

Supporting Information

9-Borabicyclo[3.3.1]nonane: a Metal-free Catalyst for the Hydroboration of Carbodiimides

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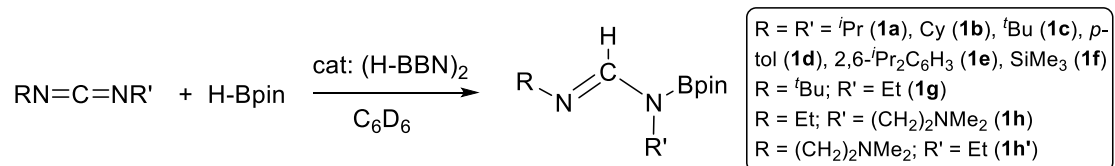
General remarks. All manipulations were carried out under dry nitrogen using standard Schlenk and glovebox techniques. Solvents were distilled from appropriate drying agents and stored under N₂ in Schlenk tubes equipped with J. Young-type Teflon stoppers and containing activated molecular sieves (4 Å). Microanalyses were carried out with a LECO CHNS-932 analyser. NMR spectra were recorded on Bruker 400 and 500 spectrometers in C₆D₆ at 298 K unless otherwise stated, using standard TOPSPIN 4.0 software. ¹H NMR and ¹³C{¹H} NMR chemical shifts are referenced to residual protons or carbons in deuterated solvent. Chemical shifts (δ) are given in ppm and coupling constants (J) in Hz. All reagents were purchased from the usual commercial suppliers. Compounds CH(N^{*i*}Pr)₂BC₈H₁₄ (**2**) and CH(N^{*i*}Pr)₂(C₈H₁₄BHBC₈H₁₄) (**3**) were prepared according to literature procedures.¹

Catalytic reactions

General procedure for the hydroboration reaction.

NMR scale: In a glovebox, the corresponding carbodiimide (0.20 mmol) was dissolved in 600 μ L of C₆D₆. Then, pinacol borane (HBpin, 30 μ L, 0.20 mmol) was added to the solution, followed by addition of a measured volume of a stock solution of 9-borabicyclo[3.3.1]nonane dimer [(H-BBN)₂, 0.10 M in C₆D₆]. The final catalyst load, as well as the reaction time and temperature for each reaction are collected in table S1 (*vide infra*). The reaction progress was monitored by ¹H and ¹¹B NMR spectroscopy until reaction completion. The NMR spectra obtained were then compared with those reported in the literature for the corresponding borylamidines.² Conversions were determined by ¹H NMR spectroscopy based on the ratio of the limiting reagent and the target borylamidine product (**1a-h'**). The reactions with the different commercial carbodiimides and HBpin were also performed in the absence of catalyst under the same conditions (see table S1 and Figure S1), to confirm that either negligible or only trace amounts of the target products were obtained.

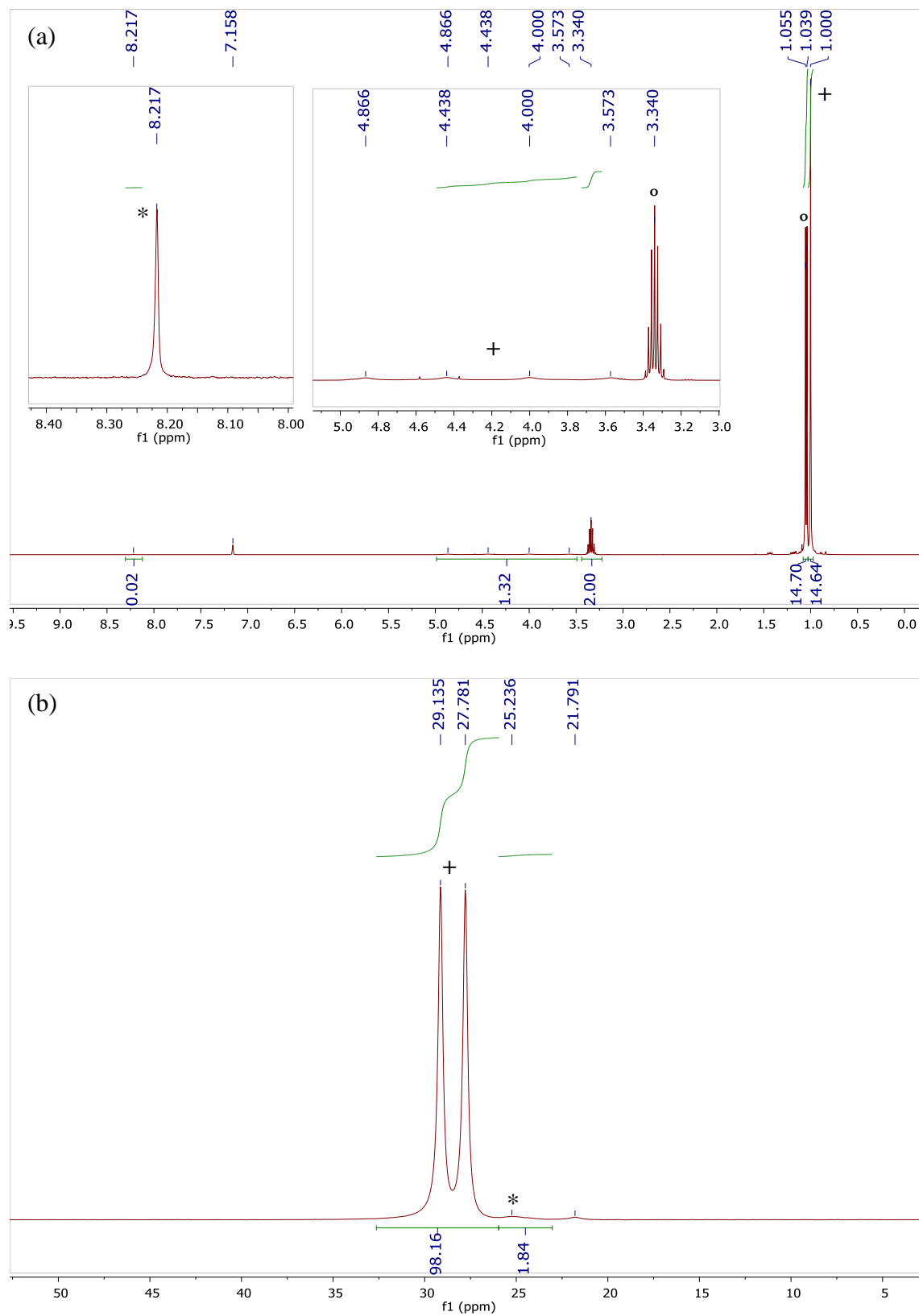
Table S1. Monohydroboration of carbodiimides (RNCNR'), 0.20 mmol) with HBpin (0.20 mmol) using (H-BBN)₂ as catalyst (NMR scale).



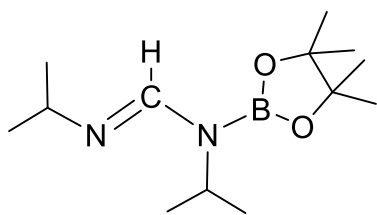
R, R' (RNCNR')	Catalyst load (mol%)	t (h)	T (°C)	Conversion (%)
<i>i</i> Pr	-	15	60	2
	2.5	0.2	25	>99
	0.5	2	25	>99
Cy	-	15	60	1
	2.5	0.2	25	>99
	0.5	2	25	>99
<i>t</i> Bu	-	15	60	-
	2.5	3.5	25	>99
	2.5	1	60	>99
	0.5	2.5	60	99
<i>p</i> -tol	2.5	15	60	-
	2.5	1	60	>99
	0.5	2.5	60	>99
Dipp	-	15	60	-
	2.5	2.5	25	>99
	0.5	2.5	60	>99
	2.5	1	60	>99
SiMe ₃	-	15	60	-
	2.5	3.5	60	23
Et, <i>t</i> Bu	-	15	60	2
	2.5	20	60	>99
	0.5	20	60	67
Et, (CH ₂) ₃ NMe ₂ ^a	-	15	60	-
	2.5	15	60	>99
	0.5	20	60	>99

^a Isomer mixture **1h/1h'** 57:43.

Figure S1. ^1H (a) and ^{11}B (b) NMR spectra in C_6D_6 of the reaction crude of $\text{C}(\text{N}^i\text{Pr})_2$ (°) with HBpin (+) in the absence of catalyst after 15 h at 60 °C. [**1a** (*)]



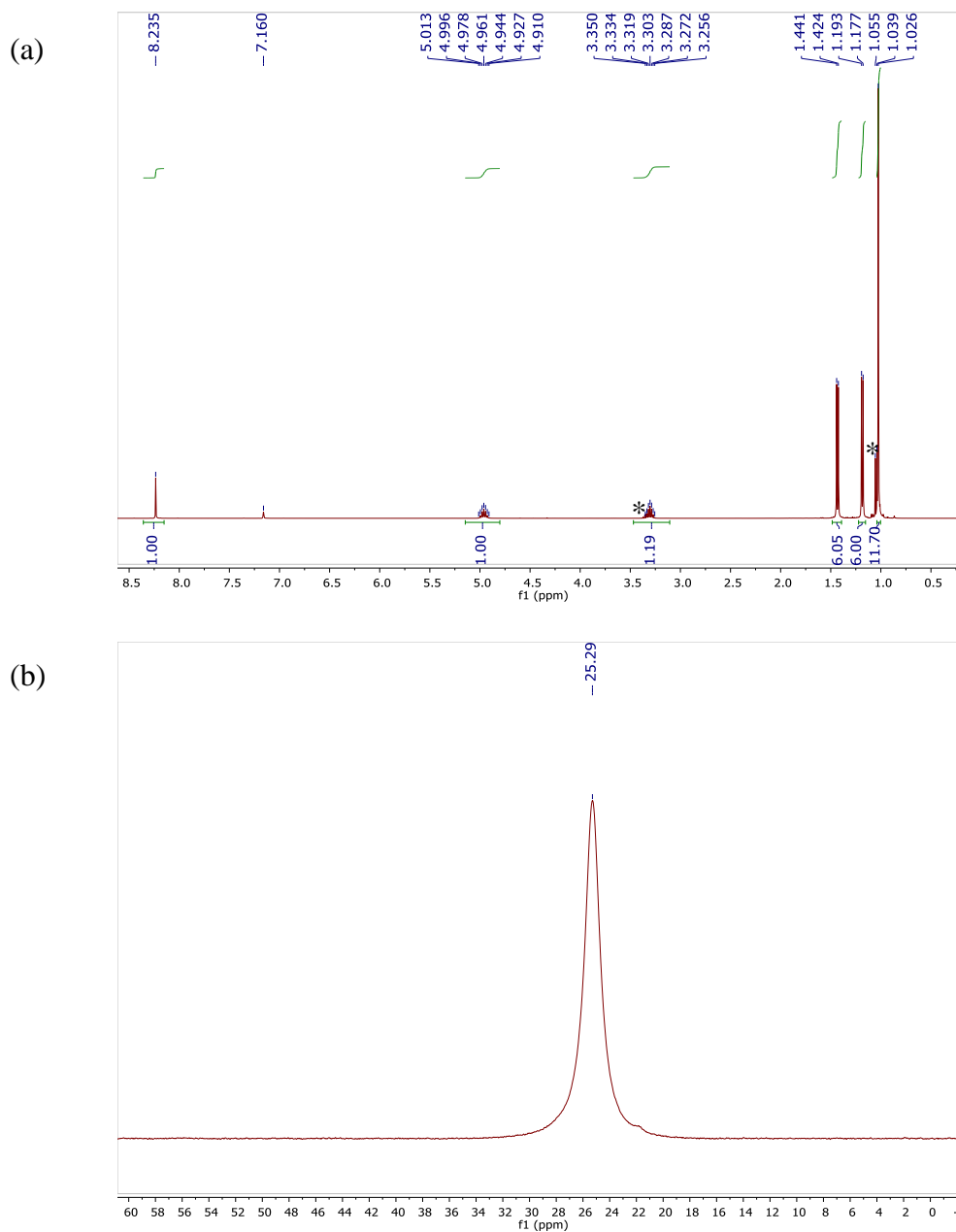
Hydroboration of *N,N'*-diisopropylcarbodiimide (1a). 31.5 μL of $\text{C}(\text{N}^i\text{Pr})_2$ (0.20



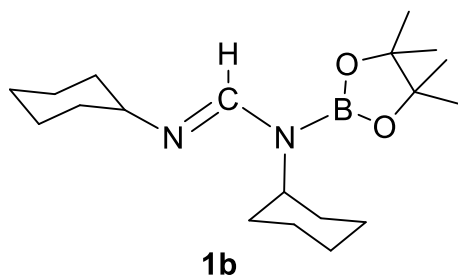
1a

mmol), 30 μL of HBpin (0.20 mmol). ^1H NMR (400 MHz) δ 8.24 (s, 1H, $\text{HC}=\text{N}$), 4.96 (sept, $J = 6.9$ Hz, 1H, CH^iPr), 3.30 (sept, $J = 6.3$ Hz, 1H, CH^iPr), 1.43 (d, $J = 6.9$ Hz, 6H, CH_3^iPr), 1.18 (d, $J = 6.3$ Hz, 6H, CH_3^iPr), 1.03 (s, 12H, Bpin). ^{11}B NMR (128 MHz) δ 25.3 (s, Bpin).

Figure S2. ^1H (a) and ^{11}B (b) NMR spectra in C_6D_6 of the reaction crude of $\text{C}(\text{N}^i\text{Pr})_2$ (*) with HBpin. [Reaction conditions: 0.5 mol% cat., 25 $^\circ\text{C}$, 2 h]

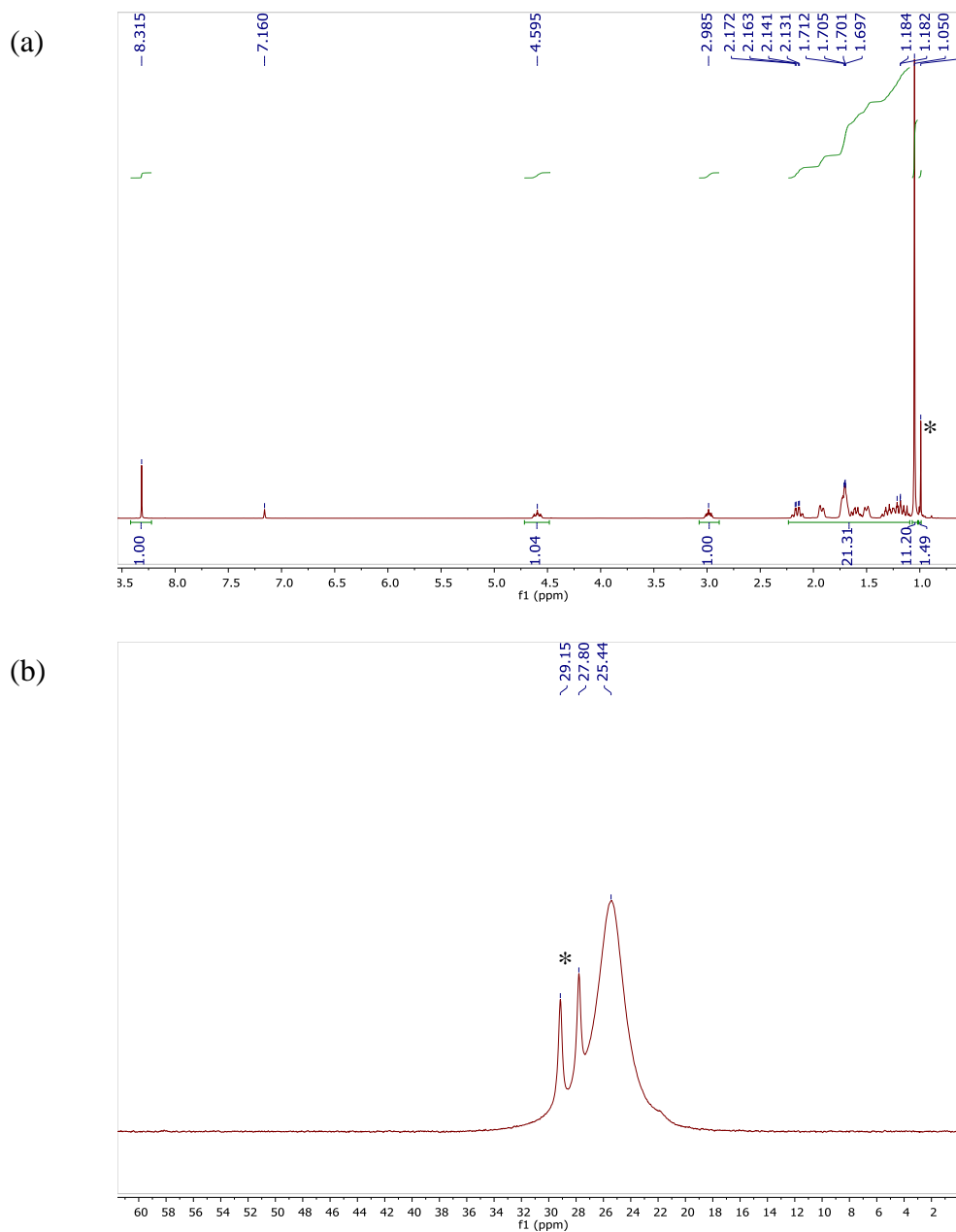


Hydroboration of *N,N'*-dicyclohexylcarbodiimide (1b). 41 mg of C(NCy)₂ (0.20

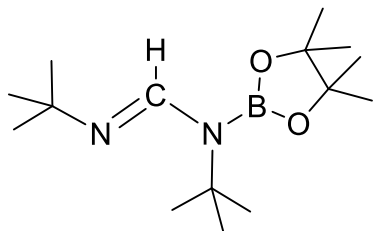


mmol), 30 μ L of HBpin (0.20 mmol). ¹H NMR (400 MHz) δ 8.32 (s, 1H, HC=N), 4.60 (m, 1H, NCH-Cy), 2.99 (m, 1H, NCH-Cy), 2.25 – 1.10 (m, 22H, Cy), 1.05 (s, 12H, Bpin). ¹¹B NMR (128 MHz) δ 25.4 (s, Bpin).

Figure S3. ¹H (a) and ¹¹B (b) NMR spectra in C₆D₆ of the reaction crude of C(NCy)₂ with HBpin (*). [Reaction conditions: 0.5 mol% cat., 25 $^{\circ}$ C, 2 h]



Hydroboration of *N,N'*-di-*tert*-butylcarbodiimide (1c). NMR scale: 39 μL of $\text{C}(\text{N}^t\text{Bu})_2$

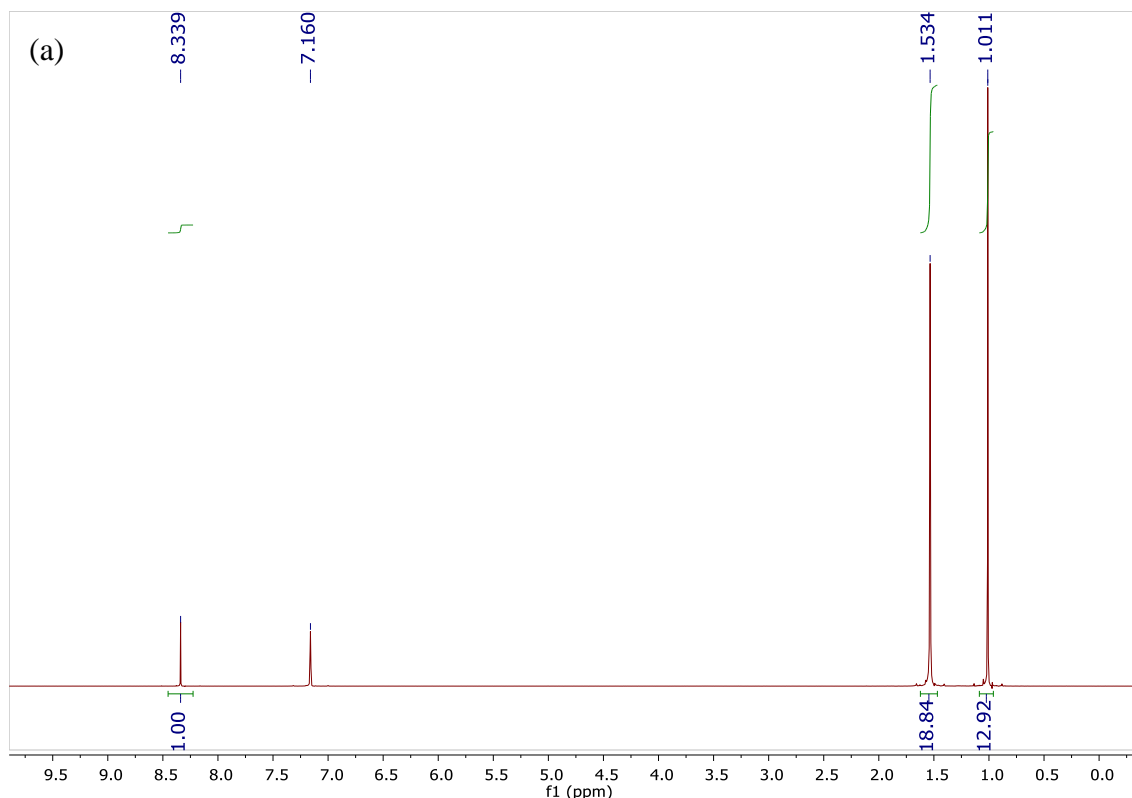


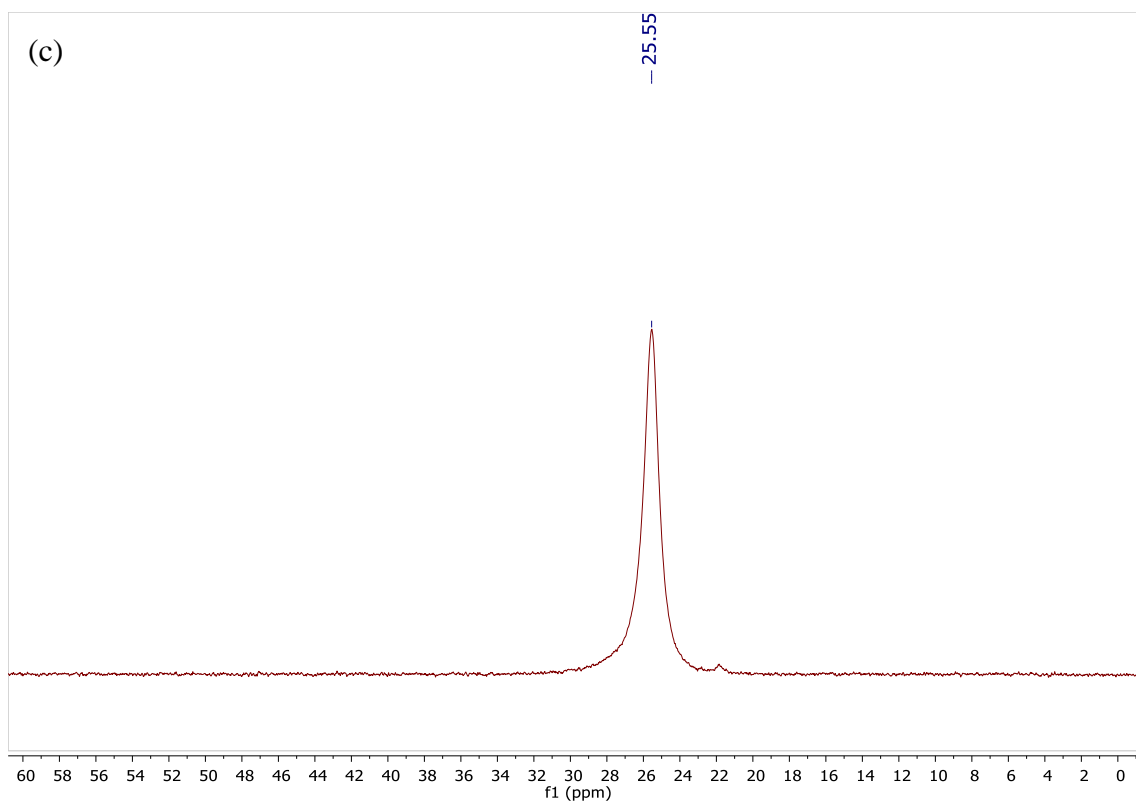
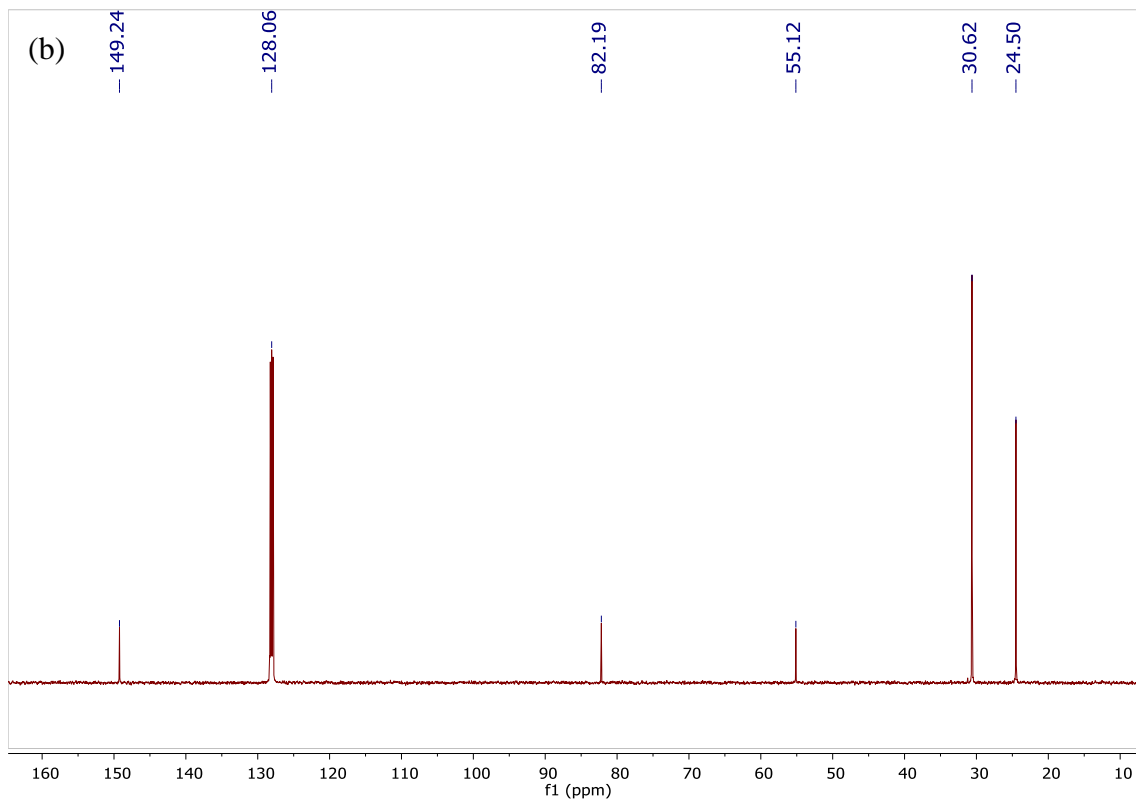
1c

(0.20 mmol), 30 μL of HBpin (0.20 mmol). Upscale reaction: Solid $(\text{H}-\text{BBN})_2$ (6 mg, 0.025 mmol, 2.5 mol%) was added to a toluene solution (6 mL) of HBpin (150 μL , 1.00 mmol) and $\text{C}(\text{N}^t\text{Bu})_2$ (195 μL , 1.00 mmol), and the solution was stirred for 1 h at 60 $^\circ\text{C}$. Then, the solvent was

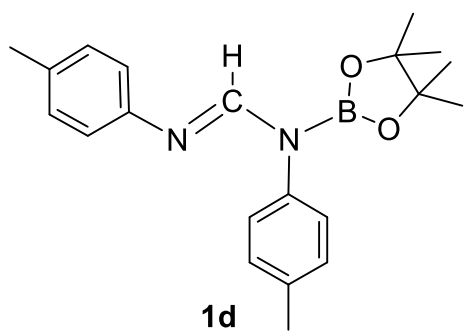
removed under vacuum and the solid residue was dissolved in the minimum amount of pentane (ca. 0.5 mL) and kept at -20 $^\circ\text{C}$ for 24 h. Thus, crystals of compound **1c** (160 mg, 60%) were obtained, which were also suitable for an X-ray analysis. Anal. Calc. for $\text{C}_{15}\text{H}_{31}\text{BN}_2\text{O}_2$: C, 63.84; H 11.07; N, 9.93. Found: C, 63.58; H, 10.99; N, 9.70. ^1H NMR (500 MHz) δ 8.34 (s, 1H, $\text{HC}=\text{N}$), 1.53 (s, 18H, ^tBu), 1.01 (s, 12H, Bpin). $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz) δ 149.2 (s, HCN_2), 82.2 (s, $\text{BO}_2\text{C}_2\text{Me}_4$), 55.1 (s, $\text{C}-^t\text{Bu}$), 30.6 (s, CH_3-^tBu), 24.5 (s, $\text{BO}_2\text{C}_2\text{Me}_4$),. ^{11}B NMR (160 MHz) δ 25.6 (s, Bpin).

