal standard were syringed into the NMR tube and mixed with the solution. The sealed NMR tube was removed from the glove box and left at room temperature for the indicated reaction times (Scheme S3). The TMS peaks are not reported due to the overlapped nature of the complex mixture.

Scheme S3. Stoichiometric reaction between complex **4** and HBpin



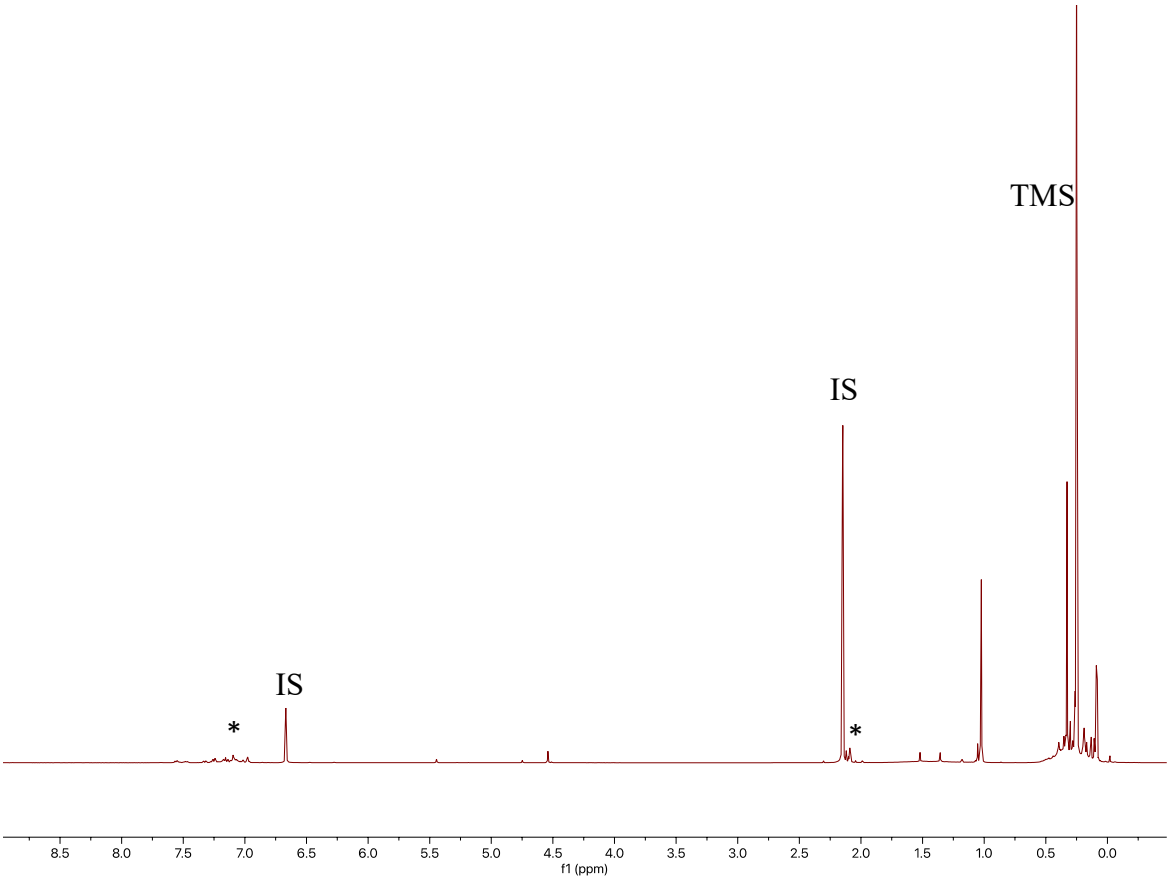


Figure S22. ^{1}H NMR spectrum of the reaction between complex **4** and HBpin in toluene-d_8. * = toluene-d_8, TMS = $SiMe_3$, IS = internal standard (mesitylene).

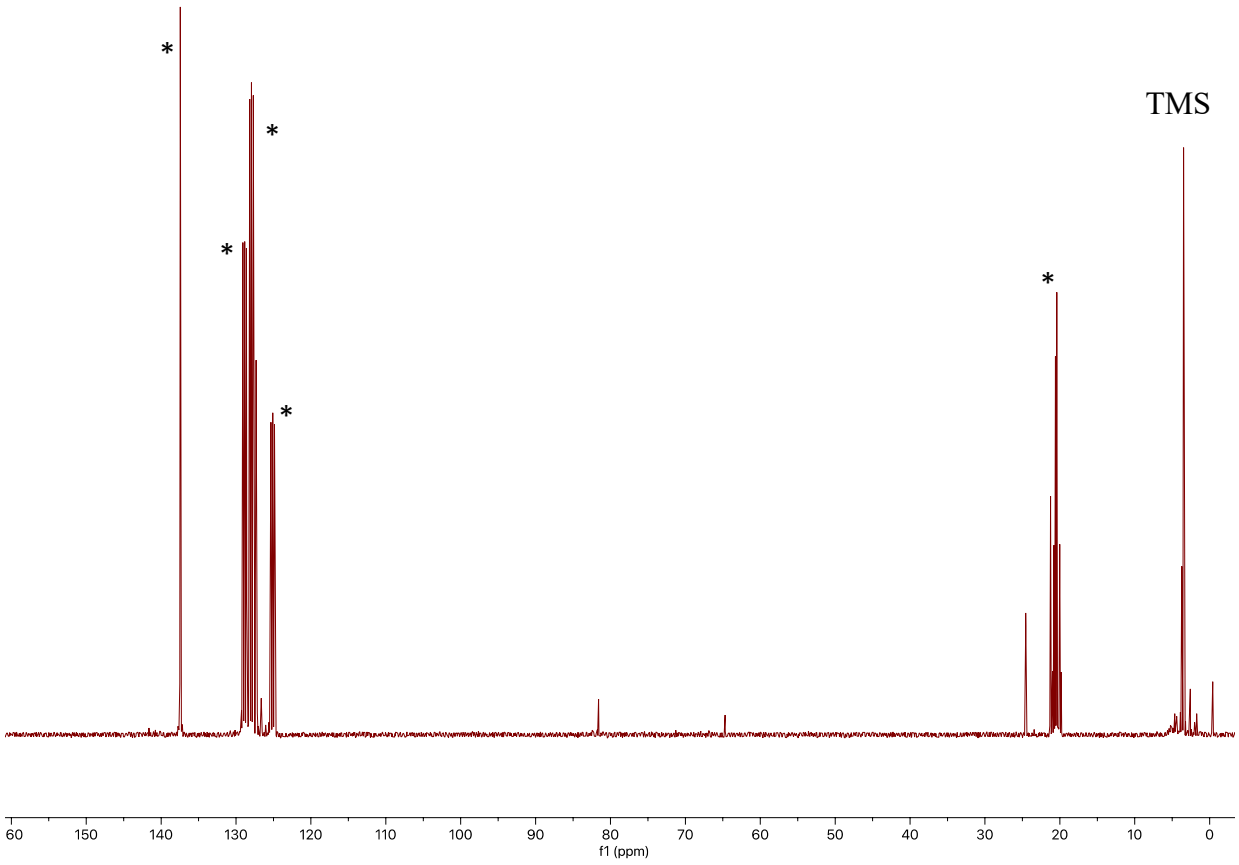


Figure S23. ^{13}C NMR spectrum of the reaction between complex **4** and HBpin in toluene-d_8. * = toluene-d_8, TMS = $SiMe_3$, IS = internal standard (mesitylene).

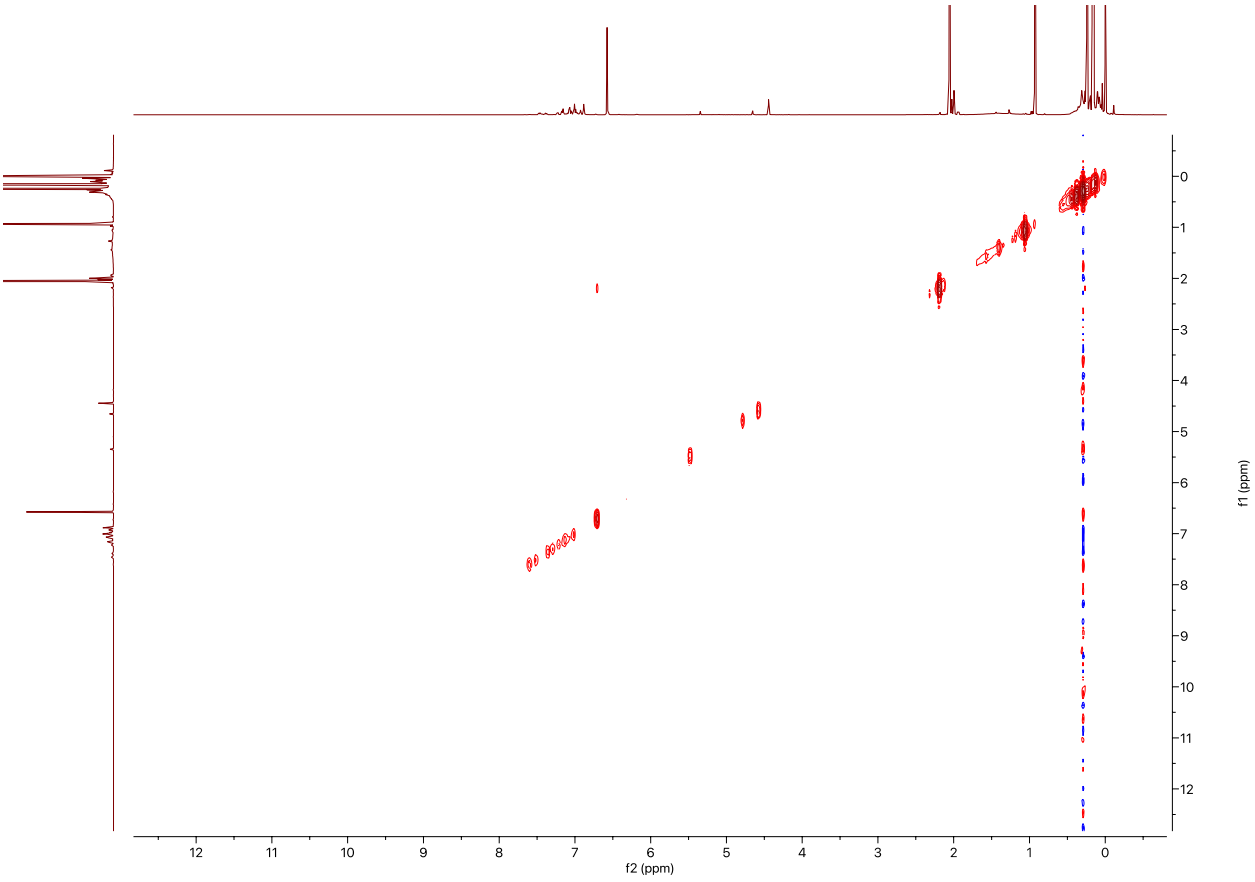


Figure S24. ^{1}H – ^{1}H COSY NMR spectrum of the reaction between complex **4** and HBpin in toluene-d_8.

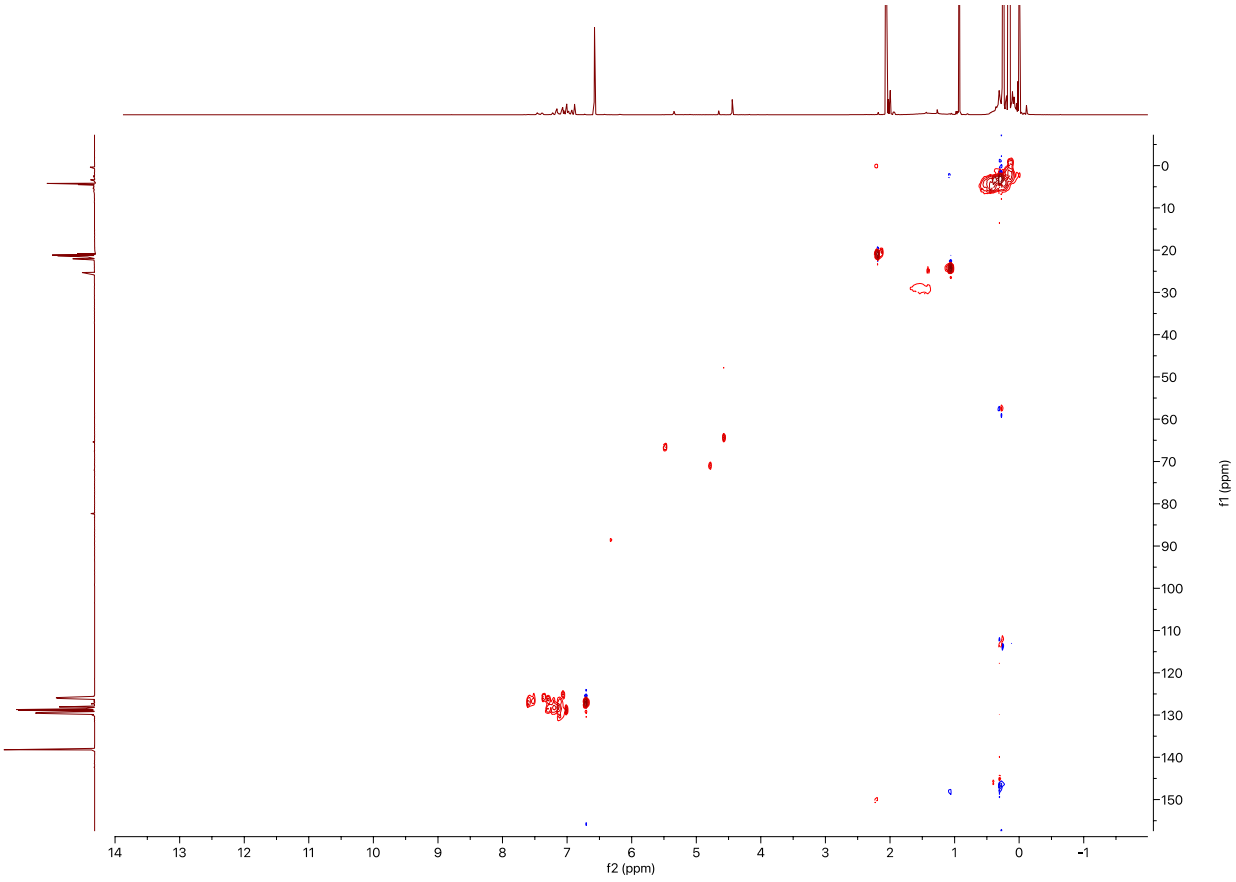


Figure S25. ^{1}H – ^{13}C HSQC NMR spectrum of the reaction between complex **4** and HBpin in toluene-d_8.

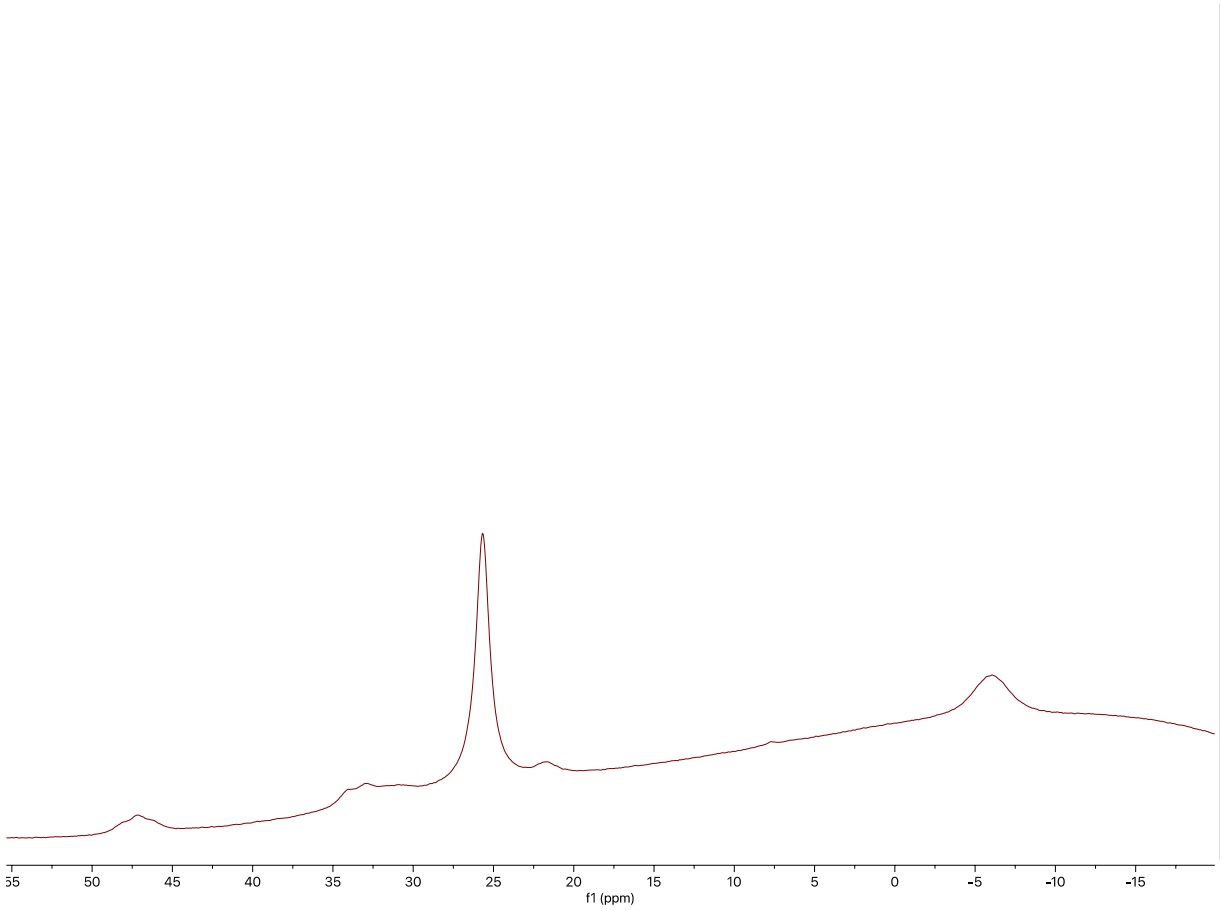
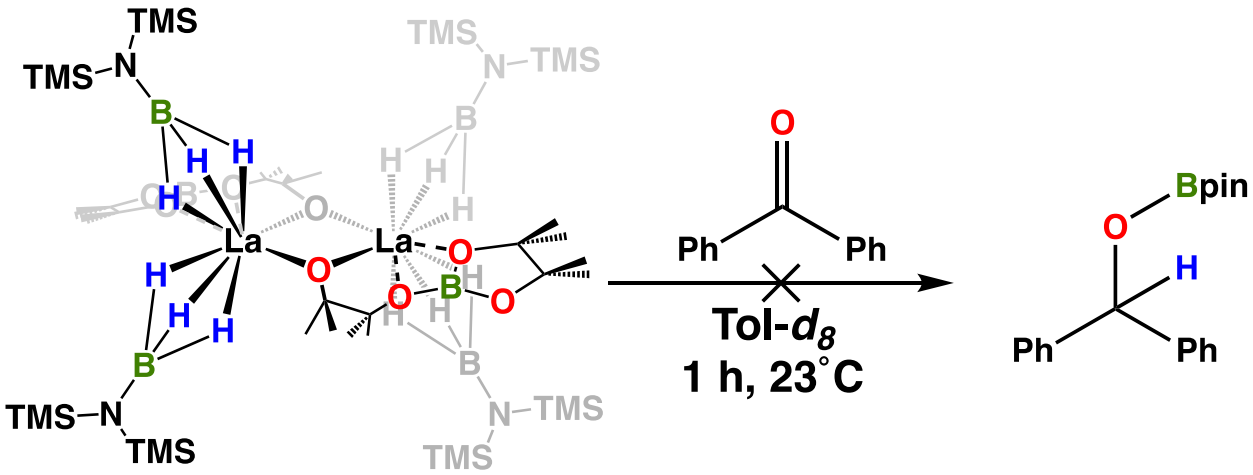


Figure S26. ^{11}B NMR spectrum of the reaction between complex **4** and HBpin in toluene-d_8.

1.9. Stoichiometric Reaction Studies of 8 with Benzophenone.

In a glovebox, complex **8** (40 mg, 0.027 mmol) was weighed into a 4 mL vial, 500 µL of toluene-d_8 was added, thoroughly mixed, and transferred to a J-Young NMR tube. Benzophenone (5.0 mg, 0.027 mmol) and mesitylene (5 µL) as the internal standard were syringed into the NMR tube and mixed with the solution. The sealed NMR tube was removed from the glove box and left at room temperature for the indicated reaction times (Scheme S4). There was little reactivity, and 82% of the starting material is leftover.

Scheme S4. Stoichiometric reaction between complex **8** and benzophenone with no turnover.



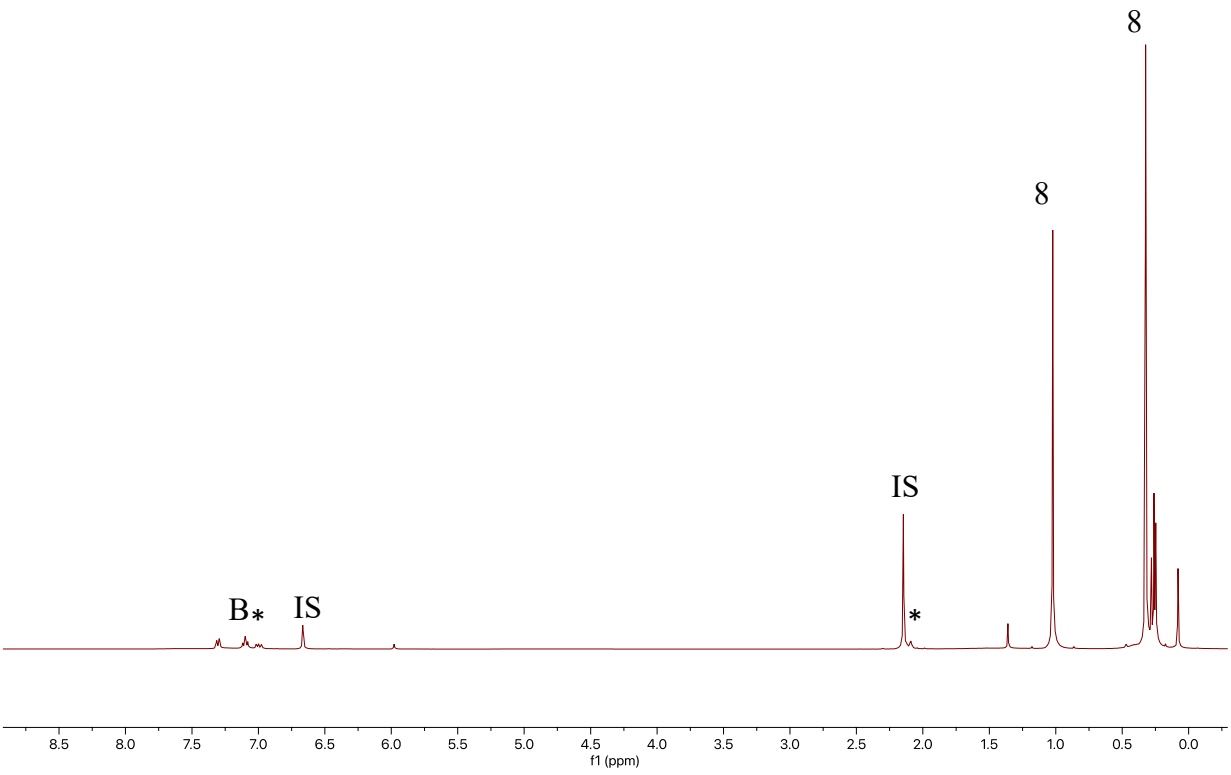


Figure S27. ^{1}H NMR spectrum of the reaction between complex **8** and benzophenone in toluene-d_8. 8 = Complex **8**, * = toluene-d_8, B = benzophenone, IS = internal standard (mesitylene).

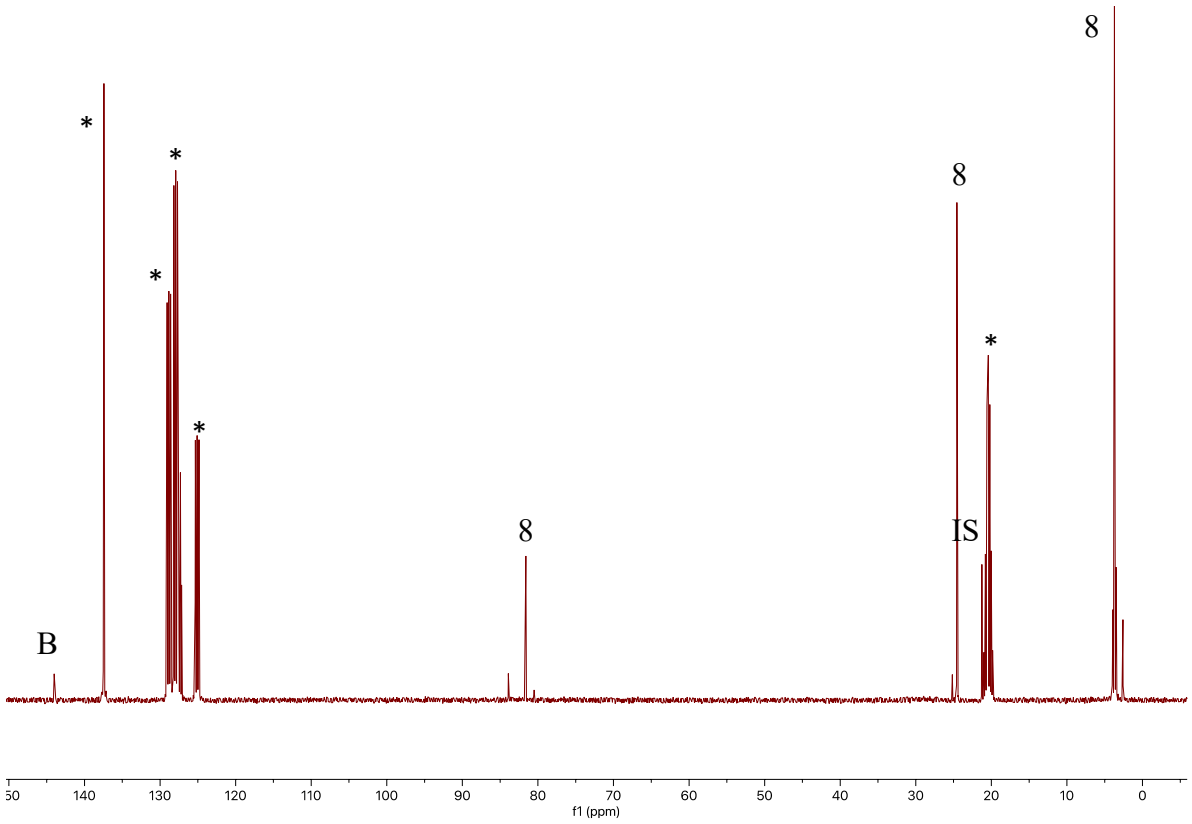


Figure S28. ^{13}C NMR spectrum of the reaction between complex **8** and benzophenone in toluene-d_8. 8 = Complex **8**, * = toluene-d_8, B = benzophenone, IS = internal standard (mesitylene).

