Electronic Supplementary Material (ESI) for Chemical Communications

Hydrogen activation with perfluorinated organoboranes: 1,2,3-*tris*(pentafluorophenyl)-4,5,6,7-tetrafluoro-1-boraindene

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General Experimental Details

Unless explicitly stated otherwise, all operations were carried out under a purified argon atmosphere using either glovebox or vacuum line techniques. Dichloromethane was dried over and distilled from CaH_2, then distilled from molecular sieves after at least three days. Toluene, hexanes and benzene were dried over and distilled from Na/benzophenone. Hydrogen and argon were purchased from PRAXAIR and passed through a Matheson TriGas® cartridge (model M641-02) prior to use. All NMR analysis (^{1}H, ^{11}B, ^{13}C, ^{19}F, ^{31}P) were performed on either a Bruker 400 MHz or 600 MHz instrument. X-ray crystallography analyses were performed on suitable crystals coated in Paratone oil and mounted on a Nonius Kappa CCD diffractometer.

Starting Materials

All reagents were purchased from either Aldrich or Strem Chemicals. 1,2,3,4-tetrafluorobenzene was dried over molecular sieves and degassed prior to use. *Bis*(pentafluorophenyl)acetylene[1] and *bis*(pentafluorophenyl)zinc[2] were prepared as previously reported. Boron tribromide was purchased from Aldrich, distilled into a Kontes bomb and stored over copper wire. All other reagents were used as received.

Synthesis of $Cp_2Zr(o\text{-}C_6HF_4)_2$. A 250 mL, two-neck round-bottom flask (rbf) was charged with 1,2,3,4-tetrafluorobenzene (3.00 g, 20.0 mmol) and THF (80 mL). The solution was cooled to -78ºC and n-butyllithium (2.5 M in hexanes, 8.0 mL, 20.0 mmol) was added via syringe pump over 1.5 hours. WARNING! Do not let the solution warm above -30ºC lest you risk the explosive elimination of LiF. The now black solution was allowed to stir for an additional 1.5 hours at -78ºC. A 250 mL, three-neck rbf was charged with zirconocene dichloride (2.915 g, 10.0 mmol) and THF (90 mL), and kept at -78ºC. A bubbler was connected to this flask, and the solution of (2,3,4,5-tetrafluorophenyl)lithium was transferred into it via cannula over one hour (the cannula was initially cooled down with a piece of dry ice). The temperature was maintained at -78ºC for 3 hours and then allowed to gradually warm to room temperature overnight (i.e. the cold bath was left in place). The solvent was removed in vacuo and the remaining grey solid was washed with hexanes (2 x 10 mL), taken up in CH_2Cl_2 (120 mL) and filtered through a swivel frit. The LiCl was washed with CH_2Cl_2, and the solvent was removed in vacuo. The resulting brown solid (4.30 g, 8.30 mmol, 83.0 % crude yield) was ~90% pure **$Cp_2Zr(o\text{-}C_6HF_4)_2$** by ^{1}H and ^{19}F NMR, which is sufficiently pure for the subsequent synthetic steps. Pure **$Cp_2Zr(o\text{-}C_6HF_4)_2$** was obtained by recrystallization from layered CH_2Cl_2 and hexanes at -30ºC as a light brown solid (2.39 g, 4.61 mmol, 46.1 % yield). Crystals suitable for X-ray analysis were obtained from CH_2Cl_2 and hexanes at -30°C. ^{1}H NMR (400 MHz, CD_2Cl_2) δ 6.57 (m, 2H, $Zr(C_6F_4\mathit{H})_2$), 6.37 (s, 10H, Cp-*H*). $^{19}F\{^{1}H\}$ NMR (376 MHz, CD_2Cl_2) δ -116.02 (ddd, J = 31.8, 16.7, 4.1 Hz), -143.25 (dd, J = 19.6, 16.8 Hz), -160.25 (dd, J = 31.8, 18.5 Hz), -161.62 (td, J = 19.1, 4.1 Hz). $^{13}C\{^{1}H\}$ NMR (101 MHz, CD_2Cl_2) δ 156.31 (m), 148.77 (dm, $^{1}J_{CF}$ =221.2 Hz), 147.27 (ddd, J = 251.5, 9.7, 2.8 Hz), 140.02 (dddd, J = 259.6, 27.2, 11.8, 2.2 Hz), 138.80 (dddd, J = 249.5, 17.6, 12.7, 5.1 Hz), 114.27 (dddd, J = 22.1, 14.3, 5.4, 1.9 Hz), 113.55 (s). Elemental analysis (%) for $C_{22}H_{12}F_8Zr$: Calculated: C 50.86, H 2.33; Found C 50.43, H 2.45.

Synthesis of 4. In a Kontes bomb, **$Cp_2Zr(o\text{-}C_6HF_4)_2$** (2.38 g, 4.60 mmol) and $[(C_6F_5)C]_2$ (1.64 g, 4.61 mmol) were taken up in toluene (30 mL). The mixture was stirred and heated at 110ºC for

40 hours, after which time it was allowed to cool to room temperature. The solvent was reduced to a volume of ca. 5 mL and decanted. The solids were washed with hexanes (3 x 6 mL) and dried in vacuo to give a yellow powder (2.10 g, 2.89 mmol, 62.7 % yield). Crystals suitable for x-ray analysis were obtained from toluene at -30ºC. ^{1}H NMR (400 MHz, CD_2Cl_2) δ 6.57 (s, 1H, Cp^{H}). ^{19}F NMR (376 MHz, CD_2Cl_2) δ -122.85 (dd, J = 34.0, 17.2 Hz, 1F), -141.01 (m, 2F, *o*-C_6F_5), -142.02 (td, J = 17.6, 2.6 Hz, 1F), -142.34 (m, 2F, *o*-C_6F_5), -156.85 (t, J = 20.7 Hz, 1F), -158.61 (t, J = 18.3 Hz, 1F), -159.09 (ddd, J = 34.0, 18.5, 2.7 Hz, 1F), -159.73 (t, J = 20.9 Hz, 1F), -162.68 (ddd, J = 23.3, 20.5, 7.4 Hz, 2F, *m*-C_6F_5), -163.74 (ddd, J = 23.3, 20.2, 7.8 Hz, 2F, *m*-C_6F_5). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 185.84 (s, Zr-C^{vinyl}), 157.00 (d, J = 62.1 Hz, Zr-C^{aryl}), 147.63 (dt, J = 6.9, 3.3 Hz), 146.54 – 145.87 (m), 145.45 (dt, J = 6.8, 3.2 Hz), 145.37 – 144.94 (m), 143.86 – 143.42 (m), 143.09 – 142.23 (m), 142.14 – 141.58 (m), 141.15 – 140.38 (m), 140.31 – 138.06 (m), 137.76 – 137.20 (m), 137.17 – 135.95 (m), 130.10 (s, Zr-C=C^{vinyl}), 126.19 (dd, J = 22.5, 5.5 Hz), 114.90 (s, C^{Cp}). Elemental analysis (%) for $C_{30}H_{10}F_{14}Zr$: Calculated: C 49.52, H 1.39; Found C 49.26, H 1.58.

Synthesis of 5. In a Kontes bomb, **4** (2.55 g, 3.51 mmol), CuCl (0. 695 g, 7.02 mmol) and Me_2SnCl_2 (0.848 g, 3.86 mmol) were taken up in THF (15 mL) and the resulting slurry was stirred at 80ºC for 48 hours. The solvent was removed in vacuo and the excess Me_2SnCl_2 was sublimed out of the flask at 55ºC for 1 hour. Under ambient conditions, the remaining brown solids were taken up in wet CH_2Cl_2 and passed through Florisil (60 mL). Removal of the solvent gave a light yellow solid. Under an argon atmosphere, this solid was recrystallized from hot (dry) hexanes, the mother liquor was decanted. the solid washed with cold hexanes (2 x 5 mL) and dried in vacuo to give an off-white solid (1.62 g, 2.47 mmol, 71.3 % yield). Crystals suitable for x-ray analysis were obtained by slow evaporation from CH_2Cl_2. ^{1}H NMR (400 MHz, CD_2Cl_2) δ 0.78 (s, $^{2}J_{SnH}$ = 64.8 Hz, 62.8 Hz, 6H). ^{19}F NMR (376 MHz, CD_2Cl_2) δ -119.53 (ddd, J = 28.3, 16.8, 3.4 Hz, Ar^{F}), -140.95 (m, 4F, *o*-C_6F_5), -141.21 (td, J = 17.6, 4.5 Hz, 1F, Ar^{F}), -152.80 (td, J = 18.3, 3.4 Hz, 1F, Ar^{F}), -153.25 (ddd, J = 28.3, 18.1, 4.6 Hz, 1F, Ar^{F}), -154.27 (t, J = 20.7 Hz, 1F, *p*-C_6F_5), -156.52 (t, J = 20.8 Hz, 1F, *p*-C_6F_5), -162.25 (m, 2F, *m*-C_6F_5), -162.55 (m, 2F, *m*-C_6F_5). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 150.83 (m), 148.48 (m), 147.96 (m), 145.36 (m), 143.99 (m), 143.54 (m), 142.95 (m), 142.21 – 141.38 (m), 140.91 (d, J = 7.7 Hz), 140.36 (m), 139.64 – 138.84 (m), 138.38 (m), 136.72 (m), 128.59 (m), -6.82 (s, $^{1}J_{SnC}$ = 189, 197 Hz, Sn-CH_3). Elemental analysis (%) for $C_{22}H_6F_{14}Sn$: Calculated: C 40.34, H 0.92; Found C 40.38, H 1.16.

Synthesis of 6. In a Kontes bomb, BBr_3 (ca. 3 mL) was condensed into a slurry of **5** (528 mg, 0.806 mmol) in CH_2Cl_2 (3 mL) and the resulting yellow mixture was allowed to stir at room temperature for 16 hours. The solvent and excess BBr_3 were removed in vacuo, and Me_2SnBr_2 was sublimed out of the product mixture at 60ºC for one hour. The crude solid was recrystallized from hot hexanes at -30ºC. The mother liquor was decanted and the solid washed with cold hexanes (2 x 2 mL). A yellow powder was obtained (440 mg, 0.738 mmol, 91.6% yield). Yellow crystals suitable for x-ray analysis were obtained from hexanes at -30ºC. ^{19}F NMR (376 MHz, CD_2Cl_2) δ = -123.84 (dt, J=21.6, 12.6, 1F, Ar^{F}), -137.98 (m, 4F, *o*-C_6F_5), -142.29 (m, 1F), -143.13 (dt, J=18.5, 13.1, 1F), -150.52 (m, 2F, Ar^{F}), -153.39 (t, J=20.8, 1F, *p*-C_6F_5), -160.78 (m, 2F, *m*-C_6F_5), -161.49 (m, 2F, *m*-C_6F_5). ^{11}B NMR (128 MHz, CD_2Cl_2) δ = 61 ppm (br). ^{13}C NMR (101 MHz, CD_2Cl2) δ, 151.83 , 150.92 (dd, J =254, 11.7 Hz), 147.48 (ddd, J = 17.8, 13.3, 4.3 Hz), 145.17 (m), 144.91 – 144.52 (m), 144.39 – 143.74 (m), 143.21 – 142.86

(m), 142.70 (m), 142.06 (m), 141.81 – 141.05 (m), 140.72 – 140.16 (m), 138.26 (dm, J = 251 Hz), 129.70 (m), 109.98 – 108.57 (m). $C_{20}BBrF_{14}$ Calculated: C 40.24; Found C 40.17. Comment: Four repeat trials found %C to be 40.17, 40.08, 40.08, 39.70, however the analysis was plagued by high %N values of 4.70, 1.29, 2.59, 2.20. The fact that the %C values are so consistent while the %N values are not, combined with the complete absence of nitrogen in the synthesis of this compound, lead us to believe that the sample is in fact pure. ^{19}F and ^{13}C NMR can be found in figures S5 and S6.

Synthesis of 3. A solution of $Zn(C_6F_5)_2$ (134 mg, 0.336 mmol) in CH_2Cl_2 (5 mL) was added dropwise over ~ 1 min to a stirred solution of **6** (400 mg, 0.671 mmol) in CH_2Cl_2 (5 mL). The orange-yellow solution quickly turned bright red and was allowed to stir at room temperature for 16 hours. The precipitated $ZnCl_2$ was filtered off via syringe filter and the solvent removed *in vacuo* to yield **3** as an orange powder (436 mg, 0.637 mmol, 95.0% yield). Red crystals suitable for x-ray analysis were obtained from hexanes at -30ºC. $^{19}F\{1H\}$ NMR (376 MHz, CD_2Cl_2) δ -119.15 (m, 1F, Ar^F), -128.11 (m, 2F, *o*-C_6F_5), -139.76 (m, 2F, *o*-C_6F_5), -141.65 (m, 2F, *o*-C_6F_5), -143.27 (m, 1F, Ar^F), -143.68 (dt, J = 18.8, 13.4 Hz, 1F, Ar^F), -147.23 (tt, J = 20.0, 5.6 Hz, 1F, *p*-C_6F_5), -152.20 (m, 2F, Ar^F and *p*-C_6F_5), -155.39 (t, J = 20.8 Hz 1F, *p*-C_6F_5), -162.27 (m, 2F, *m*-C_6F_5), -162.47 (m, 2F, *m*-C_6F_5), -163.06 (m, 2F, *m*-C_6F_5). ^{11}B NMR (128 MHz, CD_2Cl_2) δ 62.3 (br). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 154.50 (m), 152.91 (m), 151.15 (m), 148.81 (m), 147.24 (m), 145.78 (m), 144.75 (m), 144.42 (m), 144.01, 143.58 (m), 143.14 (m), 142.83 (m), 141.93 (m), 140.57 (d, J = 13.6 Hz), 138.88 (m), 137.25 (m), 130.11, 110.84 (m), 109.11 , 100.43 (m). $C_{26}BF_{19}$: Calculated: C 45.65; Found C 45.55.

Synthesis of 7. A 1-neck rbf was charged with a solution of **3** (207 mg, 0.303 mmol) in CH_2Cl_2 (15 mL) and equipped with a constant volume bulb (19.1 mL). The solution was cooled to -94ºC and the system evacuated. HCl gas was introduced into the bulb (290 mmHg), and the valve in between the bulb and the rbf was opened. The system was allowed to stir and gradually reach room temperature overnight, resulting in a pale yellow solution. The solvent was removed *in vacuo*, the remaining pale yellow solids were taken up in hot hexanes and allowed to recrystallize at -30ºC to give an off-white solid (192 mg, 0.271 mmol, 89.4% yield). Crystals suitable for x-ray analysis were obtained from hexanes at -30ºC. ^1H NMR (400 MHz, CD_2Cl_2) δ 6.76 (s, 1H). ^{19}F NMR (376 MHz, CD_2Cl_2) δ -128.54 (m, 2F, *o*-C_6F_5), -130.17 (ddd, J = 22.3, 12.5, 5.8 Hz, 1F, Ar^F), -138.19 (ddd, J = 19.3, 12.5, 6.0 Hz, 1F, Ar^F), -139.11 (d, J = 20.3 Hz, 2F, *o*-C_6F_5), -140.14 (m, 2F, *o*-C_6F_5), -143.02 (m, 1F, Ar^F), -150.57 (td, J = 19.9, 5.8 Hz, 1F, *p*-C_6F_5), -150.78 (m, 1F, *p*-C_6F_5), -151.35 (m, 1F, *p*-C_6F_5), -152.48 (ddd, J = 22.4, 19.7, 6.1 Hz, 1F, Ar^F), -160.63 (m, 2F, *m*-C_6F_5), -161.22 (m, 4F, *m*-C_6F_5). ^{11}B NMR (128 MHz, CD_2Cl_2) δ 61.5 (br). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 151.1 – 150.3 (m), 149.2 , 148.4 – 148.0 (m), 147.4 (d, J = 10.3 Hz), 147.0 (m) , 146.7 (m), 145.7 (m), 144.9 (m), 144.7 – 142.7 (m), 141.5 - 140.9 (m), 140.5 - 140.1 (m), 139.8 – 139.0 (m), 137.4 – 136.6 (m), 129.9 (s, C^{vinyl}), 127.0 (s, *C*H), 125.0 (m) , 112.6 (m), 110.1 (m). $C_{26}HBClF_{19}$ Calculated: C 43.34, H 0.14; Found C 43.56, 0.32

Synthesis of 8. To a solution of **7** (0.176 mg, 0.248 mmol) and cyclohexene (60 μL, 0.60 mmol) in CH_2Cl_2 (5 mL) was added $Me_2Si(H)Cl$ (0.56 mL, 6.8 mmol) and the solution was allowed to stir at room temperature for 33 hours. The volatiles were removed in vacuo, and the solids were recrystallized from pentane (< 2 mL) to give an off-white solid (132 mg, 0.172 mmol, 69.3% yield). ^1H NMR (600 MHz, C_6D_6) δ 6.35 (s, 1H), 1.88 – 1.59 (m, 6H), 1.42 (q, J = 12.4 Hz, 2H),

1.29 – 1.15 (m, 3H), ^{19}F NMR (376 MHz, C_6D_6) δ -129.23 (d, J = 21.3 Hz, 2F, *o*-C_6F_5), -130.08 (dd, J = 24.6, 12.2 Hz, 1F, Ar^F), -137.77 (ddd, J = 19.4, 12.2, 5.7 Hz, 1F, Ar^F), -140.15 (d, J = 19.0 Hz, 2F, *o*-C_6F_5), -140.64 (d, J = 15.8 Hz, 2F, *o*-C_6F_5), -146.42 (tt, J = 21.2, 5.5 Hz, 1F, Ar^F), -149.46 (q, J = 21.8 Hz, 2F, Ar^F), -151.93 (td, J = 20.5, 4.3 Hz, 1F, Ar^F), -152.91 (ddd, J = 25.3, 20.5, 5.8 Hz, 1F, Ar^F), -159.98 (td, J = 22.1, 20.4, 7.1 Hz, 2F, *m*-C_6F_5), -160.09 – -160.37 (m, 2F, *m*-C_6F_5), -161.05 – -161.38 (m, 2F, *m*-C_6F_5).^{13}C NMR (151 MHz, C_6D_6) δ 148.80 (t, J = 11.3 Hz), 147.15 (dd, J = 14.1, 8.9 Hz), 146.94 – 146.56 (m), 145.16 (dd, J = 10.9, 4.2 Hz), 144.68 (m), 143.74 – 143.22 (m), 142.96 (m), 142.38 – 141.99 (m), 141.75 (m), 141.52 – 141.03 (m), 140.74 – 140.23 (m), 140.08 (m), 138.76 (m), 137.07 (m), 130.63 (s, C^{vinyl}), 124.10 (s, H C^{vinyl}) 123.52 (m), 112.64 (m), 109.83 (m), 42.41 (s, B*C*H 29.08 (s, *C*H_2), 28.22 (s, *C*H_2), 26.59 (s, *C*H_2). $C_{32}H_{12}BF_{19}$ Calculated: C 50.03, H 1.57; Found C 50.03, H 1.78.

