Supporting Information

$La[N(SiMe_3)_2]_3$ – Catalyzed Deoxygenative Reduction of Amides with Pinacolborane. Scope and Mechanism.

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Materials and Methods. All manipulations of air-sensitive materials were carried out with rigorous exclusion of oxygen and moisture in flame- or oven-dried Schlenk-type glassware on a dual-manifold Schlenk line or in an argon-filled glovebox with a high capacity recirculator (<1 ppm O_2). Benzene-d_6 (Cambridge Isotope Laboratories; 99+ atom % D) was stored over Na/K alloy and vacuum transferred prior to use. $La[N(SiMe_3)_2]_3$ (La^{NTMS})* and hexamethylbenzene were purchased from Sigma-Aldrich Co. and sublimed under high-vacuum (10^{-6} Torr). Pinacolborane ("HBpin") was purchased from Sigma-Aldrich Co. and distilled under high-vacuum (10^{-6} Torr) to remove trace boronic acid impurities. Amide substrates were purchased from Sigma-Aldrich Co. and used as received or prepared according to established procedures. The products of amide deoxygenation were isolated as the amine hydrochlorides and then characterized by ^{1}H NMR and ^{13}C NMR, unless otherwise noted.

*The La^{NTMS} precatalyst can also be used as received without further purification.

Physical and Analytical Measurements. NMR spectra were recorded on a Bruker Avance III (500 MHz, ^{1}H; 125 MHz, ^{13}C; 125 MHz, ^{29}Si), Varian Inova 500 (500 MHz, ^{1}H; 125 MHz, ^{13}C), Agilent DD MR-400 (400 MHz, ^{1}H; 100 MHz, ^{13}C; 128 MHz, ^{11}B;), or Agilent DD2 500 (500 MHz, ^{1}H; 125 MHz, ^{13}C). Chemical shifts (δ) for ^{1}H are referenced to residual solvent resonances (δ 7.16 for benzene-d_6; 4.79 ppm for D_2O). ^{13}C shifts are referenced to residual solvent resonances (δ 128.06 ppm for benzene-d_6) or external $SiMe_4$ standard. ^{11}B shifts are referenced to an external $BF_3{\cdot}OEt_2$ standard. ^{29}Si shifts are referenced to an external $SiMe_4$ standard. NMR scale reactions were carried out either in Teflon-sealed J. Young tubes or rubber septum-sealed tubes (*vide infra*).

Typical NMR-scale reaction involving solid amides. In a glovebox, the amide (0.25 mmol), internal standard hexamethylbenzene (50 μmol), and HBpin (1.25 mmol) were dissolved in benzene-d_6 (total volume 1.0 mL). This solution as injected into a vial containing La^{NTMS} (12.5 μmol), shaken to dissolve the catalyst. The reaction mixture was transferred to a J. Young capped NMR tube, and the reaction was monitored by ^{1}H-NMR spectroscopy.

Typical NMR-scale reaction involving liquid amides. In a glovebox, La^{NTMS} (12.5 μmol) was placed in a septum-sealed NMR tube, and the cap was wrapped in film. Internal standard (50 μmol), HBpin (1.25 mmol) and benzene-d_6 were added to a septum-sealed vial. Outside the glovebox (to prevent amine poisoning of the glovebox circulation catalyst), the liquid amide (0.25 mmol) was injected into the vial with HBpin and internal standard, the vial was shaken, and the contents were injected into the NMR tube containing the catalyst, all under N_2. The tube was shaken to dissolve the catalyst, and the reaction was monitored by ^{1}H NMR spectroscopy.

Scale-Up/ Isolation of Amine Hydrochlorides. In a glovebox, La^{NTMS} (0.125mmol) was weighed into a 25 mL round bottom and dissolved in 5 mL benzene. HBpin (12.5 mmol) and amide (2.5 mmol) were dissolved in 5 mL benzene, and the solution was injected into the stirred catalyst solution at 25 °C or 60 °C. Low boiling amines (trimethylamine, *N,N*-dimethylethylamine, *N*-methylpyrrolidine, *N*-methylethylamine,) were isolated by evaporation. Nitrogen was bubbled into a solution containing the reaction mixture. A cannula needle was used to bubble the volatile

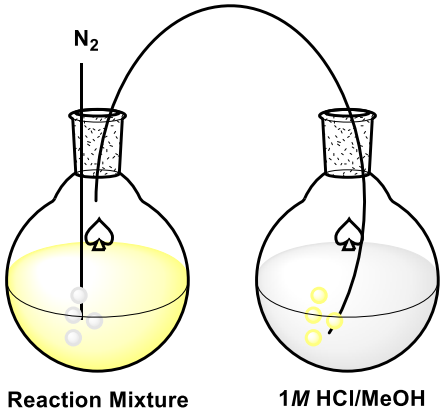


Figure S1. Schematic of reaction apparatus to trap volatile amine products from large-scale amide reductions.

amine product into a 1M HCl/methanol solution cooled to 0 °C (Figure S1). The methanol was then removed by rotary evaporation, and the remaining solid was washed with pentanes. Amines with boiling points similar to HBpin (*N*-methylpiperidine and *N,N*-diisopropylmethylamine) were first isolated by distillation under vacuum. To the distillate, 1M HCl/methanol was added, precipitating a solid that was subsequently collected and washed with pentanes. The remaining high-boiling or solid amines were isolated by first removing HBpin under vacuum, re-dissolving the amine in benzene, and filtering the solution through a basic alumina plug to remove trace HBpin, pinB-O-Bpin, and the catalyst. A 1M HCl/methanol solution was then added, precipitating a solid that was collected and washed with ether or pentanes.

Typical NMR-Scale Reaction for Kinetic Monitoring by ^{1}H NMR Arrays. In a glovebox, amide, HBpin, and the internal standard were mixed in a vial and dissolved in C_6D_6 (V_{total} =1.0 mL). This solution was then added to a rubber septum-sealed NMR tube, wrapped with film, and removed from the box. At the NMR, the magnet was locked, tuned, and shimmed to the sample, then a stock solution containing an appropriate loading of $La[N(SiMe_3)_2]_3$ was injected into the tube. The tube was shaken and reinserted into the instrument and the experiment was started. Single (^{1}H NMR) scans were collected at regular intervals. Substrate and/or product concentrations were determined relative to the intensity of the internal standard resonance and plotted versus time.

Kinetic Analysis. Kinetic analysis of the NMR-scale reactions described above was carried out by collecting multiple (> 15) data points early in the reaction (< 20% conversion). Under these conditions, the reaction can be approximated as pseudo-zero-order with respect to the substrate concentrations. The product concentration was measured from the area of the RC*H*$_2$NR'R" product peaks relative to the C_6Me_6 internal standard. Data were fit by least-squares analysis ($R^2 > 0.98$) according to eq S1, where "t" is time, "[product]" is the concentration of product at time t, and "m" is the rate of reaction.

$$[product] = mt \qquad \text{(S1)}$$

Reaction orders for HBpin and *N,N*-dimethylbenzamide were determined by running reaction under pseudo-first-order conditions (10-fold excess of non-measured reactant). The order of the reactant not in excess was determined from the linearity of plots of [A] vs. time (zeroth-order), ln[A] vs. time (first-order), and $[A]^{-1}$ vs. time (second-order).[1] As discussed in the paper, the order in HBpin for amide reduction was not amenable to determination under pseudo-first-order conditions (Figure S3) and instead had to be determined by initial rates analysis (Figure S4).

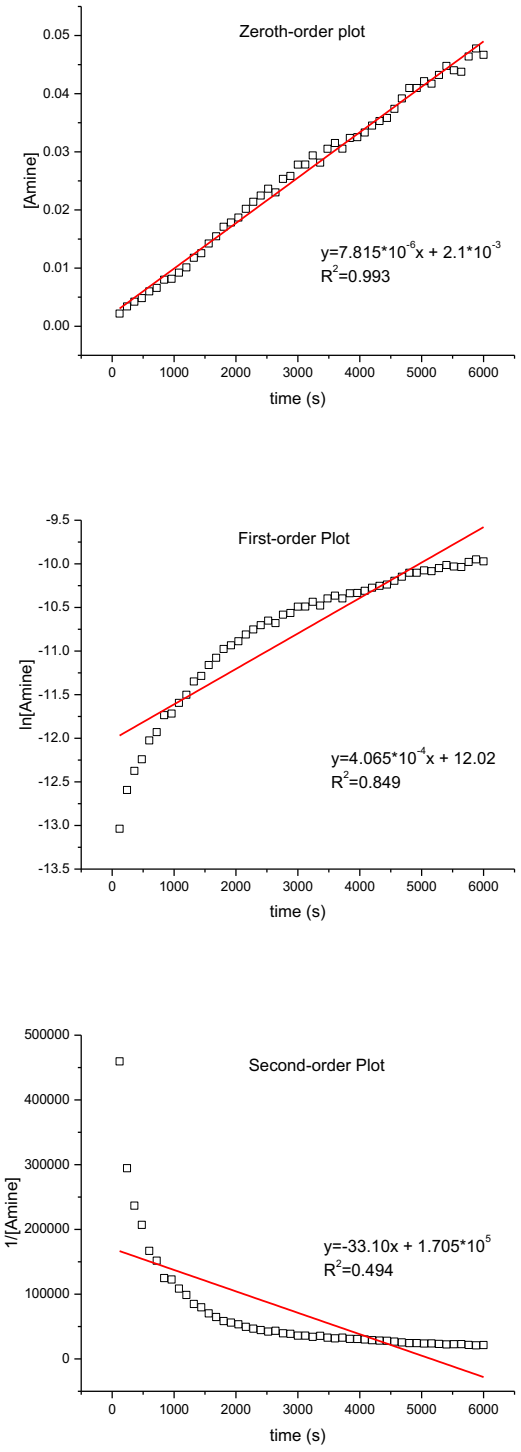


Figure S2. Pseudo-first-order plots for reaction order in *N,N*-dimethylbenzamide (HBpin in 10-fold excess). The zeroth-order plot ([Amine] vs. time) is linear, while the other two plots are not. Reaction conditions: 6.25 μmol La^{NTMS}, 0.125 mmol *N,N*-dimethylbenzamide, 1.25 mmol HBpin, 0.0330 mmol C_6Me_6, C_6D_6 (total volume 1.00 mL).

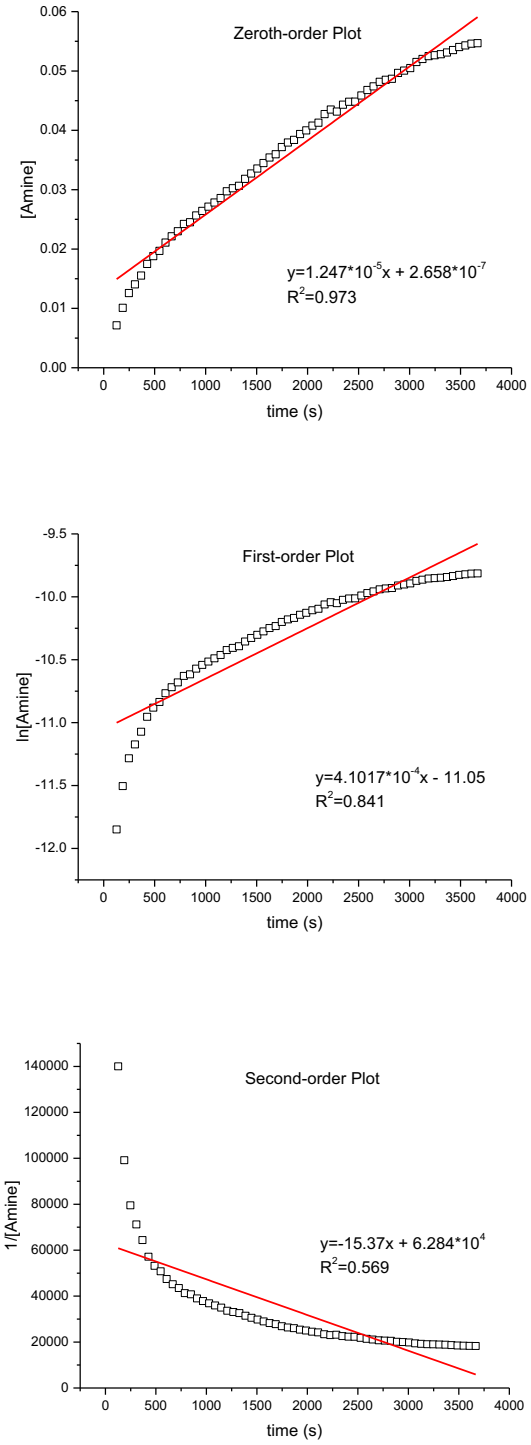


Figure S3. Pseudo-first-order plots for reaction order in HBpin for amide reduction (10-fold excess of amide). None of the plots are linear, indicating HBpin consumption is likely mixed-order for amide reduction. Reaction conditions: 6.25 μmol La^{NTMS}, 1.25 mmol *N,N*-dimethylbenzamide, 0.125 mmol HBpin, 0.0330 mmol C_6Me_6, C_6D_6 (total volume 1.00 mL).

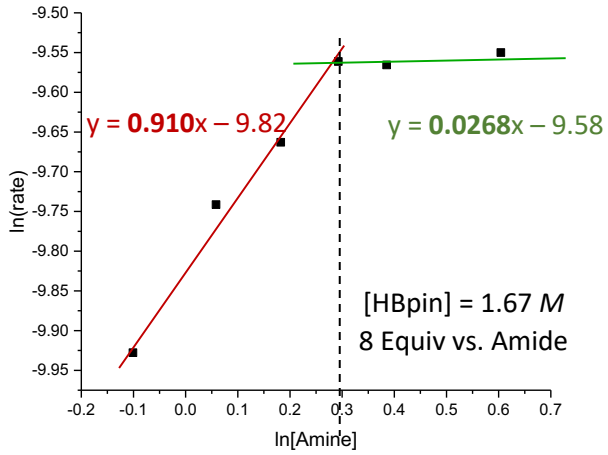


Figure S4. Ln vs. ln plot for the determination of reaction order of HBpin in amide reduction. A mixed-order system is observed, wherein at [HBpin] < 1.67 *M*, the order in HBpin = 1 (slope = 0.910 ≈ 1, *vide infra* for derivation and explanation). At [HBpin] ≥ 1.67 *M*, the order in HBpin = 0 (slope = 0.0268 ≈ 0).

The order for La^{NTMS} was determined from the rates of reduction of *N,N*-dimethylbenzamide at 5 different catalyst loadings (0.5-2.5%). The rates were measured as the slope of the line for [Product] vs. time at conversion < 20%. These rates were then plotted as ln(rate) vs. ln[La^{NTMS}]. The negative rate of disappearance of La^{NTMS} is proportional to the concentration of La^{NTMS} to the order (α) (see eq. S2). Therefore, the order is the slope of a plot of ln(rate) vs. ln[amide] (eq. S3).[2]

$$\frac{-d[LaNTMS]}{dt} = k_{obs}[LaNTMS]^{\alpha} \quad \text{(S2)}$$

$$\ln(rate) = lnk_{obs} + \propto \ln[LaNTMS] \quad \text{(S3)}$$

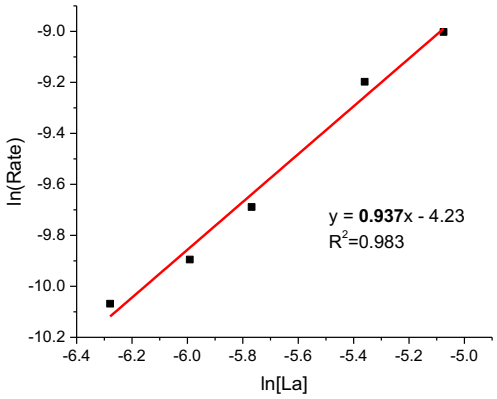


Figure S5. Ln vs. ln plot for the determination of the reaction order of La^{NTMS} for reduction of *N,N*-dimethylbenzamide.

Isotopic Labeling Studies. DBpin was synthesized according to literature procedures.[3] BD_3•SMe_2 (Cambridge Isotope Laboratories, 8.5 mmol, 10 *M*) was diluted in 10 mL DCM in an addition funnel under N_2. This solution was added dropwise over 30 min to a 0 °C solution of pinacol (8.5 mmol, 1.0 g) in 20 mL DCM. After addition was complete, the solution was brought to room temperature and stirred until bubbling was no longer observed (1 h). DBpin was purified by distillation (0 °C at 10 mmHg). **^{1}H NMR (400 MHz, C_6D_6)**: 1.00 (s, 12H, DB*pin*) **^{11}B{^{1}H NMR (128 MHz, C_6D_6)**: 28.37 (t, $^2J_{DB}$=22.8 Hz, D*B*pin).

Rate studies were carried out with HBpin and DBpin under the same ^{1}H NMR kinetic monitoring conditions outlined above using *N,N*-dimethylbenzamide.

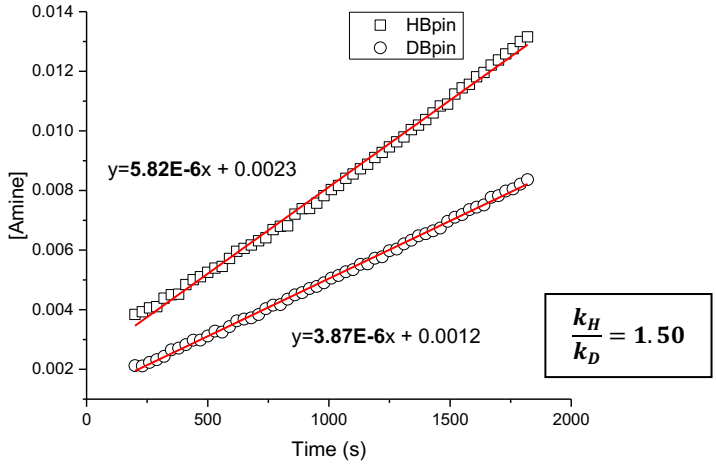


Figure S6. Plots for the determination of the kinetic isotope effect for reduction of *N,N*-dimethylbenzamide using HBpin and DBpin.

Variable-Temperature Kinetic Analysis. Temperature-dependent rate data were obtained *via* arrayed NMR scans as described above. Temperatures were set on the NMR instrument using an external temperature controller and calibrated using ethylene glycol (> 25 °C) or methanol (< 25 °C) standards. Rates at each temperature were determined from the average of three trials.

These data were then plotted as 1000/T vs. ln(k/T) from which the enthalpy and entropy of the transition state could be obtained using the Eyring equation (see eq S4). $\Delta H^{\neq}$ is the negative slope times R and $\Delta S^{\neq}$ is the intercept minus the natural log of k_b/h times R.

$$\ln\frac{k}{T} = \frac{\Delta H^{\neq}}{RT}\left[\frac{\Delta S^{\neq}}{R} - \ln\frac{k_b}{h}\right] \quad \text{(S4)}$$

From a plot of 1000/T vs. ln(k), the activation energy can be obtained using the Arrhenius equation (eq S5). E_a is the negative slope times R.

$$\ln k = -\frac{E_a}{RT} - \ln A \tag{S5}$$

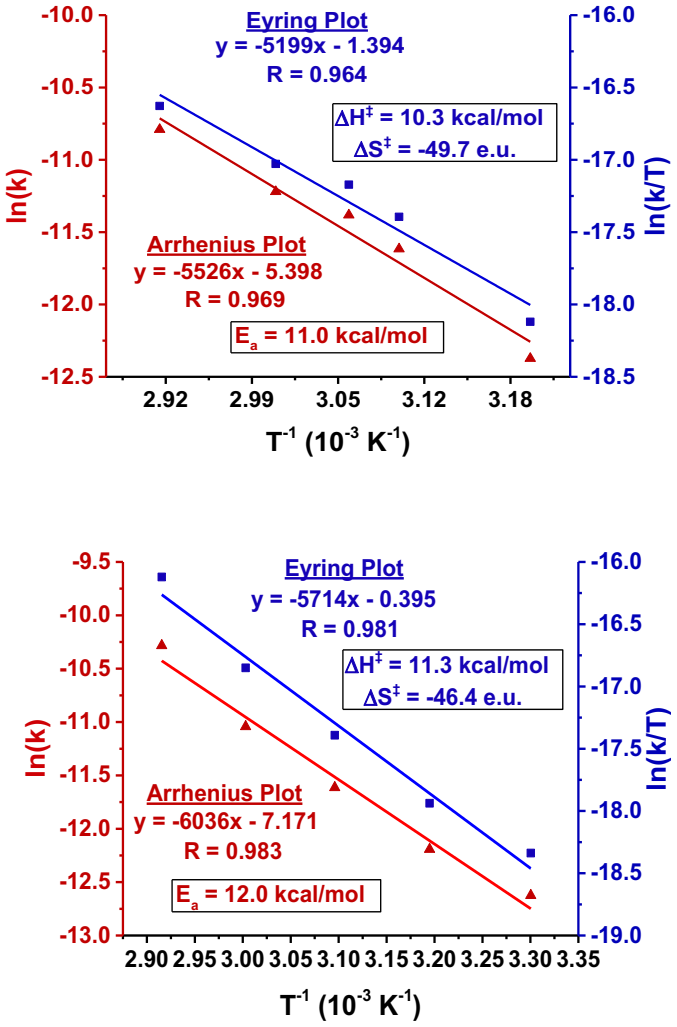


Figure S7. Eyring (blue) and Arrhenius (red) plots for the reduction of *N,N*-dimethylbenzamide at low [HBpin] (5 equiv, top) and high [HBpin] (10 equiv, bottom).

Hammett Analysis. A series of *para*-substituted *N*-benzoyl piperidines was synthesized from the corresponding benzaldehydes and piperidine according to literature procedures (^{1}H and ^{13}C NMR spectra were identical to those previously reported).[4] Rates were determined by ^{1}H NMR spectroscopy (*vide supra*). The rates of reduction for each substrate were plotted according to the Hammett equation (eq S6), so that the slope of the line gives rho (ρ), which indicates the sensitivity of the reaction to the electron density at the carbonyl carbon of the substrate.[5]

$$log\frac{k}{k_H} = \sigma\rho \tag{S6}$$

Competition Studies. To gauge the selectivity of La^{NTMS} for amide hydroboration over olefin/alkyne hydroboration, intermolecular competition experiments were performed using 1-octene and 1-octyne. *N,N*-dimethylbenzamide (0.125 mmol), 1-octene/1-octyne (0.125 mmol), and HBpin (0.625 mmol) were dissolved in C_6D_6 in a J. Young capped NMR tube. La^{NTMS} (6.25 μmol) was added and the tube was shaken. After 2 h at 60 °C, complete conversion of the *N,N*-dimethylbenzamide was observed, with no concomitant reduction of olefin.

Secondary Amide Reduction. To determine the active catalyst for secondary amide reduction, La^{NTMS} (2.08 μmol) and benzanilide (6.25 μmol, 3 equiv) were dissolved in C_6D_6 in a J. Young capped NMR tube. After 15 min at 25 °C, no La^{NTMS} was observed in the ^1H NMR spectrum (ligand methyl signals appear at 0.30 ppm), and only free $HN(SiMe_3)_2$ (0.10 ppm) was present, indicating complete conversion of the precatalyst to a lanthanide tris-amidate species had occurred. Introducing additional benzanilide (0.125 mmol) and HBpin (0.625 mmol) to this in situ generated catalyst results in ~90% conversion of the amide.

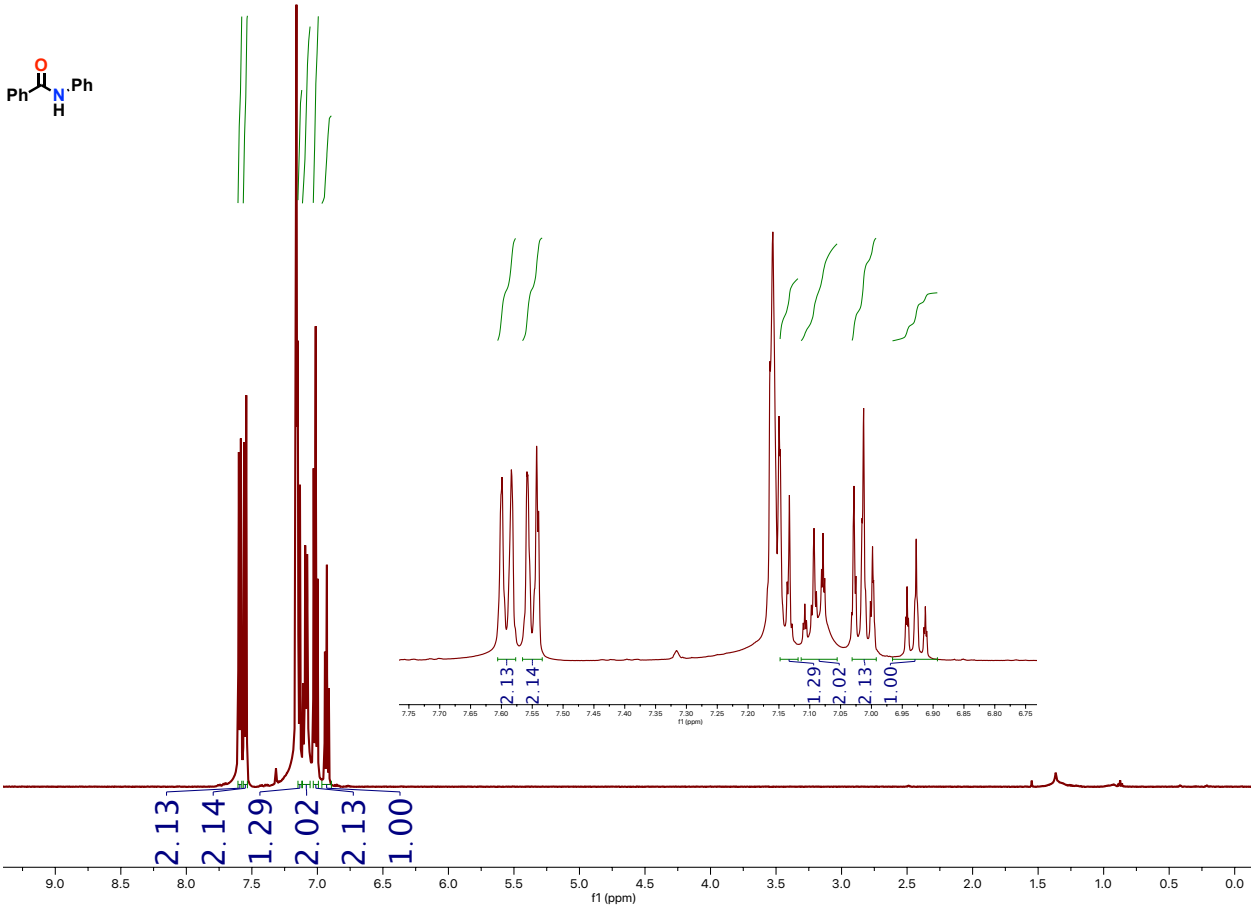


Figure S8. ^1H NMR (500 MHz) spectrum of benzanilide in benzene-d_6.

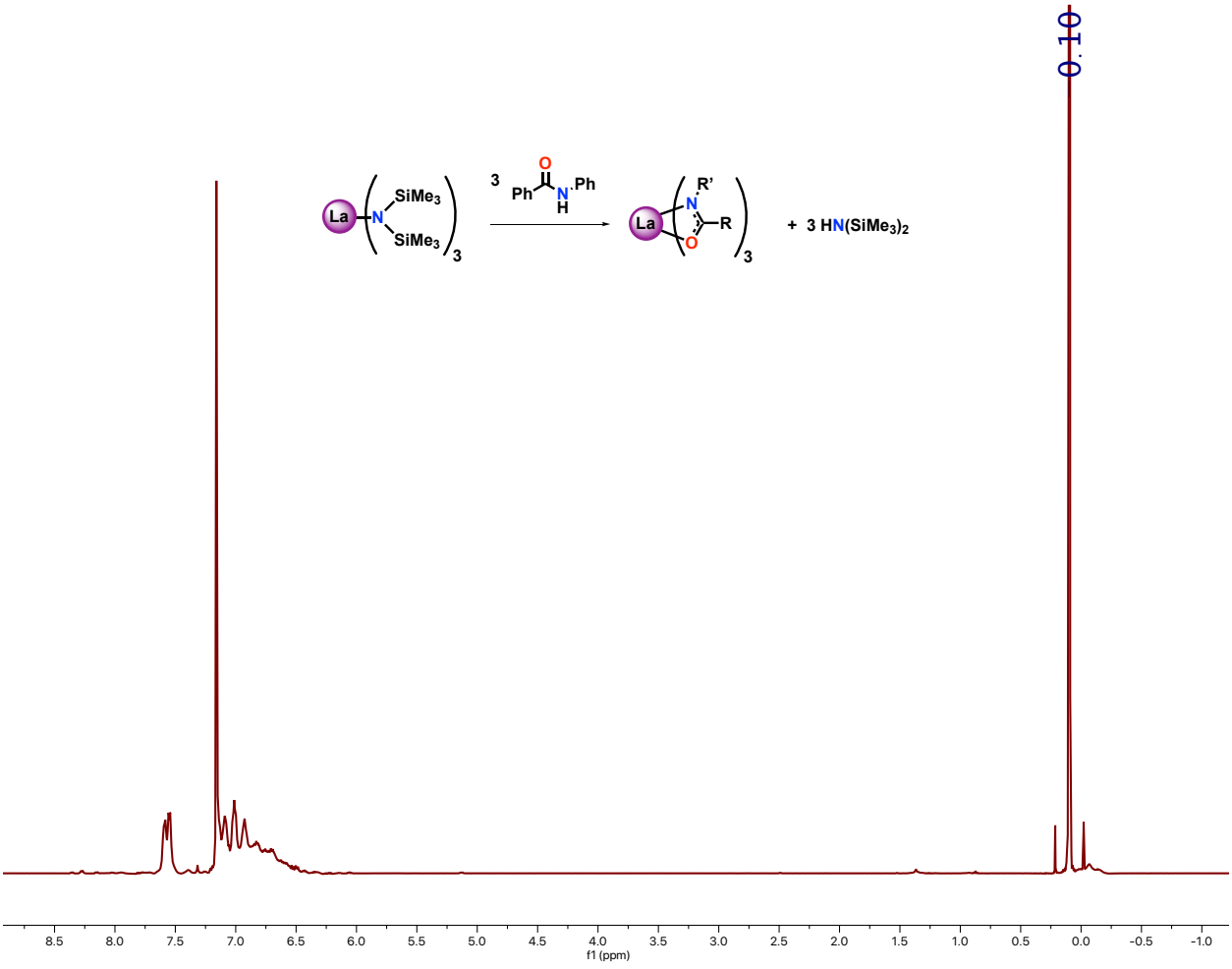


Figure S9. ^{1}H NMR (500 MHz) spectrum of *in situ* formed lanthanum tris-amidate catalyst obtained from benzanilide and La^{NTMS} (3:1 molar ratio) in benzene-d_6.

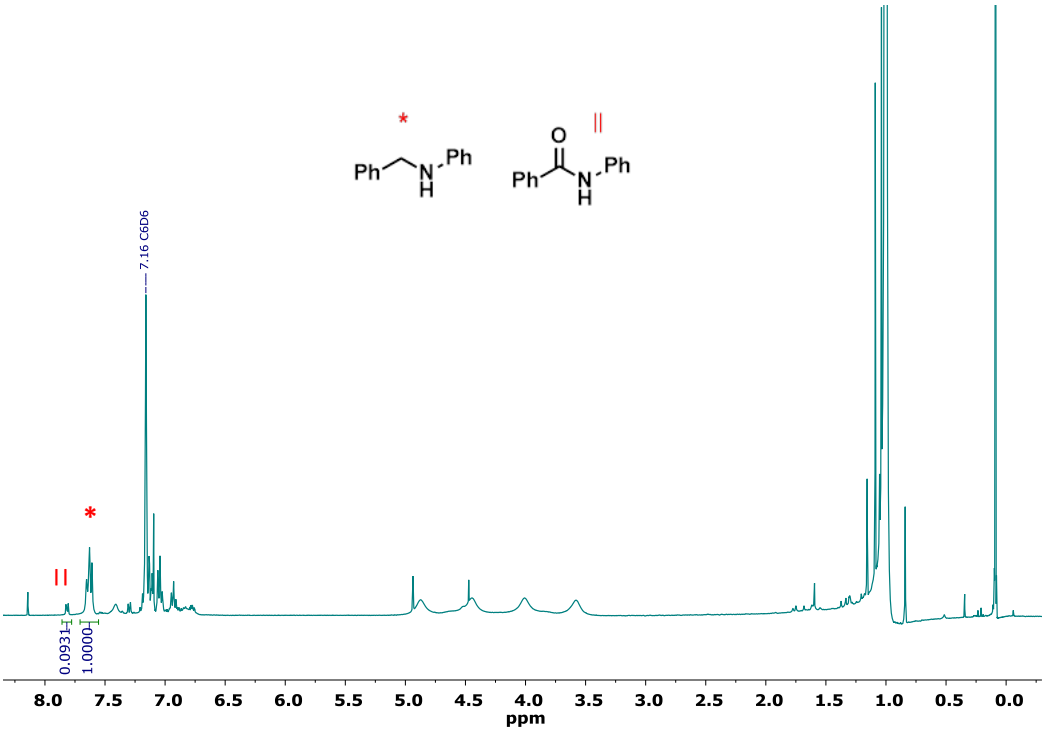


Figure S10. ^{1}H NMR (500 MHz) spectrum of the reduction of benzanilide with HBpin using an *in situ* formed lanthanum tris-amidate catalyst.

Primary Amide Reduction. Reduction does not occur with the two primary amides tested (acetamide and benzamide), and instead an intractable, off-white precipitate is observed. To determine the identity of the precipitate formed during primary amide reduction, first La^{NTMS} (50 μmol) and benzamide (50 μmol, 1 equiv) were dissolved in C_6D_6 in a J. Young capped NMR tube at rt in an inert atmosphere glovebox. A white precipitate was immediately formed and allowed to settle to the bottom of the NMR tube. The solvent was decanted and the J. Young capped NMR tube containing the white precipitate was sealed, removed from the glovebox, and dried on a high vacuum line. After drying, the NMR tube was again sealed and taken into the glovebox where the precipitate was dissolved in THF to give a pale yellow solution. A sealed capillary containing d_6-DMSO was added in to provide a solvent lock. NMR spectroscopic experiments were then performed (Figures S12, S13). After all data were collected, the NMR tube containing the precipitate dissolved in THF was opened under strong flow of argon and 1 drop of D_2O was added in order to confirm ligand identities by hydrolyzing/quenching the metal complex. The tube was gently inverted to obtain a homogeneous solution before additional NMR experiments were performed, again using a d_6-DMSO solvent lock (Figures S14 and S15). The spectroscopic experiments support the identity of the precipitate to be the unsymmetrical La-hemiaminalate complex $[(Me_3Si)_2N]_2La\{\eta^2\text{-}OC(NH)Ph\}$ which is not catalytically active under the reaction conditions described. Based on the low solubility of this complex, it is plausible that it may exist as an oligomeric species, having bridging hemiaminalate ligands. There is no spectroscopic evidence of a ligand insertion reaction between the La^{NTMS} precatalyst and the primary amide (i.e. $-N(SiMe_3)_2$ insertion into the amide C=O bond).

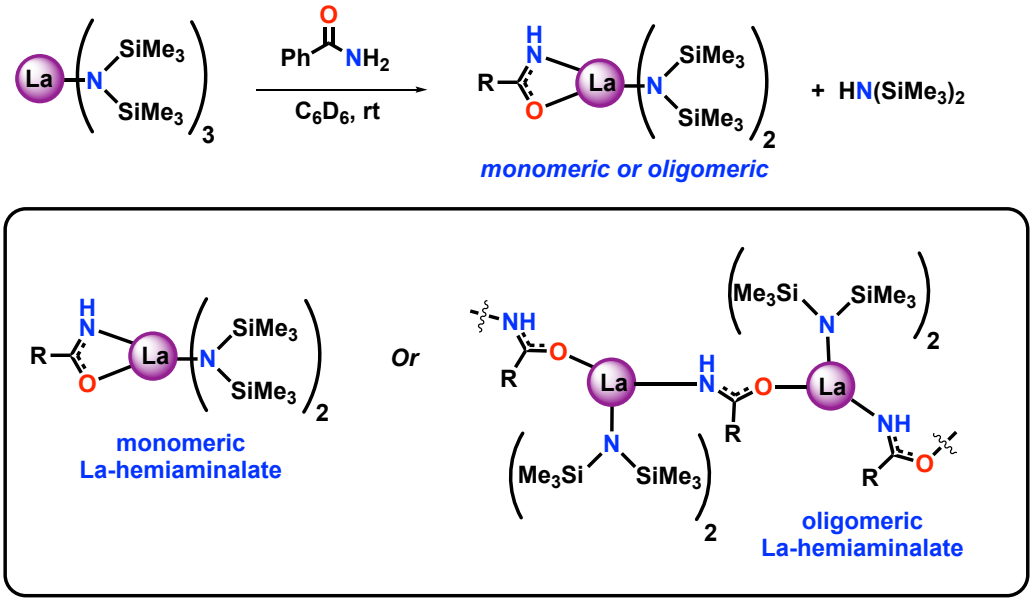


Figure S11. Proposed monomeric or oligomeric La-hemiaminalate complex $[(Me_3Si)_2N]_2La\{\eta^2\text{-}OC(NH)Ph\}$ obtained from the reaction of La^{NTMS} with the primary amide benzamide.