Figure S4. ^1H (a), $^{13}\text{C}\{^1\text{H}\}$ (b), ^{11}B (c) NMR spectra in C_6D_6 of compound **1c**.



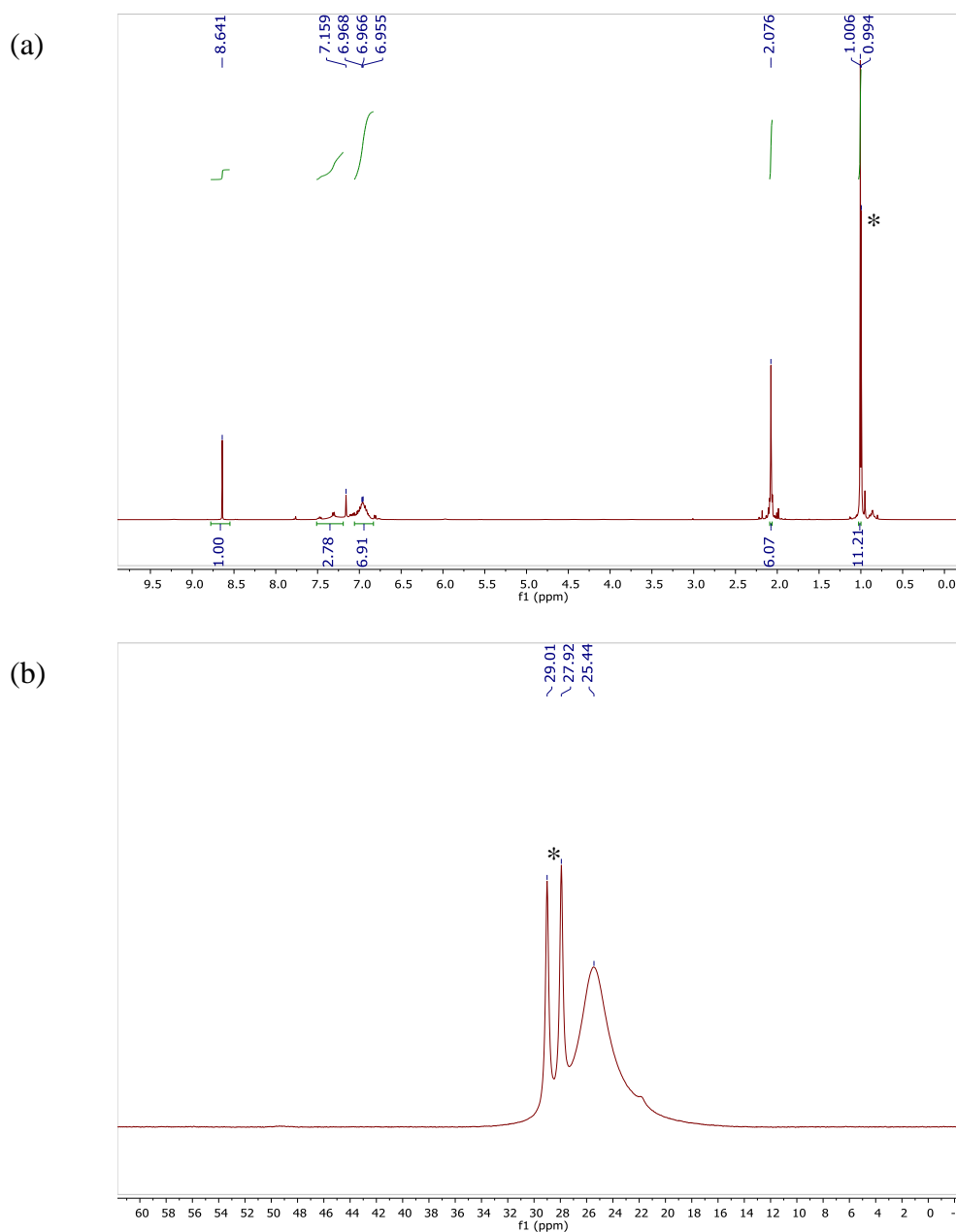


Hydroboration of *N,N'*-di-*p*-tolylcarbodiimide (1d). 45 mg of $C\{N(p\text{-tol})\}_2$ (0.20

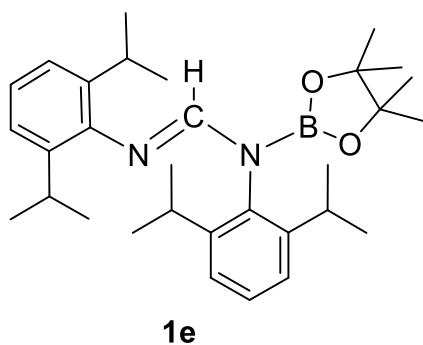


mmol), 30 μL of HBpin (0.20 mmol). ^1H NMR (500 MHz) δ 8.64 (s, 1H, $\text{HC}=\text{N}$), 7.50 – 6.80 (m, br, 8H, C_6H_4), 2.08 (s, 6H, $\text{CH}_3\text{-Ar}$), 2.25 – 1.10 (m, 22H, Cy), 1.01 (s, 12H, Bpin). ^{11}B NMR (160 MHz) δ 25.4 (s, Bpin).

Figure S5. ^1H (a) and ^{11}B (b) NMR spectra in C_6D_6 of the reaction crude of $C\{N(p\text{-tol})\}_2$ with HBpin (*). [Reaction conditions: 0.5 mol% cat., 60 $^\circ\text{C}$, 2.5 h]

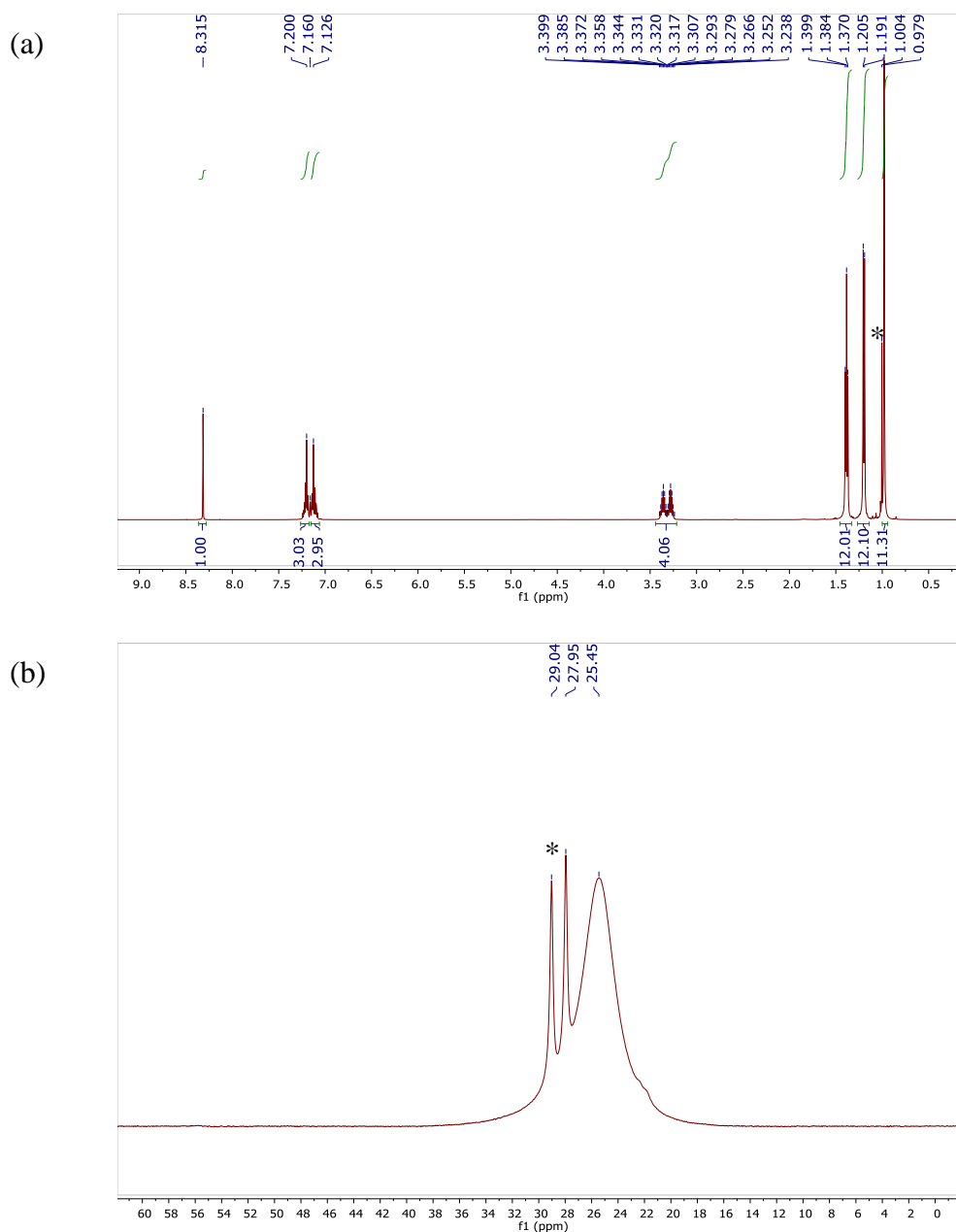


Hydroboration of *N,N'*-diisopropylphenylcarbodiimide (1e). 73 mg of C{N(Dipp)}₂

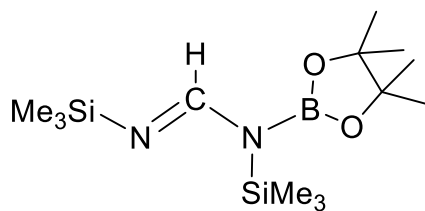


(0.20 mmol), 30 μ L of HBpin (0.20 mmol). ¹H NMR (500 MHz) δ 8.32 (s, 1H, HC=N), 7.25 – 7.05 (m, 6H, C₆H₃), 2.08 (s, 6H, CH₃-Ar), 3.36 (\approx sept, $J \approx 7.0$ Hz, 2H, CH-^{*i*}Pr), 3.27 (\approx sept, $J \approx 7.0$ Hz, 2H, CH-^{*i*}Pr), 1.39 (d, $J = 7.0$ Hz, 6H, CH₃-^{*i*}Pr), 1.38 (d, $J = 7.0$ Hz, 6H, CH₃-^{*i*}Pr), 1.20 (d, $J = 7.0$ Hz, 12H, CH₃-^{*i*}Pr), 0.98 (s, 12H, Bpin). ¹¹B NMR (160 MHz) δ 25.5 (s, Bpin).

Figure S6. ¹H (a) and ¹¹B (b) NMR spectra in C₆D₆ of the reaction crude of C{N(Dipp)}₂ with HBpin (*). [Reaction conditions: 0.5 mol% cat., 60 °C, 2.5 h]



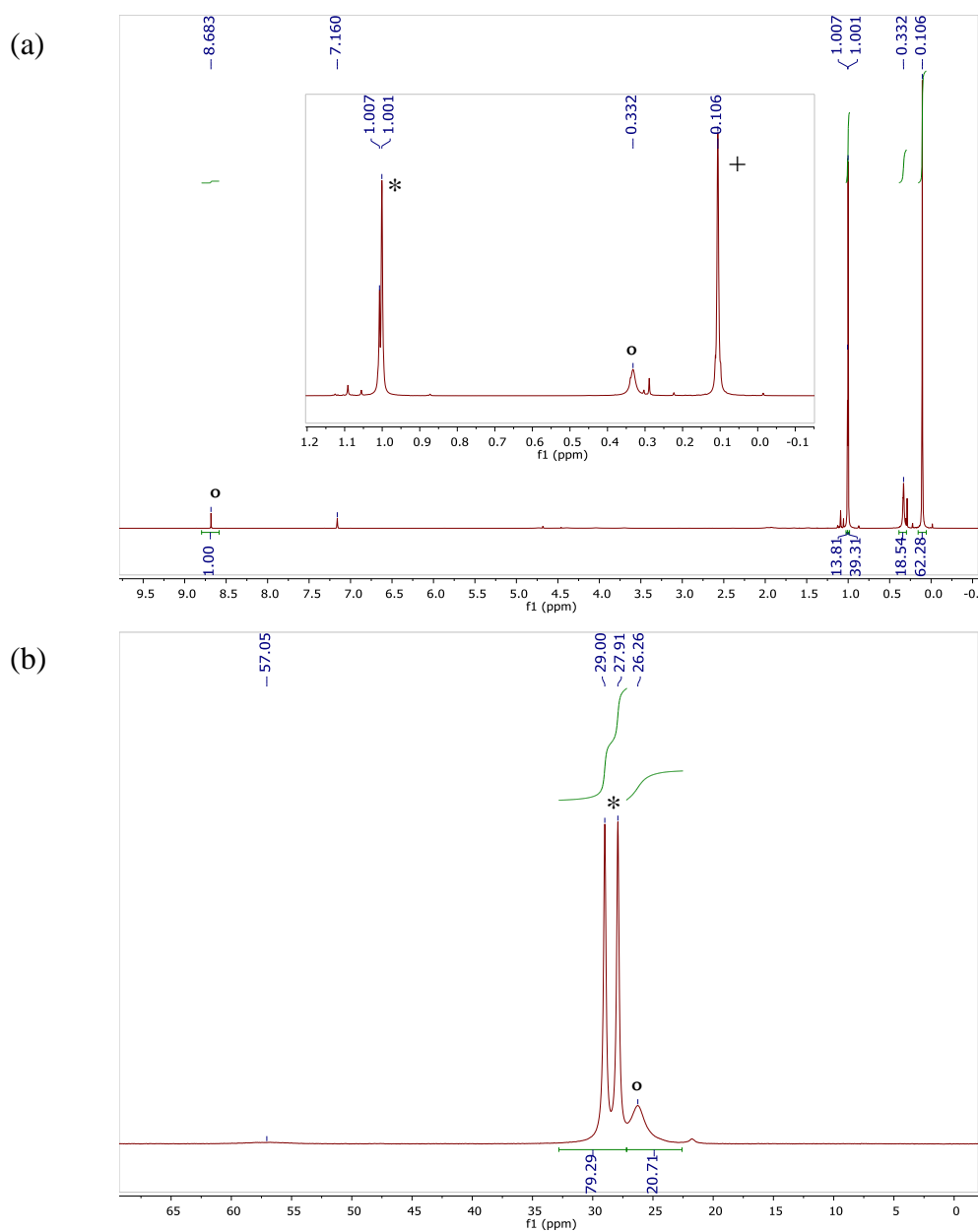
Hydroboration of *N,N'*-bis(trimethylsilyl)carbodiimide (1f). 46 μL of $\text{C}\{\text{N}(\text{SiMe}_3)\}_2$



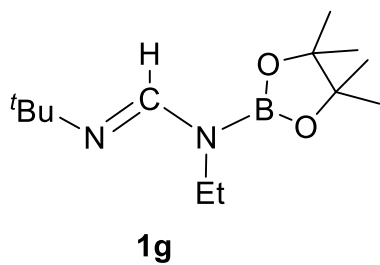
(0.20 mmol), 30 μL of HBpin (0.20 mmol). ^1H NMR (500 MHz) δ 8.68 (s, 1H, $\text{HC}=\text{N}$), 1.01 (s, 12H, Bpin), 0.33 (s, br, 18H, SiMe_3). ^{11}B NMR (160 MHz) δ 26.3 (s, Bpin).

1f

Figure S7. ^1H (a) and ^{11}B (b) NMR spectra in C_6D_6 of the reaction crude of $\text{C}\{\text{N}(\text{SiMe}_3)\}_2$ (+) with HBpin (*). [Reaction conditions: 2.5 mol% cat., 60 $^\circ\text{C}$, 3.5 h; 23% conv. to **1f** ($^\circ$)].

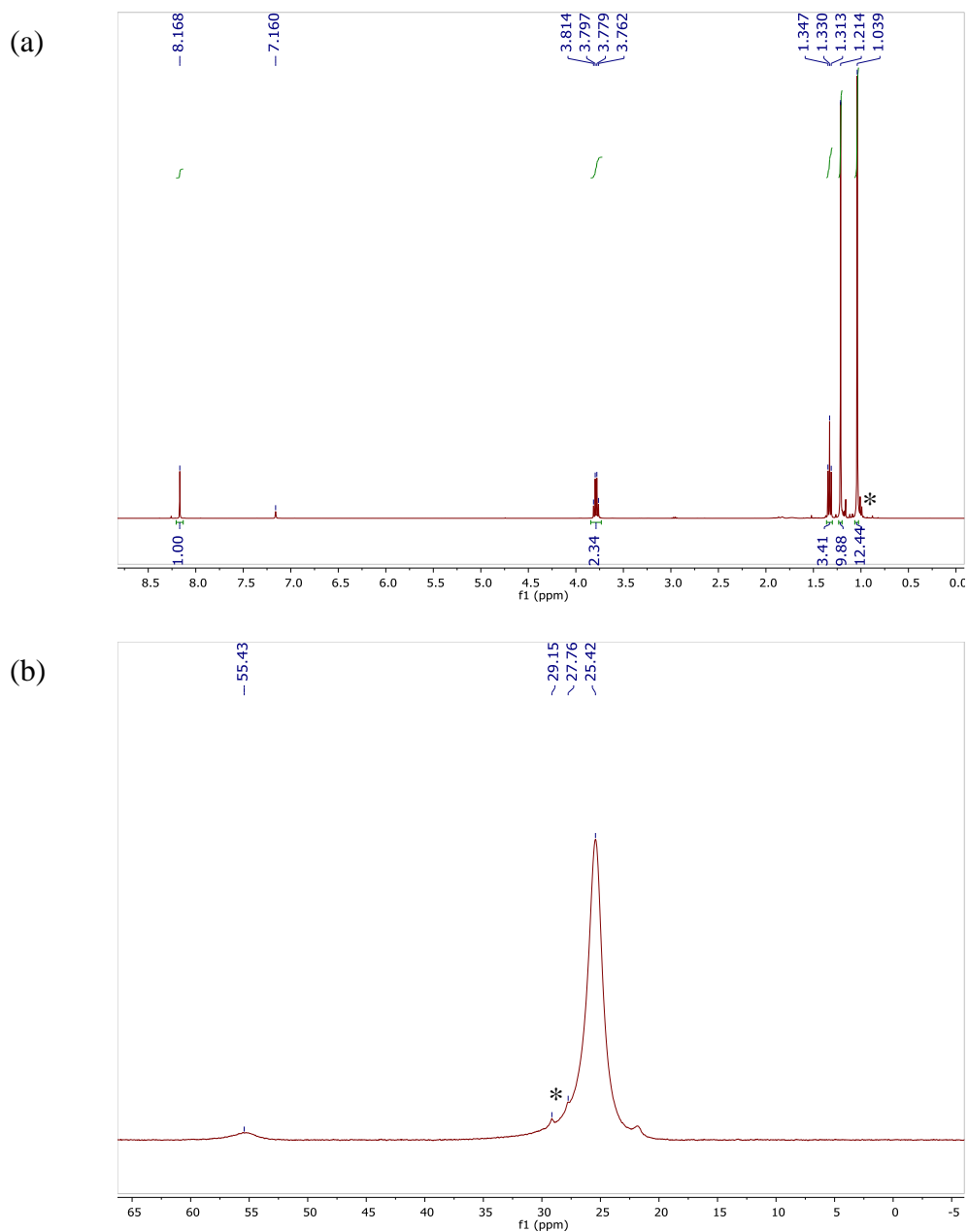


Hydroboration of *N*-tert-butyl-*N'*-ethylcarbodiimide (1g**).** 31 μL of ${}^t\text{BuNCNEt}$ (0.20

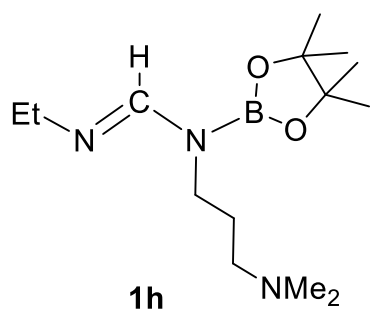


mmol), 30 μL of HBpin (0.20 mmol). ${}^1\text{H}$ NMR (400 MHz) δ 8.17 (s, 1H, $\text{HC}=\text{N}$), 3.79 (q, $J = 7.0$ Hz, 2H, $\text{CH}_2\text{-Et}$), 1.33 (t, $J = 7.0$ Hz, 3H, $\text{CH}_3\text{-Et}$), 1.21 (s, 9H, ${}^t\text{Bu}$), 1.04 (s, 12H, Bpin). ${}^{11}\text{B}$ NMR (128 MHz) δ 25.4 (s, Bpin).

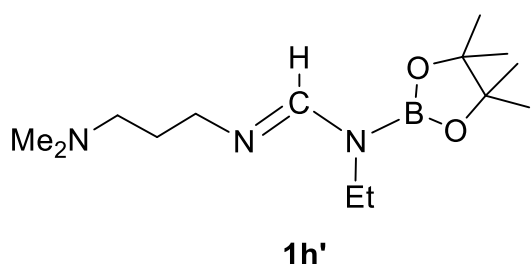
Figure S8. ${}^1\text{H}$ (a) and ${}^{11}\text{B}$ (b) NMR spectra in C_6D_6 of the reaction crude of ${}^t\text{BuNCNEt}$ with HBpin (*). [Reaction conditions: 2.5 mol% cat., 60 $^\circ\text{C}$, 20 h]



Hydroboration of *N*-(3-dimethylaminopropyl)-*N*'-ethylcarbodiimide (1h/1h'**). 36.5**

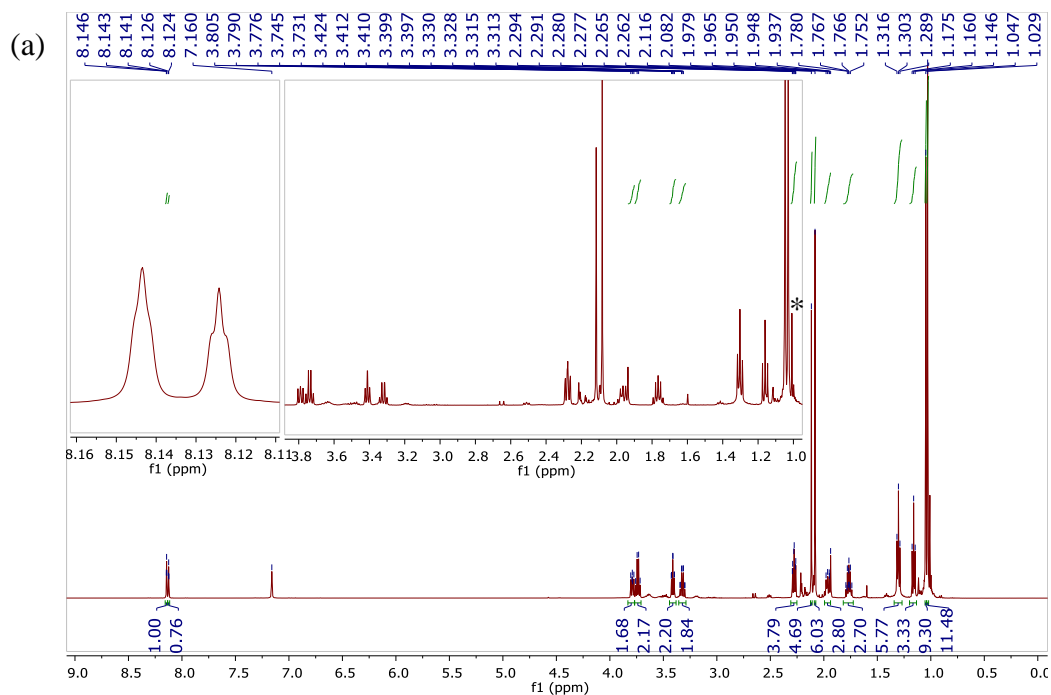


μL of $\text{EtNCN}(\text{CH}_2)_3\text{NMe}_2$ (0.20 mmol), 30 μL of HBpin (0.20 mmol). Compounds **1h** and **1h'** were obtained as an isomer mixture in a ratio **1h:1h'** ca. 43:57. Spectroscopic data for **1h**: ^1H NMR (500 MHz) δ 8.12 (t, $J = 1.1$ Hz, 1H, $\text{HC}=\text{N}$), 3.79 (m, 2H, $\text{BNCH}_2\text{CH}_2\text{CH}_2$), 3.32 (qd, $J = 7.2$, 1.1 Hz, 2H, $\text{CH}_2\text{-Et}$), 2.28 (m, 4H, $\text{BNCH}_2\text{CH}_2\text{CH}_2$), 2.12 (s, 6H, NMe_2), 1.16 (t, $J = 7.2$ Hz, 3H, $\text{CH}_3\text{-Et}$), 1.05 (s, 12H, Bpin). ^{11}B NMR (160 MHz) δ 25.1 (s, Bpin).

