# Supporting Information

## Metal-Free Borylation of Heteroarenes using Ambiphilic Aminoboranes: On the Importance of Sterics in Frustrated Lewis Pair C-H Bond Activation

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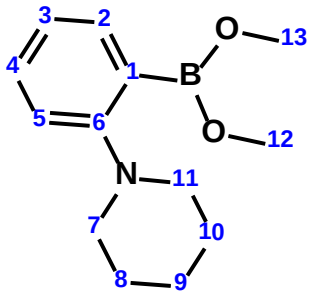
## Contents

## General experimental

The synthesis of -$BH_2$, -$B(OH)_2$ and -$B(OMe)_2$ derivatives (**2, $2_{OMe}$, $2_{OH}$, 3, $3_{OH}$**) were done using standard Schlenk techniques. The synthesis of the trifluoroborate derivatives and the borylation reactions using precatalysts **1F-4F** were performed in oven-dried glassware under a nitrogen atmosphere. Toluene, hexanes, ethyl ether and tetrahydrofuran were purified by distillation over Na/benzophenone. Deuterated-chloroform ($CDCl_3$) and dichloromethane were dried by distillation over $P_2O_5$ and deuterated-benzene ($C_6D_6$) by vacuum distillation from NaK alloy. Unless otherwise stated, all reagents were used as received. Pinacolborane (HBpin) with 1% $NEt_3$ additive obtained commercially from BASF for the 2 gram scale reactions was distilled prior to use. NMR spectra were recorded on Agilent Technologies NMR spectrometer at 500.00 MHz ($^1$H), 125.757 MHz ($^{13}$C), 160.46 MHz ($^{11}$B) and 470.385 MHz ($^{19}$F) or on Varian Inova NMR AS400 spectrometer, at 400.0 MHz ($^1$H), 100.580 MHz ($^{13}$C) and 376.29 ($^{19}$F). $^1$H NMR and $^{13}$C{$^1$H} NMR chemical shifts are referenced respectively to the residual hydrogen and carbon atoms in the deuterated solvents. $^{11}$B{$^1$H} NMR calibration was performed using $F_3B{\bullet}OEt_2$ as an external reference. $^{19}$F NMR was calibrated using $CFCl_3$ as external standard. Multiplicities are reported as singlet (s), broad singlet (s, br) doublet (d), triplet (t), multiplet (m). Chemical shifts are reported in ppm. Coupling constants are reported in Hz. Note: In the $^{13}$C{$^1$H} spectroscopy, the signal corresponds to the carbon that is directly attached to boron is obscured for most of the compounds. Mass Spectrometry analyses were carried out on an Agilent 6210 LC Time of Flight Mass Spectrometer, using electrospray ionization (ESI) method. Microanalyses for C, H, and N were carried out on a Thermo Scientific FLASH 2000 Series CHNS. Column chromatography was performed using the silica gel (230–400 mesh) stationary phase and the mobile phases were dried over alumina prior to use.

## Synthesis and NMR characterization

### 1-piperidyl-2-$B(OMe)_2$-$C_6H_4$ ($2_{OMe}$)



In a 250 mL Schlenk flask, 6.9 g (28.7 mmol, 1 equiv) of 1-(2-bromophenyl)piperidine was added and dissolved in hexanes (100 mL) and cooled to -78 °C. Then, 11.5 mL of a 2.5 M solution of *n*-BuLi in hexanes (30.1 mmol, 1.05 equiv) was added dropwise, the ice bath was removed and the reaction left to room temperature for 2 hours. The resulting solution was again cooled to -78 °C, and 9.6 mL (86.1 mmol, 3 equiv) of $B(OMe)_3$ was added. Then this new mixture was stirred for 12 hours by gradually warming the reaction flask to room temperature. From the resulting reaction solution, the salts were removed by filtration and the volatiles were removed under reduced pressure. Afterwards, purification by vacuum distillation at 90°C gave the desired product as a colorless oil (3.0 g (44% yield). Since the product is air-sensitive, no elemental analysis was performed.

$^{1}$H NMR (500 MHz, chloroform-*d*) δ 7.32-7.26 (m, 2H), 6.99-6.95 (m, 2H), 3.64 (s, 6H), 3.00 (m, 4H), 1.7 (m, 4H), 1.6 (m, 2H) .

$^{13}$C{$^{1}$H} NMR (126 MHz, chloroform-*d*) δ 156.8 (s, 1C), 132.5 (s, 1C), 129.6 (s, 1C), 121.5 (s, 1C), 117.2 (s, 1C), 54.2 (s, 2C), 52.4 (s, 2C), 26.6 (s, 2C), 24.3 (s, 1C). The carbon linked directly to boron was not observed.

$^{11}$B{$^{1}$H} NMR (160 MHz, chloroform-*d*) δ 30.4 (s).

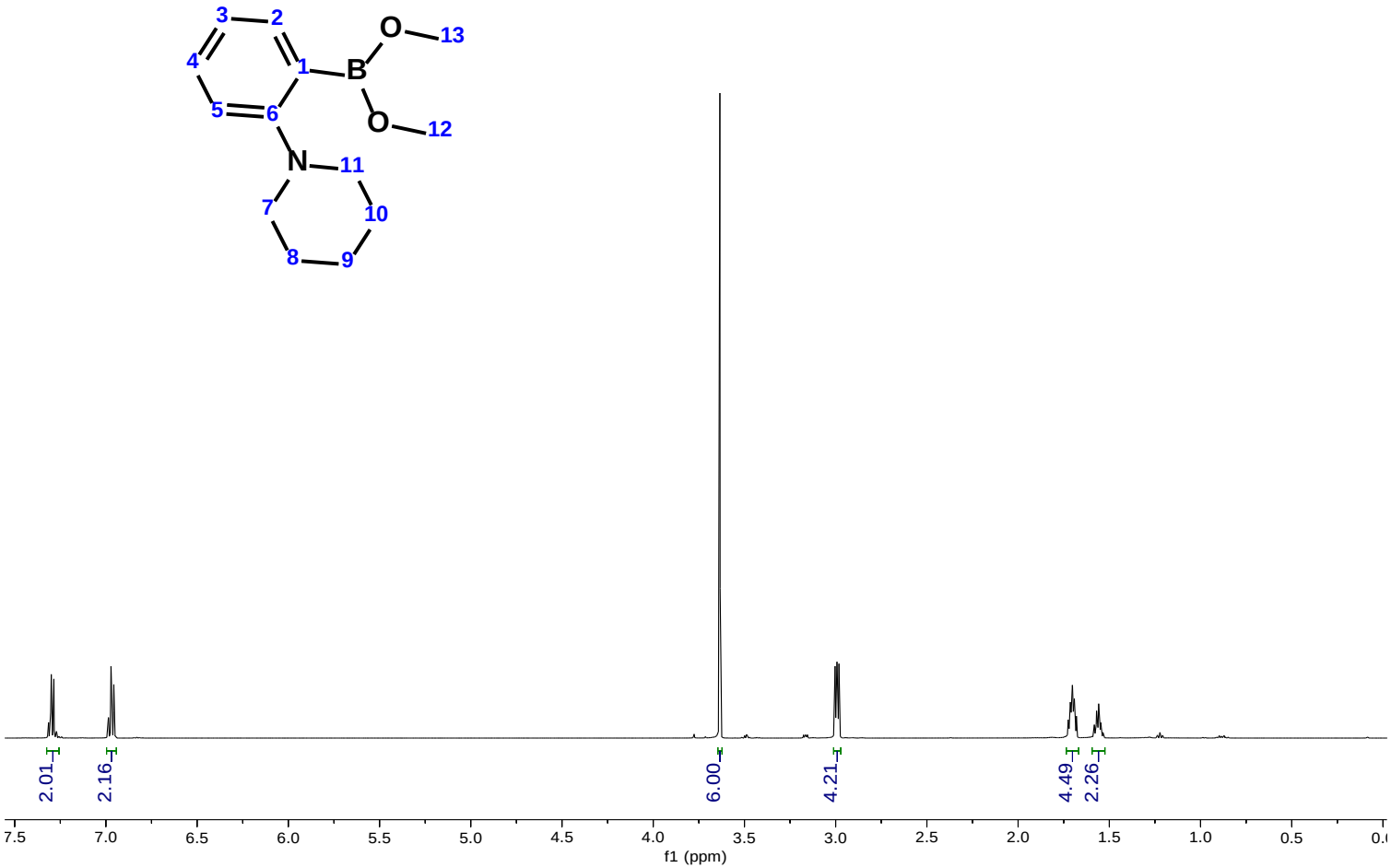



**Figure S1:** $^{1}$H NMR (500 MHz, chloroform-*d*) of 1-piperidyl-2-B(OMe)$_2$-C$_6$H$_4$ (**2$_{OMe}$**)

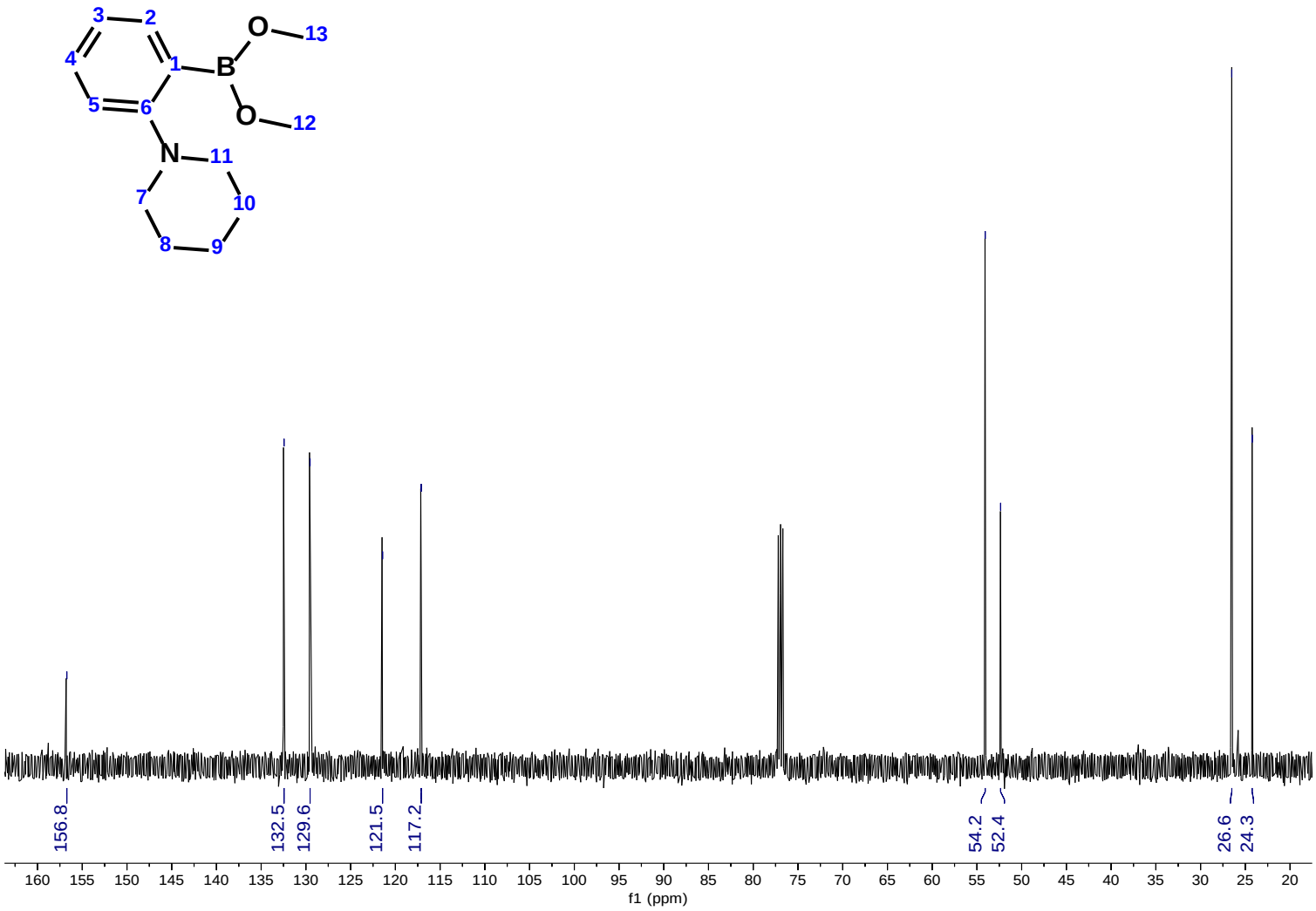
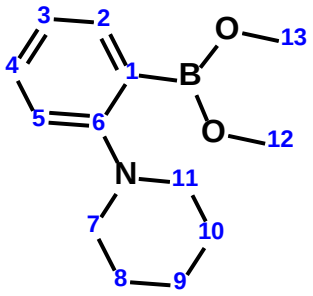