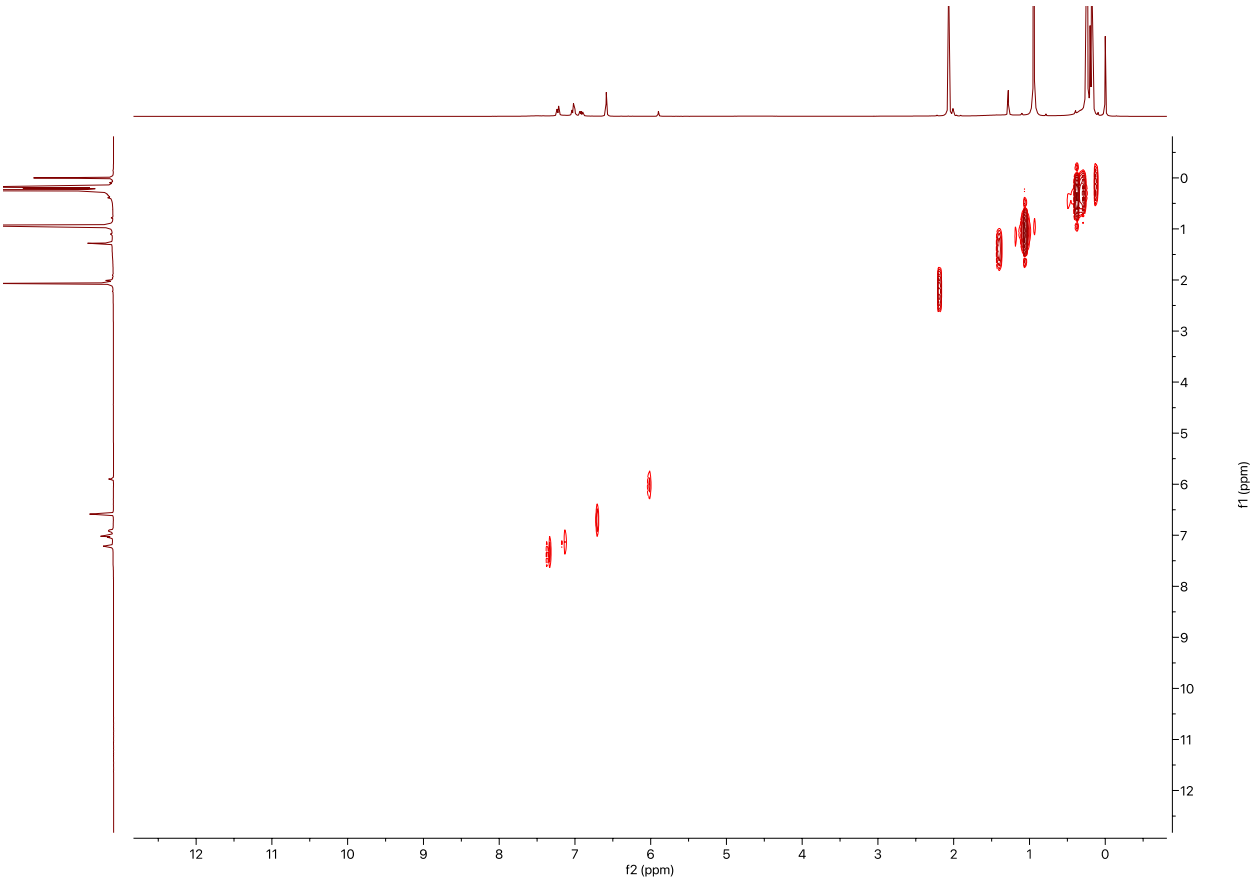


Figure S29. $^{1}H - {}^{1}H$ COSY NMR spectrum of the reaction between complex **8** and benzophenone in toluene-d_8.

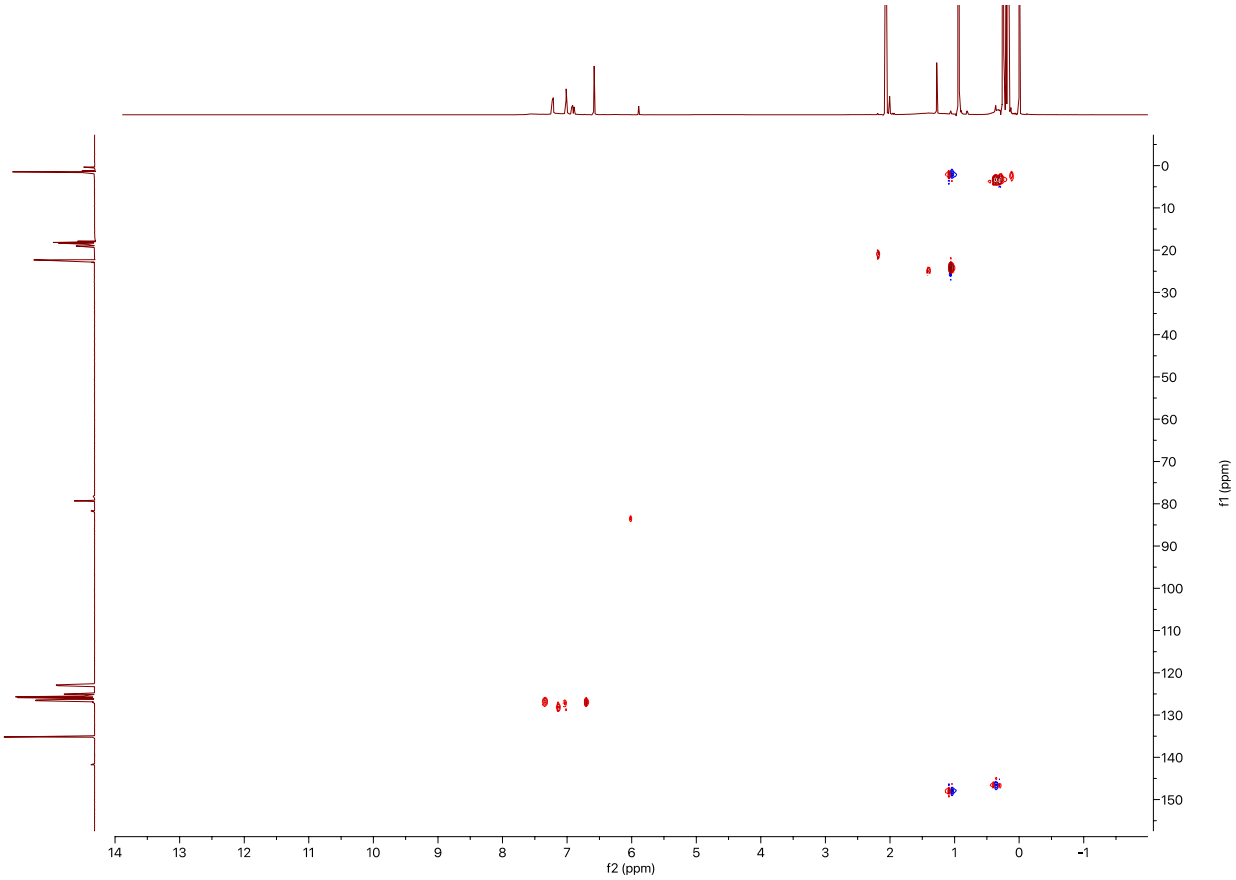


Figure S30. $^{1}H - ^{13}C$ HSQC NMR spectrum of the reaction between complex **8** and benzophenone in toluene-d_8.

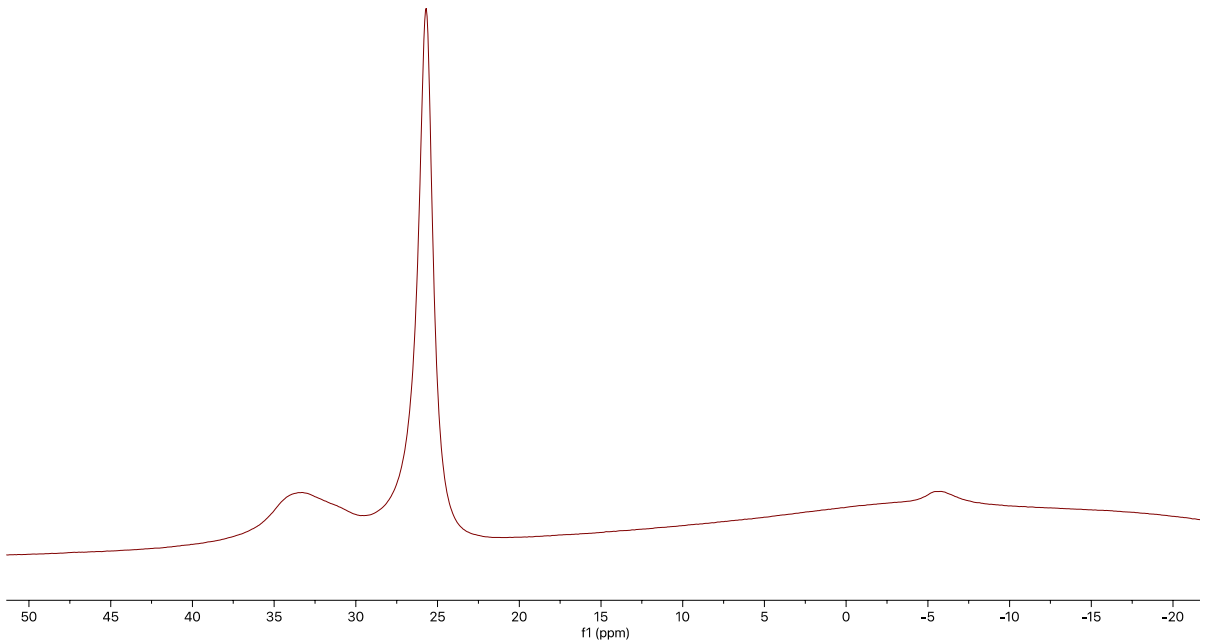
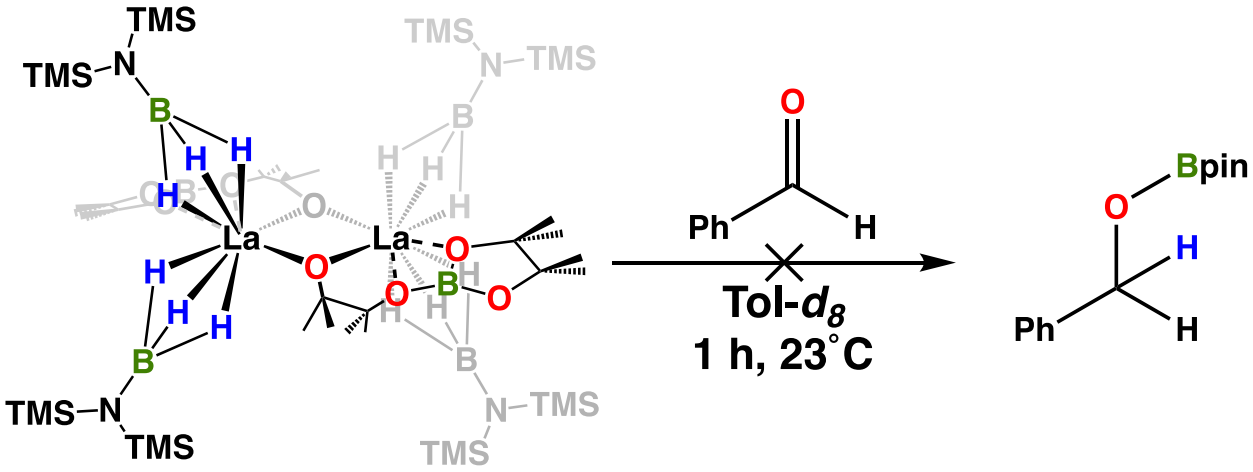


Figure S31. ^{11}B NMR spectrum of the reaction between complex **8** and benzophenone in toluene-d_8. 8 = Complex **8**, # = unidentified side product.

1.10. Stoichiometric Reaction Studies of 8 with Benzaldehyde.

In a glovebox, complex **8** (40 mg, 0.027 mmol) was weighed into a 4 mL vial, 500 µL of toluene-d_8 was added, thoroughly mixed, and transferred to a J-Young NMR tube. Benzaldehyde (2.8 µL, 0.027 mmol) and mesitylene (5 µL) as the internal standard were syringed into the NMR tube and mixed with the solution. The sealed NMR tube was removed from the glove box and left at room temperature for the indicated reaction times (Scheme S5).

Scheme S5. Stoichiometric reaction between complex **8** and benzaldehyde with no turnover.



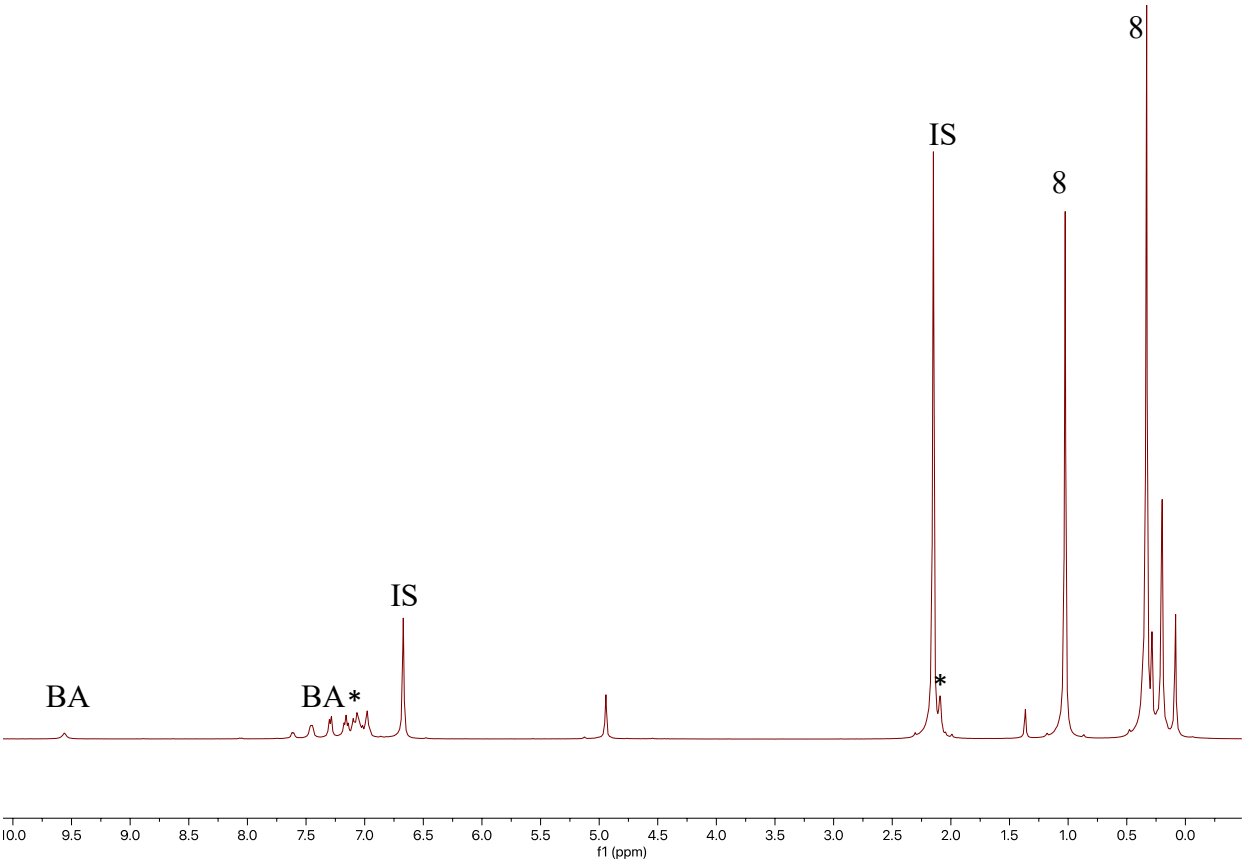


Figure S32. ^{1}H NMR spectrum of the reaction between complex **8** and benzophenone in toluene-d_8. 8 = Complex **8**, * = toluene-d_8, BA = benzaldehyde, IS = internal standard (mesitylene).

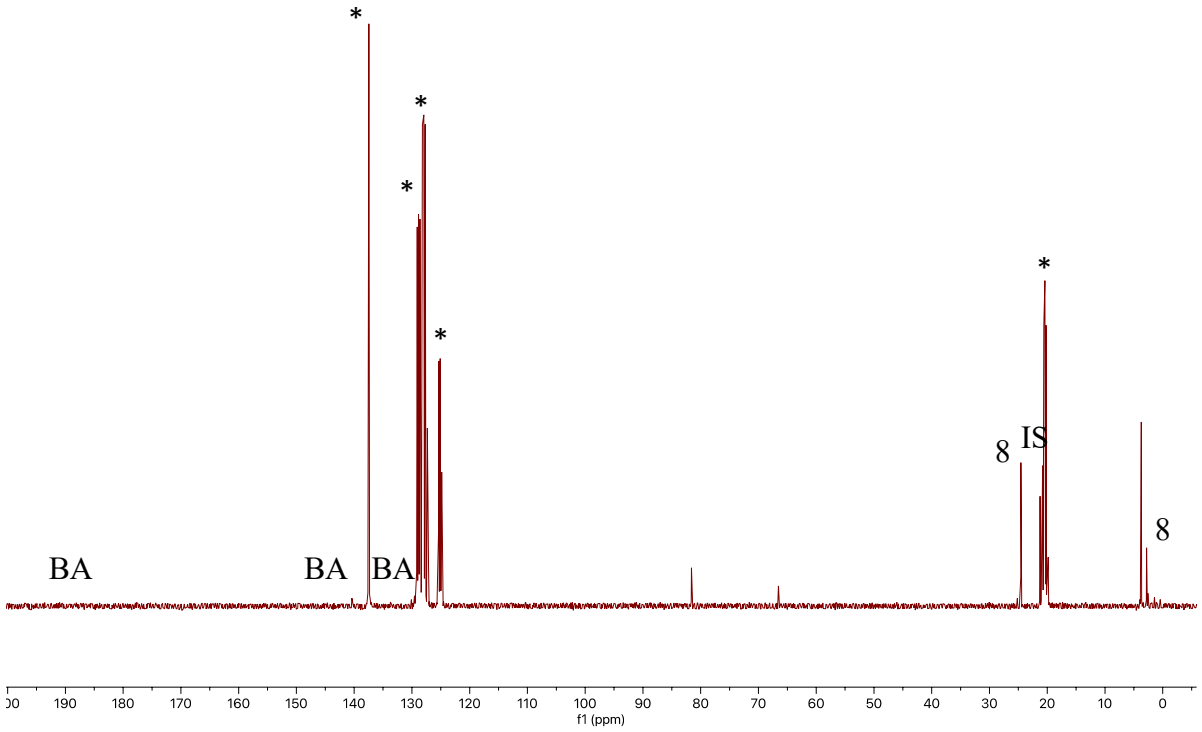


Figure S33. ^{13}C NMR spectrum of the reaction between complex **8** and benzophenone in toluene-d_8. 8 = Complex **8**, * = toluene-d_8, BA = benzaldehyde, IS = internal standard (mesitylene).

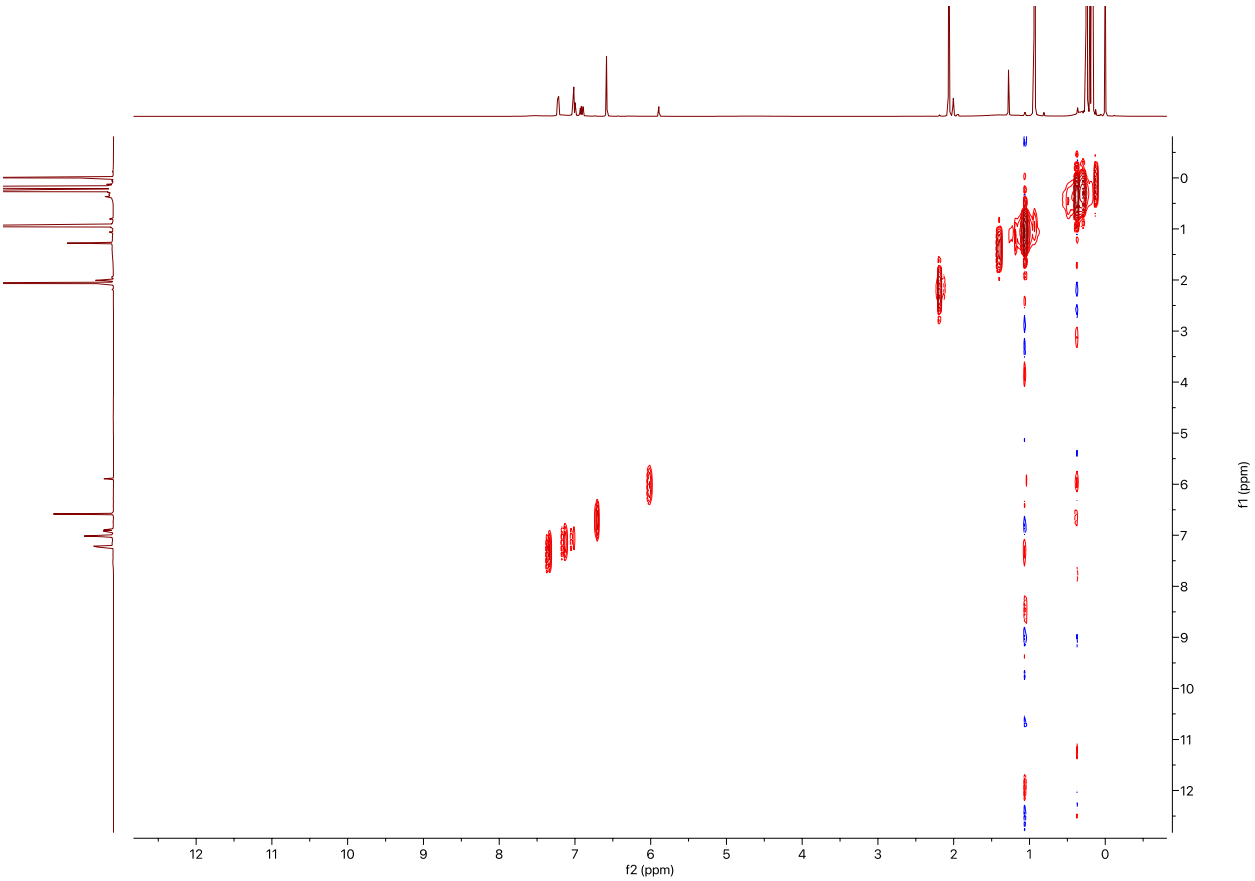


Figure S34. $^{1}H - {}^{1}H$ COSY NMR spectrum of the reaction between complex **8** and benzaldehyde in toluene-d_8.

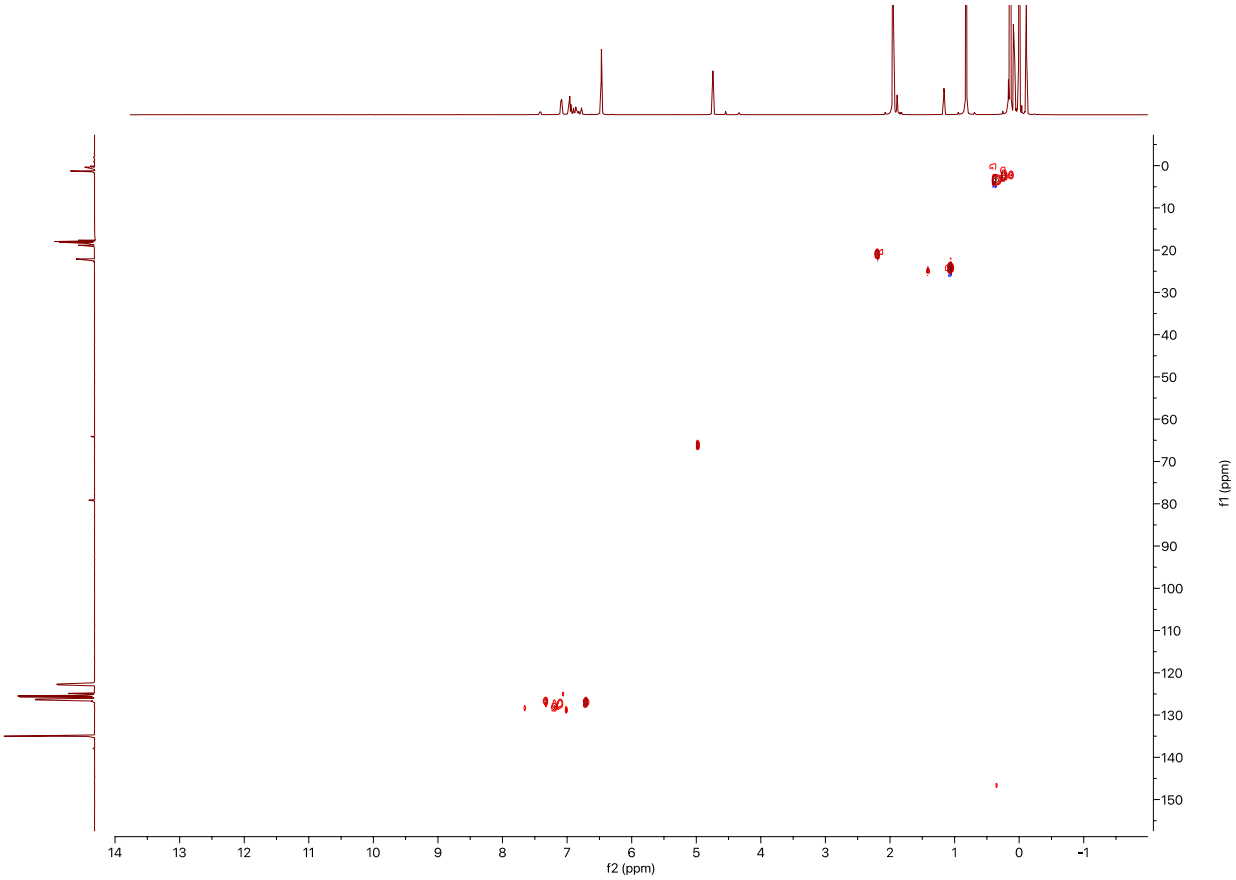


Figure S35. $^{1}H - {}^{13}C$ HSQC NMR spectrum of the reaction between complex **8** and benzaldehyde in toluene-d_8.