Gutmann-Beckett. Excess Lewis acid was used in all cases. $^{31}P\{^1H\}$ NMR: Et_3PO reference: δ 50.3. $(Et_3PO)B(C_6F_5)_3$ reference adduct: δ 76.9. Reference Δδ 26.6. (Et_3PO)-**3** adduct: δ 81.4. Δδ 31.1. Lewis-acidity relative to $B(C_6F_5)_3$: 1.17. $^{11}B\{^1H\}$ (adduct check) δ 2.0.

Reaction between 3 and H_2: In a J-Young tube, a solution of **3** in toluene-d_8 was degassed at -78°C and then placed under an atmosphere of dihydrogen. The solution was held at 125°C for 20 hours, and then the NMR spectra were recorded. ^{1}H NMR (400 MHz, tol-d_8) δ 6.56 (C^{vinyl}H). $^{19}F\{^1H\}$ NMR shown in figure S14.

Reaction between 7 and $Me_2Si(H)Cl$. In a J-Young NMR tube, **7** (57 mg, 0.080 mmol) was combined with $Me_2Si(H)Cl$ (0.3 mL) and the mixture was allowed to stand at room temperature. After 20 hours, the volatiles were removed in vacuo and the resulting red solids were taken up in toluene-d_8. The ^{1}H and ^{19}F NMR are shown in figures S15 and S16.

Heating 8. A solution of **8** in C_6D_6 was heated at 140°C for 2.5 hours, during which the solution changed from pale yellow to orange. $^{19}F\{^1H\}$ and ^{1}H NMR are shown in figures S17 and S18, respectively.

Reaction of 3 with cyclohexene. A J. Young tube was charged with **3** (29 mg, 0.042 mmol) and a stock solution of cyclohexene (0.44 M) and toluene (1.3 M, internal standard) in C_6D_6 (0.50 mL). The solution was heated to 140°C for 90 minutes, after which it changed from orange-red to yellow. $^{19}F\{^1H\}$ NMR is shown in figure S18.

Hydrogenation of cyclohexene (20% loading). A Kontes bomb (30 mL) was charged with **3** (29 mg, 0.042 mmol) and a stock solution of cyclohexene (0.44 M) and toluene (1.3 M, internal standard) in C_6D_6 (0.50 mL). After three freeze-pump-thaw cycles, the mixture was subjected to H_2 (ca. 1 ATM) at -193°C and then heated to 140°C for 72 hours. The yield of cyclohexane was determined by ^{1}H NMR, using a delay of 20 seconds.

Hydrogenation of cyclohexene (10% loading). A Kontes bomb (30 mL) was charged with **3** (15 mg, 0.022 mmol) and a stock solution of cyclohexene (0.44 M) and toluene (1.3 M, internal standard) in C_6D_6 (0.50 mL). After three freeze-pump-thaw cycles, the mixture was subjected to H_2 (ca. 1 ATM) at -193°C and then heated to 140°C for 48 hours. The yield of cyclohexane was determined by ^{1}H NMR, using a delay of 20 seconds.

Table S1: Data Collection and Structure Refinement Details for **3**, **$Cp_2Zr(o\text{-}C_6HF_4)_2$**, **4**

Compound	**3**	**$Cp_2Zr(o\text{-}C_6HF_4)_2$**	**4**
Formula	$C_{26}BF_{19}$	$C_{22}H_{12}F_8Zr$	$C_{30}H_{10}F_{14}Zr$
Mol. Wt.	684.07	519.54	727.60
CCDC	956378	956379	956380
Crystal System	Monoclinic	Orthorhombic	Monoclinic
Space Group	P $2_1/c$	P bca	P $2_1/n$
a/Å	11.0400(4)	13.7831(3)	8.4552(3)
b/Å	8.8720(3)	13.7152(3)	16.9172(5)
c/Å	23.965(9)	20.0961(5)	17.7991(4)
α/°	90	90	90
β/°	101.614(1)	90	94.924
γ/°	90	90	90
V/Å^{-3}	2299.24(14)	3798.829(15)	2536.53(13)
Z	4	8	4
T/K	173	173	173
λ/Å	0.71073	0.71073	0.71073
ρ_{calc}/g*cm^{-3}	1.976	1.817	1.905
F(000)	1328.0	2048.0	1424.0
μ/mm^{-1-}	0.223	0.662	0.559
Crystal size/mm^3	0.08x0.08x0.06	0.08x0.08x0.06	0.1x0.08x0.06
Transmission factors	0.8514 & 0.5561	0.9614 & 0.9490	0.9673 & 0.9463
θ range/°	1.74-27.37	2.03-27.51	27.47
Data/restraints/param	5161 / 0 / 415	4350 / 0 / 280	5779 / 0 / 446
GoF	1.164	1.232	1.134
R_1 ($I > 2\sigma(I)$)	0.0653 (4054)	0.0593 (3209)	0.0532 (4351)
wR_2 (all data)	0.2005 (5161)	0.1449 (4350)	0.1057 (5779)
Residual density/e*Å^{-3}	0.366 & -0.433	0.540 & -0.415	0.446 & -0.489

Table S2: Data Collection and Structure Refinement Details for **5, 6** and **7**

Compound	**5**	**6**	**7**

Formula	$C_{22}H_6F_{14}Sn$	$C_{20}BBrF_{14}$	$C_{26}HBClF_{19}$
Mol. Wt.	654.98	596.91	720.53
CCDC	956381	956382	956383
Crystal System	Monoclinic	Triclinic	Monoclinic
Space Group	P 2_1	P -1	P $2_1/c$
a/Å	7.8081(4)	9.0742(3)	11.2301(3)
b/Å	14.4792(9)	10.2272(4)	17.6492(4)
c/Å	9.4551(5)	10.9121(3)	15.5641(5)
α/°	90	71.095(2)	90
β/°	90.521(3)	79.247(2)	126.554(2)
γ/°	90	84.755(2)	90
V/Å^{-3}	1068.90(10)	940.71(5)	2478.04(13)
Z	2	2	4
T/K	173	173	173
λ/Å	0.71073	0.71073	0.71073
ρ_{calc}/g*cm^{-3}	2.035	2.107	1.931
F(000)	628.0	572.0	1400.0
μ/mm^{-1-}	1.326	2.330	0.317
Crystal size/mm^3	0.1x0.08x0.06	0.1x0.08x0.06	0.1x0.08x0.06
Transmission factors	0.9247 & 0.8788	0.8729 & 0.8004	0.9812 & 0.9690
θ range/°	2.57-27.46	3.03-27.58	2.00-27.57
Data/restraints/param	3452 / 1 / 336	4291 / 0 / 325	5731 / 0 / 424
GoF	1.063	1.081	1.176
R_1 (I > 2σ(I))	0.0236 (3397)	0.0351 (3859)	0.0790 (3745)
wR_2 (all data)	0.0604 (3452)	0.0885 (4291)	0.1187
Residual density/e*Å^{-3}	0.770 & -0.471	0.575 & -0.419	0.243 &-0.357

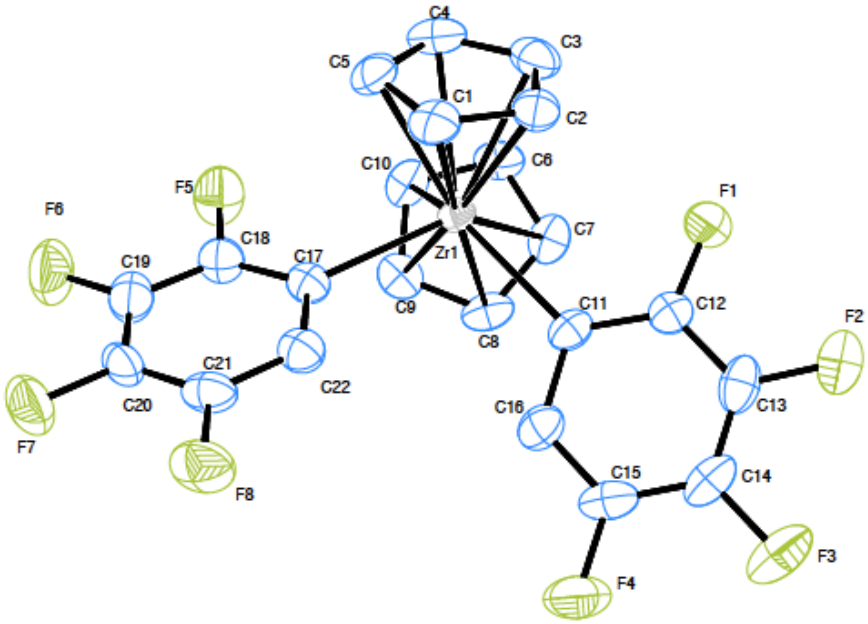

Figure S1. Thermal ellipsoid (50%) diagram of *bis*(2,3,4,5-tetrafluorophenyl) zirconocene. Selected bond lengths (Å): Zr1-C11 2.348(5), Zr1-C17 2.336(5); Selected bond angle (°): C11-Zr1-C17 101.19(17)

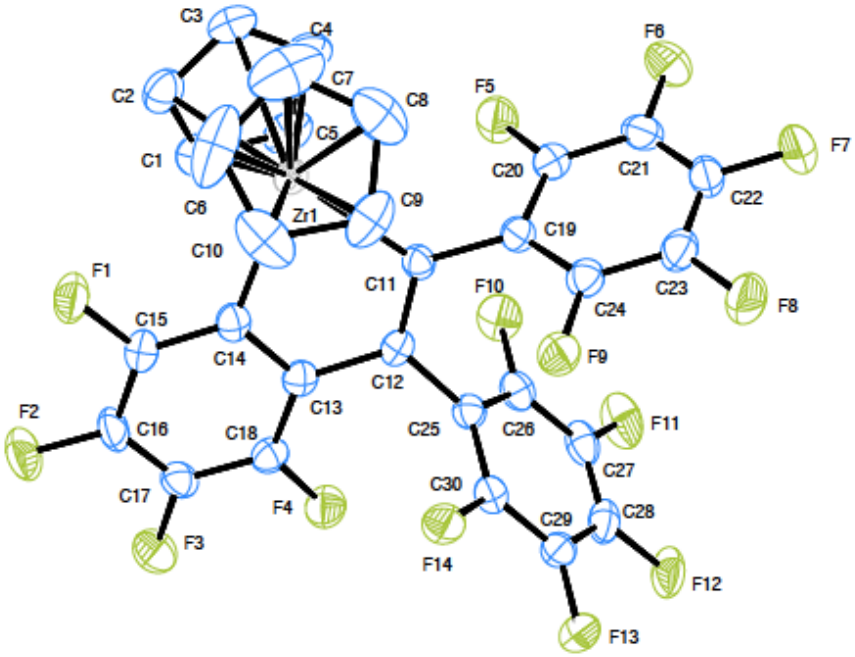

Figure S2. Thermal ellipsoid (50%) diagram of zirconocycle **4.** Selected bond lengths (Å): Zr1-C14 2.282(4), C14-C13 1.414(5), C13-C12 1.483(5), C12-C11 1.350(5), Zr1-C11 2.307(4); Selected bond angles (°)C14-Zr1-C11 75.14(14), C12-C11-Zr1 114.1(3), C11-C12-C13 119.1(3), C14-C13-C12 117.4(3), C13-C14-Zr1 113.1(3); Selected torsion angle (°): C11-C12-C13-C14 10.10

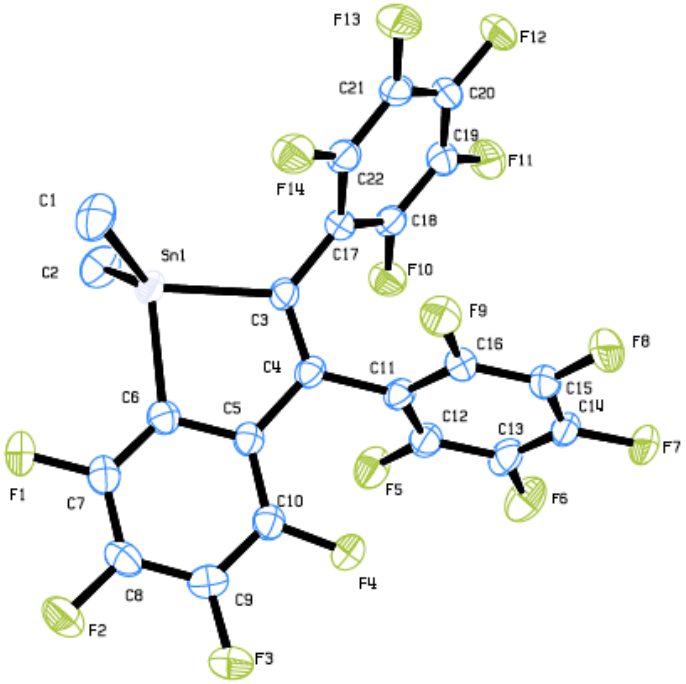

Figure S3. Thermal ellipsoid (50%) diagram of stannacycle **5.** Selected bond lengths (Å): Sn1-C3 2.162(3), C3-C4 1.335(5), C4-C5 1.493(6), C5-C6 1.403(5) Sn1-C6 2.138(4); Selected bond angles (°): C6-Sn1-C3 81.71(14), C4-C3-Sn1 110.7(3), C3-C4-C5 119.5(3), C4-C5-C6 118.1(3), C5-C6-Sn1 109.8(3); Selected torsion angle (°): C3-C4-C5-C6 3.27

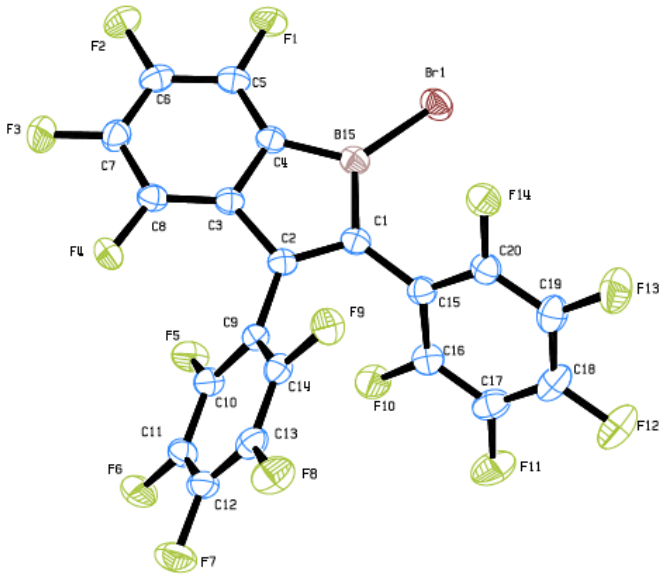

Figure S4. Thermal ellipsoid (50%) diagram of boraindene **6.** Selected bond lengths (Å): B15-C1 1.562(4), C2-C1 1.352(3), C3-C2 1.492(3), C3-C4 1.417(3), B15-C4 1.548(4), Br1-B15 1.878(3); Selected bond angles (°):C4-B15-C1 105.2(2), C2-C1-B15 107.4(2), C1-C2-C3 111.7(2), C2-C3-C4 109.7(2), C3-C4-B15 106.1(2); Selected torsion angle (°): C1-C2-C3-C4 1.47.