**Figure S2:** $^{13}C\{^{1}H\}$ NMR (126 MHz, chloroform-*d*) of 1-piperidyl-2-B$(OMe)_2$-$C_6H_4$ (**2$_{OMe}$**)



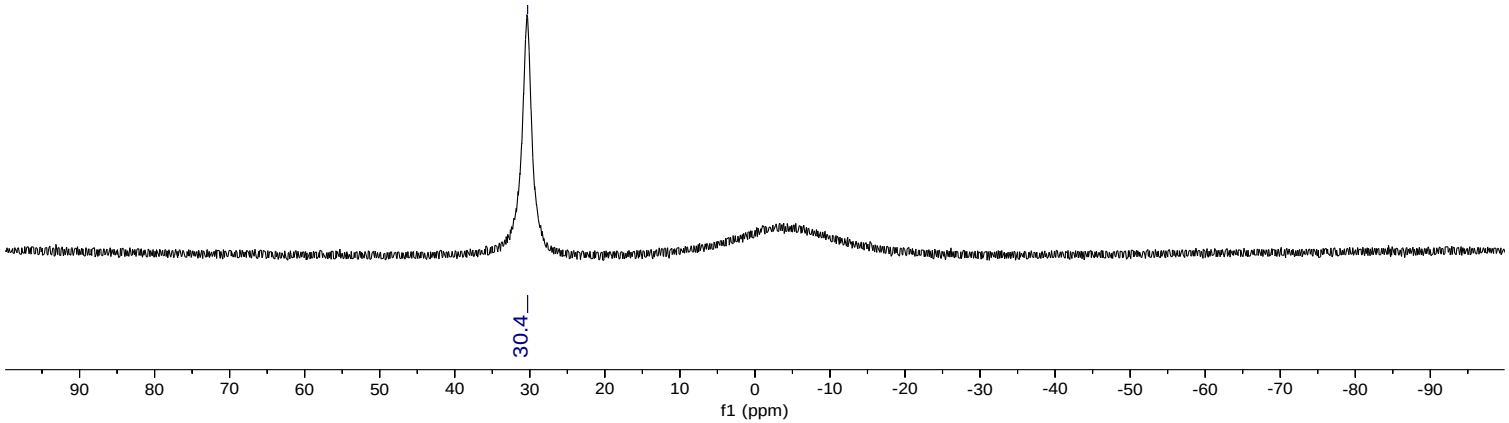
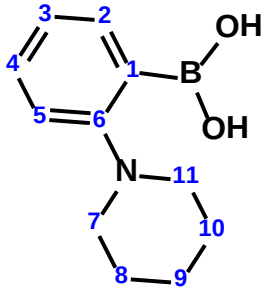




**Figure S3:** $^{11}B\{^{1}H\}$ NMR (160 MHz, chloroform-*d*) of 1-piperidyl-2-B(OMe)$_2$-C$_6$H$_4$ (**2$_{OMe}$**)

## 1-piperidyl-2-B(OH)$_2$-C$_6$H$_4$ (2$_{OH}$)




In a 250 mL Schlenk flask, 9.1 g (37.9 mmol, 1 equiv) of 1-(2-bromophenyl)piperidine was added and dissolved in THF (100 mL) and cooled to -78 °C. Then, 19.7 mL of a 2.5 M solution of *n*-BuLi in hexanes (49.3 mmol, 1.3 equiv) was added dropwise, the ice bath was removed and the reaction left to room temperature for 2 hours. The resulting solution was again cooled to -78 °C, and 9.6 mL (78.0 mmol, 2 equiv) of $B(OMe)_3$ was added. Then this new mixture was stirred for 2 hours by gradually warming the reaction flask to room temperature. Approximately 20 mL of water was added to quench the reaction, and it was left stirring for 16 hours. The mixture was acidified with HCl 1 M and the organic impurities were extracted with chloroform (3 x 30 mL). The aqueous phase was recovered and basified with NaOH to pH 11. The compound was extracted with chloroform (3 x 30 mL). The organic phase was evaporated and dried under vacuum. The solid obtained was dissolved in a minimum of dichloromethane and hexanes and cooled to -80 °C for 16 hours. The titled compound precipitated as a white powder. It was isolated and dried to obtain 5.44 g (70 % yield).

$^1$H NMR (500 MHz, chloroform-*d*) δ 9.55 (br s, 2H), 7.96 (d, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.7 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.25 (t, 1H), 2.93 (m, 4H), 1.81 (m, 4H), 1.63 (br s, 2H).

$^{13}$C{$^1$H} NMR (126 MHz, chloroform-*d*) δ 159.8 (s, 1C), 135.8 (s, 1C), 131.8 (s, 1C), 125.6 (s, 1C), 121.0 (s, 1C), 55.4 (s, 2C), 26.6 (s, 2C), 23.6 (s, 1C). The carbon linked directly to boron was not observed.

$^{11}$B{$^1$H} NMR (160 MHz, chloroform-*d*) δ (s).

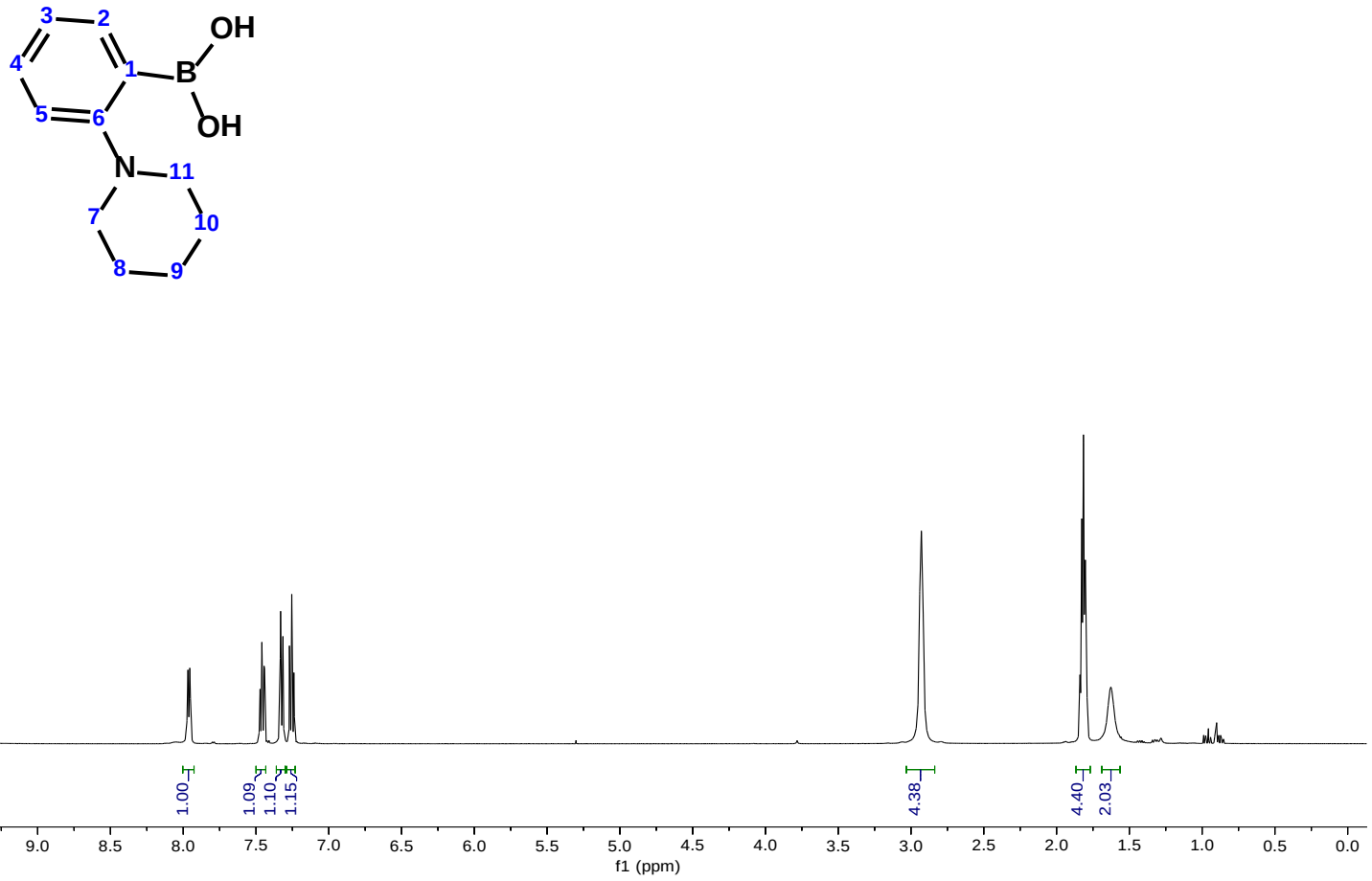



**Figure S4:** $^{1}$H NMR (500 MHz, chloroform-*d*) of (1-piperidyl-2-B(OH)$_2$-C$_6$H$_4$)$_2$ (**2**$_{OH}$)

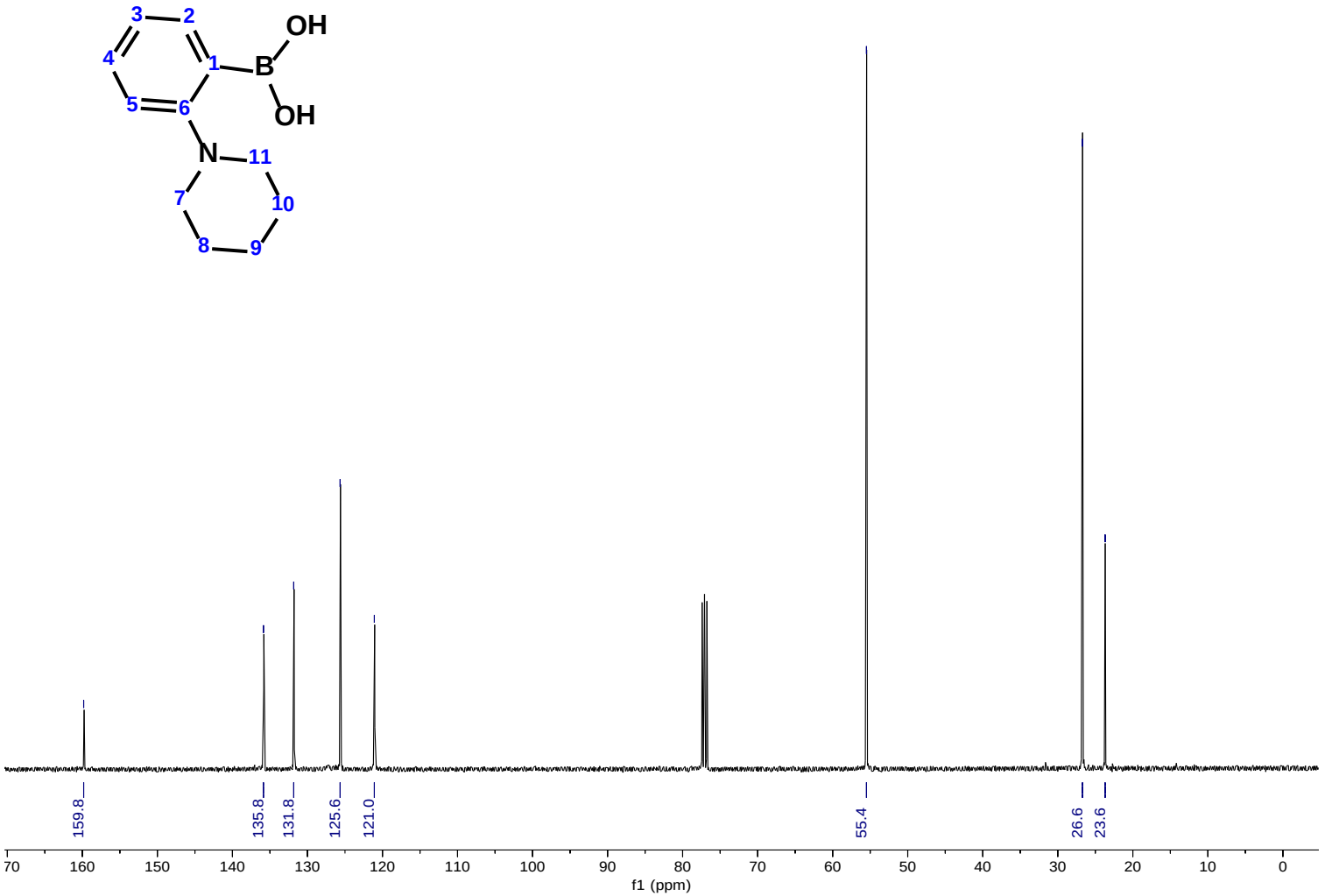
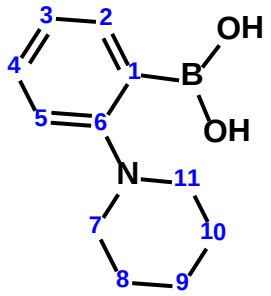



**Figure S5:** $^{13}C\{^{1}H\}$ NMR (126 MHz, chloroform-*d*) of 1-piperidyl-2-$B(OH)_2$-$C_6H_4$ (**2**$_{OH}$)



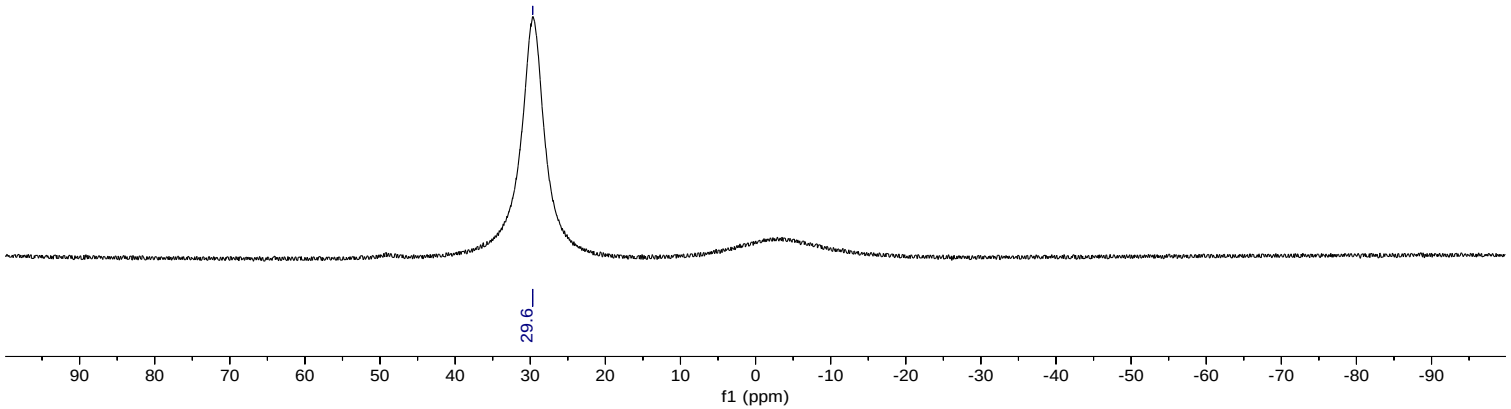
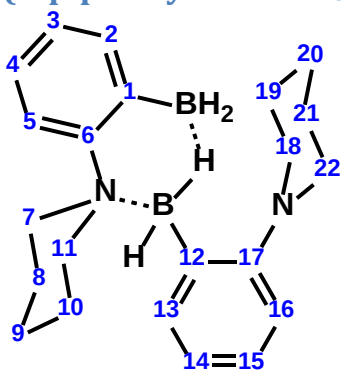