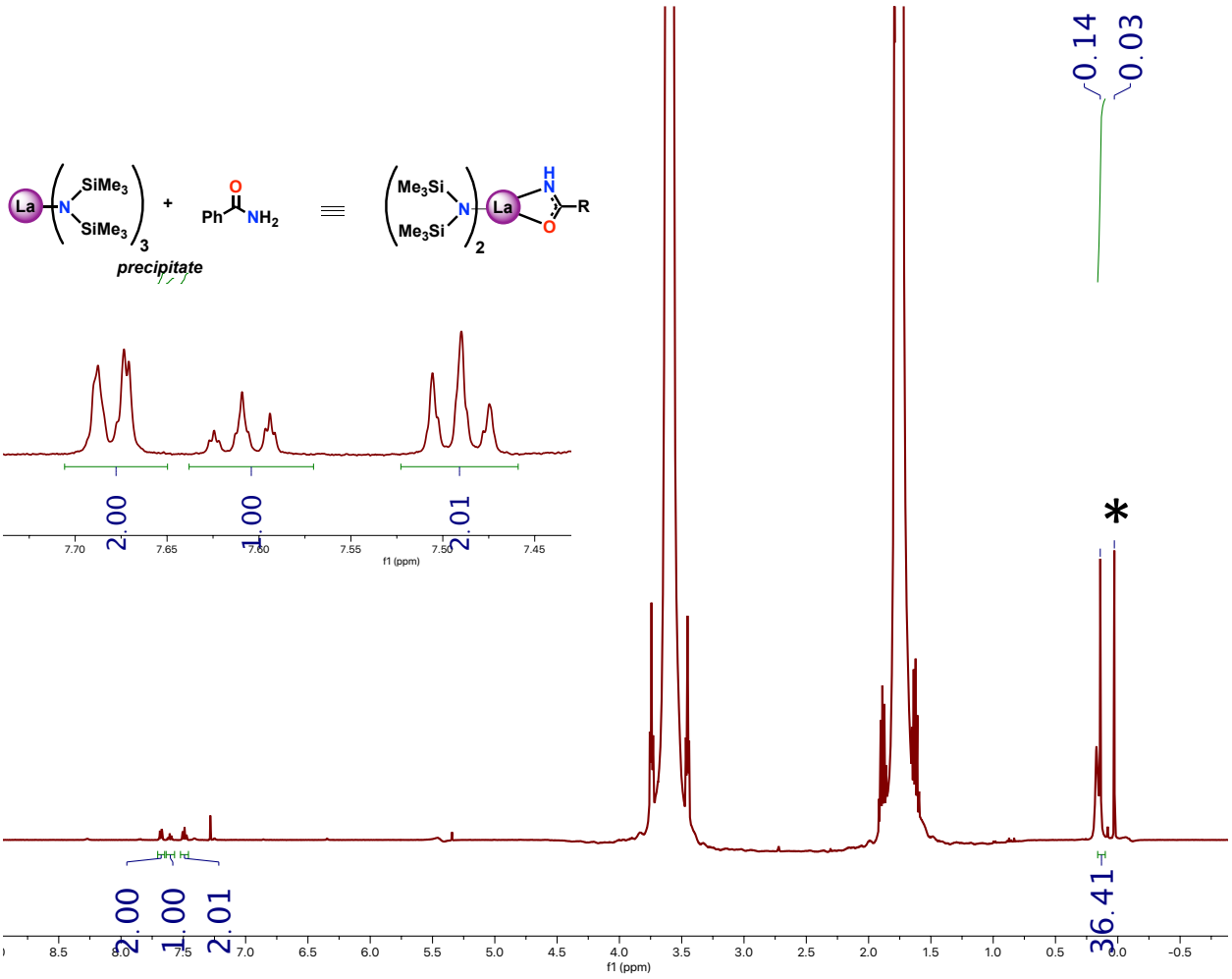


Figure S12. ^{1}H NMR (500 MHz) spectrum of a proposed La-hemiaminalate complex $[(Me_3Si)_2N]_2La\{\eta^2\text{-}OC(NH)Ph\}$ obtained as a precipitate from the reaction of benzamide and La^{NTMS} (1:1 molar ratio) in benzene-d_6. Spectrum obtained from a solution of precipitate in THF with a sealed capillary containing d_6-DMSO. * = $HN(SiMe_3)_2$

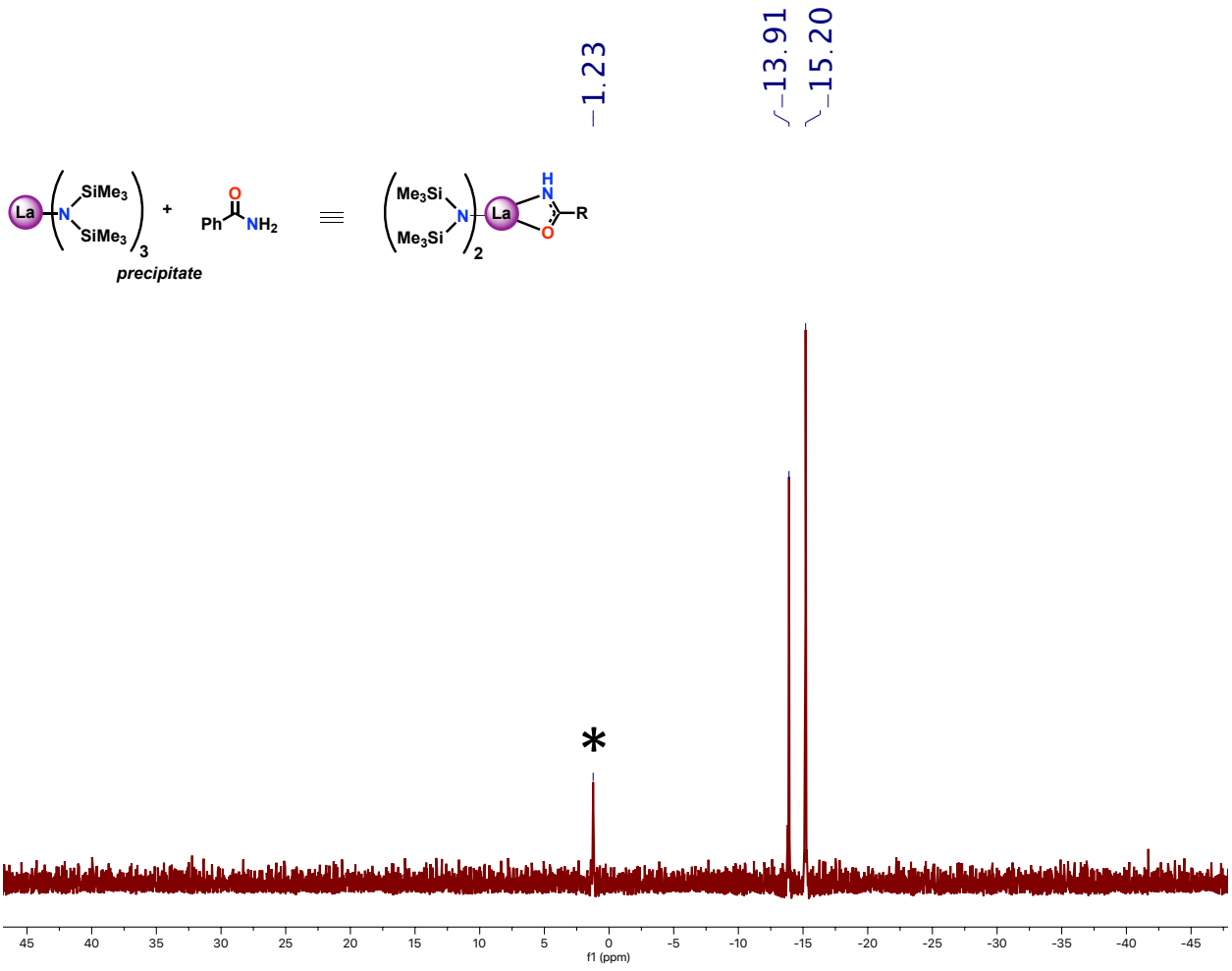


Figure S13. ^{29}Si NMR (125 MHz) spectrum of a proposed La-hemiaminalate complex $[(Me_3Si)_2N]_2La\{\eta^2\text{-}OC(NH)Ph\}$ obtained as a precipitate from the reaction of benzamide and La^{NTMS} (1:1 molar ratio) in benzene-d_6. Spectrum obtained from a solution of precipitate in THF with a sealed capillary containing d_6-DMSO. * = $HN(SiMe_3)_2$

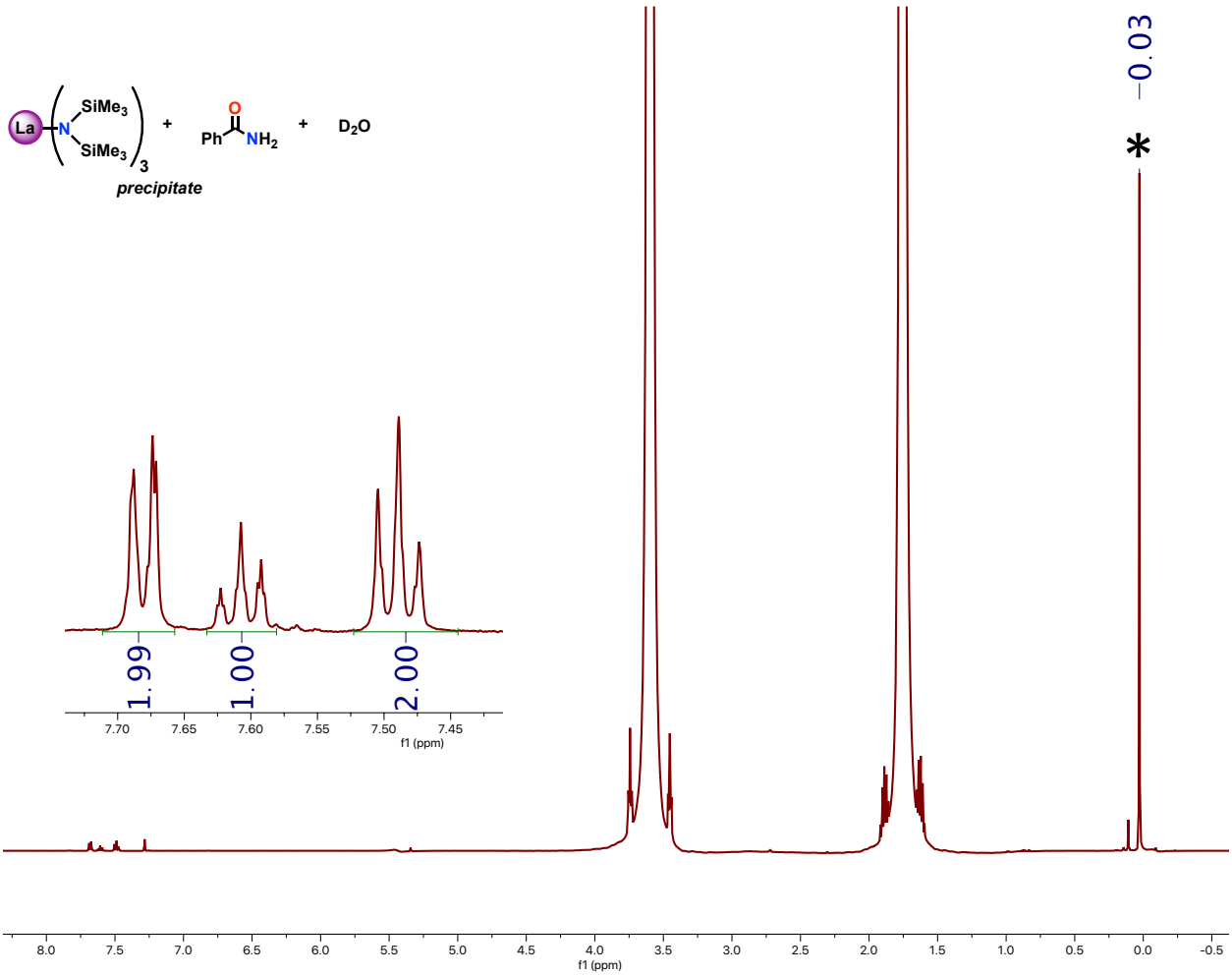


Figure S14. ^{1}H NMR (500 MHz) spectrum of the D_2O-*quenched* proposed La-hemiaminalate complex $[(Me_3Si)_2N]_2La\{\eta^2\text{-}OC(NH)Ph\}$ obtained as a precipitate from the reaction of benzamide and La^{NTMS} (1:1 molar ratio) in benzene-d_6. Spectrum obtained from a solution of precipitate in THF with a sealed capillary containing d_6-DMSO. * = $HN(SiMe_3)_2$

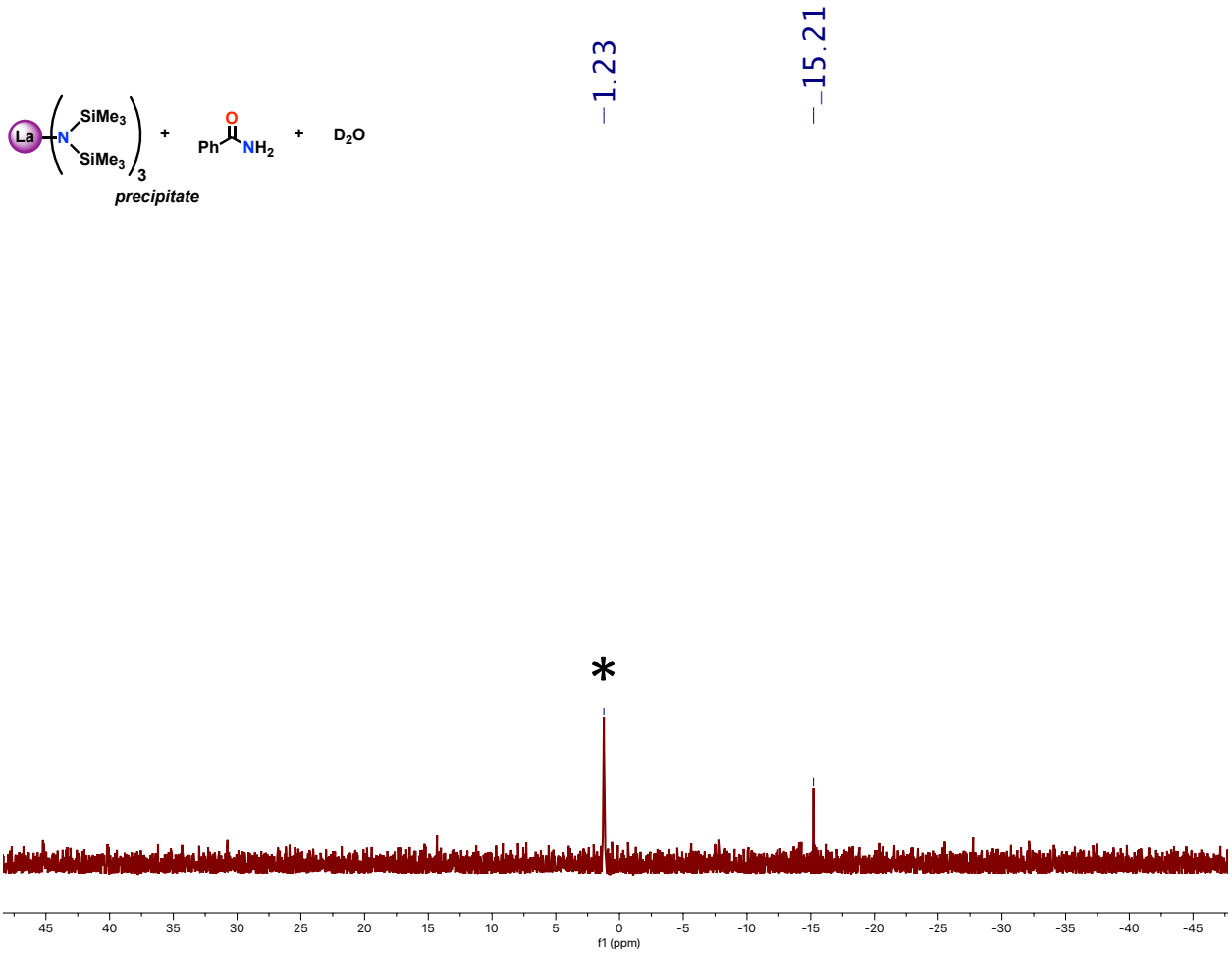


Figure S15. ^{29}Si NMR (125 MHz) spectrum of the D_2O-*quenched* proposed La-hemiaminalate complex $[(Me_3Si)_2N]_2La\{\eta^2\text{-}OC(NH)Ph\}$ obtained as a precipitate from the reaction of benzamide and La^{NTMS} (1:1 molar ratio) in benzene-d_6. Spectrum obtained from a solution of precipitate in THF with a sealed capillary containing d_6-DMSO. * = $HN(SiMe_3)_2$

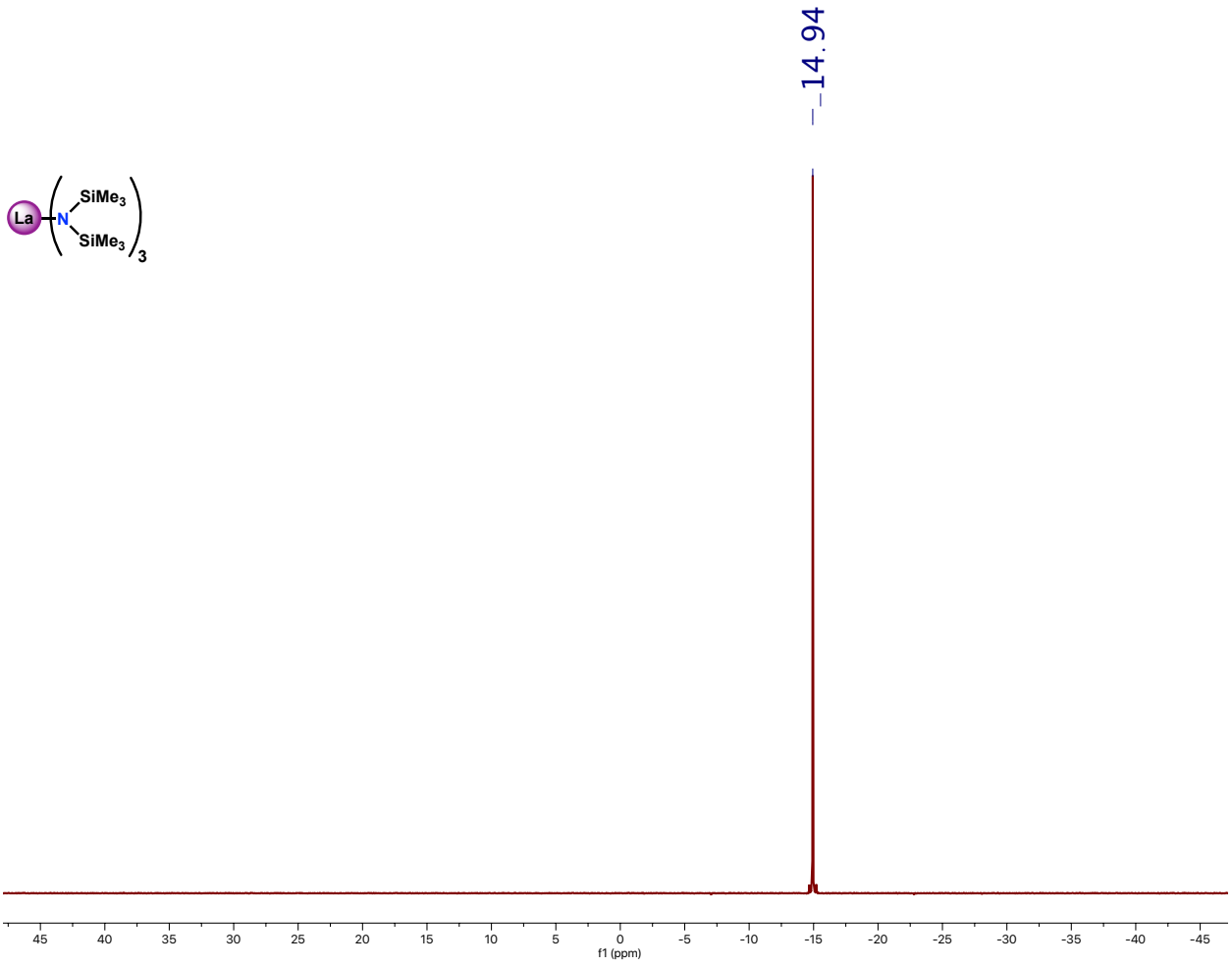


Figure S16. ^{29}Si NMR (125 MHz) spectrum of La^{NTMS} precatalyst in benzene-d_6 included for reference. (For ^{1}H NMR spectrum of La^{NTMS} precatalyst in benzene-d_6, see Figure S24).

DFT Examination of Primary Amide Reduction. DFT calculations were performed to assess the feasibility of a ligand insertion reaction between the La^{NTMS} precatalyst and the primary amide benzamide (i.e., La-N($SiMe_3$)$_2$ insertion into the amide C=O bond) (Figure S17). The insertion of the La-silylamide group (-N($SiMe_3$)$_2$) into the primary amide C=O bond and subsequent silyl migration to yield a La-siloxide complex was modeled. First, the approach of the primary amide produces a stabilization of 17.4 kcal/mol due to an interaction between the carbonyl group of the amide and the La metal center. However, the insertion of the La-silylamide (La-N($SiMe_3$)$_2$) into the primary amide C=O bond is very endoergonic (+22.8 kcal/mol) with an energy barrier of +32.6 kcal/mol. Finally, the silyl migration and formation of a La-siloxide complex is exoergonic (-0.6 kcal/mol with an energy barrier of +21.2 kcal/mol). Thus, the overall reaction is slightly endoergonic (+4.8 kcal/mol) with an energy barrier of +44.0 kcal/mol.

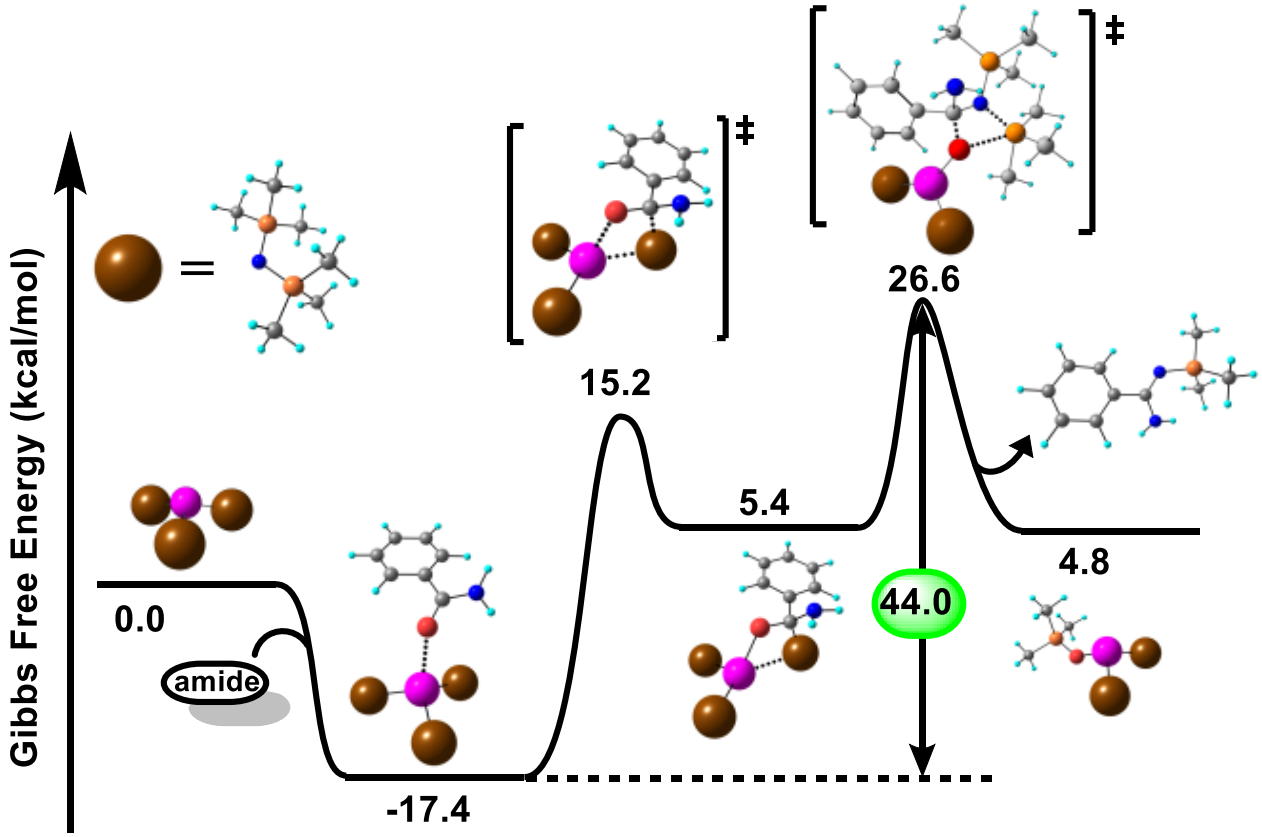


Figure S17. Gibbs free energy profile for a La-silylamide group (La-N($SiMe_3$)$_2$) insertion of the La^{NTMS} precatalyst into the benzamide C=O bond and subsequent silyl migration to yield a La-siloxide complex.

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. *N,N*-dimethylbenzamide was adopted as substrate model. Frequency analysis was performed to obtain thermochemical information about the reaction pathways at 298 K using the harmonic approximation. The difference in translational and rotational entropy when moving from gas to solvent are accounted for by adding an energy contribution of 8RT to the Gibbs free energy of each species as detailed in the literature.[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.

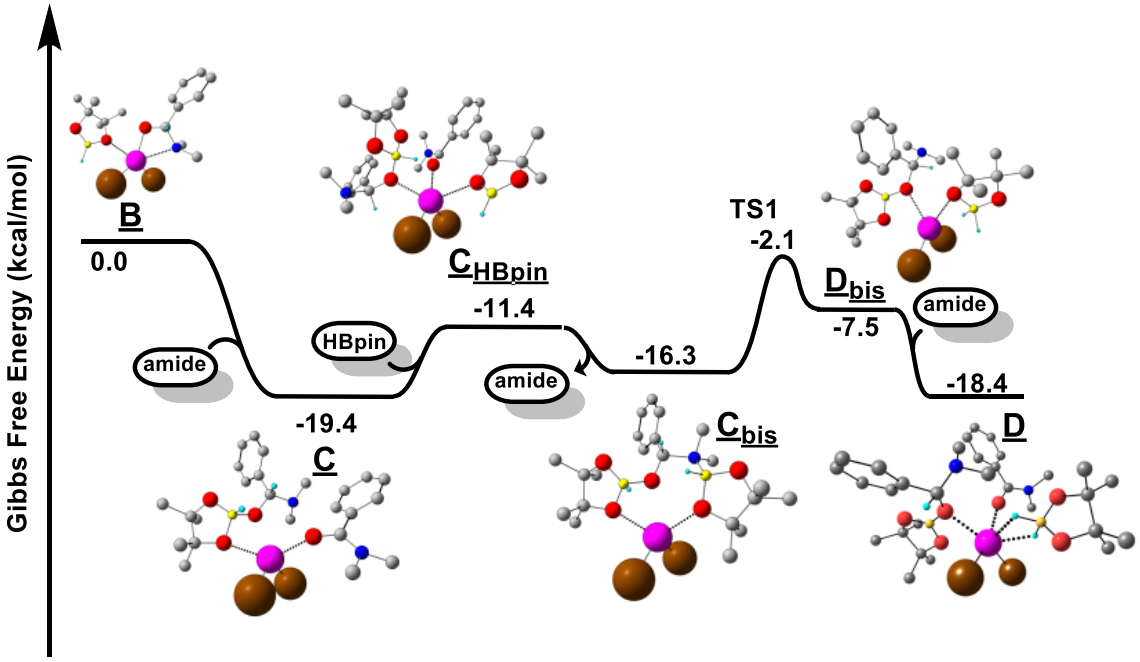


Figure S18. Gibbs free energy profile/catalytic cycle for the hydroboration/reduction of amides catalyzed by La^{NTMS}, and conversion of active catalyst **B** to species **D**.

Stoichiometric Reactivity Studies

Catalyst activation intermediate **I-$_{act}$-1** was obtained from a 1:1 mixture of the La^{NTMS} precatalyst and *N,N*-dimethylbenzamide. This intermediate was characterized using ^{1}H and ^{13}C NMR spectroscopy (Figures S17–S23). Attempts to experimentally characterize additional catalyst activation intermediates were carried out by monitoring stoichiometric mixtures of La^{NTMS} and substrates HBpin and *N,N*-dimethylbenzamide via ^{1}H and ^{11}B NMR. However, only the proposed off-cycle/deactivation product described in the main text is observed. When various mixtures of La^{NTMS} and HBpin are examined (0.5-6 equiv HBpin), the spectrum below is obtained with varying degrees of conversion of La^{NTMS}. Full conversion is observed at 4 equiv HBpin, which matches what would be expected given the proposed deactivation pathway. However, additional, uncharacterized decomposition products are observed at such high HBpin ratios, and therefore 1:3 La^{NTMS}:HBpin mixtures were studied further (Figures S14–S16). A solution of La^{NTMS}, HBpin and *N,N*-dimethylbenzamide (1:3:1) yields incomplete reduction of the amide, as evidenced by the appearance of O(Bpin)$_2$ and amine, but primarily the off-cycle product described below.

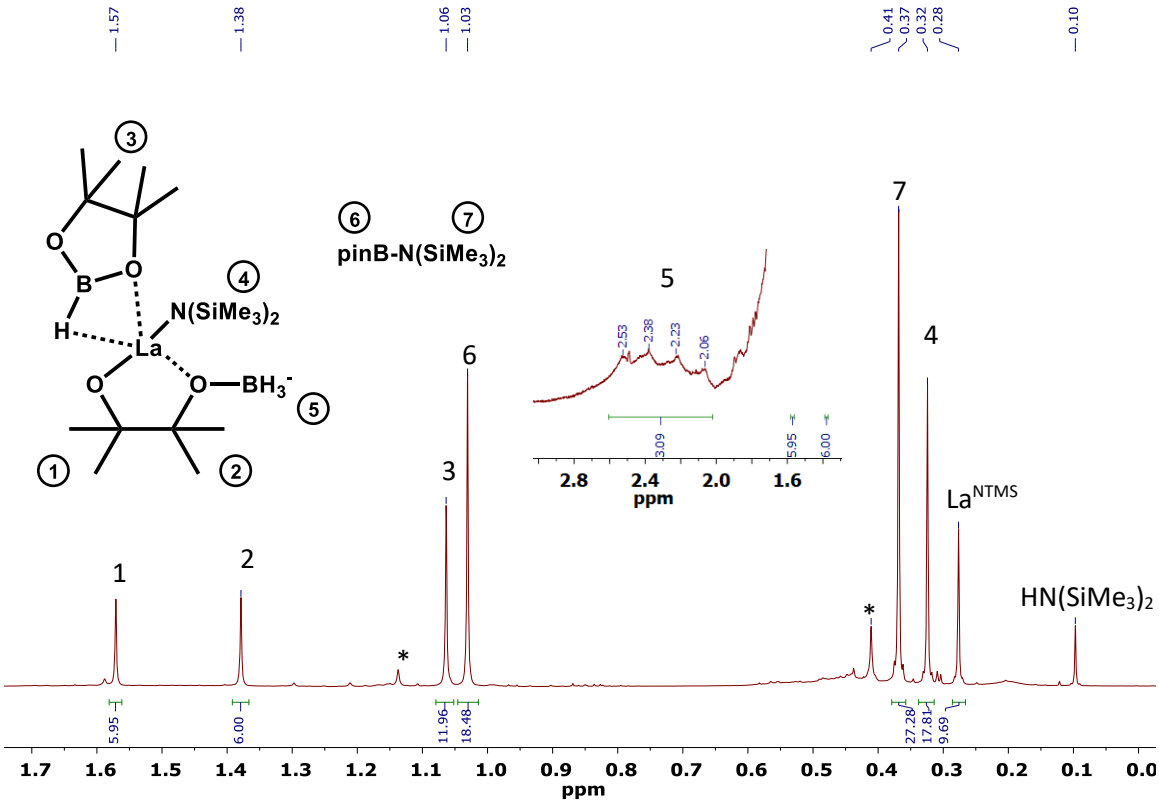


Figure S19. ^{1}H NMR (500 MHz) spectrum of the catalyst deactivation product (Figure 4A) obtained from 1:3 mixture of La^{NTMS} and HBpin in benzene-d$_6$.

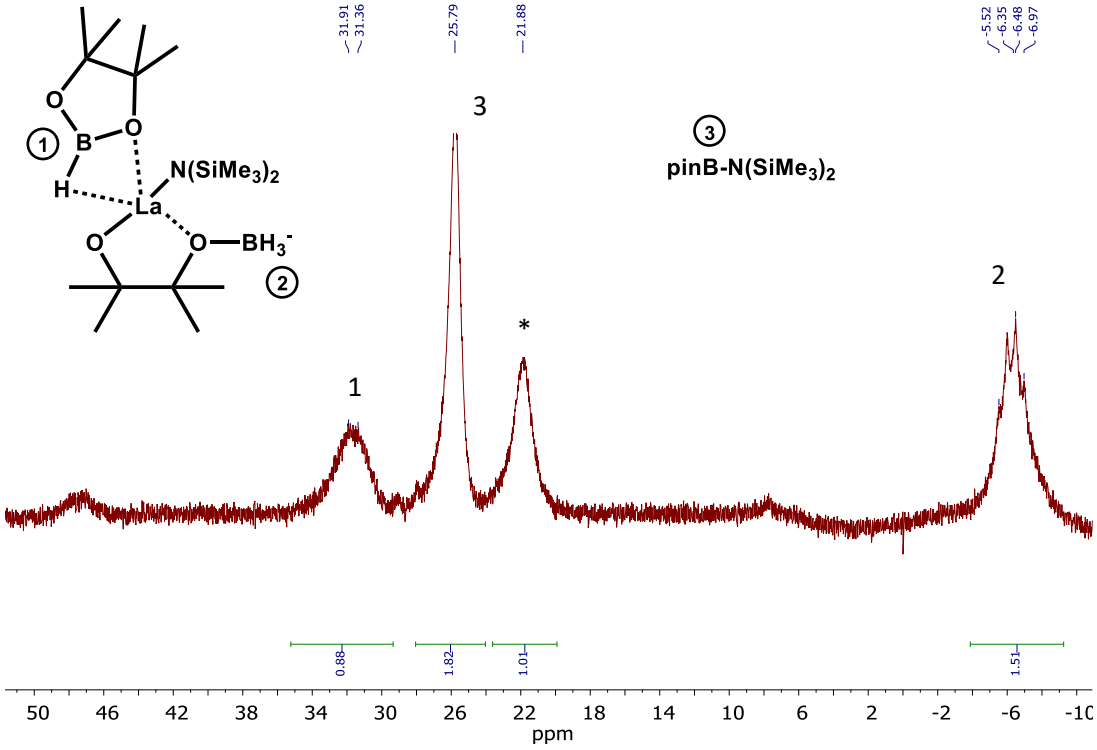


Figure S20. ^{11}B NMR (128 MHz) spectrum of the catalyst deactivation product (Figure 4A) obtained from 1:3 mixture of La^{NTMS} and HBpin in benzene-d_6. * = Unidentified side product, possibly weakly and reversibly coordinated pinB-N($SiMe_3$)$_2$ or B_2pin_3. The peak at δ 31.6 ppm is a broad doublet, likely due to coordination of the B-H to the metal center or exchange with RBH_3^-. The downfield shift is similar to previously reported coordinated boranes.[11]

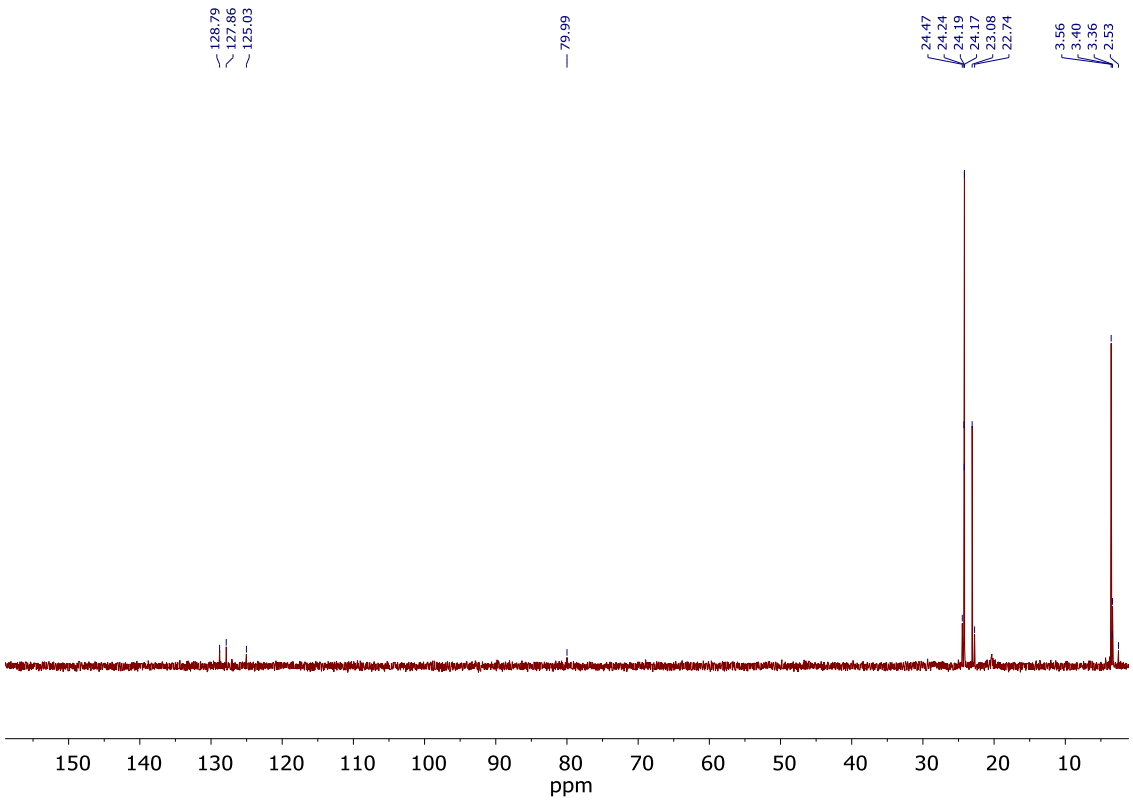


Figure S21. ^{13}C NMR (125 MHz) spectrum of the catalyst deactivation product (Figure 4A) obtained from 1:3 mixture of La^{NTMS} and HBpin in benzene-d_6.