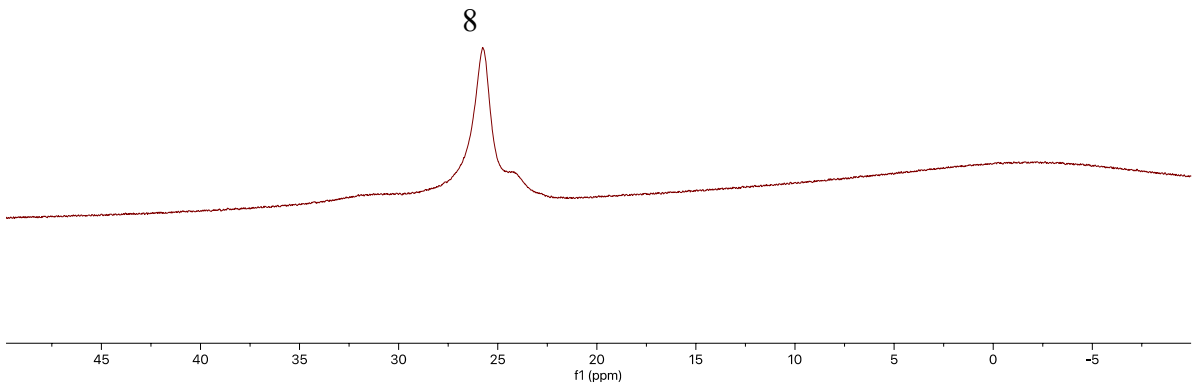
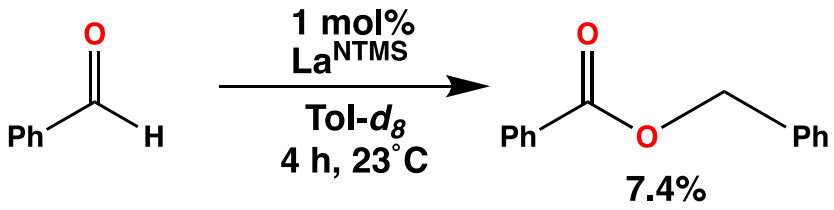


Figure S36. ^{11}B NMR spectrum of the reaction between complex **8** and benzaldehyde in toluene-d_8. 8 = Complex **8**.

1.11. Procedure for NMR-Scale Catalytic Reactions

In a glovebox, La^{NTMS} (3 mg, 0.005 mmol) was weighed into a 4 mL vial, 500 µL of toluene-d_8 was added, thoroughly mixed, and transferred to a J-Young NMR tube. Benzaldehyde (49.4 µL, 0.484 mmol) and mesitylene (5 µL) as the internal standard were syringed into the NMR tube and mixed with the solution. The sealed NMR tube was removed from the glove box and left at room temperature for the indicated reaction times (Scheme S6). After 4 h, HBpin was added to the solution (Fig. S38).



Scheme S6. Catalytic reaction between La^{NTMS} and benzaldehyde

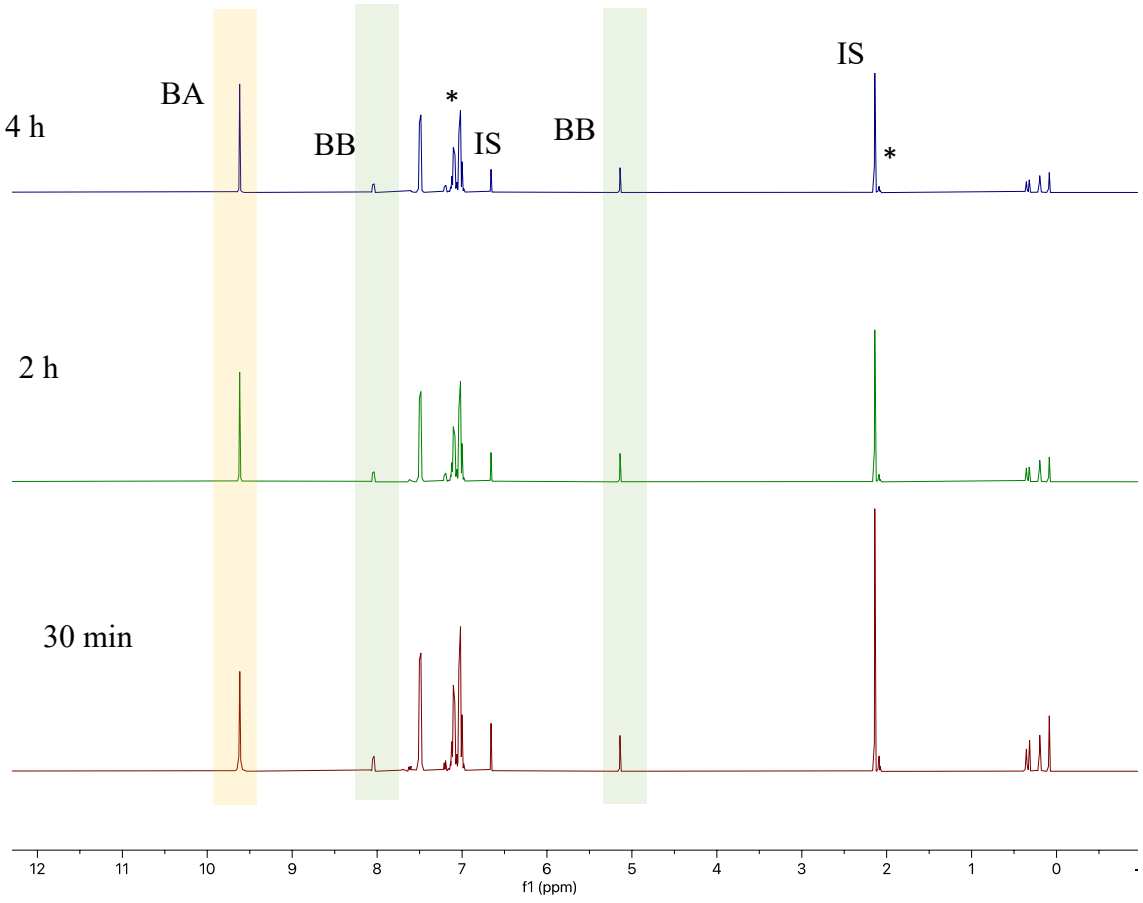


Figure S37. Stacked ^{1}H NMR spectra of the reaction in Scheme S6 after 30 minutes, 2 hours, and 4 hours. BA = benzaldehyde (highlighted in yellow), BB = benzyl benzoate (highlighted in blue), IS = internal standard (mesitylene), * = toluene-d_8.

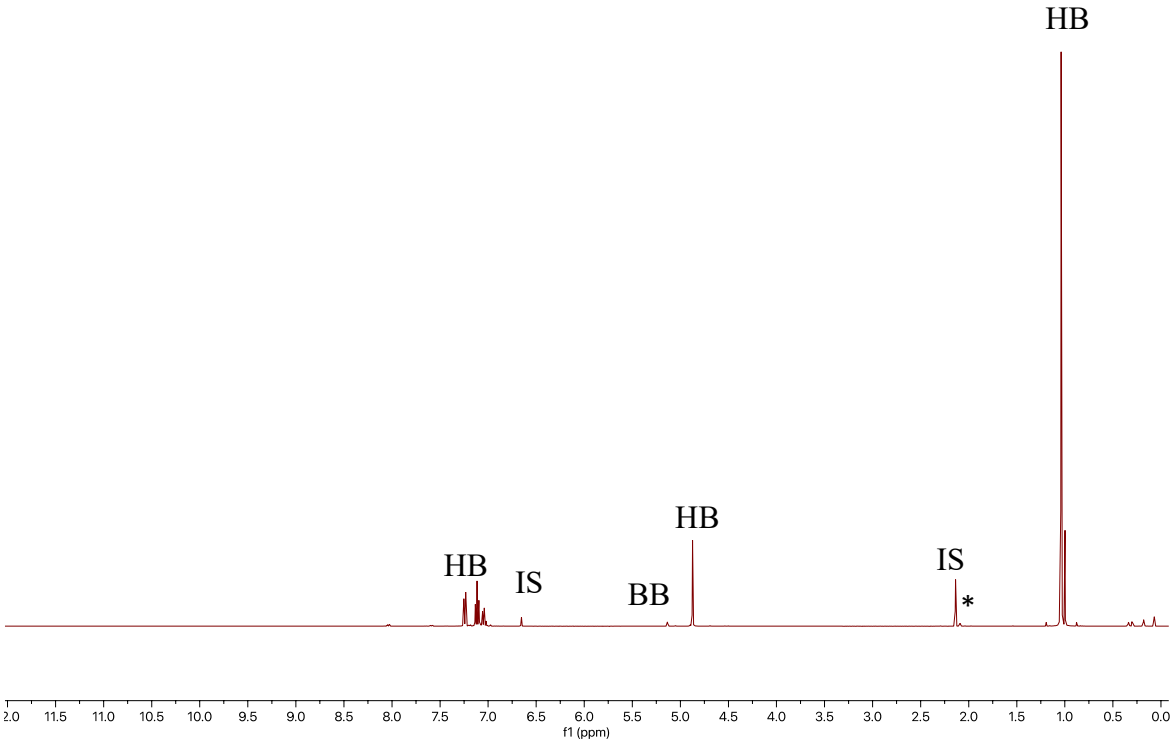


Figure S38. ^{1}H NMR of the reaction from addition of HBpin to Scheme S6 after 1 h. BB = benzyl benzoate, IS = internal standard (mesitylene)., HB = hydroborated product (**6**), * = toluene-d_8.

1.12. X-ray Data Collection, Structure Solution, and Refinement

Single crystals of $C_{31}H_{64}LaN_3OSi_6$ suitable for diffraction were grown by cooling a concentrated toluene solution and were then washed with cold toluene. A suitable crystal was selected, and the crystal was mounted on a MITIGEN holder with Paratone oil on a XtaLAB Synergy, Single source at offset/far, HyPix diffractometer. The crystal was kept at 100.00(10) K during data collection. Using Olex2,[3] the structure was solved with the ShelXT[4] structure solution program using Intrinsic Phasing and refined with the XL[5] refinement package using Least Squares minimization. Crystallographic and experimental details of the structure determination are summarized in Table S1. (CCDC 2196153)

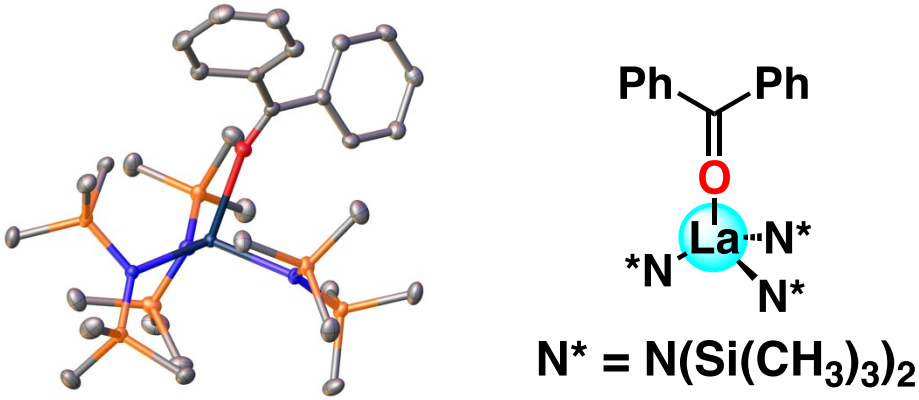
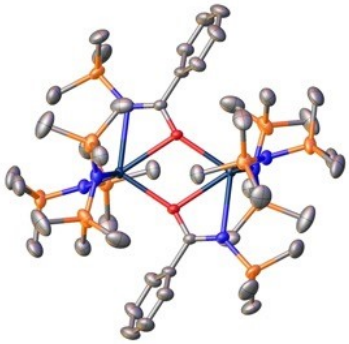


Table S1: Crystal data and structure refinement for $C_{31}H_{64}LaN_3OSi_6$

Empirical formula	$C_{31}H_{64}LaN_3OSi_6$
Formula weight	802.30
Temperature / K	100.00(10)
Crystal system	monoclinic

Space group	$P2_1/n$
a / Å, b / Å, c / Å	11.6736(2), 18.4590(3), 20.0226(3)
α/°, β/°, γ/°	90, 93.0920(10), 90
Volume / Å^3	4308.25(12)
Z	4
ρ_{calc} / mg mm^{-3}	1.237
μ / mm^{-1}	1.184
F(000)	1680
Crystal size / mm^3	0.229 × 0.154 × 0.031
2Θ range for data collection	4.074 to 67.476°
Index ranges	$-16 \leq h \leq 17$, $-26 \leq k \leq 28$, $-28 \leq l \leq 31$
Reflections collected	61050
Independent reflections	15032[R(int) = 0.0360]
Data/restraints/parameters	15032/0/397
Goodness-of-fit on F^2	1.022
Final R indexes [I>2σ (I)]	R_1 = 0.0315, wR_2 = 0.0583
Final R indexes [all data]	R_1 = 0.0451, wR_2 = 0.0619
Largest diff. peak/hole / e Å^{-3}	0.545/-0.583

Single crystals of $C_{22}H_{50}LaN_3OSi_5$ suitable for diffraction analysis were grown by slow cooling a concentrated toluene solution and were then washed with cold toluene. A suitable crystal was selected, and the crystal was mounted on a MITIGEN holder in paratone oil on a XtaLAB Synergy, Single source at offset/far, HyPix diffractometer. The crystal was kept at 100.0(2) K during data collection. Using Olex2[3] the structure was solved with the SHELXT[4] structure solution program using Intrinsic Phasing and refined with the XL[5] refinement package using Least Squares minimizations. Crystallographic and experimental details of the structure determination are summarized in Table S2. (CCDC 2196157)



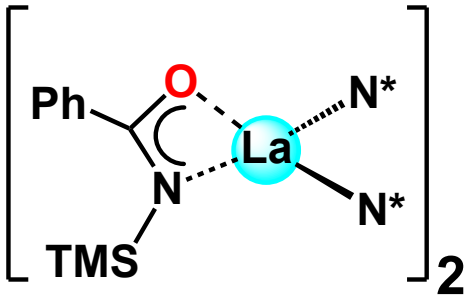
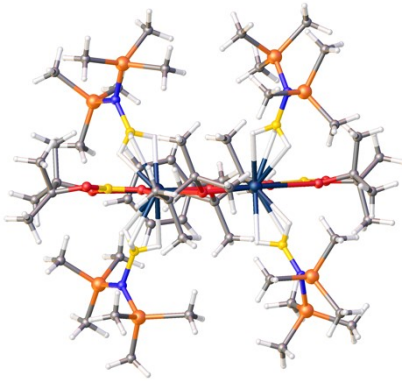


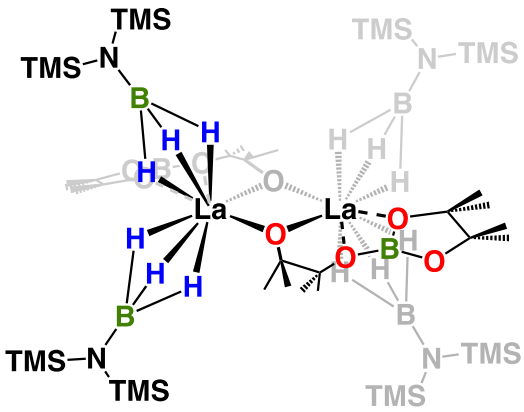
Table S2: Crystal data and structure refinement for $C_{22}H_{50}LaN_3OSi_5$

Empirical formula	$C_{22}H_{50}LaN_3OSi_5$
Formula weight	652.01
Temperature / K	100.0(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a / Å, b / Å, c / Å	21.1647(3), 15.1053(2), 21.1116(3)
α/°, β/°, γ/°	90, 90.8294(13), 90

Volume / $Å^3$	6748.65(17)
Z	8
ρ_{calc} / mg mm^{-3}	1.283
μ / mm^{-1}	1.461
F(000)	2704
Crystal size / mm^3	0.165 × 0.086 × 0.05
2Θ range for data collection	4.288 to 61.968°
Index ranges	$-30 \leq h \leq 27$, $-21 \leq k \leq 21$, $-28 \leq l \leq 28$
Reflections collected	80750
Independent reflections	17623[R(int) = 0.0556]
Data/restraints/parameters	17623/210/695
Goodness-of-fit on F^2	1.048
Final R indexes [I>2σ (I)]	R_1 = 0.0372, wR_2 = 0.0842
Final R indexes [all data]	R_1 = 0.0562, wR_2 = 0.0934
Largest diff. peak/hole / e $Å^{-3}$	1.736/-1.080

Single crystals of $C_{55}H_{140}B_6La_2N_4O_8Si_8$ suitable for diffraction were grown by slow cooling a concentrated toluene solution and were then washed with cold toluene. A suitable crystal was selected, and the crystal was mounted on a MITIGEN holder in paratone oil on a XtaLAB Synergy, Single source at offset/far, HyPix diffractometer. The crystal was kept at 100.00(10) K during data collection. Using Olex2[3], the structure was solved with the SHELXT[4] structure solution program using Intrinsic Phasing and refined with the XL[5] refinement package using Least Squares minimization. Crystallographic and experimental details of the structure determination are





summarized in Table S3. (CCDC 2196158)

Table S3: Crystal data and structure refinement for $C_{55}H_{140}B_6La_2N_4O_8Si_8$

Empirical formula	$C_{55}H_{140}B_6La_2N_4O_8Si_8$
Formula weight	1553.10
Temperature / K	100.00(10)
Crystal system	monoclinic
Space group	Cc
a / Å, b / Å, c / Å	27.6404(7), 15.2264(3), 24.7520(7)

α/°, β/°, γ/°	90, 123.939(4), 90
Volume / $Å^3$	8642.5(5)
Z	4
ρ_{calc} / mg mm^{-3}	1.194
μ / mm^{-1}	1.128
F(000)	3272
Crystal size / mm^3	0.133 × 0.127 × 0.058
2Θ range for data collection	4.264 to 56.674°
Index ranges	$-36 \leq h \leq 36$, $-20 \leq k \leq 20$, $-33 \leq l \leq 33$
Reflections collected	139797
Independent reflections	21472[R(int) = 0.0684]
Data/restraints/parameters	21472/835/810
Goodness-of-fit on F^2	1.039
Final R indexes [I>2σ (I)]	R_1 = 0.0536, wR_2 = 0.1334
Final R indexes [all data]	R_1 = 0.0673, wR_2 = 0.1415
Largest diff. peak/hole / e $Å^{-3}$	1.758/-0.766

2. Computational Details

Geometry optimizations of all reactants, products, intermediates, and transition states were carried out along the entire catalytic cycle. Calculations were performed adopting the M06 hybrid meta-GGA functional. The effective core potential of Hay and Wadt,[6, 7] (LANL2DZ) and the relative basis set were used for the La and Si atoms. The standard all-electron 6-31G** basis[8] was used for all the remaining atoms. Molecular geometry optimization of stationary points was carried out without symmetry constraints and used analytical gradient techniques. The transition states were searched with the "distinguished reaction coordinate procedure" along the emerging bonds. Cyclohexylaldehyde and dicyclohexylketone were adopted as substrate models. Frequency analysis was performed to obtain thermochemical information about the reaction pathways at 298 K using the harmonic approximation. The Gibbs free energy of solvation is taken into account within the SMD model.[9] Moreover, the effect of concentration on moving from 1 atm to 1 *M* is accounted for by adding an energy contribution of 1.89 kcal/mol ($RTln(P_{1M}/P_{1atm})$) to each species. All calculations were performed using the G16 code[10] on a Linux cluster system.

Table S4. DFT derived and solid-state bond lengths (Å) from complex **1**

Complex **1**	La(1) - O(1)	La(1) - N(1)	O(1) - C(1)
DFT	2.536	2.383	1.241
Solid-State	2.502	2.393	1.241

Table S5. DFT derived and solid-state bond lengths (Å) from complex **4**

Complex **4**	La(1) - O(1)	La(1) - N(1)	O(1) - C(1)	La(1) - N(2)	N(1) - C(1)
DFT	2.680	2.628	1.308	2.382	1.300
Solid-State	2.627	2.591	1.327	2.370	1.290

2.1 DFT Examination of Catalyst Decomposition Pathway

DFT calculations were performed to better understand the decomposition pathway of the La^{NTMS} precatalyst induced by HBpin without the presence of either ketone or aldehyde (Figure S39). In particular, the first insertion of HBpin (**1**) leads to the formation of the pinBN(TMS)$_2$ and a La-H hydride forms as a result. This step was previously reported in the activation step of amide reduction catalyzed by La^{NTMS} complex[11]. The second (**2**) and third (**3**) HBpin insertions are reminiscent of the deactivation path reported in the B-N bond forming 1,2-dearomatization process described elsewhere.[12] In this case, the third insertion forms the N(TMS)$_2$-BH$_3^-$ ligand (**3a**). This intermediate then undergoes ligand exchange with another equivalent of itself to form the monomer of complex **8**. This reaction is computed to be exergonic (ΔG = -18.8 kcal/mol) and complex **8** spontaneously forms a dimer ($\Delta G_{dimerization}$ = -35.1 kcal/mol).

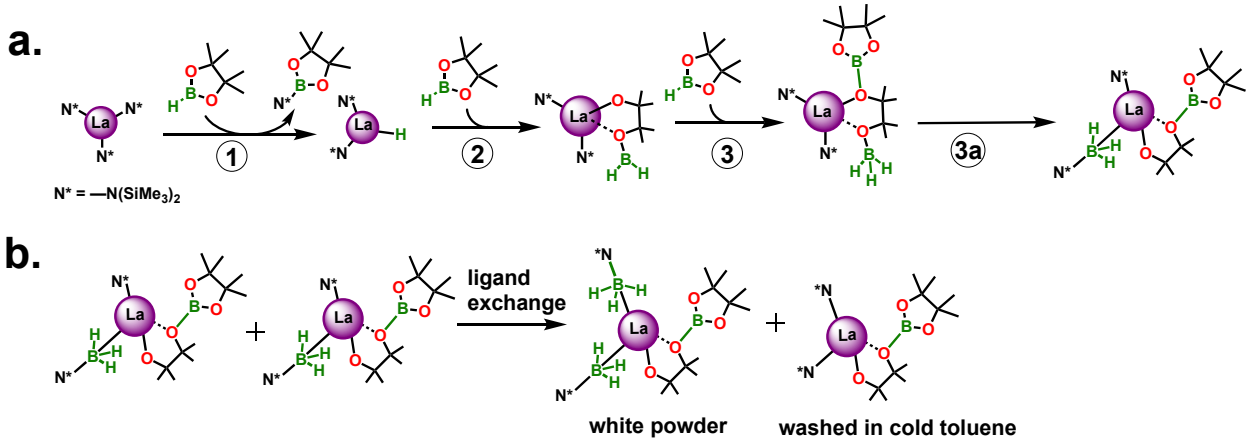


Figure S39. Plausible mechanistic pathway associated with the decomposition pathway of La^{NTMS} precatalyst in the presence of HBpin in the absence of ketone/aldehyde. **a.** Initial formation of deactivated complex after three additions of HBpin. **b.** Ligand exchange between two complexes to yield complex **8**.