**Figure S6:** $^{11}B\{^{1}H\}$ NMR (160 MHz, chloroform-*d*) of 1-piperidyl-2-$B(OH)_2$-$C_6H_4$ (**2**$_{OH}$)

## (1-piperidyl-2-$BH_2$-$C_6H_4$)$_2$ (2)




In a 100 ml Schlenk, 1.2 g (5.2 mmol, 1 equiv) of 1-piperidyl-2-B(OMe)$_2$-$C_6H_4$ was dissolved in toluene (60 mL), cooled in an ice bath, and 254 mg of $LiAlH_4$ (6.7 mmol, 1.3 equiv according to Li) was added, followed by 1.1 mL of DME (10.3 mmol, 2 equiv). A certain amount of $H_2$ is liberated. The reaction was stirred for 2 hours at room temperature, then the mixture was filtered on fritted glass and the volatiles were removed under reduced pressure. The remaining white oil was then dissolved in toluene (50 mL) and 0.8 mL (5.7 mmol, 1.1 equiv) of TMSBr was added. The reaction was stirred at room temperature for 16 hours. Afterwards, the solution was separated from the precipitated salts by filtration and the volatiles were removed under reduced pressure. This gave 0.7 g of **2** (79% yield) as a white powder. Single crystals of **2** were obtained from a toluene/hexanes solution at -35°C. Since the product is extremely air-sensitive, no elemental analysis was performed.

$^1$H NMR (500 MHz, benzene-$d_6$): δ 7.79 (d, $J$ = 6.5Hz, 1H), 7.19 (d, $J$ = 9.0Hz, 1H), 7.15-7.08 (m, 2H), 7.01-6.96 (m, 2H), 6.76-6.69 (m, 2H), 4.84-3.64 (m, 3H, $BH_2$), 3.59 (m, 1H), 3.07 (s, 2H), 2.84 (m, 1H), 2.75 (m, 1H), 2.65 (s, 2H), 2.40 (m, 1H), 2.08 (m, 2H), 1.68 (s, 2H), 1.53 (s, 2H), 1.41 (m, 2H), 1.19, (m, 1H), 1.10 (m, 1H), 0.92 (m, 1H), 0.79 (m, 1H), -0.95 (s, 1H, $BH_2$).

$^{13}$C{$^1$H} NMR (126 MHz, benzene-$d_6$): δ 159.6 (s), 152.4 (s), 135.6 (s), 133.7 (s), 128.7 (s), 127.3 (s), 125.5 (s), 122.7 (s), 119.0 (s), 117.0 (s), 61.7 (s), 54.4 (s), 26.7 (s), 24.5 (s), 22.3 (s), 22.0 (s), 20.3 (s). The carbon linked directly to boron was not observed.

$^{11}$B{$^1$H} NMR (160 MHz, benzene-$d_6$) δ 0.5 (s, 1B), -7.7 (s, 1B).

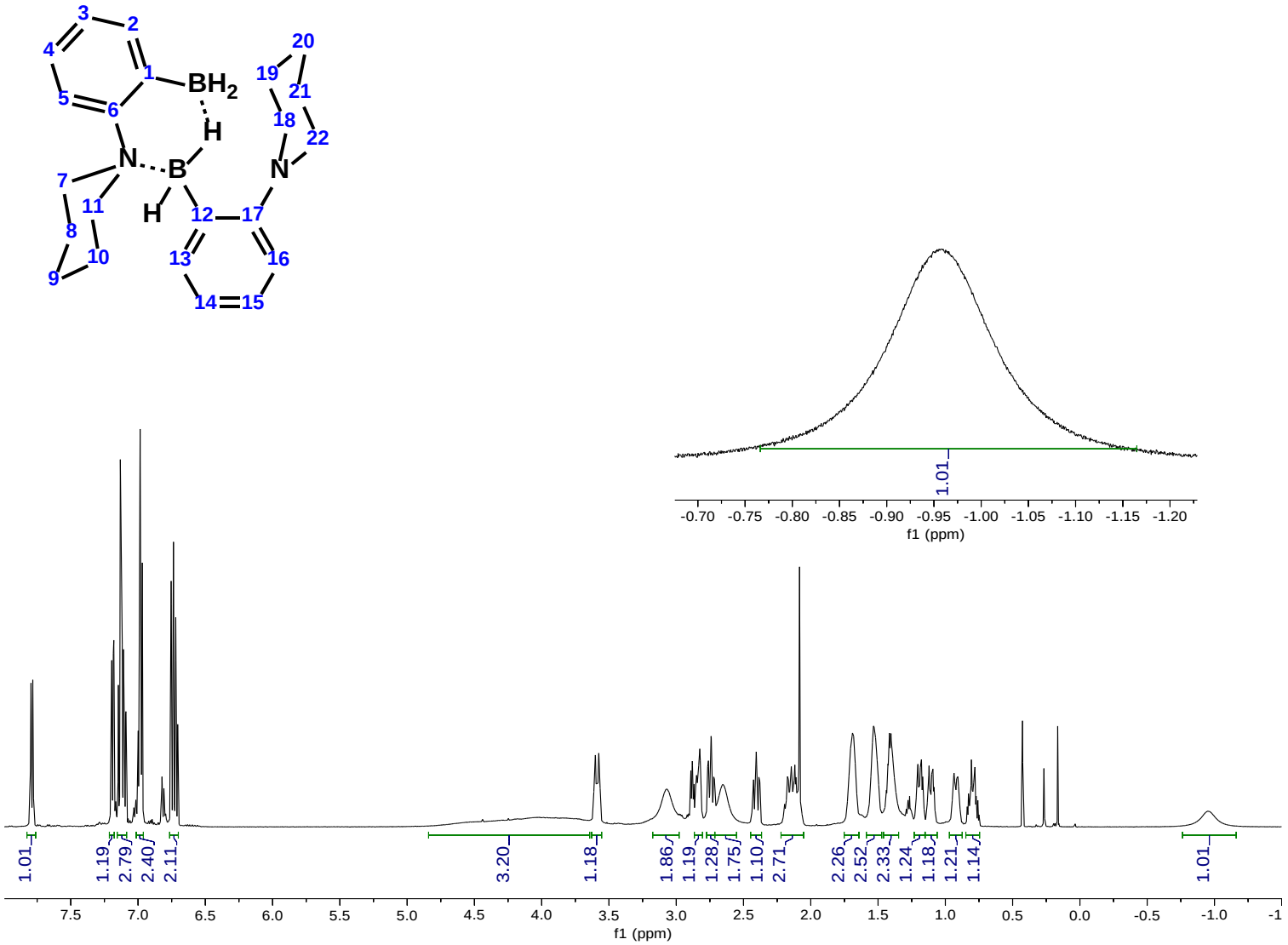



**Figure S7:** $^{1}$H NMR (500 MHz, benzene-$d_6$) of (1-piperidyl-2-$BH_2$-$C_6H_4$)$_2$ (**2**)

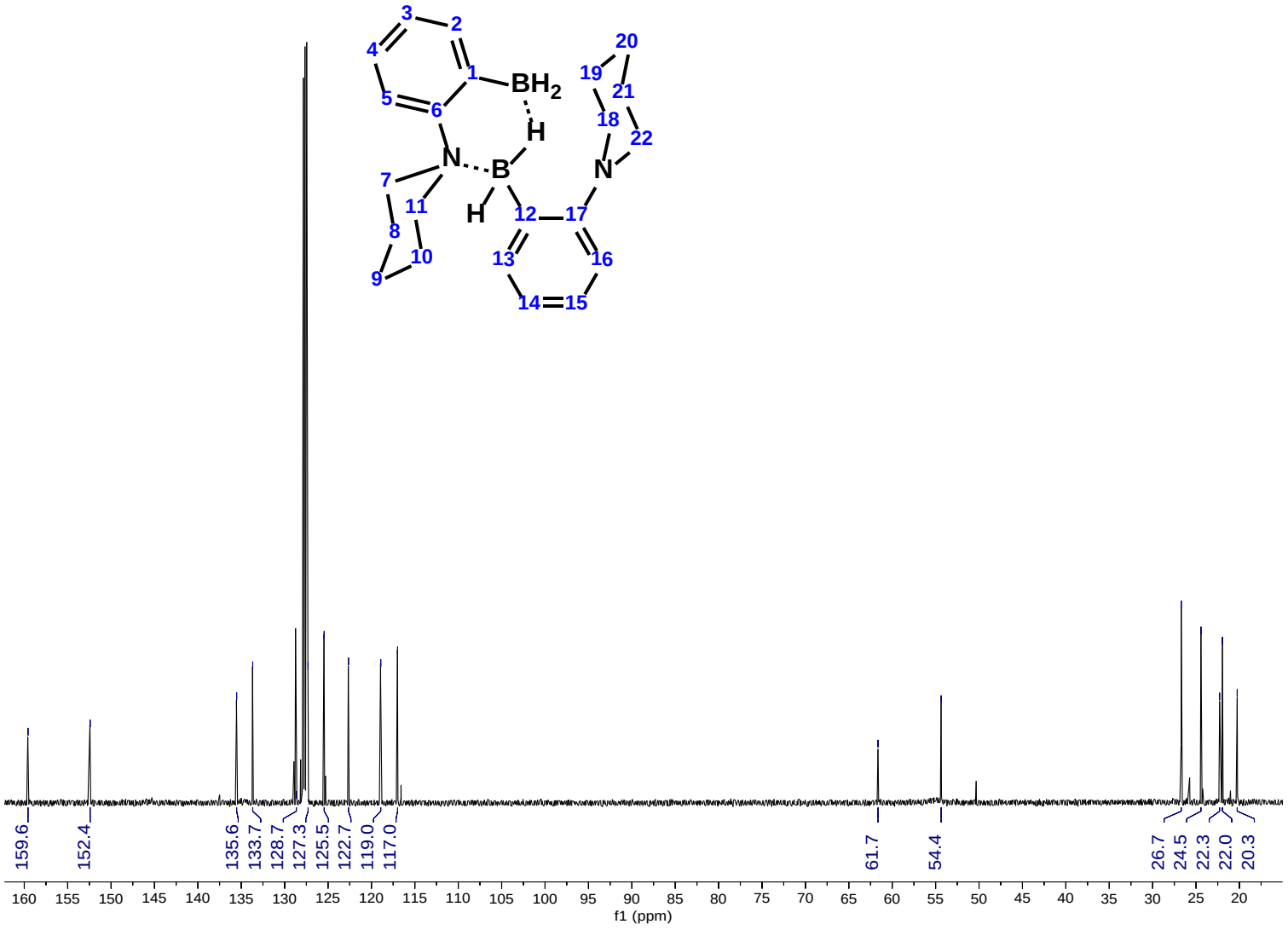
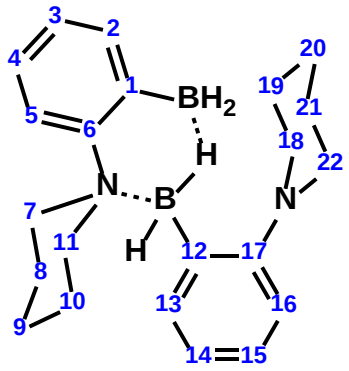