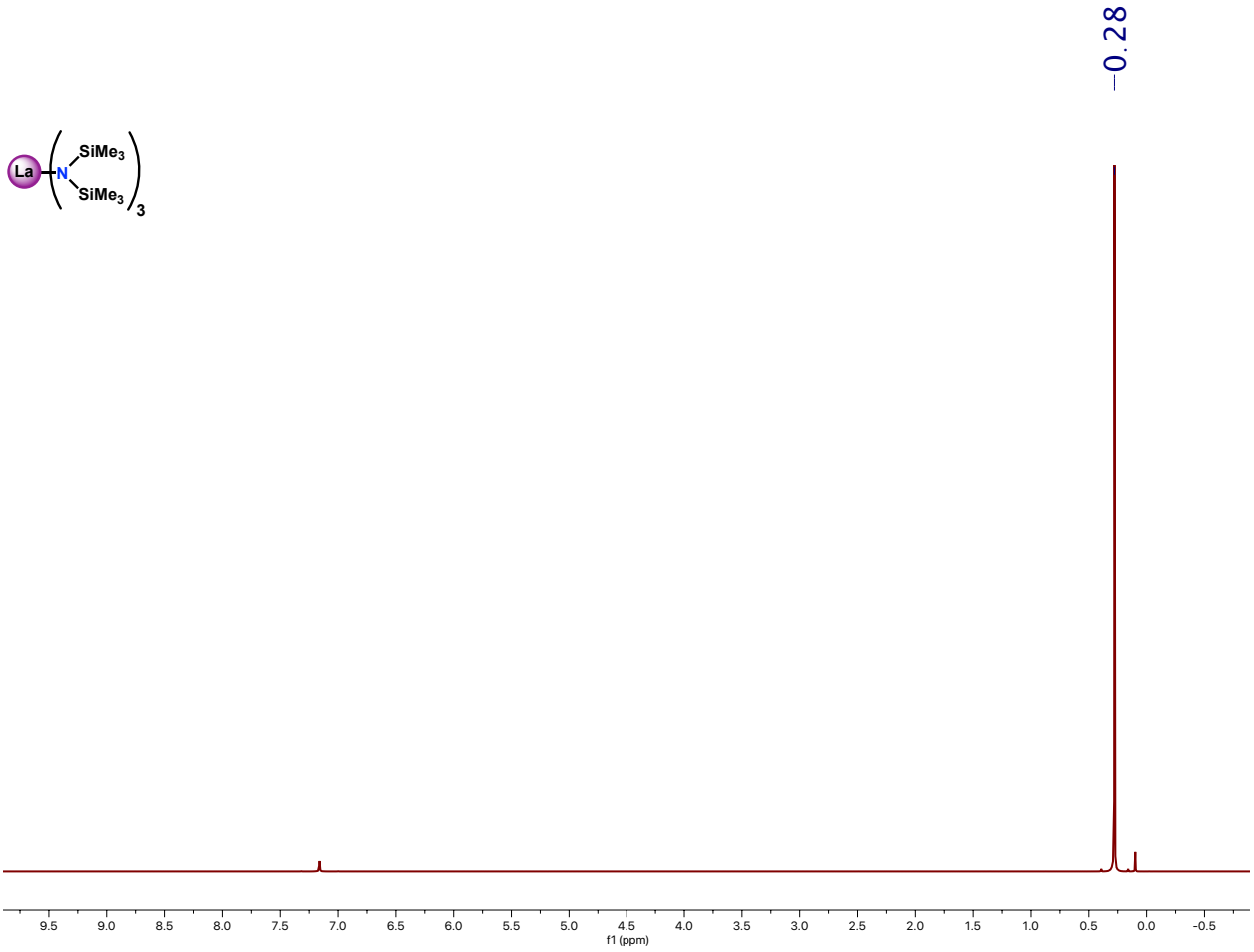


Figure S22. ^{1}H NMR (500 MHz) spectrum of the La^{NTMS} precatalyst in benzene-d_6 included for reference.

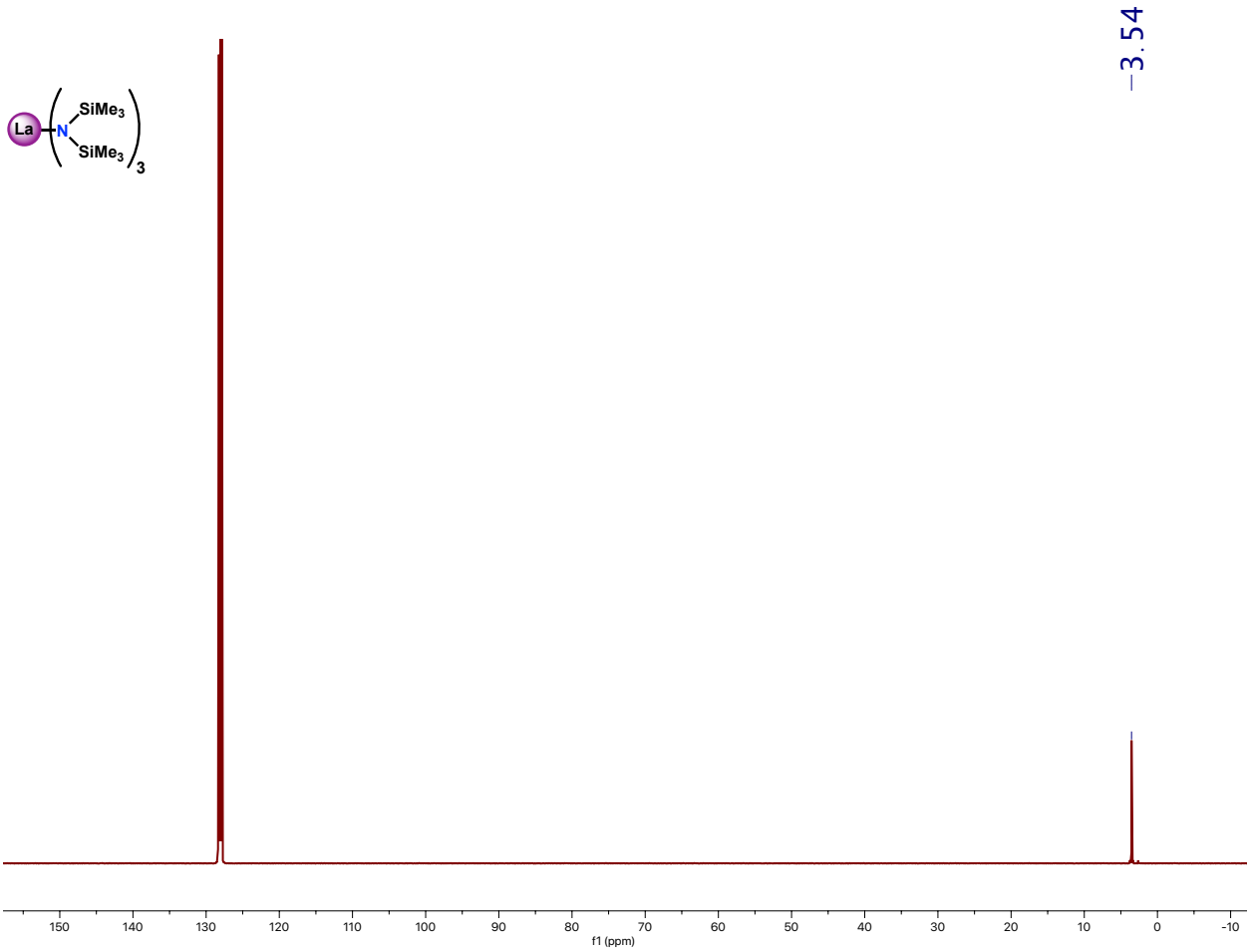


Figure S23. ^{13}C NMR (125 MHz) spectrum of the La^{NTMS} precatalyst in benzene-d_6 included for reference.

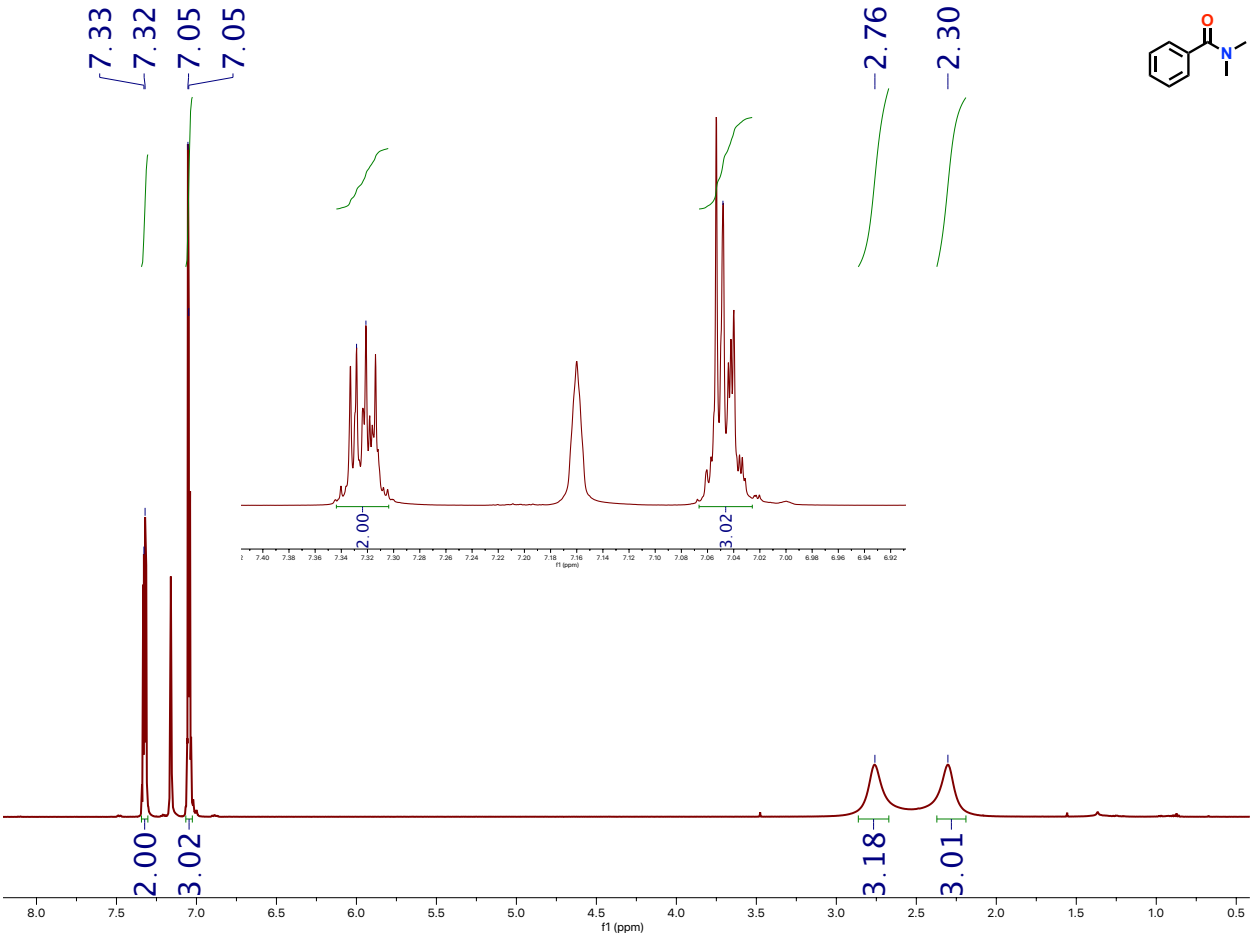


Figure S24. ^{1}H NMR (500 MHz) spectrum of *N,N*-dimethylbenzamide in benzene-d_6 included for reference.

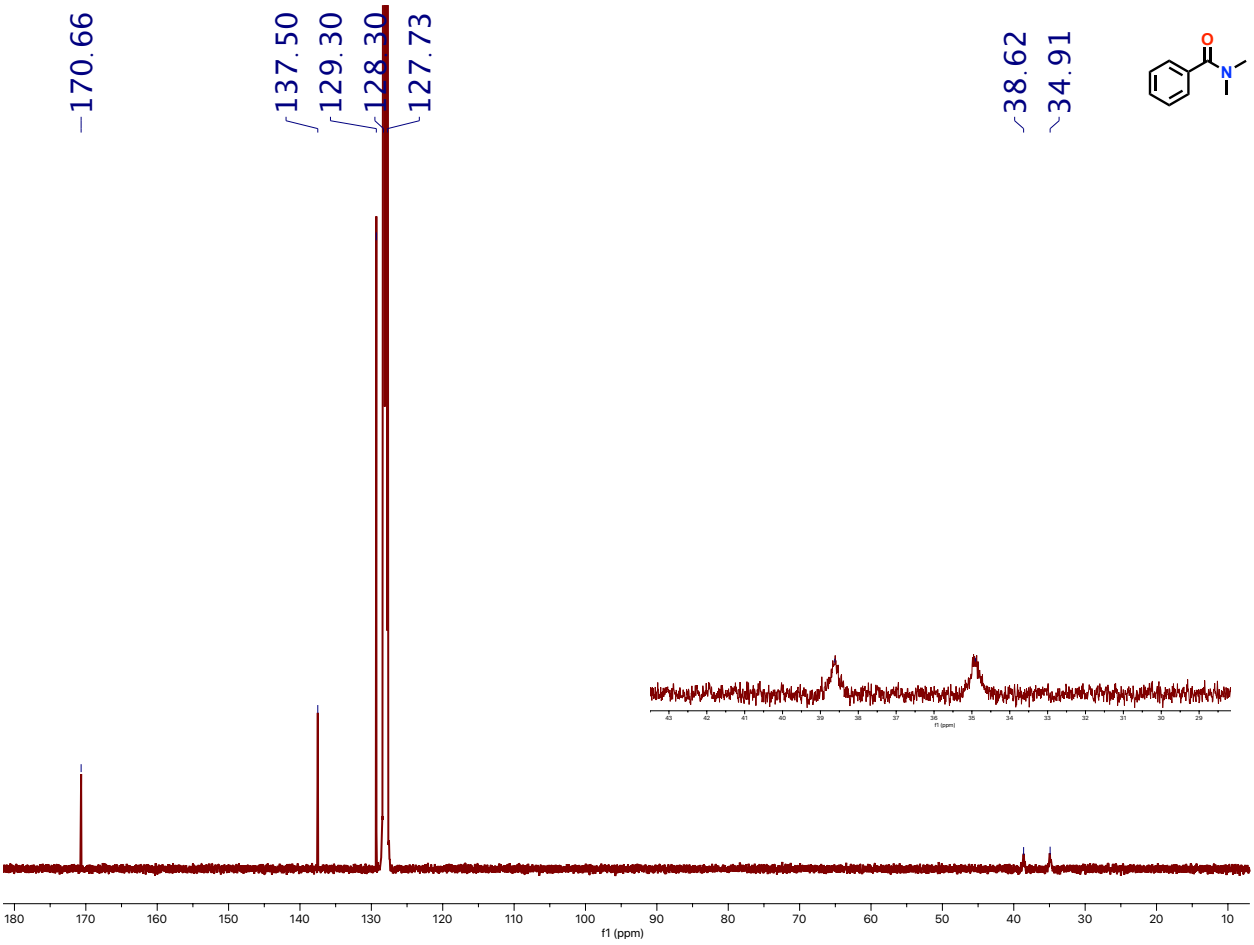


Figure S25. ^{13}C NMR (125 MHz) spectrum of *N,N*-dimethylbenzamide in benzene-d_6 included for reference.

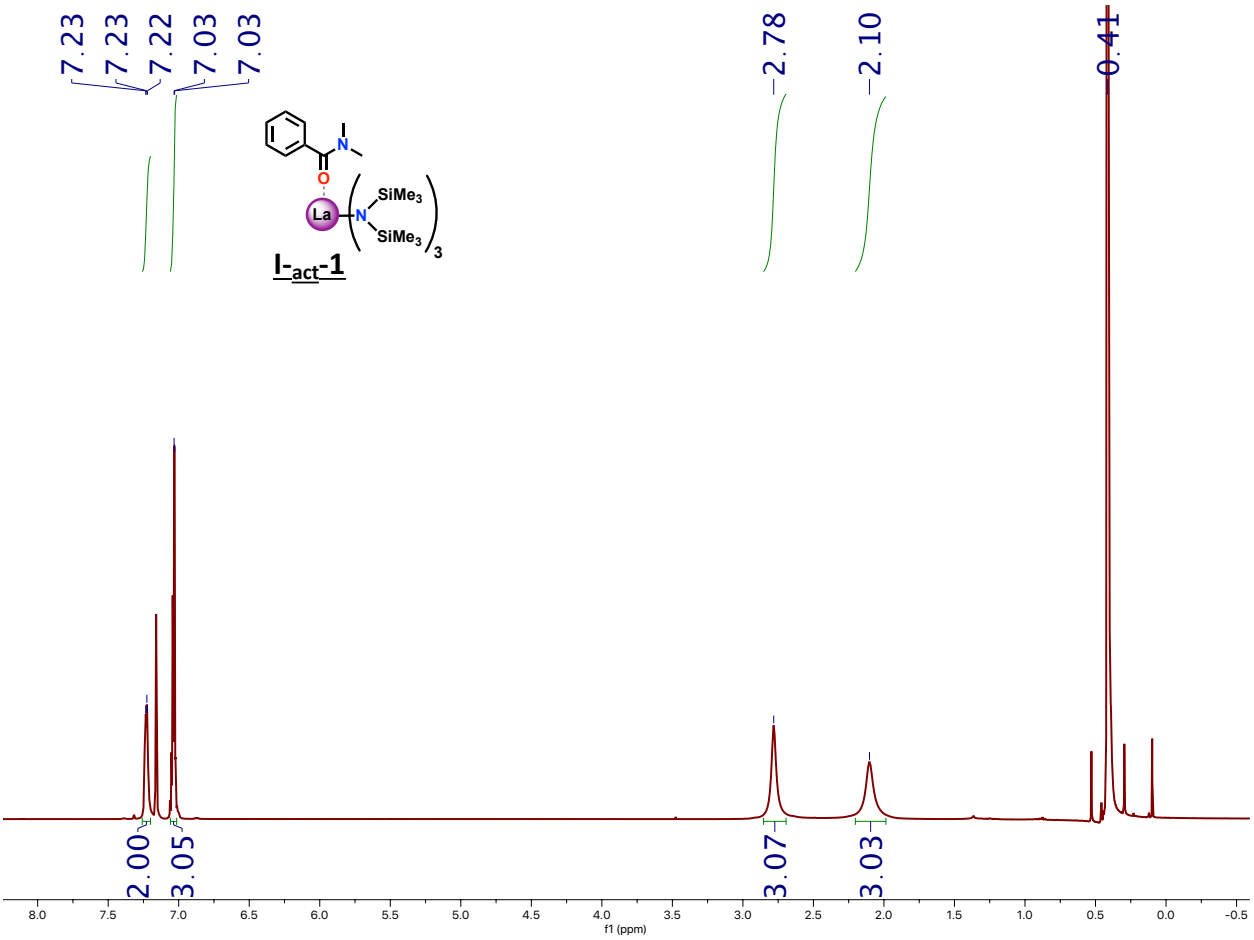


Figure S26. ^{1}H NMR (500 MHz) spectrum of the proposed catalyst activation intermediate **I-$_{act}$-1** in benzene-d_6.

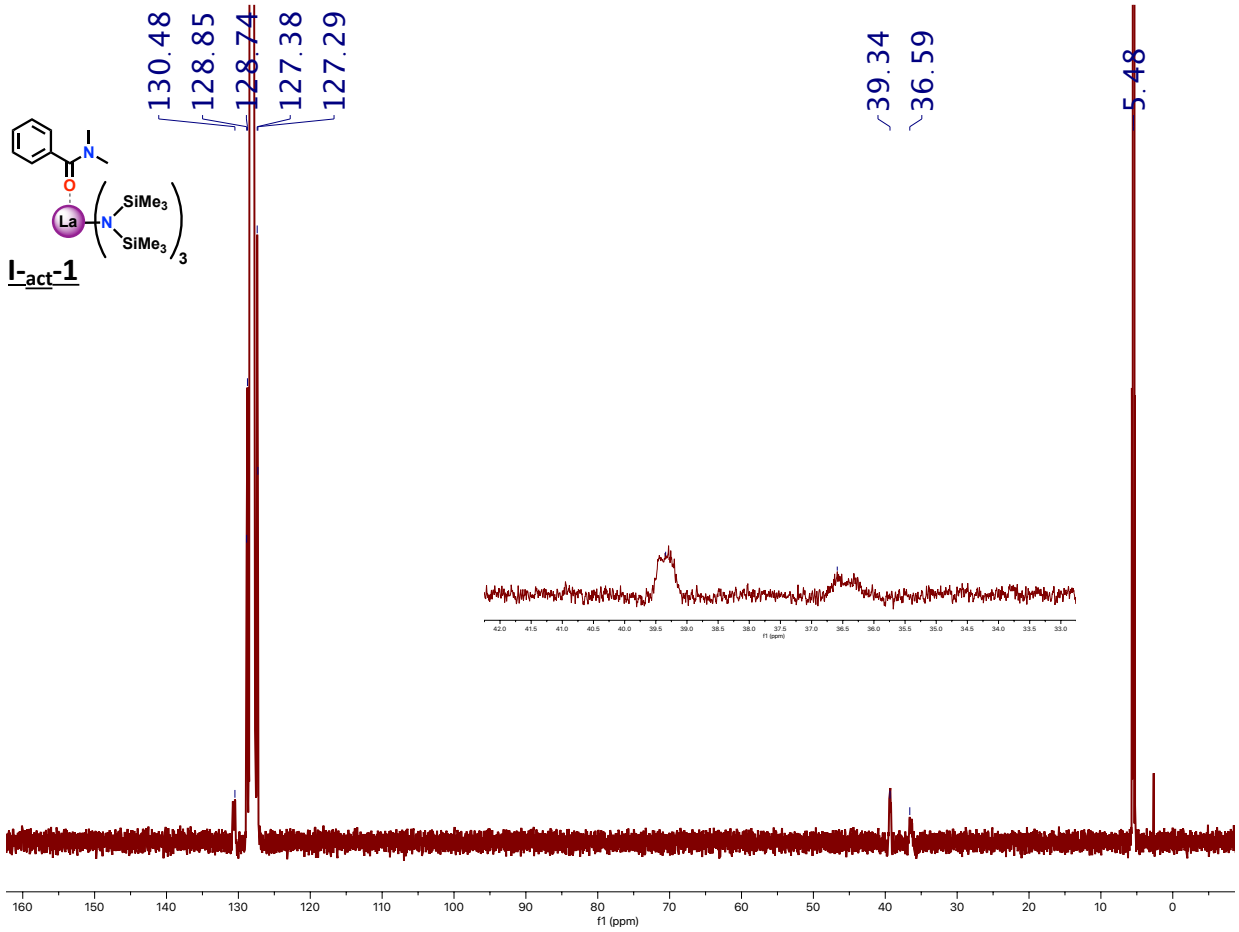


Figure S27. ^{13}C NMR (125 MHz) spectrum of the proposed catalyst activation intermediate **I-$_{act}$-1** in benzene-d_6.

DFT Examination of Catalyst Decomposition Pathway. DFT calculations were performed to better understand the decomposition path of the La^{NTMS} precatalyst induced by HBpin (Figure S28). The decomposition path involves four main steps. The coordination of the first HBpin leads to the formation of the pinBH-$N(SiMe_3)_2^-$ borate species (**I_{deact}-1**, -7.0 kcal/mol). The second step is promoted by the approach of a second HBpin leading to hydride transfer from the pinBH-$N(SiMe_3)_2^-$ species to the coordinated HBpin, producing a new H_2Bpin^- species and releasing pinB-$N(SiMe_3)_2$. This intermediate is stabilized by the coordination of a third HBpin (**I_{deact}-2,** -28.5 kcal/mol). The third step is analogous to the first one involving the formation of a new pinBH-$N(SiMe_3)_2^-$ borate species (**I_{deact}-3,** -29.4 kcal/mol). The last step involves the ring-opening of the H_2Bpin^- species and the subsequent hydride transfer from pinBH-$N(SiMe_3)_2^-$ to the opened H_2Bpin^-, leading to the final product. A second pinB-$N(SiMe_3)_2$ molecule is released and a new HBpin coordinates and stabilizes the final product (-34.5 kcal/mol). This last step is the rate determining step with a Gibbs free energy barrier of 14.9 kcal/mol.

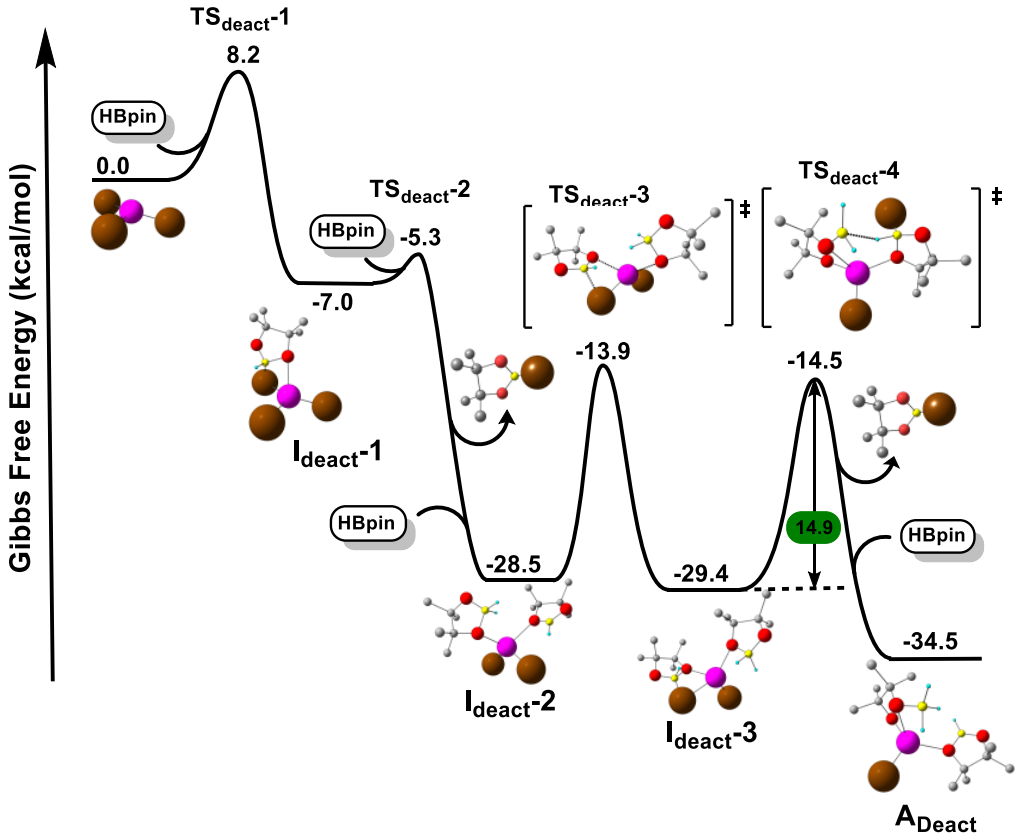


Figure S28. Energy profile associated with the decomposition pathway of La^{NTMS} precatalyst induced by HBpin.

Evaluation of the Effect of Different Basis Sets on the Accuracy of the Theoretical Model. It is well known that while 4f electrons must be considered when spectroscopic properties are being studied, it has been shown that the atomic 4f shells of the lanthanides are strongly stabilized and do not contribute significantly to the chemical bonding or reactivity.[12] For this reason, it is expected that adding a polarization function (*f* function) to the basis set used on the lanthanum atom should not have a significant effect on the calculated energetic profile corresponding to the catalytic cycle discussed in this work. Nevertheless, in order to investigate the effects of different basis sets a series of calculations on the key steps of the catalytic cycle were performed. In particular, to evaluate the first hydrogen exchange step we have applied alternative basis sets to the formation of complex **C** and **TS1**. Similarly, to evaluate the second hydrogen exchange step we have applied alternative basis sets to the formation of complex **E** and **TS2**. The data reported in **Table S1** show the stabilization energy for the formation of complex **C**, **TS1**, complex **E** and **TS2** computed at the SCF level of theory (at zero kelvin, without considering temperature and pressure) using different basis sets.

Table S1. Stabilization energy (kcal/mol) obtained using different basis sets computed at the SCF level of theory.

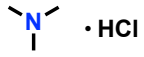
	LANL2DZ[a]	LANL2DZ + pol[b]	Def2-SVP[c]
C	–32.2	–32.0	–32.7
TS1	–11.0	–11.0	–13.6
E	–72.4	–72.4	–73.9
TS2	–61.1	–62.2	–62.6

[a]ECP and basis set applied to the lanthanum atom in the present work. [b]Geometry optimization using a polarization function (*f* function) added only to the basis set of the lanthanum atom.[13] [c]Geometry optimization using the Def2-SVP basis set reported by Ahlrich and coworkers on all atoms.[14]

It is evident that adding the polarization function to the LANL2DZ basis set (see **Table S1**, LANL2DZ + pol) produces negligible changes in the stabilization energies of complex **C**, **TS1** as well as complex **E**. Only **TS2** becomes slightly more stabilized, experiencing a decrease in energy by approximately 1 kcal/mol. Additionally, upon using a full electron basis set plus polarization for all atoms (see **Table S1**, Def2-SVP) we obtain a slightly greater stabilization for all intermediates and transition states shown above. Ultimately, these additional calculations suggest that adding the polarization function to the lanthanum atom does not significantly modify the stabilization energies along the catalytic cycle and it does not produce any significant improvement in the accuracy of the calculations.

Characterization of Amide Hydroboration/Reduction Products

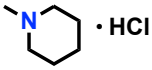
Characterization data for the products of amide reduction are given below. Products were converted to amine•HCls (unless otherwise noted) and characterized by ^{1}H and $^{13}C\{^{1}H\}$ NMR. Previously unreported products were compared to amine•HCls synthesized from commercially available amines.

1.  (white powder in 50% yield – low yield due to volatility of amine)

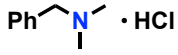
NMR spectra are identical to those reported in the literature.[15]
^{1}H NMR (D_2O, 500 MHz): 2.93 (9 H) **$^{13}C\{^{1}H\}$ NMR (D_2O, 125 MHz):** 44.76

2.  (white powder in 56% yield)

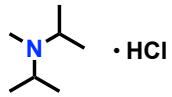
NMR spectra are identical to those reported in the literature.[15]
^{1}H NMR (D_2O, 500 MHz): 1.32 (t, 3H, $^{3}J_{HH}$=7.3 Hz, N-CH_2CH_3), 2.87 (s, 6H, N-CH_3), 3.20 (q, 2H, $^{3}J_{HH}$=7.2 Hz, N-CH_2CH_3). **$^{13}C\{^{1}H\}$ NMR (D_2O, 125 MHz):** 9.02 (N-CH_2CH_3), 42.01 (N-CH_3), 53.01 (N-CH_2CH_3)

3.  (white powder in 88% yield)

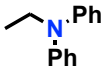
NMR spectra are identical to samples prepared from commercially available amine.
^{1}H NMR (D_2O, 500 MHz): 1.40-1.54 (m, 1H, N-C_5H_{10}), 1.65-1.88 (m, 3H, N-C_5H_{10}), 1.89-2.02 (m, 2H, N-C_5H_{10}), 2.84 (s, 3H, Me), 2.95 (t, 2H, $^{3}J_{HH}$=12.5 Hz, N-C_5H_{10}), 3.48 (d, 2H, $^{3}J_{HH}$=12.7 Hz, N-C_5H_{10}).**$^{13}C\{^{1}H\}$ NMR (D_2O, 125 MHz):** 20.61 (N-C_5H_{10}), 22.98 (N-C_5H_{10}), 43.19 (N-*Me*), 54.92 (N-C_5H_{10}).

4.  (white powder in 79% yield)

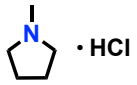
NMR spectra are identical to those reported in the literature.[15]
^{1}H NMR (D_2O, 500 MHz): 2.87 (s, 6H, N-CH_3), 4.33 (s, 2H, N-CH_2Ph), 7.49-7.58 (m, 5H, N-CH_2Ph). **$^{13}C\{^{1}H\}$ NMR (D_2O, 125 MHz):** 42.07 (N-CH_3), 61.12 (N-CH_2Ph), 129.30 (N-CH_2Ph), 130.15 (N-CH_2Ph), 130.77 (N-CH_2Ph)

5.  (white powder in 92% yield)

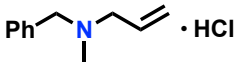
NMR spectra are identical to samples prepared from commercially available amine.
^{1}H NMR (D_2O, 500 MHz): 1.33 (dd, 12H, $^{3}J_{HH}$=6.7 Hz, $^{4}J_{HH}$=19.2 Hz, N-(CH(CH_3)$_2$)$_2$), 2.70 (s, 3H, N-CH_3), 3.70 (septet, 2H, $^{3}J_{HH}$=6.7 Hz, N-(C*H*(CH_3)$_2$)$_2$). **$^{13}C\{^{1}H\}$ NMR (D_2O, 125 MHz):** 15.57 (N-CH(CH_3)$_2$), 18.06 (N-CH(CH_3)$_2$), 30.68 (N-*Me*), 54.92 (N-CH(CH_3)$_2$),

6. 

NMR spectra are in accordance with those in the literature.[16]
^{1}H NMR (C_6D_6, 500 MHz): 0.97 (t, 3H, $^3J_{HH}$=7.0 Hz, NCH$_2$C*H$_3$*), 3.47 (q, 2H, $^3J_{HH}$=7.0 Hz, NC*H$_2$*CH$_3$), 6.81-6.86 (m, 2H, N-*Ph*), 6.89-6.93 (m, 4H, N-*Ph*), 7.08-7.13 (m, 4H, N-*Ph*)
^{13}C{^{1}H} NMR (C_6D_6, 125 MHz): 12.77 (N-CH$_2$*C*H$_3$), 46.51 (N-*C*H$_2$CH$_3$), 121.38 (N-*Ph*), 121.46 (N-*Ph*), 129.58 (N-*Ph*), 148.28 (N-*Ph*)

7.  (oily solid in 91% yield)

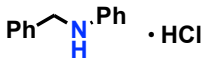
NMR spectra are identical to samples prepared from commercially available amine.
^{1}H NMR (D_2O, 500 MHz): 1.98-2.08 (m, 2H, N-C$_4$*H$_8$*), 2.13-2.22 (m, 2H, N-C$_4$*H$_8$*), 2.93 (s, 3H, N-*Me*), 3.03-3.11 (m, 2H, N-C$_4$*H$_8$*), 3.62-3.69 (m, 2H, N-C$_4$*H$_8$*). **^{13}C{^{1}H} NMR (D_2O, 125 MHz):** 22.83 (N-*Me*), 40.56 (N-*C*$_4$H$_8$), 55.76 (N-*C*$_4$H$_8$)

8.  (white powder in 93% yield)

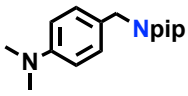
NMR spectra are in accordance with those in the literature.[17]
^{1}H NMR ($CDCl_3$, 500 MHz): 2.63 (d, 3H, N-C*H$_3$* coupling to N-*H*), 3.77-3.40 (m, 2H, PhC*H$_2$*), 4.20-4.00 (m, 2H, N-C*H$_2$*), 5.49 (d, 1H, $^3J_{HH}$ = 17.2 Hz, NCH$_2$CH=C*H$_2$*), 5.59 (d, 1H, $^3J_{HH}$ = 10.1 Hz, NCH$_2$CH=C*H$_2$*), 6.29-6.17 (m, 1H, NCH$_2$C*H*=CH$_2$), 7.48-7.42 (m, 3H, *Ph*), 7.65-7.59 (m, 2H, *Ph*). **^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz):** 131.30, 130.34, 129.60, 128.50, 126.65, 126.09, 59.01, 57.77, 38.89.

9.  (white powder in 66% yield)

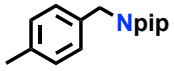
NMR spectra are identical to samples prepared from commercially available amine.
^{1}H NMR (D_2O, 500 MHz): 1.28 (t, 3H, $^3J_{HH}$=7.5 Hz, N-CH$_2$C*H$_3$*), 2.70 (s, 3H, N-C*H$_3$*), 3.09 (q, 2H, $^3J_{HH}$=7.5 Hz, N-C*H$_2$*CH$_3$). **^{13}C{^{1}H} NMR (D_2O, 125 MHz):** 10.33 (N-CH$_2$*C*H$_3$), 32.12 (N-*C*H$_3$), 44.23 (N-*C*H$_2$CH$_3$)

10.  (gray powder in 75% yield)

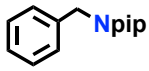
NMR spectra are identical to samples prepared from commercially available amine.
^{1}H NMR ($CDCl_3$, 500 MHz): 4.36 (s, 2H, PhC*H$_2$*-N), 7.20-7.28 (m, 3H, *Ph*), 7.29-7.40 (m, 7H, *Ph*). **^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz):** 56.09 (Ph*C*H$_2$-N), 124.00 (Ph), 128.84 (Ph), 129.29 (Ph), 129.55 (Ph), 129.82 (Ph), 131.17 (Ph), 134.45 (Ph), 133.93 (Ph)

11. 

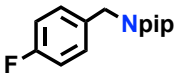
NMR spectra are in accordance with those in the literature.[18]
^{1}H NMR (C_6D_6, 500 MHz): 1.29-1.39 (m, 2H, *pip*), 1.56 (p, 4H, $^3J_{HH}$=5.9 Hz, *pip*), 2.31 (br s, 4H, *pip*), 2.48 (s, 6H, PhN*Me*$_2$), 3.45 (br s, 2H, PhC*H*$_2$Npip), 6.46 (d, 2H, $^3J_{HH}$=8.1 Hz, *Ph*), 7.54 (d, 2H, $^3J_{HH}$=8.1 Hz, *Ph*). **^{13}C{^{1}H} NMR (C_6D_6, 125 MHz):** 17.02 (N-*pip*), 23.25 (N-*pip*), 48.72 (PhN*Me*$_2$), 55.58 (N-*pip*), 62.96 (Ph*C*H$_2$-Npip), 121.25 (*Ph*), 131.86 (*Ph*), 134.86 (*Ph*), 136.24 (*Ph*).

12. 

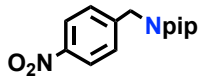
NMR spectra are in accordance with those in the literature.[19]
^{1}H NMR (C_6D_6, 500 MHz): 1.28-1.39 (m, 2H, *pip*), 1.54 (p, 4H, $^3J_{HH}$=5.9 Hz, *pip*), 2.15 (s, 3H, Ph*CH*$_3$), 2.29 (br s, 4H, *pip*), 3.35 (br s, 2H, PhC*H*$_2$Npip), 7.02 (d, 2H, $^3J_{HH}$=8.1 Hz, *Ph*), 7.28 (d, 2H, $^3J_{HH}$=8.1 Hz, *Ph*). **^{13}C{^{1}H} NMR (C_6D_6, 125 MHz):** 16.94 (N-*pip*), 21.15 (*Me*Ph), 26.55 (N-*pip*), 54.85 (N-*pip*), 63.97 (Ph*C*H$_2$-Npip), 129.26 (*Ph*), 131.76 (*Ph*), 136.32 (*Ph*), 136.81 (*Ph*).

13. 

NMR spectra are in accordance with those in the literature.[20]
^{1}H NMR (C_6D_6, 500 MHz): 1.25-1.35 (m, 2H, *pip*), 1.47 (p, 4H, $^3J_{HH}$=5.6 Hz, *pip*), 2.26 (br s, 4H, *pip*), 3.33 (s, 2H, PhC*H*$_2$Npip), 7.07-7.12 (m, 1H, *Ph*), 7.15-7.22 (m, 2H, *Ph*), 7.33-7.38 (m, 2H, *Ph*). **^{13}C{^{1}H} NMR (C_6D_6, 125 MHz):** 16.94 (N-*pip*), 26.52 (N-*pip*), 54.86 (N-*pip*), 64.17 (Ph*C*H$_2$-Npip), 127.10 (*Ph*), 129.21 (*Ph*), 131.76 (*Ph*), 139.86 (*Ph*).

14. 

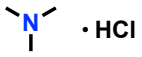
NMR spectra are in accordance with those in the literature.[21]
^{1}H NMR (C_6D_6, 500 MHz): 1.24-1.32 (m, 2H, *pip*), 1.45 (p, 4H, $^3J_{HH}$=5.4 Hz, *pip*), 2.20 (br s, 4H, *pip*), 3.19 (s, 2H, PhC*H*$_2$Npip), 6.80-6.87 (m, 2H, *Ph*), 7.08-7.20 (m, 2H, *Ph*). **^{13}C{^{1}H} NMR (C_6D_6, 125 MHz):** 16.94 (N-*pip*), 26.48 (N-*pip*), 54.71 (N-*pip*), 63.17 (Ph*C*H$_2$-Npip), 115.07 (*Ph*), 115.24 (*Ph*), 130.62 (*Ph*), 131.76 (*Ph*).

15. 