2.2 Cartesian coordinates (Å) of all the investigated species described in the text

Complex 1 formed with benzophenone (for comparison with XRD)

La	-0.570746000	-0.040918000	-0.055651000
Si	-1.364304000	-2.535399000	-2.518660000
Si	-3.688095000	-1.529732000	-0.817027000
Si	-1.513258000	2.936367000	-1.437453000
Si	-2.724346000	2.704473000	1.331419000
Si	1.339398000	0.411255000	2.897361000
Si	0.020390000	-2.325896000	2.745812000
O	1.773626000	0.388216000	-0.922356000
N	-1.983005000	-1.583531000	-1.198294000
N	-1.762232000	2.031308000	0.032329000
N	0.365779000	-0.763105000	2.035183000
C	3.006942000	0.259724000	-0.981974000
C	3.603315000	-1.084339000	-0.860320000
C	3.009824000	-2.010609000	0.009725000
H	2.179568000	-1.698150000	0.651826000
C	3.507976000	-3.303471000	0.083166000
H	3.056156000	-4.016470000	0.770183000
C	4.574396000	-3.689415000	-0.727040000
H	4.951366000	-4.708175000	-0.677172000
C	5.157852000	-2.777169000	-1.601292000
H	5.981470000	-3.083423000	-2.240978000
C	4.684781000	-1.472287000	-1.659927000
H	5.127507000	-0.761681000	-2.354787000
C	3.838267000	1.462122000	-1.160836000
C	5.180649000	1.501271000	-0.761533000
H	5.645234000	0.614868000	-0.335730000
C	5.902035000	2.683100000	-0.869014000
H	6.938987000	2.715074000	-0.545264000
C	5.293285000	3.826890000	-1.377707000
H	5.861610000	4.750379000	-1.460034000
C	3.955794000	3.797922000	-1.771257000
H	3.476937000	4.693936000	-2.158498000
C	3.229629000	2.624278000	-1.656576000
H	2.181583000	2.589825000	-1.947741000
C	-1.493921000	-4.412876000	-2.281851000
H	-1.068794000	-4.716049000	-1.317396000
H	-0.941716000	-4.930856000	-3.076639000
H	-2.532550000	-4.760094000	-2.315198000
C	0.499610000	-2.175749000	-2.711092000

H	0.729547000	-1.120096000	-2.913235000
H	0.881578000	-2.749048000	-3.565567000
H	1.080759000	-2.497303000	-1.834847000
C	-2.174319000	-2.119447000	-4.185485000
H	-3.251411000	-2.327756000	-4.174286000
H	-1.729755000	-2.715611000	-4.992432000
H	-2.043397000	-1.059230000	-4.435391000
C	-4.609625000	-3.150937000	-1.159983000
H	-4.632184000	-3.410222000	-2.225242000
H	-5.648637000	-3.066258000	-0.817745000
H	-4.142027000	-3.981823000	-0.616641000
C	-3.852986000	-1.234384000	1.056234000
H	-3.432294000	-2.081795000	1.613960000
H	-4.908344000	-1.138862000	1.342369000
H	-3.360151000	-0.314312000	1.403940000
C	-4.566564000	-0.112510000	-1.717002000
H	-4.085345000	0.836664000	-1.443380000
H	-5.627726000	-0.046965000	-1.445692000
H	-4.495040000	-0.231971000	-2.805384000
C	-0.832304000	1.735897000	-2.770000000
H	0.206829000	1.409105000	-2.612147000
H	-0.835182000	2.261900000	-3.733007000
H	-1.471692000	0.848168000	-2.893582000
C	-3.065243000	3.713037000	-2.197725000
H	-3.809162000	2.948268000	-2.451817000
H	-2.800898000	4.248233000	-3.118691000
H	-3.539140000	4.433815000	-1.520609000
C	-0.205714000	4.307653000	-1.258935000
H	-0.611544000	5.184763000	-0.741841000
H	0.160972000	4.635930000	-2.241329000
H	0.648269000	3.947462000	-0.668546000
C	-4.590552000	2.525828000	1.036653000
H	-4.897298000	3.017091000	0.105185000
H	-5.149264000	2.986811000	1.861290000
H	-4.891942000	1.473540000	0.970929000
C	-2.392601000	4.555347000	1.612340000
H	-1.326785000	4.741514000	1.795909000
H	-2.951221000	4.904656000	2.489952000
H	-2.702191000	5.171573000	0.759025000
C	-2.307713000	1.853597000	2.981258000
H	-2.096950000	0.778075000	2.898166000
H	-3.142071000	1.971398000	3.683975000
H	-1.423667000	2.320662000	3.434187000
C	1.272254000	2.100572000	2.011778000
H	1.863553000	2.097224000	1.084176000
H	1.725252000	2.853051000	2.670537000

H	0.261923000	2.449412000	1.761235000
C	0.830092000	0.658064000	4.708592000
H	-0.235095000	0.896840000	4.803801000
H	1.406106000	1.479369000	5.153803000
H	1.027917000	-0.241704000	5.304706000
C	3.199855000	-0.001390000	2.937782000
H	3.406948000	-0.965314000	3.416645000
H	3.728966000	0.776486000	3.503878000
H	3.635811000	-0.029070000	1.930140000
C	-1.381887000	-2.270564000	4.019843000
H	-1.110369000	-1.641549000	4.876132000
H	-1.606938000	-3.276498000	4.396171000
H	-2.301234000	-1.858208000	3.585907000
C	1.517670000	-3.112243000	3.618340000
H	2.390149000	-3.177174000	2.955504000
H	1.263060000	-4.129971000	3.940641000
H	1.820288000	-2.551368000	4.511108000
C	-0.475064000	-3.538172000	1.368444000
H	-1.341197000	-3.201207000	0.780834000
H	-0.720638000	-4.516119000	1.802286000
H	0.353826000	-3.691240000	0.660888000

Precatalyst La[N(TMS)$_2$]$_3$

La	-0.000115000	0.000539000	-0.514255000
N	2.136038000	0.834770000	0.040670000
N	-0.344546000	-2.266572000	0.040469000
N	-1.791525000	1.431857000	0.040448000
Si	-1.795844000	2.845805000	-0.973264000
Si	0.603775000	-3.155403000	1.211356000
Si	3.361738000	0.132262000	-0.974571000
Si	2.431952000	2.099833000	1.211986000
Si	-3.035363000	1.053991000	1.211117000
Si	-1.566494000	-2.977004000	-0.974006000
C	2.603717000	3.801303000	0.389333000
H	2.651406000	4.602154000	1.137682000
H	3.513734000	3.855974000	-0.220427000
H	1.750708000	4.008247000	-0.270310000
C	0.948086000	2.151749000	2.394422000
H	0.887185000	1.221539000	2.976712000
H	1.046212000	2.980179000	3.106854000
H	-0.004834000	2.286294000	1.859999000
C	3.994937000	1.785167000	2.235817000
H	3.950848000	0.802752000	2.721940000
H	4.899136000	1.815122000	1.614416000
H	4.106585000	2.546146000	3.017742000
C	4.362620000	1.413050000	-1.944598000

H	4.986748000	2.021787000	-1.278810000
H	5.026333000	0.930178000	-2.672242000
H	3.692241000	2.091931000	-2.487062000
C	4.555318000	-1.034935000	-0.084325000
H	5.236681000	-0.478687000	0.570042000
H	4.010297000	-1.753683000	0.540452000
H	5.163843000	-1.599045000	-0.802153000
C	2.439942000	-0.923738000	-2.298756000
H	3.187864000	-1.363978000	-2.969610000
H	1.871934000	-1.777430000	-1.891853000
H	1.787504000	-0.321902000	-2.956021000
C	-2.021542000	-1.650686000	-2.297453000
H	-1.174454000	-1.386607000	-2.955099000
H	-2.777541000	-2.078056000	-2.967593000
H	-2.476023000	-0.731699000	-1.890143000
C	-0.958121000	-4.484132000	-1.944564000
H	-0.035973000	-4.242587000	-2.488528000
H	-0.741167000	-5.328508000	-1.278687000
H	-1.708971000	-4.818336000	-2.670966000
C	-3.173042000	-3.427747000	-0.082037000
H	-3.966000000	-3.674935000	-0.798894000
H	-3.030063000	-4.294749000	0.573473000
H	-3.523814000	-2.595872000	0.541781000
C	1.991005000	-4.154016000	0.387090000
H	2.596827000	-3.518057000	-0.271749000
H	2.660728000	-4.597324000	1.134512000
H	1.582328000	-4.967974000	-0.223879000
C	-0.448692000	-4.352579000	2.235706000
H	-0.872957000	-5.152302000	1.615217000
H	0.155148000	-4.827812000	3.018327000
H	-1.278431000	-3.824163000	2.721229000
C	1.390646000	-1.896738000	2.394103000
H	2.059961000	-2.396093000	3.105541000
H	1.982543000	-1.137960000	1.859693000
H	0.615742000	-1.379778000	2.977493000
C	-2.337349000	-0.255900000	2.394270000
H	-1.501628000	0.157632000	2.976212000
H	-3.103493000	-0.585373000	3.106981000
H	-1.976627000	-1.148518000	1.860468000
C	-4.592961000	0.349885000	0.386987000
H	-4.344048000	-0.492615000	-0.271766000
H	-5.311062000	-0.009367000	1.134621000
H	-5.095058000	1.109780000	-0.224105000
C	-3.546493000	2.564524000	2.234352000
H	-4.262065000	2.280664000	3.015567000
H	-2.674263000	3.017804000	2.721320000

H	-4.024083000	3.332355000	1.612335000
C	-3.404854000	3.072356000	-1.944395000
H	-3.656422000	2.152964000	-2.488435000
H	-4.244823000	3.306539000	-1.278884000
H	-3.318670000	3.889732000	-2.670741000
C	-1.383616000	4.462075000	-0.080315000
H	-2.206950000	4.772350000	0.573581000
H	-0.489201000	4.349140000	0.545306000
H	-1.199117000	5.272278000	-0.796764000
C	-0.418804000	2.577853000	-2.296022000
H	0.603829000	2.511137000	-1.887581000
H	-0.613216000	1.712985000	-2.954774000
H	-0.410061000	3.446870000	-2.965355000

HBpin

O	1.062414000	1.182413000	-0.419543000
C	0.777871000	-0.186473000	-0.054681000
B	0.000001000	1.927385000	-0.000001000
C	-0.777871000	-0.186473000	0.054681000
O	-1.062416000	1.182416000	0.419534000
H	-0.000001000	3.113173000	-0.000014000
C	1.473588000	-0.433207000	1.275783000
H	2.536552000	-0.194343000	1.164338000
H	1.065196000	0.207304000	2.065878000
H	1.386828000	-1.478933000	1.592510000
C	1.347049000	-1.104827000	-1.115767000
H	1.089520000	-2.150124000	-0.902173000
H	0.982368000	-0.850272000	-2.114914000
H	2.439130000	-1.020944000	-1.124508000
C	-1.347047000	-1.104819000	1.115774000
H	-0.982364000	-0.850257000	2.114918000
H	-2.439128000	-1.020938000	1.124518000
H	-1.089517000	-2.150117000	0.902187000
C	-1.473590000	-0.433217000	-1.275781000
H	-2.536550000	-0.194336000	-1.164344000
H	-1.065184000	0.207274000	-2.065885000
H	-1.386844000	-1.478950000	-1.592490000

dicyclohexylketone

O	0.338059000	0.000494000	2.345752000
C	0.007645000	0.000214000	1.175476000
C	1.937090000	-1.257748000	0.214533000
C	1.069695000	0.000018000	0.089329000
C	1.937107000	1.257815000	0.214103000
C	3.068264000	1.255884000	-0.805852000
C	3.922871000	-0.000130000	-0.677717000

C	3.068249000	-1.256177000	-0.805422000
H	1.315542000	-2.158092000	0.102976000
H	2.345249000	-1.281695000	1.236096000
H	0.596961000	-0.000150000	-0.907412000
H	1.315566000	2.158127000	0.102242000
H	2.345266000	1.282105000	1.235657000
H	3.684531000	2.156473000	-0.687644000
H	2.642205000	1.301121000	-1.821594000
H	4.722509000	-0.000265000	-1.429565000
H	4.416964000	0.000036000	0.307075000
H	3.684504000	-2.156734000	-0.686905000
H	2.642188000	-1.301757000	-1.821147000
C	-1.820353000	1.261065000	-0.020076000
C	-3.299180000	1.256520000	-0.391853000
C	-3.666200000	-0.000186000	-1.173041000
C	-3.299157000	-1.256673000	-0.391511000
C	-1.820327000	-1.261096000	-0.019741000
C	-1.449993000	0.000089000	0.770583000
H	-1.570548000	2.156326000	0.565761000
H	-1.217980000	1.308332000	-0.942422000
H	-3.546480000	2.156904000	-0.968529000
H	-3.901753000	1.299216000	0.529330000
H	-4.735301000	-0.000230000	-1.420708000
H	-3.122956000	-0.000312000	-2.132202000
H	-3.546447000	-2.157219000	-0.967940000
H	-3.901725000	-1.299126000	0.529687000
H	-1.570507000	-2.156203000	0.566325000
H	-1.217961000	-1.308599000	-0.942080000
H	-2.018562000	0.000214000	1.714121000

Intermediate A

La	-0.720192000	-0.054169000	0.013506000
N	-0.650684000	-1.775274000	-1.656135000
N	-1.831689000	1.980386000	-0.585083000
N	-1.391915000	-0.786575000	2.194705000
Si	-0.205507000	-1.272733000	3.372060000
Si	-3.080414000	2.212120000	-1.792332000
Si	0.165185000	-1.326783000	-3.136567000
Si	-1.435183000	-3.343988000	-1.554765000
Si	-3.115099000	-0.740515000	2.463684000
Si	-1.246093000	3.367514000	0.305763000
C	-0.467135000	-4.735811000	-2.414672000
H	-0.968701000	-5.693807000	-2.227088000
H	-0.403502000	-4.605280000	-3.501702000
H	0.553334000	-4.808779000	-2.018654000
C	-1.609439000	-3.896370000	0.253049000

H	-1.815397000	-3.073028000	0.950105000
H	-2.419035000	-4.632022000	0.345389000
H	-0.680931000	-4.376958000	0.586480000
C	-3.163637000	-3.326096000	-2.342643000
H	-3.835355000	-2.617749000	-1.841754000
H	-3.112107000	-3.038476000	-3.399838000
H	-3.622072000	-4.321518000	-2.283766000
C	1.818368000	-2.238273000	-3.384216000
H	1.673597000	-3.258874000	-3.755674000
H	2.454308000	-1.704530000	-4.103203000
H	2.358387000	-2.308493000	-2.431066000
C	-0.820446000	-1.607407000	-4.733330000
H	-1.005129000	-2.676077000	-4.899219000
H	-1.790182000	-1.098528000	-4.723139000
H	-0.247632000	-1.236693000	-5.593126000
C	0.657515000	0.521052000	-3.051839000
H	0.970881000	0.838619000	-4.054734000
H	-0.139173000	1.212034000	-2.736510000
H	1.523176000	0.678679000	-2.392247000
C	-0.428749000	2.780574000	1.922531000
H	-1.119560000	2.202943000	2.551302000
H	0.476114000	2.176375000	1.770876000
H	-0.111804000	3.662235000	2.495388000
C	0.105016000	4.309247000	-0.645341000
H	0.902681000	3.614175000	-0.945082000
H	-0.286151000	4.774411000	-1.557509000
H	0.552860000	5.096554000	-0.024214000
C	-2.571241000	4.620726000	0.824196000
H	-2.109024000	5.410564000	1.429990000
H	-3.056042000	5.102420000	-0.033059000
H	-3.350666000	4.143511000	1.430402000
C	-2.714294000	3.656845000	-2.971043000
H	-1.746703000	3.514457000	-3.469203000
H	-3.487432000	3.715591000	-3.747482000
H	-2.689265000	4.624822000	-2.455684000
C	-4.788398000	2.533529000	-1.026089000
H	-4.833003000	3.518728000	-0.547880000
H	-5.567764000	2.499601000	-1.797818000
H	-5.033064000	1.783475000	-0.263980000
C	-3.208118000	0.677541000	-2.900537000
H	-4.124766000	0.727996000	-3.501576000
H	-2.359403000	0.646508000	-3.595379000
H	-3.222005000	-0.276400000	-2.356809000
C	-3.952271000	-0.841527000	0.752077000
H	-3.769985000	-1.810317000	0.267385000
H	-5.038769000	-0.739086000	0.870010000

H	-3.656994000	-0.031106000	0.068723000
C	-3.699895000	0.880261000	3.253556000
H	-3.510598000	1.719313000	2.569435000
H	-4.775388000	0.857064000	3.468393000
H	-3.168483000	1.083384000	4.192235000
C	-3.821678000	-2.194696000	3.454883000
H	-3.636489000	-2.100963000	4.530209000
H	-4.907695000	-2.244229000	3.305543000
H	-3.391776000	-3.145768000	3.115062000
C	-0.877867000	-1.770231000	5.072345000
H	-1.508995000	-0.985041000	5.506940000
H	-1.463919000	-2.694496000	5.028951000
H	-0.036482000	-1.936658000	5.756906000
C	0.792462000	-2.752795000	2.707219000
H	0.158226000	-3.645935000	2.655419000
H	1.165736000	-2.566716000	1.687331000
H	1.654985000	-2.978875000	3.348734000
C	1.074546000	0.097496000	3.718745000
H	1.582859000	0.442881000	2.808188000
H	0.600492000	0.973273000	4.178269000
H	1.842799000	-0.277551000	4.408646000
O	1.737045000	0.631994000	0.198068000
C	2.950488000	0.404879000	0.153793000
C	3.535743000	2.561337000	1.302008000
C	3.907757000	1.559230000	0.204313000
C	3.918300000	2.258343000	-1.169819000
C	4.884428000	3.436848000	-1.159829000
C	4.544994000	4.424143000	-0.049202000
C	4.509773000	3.732381000	1.309147000
H	3.514246000	2.058785000	2.280219000
H	2.515429000	2.927895000	1.111785000
H	4.922962000	1.177004000	0.398356000
H	4.181804000	1.547220000	-1.965284000
H	2.895824000	2.610479000	-1.381657000
H	4.869528000	3.933316000	-2.137826000
H	5.910022000	3.060462000	-1.015276000
H	5.266359000	5.250549000	-0.040799000
H	3.558730000	4.869990000	-0.253411000
H	4.231082000	4.442570000	2.097075000
H	5.519211000	3.368247000	1.560485000
C	4.538216000	-1.238960000	-0.971027000
C	5.000389000	-2.692068000	-0.948111000
C	5.498525000	-3.092169000	0.435755000
C	4.425645000	-2.853924000	1.491281000
C	3.954846000	-1.404279000	1.487829000
C	3.452072000	-1.004659000	0.084813000

H	4.157919000	-0.974752000	-1.968059000
H	5.401158000	-0.584243000	-0.770284000
H	5.782214000	-2.842719000	-1.702302000
H	4.160030000	-3.343171000	-1.237146000
H	5.811951000	-4.143143000	0.440197000
H	6.392418000	-2.497709000	0.685597000
H	4.793708000	-3.117546000	2.490698000
H	3.562909000	-3.509465000	1.293587000
H	3.154839000	-1.255538000	2.227254000
H	4.789539000	-0.744298000	1.776505000
H	2.577796000	-1.637305000	-0.156285000

TS1 between A and B

La	-0.711216000	-0.229027000	-0.044125000
N	-0.855048000	1.176940000	2.049424000
N	-1.165681000	-2.595481000	0.132383000
N	-2.281991000	0.335248000	-1.747306000
Si	-1.842239000	1.143543000	-3.234744000
Si	-2.017267000	-3.463461000	1.400434000
Si	-0.026714000	0.504782000	3.481840000
Si	-2.265396000	2.216427000	2.382603000
Si	-3.920720000	-0.286099000	-1.606180000
Si	-0.495529000	-3.572669000	-1.163927000
C	-1.746972000	3.767196000	3.349617000
H	-2.538029000	4.527025000	3.325677000
H	-1.564718000	3.514783000	4.402343000
H	-0.819777000	4.196658000	2.954655000
C	-3.180460000	2.728662000	0.782472000
H	-2.773827000	2.289158000	-0.138759000
H	-4.226724000	2.407848000	0.854843000
H	-3.192805000	3.817319000	0.660046000
C	-3.647871000	1.416442000	3.420567000
H	-3.940610000	0.427123000	3.046368000
H	-3.394435000	1.315743000	4.479302000
H	-4.528998000	2.068351000	3.350403000
C	1.333384000	1.592239000	4.242674000
H	0.949916000	2.580691000	4.519530000
H	1.683812000	1.095279000	5.157396000
H	2.191487000	1.751583000	3.583692000
C	-1.104361000	0.124489000	5.001383000
H	-1.395982000	1.046793000	5.518581000
H	-2.004208000	-0.460694000	4.798370000
H	-0.477634000	-0.448835000	5.698317000
C	0.866077000	-1.113164000	2.993278000
H	1.119742000	-1.665489000	3.908282000
H	0.295046000	-1.804550000	2.356487000

H	1.807305000	-0.878206000	2.482628000
C	-0.154331000	-2.489680000	-2.690095000
H	-1.048364000	-1.928404000	-2.991087000
H	0.672015000	-1.783219000	-2.543334000
H	0.133362000	-3.142024000	-3.524724000
C	1.164279000	-4.377478000	-0.681547000
H	1.705864000	-3.729896000	0.017937000
H	1.016601000	-5.344113000	-0.185584000
H	1.791675000	-4.546012000	-1.567996000
C	-1.567526000	-5.006784000	-1.799693000
H	-1.037802000	-5.479458000	-2.637540000
H	-1.728943000	-5.779356000	-1.038854000
H	-2.546702000	-4.678266000	-2.165986000
C	-0.987098000	-4.883699000	2.135113000
H	-0.006553000	-4.522137000	2.471585000
H	-1.506197000	-5.311913000	3.002069000
H	-0.817667000	-5.695993000	1.417848000
C	-3.669418000	-4.224300000	0.850607000
H	-3.537705000	-5.030434000	0.121740000
H	-4.181838000	-4.644721000	1.725847000
H	-4.330718000	-3.473423000	0.402118000
C	-2.419376000	-2.301258000	2.855119000
H	-3.450563000	-2.458013000	3.197515000
H	-1.751311000	-2.501380000	3.701935000
H	-2.326131000	-1.234295000	2.614415000
C	-4.364376000	-0.589662000	0.215592000
H	-4.430892000	0.336788000	0.795132000
H	-5.347415000	-1.077105000	0.261335000
H	-3.663577000	-1.268777000	0.716009000
C	-4.150246000	-1.956472000	-2.473895000
H	-3.462729000	-2.690146000	-2.033820000
H	-5.174031000	-2.326772000	-2.333653000
H	-3.951448000	-1.900623000	-3.550240000
C	-5.238956000	0.909228000	-2.267666000
H	-5.142724000	1.095835000	-3.343823000
H	-6.235088000	0.481816000	-2.095515000
H	-5.192965000	1.875698000	-1.751565000
C	-2.405165000	0.256107000	-4.820045000
H	-1.994913000	-0.758877000	-4.885949000
H	-3.496423000	0.187449000	-4.902884000
H	-2.045018000	0.820034000	-5.690746000
C	-2.530386000	2.918710000	-3.374186000
H	-3.409556000	2.938567000	-4.029816000
H	-2.846535000	3.308299000	-2.399772000
H	-1.789426000	3.610342000	-3.795890000
C	0.056924000	1.188390000	-3.385291000

H	0.573805000	1.493796000	-2.465844000
H	0.417592000	0.194671000	-3.681695000
H	0.352852000	1.892084000	-4.175174000
O	1.773190000	-0.749688000	-0.613159000
C	2.984380000	-0.976598000	-0.574944000
C	3.856127000	1.166327000	-1.444233000
C	3.879824000	-0.359665000	-1.613973000
C	3.430993000	-0.761030000	-3.024068000
C	4.275110000	-0.066412000	-4.084256000
C	4.220530000	1.448364000	-3.914772000
C	4.684764000	1.853853000	-2.520850000
H	4.226517000	1.430421000	-0.442699000
H	2.807982000	1.501775000	-1.491277000
H	4.913601000	-0.707286000	-1.460299000
H	3.468934000	-1.855426000	-3.133611000
H	2.379394000	-0.464567000	-3.145918000
H	3.927832000	-0.356715000	-5.083400000
H	5.320913000	-0.405165000	-4.005240000
H	4.829490000	1.943358000	-4.681299000
H	3.182830000	1.790534000	-4.063618000
H	4.629581000	2.943911000	-2.391095000
H	5.745150000	1.581140000	-2.395558000
C	4.453188000	-2.960299000	0.014040000
C	4.937152000	-3.796968000	1.192872000
C	5.710373000	-2.940833000	2.190376000
C	4.882426000	-1.750687000	2.663346000
C	4.380052000	-0.917974000	1.488348000
C	3.576432000	-1.808326000	0.522106000
H	3.892012000	-3.580531000	-0.697287000
H	5.325006000	-2.557511000	-0.524829000
H	5.558150000	-4.626487000	0.833226000
H	4.065053000	-4.251554000	1.689837000
H	6.031070000	-3.545439000	3.047620000
H	6.629898000	-2.571172000	1.708017000
H	5.466301000	-1.118495000	3.343540000
H	4.015071000	-2.111805000	3.238285000
H	3.760235000	-0.079830000	1.841924000
H	5.237982000	-0.478476000	0.953421000
H	2.726668000	-2.231780000	1.082032000
O	1.262781000	3.337337000	1.780830000
C	1.561801000	4.324117000	0.785030000
C	0.709578000	3.860306000	-0.436906000
O	0.646336000	2.420949000	-0.237219000
C	3.063583000	4.261497000	0.529883000
H	3.584597000	4.417863000	1.480402000
H	3.359477000	3.280751000	0.141702000

C	1.207802000	5.698410000	1.319651000
H	1.388095000	6.468228000	0.558337000
H	0.164759000	5.763323000	1.640548000
H	1.840893000	5.923381000	2.184833000
C	-0.694744000	4.421050000	-0.408619000
H	-1.308855000	3.886973000	-1.140970000
H	-1.150904000	4.301930000	0.577426000
H	-0.699637000	5.485960000	-0.670056000
B	0.959409000	2.166044000	1.110106000
H	1.531140000	1.127517000	1.330065000
H	0.651926000	3.843078000	-2.589340000
C	1.335512000	4.147447000	-1.788079000
H	2.284072000	3.618979000	-1.930098000
H	1.518497000	5.224410000	-1.895104000
H	3.395096000	5.032127000	-0.176288000

Intermediate B

La	-0.715480000	-0.192537000	0.025352000
N	-0.854042000	2.489027000	0.552779000
N	-1.427677000	-1.734321000	1.752741000
N	-2.034443000	-1.003877000	-1.761519000
Si	-1.341952000	-1.444759000	-3.306875000
Si	-2.489813000	-1.433023000	3.118881000
Si	-0.294274000	2.866347000	2.238960000
Si	-2.228878000	3.436013000	-0.149452000
Si	-3.746669000	-1.277392000	-1.493328000
Si	-0.783907000	-3.364951000	1.608247000
C	-1.718054000	5.240569000	-0.393160000
H	-2.449243000	5.774552000	-1.012067000
H	-1.654695000	5.760936000	0.570969000
H	-0.730339000	5.297203000	-0.862902000
C	-2.807900000	2.680171000	-1.796641000
H	-2.483598000	1.643477000	-1.961251000
H	-3.904858000	2.697750000	-1.828090000
H	-2.446999000	3.264824000	-2.647383000
C	-3.774526000	3.435121000	0.952446000
H	-4.031389000	2.443408000	1.343167000
H	-3.701455000	4.125782000	1.796524000
H	-4.615289000	3.765382000	0.328418000
C	1.193888000	4.031459000	2.322485000
H	0.993914000	4.987857000	1.828645000
H	1.416533000	4.221683000	3.381572000
H	2.078467000	3.598156000	1.843846000
C	-1.594524000	3.696550000	3.334429000
H	-1.817615000	4.715079000	2.995754000
H	-2.532802000	3.145043000	3.431193000