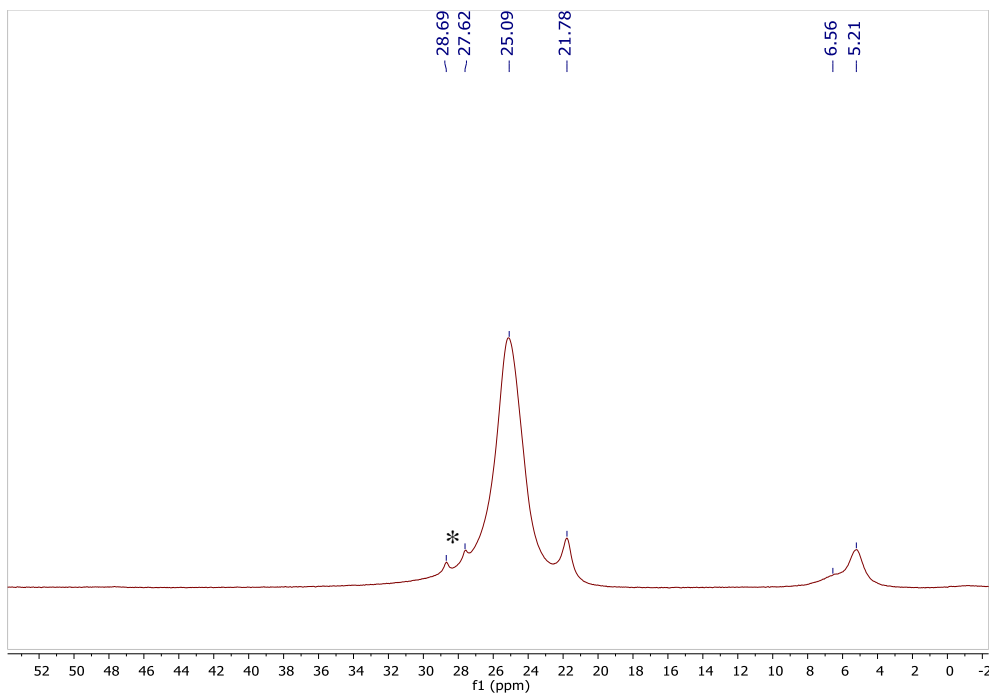


Spectroscopic data for **1h'**: ^1H NMR (500 MHz) δ 8.14 (t, $J = 1.1$ Hz, 1H, $\text{HC}=\text{N}$), 3.74 (q, $J = 7.0$ Hz, 2H, BNCH_2CH_3), 3.41 (td, $J = 6.8$, 1.1 Hz, 2H, $\text{NCH}_2\text{CH}_2\text{CH}_2$), 2.08 (s, 6H, NMe_2), 2.01 – 1.92 (m, 2H, $\text{NCH}_2\text{CH}_2\text{CH}_2$), 1.77 (m, 2H, $\text{NCH}_2\text{CH}_2\text{CH}_2$), 1.30 (t, $J = 7.0$ Hz, 3H, $\text{CH}_3\text{-Et}$), 1.03 (s, 12H, Bpin). ^{11}B NMR (160 MHz) δ 25.1 (s, Bpin).

Figure S9. ^1H (a) and ^{11}B (b) NMR spectra in C_6D_6 of the reaction crude of $\text{EtNCN}(\text{CH}_2)_3\text{NMe}_2$ with HBpin (*). [Reaction conditions: 0.5 mol% cat., 60 $^\circ\text{C}$, 20 h]



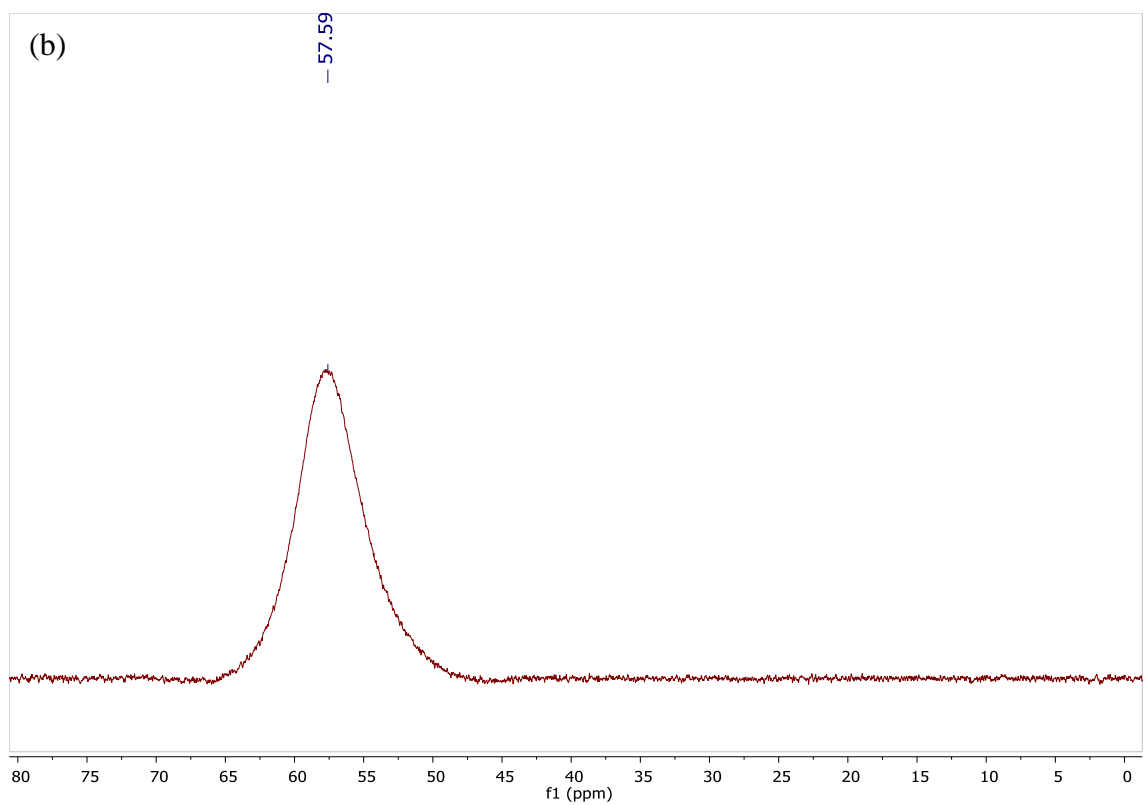
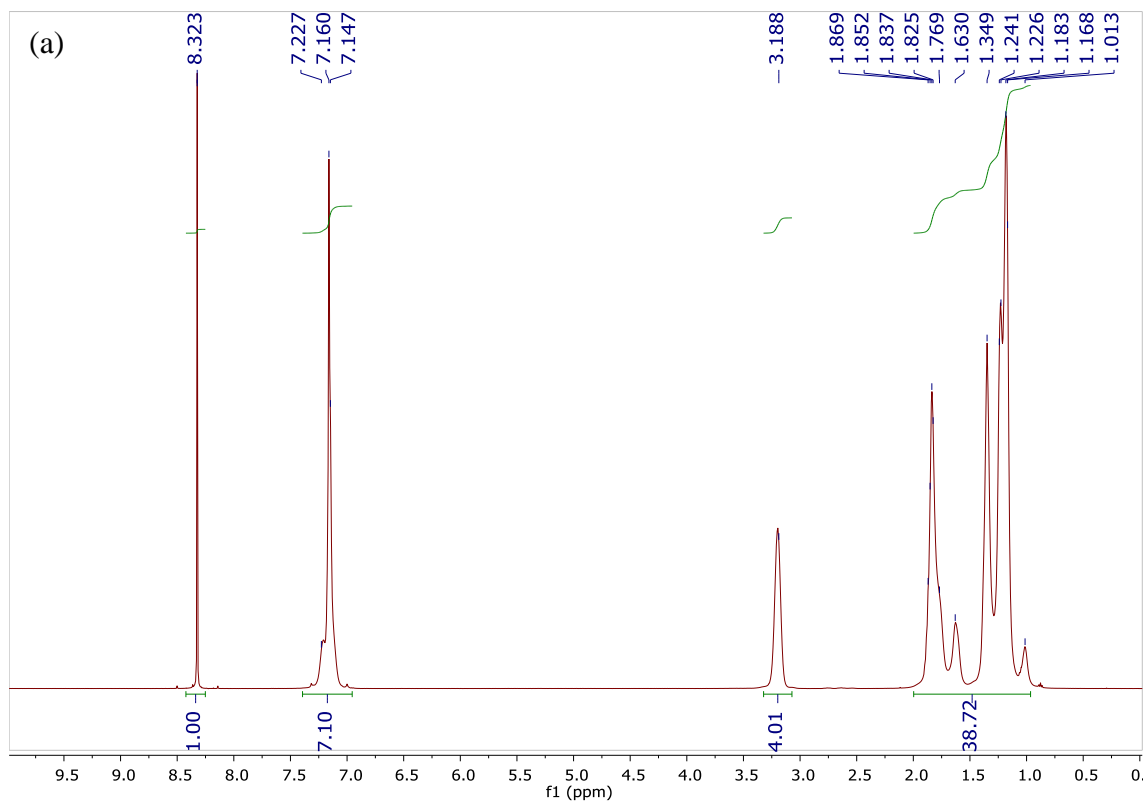
(b)

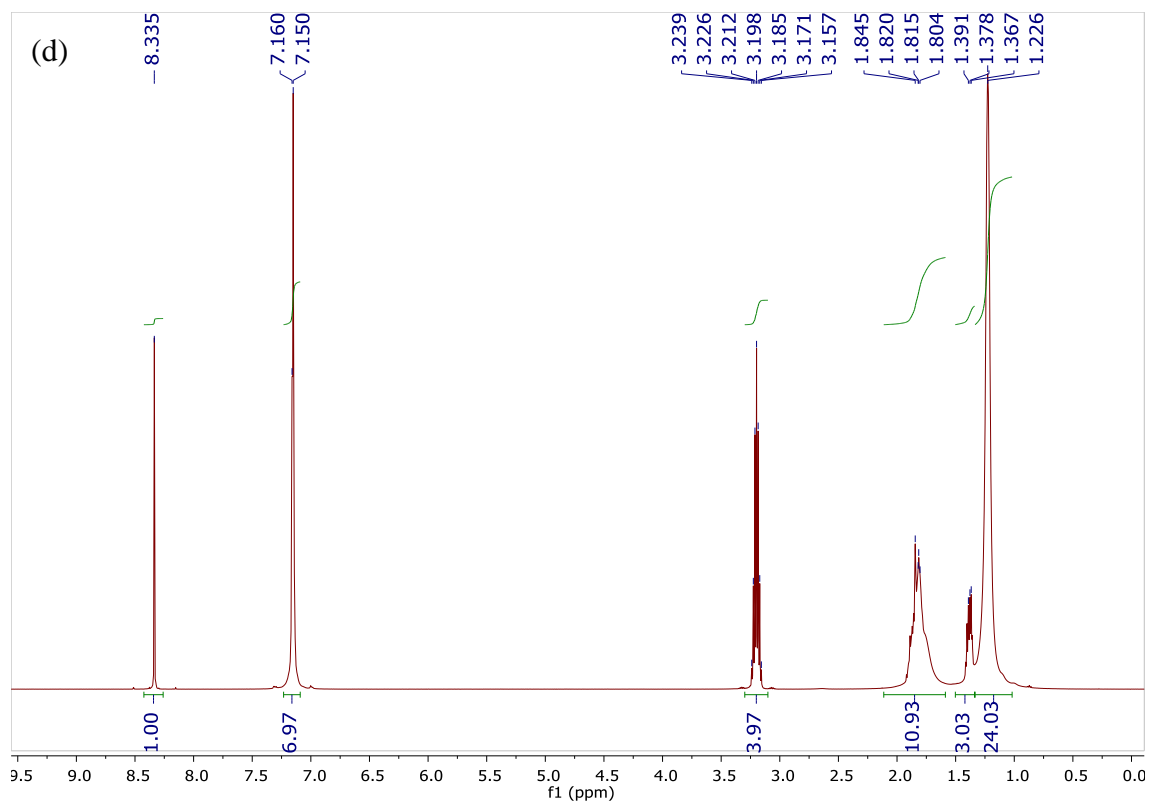
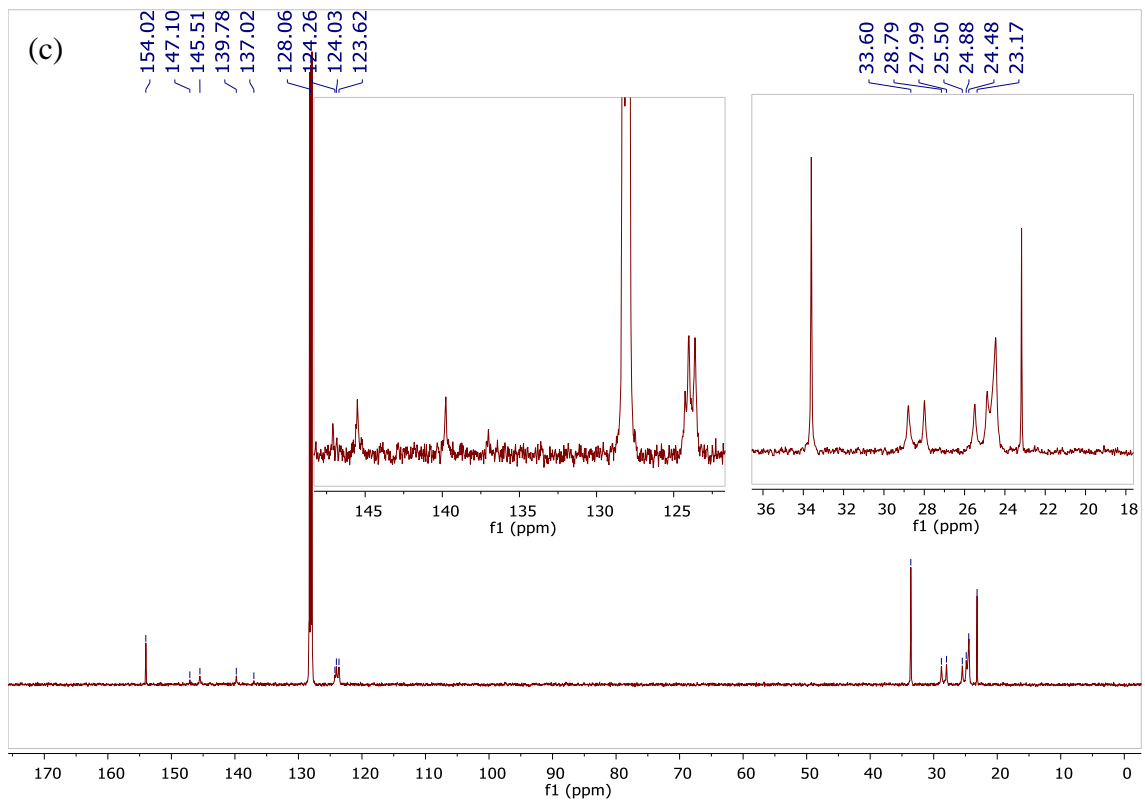


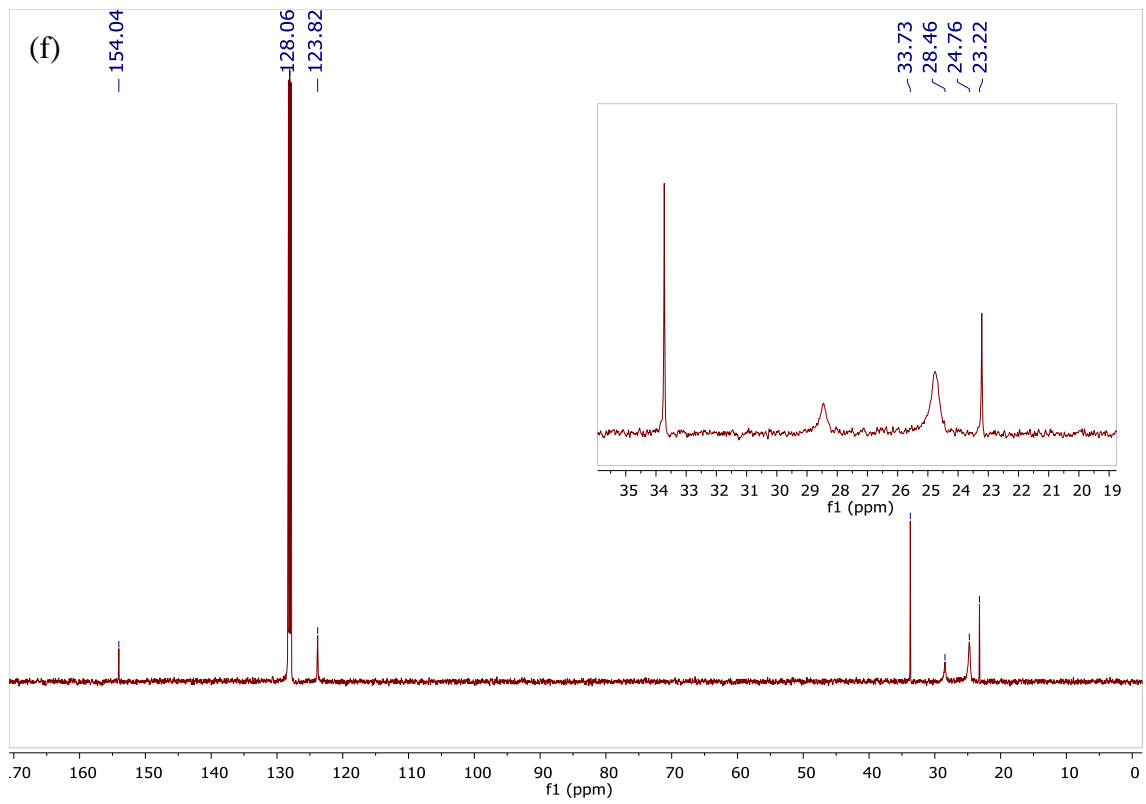
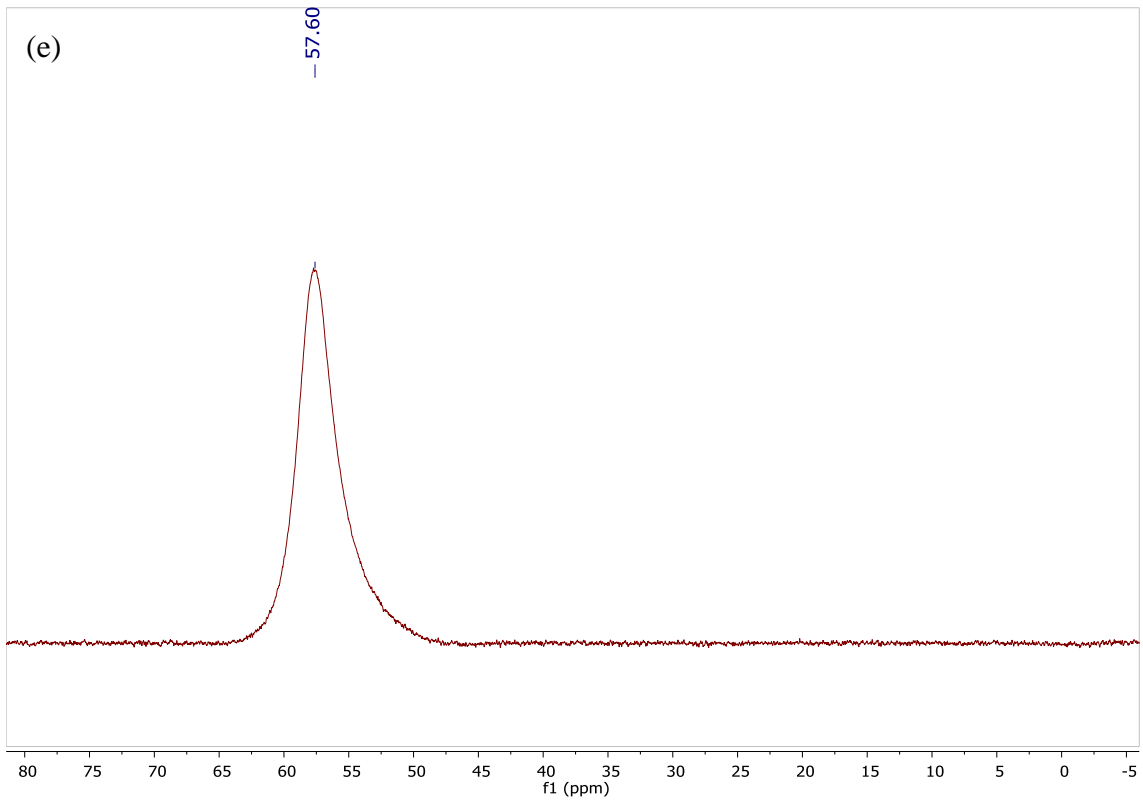
Preparation of compound (2,6-ⁱPr₂C₆H₃)N=CH-N(2,6-ⁱPr₂C₆H₃)BC₈H₁₄ (4). (H-BBN)₂ (122 mg, 0.5 mmol) was added to a solution of C{N(2,6-ⁱPr₂C₆H₃)₂}₂ (365 mg, 1.0 mmol) in toluene (10 mL). The solution thus formed was stirred for 1h at 60 °C. Then, the solvent was removed under vacuum and compound **4** was obtained as a white solid (410 mg, 85%). Suitable crystals for an X-ray diffractometric analysis were grown from a concentrated solution of **4** in pentane at -20 °C. Anal. Calc. for C₃₃H₄₉BN₂: C, 81.80; H 10.19; N, 5.78. Found: C, 81.63; H, 10.44; N, 5.72. ¹H NMR (500 MHz, 298 K) δ 8.32 (s, 1H, HC=N), 7.30 – 7.05 (br, 6H, C₆H₃), 3.19 (br, 4H, CH-ⁱPr), 2.00 – 0.95 (m, br, 38H, BC₈H₁₄ + CH₃-ⁱPr). ¹³C{¹H} NMR (126 MHz, 298 K) δ 154.0 (s, HC=N), 147.1 (br, *ipso*-C-Ar), 145.5, 139.8 (2 x br, *o*-C-Ar), 137.0 (br, *ipso*-C-Ar), 124.3, 124.0, 123.6 (3 x br, *m,p*-CH-Ar) 33.6 (s, CH₂-BC₈H₁₄), 28.8, 28.0, (2 x br, CH-ⁱPr) 25.5, 24.9, 24.5 (3 x br, CH₃-ⁱPr), 23.2 (s, CH₂-BC₈H₁₄). ¹¹B NMR (160 MHz, 298 K) δ 57.6 (s, Δv_{1/2} ca. 890 Hz, BC₈H₁₄).

¹H NMR (500 MHz, 333 K) δ 8.34 (s, 1H, HC=N), 7.15 (s, 6H, C₆H₃), 3.20 (sept, *J* = 6.8 Hz, 4H, CH-ⁱPr), 2.00 – 1.30 (m, 14H, BC₈H₁₄), 1.23 (br, 24H, CH₃-ⁱPr). ¹³C{¹H} NMR (126 MHz, 333 K) δ 154.0 (s, HC=N), 123.8 (s, *m,p*-CH-Ar), 33.7 (s, CH₂-BC₈H₁₄), 28.5, (br, CH-ⁱPr), 24.8 (br, CH₃-ⁱPr), 23.2 (s, CH₂-BC₈H₁₄). ¹¹B NMR (160 MHz, 298 K) δ 57.6 (s, Δv_{1/2} ca. 540 Hz, BC₈H₁₄).

Figure S10. ^1H , ^{11}B and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **4** in C_6D_6 at 25 (a-c) and 60 $^\circ\text{C}$ (d-f).







Stoichiometric reactions

Figure S11. Stoichiometric reaction between $C(N^iPr)_2$, $(H-BBN)_2$ (°) and HBpin (*) in C_6D_6 at 25 °C after 4 h (ratio **1a**:**3**:HBpin \approx 3:1:1): 1H (a) and ^{11}B (b) NMR spectra.