NMR spectra are in accordance with those in the literature.[18]

^{1}H NMR (C_6D_6, 500 MHz): 1.19-1.23 (m, 2H, *pip*), 1.43 (p, 4H, $^{3}J_{HH}$=5.4 Hz, *pip*), 2.10 (br s, 4H, *pip*), 3.05 (s, 2H, PhC*H*$_2$Npip), 7.01 (d, 2H, $^{3}J_{HH}$=7.9 Hz, *Ph*), 7.88 (d, 2H, $^{3}J_{HH}$=7.9 Hz, *Ph*).

^{13}C{^{1}H} NMR (C_6D_6, 125 MHz): 22.22 (N-*pip*), 23.92 (N-*pip*), 52.28 (N-*pip*), 60.45 (Ph*C*H$_2$-Npip), 121.04 (*Ph*), 126.75 (*Ph*), 144.58 (*Ph*), 145.02 (*Ph*).

1. 

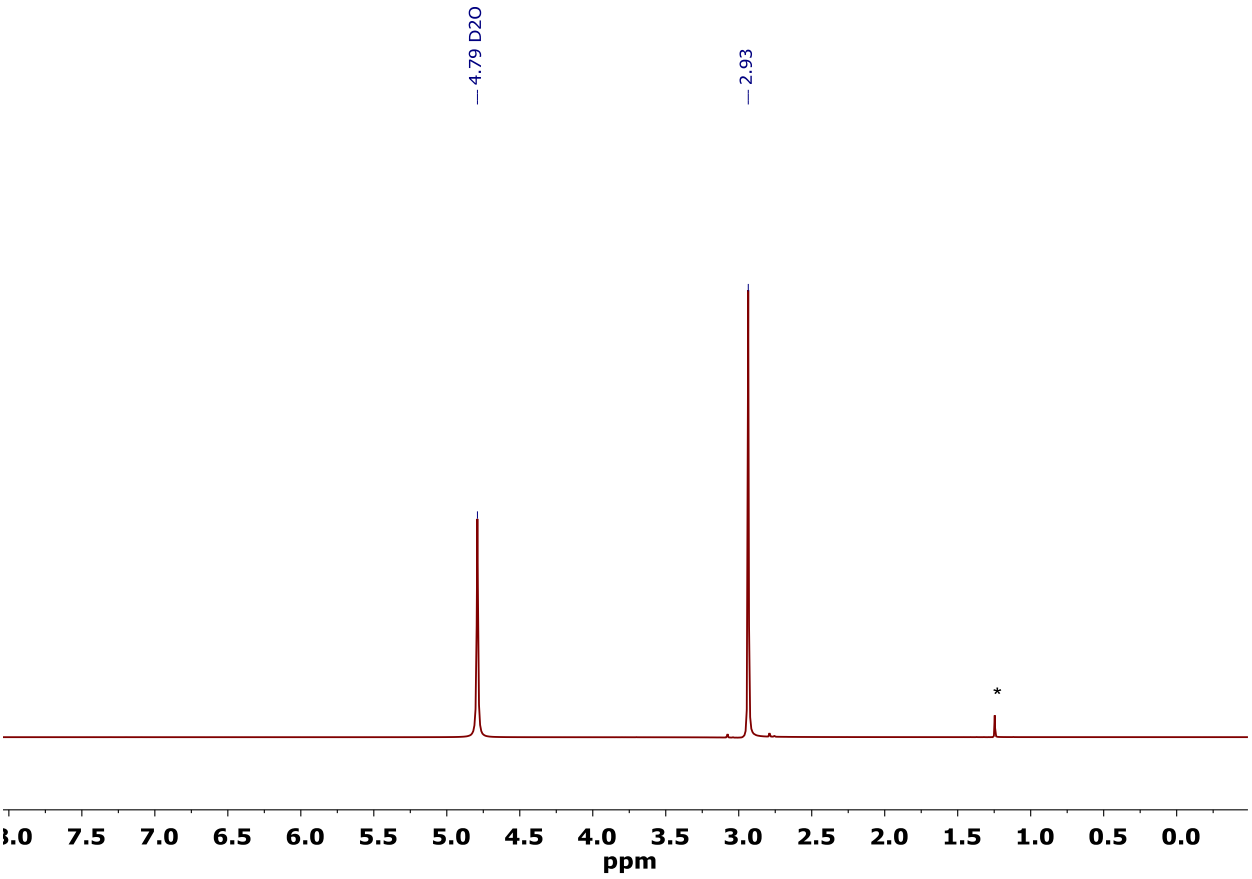
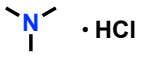


Figure S29. ^{1}H NMR (500 MHz) spectrum of trimethylamine hydrochloride in D_2O. * = residual $O(Bpin)_2$.

1. 

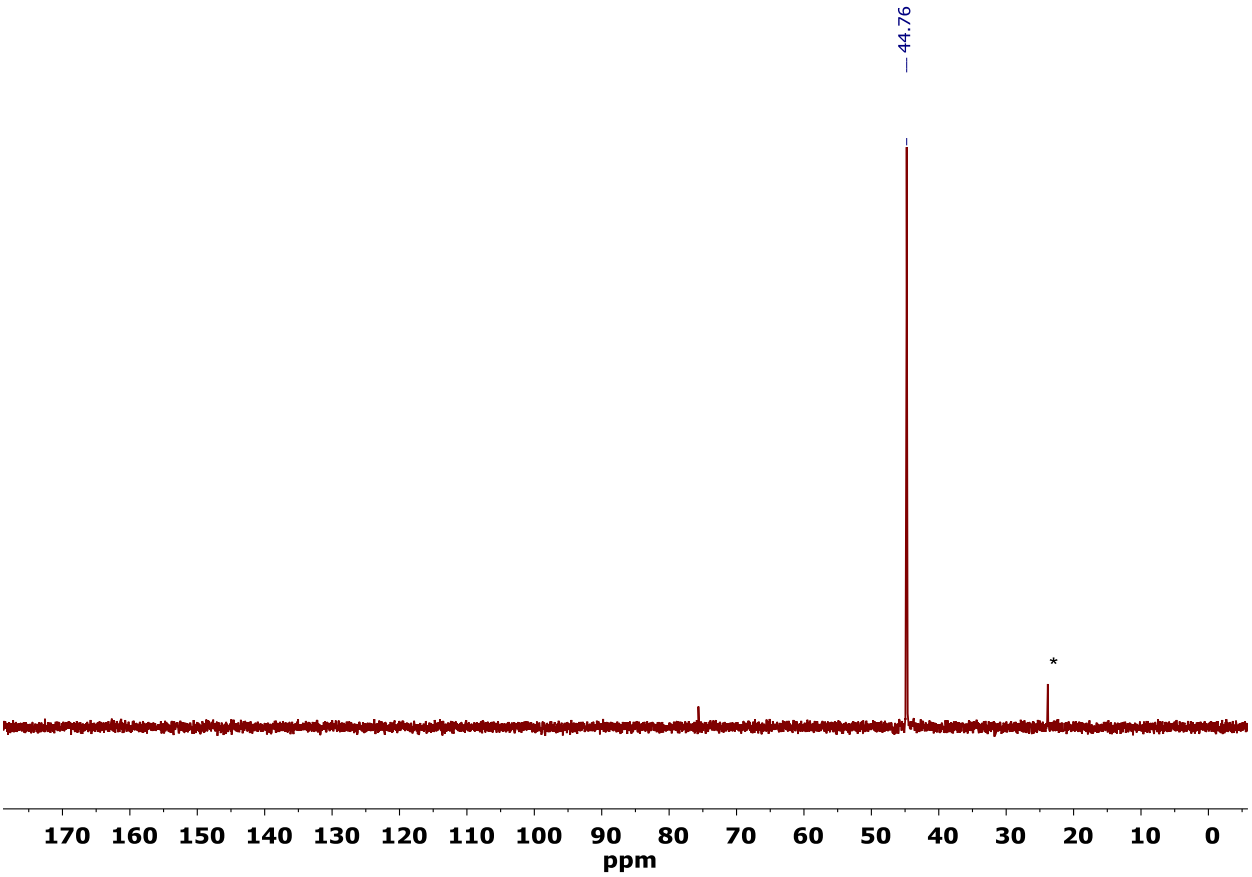


Figure S30. ^{13}C NMR (125 MHz) spectrum of trimethylamine hydrochloride in D_2O. * = residual $O(Bpin)_2$.

2. 

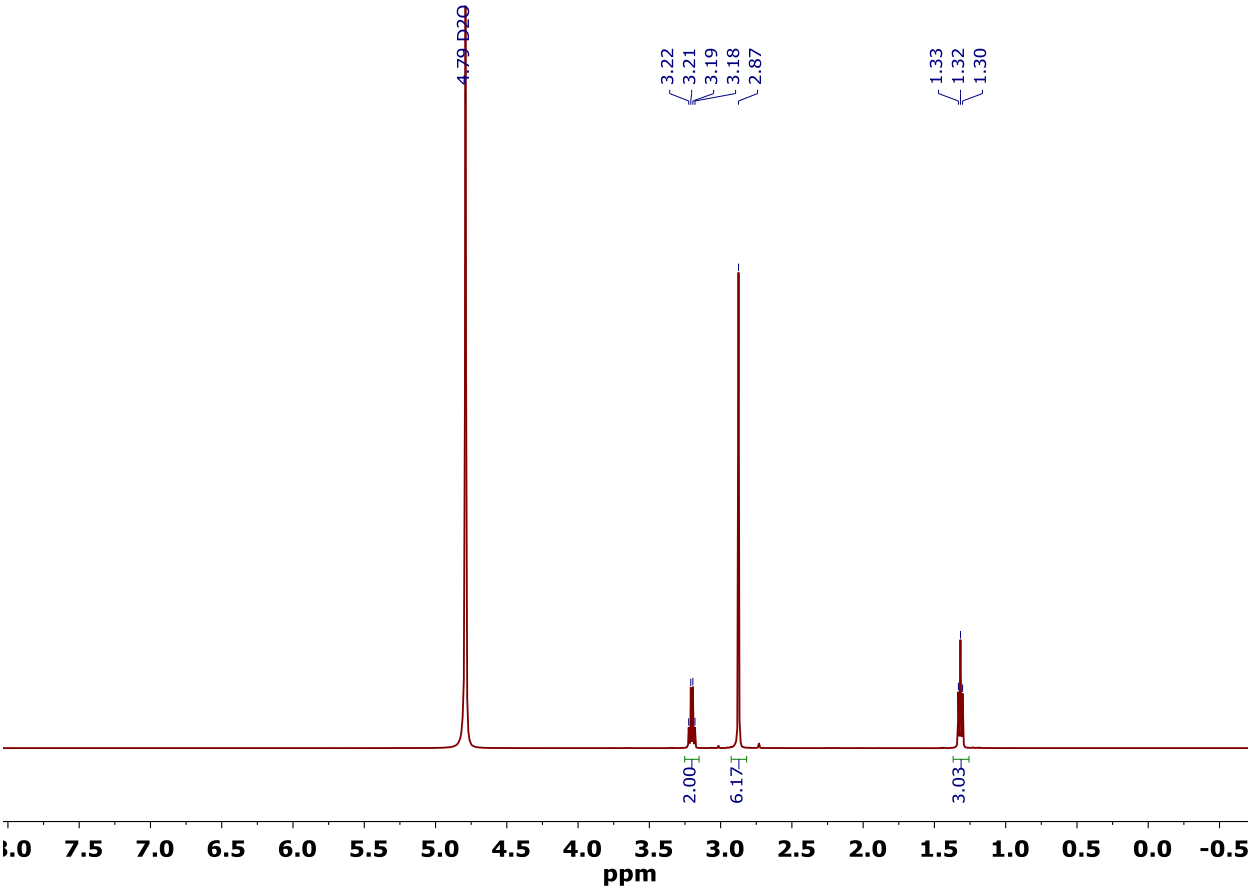


Figure S31. ^{1}H NMR (500 MHz) spectrum of *N,N*-dimethylethylamine hydrochloride in D_2O.

2. 

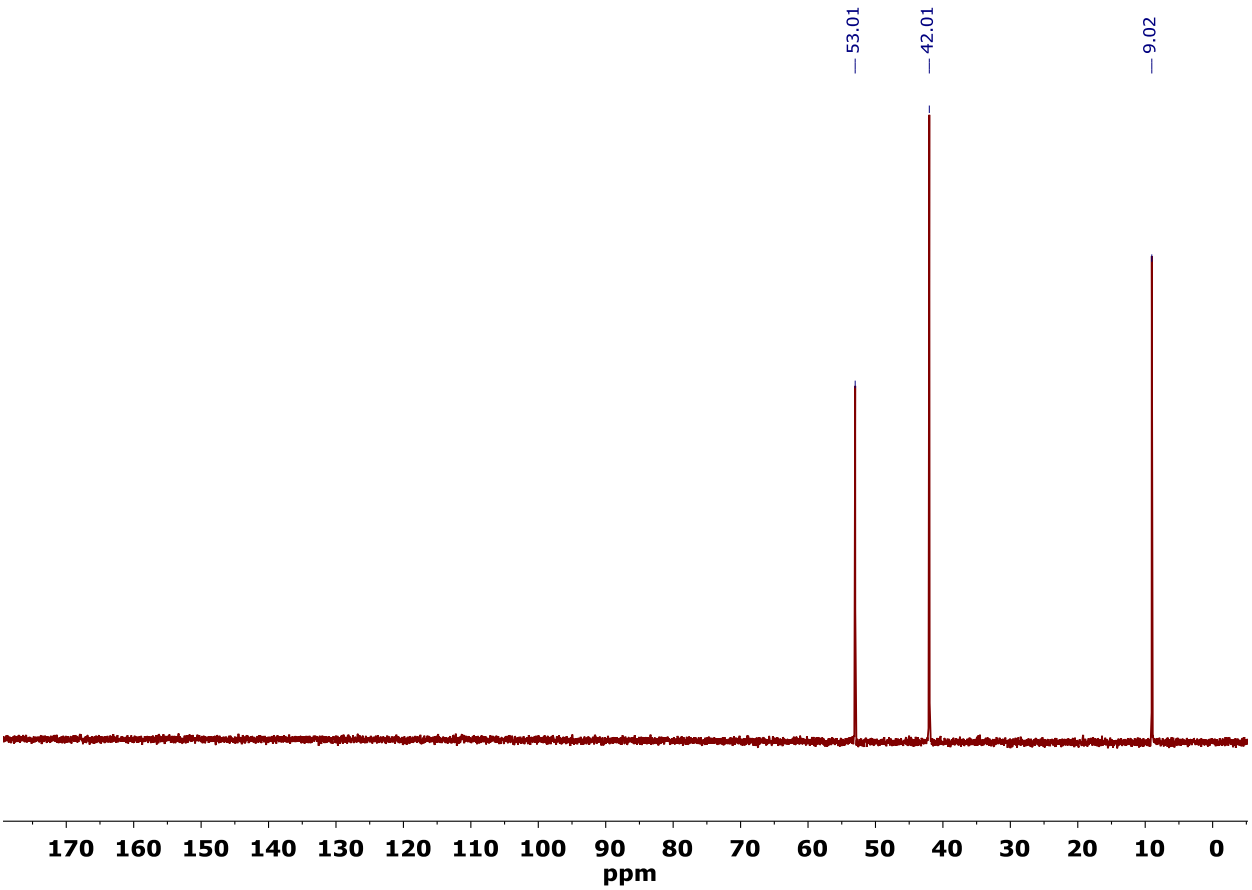
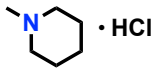


Figure S32. ^{13}C NMR (125 MHz) spectrum of *N,N*-dimethylethylamine hydrochloride in D_2O.

3. 

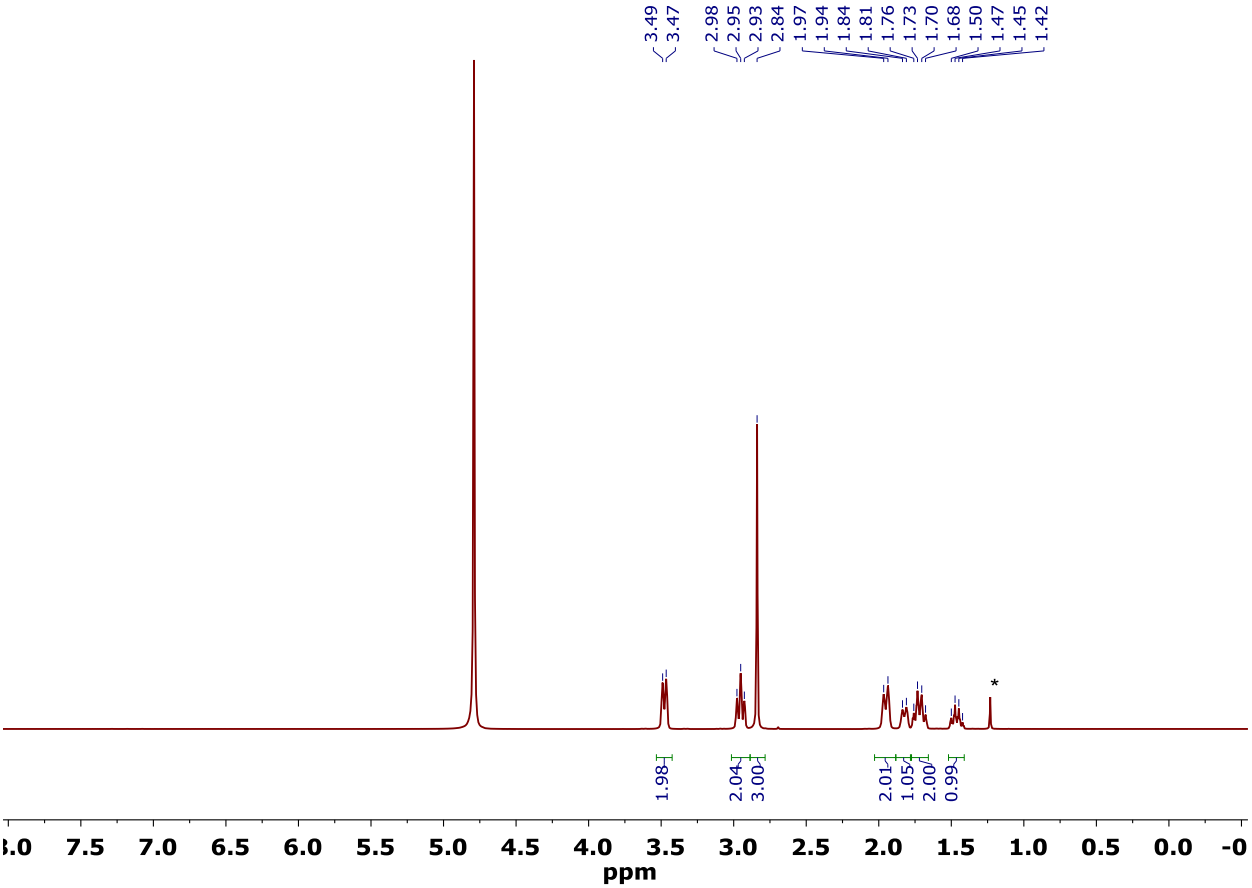
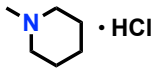


Figure S33. ^{1}H NMR (500 MHz) spectrum of *N*-methylpiperidine hydrochloride in D_2O. * = residual $O(Bpin)_2$.

3. 

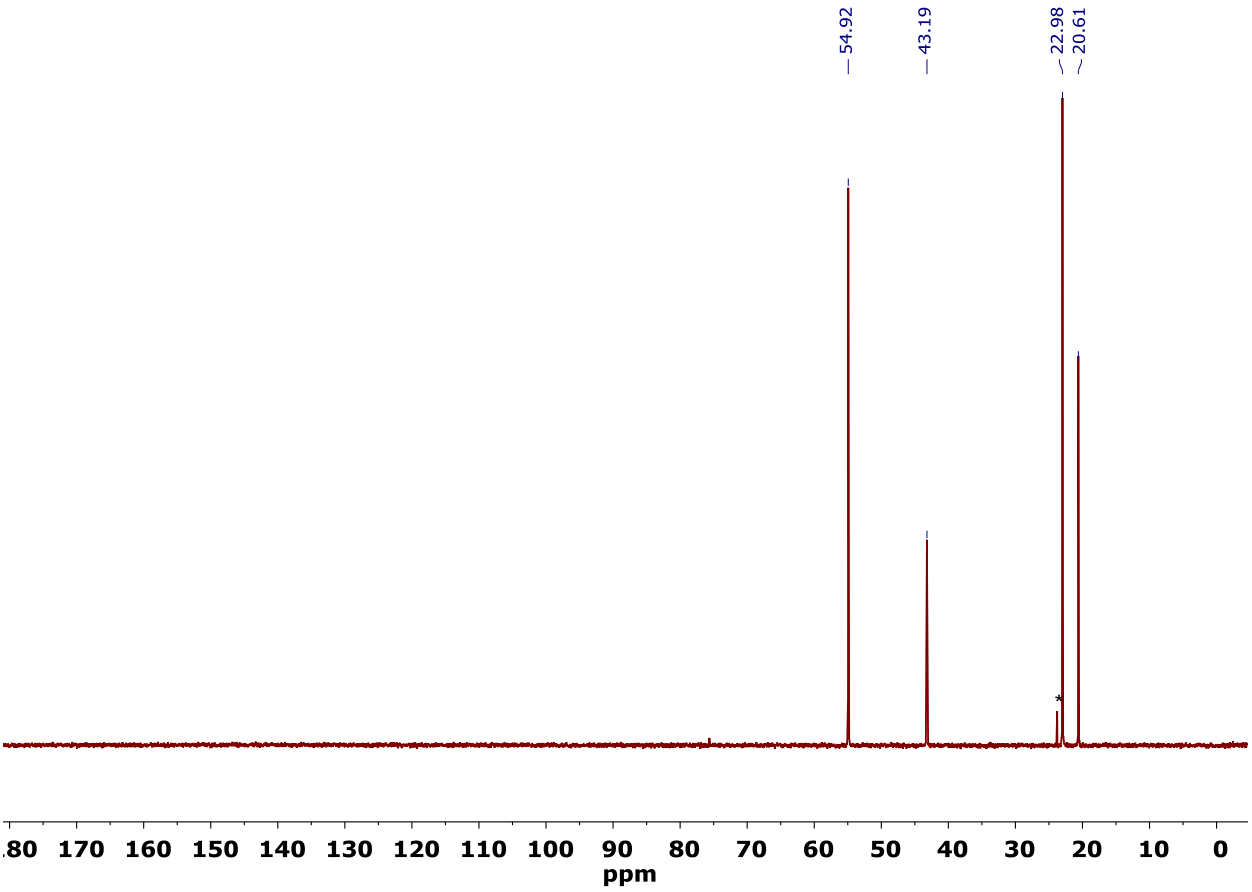
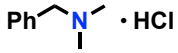


Figure S34. ^{13}C NMR (125 MHz) spectrum of *N*-methylpiperidine hydrochloride in D_2O. * = residual $O(Bpin)_2$.

4. 

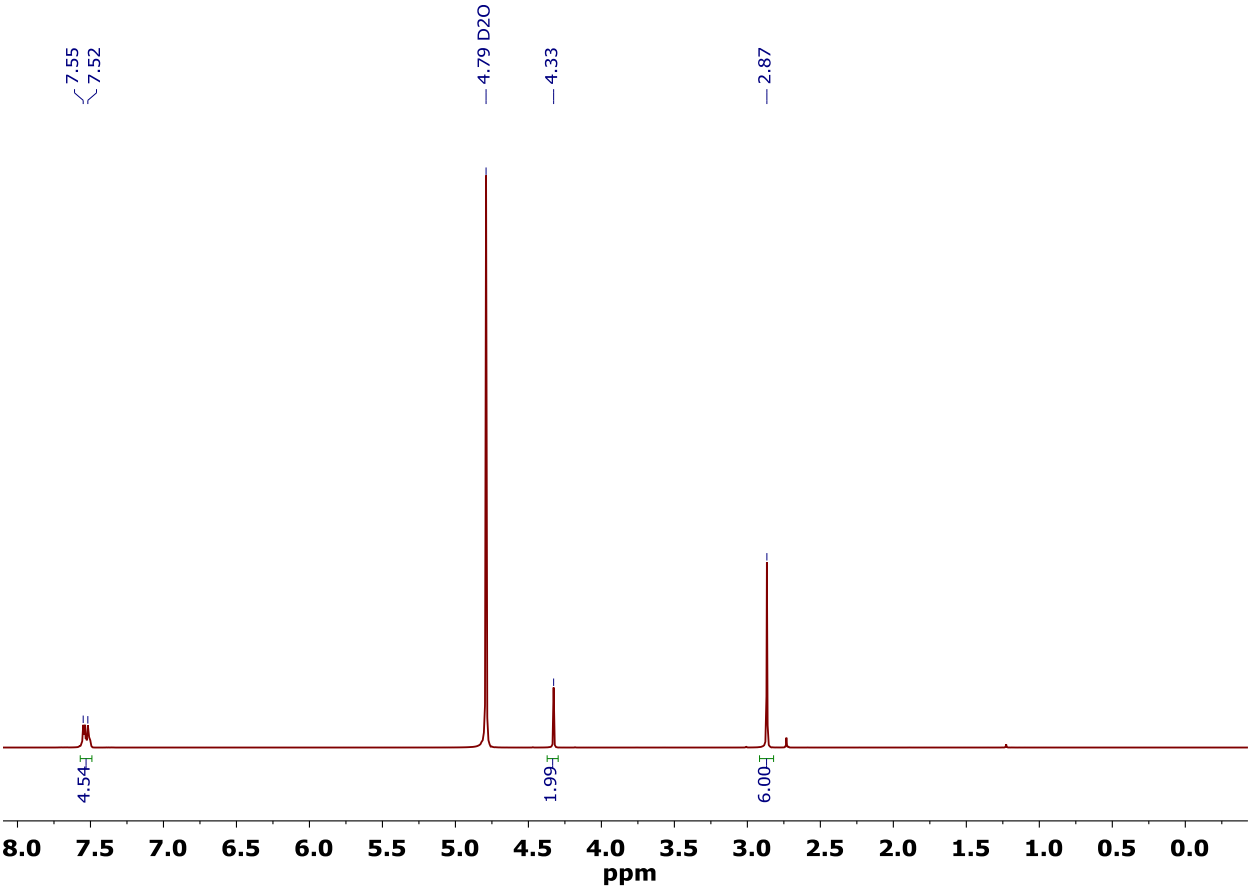
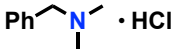


Figure S35. ^{1}H NMR (500 MHz) spectrum of *N,N*-dimethylbenzylamine hydrochloride in D_2O.

4. 

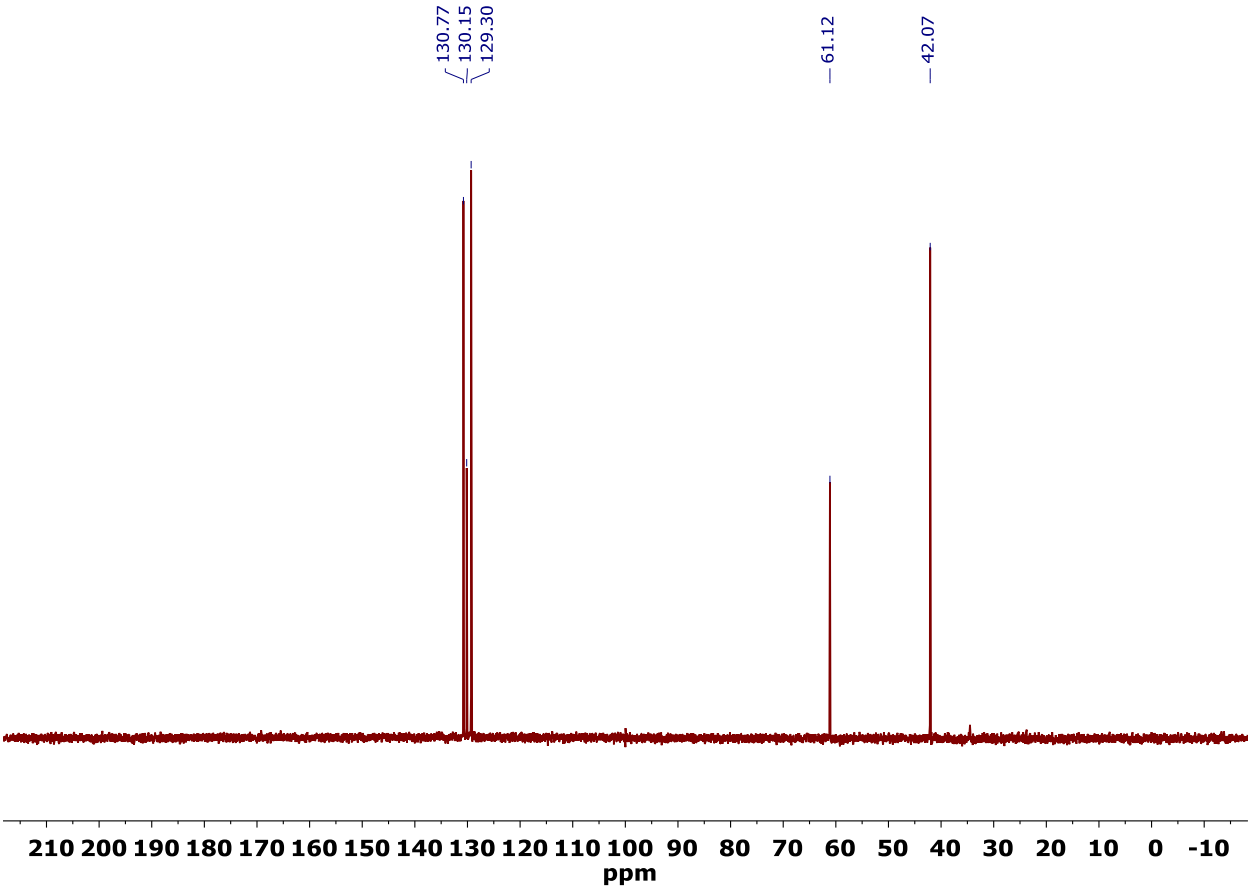
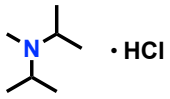


Figure S36. ^{13}C NMR (125 MHz) spectrum of *N,N*-dimethylbenzylamine hydrochloride in D_2O.

5. 

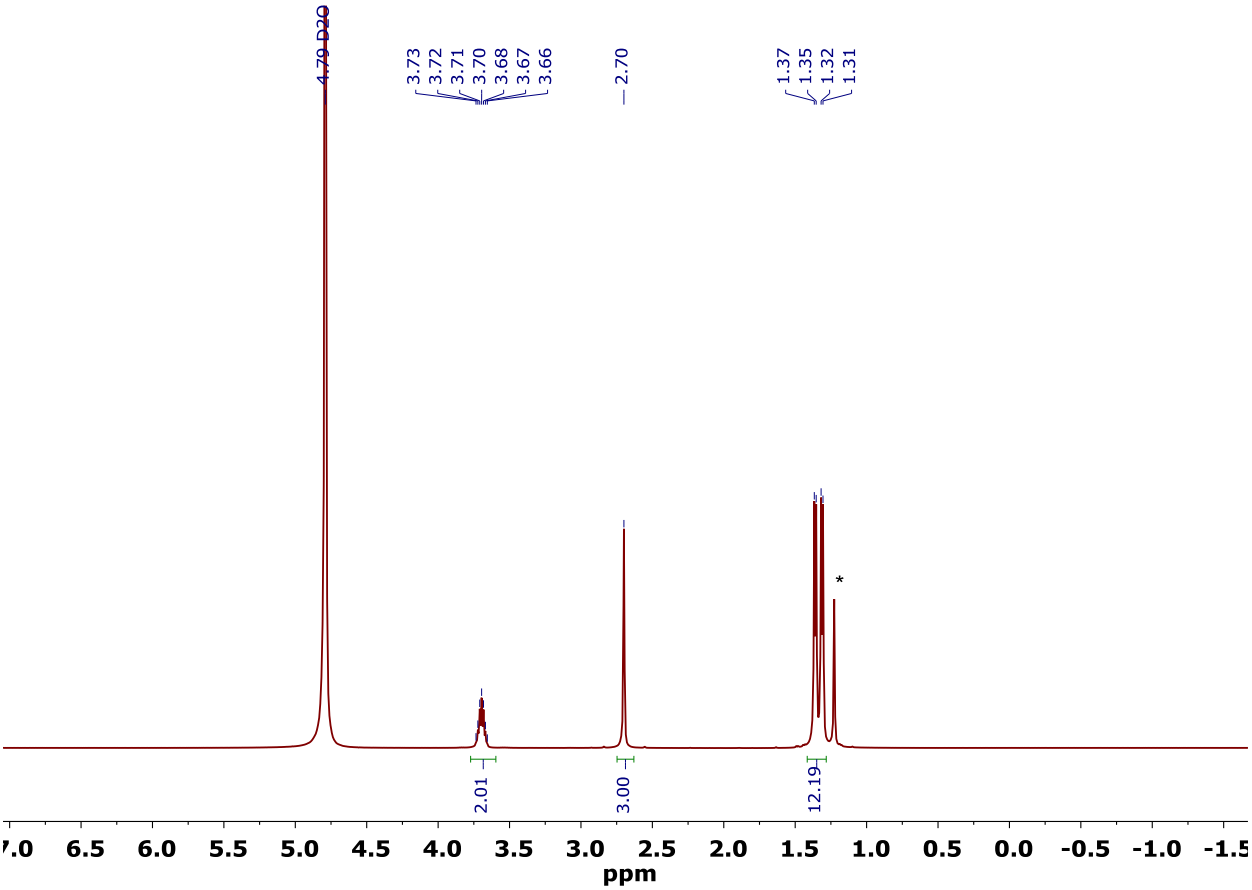
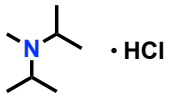


Figure S37. ^{1}H NMR (500 MHz) spectrum of *N,N*-diisopropylmethylamine hydrochloride in D_2O. * = residual $O(Bpin)_2$.

5. 

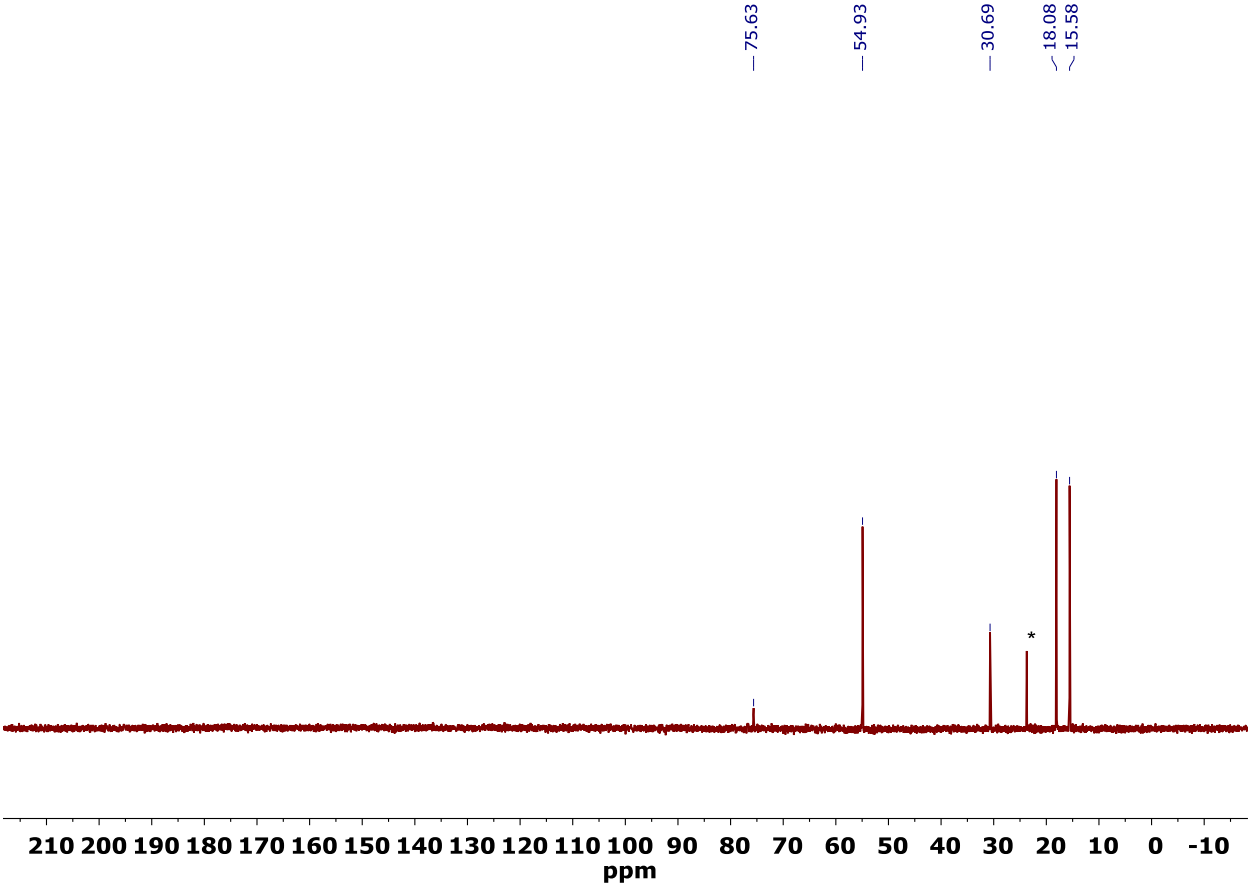
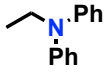


Figure S38. ^{13}C NMR (125 MHz) spectrum of *N,N*-diisopropylmethylamine hydrochloride in D_2O. * = residual $O(Bpin)_2$.

6. 

