Supporting Information

Syntheses, formation mechanisms and structures of a series of linear diborazanes

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Table of Contents

1. Synthesis of diborazanes........4
2. Supporting results........11
Table S1 The reactions of ADB with alkylamines. 11
Figure S1 Predicted pathways of the reaction between ADB and NH_3 based on density functional theory (DFT) calculations. 12
Table S2a The relative energies {Δ(E+ZPE)/(kcal·mol^{-1})}, enthalpies {ΔH (298 K)/(kcal·mol^{-1})}, free energy changes {ΔG (298 K)/(kcal·mol^{-1})} and entropy {S (298 K)(cal·mol-1)} for the reactions of ADB with alkylamines. 13
Table S2b The calculated rate constants (ml·mol^{-1}·s^{-1}) of the reactions of ADB with alkylamines. 14
Figure S2 Energy profile of the reaction of ADB with alkylamines. 15
Table S3 The nomenclature of the diborazanes........15
Table S4 FTIR spectra assignments of the diborazanes. 16
Figure S3a ^{11}B NMR spectra of **1a** in THF-d_8. 17
Figure S3b ^{1}H{^{11}B} NMR spectra of **1a** in THF-d_8. 17
Figure S3c ^{13}C{^{1}H} NMR spectra of **1a** in THF-d_8. 17
Figure S3d ^{11}B NMR spectra of **1b** in THF-d_8........18
Figure S3e ^{1}H{^{11}B} NMR spectra of **1b** in THF-d_8. 18
Figure S3f ^{13}C{^{1}H} NMR spectra of **1b** in THF-d_8. 18
Figure S3g ^{11}B NMR spectra of **1c** in THF-d_8. 19
Figure S3h ^{1}H{^{11}B} NMR spectra of **1c** in THF-d_8. 19
Figure S3i ^{13}C{^{1}H} NMR spectra of **1c** in THF-d_8. 19
Figure S3j ^{11}B NMR spectra of **2a** in THF-d_8........20
Figure S3k ^{1}H{^{11}B} NMR spectra of **2a** in THF-d_8. 20
Figure S3l ^{13}C{^{1}H} NMR spectra of **2a** in THF-d_8........20
Figure S3m ^{11}B NMR spectra of **2c** in THF-d_8. 21
Figure S3n ^{1}H{^{11}B} NMR spectra of **2c** in THF-d_8. 21
Figure S3o ^{13}C{^{1}H} NMR spectra of **2c** in THF-d_8. 21
Figure S3p ^{11}B NMR spectra of **3a** in THF-d_8. 22
Figure S3q ^{1}H{^{11}B} NMR spectra of **3a** in THF-d_8. 22
Figure S3r ^{13}C{^{1}H} NMR spectra of **3a i**n THF-d_8. 22
Figure S3s ^{11}B NMR spectra of **3c** in THF-d_8. 23
Figure S3t ^{1}H{^{11}B} NMR spectra of **3c** in THF-d_8. 23
Figure S3u ^{13}C{^{1}H} NMR spectra of **3c** in THF-d_8. 23
Figure S3v ^{11}B NMR spectra of **3d** in THF-d_8........24
Figure S3w ^{1}H{^{11}B} NMR spectra of **3d** in THF-d_8........24
Figure S3x ^{13}C{^{1}H} NMR spectra of **3d** in THF-d_8. 24
Figure S3y X-ray powder diffraction data of **1a.** 25
Figure S3z X-ray powder diffraction data of **1b**. 25
Figure S3aa X-ray powder diffraction data of **1c**. 26
Figure S3ab X-ray powder diffraction data of **2a**. 26
Figure S3ac X-ray powder diffraction data of **3a**........27

Figure S3ad X-ray powder diffraction data of **3c**..27
Figure S3ae X-ray powder diffraction data of **3d.** 28
Figure S4 The ^{11}B NMR chemical shift of the diborazanes...28
Table S5 The experiment and calculated chemical shifts of B in the diborazanes.........................29
Table S6 The chemical shifts of H in the diborazanes. 30
Table S7 Bond angles and dihedral angles of the diborazanes...31
Table S8 Bond lengths of the diborazanes. 31
Table S9 The inter-/intramolecular DHBs and hydrogen bond (HB) of the diborazanes.* 32
Figure S5a Intermolecular DHBs of **1a**. 33
Figure S5b Intramolecular DHBs of **1a** 33
Figure S5c Intermolecular DHBs of **1b**. 34
Figure S5d Intramolecular DHBs of **1b**. 34
Figure S5e Intermolecular DHBs of 1c...35
Figure S5f Intramolecular DHBs of 1c. 35
Figure S5g Intermolecular DHBs of $C_{12}H_{24}O_6$·2a. 36
Figure S5h Intramolecular DHBs of $C_{12}H_{24}O_6$·2a. 36
Figure S5i Intermolecular DHBs of 2c. 37
Figure S5j Intramolecular DHBs of 2c 37
Figure S5k Intermolecular DHBs of C_4H_8O·3c. 38
Figure S5l Intramolecular DHBs of C_4H_8O·3c. 38
Figure S5m Intermolecular DHBs of 3d. 39
Figure S5n Intramolecular DHBs of 3d 39
Figure S6a The NPA value and CPs of mono-molecule **1a**, **1b** and **1c**. 40
Figure S6b The CPs of **1a** intermolecular DHB interaction. 40
Figure S6c The BCPs of **1b** intermolecular DHB interaction...41
Figure S6d The BCPs of **1c** intermolecular DHB interaction. 41
Figure S6e The NPA value and BCPs of mono-molecule **2a** and **2c**. 42
Figure S6f The BCPs of **2a** intermolecular DHB interaction..42
Figure S6g The BCPs of **2c** intermolecular DHB interaction 43
Figure S6h The NPA value and BCPs of mono-molecule **3c** and **3d** 44
Figure S6i The BCPs of **3c** intermolecular DHB interaction. 45
Figure S6j The BCPs of **3d** intermolecular DHB interaction 45
Table S10 The energy difference (ΔE) of *anti* configuration and *gauch* configuration of the diborazanes. 46
Table S11 The melting points of the diborazanes and the isoelectronic analogs. 46
3. The optimized cartesian coordinates of all species...47

1. Synthesis of diborazanes

Synthesis of $Me_2NHBH_2NH_2BH_3$ (1b)

1b was prepared in the same way as compound **1a**. The reaction was completed as soon as Me_2NH was dropped into ADB solution and a clear solution was obtained. The clear solution was kept in a refrigerator at -10 °C, and colorless transparent block crystals were obtained. The yield/conversion (%) of **1b** are 68/100. ^{11}B NMR (d_8-THF, 128 MHz, δ) -4.0 (t, $B1H_2$, $J_{B\text{-}H}$ = 104 Hz), -21.9 (*q*, $B2H_3$, $J_{B\text{-}H}$ = 87 Hz). $^{11}B\{^1H\}$ NMR (d_8-THF, 128 MHz, δ) -4.0 (*s*, $B1H_2$), -21.9 (*s*, $B2H_3$). ^1H NMR (d_8-THF, 400 MHz, δ) 5.3 (*br*, H of N1H), 2.5 (*br*, 2H of $N2H_2$), 2.3 (*d*, 6H of $C1H_3$ and $C2H_3$, $J_{H\text{-}H}$ = 6 Hz), 1.8 (*q*, 2H of $B1H_2$), 1.2 (*q*, 3H of $B2H_3$, $J_{B\text{-}H}$ = 4 Hz). $^1H\{^{11}B\}$ NMR (d_8-THF, 400 MHz, δ) 5.3 (*br*, H of N1H), 2.5 (*br*, 2H of $N2H_2$), 2.3 (d, 6H of $C1H_3$ and $C2H_3$, $J_{H\text{-}H}$ = 6 Hz), 1.8 (*q*, 2H of $B1H_2$, $^3J_{H\text{-}H}$ = 4 Hz), 1.2 (*t*, 3H of $B2H_3$, $^3J_{H\text{-}H}$ = 4 Hz). $^{13}C\{^1H\}$ NMR (d_8-THF, 400 MHz, δ) 39.6 (*s*, CH_3). Anal. Calcd for $C_2H_{14}B_2N_2$ (87.77): C, 27.37; H, 16.08; N, 31.92. Found: C, 27.61; H, 16.42; N, 32.10.

Synthesis of $Me_3NBH_2NH_2BH_3$ (1c)

1c was prepared in the same way as compound **1a**. The reaction was completed as soon as Me_3N was dropped into ADB solution and white precipitation was obtained. The yield/conversion (%) are 67/100. The white precipitation was re-dissolved by more THF, and kept in a refrigerator at -10 °C, and colorless transparent block crystals were obtained. ^{11}B NMR (d_8-THF, 128 MHz, δ) -1.34 (*t*, $B1H_2$, $J_{B\text{-}H}$ = 109.40 Hz), -20.44 (*q*, $B2H_3$, $J_{B\text{-}H}$ = 88.10 Hz). $^{11}B\{^1H\}$ NMR (d_8-THF, 128 MHz, δ) -1.3 (*s*, $B1H_2$), -20.4 (*s*, $B2H_3$). ^1H NMR (d_8-THF, 400 MHz, δ) 2.6 (*br*, 2H of $N2H_2$), 2.5 (*s*, 9H of $C1H_3$, $C2H_3$ and $C3H_3$), 1.9 (*q*, 2H of $B1H_2$), 1.2 (*q*, 3H of $B2H_3$, $J_{B\text{-}H}$ = 4 Hz). $^1H\{^{11}B\}$ NMR (d_8-THF, 400 MHz, δ) 2.6 (*br*, 2H of $N2H_2$), 2.5 (*s*, 9H of $C1H_3$, $C2H_3$

and C3H$_3$), 1.9 (*t*, 2H of B1H$_2$, $^3J_{H\text{-}H}$ = 5 Hz), 1.2 (*t*, 3H of B2H$_3$, $^3J_{H\text{-}H}$ = 4 Hz). ^{13}C{^{1}H} NMR (*d*$_8$-THF, 400 MHz, δ) 49.6 (*s*, CH$_3$). Anal. Calcd for $C_3H_{16}B_2N_2$ (101.80): C, 35.39; H, 15.84; N, 27.70. Found: C, 35.57; H, 16.20; N, 27.40.

Synthesis of EtNH$_2$BH$_2$NH$_2$BH$_3$ (2a)

2a was prepared in the same way as compound **1a**. The reaction was completed as soon as EtNH$_2$ was dropped into ADB solution and a clear solution was obtained. The clear solution was kept in a refrigerator at -10 ^{o}C, and colorless transparent block crystals were obtained. While the crystal is not suitable for X-Ray analysis. The yield/conversion (%) of **2a** are 68/100. ^{11}B NMR (*d*$_8$-THF, 128 MHz, δ) -8.3 (*t*, B1H$_2$, $J_{B\text{-}H}$ = 104 Hz), -21.8 (*q*, B2H$_3$, $J_{B\text{-}H}$ = 94 Hz). ^{11}B{^{1}H} NMR (*d*$_8$-THF, 128 MHz, δ) -8.3 (*s*, B1H$_2$), -21.8 (*s*, B2H$_3$). ^{1}H NMR (*d*$_8$-THF, 400 MHz, δ) 4.9 (*br*, 2H of N1H$_2$), 2.6 (*m*, 2H of C1H$_2$), 2.4 (*br*, 2H of N2H$_2$), 1.9 (*q*, 2H of B1H$_2$), 1.2 (*q*, 3H of B2H$_3$), 1.1 (*t*, 3H of C2H$_3$, $J_{H\text{-}H}$ = 7 Hz). ^{1}H{^{11}B} NMR (*d*$_8$-THF, 400 MHz, δ) 4.9 (*br*, 2H of N1H$_2$), 2.6 (*m*, 2H of C1H$_2$), 2.4 (*br*, 2H of N2H$_2$), 1.90 (*quint*, 2H of B1H$_2$, $^3J_{H\text{-}H}$ = 4 Hz), 1.2 (*t*, 3H of B2H$_3$, $^3J_{H\text{-}H}$ = 4 Hz), 1.1 (*t*, 3H of C2H$_3$, $J_{H\text{-}H}$ = 7 Hz). ^{13}C{^{1}H} NMR (*d*$_8$-THF, 400 MHz, δ) 39.0 (*s*, C1H$_2$), 13.3 (*s*, C2H$_3$). Anal. Calcd for $C_2H_{14}B_2N_2$ (87.77): C, 27.37; H, 16.08; N, 31.92. Found: C, 27.64; H, 16.45; N, 32.15.

We utilized 18-crown-6 ether to bind **2a** by weak hydrogen bonds. A 10 mL THF solution of **2a** (0.088g, 1 mmol) was prepared and 0.185 g (0.7 mmol) of 18-crown-6 was added to the solution in a dry box. The mixture was stirred for 5 min and filtered. The clear solution was kept in a refrigerator at -10 ^{o}C, and colorless transparent block crystals ($C_{12}H_{24}O_6$·**2a**) were obtained. ^{11}B NMR (*d*$_8$-THF, 128 MHz, δ) -8.3 (*t*, B1H$_2$, $J_{B\text{-}H}$ = 104 Hz), -21.0 (*q*, B2H$_3$, $J_{B\text{-}H}$ = 94 Hz). ^{11}B{^{1}H} NMR (*d*$_8$-THF, 128 MHz, δ) -8.3 (*s*, B1H$_2$), -21.8 (*s*, B2H$_3$). ^{1}H NMR (*d*$_8$-THF, 400 MHz, δ) 4.9 (*br*, 2H of N1H$_2$), 3.5 (*s*, 24H of CH_2, 18-C-6), 2.6 (*m*, 2H of $C1H_2$), 2.4 (*br*, 2H of $N2H_2$), 1.9 (*q*, 2H of $B1H_2$), 1.2 (*q*, 3H of $B2H_3$), 1.1 (*t*, 3H of $C2H_3$, $J_{H\text{-}H}$ = 7 Hz). $^1H\{^{11}B\}$ NMR (d_8-THF, 400 MHz, δ) 4.9 (*br*, 2H of $N1H_2$), 3.5 (*s*, 24H of CH_2, 18-C-6), 2.6 (*m*, 2H of $C1H_2$), 2.4 (*br*, 2H of $N2H_2$), 1.9 (*quint*, 2H of $B1H_2$, $^3J_{H\text{-}H}$ = 4 Hz), 1.2 (*t*, 3H of $B2H_3$, $^3J_{H\text{-}H}$ = 4 Hz), 1.1 (*t*, 3H of $C2H_3$, $J_{H\text{-}H}$ = 7 Hz). $^{13}C\{^1H\}$ NMR (d_8-THF, 400 MHz, δ) 70.6 (*s*, CH_2 of 18-Crown-6), 39.0 (*s*, $C1H_2$), 13.3 (*s*, $C2H_3$).

Synthesis of $Et_2NHBH_2NH_2BH_3$ (2b)

2b was prepared in the same way as compound **1a**. The reaction was completed as soon as Et_2NH was dropped into ADB solution and a clear solution was obtained. Several crystal growing techniques had been tried to prepare **2b** crystal, no crystal had been obtained yet. The product was characterized by its solution of THF. ^{11}B NMR (d_8-THF, 128 MHz, δ) -7.1 (*t*, $B1H_2$, $J_{B\text{-}H}$ = 107 Hz), -21.3 (*q*, $B2H_3$, $J_{B\text{-}H}$ = 91 Hz).

Synthesis of $Et_3NBH_2NH_2BH_3$ (2c)

2c was prepared in the same way as compound **1a**. The reaction was completed as soon as Et_3N was dropped into ADB solution and a clear solution was obtained. The clear solution was kept in a refrigerator at -10 ^{o}C, and colorless transparent block crystals were obtained. The yield/conversion (%) of **2c**, are 67/100. ^{11}B NMR (d_8-THF, 128 MHz, δ) -6.0 (*t*, $B1H_2$, $J_{B\text{-}H}$ = 102 Hz), -20.2 (*q*, $B2H_3$, $J_{B\text{-}H}$ = 85 Hz), -27.4 (br, *t*, $NH_2B_2H_5$). $^{11}B\{^1H\}$ NMR (d_8-THF, 128 MHz, δ) -6.0 (*s*, $B1H_2$), -20.2 (*s*, $B2H_3$), -27.4 (*s*, $NH_2B_2H_5$). ^1H NMR (d_8-THF, 400 MHz, δ) 3.9 (*br t*, 2H of NH_2, $J_{N\text{-}H}$ = 53 Hz), 2.8 (*q*, 6H of CH_2, $J_{H\text{-}H}$ = 7 Hz), 2.9 (*q*, 6H of CH_2, $J_{H\text{-}H}$ = 7 Hz), 2.4 (*br*, 2H of NH_2), 2.2 (*t*, 2H, $J_{H\text{-}H}$ = 7 Hz), 1.8 (*q*, 2H of BH_2), 1.3 (*q*, 3H of BH_3), 1.0 (*t*, 9H of CH_3, $J_{H\text{-}H}$ = 7 Hz), 0.9 (*t*, 9H of CH_3, $J_{H\text{-}H}$ = 7 Hz). $^1H\{^{11}B\}$ NMR (d_8-THF, 400 MHz, δ) 3.9 (*br t*, 2H of NH_2, $J_{N\text{-}H}$ = 53 Hz), 2.8 (*q*, 6H of CH_2, $J_{H\text{-}H}$ = 7 Hz), 2.8 (*q*, 6H of CH_2, $J_{H\text{-}H}$ = 7 Hz), 2.4 (*br*, 2H of NH_2), 2.2 (*t*, 2H, $J_{H\text{-}H}$ = 7 Hz), 1.8 (*t*, 2H of BH_2,

$^{3}J_{H\text{-}H}$ = 5 Hz), 1.3 (*t*, 3H of BH_3, $^{3}J_{H\text{-}H}$ = 4 Hz), 1.0 (*t*, 9H of CH_3, $J_{H\text{-}H}$ = 7 Hz), 0.9 (*t*, 9H of CH_3, $J_{H\text{-}H}$ = 7 Hz). $^{13}C\{^{1}H\}$ NMR (d_8-THF, 400 MHz, δ) 48.4 (*s*, $C1H_2$), 46.4 (*s*, CH_2 of $N(\underline{CH_2}CH_3)_3$), 11.7 (*s*, CH_3 of $N(CH_2\underline{CH_3})_3$), 7.3(*s*, $C2H_3$). Anal. Calcd for $C_6H_{22}B_2N_2$ (143.88): C, 50.08; H, 15.52; N, 19.48. Found: C, 50.25; H, 15.55; N, 19.34.

Synthesis of $^{n}PrNH_2BH_2NH_2BH_3$ (3a)

3a was prepared in the same way as compound **1a**. The reaction was completed as soon as $^{n}PrNH_2$ was dropped into ADB solution and a clear solution was obtained. The clear solution was kept in a refrigerator at -10 °C, and colorless transparent block crystals were obtained. The yield/conversion (%) of **3a** are 68/100. Several crystal growing techniques had been tried to prepare 2b crystal, no crystal had been obtained yet. ^{11}B NMR (d_8-THF, 128 MHz, δ) -8.61 (*t*, $B1H_2$, $J_{B\text{-}H}$ = 106.50 Hz), -22.34 (*q*, $B2H_3$, $J_{B\text{-}H}$ = 95.20 Hz). $^{11}B\{^{1}H\}$ NMR (d_8-THF, 128 MHz, δ) -8.61 (*s*, $B1H_2$), -22.34 (*s*, $B2H_3$). ^{1}H NMR (d_8-THF, 400 MHz, δ) 4.88 (*br*, 2H of $N1H_2$), 2.51 (*m*, 2H of $C1H_2$), 2.38 (*br*, 2H of $N2H_2$), 1.90 (*q*, 2H of $B1H_2$), 1.61 (*m*, 2H of $C2H_2$), 1.20 (*q*, 3H of $B2H_3$), 0.85 (*t*, 3H of $C3H_3$, $J_{H\text{-}H}$ = 7.50 Hz). $^{1}H\{^{11}B\}$ NMR (d_8-THF, 400 MHz, δ) 4.88 (*br*, 2H of $N1H_2$), 2.51 (*m*, 2H of $C1H_2$), 2.38 (*br*, 2H of $N2H_2$), 1.90 (*quint*, 2H of $B1H_2$, $^{3}J_{H\text{-}H}$ = 4.00 Hz), 1.61 (*m*, 2H of $C2H_2$), 1.20 (*t*, 3H of $B2H_3$, $^{3}J_{H\text{-}H}$ = 4.50 Hz), 0.85 (*t*, 3H of $C3H_3$, $J_{H\text{-}H}$ = 7.50 Hz). $^{13}C\{^{1}H\}$ NMR (d_8-THF, 400 MHz, δ) 44.04 (*s*, $C1H_2$), 20.06 (*s*, $C2H_2$), 8.64 (*s*, $C3H_3$). Anal. Calcd for $C_3H_{16}B_2N_2$ (101.80): C, 35.39; H, 15.84; N, 27.53. Found: C, 35.58; H, 16.18; N, 27.18.