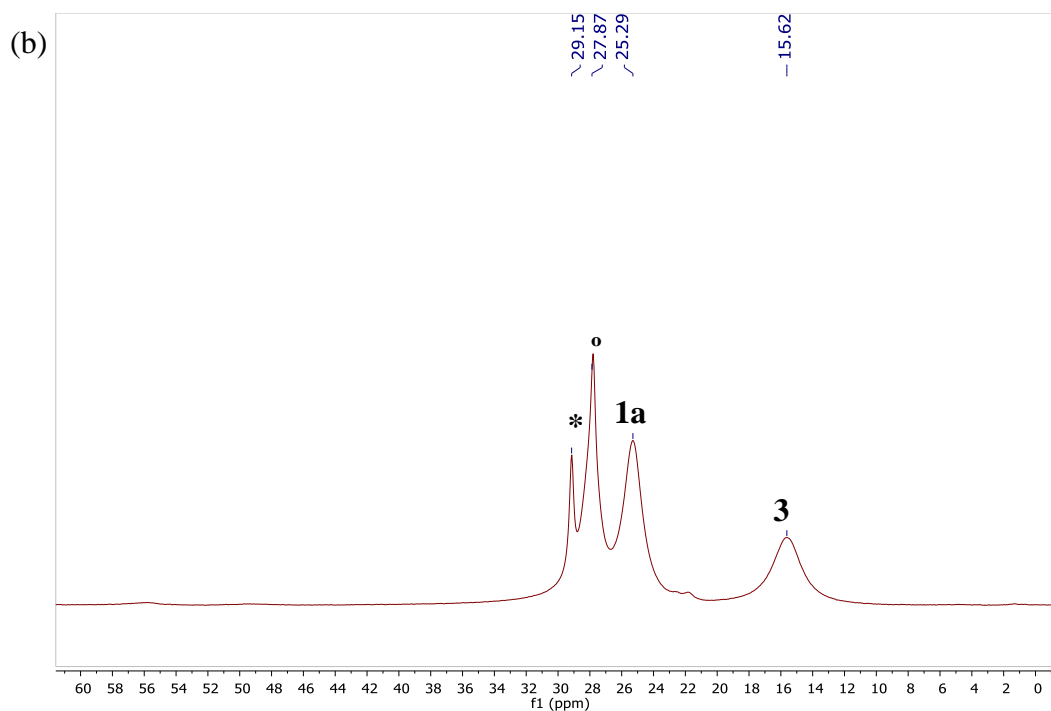
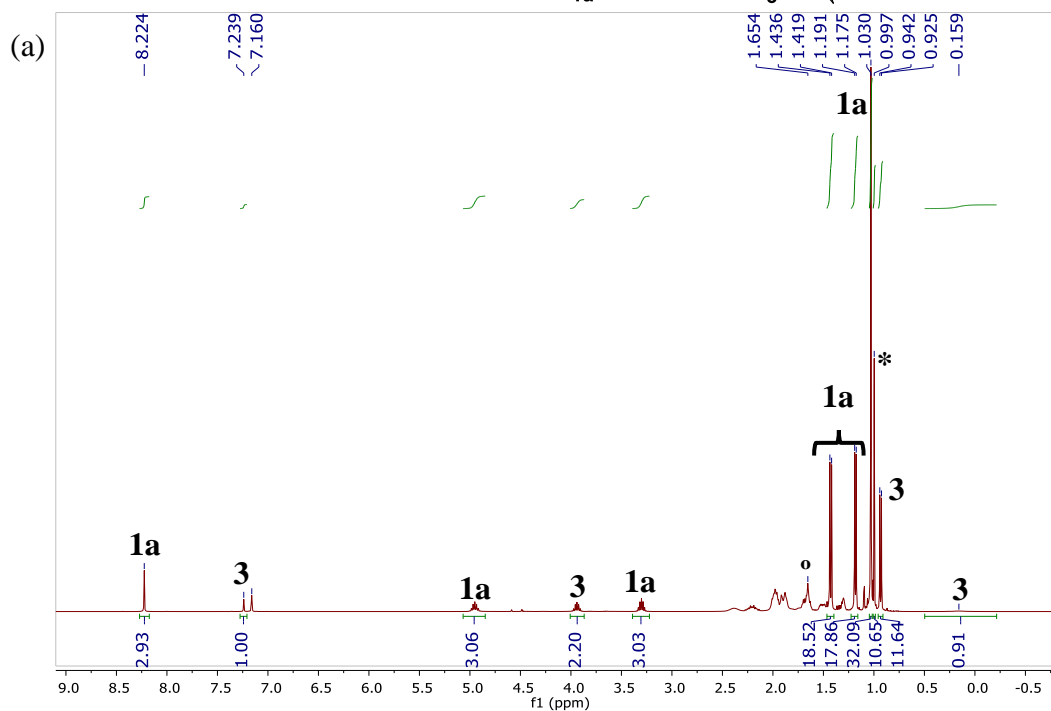
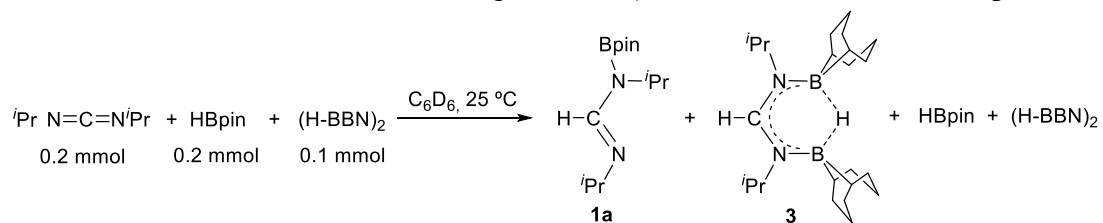
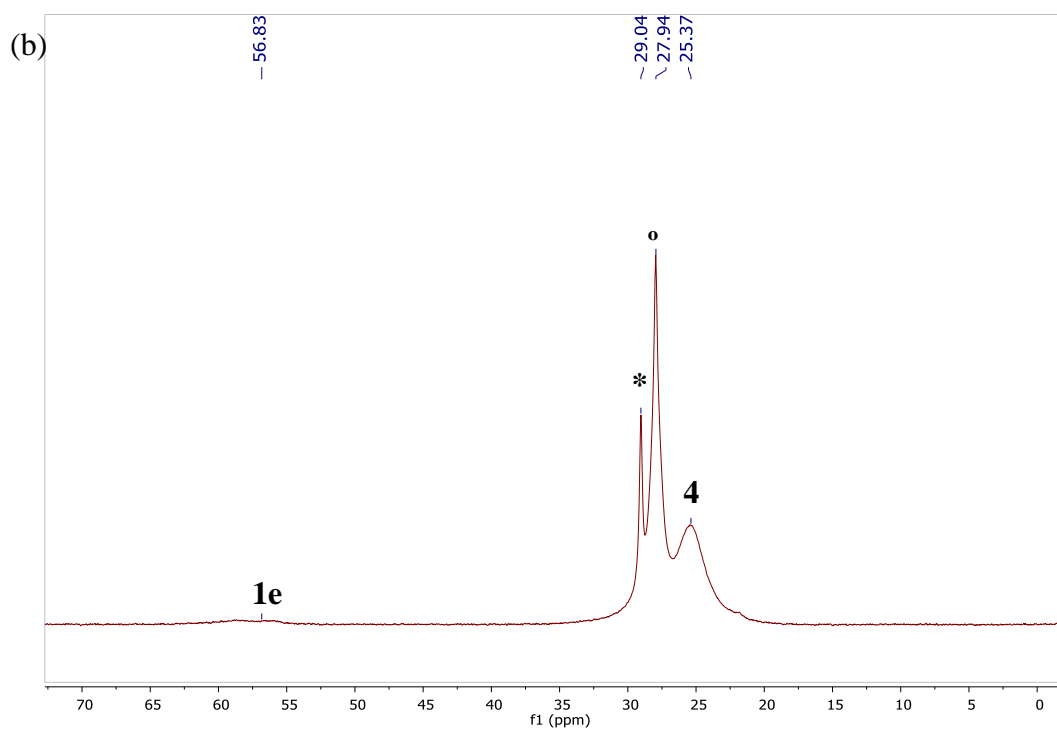
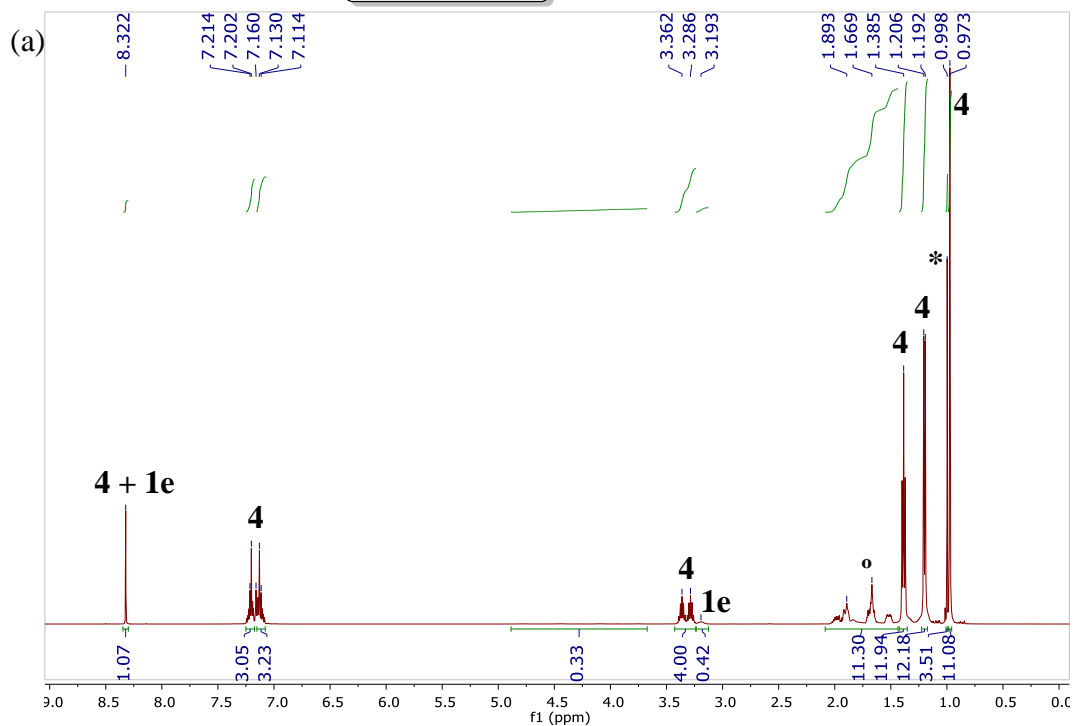
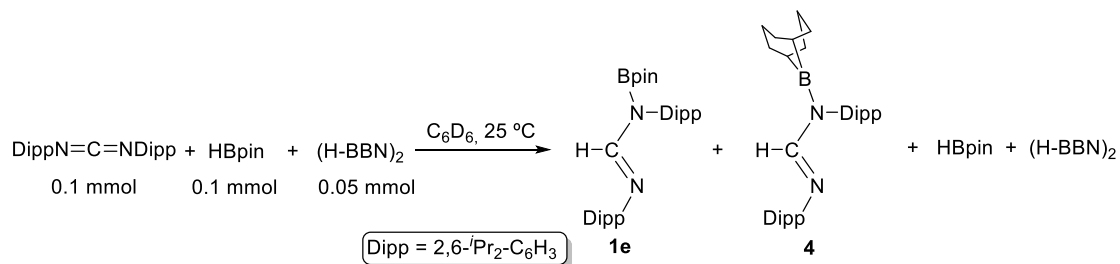


Figure S12. Stoichiometric reaction between $C\{N(\text{Dipp})\}_2$, $(\text{H-BBN})_2$ (°) and HBpin (*) in C_6D_6 at 25 °C after 4 h (ratio **1e**:**4**:HBpin \approx 10:1:3): ^1H (a) and ^{11}B (b) NMR spectra.



Kinetic studies. All kinetics experiments were performed in a similar fashion. In order to determine the *pseudo*-order in [carbodiimide], C(NDipp)₂ (36 mg, 0.10 mmol) was dissolved in ca. 400 μ L of C₆D₆. Then, HBpin (150 μ L, 1.00 mmol) and the internal standard, tetrakis(trimethylsilyl)silane (TKS, 50 μ L of a 0.2 M solution in C₆D₆, 0.01 mmol) were added to the latter solution, followed by the appropriate volume of catalyst, (H-BBN)₂ (0.025 M stock solution in C₆D₆), or compound **4** (0.05 M stock solution in C₆D₆). The typical catalyst loads were 0.5-2.5 mol% for (H-BBN)₂ and 1.0-5.0 mol% for compound **4**. The solution was then transferred to a J. Young-NMR tube and the final volume was made up to 0.8 mL (i.e. [C(NDipp)₂]₀ = 0.125 M; [HBpin]₀ = 1.25 M). The sample was taken out of the glovebox, frozen immediately in a cold acetone bath and subsequently introduced in the NMR spectrometer, set at 25 °C. The reaction was followed by ¹H NMR, collecting data after fixed intervals of time (15 – 300 s) up to, at least, four half-lives. To determine the *pseudo*-order in [HBpin], an analogous procedure was followed, but inverting the reagents' concentration (i.e. [C(NDipp)₂]₀ = 1.25 M; [HBpin]₀ = 0.125 M). A blank experiment without HBpin was also conducted to ascertain the origin of the induction period in the reactions using (H-BBN)₂ as catalyst (*vide infra*).

Figure S13. Reaction progress using (H-BBN)₂ (●) or compound **4** (●) as catalyst: (a) [C(NDipp)₂] vs t ([C(NDipp)₂]₀ = 0.125 M; [HBpin]₀ = 1.25 M); (b) [HBpin] vs t ([C(NDipp)₂]₀ = 1.25 M; [HBpin]₀ = 0.125 M).

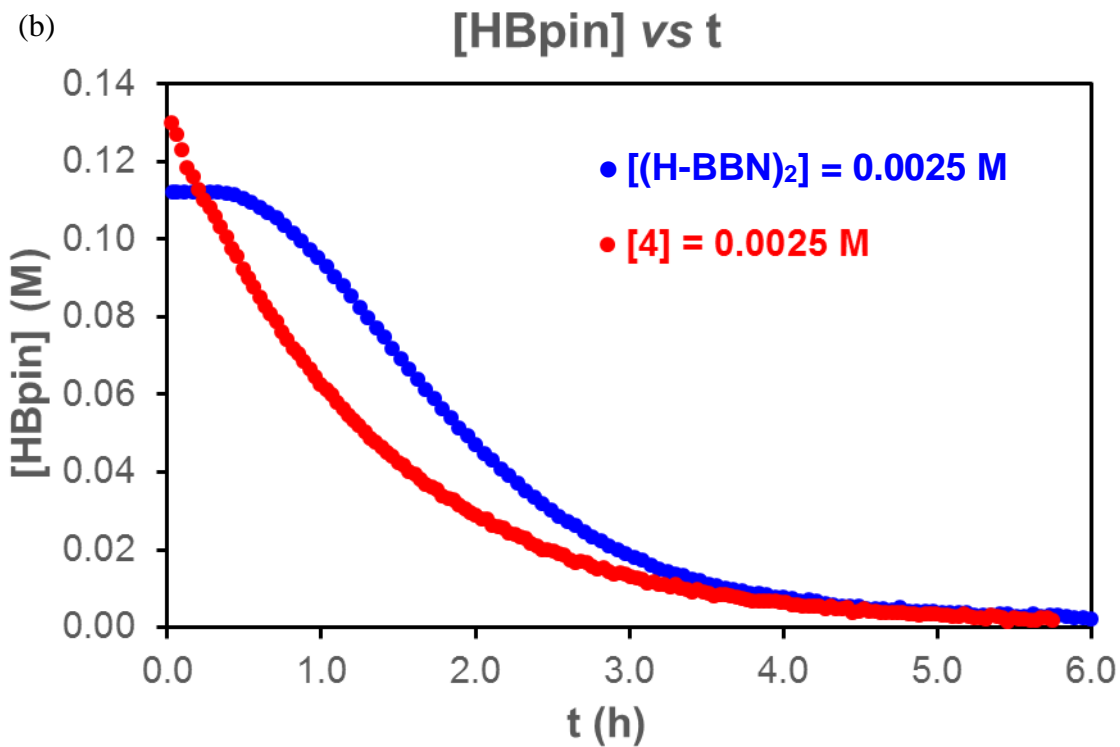
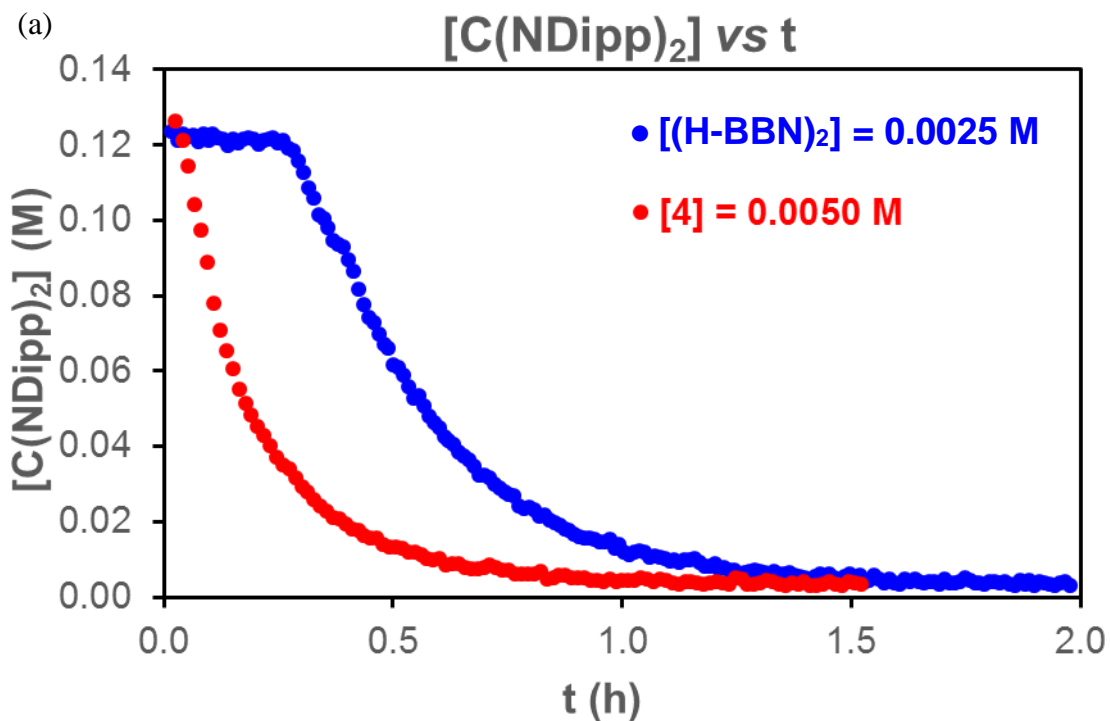


Figure S14. Reaction progress for the blank experiment. Reaction conditions:
[C(NDipp)₂]₀ = 0.125 M, [(H-BBN)₂] = 0.00313 M.

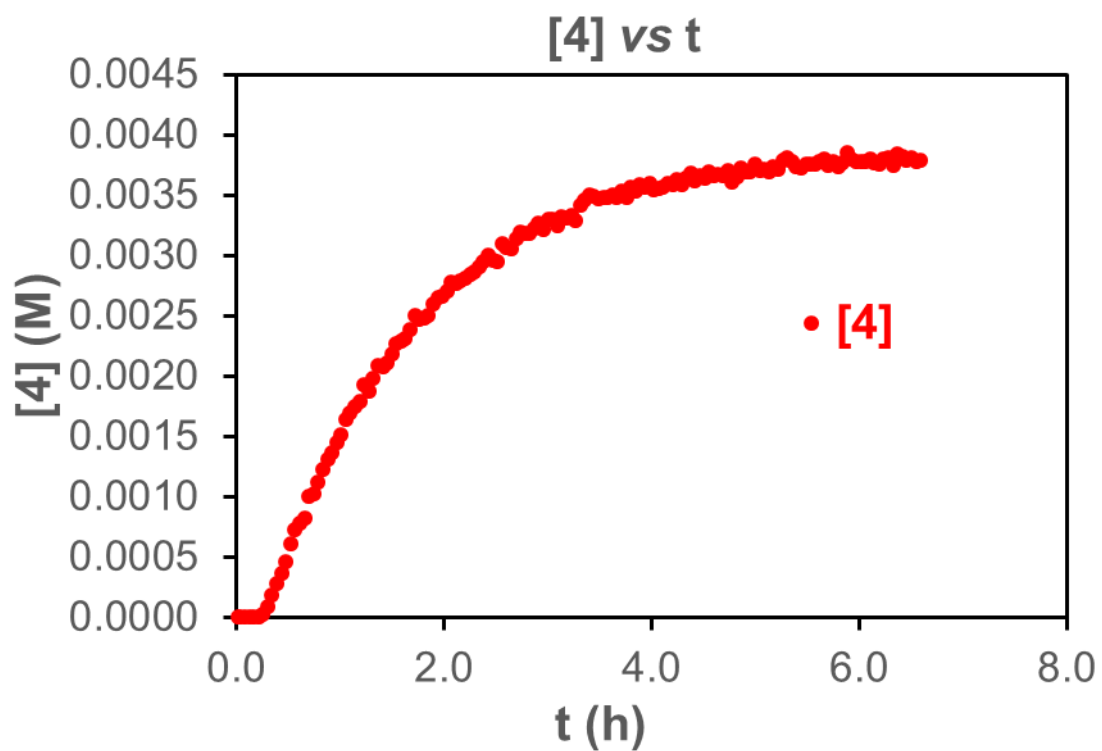
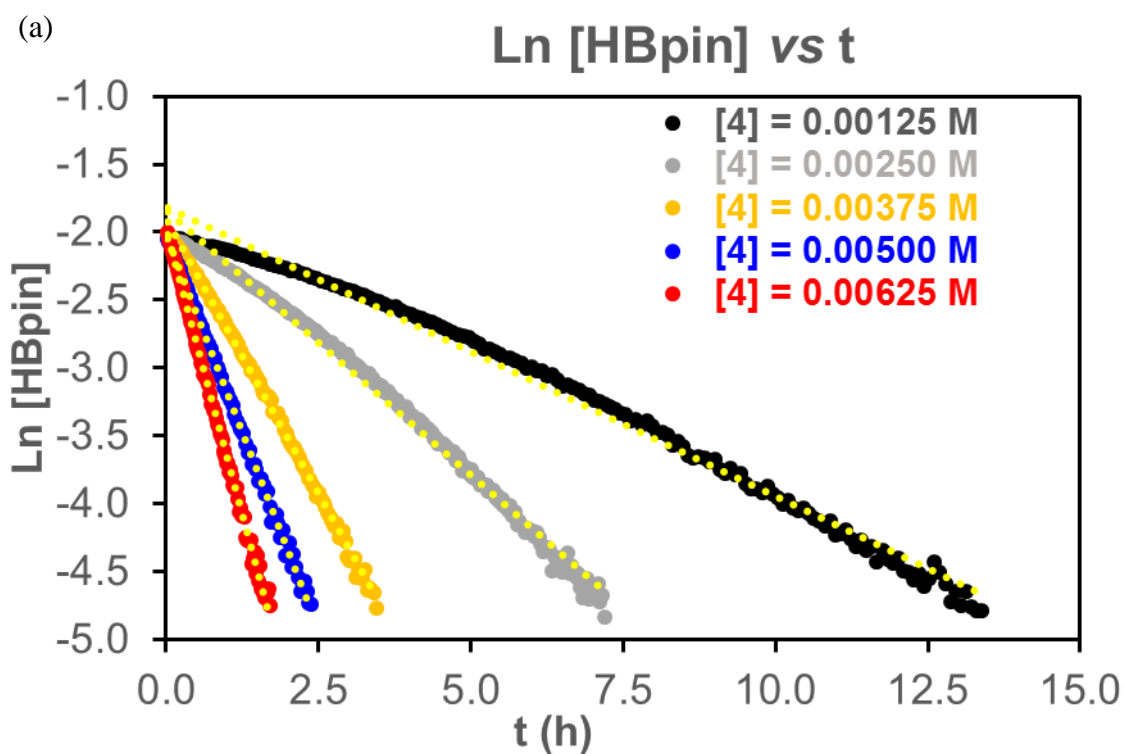


Figure S15. (a) *Pseudo*-first order kinetics of [HBpin], at different [4]. (b) k_{obs} vs [4] showing first order dependence on the [catalyst].



[4] (M)	a	b	R ²
0.00125	-1.665	-1.9913	0.997
0.0025	-1.1594	-2.0242	0.9982
0.00375	-0.8106	-1.904	0.9981
0.005	-0.3894	-1.8447	0.992
0.00625	-0.2124	-1.8207	0.9903

$$\text{Ln [HBpin]} = \text{Ln [HBpin]}_0 - k_{obs}t$$

$$a = -k_{obs}$$

$$b = \text{Ln [HBpin]}_0$$

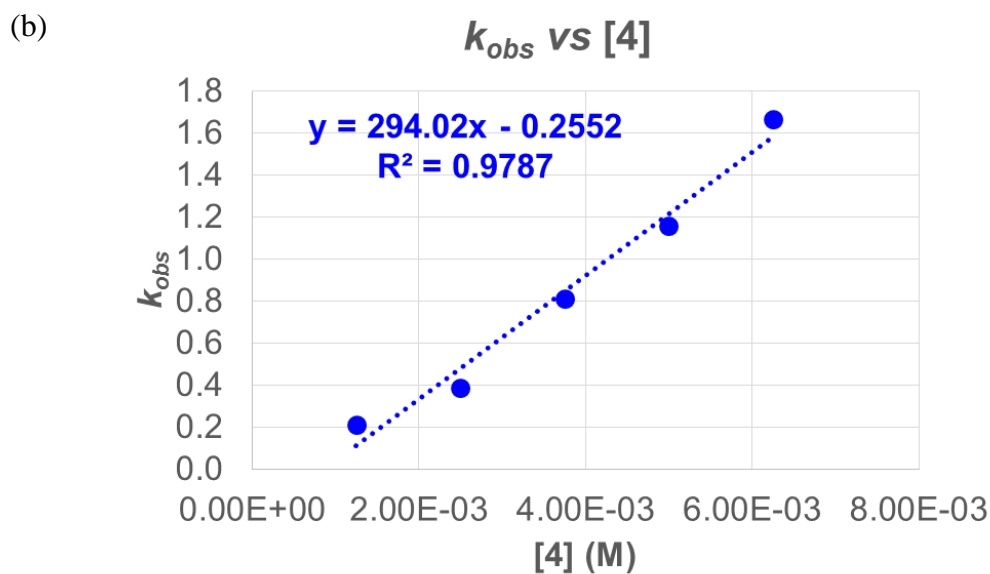


Figure S16. Non-linear kinetics: (a) [HBpin] vs t, (b) 1/[HBpin] vs t.