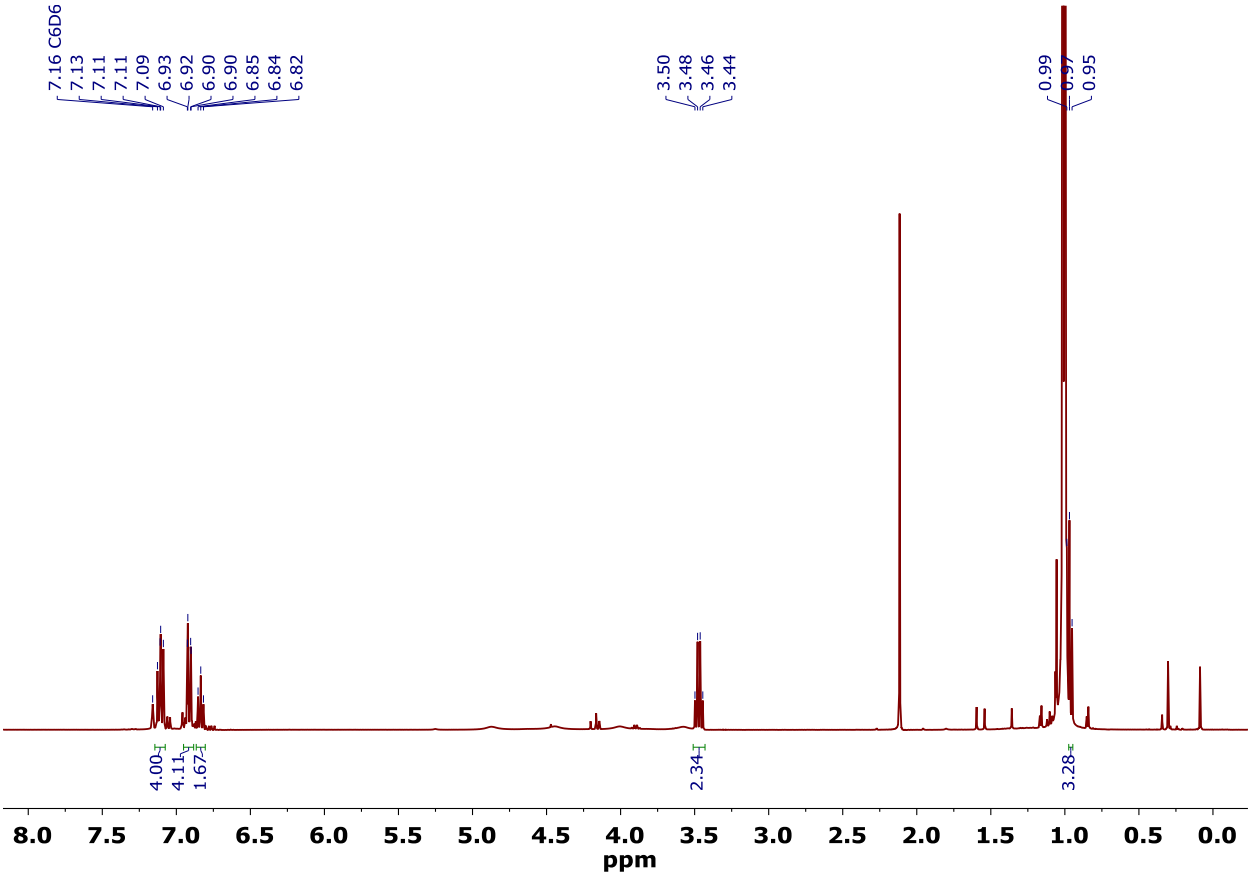
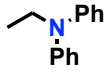


Figure S39. ^{1}H NMR (500 MHz) spectrum of *N,N*-diphenylethylamine in C_6D_6.

6. 

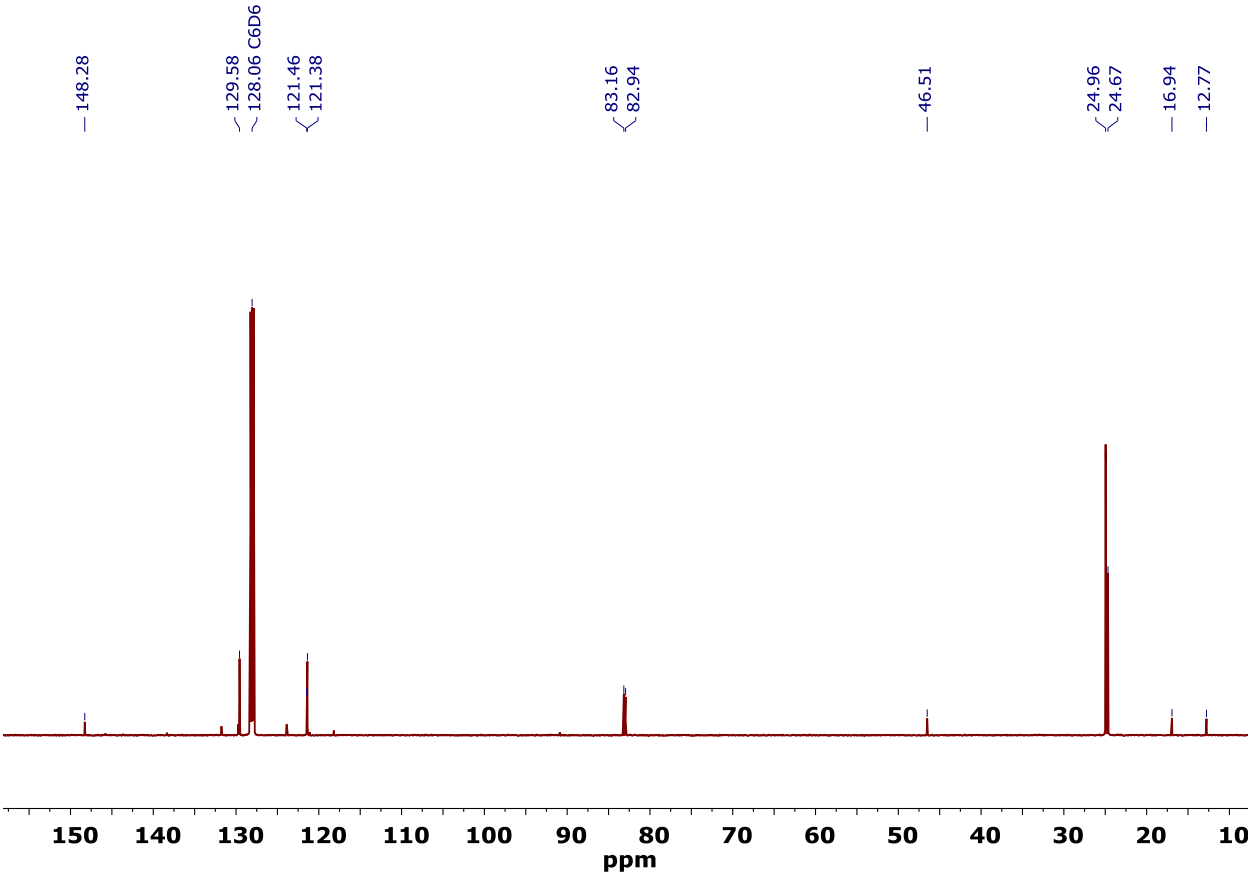
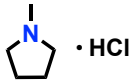


Figure S40. ^{13}C NMR (125 MHz) spectrum of *N,N*-diphenylethylamine in C_6D_6.

7. 

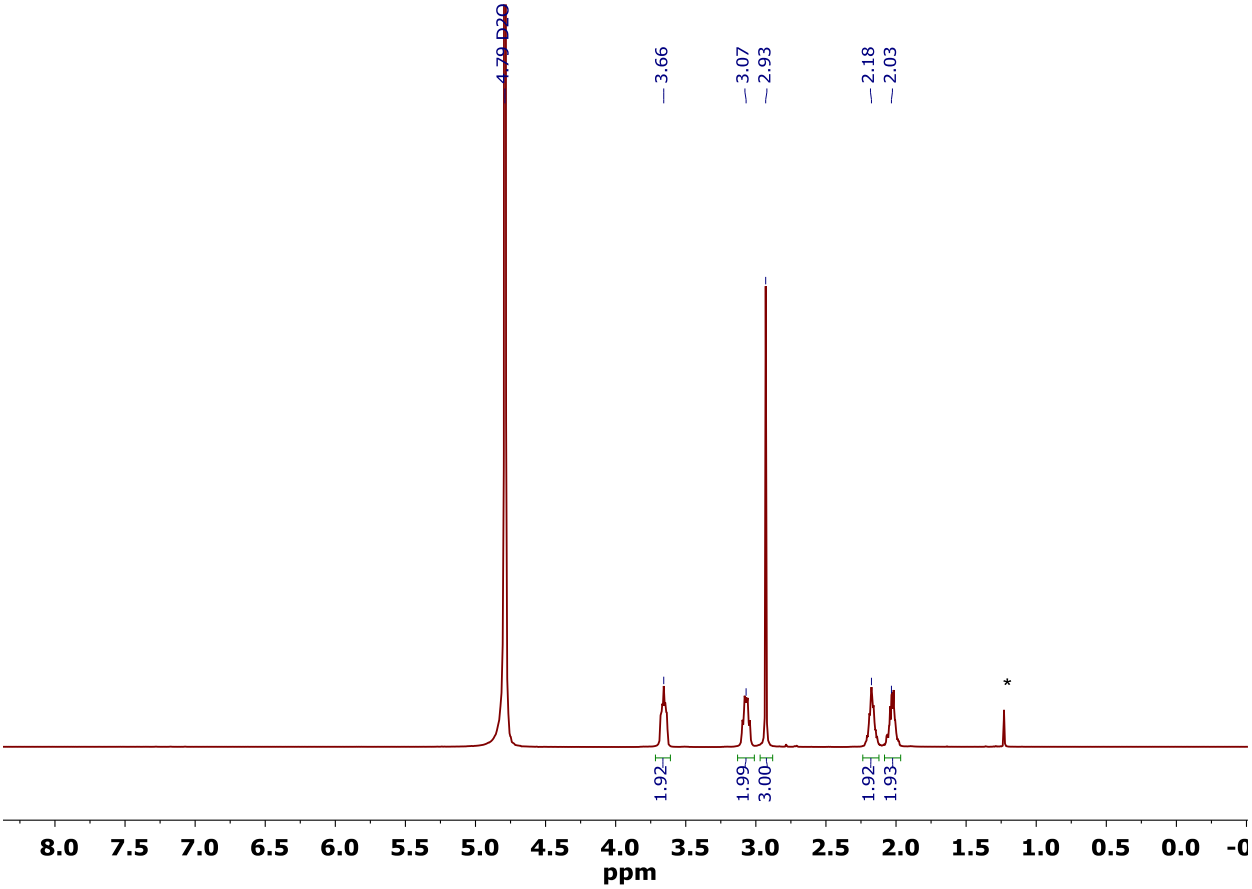
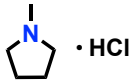


Figure S41. ^{1}H NMR (500 MHz) spectrum of *N*-methylpyrrolidine hydrochloride in D_2O. * = residual $O(Bpin)_2$.

7. 

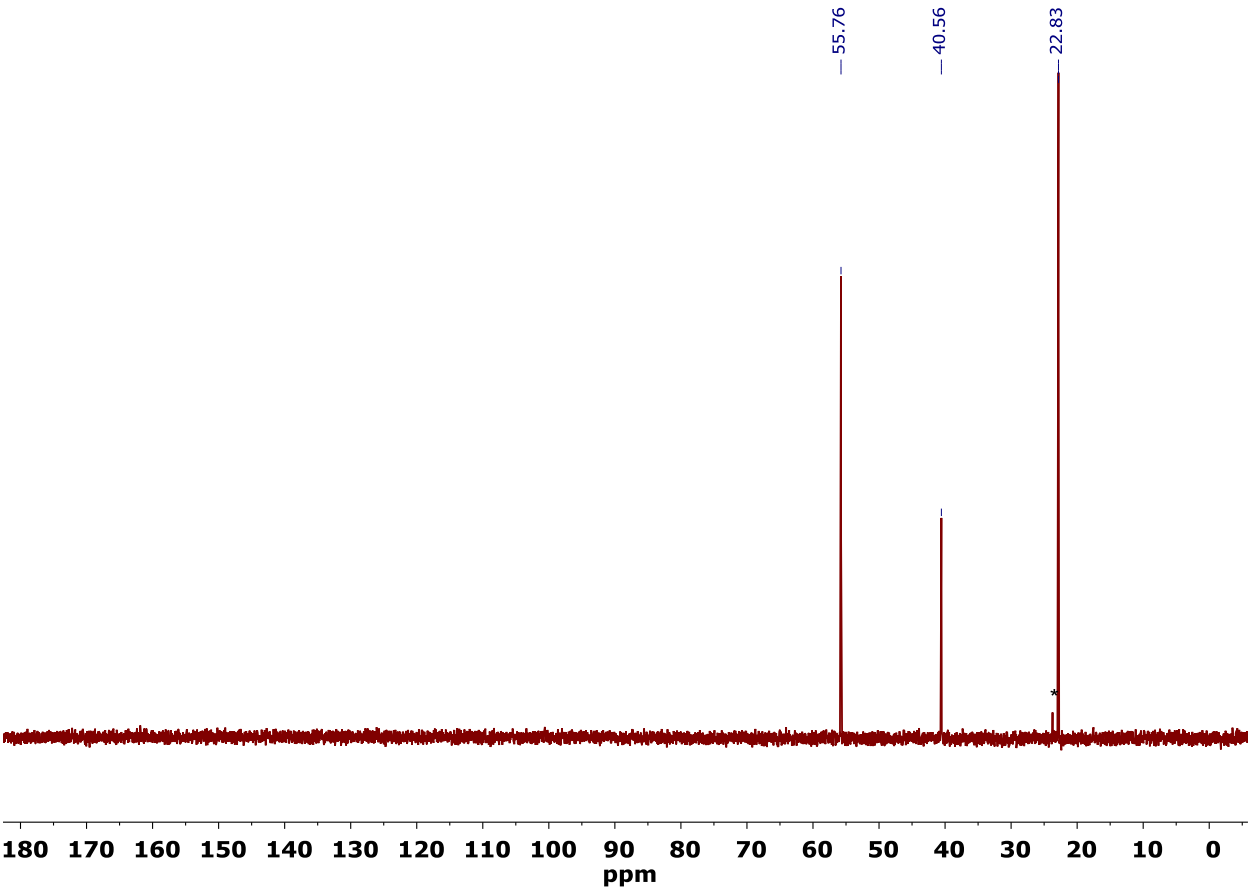
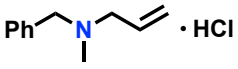


Figure S42. ^{13}C NMR (125 MHz) spectrum of *N*-methylpyrrolidine hydrochloride in D_2O. * = residual $O(Bpin)_2$.

8. 

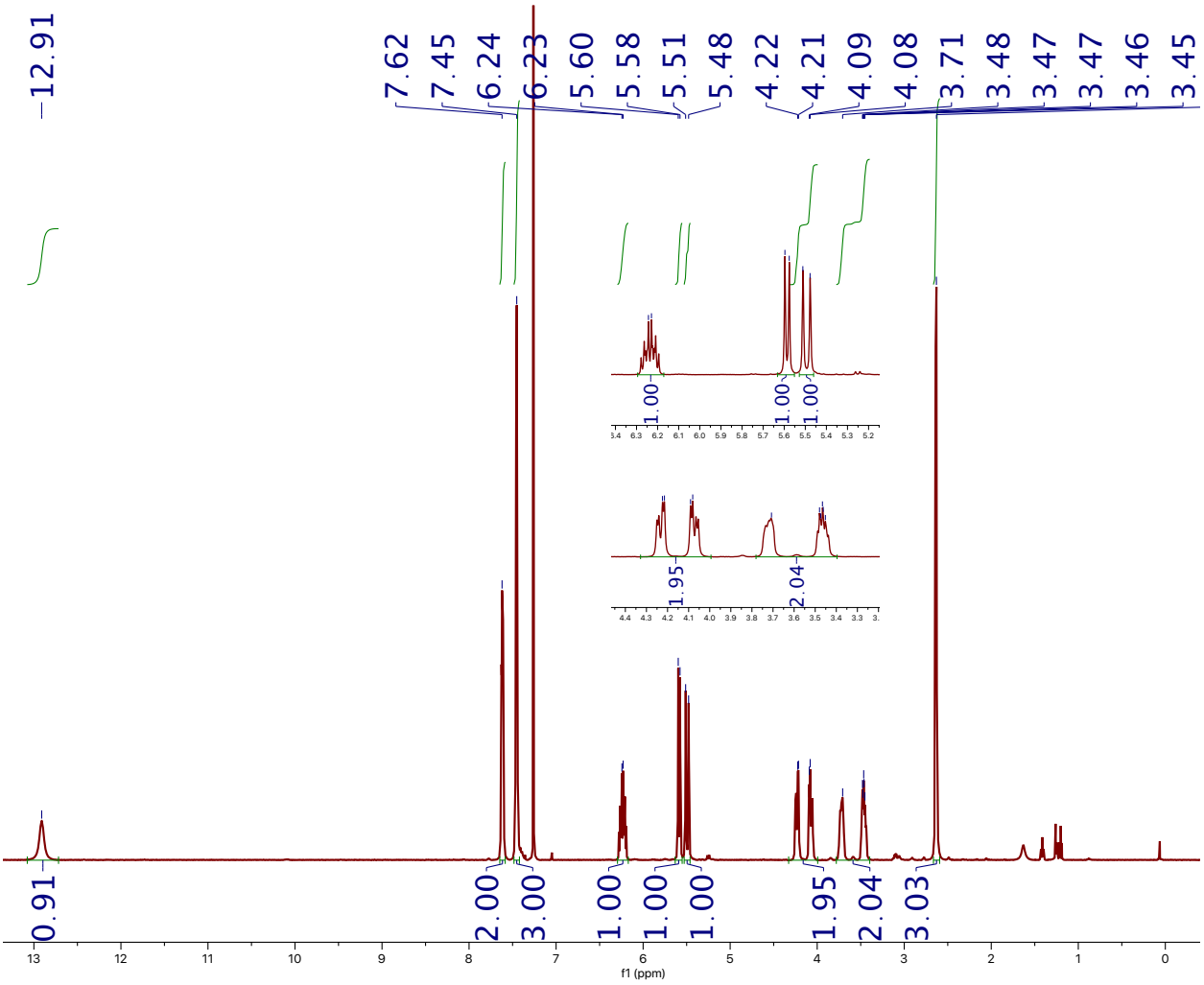
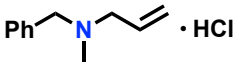


Figure S43. [1]H NMR (500 MHz) spectrum of *N*-methyl-*N*-allylbenzamide hydrochloride in $CDCl_3$.

8. 

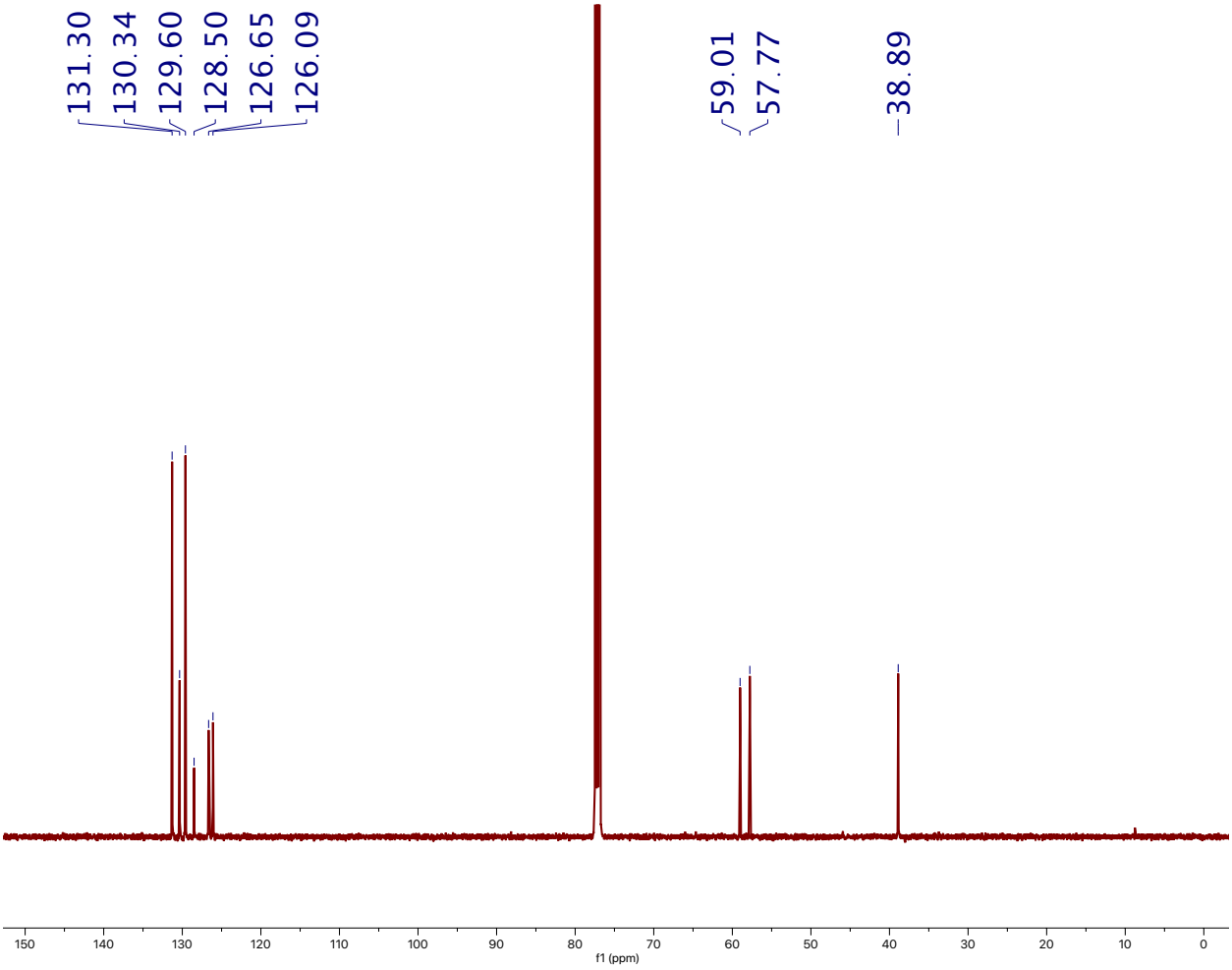


Figure S44. ^{13}C NMR (125 MHz) spectrum of *N*-methyl-*N*-allylbenzamide hydrochloride in $CDCl_3$.

9. 

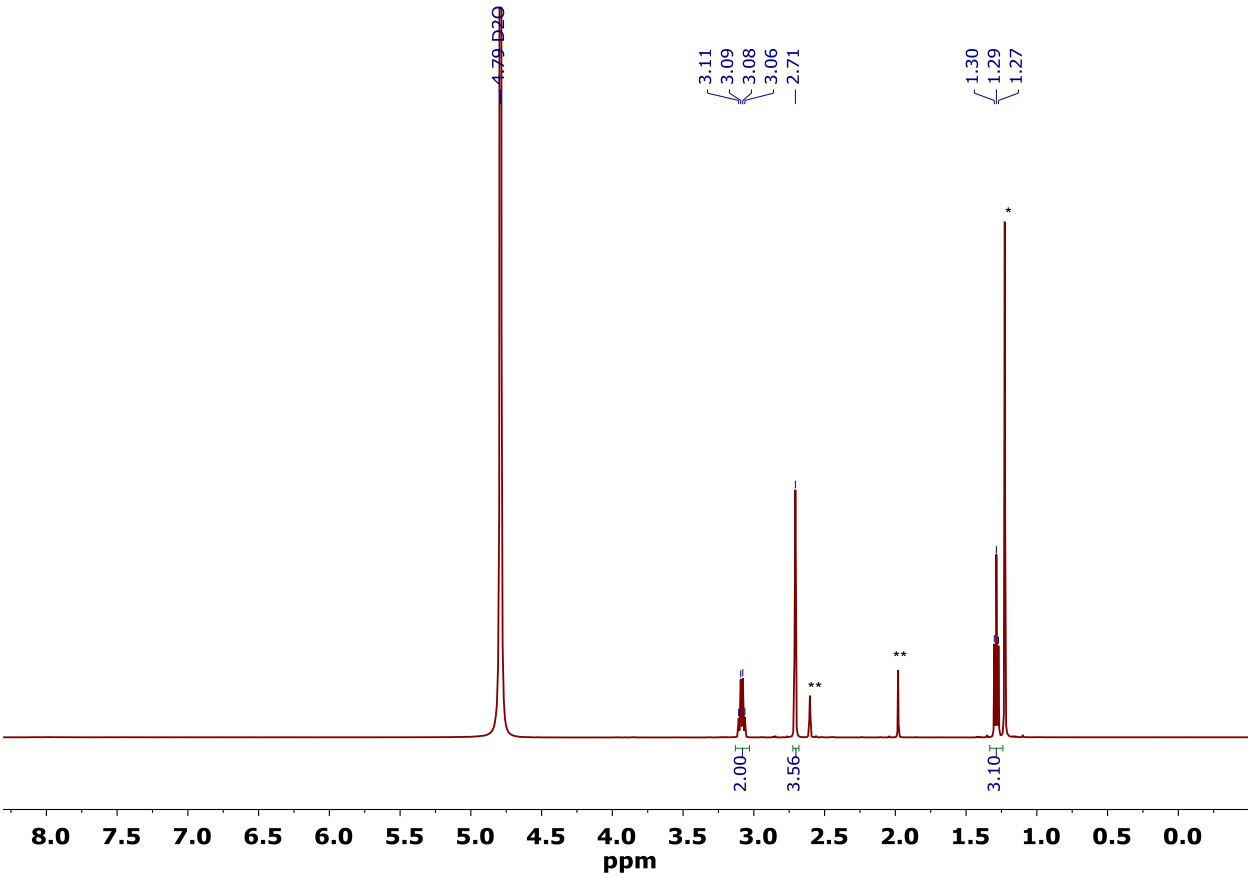


Figure S45. ^{1}H NMR (500 MHz) spectrum of *N*-methylethylamine hydrochloride in D_2O. * = residual $O(Bpin)_2$. ** = trace starting material.

9. 

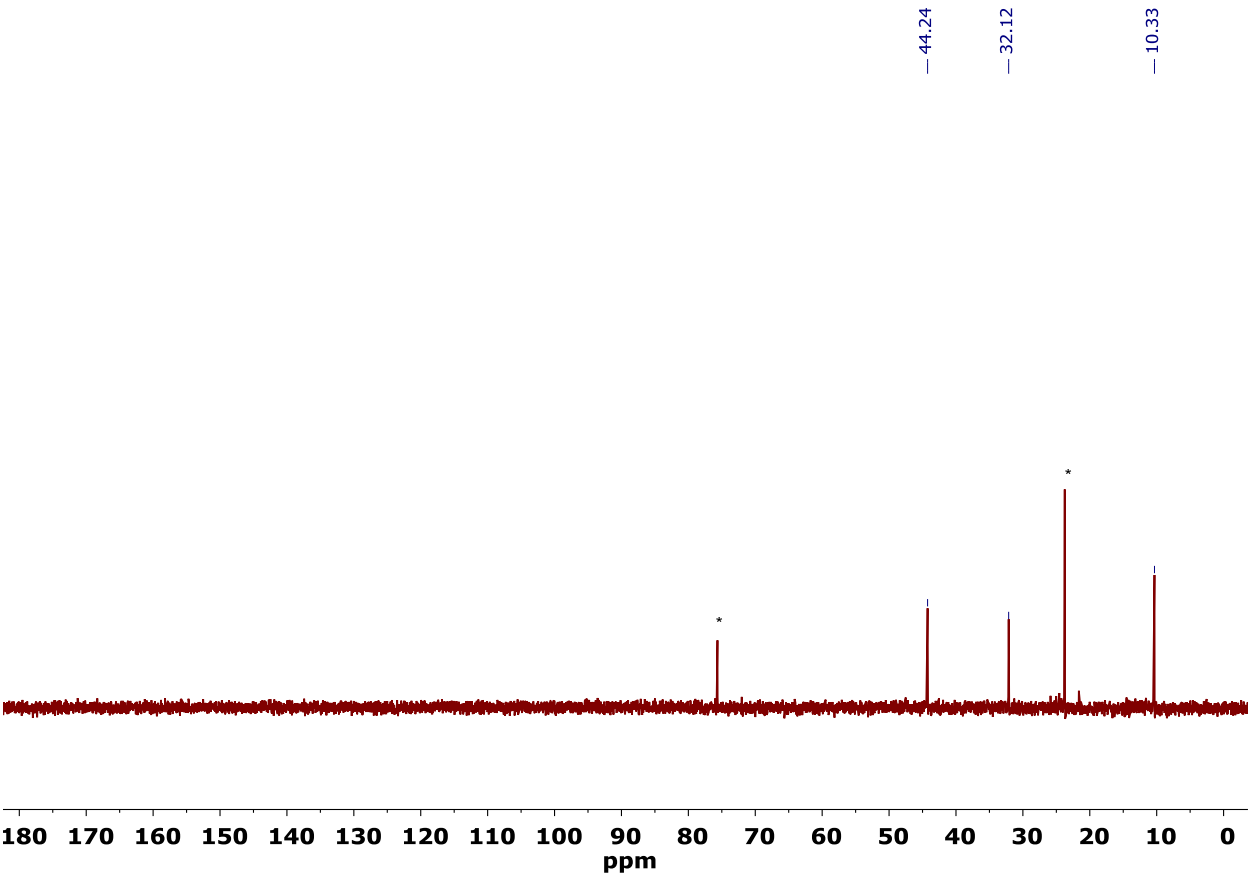
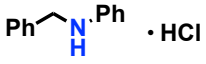


Figure S46. ^{13}C NMR (125 MHz) spectrum of *N*-methylethylamine hydrochloride in D_2O. * = residual $O(Bpin)_2$.

10. 

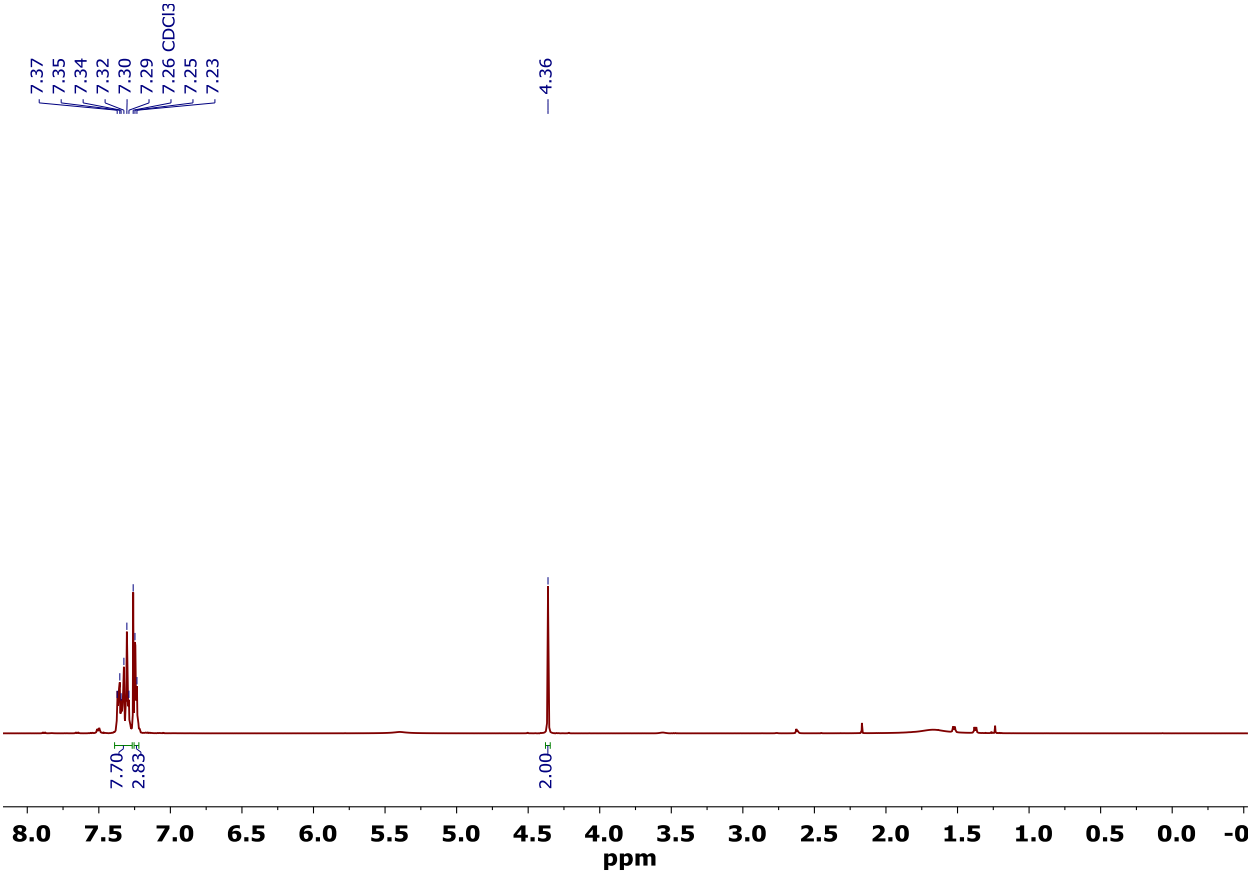
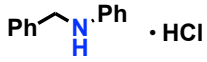


Figure S47. ^{1}H NMR (500 MHz) spectrum of *N*-phenylbenzylamine hydrochloride in $CDCl_3$.

10. 

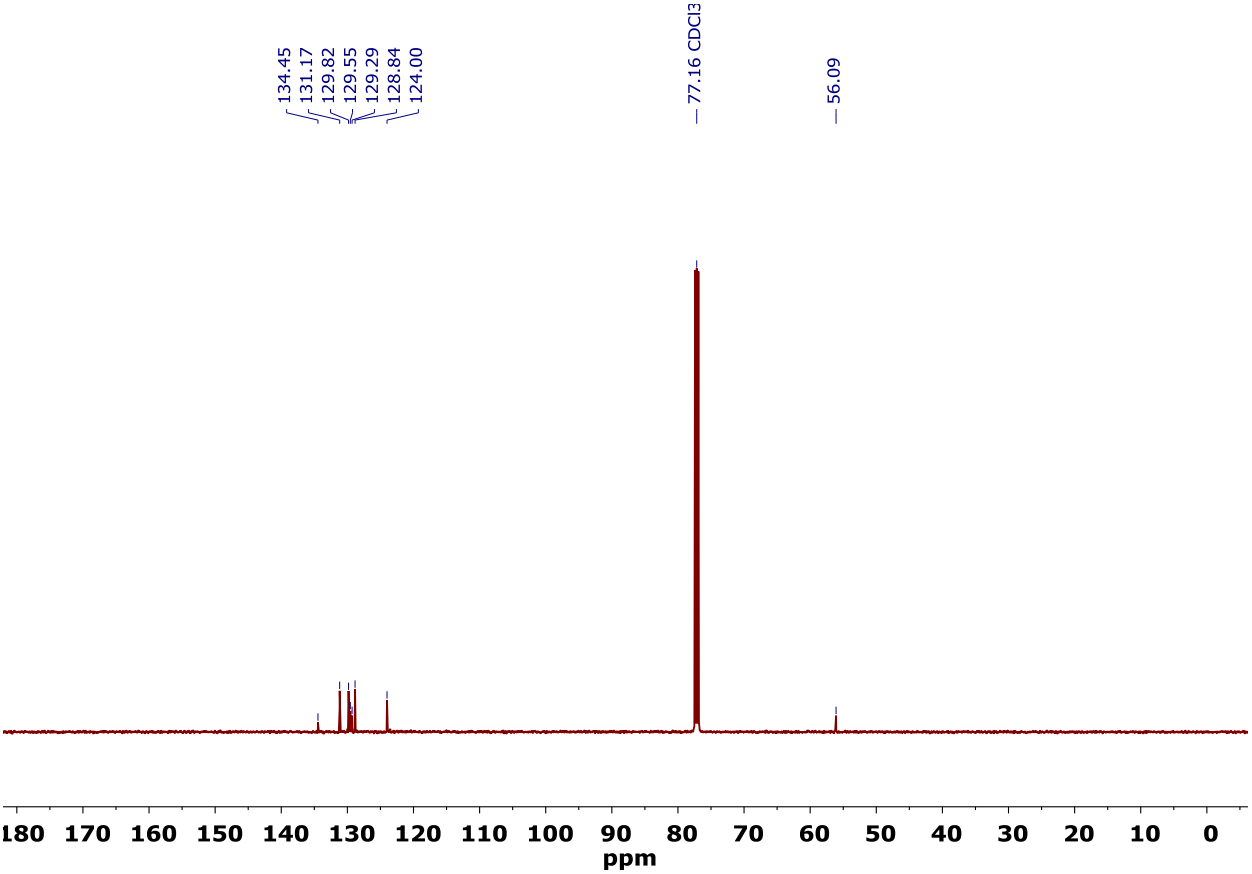
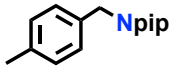


Figure S48. ^{13}C NMR (125 MHz) spectrum of *N*-phenylbenzylamine hydrochloride in $CDCl_3$.

12. 

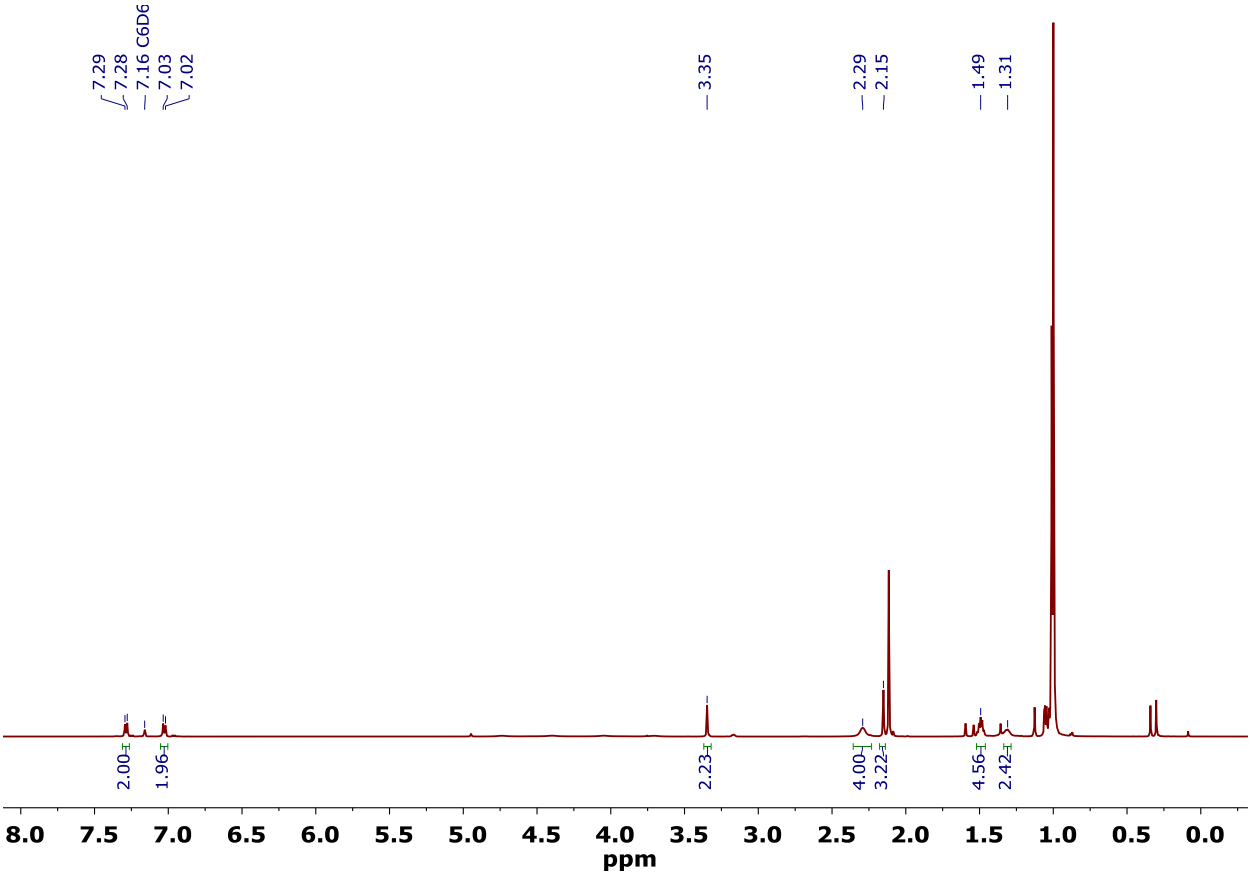
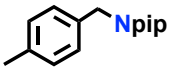


Figure S49. ^{1}H NMR (500 MHz) spectrum of *N,N*-piperidyl-1-*p*-tolylmethanamine in C_6D_6.