Synthesis of $^{n}Pr_2NHBH_2NH_2BH_3$ (3b)

3b was prepared in the same way as compound **1a**. The reaction was completed as soon as $^{n}Pr_2NH$ was dropped into ADB solution and a clear solution was obtained. The solvent THF was evaporated under a dynamic vacuum to leave a wax. Several crystal growing techniques had been tried to prepare **3b** crystal, no crystal had been obtained yet. The product was characterized by its solution of THF. ^{11}B NMR (d_8-THF, 128 MHz, δ) -6.65 (*t*, B1H_2, J_{B-H} = 94.65 Hz), -21.58 (*q*, B2H_3, J_{B-H} = 90.90 Hz).

Synthesis of ^{n}Pr$_3$NBH$_2$NH$_2$BH$_3$ (3c)

3c was prepared in the same way as compound **1a**. The reaction was completed as soon as ^{n}Pr$_3$N was dropped into ADB solution and a clear solution was obtained. The clear solution was kept in a refrigerator at -10 ^{o}C, and colorless transparent block crystals (C_4H_8O·**3c**)were obtained. The yield/conversion (%) of **3c**, are 67/93. ^{11}B NMR (d_8-THF, 128 MHz, δ) -4.49 (*t*, B1H_2, J_{B-H} = 99.66 Hz), -19.68 (*q*, B2H_3, J_{B-H} = 88.2 Hz), -27.43 (br, *t*, $NH_2B_2H_5$). ^{11}B{^{1}H} NMR (d_8-THF, 128 MHz, δ) -4.49 (*s*, B1H_2), -19.68 (*s*, B2H_3), -27.43 (*s*, $NH_2B_2H_5$). ^{1}H NMR (d_8-THF, 400 MHz, δ) 3.90 (*br t*, 2H of NH_2, $NH_2B_2H_5$, J_{N-H} = 52.91 Hz), 3.51 (*m*, 4α-H of THF), 2.65 (*m*, 6H of C1H_2), 2.40 (*br*, 2H of N2H_2), 2.21 (*t*, 6H of C1H_2, J_{H-H} = 7.01 Hz), 1.86 (*q*, 2H of B1H_2), 1.67 (*m*, 4*β*-H of THF), 1.64 (*m*, 6H of C2H_2), 1.31 (*sext*, 6H of C2H_2, J_{H-H} = 7.88 Hz), 1.28 (*q*, 3H of B2H_3), 0.77 (*m*, 18H of C3H_3). ^{1}H{^{11}B} NMR (d_8-THF, 400 MHz, δ) 3.90 (*br t*, 2H of NH_2, $NH_2B_2H_5$, J_{N-H} = 52.91 Hz), 3.51 (*m*, 4α-H of THF), 2.65 (*m*, 6H of C1H_2), 2.40 (*br*, 2H of N2H_2), 2.21 (*t*, 6H of C1H_2, J_{H-H} = 7.01 Hz), 1.86 (*t*, 2H of B1H_2, $^3J_{H-H}$ = 4.56 Hz), 1.67 (*m*, 4*β*-H of THF), 1.64 (*m*, 6H of C2H_2), 1.31 (*sext*, 6H of C2H_2, J_{H-H} = 7.88 Hz), 1.28 (*t*, 3H of B2H_3), 0.77 (*m*, 18H of C3H_3). ^{13}C{^{1}H} NMR (d_8-THF, 400 MHz, δ) 67.23 (*s*, CH_2 of THF), 57.11 (*s*, CH_2 of $N(\underline{CH_2}CH_2CH_3)_3$), 56.25 (*s*, C1$H_2$), 25.13 (*s*, CH_2 of THF), 20.62 (*s*, C2H_2), 15.53 (*s*, CH_2 of $N(CH_2\underline{CH_2}CH_3)_3$), 11.22 (*s*, C3$H_3$), 10.71 (*s*, CH_3 of $N(CH_2CH_2\underline{CH_3})_3$). Anal. Calcd for $C_9H_{28}B_2N_2$ (185.95): C, 58.37; H, 15.56; N, 15.27. Found: C, 58.37; H, 15.56; N, 15.27.

Synthesis of $^{i}PrNH_2BH_2NH_2BH_3$ (3d)

3d was prepared in the same way as compound **1a**. The reaction was completed as soon as $^{i}PrNH_2$ was dropped into ADB solution and a clear solution was obtained. The clear solution was kept in a refrigerator at -10 °C, and colorless transparent block crystals were obtained. The yield/conversion (%) of **3d** are 67/100. ^{11}B NMR (d_8-THF, 128 MHz, δ) -10.27 (*t*, $B1H_2$, $J_{B\text{-}H}$ = 104.3 Hz), -22.85 (*q*, $B2H_3$, $J_{B\text{-}H}$ = 92.97 Hz). $^{11}B\{^1H\}$ NMR (d_8-THF, 128 MHz, δ) -10.27 (*s*, $B1H_2$), -22.85 (*s*, $B2H_3$). ^1H NMR (d_8-THF, 400 MHz, δ) 4.86 (*br*, 2H of $N1H_2$), 2.92 (*m*, H of C1H), 2.34 (*br*, 2H of $N2H_2$), 1.94 (*q*, 2H of $B1H_2$), 1.20 (*q*, 3H of $B2H_3$), 1.11 (*t*, 6H of $C2H_3$ and $C3H_3$, $J_{H\text{-}H}$ = 6.5 Hz). $^1H\{^{11}B\}$ NMR (d_8-THF, 400 MHz, δ) 4.86 (*br*, 2H of NH_2), 2.92 (*m*, H of C1H), 2.34 (*br*, 2H of $N2H_2$), 1.94 (*quint*, 2H of $B1H_2$, $^3J_{H\text{-}H}$ = 4.29 Hz), 1.20 (*t*, 3H of $B2H_3$, $^3J_{H\text{-}H}$ = 4.5 Hz), 1.11 (*t*, 6H of $C2H_3$ and $C3H_3$, $J_{H\text{-}H}$ = 6.5 Hz). $^{13}C\{^1H\}$ NMR (d_8-THF, 400 MHz, δ) 46.17 (*s*, $C1H_2$), 20.74 (*s*, $C2H_3$ and $C3H_3$). Anal. Calcd for $C_3H_{16}B_2N_2$ (101.80): C, 35.39; H, 15.84; N, 27.53. Found: C, 35.54; H, 16.10; N, 27.18.

Synthesis of $^{i}Pr_2NHBH_2NH_2BH_3$ (3e)

3e was prepared in the same way as compound **1a**. The reaction was completed as soon as $^{i}Pr_2NH$ was dropped into ADB solution and a clear solution was obtained. The THF solution of **3e** was subjected to fractional distillation to remove the excess solvent to further purify the products, but only a wax was obtained, and no crystal had been obtained yet. The product was characterized by its solution of THF. ^{11}B NMR (d_8-THF, 128 MHz, δ) -9.80 (*t*, $B1H_2$, $J_{B\text{-}H}$ = 110.80 Hz), -22.27 (*q*, $B2H_3$, $J_{B\text{-}H}$ = 92.70 Hz).

Synthesis of $^{i}Pr_2MeNBH_2NH_2BH_3$ (3f)

3f was tried to be prepared in the same way as compound **1a**. A very slow reaction occurred when iPr$_2$Me was dropped into the ADB solution of THF at room temperature. The conversion was only 0.60% after 24 h. The product was characterized by its solution of THF. ^{11}B NMR (d_8-THF, 128 MHz, δ) -11.50 (t, B1H$_2$, J_{B-H} = 88.22 Hz), -22.20 (q, B2H$_3$, J_{B-H} = 97.51 Hz).

Synthesis of ^{i}Pr$_2$EtNBH$_2$NH$_2$BH$_3$ (3g)

3g was tried to be prepared in the same way as compound **1a**. No reaction occurred when ^{i}Pr$_2$Et was dropped into the ADB solution at room temperature.

2. Supporting results

Table S1 The reactions of ADB with alkylamines.

Entry	alkylamines	Reaction speed*	Product		Yield[a]/conversion[b] (%)
1	$MeNH_2$	fast	$MeNH_2BH_2NH_2BH_3$ (**1a**)	white powder	68/100
2	Me_2NH	fast	$Me_2NHBH_2NH_2BH_3$ (**1b**)	white powder	68/100
3	Me_3N	fast	$Me_3NBH_2NH_2BH_3$ (**1c**)	white powder	67/100
4	$EtNH_2$	fast	$EtNH_2BH_2NH_2BH_3$ (**2a**)	white powder	68/100
5	Et_2NH	fast	$Et_2NHBH_2NH_2BH_3$ (**2b**)	wax	-[c]/100
6	Et_3N	fast	$Et_3NBH_2NH_2BH_3$ (**2c**)	white powder	67/100
7	$^nPrNH_2$	fast	$^nPrNH_2BH_2NH_2BH_3$ (**3a**)	white powder	68/100
8	$^nPr_2NH$	fast	$^nPr_2NHBH_2NH_2BH_3$ (**3b**)	wax	-/100
9	$^nPr_3N$	fast	$^nPr_3NBH_2NH_2BH_3$ (**3c**)	white powder	67/93
10	$^iPrNH_2$	fast	$^iPrNH_2BH_2NH_2BH_3$ (**3d**)	white powder	67/100
11	$^iPr_2NH$	fast	$^iPr_2NHBH_2NH_2BH_3$ (**3e**)	wax	-[c]/100
12	$^iPr_2MeN$	slow	$^iPr_2MeNBH_2NH_2BH_3$ (**3f**)	-[c]	-[c]/0.6
13	$^iPr_2EtN$	NR	-	-	-

*Fast: the reaction was completed as soon as alkylamine was added to ADB solution.

*Slow: the reaction of $^iPr_2MeN$ with ADB is very slow, only 0.6 % of $^iPr_2MeNBH_2NH_2BH_3$ was formed after 24 h.

*NR: No Reaction.

a: isolated yield;

b: calculated by the resonance intensities of boron signals in the ^{11}B NMR spectra of the reaction mixture;

c: The product could not be isolated.

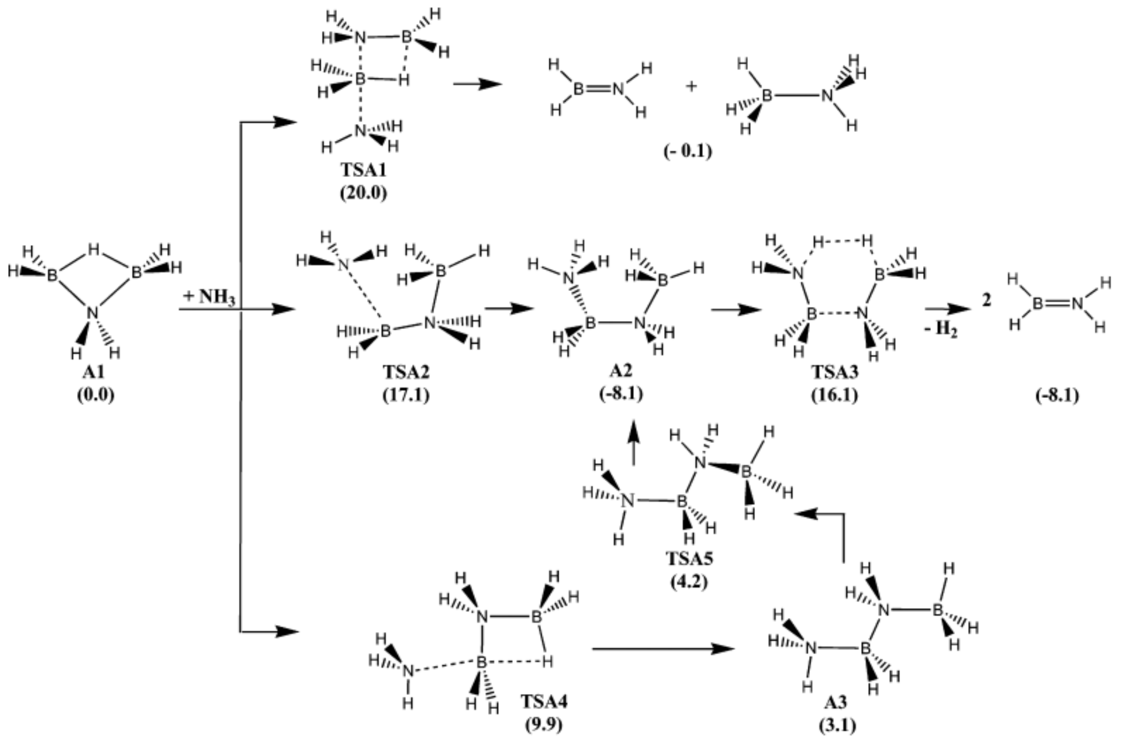


Figure S1 Predicted pathways of the reaction between ADB and NH_3 based on density functional theory (DFT) calculations (Inorg. Chem. 2007, 46, 7633−7645). Enthalpies (kcal/mol) are relative to ADB + NH_3 at 298.15 K. Pathway 1: A1 → TSA4 → A3; Pathway 2: A1 → TSA2 → A2. The reaction depicted in our manscript (reaction 1) ends the formation of the linear diborazanes without further reactions at room temperature.

Table S2a The relative energies {Δ(E+ZPE)/(kcal·mol^{-1})}, enthalpies {ΔH (298 K)/(kcal·mol^{-1})}, free energy changes {ΔG (298 K)/(kcal·mol^{-1})} and entropy {S (298 K)(cal·mol-1)} for the reactions of ADB with alkylamines.

Species	**Δ(*E* + ZPE)**	**Δ*H***	**Δ*G***	**S**
1) ADB + $MeNH_2$	0.0	0.0	0.0	119.9
TS1	4.7	4.5	14.8	85.6
P1	-18.4	-18.7	-8.1	84.3
2) ADB + Me_2NH	0.0	0.0	0.0	127.5
TS2	2.9	2.8	13.5	91.6
P2	-20.5	-20.8	-9.3	89.1
3) ADB + NMe_3	0.0	0.0	0.0	133.4
TS3	1.9	1.8	13.2	95.0
P3	-20.4	-20.6	-9.0	94.7
4) ADB + $EtNH_2$	0.0	0.0	0.0	127.3
TS4	4.5	4.4	14.7	92.8
P4	-18.8	-18.9	-8.1	91.2
5) ADB + Et_2NH	0.0	0.0	0.0	142.2
TS5	3.6	3.5	15.1	103.3
P5	-17.3	-17.9	-4.9	98.8
6) ADB + Et_3N	0.0	0.0	0.0	155.2
TS6	1.6	1.2	14.3	111.3
P6	-18.1	-18.9	-4.7	107.7
7) ADB + $PrNH_2$	0.0	0.0	0.0	135.2
TS7	5.0	4.9	15.5	99.7
P7	-18.3	-18.4	-7.7	99.3
8) ADB + Pr_2NH	0.0	0.0	0.0	157.8
TS8	3.4	3.3	14.6	119.7
P8	-17.0	-17.5	-4.7	115.1
9) ADB + Pr_3N	0.0	0.0	0.0	177.9
TS9	2.5	2.3	15.0	135.2
P9	-17.1	-17.5	-3.8	132.1
10) ADB + $^{i}PrNH_2$	0.0	0.0	0.0	133.9
TS10	5.2	5.1	16.0	97.5
P10	-17.9	-18.0	-6.9	96.8
11) ADB + $^{i}Pr_2NH$	0.0	0.0	0.0	153.8
TS11	1.9	1.8	13.7	114.1
P11	-17.6	-18.0	-5.3	111.2
12) ADB + $^{i}Pr_2MeN$	0.0	0.0	0.0	159.1
TS12	4.4	4.3	16.3	119.1
P12	-13.9	-14.5	-0.7	112.7
13) ADB + $^{i}Pr_2EtN$	0.0	0.0	0.0	164.2
TS13	9.4	9.3	21.5	123.2
P13	-8.4	-9.2	5.1	116.0

Table S2b The calculated rate constants (ml·mol^{-1}·s^{-1}) of the reactions of ADB with alkylamines.

T/K	240	250	278	288	298	308	325	375
k_1	5.97E-19	9.18E-19	2.66E-18	3.73E-18	5.13E-18	6.94E-18	1.12E-17	3.71E-17
k_2	1.12E-17	1.49E-17	3.00E-17	3.76E-17	4.67E-17	5.72E-17	7.93E-17	1.82E-16
k_3	2.45E-17	2.99E-17	4.95E-17	5.84E-17	6.83E-17	7.94E-17	1.01E-16	1.90E-16
k_4	6.82E-19	1.04E-18	2.94E-18	4.10E-18	5.60E-18	7.53E-18	1.20E-17	3.90E-17
k_5	5.76E-19	8.08E-19	1.88E-18	2.47E-18	3.19E-18	4.06E-18	5.97E-18	1.58E-17
k_6	5.24E-18	6.10E-18	8.99E-18	1.02E-17	1.16E-17	1.30E-17	1.58E-17	2.61E-17
k_7	1.47E-19	2.34E-19	7.35E-19	1.06E-18	1.49E-18	2.06E-18	3.44E-18	1.24E-17
k_8	2.63E-18	3.59E-18	7.83E-18	1.01E-17	1.28E-17	1.60E-17	2.29E-17	5.70E-17
k_9	9.59E-19	1.22E-18	2.25E-18	2.74E-18	3.31E-18	3.96E-18	5.27E-18	1.10E-17
k_{10}	2.07E-19	3.24E-19	9.88E-19	1.41E-18	1.97E-18	2.70E-18	4.46E-18	1.57E-17
k_{11}	1.16E-17	1.42E-17	2.37E-17	2.81E-17	3.29E-17	3.84E-17	4.91E-17	9.28E-17
k_{12}	5.18E-20	7.81E-20	2.17E-19	3.00E-19	4.09E-19	5.47E-19	8.70E-19	2.79E-18
k_{13}	9.26E-25	2.13E-24	1.64E-23	3.10E-23	5.66E-23	9.96E-23	2.42E-22	2.17E-21

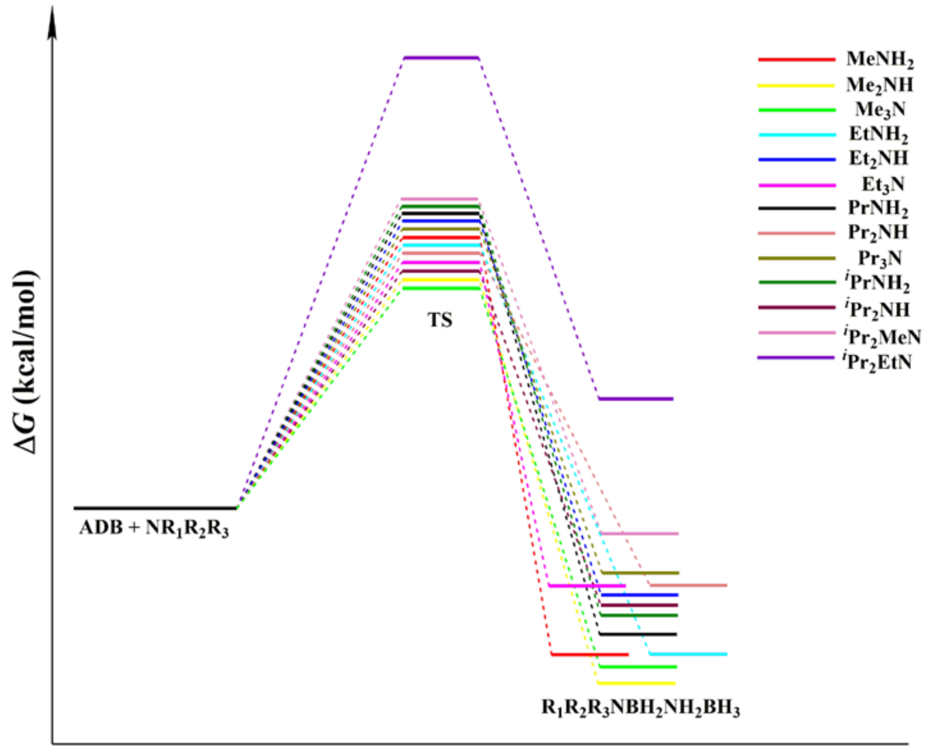


Figure S2 Energy profile of the reaction of ADB with alkylamines.

Table S3 The nomenclature of the diborazanes.