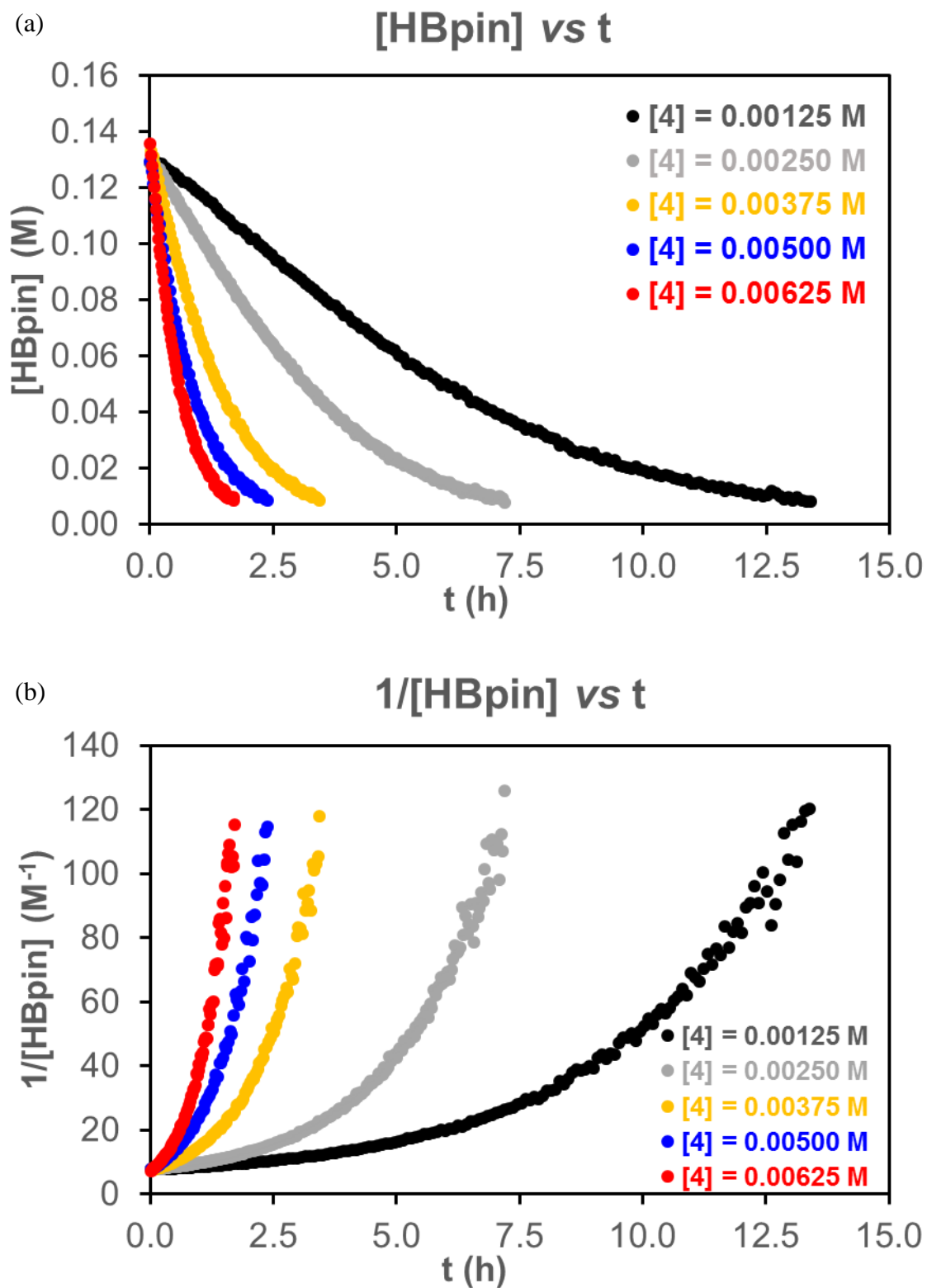
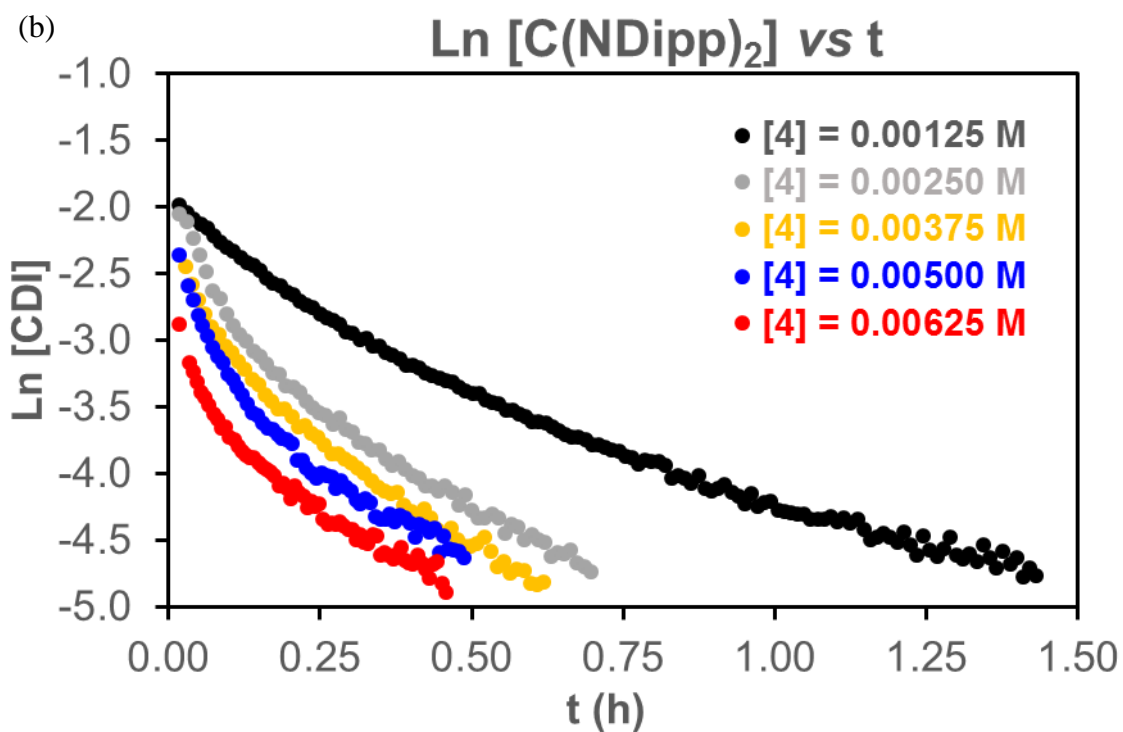
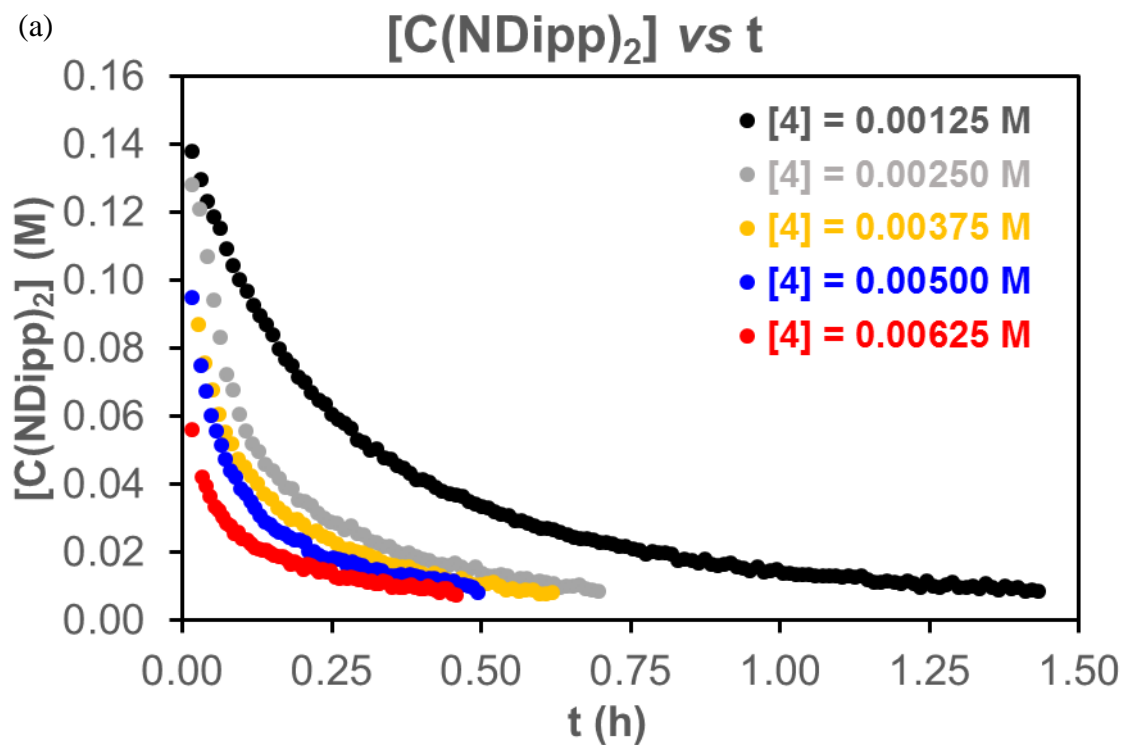
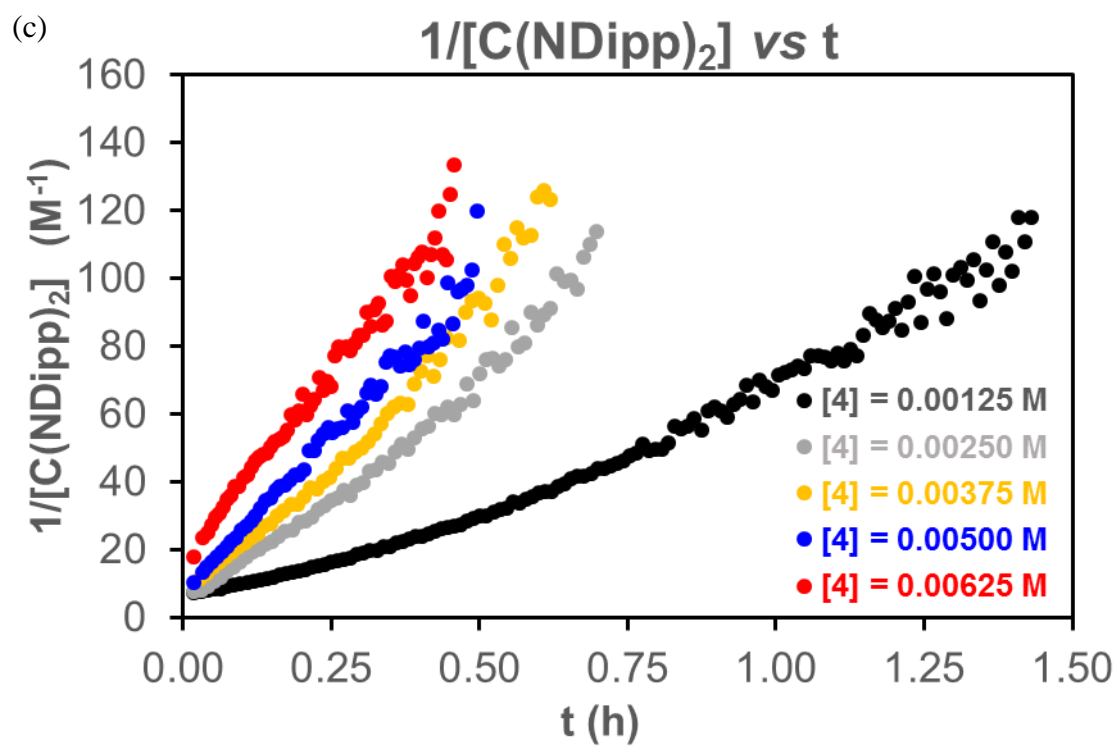


Figure S17. Non-linear kinetics: (a) $[C(NDipp)_2]$ vs t ; (b) $\ln [C(NDipp)_2]$ vs t ; (c) $1/[C(NDipp)_2]$ vs t .





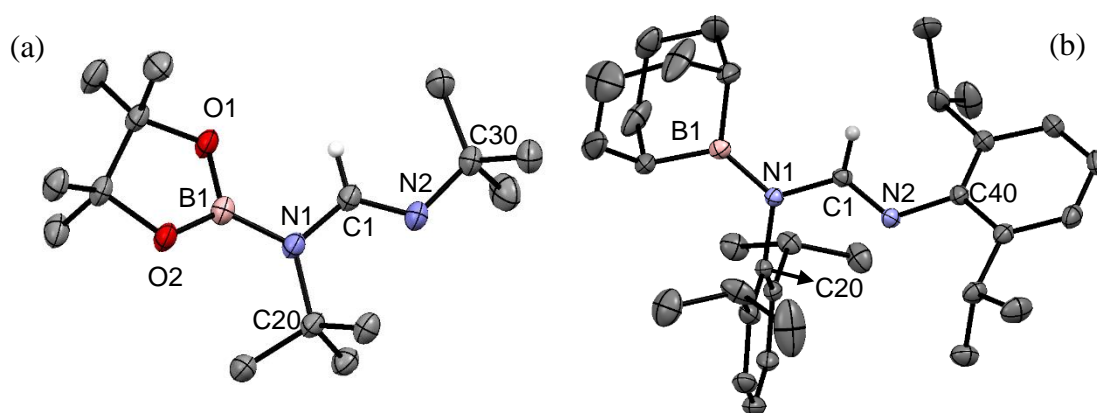
X-ray crystal determination. X-ray data collection for compounds **1c** and **4** was performed on an Oxford Diffraction Xcalibur Nova single crystal diffractometer at 155 K (**1c**) or 136 K (**4**), using Cu K α radiation. Images were collected at a 62 mm fixed crystal-detector distance using the oscillation method, with 1.1° (**1c**) and 1.2° (**4**) oscillation and variable exposure time per image [2.5-7.5 s (**1c**) and 11.0-60.0 s (**4**)]. Data collection strategy was calculated with the program CrysAlis Pro CCD,³ and data reduction and cell refinement was performed with the program CrysAlis Pro RED.³ An empirical absorption correction was applied using the SCALE3 ABSPACK algorithm as implemented in the program CrysAlis Pro RED.³ Using the program suite WINGX,⁴ the structure was solved by SUPERFLIP and refined with full-matrix least squares on F^2 using SHELXL2016.⁵ Positional parameters and anisotropic temperature factors for all non-H atoms were refined anisotropically, and all hydrogen atoms were geometrically placed and refined using a riding model.

Table S2. Crystallographic data and structure refinement details for all compounds.

Compound	1c	4
Chem. form.	C15 H31 B N2 O2	C33 H49 B N2
CCDC	1882207	1882208
Form. Weight	282.23	484.55
Cryst. system	monoclinic	monoclinic
Space group	P 2 ₁ /n	P 2 ₁ /c
<i>a</i> (Å)	6.05230(10)	15.1308(17)
<i>b</i> (Å)	15.6534(4)	10.9346(11)
<i>c</i> (Å)	18.9600(4)	19.7707(18)
α (°)	90	90
β (°)	97.070(2)	111.704(11)
γ (°)	90	90
<i>V</i> (Å ³)	1782.59(7)	3039.2(6)
<i>Z</i>	4	4
GOF ^a	1.047	1.096
<i>R</i> _{int}	0.0439	0.0460
<i>R</i> ₁ ^b / <i>wR</i> ₂ ^c [<i>I</i> > 2 σ (<i>I</i>)]	0.0517 / 0.1442 ^d	0.0708 / 0.1998 ^e
<i>R</i> ₁ ^b / <i>wR</i> ₂ ^c [all data]	0.0600 / 0.1544	0.0823 / 0.2201

^a $S = [\sum w(F_0^2 - F_c^2)^2 / (N_{\text{obs}} - N_{\text{param}})]^{1/2}$, $w = 1/[\sigma^2(F_0^2) + (aP)^2 + bP]$ where $P = F_0^2 + 2F_c^2 / 3$. ^b $R_1 = \sum ||F_0| - |F_c|| / \sum |F_0|$ ^c $wR_2 = [\sum w(F_0^2 - F_c^2)^2 / \sum wF_0^2]^{1/2}$. ^d $a = 0.0913$, $b = 0.1830$. ^e $a = 0.1235$, $b = 1.4411$.

Fig S18. Molecular structures of compounds **1c** (a) and **4** (b) with thermal ellipsoid shown at 30% probability. H atoms are omitted for clarity except for those attached to C1 (**1c**) and C9 (**3**). Selected bond lengths (Å) and angles (°) for **1c**: N1–C1 1.400(2), N2–C1 1.266(2), N1–B1 1.440(2), N1–C20 1.503(2), N2–C30 1.473(2), B1–N1–C1 114.4(1), B1–N1–C20 126.2(1), C1–N1–C20 119.3(1), N1–C1–N2 124.7(1), C1–N2–C30 120.1(1). Selected bond lengths (Å) and angles (°) for **4**: N1–C1 1.397(2), N2–C1 1.267(3), N1–B1 1.427(3), N1–C20 1.454(3), N2–C40 1.420(2), B1–N1–C20 123.8(2), B1–N1–C1 121.7(2), C1–N1–C20 114.4(1), N1–C1–N2 121.9(2), C1–N2–C40 120.3(2).



DFT calculations. All the calculations were carried out by using the Gaussian09 suite of programs.⁶ The M05–2X functional of Truhlar and co-workers⁷ was employed to optimize all the equilibrium structures (catalysts, intermediates and transition states). This functional was parametrized for organic systems with non-covalent interactions and proved to be efficient and reliable for investigating reaction mechanisms. In particular, Cantat and co-workers have recently demonstrated the accuracy of this functional for the computation of reaction mechanisms for the metal-free reduction of CO₂ using highly related guanidines and amidines,⁸ and we used extensively for the calculation of reaction mechanisms in the carbodiimide catalyzed reduction of CO₂ with H-BBN or BH₃.¹ The 6–31G* split-valence basis set of Pople and co-workers was used for all the atoms.⁹ Geometry optimizations were performed under no symmetry restrictions, and frequency analyses were performed for all the stationary points to ensure that minimum structures with no imaginary frequencies were achieved. Transition states were optimized through the Synchronous Transit-Guided Quasi-Newton (STQN) Method as implemented in Gaussian, with the initial guess structures derived in general from previous *relaxed* potential energy surface scans using single and multiple internal coordinates. The corresponding transition states were characterized by frequency analysis (one imaginary frequency) and their connectivity was typically corroborated through Intrinsic-Reaction-Coordinate (IRC) calculations, or when the PES around the TS was relatively flat through manual displacement of atomic coordinates along the imaginary frequency and re-optimization of the resulting structure. The free energies were calculated within the harmonic approximation for vibrational frequencies.

Fig S19. Computed reaction profile for the hydroboration of *i*PrCDI with HBpin using (H-BBN)₂ as catalyst, Gibbs free energies expressed in kcal mol⁻¹ relative to *i*PrCDI + 1/2 (HBBN)₂ + HBpin.

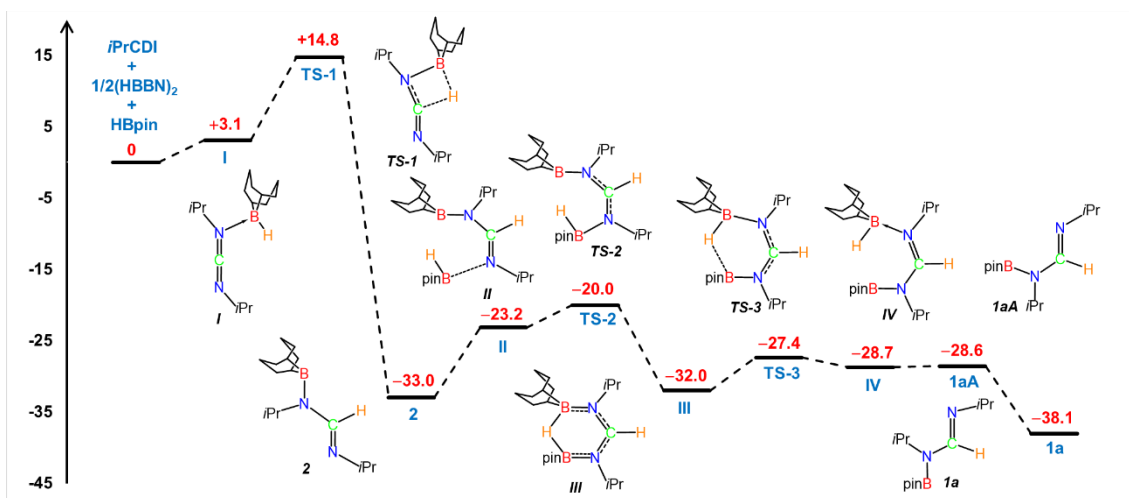


Fig S20. Computed reaction profile for the hydroboration of DippCDI with HBpin using (H-BBN)₂ as catalyst, Gibbs free energies expressed in kcal mol⁻¹ relative to DippCDI + 1/2 (HBBN)₂ + HBpin.

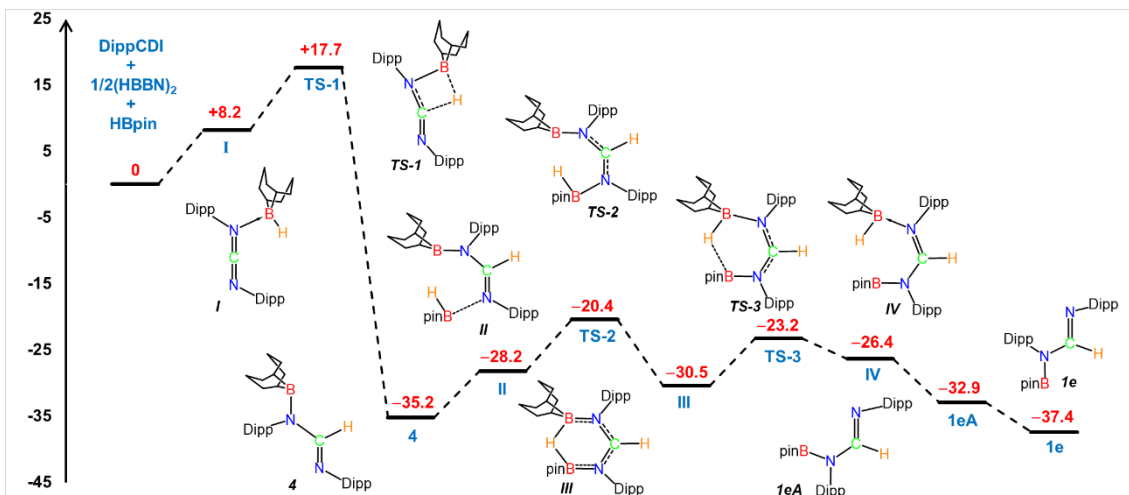


Table S3. Cartesian coordinates for the optimized structures.

48				H	-0.5376630	11.0108360	-2.4589220
				H	-1.5417950	9.6278980	-2.0677360
				C	-1.4711110	11.1159080	-0.5139010
(HBBN)2				H	-2.4537720	11.4523310	-0.8566570
B	0.0000000	8.5993370	0.0000000	H	-0.9051900	12.0248980	-0.3171980
C	-0.4318270	9.4894310	1.2371960	H	2.4936310	9.6298530	-0.6602720
H	-0.7352390	8.8967220	2.1054340	H	1.9489640	11.0129010	-1.5900350
C	0.8025120	10.3215210	1.6499090	H	0.7352420	6.5103190	-2.1054320
H	0.5376630	11.0108360	2.4589220	C	-0.8025090	5.0855210	-1.6499110
H	1.5417950	9.6278980	2.0677360	H	-0.5376590	4.3962050	-2.4589230
C	1.4711110	11.1159080	0.5139010	H	-1.5417910	5.7791430	-2.0677390
H	2.4537720	11.4523310	0.8566570	C	-1.4711120	4.2911340	-0.5139040
H	0.9051900	12.0248980	0.3171980	H	-2.4537730	3.9547180	-0.8566630
C	-1.6541360	10.3227200	0.7922130	H	-0.9052010	3.3821370	-0.3172020
H	-2.4936310	9.6298530	0.6602720	C	-1.6541380	5.0843230	0.7922090
H	-1.9489640	11.0129010	1.5900350	H	-2.4936320	5.7771910	0.6602670
H	0.9299100	7.7035200	0.3251710	H	-1.9489690	4.3941420	1.5900310
B	0.0000000	6.8077050	0.0000000	H	2.4936320	5.7771910	-0.6602670
C	-0.4318290	5.9176100	1.2371950	H	1.9489690	4.3941420	-1.5900310
H	-0.7352420	6.5103190	2.1054320	22			
C	0.8025090	5.0855210	1.6499110	HBpin			
H	0.5376590	4.3962050	2.4589230	O	-5.6084370	21.2233090	12.5914750
H	1.5417910	5.7791430	2.0677390	O	-5.3378100	19.2061920	13.6402100
C	1.4711120	4.2911340	0.5139040	C	-6.9185430	20.6005880	12.6143450
H	2.4537730	3.9547180	0.8566630	C	-7.6891410	21.2471050	13.7619270
H	0.9052010	3.3821370	0.3172020	H	-7.2023970	21.0455010	14.7178310
C	1.6541380	5.0843230	-0.7922090	H	-8.7174200	20.8843670	13.8055050
C	0.4318290	5.9176100	-1.2371950	H	-7.7037020	22.3260700	13.6051090
C	1.6541360	10.3227200	-0.7922130	C	-7.6157810	20.8692940	11.2922510
C	0.4318270	9.4894310	-1.2371960	H	-7.8125610	21.9380170	11.1989780
H	-0.9299100	7.7035200	-0.3251710	H	-8.5696790	20.3382080	11.2501800
H	0.7352390	8.8967220	-2.1054340				
C	-0.8025120	10.3215210	-1.6499090				

H	-6.9998030	20.5600380	10.4497490	H	-3.0289860	-0.3439730	-2.9745910
C	-6.5711230	19.1057560	12.8829920	H	-2.2811000	0.7057110	-1.7548250
C	-7.5962780	18.3471850	13.7076100	N	0.1125880	-1.0327060	1.3459210
H	-7.2620150	17.3174320	13.8398920	N	-2.0031400	-1.1823580	0.1382870
H	-8.5614620	18.3331920	13.1957870	H	1.4298320	-0.8632980	3.6450900
H	-7.7226430	18.7948110	14.6917580	61			
C	-6.2393540	18.3347870	11.6085220	DippCDI			
H	-5.5135730	18.8808590	11.0032260	N	9.0982960	1.0037290	4.0387550
H	-7.1329820	18.1520260	11.0094690	N	11.2227910	2.1627600	3.9325410
H	-5.8012840	17.3760470	11.8875600	C	8.4356050	4.2763560	3.8876240
B	-4.7767580	20.4126140	13.3166390	H	8.7528220	3.5957140	3.0971450
H	-3.6746610	20.7259470	13.6348820	H	9.1825890	5.0682290	3.9778770
23				H	7.4871960	4.7256130	3.5839950
iPrCDI				C	8.2533740	3.5553860	5.2330470
C	-0.9232370	-1.1630300	0.7103840	H	9.2300390	3.1823000	5.5566690
C	0.8033590	-2.1370980	2.0274870	C	7.7960810	4.5559810	6.2959590
H	0.2416780	-3.0679470	1.8994180	H	6.8930950	5.0847020	5.9831440
C	2.1886990	-2.2946140	1.4111170	H	8.5753780	5.3045170	6.4485070
H	2.1160600	-2.5366760	0.3501660	H	7.5971950	4.0659300	7.2505330
H	2.7401370	-3.0900460	1.9160640	C	7.3244670	2.3668110	5.0715370
H	2.7439560	-1.3607650	1.5139900	C	5.9888760	2.4304560	5.4668740
C	0.8908300	-1.8028700	3.5121190	H	5.6143470	3.3330700	5.9301830
H	1.4211700	-2.5927400	4.0475920	C	5.1294110	1.3551700	5.2826840
H	-0.1047080	-1.6927990	3.9427650	H	4.0965140	1.4288750	5.5986470
C	-2.1643820	-1.4095890	-1.3052520	C	5.5972410	0.1842030	4.6997210
H	-1.1845490	-1.5267980	-1.7791620	H	4.9230540	-0.6515830	4.5690370
C	-2.9778010	-2.6830920	-1.5063890	C	6.9229040	0.0691690	4.2895560
H	-2.4634490	-3.5437930	-1.0772650	C	7.4521280	-1.1866980	3.6224600
H	-3.1401050	-2.8653700	-2.5704430	H	8.4784310	-1.3274810	3.9693320
H	-3.9466110	-2.5807110	-1.0145610	C	6.6547660	-2.4443600	3.9703380
C	-2.8709280	-0.1989730	-1.9041160	H	5.6586270	-2.4232220	3.5220190
H	-3.8393670	-0.0630960	-1.4197030	H	6.5439410	-2.5658200	5.0494750