**Figure S8:** $^{13}C\{^{1}H\}$ NMR (126 MHz, benzene-$d_6$) of (1-piperidyl-2-$BH_2$-$C_6H_4$)$_2$ (**2**)



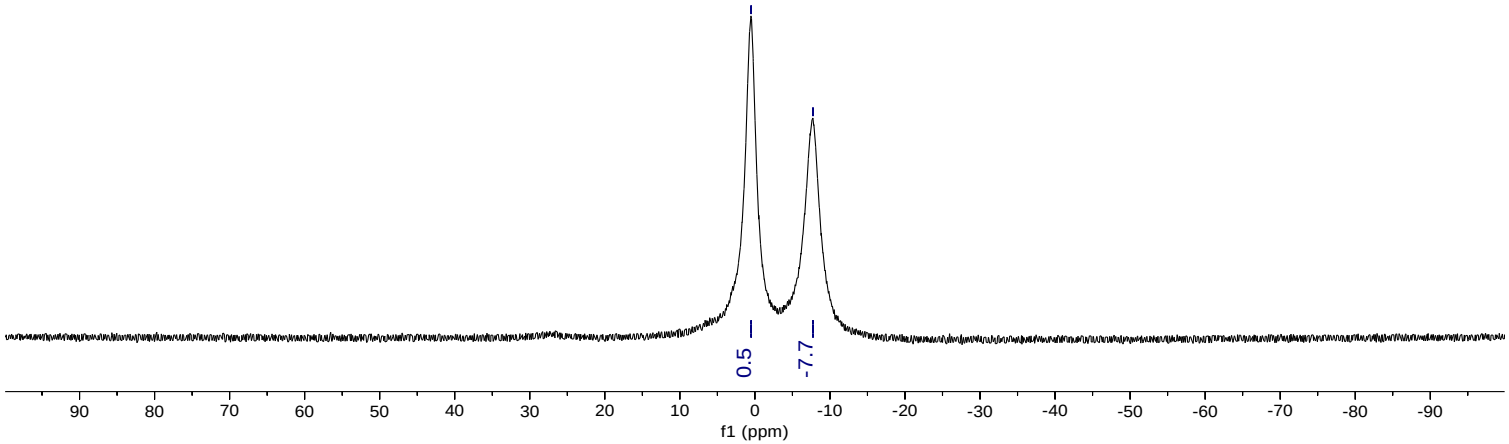




**Figure S9:** $^{11}B\{^{1}H\}$ NMR (160 MHz, benzene-$d_6$) of (1-piperidyl-2-$BH_2$-$C_6H_4$)$_2$ (**2**)

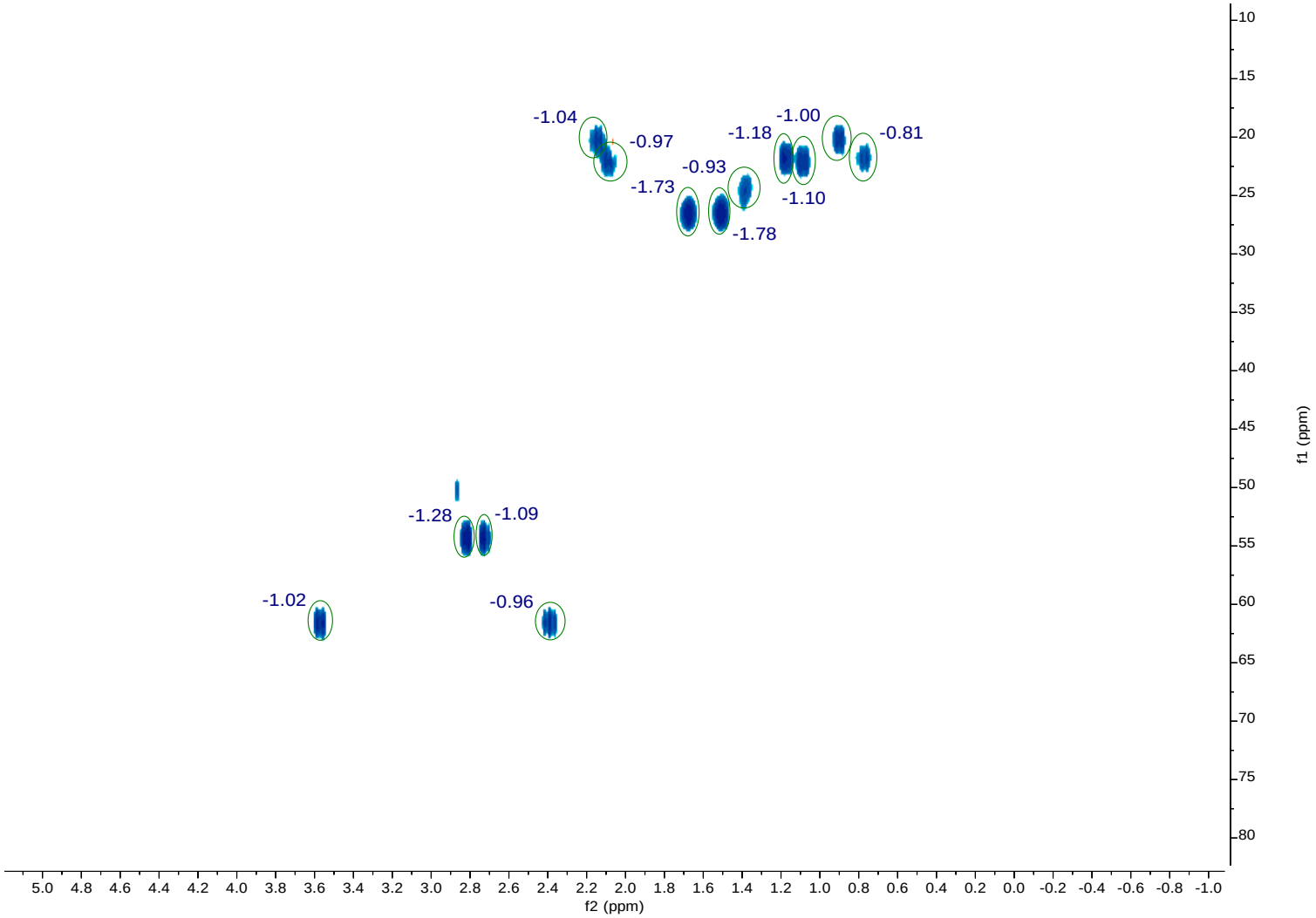
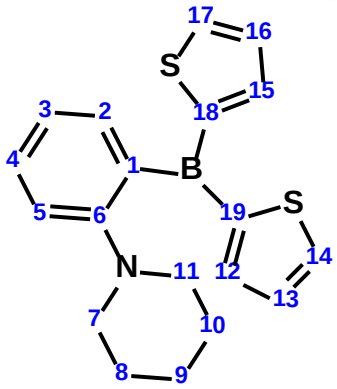



**Figure S10:** $^{13}C$-$^{1}H$ HSQC (126 MHz-500 MHz, benzene-$d_6$) of (1-piperidyl-2-$BH_2$-$C_6H_4$)$_2$ (**2**)

## 1-piperidyl-2-B(thiophenyl)$_2$-C$_6$H$_4$ (6)




13.0 mg (0.075 mmol, 1 equiv) of (1-piperidyl-2-BH$_2$-C$_6$H$_4$)$_2$ was dissolved in 0.3 mL (3.7 mmol, 50 equiv) of thiophene in a J-Young tube. The mixture was heated for 4 hours at 40°C. The remaining thiophene was evaporated under reduced pressure and 0.4 mL of chloroform-*d* was added to the tube for NMR analysis. Since compound **6** is extremely air-sensitive, elemental analysis was not performed.

$^1$H NMR (500 MHz, chloroform-*d*) δ 7.88 (m, 2H, H17 and H14, H16 and H13 or H15 and H12), 7.85 (m, 2H, H17 and H14, H16 and H13 or H15 and H12), 7.40 (m, 2H, H2, H3, H4 or H5), 7.31 (m, 2H, H14, H16 and H13 or H15 and H12), 7.07 (m, 2H, H2, H3, H4 or H5), 2.91 (m, 4H, H7 and H11 or H8 and H10), 1.32 (m, 2H, H9), 1.22 (m, 4H, H7 and H11 or H8 and H10).

$^{13}$C{$^1$H} NMR (126 MHz, chloroform-*d*) δ 157.2 (s, 1C), 141.1 (s, 2C), 135.8 (s, 2C), 133.9 (s, 1C), 129.8 (s, 1C), 128.5 (s, 2C), 121.2 (s, 1C), 117.3 (s, 1C), 54.0 (s, 2C), 25.5 (s, 2C), 23.9 (s, 1C). The carbon linked directly to boron was not observed. * Residual thiophene.

$^{11}$B{$^1$H} NMR (160 MHz, chloroform-*d*) δ 49.7 (s, 1B).