Diborazanes	Nomenclature
$MeNH_2BH_2NH_2BH_3$ (**1a**)	1-N-methyl-1,3-diaza-2,4-diborabutane analogue
$Me_2NHBH_2NH_2BH_3$ (**1b**)	1-N,N-dimethyl-1,3-diaza-2,4-diborabutane analogue
$Me_3NBH_2NH_2BH_3$ (**1c**)	1-N,N,N-trimethyl-1,3-diaza-2,4-diborabutane analogue
$EtNH_2BH_2NH_2BH_3$ (**2a**)	1-N-ethyl-1,3-diaza-2,4-diborabutane analogue
$Et_2NHBH_2NH_2BH_3$ (**2b**)	1-N,N-diethyl-1,3-diaza-2,4-diborabutane analogue
$Et_3NBH_2NH_2BH_3$ (**2c**)	1-N,N,N-triethyl-1,3-diaza-2,4-diborabutane analogue
$^nPrNH_2BH_2NH_2BH_3$ (**3a**)	1-N-propyl-1,3-diaza-2,4-diborabutane analogue
$^nPr_2NHBH_2NH_2BH_3$ (**3b**)	1-N,N-dipropyl-1,3-diaza-2,4-diborabutane analogue
$^nPr_3NBH_2NH_2BH_3$ (**3c**)	1-N,N,N-tripropyl-1,3-diaza-2,4-diborabutane analogue
$^iPrNH_2BH_2NH_2BH_3$ (**3d**)	1-N-isopropyl-1,3-diaza-2,4-diborabutane analogue
$^iPr_2NHBH_2NH_2BH_3$ (**3e**)	1-N,N-diisopropyl-1,3-diaza-2,4-diborabutane analogue
$^iPr_2MeNBH_2NH_2BH_3$ (**3f**)	1-N,N- methyl-diisopropyl-1,3-diaza-2,4-diborabutane analogue

Table S4 FTIR spectra assignments of the diborazanes.

Diborazanes	B-H (cm^{-1})	N-H (cm^{-1})	B-N (cm^{-1})	C-N (cm^{-1})
$MeNH_2HBH_2NH_2BH_3$ (**1a**)	2294.16	3297.80	1345.21	1151.03
$Me_2NHBH_2NH_2BH_3$ (**1b**)	2317.50	3277.49	1319.42	1159.62
$Me_3NBH_2NH_2BH_3$(**1c**)	2312.28	3299.97	1471.56	1148.88
$EtNH_2BH_2NH_2BH_3$(**2a**)	2298.47	3208.26	1353.24	1104.91
$Et_3NBH_2NH_2BH_3$(**2c**)	2284.00	3301.54	1396.90	1160.31
$^{n}PrNH_2BH_2NH_2BH_3$(**3a**)	2291.29	3291.46	1339.29	1142.13
$^{n}Pr_3NBH_2NH_2BH_3$(**3c**)	2282.76	3247.52	1380.89	1160.44
$^{i}PrNH_2BH_2NH_2BH_3$(**3d**)	2298.43	3298.06	1378.02	1164.90

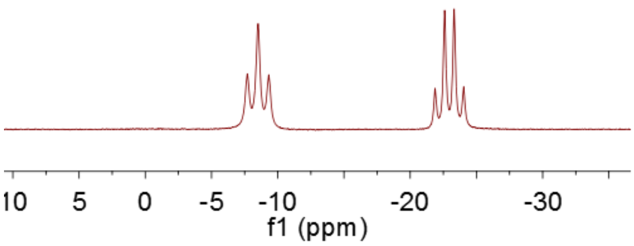


Figure S3a ^{11}B NMR spectra of **1a** in THF-d_8.

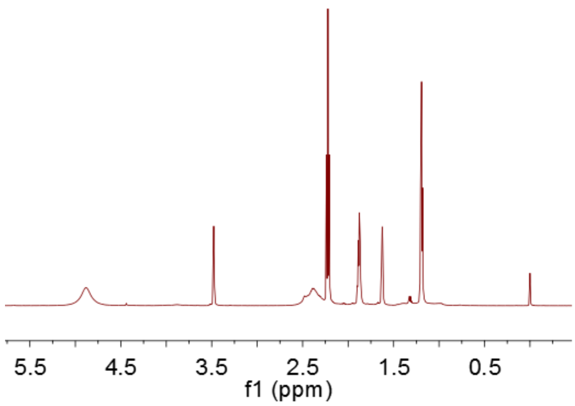


Figure S3b ^{1}H{^{11}B} NMR spectra of **1a** in THF-d_8.

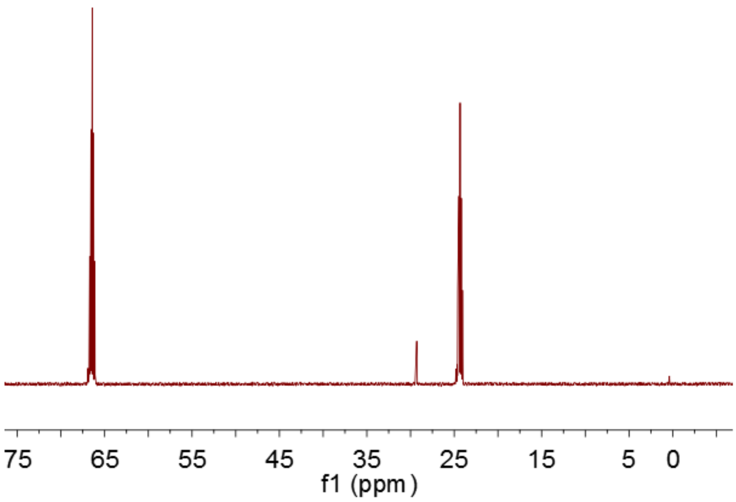


Figure S3c ^{13}C{^{1}H} NMR spectra of **1a** in THF-d_8.

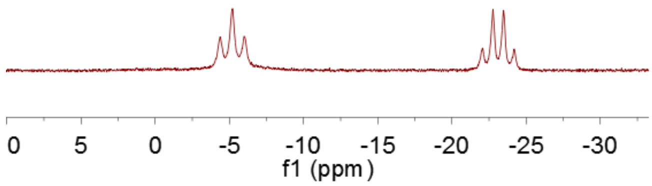


Figure S3d ^{11}B NMR spectra of **1b** in THF-d_8.

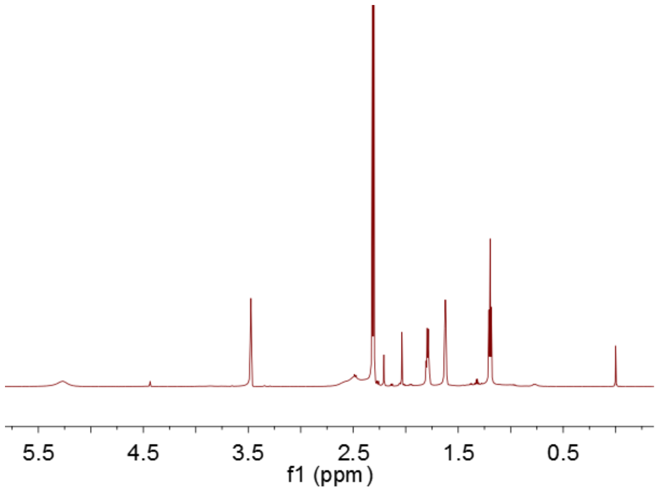


Figure S3e ^{1}H{^{11}B} NMR spectra of **1b** in THF-d_8.

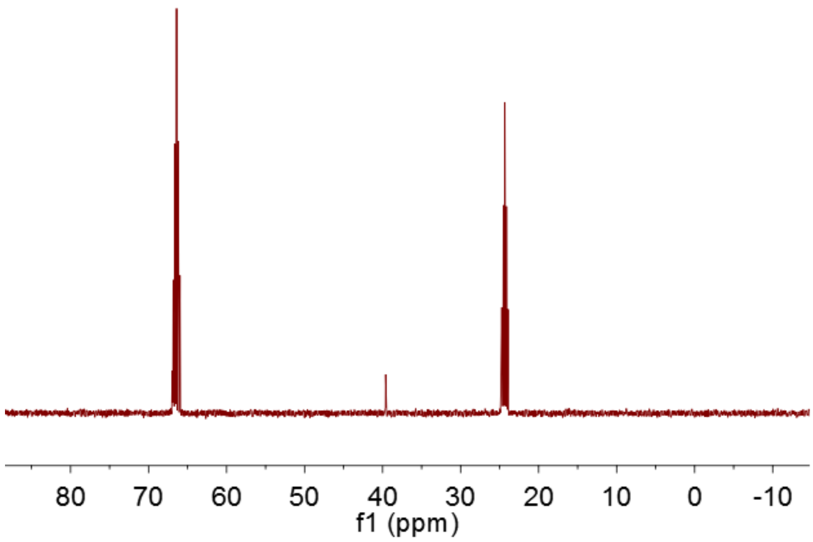


Figure S3f ^{13}C{^{1}H} NMR spectra of **1b** in THF-d_8.

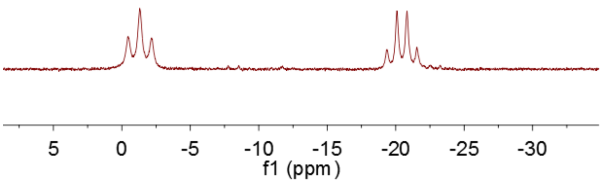


Figure S3g ^{11}B NMR spectra of **1c** in THF-d_8.

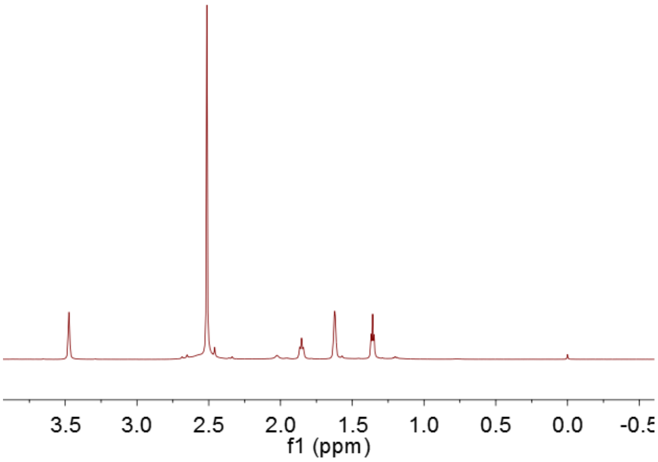


Figure S3h ^{1}H{^{11}B} NMR spectra of **1c** in THF-d_8.

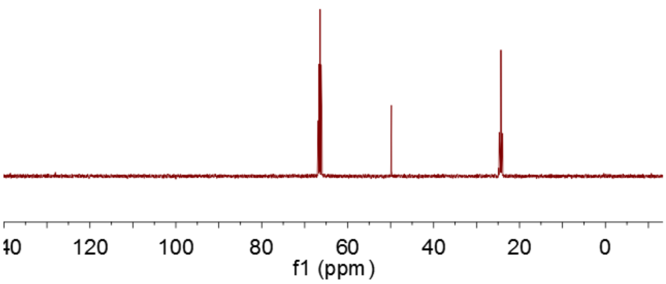


Figure S3i ^{13}C{^{1}H} NMR spectra of **1c** in THF-d_8.

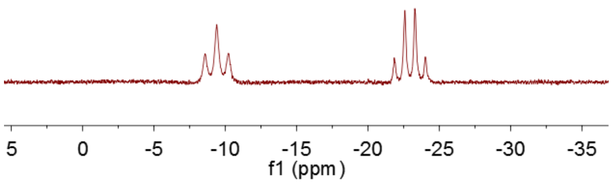


Figure S3j ^{11}B NMR spectra of **2a** in THF-d_8.

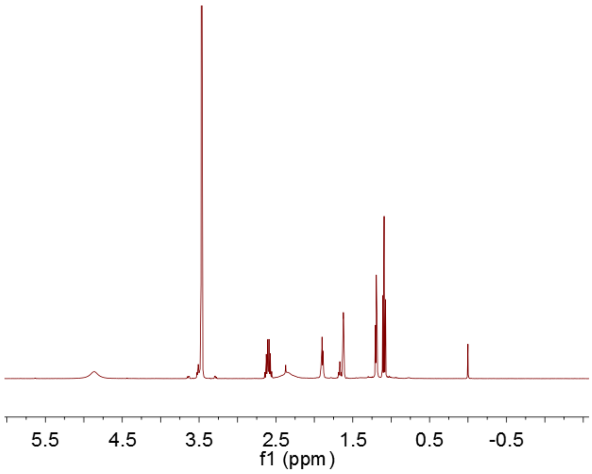


Figure S3k $^{1}H\{^{11}B\}$ NMR spectra of **2a** in THF-d_8.

Figure S3l $^{13}C\{^{1}H\}$ NMR spectra of **2a** in THF-d_8.

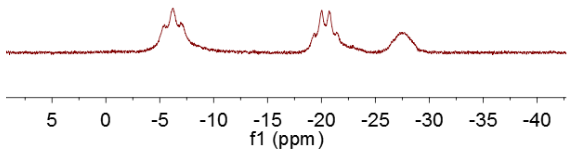


Figure S3m ^{11}B NMR spectra of **2c** in THF-d_8.

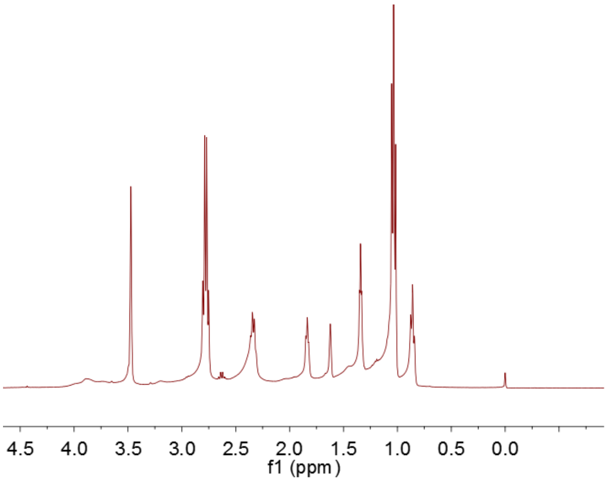


Figure S3n $^{1}H\{^{11}B\}$ NMR spectra of **2c** in THF-d_8.

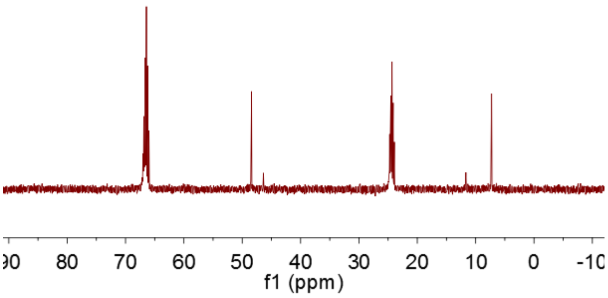


Figure S3o $^{13}C\{^{1}H\}$ NMR spectra of **2c** in THF-d_8.

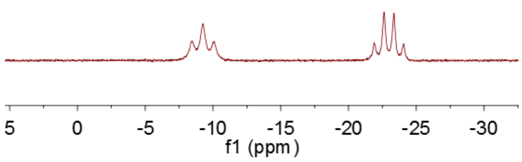


Figure S3p ^{11}B NMR spectra of **3a** in THF-d_8.

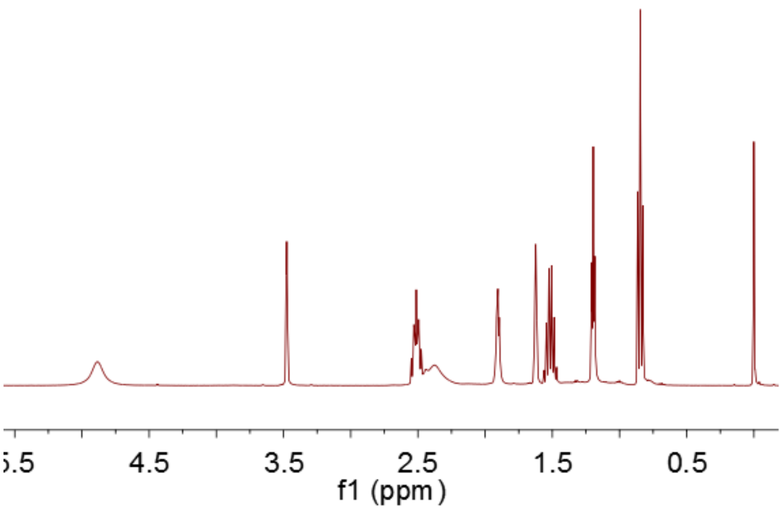


Figure S3q ^{1}H{^{11}B} NMR spectra of **3a** in THF-d_8.

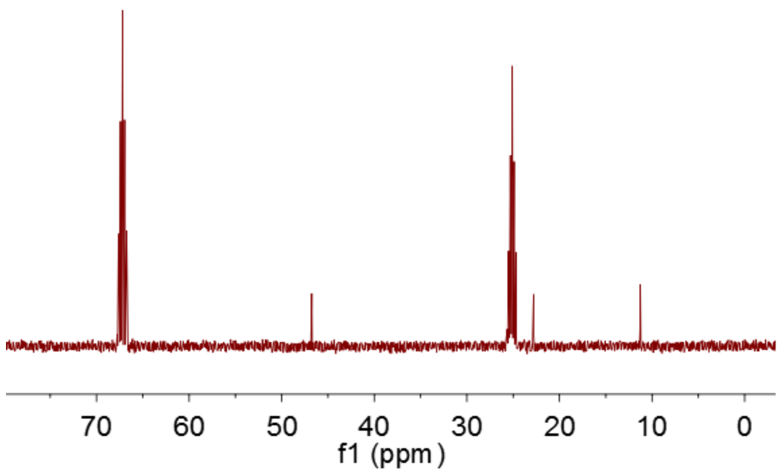


Figure S3r ^{13}C{^{1}H} NMR spectra of **3a** in THF-d_8.

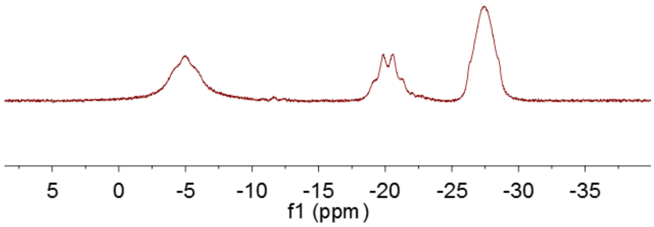


Figure S3s ^{11}B NMR spectra of **3c** in THF-d_8.

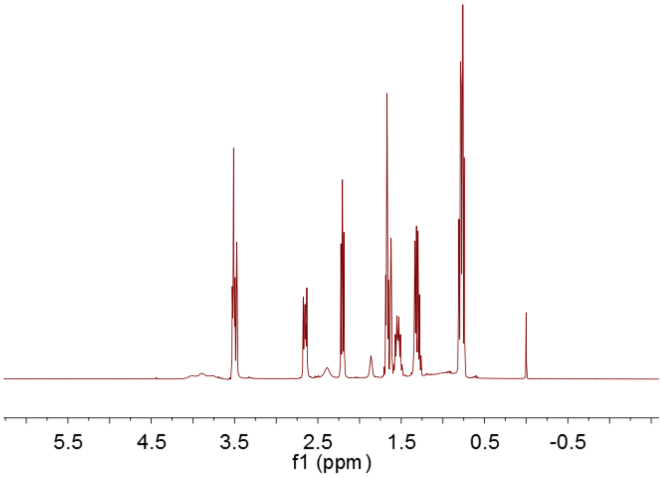


Figure S3t $^{1}H\{^{11}B\}$ NMR spectra of **3c** in THF-d_8.

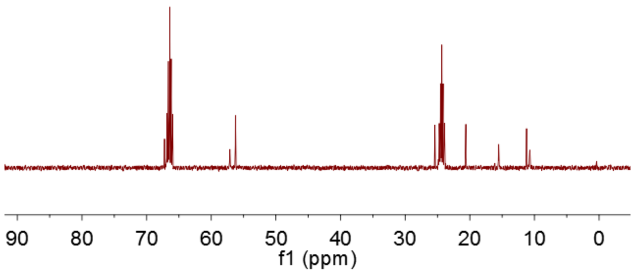


Figure S3u $^{13}C\{^{1}H\}$ NMR spectra of **3c** in THF-d_8.

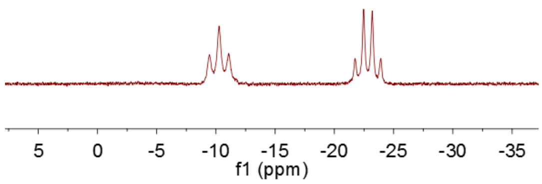


Figure S3v ^{11}B NMR spectra of **3d** in THF-d_8.

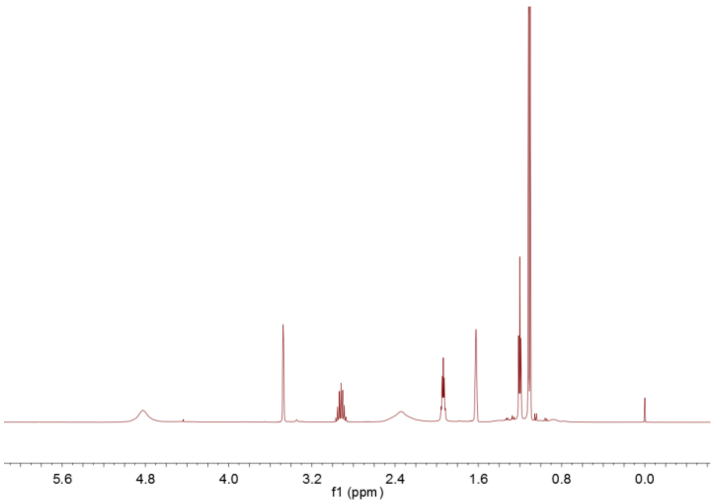


Figure S3w $^{1}H\{^{11}B\}$ NMR spectra of **3d** in THF-d_8.