12. 

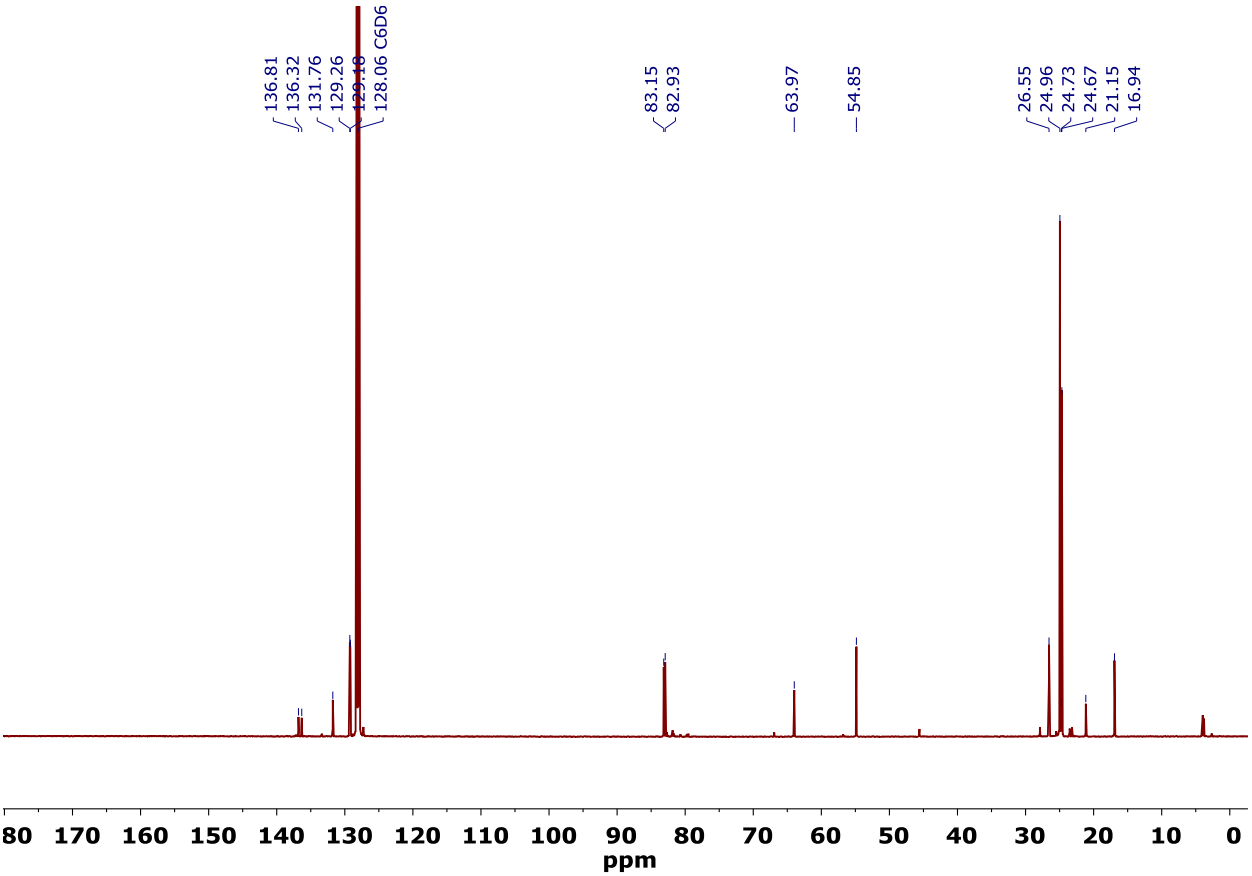
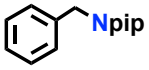


Figure S50. ^{13}C NMR (125 MHz) spectrum of *N,N*-piperidyl-1-*p*-tolylmethanamine in C_6D_6.

13. 

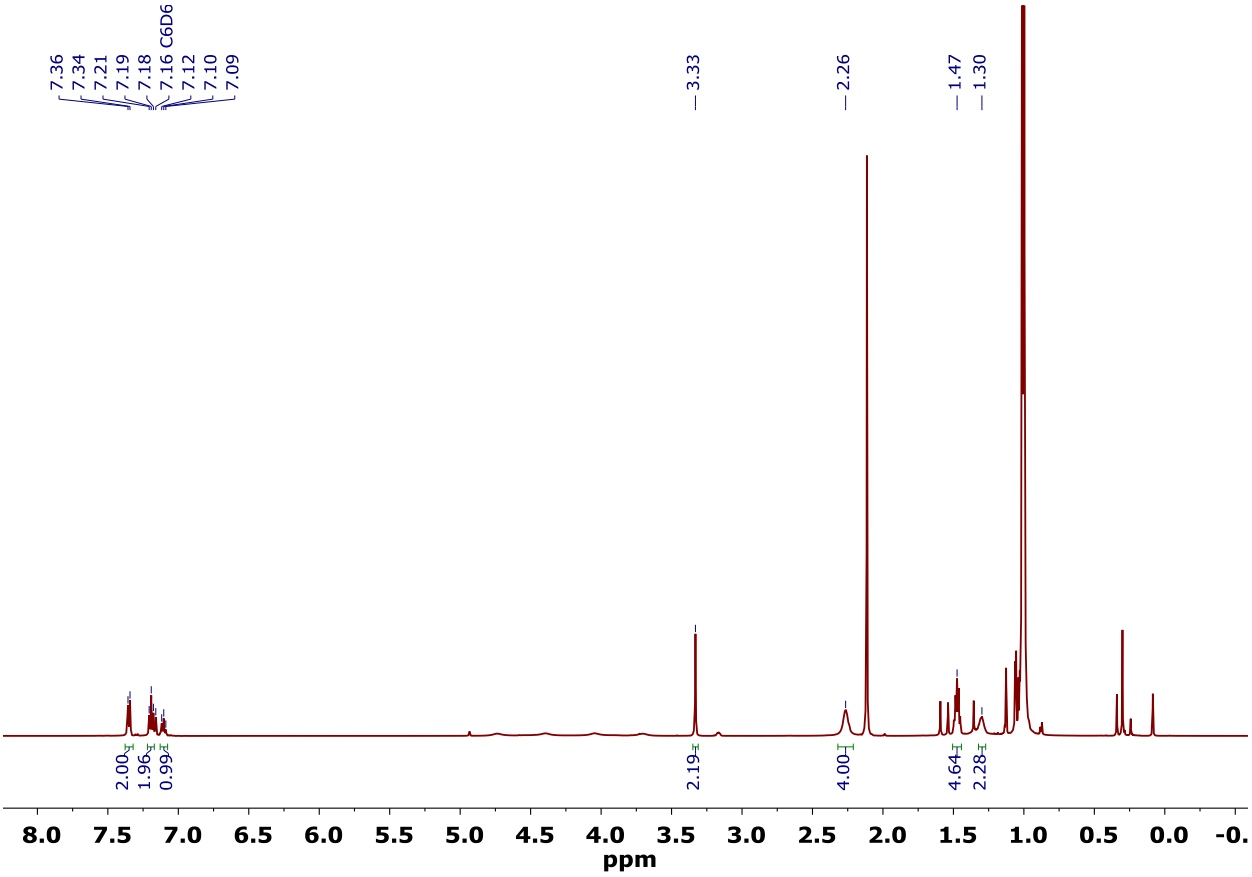
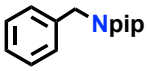


Figure S51. ^{1}H NMR (500 MHz) spectrum of *N,N*-piperidylbenzylamine in C_6D_6.

13. 

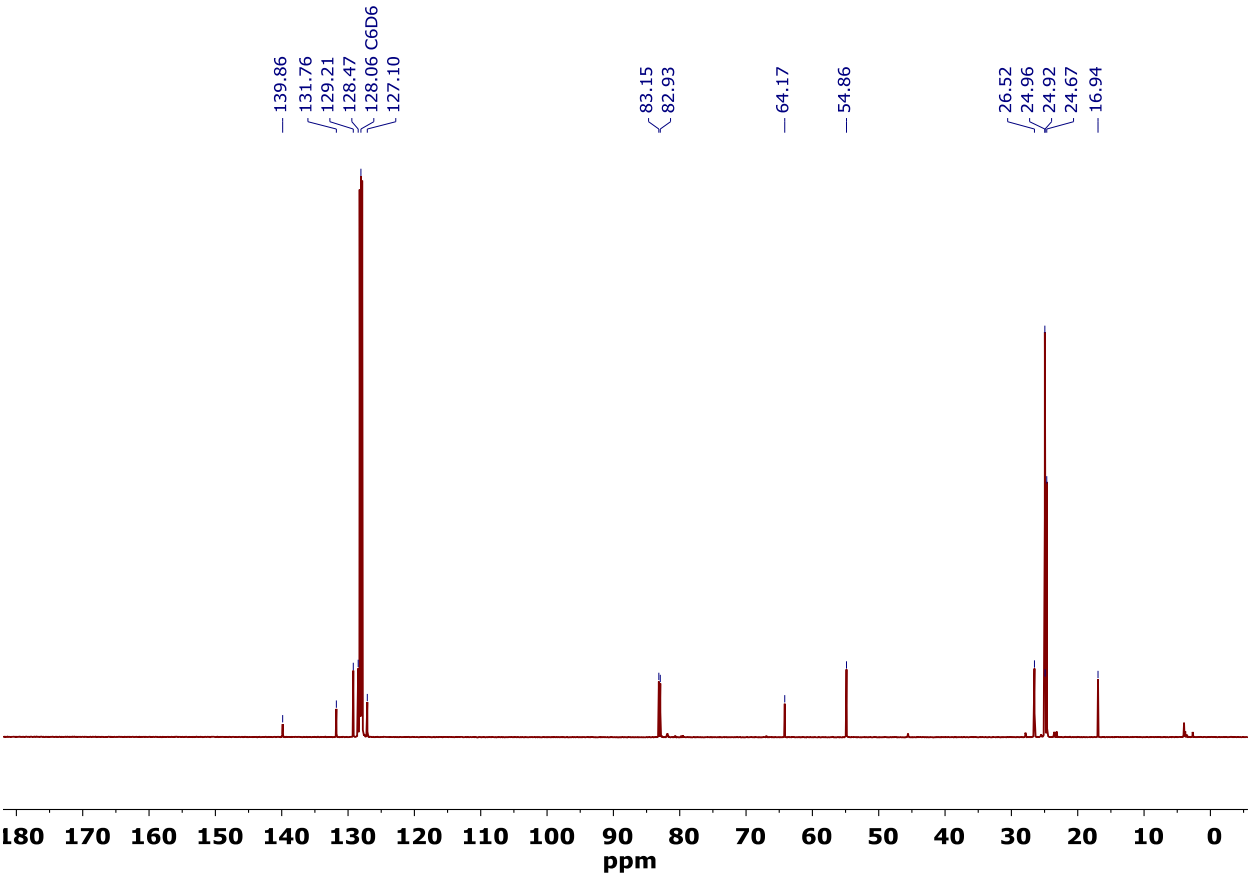
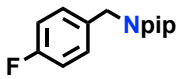


Figure S52. ^{13}C NMR (125 MHz) spectrum of *N,N*-piperidylbenzylamine in C_6D_6.

14. 

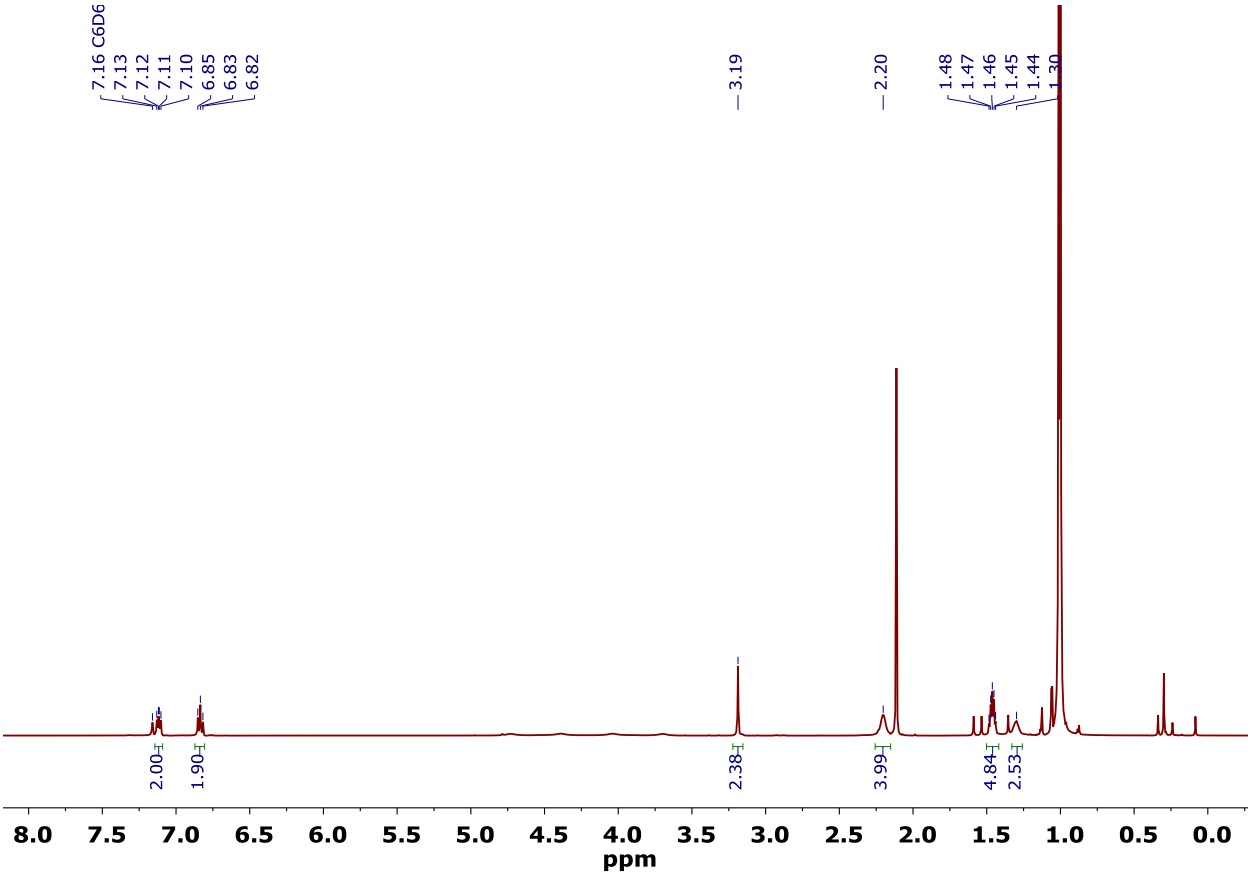
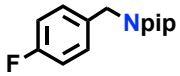


Figure S53. ^{1}H NMR (500 MHz) spectrum of *N,N*-piperidyl-1-(4-fluorobenzyl)amine in C_6D_6.

14. 

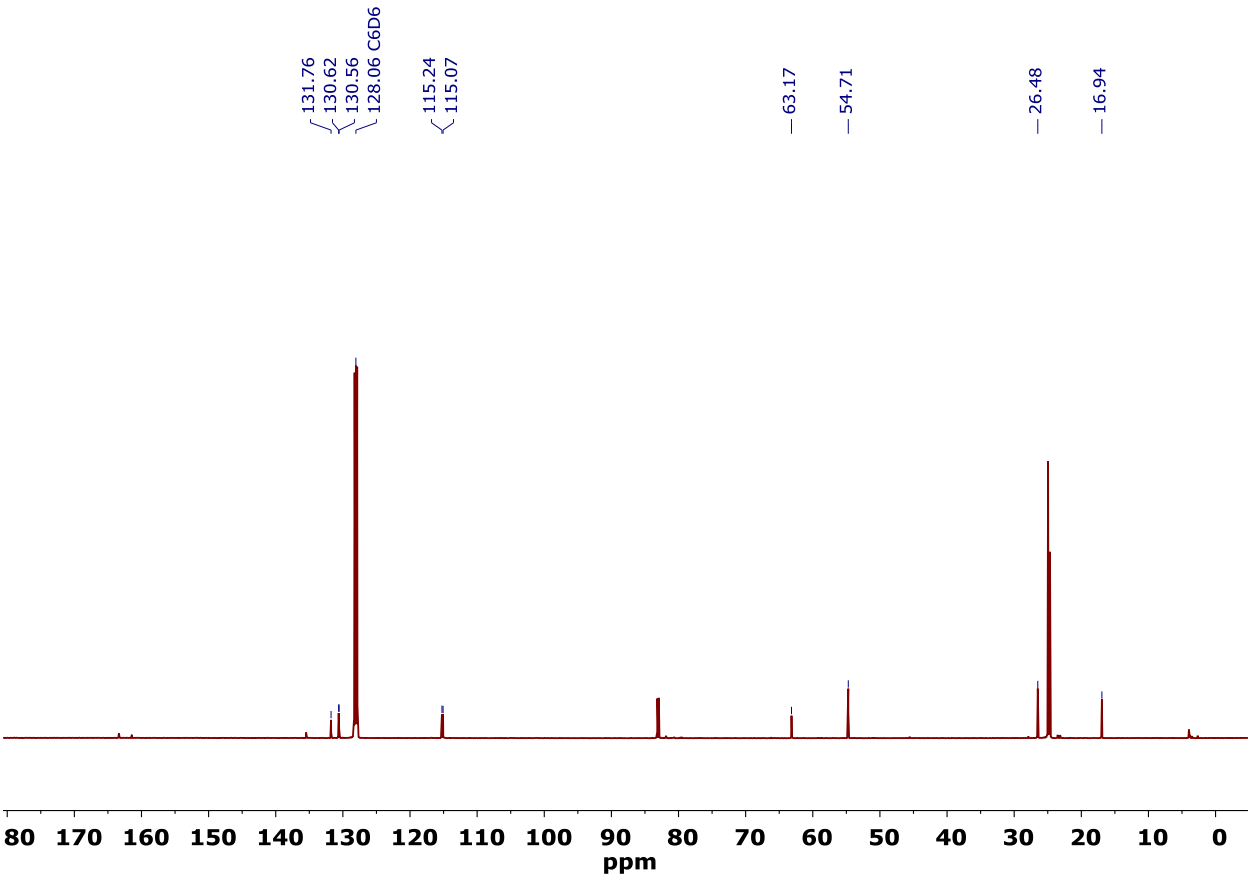
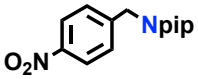


Figure S54. ^{13}C NMR (125 MHz) spectrum of *N,N*-piperidyl-1-(4-fluorobenzyl)amine in C_6D_6.

15. 

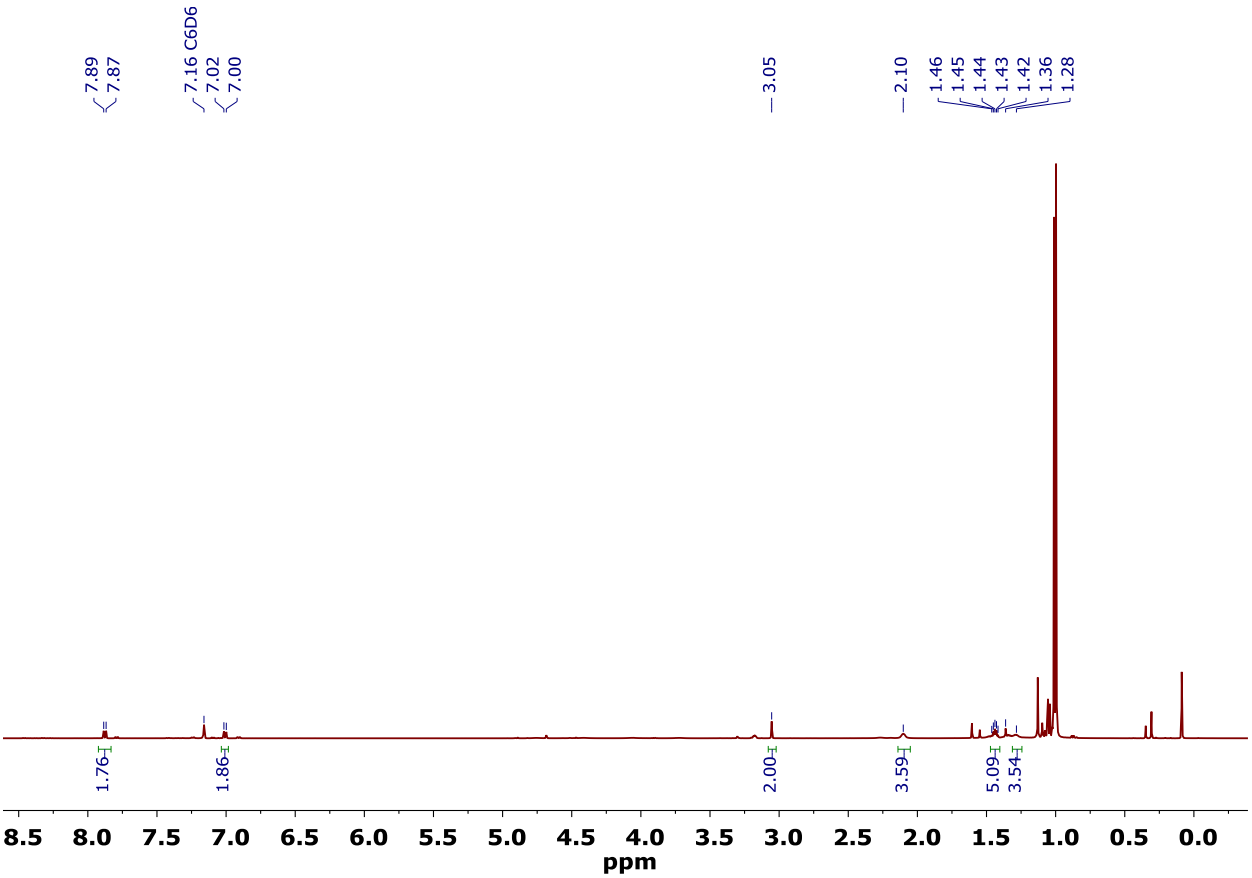
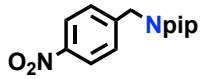


Figure S55. ^{1}H NMR (500 MHz) spectrum of *N,N*-piperidyl-1-(4-nitrobenzyl)amine in C_6D_6.

15. 

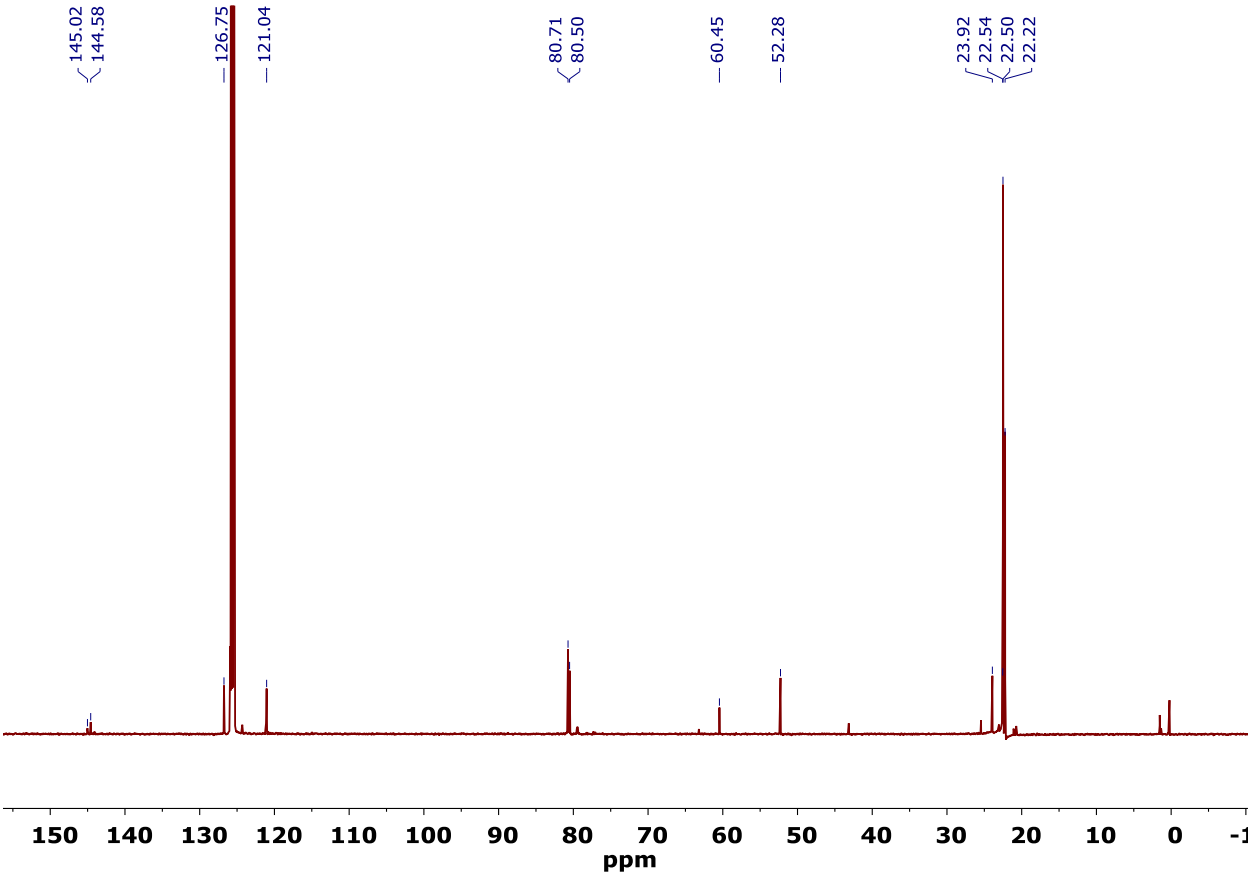


Figure S56. ^{13}C NMR (125 MHz) spectrum of *N,N*-piperidyl-1-(4-nitrobenzyl)amine in C_6D_6.

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

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

N,N-dimethylbenzamide

O	1.276849000	-1.790660000	0.493372000
C	0.991649000	-0.644113000	0.177598000
N	1.956401000	0.311201000	-0.043977000
C	3.337851000	-0.056041000	0.188128000
H	3.870932000	0.788425000	0.642512000
H	3.371478000	-0.919175000	0.853743000
H	3.845242000	-0.319241000	-0.751753000
C	1.776628000	1.515470000	-0.826795000
H	2.022842000	2.413860000	-0.242844000
H	2.441807000	1.491585000	-1.702202000
H	0.749985000	1.602691000	-1.185104000
C	-0.444964000	-0.234550000	0.071216000
C	-0.935121000	0.965530000	0.590973000
C	-1.339082000	-1.164238000	-0.462672000
C	-2.297682000	1.241290000	0.552829000
C	-2.696710000	-0.879412000	-0.520436000
C	-3.178170000	0.324891000	-0.013370000
H	-0.250075000	1.675911000	1.050685000
H	-0.947507000	-2.113819000	-0.819453000
H	-2.673095000	2.172286000	0.971335000
H	-3.384763000	-1.603021000	-0.951306000
H	-4.242833000	0.544417000	-0.049578000

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

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La	0.418843000	0.061656000	0.154377000
N	-0.141029000	1.954859000	-1.234349000
N	0.394654000	-2.022649000	-1.012322000
N	2.520815000	0.138567000	1.289148000
Si	2.582426000	0.642215000	2.954195000
Si	0.842887000	-2.361874000	-2.670023000
Si	-1.578060000	1.829508000	-2.222965000
Si	0.917864000	3.341768000	-1.393145000
Si	3.912629000	-0.553795000	0.484958000
Si	-0.242208000	-3.287996000	0.007978000
C	-0.010505000	4.999160000	-1.494894000
H	0.712461000	5.823729000	-1.535667000
H	-0.645612000	5.073855000	-2.385940000
H	-0.644668000	5.157003000	-0.613046000
C	2.020428000	3.461823000	0.147523000
H	2.612835000	2.553320000	0.329586000
H	2.716548000	4.304087000	0.043958000
H	1.415477000	3.646479000	1.047935000
C	2.044258000	3.238520000	-2.914731000
H	2.618902000	2.303773000	-2.916352000
H	1.463088000	3.269709000	-3.844056000
H	2.755382000	4.074029000	-2.931448000
C	-3.014557000	2.962547000	-1.676467000
H	-2.720767000	4.016958000	-1.616292000
H	-3.833768000	2.882044000	-2.403266000
H	-3.406182000	2.659716000	-0.696790000
C	-1.314047000	2.218760000	-4.061467000
H	-1.089824000	3.281179000	-4.219258000
H	-0.492521000	1.633592000	-4.488853000
H	-2.227013000	1.989091000	-4.625829000
C	-2.306956000	0.074465000	-2.085478000
H	-3.210033000	0.017459000	-2.708028000
H	-1.621559000	-0.716092000	-2.413414000

H	-2.620709000	-0.175267000	-1.060853000
C	-0.065657000	-2.722502000	1.830986000
H	0.972383000	-2.450955000	2.074378000
H	-0.729270000	-1.893052000	2.116795000
H	-0.339297000	-3.563109000	2.481442000
C	-2.095206000	-3.597424000	-0.273732000
H	-2.661740000	-2.658928000	-0.190835000
H	-2.282518000	-4.010770000	-1.271878000
H	-2.497147000	-4.300716000	0.467858000
C	0.648958000	-4.957478000	-0.098103000
H	0.185151000	-5.667282000	0.598800000
H	0.592745000	-5.395615000	-1.101723000
H	1.707561000	-4.862170000	0.171621000
C	-0.430612000	-3.452191000	-3.569569000
H	-1.428007000	-2.995010000	-3.556605000
H	-0.134261000	-3.583741000	-4.618008000
H	-0.512007000	-4.451113000	-3.122955000
C	2.510873000	-3.253910000	-2.827483000
H	2.508909000	-4.218077000	-2.305292000
H	2.734032000	-3.443561000	-3.885404000
H	3.328310000	-2.652454000	-2.411997000
C	0.969548000	-0.740945000	-3.671045000
H	1.876688000	-0.735612000	-4.288357000
H	0.107815000	-0.645807000	-4.344528000
H	0.989682000	0.167559000	-3.051922000
C	3.872809000	-0.004558000	-1.335628000
H	3.987707000	1.085726000	-1.400952000
H	4.694163000	-0.462187000	-1.901955000
H	2.945020000	-0.280817000	-1.856566000
C	3.885450000	-2.447896000	0.548081000
H	2.954934000	-2.810921000	0.091035000
H	4.729097000	-2.889523000	0.002736000
H	3.921333000	-2.804833000	1.585322000
C	5.582592000	0.044108000	1.157442000
H	5.752139000	-0.248902000	2.200486000
H	6.392354000	-0.389246000	0.556918000
H	5.662186000	1.136334000	1.091728000
C	3.015170000	-0.767793000	4.150224000
H	2.288748000	-1.586256000	4.071327000
H	4.008260000	-1.183302000	3.938891000
H	3.017042000	-0.413297000	5.188736000
C	3.758760000	2.083209000	3.327465000
H	4.810648000	1.787009000	3.254317000
H	3.592619000	2.915690000	2.632812000
H	3.584919000	2.450674000	4.347183000
C	0.853517000	1.277031000	3.455057000
H	0.572905000	2.163579000	2.868415000
H	0.050799000	0.533109000	3.362421000
H	0.882985000	1.586603000	4.507496000
O	-1.677290000	0.357179000	1.532720000
C	-2.870063000	0.729188000	1.591081000
C	-3.939576000	-0.298418000	1.494878000
C	-4.987831000	-0.182665000	0.577489000
C	-3.802853000	-1.463685000	2.252854000
C	-5.896531000	-1.223992000	0.431216000
C	-4.731130000	-2.487933000	2.124841000

C	-5.774681000	-2.370579000	1.210963000
H	-5.068565000	0.707757000	-0.045751000
H	-2.964466000	-1.557188000	2.940024000
H	-6.698965000	-1.141683000	-0.297285000
H	-4.628968000	-3.388427000	2.725029000
H	-6.490584000	-3.180898000	1.097803000
N	-3.175695000	2.029776000	1.717875000
C	-4.489728000	2.544727000	2.068225000
H	-4.397630000	3.188939000	2.950374000
H	-4.902422000	3.140522000	1.243614000
H	-5.176920000	1.731206000	2.302003000
C	-2.095379000	3.013208000	1.675646000
H	-1.396234000	2.778541000	0.861270000
H	-2.535572000	3.995060000	1.478291000
H	-1.555368000	3.040542000	2.630570000

TS_{act}-1

La	-0.647491000	-0.141407000	-0.101846000
N	0.691303000	-2.228470000	-0.627422000
N	-2.879286000	0.097323000	-0.934193000
N	-1.051408000	0.046725000	2.225359000
Si	-0.016334000	1.089208000	3.172023000
Si	-3.976849000	-1.133930000	-1.528208000
Si	0.703711000	-2.570248000	-2.373192000
Si	0.838384000	-3.617902000	0.471998000
Si	-2.443244000	-0.715881000	2.972366000
Si	-3.387234000	1.773798000	-1.033365000
C	2.440881000	-4.572384000	0.095195000
H	2.759968000	-5.174378000	0.955281000
H	2.300664000	-5.256036000	-0.751856000
H	3.247931000	-3.878639000	-0.171965000
C	0.833716000	-3.038088000	2.274615000
H	0.096120000	-2.243543000	2.449306000
H	0.587123000	-3.883997000	2.929678000
H	1.800902000	-2.634550000	2.580368000
C	-0.571494000	-4.889753000	0.367136000
H	-1.560932000	-4.429833000	0.475936000
H	-0.566279000	-5.462373000	-0.565231000
H	-0.447361000	-5.600686000	1.195015000
C	2.398275000	-2.579441000	-3.230716000
H	3.041689000	-3.360814000	-2.810042000
H	2.232944000	-2.810147000	-4.291910000
H	2.951960000	-1.640957000	-3.150655000
C	-0.024993000	-4.244181000	-2.898548000
H	0.618314000	-5.079833000	-2.597545000
H	-1.032842000	-4.428251000	-2.515835000
H	-0.073146000	-4.250850000	-3.995864000
C	-0.355025000	-1.269046000	-3.297855000
H	-0.190775000	-1.421853000	-4.373324000
H	-1.428038000	-1.407779000	-3.116951000
H	-0.122203000	-0.214646000	-3.098400000
C	-2.511289000	2.782699000	0.325825000
H	-2.766701000	2.399125000	1.321075000
H	-1.417025000	2.804810000	0.239483000
H	-2.842180000	3.828866000	0.265237000
C	-2.927036000	2.549621000	-2.707372000

H	-1.858956000	2.402739000	-2.914298000
H	-3.489396000	2.079315000	-3.523008000
H	-3.145233000	3.626207000	-2.725767000
C	-5.236605000	2.109885000	-0.769417000
H	-5.403815000	3.193663000	-0.823190000
H	-5.868192000	1.641267000	-1.533059000
H	-5.577814000	1.767151000	0.214574000
C	-4.574870000	-0.786385000	-3.299577000
H	-3.726114000	-0.668834000	-3.985195000
H	-5.191347000	-1.618860000	-3.661934000
H	-5.182453000	0.125118000	-3.360400000
C	-5.533299000	-1.355506000	-0.462737000
H	-6.188343000	-0.478304000	-0.493065000
H	-6.108116000	-2.216083000	-0.829177000
H	-5.274244000	-1.545714000	0.585983000
C	-3.113019000	-2.836244000	-1.570191000
H	-3.703422000	-3.582589000	-1.023326000
H	-3.009432000	-3.188706000	-2.604382000
H	-2.107799000	-2.843559000	-1.127404000
C	-2.849940000	-2.342290000	2.080247000
H	-2.067687000	-3.093112000	2.247457000
H	-3.791593000	-2.750642000	2.470433000
H	-2.988116000	-2.216918000	0.998782000
C	-4.002486000	0.361090000	2.901430000
H	-4.248395000	0.589145000	1.855804000
H	-4.858083000	-0.166262000	3.342636000
H	-3.871653000	1.307502000	3.440158000
C	-2.154768000	-1.218968000	4.781777000
H	-1.928970000	-0.371522000	5.439438000
H	-3.058368000	-1.707049000	5.168917000
H	-1.329239000	-1.937869000	4.857770000
C	-0.962533000	2.339374000	4.245799000
H	-1.590869000	2.986856000	3.621427000
H	-1.608235000	1.859455000	4.990379000
H	-0.252132000	2.978745000	4.785633000
C	1.201547000	0.151059000	4.281308000
H	0.691140000	-0.476310000	5.020561000
H	1.824902000	-0.498505000	3.654261000
H	1.853556000	0.851876000	4.819841000
C	1.041994000	2.160494000	2.003848000
H	1.653580000	1.571326000	1.304374000
H	0.439548000	2.893356000	1.450641000
H	1.753777000	2.735529000	2.612785000
O	0.359554000	1.791031000	-1.599001000
C	1.259761000	2.635998000	-1.783869000
O	3.616585000	-1.301112000	-0.858989000
C	4.679197000	-0.783503000	-0.050359000
C	4.043202000	-0.732868000	1.380451000
O	2.639114000	-0.576095000	1.088097000
C	5.011883000	0.602187000	-0.605450000
H	5.291248000	0.491017000	-1.660354000
H	4.137702000	1.269159000	-0.558354000
C	5.888250000	-1.685806000	-0.183768000
H	6.705042000	-1.342963000	0.464380000
H	5.648463000	-2.721827000	0.071448000
H	6.245321000	-1.668548000	-1.219360000

C	4.263840000	-2.007647000	2.177442000
H	3.699537000	-1.951608000	3.115154000
H	3.933386000	-2.896533000	1.630334000
H	5.322347000	-2.128714000	2.436500000
B	2.454386000	-0.811050000	-0.271678000
H	1.781365000	-0.009134000	-0.867621000
H	3.973270000	0.430190000	3.188281000
C	4.480640000	0.457318000	2.216893000
H	4.227099000	1.408874000	1.737914000
H	5.563588000	0.428956000	2.396405000
H	5.845978000	1.076713000	-0.075686000
C	1.239620000	3.909091000	-1.011957000
C	2.336241000	4.316924000	-0.248128000
C	0.053420000	4.642725000	-0.974152000
C	2.243479000	5.450525000	0.548822000
C	-0.030631000	5.784517000	-0.186482000
C	1.061263000	6.185729000	0.577658000
H	3.250640000	3.723380000	-0.252058000
H	-0.801024000	4.306268000	-1.559247000
H	3.091189000	5.755126000	1.157353000
H	-0.955517000	6.355557000	-0.161422000
H	0.989493000	7.072201000	1.203071000
N	2.265053000	2.429212000	-2.659635000
C	2.368072000	1.177016000	-3.393228000
H	1.910065000	0.367545000	-2.829443000
H	1.880980000	1.256886000	-4.374436000
H	3.428211000	0.941056000	-3.539537000
C	3.180504000	3.460609000	-3.123225000
H	3.163526000	3.483037000	-4.219668000
H	2.891813000	4.443238000	-2.750989000
H	4.206215000	3.240235000	-2.799294000