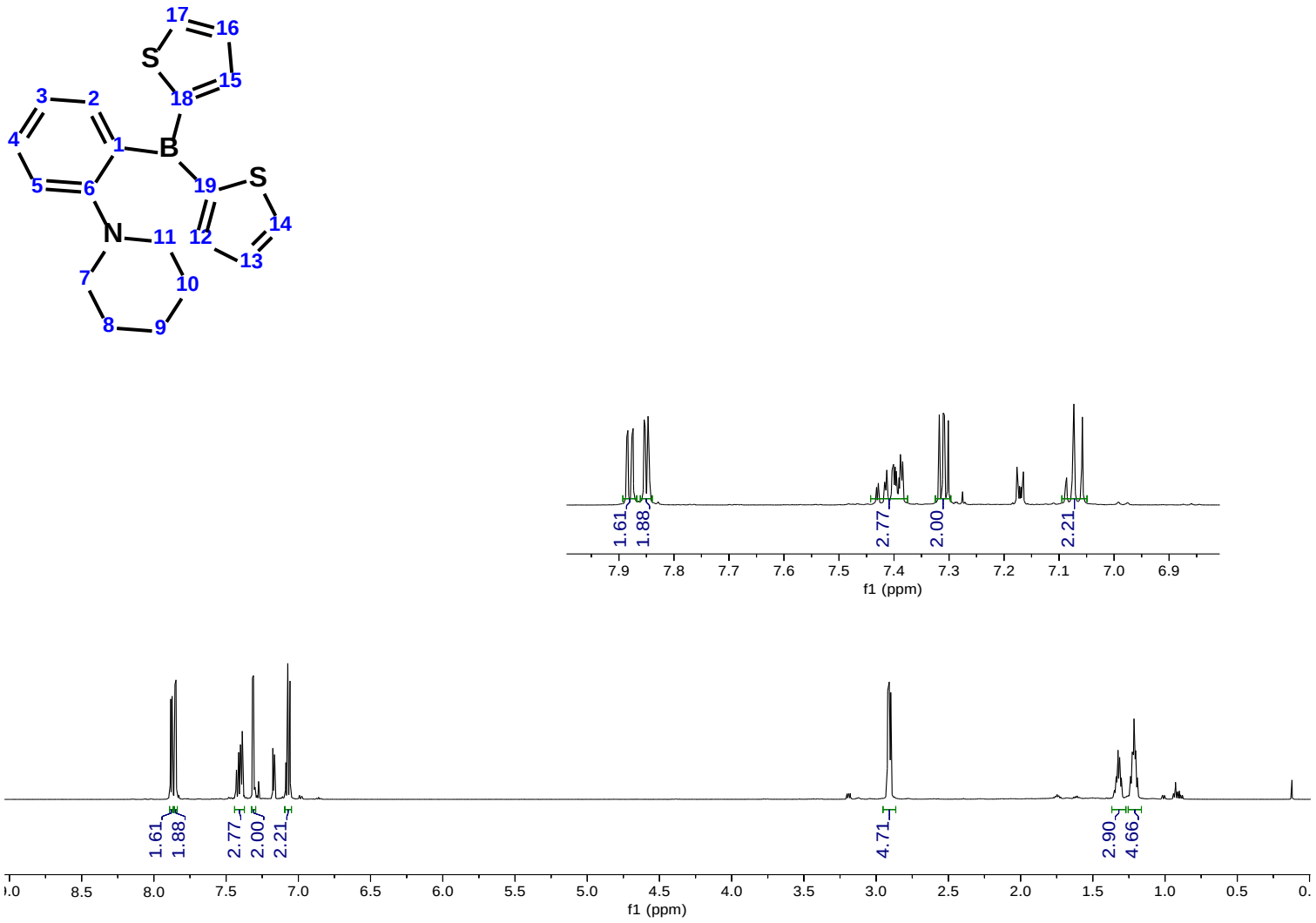



**Figure S11:** $^{1}$H NMR (500 MHz, chloroform-*d*) of 1-piperidyl-2-B(thiophenyl)$_2$-C$_6$H$_4$ (**6**)

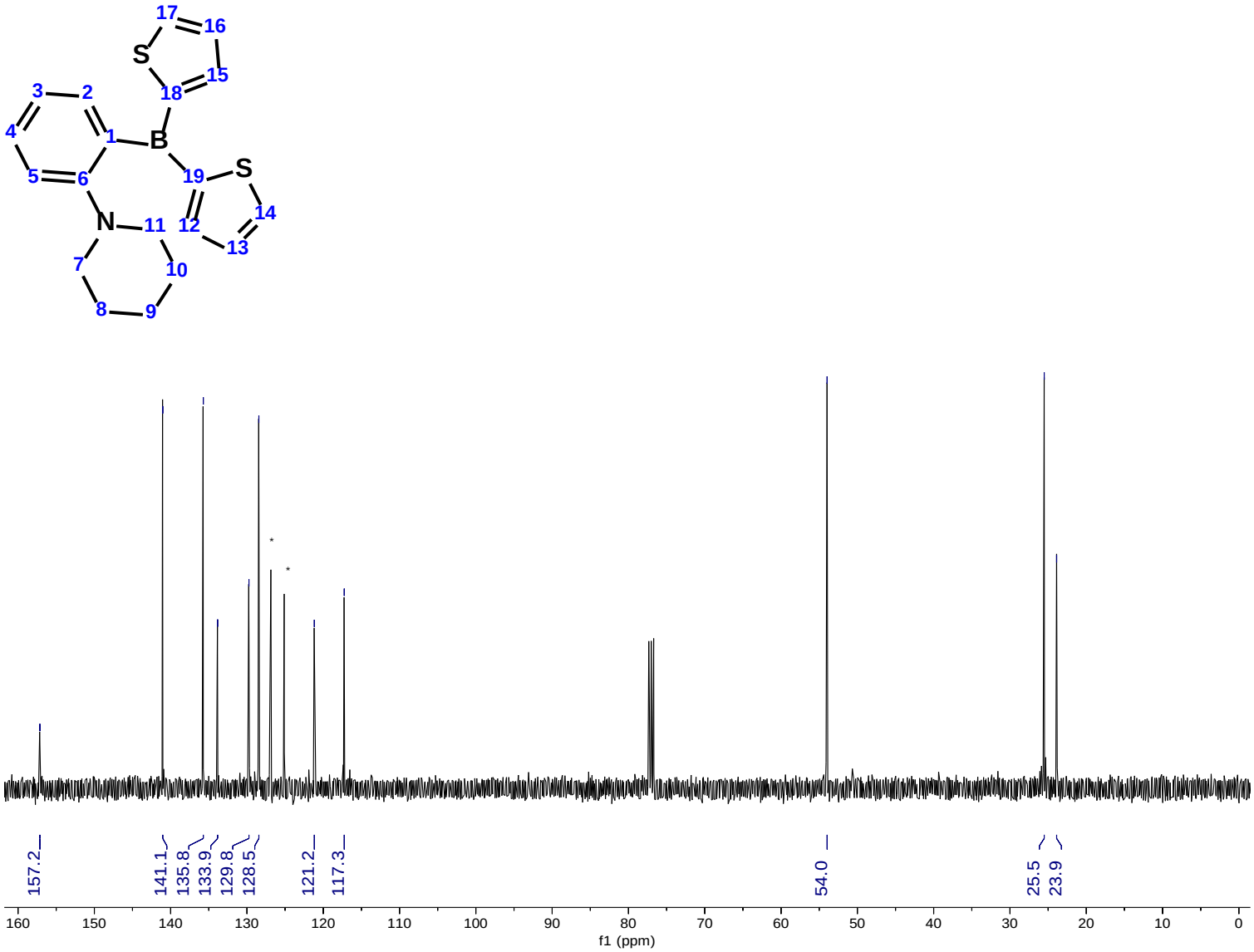



**Figure S12:** $^{13}C\{^{1}H\}$ NMR (126 MHz, chloroform-*d*) of 1-piperidyl-2-B(thiophenyl)$_2$-$C_6H_4$ (**6**)

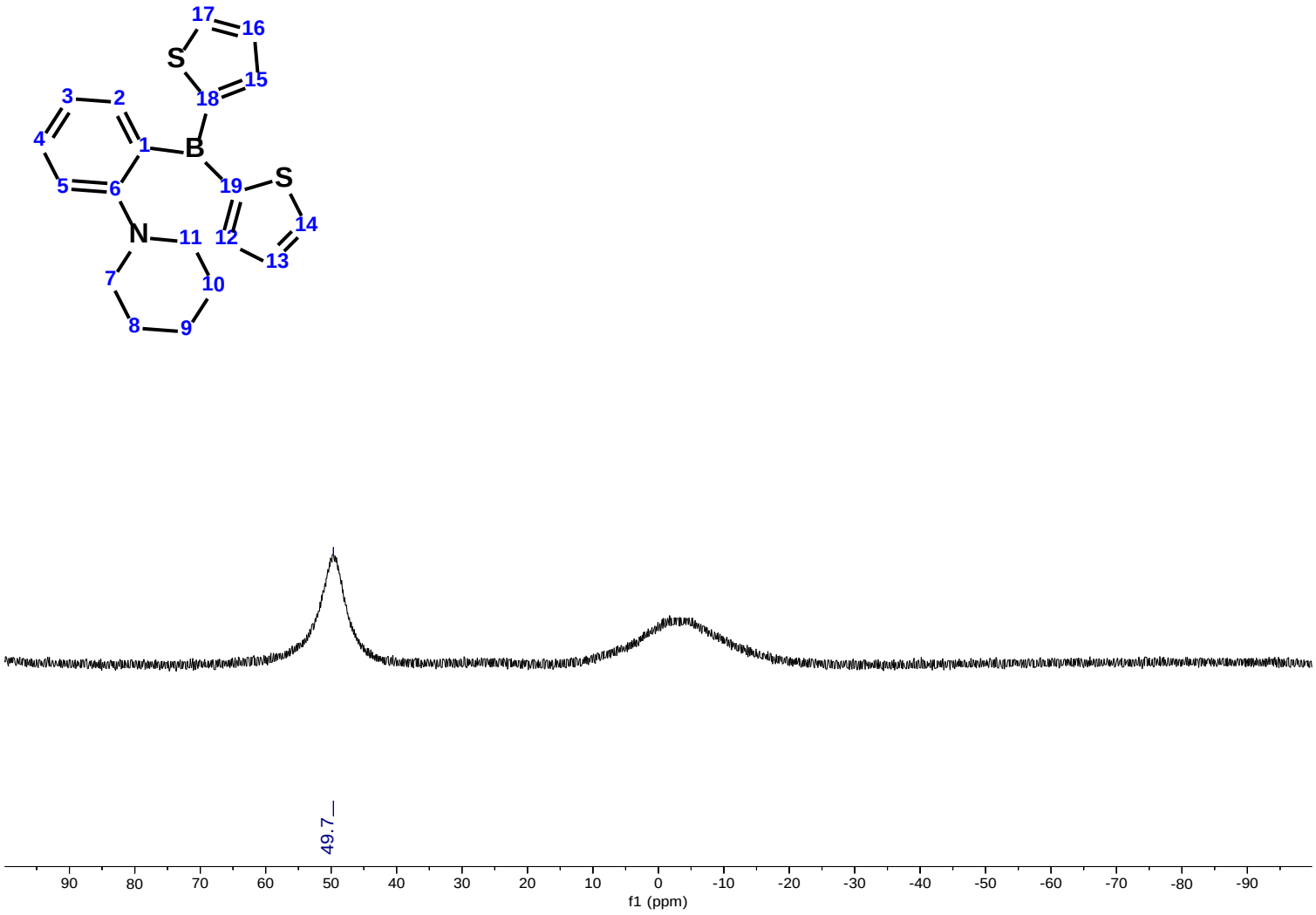



**Figure S13:** $^{11}B\{^{1}H\}$ NMR (160 MHz, chloroform-*d*) of 1-piperidyl-2-B(thiophenyl)$_2$-$C_6H_4$ (**6**)

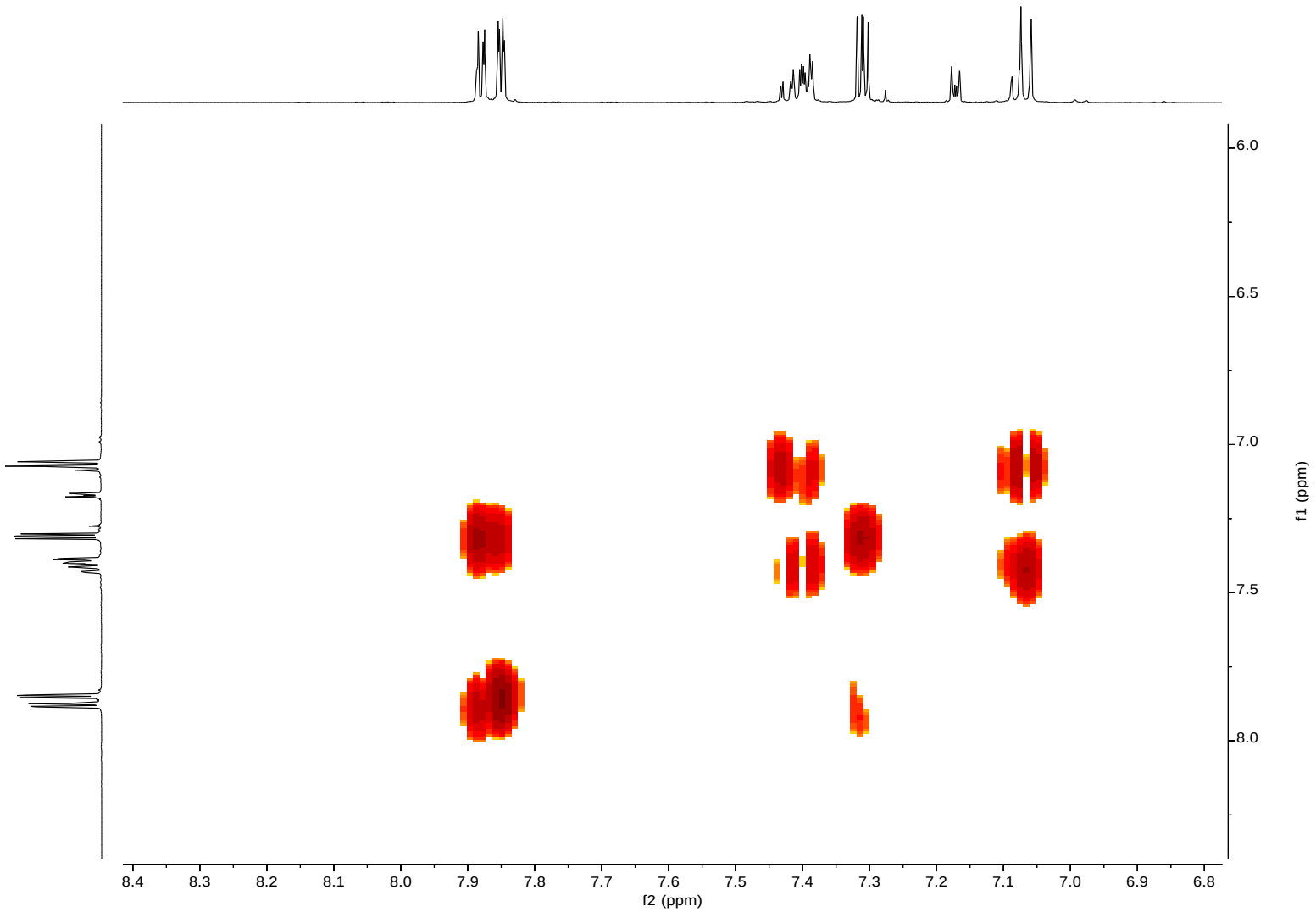
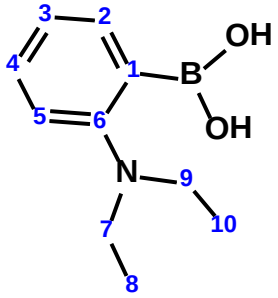



**Figure S14:** COSY NMR (500 MHz, chloroform-*d*) of the aromatic region of 1-piperidyl-2-B(thiophenyl)$_2$-C$_6$H$_4$ (**6**)

## 1-diethylamino-2-B(OH)$_2$-C$_6$H$_4$ ($3_{OH}$)




1-diethylamino-2-B(OH)$_2$-C$_6$H$_4$ was prepared using a method inspired from Kaufmann et al [1] In a 250 mL Schlenk flask, 9.6 mL (60.0 mmol, 1 equiv) of N,N-diethylaniline, 9.0 mL (60.0 mmol, 1 equiv) of TMEDA and *ca*. 80 mL of hexanes were added and cooled to -78 °C, followed by 26.9 mL of a 2.5 M solution of *n*-BuLi in hexanes (66.0 mmol, 1.1 equiv) was added dropwise. The reaction mixture was then stirred at room temperature for *ca* 16 hours, after which it was again cooled to -78 °C. Then, 13.4 mL (120 mmol, 2 equiv) of B(OMe)$_3$ was added. The mixture was then left to warm to room temperature and reacted at that temperature for 2 hours. The salts were then removed by filtration and the volatiles removed under reduced pressure. The residual oil was dissolved in about 100 mL of chloroform in a round-bottom flask and 100 mL of water was added before the reaction solution was left stirring for 1 hour. The resulting solution was then extracted with chloroform, then the organic extracts were combined and the solvent was removed under reduced pressure. The *ortho*-aminoboronic acid synthesized from their methoxy derivatives tend to stay partially under the form of a methanol adduct at this step. To obtain the title compound, about 10 mL of water was added to the oil and evaporated under reduced pressure right away. The yellowish solid was then washed with hexanes ( 2 x 30 mL) to remove the unreacted N,N-diethylaniline and the white solid was dried under reduced pressure to give 4.7g (41 % yield) of the title compound as a white powder. The solid can be further purified by dissolution in toluene at 50 °C and recrystallization at -35°C.

$^1$H NMR (500 MHz, chloroform-*d*) δ 9.13 (s, br, 2H, BOH), 7.93 (d, *J* = 7.5, 1H), 7.47 (t, *J* = 7.7 Hz, 1H), 7.30 – 7.25 (m, 2H), 3.02 (q, *J* = 7.2 Hz, 4H), 1.00 (t, *J* = 6.6 Hz, 6H).

$^{13}$C{$^1$H} NMR (126 MHz, chloroform-*d*) δ 156.1 (s, 1C), 135.2 (s, 1C), 131.9 (s, 1C), 125.9 (s, 1C), 122.1 (s, 1C), 50.9 (s, 2C), 12.6 (s, 2C). The carbon linked directly to boron was not observed.

$^{11}$B{$^1$H} NMR (160 MHz, chloroform-*d*) δ 29.6 (s).