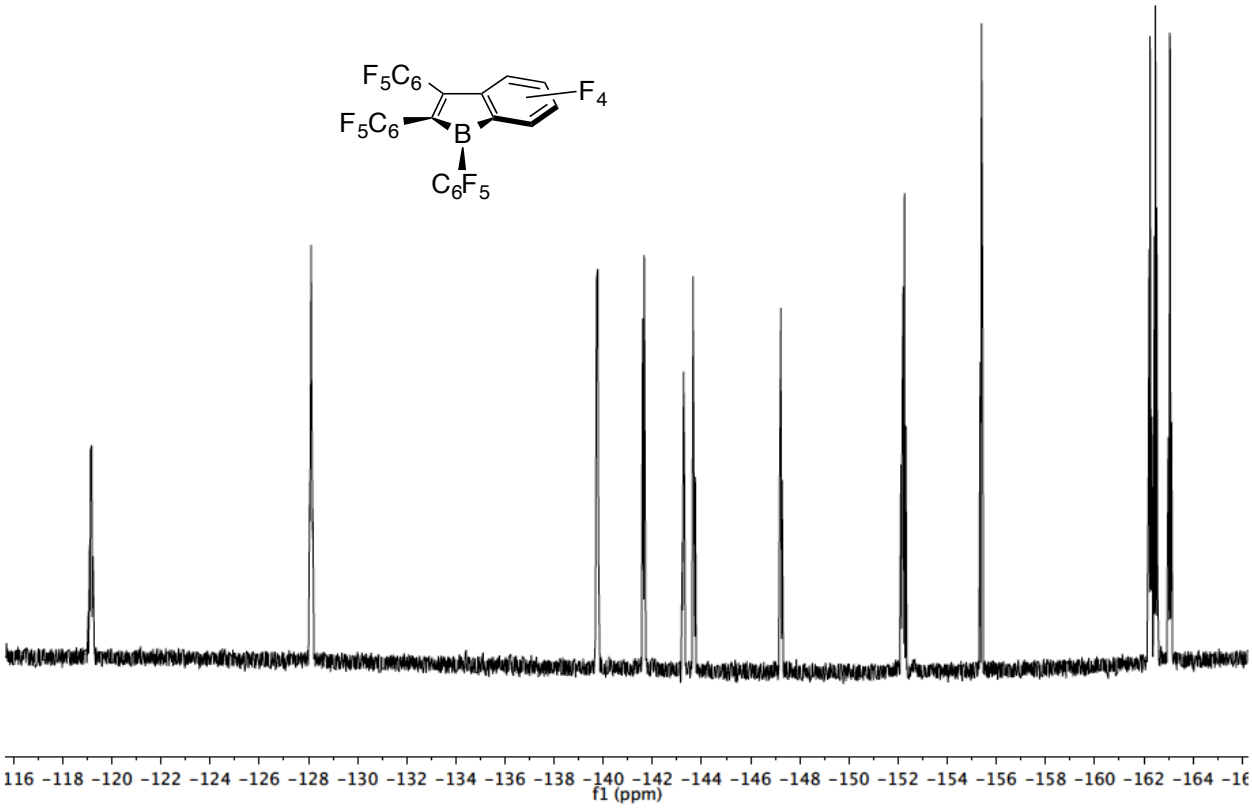

Figure S5. $^{19}F\{^{1}H\}$ spectrum of compound **3** in CD_2Cl_2

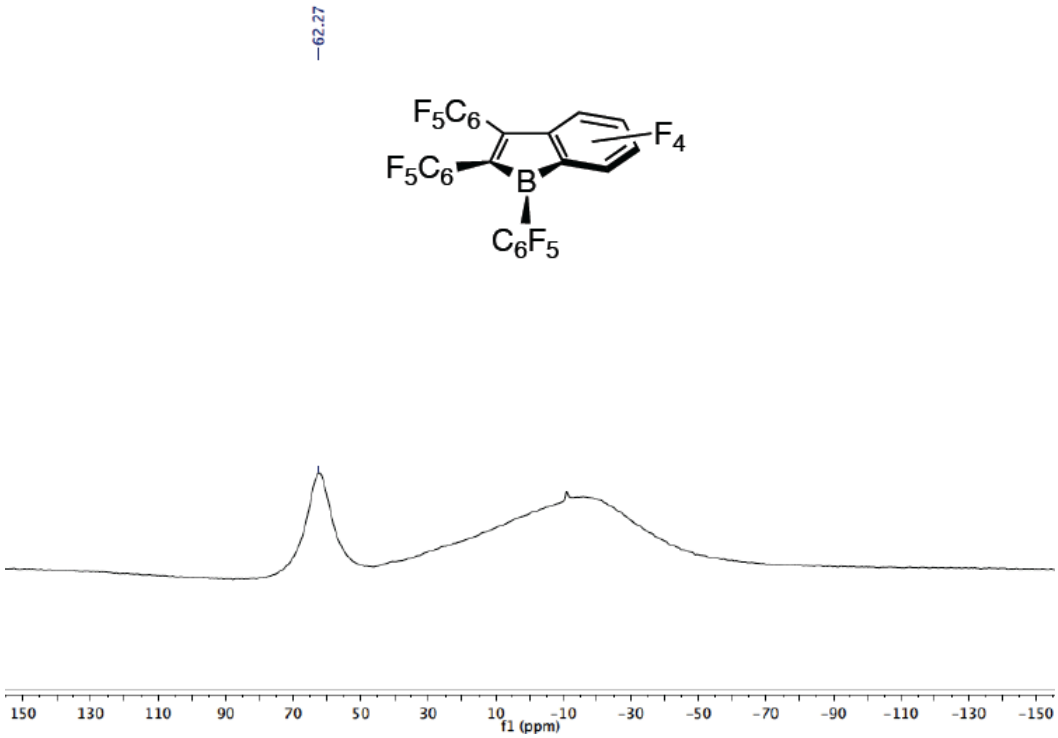

Figure S6. $^{11}B\{^{1}H\}$ spectrum of compound **3** in CD_2Cl_2

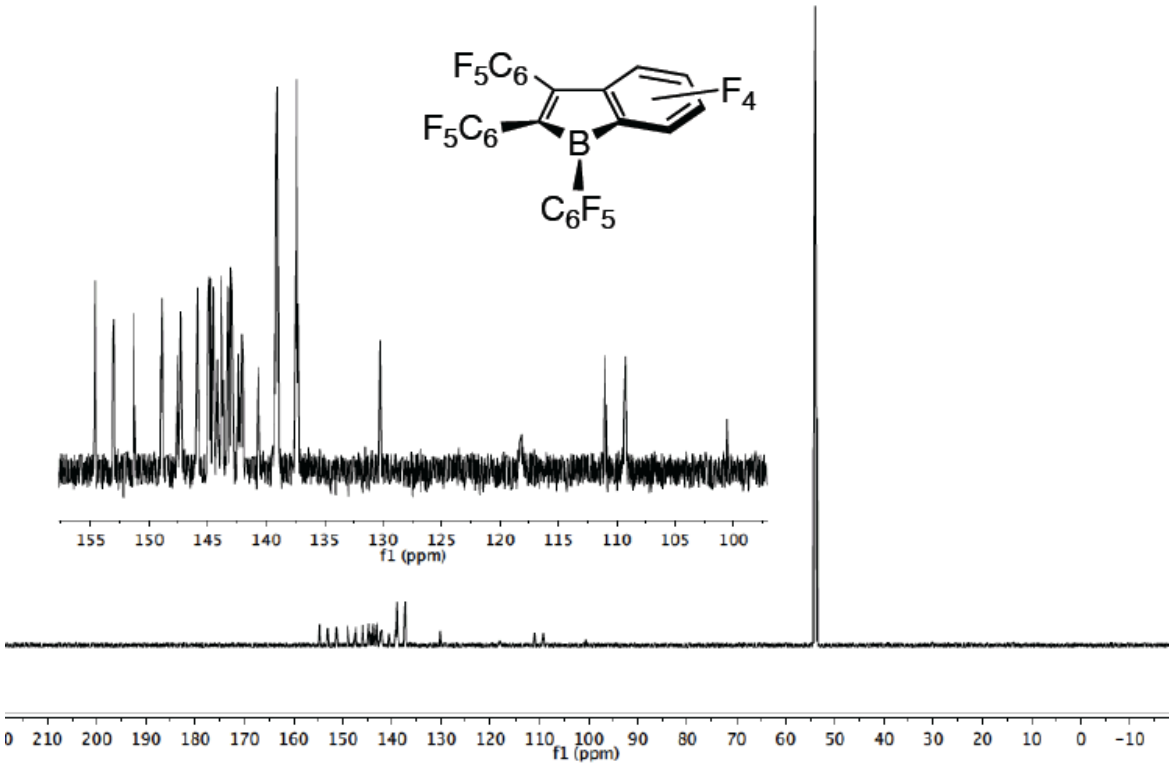

Figure S7. $^{13}C\{^{1}H\}$ spectrum of compound **3** in CD_2Cl_2

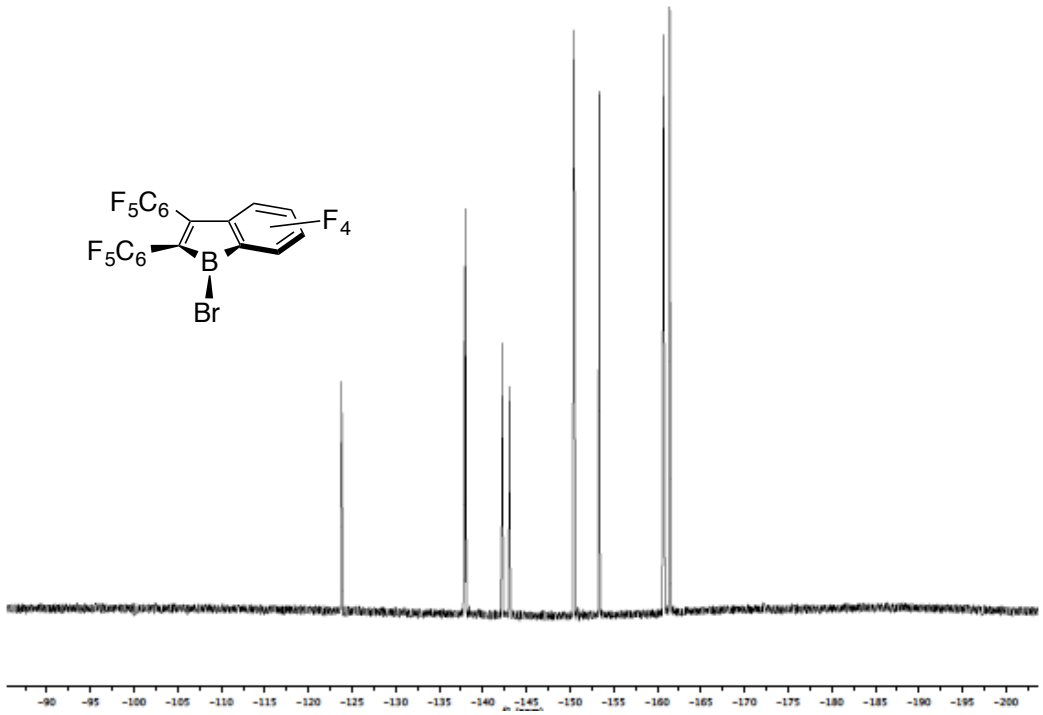

Figure S5. $^{19}F\{^{1}H\}$ of purified **6** in CD_2Cl_2

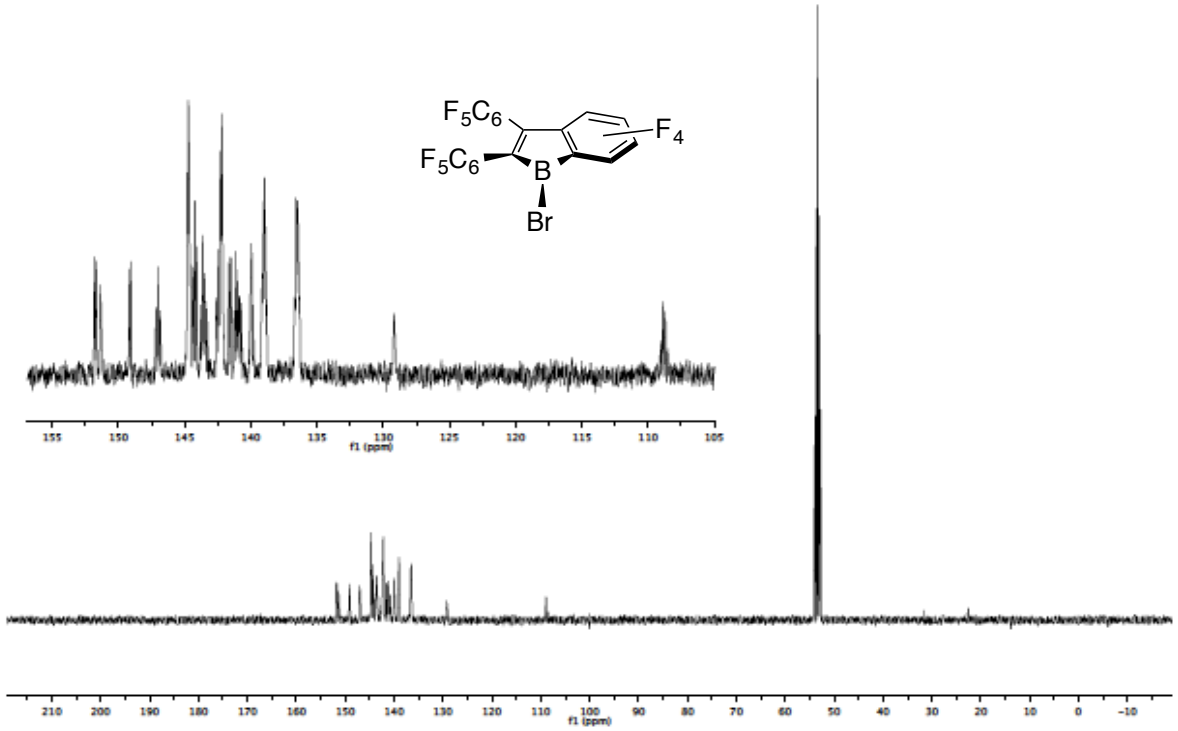

Figure S6. $^{13}C\{^{1}H\}$ of purified **6** in CD_2Cl_2

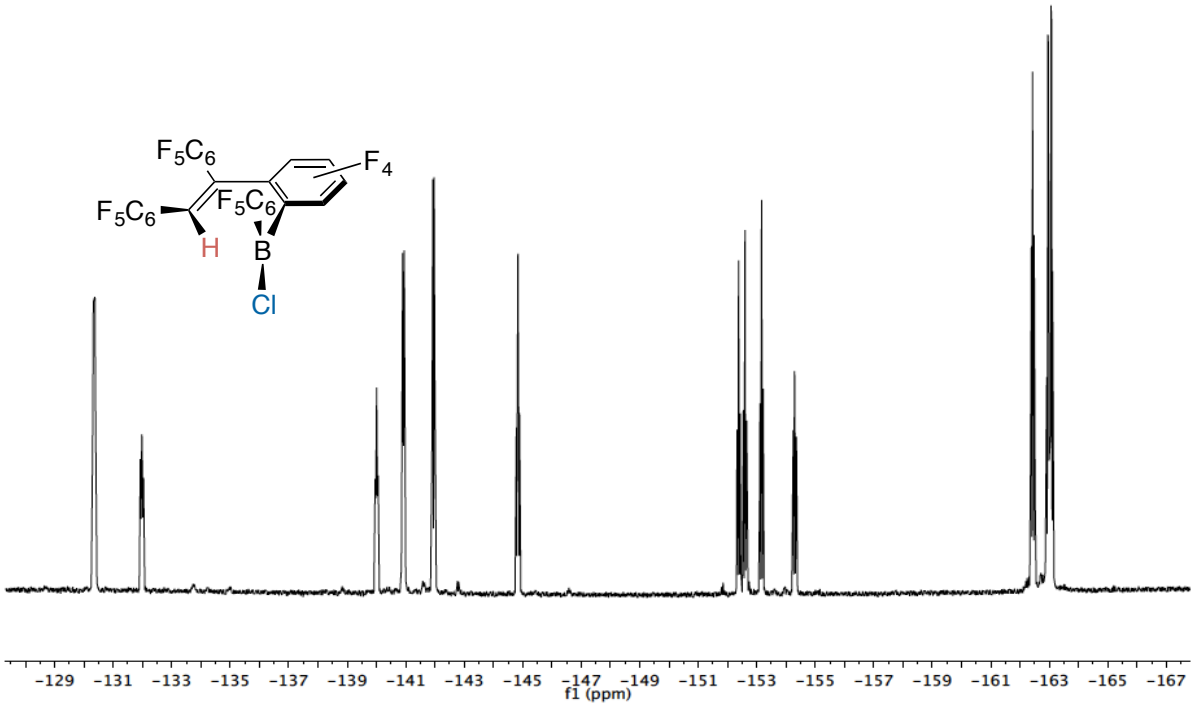

Figure S7. $^{19}F\{1H\}$ spectrum of **7** in CD_2Cl_2

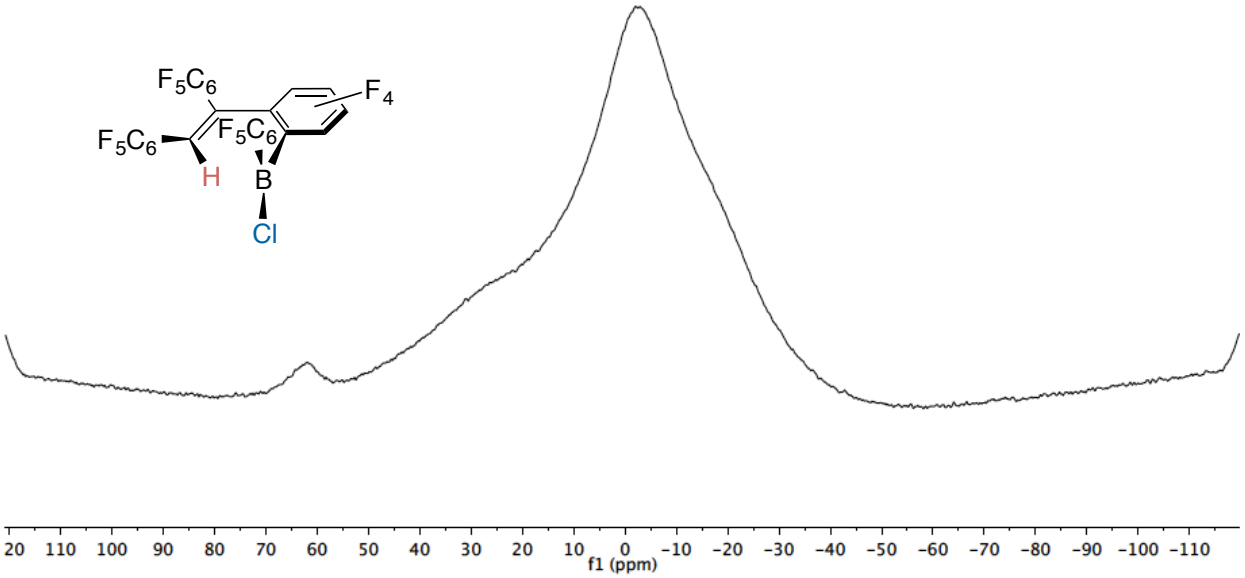

Figure S8. ^{11}B spectrum of **7** in CD_2Cl_2

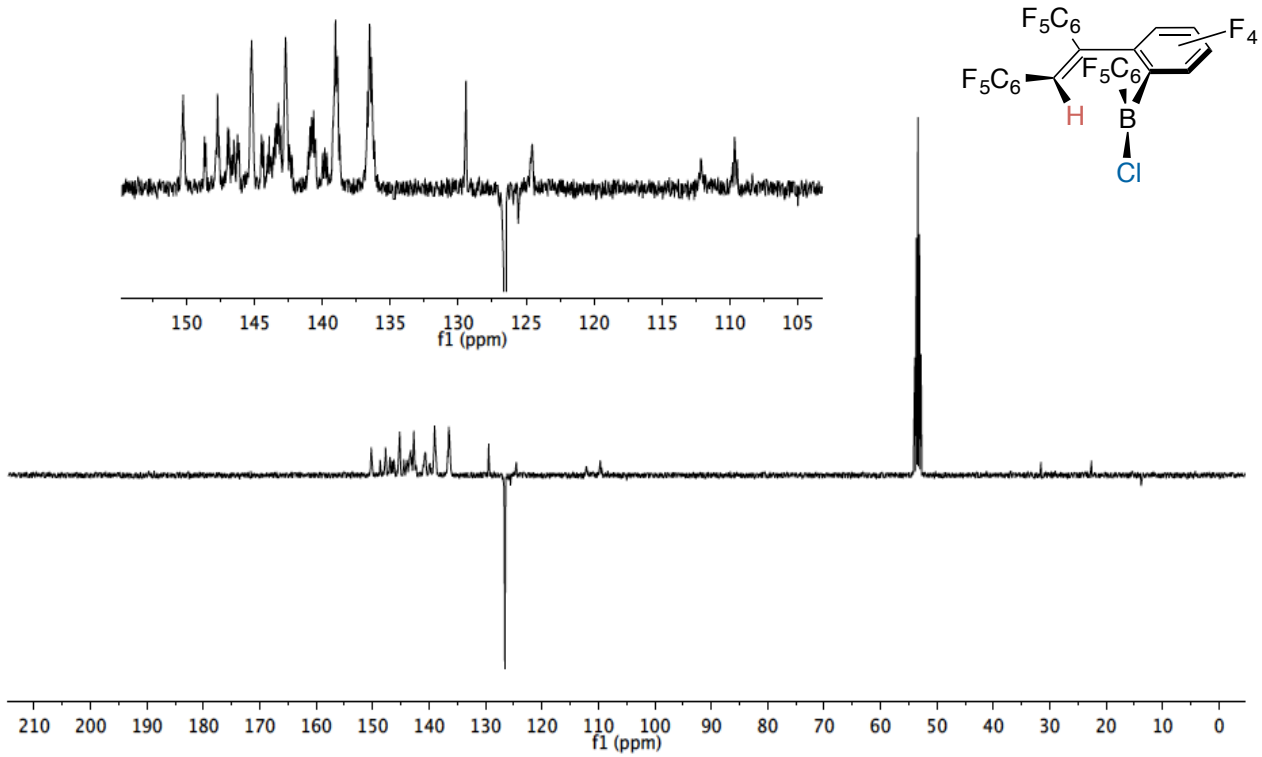