H	-1.148856000	3.781229000	4.334766000
C	0.300090000	1.277352000	3.106602000
H	0.304732000	1.454538000	4.191114000
H	-0.291839000	0.367707000	2.944438000
H	1.330592000	1.061915000	2.806656000
C	-0.417950000	-3.771102000	-0.210443000
H	-1.337500000	-3.787065000	-0.807378000
H	0.278372000	-3.064817000	-0.676788000
H	0.055048000	-4.761176000	-0.266319000
C	0.858288000	-3.577762000	2.544077000
H	1.634943000	-2.944054000	2.098739000
H	0.762416000	-3.300124000	3.600903000
H	1.202606000	-4.619361000	2.493135000
C	-1.904624000	-4.778294000	2.203225000
H	-1.389016000	-5.725179000	1.995413000
H	-2.109006000	-4.745728000	3.279547000
H	-2.862986000	-4.798359000	1.671348000
C	-1.674964000	-1.864983000	4.781133000
H	-0.728135000	-1.322894000	4.903134000
H	-2.335216000	-1.586299000	5.612197000
H	-1.461905000	-2.937112000	4.873014000
C	-4.149933000	-2.355752000	3.062130000
H	-4.045258000	-3.434594000	3.212710000
H	-4.798251000	-1.968766000	3.859344000
H	-4.664758000	-2.197272000	2.106284000
C	-2.957272000	0.417859000	3.220213000
H	-4.047756000	0.536149000	3.261294000
H	-2.536995000	0.868535000	4.128074000
H	-2.608581000	1.022861000	2.373588000
C	-4.355899000	-0.154394000	-0.086864000
H	-4.311855000	0.905416000	-0.365299000
H	-5.404581000	-0.390914000	0.136766000
H	-3.805332000	-0.301254000	0.850552000
C	-4.150504000	-3.058250000	-0.982475000
H	-3.600256000	-3.321141000	-0.069419000
H	-5.222730000	-3.165233000	-0.773050000
H	-3.884044000	-3.780312000	-1.763437000
C	-4.828462000	-0.830089000	-2.987347000
H	-4.642679000	-1.467885000	-3.859412000
H	-5.886625000	-0.940201000	-2.717706000
H	-4.663755000	0.212110000	-3.287795000
C	-1.935569000	-3.120481000	-3.976165000
H	-1.693985000	-3.930747000	-3.277130000
H	-3.014659000	-3.147953000	-4.167674000
H	-1.426769000	-3.333581000	-4.925248000
C	-1.672763000	-0.153645000	-4.654875000

H	-2.730529000	-0.141002000	-4.941962000
H	-1.416138000	0.849293000	-4.293439000
H	-1.080008000	-0.359787000	-5.555503000
C	0.546295000	-1.646164000	-3.132957000
H	1.020401000	-0.868319000	-2.519427000
H	0.787472000	-2.626416000	-2.702353000
H	1.018337000	-1.593346000	-4.123394000
O	1.730140000	-1.069900000	0.084021000
C	2.946762000	-1.032850000	0.295507000
C	4.196336000	-1.405268000	-1.799147000
C	3.853955000	-1.998078000	-0.414570000
C	3.255139000	-3.394827000	-0.579030000
C	4.223087000	-4.306642000	-1.322665000
C	4.582770000	-3.726742000	-2.686136000
C	5.155702000	-2.321001000	-2.549509000
H	4.618533000	-0.395102000	-1.701271000
H	3.256158000	-1.306221000	-2.365542000
H	4.793513000	-2.080997000	0.155509000
H	2.991121000	-3.813879000	0.402667000
H	2.317619000	-3.315285000	-1.146975000
H	3.783823000	-5.305698000	-1.432313000
H	5.141139000	-4.433818000	-0.726045000
H	5.292933000	-4.379870000	-3.208348000
H	3.675387000	-3.685160000	-3.310210000
H	5.377260000	-1.894537000	-3.535778000
H	6.112619000	-2.365472000	-2.004795000
C	3.436221000	-0.703223000	2.679964000
C	3.937296000	0.246479000	3.763632000
C	5.334365000	0.771776000	3.461623000
C	5.373483000	1.432722000	2.090010000
C	4.932809000	0.456159000	1.005591000
C	3.513537000	-0.046504000	1.282918000
H	2.400351000	-1.007723000	2.888727000
H	4.045588000	-1.623858000	2.680835000
H	3.911193000	-0.263546000	4.734618000
H	3.244149000	1.099822000	3.840369000
H	5.652649000	1.475693000	4.240335000
H	6.053107000	-0.063621000	3.480519000
H	6.379691000	1.807759000	1.866277000
H	4.703228000	2.308144000	2.084141000
H	4.982646000	0.938745000	0.020604000
H	5.640725000	-0.387699000	0.986178000
H	2.826045000	0.816941000	1.278222000
O	1.139382000	3.651482000	-0.587269000
C	1.951832000	3.401102000	-1.714888000
C	1.030428000	2.504549000	-2.602335000

O	0.279486000	1.757559000	-1.630296000
C	3.225672000	2.672210000	-1.277688000
H	3.679912000	3.237642000	-0.453096000
H	3.008129000	1.660599000	-0.915948000
C	2.345292000	4.729284000	-2.336833000
H	2.884338000	4.584804000	-3.282130000
H	1.471566000	5.360598000	-2.523056000
H	3.006371000	5.268778000	-1.648853000
C	0.077240000	3.345866000	-3.439796000
H	-0.677594000	2.697321000	-3.897326000
H	-0.436654000	4.095298000	-2.828488000
H	0.609544000	3.861970000	-4.248030000
B	0.472748000	2.414002000	-0.298074000
H	1.187529000	1.627706000	0.390320000
H	1.077188000	0.996893000	-4.144878000
C	1.783289000	1.564553000	-3.526245000
H	2.402449000	0.849413000	-2.973151000
H	2.435616000	2.134386000	-4.201389000
H	3.958197000	2.597941000	-2.092117000

TS2 between B and C

La	-1.035804000	-0.180845000	-0.288590000
N	1.846927000	0.537067000	-1.935849000
N	-2.368665000	1.771074000	0.134712000
N	-2.550333000	-1.986214000	-0.032748000
Si	-2.354658000	-3.321510000	1.099077000
Si	-2.480094000	3.127506000	-0.963766000
Si	3.186207000	1.734567000	-2.205204000
Si	1.206389000	-0.042687000	-3.509041000
Si	-4.045495000	-1.917283000	-0.961629000
Si	-3.227637000	1.856848000	1.663446000
C	2.301167000	-1.273133000	-4.461161000
H	1.737700000	-2.152371000	-4.795781000
H	2.708975000	-0.788539000	-5.355743000
H	3.143713000	-1.602926000	-3.847904000
C	-0.526869000	-0.824491000	-3.314765000
H	-0.609095000	-1.672278000	-2.620403000
H	-1.300700000	-0.068392000	-3.114920000
H	-0.803572000	-1.232936000	-4.295822000
C	0.884573000	1.356834000	-4.747012000
H	0.272916000	2.168920000	-4.344953000
H	1.806934000	1.785346000	-5.152243000
H	0.340103000	0.911236000	-5.590767000
C	4.369847000	1.911273000	-0.741061000
H	4.686400000	0.935555000	-0.357763000
H	5.260187000	2.432006000	-1.116934000

H	3.966603000	2.510887000	0.078994000
C	4.343304000	1.222857000	-3.620947000
H	4.843158000	0.280222000	-3.370937000
H	3.865366000	1.110085000	-4.598588000
H	5.113020000	1.999375000	-3.719985000
C	2.537429000	3.468917000	-2.611510000
H	2.102021000	3.534372000	-3.613684000
H	1.786635000	3.820247000	-1.895429000
H	3.384419000	4.166546000	-2.571411000
C	-2.972565000	0.245961000	2.634571000
H	-3.295444000	-0.643926000	2.080996000
H	-1.917474000	0.119179000	2.921412000
H	-3.553403000	0.296525000	3.564513000
C	-2.605617000	3.210346000	2.843255000
H	-1.535621000	3.079697000	3.051755000
H	-2.752346000	4.223724000	2.454183000
H	-3.142164000	3.135046000	3.798007000
C	-5.089647000	2.146993000	1.427310000
H	-5.645007000	1.898389000	2.340350000
H	-5.297847000	3.198450000	1.190278000
H	-5.484546000	1.534719000	0.606441000
C	-2.129527000	4.828107000	-0.192511000
H	-1.248281000	4.832927000	0.458496000
H	-1.967624000	5.562671000	-0.992186000
H	-2.986571000	5.175581000	0.398228000
C	-4.156451000	3.341805000	-1.832264000
H	-4.958444000	3.572777000	-1.122147000
H	-4.088000000	4.177608000	-2.541180000
H	-4.453514000	2.448886000	-2.394466000
C	-1.228415000	2.835406000	-2.364250000
H	-1.622970000	2.111273000	-3.091643000
H	-1.055330000	3.767532000	-2.918289000
H	-0.243452000	2.487194000	-2.019004000
C	-3.958828000	-0.497505000	-2.225423000
H	-3.309035000	-0.723865000	-3.078932000
H	-4.968152000	-0.338949000	-2.626974000
H	-3.661465000	0.455961000	-1.765270000
C	-5.586636000	-1.565985000	0.088680000
H	-5.398950000	-0.754216000	0.803093000
H	-6.416627000	-1.257688000	-0.559576000
H	-5.914255000	-2.441161000	0.659048000
C	-4.343436000	-3.495900000	-1.968210000
H	-4.588733000	-4.357294000	-1.335711000
H	-5.174281000	-3.351915000	-2.670031000
H	-3.445208000	-3.748249000	-2.547207000
C	-3.906258000	-3.753885000	2.106771000

H	-4.312021000	-2.887004000	2.641199000
H	-4.705472000	-4.185271000	1.492578000
H	-3.627069000	-4.507716000	2.855010000
C	-1.891298000	-4.955957000	0.239942000
H	-2.787958000	-5.418907000	-0.189687000
H	-1.171661000	-4.825117000	-0.575742000
H	-1.465452000	-5.666414000	0.960497000
C	-1.060134000	-2.861206000	2.416041000
H	-0.217166000	-2.267022000	2.043098000
H	-1.549042000	-2.278237000	3.207179000
H	-0.643903000	-3.767626000	2.875518000
O	0.363440000	0.181691000	1.605036000
C	1.574222000	0.500679000	1.812394000
C	1.636236000	-0.727898000	4.003379000
C	2.361437000	-0.475633000	2.666721000
C	3.832548000	-0.136534000	2.892678000
C	4.532450000	-1.203345000	3.733780000
C	3.795841000	-1.465438000	5.042211000
C	2.339579000	-1.831619000	4.781398000
H	0.589980000	-0.988743000	3.805240000
H	1.627149000	0.186812000	4.613978000
H	2.288789000	-1.427891000	2.120535000
H	4.343837000	-0.009293000	1.926695000
H	3.911999000	0.828668000	3.418053000
H	5.569707000	-0.901563000	3.926620000
H	4.586747000	-2.145032000	3.165143000
H	4.300695000	-2.255702000	5.612259000
H	3.828251000	-0.558269000	5.667987000
H	1.811233000	-2.021783000	5.724232000
H	2.291263000	-2.769168000	4.200784000
C	1.148670000	2.763054000	0.769520000
C	1.486345000	4.247899000	0.811604000
C	1.177495000	4.832919000	2.183759000
C	1.903877000	4.053990000	3.271944000
C	1.589810000	2.561826000	3.220164000
C	1.913116000	1.977745000	1.829589000
H	1.354020000	2.340002000	-0.223164000
H	0.066739000	2.638797000	0.947034000
H	0.927446000	4.780274000	0.027857000
H	2.555196000	4.396144000	0.581526000
H	1.451067000	5.894836000	2.224995000
H	0.091178000	4.780837000	2.366076000
H	1.652758000	4.448453000	4.264893000
H	2.991139000	4.188941000	3.148334000
H	2.159354000	2.048558000	4.004177000
H	0.522616000	2.384463000	3.434733000

H	2.995172000	2.091016000	1.671737000
O	3.472242000	-1.218190000	-1.262190000
C	3.422735000	-2.576651000	-0.880624000
C	1.881401000	-2.886666000	-0.737511000
O	1.266907000	-1.582845000	-0.629744000
C	4.216209000	-2.730863000	0.412800000
H	5.229016000	-2.349295000	0.236325000
H	3.781046000	-2.137075000	1.215992000
C	4.119532000	-3.423251000	-1.938036000
H	4.131438000	-4.481066000	-1.644175000
H	3.651651000	-3.347506000	-2.922718000
H	5.158659000	-3.087837000	-2.031234000
C	1.266771000	-3.576288000	-1.949514000
H	0.176866000	-3.617454000	-1.815710000
H	1.474712000	-3.043140000	-2.880448000
H	1.627496000	-4.606355000	-2.054081000
B	2.269792000	-0.529315000	-0.895308000
H	2.341962000	0.115579000	0.310672000
H	0.491732000	-3.936218000	0.537255000
C	1.565270000	-3.736898000	0.479861000
H	1.872913000	-3.270523000	1.420900000
H	2.076791000	-4.704889000	0.397260000
H	4.293660000	-3.772438000	0.747377000

Intermediate C

La	-0.398330000	0.566863000	0.214033000
N	3.730475000	-0.681107000	-0.566789000
N	-0.650049000	0.439931000	2.597774000
N	-0.888086000	2.798813000	-0.559362000
Si	-2.165159000	3.381760000	-1.614546000
Si	0.590860000	-0.228792000	3.618117000
Si	4.458069000	-2.314409000	-0.287887000
Si	4.603253000	0.793156000	-0.032144000
Si	0.178426000	3.954464000	0.205143000
Si	-2.118624000	1.105046000	3.277951000
C	6.441211000	0.634559000	-0.446280000
H	6.943401000	1.576249000	-0.191563000
H	6.949790000	-0.166859000	0.099982000
H	6.583600000	0.461200000	-1.519567000
C	3.998185000	2.288726000	-1.018760000
H	2.910804000	2.343874000	-1.125814000
H	4.330835000	3.209716000	-0.522617000
H	4.436497000	2.278414000	-2.024584000
C	4.436129000	1.077596000	1.823966000
H	3.393988000	1.062688000	2.158318000
H	4.980176000	0.316979000	2.395326000

H	4.854968000	2.058069000	2.084269000
C	5.726363000	-2.741943000	-1.615790000
H	6.597878000	-2.079226000	-1.578324000
H	6.080825000	-3.770972000	-1.480669000
H	5.271986000	-2.661866000	-2.608587000
C	5.281804000	-2.374154000	1.409438000
H	6.126353000	-1.684900000	1.515130000
H	4.561795000	-2.166312000	2.208625000
H	5.667841000	-3.388841000	1.567208000
C	3.056559000	-3.574949000	-0.299194000
H	3.424099000	-4.555928000	0.024907000
H	2.260434000	-3.271605000	0.392917000
H	2.623272000	-3.686388000	-1.298867000
C	-3.211077000	1.690920000	1.836941000
H	-2.737406000	2.468240000	1.222081000
H	-3.493114000	0.851080000	1.181914000
H	-4.147411000	2.104731000	2.232330000
C	-3.192347000	-0.119909000	4.251458000
H	-3.450403000	-0.991395000	3.637415000
H	-2.702465000	-0.479570000	5.162877000
H	-4.127628000	0.373641000	4.546075000
C	-1.774328000	2.568897000	4.437031000
H	-2.697151000	3.111050000	4.678212000
H	-1.340061000	2.219433000	5.383137000
H	-1.066399000	3.277852000	3.988820000
C	-0.037532000	-1.357169000	5.010497000
H	-0.830867000	-2.035511000	4.676106000
H	0.788466000	-1.964566000	5.403386000
H	-0.431833000	-0.761825000	5.844157000
C	1.669019000	1.054781000	4.518800000
H	1.065597000	1.622516000	5.238122000
H	2.462504000	0.543407000	5.080256000
H	2.146405000	1.777666000	3.847958000
C	1.749628000	-1.282354000	2.525951000
H	2.642226000	-1.550228000	3.107986000
H	1.261713000	-2.219761000	2.227508000
H	2.129190000	-0.790687000	1.613730000
C	1.424688000	2.971833000	1.271612000
H	1.960237000	2.165693000	0.746726000
H	2.211921000	3.651756000	1.623859000
H	0.933895000	2.554082000	2.161980000
C	-0.646075000	5.125158000	1.449237000
H	-1.353865000	4.576634000	2.084586000
H	0.114401000	5.573853000	2.101499000
H	-1.194992000	5.938452000	0.963188000
C	1.172817000	5.017100000	-1.012293000

H	0.526167000	5.723914000	-1.547223000
H	1.931740000	5.602280000	-0.476928000
H	1.686545000	4.399080000	-1.759571000
C	-3.024575000	4.960145000	-0.999278000
H	-3.394120000	4.854814000	0.027601000
H	-2.367415000	5.837740000	-1.038605000
H	-3.886542000	5.167755000	-1.646576000
C	-1.549149000	3.833293000	-3.360516000
H	-0.726189000	4.557002000	-3.308584000
H	-1.197037000	2.970689000	-3.937546000
H	-2.366292000	4.298544000	-3.926887000
C	-3.510077000	2.052142000	-1.763653000
H	-3.106184000	1.039046000	-1.643283000
H	-4.273679000	2.188697000	-0.987525000
H	-4.009258000	2.098076000	-2.740240000
O	-1.661165000	-1.071248000	-0.643501000
C	-2.329357000	-2.270901000	-0.877003000
C	-2.596086000	-2.759376000	1.629271000
C	-2.118463000	-3.264711000	0.270169000
C	-0.657543000	-3.698904000	0.359819000
C	-0.448153000	-4.759277000	1.434327000
C	-0.964425000	-4.287116000	2.788715000
C	-2.415600000	-3.824780000	2.706521000
H	-3.649131000	-2.441854000	1.575748000
H	-2.016419000	-1.861988000	1.907760000
H	-2.692910000	-4.175611000	0.021650000
H	-0.316186000	-4.073707000	-0.618489000
H	-0.033340000	-2.814232000	0.584660000
H	0.614120000	-5.035402000	1.502015000
H	-0.988231000	-5.673666000	1.138815000
H	-0.853078000	-5.079416000	3.540780000
H	-0.343033000	-3.444813000	3.133643000
H	-2.748778000	-3.443889000	3.683111000
H	-3.059730000	-4.689551000	2.474209000
O	2.865475000	-1.430510000	-2.743130000
C	1.673302000	-1.257386000	-3.526612000
C	1.178368000	0.140298000	-3.069080000
O	1.611715000	0.153850000	-1.658246000
C	0.710534000	-2.376032000	-3.159366000
H	1.215638000	-3.338073000	-3.304555000
H	0.386918000	-2.307660000	-2.112268000
C	2.041042000	-1.336566000	-4.993468000
H	1.172756000	-1.107874000	-5.623737000
H	2.851255000	-0.646029000	-5.244357000
H	2.374316000	-2.351878000	-5.233501000
C	1.887746000	1.301059000	-3.745169000

H	1.612692000	2.230382000	-3.229658000
H	2.978518000	1.193276000	-3.713689000
H	1.577175000	1.393077000	-4.791975000
B	2.773019000	-0.647927000	-1.617983000
H	-1.881274000	-2.766817000	-1.773018000
H	-0.580076000	1.322289000	-2.776487000
C	-0.315138000	0.332067000	-3.167666000
H	-0.882274000	-0.428426000	-2.621422000
H	-0.621583000	0.305638000	-4.221506000
H	-0.186142000	-2.362604000	-3.791090000
C	-4.735121000	-3.194574000	-1.159878000
C	-3.795537000	-1.991406000	-1.253392000
C	-3.857773000	-1.432898000	-2.677398000
C	-5.269950000	-1.035686000	-3.082902000
C	-6.212727000	-2.227759000	-2.970927000
C	-6.159055000	-2.828360000	-1.571532000
H	-4.746949000	-3.608267000	-0.142379000
H	-4.356058000	-3.996739000	-1.818501000
H	-4.164427000	-1.212208000	-0.558890000
H	-3.168618000	-0.586330000	-2.784024000
H	-3.492544000	-2.218513000	-3.364663000
H	-5.278644000	-0.627329000	-4.102662000
H	-5.619635000	-0.227064000	-2.419798000
H	-7.240775000	-1.939277000	-3.226626000
H	-5.910627000	-2.993722000	-3.704130000
H	-6.810816000	-3.709514000	-1.504668000
H	-6.555633000	-2.093737000	-0.851715000

TS3 between C and D

La	-1.290330755	0.039797000	-0.315143000
N	3.129609980	0.558026000	-0.931169225
N	-2.510399245	2.024035245	0.085298000
N	-2.757632000	-1.831929245	-0.052075245
Si	-2.740463245	-3.187194000	1.079003000
Si	-2.317838245	3.361088000	-1.031225000
Si	4.797435225	-0.094955000	-0.830107755
Si	3.017413000	2.292937735	-1.316691245
Si	-4.086660000	-1.749523000	-1.202632000
Si	-3.685574000	2.121756000	1.386597000
C	4.418258245	3.320541000	-0.554325755
H	4.262043245	4.359981000	-0.871836755
H	4.375331000	3.311390755	0.541071245
H	5.428958245	3.038354755	-0.859816755
C	3.055001000	2.700509755	-3.171595245
H	3.219637510	3.781003755	-3.279389735
H	3.852464245	2.186754755	-3.716661000

H	2.101759000	2.463535265	-3.656215000
C	1.438221000	3.111542265	-0.654489510
H	0.745559469	2.390720775	-0.206607286
H	1.695610755	3.838064245	0.128399510
H	0.922986531	3.651798041	-1.452264510
C	5.015620490	-1.970926000	-0.811925000
H	4.710216490	-2.448664755	-1.748570000
H	6.092386245	-2.152186490	-0.666656755
H	4.475771000	-2.454343755	0.003608000
C	5.810512735	0.473631000	-2.333850000
H	5.394393245	0.048115000	-3.257094755
H	5.875242490	1.559023000	-2.463680000
H	6.835399735	0.087454245	-2.232526490
C	5.715017000	0.443984245	0.746863490
H	5.627128755	1.505615245	0.995176245
H	5.361252510	-0.135359755	1.610275245
H	6.782691000	0.215275245	0.621323980
C	-3.556999755	0.555963000	2.451812000
H	-3.787660245	-0.348238000	1.875387000
H	-2.568949510	0.424676755	2.923805020
H	-4.281999265	0.622072000	3.271947490
C	-3.401134000	3.617950000	2.508289245
H	-2.365920000	3.635005000	2.872706245
H	-3.586844000	4.562359000	1.981772245
H	-4.070330000	3.578802245	3.376820245
C	-5.486065000	2.186485000	0.779066245
H	-6.165157245	1.979190000	1.612074245
H	-5.749778000	3.166434000	0.365839245
H	-5.670611000	1.436079000	-0.000550755
C	-1.420982000	4.854658000	-0.277627245
H	-0.621269000	4.545502000	0.399823000
H	-0.987449755	5.492496000	-1.060655000
H	-2.128559000	5.468612000	0.293111755
C	-3.948216000	4.043408245	-1.726082245
H	-4.534469000	4.569705000	-0.959796245
H	-3.722844000	4.770364245	-2.517309245
H	-4.577553000	3.256449245	-2.158800245
C	-1.403921000	2.708445755	-2.581169000
H	-2.096556245	2.123058000	-3.201858000
H	-1.076474000	3.560924755	-3.191374000
H	-0.495936245	2.105709755	-2.404944000
C	-3.867753490	-0.193399000	-2.293999245
H	-3.006448490	-0.212772000	-2.975281245
H	-4.752008490	-0.143536000	-2.947197000
H	-3.859510245	0.746495755	-1.719328000
C	-5.813568000	-1.541773000	-0.442077000

H	-5.780297000	-0.884628000	0.436620000
H	-6.484985245	-1.084330000	-1.175566000
H	-6.251826000	-2.495242000	-0.131191000
C	-4.118252245	-3.222955000	-2.391936245
H	-4.310019000	-4.167901000	-1.872832000
H	-4.907017245	-3.091603245	-3.149007000
H	-3.158979245	-3.320478000	-2.917178245
C	-4.459767000	-3.936103245	1.412523755
H	-5.155395000	-3.197864245	1.823659000
H	-4.917257245	-4.385366245	0.520878000
H	-4.337377000	-4.733074245	2.152684000
C	-1.663420000	-4.642420000	0.516762000
H	-1.904735000	-4.948902000	-0.508885000
H	-0.594381000	-4.411863755	0.560621000
H	-1.847087755	-5.500985000	1.176772000
C	-2.146817245	-2.661137000	2.808269755
H	-1.254629490	-2.027546510	2.808987265
H	-2.939874245	-2.121943245	3.339445000
H	-1.903791510	-3.561838755	3.388679755
O	1.010969897	-0.074233490	0.466690347
C	1.183266306	-0.380968245	1.861940388
C	0.291999000	1.834847490	2.792999204
C	1.461738755	0.844653490	2.745101184
C	2.762877265	1.562553755	2.396210735
C	3.039212245	2.739177490	3.323941510
C	1.878651245	3.726820490	3.325253000
C	0.581882245	3.020657225	3.711553980
H	-0.614811245	1.314079980	3.136362694
H	0.073633000	2.213552510	1.778149959
H	1.556069980	0.451606204	3.774814674
H	3.603651265	0.857615755	2.423435245
H	2.698245041	1.907139020	1.357898490
H	3.973749000	3.241125245	3.025239775
H	3.200211980	2.368766980	4.346502755
H	2.075969980	4.558755980	4.011991265
H	1.768504755	4.166697000	2.321501755
H	-0.261213510	3.726068469	3.690406735
H	0.664743490	2.659199204	4.750945225
O	2.174474959	-1.699269245	-1.157606184
C	1.467652755	-2.203959980	-2.273162959
C	0.894209755	-0.920522980	-2.963005959
O	0.791330204	0.007799000	-1.864325204
C	0.386562245	-3.167450000	-1.786175000
H	0.868007490	-3.946213755	-1.186071755
H	-0.381921020	-2.699374265	-1.154441755
C	2.414875265	-2.998740469	-3.160928959