I_{act}-2

La	-0.136886000	0.404108000	0.116436000
N	-2.801936000	-0.233471000	-0.576817000
N	0.905422000	2.325360000	-0.970965000
N	0.472212000	0.769861000	2.378710000
Si	1.319740000	-0.381135000	3.396302000
Si	0.011978000	3.667757000	-1.664308000
Si	-3.396049000	0.116278000	-2.257754000
Si	-3.972871000	-0.017609000	0.782851000
Si	0.016949000	2.316496000	3.065331000
Si	2.656701000	2.461625000	-0.915959000
C	-5.378812000	-1.276573000	0.640443000
H	-5.912209000	-1.385459000	1.592432000
H	-6.110089000	-0.972699000	-0.119032000
H	-4.972721000	-2.250197000	0.340636000
C	-3.139299000	-0.193197000	2.481266000
H	-2.090216000	0.129351000	2.531860000
H	-3.702653000	0.420341000	3.197322000
H	-3.163758000	-1.225697000	2.836202000
C	-4.722709000	1.728938000	0.805170000
H	-3.995613000	2.507902000	0.544359000
H	-5.580785000	1.835288000	0.136129000
H	-5.071222000	1.936084000	1.824832000
C	-4.189641000	-1.375051000	-3.106284000

H	-5.017114000	-1.787155000	-2.518699000
H	-4.582919000	-1.048886000	-4.078602000
H	-3.468244000	-2.182576000	-3.259610000
C	-4.730368000	1.457819000	-2.360666000
H	-5.687767000	1.109959000	-1.956438000
H	-4.473358000	2.407638000	-1.885238000
H	-4.886470000	1.648569000	-3.431161000
C	-1.966411000	0.642744000	-3.403164000
H	-2.356602000	1.328004000	-4.167274000
H	-1.138912000	1.162490000	-2.905123000
H	-1.561982000	-0.234766000	-3.920013000
C	3.387280000	1.373784000	0.458050000
H	2.993280000	1.657677000	1.442159000
H	3.193366000	0.303305000	0.320670000
H	4.478022000	1.504850000	0.470925000
C	3.517997000	1.929055000	-2.536825000
H	3.402795000	0.858237000	-2.743055000
H	3.123911000	2.478737000	-3.400839000
H	4.593076000	2.144088000	-2.466109000
C	3.358803000	4.200142000	-0.600205000
H	4.441631000	4.103034000	-0.445999000
H	3.208746000	4.872668000	-1.453223000
H	2.935632000	4.678158000	0.290405000
C	0.398121000	3.921313000	-3.507679000
H	0.234587000	2.999998000	-4.081439000
H	-0.244279000	4.703601000	-3.931481000
H	1.439880000	4.231928000	-3.658344000
C	0.271664000	5.353648000	-0.822429000
H	1.238688000	5.811311000	-1.049901000
H	-0.512724000	6.040005000	-1.167825000
H	0.185589000	5.271296000	0.269098000
C	-1.876114000	3.387968000	-1.511445000
H	-2.316285000	4.149726000	-0.855198000
H	-2.350088000	3.485154000	-2.496304000
H	-2.186607000	2.414148000	-1.111514000
C	-1.350510000	3.076129000	1.982703000
H	-2.280676000	2.493837000	2.016805000
H	-1.588678000	4.082358000	2.351232000
H	-1.041822000	3.209127000	0.937789000
C	1.429789000	3.579837000	3.089908000
H	1.826848000	3.716690000	2.075161000
H	1.069876000	4.553536000	3.446394000
H	2.256188000	3.265519000	3.737549000
C	-0.733303000	2.207269000	4.804881000
H	-0.029597000	1.828249000	5.554664000
H	-1.057084000	3.204842000	5.128249000
H	-1.612616000	1.551222000	4.804797000
C	2.572766000	0.416069000	4.583416000
H	3.350016000	0.956999000	4.029390000
H	2.118028000	1.111152000	5.298498000
H	3.067693000	-0.375043000	5.161590000
C	0.110864000	-1.395010000	4.449508000
H	-0.417561000	-0.758108000	5.168926000
H	-0.646571000	-1.864779000	3.809717000
H	0.629965000	-2.184556000	5.007883000
C	2.357607000	-1.586873000	2.357226000

H	1.865177000	-1.919378000	1.436381000
H	3.312365000	-1.125822000	2.071546000
H	2.584433000	-2.485233000	2.947339000
O	1.551729000	-1.145911000	-0.936286000
C	2.466578000	-1.541790000	-1.689120000
O	-2.784049000	-2.791906000	-0.954052000
C	-1.982075000	-3.863973000	-0.501798000
C	-1.436429000	-3.323296000	0.858832000
O	-1.307804000	-1.913722000	0.610532000
C	-0.864210000	-4.146995000	-1.512706000
H	-1.322835000	-4.261016000	-2.502889000
H	-0.135646000	-3.329761000	-1.570382000
C	-2.854363000	-5.102009000	-0.389449000
H	-2.313000000	-5.934048000	0.079543000
H	-3.761259000	-4.899520000	0.188070000
H	-3.161581000	-5.420281000	-1.392291000
C	-2.429366000	-3.548376000	1.991448000
H	-2.085041000	-3.022732000	2.889096000
H	-3.428250000	-3.179373000	1.733880000
H	-2.506196000	-4.613256000	2.242576000
B	-2.036456000	-1.599012000	-0.669582000
H	-1.157821000	-1.371129000	-1.554837000
H	0.195800000	-3.519070000	2.258855000
C	-0.095720000	-3.900432000	1.271793000
H	0.690993000	-3.626232000	0.562201000
H	-0.148501000	-4.995576000	1.336270000
H	-0.328971000	-5.074788000	-1.272448000
C	3.667832000	-2.189734000	-1.092213000
C	3.518741000	-3.391050000	-0.400169000
C	4.905661000	-1.544458000	-1.120278000
C	4.608360000	-3.951419000	0.254686000
C	5.986895000	-2.098617000	-0.444850000
C	5.838984000	-3.301507000	0.239850000
H	2.547140000	-3.882827000	-0.380408000
H	5.011531000	-0.597931000	-1.651080000
H	4.492792000	-4.891250000	0.788448000
H	6.946967000	-1.588835000	-0.452466000
H	6.686964000	-3.733617000	0.765523000
N	2.383180000	-1.376745000	-3.015556000
C	3.359660000	-1.861856000	-3.975664000
H	2.849626000	-2.440787000	-4.753413000
H	3.880585000	-1.018989000	-4.448767000
H	4.093543000	-2.502852000	-3.486074000
C	1.219788000	-0.668644000	-3.540668000
H	0.301165000	-1.219006000	-3.305366000
H	1.148658000	0.334861000	-3.098947000
H	1.325755000	-0.571401000	-4.623592000

TS_{act}-2

La	0.985205000	-0.113499000	-0.081805000
N	-3.368249000	0.002344000	0.733502000
N	2.427268000	1.773313000	0.348001000
N	2.512809000	-1.899993000	0.108265000
Si	3.095192000	-2.993720000	-1.132487000
Si	2.466742000	3.054489000	1.559976000
Si	-5.107740000	-0.148275000	0.420174000

Si	-2.858783000	1.023379000	2.082630000
Si	3.156613000	-1.931696000	1.740432000
Si	3.546638000	1.979841000	-0.998142000
C	-2.836032000	0.192372000	3.786097000
H	-2.727484000	0.964398000	4.558783000
H	-3.751776000	-0.370341000	3.997581000
H	-1.984814000	-0.492077000	3.878665000
C	-1.083736000	1.668521000	1.847334000
H	-0.875999000	1.998206000	0.820295000
H	-0.931237000	2.548518000	2.485263000
H	-0.362971000	0.914276000	2.194370000
C	-3.920775000	2.585247000	2.279733000
H	-3.850514000	3.239492000	1.403732000
H	-4.979614000	2.380902000	2.469170000
H	-3.536239000	3.147474000	3.140276000
C	-5.630887000	-1.595565000	-0.676845000
H	-5.461862000	-2.554813000	-0.176942000
H	-6.708771000	-1.495502000	-0.863215000
H	-5.104898000	-1.635839000	-1.634780000
C	-6.061805000	-0.409525000	2.042029000
H	-5.771653000	-1.356682000	2.513861000
H	-5.922428000	0.387908000	2.780214000
H	-7.134878000	-0.468004000	1.819253000
C	-5.839716000	1.403231000	-0.405560000
H	-6.926770000	1.276000000	-0.490045000
H	-5.657274000	2.319966000	0.165611000
H	-5.452407000	1.557575000	-1.420360000
C	3.161224000	0.730224000	-2.386993000
H	3.334783000	-0.307017000	-2.072396000
H	2.168716000	0.800555000	-2.848717000
H	3.893347000	0.923942000	-3.181958000
C	3.432260000	3.682966000	-1.836119000
H	2.405812000	3.875947000	-2.171089000
H	3.729785000	4.508642000	-1.180274000
H	4.086751000	3.704980000	-2.716912000
C	5.372680000	1.631079000	-0.624981000
H	5.969143000	1.844043000	-1.522008000
H	5.774839000	2.230581000	0.197573000
H	5.512487000	0.572319000	-0.373706000
C	1.280461000	4.474262000	1.123020000
H	0.262121000	4.117938000	0.923930000
H	1.236665000	5.206688000	1.939513000
H	1.625127000	4.995387000	0.220778000
C	4.181007000	3.853103000	1.789651000
H	4.600933000	4.297956000	0.881148000
H	4.088309000	4.653391000	2.535529000
H	4.903886000	3.124493000	2.177587000
C	2.080294000	2.491488000	3.335093000
H	2.863695000	1.818575000	3.707011000
H	2.097127000	3.388344000	3.968843000
H	1.111190000	2.006247000	3.484356000
C	1.894680000	-1.005961000	2.846949000
H	0.872150000	-1.406808000	2.815481000
H	2.229512000	-1.074691000	3.889765000
H	1.876172000	0.073397000	2.638975000
C	4.773975000	-0.977635000	1.971718000

H	4.622422000	0.077063000	1.705888000
H	5.099849000	-1.025550000	3.018864000
H	5.583468000	-1.373773000	1.346688000
C	3.399063000	-3.662596000	2.471164000
H	4.249902000	-4.176062000	2.006719000
H	3.616321000	-3.575172000	3.543317000
H	2.513090000	-4.296370000	2.352326000
C	4.969308000	-2.816872000	-1.379010000
H	5.247869000	-1.781076000	-1.611933000
H	5.514103000	-3.113286000	-0.473144000
H	5.318340000	-3.456398000	-2.199330000
C	2.777901000	-4.828167000	-0.754881000
H	3.357049000	-5.186846000	0.102765000
H	1.717953000	-5.023758000	-0.549033000
H	3.064450000	-5.429394000	-1.627408000
C	2.231304000	-2.654391000	-2.804961000
H	1.637845000	-3.528172000	-3.103261000
H	1.559072000	-1.787059000	-2.817830000
H	2.980748000	-2.480016000	-3.587224000
O	-0.021295000	0.090951000	-2.304480000
C	-1.194386000	0.602977000	-2.343551000
O	-2.732040000	-1.886027000	-0.807784000
C	-2.070300000	-3.072145000	-0.399931000
C	-1.508864000	-2.716262000	1.005649000
O	-1.175751000	-1.315124000	0.838395000
C	-0.956283000	-3.407088000	-1.387333000
H	-1.382566000	-3.553258000	-2.385645000
H	-0.217025000	-2.599646000	-1.466304000
C	-3.068200000	-4.219731000	-0.403430000
H	-2.595957000	-5.162012000	-0.096368000
H	-3.919190000	-4.026018000	0.255248000
H	-3.457562000	-4.350649000	-1.420818000
C	-2.552421000	-2.857158000	2.107126000
H	-2.156523000	-2.416423000	3.028444000
H	-3.486805000	-2.343343000	1.861826000
H	-2.763087000	-3.914754000	2.306083000
B	-2.285815000	-0.752794000	-0.034934000
H	-1.697035000	0.076755000	-0.862695000
H	-0.024843000	-3.321209000	2.453101000
C	-0.285658000	-3.518934000	1.405720000
H	0.591265000	-3.293487000	0.788338000
H	-0.502589000	-4.592861000	1.327315000
H	-0.427538000	-4.328550000	-1.115142000
C	-1.334221000	2.054583000	-1.966050000
C	-2.411145000	2.578944000	-1.246622000
C	-0.312296000	2.909643000	-2.390621000
C	-2.474629000	3.942269000	-0.981736000
C	-0.383235000	4.272965000	-2.124855000
C	-1.465267000	4.793117000	-1.423544000
H	-3.170857000	1.905603000	-0.852554000
H	0.533817000	2.499922000	-2.939812000
H	-3.321057000	4.341560000	-0.425657000
H	0.415127000	4.930550000	-2.462902000
H	-1.516168000	5.858236000	-1.211030000
N	-2.108213000	0.082362000	-3.200556000
C	-3.457946000	0.585399000	-3.356743000

H	-3.800755000	0.346265000	-4.368926000
H	-4.144267000	0.106836000	-2.641357000
H	-3.501121000	1.668129000	-3.228721000
C	-1.904805000	-1.226747000	-3.795283000
H	-0.871651000	-1.542552000	-3.651685000
H	-2.581688000	-1.954635000	-3.329145000
H	-2.116161000	-1.164050000	-4.869676000

I_{act}-3

La	0.212339000	-0.314900000	-0.064317000
N	2.412514000	-1.168278000	-0.431983000
N	0.080794000	2.030222000	0.162055000
Si	-0.726044000	3.038431000	-1.009834000
Si	2.640318000	-2.805797000	0.108515000
Si	3.737351000	-0.162188000	-0.973588000
Si	0.793414000	2.548423000	1.655000000
C	4.931367000	-1.061083000	-2.140169000
H	5.688503000	-0.364708000	-2.521374000
H	5.461521000	-1.877003000	-1.632750000
H	4.398403000	-1.486523000	-2.998588000
C	3.013982000	1.321198000	-1.913058000
H	2.286976000	1.884297000	-1.308291000
H	3.811278000	2.018731000	-2.199176000
H	2.517012000	0.994778000	-2.836685000
C	4.771175000	0.519946000	0.467828000
H	4.140114000	1.017429000	1.215915000
H	5.321395000	-0.279696000	0.978033000
H	5.503260000	1.254355000	0.108401000
C	2.951623000	-4.068731000	-1.264549000
H	3.905617000	-3.884477000	-1.771246000
H	2.976420000	-5.087963000	-0.859303000
H	2.157940000	-4.019928000	-2.019186000
C	3.994323000	-2.987783000	1.422635000
H	4.990429000	-2.783996000	1.011201000
H	3.824412000	-2.285789000	2.249047000
H	4.007690000	-4.004809000	1.833655000
C	1.003733000	-3.334094000	0.957691000
H	1.114201000	-4.355453000	1.342534000
H	0.746378000	-2.713098000	1.831529000
H	0.145967000	-3.361857000	0.268117000
C	1.267242000	0.933603000	2.602240000
H	2.034205000	0.317443000	2.101587000
H	1.708606000	1.213206000	3.566492000
H	0.397485000	0.302592000	2.859217000
C	-0.395873000	3.499179000	2.780806000
H	-1.325357000	2.936929000	2.935040000
H	0.054803000	3.696044000	3.761244000
H	-0.663105000	4.467166000	2.338354000
C	2.379376000	3.563578000	1.469816000
H	2.893880000	3.676208000	2.432306000
H	3.072786000	3.088249000	0.764868000
H	2.157048000	4.567273000	1.088215000
C	-2.490728000	3.512833000	-0.495929000
H	-3.147862000	2.633822000	-0.460216000
H	-2.507735000	3.984061000	0.494314000
H	-2.925647000	4.220448000	-1.212735000

C	0.227166000	4.636471000	-1.362631000
H	0.252103000	5.287392000	-0.478957000
H	1.263061000	4.418612000	-1.649767000
H	-0.241069000	5.203188000	-2.176459000
C	-0.857270000	2.020111000	-2.608557000
H	0.136096000	1.781631000	-3.012877000
H	-1.412096000	1.080284000	-2.460171000
H	-1.392790000	2.579785000	-3.384868000
H	-2.289694000	-2.848329000	-0.110710000
O	-1.646406000	-1.184286000	-1.137061000
C	-2.448042000	-1.750911000	-0.200406000
N	-2.016816000	-1.236294000	1.191277000
C	-2.640304000	0.035108000	1.570761000
H	-2.150023000	0.423580000	2.474518000
H	-2.518853000	0.784336000	0.778164000
H	-3.717038000	-0.071918000	1.778754000
C	-2.206482000	-2.209026000	2.259196000
H	-1.747968000	-3.166401000	1.987114000
H	-1.726162000	-1.848563000	3.178806000
H	-3.273976000	-2.378116000	2.481161000
C	-3.924063000	-1.515573000	-0.431947000
C	-4.873107000	-2.373397000	0.125301000
C	-4.357363000	-0.412267000	-1.166773000
C	-6.233161000	-2.119351000	-0.024130000
C	-5.715155000	-0.155964000	-1.317754000
C	-6.656604000	-1.005022000	-0.741336000
H	-4.542922000	-3.261427000	0.665514000
H	-3.610063000	0.231598000	-1.628000000
H	-6.963302000	-2.798117000	0.411350000
H	-6.042046000	0.707217000	-1.893776000
H	-7.718954000	-0.805571000	-0.862684000

pinB-N(SiMe$_3$)$_2$

N	0.926985000	0.014099000	0.006437000
Si	1.716392000	-1.590211000	-0.096987000
Si	1.860532000	1.535735000	0.098944000
C	0.805831000	2.931460000	0.802326000
H	0.332676000	2.628696000	1.744273000
H	1.448187000	3.795986000	1.010374000
H	0.013266000	3.232712000	0.113217000
C	2.508084000	2.038335000	-1.599876000
H	1.673672000	2.154833000	-2.300955000
H	3.038476000	2.996364000	-1.542624000
H	3.196781000	1.292545000	-2.010919000
C	3.292619000	1.311964000	1.318299000
H	3.864430000	2.246064000	1.381329000
H	2.897056000	1.099786000	2.319135000
H	3.994202000	0.512890000	1.057319000
C	3.346636000	-1.442098000	-1.047031000
H	3.152245000	-1.164313000	-2.090035000
H	4.052043000	-0.717658000	-0.628417000
H	3.841028000	-2.421346000	-1.054025000
C	2.020007000	-2.293738000	1.626153000
H	2.688703000	-1.652128000	2.211066000
H	1.069301000	-2.377497000	2.164927000
H	2.469534000	-3.292059000	1.567676000

C	0.653712000	-2.778722000	-1.108777000
H	-0.276958000	-3.035394000	-0.596309000
H	0.399450000	-2.330364000	-2.077476000
H	1.217194000	-3.698738000	-1.306887000
O	-1.268576000	1.126078000	-0.363451000
C	-2.613812000	0.640271000	-0.497064000
B	-0.495058000	0.047111000	0.027726000
C	-2.631534000	-0.557627000	0.496570000
O	-1.275369000	-1.023770000	0.430142000
C	-2.787422000	0.202056000	-1.945403000
H	-2.536119000	1.043539000	-2.599812000
H	-2.115594000	-0.630399000	-2.189167000
H	-3.817705000	-0.106710000	-2.158550000
C	-3.580577000	1.759139000	-0.170509000
H	-4.615405000	1.393473000	-0.176211000
H	-3.369569000	2.203349000	0.806589000
H	-3.496904000	2.548964000	-0.925249000
C	-3.559442000	-1.692872000	0.115184000
H	-3.284759000	-2.129024000	-0.850167000
H	-3.501717000	-2.484011000	0.871050000
H	-4.600298000	-1.348219000	0.064489000
C	-2.891182000	-0.128103000	1.933925000
H	-2.663078000	-0.967855000	2.599002000
H	-2.249514000	0.714417000	2.218594000
H	-3.937126000	0.161661000	2.090352000

Structure A

La	0.088740000	0.059472000	0.131366000
N	0.230716000	2.434417000	0.101817000
N	2.075214000	-1.229908000	-0.024291000
Si	2.742662000	-1.780151000	1.483745000
Si	-1.310345000	3.256973000	0.181309000
Si	1.722492000	3.313217000	-0.170305000
Si	2.767579000	-1.556023000	-1.594850000
C	1.853145000	4.925153000	0.823335000
H	2.848108000	5.367310000	0.687177000
H	1.115218000	5.668982000	0.498037000
H	1.704913000	4.746309000	1.894882000
C	3.178195000	2.221703000	0.375125000
H	3.175328000	1.222864000	-0.084109000
H	4.131905000	2.702384000	0.123131000
H	3.155970000	2.082607000	1.465105000
C	1.959076000	3.772335000	-1.996576000
H	1.816084000	2.900456000	-2.646492000
H	1.232370000	4.533617000	-2.305031000
H	2.964133000	4.173939000	-2.176653000
C	-1.536758000	4.323455000	1.733702000
H	-0.869251000	5.192202000	1.737292000
H	-2.568797000	4.691072000	1.796788000
H	-1.328632000	3.738726000	2.637885000
C	-1.668259000	4.338849000	-1.332407000
H	-0.984720000	5.194959000	-1.389706000
H	-1.555399000	3.755885000	-2.254352000
H	-2.691457000	4.733041000	-1.296164000
C	-2.679995000	1.931427000	0.261565000
H	-3.655363000	2.433484000	0.296371000

H	-2.703634000	1.273293000	-0.619914000
H	-2.635437000	1.303396000	1.164199000
C	2.234511000	-0.157000000	-2.763690000
H	2.675997000	0.800523000	-2.456089000
H	2.573894000	-0.359890000	-3.786871000
H	1.139701000	-0.045666000	-2.817187000
C	2.138883000	-3.191048000	-2.327361000
H	1.056599000	-3.136081000	-2.504866000
H	2.626371000	-3.408157000	-3.285801000
H	2.333542000	-4.032726000	-1.650186000
C	4.662892000	-1.605691000	-1.593414000
H	5.037281000	-1.721411000	-2.618109000
H	5.079453000	-0.677321000	-1.183663000
H	5.054081000	-2.443144000	-1.002394000
C	2.897386000	-3.669207000	1.612814000
H	1.938613000	-4.176368000	1.452338000
H	3.604401000	-4.052987000	0.866382000
H	3.272685000	-3.960012000	2.601968000
C	4.438639000	-1.066941000	1.935350000
H	5.229360000	-1.458284000	1.285507000
H	4.443839000	0.025939000	1.848022000
H	4.694482000	-1.329770000	2.969778000
C	1.547117000	-1.196686000	2.861486000
H	1.525599000	-0.099356000	2.955369000
H	0.517589000	-1.568493000	2.748869000
H	1.902678000	-1.569149000	3.830112000
H	-1.020919000	-0.645468000	-1.660189000
O	-1.650270000	-1.412912000	1.244982000
C	-2.383483000	-2.065971000	0.457353000
N	-1.981046000	-3.263184000	0.006718000
C	-2.696388000	-4.067186000	-0.967690000
H	-2.251254000	-3.946355000	-1.965076000
H	-2.635815000	-5.121647000	-0.679555000
H	-3.746673000	-3.776932000	-1.009728000
C	-0.637914000	-3.705050000	0.365065000
H	0.138600000	-3.079012000	-0.102119000
H	-0.504543000	-3.663660000	1.450945000
H	-0.502946000	-4.734249000	0.023502000
C	-3.717124000	-1.512731000	0.094409000
C	-4.554075000	-1.107998000	1.136251000
C	-4.088019000	-1.273615000	-1.230882000
C	-5.773628000	-0.506159000	0.854318000
C	-5.300767000	-0.652669000	-1.506421000
C	-6.147089000	-0.277672000	-0.467174000
H	-4.235677000	-1.262217000	2.165146000
H	-3.395567000	-1.519390000	-2.033962000
H	-6.428443000	-0.203182000	1.667548000
H	-5.579576000	-0.450902000	-2.537605000
H	-7.096367000	0.204968000	-0.687463000

Structure B

La	-0.240992000	-0.103261000	-0.036773000
N	-1.874990000	1.137123000	1.158409000
N	-1.208838000	-2.139203000	-0.886507000
Si	-0.881729000	-2.513736000	-2.547620000
Si	-1.458751000	1.975911000	2.637188000

Si	-3.494620000	1.248721000	0.492581000
Si	-2.263013000	-3.095625000	0.120237000
C	-4.234329000	2.998592000	0.509581000
H	-5.219368000	2.974752000	0.025732000
H	-4.383557000	3.366536000	1.532366000
H	-3.614843000	3.727955000	-0.023808000
C	-3.419312000	0.688049000	-1.327549000
H	-2.997160000	-0.322085000	-1.440803000
H	-4.433334000	0.654823000	-1.746623000
H	-2.839056000	1.387388000	-1.945561000
C	-4.779323000	0.169369000	1.379348000
H	-4.483347000	-0.883949000	1.433502000
H	-4.948873000	0.522657000	2.403484000
H	-5.737710000	0.220963000	0.845798000
C	-1.167949000	3.833284000	2.385625000
H	-2.073362000	4.345880000	2.040799000
H	-0.847592000	4.305097000	3.323052000
H	-0.384082000	4.011101000	1.636611000
C	-2.742583000	1.746132000	4.012628000
H	-3.702249000	2.219966000	3.773653000
H	-2.927557000	0.678923000	4.188790000
H	-2.380187000	2.186978000	4.949612000
C	0.174205000	1.248128000	3.274129000
H	0.468482000	1.732833000	4.212935000
H	0.072606000	0.172552000	3.482602000
H	0.996855000	1.391093000	2.558613000
C	-2.165771000	-2.436854000	1.905439000
H	-2.325532000	-1.350893000	1.982974000
H	-2.941542000	-2.916574000	2.516437000
H	-1.199550000	-2.674189000	2.367710000
C	-1.777357000	-4.931243000	0.181295000
H	-0.727023000	-5.066812000	0.469036000
H	-2.399559000	-5.469642000	0.907265000
H	-1.921501000	-5.411400000	-0.795499000
C	-4.084644000	-3.062410000	-0.421125000
H	-4.719256000	-3.524716000	0.346221000
H	-4.448318000	-2.041145000	-0.587053000
H	-4.229356000	-3.622137000	-1.353128000
C	0.241361000	-4.012849000	-2.858520000
H	1.238629000	-3.876054000	-2.423954000
H	-0.183816000	-4.929555000	-2.432907000
H	0.364169000	-4.172282000	-3.937459000
C	-2.424840000	-2.769832000	-3.618109000
H	-2.926337000	-3.712152000	-3.363592000
H	-3.149425000	-1.957879000	-3.485049000
H	-2.152674000	-2.818851000	-4.680019000
C	0.064255000	-1.007307000	-3.260625000
H	-0.508870000	-0.069268000	-3.205514000
H	1.041027000	-0.859253000	-2.772560000
H	0.283228000	-1.174900000	-4.322494000
H	2.298127000	-0.314261000	2.496937000
O	2.009868000	0.300346000	0.555211000
C	2.453749000	-0.629049000	1.441586000
N	1.557752000	-1.848041000	1.313488000
O	0.225997000	2.123218000	-1.583871000
C	1.424663000	2.676841000	-2.254618000

B	-0.489536000	3.242028000	-1.160584000
C	1.610176000	4.004971000	-1.476604000
O	0.241446000	4.376581000	-1.174282000
H	-1.629715000	3.192359000	-0.859297000
C	1.028710000	2.876352000	-3.708555000
H	0.697939000	1.917493000	-4.123440000
H	0.212736000	3.599731000	-3.818687000
H	1.883053000	3.224180000	-4.299779000
C	2.593776000	1.728164000	-2.148045000
H	3.494858000	2.226353000	-2.528680000
H	2.767910000	1.399366000	-1.118564000
H	2.423920000	0.844520000	-2.776892000
C	2.241539000	5.121561000	-2.279370000
H	1.638241000	5.386289000	-3.152216000
H	2.336808000	6.013062000	-1.650786000
H	3.245775000	4.835978000	-2.615792000
C	2.329175000	3.822066000	-0.149165000
H	2.190097000	4.728717000	0.449695000
H	1.945031000	2.963012000	0.416512000
H	3.403941000	3.668665000	-0.297384000
C	1.927312000	-2.721960000	0.200054000
H	2.106900000	-2.129774000	-0.707250000
H	2.846376000	-3.295189000	0.407417000
H	1.099353000	-3.410141000	-0.008119000
C	1.482896000	-2.639871000	2.532722000
H	0.765415000	-3.458735000	2.396790000
H	2.456626000	-3.090027000	2.794910000
H	1.147406000	-2.018604000	3.372331000
C	3.923600000	-0.971384000	1.298036000
C	4.573779000	-0.864649000	0.068034000
C	4.648652000	-1.424567000	2.401190000
C	5.910630000	-1.222392000	-0.060772000
C	5.987235000	-1.784922000	2.277087000
C	6.620732000	-1.688554000	1.042856000
H	4.015356000	-0.488058000	-0.787436000
H	4.162134000	-1.473633000	3.375876000
H	6.404953000	-1.132858000	-1.026108000
H	6.538641000	-2.131768000	3.148413000
H	7.668001000	-1.964778000	0.942450000

Structure C

La	-0.387856000	0.401230000	-0.045899000
N	-1.968238000	1.961077000	0.848228000
N	-1.466255000	-0.617342000	-1.939410000
Si	-0.560455000	-0.610432000	-3.437342000
Si	-2.311893000	2.028263000	2.560948000
Si	-2.808718000	3.035558000	-0.252823000
Si	-3.143886000	-1.131102000	-1.919743000
C	-2.583455000	4.897751000	0.058516000
H	-2.975059000	5.446833000	-0.808172000
H	-3.121412000	5.248238000	0.945326000
H	-1.527833000	5.172136000	0.176615000
C	-2.146958000	2.778941000	-2.018608000
H	-2.154446000	1.732805000	-2.344741000
H	-2.773112000	3.347811000	-2.719026000

H	-1.124078000	3.166517000	-2.120980000
C	-4.686198000	2.735633000	-0.237322000
H	-4.930115000	1.672039000	-0.350799000
H	-5.120632000	3.077699000	0.711221000
H	-5.183028000	3.287920000	-1.045395000
C	-2.818887000	3.725441000	3.243222000
H	-3.782621000	4.070579000	2.850203000
H	-2.917058000	3.648073000	4.334069000
H	-2.065397000	4.492015000	3.027821000
C	-3.747810000	0.863820000	3.031081000
H	-4.678556000	1.212170000	2.564833000
H	-3.581082000	-0.163622000	2.680326000
H	-3.906496000	0.846925000	4.118048000
C	-0.757315000	1.558502000	3.547451000
H	-1.004558000	1.423238000	4.609132000
H	-0.261963000	0.643529000	3.199279000
H	-0.018999000	2.366962000	3.475019000
C	-3.727590000	-1.209790000	-0.110708000
H	-3.528522000	-0.262431000	0.411334000
H	-4.812126000	-1.375248000	-0.076609000
H	-3.253584000	-2.027728000	0.450746000
C	-3.422656000	-2.845794000	-2.692299000
H	-2.823347000	-3.627373000	-2.211126000
H	-4.479959000	-3.123175000	-2.591871000
H	-3.186589000	-2.846495000	-3.764066000
C	-4.363950000	0.004359000	-2.831632000
H	-5.384509000	-0.363870000	-2.661676000
H	-4.322611000	1.043276000	-2.487781000
H	-4.186020000	0.002422000	-3.913067000
C	0.043171000	-2.333513000	-3.958833000
H	0.664158000	-2.791767000	-3.180504000
H	-0.805149000	-3.000580000	-4.159722000
H	0.643991000	-2.271238000	-4.875052000
C	-1.499777000	0.088311000	-4.930732000
H	-2.331726000	-0.557395000	-5.237239000
H	-1.901679000	1.087658000	-4.725014000
H	-0.814994000	0.168884000	-5.784733000
C	0.963770000	0.514254000	-3.223005000
H	0.665503000	1.569652000	-3.143979000
H	1.616322000	0.288668000	-2.366861000
H	1.588560000	0.428655000	-4.121732000
H	2.599536000	-0.884046000	1.709926000
O	2.277219000	0.134530000	-0.044580000
C	2.864724000	-0.933433000	0.633711000
C	4.375162000	-0.903186000	0.518802000
C	5.003037000	-0.426173000	-0.632831000
C	5.161192000	-1.397724000	1.558608000
C	6.387197000	-0.456224000	-0.745167000
C	6.548583000	-1.430668000	1.449041000
C	7.164386000	-0.962777000	0.293956000
H	4.392996000	-0.002639000	-1.428783000
H	4.680664000	-1.740935000	2.475351000
H	6.864146000	-0.073081000	-1.645211000
H	7.148696000	-1.811573000	2.272654000
H	8.248579000	-0.980658000	0.206981000
O	1.307929000	2.240790000	-0.165344000

C	1.786043000	3.591915000	-0.126365000
B	2.258329000	1.451435000	0.688338000
C	3.324048000	3.352999000	-0.086029000
O	3.447784000	2.225292000	0.763746000
H	1.762963000	1.189149000	1.806344000
C	1.254639000	4.246158000	1.144155000
H	0.168915000	4.082935000	1.188280000
H	1.702302000	3.797409000	2.037957000
H	1.449843000	5.325710000	1.156342000
C	1.295978000	4.346784000	-1.344741000
H	1.814391000	5.310408000	-1.431135000
H	1.465749000	3.778693000	-2.266234000
H	0.222776000	4.558919000	-1.257201000
C	4.109299000	4.506366000	0.511599000
H	3.822626000	4.685705000	1.551946000
H	5.178262000	4.265640000	0.495877000
H	3.960788000	5.430665000	-0.062488000
C	3.888833000	3.003935000	-1.460922000
H	4.908111000	2.622827000	-1.325568000
H	3.292980000	2.219284000	-1.943600000
H	3.931491000	3.874840000	-2.127566000
N	2.249572000	-2.171964000	0.140980000
C	2.633118000	-2.529043000	-1.215005000
H	2.444636000	-1.693195000	-1.897900000
H	3.695502000	-2.820090000	-1.304987000
H	2.019040000	-3.380607000	-1.536571000
C	2.487907000	-3.289072000	1.034650000
H	3.553792000	-3.581444000	1.087260000
H	2.151351000	-3.039550000	2.049894000
H	1.917162000	-4.158886000	0.688535000
O	-0.658596000	-1.449104000	1.657490000
C	-1.113244000	-2.573147000	1.960901000
N	-1.742270000	-2.757189000	3.144409000
C	-1.604477000	-1.767860000	4.201021000
H	-1.602767000	-2.295019000	5.161848000
H	-0.664556000	-1.227630000	4.083085000
H	-2.426920000	-1.042902000	4.196469000
C	-2.792845000	-3.737685000	3.366993000
H	-2.535272000	-4.421576000	4.185941000
H	-3.713793000	-3.203938000	3.638558000
H	-2.986920000	-4.315888000	2.462731000
C	-0.884135000	-3.755736000	1.089011000
C	-0.619536000	-5.008068000	1.659462000
C	-0.788517000	-3.601317000	-0.296421000
C	-0.299080000	-6.095058000	0.857883000
C	-0.483346000	-4.697161000	-1.096882000
C	-0.240491000	-5.942549000	-0.525003000
H	-0.629030000	-5.122564000	2.741246000
H	-0.954897000	-2.630141000	-0.769050000
H	-0.084747000	-7.058632000	1.313086000
H	-0.428756000	-4.566568000	-2.176667000
H	0.005281000	-6.793002000	-1.156493000

TS1

La	-1.133394000	-0.012506000	-0.080089000
N	-1.792800000	2.186528000	-0.609164000

N	-2.966651000	-1.481437000	-0.196312000
Si	-3.490203000	-2.500552000	1.136291000
Si	-0.724157000	3.070137000	-1.681276000
Si	-3.759394000	-1.538645000	-1.753200000
Si	-3.323294000	2.844218000	-0.065256000
C	-4.116513000	1.632168000	1.166054000
H	-4.262397000	0.630183000	0.737735000
H	-3.531623000	1.526094000	2.090172000
H	-5.102922000	2.013041000	1.459966000
C	-3.105532000	4.501718000	0.826668000
H	-2.423474000	4.396076000	1.680012000
H	-2.691913000	5.268948000	0.160139000
H	-4.066672000	4.871884000	1.204049000
C	-4.581954000	3.089795000	-1.464937000
H	-5.585263000	3.250301000	-1.050158000
H	-4.335783000	3.954420000	-2.091210000
H	-4.626531000	2.208281000	-2.117597000
C	0.455558000	4.257872000	-0.800980000
H	1.221248000	3.680022000	-0.265871000
H	0.967033000	4.897904000	-1.531808000
H	-0.066919000	4.906069000	-0.087773000
C	-1.624232000	4.012796000	-3.056754000
H	-2.210943000	4.853459000	-2.667095000
H	-0.891319000	4.422656000	-3.763155000
H	-2.302290000	3.355547000	-3.614552000
C	0.363704000	1.758696000	-2.540471000
H	-0.227271000	1.057883000	-3.147286000
H	1.061055000	2.258708000	-3.224588000
H	0.996595000	1.199619000	-1.834543000
C	-2.715942000	-0.489517000	-2.968852000
H	-1.699287000	-0.878929000	-3.137364000
H	-3.206770000	-0.505564000	-3.949912000
H	-2.652347000	0.569729000	-2.673583000
C	-5.497326000	-0.784214000	-1.787112000
H	-5.521139000	0.192630000	-1.288009000
H	-5.827950000	-0.640613000	-2.823859000
H	-6.228564000	-1.431171000	-1.289869000
C	-3.880960000	-3.283051000	-2.485008000
H	-4.527059000	-3.928665000	-1.877558000
H	-4.309994000	-3.243572000	-3.494103000
H	-2.897950000	-3.764344000	-2.551404000
C	-5.366116000	-2.776319000	1.160709000
H	-5.899727000	-1.818825000	1.207337000
H	-5.727914000	-3.326354000	0.283705000
H	-5.640788000	-3.357230000	2.049979000
C	-2.637794000	-4.193926000	1.115563000
H	-2.787599000	-4.709592000	0.159081000
H	-1.556983000	-4.086845000	1.281346000
H	-3.030842000	-4.836693000	1.913026000
C	-3.049973000	-1.663599000	2.780217000
H	-1.974997000	-1.465025000	2.882703000
H	-3.596892000	-0.720625000	2.907150000
H	-3.326921000	-2.323849000	3.611655000
O	3.063358000	-2.124275000	-0.076209000
C	2.358285000	-3.192119000	-0.692122000
C	1.247511000	-2.451188000	-1.496867000