Figure S9. DEPT-Q spectrum of **7** in CD_2Cl_2

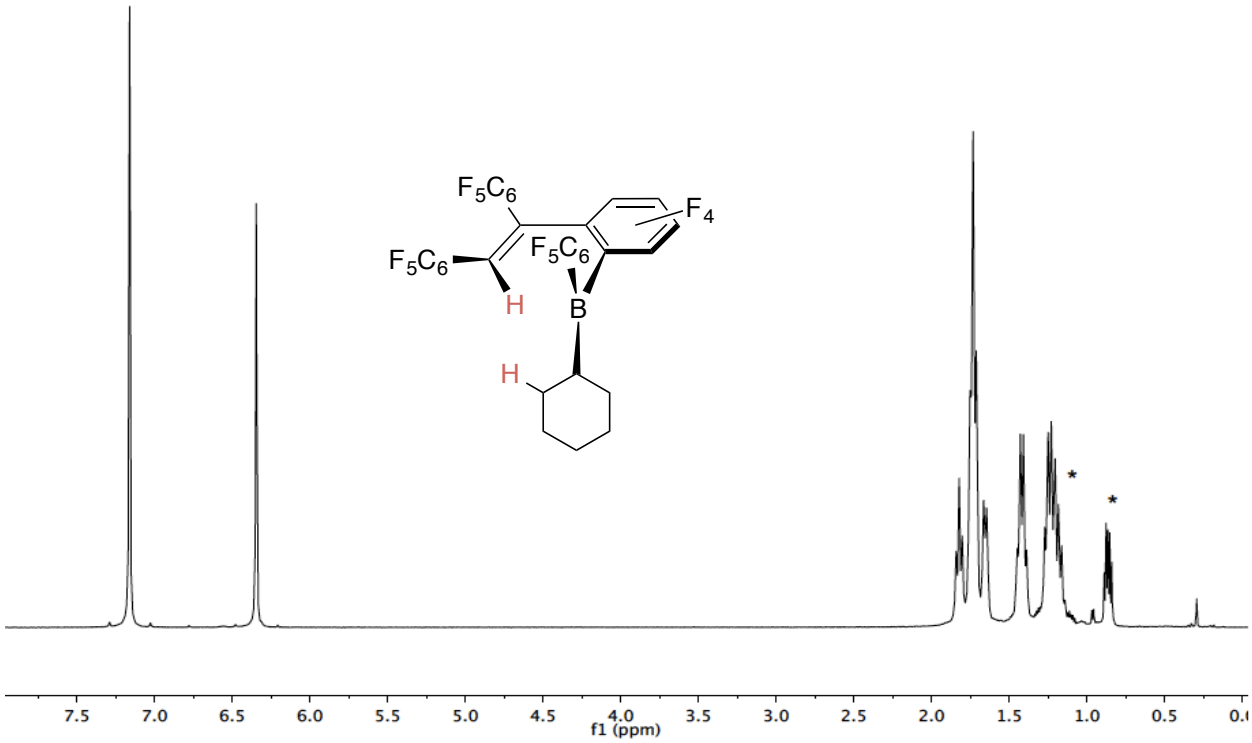

Figure S10. ^{1}H spectrum of compound **8** in C_6D_6. Pentane impurity highlighted by *.

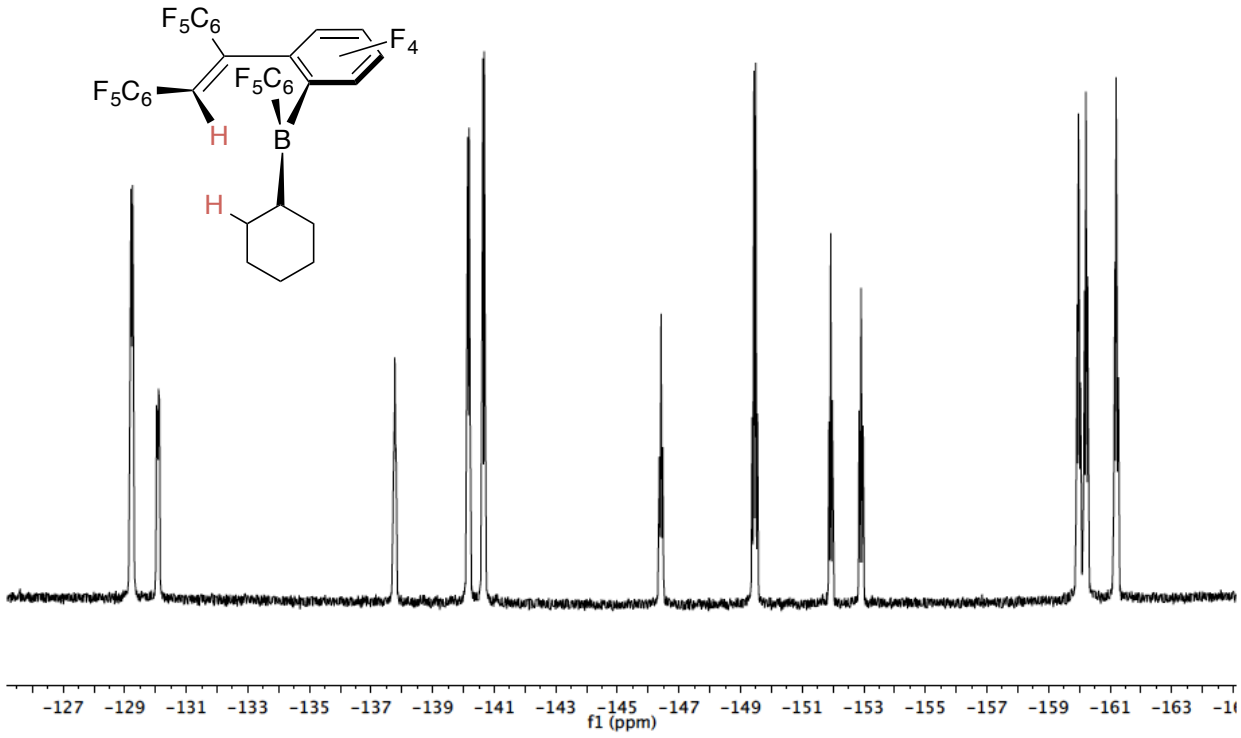

Figure S11. $^{19}F\{^{1}H\}$ spectrum of compound **8** in C_6D_6.

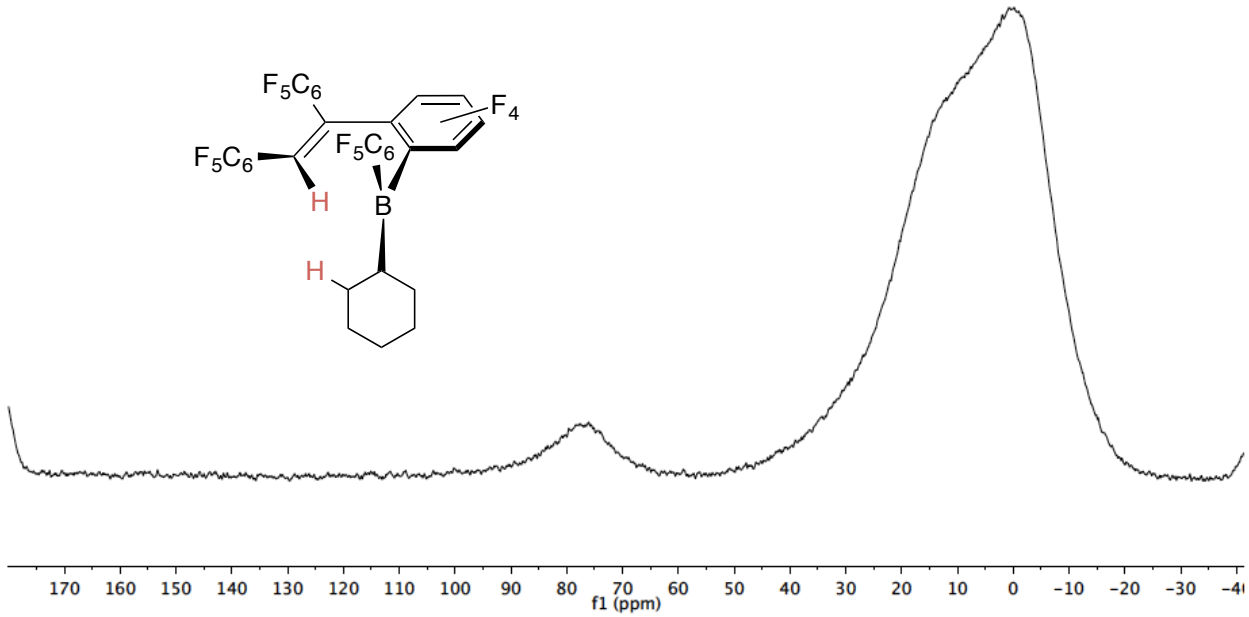

Figure S12. $^{11}B\{^{1}H\}$ spectrum of compound **8** in C_6D_6.

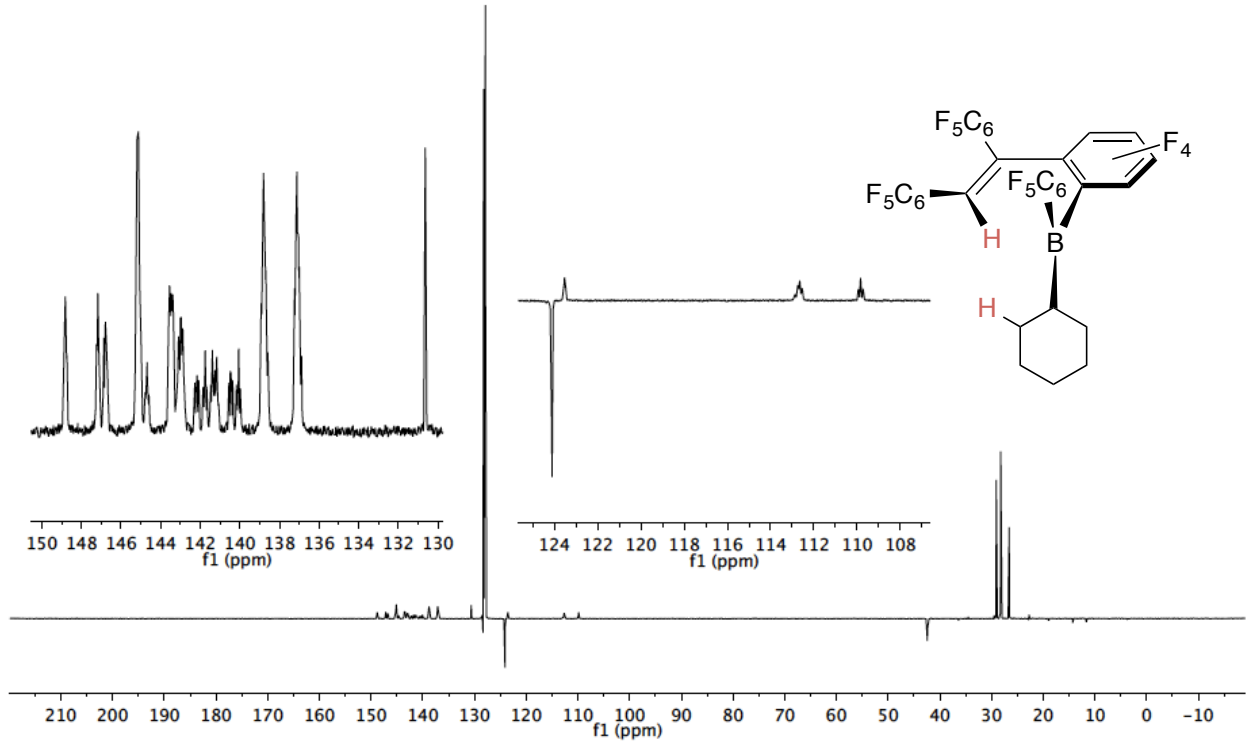

Figure S13. DEPT-Q spectrum of compound **8** in C_6D_6.

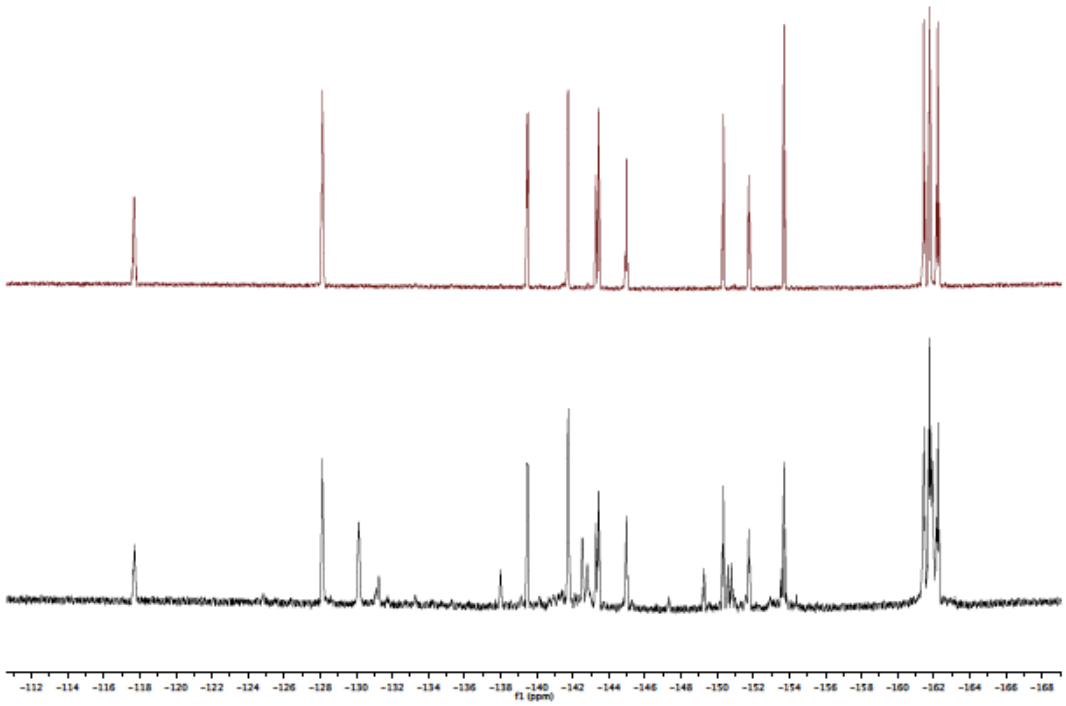

Figure S14. $^{19}F\{^{1}H\}$ spectra of **3** in toluene-d_8 (top) and of **3** after 20 hours under 1 atm H_2 at 125˚C.

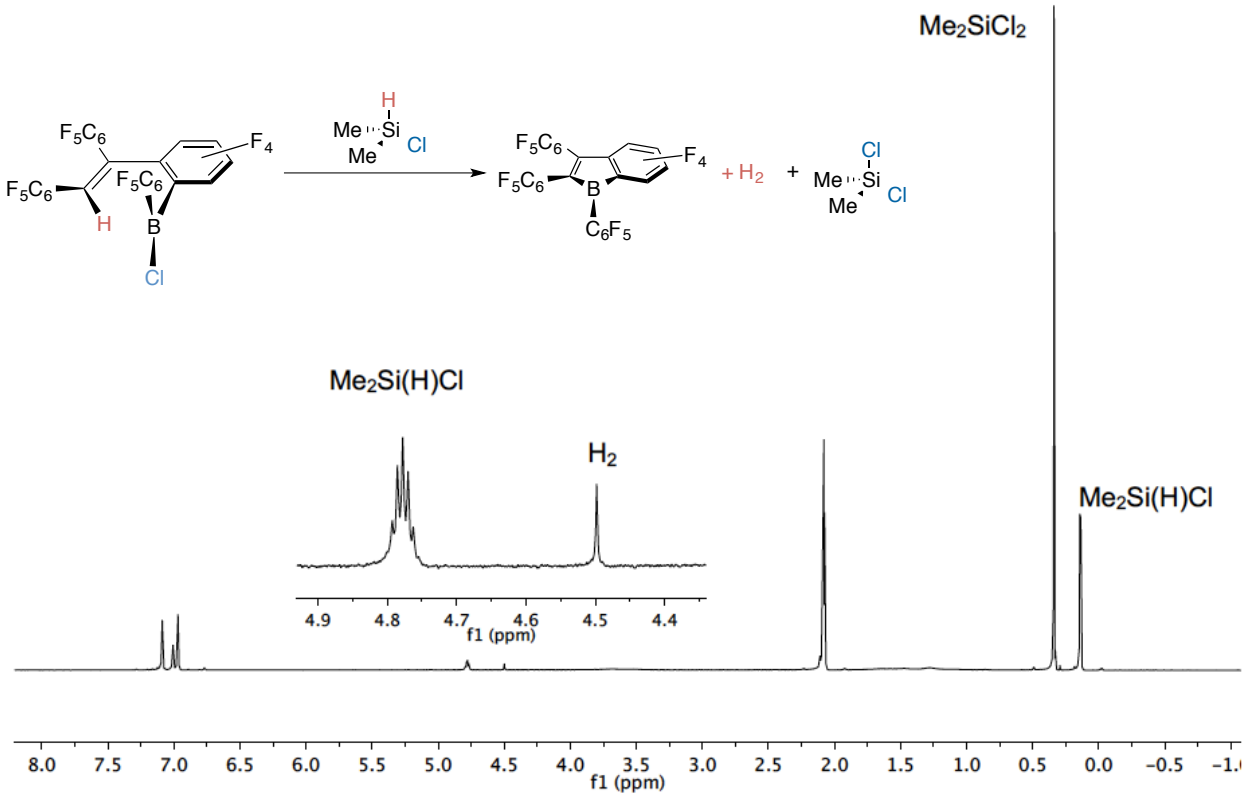

Figure S15. ^{1}H NMR spectrum of the reaction products of **7** and $Me_2Si(H)Cl$