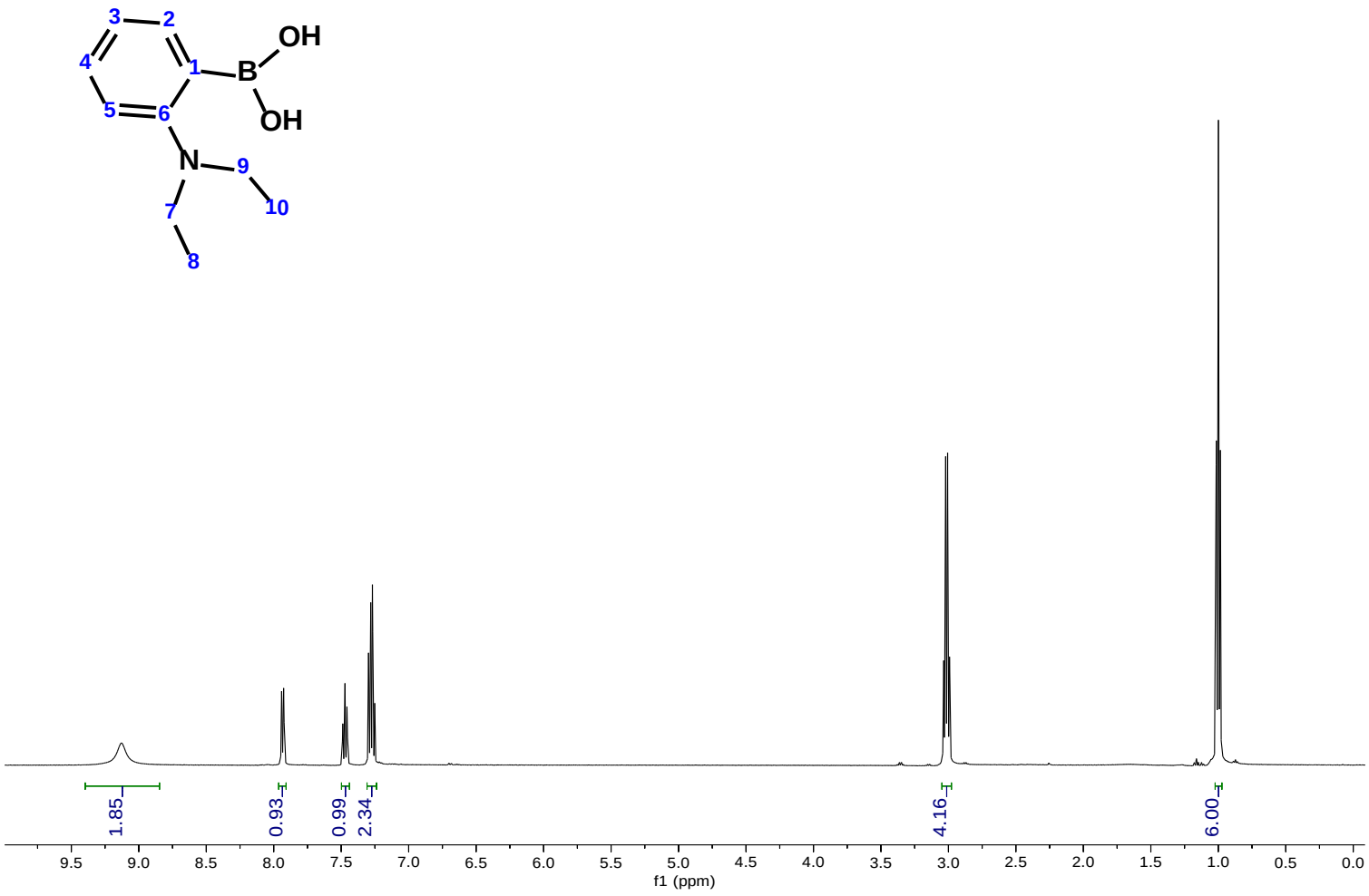



**Figure S15:** $^{1}$H NMR (500 MHz, chloroform-*d*) of 1-diethylamino-2-B(OH)$_2$-C$_6$H$_4$ (**3$_{OH}$**)

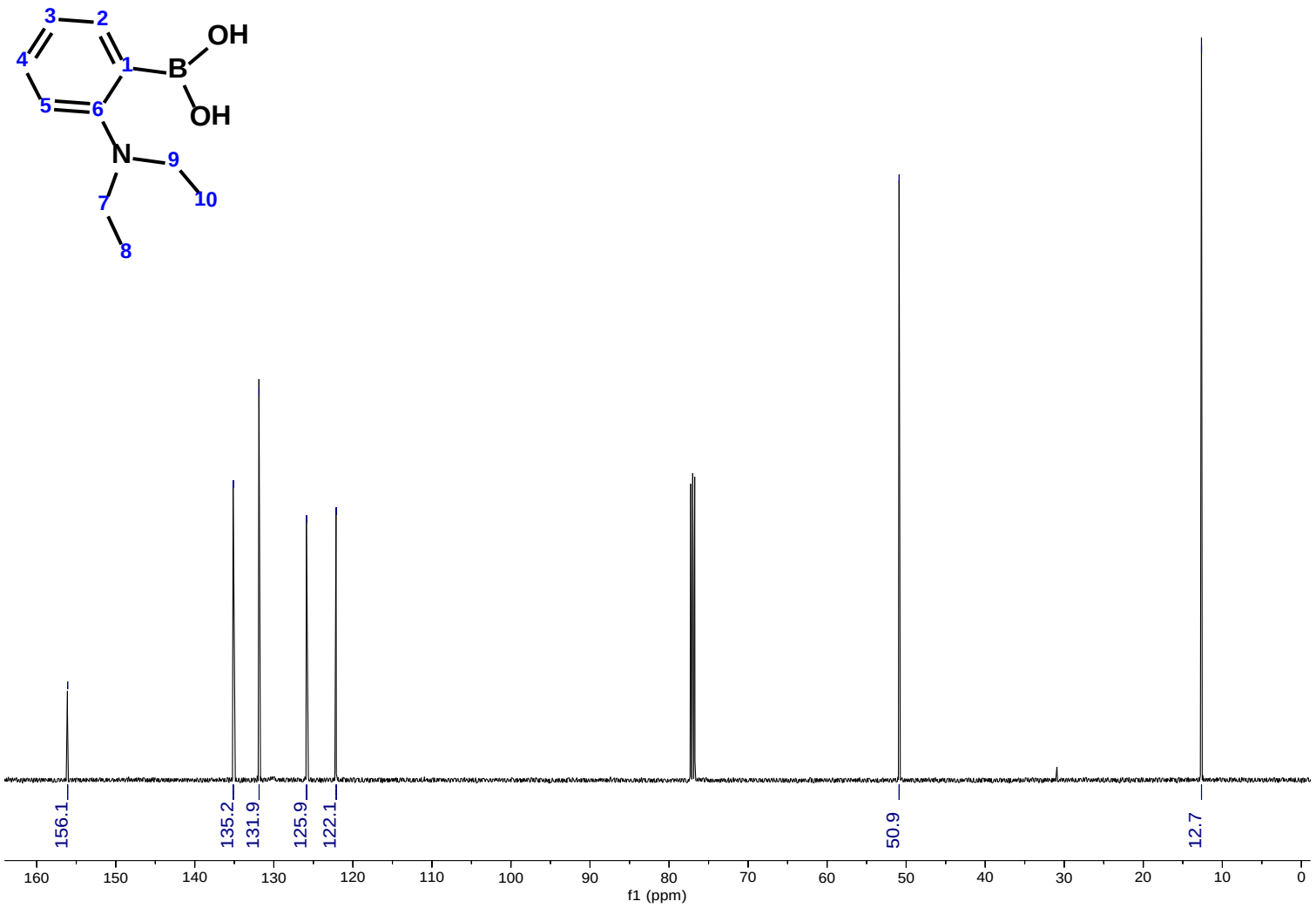



**Figure S16:** $^{13}C\{^{1}H\}$ NMR (126 MHz, chloroform-*d*) of 1-diethylamino-2-B(OH)$_2$-C$_6$H$_4$ (**3$_{OH}$**)

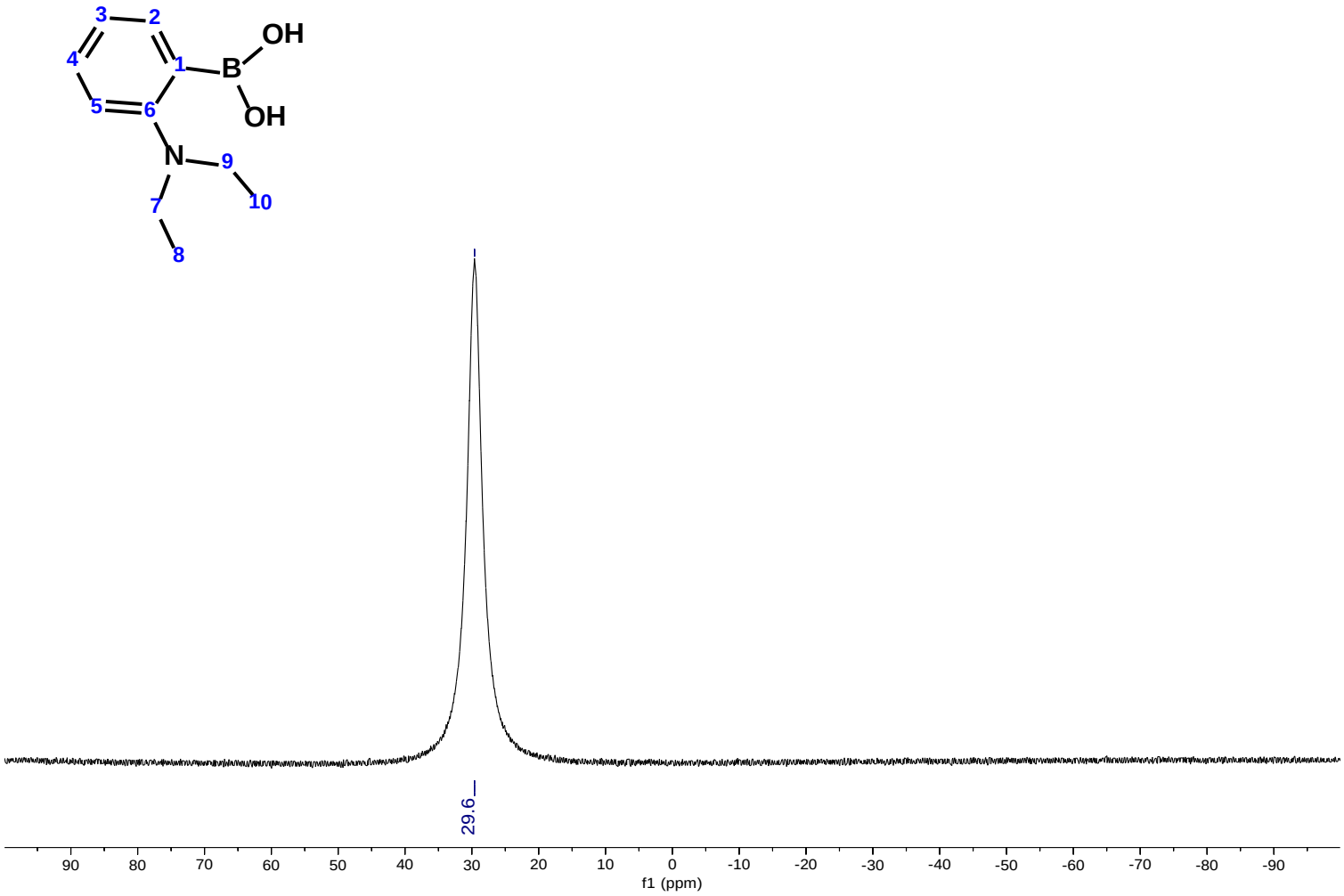
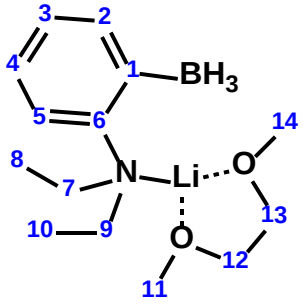



**Figure S17:** $^{11}B\{^{1}H\}$ NMR (160 MHz, chloroform-*d*) of 1-diethylamino-2-B$(OH)_2$-$C_6H_4$ (**3$_{OH}$**)

## 1-diethylamino-2-$BH_3$-$C_6H_4$-2-LiDME ($3_{LiH}$)

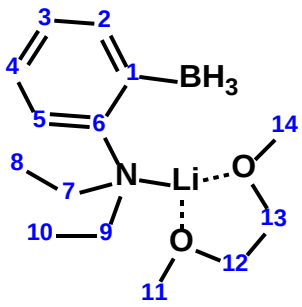



1.00 g (5.1 mmol, 1 equiv) of 1-diethylamino-2-$B(OH)_2$-$C_6H_4$ was dissolved in toluene and cooled in an ice bath, 256 mg of $LiAlH_4$ (6.73 mmol, 1.3 equiv according to Li) was added followed by 1.6 mL of DME (15.6 mmol, 3 equiv). A certain amount of $H_2$ is liberated. The reaction was stirred for 1 hour at room temperature, then the mixture was filtered and the volatiles removed under reduced pressure until almost dryness. The oil was then dissolved in hexanes and 0.55 mL (5.2 mmol, 1 equiv) of DME was added, which induced the precipitation of the title compound as a white powder. The liquid phase was removed by cannula filtration and the solid dried under reduced pressure to yield 822 mg (61 % yield) of the title compound as a white powder.

$^{1}$H NMR (400 MHz, chloroform-*d*) δ 7.63 (s, br, 1H), 7.03 (m, 3H), 3.67 (s, 4H), 3.45 (s, 6H), 3.05 (q, *J* = 7.2Hz, 4H), 1.20 (m, 3H, $BH_3$), 0.99 (t, *J* = 7.1Hz, 6H).

$^{13}$C{$^{1}$H} NMR (126 MHz, chloroform-*d*) δ 151.0 (s, 1C), 138.6 (s, 1C), 124.8 (s, 1C), 124.4 (s, 1C), 120.0 (s, 2C), 70.6 (s, 2C), 59.6 (s, 2C), 49.0 (s, 2C), 11.2 (s, 2C). The carbon linked directly to boron was not observed.

$^{11}$B{$^{1}$H} NMR (160 MHz, chloroform-*d*) δ -28.8 (s).