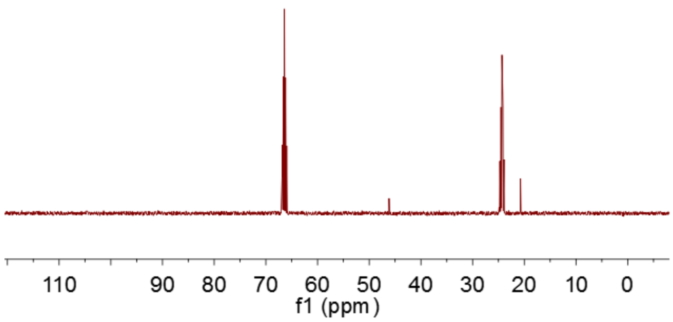


Figure S3x $^{13}C\{^{1}H\}$ NMR spectra of **3d** in THF-d_8.

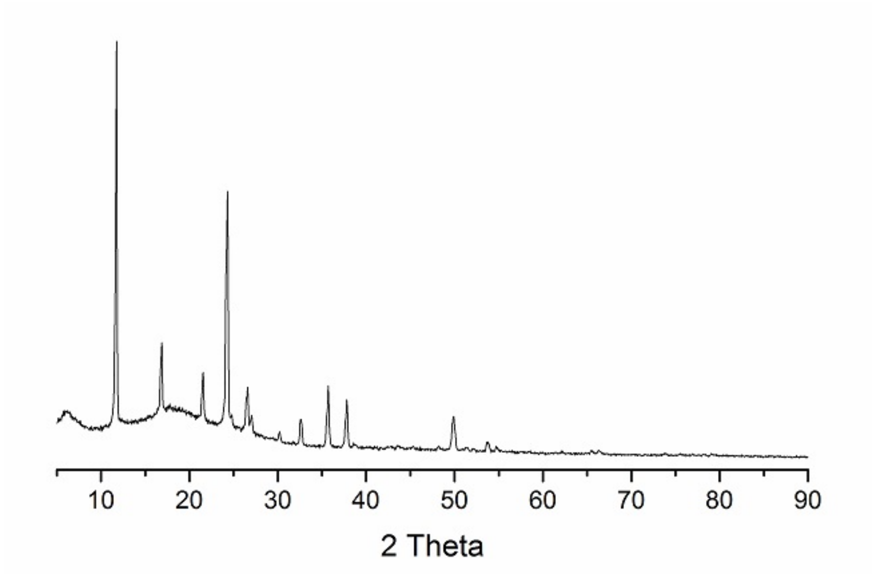


Figure S3y X-ray powder diffraction data of **1a**.

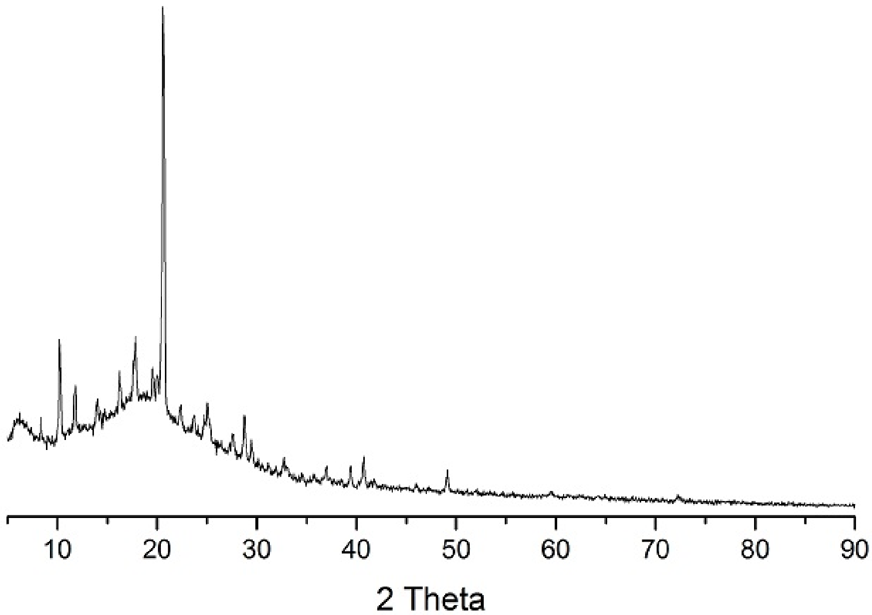


Figure S3z X-ray powder diffraction data of **1b**.

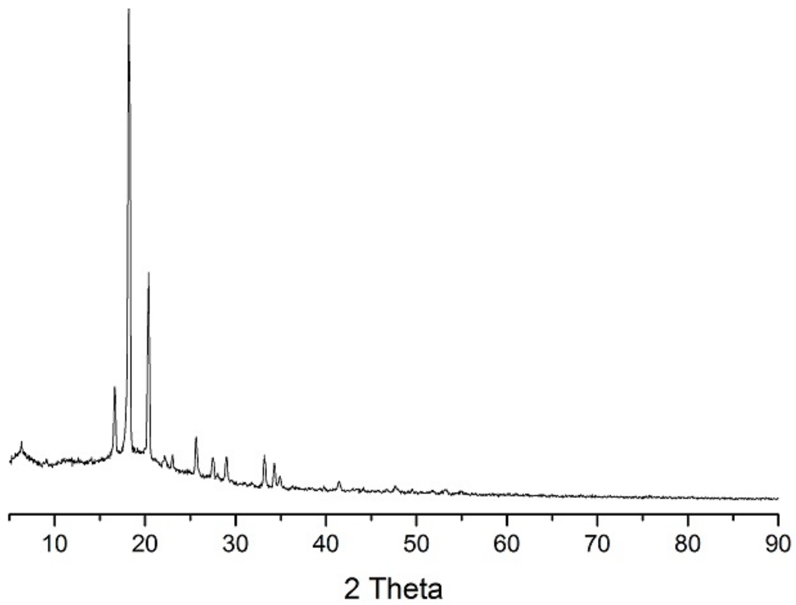


Figure S3aa X-ray powder diffraction data of 1c.

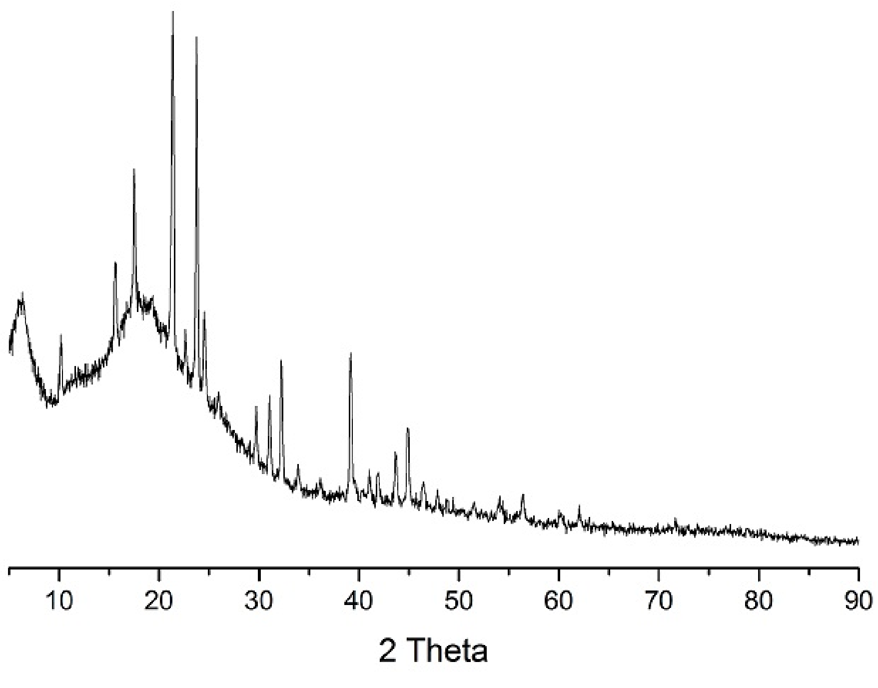


Figure S3ab X-ray powder diffraction data of **2a**.

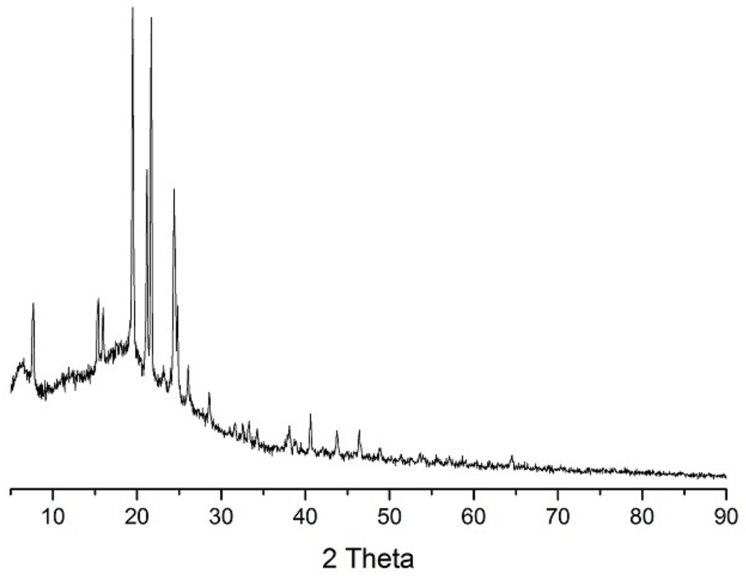


Figure S3ac X-ray powder diffraction data of **3a**.

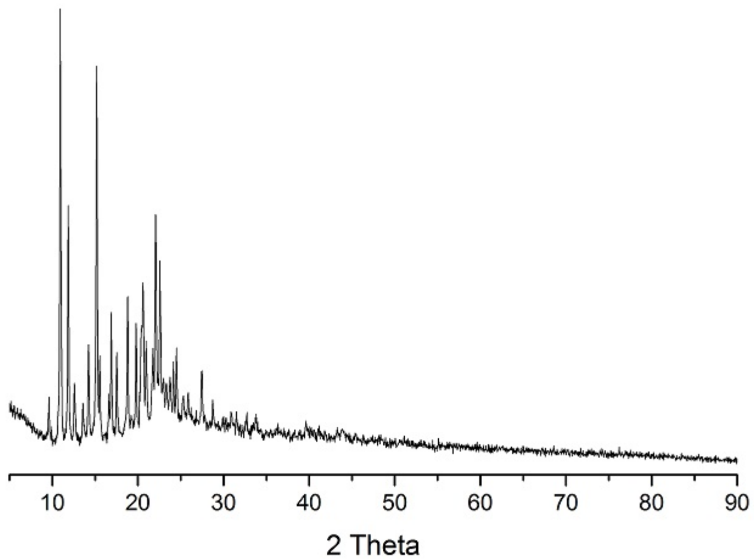


Figure S3ad X-ray powder diffraction data of **3c**.

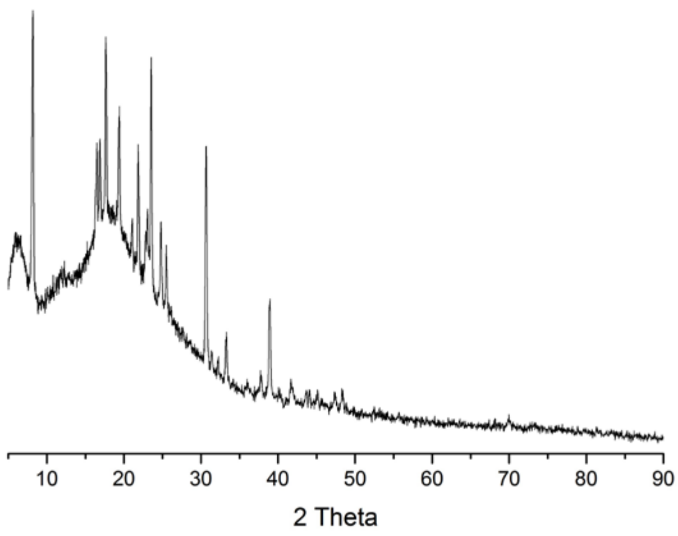


Figure S3ae X-ray powder diffraction data of **3d**.

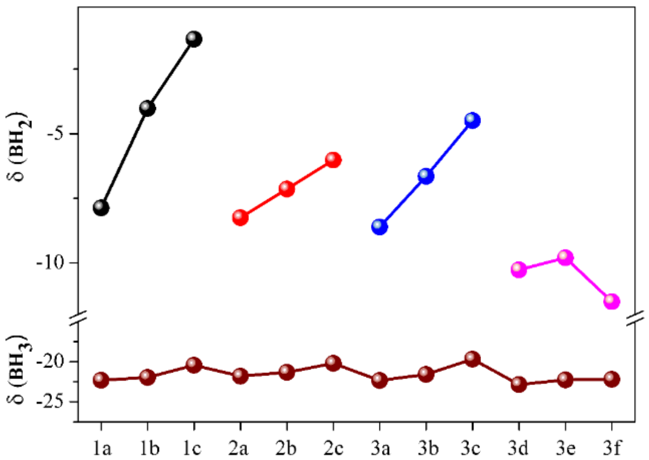


Figure S4 The ^{11}B NMR chemical shift of the diborazanes.

Table S5 The experiment and calculated chemical shifts of B in the diborazanes.

Diborazanes	δ (BH_2)	δ (BH_3)
$MeNH_2BH_2NH_2BH_3$(**1a**)	-7.87	-22.31
$Me_2NHBH_2NH_2BH_3$(**1b**)	-4.02	-21.96
$Me_3NBH_2NH_2BH_3$(**1c**)	-1.34	-20.44
$EtNH_2BH_2NH_2BH_3$(**2a**)	-8.25	-21.80
$Et_2NHBH_2NH_2BH_3$(**2b**)	-7.14	-21.32
$Et_3NBH_2NH_2BH_3$(**2c**)	-6.02	-20.21
$^nPrNH_2BH_2NH_2BH_3$(**3a**)	-8.61	-22.34
$^nPr_2NHBH_2NH_2BH_3$(**3b**)	-6.65	-21.58
$^nPr_3NBH_2NH_2BH_3$(**3c**)	-4.49	-19.68
$^iPrNH_2BH_2NH_2BH_3$(**3d**)	-10.27	-22.85
$^iPr_2NHBH_2NH_2BH_3$(**3e**)	-9.80	-22.27
$^iPr_2MeNBH_2NH_2BH_3$(**3f**)	-11.50	-22.20
$NH_3BH_2NH_2BH_3$	-11.60	-22.80

Table S6 The chemical shifts of H in the diborazanes.

$R_1R_2R_3NBH_2NH_2BH_3$	δ (B1H)	δ (B2H)	δ (N1H)	δ (N2H)
$MeNH_2BH_2NH_2BH_3$(**1a**)	1.89	1.19	4.88	2.39
$Me_2NHBH_2NH_2BH_3$(**1b**)	1.79	1.20	5.27	2.48
$Me_3NBH_2NH_2BH_3$(**1c**)	1.85	1.20	-	2.61
$EtNH_2BH_2NH_2BH_3$(**2a**)	1.90	1.19	4.87	2.37
$Et_3NBH_2NH_2BH_3$(**2c**)	1.84	1.34	-	2.40
$^{n}PrNH_2BH_2NH_2BH_3$(**3a**)	1.90	1.20	4.88	2.38
$^{n}Pr_3NBH_2NH_2BH_3$(**3c**)	1.86	1.28	-	2.40
$^{i}PrNH_2BH_2NH_2BH_3$(**3d**)	1.94	1.20	4.86	2.34
$NH_3BH_2NH_2BH_3$	2.06	1.30	4.57	2.35

Table S7 Bond angles and dihedral angles of the diborazanes.

	Angles (°)						
	$CH_{12}B_2N_2$(**1a**)	$C_2H_{14}B_2N_2$(**1b**)	$C_3H_{16}B_2N_2$(**1c**)	$C_{16}H_{52}B_4N_4O_6$ ($C_{12}H_{24}O_6$·**2a**)	$C_6H_{22}B_2N_2$(**2c**)	$C_{13}H_{36}B_4N_4$ (C_4H_8O·**3c**)	$C_3H_{16}B_2N_2$(**3d**)
N2-B1-N1	108.17(14)	109.3(2)	110.56(6)	110.05(15)	111.3(2)	111.42(10)	108.61(6)
B1-N2-B2	115.31(14)	117.5(2)	114.13(6)	114.89(16)	113.7(2)	113.37(10)	112.67(6)
N1-B1-N2-B2	180	55.59	177.33	169.49	177.93	171.14	178.60

Table S8 Bond lengths of the diborazanes.

	Bond lengths (Å)						
	B1-N1	B1-N2	B2-N2	N1-H	B1-H	N2-H	B2-H
$CH_{12}B_2N_2$(**1a**)	1.595(2)	1.560(2)	1.601(2)	0.845	1.128	0.884	1.149, 1.120
$C_2H_{14}B_2N_2$(**1b**)	1.591(3)	1.557(4)	1.596(4)	0.979	1.117, 1.125	0.890	1.135, 1.128, 1.119
$C_3H_{16}B_2N_2$(**1c**)	1.6269(11)	1.5594(11)	1.6090(11)	-	1.115, 1.112	0.897, 0.929	1.135, 1.104
$C_{16}H_{52}B_4N_4O_6$($C_{12}H_{24}O_6$·**2a**)	1.593(2)	1.546(3)	1.605(3)	0.838, 0.851	1.113	0.823, 0.903	1.113, 1.115, 1.116
$C_6H_{22}B_2N_2$(**2c**)	1.631(4)	1.563(4)	1.619(4)	-	1.111, 1.120	0.910	1.132, 1.122, 1.125
$C_{13}H_{36}B_2N_2O$(C_4H_8O·**3c**)	1.6482(16)	1.5497(17)	1.6100(17)	-	1.121, 1.103	0.884, 0.866	1.111, 1.119
$C_3H_{16}B_2N_2$(**3d**)	1.6019(11)	1.5633(11)	1.6048(11)	0.910	1.115, 1.101	0.910	1.151, 1.155, 1.140

Table S9 The inter-/intramolecular DHBs and hydrogen bond (HB) of the diborazanes.*

	Types of DHBs/HBs		H···H/O distance in Å (*amounts*)
1a	Intermolecular DHBs	NH···HB	1.972 (*4*); 2.043(*4*); 2.372 (*4*); 2.402 (*4*); 2.410 (*4*);
		CH···HB	2.180 (*2*)
	Intramolecular DHBs	CH···HN	2.335 (*2*); 2.403 (*2*)
1b	Intermolecular DHBs	NH···HB	2.115 (*2*); 2.121 (*2*); 2.401 (*2*); 2.417 (*2*); 2.431 (*2*);
		CH···HB	2.387 (*2*)
	Intramolecular DHBs	NH···HB	2.154 (*1*); 2.458 (*1*); 2.491 (*1*)
		CH···HN	2.261 (*1*); 2.348 (*1*); 2.377 (*1*); 2.386 (*1*); 2.403 (*1*)
		CH···HB	2.154 (*1*); 2.486 (*1*)
1c	Intermolecular DHBs	NH···HB	2.090 (*2*); 2.076 (*2*)
		CH···HB	2.231 (*1*); 2.449 (*2*); 2.457 (*2*); 2.491 (*2*)
	Intramolecular DHBs	NH···HB	2.458 (*1*)
		CH···HN	2.204 (*1*); 2.211 (*1*)
		CH···HB	2.369 (*1*); 2.405 (*1*); 2.479 (*1*); 2.499 (*1*)
$C_{12}H_{24}O_6$·**2a**	Hydrogen Bonds	NH···O	2.037 (*1*); 2.132 (*1*)
	Intermolecular DHBs	NH···HB	1.849 (*2*); 2.233 (*2*); 2.471 (*2*)
		CH···HB	2.47 (*1*); 2.39 (*1*); 2.47 (*1*)
	Intramolecular DHBs	NH···HB	2.490 (*1*)
		CH···HN	2.372 (*1*); 2.464 (*1*); 2.497 (*1*)
		CH···HB	2.435 (*1*)
2c	Intermolecular DHBs	NH···HB	2.091 (*2*); 2.441 (*2*)
		CH···HB	2.139 (*2*); 2.226 (*1*); 2.262 (*2*); 2.322 (*1*); 2.409 (*2*); 2.421 (*1*); 2.450(*1*); 2.497 (*1*);
	Intramolecular DHBs	CH···HN	2.121 (*1*); 2.130 (*1*); 2.425 (*1*); 2.443 (*1*)
		CH···HB	2.139 (*1*); 2.096 (*1*); 2.369 (*1*); 2.422 (*1*);
C_4H_8O·**3c**	Hydrogen Bond	NH···O	2.044 (*1*)
	Intermolecular DHBs	NH···HB	2.017 (*2*); 2.341 (*2*);
		CH···HB	2.284 (*2*); 2.343 (*1*); 2.355 (*2*); 2.373 (*1*); 2.417 (*1*); 2.461 (*2*);
	Intramolecular DHBs	NH···HB	2.476 (*1*); 2.481 (*1*); 2.490 (*1*)
		CH···HN	2.096 (*1*); 2.234 (*1*)
		CH···HB	2.151 (*1*); 2.260 (*1*); 2.278 (*1*); 2.338 (*1*)
3d	Intermolecular DHBs	NH···HB	1.995 (*2*); 2.048 (*2*); 2.091 (*2*); 2.112 (*2*); 2.160 (*2*); 2.298 (*2*); 2.331(*2*)
		NH···HN	2.353 (*1*)
		CH···HB	2.417 (*2*); 2.421 (*1*); 2.426 (*2*); 2.427 (*1*); 2.439 (*1*); 2.470 (*1*)
	Intramolecular DHBs	NH···HB	2.483 (*1*)
		CH···HN	2.322 (*1*); 2.401 (*1*); 2.469 (*1*)
		CH···HB	2.387 (*1*); 2.491 (*1*)

*the bond lengths were normalized based on an N−H bond of 1.03 Å, a B−H bond of

1.21 Å, and C-H bond of 1.09 Å. Refs: (a) T. B. Richardson, S. D. Gala and R. H. Crabtree, *J. Am. Chem. Soc.*, **1995**, 117, 12875; (b) W. T. Klooster, T. F. Koetzle, P. E. M. Siegbahn, T. B. Richardson and R. H. Crabtree, *J. Am. Chem. Soc.*, **1999**, 121, 6337. (c) G. A. Jeffrey and W. Saenger, Hydrogen bonding in biological structure, Springer, Berlin, **1994**. (d) https://cccbdb.nist.gov/exp1x.asp

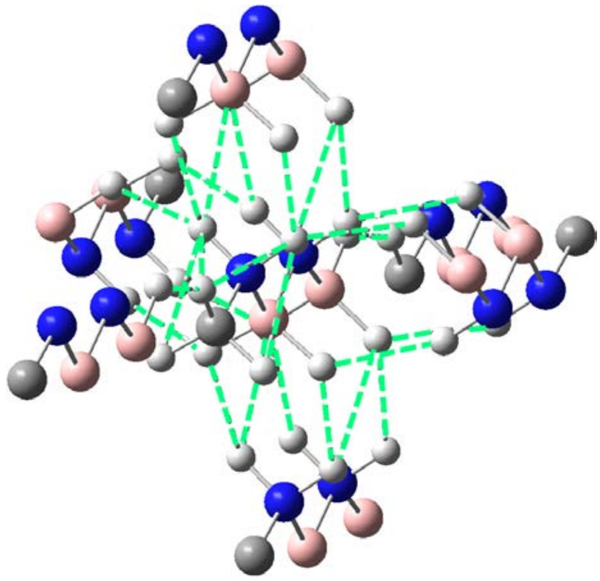


Figure S5a Intermolecular DHBs of **1a** (N, blue; B, pink; C, gray; H, light−gray).