H	7.1685390	-3.3230690	3.5761680	C	11.7550630	0.6114250	8.0207950
C	7.4936530	-0.9931420	2.0996300	H	10.9103640	0.0322800	8.3975070
H	6.4836720	-0.8284920	1.7162300	H	11.7775360	1.5688470	8.5440170
H	7.9052970	-1.8806500	1.6132850	H	12.6646250	0.0598950	8.2683960
H	8.1090860	-0.1342690	1.8315320	47			
C	7.7759760	1.1721480	4.4762270	Int-I(iPr)			
C	10.1483980	1.6148100	4.0867710	C	-0.5269830	-0.8788080	1.0378190
C	12.4048000	2.3593060	4.6621200	C	1.6215570	-1.8721430	1.2865240
C	13.3529210	3.2167090	4.0746720	H	2.3284930	-1.5527470	2.0513070
C	13.0687090	3.8364310	2.7192060	C	0.8789090	-3.1127140	1.7620430
H	12.0034790	4.0772770	2.6923470	H	0.3311620	-2.9198750	2.6860370
C	13.8549940	5.1221190	2.4594020	H	1.5952370	-3.9139540	1.9459790
H	13.7373240	5.8384070	3.2746470	H	0.1732590	-3.4609430	1.0025680
H	13.4994160	5.5876750	1.5383660	C	2.3661260	-2.1120520	-0.0208240
H	14.9208300	4.9199540	2.3295860	H	3.0900520	-2.9175900	0.1144530
C	13.3470820	2.8145570	1.6072100	H	2.8868390	-1.2110800	-0.3387390
H	13.1145580	3.2422250	0.6291130	C	-2.5980010	-1.1379130	-0.1342520
H	12.7468340	1.9148890	1.7435610	H	-3.2869640	-0.2926670	-0.1052700
H	14.4024380	2.5311200	1.6159950	C	-1.8082350	-1.1177030	-1.4366390
C	14.5480140	3.4416690	4.7528440	H	-1.2251910	-0.1992030	-1.5277790
H	15.2910970	4.0992520	4.3220590	H	-2.4871170	-1.1874620	-2.2876280
C	14.7965880	2.8400260	5.9801050	H	-1.1236940	-1.9697650	-1.4753780
H	15.7297010	3.0262900	6.4965460	C	-3.3848360	-2.4298390	0.0521280
C	13.8443920	2.0041480	6.5489110	H	-2.7077440	-3.2865530	0.0398420
H	14.0461830	1.5496050	7.5093000	H	-4.1043000	-2.5454350	-0.7595110
C	12.6328840	1.7446440	5.9093480	H	-3.9197100	-2.4223040	1.0013100
C	11.6100970	0.7984380	6.5094780	N	0.7044680	-0.7129550	1.1194810
H	10.6151670	1.2226160	6.3421420	N	-1.7285270	-0.9576430	1.0424860
C	11.6735570	-0.5689150	5.8098910	H	1.6632760	-2.4025630	-0.8055790
H	11.5823480	-0.4802370	4.7270350	C	2.5367620	1.1468740	1.7673150
H	10.8718340	-1.2180940	6.1690720	H	3.3533770	0.4165850	1.6766580
H	12.6318450	-1.0456710	6.0287240	C	3.1257950	2.4948680	1.2974650

H	3.5617400	2.3255170	0.3072500	H	2.1051590	-2.8895280	-0.8453180
H	3.9495110	2.8036940	1.9529400	C	-2.5511720	-1.0236150	1.1629670
C	2.1224620	3.6581170	1.1841740	H	-2.5807330	0.0244740	0.8382800
H	1.9486110	4.0949540	2.1669550	C	-3.7158040	-1.7880570	0.5509830
H	2.5804540	4.4550430	0.5896720	H	-3.6700400	-1.7524080	-0.5373180
C	0.7760140	3.2782820	0.5428840	H	-4.6621430	-1.3550280	0.8785260
H	0.9236110	3.1835070	-0.5379760	H	-3.6829000	-2.8328670	0.8649140
H	0.0706580	4.1047830	0.6933850	C	-2.5733180	-1.0696410	2.6887180
C	0.1691360	1.9514560	1.0445100	H	-2.4829370	-2.1019200	3.0325290
H	-0.7409660	1.7868870	0.4482220	H	-3.5107930	-0.6570410	3.0658450
C	-0.2617210	1.9878960	2.5244220	H	-1.7453940	-0.4891490	3.1009930
H	-0.9427560	2.8297840	2.7010530	N	1.0569480	-0.8967950	0.6100150
H	-0.8475110	1.0859450	2.7371270	N	-1.2958040	-1.5811040	0.6676010
C	0.8866020	2.0621780	3.5464610	H	0.9016680	-3.5826040	0.2553850
H	1.2430730	3.0878190	3.6294580	C	1.4777740	1.5085430	-0.5758810
H	0.4922870	1.8104290	4.5362910	H	1.1791360	1.0544670	-1.5272570
C	2.0707390	1.1335460	3.2340060	C	0.9122990	2.9416480	-0.5423400
H	1.7709730	0.1080810	3.4900380	H	-0.1564190	2.8711720	-0.7745750
H	2.8999930	1.3820220	3.9076820	H	1.3606960	3.5536760	-1.3338910
B	1.3077310	0.8396310	0.7691000	C	1.0599770	3.6835920	0.7997830
H	1.6170880	0.7418180	-0.4067380	H	2.0684020	4.0848630	0.8937810
47				H	0.4005430	4.5568310	0.7888090
TS1(gPr)				C	0.7275750	2.8348980	2.0397080
C	-0.2109530	-1.0262330	0.6626330	H	-0.3609960	2.7216970	2.1001760
C	2.0026480	-1.9218530	1.0882990	H	1.0340110	3.3870800	2.9359910
H	2.9892840	-1.4730400	0.9827730	C	1.3403400	1.4203520	2.0414450
C	1.7429820	-2.2621070	2.5536360	H	0.9633560	0.9021290	2.9329700
H	1.8196570	-1.3722340	3.1789780	C	2.8832270	1.4083810	2.1130240
H	2.4672010	-3.0001730	2.9029510	H	3.2277590	1.9968840	2.9718800
H	0.7412390	-2.6844310	2.6668650	H	3.2029490	0.3786850	2.3101730
C	1.9041410	-3.1529550	0.1931850	C	3.6141220	1.9054320	0.8492260
H	2.6240330	-3.9083670	0.5124630	H	3.6471430	2.9937940	0.8488680

H	4.6590080	1.5839830	0.9036230	H	7.4987350	2.2532450	3.6288900
C	3.0141530	1.4142930	-0.4806370	C	5.6225420	1.2997240	3.7970760
H	3.2885120	0.3615030	-0.6237680	H	5.4875380	1.4753340	4.8663380
H	3.4877480	1.9641390	-1.3024200	H	6.1134750	0.3323330	3.6693250
B	0.8945980	0.7104940	0.6764480	H	4.6480370	1.2698630	3.3181330
H	-0.4145600	0.6584300	0.6365510	C	6.6539540	2.2444500	1.6739880
47				H	5.6864770	2.3579250	1.1894540
Compound 2				H	7.0571340	1.2582330	1.4330800
C	8.6011110	4.4561290	4.2318510	H	7.3399740	3.0006820	1.2856050
H	8.9411960	3.5099600	3.8049130	C	2.6304510	3.9908750	2.3946400
C	9.2291940	5.5669060	3.3513950	H	2.4984540	3.9930700	1.3077330
H	8.9180840	5.3836260	2.3159060	C	1.6426260	2.9800460	2.9804310
H	10.3202440	5.4695590	3.3649230	H	1.8524860	1.9819800	2.5951520
C	8.8469380	7.0056170	3.7256720	H	0.6143640	3.2486600	2.7300800
H	9.4120800	7.3217500	4.6005970	H	1.7412730	2.9548230	4.0683330
H	9.1599450	7.6725190	2.9171710	C	2.3205600	5.3980540	2.9078590
C	7.3422810	7.2001690	3.9694080	H	2.3828600	5.4459570	3.9984030
H	6.8391050	7.2435240	2.9965760	H	1.3023480	5.6669190	2.6223460
H	7.1755610	8.1728910	4.4452600	H	2.9952060	6.1466350	2.4868140
C	6.6560990	6.0879300	4.7956690	B	7.0316600	4.6786680	4.1617610
H	5.5886530	6.3213440	4.8085870	N	6.1048480	3.7529340	3.5851100
C	7.0909140	6.0307700	6.2819100	N	3.9756450	3.4742180	2.6285580
H	6.8666080	6.9885560	6.7640310	H	4.5804930	5.1525510	3.6832320
H	6.4645590	5.2823100	6.7813820	69			
C	8.5634040	5.6757840	6.5303470	Int-II(iPr)			
H	9.1896450	6.5446770	6.3357540	O	-0.7494310	-2.5382630	-2.0125910
H	8.6941570	5.4514930	7.5928920	O	0.4856540	-0.8676330	-2.9788020
C	9.0553490	4.4744590	5.7083380	N	-0.8279770	0.8529510	1.1605740
H	8.6799930	3.5584870	6.1788900	N	1.0809850	0.0135100	0.1021790
H	10.1483540	4.4218400	5.7630340	C	-1.7121780	2.0326810	1.0597690
C	4.8031370	4.1639440	3.2954200	C	0.4321370	0.9925320	0.5816240
C	6.5138210	2.3848800	3.1889020	H	0.8011720	2.0168540	0.5529200

C	2.4347930	0.2265170	-0.4029950	H	0.7352060	-1.2432710	2.2445070
C	1.3894700	-3.5524500	-1.6549470	C	-0.5619070	-2.7850390	1.5259560
H	1.7485790	-2.6540110	-1.1496100	H	-0.1225710	-2.6125240	0.5422270
H	2.2344950	-4.0801560	-2.1009770	H	-0.0196500	-3.6246180	1.9786050
H	0.9281420	-4.1995980	-0.9080270	C	-2.0356680	-3.1813940	1.3226120
C	0.3426330	-3.1941860	-2.7045730	H	-2.0904530	-3.8670850	0.4720680
C	-0.1869930	-4.4528580	-3.3705260	H	-2.4059880	-3.7390190	2.1823050
H	-0.5063800	-5.1576340	-2.6017020	C	-2.9685680	-1.9942810	1.0351320
H	0.5954770	-4.9264060	-3.9684150	H	-4.0091790	-2.3347410	1.0819160
H	-1.0404770	-4.2354060	-4.0102830	H	-2.7958730	-1.6689450	0.0031660
C	0.8250520	-2.0848520	-3.6876540	B	-1.2697080	-0.3707300	1.7678880
C	2.3159320	-2.0904360	-3.9789880	H	-1.2193580	-0.3818400	-1.5748890
H	2.5528260	-1.2702310	-4.6581340	H	2.4386360	-0.2241470	-1.3989790
H	2.6071390	-3.0287620	-4.4571390	H	-2.5684830	1.8094520	1.6924120
H	2.8997370	-1.9628540	-3.0687040	C	3.3932650	-0.5627430	0.4918940
C	0.0339920	-2.0627010	-4.9931980	H	4.4043300	-0.5581680	0.0791050
H	-1.0392570	-2.0685030	-4.7945610	H	3.4227940	-0.1147330	1.4884300
H	0.2810600	-2.9171840	-5.6254890	H	3.0564840	-1.5950730	0.5964020
H	0.2781840	-1.1456490	-5.5304140	C	2.9083280	1.6731130	-0.5483860
B	-0.5315180	-1.1863730	-2.1111500	H	3.8953250	1.6789210	-1.0138330
C	-2.7924130	-0.7570390	1.9597640	H	2.2352690	2.2555060	-1.1812650
H	-3.4995510	-0.0040410	1.5977460	H	2.9981320	2.1692480	0.4217170
C	-3.1108190	-1.0192950	3.4462950	C	-2.2013690	2.2380950	-0.3717080
H	-4.1200640	-1.4346080	3.5467710	H	-1.3543060	2.3922860	-1.0458760
H	-3.1265850	-0.0488560	3.9566700	H	-2.7520550	1.3615870	-0.7158260
C	-2.1102660	-1.9286690	4.1782130	H	-2.8537190	3.1118840	-0.4347750
H	-2.2622690	-1.8208460	5.2564210	C	-1.0703720	3.3067870	1.6194080
H	-2.3194450	-2.9734240	3.9541090	H	-0.5966440	3.1106580	2.5826410
C	-0.6451940	-1.6164700	3.8478090	H	-0.3277970	3.7334650	0.9424320
H	-0.3728650	-0.6698900	4.3315290	H	-1.8450100	4.0621320	1.7623270
H	-0.0058160	-2.3837400	4.2987940	69			
C	-0.3218750	-1.4961910	2.3390560	TS-2(iPr)			

O	8.7085080	-0.6197840	2.4111050	C	7.5712320	-0.1331920	8.1481020
O	9.9517240	0.8089850	1.1044740	H	7.7525920	0.2362550	9.1617780
N	8.3235540	2.1673240	5.0505970	H	7.2464150	-1.1649780	8.2668260
N	10.1882500	1.6203910	3.7282490	C	8.8965770	-0.1106250	7.3680230
C	7.5692400	3.4182940	5.2966230	H	9.3872120	0.8582640	7.5265470
C	9.6017050	2.3831030	4.5591620	H	9.5684580	-0.8669810	7.7880910
H	10.0709050	3.3046140	4.9099620	C	8.7532420	-0.3393780	5.8345770
C	11.5586920	1.9989000	3.3393290	H	9.7505600	-0.2783690	5.3975680
C	10.8433940	-1.6611770	2.8156340	C	8.1570980	-1.7121540	5.4660160
H	11.2782970	-0.7192220	3.1482980	H	8.2840990	-1.8240300	4.3889830
H	11.6307510	-2.2950830	2.4027680	H	8.7371140	-2.5086160	5.9484990
H	10.4181680	-2.1614480	3.6864290	C	6.6645020	-1.9116620	5.7746590
C	9.7326560	-1.4230750	1.7936760	H	6.3044020	-2.7709180	5.2013290
C	9.1231520	-2.7559830	1.3854430	H	6.5075690	-2.1709540	6.8210440
H	8.8463020	-3.3151810	2.2810120	C	5.8149470	-0.6904310	5.4131450
H	9.8437510	-3.3511540	0.8188050	H	4.7869610	-0.8486310	5.7576630
H	8.2278090	-2.6125900	0.7831520	H	5.7712070	-0.6083530	4.3213630
C	10.1808560	-0.5222890	0.6025140	B	7.8234560	0.8759670	5.4501460
C	11.6406630	-0.6676950	0.2043950	H	8.1549350	1.5518410	2.2963890
H	11.8594790	0.0151390	-0.6180080	H	6.5746040	3.1060770	5.6008160
H	11.8457710	-1.6874410	-0.1309080	H	11.8580220	1.2580120	2.5996000
H	12.3070460	-0.4317630	1.0329820	C	8.1625000	4.2358480	6.4484620
C	9.2888220	-0.6880720	-0.6271240	H	8.3136630	3.6072680	7.3277340
H	8.2369610	-0.6032090	-0.3492380	H	9.1166470	4.6958080	6.1828350
H	9.4504760	-1.6492480	-1.1187420	H	7.4773010	5.0434550	6.7126940
H	9.5223650	0.1111270	-1.3316260	C	7.4389430	4.2471370	4.0200290
B	8.9778660	0.7099080	2.1022920	H	8.4160530	4.5922270	3.6710940
C	6.3453740	0.6480040	5.9680640	H	6.9857770	3.6537660	3.2256620
H	5.6312770	1.4162110	5.6577710	H	6.8189050	5.1267490	4.2035930
C	6.4417540	0.7074090	7.5166200	C	11.5937430	3.3574940	2.6388580
H	5.4833570	0.4162240	7.9611920	H	10.8959700	3.3537120	1.8011150
H	6.6009360	1.7560230	7.7953580	H	11.3317730	4.1722120	3.3190860

H	12.5973970	3.5541920	2.2569290	H	12.4450170	0.5374460	7.5809860
C	12.5184340	1.9245370	4.5261730	H	12.2080920	1.7407010	6.3496060
H	12.4476870	0.9508820	5.0151860	C	10.4653640	0.5085940	6.7272540
H	13.5469860	2.0725080	4.1914600	H	10.6812250	0.0641040	5.7503790
H	12.2916990	2.6953140	5.2671030	H	10.2843260	-0.3356690	7.3912620
69				C	9.1657490	1.3318870	6.6259790
Int-III(iPr)				H	9.1615260	1.9054600	5.6923800
C	10.1620680	5.6320530	7.1744690	H	8.3264670	0.6314030	6.5398470
H	10.3492700	6.3711250	6.4022780	C	8.9234220	2.2956960	7.8037680
C	10.8994310	4.0812110	5.5320810	H	8.0117840	2.8655390	7.5932170
H	10.9184530	2.9992660	5.4633130	C	8.7008950	1.5645620	9.1422700
C	12.3295250	4.5937450	5.3710910	H	8.3104240	2.3139830	9.8331340
H	12.3642210	5.6855680	5.4158670	H	7.9159930	0.8056590	9.0331360
H	12.7354220	4.2843820	4.4060660	C	9.9419920	0.8992010	9.7718020
H	12.9657140	4.1972370	6.1632980	H	9.7291640	0.6920100	10.8262420
C	9.9690960	4.5923700	4.4321970	H	10.1101910	-0.0772300	9.3170600
H	8.9521860	4.2338120	4.5974770	C	11.2385080	1.7225860	9.6812270
H	10.3147680	4.2307710	3.4623150	H	12.0806290	1.0787570	9.9623520
H	9.9486140	5.6837430	4.3850620	H	11.2077210	2.5328550	10.4157980
C	9.5588810	7.5292070	8.5276900	B	10.1971840	3.2582490	7.9652930
H	9.4075810	7.6463290	9.5991400	N	10.3743980	4.3762630	6.8823590
C	10.8021140	8.3355940	8.1554160	N	9.7560870	6.0790410	8.3452730
H	11.6780910	7.9413590	8.6712480	B	9.3605060	5.1508010	9.4982490
H	10.6627210	9.3773350	8.4489330	H	10.0175480	3.9703230	9.0698630
H	10.9925310	8.3256090	7.0793190	O	9.9094430	5.5458450	10.7374240
C	8.3124680	8.0025490	7.7824580	O	7.9878190	4.8327740	9.6621110
H	8.4556580	7.9202780	6.7012380	C	8.9804370	5.1835060	11.7696070
H	8.0993430	9.0478470	8.0149690	C	9.3911250	3.8222180	12.3269340
H	7.4536350	7.3922790	8.0628290	H	9.3211020	3.0464780	11.5654300
C	11.4886870	2.3501330	8.2967960	H	8.7719320	3.5361190	13.1795120
H	12.4070660	2.9452420	8.3716840	H	10.4302360	3.8851640	12.6538750
C	11.7203920	1.2728550	7.2103900	C	9.0629950	6.2248010	12.8770060

H	10.0490430	6.1768160	13.3414180	C	9.2866830	8.5475220	7.7945210
H	8.3105930	6.0313890	13.6454790	H	9.4219550	8.3677740	6.7251240
H	8.9190710	7.2313210	12.4863330	H	9.4939240	9.6031670	7.9785460
C	7.6111750	5.1493010	11.0123860	H	8.2440400	8.3470370	8.0459930
C	6.6334620	4.0998830	11.5239360	C	11.6824590	2.3674490	8.0913430
H	5.7250470	4.1326430	10.9204060	H	12.5694680	3.0111470	8.0152850
H	6.3641890	4.3045720	12.5633610	C	11.7440270	1.3608080	6.9204620
H	7.0478810	3.0960800	11.4596280	H	12.5549460	0.6426930	7.0992680
C	6.9032210	6.5051650	10.9889820	H	12.0412760	1.8918540	6.0107960
H	7.5706480	7.2988680	10.6520090	C	10.4530420	0.5520630	6.6364670
H	6.5143420	6.7733190	11.9732490	H	10.4692430	0.2197830	5.5928690
H	6.0683340	6.4423060	10.2892010	H	10.4766980	-0.3649760	7.2242280
69				C	9.1110030	1.2639880	6.9139380
TS-3(iPr)				H	8.8235880	1.8682790	6.0465930
C	10.1032930	5.6557210	7.3336180	H	8.3353270	0.4908630	6.9894140
H	10.2631560	6.3516300	6.5154080	C	9.0874090	2.1545280	8.1693160
C	10.4075830	4.0767620	5.6332780	H	8.1113380	2.6510740	8.2024330
H	10.4406040	2.9963920	5.5889140	C	9.2119550	1.3253900	9.4637180
C	11.7506310	4.6072550	5.1332200	H	8.9753470	1.9911740	10.2975370
H	11.7674050	5.6993430	5.0862770	H	8.4587800	0.5261180	9.4830900
H	11.9429740	4.2320020	4.1264000	C	10.5950640	0.7037620	9.7356200
H	12.5555390	4.2749990	5.7896820	H	10.6375600	0.3855150	10.7827060
C	9.2332910	4.5410300	4.7739210	H	10.7133200	-0.2094530	9.1517860
H	8.2944750	4.1606940	5.1788030	C	11.7784540	1.6418370	9.4497420
H	9.3516490	4.1684930	3.7548460	H	12.7060350	1.0578900	9.5073010
H	9.1711220	5.6311170	4.7238050	H	11.8314010	2.3977350	10.2399490
C	10.2200540	7.6788160	8.6381670	B	10.3013820	3.2319360	8.1887870
H	10.0603980	7.9194050	9.6866910	N	10.1941130	4.3941500	7.0687580
C	11.6922460	7.9256070	8.3171400	N	9.8735930	6.2390520	8.5238940
H	12.3252500	7.2808700	8.9270800	B	9.1634800	5.6297750	9.6536850
H	11.9474490	8.9664580	8.5233300	H	10.3162590	3.8676610	9.2477230
H	11.9137320	7.7324250	7.2644020	O	9.4306570	6.0857970	10.9230420

O	7.9908960	4.9214860	9.5602690	H	7.7228370	4.1125250	5.3603970
C	8.4857120	5.4298560	11.8050120	C	9.0586760	7.2567060	8.4713790
C	9.1892750	4.2018550	12.3702810	H	9.1948670	7.5646040	9.5055990
H	9.4982520	3.5308090	11.5689170	C	10.0589230	8.0228070	7.6089240
H	8.5477160	3.6612990	13.0681940	H	11.0793210	7.7791250	7.9058950
H	10.0840660	4.5309110	12.9002950	H	9.9044860	9.0967940	7.7251760
C	8.1175260	6.3878980	12.9255840	H	9.9420160	7.7834960	6.5487140
H	8.9964200	6.5729310	13.5443190	C	7.6105340	7.5374970	8.0697680
H	7.3395280	5.9516310	13.5563670	H	7.4159510	7.2564770	7.0317920
H	7.7644100	7.3415790	12.5366740	H	7.3974400	8.6034770	8.1666530
C	7.3146770	5.0856360	10.8313420	H	6.9209510	6.9855170	8.7103240
C	6.5598320	3.8120470	11.1655020	C	12.6837710	3.4391080	7.1010260
H	5.7709230	3.6571820	10.4281710	H	12.9345170	4.4264590	6.6888020
H	6.0988550	3.8931930	12.1530230	C	12.8452040	2.4109070	5.9590160
H	7.2176250	2.9459160	11.1477650	H	13.9114050	2.2890710	5.7272890
C	6.3389120	6.2464610	10.6496390	H	12.4102400	2.8235050	5.0435020
H	6.8739560	7.1714410	10.4220690	C	12.2549550	0.9999760	6.2103840
H	5.7295730	6.4028960	11.5412370	H	12.0396010	0.5322870	5.2435510
H	5.6814140	6.0152460	9.8110720	H	13.0242430	0.3730790	6.6598860
69				C	10.9915860	0.9193200	7.0960050
Int-IV(iPr)				H	10.0978000	1.0764630	6.4821710
C	9.4208890	5.1996330	7.2588900	H	10.9069410	-0.1137830	7.4577910
H	8.8833180	5.7144620	6.4667510	C	10.9511430	1.8966180	8.2846320
C	9.8491800	3.6644230	5.5501150	H	9.9719800	1.7877440	8.7630450
H	10.4632350	2.7794540	5.4530570	C	12.0132780	1.5519600	9.3497670
C	10.3381810	4.6879900	4.5257210	H	11.7983150	2.1564040	10.2362780
H	9.7063920	5.5795040	4.4985370	H	11.9223070	0.5019340	9.6594070
H	10.3192700	4.2439270	3.5288550	C	13.4752010	1.8201140	8.9459750
H	11.3608890	4.9910570	4.7528890	H	14.1008920	1.7855900	9.8440180
C	8.3960790	3.2521190	5.3259990	H	13.8380080	1.0127610	8.3091710
H	8.0835290	2.5395340	6.0905290	C	13.6956710	3.1638600	8.2334520
H	8.2906230	2.7837650	4.3457420	H	14.7214380	3.1860540	7.8432330

H	13.6180670	3.9709940	8.9685410	C	-3.1000260	18.8407500	16.8102210
B	11.2317090	3.4366670	7.8529450	H	-3.9172860	18.3423280	17.3419200
N	10.0672660	4.1286020	6.9453820	C	-2.1343420	17.7569000	16.3271840
N	9.3537290	5.8029930	8.4681960	H	-2.6407510	17.0937920	15.6264080
B	9.3544280	5.0984650	9.7393040	H	-1.7519680	17.1707570	17.1656060
H	11.2945650	4.1684220	8.8358530	H	-1.2893310	18.2187500	15.8106480
O	9.5547070	5.7955020	10.9069860	C	-2.3997550	19.7743650	17.7999720
O	8.9119510	3.8168070	9.9281920	H	-1.5326520	20.2595610	17.3432090
C	9.4932240	4.8148870	11.9755040	H	-2.0424450	19.1925780	18.6512300
C	10.9267410	4.3733690	12.2456320	H	-3.0715060	20.5473210	18.1804630
H	11.3680160	3.9330370	11.3506850	C	-3.5695370	20.6843950	15.4223380
H	10.9741090	3.6523750	13.0633660	H	-3.0392320	21.3532540	16.1011120
H	11.5133690	5.2515470	12.5184140	C	-3.9189410	22.8136400	14.2784290
C	8.8970070	5.4706340	13.2088950	H	-4.4091690	23.1354750	13.3627420
H	9.5799140	6.2382880	13.5748830	C	-2.4475190	23.2220590	14.1903440
H	8.7571030	4.7304120	14.0000350	H	-1.8970620	22.9548240	15.0951750
H	7.9392860	5.9392880	12.9887510	H	-2.3671380	24.3032090	14.0608340
C	8.6127990	3.6936900	11.3407860	H	-1.9697420	22.7330590	13.3404630
C	8.9475750	2.2855130	11.7978220	C	-4.6297240	23.4889900	15.4522870
H	8.2783920	1.5782220	11.3058520	H	-5.6741050	23.1770580	15.4933710
H	8.8119000	2.1949910	12.8784160	H	-4.5937960	24.5738510	15.3348240
H	9.9710260	2.0207010	11.5403310	H	-4.1602940	23.2436720	16.4075200
C	7.1173790	3.9612690	11.4911970	C	-5.9611630	20.5523420	11.3129560
H	6.8711160	4.9782650	11.1779900	C	-7.4084320	20.7251010	11.7663580
H	6.7873040	3.8204130	12.5217050	H	-7.5238500	20.4272580	12.8101690
H	6.5763750	3.2637980	10.8510750	H	-8.0916800	20.1345850	11.1535760
45				H	-7.6775370	21.7781760	11.6755170
Compound 1a_A				C	-5.8147490	20.9375240	9.8511990
O	-5.1557050	21.4425220	12.1174090	H	-6.2571090	21.9215430	9.6889530
O	-4.9642120	19.3551090	13.0583000	H	-6.3340750	20.2177180	9.2141170
N	-3.7063860	19.4444980	15.6300060	H	-4.7672580	20.9801880	9.5577780
N	-4.0801310	21.3464670	14.3107710	C	-5.3767290	19.1594820	11.6881750