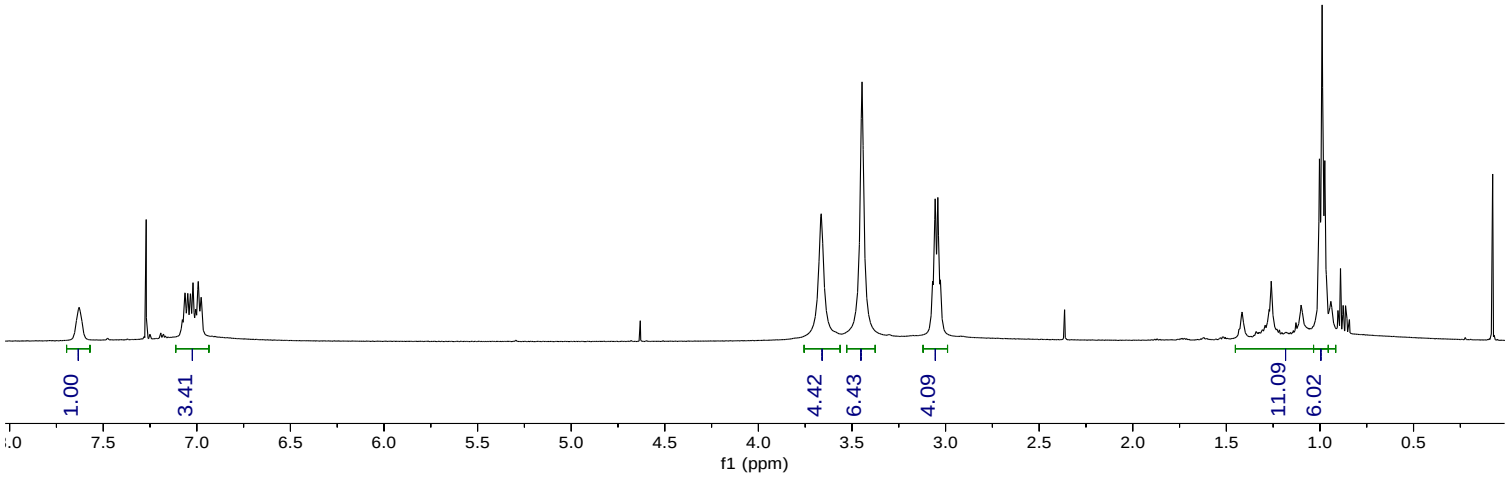




**Figure S18:** $^{1}$H NMR (500 MHz, chloroform-*d*) of 1-diethylamino-2-$BH_3$-$C_6H_4$-LiDME (**3**$_{\mathbf{LiDME}}$)

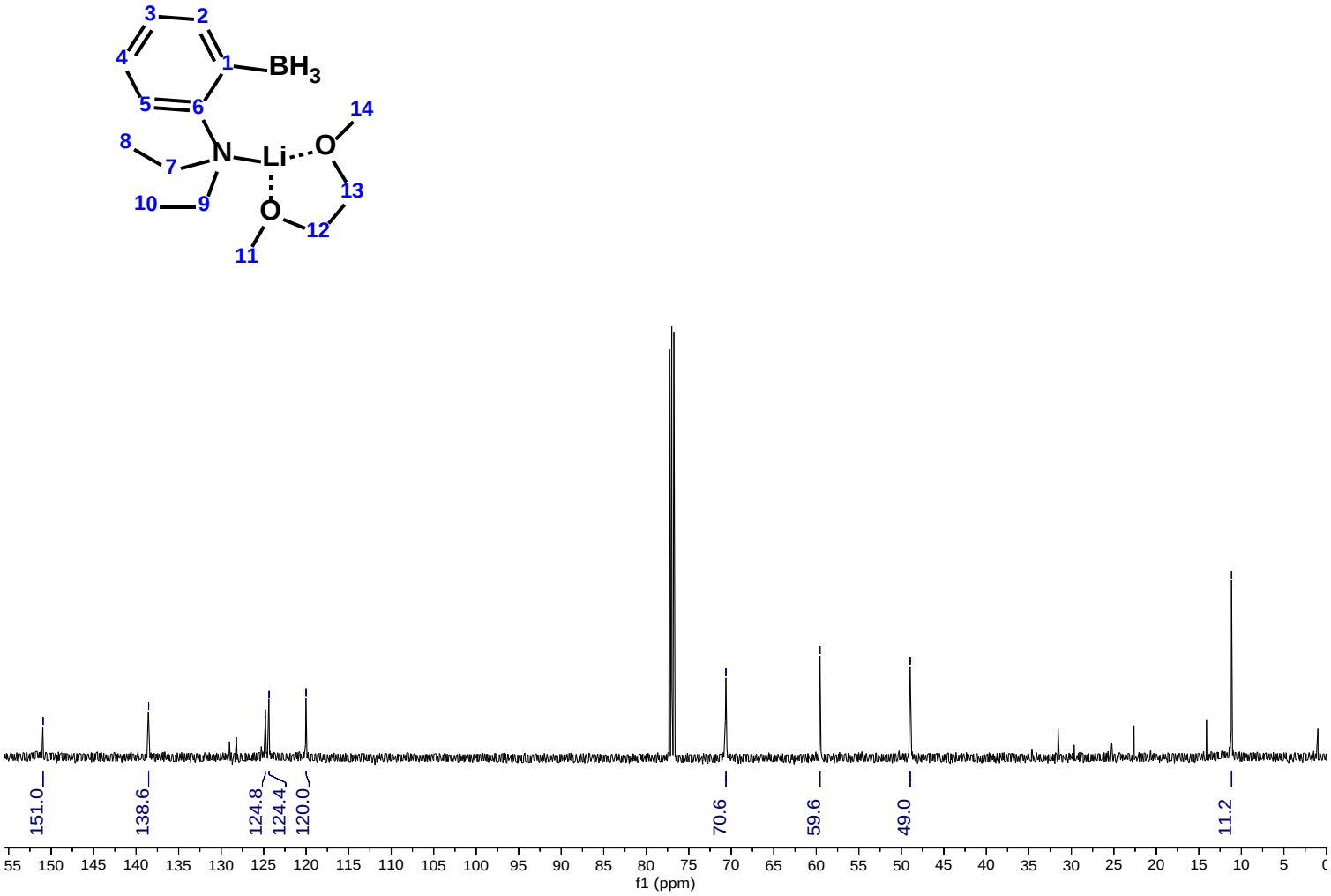



**Figure S19:** $^{13}C\{^{1}H\}$ NMR (126 MHz, chloroform-*d*) of 1-diethylamino-2-$BH_3$-$C_6H_4$-LiDME (**3**$_{\mathbf{LiDME}}$)

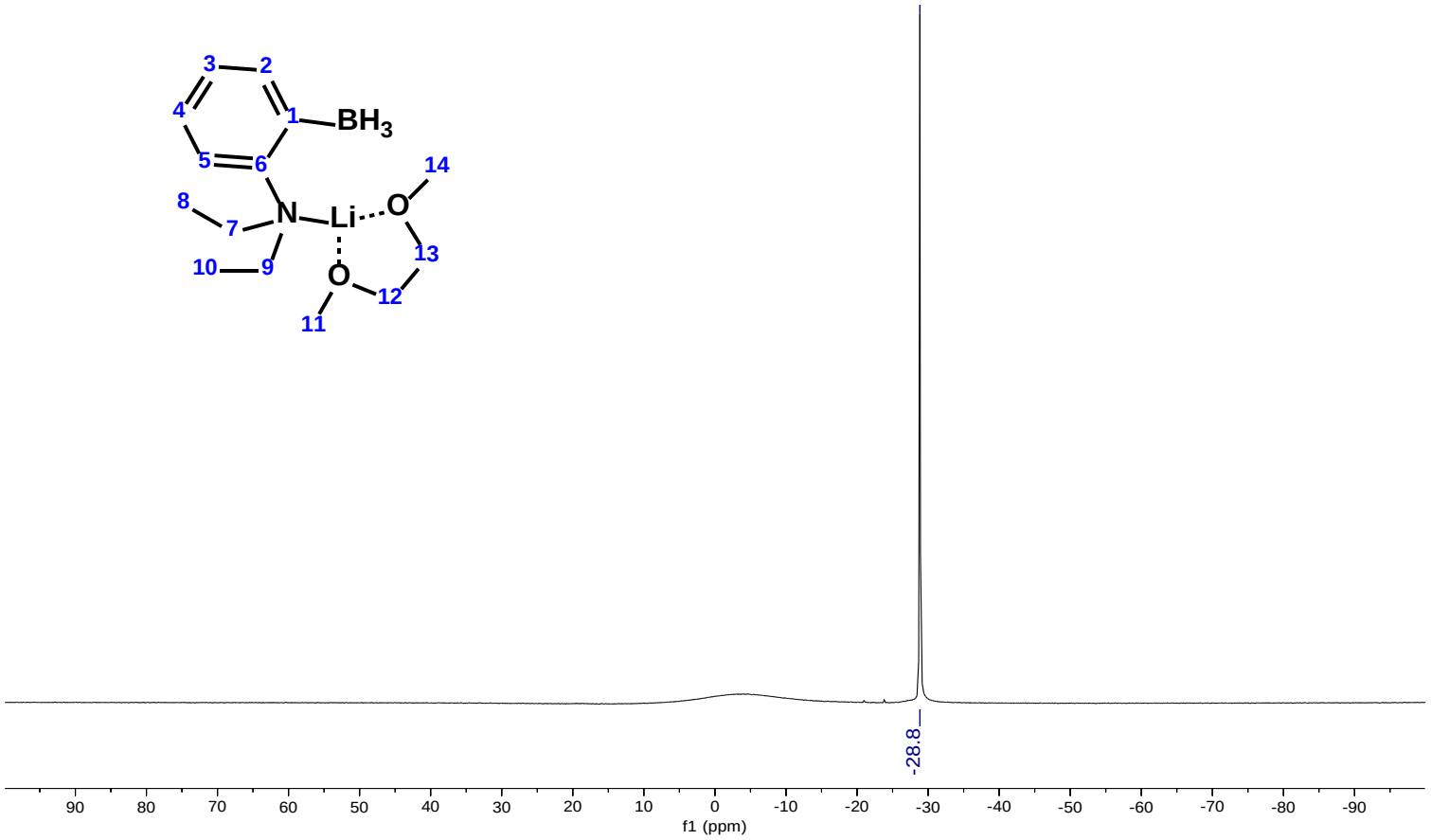
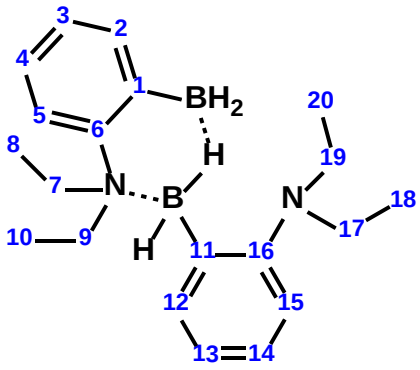



**Figure S20:** $^{11}B\{^{1}H\}$ NMR (160 MHz, chloroform-*d*) of 1-diethylamino-2-$BH_3$-$C_6H_4$-LiDME (**3**$_{\mathbf{LiDME}}$)

## (1-diethylamino-2-$BH_2$-$C_6H_4$)$_2$ (3)




750 mg (2.89 mmol, 1 equiv) of **3**-LiDME was dissolved in toluene and 0.57 mL (4.34 mmol, 1.5 eq) of TMSBr was added. The reaction was stirred at room temperature for 12 hours. The solution was separated from the precipitated salts by filtration and the volatile removed under reduced pressure to give 140 mg (30 % yield) of the title compound as a white powder. Single crystals were obtained from a toluene solution at -35°C.

Alternative synthesis from 1-diethylamino-2-B(OH)$_2$-$C_6H_4$: 2.75 g (14.2 mmol, 1 equiv) of 1-diethylamino-2-B(OH)$_2$-$C_6H_4$ was dissolved in toluene and cooled with an ice bath, 822 mg of $LiAlH_4$ (18.5 mmol, 1.3 equiv according to Li) was added followed by 3.5 mL of DME (24.4 mmol, 2 equiv). A certain amount of $H_2$ is liberated. The reaction was stirred for 1 hour at room temperature, then the mixture was filtered and the volatiles removed under reduced pressure. The remaining white oil was then dissolved in toluene and 2.42 mL (15.6 mmol, 1.1 equiv) of TMSBr was added. The reaction was stirred at room temperature for 12 hours. The solution was separated from the precipitated salts by filtration and the volatiles removed under reduced pressure to give 1.15 g (50% yield) of the compound as a white powder.

$^1$H NMR (500 MHz, chloroform-*d*) δ 7.55 (d, *J* = 6.7 Hz, 1H), 7.46 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.29-7.24 (m, 2H), 7.20 (t, *J* = 7.0 Hz, 1H), 7.11 (d, *J* = 8.0 Hz, 1H), 7.03-6.97 (m, 2H) , 3.49-3.33 (m, 2H), 3.12 (d, *J* = 5.1 Hz, 6H), 1.39-1.03 (m, 6H), 1.00 (t, *J* = 7.1 Hz, 6H), -0.69 (s, $BH_2$).

$^{13}$C{$^1$H} NMR (126 MHz, chloroform-*d*) δ 156.3 (s), 145.4 (br s), 144.3 (s), 138.1 (s), 136.5 (br s), 132.9 (s), 128.1 (s), 127.0 (s), 124.5 (s), 122.7 (s), 122.2 (s), 120.2 (s), 55.0 (br s), 50.0 (br s), 47.2 (s), 11.1 (s), 9.5 (br s).