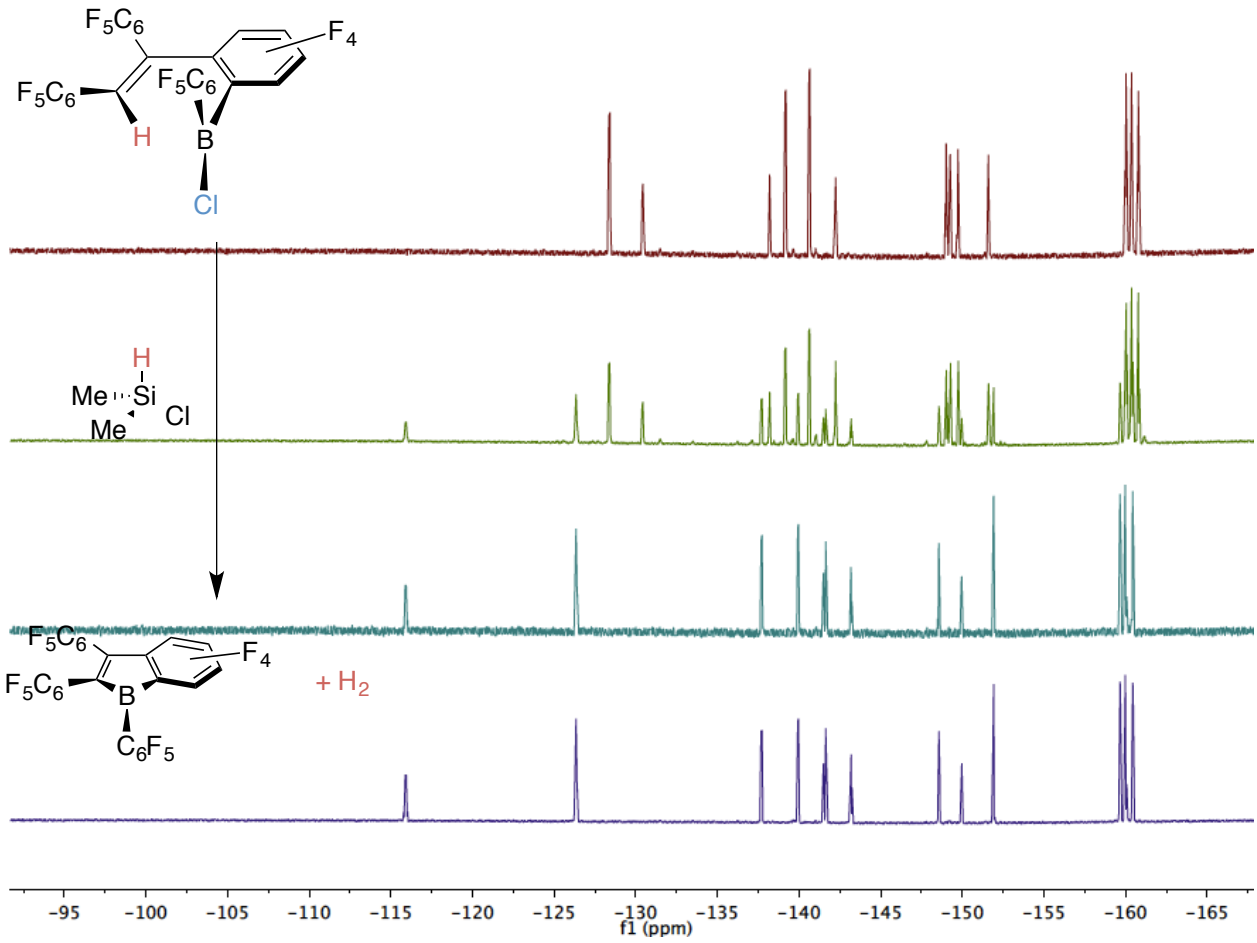

Figure S16. $^{19}F\{^{1}H\}$ spectra in toluene-d_8 of: **7** (top) the reaction mixture of **7** and $Me_2Si(H)Cl$ after 2.5 hrs (second from top) the reaction mixture of **7** and $Me_2Si(H)Cl$ after 24 hrs (second from bottom) and **3** for reference (bottom).

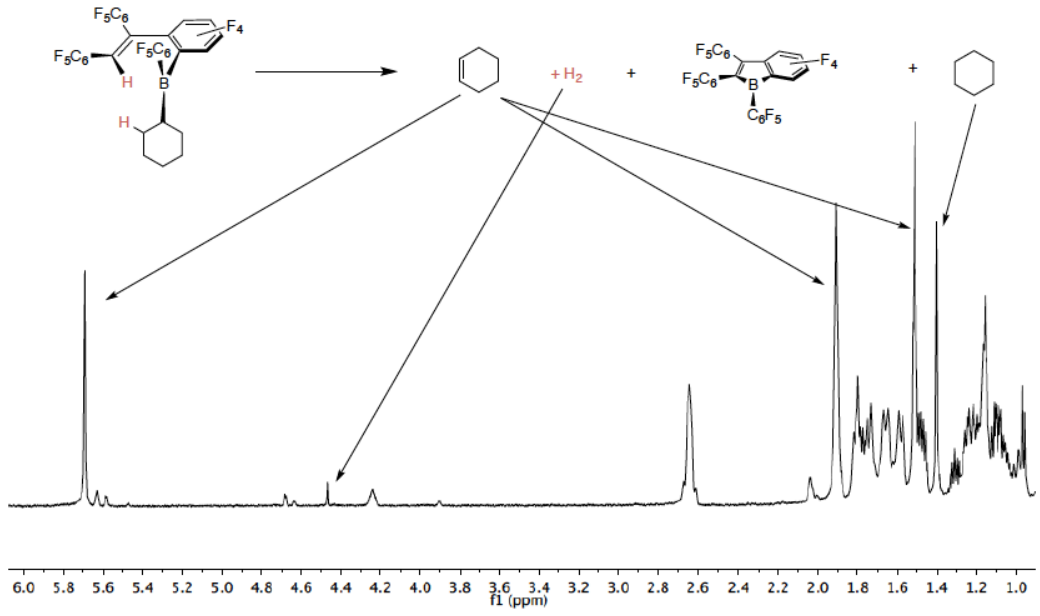

Figure S17. ^{1}H NMR spectrum (C_6D_6) of **8** after heating at 140 ˚C for 2.5 hours.

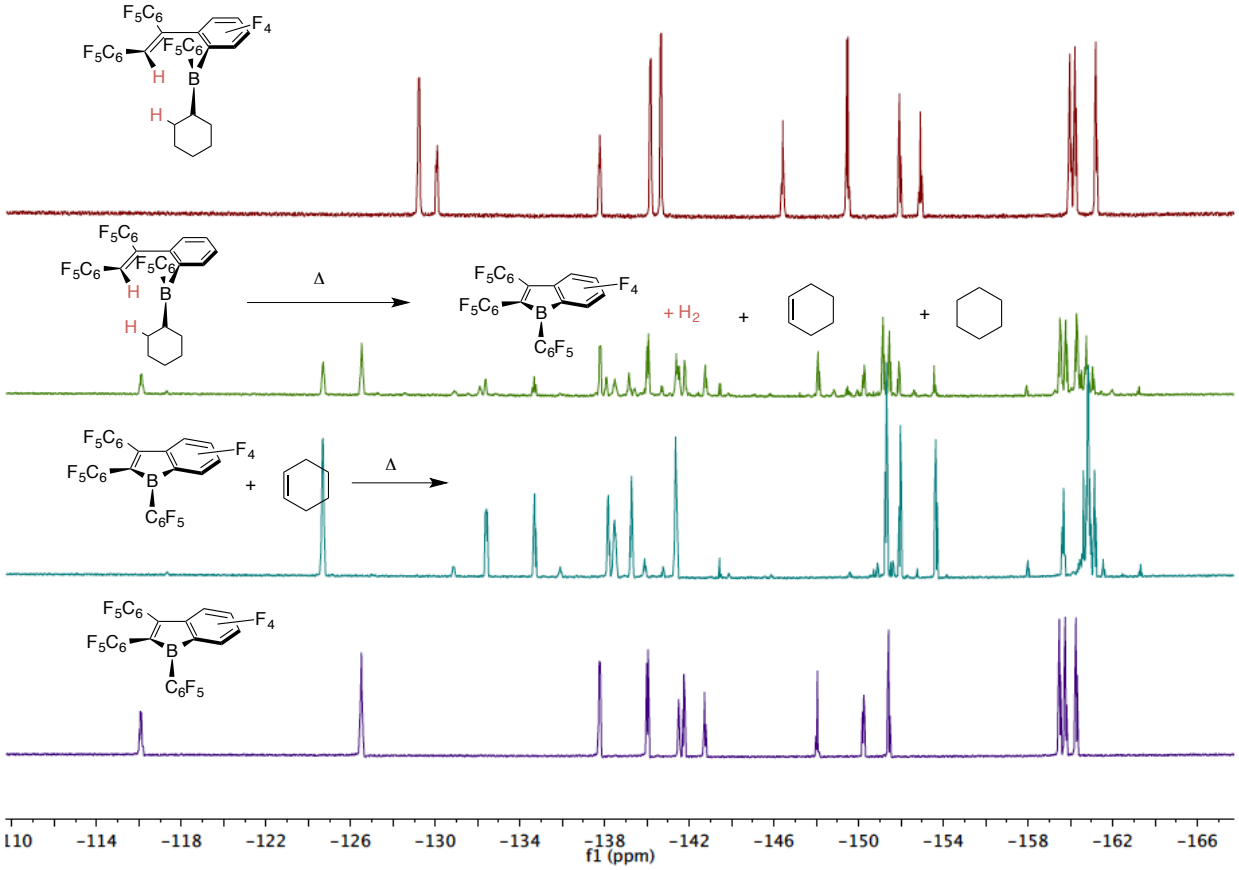

Figure S18. ^{19}F NMR spectra (C_6D_6) of **8** (top), **8** after heating at 140˚C for 2.5 hours (second from top), **3** after heating in the presence of cyclohexene at 140˚C for 1.5 hrs (second from bottom) and **3** for reference (bottom).

Computational Details

All calculations were done with the program package Gaussian09.[1] Geometries of the studied systems were optimized in methylene chloride solution using the PBE0 density functional[2-5] in combination with Ahlrichs' TZVP basis sets.[6] The polarizable continuum model, as implemented in Gaussian 09, was used for the treatment of solvent effects.[7] The nature of stationary points found was assessed by calculating the full Hessian matrices. For the calculation of nucleus independent chemical shifts (NICS(0)) of **3**, the B3LYP functional[8-11] was used in together with the 6-311+G(d,p) basis sets as found in the internal basis set library of the Gaussian program.

Although not shown explicitly in Figure 2, we also considered the possibility for H_2 to add to the other B-C bond of **3**. The transition state for this process, **TS2b**, has a relative energy of 97 kJ mol^{-1}, whereas the products ***cis*-IIIb** and ***trans*-IIIb** reside at 24 and 17 kJ mol^{-1}, respectively, on the same energy scale. Calculations were also conducted for the reaction of H_2 with ***cis*-IV** and ***trans*-IV** to eliminate ethane and generate ***cis*-III** and ***trans*-III**, respectively. For these reactions, the lowest energy pathways correspond the reaction of **IV** with H_2 from the 'inside' of the molecule to give intermediates in which a molecule of H_2 is weakly bound to the Lewis acidic boron center (***cis*-V** and ***trans*-V**, analogous to **I**). The subsequent transition states for the elimination of ethane from these adducts, **TS9** and **TS10**, reside at 65 and 71 kJ mol^{-1}, respectively.

1. Gaussian 09, Revision A.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
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Table S3. Calculated relative energies (kJ mol^{-1}) for the reaction of **3** with H_2 and ethane.

	ΔE	ΔG
TS1	20	61
I	14	62
TS2	44	90
II	17	75
TS3	18	79
cis-III	-24	25
TS4	3	56
trans-III	-35	14
TS2b	51	97
cis-IIIb	-23	24
TS4b	6	61
trans-IIIb	-31	17
TS5	-30	78
trans-IV	-173	-58
TS7	-136	-19
TS6	-23	82
cis-IV	-175	-61
TS8	-59	53
3+ethane	-182	-116
TS9	-98	65
TS10	-95	71
cis-V	-131	35
trans-V	-130	34

XYZ-coordinates of optimized structures

H_2

H	0.00000000	0.00000000	0.37311200
H	0.00000000	0.00000000	-0.37311200

3

F	3.41318900	1.71204700	1.62719200
F	5.93813300	0.81893600	1.52606700
F	6.63497200	-1.06946300	-0.28149700
F	-2.74926600	3.33258900	0.14262100
F	-1.52867400	5.69008700	0.01839600
F	1.16207200	5.86703600	-0.18161400
F	2.65479000	3.64866500	-0.25564500
C	2.74328800	0.30771200	-0.14322700
C	3.72630500	0.79823400	0.71162300
C	5.03138800	0.34297000	0.68318800
C	5.38964800	-0.62983000	-0.23684200
C	0.74241900	2.27866800	-0.06827800
C	-0.66823600	2.19669200	-0.00361000
C	-1.42324200	3.33798900	0.04739600
C	-0.79319000	4.59247500	-0.01582800
C	0.57430400	4.68214200	-0.11545400
C	1.34003300	3.50763400	-0.14986800
B	1.27369000	0.81096700	-0.08171100
C	3.14280000	-0.67683800	-1.04215600
F	2.26331600	-1.17843300	-1.90964600
C	4.44331500	-1.14061500	-1.11116400
F	4.79309300	-2.06184500	-1.99912000
C	-1.09315900	0.77474000	0.02939600
C	-0.02810200	-0.06278200	-0.02629300
C	-2.49912500	0.35290300	0.14647900
C	-2.94649400	-0.37302400	1.24520100
C	-3.42619900	0.64058500	-0.84902800
C	-4.26237700	-0.78820100	1.35588900
C	-4.74293600	0.23041200	-0.76275600
C	-5.16149000	-0.48692200	0.34697100
C	-0.12197800	-1.52700700	-0.01468900
C	-0.80785200	-2.23967700	-0.99359100
C	0.52791300	-2.27320300	0.96370500
C	-0.85192800	-3.62280500	-0.99982400
C	0.49507600	-3.65564200	0.98140300
C	-0.19897900	-4.33370600	-0.00704800
F	-1.42210900	-1.59361400	-1.98196300
F	-1.50751200	-4.27119500	-1.95426800
F	-0.23876800	-5.65716800	-0.00191400

F	1.11315600	-4.33378900	1.93988400
F	-5.60271500	0.50999400	-1.73209700
F	-6.41948400	-0.88283300	0.44184900
F	-4.66611000	-1.46674700	2.42107000
F	-2.11370400	-0.66609100	2.23824300
F	-3.04203100	1.31124000	-1.92968000
F	1.18924600	-1.64855700	1.93645400

TS1

F	-3.88709300	1.23604300	-1.79774400
F	-6.25773900	0.25979600	-1.05421200
F	-6.45569600	-1.32433400	1.13483700
F	2.56613900	3.43401200	-0.01039100
F	1.22319600	5.73305900	0.04874700
F	-1.47263800	5.78179300	-0.09122400
F	-2.85897400	3.49501800	-0.31838800
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C	-5.27662400	-0.85151000	0.76547600
C	-0.87035500	2.22421500	-0.27979500
C	0.53654400	2.20236100	-0.17312300
C	1.23721800	3.38395500	-0.08341100
C	0.54816200	4.59826600	-0.05401400
C	-0.82856000	4.62352300	-0.12709000
C	-1.53212100	3.42278600	-0.23908000
B	-1.34425600	0.72090100	-0.40152100
C	-2.91867900	-0.65741700	1.09474400
F	-1.86041700	-0.96015100	1.84975100
C	-4.14315500	-1.16121900	1.49716000
F	-4.24087800	-1.92650300	2.57701900
C	1.03532100	0.81068300	-0.18872600
C	0.02598800	-0.08420000	-0.30738800
H	-1.62107400	1.06194100	-2.18875000
H	-1.31434200	0.36002200	-2.19227500
C	2.46702700	0.46570000	-0.11078400
C	3.10766700	-0.19241300	-1.15449800
C	3.22657800	0.76640500	1.01394600
C	4.44843600	-0.53140500	-1.08845400
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C	0.83547100	-2.19185900	0.77895700
C	-0.30389100	-2.35665100	-1.28732600
C	0.96665000	-3.56847800	0.82697900
C	-0.18391100	-3.73386400	-1.26517500

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F	1.29989700	-1.49385400	1.81132900
F	1.56488500	-4.15050300	1.85845400
F	0.58380800	-5.66111700	-0.16620100
F	-0.67090900	-4.46956500	-2.25581100
F	5.26182500	0.72546000	2.19405900
F	6.45788900	-0.54200500	0.12065200
F	5.03765300	-1.14863900	-2.10408200
F	2.44149400	-0.49736500	-2.26410100
F	2.65596500	1.37635700	2.04725200
F	-0.92390900	-1.80530400	-2.33289600

I

F	-3.97896800	0.67620300	-1.98853700
F	-6.25656100	-0.21162000	-0.89223900
F	-6.25818500	-1.19840100	1.63337300
F	2.53352300	3.42112800	0.01919700
F	1.18179700	5.71996800	-0.04219300
F	-1.49031800	5.75998800	-0.41136800
F	-2.84954000	3.45659200	-0.75501400
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C	-0.86887400	2.20257800	-0.49995000
C	0.52325600	2.18141100	-0.28730200
C	1.21240700	3.37079900	-0.15233500
C	0.52254700	4.57893800	-0.19022500
C	-0.84639000	4.60051300	-0.38140100
C	-1.53281000	3.40032000	-0.54452700
B	-1.35870700	0.69134700	-0.66370900
C	-2.77995800	-0.35303900	1.23237700
F	-1.66811300	-0.40412700	1.97005800
C	-3.94916200	-0.81261800	1.81382700
F	-3.95013000	-1.29053700	3.05254800
C	1.02457700	0.79571200	-0.26628300
C	0.02981600	-0.10052600	-0.45966300
H	-1.70239800	0.96159500	-2.06370800
H	-1.34087400	0.24542600	-2.05585100
C	2.44801900	0.45119300	-0.08553800
C	3.16292500	-0.20094100	-1.08349800
C	3.12724200	0.75332800	1.08898800
C	4.49759400	-0.53410600	-0.92624000
C	4.45794900	0.42765800	1.27038600
C	5.14533100	-0.21986900	0.25599600
C	0.18842500	-1.55734200	-0.41019000