O	0.979077000	-1.301082000	-0.654234000
C	1.795567000	-4.110304000	0.387448000
H	2.620045000	-4.418596000	1.039092000
H	1.048986000	-3.606221000	1.010329000
C	3.333015000	-3.969196000	-1.558333000
H	2.814470000	-4.730632000	-2.155291000
H	3.891611000	-3.307617000	-2.227043000
H	4.057898000	-4.479330000	-0.915137000
C	1.739407000	-1.929015000	-2.838892000
H	1.003792000	-1.224604000	-3.249731000
H	2.696549000	-1.404216000	-2.737542000
H	1.867564000	-2.743854000	-3.560811000
B	2.175903000	-1.078156000	0.203993000
H	1.712974000	-1.234570000	1.512632000
H	-0.739003000	-2.686648000	-2.316575000
C	-0.028974000	-3.244154000	-1.689670000
H	-0.524730000	-3.473565000	-0.739902000
H	0.181675000	-4.188654000	-2.207496000
H	1.340831000	-5.011491000	-0.042017000
O	2.642928000	0.254145000	0.257944000
C	3.424146000	0.749901000	-0.797027000
H	2.968565000	0.482079000	-1.770794000
C	4.836324000	0.199031000	-0.787988000
C	5.505129000	0.027345000	-2.000088000
C	5.508931000	-0.092644000	0.399272000
C	6.824587000	-0.414776000	-2.031009000
C	6.826420000	-0.532287000	0.371825000
C	7.490064000	-0.691502000	-0.842296000
H	4.979562000	0.231502000	-2.934399000
H	4.981173000	-0.002815000	1.347007000
H	7.329603000	-0.549185000	-2.985195000
H	7.337166000	-0.762565000	1.304373000
H	8.520153000	-1.040355000	-0.860452000
O	0.027187000	0.153074000	2.059836000
C	0.283663000	1.094333000	3.135236000
B	0.683926000	-1.129366000	2.380095000
C	1.389643000	0.358677000	3.970217000
O	1.159341000	-1.019193000	3.689812000
C	-1.021417000	1.262116000	3.894478000
H	-1.791026000	1.639985000	3.207847000
H	-1.367934000	0.309600000	4.310482000
H	-0.921323000	1.990109000	4.707483000
C	0.700770000	2.410608000	2.509734000
H	0.993216000	3.136940000	3.278916000
H	1.532542000	2.269173000	1.811092000
H	-0.141579000	2.835580000	1.943586000
C	1.262619000	0.565575000	5.468813000
H	0.313870000	0.182172000	5.854079000
H	2.071425000	0.026436000	5.973416000
H	1.350301000	1.628774000	5.727961000
C	2.807676000	0.712082000	3.538067000
H	3.499393000	0.035940000	4.053162000
H	2.941315000	0.583570000	2.459545000
H	3.069633000	1.742678000	3.809772000
H	0.020474000	-2.104191000	2.076521000
N	3.355019000	2.205745000	-0.736158000

C	4.007702000	2.797488000	0.417357000
H	3.697621000	2.285419000	1.332961000
H	5.111570000	2.765321000	0.357484000
H	3.699797000	3.848623000	0.495472000
C	3.791365000	2.854470000	-1.953188000
H	4.883008000	2.784620000	-2.123843000
H	3.283286000	2.416450000	-2.821812000
H	3.525416000	3.918455000	-1.905287000

Structure D

La	0.559475000	-0.392268000	-0.572752000
N	0.249086000	-2.725986000	-0.018835000
N	2.248097000	-0.010926000	-2.264727000
Si	1.972001000	1.116886000	-3.560211000
Si	0.505155000	-3.625333000	1.487231000
Si	-0.016483000	-3.667922000	-1.471617000
Si	3.757095000	-0.896717000	-2.158805000
C	-1.680274000	-4.593155000	-1.531772000
H	-1.943451000	-4.837563000	-2.569667000
H	-1.642335000	-5.530181000	-0.966577000
H	-2.489473000	-3.983332000	-1.111018000
C	-0.040354000	-2.496930000	-2.992382000
H	0.926673000	-2.016215000	-3.196651000
H	-0.287191000	-3.111999000	-3.868293000
H	-0.808140000	-1.710754000	-2.944926000
C	1.330469000	-4.944006000	-1.869807000
H	2.315104000	-4.469943000	-1.969736000
H	1.408063000	-5.714215000	-1.093128000
H	1.099880000	-5.447574000	-2.817706000
C	-0.489574000	-5.253238000	1.548143000
H	-0.204217000	-5.973828000	0.772427000
H	-0.300599000	-5.728001000	2.519872000
H	-1.569931000	-5.074886000	1.473687000
C	2.315017000	-4.109366000	1.784602000
H	2.743417000	-4.687792000	0.957301000
H	2.922277000	-3.210250000	1.942652000
H	2.371049000	-4.723756000	2.693528000
C	-0.047023000	-2.704986000	3.048271000
H	0.174749000	-3.355019000	3.905827000
H	0.518204000	-1.778010000	3.185158000
H	-1.125658000	-2.507563000	3.058637000
C	3.763752000	-1.970940000	-0.600478000
H	2.902307000	-2.651779000	-0.556233000
H	4.664969000	-2.598754000	-0.596954000
H	3.760609000	-1.389369000	0.330075000
C	5.269052000	0.250440000	-2.071199000
H	5.200508000	0.912980000	-1.198235000
H	6.191768000	-0.335560000	-1.976470000
H	5.361248000	0.876294000	-2.968311000
C	4.053599000	-2.102193000	-3.601244000
H	4.916439000	-2.740547000	-3.370615000
H	3.186933000	-2.758702000	-3.754471000
H	4.257365000	-1.592724000	-4.549229000
C	2.762182000	2.843017000	-3.373679000
H	2.279594000	3.431209000	-2.582361000
H	3.834546000	2.785699000	-3.151125000

H	2.643835000	3.392126000	-4.317113000
C	2.523861000	0.501399000	-5.271131000
H	3.615918000	0.458104000	-5.363948000
H	2.126040000	-0.498947000	-5.481787000
H	2.153570000	1.186379000	-6.045130000
C	0.101679000	1.435386000	-3.734763000
H	-0.398499000	0.544500000	-4.133249000
H	-0.390735000	1.714630000	-2.791682000
H	-0.065717000	2.254952000	-4.446669000
H	-1.341856000	-0.370889000	2.525228000
O	-1.848340000	0.156926000	0.643574000
C	-2.251722000	0.043975000	2.068506000
C	-3.352761000	-0.983606000	2.180490000
C	-3.257123000	-2.165917000	1.435334000
C	-4.408822000	-0.827754000	3.073821000
C	-4.232620000	-3.148826000	1.551007000
C	-5.386350000	-1.813240000	3.185239000
C	-5.307514000	-2.970101000	2.418909000
H	-2.395461000	-2.331848000	0.780208000
H	-4.452166000	0.067523000	3.689696000
H	-4.142936000	-4.064820000	0.968585000
H	-6.211479000	-1.675392000	3.880518000
H	-6.070496000	-3.739787000	2.510000000
O	-2.232611000	-0.063453000	-1.657482000
C	-3.418341000	-0.271642000	-2.491439000
B	-2.730157000	0.190653000	-0.387663000
C	-4.478946000	0.583639000	-1.737579000
O	-4.066448000	0.443551000	-0.362459000
C	-3.740302000	-1.755897000	-2.453575000
H	-2.878784000	-2.328486000	-2.812948000
H	-3.972679000	-2.092342000	-1.435049000
H	-4.594085000	-1.988282000	-3.099993000
C	-3.149541000	0.175166000	-3.909472000
H	-4.082724000	0.149038000	-4.486552000
H	-2.735146000	1.186258000	-3.953242000
H	-2.441473000	-0.506052000	-4.395177000
C	-5.902988000	0.087599000	-1.864789000
H	-6.017140000	-0.912845000	-1.438207000
H	-6.574950000	0.762674000	-1.324164000
H	-6.216985000	0.066656000	-2.915713000
C	-4.393826000	2.064206000	-2.072521000
H	-4.987563000	2.623382000	-1.339931000
H	-3.358214000	2.422708000	-2.010091000
H	-4.782499000	2.279282000	-3.074430000
O	2.619409000	-0.857334000	2.617476000
C	3.559994000	-0.282471000	3.506892000
B	1.971474000	0.224671000	1.927702000
C	2.878550000	1.070427000	3.875165000
O	2.237477000	1.443289000	2.659841000
H	0.724857000	-0.036337000	1.813403000
C	4.879978000	-0.089632000	2.763645000
H	5.195150000	-1.060875000	2.362310000
H	4.763099000	0.600747000	1.917748000
H	5.677166000	0.286860000	3.416904000
C	3.764795000	-1.237273000	4.668897000
H	4.399161000	-0.793538000	5.448033000

H	2.807465000	-1.530708000	5.111648000
H	4.255445000	-2.149316000	4.307930000
C	3.838777000	2.173360000	4.282067000
H	4.534365000	2.416699000	3.472136000
H	3.276272000	3.081958000	4.529734000
H	4.421128000	1.885058000	5.167321000
C	1.812212000	0.900332000	4.953200000
H	1.235280000	1.830583000	5.027499000
H	1.122245000	0.085904000	4.696693000
H	2.245609000	0.688756000	5.938684000
N	-2.487788000	1.297451000	2.678526000
C	-3.478110000	2.158487000	2.053729000
H	-4.391532000	1.603914000	1.825327000
H	-3.721051000	2.976935000	2.742106000
H	-3.108305000	2.610608000	1.112305000
C	-1.261780000	2.028111000	2.958336000
H	-1.492107000	2.889719000	3.597571000
H	-0.540354000	1.388313000	3.476195000
H	-0.779158000	2.398619000	2.038330000
H	2.398120000	0.340165000	0.731689000
O	0.438393000	2.179067000	-0.377685000
C	0.672046000	3.378829000	-0.131257000
N	1.918771000	3.860621000	-0.010412000
C	2.253103000	5.268944000	0.104747000
H	2.974920000	5.526460000	-0.680407000
H	1.370930000	5.897359000	-0.017501000
H	2.712455000	5.479552000	1.078996000
C	3.064596000	2.949505000	-0.016147000
H	3.929666000	3.488973000	-0.414196000
H	3.260280000	2.599032000	1.005881000
H	2.861675000	2.085706000	-0.656524000
C	-0.499665000	4.289052000	0.037456000
C	-1.502806000	4.265061000	-0.932095000
C	-0.676182000	5.047071000	1.197008000
C	-2.655821000	5.022325000	-0.760049000
C	-1.842151000	5.782140000	1.378889000
C	-2.828603000	5.777437000	0.397238000
H	-1.362327000	3.654860000	-1.824625000
H	0.090691000	5.032699000	1.970620000
H	-3.424995000	5.019198000	-1.529389000
H	-1.981178000	6.358086000	2.290556000
H	-3.735885000	6.360595000	0.535416000

TS2

La	0.109261000	-0.798927000	-0.204659000
N	-0.877720000	-1.799337000	1.772840000
N	1.046176000	-2.428884000	-1.750738000
Si	0.766136000	-2.205303000	-3.453965000
Si	-0.499257000	-1.588684000	3.486619000
Si	-1.923233000	-3.138909000	1.334264000
Si	1.886229000	-3.840745000	-1.152972000
C	-3.742515000	-2.942175000	1.857744000
H	-4.332055000	-3.768578000	1.438300000
H	-3.888487000	-2.939098000	2.942853000
H	-4.147652000	-2.007069000	1.448635000
C	-2.068978000	-3.265496000	-0.567400000

H	-1.128077000	-3.434470000	-1.106795000
H	-2.716921000	-4.127325000	-0.778957000
H	-2.561701000	-2.382206000	-0.997323000
C	-1.327590000	-4.831690000	1.955041000
H	-0.296441000	-5.030538000	1.636413000
H	-1.356343000	-4.902442000	3.048952000
H	-1.964934000	-5.629452000	1.551482000
C	-1.894727000	-2.179646000	4.648565000
H	-2.142505000	-3.242628000	4.548053000
H	-1.564548000	-2.016043000	5.682867000
H	-2.813434000	-1.596857000	4.502279000
C	1.061540000	-2.519740000	4.022036000
H	0.984825000	-3.595043000	3.819343000
H	1.938770000	-2.115325000	3.503623000
H	1.215049000	-2.385460000	5.101328000
C	-0.292585000	0.229943000	4.001492000
H	0.007157000	0.241444000	5.058365000
H	0.498125000	0.741422000	3.443243000
H	-1.242568000	0.776293000	3.927312000
C	2.287804000	-3.605474000	0.687108000
H	1.407349000	-3.321333000	1.282429000
H	2.664832000	-4.547518000	1.107320000
H	3.052749000	-2.834189000	0.847692000
C	3.533889000	-4.175988000	-2.044014000
H	4.211284000	-3.315223000	-1.982981000
H	4.038801000	-5.033099000	-1.580331000
H	3.384887000	-4.415035000	-3.104749000
C	0.903814000	-5.465668000	-1.285959000
H	1.492311000	-6.283921000	-0.850318000
H	-0.049764000	-5.418072000	-0.745984000
H	0.684651000	-5.727762000	-2.327635000
C	2.274559000	-1.649779000	-4.474387000
H	2.607620000	-0.647225000	-4.177492000
H	3.123697000	-2.335624000	-4.371430000
H	2.000873000	-1.610689000	-5.536903000
C	0.069669000	-3.740615000	-4.331233000
H	0.801138000	-4.557218000	-4.372739000
H	-0.824680000	-4.115411000	-3.817819000
H	-0.207803000	-3.492410000	-5.363843000
C	-0.527721000	-0.827879000	-3.695050000
H	-1.485615000	-1.076765000	-3.222423000
H	-0.181889000	0.139551000	-3.300762000
H	-0.715202000	-0.690504000	-4.768505000
H	-0.869263000	1.745449000	1.939331000
O	-1.474237000	1.196505000	-0.125443000
C	-1.599816000	2.360067000	1.409240000
C	-2.995721000	2.144420000	1.842062000
C	-3.407392000	0.833220000	2.119434000
C	-3.867784000	3.204560000	2.099982000
C	-4.688805000	0.593566000	2.598101000
C	-5.152697000	2.956906000	2.569017000
C	-5.569858000	1.652139000	2.808222000
H	-2.716098000	0.000427000	1.952909000
H	-3.538327000	4.230843000	1.960934000
H	-4.997470000	-0.429289000	2.807545000
H	-5.824929000	3.789697000	2.760771000

H	-6.573537000	1.460395000	3.180372000
O	-2.878340000	-0.138373000	-1.499381000
C	-4.213454000	-0.019914000	-2.031972000
B	-2.567864000	1.071598000	-0.885303000
C	-4.347459000	1.524603000	-2.218063000
O	-3.506330000	2.043744000	-1.173319000
C	-5.165949000	-0.575320000	-0.983436000
H	-4.881479000	-1.610118000	-0.756435000
H	-5.116363000	0.003021000	-0.052011000
H	-6.202481000	-0.577144000	-1.340366000
C	-4.323078000	-0.828791000	-3.308204000
H	-5.318093000	-0.706312000	-3.755014000
H	-3.569430000	-0.541079000	-4.046799000
H	-4.183466000	-1.892959000	-3.082206000
C	-5.748593000	2.065860000	-2.024468000
H	-6.101761000	1.894243000	-1.002665000
H	-5.756084000	3.146284000	-2.207447000
H	-6.449802000	1.599311000	-2.727918000
C	-3.765220000	2.010412000	-3.538208000
H	-3.692518000	3.103316000	-3.509156000
H	-2.758358000	1.604730000	-3.701046000
H	-4.395662000	1.730406000	-4.390124000
O	2.622542000	0.065347000	2.760435000
C	3.966873000	0.428403000	2.999695000
B	2.327842000	0.392674000	1.391959000
C	4.131062000	1.673852000	2.077563000
O	3.351183000	1.327329000	0.940909000
H	1.144603000	0.860510000	1.309155000
C	4.873139000	-0.728738000	2.583753000
H	4.552315000	-1.629953000	3.120038000
H	4.788657000	-0.932971000	1.509076000
H	5.927802000	-0.542709000	2.823333000
C	4.134973000	0.692514000	4.485017000
H	5.140083000	1.068886000	4.717976000
H	3.392252000	1.409704000	4.848505000
H	3.984982000	-0.244521000	5.035166000
C	5.558337000	1.949401000	1.638152000
H	5.958260000	1.119974000	1.044330000
H	5.599365000	2.860246000	1.024023000
H	6.217166000	2.106841000	2.502447000
C	3.539243000	2.928963000	2.715292000
H	3.445633000	3.711951000	1.950337000
H	2.539857000	2.719735000	3.117768000
H	4.163673000	3.318397000	3.529335000
N	-1.107647000	3.534296000	1.021625000
C	-1.789292000	4.378337000	0.048224000
H	-2.815478000	4.047771000	-0.110008000
H	-1.763934000	5.425628000	0.371375000
H	-1.261093000	4.291422000	-0.912957000
C	0.343849000	3.660265000	0.974566000
H	0.613222000	4.721494000	1.005309000
H	0.797620000	3.147265000	1.826542000
H	0.738478000	3.214421000	0.050975000
H	2.335477000	-0.640954000	0.645043000
O	1.509215000	0.876562000	-1.607789000
C	2.527511000	1.560945000	-1.824040000

N	3.737697000	1.014357000	-2.028729000
C	4.947391000	1.768671000	-2.292778000
H	5.545729000	1.224626000	-3.031988000
H	4.720816000	2.757490000	-2.692766000
H	5.546003000	1.876703000	-1.376118000
C	3.966806000	-0.394592000	-1.740264000
H	4.646179000	-0.805033000	-2.496145000
H	4.421546000	-0.486244000	-0.743509000
H	3.028523000	-0.957554000	-1.762670000
C	2.355434000	3.042245000	-1.901603000
C	1.303762000	3.541587000	-2.672654000
C	3.107415000	3.912340000	-1.110347000
C	1.040878000	4.906579000	-2.691560000
C	2.828039000	5.274730000	-1.114272000
C	1.802603000	5.774765000	-1.912081000
H	0.691752000	2.847931000	-3.246865000
H	3.874033000	3.502266000	-0.456164000
H	0.234140000	5.293702000	-3.310186000
H	3.408719000	5.945699000	-0.484914000
H	1.591327000	6.841673000	-1.921746000

Amine product

C	1.987652000	-0.083618000	-1.442852000
H	2.673345000	-0.777169000	-1.942966000
H	0.979640000	-0.257359000	-1.834185000
H	2.287981000	0.951079000	-1.711485000
N	2.017037000	-0.308171000	-0.011515000
C	1.078771000	0.562595000	0.676064000
H	1.288217000	1.634594000	0.459429000
H	1.242353000	0.432120000	1.757335000
C	3.356481000	-0.122447000	0.502282000
H	3.733878000	0.910465000	0.348898000
H	3.382878000	-0.336364000	1.577355000
H	4.047963000	-0.809663000	0.001017000
C	-0.359174000	0.258297000	0.352994000
C	-0.816386000	-1.061646000	0.355715000
C	-1.260934000	1.283043000	0.073667000
C	-2.150258000	-1.346341000	0.091924000
C	-2.599804000	1.001415000	-0.184365000
C	-3.047566000	-0.314665000	-0.175442000
H	-0.102721000	-1.859589000	0.553487000
H	-0.907333000	2.313901000	0.057973000
H	-2.494018000	-2.378652000	0.095104000
H	-3.292074000	1.812359000	-0.400394000
H	-4.092068000	-0.538325000	-0.380881000

Structure E

La	-1.049328000	0.134341000	0.252252000
N	-0.746095000	2.168740000	-0.936711000
N	-3.218826000	-0.694345000	-0.337610000
Si	-4.205029000	-1.290942000	0.980035000
Si	0.484395000	2.594135000	-2.111045000
Si	-3.879283000	-0.631681000	-1.960380000
Si	-1.849331000	3.387114000	-0.343285000
C	-2.825153000	2.636190000	1.123155000
H	-3.446966000	1.780584000	0.815554000
H	-2.205997000	2.357799000	1.988945000

H	-3.527926000	3.398635000	1.482232000
C	-0.994444000	4.938276000	0.334261000
H	-0.245075000	4.654730000	1.083409000
H	-0.481124000	5.505393000	-0.451002000
H	-1.725098000	5.606139000	0.807776000
C	-3.177362000	3.924362000	-1.583729000
H	-3.897584000	4.597229000	-1.100888000
H	-2.749777000	4.450199000	-2.444509000
H	-3.729688000	3.053943000	-1.961089000
C	2.110076000	3.030341000	-1.234616000
H	2.506833000	2.181554000	-0.658184000
H	2.879903000	3.359409000	-1.945514000
H	1.936356000	3.845635000	-0.519619000
C	0.013218000	4.075576000	-3.206182000
H	-0.170337000	5.000833000	-2.647842000
H	0.829826000	4.272389000	-3.912716000
H	-0.884489000	3.848022000	-3.795090000
C	0.781032000	1.188826000	-3.344395000
H	-0.101543000	1.056400000	-3.980699000
H	1.624163000	1.454564000	-3.995746000
H	1.030028000	0.226538000	-2.880005000
C	-2.644334000	0.203556000	-3.130704000
H	-1.722752000	-0.386518000	-3.238188000
H	-3.090748000	0.276872000	-4.130843000
H	-2.357877000	1.211414000	-2.803470000
C	-5.513052000	0.331786000	-2.044959000
H	-5.428068000	1.297741000	-1.530587000
H	-5.796122000	0.523212000	-3.087484000
H	-6.334078000	-0.225994000	-1.576582000
C	-4.204357000	-2.345807000	-2.715488000
H	-4.983694000	-2.900309000	-2.181179000
H	-4.527145000	-2.234251000	-3.758664000
H	-3.294632000	-2.959874000	-2.711809000
C	-5.580180000	-0.108813000	1.550711000
H	-5.178741000	0.850457000	1.899050000
H	-6.302698000	0.099819000	0.753600000
H	-6.126943000	-0.564757000	2.386686000
C	-5.084148000	-2.943349000	0.660418000
H	-5.896070000	-2.824865000	-0.068001000
H	-4.410178000	-3.724012000	0.290756000
H	-5.534651000	-3.298138000	1.596449000
C	-3.077869000	-1.515716000	2.499268000
H	-2.214502000	-2.163307000	2.292639000
H	-2.707519000	-0.556893000	2.890796000
H	-3.659446000	-1.978238000	3.306896000
O	-0.496849000	0.643690000	2.644522000
C	0.622412000	0.687274000	3.216921000
C	1.596769000	1.742168000	2.828369000
C	2.842648000	1.415677000	2.289376000
C	1.204700000	3.078912000	2.931696000
C	3.704941000	2.429661000	1.889352000
C	2.086049000	4.087458000	2.560597000
C	3.338489000	3.762616000	2.045050000
H	3.119006000	0.374787000	2.130462000
H	0.212367000	3.319932000	3.311376000
H	4.656753000	2.165025000	1.433854000

H	1.787905000	5.128754000	2.660288000
H	4.019588000	4.553348000	1.739096000
N	0.915882000	-0.184772000	4.188147000
C	2.198043000	-0.260940000	4.866136000
H	2.028516000	-0.443189000	5.932522000
H	2.795854000	-1.086080000	4.455751000
H	2.752688000	0.670541000	4.752110000
C	0.008526000	-1.303242000	4.414465000
H	-1.028397000	-0.963200000	4.389980000
H	0.148208000	-2.061589000	3.630214000
H	0.228065000	-1.740325000	5.391440000
O	1.466119000	-0.598806000	-0.085083000
O	-0.090750000	-2.239285000	0.715531000
C	-0.110698000	-3.342378000	-0.213327000
B	1.327591000	-1.819379000	0.851264000
C	1.275100000	-4.004227000	0.048903000
O	2.118623000	-2.907186000	0.358073000
C	-0.251096000	-2.800456000	-1.634921000
H	-1.173514000	-2.200233000	-1.689133000
H	0.607822000	-2.190696000	-1.938324000
H	-0.372679000	-3.611946000	-2.363026000
C	-1.312241000	-4.210507000	0.103163000
H	-1.307088000	-5.121528000	-0.509361000
H	-1.337022000	-4.496984000	1.159317000
H	-2.230730000	-3.653265000	-0.123059000
C	1.850919000	-4.732138000	-1.152381000
H	2.033927000	-4.036473000	-1.978059000
H	2.809680000	-5.187354000	-0.875337000
H	1.183838000	-5.533156000	-1.497426000
C	1.250391000	-4.933271000	1.258806000
H	2.282765000	-5.200028000	1.510018000
H	0.810442000	-4.430015000	2.128464000
H	0.690913000	-5.856937000	1.065725000
O	3.852908000	-0.260728000	-0.094724000
C	4.923115000	-0.725907000	-0.936639000
B	2.674857000	-0.619086000	-0.714812000
C	4.244288000	-0.792689000	-2.345442000
O	2.862691000	-1.022805000	-2.015864000
H	1.581972000	-1.454121000	1.993900000
C	5.337152000	-2.091214000	-0.406970000
H	5.635357000	-1.981889000	0.641746000
H	4.497205000	-2.795295000	-0.438172000
H	6.186365000	-2.503056000	-0.964910000
C	6.074563000	0.253116000	-0.834962000
H	6.879674000	-0.012291000	-1.531966000
H	5.748565000	1.277078000	-1.046445000
H	6.487838000	0.228775000	0.180329000
C	4.729268000	-1.927070000	-3.225183000
H	4.558112000	-2.901660000	-2.759163000
H	4.191171000	-1.906447000	-4.179296000
H	5.801060000	-1.822036000	-3.437787000
C	4.316687000	0.519519000	-3.110717000
H	3.672386000	0.446324000	-3.993962000
H	3.957729000	1.358126000	-2.502071000
H	5.337573000	0.736965000	-3.445937000

E_{HBpin}

La	-0.814848000	-0.472473000	0.045721000
N	-0.306967000	-2.482777000	-1.123122000
N	-2.168147000	-1.140758000	1.902712000
Si	-1.946253000	-0.658434000	3.587163000
Si	-0.363472000	-2.328240000	-2.854158000
Si	0.127797000	-3.930191000	-0.244897000
Si	-3.657815000	-1.952864000	1.466183000
C	1.431530000	-5.007169000	-1.116377000
H	1.901264000	-5.685021000	-0.391655000
H	0.955040000	-5.627558000	-1.886553000
H	2.219523000	-4.421372000	-1.600275000
C	0.737033000	-3.386762000	1.469554000
H	-0.096685000	-2.950563000	2.041721000
H	1.105448000	-4.245780000	2.045002000
H	1.551440000	-2.647197000	1.439173000
C	-1.307661000	-5.142199000	0.039280000
H	-2.086762000	-4.733876000	0.692576000
H	-1.776833000	-5.423582000	-0.913009000
H	-0.926106000	-6.059806000	0.505670000
C	1.020752000	-3.119388000	-3.871611000
H	1.037493000	-4.212129000	-3.805030000
H	0.881274000	-2.847948000	-4.926413000
H	1.991602000	-2.733617000	-3.543706000
C	-1.990790000	-2.957264000	-3.611674000
H	-2.065619000	-4.046121000	-3.490527000
H	-2.872759000	-2.520506000	-3.126892000
H	-2.034962000	-2.737002000	-4.686306000
C	-0.180040000	-0.461770000	-3.222031000
H	-0.291212000	-0.273654000	-4.298855000
H	-0.897869000	0.210026000	-2.729414000
H	0.832538000	-0.147441000	-2.927250000
C	-3.652759000	-2.385480000	-0.393014000
H	-2.886975000	-3.119328000	-0.663649000
H	-4.635216000	-2.813705000	-0.637305000
H	-3.523368000	-1.510468000	-1.043495000
C	-5.199032000	-0.857796000	1.705431000
H	-5.064958000	0.106926000	1.198956000
H	-6.089747000	-1.341048000	1.282302000
H	-5.400833000	-0.646068000	2.761681000
C	-3.968783000	-3.594170000	2.375955000
H	-4.505162000	-4.298909000	1.727939000
H	-3.018360000	-4.059518000	2.667655000
H	-4.563460000	-3.451446000	3.284754000
C	-2.182074000	1.219504000	3.784178000
H	-1.519263000	1.789669000	3.121939000
H	-3.219157000	1.494427000	3.550437000
H	-1.972204000	1.532032000	4.815724000
C	-3.204668000	-1.419388000	4.800306000
H	-4.251735000	-1.207723000	4.555934000
H	-3.084481000	-2.505322000	4.887165000
H	-3.006544000	-0.987333000	5.790311000
C	-0.281443000	-1.170479000	4.329719000
H	-0.208435000	-2.265424000	4.365138000
H	0.601508000	-0.786944000	3.805502000
H	-0.241726000	-0.808422000	5.367079000

O	1.706556000	0.050788000	0.313922000
O	1.705765000	2.161193000	1.563274000
C	2.266872000	2.570055000	2.805842000
B	1.532980000	0.719233000	1.661231000
C	3.167661000	1.354198000	3.169377000
O	2.391914000	0.260956000	2.704020000
H	0.319878000	0.438149000	1.942567000
C	1.152811000	2.770783000	3.830551000
H	0.418457000	3.482947000	3.433323000
H	0.632963000	1.829793000	4.044149000
H	1.537759000	3.175911000	4.774486000
C	2.999782000	3.884488000	2.612372000
H	3.537349000	4.176102000	3.524040000
H	3.720615000	3.836367000	1.788891000
H	2.273079000	4.679185000	2.391018000
C	3.422272000	1.169455000	4.655186000
H	2.491478000	0.976796000	5.197628000
H	4.080202000	0.306189000	4.807133000
H	3.913280000	2.050693000	5.089955000
C	4.504852000	1.394278000	2.433046000
H	4.988757000	0.417181000	2.528990000
H	4.366674000	1.581725000	1.359939000
H	5.169012000	2.163958000	2.848176000
C	1.360123000	2.873311000	-1.767552000
C	2.688906000	2.989096000	-1.353269000
C	1.059551000	2.671247000	-3.113444000
C	3.706317000	2.939657000	-2.296757000
C	2.083514000	2.618010000	-4.052941000
C	3.405637000	2.761488000	-3.645573000
H	2.893835000	3.087806000	-0.288145000
H	0.020846000	2.558769000	-3.422250000
H	4.742476000	3.033518000	-1.978590000
H	4.207589000	2.725194000	-4.379848000
C	0.244497000	2.962784000	-0.787811000
H	1.847107000	2.464939000	-5.103251000
O	-0.564444000	2.016294000	-0.654811000
O	-3.170613000	0.894102000	-0.977603000
C	-4.072863000	1.283353000	-2.066708000
B	-3.296363000	1.874264000	-0.012835000
C	-4.156909000	2.827047000	-1.867807000
O	-3.974058000	2.968796000	-0.438703000
H	-2.885165000	1.733126000	1.089958000
C	-5.398515000	0.582048000	-1.814593000
H	-5.243527000	-0.501769000	-1.790392000
H	-5.838748000	0.879594000	-0.855789000
H	-6.115781000	0.804413000	-2.612351000
C	-3.496476000	0.846522000	-3.393548000
H	-4.165978000	1.154400000	-4.206721000
H	-2.507407000	1.273454000	-3.581428000
H	-3.407447000	-0.246856000	-3.428744000
C	-5.486369000	3.441567000	-2.249909000
H	-6.309229000	3.032231000	-1.658099000
H	-5.451889000	4.522660000	-2.078722000
H	-5.697598000	3.273230000	-3.313397000
C	-3.015598000	3.584850000	-2.528573000
H	-3.027533000	4.619439000	-2.167237000

H	-2.048583000	3.140903000	-2.265089000
H	-3.119193000	3.601958000	-3.619680000
N	0.074556000	4.103996000	-0.107670000
C	-0.911090000	4.132041000	0.962122000
H	-1.927029000	4.279403000	0.572427000
H	-0.872691000	3.188821000	1.514964000
H	-0.662266000	4.951034000	1.643780000
C	0.850767000	5.313260000	-0.311545000
H	1.601786000	5.437015000	0.480892000
H	1.359113000	5.290677000	-1.276103000
H	0.175543000	6.176038000	-0.292992000
O	2.950518000	-1.027231000	-1.442807000
C	4.337013000	-1.401817000	-1.588440000
B	2.805211000	-0.613531000	-0.129366000
C	4.732731000	-1.797872000	-0.135330000
O	3.884796000	-0.951706000	0.648702000
C	5.080247000	-0.168097000	-2.077548000
H	4.602344000	0.188868000	-2.996802000
H	5.028970000	0.640406000	-1.337173000
H	6.133857000	-0.384847000	-2.289823000
C	4.480193000	-2.514808000	-2.603237000
H	5.523795000	-2.852776000	-2.647021000
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H	4.202594000	-2.154134000	-3.600637000
C	6.176520000	-1.517263000	0.231732000
H	6.414831000	-0.451935000	0.155016000
H	6.355908000	-1.827500000	1.267390000
H	6.861606000	-2.081579000	-0.414121000
C	4.375708000	-3.233762000	0.217151000
H	4.484095000	-3.364098000	1.299587000
H	3.334549000	-3.454728000	-0.042197000
H	5.025794000	-3.957578000	-0.288930000

TS3

La	-0.780850000	-0.457709000	-0.077182000
N	0.083586000	-1.530671000	-2.031134000
N	-2.573515000	-1.771936000	0.828010000
Si	-2.818129000	-2.133114000	2.524443000
Si	0.460839000	-0.511535000	-3.396231000
Si	0.276566000	-3.271139000	-2.049010000
Si	-3.745750000	-2.359230000	-0.336396000
C	1.930928000	-3.857257000	-2.757238000
H	2.045278000	-4.933709000	-2.575659000
H	2.006105000	-3.692753000	-3.839017000
H	2.758920000	-3.336458000	-2.266350000
C	0.247955000	-3.841422000	-0.238366000
H	-0.644503000	-3.504968000	0.312779000
H	0.264514000	-4.936732000	-0.171382000
H	1.150142000	-3.468097000	0.266976000
C	-1.030946000	-4.248507000	-3.025829000
H	-2.028850000	-4.222120000	-2.576116000
H	-1.118458000	-3.874646000	-4.053915000
H	-0.715241000	-5.298538000	-3.080724000
C	2.232230000	-0.612039000	-4.069323000
H	2.507471000	-1.606513000	-4.436785000
H	2.338658000	0.097941000	-4.900133000
H	2.941125000	-0.310402000	-3.287061000
C	-0.712160000	-0.797158000	-4.861010000
H	-0.575084000	-1.801105000	-5.283293000
H	-1.761788000	-0.709430000	-4.553097000
H	-0.523524000	-0.070958000	-5.661684000
C	0.305984000	1.293272000	-2.819042000
H	0.253186000	1.966744000	-3.684838000
H	-0.576845000	1.525400000	-2.207392000
H	1.187007000	1.586670000	-2.230885000
C	-3.302118000	-1.741275000	-2.084414000
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H	-4.038051000	-2.152429000	-2.789170000
H	-3.379126000	-0.647575000	-2.137028000
C	-5.519220000	-1.714128000	-0.072515000
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H	-6.082499000	-1.794854000	-1.011661000
H	-6.064041000	-2.272058000	0.695746000
C	-3.850963000	-4.255476000	-0.374816000
H	-4.475392000	-4.600366000	-1.209083000
H	-2.857968000	-4.709782000	-0.480952000
H	-4.293709000	-4.640783000	0.552565000
C	-2.306595000	-0.659038000	3.610216000
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H	-3.085407000	0.112477000	3.581656000
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C	-4.610541000	-2.483333000	3.050038000
H	-5.264565000	-1.624647000	2.857347000
H	-5.044194000	-3.364412000	2.562720000
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C	-1.841320000	-3.676357000	3.053710000
H	-2.221199000	-4.558198000	2.521600000
H	-0.772384000	-3.598735000	2.820573000
H	-1.944064000	-3.860921000	4.131216000

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C	2.868129000	-0.087844000	3.519329000
B	1.835066000	0.451908000	1.552567000
C	1.646769000	-1.034971000	3.295745000
O	0.867832000	-0.308216000	2.300410000
H	1.275980000	1.773473000	1.506848000
C	2.582933000	1.024118000	4.519021000
H	3.382851000	1.770311000	4.447252000
H	1.631407000	1.523088000	4.301280000
H	2.552084000	0.651291000	5.549314000
C	4.150583000	-0.804319000	3.896544000
H	4.039427000	-1.352836000	4.840408000
H	4.455756000	-1.505500000	3.113075000
H	4.952099000	-0.067054000	4.025884000
C	0.825624000	-1.270504000	4.545453000
H	0.382642000	-0.348924000	4.933925000
H	0.015251000	-1.979431000	4.342640000
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C	2.045022000	-2.371447000	2.689800000
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H	2.572209000	-2.997777000	3.419410000
C	1.206016000	3.370498000	-0.033961000
C	2.590630000	3.256223000	-0.083719000
C	0.558872000	4.199823000	-0.953254000
C	3.317493000	3.931977000	-1.059742000
C	1.284146000	4.886089000	-1.917979000
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H	-0.523103000	4.300949000	-0.904677000
H	4.398552000	3.809269000	-1.103292000
H	3.238127000	5.271508000	-2.743213000
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H	0.767799000	5.527849000	-2.628783000
O	-0.619765000	1.898196000	0.485021000
O	-3.279409000	1.251365000	-0.587071000
C	-3.941361000	2.235466000	-1.446731000
B	-3.769893000	1.475397000	0.681591000
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H	-3.573625000	0.734204000	1.582268000
C	-5.174494000	1.561825000	-2.030753000
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H	-5.870932000	1.242778000	-1.246445000
H	-5.702489000	2.238049000	-2.712366000
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H	-6.442558000	3.479158000	-0.778573000
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H	-2.952710000	4.971680000	-1.000158000
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H	-0.496236000	1.930350000	3.521117000
H	-1.222403000	3.543123000	3.777764000
C	1.065035000	4.150729000	2.724482000
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H	0.655533000	4.779597000	3.521069000
O	3.861010000	0.667751000	-1.083454000
C	5.228603000	0.225938000	-0.982424000
B	3.113372000	-0.217118000	-0.353077000
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H	6.901717000	0.762429000	0.313392000
C	5.949809000	0.564735000	-2.269956000
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C	6.080586000	-1.852633000	0.315579000
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O	-1.466835000	0.466227000	0.562452000
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C	-3.452522000	1.643445000	1.241711000
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C	-4.009188000	-1.207499000	1.129519000
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H	-3.278136000	-1.189161000	1.946000000
H	-4.925958000	-0.712251000	1.469998000
O	0.000024000	-1.360595000	0.002857000

O	1.465587000	0.466425000	-0.559325000
C	2.794983000	0.832796000	-0.144719000
B	1.216083000	-0.758533000	0.005930000
C	3.450608000	-0.557533000	0.126430000
O	2.324876000	-1.351493000	0.546469000
C	2.648366000	1.676497000	1.113335000
H	1.983909000	2.518931000	0.894254000
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C	3.449818000	1.643700000	-1.242743000
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H	3.419571000	1.122942000	-2.203813000
H	2.924986000	2.598259000	-1.358971000
C	4.495665000	-0.566229000	1.221940000
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H	3.274014000	-1.188695000	-1.947215000
H	4.922821000	-0.711800000	-1.474617000

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