C	-6.3708960	18.0125290	11.6347250	H	-5.7216090	23.3831330	15.0594210
H	-5.8661970	17.0864720	11.9124650	C	-2.8417270	23.4017090	13.1070050
H	-6.7704870	17.8994070	10.6239540	H	-1.8933930	22.8644450	13.1605950
H	-7.1942650	18.1728440	12.3285050	H	-2.6359110	24.4715640	13.1820110
C	-4.1228210	18.8124700	10.8895430	H	-3.3058140	23.2055230	12.1398990
H	-3.4143910	19.6430010	10.9018160	C	-5.9102940	20.5264790	11.3022540
H	-4.3627330	18.5678710	9.8531890	C	-7.3432140	20.7729850	11.7659400
H	-3.6469560	17.9490650	11.3550630	H	-7.4412610	20.5871080	12.8372070
B	-4.7188570	20.6973950	13.2039990	H	-8.0506450	20.1371000	11.2310810
45				H	-7.5955750	21.8163990	11.5730390
Compound 1a				C	-5.7875470	20.7598370	9.8070910
O	-5.0704910	21.4798520	11.9962720	H	-6.2148410	21.7315700	9.5561480
O	-4.9086900	19.4914000	13.1440420	H	-6.3339130	19.9908870	9.2559280
N	-2.9077530	21.2310660	16.2888050	H	-4.7458830	20.7516780	9.4911050
N	-3.9725930	21.5056150	14.2192480	C	-5.3419200	19.1653110	11.8023610
C	-2.4854380	20.2905810	17.3155610	C	-6.3562640	18.0376620	11.8732380
H	-2.7630780	19.2602510	17.0444440	H	-5.8639940	17.1292610	12.2229700
C	-0.9669500	20.3672850	17.4594020	H	-6.7774220	17.8418450	10.8843370
H	-0.4780720	20.0963460	16.5223900	H	-7.1637580	18.2766980	12.5630160
H	-0.6169690	19.6949100	18.2456820	C	-4.1046420	18.7235250	11.0261830
H	-0.6756720	21.3882140	17.7136940	H	-3.3832360	19.5393590	10.9506880
C	-3.1739290	20.6540110	18.6294530	H	-4.3635220	18.3869550	10.0209120
H	-2.9193680	21.6797080	18.9032690	H	-3.6358700	17.8975880	11.5620950
H	-2.8555790	19.9856550	19.4324340	B	-4.6349750	20.8462300	13.1427800
H	-4.2580290	20.5874590	18.5261670	85			
C	-3.5068610	20.7449030	15.2825340	Int-I(Dipp)			
H	-3.7098470	19.6779840	15.1644320	N	8.4940860	2.0174200	5.4260070
C	-3.7604190	22.9668240	14.2467650	N	10.7361430	2.9010280	5.0588170
H	-3.2626330	23.1610750	15.1938060	C	8.9427930	3.8749520	2.1812650
C	-5.0942810	23.7103920	14.2285680	H	9.7725450	3.2248290	2.4626650
H	-5.6244070	23.5319700	13.2924930	H	9.3120410	4.9020760	2.1287490
H	-4.9218920	24.7839720	14.3291200	H	8.6093890	3.5808830	1.1829920

C	7.7745920	3.7773330	3.1750850	H	11.3291680	5.0410210	6.7329280
H	8.1242280	4.1012050	4.1559690	H	11.4286240	6.6991230	6.1255770
C	6.6580460	4.7404070	2.7541520	H	12.8864370	5.8831610	6.7177820
H	6.3589340	4.5781920	1.7165590	C	13.0653080	6.2468370	3.9740970
H	7.0163100	5.7687960	2.8326800	H	12.4751550	7.1533900	3.8305420
H	5.7765340	4.6336880	3.3870690	H	13.3565600	5.8664100	2.9934280
C	7.3054880	2.3352870	3.2865840	H	13.9691980	6.5319870	4.5170460
C	6.4921460	1.7982570	2.2887590	C	14.2863520	3.7011170	4.7966930
H	6.1720810	2.4313630	1.4712000	H	14.9205120	4.5655310	4.6550800
C	6.0828590	0.4721900	2.3277000	C	14.8603420	2.4422680	4.9239760
H	5.4398800	0.0802730	1.5498620	H	15.9368980	2.3351810	4.8831910
C	6.5125660	-0.3516190	3.3573040	C	14.0636000	1.3168580	5.0992310
H	6.2094190	-1.3913400	3.3750050	H	14.5301880	0.3457400	5.1891170
C	7.3447140	0.1285310	4.3699500	C	12.6751360	1.4199870	5.1568250
C	7.8648410	-0.8308560	5.4249630	C	11.7934170	0.2107270	5.3967260
H	8.5724090	-0.2911210	6.0504640	H	10.8868310	0.3266370	4.7918130
C	6.7407940	-1.3383030	6.3341680	C	12.4460760	-1.1078300	4.9775390
H	5.9788430	-1.8663380	5.7550390	H	12.8192450	-1.0659540	3.9528270
H	6.2661350	-0.5115590	6.8619780	H	11.7128180	-1.9125080	5.0456910
H	7.1445850	-2.0319720	7.0751160	H	13.2751420	-1.3669930	5.6394660
C	8.6036140	-2.0073130	4.7725540	C	11.3864690	0.1440550	6.8781660
H	7.9194590	-2.6456430	4.2090980	H	10.7359580	-0.7152640	7.0540810
H	9.0721070	-2.6252000	5.5427580	H	10.8551400	1.0381690	7.2087850
H	9.3785830	-1.6597460	4.0859800	H	12.2802260	0.0316220	7.4961300
C	7.7059540	1.4820820	4.3303740	C	8.6932150	3.4174140	7.7755350
C	9.6706770	2.3931670	5.2122920	H	9.7899860	3.3257730	7.7791180
H	8.2714830	1.0904300	7.5716850	C	8.2608900	3.3614510	9.2576190
C	12.1236850	2.7071840	5.0278160	H	8.6983550	4.1993610	9.8141470
C	12.9036170	3.8600220	4.8415010	H	8.6826440	2.4461180	9.6858110
C	12.2426130	5.2219560	4.7561190	C	6.7403220	3.3485660	9.4972530
H	11.2874830	5.0902840	4.2417260	H	6.5538180	3.0669870	10.5384410
C	11.9502830	5.7407780	6.1723920	H	6.3426930	4.3579810	9.3938960

C	5.9631660	2.3903800	8.5776030	C	5.6414610	1.7666710	2.5607150
H	6.1305420	1.3654110	8.9269130	H	4.8600630	1.7057500	1.8137380
H	4.8900170	2.5888460	8.6875650	C	6.0937200	0.6141080	3.1876480
C	6.3727710	2.4510050	7.0910860	H	5.6684170	-0.3440020	2.9170870
H	5.8009530	1.6730080	6.5701560	C	7.0951440	0.6673990	4.1579110
C	6.0334020	3.7828020	6.4025810	C	7.6395840	-0.6117150	4.7629660
H	6.1906720	3.6377810	5.3302560	H	8.1865490	-0.3454300	5.6668060
H	4.9668120	4.0134650	6.5187710	C	6.5440460	-1.6049520	5.1611410
C	6.8477390	5.0073970	6.8583150	H	6.0319810	-2.0111390	4.2862470
H	6.7351050	5.8006270	6.1105300	H	5.8009060	-1.1383950	5.8092140
H	6.4157370	5.4117730	7.7730880	H	6.9889220	-2.4455590	5.6974820
C	8.3492010	4.7467580	7.0790510	C	8.6227130	-1.2614700	3.7779260
H	8.7712170	5.5915400	7.6386370	H	8.1076290	-1.5267870	2.8512460
H	8.8544860	4.7652070	6.1048220	H	9.0486960	-2.1718410	4.2058000
B	7.9537400	2.1590920	7.0870130	H	9.4392420	-0.5808940	3.5264340
85				C	7.6282860	1.9237670	4.4817740
TS-1(Dipp)				C	9.8953430	1.8969720	5.3433580
N	8.6361630	2.0192190	5.5054240	H	10.1125810	2.0621210	7.0287430
N	10.9475140	1.7998790	4.7514280	C	12.2872030	1.4895020	5.0238370
C	8.9709670	4.6661600	3.0542300	C	13.2559440	2.4180440	4.5970170
H	9.6911700	3.8460660	3.0486480	C	12.8174090	3.7056200	3.9260820
H	9.5053480	5.5977450	3.2552400	H	11.9750100	3.4585550	3.2755630
H	8.5249740	4.7320560	2.0585240	C	12.3261720	4.7104000	4.9796110
C	7.8801350	4.4330010	4.1098140	H	11.5068130	4.3031790	5.5747500
H	8.3623640	4.3734540	5.0843400	H	11.9789340	5.6270550	4.4970660
C	6.9045880	5.6124770	4.1411420	H	13.1430610	4.9677450	5.6579160
H	6.4914590	5.8198180	3.1515850	C	13.9060820	4.3448930	3.0632740
H	7.4292910	6.5119060	4.4690550	H	13.4835270	5.1804470	2.5024800
H	6.0770300	5.4281500	4.8278060	H	14.3267700	3.6313370	2.3526230
C	7.2056430	3.1007130	3.8436820	H	14.7185970	4.7423830	3.6759030
C	6.2007140	2.9962880	2.8821670	C	14.5923160	2.1349390	4.8567670
H	5.8576190	3.8884490	2.3743460	H	15.3573920	2.8320280	4.5427150

C	14.9601470	0.9647690	5.5144490	H	5.0574300	2.6620650	7.9285000
H	16.0049390	0.7594990	5.7099540	H	6.0596230	2.7365850	9.3462910
C	13.9889770	0.0600000	5.9134430	C	6.8816460	3.7628910	7.6209000
H	14.2832270	-0.8515540	6.4195190	H	6.5451400	4.7094670	8.0606380
C	12.6327980	0.2936030	5.6729910	H	6.6047840	3.8005190	6.5612270
C	11.6126620	-0.7415390	6.1074560	B	8.8156510	2.2107380	7.1212310
H	10.6195690	-0.4017910	5.8101220	85			
C	11.8637460	-2.0865790	5.4142980	Compound 4			
H	11.8442240	-1.9796470	4.3286840	N	8.5999080	1.8197830	5.5642030
H	11.0976160	-2.8082190	5.7067490	N	10.3684670	1.3040040	4.1199130
H	12.8349230	-2.4975520	5.6980910	C	9.1282240	3.7046570	2.1511920
C	11.6113870	-0.9071440	7.6313890	H	9.8652150	2.9074270	2.2463630
H	10.8271370	-1.6035500	7.9366880	H	9.6444590	4.6669850	2.1089980
H	11.4364940	0.0493280	8.1245710	H	8.5947800	3.5692410	1.2069510
H	12.5683770	-1.3014750	7.9811520	C	8.1413520	3.6834950	3.3261660
C	8.4199650	3.6476850	7.6990960	H	8.6969330	3.8641410	4.2489340
H	8.8447810	4.4730990	7.1148850	C	7.1188190	4.8171530	3.1645340
C	9.0027920	3.7672400	9.1208840	H	6.6137870	4.7525280	2.1984380
H	8.7166760	4.7244320	9.5720600	H	7.6231280	5.7850370	3.2082350
H	10.0945810	3.7826240	9.0255650	H	6.3547020	4.7867950	3.9421740
C	8.6173220	2.6310340	10.0819050	C	7.4589270	2.3322650	3.4405210
H	9.2681510	2.6801940	10.9602500	C	6.5879650	1.9369420	2.4253620
H	7.6091170	2.7941730	10.4596280	H	6.4262910	2.5961550	1.5812450
C	8.7300680	1.2232500	9.4708670	C	5.9300010	0.7166040	2.4757030
H	9.7907240	0.9517560	9.4438100	H	5.2610480	0.4247260	1.6759470
H	8.2459940	0.5058050	10.1439800	C	6.1275950	-0.1228080	3.5613150
C	8.1771450	1.0648820	8.0389850	H	5.6049920	-1.0705450	3.6055750
H	8.4417260	0.0520650	7.7110470	C	6.9921280	0.2279060	4.5999000
C	6.6441390	1.2067780	7.9300730	C	7.1534930	-0.7366180	5.7620170
H	6.3577560	0.9708370	6.8987530	H	7.7819060	-0.2647250	6.5191340
H	6.1443010	0.4671200	8.5670960	C	5.8000960	-1.0663580	6.4061690
C	6.0966580	2.6054090	8.2661480	H	5.1794930	-1.6581530	5.7299970

H	5.2478360	-0.1613840	6.6627220	H	9.7911790	-1.9180930	2.0688860
H	5.9490420	-1.6530980	7.3156120	H	11.1103650	-1.0790850	1.2354590
C	7.8473420	-2.0280590	5.3114970	C	12.0797880	-2.5507910	3.3832490
H	7.2380360	-2.5517180	4.5710100	H	11.3426190	-3.3555830	3.4162420
H	7.9962000	-2.6978370	6.1615640	H	12.7441220	-2.6580600	4.2430350
H	8.8154290	-1.8164990	4.8585340	H	12.6692680	-2.6863190	2.4731340
C	7.6658540	1.4574290	4.5202290	C	6.6630590	2.6355570	7.1736640
C	9.9487690	1.6645820	5.2618240	H	5.9742280	2.2423150	6.4209460
H	10.6171500	1.8850640	6.0905200	C	6.5379350	4.1822100	7.1443480
C	11.7669010	1.2371090	3.9139720	H	5.5227350	4.4756440	7.4326020
C	12.5955450	2.3699420	4.0178460	H	6.6669140	4.5006490	6.1048010
C	12.0752580	3.7575350	4.3619720	C	7.5541660	4.9489270	8.0088630
H	10.9854150	3.7249410	4.3687110	H	7.5477190	5.9988690	7.7026730
C	12.5504900	4.2096140	5.7490440	H	7.2376710	4.9467790	9.0500150
H	12.2326720	3.5167040	6.5310240	C	8.9932380	4.4179830	7.9021750
H	12.1563940	5.2010000	5.9860610	H	9.4161770	4.7459240	6.9438440
H	13.6413850	4.2627650	5.7803790	H	9.6087390	4.8785380	8.6823270
C	12.4874660	4.7902910	3.3044200	C	9.1352160	2.8736930	7.9711050
H	12.0013960	5.7479730	3.5061940	H	10.1966010	2.6544100	7.8332420
H	12.2038200	4.4598870	2.3046260	C	8.7326050	2.2498040	9.3261900
H	13.5661720	4.9595430	3.3128440	H	9.0053730	1.1887130	9.2925490
C	13.9622380	2.2155940	3.7595440	H	9.3332040	2.6942540	10.1271230
H	14.6144320	3.0767370	3.8456930	C	7.2449070	2.3526170	9.6923930
C	14.4963690	0.9922770	3.3943160	H	7.0446350	1.6746750	10.5269320
H	15.5574130	0.8959110	3.2015940	H	7.0189270	3.3497160	10.0656210
C	13.6592790	-0.1138310	3.2697600	C	6.3040930	1.9966040	8.5328770
H	14.0816020	-1.0675220	2.9826690	H	5.2766530	2.2609690	8.8061280
C	12.2956800	-0.0116500	3.5164260	H	6.3168300	0.9085790	8.4076310
C	11.3615100	-1.2014660	3.3842150	B	8.1729690	2.3454180	6.8304380
H	10.7021650	-1.1778140	4.2543090	107			
C	10.4831770	-1.0738750	2.1304420	Int-II(Dipp)			
H	9.9031100	-0.1521930	2.1535950	O	-0.4554050	-2.9277590	-2.0879540

O	0.5381210	-1.1190280	-3.0734410	C	0.1996740	0.9119820	0.3768910
N	-1.0374610	0.7305900	0.9913570	H	0.5058840	1.9576850	0.3638710
N	0.9321890	-0.0012070	-0.1156350	C	2.1903930	0.3841690	-0.6438390
C	1.2367190	3.1628150	2.9663980	C	2.3285210	1.2714990	-1.7312110
H	1.5779710	3.0612200	1.9348090	C	1.1475130	1.9509580	-2.4064790
H	2.0478320	2.8402520	3.6231170	H	0.2433270	1.4225370	-2.1035870
H	1.0491490	4.2227450	3.1540820	C	1.0397760	3.4254720	-1.9866640
C	-0.0315730	2.3426950	3.2470250	H	0.9304590	3.5515900	-0.9079730
H	0.1801970	1.2921440	3.0385430	H	0.1825410	3.8985650	-2.4722730
C	-0.3884230	2.4585410	4.7358280	H	1.9405290	3.9652820	-2.2899190
H	-0.4677750	3.5037860	5.0419900	C	1.2166980	1.8757840	-3.9370290
H	0.3945940	1.9972850	5.3412470	H	0.2844690	2.2570040	-4.3613030
H	-1.3363830	1.9695860	4.9619960	H	1.3492710	0.8473400	-4.2655170
C	-1.1851610	2.7795400	2.3571500	H	2.0291150	2.4891700	-4.3331420
C	-1.7774200	4.0237090	2.5849070	C	3.6172380	1.5377240	-2.2021830
H	-1.3990620	4.6519920	3.3819740	H	3.7405640	2.2220840	-3.0327150
C	-2.8415950	4.4650250	1.8130350	C	4.7374000	0.9442980	-1.6407220
H	-3.2875580	5.4329360	2.0041690	H	5.7236960	1.1653300	-2.0290750
C	-3.3368850	3.6571710	0.7984860	C	4.5853500	0.0634460	-0.5755450
H	-4.1711870	4.0026640	0.2006160	H	5.4604180	-0.3961110	-0.1340460
C	-2.7713720	2.4116880	0.5260400	C	3.3236210	-0.2288620	-0.0647890
C	-3.3297440	1.5775030	-0.6136070	C	3.1593300	-1.1185040	1.1552120
H	-2.9046820	0.5756790	-0.5480030	H	2.1812280	-1.5978890	1.0822030
C	-4.8545270	1.4395710	-0.5365610	C	4.2214700	-2.2141660	1.2639470
H	-5.3527400	2.3926620	-0.7262130	H	4.3066460	-2.7799640	0.3341610
H	-5.1712580	1.0790330	0.4435070	H	3.9553630	-2.9063390	2.0653910
H	-5.2006300	0.7322980	-1.2932900	H	5.2037700	-1.8010600	1.5047680
C	-2.9105800	2.1724740	-1.9639220	C	3.1561020	-0.2564190	2.4254800
H	-3.3212640	3.1786840	-2.0808690	H	2.9994310	-0.8755640	3.3126470
H	-3.2782000	1.5534180	-2.7852150	H	2.3654530	0.4949120	2.3832610
H	-1.8245000	2.2403780	-2.0430300	H	4.1115390	0.2639920	2.5309150
C	-1.6823450	1.9873030	1.3072130	C	1.7562960	-3.4293770	-1.3460130

H	1.8867340	-2.4257210	-0.9408360	H	-2.1762060	-2.9065720	-0.2174130
H	2.7341310	-3.8425290	-1.6011990	H	-1.5595780	-4.0191360	0.9753200
H	1.2962860	-4.0568190	-0.5801820	C	-3.3745290	-3.0006790	1.5632900
C	0.8364640	-3.3902980	-2.5602600	H	-4.0781320	-3.6068550	0.9851500
C	0.6723650	-4.7802290	-3.1499600	H	-3.3132530	-3.4771450	2.5407290
H	0.3907290	-5.4748680	-2.3574840	C	-3.9495250	-1.5882220	1.7163030
H	1.6136630	-5.1205300	-3.5880200	H	-4.8386640	-1.6240880	2.3556900
H	-0.1028480	-4.8002060	-3.9140970	H	-4.2921110	-1.2437280	0.7332630
C	1.2377420	-2.2825880	-3.5830720	B	-1.6437250	-0.5235340	1.3865910
C	2.7253240	-1.9769640	-3.6426860	H	-1.3710850	-0.8767500	-1.8942460
H	2.9065530	-1.2008150	-4.3881600	107			
H	3.2826600	-2.8703510	-3.9360790	TS-2(Dipp)			
H	3.0983440	-1.6165100	-2.6850120	O	9.5434610	-1.2039410	2.8337190
C	0.6879520	-2.5380190	-4.9835170	O	9.6738850	0.5547570	1.3557820
H	-0.3800880	-2.7603670	-4.9462210	N	8.3381770	2.1980700	5.0949130
H	1.2054290	-3.3665420	-5.4700850	N	10.2297520	1.4502130	3.8563120
H	0.8299750	-1.6372330	-5.5822460	C	10.5379980	4.5990780	7.2355660
B	-0.4909090	-1.5737180	-2.2937010	H	10.9043990	4.5873800	6.2073640
C	-2.9535360	-0.5491880	2.2673250	H	11.3336840	4.2227880	7.8823190
H	-3.4653510	0.4152860	2.3208240	H	10.3427820	5.6392630	7.5067110
C	-2.4341450	-0.8598500	3.7003190	C	9.2674710	3.7538020	7.4122520
H	-3.2853460	-1.0024440	4.3755110	H	9.5055430	2.7210350	7.1586070
H	-1.9106900	0.0352600	4.0519980	C	8.8411220	3.7759300	8.8857740
C	-1.4709760	-2.0562770	3.8328100	H	8.6711490	4.7968100	9.2339620
H	-0.9581080	-1.9801830	4.7962400	H	9.6303540	3.3430530	9.5041480
H	-2.0316140	-2.9882840	3.8717400	H	7.9255240	3.2070030	9.0479960
C	-0.4194330	-2.1414710	2.7146490	C	8.1588880	4.2270720	6.4848450
H	0.3440970	-1.3706540	2.8836850	C	7.5725910	5.4724590	6.7181280
H	0.0995480	-3.1047280	2.7772960	H	7.9097150	6.0666090	7.5587230
C	-0.9882430	-1.9504360	1.2809220	C	6.5677210	5.9586250	5.8948910
H	-0.1540910	-1.9966100	0.5860600	H	6.1225520	6.9254020	6.0933320
C	-2.0105870	-3.0270100	0.8559380	C	6.1363530	5.2009880	4.8151470

H	5.3534580	5.5845740	4.1723740	H	14.7882790	1.1901370	4.0804140
C	6.6997800	3.9562560	4.5315510	C	12.6455410	1.2647020	4.0358760
C	6.2113690	3.1869740	3.3154980	C	12.4408400	0.2361730	5.1342360
H	6.6965360	2.2115630	3.3083270	H	11.5433520	-0.3308430	4.8758120
C	4.6935780	2.9638550	3.3414010	C	13.6038420	-0.7488340	5.2736600
H	4.1540030	3.9103520	3.2631770	H	13.8773110	-1.1897530	4.3138250
H	4.3723520	2.4646230	4.2560660	H	13.3212370	-1.5541130	5.9545680
H	4.3986510	2.3444300	2.4916990	H	14.4885580	-0.2640730	5.6934970
C	6.6047570	3.9167520	2.0239210	C	12.2019510	0.9351870	6.4803640
H	6.1054290	4.8870990	1.9622630	H	12.0103260	0.2001050	7.2659830
H	6.3118210	3.3266620	1.1531440	H	11.3492990	1.6138650	6.4328560
H	7.6799180	4.0878090	1.9768250	H	13.0827100	1.5190010	6.7599790
C	7.7140610	3.4784430	5.3796060	C	11.8378600	-1.6092890	2.2315900
C	9.5851320	2.3322450	4.5257190	H	12.1559200	-0.5886740	2.4398630
H	10.0173770	3.3225570	4.6639800	H	12.5103110	-2.0424480	1.4879290
C	11.5306150	1.8778190	3.4320600	H	11.9139840	-2.1938510	3.1500980
C	11.6836670	2.8591090	2.4379770	C	10.3892190	-1.6501550	1.7588460
C	10.5081140	3.5695110	1.7882170	C	10.0125600	-3.0868640	1.4225190
H	9.5982210	3.0434610	2.0731830	H	10.2638400	-3.7289940	2.2682150
C	10.4226540	5.0266060	2.2677140	H	10.5673950	-3.4367400	0.5483680
H	10.2892070	5.0999750	3.3495730	H	8.9456680	-3.1822370	1.2284490
H	9.5845630	5.5384600	1.7888590	C	10.0826580	-0.6175010	0.6276960
H	11.3372920	5.5657620	2.0092710	C	11.2770460	-0.2801860	-0.2519680
C	10.5749860	3.5262620	0.2587470	H	10.9628720	0.3864350	-1.0570140
H	9.6735210	3.9809470	-0.1595440	H	11.6863330	-1.1865910	-0.7051980
H	10.6331680	2.4956980	-0.0842090	H	12.0581130	0.2176540	0.3221830
H	11.4338080	4.0815700	-0.1251260	C	8.8945520	-1.0276640	-0.2423240
C	12.9832950	3.2138590	2.0635040	H	8.0337620	-1.2839070	0.3780780
H	13.1224700	3.9714180	1.3017400	H	9.1346950	-1.8770290	-0.8846820
C	14.0919780	2.6195090	2.6454200	H	8.6213870	-0.1782570	-0.8698620
H	15.0887690	2.9088770	2.3370360	B	9.1802180	0.1237360	2.5952710
C	13.9197890	1.6509070	3.6285610	C	6.2314620	0.9627400	6.0987410