C	0.75835900	-2.21861500	0.67713800
C	-0.29883000	-2.36566300	-1.43383900
C	0.85247400	-3.59887600	0.73158500
C	-0.21676900	-3.74415300	-1.40576800
C	0.36901000	-4.36525900	-0.31488300
F	1.20269300	-1.53193800	1.72454600
F	1.39482900	-4.19210000	1.78687700
F	0.45903400	-5.68473400	-0.27070200
F	-0.68227000	-4.47088100	-2.41252000
F	5.07785900	0.72123400	2.40550800
F	6.41964600	-0.53708000	0.41797700
F	5.15783300	-1.14744300	-1.90006900
F	2.57684100	-0.50785000	-2.23743400
F	2.48467400	1.35951500	2.08144800
F	-0.86404900	-1.79534500	-2.50359700

TS2

F	-3.79198300	-0.05392100	-2.11741700
F	-5.99382100	-0.79662100	-0.78782400
F	-6.07135200	-0.64191800	1.91628900
F	2.96888600	3.06676500	-0.21635400
F	1.97623300	5.54732600	-0.38981700
F	-0.65372200	5.96280200	-0.77443000
F	-2.34735000	3.88112300	-1.04350300
C	-2.65773300	0.49755800	-0.12271200
C	-3.78450400	0.03204700	-0.78436300
C	-4.93476700	-0.35598100	-0.11784600
C	-4.97779700	-0.27683200	1.26357100
C	-0.58733200	2.35425900	-0.67556600
C	0.78760600	2.13845000	-0.46086400
C	1.65623100	3.21937300	-0.38186700
C	1.15932400	4.50693000	-0.48702100
C	-0.19704900	4.72162900	-0.69224000
C	-1.05563600	3.63883100	-0.81218300
B	-1.33861400	0.97579000	-0.86052200
C	-2.74037100	0.55830700	1.26188200
F	-1.69503300	0.99670100	1.96580600
C	-3.87332100	0.18295800	1.96181900
F	-3.91301500	0.25772600	3.28727000
C	1.08883700	0.71402900	-0.40336300
C	0.00046800	-0.06163300	-0.66314800
H	-1.58781500	0.95217800	-2.12335700
H	-0.77262300	0.30213300	-1.82405100
C	2.41677300	0.16620400	-0.07185900
C	3.09202200	-0.67107000	-0.95404700
C	3.03717900	0.44984400	1.14032300

C	4.33567800	-1.19713000	-0.65084000
C	4.27453700	-0.07164800	1.46736100
C	4.92587900	-0.89861500	0.56572900
C	-0.06144200	-1.51945100	-0.51526500
C	0.22121600	-2.15066200	0.69430700
C	-0.45385400	-2.33817100	-1.57025400
C	0.12930200	-3.52382500	0.84185700
C	-0.55566100	-3.71052900	-1.44814700
C	-0.25793900	-4.30644700	-0.23312100
F	0.57169700	-1.43311600	1.75638800
F	0.40164100	-4.09336200	2.00775500
F	-0.34748100	-5.61907600	-0.09928100
F	-0.92325400	-4.45628800	-2.48012200
F	4.83787700	0.20699400	2.63410300
F	6.11081300	-1.40105100	0.86705500
F	4.96375200	-1.98057900	-1.51656500
F	2.56068100	-0.96896400	-2.13523800
F	2.42754200	1.22957500	2.02523900
F	-0.73459600	-1.78453700	-2.75078100

II

C	3.01761300	0.83144200	0.12682700
C	2.18886800	0.60168900	1.21775800
C	2.84323200	0.22229500	2.38455200
C	4.21893900	0.09109100	2.47547700
C	5.00046400	0.33782100	1.36027100
C	4.39550700	0.71174300	0.17291700
B	0.59679600	0.76865200	1.18225000
C	-0.05509300	1.87134400	0.24718900
F	2.14692200	-0.04224300	3.49418600
F	4.79756200	-0.27294700	3.61773200
F	6.31988600	0.21522800	1.42833300
F	5.14120900	0.94699500	-0.90434800
F	2.48756300	1.18743100	-1.05164200
C	-0.34644600	-0.61176900	0.57972000
C	0.47981100	-1.27462600	-0.48051300
C	1.43743300	-2.20051800	-0.06915100
C	2.25415300	-2.87774800	-0.95454200
C	2.13322800	-2.64239800	-2.31342000
C	1.18149900	-1.74514200	-2.76050200
C	0.37239500	-1.08191200	-1.85239000
F	1.56837100	-2.47243800	1.22921500
F	3.15012300	-3.75031200	-0.50932500
F	2.91266000	-3.27914300	-3.17575000
F	1.03836700	-1.52573000	-4.06221700

F	-0.54826900	-0.25760500	-2.35557000
C	-1.56654700	0.10185200	0.20725200
C	-2.87230000	-0.46151900	0.47170500
C	-3.92922700	0.29417000	1.00801400
C	-5.15123200	-0.27020100	1.30884700
C	-5.36476800	-1.61850200	1.05891800
C	-4.34942700	-2.39933000	0.52593400
C	-3.12348400	-1.82741300	0.25597700
F	-3.76023300	1.57087500	1.30432100
F	-6.11594300	0.45896300	1.84229000
F	-6.53189100	-2.15736600	1.33023400
F	-4.56561800	-3.67899100	0.27591000
F	-2.19267200	-2.60047600	-0.27623100
C	-1.33164900	1.43245600	-0.20029800
H	0.14437300	0.90201700	2.29667300
H	-0.55254200	-1.35143600	1.35228600
C	-2.16899800	2.27157700	-0.96078200
C	0.34345500	3.14751800	-0.09478900
C	-1.73349400	3.52421200	-1.29281000
C	-0.47652200	3.96713600	-0.84581300
F	1.51275100	3.64120000	0.31165500
F	-0.10433700	5.19080700	-1.15536700
F	-2.46860800	4.33400600	-2.03712500
F	-3.33898300	1.85114000	-1.41944400

TS3

C	-3.00507500	0.78621800	-0.39323800
C	-2.07703100	0.43941100	-1.36949000
C	-2.61865600	-0.06897000	-2.54743200
C	-3.97965300	-0.21650300	-2.75343500
C	-4.86180200	0.14737000	-1.75068800
C	-4.37208600	0.65241600	-0.55830100
B	-0.50662500	0.63047100	-1.22002700
C	0.11587800	1.75946600	-0.30465800
F	-1.82255000	-0.44936500	-3.54850700
F	-4.44886600	-0.70588300	-3.89780100
F	-6.16758500	0.01035800	-1.92956800
F	-5.21623500	0.99835900	0.40946300
F	-2.59080300	1.26905700	0.78334000
C	0.40946900	-0.81426200	-0.30321800
C	-0.55463800	-1.18862700	0.75939700
C	-1.55945700	-2.10138100	0.43117900
C	-2.48141700	-2.56446300	1.34938200
C	-2.42521000	-2.11733800	2.65879100
C	-1.43075700	-1.23022000	3.02811100
C	-0.51443900	-0.78279600	2.09121500

F	-1.63190100	-2.57252100	-0.81272300
F	-3.41767500	-3.43049500	0.98358400
F	-3.30520400	-2.54598500	3.55033800
F	-1.34946600	-0.81583800	4.28624500
F	0.44106400	0.03514400	2.52780500
C	1.58495100	-0.03922000	-0.07454700
C	2.89190200	-0.57934000	-0.39769800
C	3.88633800	0.16823500	-1.04739800
C	5.11550800	-0.37169900	-1.36557700
C	5.39772300	-1.68582300	-1.02132200
C	4.44603300	-2.45540900	-0.36946500
C	3.21335100	-1.90814500	-0.07643000
F	3.65261900	1.41420900	-1.42445800
F	6.02201400	0.34862200	-2.00447800
F	6.57126800	-2.20245700	-1.31387900
F	4.72931800	-3.70076700	-0.02620400
F	2.34892400	-2.66709200	0.57825500
C	1.35053600	1.33283500	0.23644600
H	0.07513800	0.54718200	-2.26837700
H	0.57825400	-1.66124000	-0.96306400
C	2.17672800	2.20991900	0.94839700
C	-0.27535500	3.06418500	-0.07187000
C	1.75675100	3.49671100	1.16819400
C	0.52912600	3.92682900	0.64771700
F	-1.41181000	3.54681900	-0.57565500
F	0.16934300	5.18203000	0.84177700
F	2.49183100	4.34646800	1.86898600
F	3.33209400	1.80659200	1.46428100

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F	-1.31904500	3.35833800	-1.53454900
F	-2.65018900	4.47024900	0.50312500
F	-1.60016100	4.41046400	2.99459700
F	3.02230700	-2.50085500	-0.56847700
F	5.49270300	-1.66174200	-1.10766500
F	5.95344000	0.91178500	-1.80381500
F	3.90830600	2.65616500	-1.95145800
C	0.45223200	2.65977100	-0.13726000
C	-0.77089100	3.30834900	-0.32309600
C	-1.47790600	3.88550300	0.71404000
C	-0.94365600	3.85457700	1.99296900
C	2.36545500	1.01478000	-1.26984600
C	2.12564500	-0.32722900	-0.91552400
C	3.19923900	-1.21248300	-0.86202200
C	4.48606700	-0.80067700	-1.15750400
C	4.72093700	0.51348000	-1.52686900

C	3.65412100	1.39094400	-1.59900800
B	1.21366700	2.07540200	-1.35832200
C	0.95261400	2.65815900	1.16571400
F	2.13129600	2.10778700	1.43375300
C	0.27811700	3.24158400	2.22236500
F	0.78797100	3.22992200	3.44701600
C	0.73627300	-0.76235700	-0.70032500
C	-0.23298800	-0.19431600	-1.44776700
H	0.97132600	2.55233200	-2.42598500
H	0.07076900	0.38228900	-2.32112500
C	0.43970600	-1.81636600	0.29316800
C	-0.24067300	-2.97799200	-0.06344400
C	0.85002100	-1.70825700	1.61805800
C	-0.50593500	-3.98060600	0.85284800
C	0.59155300	-2.69450300	2.55143600
C	-0.09098700	-3.83654700	2.16586800
C	-1.67728200	-0.33090200	-1.28443400
C	-2.33661800	-0.21285800	-0.06152600
C	-2.47831400	-0.50498800	-2.41309400
C	-3.71426900	-0.29668100	0.03807900
C	-3.85459700	-0.59482900	-2.33693000
C	-4.47551500	-0.49280000	-1.10202100
F	-1.65335300	0.02935300	1.05323700
F	-4.31018600	-0.17150500	1.21617700
F	-5.79202500	-0.57524600	-1.01358000
F	-4.58176700	-0.78107800	-3.42934700
F	0.98255600	-2.55104800	3.81017300
F	-0.34309300	-4.78775400	3.04911100
F	-1.14463000	-5.08114700	0.47886900
F	-0.62910400	-3.17301800	-1.31936200
F	1.49237400	-0.61856600	2.02328100
F	-1.90567900	-0.60634600	-3.60825700

TS4

C	-3.34595500	0.13838800	0.89242000
C	-3.20753000	-0.08204800	-0.48178100
C	-4.01556700	-1.08706800	-1.02587800
C	-4.90939700	-1.81859100	-0.26762100
C	-5.01306000	-1.55949100	1.09035500
C	-4.22933200	-0.57717400	1.67696200
B	-2.24170900	0.70996900	-1.39455400
C	-1.44400900	1.98564600	-0.94135400
F	-3.94837500	-1.37574500	-2.31972200
F	-5.66374800	-2.76063300	-0.81707800
F	-5.86024300	-2.24994800	1.82780100
F	-4.33506600	-0.34180800	2.97750900

F	-2.61118100	1.06034800	1.50201200
C	0.24913400	-0.37786300	-0.86747100
C	0.92853300	-1.67863500	-0.79523300
C	2.11808800	-1.96413500	-1.45776500
C	2.70658800	-3.21568100	-1.39547400
C	2.09887700	-4.22444100	-0.66725500
C	0.90311700	-3.97835400	-0.01177700
C	0.33436800	-2.72088600	-0.08840000
F	2.71098300	-1.03540400	-2.19987500
F	3.84029700	-3.45749100	-2.03986900
F	2.65494600	-5.42291900	-0.60329700
F	0.31878000	-4.94383400	0.68419800
F	-0.81470200	-2.50761500	0.54714200
C	0.71224400	0.80018500	-0.42927000
C	2.06426000	0.81255700	0.19952100
C	3.18053000	1.29363900	-0.47114000
C	4.44007100	1.27163700	0.09687100
C	4.60340900	0.75679500	1.37335400
C	3.50899500	0.27205100	2.06776300
C	2.25706800	0.30303900	1.47578400
F	3.04515300	1.81020700	-1.68793600
F	5.48930900	1.74020800	-0.56608700
F	5.80525400	0.73011400	1.92729200
F	3.66439500	-0.22017400	3.29022300
F	1.22539800	-0.17037800	2.16936400
C	-0.09750100	2.03480900	-0.51352500
H	-2.19417300	0.40211200	-2.54721100
H	-0.74400500	-0.45247600	-1.31649500
C	0.40318100	3.28430200	-0.13880400
C	-2.16699200	3.15539300	-1.02736300
C	-0.35159600	4.44455600	-0.22212700
C	-1.65338300	4.38991100	-0.67184200
F	-3.43977100	3.10626100	-1.45023400
F	-2.38528300	5.48962500	-0.75461500
F	0.18040700	5.60566900	0.13580500
F	1.64587900	3.44899100	0.31545600

***trans*-III**

C	3.95079800	-0.14294500	0.47693000
C	3.14962600	0.02938800	-0.65429500
C	3.64677900	0.90490900	-1.62465900
C	4.86402100	1.54838400	-1.49921600
C	5.62385500	1.34055200	-0.35907800
C	5.16549300	0.49448900	0.63929400
B	1.76220400	-0.63540000	-0.85199000
C	1.24301000	-1.90448100	-0.10817000

F	2.95536900	1.13848600	-2.73480100
F	5.31103600	2.35981000	-2.44911100
F	6.78561000	1.95159400	-0.22137400
F	5.89440400	0.31156500	1.73264300
F	3.54549600	-0.92614600	1.47212300
C	-0.30397800	0.44123600	0.68096800
C	-0.86718900	1.78532900	0.57307300
C	-1.48869700	2.27580100	-0.57393100
C	-1.97117900	3.57083700	-0.64683900
C	-1.83068900	4.41923600	0.43862200
C	-1.20025000	3.97004900	1.58816000
C	-0.72327800	2.67445200	1.63752400
F	-1.59978300	1.51526300	-1.65793200
F	-2.55103100	4.00939100	-1.75606900
F	-2.29062600	5.65746700	0.37594900
F	-1.06430600	4.78139200	2.62795100
F	-0.12342700	2.26601800	2.75158600
C	-0.89308300	-0.72023900	0.33398200
C	-2.31180300	-0.80542000	-0.07201900
C	-2.67705900	-1.37583400	-1.28751800
C	-3.99785700	-1.47935200	-1.68281300
C	-4.99826300	-1.01010800	-0.84737800
C	-4.66894100	-0.44338800	0.37239700
C	-3.33990700	-0.34582400	0.74549000
F	-1.73862800	-1.81557600	-2.11993700
F	-4.31179600	-2.01259900	-2.85556300
F	-6.26557300	-1.10460100	-1.21361000
F	-5.62770000	-0.00851700	1.17915500
F	-3.06848700	0.17625500	1.93715700
C	-0.08891300	-1.95085600	0.35653300
H	1.05936400	-0.18100800	-1.69907600
H	0.67240200	0.38938100	1.15669000
C	-0.59174000	-3.13774800	0.87814000
C	2.00876700	-3.05764800	-0.00760200
C	0.18991100	-4.27594400	0.94782600
C	1.49957000	-4.23994900	0.49571200
F	3.26857500	-3.07588300	-0.44984300
F	2.24403300	-5.33485800	0.55021700
F	-0.29865700	-5.39512700	1.46028700
F	-1.82859700	-3.20737000	1.37067500

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C	0.00000000	0.66249900	0.00000000
H	0.92376900	1.23253000	0.00000000
H	-0.92372100	1.23258400	0.00000000
C	0.00000000	-0.66249900	0.00000000

H	-0.92376900	-1.23253000	0.00000000
H	0.92372100	-1.23258400	0.00000000

ethane

C	0.00000000	0.00000000	0.76023500
H	0.00000000	1.01799200	1.15863200
H	-0.88160700	-0.50899600	1.15863200
H	0.88160700	-0.50899600	1.15863200
C	0.00000000	0.00000000	-0.76023500
H	0.00000000	-1.01799200	-1.15863200
H	-0.88160700	0.50899600	-1.15863200
H	0.88160700	0.50899600	-1.15863200

TS6

F	2.52055100	3.18993100	-1.19711600
F	4.47709800	4.37610100	0.16553600
F	6.04681000	2.92752800	1.83762900
F	-1.15768300	-3.54551600	-0.68837700
F	0.81981000	-5.19644700	-1.42238700
F	3.26808800	-4.19997200	-2.02930500
F	3.72746600	-1.58956600	-1.88064000
C	3.04194600	1.05392700	-0.33321900
C	3.27569400	2.42720300	-0.40323000
C	4.28277100	3.06761300	0.29336000
C	5.08507300	2.33209200	1.14951100
C	1.50622400	-1.11260900	-1.22024900
C	0.23347000	-1.64944500	-0.92212900
C	0.03598900	-3.02174600	-0.97665500
C	1.04332800	-3.89243500	-1.35323500
C	2.28861200	-3.38216400	-1.66576400
C	2.49609200	-2.01684700	-1.58473900
B	1.79396600	0.43346900	-1.07966200
C	3.86437000	0.36183000	0.55273200
F	3.69691300	-0.94298000	0.76729300
C	4.87217100	0.97212100	1.28180900
F	5.62725800	0.26494400	2.11617200
C	-0.94190900	-0.82668400	-0.51013000
C	-1.58651400	-0.07938400	-1.41026100
H	0.84845800	1.15404600	-1.10730200
H	-1.25885300	-0.13402700	-2.44358500
C	-1.39309100	-0.97412100	0.89330300
C	-2.66560800	-1.44294800	1.20832300
C	-0.54770200	-0.68883700	1.96071600
C	-3.07772200	-1.61806500	2.51852000
C	-0.93745900	-0.85513800	3.27666500
C	-2.21155200	-1.32066900	3.55638600