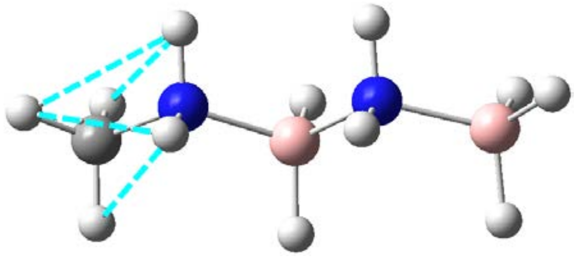


Figure S5b Intramolecular DHBs of **1a** (N, blue; B, pink; C, gray; H, light−gray).

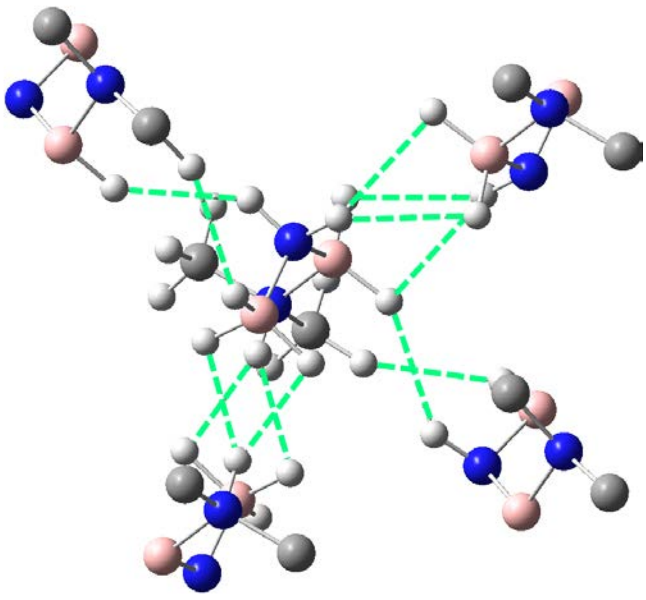


Figure S5c Intermolecular DHBs of **1b** (N, blue; B, pink; C, gray; H, light−gray).

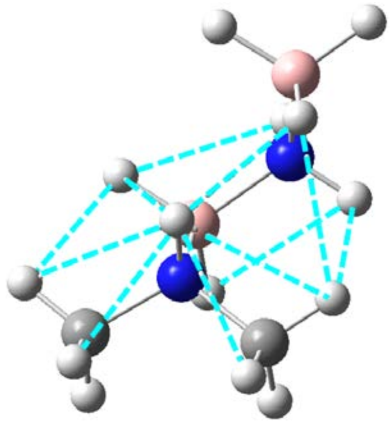


Figure S5d Intramolecular DHBs of **1b** (N, blue; B, pink; C, gray; H, light−gray).

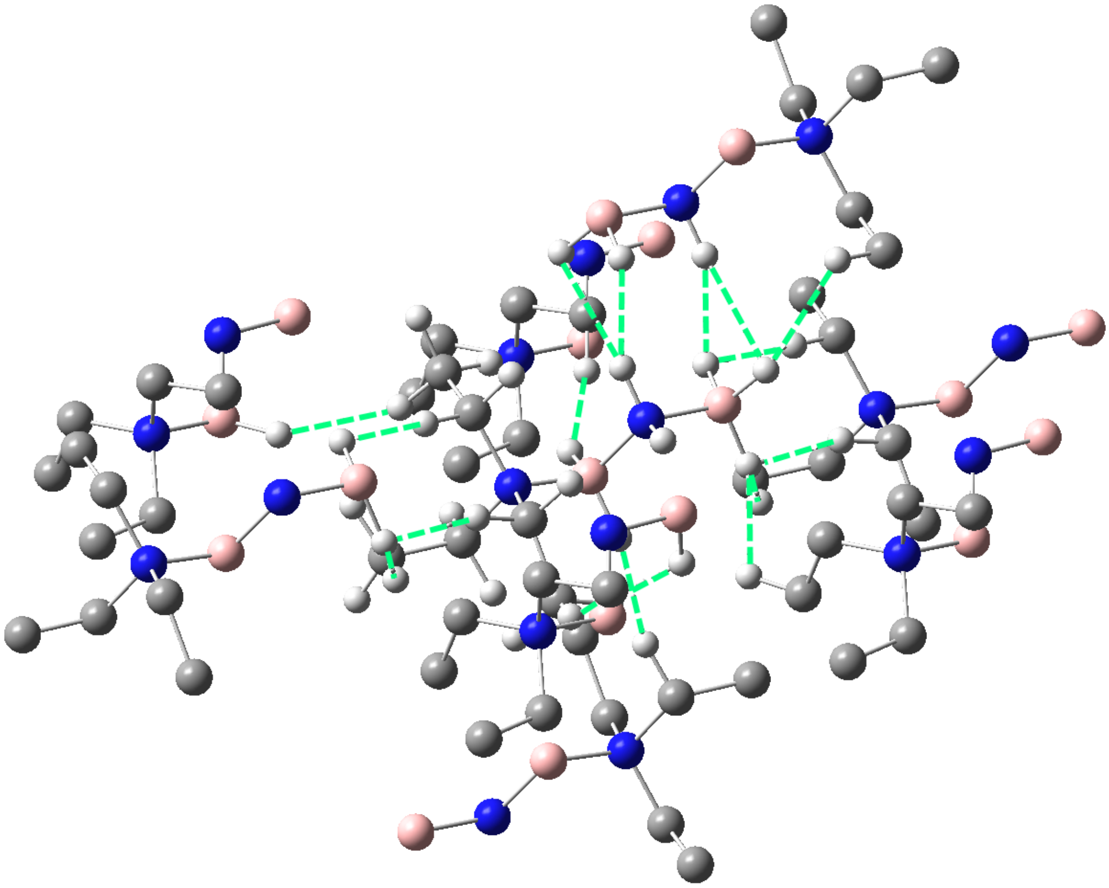


Figure S5e Intermolecular DHBs of **1c** (N, blue; B, pink; C, gray; H, light−gray).

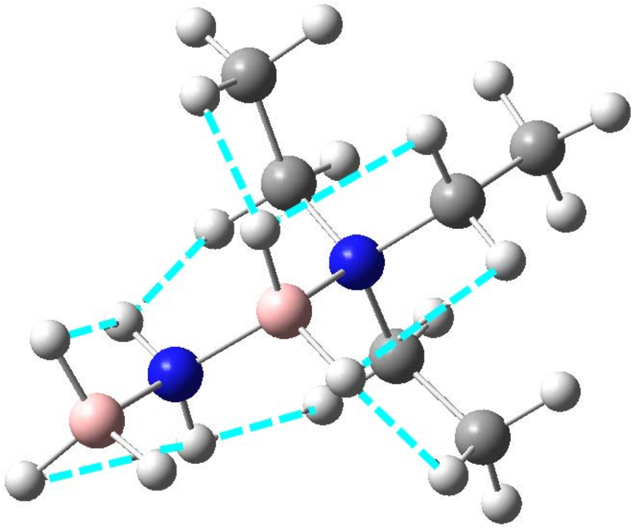


Figure S5f Intramolecular DHBs of **1c** (N, blue; B, pink; C, gray; H, light−gray).

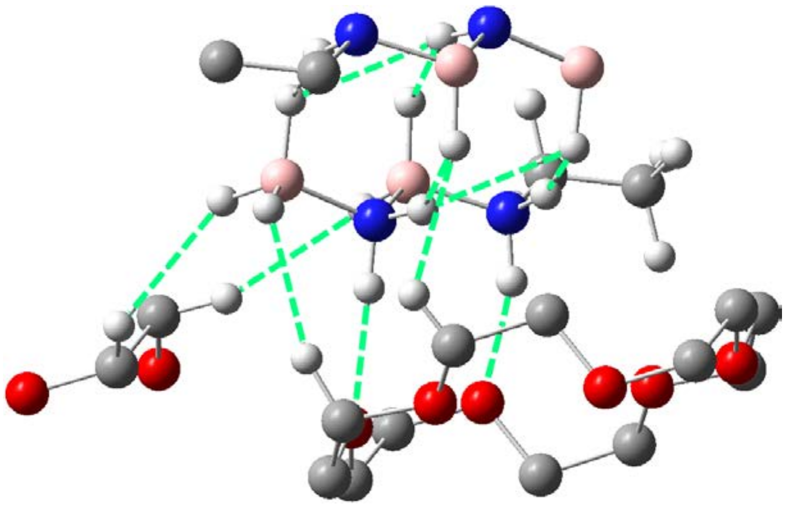


Figure S5g Intermolecular DHBs of $C_{12}H_{24}O_6$·**2a** (N, blue; B, pink; C, gray; O, red; H, light−gray).

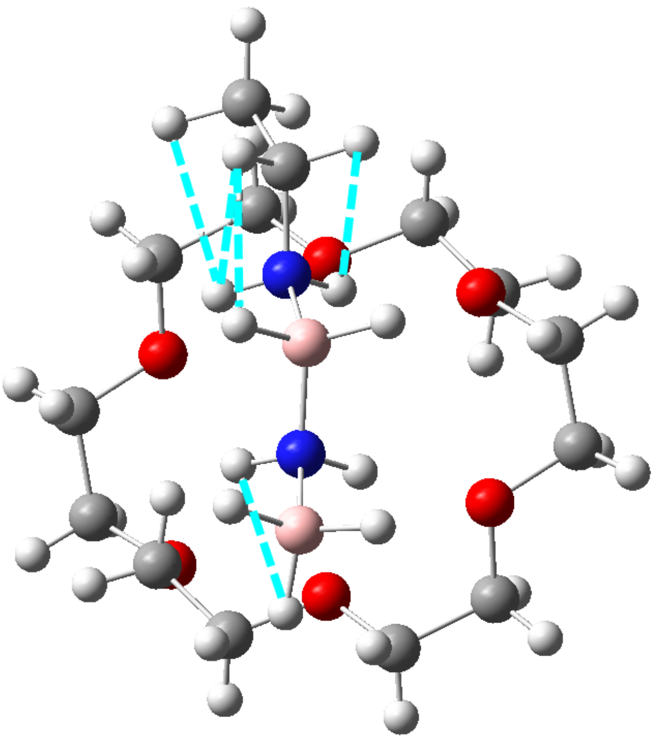


Figure S5h Intramolecular DHBs of $C_{12}H_{24}O_6$·**2a** (N, blue; B, pink; C, gray; O, red; H, light−gray).

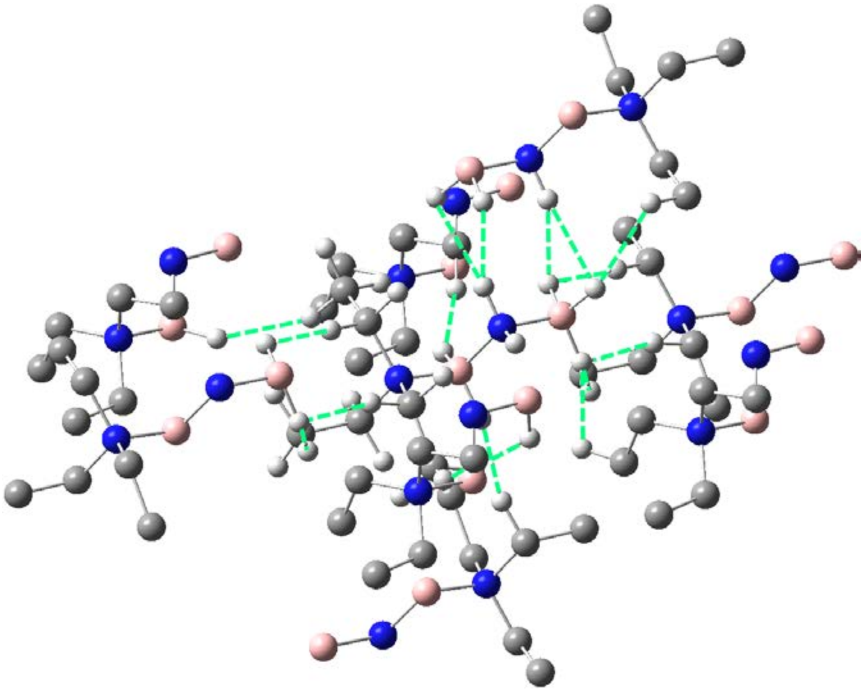


Figure S5i Intermolecular DHBs of **2c** (N, blue; B, pink; C, gray; H, light−gray).

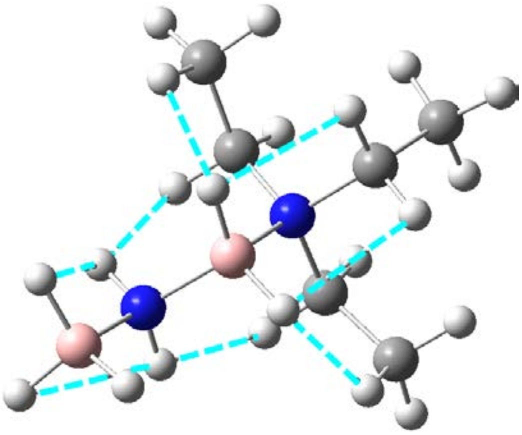


Figure S5j Intramolecular DHBs of **2c** (N, blue; B, pink; C, gray; H, light−gray).

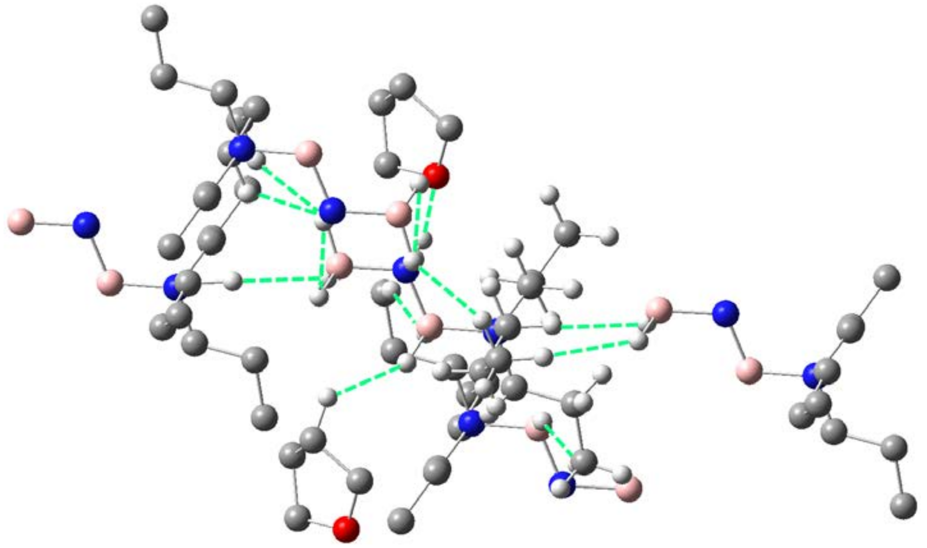


Figure S5k Intermolecular DHBs of C_4H_8O·**3c** (N, blue; B, pink; C, gray; O, red; H, light−gray).

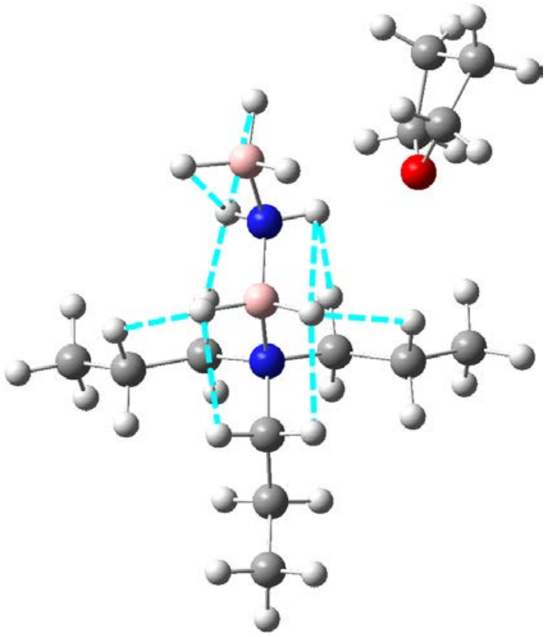


Figure S5l Intramolecular DHBs of C_4H_8O·**3c** (N, blue; B, pink; C, gray; O, red; H, light−gray).

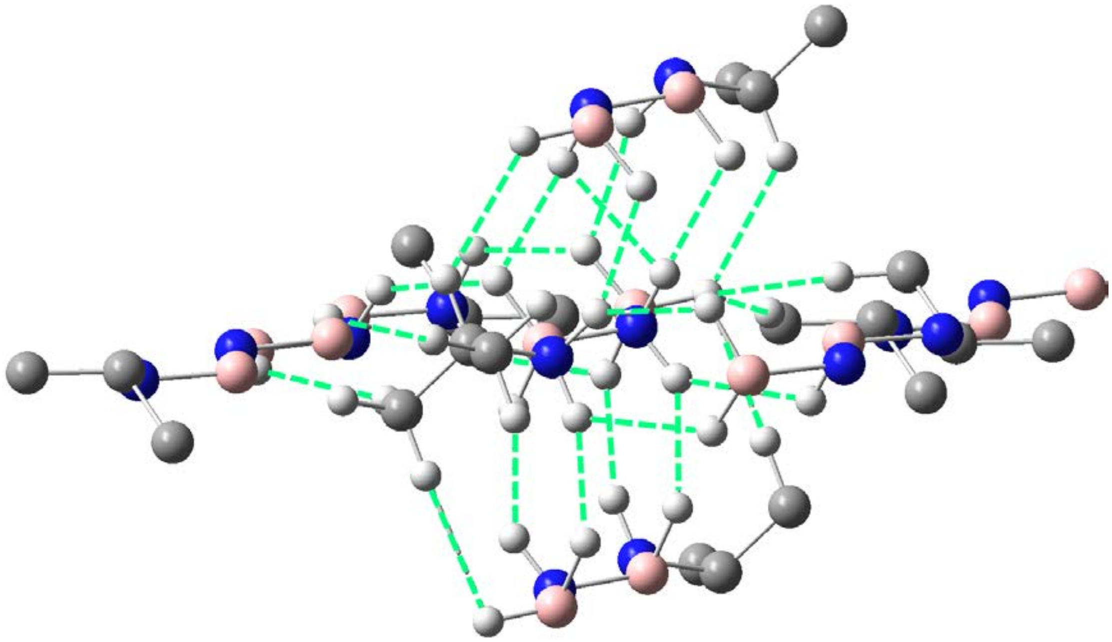


Figure S5m Intermolecular DHBs of **3d** (N, blue; B, pink; C, gray; H, light−gray).