H	1.895796020	-3.382267714	-4.053872469
H	3.271546265	-2.404400469	-3.484346449
H	2.794202510	-3.862934980	-2.595904714
C	1.816329265	-0.343868225	-4.026978449
H	1.397054510	0.604826020	-4.383360959
H	2.812549755	-0.146252469	-3.618337429
H	1.905920531	-1.015808225	-4.883953694
B	1.903640898	-0.318531490	-0.883618307
H	-0.845338735	-0.142955000	-3.972532000
C	-0.485564735	-1.105307000	-3.579918245
H	-1.223975245	-1.506622755	-2.873809510
H	-0.445386959	-1.809438245	-4.416853245
H	-0.133959490	-3.659620490	-2.622262020
H	0.178759245	-0.746402225	2.219431531
H	3.840581000	-5.028620000	2.890092265
H	2.351186000	-4.530465000	3.685539510
C	3.096260245	-4.218936000	2.935183755
C	2.405032000	-4.040049265	1.592503755
H	1.859712245	-4.954535265	1.317193265
H	3.143364245	-3.864432020	0.793428000
C	1.448021000	-2.860157265	1.647140245
H	0.667026755	-3.067207245	2.399576755
H	0.944692245	-2.726183531	0.683943245
C	2.153679020	-1.559749265	2.036836714
H	2.981886041	-1.383627306	1.330076980
H	4.582758000	-2.670084000	2.720214755
C	3.754401245	-2.922323245	3.402778000
H	4.202146735	-3.060734490	4.395367755
C	2.770373245	-1.754146245	3.427792735
H	1.968428735	-1.951579735	4.159635225
H	3.292768245	-0.846947490	3.768935980

Intermediate D

La	-0.842310000	-0.263337000	-0.008772000
N	-1.758681000	-0.112435000	2.218107000
N	0.036231000	-2.451784000	-0.590349000
N	-2.449616000	0.259077000	-1.732173000
Si	-2.476496000	1.643815000	-2.806843000
Si	-0.088085000	-3.954447000	0.320325000
Si	-0.746647000	-0.527349000	3.594425000
Si	-3.409333000	0.390102000	2.581767000
Si	-3.693375000	-0.963316000	-1.952606000
Si	0.684517000	-2.545125000	-2.216304000
C	-3.590504000	1.388804000	4.195064000
H	-4.644764000	1.677415000	4.298357000
H	-3.315550000	0.826510000	5.094614000

H	-2.998425000	2.312206000	4.180806000
C	-4.071669000	1.550725000	1.233204000
H	-3.770707000	1.258552000	0.217406000
H	-5.169237000	1.569273000	1.265074000
H	-3.727843000	2.578428000	1.411998000
C	-4.617223000	-1.066134000	2.741407000
H	-4.856786000	-1.513839000	1.769725000
H	-4.209788000	-1.856161000	3.383747000
H	-5.559191000	-0.719846000	3.185800000
C	-0.061651000	0.952357000	4.577164000
H	-0.818992000	1.690760000	4.860513000
H	0.405448000	0.577232000	5.497405000
H	0.724211000	1.460490000	4.000899000
C	-1.564838000	-1.685021000	4.858032000
H	-2.416111000	-1.223100000	5.371018000
H	-1.916335000	-2.608890000	4.384504000
H	-0.827534000	-1.959589000	5.623586000
C	0.828393000	-1.415450000	3.015226000
H	1.571654000	-1.357165000	3.822684000
H	0.650466000	-2.473872000	2.802321000
H	1.299259000	-0.966368000	2.129222000
C	0.610236000	-0.811528000	-3.003562000
H	-0.427439000	-0.526205000	-3.221108000
H	1.073672000	-0.011405000	-2.407440000
H	1.156408000	-0.838965000	-3.956142000
C	2.489483000	-3.131719000	-2.338044000
H	2.591288000	-4.177988000	-2.022571000
H	2.822728000	-3.070108000	-3.382960000
H	3.172799000	-2.531122000	-1.724973000
C	-0.281690000	-3.643731000	-3.432212000
H	-0.125901000	-3.279653000	-4.456619000
H	0.042958000	-4.689160000	-3.397636000
H	-1.358730000	-3.621593000	-3.229339000
C	1.556459000	-4.519588000	1.088977000
H	1.951686000	-3.821444000	1.833257000
H	1.415306000	-5.492316000	1.578175000
H	2.321772000	-4.645355000	0.311822000
C	-0.616155000	-5.466058000	-0.709629000
H	0.157369000	-5.783647000	-1.419058000
H	-0.785339000	-6.300227000	-0.015594000
H	-1.545482000	-5.302990000	-1.267171000
C	-1.398096000	-3.835490000	1.699333000
H	-2.350666000	-4.250627000	1.347355000
H	-1.080682000	-4.422445000	2.571760000
H	-1.600025000	-2.812418000	2.039967000
C	-3.435593000	-2.315570000	-0.641528000

H	-3.281326000	-1.946654000	0.383672000
H	-4.333223000	-2.946419000	-0.598145000
H	-2.585532000	-2.958021000	-0.902619000
C	-3.633764000	-1.860888000	-3.627212000
H	-2.603330000	-1.969125000	-3.986225000
H	-4.061804000	-2.866845000	-3.524858000
H	-4.202935000	-1.333200000	-4.400316000
C	-5.467561000	-0.316892000	-1.759813000
H	-5.721307000	0.415991000	-2.535808000
H	-6.172491000	-1.152932000	-1.855084000
H	-5.629485000	0.155407000	-0.783964000
C	-2.896154000	1.251688000	-4.619691000
H	-2.230168000	0.494700000	-5.050006000
H	-3.929330000	0.908587000	-4.748744000
H	-2.781307000	2.172957000	-5.206400000
C	-3.757798000	2.962174000	-2.316150000
H	-4.768459000	2.608320000	-2.554359000
H	-3.745877000	3.201236000	-1.248251000
H	-3.589639000	3.888767000	-2.881060000
C	-0.754687000	2.457533000	-2.909358000
H	-0.264957000	2.549097000	-1.933598000
H	-0.097737000	1.876973000	-3.569873000
H	-0.845960000	3.467003000	-3.333572000
O	1.877841000	1.027229000	0.336373000
C	3.334417000	0.942197000	0.198454000
C	5.121447000	0.535512000	-1.582164000
C	3.628657000	0.693494000	-1.280725000
C	3.070387000	1.844796000	-2.128092000
C	3.341908000	1.675358000	-3.617528000
C	4.827194000	1.490497000	-3.893299000
C	5.371954000	0.330249000	-3.072531000
H	5.548119000	-0.306495000	-1.024685000
H	5.653566000	1.441219000	-1.240901000
H	3.119297000	-0.241947000	-1.577994000
H	1.986992000	1.954415000	-1.971708000
H	3.533894000	2.784315000	-1.776673000
H	2.940881000	2.536525000	-4.168062000
H	2.795411000	0.791584000	-3.983051000
H	5.004638000	1.326920000	-4.963677000
H	5.368298000	2.411534000	-3.621426000
H	6.444968000	0.192009000	-3.255442000
H	4.876436000	-0.603405000	-3.388156000
O	1.977271000	3.396571000	0.916958000
C	1.013126000	4.468581000	0.763221000
C	-0.354573000	3.730111000	0.918333000
O	-0.028949000	2.394522000	0.406202000

C	1.230329000	5.059416000	-0.621249000
H	2.276570000	5.372073000	-0.707581000
H	1.027657000	4.331547000	-1.416528000
C	1.276765000	5.515429000	1.823599000
H	0.509635000	6.298670000	1.786462000
H	1.289766000	5.084535000	2.828000000
H	2.248919000	5.985492000	1.641717000
C	-0.783682000	3.545594000	2.359726000
H	-1.566808000	2.779152000	2.395307000
H	0.041555000	3.198287000	2.989876000
H	-1.176512000	4.478545000	2.780091000
B	1.336253000	2.252591000	0.562637000
H	-2.392644000	3.728748000	0.264847000
C	-1.483214000	4.318494000	0.106594000
H	-1.272986000	4.334354000	-0.966126000
H	-1.684871000	5.343947000	0.440607000
H	0.595190000	5.936910000	-0.785723000
H	3.729220000	1.939695000	0.455059000
C	5.262138000	0.337983000	1.743126000
C	3.859256000	-0.038099000	1.249835000
C	3.776842000	-1.515061000	0.861929000
C	4.261644000	-2.416475000	1.993614000
C	5.659946000	-2.030915000	2.459151000
C	5.702587000	-0.569091000	2.885250000
H	5.267891000	1.390348000	2.062589000
H	5.994865000	0.257783000	0.927087000
H	3.194264000	0.107906000	2.121138000
H	2.748739000	-1.782928000	0.567248000
H	4.406782000	-1.701816000	-0.022649000
H	4.235851000	-3.464776000	1.670763000
H	3.564233000	-2.337345000	2.844026000
H	5.984489000	-2.683313000	3.279708000
H	6.374489000	-2.186501000	1.633687000
H	6.707978000	-0.289189000	3.224890000
H	5.028144000	-0.423533000	3.745157000

Ketone borylated product

O	-2.132616000	-1.151461000	-1.131620000
C	-3.438842000	-1.101689000	-0.532240000
B	-1.253792000	-0.710304000	-0.173825000
C	-3.256887000	-0.013286000	0.569943000
O	-1.876327000	-0.185158000	0.939083000
C	-3.724517000	-2.481545000	0.042856000
H	-3.615362000	-3.223301000	-0.755363000
H	-3.016174000	-2.734846000	0.840084000
H	-4.742179000	-2.552310000	0.444408000

C	-4.457726000	-0.761275000	-1.599529000
H	-5.451747000	-0.620815000	-1.155815000
H	-4.183759000	0.146271000	-2.144706000
H	-4.522180000	-1.581644000	-2.322583000
C	-4.125588000	-0.192109000	1.796421000
H	-3.924705000	-1.142823000	2.298020000
H	-3.928289000	0.615138000	2.510351000
H	-5.188658000	-0.153868000	1.526427000
C	-3.392750000	1.403544000	0.029233000
H	-3.031303000	2.106073000	0.788958000
H	-2.787447000	1.541033000	-0.875785000
H	-4.433313000	1.654912000	-0.206935000
O	0.082852000	-0.782344000	-0.342504000
C	0.961240000	-0.106023000	0.557485000
C	3.002448000	-0.692588000	-0.908252000
C	2.331673000	-0.777143000	0.463441000
C	2.219138000	-2.239360000	0.906332000
C	3.564936000	-2.951643000	0.892681000
C	4.199081000	-2.877444000	-0.490400000
C	4.339901000	-1.427241000	-0.932735000
H	3.165021000	0.354905000	-1.191850000
H	2.321222000	-1.121599000	-1.659693000
H	2.984016000	-0.265152000	1.193690000
H	1.766295000	-2.286917000	1.907812000
H	1.527109000	-2.757180000	0.224997000
H	3.446132000	-3.995807000	1.210524000
H	4.239215000	-2.476992000	1.624696000
H	5.174869000	-3.380594000	-0.499470000
H	3.559866000	-3.415269000	-1.209119000
H	4.782264000	-1.368427000	-1.935813000
H	5.041807000	-0.914732000	-0.253779000
C	1.930255000	2.181870000	1.121901000
C	1.684747000	3.685603000	1.057651000
C	1.613559000	4.165315000	-0.387726000
C	0.552980000	3.395460000	-1.167111000
C	0.807138000	1.892036000	-1.110865000
C	0.864026000	1.414194000	0.342357000
H	1.956129000	1.839219000	2.167317000
H	2.924695000	1.965473000	0.697095000
H	2.468580000	4.224426000	1.605805000
H	0.733194000	3.917567000	1.562796000
H	1.415759000	5.244491000	-0.426537000
H	2.594373000	4.009478000	-0.866369000
H	0.517982000	3.736409000	-2.210004000
H	-0.437805000	3.613136000	-0.734293000
H	0.025669000	1.347660000	-1.657997000

H	1.752085000	1.672803000	-1.628733000
H	-0.112304000	1.692197000	0.782609000
H	0.607759000	-0.285746000	1.590055000

cyclohexanecarboxaldehyde

O	-3.094940000	-0.000003000	-0.312343000
C	-2.072477000	0.000029000	0.326505000
C	0.062319000	-1.258367000	0.221409000
C	-0.681560000	0.000008000	-0.241480000
C	0.062332000	1.258374000	0.221416000
C	1.510239000	1.255347000	-0.254646000
C	2.240248000	-0.000008000	0.208056000
C	1.510226000	-1.255354000	-0.254651000
H	-0.462053000	-2.155963000	-0.131757000
H	0.040880000	-1.294049000	1.324347000
H	-0.770281000	0.000015000	-1.338614000
H	-0.462032000	2.155976000	-0.131746000
H	0.040894000	1.294052000	1.324355000
H	2.024944000	2.156810000	0.101034000
H	1.526560000	1.299376000	-1.355221000
H	3.274823000	-0.000013000	-0.157562000
H	2.296970000	-0.000011000	1.308704000
H	2.024922000	-2.156824000	0.101025000
H	1.526548000	-1.299379000	-1.355227000
H	-2.090627000	-0.000135000	1.449753000

intermediate E

La	-0.601483000	-0.011455000	0.096536000
N	2.101839000	0.210088000	0.880427000
N	-2.000991000	-1.915164000	-0.197761000
N	-1.728622000	2.039954000	-0.290093000
Si	-1.241231000	3.305360000	-1.398477000
Si	-2.707043000	-2.975854000	0.995358000
Si	2.280998000	-1.315245000	1.828744000
Si	2.308780000	1.791780000	1.726208000
Si	-3.224208000	2.157762000	0.606717000
Si	-2.188938000	-2.248104000	-1.909444000
C	2.733728000	3.183712000	0.526247000
H	2.757026000	4.118275000	1.102950000
H	3.716996000	3.052705000	0.061564000
H	1.990305000	3.311371000	-0.269758000
C	0.664223000	2.277611000	2.542799000
H	0.308132000	1.545107000	3.277854000
H	0.800943000	3.226138000	3.078653000
H	-0.126920000	2.464317000	1.796762000
C	3.665430000	1.768780000	3.042527000

H	3.500818000	1.040194000	3.843086000
H	4.646308000	1.569653000	2.594823000
H	3.711347000	2.761564000	3.507542000
C	4.040032000	-1.803030000	2.312222000
H	4.560421000	-1.008832000	2.858277000
H	3.981654000	-2.677582000	2.973076000
H	4.651653000	-2.081150000	1.447597000
C	1.317744000	-1.081784000	3.448166000
H	1.748503000	-0.313173000	4.099195000
H	0.254683000	-0.842837000	3.307973000
H	1.344954000	-2.030271000	4.000110000
C	1.504360000	-2.793936000	0.931454000
H	1.573099000	-3.657151000	1.608464000
H	0.443459000	-2.691865000	0.657953000
H	2.039807000	-3.043425000	0.009819000
C	-1.737596000	-0.655209000	-2.863235000
H	-2.299725000	0.228436000	-2.523359000
H	-0.660603000	-0.428341000	-2.856675000
H	-2.000549000	-0.808404000	-3.917596000
C	-0.994216000	-3.580290000	-2.530736000
H	0.037010000	-3.283004000	-2.298819000
H	-1.181670000	-4.552550000	-2.060995000
H	-1.073844000	-3.705771000	-3.617776000
C	-3.954275000	-2.712460000	-2.417281000
H	-4.013199000	-2.823359000	-3.507226000
H	-4.280565000	-3.659656000	-1.971155000
H	-4.665647000	-1.933897000	-2.116735000
C	-2.406277000	-4.814929000	0.635890000
H	-1.332398000	-5.020117000	0.539509000
H	-2.797203000	-5.430680000	1.455722000
H	-2.895404000	-5.146249000	-0.288097000
C	-4.576229000	-2.725886000	1.206304000
H	-5.117508000	-2.969667000	0.284980000
H	-4.963877000	-3.370684000	2.005243000
H	-4.815852000	-1.686883000	1.465222000
C	-1.915045000	-2.660735000	2.699154000
H	-2.420344000	-3.282982000	3.448701000
H	-0.854017000	-2.941639000	2.709885000
H	-2.009404000	-1.621588000	3.043860000
C	-3.104723000	0.933245000	2.071398000
H	-2.239239000	1.124877000	2.724713000
H	-3.996713000	1.029267000	2.702855000
H	-3.093341000	-0.113292000	1.734530000
C	-4.736644000	1.605929000	-0.387511000
H	-4.583540000	0.575056000	-0.735515000
H	-5.647769000	1.624860000	0.223390000

H	-4.900460000	2.238605000	-1.267367000
C	-3.534893000	3.863154000	1.370366000
H	-3.701936000	4.637578000	0.612653000
H	-4.421875000	3.833071000	2.015247000
H	-2.678292000	4.170388000	1.983748000
C	-2.652240000	3.868227000	-2.536263000
H	-3.042196000	3.021283000	-3.114729000
H	-3.487796000	4.309723000	-1.979032000
H	-2.292395000	4.623479000	-3.246058000
C	-0.610148000	4.848785000	-0.484185000
H	-1.430767000	5.375925000	0.016527000
H	0.130983000	4.589040000	0.282530000
H	-0.138857000	5.550180000	-1.184350000
C	0.140618000	2.682869000	-2.539856000
H	0.949849000	2.149029000	-2.025119000
H	-0.262428000	1.991928000	-3.291065000
H	0.586958000	3.531678000	-3.073541000
O	1.217709000	-0.308665000	-1.253209000
C	2.338731000	0.165868000	-0.631825000
H	2.528776000	1.220942000	-0.925151000
C	4.949299000	-1.409056000	-3.013475000
C	3.676508000	-0.706800000	-2.556123000
C	3.610158000	-0.585893000	-1.034212000
C	4.866685000	0.106702000	-0.510457000
C	6.139682000	-0.603023000	-0.957594000
C	6.196067000	-0.716379000	-2.476490000
H	4.980020000	-1.463498000	-4.109316000
H	4.934670000	-2.450752000	-2.652239000
H	2.782590000	-1.227807000	-2.916072000
H	3.636953000	0.309684000	-2.987489000
H	3.571808000	-1.612317000	-0.625474000
H	4.837538000	0.189077000	0.585544000
H	4.879207000	1.139210000	-0.903051000
H	7.024206000	-0.078130000	-0.573715000
H	6.165376000	-1.615441000	-0.520061000
H	7.102931000	-1.249538000	-2.790203000
H	6.261695000	0.295383000	-2.908897000

TS4 between E and F

La	0.674278000	0.480705000	-0.310014000
N	2.194469000	-0.045021000	1.581327000
N	0.333298000	2.704916000	-1.091370000
Si	0.684476000	2.951646000	-2.765772000
Si	1.618528000	-0.603142000	3.172482000
Si	3.660537000	0.940257000	1.516322000
Si	-0.297240000	3.819881000	0.078292000

C	5.259693000	-0.074820000	1.643314000
H	6.080156000	0.401109000	1.091103000
H	5.571866000	-0.153951000	2.691746000
H	5.114090000	-1.093947000	1.270082000
C	3.648032000	1.920857000	-0.126133000
H	3.542452000	1.321223000	-1.039198000
H	2.868254000	2.697243000	-0.139222000
H	4.611452000	2.439314000	-0.218956000
C	3.794932000	2.310568000	2.820018000
H	2.873024000	2.899301000	2.903519000
H	4.044317000	1.920198000	3.813242000
H	4.603215000	2.991825000	2.522832000
C	2.870134000	-1.797798000	3.938229000
H	3.793804000	-1.272409000	4.214062000
H	2.465371000	-2.258715000	4.847340000
H	3.138190000	-2.592298000	3.231676000
C	1.297018000	0.774956000	4.440077000
H	2.186878000	1.339025000	4.732417000
H	0.541576000	1.488072000	4.086261000
H	0.893346000	0.299711000	5.344057000
C	-0.074193000	-1.451044000	3.034003000
H	-0.522806000	-1.495506000	4.035454000
H	-0.758263000	-0.881487000	2.388254000
H	-0.021857000	-2.471534000	2.638823000
C	-0.738325000	2.732555000	1.588189000
H	0.161416000	2.277512000	2.038859000
H	-1.193214000	3.329881000	2.388335000
H	-1.457683000	1.932519000	1.345789000
C	-1.834882000	4.769236000	-0.487391000
H	-2.583392000	4.100980000	-0.929767000
H	-2.301698000	5.293178000	0.356242000
H	-1.569059000	5.522842000	-1.239511000
C	0.979878000	5.095115000	0.657918000
H	1.325319000	5.711742000	-0.181345000
H	0.558899000	5.766190000	1.416662000
H	1.860367000	4.604008000	1.092363000
C	-0.743912000	3.607858000	-3.818059000
H	-1.624615000	2.960525000	-3.735546000
H	-1.038659000	4.616237000	-3.504154000
H	-0.449867000	3.659540000	-4.873905000
C	2.189379000	4.057449000	-3.082351000
H	1.989562000	5.080955000	-2.741148000
H	3.069937000	3.693304000	-2.539365000
H	2.435460000	4.105002000	-4.150348000
C	1.107920000	1.201973000	-3.450837000
H	2.021726000	0.767216000	-3.012653000

H	0.276301000	0.485030000	-3.340141000
H	1.303427000	1.262321000	-4.528330000
O	3.420634000	-2.708866000	0.569538000
C	3.784599000	-3.217446000	-0.723858000
C	3.320797000	-2.085630000	-1.697428000
O	2.200404000	-1.513657000	-0.968056000
C	3.014078000	-4.518136000	-0.925400000
H	3.245202000	-5.189580000	-0.092112000
H	1.929918000	-4.348920000	-0.927441000
C	5.272967000	-3.497660000	-0.742488000
H	5.591772000	-3.837451000	-1.736176000
H	5.861065000	-2.617909000	-0.465886000
H	5.498999000	-4.293084000	-0.024605000
C	4.380947000	-1.022208000	-1.917731000
H	3.957685000	-0.191832000	-2.497120000
H	4.773593000	-0.627303000	-0.974492000
H	5.217354000	-1.426347000	-2.499364000
B	2.265742000	-1.974992000	0.388418000
H	1.223326000	-2.243524000	0.905633000
H	2.501202000	-1.711052000	-3.652235000
C	2.797963000	-2.569206000	-3.036347000
H	1.925011000	-3.218511000	-2.920695000
H	3.577100000	-3.118527000	-3.579992000
H	3.291513000	-5.018578000	-1.860251000
N	-3.572407000	-0.529578000	0.545653000
Si	-4.224414000	0.696192000	-0.571262000
Si	-4.187621000	-0.668637000	2.206543000
C	-3.763739000	-2.352288000	2.956486000
H	-4.265564000	-2.426893000	3.929905000
H	-4.126702000	-3.175553000	2.330279000
H	-2.690519000	-2.492344000	3.126422000
C	-3.495853000	0.655923000	3.371916000
H	-3.771515000	1.669514000	3.059830000
H	-3.875739000	0.499173000	4.389457000
H	-2.399619000	0.602594000	3.412499000
C	-6.079134000	-0.579268000	2.196831000
H	-6.484859000	0.356004000	1.797306000
H	-6.486541000	-1.406517000	1.601856000
H	-6.453082000	-0.690332000	3.222150000
C	-5.784987000	0.051377000	-1.432407000
H	-6.546602000	-0.267358000	-0.711739000
H	-6.223393000	0.831911000	-2.066819000
H	-5.550078000	-0.808381000	-2.072655000
C	-4.656941000	2.287206000	0.365899000
H	-5.407096000	2.155902000	1.152792000
H	-3.757124000	2.721600000	0.822043000

H	-5.052855000	3.022276000	-0.346996000
C	-3.036153000	1.251399000	-1.939691000
H	-3.584167000	1.961509000	-2.576388000
H	-2.155637000	1.768273000	-1.536540000
H	-2.687637000	0.431302000	-2.577664000
O	-1.291992000	-0.462180000	-0.039803000
C	-2.379236000	-1.286659000	0.167368000
H	-2.147078000	-1.977322000	1.006147000
C	-1.563330000	-3.854300000	-2.652498000
C	-1.333841000	-2.902772000	-1.483247000
C	-2.618917000	-2.198333000	-1.049378000
C	-3.704646000	-3.231197000	-0.753859000
C	-3.948262000	-4.157214000	-1.938587000
C	-2.662451000	-4.865524000	-2.348636000
H	-0.627960000	-4.369057000	-2.915563000
H	-1.854337000	-3.266374000	-3.538816000
H	-0.562710000	-2.163065000	-1.752424000
H	-0.932132000	-3.462544000	-0.617438000
H	-2.961344000	-1.570719000	-1.893056000
H	-4.630010000	-2.719970000	-0.452847000
H	-3.383291000	-3.834766000	0.114139000
H	-4.732098000	-4.887806000	-1.699867000
H	-4.323769000	-3.564400000	-2.789732000
H	-2.834974000	-5.518704000	-3.214056000
H	-2.334004000	-5.517873000	-1.522963000

Intermediate F

La	0.362028000	-0.417038000	0.048577000
N	0.475122000	2.366885000	0.289230000
N	0.783973000	-1.813657000	-1.832378000
N	-0.249880000	-1.864897000	1.847362000
Si	-1.646862000	-2.900780000	1.618242000
Si	1.684394000	-3.305222000	-1.604376000
Si	-0.401230000	3.038779000	1.712974000
Si	0.269171000	3.269845000	-1.260965000
Si	0.626048000	-1.924999000	3.372438000
Si	0.150719000	-1.450639000	-3.424900000
C	0.729013000	5.096439000	-1.127456000
H	0.658524000	5.561262000	-2.119035000
H	0.061072000	5.650270000	-0.456802000
H	1.756696000	5.195786000	-0.764410000
C	1.309915000	2.506651000	-2.643412000
H	1.339627000	1.410618000	-2.618477000
H	0.897720000	2.793198000	-3.619636000
H	2.338283000	2.873254000	-2.570190000
C	-1.540755000	3.211148000	-1.859864000