H	5.6964740	1.8962020	5.9132670	H	9.9739150	5.5039050	8.0390270
C	6.3225390	0.8018770	7.6388310	C	9.1908660	3.5112600	7.6637810
H	5.3239230	0.6104910	8.0473700	H	9.5798890	2.5799680	7.2536840
H	6.6331810	1.7729570	8.0371790	C	8.7557910	3.2472890	9.1107900
C	7.3021090	-0.2690000	8.1581160	H	8.5103900	4.1786260	9.6256510
H	7.5266910	-0.0536800	9.2071420	H	9.5684560	2.7699720	9.6622950
H	6.8294560	-1.2496590	8.1535350	H	7.8813160	2.5963470	9.1507700
C	8.6188420	-0.3455640	7.3727850	C	8.0360550	3.9648920	6.7901620
H	9.2407920	0.5202020	7.6323550	C	7.2319140	5.0203440	7.2266400
H	9.1804850	-1.2287960	7.6959520	H	7.4241850	5.4651980	8.1950670
C	8.4385310	-0.3950630	5.8285760	C	6.1938790	5.5038000	6.4452290
H	9.4260260	-0.4729820	5.3757070	H	5.5714290	6.3120370	6.8079460
C	7.6112470	-1.6113400	5.3507090	C	5.9739070	4.9668900	5.1835440
H	7.7777480	-1.7030790	4.2770680	H	5.1903700	5.3766940	4.5589200
H	8.0231390	-2.5224480	5.8000540	C	6.7612070	3.9251080	4.6951640
C	6.0938740	-1.5624270	5.6103100	C	6.6089510	3.4952880	3.2447400
H	5.6067110	-2.2794770	4.9433300	H	7.1164730	2.5397490	3.1030670
H	5.8577640	-1.8959300	6.6204110	C	5.1517300	3.3346020	2.7976030
C	5.4761920	-0.1787170	5.3846210	H	4.6414790	4.2992560	2.7531180
H	4.4297780	-0.1894540	5.7095170	H	4.5886230	2.6833110	3.4665080
H	5.4641520	0.0343890	4.3084460	H	5.1233960	2.9053980	1.7942550
B	7.7061770	0.9666780	5.5437820	C	7.3043790	4.5420180	2.3614250
H	8.1445620	0.5318250	3.0458410	H	6.7675760	5.4929670	2.4103600
107				H	7.3344390	4.2127070	1.3196900
Int-III(Dipp)				H	8.3249600	4.7224710	2.6989750
O	10.2767320	-0.8248230	3.2774410	C	7.7658680	3.4028610	5.5318960
O	9.3360150	0.6256300	1.7446390	C	9.6825570	2.5217540	4.5060290
N	8.5232370	2.2659060	5.0635080	H	10.1194380	3.5105770	4.6303970
N	10.3414210	1.6396880	3.7785150	C	11.6732530	1.9553000	3.3208890
C	10.3226860	4.5488230	7.6391580	C	11.8650550	2.8139900	2.2289750
H	10.6875660	4.7278540	6.6253990	C	10.7291680	3.5400010	1.5328940
H	11.1624750	4.2081830	8.2491380	H	9.7879190	3.1753560	1.9413580

C	10.8395670	5.0508660	1.7816370	H	10.2961870	-3.3816910	1.0925180
H	10.8105360	5.2892430	2.8478580	H	9.3076320	-3.1678750	2.5527480
H	10.0219660	5.5802840	1.2879930	C	9.3633160	-0.6778810	1.1302370
H	11.7799810	5.4381220	1.3829940	C	9.6966450	-0.5339420	-0.3453350
C	10.6966590	3.2500360	0.0299570	H	8.9042670	0.0290550	-0.8417090
H	9.8391110	3.7526540	-0.4236580	H	9.7640650	-1.5187460	-0.8141790
H	10.5993400	2.1804530	-0.1442790	H	10.6393510	-0.0114890	-0.4955720
H	11.5980160	3.6115370	-0.4701500	C	7.9815020	-1.3088210	1.2863070
C	13.1754320	3.0323010	1.7922680	H	7.7611170	-1.5070080	2.3351250
H	13.3487810	3.6932820	0.9518760	H	7.9070140	-2.2456430	0.7307720
C	14.2509390	2.4165290	2.4116960	H	7.2348460	-0.6115170	0.9026610
H	15.2571130	2.5928490	2.0523140	B	9.6499370	0.4247610	3.1091430
C	14.0386310	1.5763140	3.4990190	C	6.3742150	0.6148680	5.1087180
H	14.8849300	1.1039970	3.9792350	H	5.8369030	1.3221220	4.4739420
C	12.7528910	1.3296130	3.9737550	C	5.9137870	0.8925910	6.5598990
C	12.5204780	0.4571370	5.1935640	H	4.8338380	0.7159220	6.6333040
H	11.5779240	-0.0646180	5.0410500	H	6.0602210	1.9550590	6.7751290
C	13.6002420	-0.6063720	5.4010140	C	6.6234640	0.0725970	7.6492370
H	13.7582550	-1.1950010	4.4955750	H	6.4036400	0.5204820	8.6243740
H	13.2913090	-1.2839620	6.1988630	H	6.2033540	-0.9310960	7.6912900
H	14.5549260	-0.1660130	5.6988110	C	8.1474070	-0.0123530	7.4734110
C	12.4064590	1.3353860	6.4476110	H	8.5873790	0.9290790	7.8068440
H	12.1677590	0.7248370	7.3218670	H	8.5389440	-0.7834630	8.1479750
H	11.6262270	2.0908320	6.3387250	C	8.6236250	-0.2910620	6.0356220
H	13.3503800	1.8544110	6.6337700	H	9.7192370	-0.2471880	6.0454130
C	11.8659790	-1.1011590	1.5022080	C	8.2367810	-1.7058920	5.5490750
H	12.0094280	-0.0278760	1.3661070	H	8.7811660	-1.8881350	4.6221610
H	12.0934760	-1.6140900	0.5651920	H	8.5969920	-2.4507030	6.2693900
H	12.5667360	-1.4439540	2.2651260	C	6.7352300	-1.9526980	5.3055150
C	10.4467010	-1.4134930	1.9727650	H	6.6288170	-2.8502350	4.6867470
C	10.2571610	-2.9185720	2.0816490	H	6.2419950	-2.1945750	6.2460760
H	11.0601350	-3.3388530	2.6893690	C	5.9871550	-0.7935970	4.6222900

H	4.9090770	-0.9482180	4.7512730	H	6.6485290	5.7087240	5.2232520
H	6.1717190	-0.8316300	3.5451960	H	8.0729320	6.7548930	5.1002610
B	7.9720480	0.7754170	5.0161890	C	9.7749860	5.1786980	6.6419830
H	8.3716480	0.4146670	3.7855720	H	9.5200900	5.5172960	7.6487770
107				H	10.2879610	5.9957290	6.1293020
TS-3(Dipp)				H	10.4733080	4.3444500	6.7411790
O	10.0095000	0.2062340	1.4946130	C	7.7434950	2.3263650	6.0102420
O	9.6370550	-1.0041690	3.4115990	C	9.5919930	1.9447720	4.6763350
N	8.2969060	2.0295270	4.7099940	H	10.1638670	2.3619290	5.5016290
N	10.3057430	1.3870810	3.6879920	C	11.7303610	1.6770550	3.6580760
C	8.5819610	-0.7971590	6.7913330	C	12.1615210	2.7881020	2.9118230
H	9.4549450	-0.1936560	6.5399670	C	11.1877020	3.7278150	2.2276340
H	8.7364070	-1.7991490	6.3844270	H	10.2077450	3.5717610	2.6733730
H	8.5187360	-0.8628190	7.8808760	C	11.5473620	5.2017520	2.4457850
C	7.3011060	-0.1786490	6.2145670	H	11.6935250	5.4228000	3.5054400
H	7.4077650	-0.1597320	5.1306520	H	10.7368570	5.8298840	2.0706070
C	6.0955570	-1.0585920	6.5549150	H	12.4553920	5.4849810	1.9093420
H	6.0368570	-1.2666800	7.6259000	C	11.0783700	3.4064610	0.7322180
H	6.1903540	-2.0181140	6.0428240	H	10.3526800	4.0709650	0.2573460
H	5.1589820	-0.5939150	6.2428770	H	10.7595910	2.3754150	0.5790370
C	7.1704160	1.2515900	6.7161930	H	12.0469450	3.5496960	0.2449620
C	6.5830390	1.5177040	7.9506550	C	13.5322770	3.0280700	2.8137700
H	6.1261910	0.7102540	8.5078560	H	13.8813260	3.8672300	2.2258350
C	6.5918520	2.8003410	8.4872330	C	14.4490790	2.2150680	3.4629860
H	6.1294320	2.9898880	9.4477270	H	15.5099730	2.4129220	3.3744050
C	7.2150110	3.8304220	7.8011780	C	14.0018300	1.1639670	4.2502530
H	7.2452270	4.8216590	8.2369770	H	14.7208030	0.5596450	4.7876180
C	7.8059670	3.6181410	6.5520380	C	12.6411640	0.8740780	4.3725090
C	8.5106400	4.7772200	5.8688860	C	12.2061820	-0.2061820	5.3498020
H	8.8160410	4.4559880	4.8730980	H	11.2153330	-0.5564020	5.0634320
C	7.5846890	5.9892410	5.7071210	C	13.1492660	-1.4169010	5.3721170
H	7.3474660	6.4337310	6.6761300	H	13.3953420	-1.7641250	4.3690420

H	12.6752820	-2.2369820	5.9153660	H	4.7238190	2.3529750	0.9812300
H	14.0824850	-1.1847060	5.8900720	C	6.8802400	2.1577420	0.9481080
C	12.1420480	0.3813110	6.7702370	H	7.5589330	1.3703660	0.6186730
H	11.8361640	-0.3864580	7.4845720	H	6.8528960	2.8974740	0.1372010
H	11.4393480	1.2121680	6.8488320	C	7.5119610	2.7840320	2.2077370
H	13.1277690	0.7512810	7.0629960	H	8.5515650	2.9852710	1.9338430
C	8.2993320	-1.1705080	0.4850010	C	6.8679990	4.1245550	2.5891250
H	7.5666550	-0.8633590	1.2307460	H	7.4446610	4.5696360	3.4042640
H	8.0492530	-2.1704480	0.1259530	H	6.9359300	4.8306420	1.7511710
H	8.2431550	-0.4793520	-0.3561610	C	5.4011940	4.0182860	3.0275830
C	9.7140270	-1.1459630	1.0506330	H	5.0904940	4.9664220	3.4806200
C	10.7061000	-1.5031810	-0.0453370	H	4.7695070	3.8989630	2.1477840
H	10.5306020	-0.8562550	-0.9056400	C	5.1355930	2.8794820	4.0251050
H	10.5685640	-2.5397460	-0.3613820	H	4.0507130	2.7450790	4.1221950
H	11.7342380	-1.3631720	0.2830160	H	5.4873420	3.1988510	5.0120010
C	9.8629160	-1.9831820	2.3684150	B	7.3855950	1.6782450	3.3923720
C	8.8502950	-3.1035820	2.5364710	H	7.8614170	0.5995070	3.0101590
H	9.0301810	-3.6033600	3.4895730	107			
H	8.9529090	-3.8403830	1.7366840	Int-IV(Dipp)			
H	7.8327790	-2.7165390	2.5390790	O	10.7923570	0.1277880	1.5599300
C	11.2767370	-2.5140850	2.5750830	O	9.2208320	-0.7568070	2.9842060
H	12.0059330	-1.7057180	2.4901770	N	8.2194190	1.7650310	4.7664640
H	11.5227410	-3.2918190	1.8502580	N	10.2704730	1.4263130	3.5743220
H	11.3464500	-2.9362240	3.5783660	C	8.3634980	-1.3041930	7.3124560
B	9.8189700	0.2410260	2.8482610	H	9.3615700	-0.8622870	7.3607060
C	5.8007230	1.5270340	3.6927260	H	8.4530990	-2.3158050	6.9095910
H	5.5803540	0.8652130	4.5364310	H	7.9818390	-1.3830230	8.3330480
C	5.2002400	0.8444220	2.4471340	C	7.4329920	-0.4677270	6.4237640
H	4.1160880	0.7217630	2.5633900	H	7.8405170	-0.4779770	5.4152810
H	5.6193830	-0.1670170	2.3955710	C	6.0348730	-1.0902040	6.3576180
C	5.4656590	1.5652200	1.1115770	H	5.5626580	-1.1094490	7.3432800
H	5.2849640	0.8625690	0.2905650	H	6.1014500	-2.1187950	5.9954860

H	5.3960680	-0.5275520	5.6766260	H	11.7623470	2.2835020	0.1352350
C	7.3837880	0.9702140	6.9159110	H	12.5418140	3.8753450	0.1746610
C	6.9564210	1.2300660	8.2182400	C	13.3090370	3.4648540	2.8834550
H	6.6055170	0.4088180	8.8315240	H	13.6211960	4.2732150	2.2334310
C	6.9936250	2.5134370	8.7437180	C	14.1995320	2.9474240	3.8137640
H	6.6596420	2.6975760	9.7570260	H	15.1996460	3.3547000	3.8924590
C	7.4821960	3.5576120	7.9717160	C	13.8107700	1.8985140	4.6359230
H	7.5366230	4.5523060	8.3958020	H	14.5156390	1.4877230	5.3485070
C	7.9037310	3.3571530	6.6555500	C	12.5288300	1.3534470	4.5502370
C	8.4831800	4.5392810	5.8868770	C	12.1676000	0.1664650	5.4304190
H	8.5014060	4.2826000	4.8274410	H	11.1806320	-0.2005560	5.1398370
C	7.6491570	5.8206380	6.0380680	C	13.1624910	-0.9844730	5.2251790
H	7.7511550	6.2429670	7.0400830	H	13.2846400	-1.2151050	4.1656830
H	6.5909780	5.6462280	5.8466590	H	12.8108690	-1.8804300	5.7410460
H	8.0081810	6.5713800	5.3309320	H	14.1455560	-0.7319960	5.6279440
C	9.9187510	4.8479360	6.3475660	C	12.1168570	0.5569530	6.9141130
H	9.9242840	5.0816580	7.4149200	H	11.8837690	-0.3166170	7.5266770
H	10.3066100	5.7156290	5.8085760	H	11.3617060	1.3203700	7.1132810
H	10.6120470	4.0205790	6.1863870	H	13.0830460	0.9493220	7.2393590
C	7.8156990	2.0522130	6.1327930	C	9.3234770	-0.5900180	-0.1857090
C	9.5035360	1.8018220	4.6297220	H	8.4777860	-0.0518150	0.2418990
H	10.0777290	2.1966150	5.4607350	H	8.9482040	-1.4300720	-0.7726340
C	11.6345420	1.9216260	3.6276800	H	9.8605270	0.0884580	-0.8502630
C	12.0103720	2.9660600	2.7733820	C	10.2841900	-1.0633380	0.8988220
C	11.0630200	3.5538980	1.7463700	C	11.4547670	-1.8042400	0.2755810
H	10.1140560	3.0259910	1.8188480	H	11.8834260	-1.1927720	-0.5194250
C	10.7997390	5.0378530	2.0271210	H	11.1175270	-2.7475580	-0.1598410
H	10.4191820	5.1849680	3.0406710	H	12.2337030	-2.0086570	1.0081220
H	10.0603440	5.4274400	1.3246010	C	9.5749210	-1.8260300	2.0681480
H	11.7138070	5.6271080	1.9206140	C	8.3090680	-2.5651040	1.6731490
C	11.5984970	3.3446580	0.3252350	H	7.8855660	-3.0451450	2.5561510
H	10.8785300	3.7251080	-0.4027900	H	8.5340770	-3.3359680	0.9322570

H	7.5639600	-1.8829170	1.2688140	O	8.0953640	1.2950980	2.6682460
C	10.5123430	-2.7504840	2.8380460	O	9.9974760	0.6569490	1.5435330
H	11.4246120	-2.2266260	3.1277510	N	8.6142970	1.7767000	5.4582760
H	10.7810480	-3.6286990	2.2489260	N	10.2738640	1.2078080	3.9061370
H	10.0029650	-3.0781230	3.7453890	C	10.2241670	-0.3931550	8.4595190
B	10.0332760	0.2941060	2.6857590	H	11.0181760	0.2540930	8.0804270
C	5.6002940	2.0050750	4.0647360	H	10.5447240	-1.4325800	8.3568170
H	5.3076270	1.7253490	5.0846050	H	10.1051530	-0.1831040	9.5248980
C	4.5694300	1.3575140	3.1207780	C	8.9075110	-0.1591720	7.7090610
H	3.5581520	1.7150910	3.3520000	H	9.0806670	-0.3519350	6.6496680
H	4.5736650	0.2776240	3.3054910	C	7.8387470	-1.1530150	8.1817090
C	4.8447990	1.5971640	1.6286510	H	7.6515350	-1.0520700	9.2529780
H	4.2121890	0.9291220	1.0349690	H	8.1677510	-2.1781770	7.9949850
H	4.5362690	2.6064250	1.3570280	H	6.8969110	-0.9885580	7.6567060
C	6.3110290	1.3701600	1.2243370	C	8.4279710	1.2751260	7.8654750
H	6.4795640	0.2870970	1.2009750	C	8.0566300	1.7282260	9.1352080
H	6.4567760	1.7359840	0.1991150	H	8.1547560	1.0589990	9.9823500
C	7.3729230	1.9693030	2.1718680	C	7.5606330	3.0069690	9.3324120
H	8.3399510	1.6448450	1.7579440	H	7.2814280	3.3363550	10.3253380
C	7.4120880	3.5063080	2.1819950	C	7.4105230	3.8605630	8.2431420
H	8.2717260	3.8122010	2.7898370	H	7.0096640	4.8545270	8.3966230
H	7.6077440	3.8999140	1.1748670	C	7.7640450	3.4527520	6.9618600
C	6.1541840	4.1916020	2.7410890	C	7.6453460	4.3766600	5.7644480
H	6.3929460	5.2391690	2.9588510	H	7.4751390	3.7415200	4.8919220
H	5.3912420	4.2269260	1.9639730	C	6.4878890	5.3709860	5.8736970
C	5.5786000	3.5410810	4.0126520	H	6.6730410	6.1210590	6.6463670
H	4.5581060	3.9173880	4.1635320	H	5.5496550	4.8643070	6.1059120
H	6.1532880	3.8936630	4.8702020	H	6.3676540	5.9035420	4.9279140
B	7.0381000	1.3750140	3.6476390	C	8.9671030	5.1288010	5.5519640
H	6.9877290	0.1623710	3.6517960	H	9.1736410	5.7756780	6.4085880
83				H	8.9208370	5.7509230	4.6540290
Compound 1eA				H	9.8021300	4.4337940	5.4477420

C	8.3001960	2.1600230	6.7802730	C	7.2220000	-0.6906010	1.6726940
C	9.8313400	1.5741010	5.1682670	H	8.0607770	-1.2948510	2.0264230
H	10.6463140	1.6768240	5.8929870	H	6.8040370	-1.1570020	0.7789310
C	11.6863690	0.9528820	3.7814080	H	6.4598100	-0.6733730	2.4519350
C	12.5589680	2.0276860	3.5575510	C	7.6638500	0.7447180	1.3998430
C	12.0563580	3.4477380	3.3726760	C	6.5002420	1.5690520	0.8792730
H	10.9792000	3.4530450	3.5414840	H	5.6457220	1.4455570	1.5454680
C	12.6906940	4.4153980	4.3773980	H	6.2118880	1.2334620	-0.1197170
H	12.5190600	4.0864220	5.4041450	H	6.7531710	2.6271610	0.8408560
H	12.2613430	5.4128820	4.2605390	C	8.9624630	0.8229180	0.5431040
H	13.7692710	4.4944950	4.2240570	C	9.1075070	-0.2700710	-0.5009770
C	12.3014410	3.9100600	1.9307620	H	10.0473660	-0.1349710	-1.0378480
H	11.8809770	4.9058680	1.7726230	H	8.2878760	-0.2184120	-1.2215270
H	11.8414700	3.2171020	1.2244180	H	9.1137700	-1.2576270	-0.0424140
H	13.3713480	3.9551870	1.7137960	C	9.1695340	2.1953250	-0.0904780
C	13.9251430	1.7594810	3.4628980	H	9.0634070	2.9860990	0.6551350
H	14.6163200	2.5753650	3.2882500	H	8.4563100	2.3726840	-0.8970950
C	14.4080130	0.4631030	3.5789660	H	10.1790480	2.2405500	-0.5009560
H	15.4709410	0.2717660	3.5005740	B	9.4426820	1.0652550	2.7392130
C	13.5264650	-0.5889040	3.7900390	83			
H	13.9083320	-1.5995310	3.8705460	Compound 1e			
C	12.1537900	-0.3648070	3.8986000	O	12.7020030	1.3189480	4.7992610
C	11.2130120	-1.5385600	4.1018240	O	12.4536670	0.8848610	2.5496190
H	10.2115060	-1.1439830	4.2794720	N	8.6330230	1.7734710	5.2997670
C	11.1622930	-2.4058570	2.8370910	N	10.4290070	1.4284200	3.8580630
H	10.8761860	-1.8047850	1.9731350	C	10.3283860	-0.4150390	8.1034610
H	10.4429130	-3.2190980	2.9618240	H	11.0393010	0.3276540	7.7356510
H	12.1412350	-2.8483280	2.6363510	H	10.7505600	-1.4085180	7.9327400
C	11.6037330	-2.3763600	5.3243050	H	10.2234310	-0.2727760	9.1818110
H	10.8531030	-3.1492070	5.5048390	C	8.9678970	-0.2831800	7.4073750
H	11.6825240	-1.7545950	6.2172970	H	9.1239700	-0.4006670	6.3352030
H	12.5636160	-2.8752380	5.1732420	C	8.0277520	-1.4108030	7.8511080

H	7.8750550	-1.4016910	8.9324150	C	10.1005910	-2.3074260	2.5713500
H	8.4538060	-2.3811680	7.5846080	H	10.3812880	-3.1338110	3.2287320
H	7.0532740	-1.3167610	7.3696320	H	11.0039980	-1.8930960	2.1207550
C	8.3497220	1.0850390	7.6468070	H	9.4777410	-2.7124270	1.7704710
C	7.8814090	1.4094740	8.9229820	C	8.1978480	-0.1976660	1.3700280
H	7.9974850	0.6901850	9.7254990	H	7.7959290	-1.1786470	1.1460200
C	7.2689460	2.6261150	9.1817020	C	7.8746800	0.8792370	0.5578870
H	6.9144090	2.8566570	10.1784740	H	7.2281900	0.7372040	-0.2991850
C	7.1024130	3.5442390	8.1495170	C	8.3738740	2.1430030	0.8489620
H	6.6146090	4.4899500	8.3503890	H	8.1098310	2.9787060	0.2137890
C	7.5554600	3.2653270	6.8642240	C	9.2066650	2.3492680	1.9475300
C	7.4342710	4.2756410	5.7398280	C	9.7753540	3.7253700	2.2412920
H	7.4198350	3.7088250	4.8060030	H	10.0418170	3.7560820	3.2989760
C	6.1592690	5.1184730	5.8098560	C	11.0504160	3.9493510	1.4150340
H	6.1800990	5.8121310	6.6536990	H	11.7725330	3.1485030	1.5810080
H	5.2727520	4.4894450	5.9048380	H	11.5113500	4.9073200	1.6691730
H	6.0624520	5.7169310	4.9011040	H	10.8053930	3.9594920	0.3496890
C	8.6696510	5.1867320	5.7262930	C	8.7737680	4.8553620	1.9878060
H	8.7269310	5.7534810	6.6592620	H	9.1920540	5.8015770	2.3375760
H	8.6216520	5.8950580	4.8953900	H	7.8330520	4.6775260	2.5121680
H	9.5882000	4.6037150	5.6320920	H	8.5577330	4.9706190	0.9235170
C	8.2045160	2.0379200	6.6220800	C	14.4197490	2.7833920	4.0113320
C	9.8854630	1.7068350	5.0992960	H	13.7446180	3.2640340	3.3000470
H	10.6320980	1.8583080	5.8803530	H	15.4427050	2.8752640	3.6429820
C	9.5397540	1.2409190	2.7402200	H	14.3423890	3.3068180	4.9647910
C	9.0310100	-0.0356030	2.4779780	C	14.0354450	1.3227290	4.2277370
C	9.3476400	-1.2286700	3.3581540	C	14.9898090	0.6609380	5.2052880
H	9.9985520	-0.8917230	4.1667070	H	15.0752110	1.2775080	6.1009020
C	8.0697570	-1.7887990	3.9940500	H	15.9822130	0.5622170	4.7593780
H	7.5338330	-1.0027350	4.5284970	H	14.6324740	-0.3241110	5.5000670
H	8.3131310	-2.5901220	4.6963130	C	13.8228700	0.5474330	2.8910120
H	7.4032580	-2.2005800	3.2325500	C	14.7301810	0.9795090	1.7529930

H	14.5062710	0.3841770	0.8671410	H	13.5297140	-1.4390270	2.1527620
H	15.7775460	0.8208180	2.0202590	B	11.8382210	1.2141240	3.7315210
H	14.5812180	2.0294500	1.5061020				
C	13.8759170	-0.9661820	3.0723290				
H	13.2237600	-1.2829870	3.8890930				
H	14.8918700	-1.3065690	3.2788140				

Table S4. DFT computed energies (hartrees) for *i*PrCDI reaction.

Compound	(HBBN) ₂	HBpin	<i>i</i> PrCDI	I	TS1	2	II	TS2	III	TS3	IV	1aA	1a
E_{elec}	-677.4056798	-411.8154149	-384.5936098	-723.3046049	-723.2835024	-723.3649732	-1135.186035	-1135.183497	-1135.207398	-1135.200594	-1135.200755	-796.4820714	-796.4973398
G_{gas}	-676.996354	-411.653109	-384.424133	-722.91733	-722.898767	-722.974837	-1134.612314	-1134.607319	-1134.626456	-1134.619045	-1134.621195	-796.122775	-796.137887
H_{gas}	-676.935966	-411.610136	-384.373035	-722.848682	-722.83029	-722.905029	-1134.519207	-1134.517955	-1134.540433	-1134.534223	-1134.53327	-796.050851	-796.065991

Table S5. DFT computed energies (hartrees) for DippCDI reaction.

Compound	(HBBN) ₂	HBpin	DippCDI	I	TS1	2	II	TS2	III	TS3	IV	1eA	1e
E_{elec}	-677.4056798	-411.8154149	-1082.518723	-1421.222891	-1421.20367	-1421.294026	-1833.119253	-1833.111443	-1833.130564	-1833.11908	-1833.122147	-1494.411568	-1494.420238
G_{gas}	-676.996354	-411.653109	-1082.031762	-1420.516885	-1420.501782	-1420.586099	-1832.228013	-1832.215591	-1832.231589	-1832.220083	-1832.225097	-1493.737319	-1493.744498
H_{gas}	-676.935966	-411.610136	-1081.942663	-1420.411628	-1420.39483	-1420.479293	-1832.097552	-1832.090378	-1832.108787	-1832.097711	-1832.099726	-1493.625359	-1493.633967

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