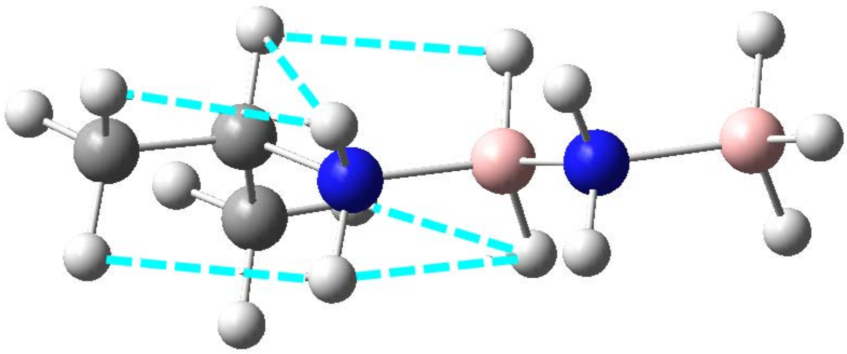


Figure S5n Intramolecular DHBs of **3d** (N, blue; B, pink; C, gray; H, light−gray).

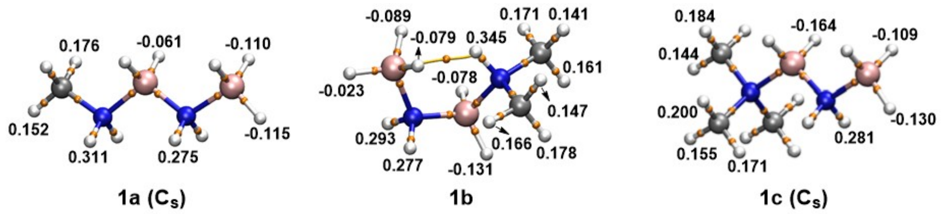


Figure S6a The NPA value and CPs of mono-molecule 1a, 1b and 1c. (Because the C_S symmetry of 1a and 1c, here the charge value of hydrogen atoms show only half. Bond critical point, orange; N, blue; B, pink; C, gray; H, light−gray).

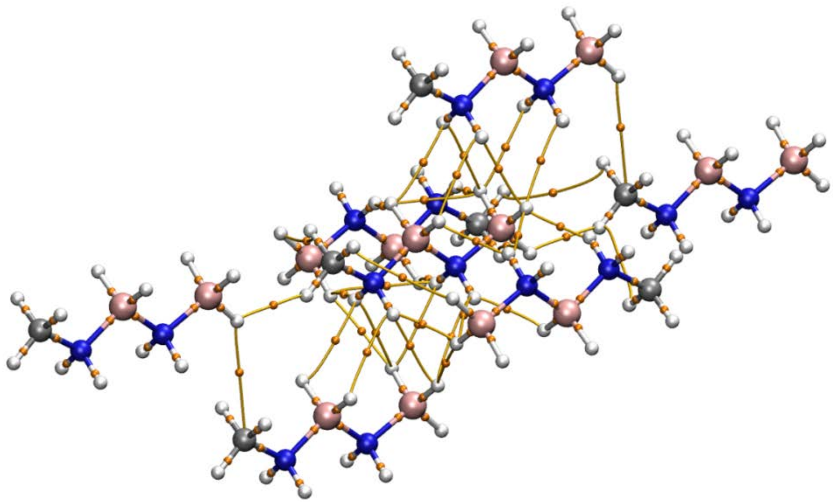


Figure S6b The CPs of 1a intermolecular DHB interaction (Bond critical point, orange; N, blue; B, pink; C, gray; H, light−gray).

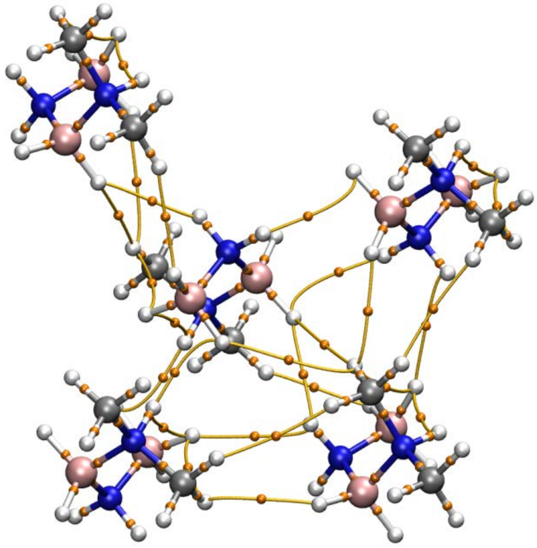


Figure S6c The BCPs of 1b intermolecular DHB interaction (Bond critical point, orange; N, blue; B, pink; C, gray; H, light−gray).

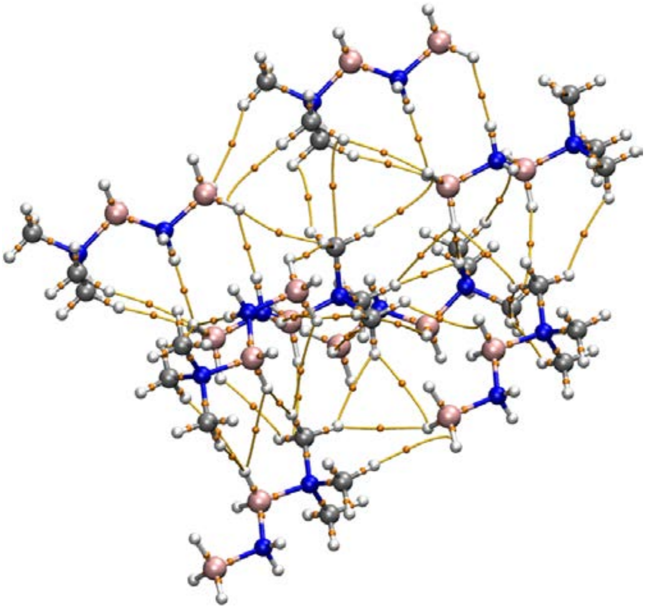


Figure S6d The BCPs of 1c intermolecular DHB interaction (Bond critical point, orange; N, blue; B, pink; C, gray; H, light−gray).

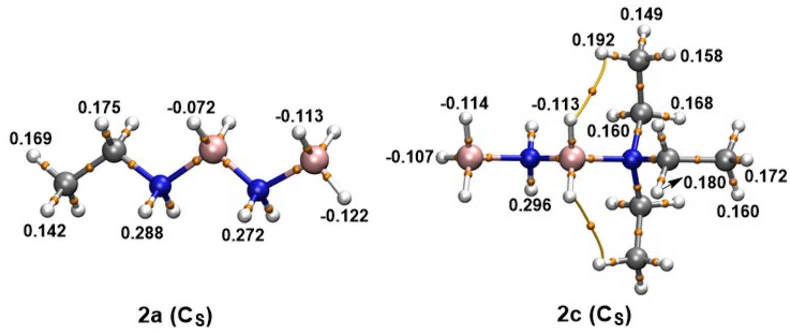


Figure S6e The NPA value and BCPs of mono-molecule 2a and 2c. (Because the C_S symmetry of 2a and 2c, here the charge value of hydrogen atoms show only half. Bond critical point, orange; N, blue; B, pink; C, gray; H, light−gray).

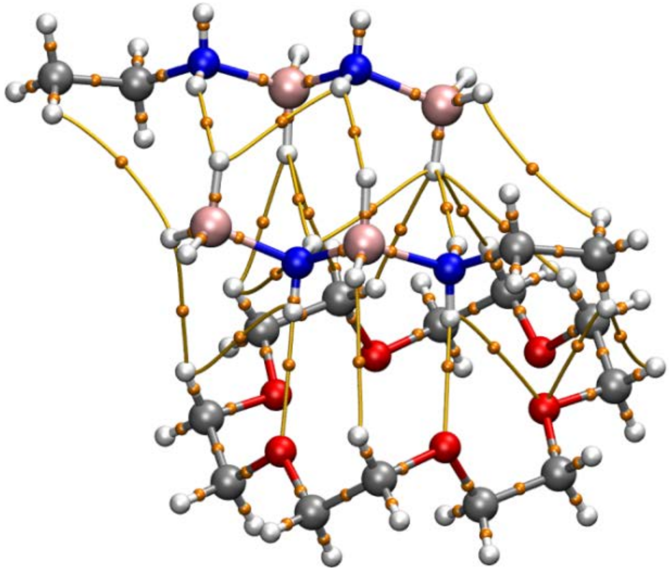


Figure S6f The BCPs of 2a intermolecular DHB interaction (Bond critical point, orange; N, blue; B, pink; C, gray; H, light−gray).

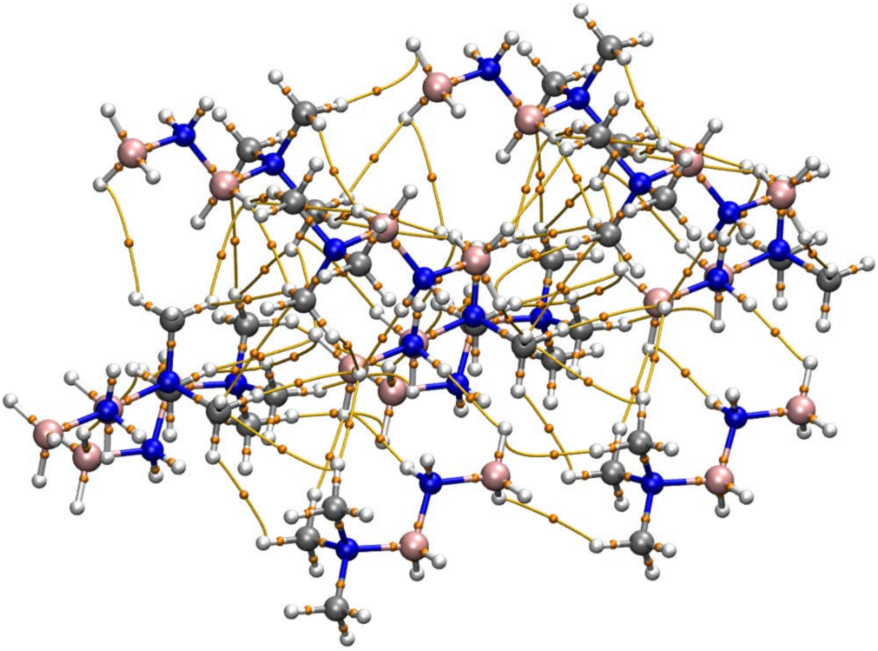
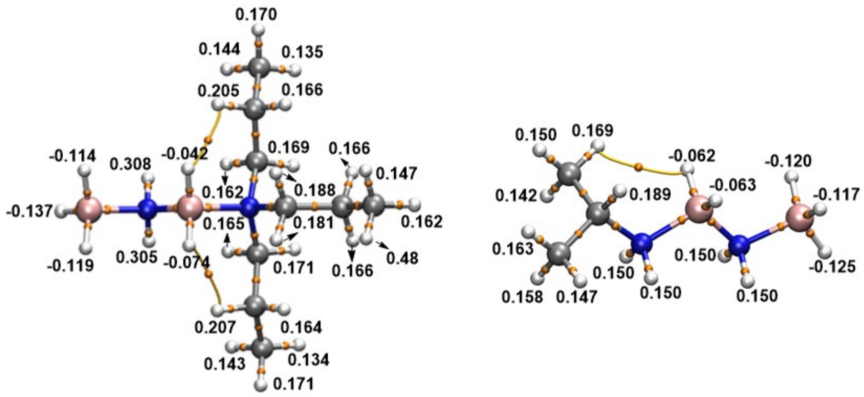


Figure S6g The BCPs of 2c intermolecular DHB interaction (Bond critical point, orange; N, blue; B, pink; C, gray; H, light−gray).



3c 3d

Figure S6h The NPA value and BCPs of mono-molecule 3c and 3d (Bond critical point, orange; N, blue; B, pink; C, gray; H, light−gray).

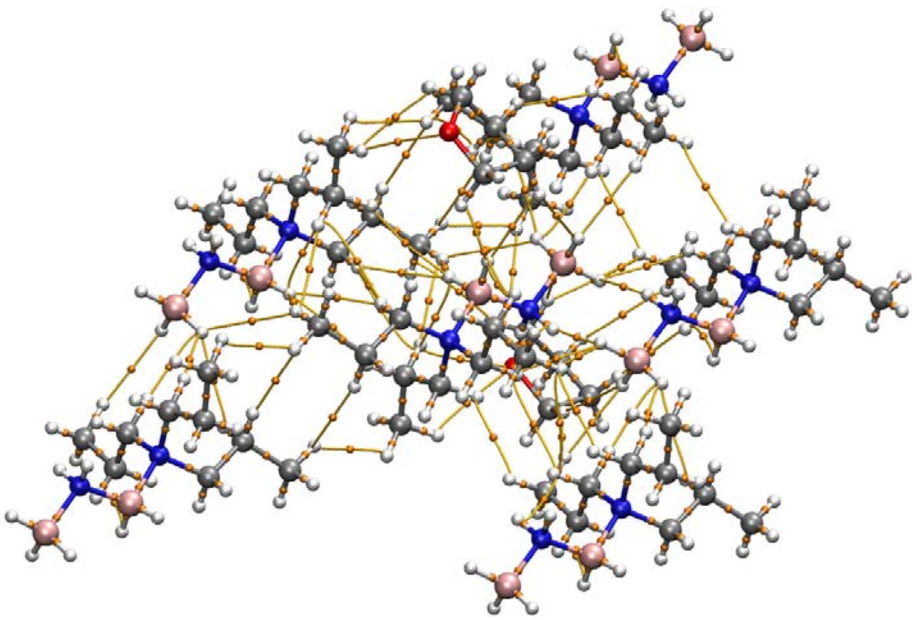


Figure S6i The BCPs of 3c intermolecular DHB interaction (Bond critical point, orange; N, blue; B, pink; C, gray; H, light−gray).

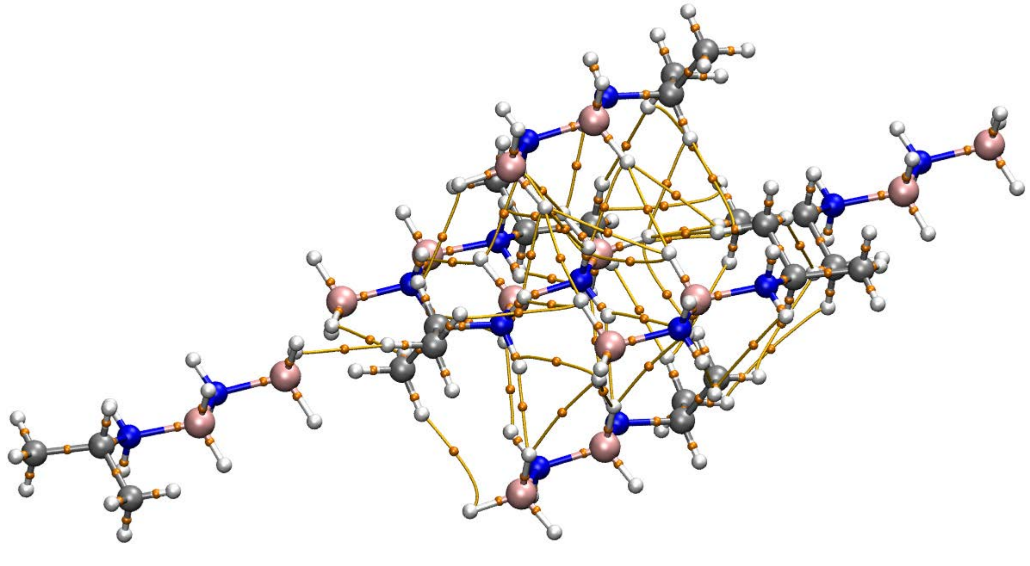


Figure S6j The BCPs of 3d intermolecular DHB interaction (Bond critical point, orange; N, blue; B, pink; C, gray; H, light−gray).

Table S10 The energy difference (ΔE) of *anti* configuration and *gauch* configuration of the diborazanes.

	E_{anti} (au)[a]	E_{gauch} (au)[a]	ΔE (kcal/mol)[b]
1a	-204.5506285	-204.5550631	2.78
1b	-243.8483385	-243.8537686	3.41
1c	-283.1467220	-283.1459078	-0.51
2a	-243.8580352	-243.8637242	3.57
2b	-322.4570357	-322.4634588	4.03
2c	-401.0576854	-401.0517219	-3.74
3a	-283.1622115	-283.1665749	2.74
3b	-401.0651287	-401.0715685	4.04
3c	-518.9683671	-518.9639863	-2.75
3d	-283.1649786	-283.1692102	2.66
3e	-401.0676821	-401.0735694	3.69
3f	-440.3567103	-440.3514900	-3.28
3g	-479.6537497	-479.6442337	-5.97

[a] The E_{anti} and E_{gauch} are the electronic energies.

[b]$\Delta E = E_{anti} - E_{gauch}$.

Table S11 The melting points of the diborazanes and the isoelectronic analogs.

diborazanes	mp (°C)	Isoelectronic analogs	mp (°C)
$MeNH_2BH_2NH_2BH_3$ (**1a**)	99	$CH_3CH_2CH_2CH_2CH_3$	-130
$Me_3NBH_2NH_2BH_3$ (**1c**)	119	$(CH_3)_3CH_2CH_2CH_2CH_3$	-124
$EtNH_2BH_2NH_2BH_3$(**2a**)	89	$CH_3CH_2CH_2CH_2CH_2CH_3$	-94
$^nPrNH_2BH_2NH_2BH_3$(**3a**)	91	$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$	-91
$^iPrNH_2BH_2NH_2BH_3$(**3d**)	102	$(CH_3)_2CH_2CH_2CH_2CH_2CH_3$	-118

3. The optimized cartesian coordinates of all species

ADB

5	0.957279	-0.441086	-0.000003
1	1.520344	-0.611932	-1.037679
1	1.520277	-0.611995	1.037698
5	-0.957279	-0.441085	-0.000002
1	-1.520273	-0.612003	1.037699
1	-1.520337	-0.611935	-1.037680
1	0.000002	-1.379748	-0.000066
7	-0.000004	0.788341	0.000007
1	0.000012	1.360043	0.835884
1	0.000002	1.360038	-0.835874

NH_2Me

7	0.749448	-0.000027	-0.125717
1	1.139224	-0.811656	0.346410
1	1.138482	0.812002	0.346397
6	-0.703808	-0.000057	0.017913
1	-1.111134	0.880816	-0.485709
1	-1.111540	-0.879413	-0.487793
1	-1.078319	-0.001214	1.053234

TS1

7	-1.490595	-0.606193	-0.051027
1	-1.609882	-1.110754	-0.926926
1	-1.620220	-1.283168	0.698173
6	-2.493263	0.457484	0.054745
1	-2.365373	0.961948	1.014676
1	-2.303428	1.192543	-0.730973
1	-3.528031	0.104583	-0.028093
5	0.456320	0.511129	-0.071830
1	0.186739	0.883397	-1.171498
1	0.129033	1.066072	0.930198
5	2.623599	0.423005	0.003274
1	3.201757	0.415001	1.058373
1	3.275315	0.228498	-0.988956
1	1.983578	1.478067	-0.115606
7	1.406711	-0.661065	0.058908
1	1.371433	-1.167386	0.936326
1	1.426250	-1.313574	-0.716547

P1

7	-1.287721	-0.502497	0.000253
1	-1.291941	-1.113527	-0.818355
1	-1.291731	-1.112682	0.819490
6	-2.511777	0.332365	-0.000013
1	-2.483708	0.967877	0.884734
1	-2.484595	0.966052	-0.886099
1	-3.413765	-0.282208	0.001059
5	0.078713	0.441305	-0.000266
1	0.000832	1.073254	-1.021160
1	0.001196	1.073653	1.020406
5	2.738329	0.360482	0.000302
1	3.606156	-0.490804	-0.000171
1	2.725998	1.024385	-1.012552
1	2.725718	1.023193	1.013886
7	1.310679	-0.489832	-0.000306
1	1.365165	-1.093260	0.819343
1	1.365416	-1.092759	-0.820306