H	-2.037993000	2.262787000	-1.626655000
H	-2.138173000	4.025636000	-1.437535000
H	-1.551309000	3.327132000	-2.951308000
C	0.477071000	4.500863000	2.528331000
H	0.834849000	5.212851000	1.775474000
H	-0.220872000	5.029436000	3.190012000
H	1.341389000	4.178613000	3.116044000
C	-2.122191000	3.714928000	1.263531000
H	-2.060728000	4.699473000	0.785564000
H	-2.702671000	3.065656000	0.601262000
H	-2.687483000	3.843427000	2.196786000
C	-0.684977000	1.692795000	3.019055000
H	-1.455072000	2.032938000	3.724669000
H	-1.015854000	0.722874000	2.616424000
H	0.227803000	1.506283000	3.596231000
C	-1.195661000	-0.121954000	-3.245907000
H	-2.010949000	-0.460797000	-2.592920000
H	-0.821992000	0.833576000	-2.859160000
H	-1.629845000	0.093790000	-4.230506000
C	1.449416000	-0.800708000	-4.645643000
H	2.052113000	0.004997000	-4.209482000
H	2.135485000	-1.597024000	-4.956222000
H	0.961440000	-0.407852000	-5.546922000
C	-0.707955000	-2.921299000	-4.264212000
H	-1.154331000	-2.592574000	-5.211500000
H	-0.015479000	-3.739834000	-4.494235000
H	-1.511129000	-3.322794000	-3.633737000
C	3.018834000	-3.577328000	-2.925955000
H	3.682130000	-2.707800000	-3.010580000
H	3.632035000	-4.447832000	-2.660755000
H	2.587468000	-3.768867000	-3.916161000
C	0.612587000	-4.872184000	-1.561148000
H	0.036774000	-5.014421000	-2.482307000
H	1.256560000	-5.750919000	-1.426788000
H	-0.095967000	-4.847691000	-0.723339000
C	2.551083000	-3.247522000	0.081487000
H	1.821909000	-3.138233000	0.896460000
H	3.090962000	-4.187671000	0.251783000
H	3.285261000	-2.434940000	0.149643000
C	2.133045000	-0.774309000	3.291852000
H	1.954303000	0.249417000	2.939660000
H	2.566292000	-0.702429000	4.298242000
H	2.901687000	-1.215276000	2.643412000
C	1.386989000	-3.612038000	3.810181000
H	2.008644000	-4.007796000	2.998353000
H	2.033069000	-3.478586000	4.688148000

H	0.638072000	-4.369456000	4.063278000
C	-0.454205000	-1.473225000	4.867794000
H	-1.179035000	-2.270900000	5.076470000
H	0.171592000	-1.359530000	5.762125000
H	-1.009593000	-0.540655000	4.717762000
C	-1.362057000	-4.713993000	2.098716000
H	-0.423305000	-5.102273000	1.685037000
H	-1.327759000	-4.842024000	3.187238000
H	-2.184279000	-5.333387000	1.718660000
C	-3.163177000	-2.321689000	2.620124000
H	-3.065898000	-2.569766000	3.683408000
H	-3.292908000	-1.232193000	2.560439000
H	-4.078986000	-2.798757000	2.246560000
C	-2.217118000	-2.896134000	-0.203535000
H	-2.879805000	-2.051667000	-0.427505000
H	-1.390923000	-2.882311000	-0.927847000
H	-2.789545000	-3.814855000	-0.386211000
O	-2.174627000	0.304723000	-0.036646000
C	-3.167947000	0.596027000	0.611952000
C	-4.663556000	0.252819000	-1.400217000
C	-4.559703000	0.572437000	0.085049000
C	-5.293359000	1.878016000	0.433714000
C	-6.751240000	1.800309000	-0.003499000
C	-6.860013000	1.484494000	-1.491227000
C	-6.123634000	0.194605000	-1.835307000
H	-4.150763000	-0.691098000	-1.626029000
H	-4.133885000	1.036434000	-1.966506000
H	-5.046437000	-0.234934000	0.672757000
H	-5.209779000	2.091826000	1.508583000
H	-4.798422000	2.709661000	-0.094660000
H	-7.260963000	2.742474000	0.231856000
H	-7.259954000	1.013689000	0.576486000
H	-7.913031000	1.416833000	-1.790823000
H	-6.422937000	2.315181000	-2.067939000
H	-6.185141000	-0.010418000	-2.910703000
H	-6.617099000	-0.650659000	-1.328899000
O	2.890931000	3.041322000	0.043220000
C	4.162800000	2.433714000	0.122050000
C	3.863447000	0.888915000	-0.029181000
O	2.481627000	0.780946000	0.364799000
C	4.795027000	2.800042000	1.467452000
H	4.810594000	3.893299000	1.540539000
H	4.211378000	2.420527000	2.312163000
C	5.043051000	2.991990000	-0.983882000
H	6.028110000	2.507323000	-0.990852000
H	4.589021000	2.869689000	-1.972079000

H	5.195194000	4.063822000	-0.814348000
C	3.977489000	0.368350000	-1.455337000
H	3.545842000	-0.641723000	-1.508612000
H	3.430306000	0.995838000	-2.163854000
H	5.023311000	0.306854000	-1.779825000
B	1.969462000	2.185624000	0.741970000
H	2.019114000	2.251997000	1.971800000
H	4.532383000	-1.033296000	0.708474000
C	4.735185000	0.031355000	0.874087000
H	4.566219000	0.247994000	1.932685000
H	5.796181000	0.198796000	0.647063000
H	5.824820000	2.435219000	1.558864000
H	-3.060552000	0.892488000	1.680356000

TS5 between F and G

La	0.721045000	0.031033000	-0.123856000
N	-1.135140000	-0.724768000	1.740227000
N	2.333081000	1.699382000	0.387424000
N	2.019862000	-1.556246000	-1.278396000
Si	1.525470000	-2.141440000	-2.851224000
Si	3.124911000	2.077526000	1.905112000
Si	-1.676761000	0.682545000	2.767194000
Si	-0.646523000	-2.269333000	2.579748000
Si	3.584495000	-1.985884000	-0.617278000
Si	2.617600000	2.782549000	-0.972071000
C	-2.128356000	-3.106587000	3.395667000
H	-1.837180000	-4.085553000	3.795797000
H	-2.498565000	-2.500472000	4.232259000
H	-2.956914000	-3.227726000	2.692739000
C	0.244646000	-3.457049000	1.384534000
H	0.634173000	-3.004873000	0.460865000
H	1.099716000	-3.890495000	1.919165000
H	-0.397490000	-4.286204000	1.079462000
C	0.656993000	-2.042599000	3.937926000
H	1.611612000	-1.666903000	3.553436000
H	0.356360000	-1.424146000	4.785629000
H	0.847159000	-3.055516000	4.319500000
C	-3.549258000	0.948254000	2.735710000
H	-4.071713000	0.053935000	3.090811000
H	-3.785177000	1.785325000	3.406160000
H	-3.939742000	1.175548000	1.738939000
C	-1.257664000	0.552121000	4.608100000
H	-1.677632000	-0.335184000	5.094387000
H	-0.183912000	0.596135000	4.814344000
H	-1.718248000	1.429514000	5.081728000
C	-0.812660000	2.273656000	2.194445000

H	-1.347341000	3.124486000	2.638574000
H	0.220198000	2.321910000	2.555916000
H	-0.800569000	2.439091000	1.110924000
C	2.177967000	1.874417000	-2.588506000
H	2.637920000	0.878540000	-2.650108000
H	1.093941000	1.786409000	-2.743293000
H	2.559115000	2.465707000	-3.430664000
C	1.500235000	4.313647000	-0.922514000
H	0.448952000	3.997636000	-0.933134000
H	1.665817000	4.918086000	-0.023668000
H	1.673357000	4.950238000	-1.799573000
C	4.410558000	3.371930000	-1.162056000
H	4.487930000	3.986017000	-2.068386000
H	4.743700000	3.988000000	-0.318664000
H	5.106588000	2.531056000	-1.265577000
C	2.938154000	3.897831000	2.417320000
H	1.883310000	4.195044000	2.467514000
H	3.380849000	4.048188000	3.410344000
H	3.446870000	4.579741000	1.725206000
C	4.985108000	1.702168000	1.914312000
H	5.540574000	2.358018000	1.235067000
H	5.387893000	1.847072000	2.925200000
H	5.185614000	0.665831000	1.616212000
C	2.371650000	1.035302000	3.321228000
H	3.088498000	0.295011000	3.697532000
H	2.095756000	1.684153000	4.163086000
H	1.460350000	0.491124000	3.039464000
C	3.517363000	-1.784350000	1.273862000
H	2.854999000	-2.525697000	1.736744000
H	4.518975000	-1.924364000	1.700709000
H	3.198210000	-0.778862000	1.580616000
C	4.969759000	-0.856028000	-1.242556000
H	4.724040000	0.185524000	-0.994383000
H	5.928781000	-1.101351000	-0.769012000
H	5.096411000	-0.928323000	-2.329185000
C	4.055415000	-3.795681000	-0.926960000
H	4.206663000	-4.019278000	-1.989693000
H	4.988798000	-4.034997000	-0.402289000
H	3.272250000	-4.464315000	-0.547238000
C	2.867268000	-1.982145000	-4.183378000
H	3.169752000	-0.936862000	-4.320974000
H	3.764714000	-2.564649000	-3.942140000
H	2.483759000	-2.349707000	-5.143666000
C	0.972281000	-3.954409000	-2.813442000
H	1.826189000	-4.631385000	-2.694328000
H	0.294769000	-4.125979000	-1.967706000

H	0.448929000	-4.230763000	-3.737750000
C	0.053114000	-1.094125000	-3.447396000
H	-0.755634000	-1.056812000	-2.705474000
H	0.358287000	-0.072506000	-3.705728000
H	-0.376596000	-1.543821000	-4.351972000
O	-0.893582000	1.570286000	-1.230469000
C	-2.100840000	1.233223000	-1.316001000
C	-3.441763000	2.649348000	-2.757032000
C	-3.210288000	2.243357000	-1.287404000
C	-2.948173000	3.466598000	-0.420320000
C	-4.081755000	4.478163000	-0.548110000
C	-4.306080000	4.884215000	-1.999643000
C	-4.574283000	3.662609000	-2.870203000
H	-3.654160000	1.757860000	-3.365794000
H	-2.508249000	3.087502000	-3.145882000
H	-4.124744000	1.737731000	-0.935596000
H	-2.828933000	3.159845000	0.626640000
H	-1.996219000	3.927407000	-0.727930000
H	-3.869503000	5.358590000	0.070933000
H	-5.008300000	4.033387000	-0.149210000
H	-5.135311000	5.598641000	-2.076720000
H	-3.408657000	5.403216000	-2.372695000
H	-4.710703000	3.953531000	-3.919406000
H	-5.515372000	3.186798000	-2.550978000
O	-3.469738000	-1.478348000	1.020754000
C	-4.061250000	-2.085182000	-0.113731000
C	-2.821593000	-2.618844000	-0.913361000
O	-1.762647000	-1.719362000	-0.526505000
C	-4.881078000	-1.048721000	-0.883040000
H	-5.529949000	-0.526932000	-0.168973000
H	-4.260320000	-0.301146000	-1.384085000
C	-5.022625000	-3.163187000	0.362688000
H	-5.444791000	-3.720568000	-0.483375000
H	-4.543931000	-3.872650000	1.043246000
H	-5.851360000	-2.690528000	0.901969000
C	-2.450418000	-4.034490000	-0.498489000
H	-1.477581000	-4.294852000	-0.929244000
H	-2.385621000	-4.133044000	0.589524000
H	-3.186045000	-4.759532000	-0.866527000
B	-2.218575000	-0.925137000	0.611194000
H	-2.405299000	0.308472000	0.138180000
H	-2.106231000	-3.023271000	-2.906075000
C	-2.997448000	-2.604061000	-2.422563000
H	-3.156015000	-1.596483000	-2.822351000
H	-3.856778000	-3.223638000	-2.710762000
H	-5.514097000	-1.518616000	-1.645530000

H	-2.349002000	0.285541000	-1.829577000

Intermediate G

La	-0.875257000	-0.119689000	0.194724000
N	3.355518000	-0.548758000	-0.821579000
N	-1.790907000	1.529147000	-1.286595000
N	-2.198359000	-2.117623000	0.158572000
Si	-3.140952000	-2.836791000	1.453651000
Si	-0.642977000	2.460770000	-2.192544000
Si	4.658676000	0.703664000	-0.759217000
Si	3.099792000	-1.530074000	-2.300905000
Si	-2.246578000	-2.792803000	-1.452943000
Si	-3.515897000	1.783139000	-1.374622000
C	4.766905000	-2.093280000	-2.989959000
H	4.592077000	-2.759075000	-3.844233000
H	5.398673000	-1.269762000	-3.339354000
H	5.327615000	-2.658508000	-2.236120000
C	2.164822000	-3.115450000	-1.866220000
H	1.314663000	-2.960192000	-1.194321000
H	1.785142000	-3.577325000	-2.786868000
H	2.841573000	-3.834795000	-1.388548000
C	2.197082000	-0.560990000	-3.642663000
H	1.241506000	-0.152700000	-3.298370000
H	2.800602000	0.276337000	-4.011424000
H	1.983695000	-1.223463000	-4.491387000
C	6.329136000	-0.067699000	-0.349780000
H	6.665560000	-0.755702000	-1.132857000
H	7.090172000	0.714128000	-0.238989000
H	6.266128000	-0.620861000	0.593044000
C	4.767162000	1.594243000	-2.421423000
H	5.092257000	0.948587000	-3.244271000
H	3.809743000	2.049597000	-2.698875000
H	5.504205000	2.401779000	-2.331752000
C	4.207696000	1.975847000	0.559848000
H	4.879446000	2.839715000	0.488519000
H	3.181368000	2.340823000	0.426128000
H	4.299238000	1.554896000	1.566091000
C	-4.329476000	0.720529000	-0.027822000
H	-4.101603000	-0.349164000	-0.128907000
H	-3.995293000	1.050041000	0.968446000
H	-5.420079000	0.837223000	-0.058245000
C	-4.078496000	3.562861000	-1.028586000
H	-3.698623000	3.913329000	-0.060861000
H	-3.745974000	4.268697000	-1.798022000
H	-5.174983000	3.599329000	-0.993709000
C	-4.208991000	1.309573000	-3.077542000

H	-5.305874000	1.291897000	-3.079489000
H	-3.886728000	2.037287000	-3.834164000
H	-3.848905000	0.322562000	-3.394693000
C	-0.890256000	4.340456000	-2.178245000
H	-1.095649000	4.722834000	-1.171495000
H	0.011446000	4.839501000	-2.556814000
H	-1.725234000	4.632980000	-2.826837000
C	-0.512775000	1.985265000	-4.028438000
H	-1.366039000	2.393024000	-4.584851000
H	0.402795000	2.393588000	-4.476962000
H	-0.511256000	0.899576000	-4.181978000
C	1.053394000	2.146334000	-1.363169000
H	1.827128000	2.748606000	-1.858586000
H	1.029446000	2.476645000	-0.312706000
H	1.430321000	1.110797000	-1.396222000
C	-1.089293000	-1.735584000	-2.554587000
H	-0.057512000	-1.649454000	-2.181078000
H	-0.996731000	-2.216619000	-3.537170000
H	-1.493415000	-0.726242000	-2.726846000
C	-3.928020000	-2.705394000	-2.325340000
H	-4.380470000	-1.712742000	-2.203810000
H	-3.801890000	-2.889248000	-3.400214000
H	-4.638215000	-3.444399000	-1.939050000
C	-1.633554000	-4.584998000	-1.552890000
H	-2.352248000	-5.278475000	-1.098319000
H	-1.494756000	-4.889444000	-2.598124000
H	-0.675854000	-4.705421000	-1.030823000
C	-4.901591000	-3.327922000	0.938128000
H	-5.447972000	-2.493208000	0.483547000
H	-4.902308000	-4.163600000	0.226974000
H	-5.459749000	-3.652849000	1.825631000
C	-2.376039000	-4.450704000	2.117786000
H	-2.302887000	-5.201616000	1.321434000
H	-1.373148000	-4.318732000	2.540406000
H	-3.017031000	-4.865493000	2.906589000
C	-3.324021000	-1.619915000	2.896213000
H	-2.373494000	-1.188700000	3.232970000
H	-3.975625000	-0.784232000	2.610164000
H	-3.790920000	-2.129484000	3.748701000
O	-1.012515000	0.862126000	2.172853000
C	-1.230872000	1.669874000	3.272767000
C	-1.586464000	3.779004000	1.926014000
C	-0.789821000	3.114820000	3.047522000
C	0.710225000	3.217119000	2.780263000
C	1.156732000	4.652394000	2.529475000
C	0.358169000	5.285187000	1.395514000

C	-1.138653000	5.215572000	1.680202000
H	-2.659925000	3.744319000	2.170881000
H	-1.466594000	3.193312000	0.997506000
H	-0.999781000	3.663801000	3.985309000
H	1.269845000	2.778490000	3.621402000
H	0.951666000	2.602394000	1.894578000
H	2.233078000	4.686198000	2.311192000
H	1.005644000	5.242826000	3.448206000
H	0.672979000	6.324667000	1.234738000
H	0.575418000	4.746290000	0.456648000
H	-1.711787000	5.659754000	0.853321000
H	-1.360177000	5.825836000	2.571466000
O	3.691057000	-1.029318000	1.565997000
C	2.871735000	-1.344776000	2.704147000
C	1.666351000	-2.067703000	2.048445000
O	1.566766000	-1.354006000	0.762796000
C	2.482017000	-0.035325000	3.371863000
H	3.392967000	0.529031000	3.602623000
H	1.850088000	0.583323000	2.721044000
C	3.673898000	-2.207777000	3.655196000
H	3.048130000	-2.553742000	4.487170000
H	4.100296000	-3.078027000	3.148198000
H	4.498903000	-1.621902000	4.074394000
C	1.932163000	-3.524853000	1.708650000
H	1.115891000	-3.895053000	1.075086000
H	2.877862000	-3.655985000	1.169191000
H	1.961519000	-4.140046000	2.614939000
B	2.887717000	-0.966835000	0.453049000
H	-0.685852000	1.268969000	4.155736000
H	-0.426947000	-2.447334000	2.257803000
C	0.374960000	-1.953368000	2.819573000
H	0.079118000	-0.917129000	3.016053000
H	0.469930000	-2.479500000	3.778014000
H	1.940073000	-0.204225000	4.309839000
H	-2.305474000	1.667427000	3.545356000

TS6 between G and H

La	-0.779641000	-0.220595000	-0.398873000
N	3.352064000	-0.380548000	-0.369731000
N	-1.521348000	1.826446000	-1.326056000
N	-2.677495000	-1.528529000	0.270555000
Si	-3.415750000	-1.955090000	1.806804000
Si	-0.391815000	2.519989000	-2.463195000
Si	4.200770000	0.818760000	0.663475000
Si	4.036753000	-0.715454000	-1.985748000
Si	-3.433778000	-2.070616000	-1.212194000
Si	-3.071702000	2.586939000	-1.024601000
C	5.555332000	-1.843498000	-1.867941000
H	5.956900000	-2.016225000	-2.874861000
H	6.352684000	-1.408192000	-1.257511000
H	5.301795000	-2.821492000	-1.441773000
C	2.846557000	-1.560786000	-3.209763000
H	2.704466000	-0.925449000	-4.091630000
H	3.282474000	-2.508471000	-3.549833000
H	1.867344000	-1.778059000	-2.777033000
C	4.596753000	0.882930000	-2.839656000
H	3.775283000	1.601251000	-2.936939000
H	5.428520000	1.390080000	-2.342428000
H	4.931131000	0.621042000	-3.851874000
C	4.063254000	0.467424000	2.515300000
H	4.569498000	-0.474138000	2.752562000
H	4.578887000	1.277731000	3.048313000
H	3.043245000	0.397656000	2.896098000
C	6.083541000	0.795695000	0.410154000
H	6.501797000	-0.167107000	0.727519000
H	6.432443000	1.003303000	-0.605021000
H	6.509378000	1.566207000	1.066231000
C	3.560307000	2.549102000	0.248952000
H	2.466278000	2.552575000	0.319885000
H	3.959127000	3.297912000	0.945378000
H	3.839894000	2.848750000	-0.768306000
C	-3.848371000	1.836560000	0.535361000
H	-3.864371000	0.739155000	0.501235000
H	-3.297940000	2.143042000	1.436013000
H	-4.882713000	2.185808000	0.649927000
C	-2.922220000	4.452923000	-0.720335000
H	-2.214648000	4.657007000	0.093784000
H	-2.577843000	4.991600000	-1.611981000
H	-3.895740000	4.871446000	-0.436411000
C	-4.274906000	2.343876000	-2.475815000
H	-5.310217000	2.546216000	-2.173591000
H	-4.030760000	3.015883000	-3.307083000

H	-4.228674000	1.316485000	-2.858950000
C	0.515011000	4.084584000	-1.898074000
H	1.090310000	3.915832000	-0.979464000
H	1.220169000	4.402421000	-2.677387000
H	-0.177306000	4.914175000	-1.713404000
C	-1.160324000	2.883994000	-4.157320000
H	-1.870448000	3.718731000	-4.112743000
H	-0.380947000	3.151610000	-4.881834000
H	-1.697635000	2.007218000	-4.540248000
C	0.946110000	1.191118000	-2.747850000
H	0.543090000	0.243115000	-3.140629000
H	1.636394000	1.546684000	-3.523397000
H	1.568775000	0.985137000	-1.860680000
C	-2.265487000	-1.591309000	-2.675990000
H	-1.253201000	-2.031198000	-2.641068000
H	-2.716814000	-2.013910000	-3.582145000
H	-2.200608000	-0.506684000	-2.867796000
C	-5.097322000	-1.265239000	-1.631615000
H	-5.102224000	-0.195854000	-1.389774000
H	-5.311964000	-1.371463000	-2.702970000
H	-5.918975000	-1.734294000	-1.078905000
C	-3.680197000	-3.945176000	-1.344643000
H	-4.457132000	-4.290770000	-0.651542000
H	-4.005491000	-4.210010000	-2.358703000
H	-2.761289000	-4.500241000	-1.122738000
C	-5.300177000	-1.715166000	1.822108000
H	-5.591347000	-0.693204000	1.552524000
H	-5.806094000	-2.404978000	1.135021000
H	-5.682644000	-1.920464000	2.830085000
C	-3.144011000	-3.774844000	2.282706000
H	-3.594868000	-4.453033000	1.548403000
H	-2.081699000	-4.031094000	2.363749000
H	-3.611549000	-3.977276000	3.254764000
C	-2.729234000	-0.897751000	3.224958000
H	-1.681393000	-1.120546000	3.462890000
H	-2.817838000	0.176854000	3.015115000
H	-3.316359000	-1.102652000	4.129296000
O	1.087332000	0.298975000	0.917251000
C	0.596013000	0.556432000	2.190491000
C	0.402800000	2.179312000	4.105003000
C	0.762317000	2.003286000	2.633266000
C	-0.060209000	2.956400000	1.773978000
C	0.147032000	4.404596000	2.195330000
C	-0.203283000	4.590851000	3.667992000
C	0.585356000	3.627243000	4.549993000
H	1.015099000	1.506924000	4.724616000

H	-0.648674000	1.873676000	4.255841000
H	1.828193000	2.263384000	2.505763000
H	0.171025000	2.819697000	0.708440000
H	-1.131871000	2.697216000	1.888534000
H	-0.447827000	5.079980000	1.564446000
H	1.203434000	4.675269000	2.027797000
H	-0.026550000	5.627852000	3.981479000
H	-1.281168000	4.402982000	3.802958000
H	0.295924000	3.744957000	5.602266000
H	1.655904000	3.882239000	4.490901000
O	2.592654000	-1.932421000	1.437262000
C	1.752516000	-3.080799000	1.485807000
C	1.338738000	-3.268761000	-0.005441000
O	1.326124000	-1.900053000	-0.488834000
C	0.570008000	-2.816627000	2.407113000
H	0.947763000	-2.450465000	3.368579000
H	-0.122665000	-2.063914000	2.012828000
C	2.556863000	-4.236285000	2.056911000
H	1.992725000	-5.176352000	2.002490000
H	3.508164000	-4.361592000	1.533245000
H	2.780011000	-4.036752000	3.110741000
C	2.386406000	-4.026216000	-0.808857000
H	2.143542000	-3.958790000	-1.874833000
H	3.387321000	-3.604256000	-0.658460000
H	2.412706000	-5.085661000	-0.530559000
B	2.338541000	-1.194631000	0.279975000
H	1.043200000	-0.126944000	2.938127000
H	-0.204033000	-4.009737000	-1.305718000
C	-0.020144000	-3.900313000	-0.227669000
H	-0.846707000	-3.320370000	0.204736000
H	-0.050771000	-4.906041000	0.211958000
H	-0.003096000	-3.732993000	2.592400000
H	-0.512275000	0.340308000	2.260061000

Intermediate H

La	-0.577272000	-0.174754000	0.005814000
N	-0.738736000	0.431947000	2.349592000
N	0.282923000	-2.413391000	-0.266423000
N	-2.648022000	0.011145000	-1.207631000
Si	-3.054820000	1.222632000	-2.405401000
Si	0.609939000	-3.573584000	1.017813000
Si	0.749532000	0.413049000	3.277062000
Si	-2.259377000	0.902744000	3.102988000
Si	-3.836054000	-1.227847000	-0.842302000
Si	0.340340000	-2.964203000	-1.930384000
C	-2.075127000	1.966566000	4.666364000

H	-3.079489000	2.265262000	4.993668000
H	-1.610894000	1.417648000	5.494839000
H	-1.494777000	2.879717000	4.492427000
C	-3.250252000	1.954018000	1.872398000
H	-3.305012000	1.494667000	0.874690000
H	-4.279068000	2.105339000	2.225091000
H	-2.789685000	2.946837000	1.769428000
C	-3.356732000	-0.554328000	3.641363000
H	-3.908107000	-1.002397000	2.806611000
H	-2.768584000	-1.347374000	4.120039000
H	-4.097609000	-0.198420000	4.368598000
C	1.177481000	1.954590000	4.315086000
H	0.672602000	1.936992000	5.286707000
H	2.258879000	1.929905000	4.508781000
H	0.945837000	2.909925000	3.834878000
C	0.936357000	-1.002644000	4.530223000
H	0.017283000	-1.140402000	5.114994000
H	1.175249000	-1.960860000	4.057178000
H	1.745299000	-0.758615000	5.230858000
C	2.197720000	0.262189000	2.041618000
H	3.117218000	0.040358000	2.600556000
H	2.087500000	-0.549024000	1.308385000
H	2.374156000	1.201169000	1.497669000
C	-0.080572000	-1.519285000	-3.103368000
H	-1.125611000	-1.195329000	-2.994491000
H	0.567971000	-0.639468000	-2.991003000
H	0.045661000	-1.876256000	-4.133927000
C	2.035405000	-3.616540000	-2.492325000
H	2.447391000	-4.354692000	-1.792988000
H	1.939617000	-4.101916000	-3.472223000
H	2.769535000	-2.807958000	-2.589602000
C	-0.915271000	-4.318926000	-2.387552000
H	-1.081058000	-4.307002000	-3.473206000
H	-0.562897000	-5.319310000	-2.115401000
H	-1.886431000	-4.160078000	-1.902592000
C	2.398601000	-3.504733000	1.665532000
H	2.671462000	-2.532062000	2.092912000
H	2.527360000	-4.259991000	2.452194000
H	3.112328000	-3.733307000	0.862935000
C	0.357728000	-5.392544000	0.521311000
H	1.017664000	-5.722045000	-0.290002000
H	0.576567000	-6.016118000	1.398096000
H	-0.678593000	-5.591750000	0.223797000
C	-0.553952000	-3.335754000	2.500872000
H	-1.535064000	-3.774674000	2.283801000
H	-0.143461000	-3.851038000	3.379255000