C	-2.71872100	0.81623700	-1.15922600
C	-2.74296000	1.76603200	-0.14092700
C	-3.81871700	0.78667300	-2.01369300
C	-3.81875900	2.61879900	0.03897700
C	-4.90375200	1.62725500	-1.85344400
C	-4.90409100	2.54721700	-0.81725000
F	-1.70328000	1.90868500	0.67589100
F	-3.80701600	3.51640800	1.01616500
F	-5.93529100	3.35988300	-0.65164900
F	-5.94139300	1.55757400	-2.67681900
F	-0.10858100	-0.55859800	4.26910800
F	-2.59860100	-1.48207500	4.81154400
F	-4.29407700	-2.07706100	2.78448000
F	-3.52447200	-1.76258100	0.24589700
F	0.67302800	-0.21311000	1.72888500
F	-3.84395300	-0.08992900	-3.01416700
C	2.84841000	0.84840700	-3.42030600
H	3.12703000	-0.15813100	-3.70425000
H	3.65813500	1.52755200	-3.17953800
C	1.57623700	1.25439400	-3.43610200
H	1.30246600	2.27865600	-3.21645700
H	0.77789100	0.58332200	-3.73228600

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F	0.59511200	-3.11061700	-0.88559100
F	1.23083600	-4.38856500	1.36458500
F	-0.38490400	-4.22155800	3.53289100
F	-1.65109800	3.41762200	-0.48261800
F	-4.25597000	3.63974800	-1.00603400
F	-5.70497300	1.46271600	-1.71080800
F	-4.53129300	-0.94007200	-1.87820600
C	-1.38866900	-2.22317600	0.04625800
C	-0.24586900	-3.01154100	0.14745200
C	0.11297700	-3.67427900	1.30633000
C	-0.70660000	-3.58467100	2.41913100
C	-2.44012200	-0.05961700	-1.23177900
C	-1.69460300	1.07247600	-0.85322100
C	-2.32979800	2.30979200	-0.78506200
C	-3.67543900	2.44956400	-1.07012500
C	-4.41228600	1.34005700	-1.44559800
C	-3.78002700	0.11330700	-1.53324800
B	-1.82200100	-1.51532100	-1.29779300
C	-2.17628500	-2.15531500	1.19223900
F	-3.30544800	-1.44612900	1.19098200
C	-1.85978600	-2.82076300	2.36347100
F	-2.64913600	-2.73835400	3.42771800

C	-0.24128100	0.96319300	-0.60889400
C	0.50586300	0.22026800	-1.44582200
H	-2.70553300	-0.87605300	-3.99188000
H	0.03046600	-0.14413800	-2.35264300
C	0.34318700	1.71816300	0.52150200
C	1.36248500	2.64716800	0.33298400
C	-0.12716400	1.55453500	1.82016300
C	1.89661400	3.37066800	1.38479300
C	0.39385700	2.26297000	2.88705600
C	1.41179600	3.17601700	2.66709600
C	1.93019700	-0.09041100	-1.33547100
C	2.55351600	-0.52494500	-0.16751800
C	2.72655900	-0.02196600	-2.47825500
C	3.89939700	-0.84338700	-0.12890600
C	4.07279300	-0.33220000	-2.46351000
C	4.66348700	-0.74264000	-1.27924400
F	1.85130300	-0.69497100	0.94959200
F	4.45643900	-1.26375900	0.99896000
F	5.95065600	-1.04480400	-1.24936900
F	4.80093800	-0.23564100	-3.56737700
F	-0.06619500	2.06815600	4.11538700
F	1.91747100	3.86182000	3.67867500
F	2.85873100	4.25818800	1.17021900
F	1.83168200	2.89300700	-0.88608800
F	-1.09232700	0.67411500	2.06842000
F	2.18541500	0.37212400	-3.62750200
C	-1.84166200	-2.34065500	-2.62301500
H	-2.77423100	-2.92032900	-2.48397800
H	-1.06112000	-3.10533500	-2.62672800
C	-1.90049500	-1.61317300	-3.96137800
H	-0.96527400	-1.08712900	-4.17248800
H	-2.06531600	-2.31423600	-4.78242500

TS8

F	2.90312900	-1.63521600	1.45537700
F	4.90952100	-2.58689000	0.00168700
F	5.72856600	-1.28492400	-2.23621000
F	-2.73043700	3.22363200	-0.00570900
F	-1.57577600	5.63660200	0.17699000
F	1.06039400	5.86993800	0.67268900
F	2.58811100	3.67986000	1.03702300
C	2.60745000	0.24299800	0.04519800
C	3.26997000	-0.93464700	0.37397000
C	4.31369400	-1.45830500	-0.36832500
C	4.73217200	-0.79952700	-1.51050100
C	0.74104000	2.27010400	0.63107000

C	-0.63345000	2.15388700	0.36266400
C	-1.41916200	3.29101800	0.22132400
C	-0.84023000	4.54263900	0.32823300
C	0.51791100	4.66314700	0.59159100
C	1.28901000	3.52392900	0.76312900
B	1.39658700	0.85137400	0.89494500
C	3.05247400	0.86035900	-1.12025700
F	2.47851300	1.98067600	-1.56268200
C	4.09558900	0.36806600	-1.88820900
F	4.48406100	1.00587800	-2.98705200
C	-1.03890200	0.75561000	0.31546500
C	-0.03928800	-0.09782000	0.66221400
H	1.27674500	1.51481000	4.62829400
H	0.73412000	0.20661100	1.80962400
C	-2.37149100	0.30444400	-0.12857200
C	-3.19281200	-0.45751700	0.69555800
C	-2.84994600	0.61068200	-1.39812100
C	-4.43918500	-0.89313000	0.28049300
C	-4.08748700	0.17888000	-1.83676300
C	-4.88502200	-0.57618900	-0.99155900
C	-0.12022800	-1.55746400	0.51351600
C	-0.25278600	-2.14977600	-0.73989800
C	-0.03978400	-2.41399400	1.60619600
C	-0.31145100	-3.52344200	-0.89808500
C	-0.09539200	-3.78831100	1.47528200
C	-0.23348800	-4.34510800	0.21407500
F	-0.31825200	-1.39163700	-1.83021800
F	-0.43628800	-4.05727500	-2.10587600
F	-0.28923800	-5.65928600	0.07241300
F	-0.02303000	-4.57298300	2.54154300
F	-4.51256800	0.47586700	-3.05652800
F	-6.07140400	-0.99342200	-1.39954800
F	-5.20713900	-1.60738400	1.09174800
F	-2.80174500	-0.76854200	1.92727300
F	-2.10125400	1.32561600	-2.23023500
F	0.09072600	-1.90010700	2.82869600
C	1.78565000	0.85699900	2.64850800
H	2.66144100	1.49538700	2.51777500
H	2.15036700	-0.10741400	3.00012100
C	0.81002100	1.47211900	3.64209600
H	0.52835700	2.48817100	3.36292600
H	-0.10620600	0.88403000	3.74234100

TS5

C	-3.90791400	0.09592700	-0.59541300
C	-3.16203900	0.18686700	0.57696500

C	-3.57983200	1.17767700	1.46495100
C	-4.67916500	1.98599500	1.24653500
C	-5.39786700	1.84628800	0.07072300
C	-5.00607100	0.89967300	-0.85778800
B	-1.83391400	-0.62715600	0.86857300
C	-1.30291800	-1.82057900	-0.02877700
F	-2.91516600	1.36604200	2.60772100
F	-5.04459000	2.89954300	2.13991300
F	-6.44779900	2.61823400	-0.16414800
F	-5.68021700	0.77384900	-1.99624900
F	-3.57387000	-0.76722600	-1.55564700
C	0.45978300	0.55672100	-0.75581400
C	1.14765500	1.83962700	-0.61367500
C	1.77872900	2.25793100	0.55600300
C	2.38391200	3.49873100	0.65770300
C	2.35878600	4.36686400	-0.42048200
C	1.72065300	3.99166000	-1.59187900
C	1.12186200	2.74896500	-1.66989200
F	1.78372300	1.48185900	1.63592400
F	2.97133300	3.86816500	1.78867500
F	2.93545200	5.55432100	-0.33019700
F	1.69337600	4.82221600	-2.62561400
F	0.51845000	2.41137800	-2.80609300
C	0.91728500	-0.65416600	-0.40355800
C	2.30635700	-0.87741800	0.05644200
C	2.57674800	-1.51311800	1.26332000
C	3.86672700	-1.74920200	1.70185500
C	4.93666400	-1.34607600	0.92074100
C	4.70415000	-0.71683500	-0.29038500
C	3.40414500	-0.49049600	-0.70745800
F	1.57342000	-1.89601600	2.04992800
F	4.08511000	-2.34508900	2.86698300
F	6.17632100	-1.56501100	1.32871000
F	5.72771900	-0.34755600	-1.04968500
F	3.22999500	0.08216700	-1.89447600
C	0.02222000	-1.82753700	-0.52823600
H	-0.99440400	0.01787300	1.41312600
H	-0.51928800	0.61023000	-1.22197500
C	0.48470400	-2.93522100	-1.23143500
C	-2.08871200	-2.92722600	-0.32480700
C	-0.31683000	-4.03520300	-1.47164600
C	-1.62006100	-4.03204900	-1.01200300
F	-3.36432400	-2.98286400	0.07373500
F	-2.40742400	-5.07381100	-1.24615200
F	0.14439400	-5.06971300	-2.15992800
F	1.71374800	-2.95208100	-1.75356700

C	-1.65000100	-1.44041000	3.11477700
H	-0.76769600	-2.04796700	2.95202300
H	-1.50844300	-0.50069500	3.63364800
C	-2.86866900	-1.87233800	2.76914200
H	-3.75710900	-1.29119300	2.98640300
H	-3.02212300	-2.84843200	2.32995100

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C	-3.54883600	0.52980700	-0.75600300
C	-3.25401900	0.19819300	0.56345400
C	-4.25794500	0.47735600	1.48792600
C	-5.46688700	1.05107300	1.13726300
C	-5.70484300	1.38050400	-0.18660500
C	-4.73658100	1.12395100	-1.14230900
B	-1.88823400	-0.48582600	0.97628500
C	-1.36564900	-1.68788400	0.09454000
F	-4.09975900	0.15622500	2.77261900
F	-6.40036200	1.28240400	2.05226500
F	-6.85223000	1.93718900	-0.53627700
F	-4.95911800	1.44166200	-2.41157800
F	-2.65322800	0.29918100	-1.72135300
C	0.47181200	0.59014200	-0.52428100
C	1.22577400	1.83344200	-0.37457600
C	2.03519300	2.14299700	0.71757400
C	2.69709700	3.35427900	0.81939700
C	2.55261300	4.30437800	-0.17742300
C	1.74020300	4.03868800	-1.26796200
C	1.08776100	2.82367100	-1.34776200
F	2.16260400	1.28971200	1.72942800
F	3.45221400	3.61799400	1.87749900
F	3.18177200	5.46402400	-0.08546700
F	1.59857800	4.94645200	-2.22393400
F	0.31738100	2.59325900	-2.40673700
C	0.90151700	-0.66494600	-0.30251700
C	2.31596000	-0.97921200	0.00174500
C	2.66978800	-1.72576200	1.12106300
C	3.98392200	-2.04213400	1.41221200
C	4.99195900	-1.61566000	0.56403600
C	4.67434300	-0.88142800	-0.56607100
C	3.35221900	-0.57379000	-0.83500100
F	1.72963900	-2.14090300	1.96615700
F	4.28456800	-2.74043000	2.49886500
F	6.25329900	-1.91244700	0.82986500
F	5.63655000	-0.48953900	-1.39077100
F	3.09201800	0.09854900	-1.95180100
C	-0.05327200	-1.78692100	-0.41750400

H	-0.62280600	1.97291500	2.05551300
H	-0.52870500	0.71230600	-0.92759800
C	0.31548600	-2.93714300	-1.10951400
C	-2.22492200	-2.75698200	-0.11720200
C	-0.56029900	-3.99242300	-1.29036100
C	-1.84315300	-3.90816400	-0.78233100
F	-3.47055600	-2.73065200	0.37145800
F	-2.68569800	-4.91928300	-0.93589000
F	-0.18160200	-5.07093200	-1.95988800
F	1.52057200	-3.04961500	-1.67068700
C	-1.16783700	-0.11665300	2.31255100
H	-1.72327000	-0.72051500	3.05241200
H	-0.15555300	-0.52399900	2.33002500
C	-1.16649800	1.34300800	2.76330600
H	-0.68231500	1.44987800	3.73640300
H	-2.17538000	1.74856200	2.85198800

TS7

C	-2.81840200	-0.53458200	1.12496800
C	-3.16298200	-0.47689100	-0.22735500
C	-4.34774800	-1.13278700	-0.56854700
C	-5.12233700	-1.81815000	0.34963200
C	-4.72115500	-1.86981100	1.67377800
C	-3.55870600	-1.22751400	2.06514100
B	-2.32579100	0.34817900	-1.27433100
C	-1.63882000	1.70249400	-0.80501000
F	-4.81296400	-1.08925200	-1.81531500
F	-6.24794200	-2.41519100	-0.02206100
F	-5.44777600	-2.52492100	2.56121800
F	-3.17531300	-1.27282300	3.33458700
F	-1.72227600	0.07425000	1.56439400
C	0.43042900	-0.39350700	-0.88169100
C	1.32857000	-1.56357200	-0.80066300
C	2.29914600	-1.80556600	-1.76564400
C	3.11719500	-2.92129800	-1.71835000
C	2.95984300	-3.83990200	-0.69433500
C	1.98736600	-3.63790000	0.27081300
C	1.18165500	-2.51438600	0.20284400
F	2.45966300	-0.95405400	-2.77340700
F	4.04236800	-3.11921300	-2.64825300
F	3.73523500	-4.91110500	-0.63980400
F	1.83154900	-4.52206300	1.24740500
F	0.24497100	-2.35659000	1.13284500
C	0.69430800	0.82387400	-0.39667900
C	2.01699800	1.02274900	0.26893700
C	3.13631900	1.42668000	-0.44582400

C	4.37506100	1.56638300	0.15313000
C	4.51174000	1.30415000	1.50667600
C	3.41139600	0.90838800	2.24657100
C	2.18114200	0.77556600	1.62383600
F	3.02578500	1.72223400	-1.73721100
F	5.42699600	1.95860700	-0.55401900
F	5.69249600	1.43512400	2.09105700
F	3.54070300	0.65829500	3.54320900
F	1.14280700	0.39992000	2.36342300
C	-0.28401000	1.93277600	-0.46875600
H	-1.17794600	-1.77346400	-3.13945500
H	-0.50474900	-0.58921900	-1.40242200
C	0.08614200	3.24597500	-0.17169200
C	-2.50764400	2.77244700	-0.83146900
C	-0.81361300	4.30103700	-0.19928400
C	-2.13076100	4.06994700	-0.52899800
F	-3.79395900	2.56462500	-1.15915300
F	-3.00503600	5.06376200	-0.55584300
F	-0.40323000	5.52876400	0.09033500
F	1.33905700	3.57704600	0.14474000
C	-2.32587800	0.04840600	-2.81711600
H	-3.30370000	0.44736300	-3.13683900
H	-1.58813500	0.68441600	-3.31545000
C	-2.18641800	-1.39045500	-3.31739000
H	-2.35952100	-1.44100600	-4.39439900
H	-2.88819800	-2.07303600	-2.83823800

TS2b

F	-3.75159700	-0.98428600	-2.10523700
F	-5.94774900	-1.74352800	-0.77980400
F	-6.15130800	-1.30689300	1.88683500
F	2.05886400	3.61397200	-0.05430900
F	0.43907700	5.71331800	-0.28465500
F	-2.16839600	5.42498500	-0.88481400
F	-3.18314900	2.95686500	-1.33987300
C	-2.74809500	-0.12733600	-0.14778100
C	-3.80768600	-0.74916000	-0.79181900
C	-4.95436600	-1.15049000	-0.12667100
C	-5.06118300	-0.92915300	1.23554300
C	-1.08852800	1.97683900	-0.88151300
C	0.27225700	2.11986000	-0.53161400
C	0.78160700	3.39475700	-0.35665400
C	-0.05046300	4.50083400	-0.47751000
C	-1.39443100	4.35447200	-0.78891900
C	-1.90560500	3.08457800	-1.00075700
B	-1.41235200	0.31036500	-0.88441900

C	-2.89506300	0.07561200	1.21787300
F	-1.91695500	0.66892400	1.90498300
C	-4.02466200	-0.31182500	1.91633000
F	-4.12599400	-0.09945000	3.22367300
C	0.92286200	0.82204100	-0.35935700
C	0.04831600	-0.19841600	-0.51653600
H	-1.38874800	1.12001900	-1.92140200
H	-1.54141900	0.01486100	-2.11722900
C	2.36543900	0.65957100	-0.08242500
C	3.21764600	0.07812700	-1.01298300
C	2.91909200	1.05185700	1.13012900
C	4.56583400	-0.10318100	-0.75481800
C	4.26175900	0.88058800	1.41131700
C	5.08766000	0.29896700	0.46270700
C	0.40373500	-1.61792000	-0.38065300
C	0.89939400	-2.13986000	0.81186600
C	0.20124000	-2.52253900	-1.41973500
C	1.18446100	-3.48577500	0.96462600
C	0.48463700	-3.87017500	-1.29265400
C	0.98063400	-4.35430700	-0.09360800
F	1.08557300	-1.34562600	1.86295100
F	1.64642800	-3.94792000	2.11949400
F	1.25668600	-5.64214600	0.03996400
F	0.29486300	-4.69778400	-2.31201000
F	4.76197700	1.26080800	2.57944100
F	6.37452400	0.12924500	0.72058100
F	5.35838800	-0.65475900	-1.66484200
F	2.75011100	-0.31211600	-2.19552200
F	2.14473700	1.60167800	2.05953900
F	-0.26019400	-2.09245400	-2.59257000

***cis*-IIIb**

F	-3.50655900	-2.29472200	-2.14200300
F	-5.81223200	-2.54671900	-0.82854900
F	-5.97909200	-1.81162600	1.76741300
F	-0.44899100	2.57201000	1.56741700
F	-2.58511200	4.12767700	1.16441100
F	-4.00744900	3.95359800	-1.12405900
F	-3.27170700	2.19497700	-3.04133100
C	-2.39294000	-1.39980700	-0.25512700
C	-3.53849300	-1.92098200	-0.86756100
C	-4.74551300	-2.05895500	-0.20875700
C	-4.83529500	-1.68331300	1.12211600
C	-1.46342300	1.45901200	-1.72598100