$NHMe_2$

7	-0.000001	0.571923	-0.151237
1	-0.000006	1.326724	0.529483
6	1.202907	-0.224266	0.020611
1	1.258311	-0.965336	-0.784124
1	2.085436	0.416516	-0.054585
1	1.246722	-0.770669	0.979634
6	-1.202908	-0.224264	0.020610
1	-2.085455	0.416453	-0.054939
1	-1.258121	-0.965573	-0.783918
1	-1.246879	-0.770399	0.979782

TS2

5	0.821330	0.672778	0.162200
1	0.698908	1.595129	-0.582382
1	0.456296	0.656674	1.298285
5	2.927485	0.236394	0.217168
1	3.407656	-0.400683	1.116977
1	3.636447	0.513752	-0.713307
1	2.411483	1.271544	0.670356
7	1.601302	-0.531125	-0.332548
1	1.427990	-1.407788	0.146542
1	1.617103	-0.679202	-1.335179
7	-1.239007	-0.026575	-0.391280
1	-1.335512	-0.136049	-1.398668
6	-1.550420	-1.282655	0.276667
1	-2.612783	-1.560168	0.210847
1	-0.954017	-2.090953	-0.156892
1	-1.284610	-1.186976	1.335047
6	-2.092439	1.066954	0.059216
1	-3.163955	0.854310	-0.065466
1	-1.892245	1.247899	1.119586
1	-1.835750	1.974753	-0.491083

P2

5	-0.378763	-0.618700	0.184486
1	-0.484063	-1.667718	-0.395438
1	-0.260988	-0.684982	1.382394
5	-3.012088	-0.257653	0.134489
1	-3.785688	0.638672	-0.141901
1	-3.140679	-1.230088	-0.576064
1	-2.996682	-0.521525	1.316389
7	-1.508132	0.356982	-0.214328
1	-1.466602	1.246601	0.280215
1	-1.540737	0.569563	-1.211014
7	1.081382	-0.015846	-0.328433
1	1.054745	0.025852	-1.349448
6	1.367749	1.337888	0.187804
1	2.372991	1.660933	-0.096823
1	0.634579	2.041092	-0.208665
1	1.281452	1.303676	1.275888
6	2.147383	-0.967717	0.054476
1	3.118885	-0.630172	-0.316202

1	2.163309	-1.030855	1.143652
1	1.900191	-1.948267	-0.352213

NMe_3

7	-0.000257	0.000002	-0.390324
6	0.692405	1.190521	0.063396
1	1.717369	1.189963	-0.319654
1	0.184298	2.081594	-0.317621
1	0.736113	1.262982	1.167492
6	0.685221	-1.194669	0.063395
1	0.171707	-2.082662	-0.317566
1	1.710149	-1.200327	-0.319708
1	0.728541	-1.267360	1.167491
6	-1.377551	0.004147	0.063528
1	-1.889546	0.892447	-0.318807
1	-1.894913	-0.881012	-0.318870
1	-1.462366	0.004365	1.167601

TS3

5	-1.056831	0.749615	0.000292
1	-0.845902	1.256105	1.059859
1	-0.846014	1.256300	-1.059202
5	-3.148150	0.247990	0.000043
1	-3.733612	0.041354	-1.029700
1	-3.734106	0.040732	1.029378
1	-2.703290	1.407464	0.000487
7	-1.755291	-0.597752	0.000096
1	-1.642993	-1.166784	-0.831593
1	-1.643173	-1.167024	0.831648
7	1.057509	0.015526	0.000028
6	1.319494	-0.760683	-1.201809
1	0.727366	-1.681538	-1.180656
1	1.026442	-0.176135	-2.078769
1	2.382086	-1.038116	-1.297671
6	1.321501	-0.755954	1.204470
1	1.030750	-0.167653	2.079652
1	0.728574	-1.676379	1.188331
1	2.384088	-1.033800	1.299148
6	1.819422	1.256737	-0.003014
1	1.555009	1.838318	-0.890069
1	1.555804	1.841980	0.881871
1	2.905843	1.072126	-0.003146

P3

5	-0.581412	0.712281	0.000857
1	-0.611145	1.349347	1.022574
1	-0.611510	1.351113	-1.019719
5	-3.199230	0.268274	-0.000122
1	-3.278385	0.926276	-1.013709
1	-3.942600	-0.693776	0.000157
1	-3.278579	0.927019	1.012956
7	-1.668343	-0.382992	0.000176
1	-1.648152	-0.986457	-0.820470
1	-1.648489	-0.986941	0.820473
7	0.943932	0.027452	-0.000006
6	1.160538	-0.793217	-1.210526
1	0.479818	-1.646438	-1.196033
1	0.951767	-0.180040	-2.088531
1	2.192254	-1.159265	-1.242588
6	1.160772	-0.795830	1.208681
1	0.952222	-0.184542	2.088061
1	0.480002	-1.648980	1.192481
1	2.192484	-1.161975	1.239743
6	1.905193	1.153574	0.001108
1	1.726787	1.762361	-0.885969
1	1.727348	1.760119	0.889830
1	2.931249	0.771010	0.000305

NH_2Et

7	1.293614	-0.185219	0.000009
1	1.312067	-0.799370	-0.812310
1	1.312007	-0.799482	0.812245
6	0.045401	0.575899	0.000006
1	0.058303	1.233118	0.876325
1	0.058315	1.233114	-0.876314
6	-1.232488	-0.262919	-0.000005
1	-2.128649	0.365958	-0.000013
1	-1.272400	-0.907341	-0.885235
1	-1.272417	-0.907339	0.885226

TS4

5	1.296929	0.790470	0.283808
1	1.480324	1.785422	-0.342673
1	0.961973	0.755740	1.427451
5	3.172810	-0.303784	0.195296
1	3.425739	-1.176607	0.983899
1	3.919853	-0.163621	-0.737061
1	3.038598	0.774610	0.792012
7	1.659086	-0.525942	-0.370795
1	1.215296	-1.353483	0.012086
1	1.614167	-0.546836	-1.383393
7	-0.881632	0.808669	-0.264992
1	-1.180661	1.586652	0.321006
1	-1.110063	1.065843	-1.224349
6	-1.586596	-0.414970	0.122781
1	-1.253803	-1.212908	-0.551662
1	-1.236403	-0.682255	1.126620
6	-3.108611	-0.315245	0.100991
1	-3.569799	-1.260351	0.402842
1	-3.455177	0.463623	0.788148
1	-3.469672	-0.067059	-0.902572

P4

5	0.836021	0.843932	0.264408
1	1.237273	1.851586	-0.254638
1	0.776846	0.856401	1.466851
5	3.218886	-0.323585	0.083961
1	3.666507	-1.386419	-0.300686
1	3.637257	0.622607	-0.546133
1	3.305041	-0.181001	1.283731
7	1.593804	-0.400197	-0.248995
1	1.277291	-1.269487	0.177891
1	1.538914	-0.525664	-1.259333
7	-0.750694	0.746374	-0.216930
1	-1.183661	1.604320	0.132286
1	-0.819070	0.799594	-1.236160

6	-1.516309	-0.425116	0.277442
1	-1.059435	-1.314218	-0.164585
1	-1.346005	-0.466877	1.356128
6	-2.996306	-0.345559	-0.061179
1	-3.517470	-1.228338	0.316979
1	-3.458722	0.536519	0.393054
1	-3.155391	-0.299951	-1.143329

$NHEt_2$

7	-0.079891	-0.701180	0.197634
1	-0.109341	-0.695946	1.216598
6	1.307870	-0.620927	-0.242393
1	1.825562	-1.507744	0.140287
1	1.309274	-0.708929	-1.336169
6	2.075791	0.637003	0.172633
1	3.120649	0.578254	-0.147935
1	1.642475	1.539540	-0.268366
1	2.064340	0.755180	1.262280
6	-0.935556	0.365969	-0.304767
1	-0.622962	1.373866	0.019521
1	-0.861219	0.354241	-1.399879
6	-2.378414	0.124232	0.115639
1	-2.470998	0.137561	1.207519
1	-3.040974	0.897139	-0.284126
1	-2.715710	-0.852574	-0.239837

TS5

5	1.318301	-0.694209	0.517013
1	1.158311	0.023606	1.455727
1	0.976442	-1.833716	0.472059
5	3.471594	-0.717960	0.200964
1	4.019406	-1.579627	-0.435145
1	4.131080	0.233082	0.529754
1	2.924178	-1.212574	1.196501
7	2.170118	-0.189256	-0.629698
1	2.052094	-0.671408	-1.513772
1	2.180769	0.812801	-0.784284
7	-0.713995	-0.051858	-0.239051
1	-0.733023	0.040574	-1.256046
6	-1.598113	-1.155128	0.153518
1	-1.212284	-2.060035	-0.325910
1	-1.465270	-1.298205	1.232481
6	-3.075903	-0.973059	-0.185760
1	-3.631447	-1.884528	0.052674
1	-3.530643	-0.153092	0.376605
1	-3.210176	-0.768992	-1.254251
6	-1.078321	1.236942	0.355449
1	-2.098944	1.541852	0.082138
1	-1.059610	1.101785	1.443479
6	-0.096157	2.328236	-0.046257
1	-0.000525	2.388463	-1.137295
1	-0.441942	3.302885	0.307603
1	0.890210	2.143830	0.387324

P5

5	0.747329	-0.899413	0.417323
1	0.902551	-0.402330	1.501622
1	0.510862	-2.080879	0.437750
5	3.379747	-0.494273	0.228782
1	4.227707	-0.456985	-0.641335
1	3.309527	0.544382	0.861125
1	3.467209	-1.468564	0.942884
7	1.934862	-0.618193	-0.555176
1	2.028089	-1.370718	-1.234783
1	1.858095	0.242188	-1.094153
7	-0.624336	-0.169259	-0.169288
1	-0.585032	-0.168705	-1.193199
6	-1.812064	-0.980039	0.229558
1	-1.653610	-1.974354	-0.190990
1	-1.756037	-1.079695	1.317678
6	-3.151648	-0.410985	-0.215831
1	-3.931913	-1.154030	-0.032625
1	-3.426402	0.495629	0.327667
1	-3.153951	-0.187334	-1.288684
6	-0.743046	1.248534	0.282633
1	-1.644054	1.685247	-0.158525
1	-0.875405	1.201091	1.367252
6	0.473471	2.090551	-0.066591
1	0.632464	2.131565	-1.151003
1	0.300231	3.115904	0.270184
1	1.380328	1.719805	0.421248

NEt_3

7	0.090744	0.011841	0.377461
6	1.495421	0.210941	0.714557
1	1.595897	1.225459	1.117801
1	1.741331	-0.474059	1.535592
6	2.493853	0.009709	-0.430557
1	3.510875	0.243443	-0.101005
1	2.487573	-1.025197	-0.785950
1	2.258507	0.658694	-1.281268
6	-0.198487	-1.343156	-0.069985
1	0.182223	-1.534770	-1.091286
1	0.335027	-2.029461	0.599500
6	-1.687672	-1.664536	-0.028880
1	-2.248635	-1.057973	-0.747153
1	-1.858504	-2.715590	-0.280288
1	-2.087929	-1.470070	0.970216
6	-0.456658	1.049723	-0.499519
1	0.312900	1.809842	-0.682770
1	-0.706273	0.631847	-1.487967
6	-1.679891	1.729447	0.110577
1	-1.413890	2.176408	1.072854
1	-2.061815	2.517125	-0.547641
1	-2.481899	1.008651	0.289979

TS6

5	-1.452493	-0.239918	-0.991049
1	-1.365260	0.797531	-1.571446
1	-1.060386	-1.280999	-1.415255
5	-3.593596	-0.517777	-0.673464
1	-4.071151	-1.592510	-0.419371
1	-4.308984	0.444510	-0.573436
1	-3.073487	-0.541417	-1.795906
7	-2.280638	-0.286925	0.274476
1	-2.107590	-1.073730	0.891261

1	-2.339348	0.566588	0.819175
7	0.596415	0.170997	-0.083957
6	1.472332	-0.415870	-1.111571
1	1.192006	-1.465902	-1.228036
1	1.208964	0.071931	-2.056849
6	2.975120	-0.301230	-0.857094
1	3.521912	-0.789371	-1.668713
1	3.307660	0.739856	-0.812978
1	3.265558	-0.790622	0.078652
6	0.797868	1.626115	-0.007514
1	1.776129	1.852019	0.448266
1	0.827309	1.998002	-1.037499
6	-0.288837	2.382803	0.748740
1	-0.399586	2.040076	1.781965
1	-0.023865	3.443038	0.789852
1	-1.250474	2.304131	0.235429
6	0.755733	-0.452638	1.235395
1	1.705245	-0.141455	1.704439
1	-0.041904	-0.065253	1.878588
6	0.671904	-1.975161	1.210038
1	1.560737	-2.427025	0.761169
1	0.589624	-2.355850	2.231631
1	-0.197831	-2.317701	0.640021

P6

5	-0.901369	-0.298036	-0.950399
1	-1.134873	0.666312	-1.630333
1	-0.615649	-1.283416	-1.581720
5	-3.538719	-0.344721	-0.672595
1	-4.359313	-0.833274	0.079323
1	-3.622110	0.868278	-0.736917
1	-3.515661	-0.870315	-1.763515
7	-2.068877	-0.632366	0.022189
1	-2.053915	-1.613028	0.297673
1	-2.093601	-0.095655	0.886065
7	0.486359	0.143679	-0.119765
6	1.600480	-0.066456	-1.102518
1	1.572317	-1.118258	-1.387725
1	1.315445	0.503919	-1.990851
6	2.992664	0.323348	-0.624641
1	3.704182	0.096270	-1.423030
1	3.081695	1.389357	-0.402258
1	3.302202	-0.244186	0.258256
6	0.425621	1.604415	0.223861
1	1.308062	1.845654	0.827316
1	0.503782	2.138308	-0.726581
6	-0.835627	2.058957	0.943848
1	-0.967394	1.571195	1.915351
1	-0.741038	3.130461	1.140987
1	-1.728977	1.909875	0.329762
6	0.710444	-0.647525	1.127019
1	1.562381	-0.213103	1.662973
1	-0.168230	-0.499762	1.757850
6	0.932805	-2.134173	0.891067
1	1.907600	-2.334792	0.438686
1	0.901447	-2.653511	1.852247
1	0.161394	-2.557135	0.242626

$^{n}PrNH_2$

7	-1.952450	0.024371	-0.000004
1	-2.079097	0.624827	-0.812688
1	-2.079133	0.624721	0.812752
6	-0.592713	-0.509045	-0.000009
1	-0.487901	-1.160340	0.876868
1	-0.487899	-1.160330	-0.876893
6	0.532590	0.526823	0.000001
1	0.420926	1.175390	-0.879513
1	0.420918	1.175381	0.879519
6	1.916943	-0.115998	0.000003
1	2.053825	-0.748273	-0.883753
1	2.710888	0.635833	0.000150
1	2.053708	-0.748492	0.883621

TS7

5	1.687921	0.513506	-0.083280
1	1.386567	0.819047	-1.194821
1	1.312184	1.074511	0.897806
5	3.859062	0.627064	-0.022240
1	4.447088	0.705754	1.024511
1	4.515847	0.453191	-1.015171
1	3.129001	1.617315	-0.169684
7	2.743426	-0.558271	0.086780
1	2.758358	-1.029085	0.984376
1	2.817628	-1.238144	-0.661401
7	-0.147442	-0.784938	-0.020390
1	-0.216730	-1.314587	-0.888768
1	-0.217739	-1.461904	0.738661
6	-1.259480	0.168441	0.063828
1	-1.164883	0.693954	1.020688
1	-1.100967	0.920901	-0.717441
6	-2.650757	-0.445463	-0.067551
1	-2.723954	-0.969765	-1.029611
1	-2.786571	-1.204991	0.713597
6	-3.751085	0.608116	0.033728
1	-3.640440	1.363712	-0.750716
1	-4.742848	0.160273	-0.068374
1	-3.711416	1.122880	0.999190

P7

5	1.340656	-0.472816	-0.000056
1	1.264818	-1.105647	1.020495
1	1.264622	-1.105502	-1.020680
5	4.003753	-0.392304	-0.000027
1	4.871511	0.459489	-0.000466
1	3.993269	-1.055609	1.013426
1	3.992814	-1.056411	-1.012930
7	2.576528	0.455452	-0.000068
1	2.629583	1.059299	-0.819573
1	2.629534	1.059351	0.819404
7	-0.019403	0.476155	0.000144
1	-0.022768	1.089342	0.818686
1	-0.022889	1.089667	-0.818156
6	-1.263317	-0.336491	0.000111
1	-1.210686	-0.982489	-0.880424
1	-1.210852	-0.982306	0.880794
6	-2.529984	0.507733	-0.000097

1	-2.535263	1.161881	0.881283
1	-2.535139	1.161603	-0.881685
6	-3.779345	-0.370894	-0.000046
1	-3.804327	-1.013999	0.884850
1	-4.686156	0.238008	-0.000298
1	-3.804112	-1.014412	-0.884647

^{n}Pr$_2$NH

7	-0.047766	1.010977	-0.092293
1	-0.059674	1.245058	-1.084032
6	1.322210	0.735644	0.319075
1	1.910445	1.646221	0.146043
1	1.316093	0.573614	1.405876
6	2.021692	-0.445728	-0.361954
1	1.485933	-1.375947	-0.138574
1	1.972259	-0.309516	-1.451035
6	-0.985239	-0.076537	0.150015
1	-0.755070	-0.998204	-0.414998
1	-0.915796	-0.340883	1.214558
6	-2.410523	0.357968	-0.170655
1	-2.462022	0.662128	-1.224985
1	-2.643333	1.248654	0.422332
6	-3.426577	-0.749390	0.094051
1	-4.442981	-0.425517	-0.145990
1	-3.206780	-1.637749	-0.507792
1	-3.411257	-1.050143	1.147097
6	3.476664	-0.573222	0.082070
1	3.974250	-1.417669	-0.402618
1	4.040990	0.333643	-0.160652
1	3.541933	-0.722941	1.165216

TS8

5	1.315319	-1.425308	0.515561
1	1.404369	-0.672034	1.435783
1	0.579022	-2.360021	0.475777
5	3.318841	-2.244177	0.284006
1	3.540808	-3.262186	-0.317590
1	4.265121	-1.585186	0.627384
1	2.596410	-2.481310	1.262189
7	2.325451	-1.304295	-0.606910
1	2.062855	-1.738935	-1.484506
1	2.707426	-0.381281	-0.781852
7	-0.319243	-0.103211	-0.322617
1	-0.297066	-0.068696	-1.342822
6	-1.550844	-0.776094	0.103596
1	-1.544653	-1.776622	-0.343937
1	-1.474632	-0.925336	1.188772
6	-2.862466	-0.069399	-0.239541
1	-2.925518	0.888680	0.288359
1	-2.879401	0.160741	-1.313771
6	-0.183294	1.260153	0.194687
1	-1.001762	1.914574	-0.144634
1	-0.253076	1.197740	1.288430
6	1.149711	1.888543	-0.195790
1	1.295682	1.785095	-1.280955
1	1.959461	1.340981	0.298270
6	1.213540	3.363612	0.191425
1	2.179258	3.802131	-0.072375
1	0.431546	3.937133	-0.316714
1	1.072832	3.487765	1.269956
6	-4.067600	-0.932206	0.128350
1	-5.007555	-0.424906	-0.103953
1	-4.052280	-1.881161	-0.417608
1	-4.067374	-1.164858	1.198286

P8

5	0.771795	-1.381068	0.442823
1	1.075326	-0.893317	1.499857
1	0.194379	-2.435866	0.524735
5	3.402652	-1.798198	0.264544
1	4.218197	-2.068905	-0.595282
1	3.653181	-0.752211	0.836482
1	3.194993	-2.710628	1.033729
7	1.984397	-1.523810	-0.529802
1	1.843232	-2.305502	-1.166796
1	2.169572	-0.710793	-1.114121
7	-0.323268	-0.308879	-0.198215
1	-0.299188	-0.386233	-1.219529
6	-1.694368	-0.696552	0.242346
1	-1.846594	-1.722105	-0.103215
1	-1.664754	-0.729470	1.336729
6	-2.818896	0.203234	-0.257106
1	-2.760081	1.191875	0.209128
1	-2.716867	0.353629	-1.340847
6	-0.003360	1.104793	0.158644
1	-0.732729	1.767443	-0.320246
1	-0.132533	1.175279	1.243643
6	1.406421	1.530245	-0.226369
1	1.546855	1.401960	-1.309582
1	2.142339	0.901119	0.286774
6	1.637232	2.995600	0.138970
1	2.648961	3.304597	-0.132550
1	0.931030	3.654867	-0.376911
1	1.520138	3.149198	1.216260
6	-4.178138	-0.422388	0.052028
1	-4.992277	0.223842	-0.284325
1	-4.288014	-1.391647	-0.443994
1	-4.298646	-0.581577	1.128262