H	-0.709879000	-2.283837000	2.771039000
C	-3.105344000	-2.372400000	0.486006000
H	-2.650080000	-1.857821000	1.343914000
H	-3.908873000	-2.990790000	0.908098000
H	-2.349176000	-3.045209000	0.062635000
C	-4.267516000	-2.379923000	-2.290439000
H	-3.373305000	-2.629244000	-2.875920000
H	-4.682835000	-3.318307000	-1.899613000
H	-5.005666000	-1.944883000	-2.972279000
C	-5.469244000	-0.533090000	-0.170407000
H	-5.970532000	0.108136000	-0.906435000
H	-6.155738000	-1.353274000	0.075589000
H	-5.309398000	0.060762000	0.738110000
C	-4.145753000	0.597836000	-3.829672000
H	-3.698817000	-0.266537000	-4.335269000
H	-5.153981000	0.318493000	-3.501769000
H	-4.251784000	1.403021000	-4.568579000
C	-3.987322000	2.712191000	-1.683138000
H	-4.955709000	2.396714000	-1.274709000
H	-3.438832000	3.198643000	-0.869496000
H	-4.178117000	3.458654000	-2.465464000
C	-1.489715000	1.870325000	-3.277173000
H	-0.688440000	2.135012000	-2.578995000
H	-1.100856000	1.118540000	-3.974864000
H	-1.739092000	2.770000000	-3.856546000
O	1.847790000	0.746874000	-1.350914000
C	3.062858000	0.396436000	-2.045153000
O	2.446319000	3.114526000	-1.226531000
C	1.623650000	4.297586000	-1.032207000
C	0.446217000	3.773361000	-0.140754000
O	0.390279000	2.361543000	-0.517023000
C	1.182297000	4.748160000	-2.415220000
H	2.073159000	4.920144000	-3.028116000
H	0.567283000	3.990914000	-2.916280000
C	2.466704000	5.368975000	-0.376533000
H	1.854245000	6.249526000	-0.146528000
H	2.931852000	5.014254000	0.546907000
H	3.262472000	5.680063000	-1.061243000
C	0.733240000	3.804986000	1.346172000
H	-0.028309000	3.200295000	1.857269000
H	1.714210000	3.373125000	1.580537000
H	0.699273000	4.826811000	1.740755000
B	1.622869000	2.052467000	-1.055746000
H	-1.653243000	3.961163000	0.225957000
C	-0.895324000	4.404563000	-0.430759000
H	-1.214167000	4.252287000	-1.466316000

H	-0.859526000	5.481745000	-0.225916000
H	0.611980000	5.682360000	-2.368869000
H	3.299816000	1.210835000	-2.743472000
C	5.556306000	0.447621000	-1.762046000
C	4.216842000	0.149396000	-1.089903000
C	4.216874000	-1.273778000	-0.537597000
C	5.352592000	-1.481234000	0.454450000
C	6.696277000	-1.176210000	-0.199763000
C	6.715143000	0.228284000	-0.794801000
H	5.562408000	1.479674000	-2.142052000
H	5.673751000	-0.214064000	-2.637787000
H	4.102610000	0.857901000	-0.248745000
H	3.240721000	-1.529176000	-0.099994000
H	4.355750000	-1.968258000	-1.385035000
H	5.334369000	-2.506279000	0.846571000
H	5.204755000	-0.814561000	1.320560000
H	7.515168000	-1.295034000	0.521115000
H	6.877343000	-1.909961000	-1.001855000
H	7.671415000	0.422454000	-1.297007000
H	6.636443000	0.965133000	0.021012000
H	2.831146000	-0.503212000	-2.631975000

Aldehyde borylated product

O	1.931089000	-1.266580000	-0.346787000
C	3.222773000	-0.635246000	-0.317077000
B	1.011212000	-0.254496000	-0.237075000
C	2.932976000	0.686103000	0.461232000
O	1.565715000	0.959696000	0.099975000
C	3.635415000	-0.391924000	-1.762071000
H	3.602111000	-1.344796000	-2.300697000
H	2.949312000	0.302485000	-2.260827000
H	4.652517000	0.010798000	-1.833539000
C	4.211239000	-1.565202000	0.354700000
H	5.185587000	-1.074316000	0.474459000
H	3.857440000	-1.889924000	1.337104000
H	4.355003000	-2.458092000	-0.263407000
C	3.795106000	1.864857000	0.061443000
H	3.664226000	2.122573000	-0.993192000
H	3.522844000	2.741382000	0.659652000
H	4.855587000	1.647279000	0.241960000
C	2.965744000	0.503165000	1.971815000
H	2.538717000	1.394796000	2.443283000
H	2.369527000	-0.363287000	2.280510000
H	3.988592000	0.372886000	2.343846000
O	-0.307933000	-0.453494000	-0.445898000
C	-1.211514000	0.623447000	-0.265859000

C	-2.989192000	-0.939116000	0.586617000
C	-4.429706000	-1.409813000	0.427212000
C	-5.402866000	-0.238728000	0.506321000
C	-5.053974000	0.830405000	-0.523401000
C	-3.611429000	1.297080000	-0.364881000
C	-2.630423000	0.129859000	-0.442716000
H	-2.287445000	-1.778060000	0.508466000
H	-2.855829000	-0.507295000	1.594736000
H	-4.671820000	-2.165046000	1.186081000
H	-4.540580000	-1.905297000	-0.551045000
H	-6.436084000	-0.582952000	0.367961000
H	-5.352542000	0.203469000	1.514879000
H	-5.741866000	1.682275000	-0.445545000
H	-5.186673000	0.413098000	-1.534731000
H	-3.363515000	2.053215000	-1.123873000
H	-3.495513000	1.790413000	0.616222000
H	-2.703632000	-0.322251000	-1.448092000
H	-1.088355000	1.057833000	0.741251000
H	-0.989536000	1.425009000	-0.988414000

TS7 between E and I (aldehyde off cycle)

La	-0.478710000	-0.008727000	-0.172959000
N	1.781396000	0.289354000	0.995422000
N	-1.957030000	-1.893575000	-0.139369000
N	-1.729413000	1.989292000	-0.304997000
Si	-1.347559000	3.265844000	-1.434929000
Si	-2.675175000	-2.920842000	1.091351000
Si	2.085971000	-1.153316000	1.969167000
Si	2.097670000	1.876114000	1.717907000
Si	-3.188522000	2.030741000	0.664487000
Si	-2.285333000	-2.270944000	-1.820214000
C	2.567278000	3.179028000	0.418497000
H	2.639727000	4.150114000	0.926205000
H	3.540121000	2.981245000	-0.047522000
H	1.819569000	3.292905000	-0.376449000
C	0.551709000	2.553122000	2.589381000
H	0.240305000	1.908865000	3.421648000
H	0.759243000	3.550449000	2.999428000
H	-0.289628000	2.655092000	1.887624000
C	3.504855000	1.914587000	2.992922000
H	3.330191000	1.252886000	3.849059000
H	4.474420000	1.653400000	2.552097000
H	3.586346000	2.937704000	3.381930000
C	3.885328000	-1.581370000	2.390313000
H	4.412870000	-0.760153000	2.887525000
H	3.874979000	-2.434227000	3.081659000

H	4.467473000	-1.881041000	1.511694000
C	1.185221000	-1.021508000	3.638245000
H	1.669931000	-0.287383000	4.293766000
H	0.137116000	-0.715843000	3.519749000
H	1.187443000	-1.986602000	4.160789000
C	1.426536000	-2.681851000	1.038858000
H	1.565784000	-3.559690000	1.684440000
H	0.361719000	-2.671310000	0.761762000
H	1.993361000	-2.861374000	0.116553000
C	-1.773171000	-0.751740000	-2.882815000
H	-2.232496000	0.195651000	-2.557638000
H	-0.688702000	-0.618245000	-3.017855000
H	-2.158666000	-0.940247000	-3.892636000
C	-1.243090000	-3.702169000	-2.494510000
H	-0.179842000	-3.520436000	-2.288753000
H	-1.513276000	-4.660290000	-2.037318000
H	-1.366117000	-3.796264000	-3.580890000
C	-4.104854000	-2.587795000	-2.239435000
H	-4.213818000	-2.727757000	-3.322354000
H	-4.495171000	-3.487433000	-1.749570000
H	-4.734212000	-1.740383000	-1.941683000
C	-2.499105000	-4.768519000	0.687454000
H	-1.444045000	-5.031590000	0.537274000
H	-2.882159000	-5.370642000	1.520973000
H	-3.051847000	-5.063114000	-0.212856000
C	-4.520524000	-2.561915000	1.354821000
H	-5.102591000	-2.726958000	0.441055000
H	-4.925727000	-3.217871000	2.135857000
H	-4.684624000	-1.523801000	1.669427000
C	-1.841961000	-2.701268000	2.781914000
H	-2.356174000	-3.349374000	3.503481000
H	-0.787673000	-3.001252000	2.767228000
H	-1.905722000	-1.678542000	3.173101000
C	-2.886488000	0.899542000	2.166402000
H	-2.046596000	1.247296000	2.783158000
H	-3.774455000	0.867868000	2.810344000
H	-2.709239000	-0.140529000	1.858217000
C	-4.681033000	1.321448000	-0.260022000
H	-4.451125000	0.297844000	-0.587426000
H	-5.569696000	1.277722000	0.381921000
H	-4.928918000	1.914599000	-1.148103000
C	-3.610077000	3.747958000	1.341813000
H	-3.860845000	4.463076000	0.549389000
H	-4.474736000	3.682742000	2.013771000
H	-2.767481000	4.155873000	1.913748000
C	-2.799567000	3.714290000	-2.570241000

H	-3.148179000	2.832822000	-3.122871000
H	-3.652426000	4.119192000	-2.011917000
H	-2.493688000	4.472421000	-3.302037000
C	-0.762544000	4.862413000	-0.594621000
H	-1.590873000	5.364379000	-0.081197000
H	0.017201000	4.662791000	0.150643000
H	-0.353846000	5.562292000	-1.334412000
C	0.039028000	2.659979000	-2.592703000
H	0.919408000	2.254945000	-2.075658000
H	-0.324157000	1.889955000	-3.285959000
H	0.397513000	3.500341000	-3.200465000
O	1.426522000	-0.424347000	-1.693195000
C	2.444524000	0.102241000	-1.177974000
H	2.526215000	1.204994000	-1.148973000
C	5.497169000	-1.633653000	-2.657485000
C	4.148790000	-0.927359000	-2.591304000
C	3.756839000	-0.622500000	-1.132866000
C	4.853071000	0.185620000	-0.448153000
C	6.204038000	-0.514885000	-0.525965000
C	6.586369000	-0.819857000	-1.969353000
H	5.762896000	-1.832276000	-3.703442000
H	5.411789000	-2.615442000	-2.164429000
H	3.360106000	-1.525623000	-3.061969000
H	4.204439000	0.022606000	-3.150138000
H	3.612764000	-1.587683000	-0.620897000
H	4.574372000	0.385977000	0.594243000
H	4.927086000	1.165144000	-0.952333000
H	6.974155000	0.097718000	-0.040860000
H	6.157066000	-1.458757000	0.042207000
H	7.546593000	-1.349231000	-2.010276000
H	6.727411000	0.127792000	-2.514033000

Intermediate I (aldehyde off cycle)

La	-0.601483000	-0.011455000	0.096536000
N	2.101839000	0.210088000	0.880427000
N	-2.000991000	-1.915164000	-0.197761000
N	-1.728622000	2.039954000	-0.290093000
Si	-1.241231000	3.305360000	-1.398477000
Si	-2.707043000	-2.975854000	0.995358000
Si	2.280998000	-1.315245000	1.828744000
Si	2.308780000	1.791780000	1.726208000
Si	-3.224208000	2.157762000	0.606717000
Si	-2.188938000	-2.248104000	-1.909444000
C	2.733728000	3.183712000	0.526247000
H	2.757026000	4.118275000	1.102950000
H	3.716996000	3.052705000	0.061564000

H	1.990305000	3.311371000	-0.269758000
C	0.664223000	2.277611000	2.542799000
H	0.308132000	1.545107000	3.277854000
H	0.800943000	3.226138000	3.078653000
H	-0.126920000	2.464317000	1.796762000
C	3.665430000	1.768780000	3.042527000
H	3.500818000	1.040194000	3.843086000
H	4.646308000	1.569653000	2.594823000
H	3.711347000	2.761564000	3.507542000
C	4.040032000	-1.803030000	2.312222000
H	4.560421000	-1.008832000	2.858277000
H	3.981654000	-2.677582000	2.973076000
H	4.651653000	-2.081150000	1.447597000
C	1.317744000	-1.081784000	3.448166000
H	1.748503000	-0.313173000	4.099195000
H	0.254683000	-0.842837000	3.307973000
H	1.344954000	-2.030271000	4.000110000
C	1.504360000	-2.793936000	0.931454000
H	1.573099000	-3.657151000	1.608464000
H	0.443459000	-2.691865000	0.657953000
H	2.039807000	-3.043425000	0.009819000
C	-1.737596000	-0.655209000	-2.863235000
H	-2.299725000	0.228436000	-2.523359000
H	-0.660603000	-0.428341000	-2.856675000
H	-2.000549000	-0.808404000	-3.917596000
C	-0.994216000	-3.580290000	-2.530736000
H	0.037010000	-3.283004000	-2.298819000
H	-1.181670000	-4.552550000	-2.060995000
H	-1.073844000	-3.705771000	-3.617776000
C	-3.954275000	-2.712460000	-2.417281000
H	-4.013199000	-2.823359000	-3.507226000
H	-4.280565000	-3.659656000	-1.971155000
H	-4.665647000	-1.933897000	-2.116735000
C	-2.406277000	-4.814929000	0.635890000
H	-1.332398000	-5.020117000	0.539509000
H	-2.797203000	-5.430680000	1.455722000
H	-2.895404000	-5.146249000	-0.288097000
C	-4.576229000	-2.725886000	1.206304000
H	-5.117508000	-2.969667000	0.284980000
H	-4.963877000	-3.370684000	2.005243000
H	-4.815852000	-1.686883000	1.465222000
C	-1.915045000	-2.660735000	2.699154000
H	-2.420344000	-3.282982000	3.448701000
H	-0.854017000	-2.941639000	2.709885000
H	-2.009404000	-1.621588000	3.043860000
C	-3.104723000	0.933245000	2.071398000

H	-2.239239000	1.124877000	2.724713000
H	-3.996713000	1.029267000	2.702855000
H	-3.093341000	-0.113292000	1.734530000
C	-4.736644000	1.605929000	-0.387511000
H	-4.583540000	0.575056000	-0.735515000
H	-5.647769000	1.624860000	0.223390000
H	-4.900460000	2.238605000	-1.267367000
C	-3.534893000	3.863154000	1.370366000
H	-3.701936000	4.637578000	0.612653000
H	-4.421875000	3.833071000	2.015247000
H	-2.678292000	4.170388000	1.983748000
C	-2.652240000	3.868227000	-2.536263000
H	-3.042196000	3.021283000	-3.114729000
H	-3.487796000	4.309723000	-1.979032000
H	-2.292395000	4.623479000	-3.246058000
C	-0.610148000	4.848785000	-0.484185000
H	-1.430767000	5.375925000	0.016527000
H	0.130983000	4.589040000	0.282530000
H	-0.138857000	5.550180000	-1.184350000
C	0.140618000	2.682869000	-2.539856000
H	0.949849000	2.149029000	-2.025119000
H	-0.262428000	1.991928000	-3.291065000
H	0.586958000	3.531678000	-3.073541000
O	1.217709000	-0.308665000	-1.253209000
C	2.338731000	0.165868000	-0.631825000
H	2.528776000	1.220942000	-0.925151000
C	4.949299000	-1.409056000	-3.013475000
C	3.676508000	-0.706800000	-2.556123000
C	3.610158000	-0.585893000	-1.034212000
C	4.866685000	0.106702000	-0.510457000
C	6.139682000	-0.603023000	-0.957594000
C	6.196067000	-0.716379000	-2.476490000
H	4.980020000	-1.463498000	-4.109316000
H	4.934670000	-2.450752000	-2.652239000
H	2.782590000	-1.227807000	-2.916072000
H	3.636953000	0.309684000	-2.987489000
H	3.571808000	-1.612317000	-0.625474000
H	4.837538000	0.189077000	0.585544000
H	4.879207000	1.139210000	-0.903051000
H	7.024206000	-0.078130000	-0.573715000
H	6.165376000	-1.615441000	-0.520061000
H	7.102931000	-1.249538000	-2.790203000
H	6.261695000	0.295383000	-2.908897000

HTMS

Si	0.000062000	-0.000062000	0.400181000

C	-1.330875000	-1.191580000	-0.231258000
H	-1.342593000	-1.201649000	-1.327224000
H	-1.147460000	-2.215873000	0.109856000
H	-2.328615000	-0.896597000	0.110347000
C	-0.366622000	1.748306000	-0.231257000
H	0.387758000	2.464979000	0.110064000
H	-0.369922000	1.763464000	-1.327231000
H	-1.345311000	2.101515000	0.110231000
C	1.697416000	-0.556652000	-0.231363000
H	2.492591000	0.114616000	0.109640000
H	1.941143000	-1.568085000	0.110387000
H	1.711901000	-0.561902000	-1.327327000
H	0.000120000	-0.000042000	1.881986000

Complex 2 formed with benzaldehyde – dimer - (for comparison with XRD)

La	-2.070743000	0.385814000	-0.270743000
Si	-2.092222000	4.347115000	-0.117404000
Si	-3.157597000	0.913335000	3.015400000
Si	-5.450668000	0.132800000	1.184954000
Si	-3.189741000	-2.125919000	-2.566504000
Si	-2.672032000	0.564829000	-3.838986000
O	0.436550000	1.293609000	-0.537046000
N	-1.138499000	2.841815000	-0.193505000
N	-3.744078000	0.467999000	1.428905000
N	-2.729050000	-0.440045000	-2.406297000
C	0.080741000	2.551956000	-0.537221000
C	1.122033000	3.509788000	-0.995920000
C	1.964416000	3.138531000	-2.049107000
H	1.843191000	2.159918000	-2.512982000
C	2.951723000	4.006414000	-2.497793000
H	3.597790000	3.709548000	-3.321758000
C	3.125904000	5.241394000	-1.878317000
H	3.906750000	5.916255000	-2.220424000
C	2.308146000	5.606163000	-0.812275000
H	2.456119000	6.560654000	-0.312763000
C	1.305982000	4.746502000	-0.376482000
H	0.687491000	5.018546000	0.477007000
C	-1.740608000	5.589570000	-1.495932000
H	-0.807768000	6.141428000	-1.345955000
H	-2.563268000	6.313474000	-1.541182000
H	-1.680654000	5.090152000	-2.470258000
C	-1.864408000	5.128629000	1.588371000
H	-1.736959000	4.352284000	2.353358000
H	-2.744092000	5.724236000	1.860172000
H	-0.990769000	5.789063000	1.633058000
C	-3.864496000	3.722605000	-0.307933000

H	-4.042703000	3.335567000	-1.322193000
H	-4.591325000	4.526192000	-0.138579000
H	-4.079882000	2.918039000	0.411346000
C	-1.257390000	1.053059000	2.936895000
H	-0.748328000	0.100128000	2.728108000
H	-0.893440000	1.401259000	3.912441000
H	-0.912298000	1.799783000	2.205599000
C	-3.785453000	2.597241000	3.631811000
H	-3.772691000	3.345900000	2.829800000
H	-3.151309000	2.965714000	4.448718000
H	-4.813065000	2.534183000	4.006908000
C	-3.563761000	-0.347973000	4.375178000
H	-4.642357000	-0.393055000	4.570744000
H	-3.067869000	-0.069558000	5.313679000
H	-3.231852000	-1.358158000	4.104061000
C	-6.605916000	1.343798000	2.086242000
H	-6.557191000	1.236159000	3.176706000
H	-7.641507000	1.142012000	1.783018000
H	-6.380578000	2.387677000	1.836053000
C	-5.953717000	-1.590461000	1.808431000
H	-5.274823000	-2.374800000	1.455569000
H	-6.970120000	-1.841843000	1.478738000
H	-5.946880000	-1.609969000	2.905917000
C	-5.873834000	0.333175000	-0.659320000
H	-6.001599000	1.399665000	-0.890827000
H	-6.825422000	-0.165442000	-0.886642000
H	-5.118402000	-0.066135000	-1.350132000
C	-3.961939000	-2.725859000	-0.940994000
H	-3.423208000	-2.423818000	-0.031258000
H	-3.993106000	-3.823007000	-0.922982000
H	-4.991336000	-2.358304000	-0.852835000
C	-4.522178000	-2.455222000	-3.876510000
H	-5.429739000	-1.882258000	-3.647110000
H	-4.787793000	-3.519989000	-3.861809000
H	-4.210326000	-2.205022000	-4.896736000
C	-1.701561000	-3.249816000	-2.930774000
H	-1.222853000	-2.997236000	-3.884467000
H	-2.010822000	-4.303086000	-2.969207000
H	-0.941990000	-3.148977000	-2.142080000
C	-1.834557000	-0.245917000	-5.335759000
H	-1.844299000	0.447798000	-6.186004000
H	-2.330946000	-1.169157000	-5.656065000
H	-0.788357000	-0.485022000	-5.109298000
C	-1.662727000	2.136349000	-3.478684000
H	-2.097571000	2.751588000	-2.680665000
H	-1.639640000	2.759267000	-4.382084000

H	-0.621591000	1.911874000	-3.209297000
C	-4.391143000	1.166524000	-4.367928000
H	-4.889369000	1.680446000	-3.535545000
H	-5.037058000	0.336674000	-4.676443000
H	-4.317852000	1.869172000	-5.207641000
La	2.070632000	-0.385752000	0.270583000
Si	2.091708000	-4.347080000	0.117498000
Si	3.158210000	-0.912907000	-3.015162000
Si	5.451261000	-0.134156000	-1.184102000
Si	3.190387000	2.125447000	2.565733000
Si	2.671582000	-0.564809000	3.839097000
O	-0.436555000	-1.293161000	0.536986000
N	1.138181000	-2.841675000	0.193478000
N	3.744654000	-0.468846000	-1.428353000
N	2.729121000	0.439687000	2.406145000
C	-0.081058000	-2.551606000	0.537097000
C	-1.122565000	-3.509212000	0.995767000
C	-1.965265000	-3.137535000	2.048564000
H	-1.844218000	-2.158729000	2.512061000
C	-2.952701000	-4.005235000	2.497302000
H	-3.599039000	-3.708095000	3.320936000
C	-3.126697000	-5.240460000	1.878265000
H	-3.907626000	-5.915200000	2.220426000
C	-2.308670000	-5.605635000	0.812567000
H	-2.456551000	-6.560291000	0.313343000
C	-1.306389000	-4.746147000	0.376722000
H	-0.687737000	-5.018487000	-0.476537000
C	1.739921000	-5.589533000	1.495996000
H	0.807231000	-6.141584000	1.345816000
H	2.562721000	-6.313266000	1.541506000
H	1.679641000	-5.090077000	2.470287000
C	1.864205000	-5.128627000	-1.588321000
H	1.738006000	-4.352263000	-2.353484000
H	2.743567000	-5.725066000	-1.859356000
H	0.990044000	-5.788318000	-1.633585000
C	3.864032000	-3.722765000	0.308182000
H	4.041952000	-3.335239000	1.322326000
H	4.590834000	-4.526505000	0.139486000
H	4.079616000	-2.918498000	-0.411343000
C	1.257846000	-1.051286000	-2.937244000
H	0.749591000	-0.098142000	-2.727458000
H	0.893910000	-1.397938000	-3.913345000
H	0.911917000	-1.798592000	-2.206925000
C	3.785125000	-2.596822000	-3.632468000
H	3.772711000	-3.345658000	-2.830614000
H	3.150334000	-2.964927000	-4.449030000

H	4.812514000	-2.533954000	-4.008234000
C	3.565683000	0.349422000	-4.373654000
H	4.644229000	0.392601000	-4.569974000
H	3.068463000	0.073689000	-5.312224000
H	3.236286000	1.359873000	-4.100416000
C	6.606182000	-1.345655000	-2.085072000
H	6.557039000	-1.238544000	-3.175573000
H	7.641911000	-1.143811000	-1.782366000
H	6.380856000	-2.389391000	-1.834293000
C	5.954448000	1.589070000	-1.807772000
H	5.271696000	2.372291000	-1.459840000
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H	5.953407000	1.606787000	-2.905308000
C	5.873948000	-0.334359000	0.660326000
H	6.001937000	-1.400800000	0.891896000
H	6.825332000	0.164529000	0.887915000
H	5.118182000	0.064786000	1.350865000
C	3.961777000	2.724545000	0.939474000
H	3.422444000	2.422229000	0.030176000
H	3.993176000	3.821679000	0.920863000
H	4.991043000	2.356736000	0.850807000
C	4.523529000	2.454547000	3.875050000
H	5.430395000	1.880350000	3.645995000
H	4.790305000	3.519006000	3.859413000
H	4.211531000	2.205523000	4.895535000
C	1.702865000	3.250000000	2.930584000
H	1.224740000	2.998015000	3.884733000
H	2.012591000	4.303153000	2.968401000
H	0.942716000	3.149095000	2.142460000
C	1.834330000	0.246760000	5.335519000
H	1.843706000	-0.446652000	6.186003000
H	2.331093000	1.169920000	5.655494000
H	0.788249000	0.486209000	5.108857000
C	1.661789000	-2.135985000	3.478640000
H	2.096781000	-2.751227000	2.680689000
H	1.638209000	-2.759023000	4.381940000
H	0.620841000	-1.911167000	3.208808000
C	4.390441000	-1.166878000	4.368313000
H	4.888013000	-1.682402000	3.536528000
H	5.036956000	-0.336917000	4.675289000
H	4.317104000	-1.868199000	5.209121000

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