C	-0.71627000	1.53694600	-0.54765900
C	-1.10489300	2.46421900	0.41403500
C	-2.21493100	3.26927200	0.22558800
C	-2.95378300	3.17246900	-0.94417600
C	-2.56769200	2.26205300	-1.91341300
B	-1.06355800	-1.35016600	-1.05127700
C	-2.53587600	-1.03451200	1.08706000
F	-1.50651600	-0.54432600	1.76707700
C	-3.72631800	-1.16887600	1.77583700
F	-3.82107300	-0.81408700	3.05063900
C	0.42530900	0.62783600	-0.33368000
C	0.28148200	-0.68619400	-0.60437800
C	1.69245800	1.21887500	0.15223600
C	2.31379800	2.25932600	-0.53202200
C	2.30117200	0.78291100	1.32585400
C	3.48978300	2.83412100	-0.08582100
C	3.47440600	1.34740700	1.79455500
C	4.07203300	2.37474700	1.08403900
C	1.44562000	-1.60303400	-0.60832100
C	1.43047400	-2.76469400	0.15684600
C	2.56167700	-1.40104200	-1.41638900
C	2.47852000	-3.66669200	0.15730000
C	3.62083000	-2.29152900	-1.43905400
C	3.58159500	-3.42525900	-0.64456200
F	0.37679300	-3.02457500	0.92984900
F	2.43539000	-4.75421400	0.91510900
F	4.59195700	-4.27970600	-0.65846500
F	4.66850400	-2.07119300	-2.22279500
F	4.02373300	0.91837100	2.92319200
F	5.19569900	2.91770400	1.52248700
F	4.06660600	3.81153900	-0.77219900
F	1.79047800	2.70969000	-1.66824900
F	1.74596700	-0.18042100	2.05273500
F	2.62739400	-0.34212000	-2.21866900
H	-1.03027900	-1.95836800	-2.07875600
H	-1.14842300	0.80665600	-2.53234900

TS4b

F	-2.16510000	2.11017000	2.16308600
F	-4.84826400	1.98075000	2.36626000
F	-6.35683900	1.57305000	0.14979400
F	-0.59784900	-1.94053100	-2.10761200
F	-2.89844100	-3.32561000	-2.02144100
F	-4.46583000	-3.23265800	0.18232000
F	-3.72517500	-1.74014000	2.30488900
C	-2.24325700	1.78096700	-0.16272600

C	-2.88959700	1.91579500	1.05473900
C	-4.26581100	1.85199900	1.18076600
C	-5.03822400	1.64652300	0.04892100
C	-1.77184800	-1.04414200	1.19357400
C	-0.96198100	-1.07933500	0.06083900
C	-1.34878600	-1.87402700	-1.00960200
C	-2.53212900	-2.59275100	-0.98006000
C	-3.33630300	-2.54277200	0.14648300
C	-2.94256300	-1.76829100	1.22731100
B	-0.69287800	1.99660300	-0.30516600
C	-3.04988500	1.60403000	-1.27493100
F	-2.48504400	1.49329600	-2.48103200
C	-4.42816700	1.51369000	-1.18812000
F	-5.16709500	1.31542400	-2.27244100
C	0.33488200	-0.36094600	0.00898300
C	0.45689600	0.98850400	-0.02774500
C	1.52294300	-1.25300700	-0.03048800
C	1.77778800	-2.15342500	1.00026300
C	2.40109400	-1.26045500	-1.11087600
C	2.86389400	-3.00924600	0.97352800
C	3.48647200	-2.11679700	-1.16306700
C	3.72074000	-2.99081300	-0.11462800
C	1.81131900	1.59441600	0.08463800
C	2.36973700	2.34548800	-0.94494500
C	2.54966700	1.49443100	1.25941200
C	3.60095000	2.96401200	-0.81932300
C	3.78153900	2.10682200	1.41022700
C	4.31054700	2.84289900	0.36393600
F	1.72539400	2.46992200	-2.10148500
F	4.11044400	3.66157300	-1.82617600
F	5.49007100	3.42959900	0.49377800
F	4.45467000	1.99561800	2.54834700
F	4.29740500	-2.11042300	-2.21151400
F	4.75879900	-3.80790200	-0.15345600
F	3.09215500	-3.83922600	1.98122400
F	0.98433100	-2.18469900	2.06515700
F	2.19759200	-0.45372900	-2.14490800
F	2.06837200	0.80399800	2.29122200
H	-0.36216900	3.07689500	-0.69273400
H	-1.47928600	-0.46766300	2.06179100

***trans*-IIIb**

F	3.71846900	1.68493100	-2.14079100
F	6.24024500	1.31151200	-1.34575800
F	6.74979700	0.06612100	0.99828800
F	-2.97151400	2.23660800	-1.52794400

F	-2.95467400	4.90523800	-1.41611600
F	-1.12608900	6.21359300	0.07636000
F	0.71467500	4.82179000	1.48608100
C	2.83810300	0.60789400	-0.22928100
C	3.92256900	1.06447200	-0.98384800
C	5.23586900	0.88153100	-0.59339800
C	5.50140600	0.24100500	0.60687200
C	-0.17561000	2.78612400	0.70903000
C	-1.11895900	2.09165500	-0.05423400
C	-2.06604600	2.83377400	-0.75603200
C	-2.06320700	4.21636300	-0.71950800
C	-1.11466700	4.89096700	0.03603300
C	-0.17502200	4.16428500	0.74598400
B	1.38864000	0.87351400	-0.72039600
C	3.15793500	-0.02647400	0.97235000
F	2.19055900	-0.45109300	1.78230900
C	4.45862900	-0.21330800	1.39944700
F	4.72112700	-0.81107400	2.55435100
C	-1.06332000	0.62445300	-0.14008800
C	0.13896200	0.02435400	-0.32135300
C	-2.33513200	-0.11914500	-0.00348400
C	-3.14887400	0.04519500	1.11345400
C	-2.78718500	-0.98866400	-0.99227800
C	-4.34874700	-0.62760500	1.25418300
C	-3.98774000	-1.66645600	-0.87636000
C	-4.76925000	-1.48749100	0.25302400
C	0.27809400	-1.44639600	-0.25399600
C	0.87615300	-2.13395400	-1.30526300
C	-0.11497500	-2.20559300	0.84463300
C	1.05497700	-3.50445200	-1.29170000
C	0.05746900	-3.57822700	0.88599200
C	0.63984000	-4.23077000	-0.18775300
F	1.28464100	-1.45575400	-2.37815100
F	1.61487100	-4.12523100	-2.32154200
F	0.80664800	-5.54335100	-0.15568500
F	-0.31940300	-4.27117000	1.95312300
F	-4.39933100	-2.47654100	-1.84251700
F	-5.91628500	-2.13433300	0.37381100
F	-5.09200200	-0.46281600	2.33988100
F	-2.76408900	0.84812900	2.10043800
F	-2.08214400	-1.16386700	-2.10470600
F	-0.64300700	-1.61707500	1.91378100
H	1.23658400	1.74363000	-1.52014900
H	0.52014900	2.24702700	1.34066400

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F	-1.89223700	-2.91144600	-1.95337100
F	-3.36466500	-4.68661600	-0.61511500
F	-5.12109900	-3.85209000	1.28363400
F	0.76005000	3.56226300	0.62507200
F	-1.24980000	5.30309200	0.29580800
F	-3.51835600	4.51589200	-0.97756000
F	-3.76272100	2.03976700	-1.87935600
C	-2.84287600	-1.07667100	-0.81165800
C	-2.75810100	-2.44644600	-1.03986400
C	-3.49971300	-3.39041600	-0.35404400
C	-4.39224300	-2.96908700	0.61584300
C	-1.61173500	1.41019900	-1.12026700
C	-0.44163500	1.83819500	-0.45770100
C	-0.35278800	3.14344800	0.01627700
C	-1.37161400	4.05989800	-0.15038000
C	-2.51953200	3.65991900	-0.80526200
C	-2.61147700	2.36252100	-1.27551900
B	-1.95869100	-0.05956000	-1.70551500
C	-3.74085500	-0.70531900	0.18081900
F	-3.90228300	0.57628700	0.51785800
C	-4.51067600	-1.61833900	0.88509700
F	-5.35868700	-1.20491000	1.82170600
C	0.76524800	0.98892500	-0.23302900
C	1.51654100	0.61339000	-1.27709800
H	-1.25262500	1.69756100	-3.92095600
H	1.24562600	0.99806100	-2.25628400
C	1.14012100	0.70264400	1.17136000
C	2.36745000	1.09477500	1.69900300
C	0.26005300	0.06278600	2.03682200
C	2.70142500	0.86117700	3.02206300
C	0.57178200	-0.18377100	3.36065700
C	1.80204900	0.21725200	3.85475200
C	2.69738600	-0.25273300	-1.24887100
C	2.74239500	-1.47816600	-0.58898600
C	3.83143300	0.11255000	-1.97146900
C	3.86686400	-2.28454800	-0.61752400
C	4.96695100	-0.67406300	-2.01140700
C	4.98436800	-1.87932800	-1.32768400
F	1.67412400	-1.93326600	0.06137700
F	3.87299900	-3.45008000	0.01503900
F	6.06279100	-2.64413700	-1.35981200
F	6.03525700	-0.28504800	-2.69319500
F	-0.28764200	-0.81121900	4.15190300
F	2.11585400	-0.01243000	5.11903900
F	3.87358100	1.25931300	3.49867100
F	3.25174200	1.73863300	0.94514800

F	-0.91631900	-0.35927800	1.58064000
F	3.83931300	1.26550900	-2.63343900
C	-2.27070500	-0.12754100	-3.29488200
H	-3.28487500	0.27099000	-3.39286300
H	-2.33996200	-1.16632900	-3.63000200
C	-1.32347700	0.64510700	-4.20727200
H	-0.30993300	0.23038400	-4.18647800
H	-1.65964000	0.60856800	-5.24620900
H	-0.61989000	-0.61829600	-1.31595000
H	-0.79219300	-0.83341100	-2.05876700

TS9

F	-1.96684100	-3.06977500	-1.66294400
F	-3.52399800	-4.71992100	-0.25417300
F	-5.25533200	-3.72437900	1.58971600
F	0.86000100	3.64318800	0.19529500
F	-1.15424400	5.34868300	-0.26036900
F	-3.48202800	4.43941300	-1.32476300
F	-3.77913400	1.86821300	-1.90513800
C	-2.85934800	-1.14832300	-0.62565100
C	-2.82048000	-2.52994800	-0.77929500
C	-3.60769600	-3.40753600	-0.05777900
C	-4.48784700	-2.90409700	0.88438900
C	-1.59661400	1.32194300	-1.17484700
C	-0.39566900	1.81165300	-0.61928000
C	-0.27842200	3.16302700	-0.31294500
C	-1.30164100	4.06165800	-0.54573600
C	-2.48173200	3.59849700	-1.09375700
C	-2.60190800	2.25357200	-1.39474600
B	-1.89285300	-0.21703900	-1.50418900
C	-3.74727000	-0.69197500	0.33882600
F	-3.85615400	0.61152400	0.60870000
C	-4.55457800	-1.53811100	1.08440100
F	-5.39001900	-1.04479600	1.99382000
C	0.79848100	0.96716600	-0.33347400
C	1.49119200	0.42468700	-1.34210000
H	-1.45160400	1.43534100	-3.96393300
H	1.19348700	0.68003500	-2.35487000
C	1.21672600	0.85551600	1.08320600
C	2.47195000	1.27652000	1.51404100
C	0.35259100	0.36149400	2.05474000
C	2.85008900	1.20774000	2.84394900
C	0.70882500	0.28170600	3.38825500
C	1.96643600	0.70585400	3.78396500
C	2.64966600	-0.46608700	-1.23996900
C	2.69608300	-1.59028700	-0.41909000

C	3.75928100	-0.23672900	-2.05114400
C	3.80006700	-2.42482900	-0.38295900
C	4.87338900	-1.05364200	-2.02978000
C	4.89393000	-2.15349800	-1.18714500
F	1.65071100	-1.91989900	0.33466900
F	3.80893200	-3.49179700	0.40535100
F	5.95275300	-2.94622600	-1.15697400
F	5.91927000	-0.79194800	-2.80204800
F	-0.13650600	-0.20975800	4.28473000
F	2.32106700	0.63390700	5.05674600
F	4.04922500	1.62986300	3.22431400
F	3.34325700	1.79132600	0.65263700
F	-0.85182200	-0.07868500	1.70332600
F	3.76451100	0.81440000	-2.86625400
C	-2.32722100	-0.41240400	-3.22194000
H	-3.34252900	-0.03328200	-3.12028300
H	-2.42851600	-1.45687700	-3.52836900
C	-1.53915300	0.38531400	-4.24858000
H	-0.52893500	-0.00941000	-4.38891000
H	-2.03983200	0.34375300	-5.21812000
H	-0.75991300	-0.80186700	-1.39587600
H	-1.21549900	-0.83575900	-2.35180800

***trans*-V**

C	-3.17520800	1.64052000	-0.03235500
C	-3.35960100	0.44788600	0.65366700
C	-4.67922800	0.18373900	1.00741400
C	-5.73120800	1.03146000	0.69603100
C	-5.48889800	2.20681100	0.00914500
C	-4.19237500	2.51943700	-0.35640600
B	-2.13464700	-0.56511100	0.97814000
C	-1.54790700	-1.42805600	-0.26899300
F	-5.00581500	-0.92281700	1.67718600
F	-6.97322400	0.72404800	1.05609500
F	-6.48594300	3.02684300	-0.28975300
F	-3.93733700	3.64894400	-1.00840100
F	-1.93558000	2.00156900	-0.40303200
C	0.79271200	0.74161000	-0.74108600
C	1.76945000	1.78920100	-0.43680000
C	2.36324400	1.96651300	0.81042400
C	3.25694500	2.99426500	1.05711000
C	3.57290500	3.88746700	0.04749700
C	2.98542000	3.75221300	-1.20021300
C	2.09323500	2.72069300	-1.42190400
F	2.05487900	1.16301400	1.82555100
F	3.79934400	3.13732900	2.25931200

F	4.42799700	4.87074900	0.27506000
F	3.28588100	4.60629000	-2.16886100
F	1.54664500	2.61015700	-2.62893400
C	0.87813100	-0.56056200	-0.43656200
C	2.11509500	-1.16833400	0.11060800
C	2.11059800	-1.93009900	1.27300900
C	3.25198600	-2.52998100	1.77212400
C	4.45159300	-2.37707200	1.09791000
C	4.49301000	-1.63148200	-0.06779700
C	3.33731700	-1.03892300	-0.54623500
F	0.98080400	-2.07753600	1.95915200
F	3.20752800	-3.23552800	2.89441000
F	5.55253700	-2.94335000	1.56384000
F	5.63728200	-1.49875300	-0.72581500
F	3.42330700	-0.36082600	-1.68541800
C	-0.24208100	-1.47698900	-0.80659000
H	-1.66929700	0.13289800	3.83608000
H	-0.07368600	1.07037900	-1.30372800
C	0.05497200	-2.40830500	-1.79804200
C	-2.46356300	-2.32965400	-0.79666700
C	-0.88295200	-3.29250700	-2.29423800
C	-2.16398000	-3.25188900	-1.78341800
F	-3.71921100	-2.35627700	-0.32975200
F	-3.08919500	-4.08826500	-2.23459700
F	-0.56643300	-4.15366000	-3.25232600
F	1.27518100	-2.44596000	-2.34053600
C	-2.20487500	-1.38917300	2.36433700
H	-2.99744500	-2.12948500	2.22378300
H	-1.28609000	-1.96622800	2.48797900
C	-2.47640800	-0.57930700	3.62975600
H	-2.55804900	-1.22915000	4.50414700
H	-3.40374400	-0.00676300	3.55792900
H	-1.02439000	0.44125600	0.90495400
H	-1.13186100	0.22199700	1.65917900

TS10

C	-3.03325400	1.72961900	0.09485600
C	-3.27604400	0.45559300	0.59891200
C	-4.61842000	0.17629700	0.83924500
C	-5.64014200	1.07975400	0.59020700
C	-5.34320800	2.32920500	0.07909000
C	-4.02374400	2.65920400	-0.16941000
B	-2.05197200	-0.56630600	0.82433700
C	-1.51609100	-1.54335800	-0.33865900
F	-4.99968900	-0.99683300	1.35006900
F	-6.90417100	0.75452400	0.84363600

F	-6.31043400	3.20216500	-0.16349100
F	-3.71929800	3.86024600	-0.65142100
F	-1.77789200	2.12268300	-0.15470700
C	0.75349300	0.66022300	-0.84753900
C	1.67904100	1.75720300	-0.55791700
C	2.20699000	2.01689300	0.70424900
C	3.04769800	3.09079000	0.94057500
C	3.37498100	3.94832900	-0.09583500
C	2.85197800	3.73076100	-1.36038300
C	2.01237500	2.65376700	-1.57143500
F	1.88211900	1.25052100	1.74290100
F	3.52725200	3.31265600	2.15783800
F	4.17922400	4.97629200	0.12199700
F	3.16326000	4.55109800	-2.35496200
F	1.52617400	2.46544200	-2.79491300
C	0.87931500	-0.62042000	-0.48133400
C	2.10984500	-1.15519400	0.14824300
C	2.07621000	-1.82898400	1.36304100
C	3.20889700	-2.36197900	1.94941100
C	4.43148900	-2.22509200	1.31357600
C	4.50339600	-1.56263900	0.10026500
C	3.35433400	-1.03715500	-0.46567800
F	0.92137500	-1.95215000	2.01610900
F	3.13515000	-2.98549300	3.11807500
F	5.52564700	-2.72763500	1.86238200
F	5.67111000	-1.44431500	-0.51842200
F	3.47134800	-0.43503800	-1.64409100
C	-0.19619300	-1.59015400	-0.84041200
H	-1.85346100	-0.20031500	3.99806000
H	-0.11493700	0.93304800	-1.43657100
C	0.14844500	-2.55922900	-1.77656400
C	-2.40693300	-2.46987400	-0.86208600
C	-0.76477000	-3.47451900	-2.26497200
C	-2.06382300	-3.42641100	-1.80201000
F	-3.67817200	-2.48695200	-0.44265500
F	-2.96444600	-4.29035400	-2.25329300
F	-0.40774700	-4.37192000	-3.17454700
F	1.38699300	-2.60459800	-2.27603700
C	-2.26331400	-1.52088700	2.30631100
H	-3.08080200	-2.13621300	1.93605900
H	-1.42370900	-2.19847400	2.47300400
C	-2.66590400	-0.80986900	3.59221200
H	-2.93638400	-1.54267000	4.35491800
H	-3.52609700	-0.15633900	3.43918500
H	-1.06278500	0.19747200	1.08309600
H	-1.35206000	-0.47927100	1.85460600