^{n}Pr$_3$N

7	0.000373	-0.000143	0.175220
6	-0.998585	-0.965813	-0.275241
1	-1.972677	-0.635697	0.099793
1	-1.072023	-0.977851	-1.383593
6	1.336746	-0.381545	-0.273904
1	1.537704	-1.390814	0.099429
1	1.386019	-0.436217	-1.382317
6	-0.336857	1.348374	-0.273072
1	0.434827	2.027287	0.103801
1	-0.310054	1.420108	-1.381274
6	-0.770567	-2.388501	0.232369
1	0.074274	-2.855329	-0.285107
1	-0.508710	-2.337848	1.296045
6	2.454371	0.525696	0.237846
1	2.432874	1.494591	-0.272366
1	2.281646	0.718483	1.303454

6	-1.683940	1.860757	0.233722
1	-2.509500	1.360040	-0.283162
1	-1.770885	1.610958	1.297973
6	-2.013640	-3.252152	0.030331
1	-1.841137	-4.281519	0.356252
1	-2.863068	-2.857490	0.597557
1	-2.303529	-3.280301	-1.025726
6	-1.812043	3.368649	0.028442
1	-2.790008	3.734055	0.353231
1	-1.045781	3.908798	0.594087
1	-1.691507	3.631019	-1.028362
6	3.824261	-0.115654	0.026809
1	4.629519	0.545159	0.359026
1	3.908776	-1.054968	0.583072
1	3.992137	-0.340336	-1.032161

TS9

7	0.342807	0.001313	-0.352976
6	1.476224	-0.938621	-0.365103
1	1.094916	-1.912659	-0.044076
1	1.856404	-1.058280	-1.398123
6	0.808553	1.368316	-0.625817
1	1.503647	1.641635	0.173151
1	1.375102	1.390011	-1.576997
6	-0.671323	-0.409356	-1.331667
1	-1.547303	0.235305	-1.195749
1	-0.306124	-0.230373	-2.361336
6	2.632247	-0.561286	0.558153
1	3.178869	0.298859	0.157202
1	2.233039	-0.267385	1.534853
6	-0.282247	2.433706	-0.670758
1	-0.964441	2.263833	-1.510574
1	-0.872672	2.382809	0.251770
6	-1.123886	-1.864642	-1.208032
1	-0.356074	-2.535207	-1.606850
1	-1.239838	-2.128373	-0.149127
6	3.593612	-1.737313	0.717727
1	4.452999	-1.463066	1.334850
1	3.094503	-2.587048	1.194344
1	3.972688	-2.072367	-0.254052
6	-2.433294	-2.092883	-1.960309
1	-2.733543	-3.143036	-1.925287
1	-3.246808	-1.496790	-1.531096
1	-2.335243	-1.806422	-3.012853
6	0.333549	3.825930	-0.800287
1	-0.439853	4.596359	-0.854158
1	0.974957	4.051614	0.057332
1	0.944668	3.899893	-1.706046
5	-0.504983	-0.086374	1.778382
1	-0.092559	-1.199886	1.881058
1	0.109655	0.897579	2.050257
5	-2.253513	-0.027896	3.091995
1	-2.704040	1.021605	3.470213
1	-2.903067	-1.018152	3.304558
1	-1.104303	-0.174902	3.523135
7	-1.978931	0.076996	1.480085
1	-2.274376	0.970232	1.101231
1	-2.426460	-0.675706	0.967280

P9

7	0.308718	0.018322	-0.216953
6	1.790441	-0.221881	-0.195013
1	1.932002	-1.204964	0.257153
1	2.134379	-0.272189	-1.238981
6	0.048192	1.355210	-0.842277
1	0.633250	2.080366	-0.275691
1	0.439371	1.324167	-1.869943
6	-0.313460	-1.042202	-1.068104
1	-1.389351	-0.858528	-1.082438
1	0.049779	-0.903401	-2.096060
6	2.626882	0.787522	0.584487
1	2.637708	1.759200	0.080870
1	2.194357	0.934267	1.577399
6	-1.401251	1.829858	-0.839864
1	-2.054883	1.127006	-1.369982
1	-1.755967	1.916273	0.193642
6	-0.060500	-2.478910	-0.616075
1	0.961678	-2.780134	-0.865504
1	-0.153510	-2.551851	0.472596
6	4.061806	0.274030	0.705556
1	4.689338	0.999463	1.228644
1	4.095681	-0.665099	1.266527
1	4.505974	0.095813	-0.279864
6	-1.047456	-3.425446	-1.297657
1	-0.840805	-4.464185	-1.029868
1	-2.077436	-3.200086	-1.001449
1	-0.986756	-3.341888	-2.387979
6	-1.494363	3.196538	-1.519263
1	-2.524695	3.559141	-1.514446
1	-0.878527	3.934879	-0.996316
1	-1.157107	3.149268	-2.559969
5	-0.256202	0.005357	1.363156
1	0.410418	-0.812096	1.948156
1	-0.104471	1.133911	1.747090
5	-2.493963	0.149561	2.782870
1	-3.575218	-0.405524	2.819750
1	-1.773721	-0.144287	3.711438
1	-2.588120	1.351805	2.618842
7	-1.755830	-0.407043	1.414955
1	-2.332280	-0.043763	0.658828
1	-1.872225	-1.419424	1.400668

^{i}PrNH$_2$

7	0.015708	-0.657041	0.072881
1	-0.145314	-1.340553	-0.668068
6	-1.219085	0.108223	0.258416
1	-1.095700	0.699268	1.175160
6	-1.558523	1.062814	-0.891499
1	-2.511003	1.570455	-0.707205
1	-0.791186	1.831518	-1.026004
1	-1.648306	0.506190	-1.832862
6	1.223572	0.100167	-0.257569
1	1.114422	0.667612	-1.199748
6	2.366141	-0.894661	-0.434764
1	2.138735	-1.620510	-1.223661
1	3.292838	-0.380741	-0.707431

1	2.526352	-1.444787	0.497638
6	1.546444	1.091744	0.856367
1	0.796081	1.884842	0.933193
1	1.589294	0.564805	1.815717
1	2.514815	1.567005	0.672924
6	-2.354073	-0.883906	0.491015
1	-3.285211	-0.366578	0.739689
1	-2.533996	-1.476914	-0.414896
1	-2.098634	-1.568604	1.303588

TS10

5	-1.419718	0.477709	-0.021572
1	-1.260359	1.160410	0.940322
1	-1.008753	0.727555	-1.111911
5	-3.580609	0.311800	-0.246173
1	-4.071402	-0.033071	-1.289132
1	-4.308372	0.398951	0.707700
1	-2.963302	1.373908	-0.402753
7	-2.354657	-0.704479	0.118371
1	-2.249047	-1.444425	-0.566524
1	-2.440499	-1.101302	1.047361
7	0.520797	-0.618601	0.408831
1	0.719792	-0.582379	1.409633
1	0.468371	-1.607789	0.164013
6	1.634601	0.008109	-0.326712
1	1.321073	0.038952	-1.377428
6	2.934722	-0.786302	-0.214396
1	3.731508	-0.320378	-0.802728
1	3.267740	-0.829070	0.829593
1	2.806781	-1.813098	-0.574316
6	1.806879	1.437843	0.169957
1	2.605682	1.941119	-0.381724
1	0.881954	2.005661	0.050354
1	2.080287	1.441074	1.232758

P10

5	-1.008696	0.374569	-0.136513
1	-0.989579	1.326942	0.595203
1	-0.909654	0.609342	-1.313939
5	-3.671809	0.257782	-0.139471
1	-3.638576	0.577821	-1.307121
1	-4.529862	-0.569467	0.101476
1	-3.699230	1.201293	0.619867
7	-2.236251	-0.519659	0.158844
1	-2.269973	-1.362784	-0.413488
1	-2.296723	-0.817514	1.131921
7	0.352614	-0.504990	0.228551
1	0.461322	-0.568081	1.244839
1	0.227326	-1.465193	-0.102136
6	1.625118	0.024240	-0.355220
1	1.440414	0.065265	-1.432849
6	2.776247	-0.926579	-0.052103
1	3.694013	-0.567728	-0.525106
1	2.958433	-0.986161	1.027275
1	2.578900	-1.936503	-0.427419
6	1.881099	1.429631	0.167913
1	2.824796	1.802941	-0.238386
1	1.078445	2.110736	-0.117064
1	1.963148	1.426127	1.261551

$^{i}Pr_2NH$

7	0.015708	-0.657041	0.072881
1	-0.145314	-1.340553	-0.668068
6	-1.219085	0.108223	0.258416
1	-1.095700	0.699268	1.175160
6	-1.558523	1.062814	-0.891499
1	-2.511003	1.570455	-0.707205
1	-0.791186	1.831518	-1.026004
1	-1.648306	0.506190	-1.832862
6	1.223572	0.100167	-0.257569
1	1.114422	0.667612	-1.199748
6	2.366141	-0.894661	-0.434764
1	2.138735	-1.620510	-1.223661
1	3.292838	-0.380741	-0.707431
1	2.526352	-1.444787	0.497638
6	1.546444	1.091744	0.856367
1	0.796081	1.884842	0.933193
1	1.589294	0.564805	1.815717
1	2.514815	1.567005	0.672924
6	-2.354073	-0.883906	0.491015
1	-3.285211	-0.366578	0.739689
1	-2.533996	-1.476914	-0.414896
1	-2.098634	-1.568604	1.303588

TS11

5	1.498560	-1.046913	0.018830
1	1.081272	-1.346456	1.092411
1	1.362636	-1.685311	-0.974814
5	3.712792	-1.024267	0.307697
1	4.464912	-1.059251	-0.631864
1	4.182193	-0.713616	1.372186
1	3.091781	-2.081690	0.402704
7	2.517461	0.057483	-0.045442
1	2.661492	0.478089	-0.956700
1	2.458961	0.781572	0.662025
7	-0.534488	-0.019433	-0.416237
1	-0.628371	-0.169495	-1.422763
6	-1.529217	-0.892404	0.254150
1	-1.224660	-0.958196	1.305984
6	-2.970099	-0.375790	0.184114
1	-3.645531	-1.114364	0.625414
1	-3.115380	0.564276	0.723121
1	-3.275661	-0.224269	-0.858698
6	-0.705983	1.423965	-0.159992
1	-1.735042	1.728154	-0.403235
6	0.214575	2.236345	-1.066726
1	0.137362	1.908567	-2.109460
1	-0.064477	3.293171	-1.028461
1	1.259789	2.160594	-0.758790
6	-0.456162	1.734768	1.312238
1	-1.203777	1.270530	1.961913
1	0.526160	1.363720	1.622418
1	-0.489569	2.814973	1.481776
6	-1.457244	-2.291350	-0.352931
1	-2.187635	-2.945770	0.130887
1	-1.701355	-2.255182	-1.422575

1	-0.467893	-2.733712	-0.239485

P11

5	0.941504	-0.982376	0.120893
1	0.773285	-1.192212	1.295270
1	0.892304	-1.946494	-0.592035
5	3.572525	-1.263957	0.227154
1	3.510725	-2.175928	-0.567926
1	4.555529	-0.564891	0.070129
1	3.424041	-1.615072	1.377290
7	2.290403	-0.268921	-0.118349
1	2.435392	0.021349	-1.083806
1	2.436382	0.552885	0.463907
7	-0.410124	-0.077075	-0.342097
1	-0.497209	-0.209358	-1.354462
6	-1.633299	-0.735495	0.263090
1	-1.445911	-0.744430	1.340059
6	-2.929461	0.020547	-0.032401
1	-3.772121	-0.589475	0.302243
1	-3.001914	0.979957	0.484888
1	-3.054688	0.191120	-1.108813
6	-0.383501	1.411626	-0.120294
1	-1.373746	1.779003	-0.400705
6	0.596263	2.120994	-1.055979
1	0.548350	1.716472	-2.073406
1	0.316489	3.176741	-1.111693
1	1.630092	2.076754	-0.714629
6	-0.144178	1.743595	1.346120
1	-0.937781	1.348351	1.986472
1	0.805602	1.337035	1.702428
1	-0.123633	2.830076	1.468962
6	-1.749793	-2.178260	-0.225209
1	-2.683764	-2.602801	0.151976
1	-1.783783	-2.217231	-1.321181
1	-0.921931	-2.796245	0.115959

$^{i}Pr_2MeN$

7	0.043653	0.436741	-0.269119
6	-0.159365	1.726378	0.377189
1	0.595070	2.441200	0.041183
1	-1.131093	2.137159	0.098179
1	-0.111269	1.673202	1.480163
6	1.266923	-0.209642	0.230533
1	1.221334	-0.318550	1.332943
6	2.488077	0.654517	-0.097848
1	2.494339	1.599993	0.449004
1	3.405816	0.120799	0.165484
1	2.504915	0.872916	-1.170944
6	1.468634	-1.599617	-0.374252
1	2.464753	-1.969406	-0.115731
1	0.744483	-2.331858	-0.007567
1	1.392659	-1.548413	-1.466057
6	-1.155956	-0.417289	-0.221615
1	-0.898331	-1.323500	-0.776792
6	-1.590019	-0.828148	1.191346
1	-2.457357	-1.494658	1.146406
1	-0.790837	-1.352578	1.725776
1	-1.875226	0.048609	1.783321
6	-2.319698	0.219808	-0.982861
1	-1.967326	0.633476	-1.931935
1	-3.080881	-0.538179	-1.191658
1	-2.808200	1.016567	-0.412892

TS12

7	-0.432709	-0.013034	0.269636
6	-0.275024	0.207856	1.706994
1	0.335665	-0.587744	2.139073
1	0.237854	1.152707	1.891832
1	-1.236574	0.224490	2.244882
6	-1.252569	-1.235265	0.033221
1	-2.252849	-1.069035	0.468402
6	-0.674321	-2.464234	0.740916
1	-0.742478	-2.389609	1.828811
1	-1.251285	-3.344613	0.444643
1	0.368485	-2.634302	0.462444
6	-1.420310	-1.520483	-1.459787
1	-1.940996	-2.473557	-1.586789
1	-2.012233	-0.757418	-1.971383
1	-0.447210	-1.593219	-1.952760
6	-1.007526	1.178855	-0.421133
1	-0.899590	0.966911	-1.488952
6	-2.487769	1.440800	-0.116362
1	-2.802366	2.361284	-0.617098
1	-3.141894	0.637344	-0.464284
1	-2.654349	1.578201	0.957941
6	-0.206477	2.453763	-0.151589
1	0.866917	2.296138	-0.279280
1	-0.510262	3.217011	-0.873536
1	-0.396196	2.861471	0.846459
5	1.658235	-0.295841	-0.715034
1	1.535372	-1.471130	-0.821241
1	1.352626	0.484077	-1.558335
5	3.865798	-0.011131	-0.520490
1	4.336201	1.081105	-0.709899
1	4.575423	-0.827173	0.008861
1	3.392228	-0.461546	-1.563336
7	2.524627	0.182468	0.419931
1	2.414644	1.147338	0.713414
1	2.553251	-0.417665	1.237232

P12

7	0.361772	-0.029906	0.203679
6	0.310713	-0.198040	1.675554
1	0.117129	0.769494	2.139370
1	-0.499040	-0.880836	1.935992
1	1.251690	-0.603820	2.056956
6	1.676223	0.649245	-0.186406
1	2.442624	-0.127196	-0.091909
6	2.067356	1.790891	0.752296
1	2.274646	1.457905	1.771362
1	2.987450	2.237122	0.365057
1	1.300222	2.567581	0.775793
6	1.676012	1.158516	-1.628249
1	2.703165	1.435722	-1.882930
1	1.342484	0.417020	-2.355911
1	1.041028	2.039867	-1.730413

6	0.298554	-1.397334	-0.471987
1	0.580350	-1.197105	-1.507000
6	1.268980	-2.419559	0.127148
1	1.293385	-3.291775	-0.531493
1	2.295604	-2.060126	0.226047
1	0.927765	-2.764868	1.108148
6	-1.105856	-1.998758	-0.495207
1	-1.839575	-1.349873	-0.979073
1	-1.057964	-2.931548	-1.064663
1	-1.452772	-2.268265	0.509702
5	-0.904601	0.938883	-0.306937
1	-0.569621	2.073734	-0.083674
1	-1.040310	0.683589	-1.471914
5	-3.555050	1.012840	-0.364260
1	-3.607402	0.160590	-1.232536
1	-4.482216	0.940902	0.418957
1	-3.392497	2.126319	-0.812957
7	-2.203199	0.655377	0.509280
1	-2.341755	-0.305870	0.810816
1	-2.238031	1.224763	1.352646

$^{i}Pr_2EtN$

7	0.044896	0.133941	-0.129303
6	-0.235936	1.323416	0.685639
1	-1.222693	1.237853	1.155081
1	0.473327	1.383507	1.522343
6	1.310147	-0.512859	0.245071
1	1.317557	-0.760984	1.325149
6	2.474475	0.443568	-0.024827
1	2.387448	1.377804	0.536237
1	3.422455	-0.024852	0.257790
1	2.506300	0.688392	-1.091900
6	1.554286	-1.804413	-0.534774
1	2.571313	-2.157945	-0.342034
1	0.868851	-2.608503	-0.254582
1	1.454554	-1.618448	-1.610000
6	-1.109266	-0.766455	-0.264547
1	-0.807072	-1.546422	-0.970006
6	-1.534826	-1.454364	1.040243
1	-2.350801	-2.160513	0.855096
1	-0.703383	-2.009968	1.486927
1	-1.887654	-0.727158	1.779729
6	-2.284852	-0.041469	-0.919758
1	-1.963837	0.428101	-1.853861
1	-3.085393	-0.754088	-1.141774
1	-2.707340	0.733430	-0.271066
6	-0.185183	2.610135	-0.133287
1	-0.385458	3.485817	0.493722
1	0.795648	2.732324	-0.601379
1	-0.931163	2.578708	-0.932911

TS13

7	0.547568	-0.006978	0.153335
6	0.688709	-0.036315	1.632992
1	0.760276	-1.072568	1.970386
1	1.646497	0.423505	1.912735
6	1.464978	1.045918	-0.388591
1	2.486204	0.811164	-0.042677
6	1.134615	2.433926	0.164807
1	1.204920	2.479237	1.254522
1	1.857175	3.151315	-0.234840
1	0.135061	2.756828	-0.134458
6	1.493428	1.095631	-1.916263
1	2.102241	1.949981	-2.225880
1	1.942273	0.203571	-2.360575
1	0.491282	1.226422	-2.330977
6	0.848632	-1.347233	-0.437319
1	0.737217	-1.223701	-1.516918
6	2.271985	-1.849971	-0.164279
1	2.419826	-2.813018	-0.661392
1	3.032593	-1.163961	-0.547076
1	2.455991	-2.000569	0.905023
6	-0.187011	-2.397980	-0.029931
1	-1.159230	-2.192157	-0.483201
1	0.133205	-3.378513	-0.393930
1	-0.308518	-2.483726	1.055043
6	-0.447291	0.636098	2.400398
1	-0.133678	0.842870	3.428349
1	-0.746109	1.580813	1.937782
1	-1.323471	-0.015535	2.453996
5	-3.838510	0.037690	-0.934181
1	-4.039584	-1.101289	-1.277690
1	-4.754129	0.598085	-0.385806
5	-1.573346	0.451168	-0.854709
1	-1.413101	1.624460	-0.921435
1	-1.250072	-0.304195	-1.710314
1	-3.395547	0.708394	-1.857591
7	-2.578609	-0.020498	0.147992
1	-2.744481	0.620270	0.916235
1	-2.468543	-0.960084	0.514962

P13

7	-0.360876	0.087430	0.048307
6	-0.346732	-0.163915	1.531789
1	0.358353	0.552908	1.956786
1	-1.334280	0.113144	1.914991
6	-1.696563	-0.362945	-0.550136
1	-2.426893	0.372921	-0.199529
6	-2.175024	-1.729139	-0.061876
1	-2.314851	-1.778018	1.019696
1	-3.149912	-1.914431	-0.521929
1	-1.499669	-2.527284	-0.376982
6	-1.706721	-0.360596	-2.080455
1	-2.742151	-0.508383	-2.401828
1	-1.353356	0.570169	-2.525924
1	-1.100851	-1.176282	-2.477791
6	-0.242754	1.601099	-0.172883
1	-0.499062	1.735231	-1.224048
6	-1.203776	2.435563	0.682074
1	-1.177925	3.461607	0.305376
1	-2.244600	2.106606	0.646040
1	-0.889096	2.469168	1.729446
6	1.176311	2.138897	0.007971
1	1.903605	1.655894	-0.648711
1	1.158274	3.203531	-0.243475
1	1.515960	2.074730	1.048869

6	0.037263	-1.578959	1.995594
1	-0.699650	-1.960076	2.706665
1	0.098597	-2.285557	1.168554
1	1.005528	-1.571044	2.501753
5	3.532561	-0.666673	-0.907728
1	3.548955	0.444035	-1.405608
1	4.476930	-0.859262	-0.166169
5	0.869959	-0.685343	-0.778140
1	0.511291	-1.820008	-0.969449
1	0.993706	-0.051564	-1.789799
1	3.387010	-1.541974	-1.733042
7	2.194468	-0.710938	0.050700
1	2.264034	-1.570047	0.591216
1	2.310288	0.048589	0.718712