$^{11}$B{$^1$H} NMR (160 MHz, chloroform-*d*) δ 1.0 (s, 1B, B1 or B2), -10.7 (s, 1B, B1 or B2).

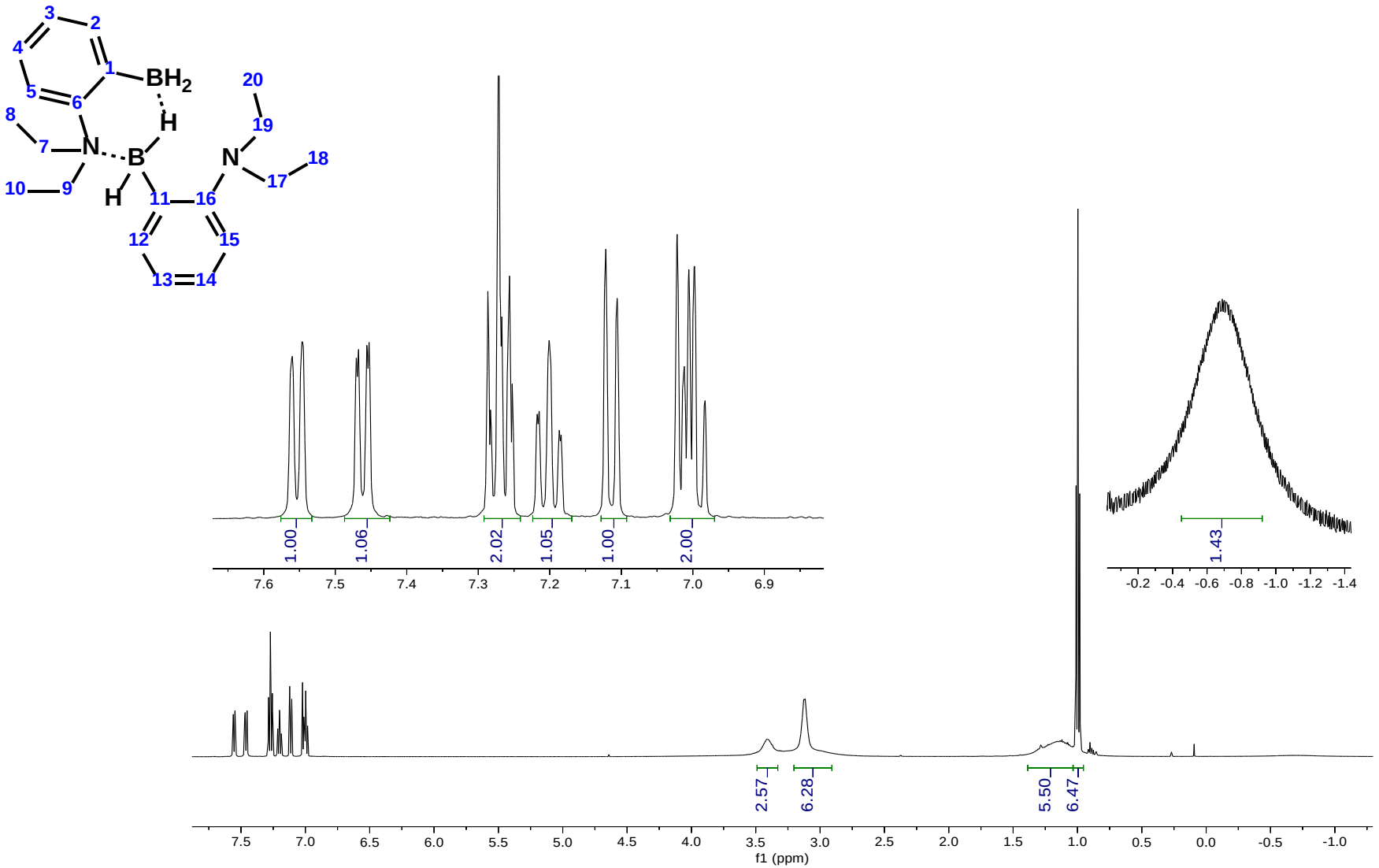



**Figure S21:** $^{1}$H NMR (500 MHz, chloroform-*d*) of (1-diethylamino-2-$BH_2$-$C_6H_4$)$_2$ (**3**)

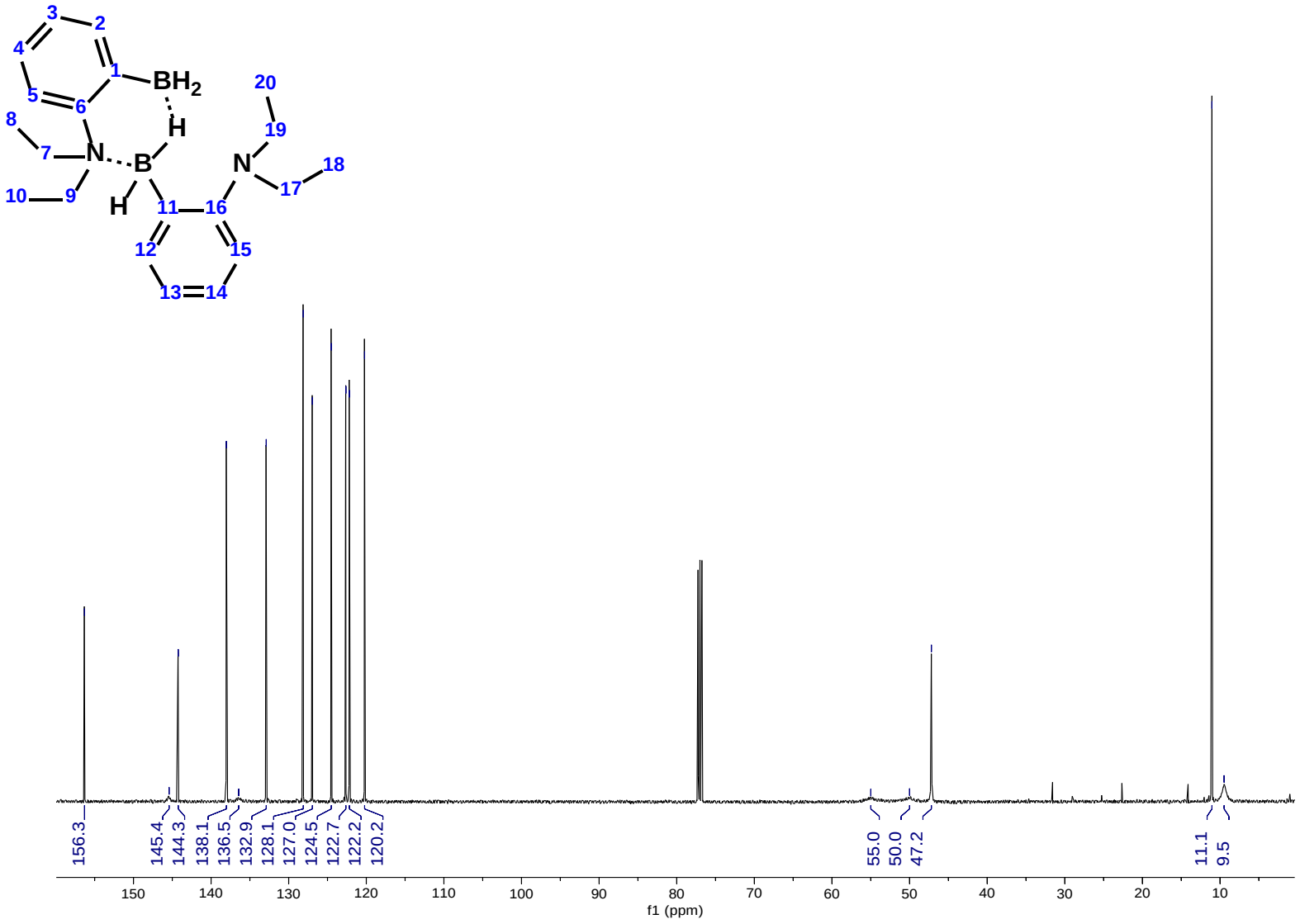



**Figure S22:** $^{13}C\{^{1}H\}$ NMR (126 MHz, chloroform-*d*) of (1-diethylamino-2-$BH_2$-$C_6H_4$)$_2$ (**3**)

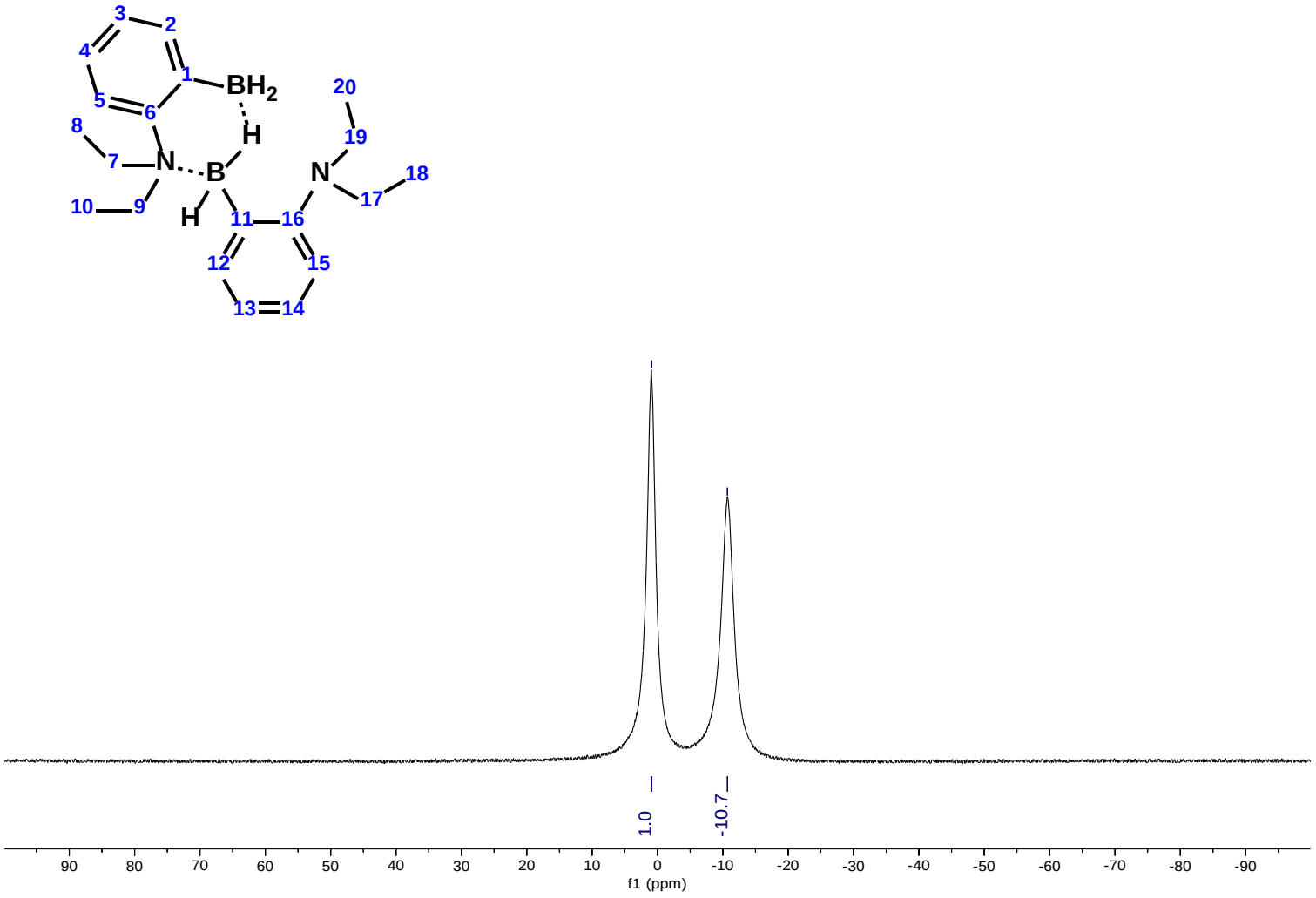
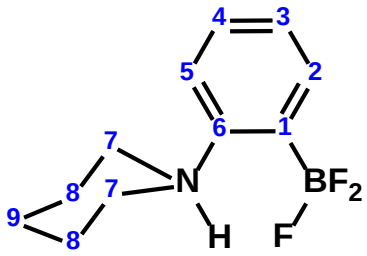



**Figure S23:** $^{11}B\{^{1}H\}$ NMR (160 MHz, chloroform-*d*) of (1-diethylamino-2-$BH_2$-$C_6H_4$)$_2$ (**3**)

## 1-piperidyl(H)-2-$BF_3$-$C_6H_4$ (2F)




To a solution of 1-piperidyl-2-$B(OH)_2$-$C_6H_4$ (6.0 g, 29.3 mmol, 1 equiv) in ethanol (250 mL) were added $KHF_2$ (13.7g, 175.6 mmol, 6 equiv) and 32 mL of a 2M HCl solution in water. The reaction mixture was sonicated for 30 minutes and stirred at room temperature for 16 hours. After evaporation of the volatiles under reduced pressure, the resulting white residue was extracted with chloroform (3 x 100 mL). The combined organic fractions were dried ($MgSO_4$), filtered and evaporated to yield the target compound **2F** (5.4 g, 81% yield).

$^1$H NMR (500 MHz, chloroform-*d*) δ 9.25 (s, br, 1H, NH), 7.77 (d, *J* = 7.3 Hz, 1H, H2 or H5), 7.39 (t, *J* = 7.3 Hz, 1H, H3 or H4), 7.33 (t, 1H, *J* = 8.0 Hz, H3 or H4), 7.24 (d, 1H, *J* = 8.0 Hz, H2 or H5), 3.67 (m, 2H, H7), 3.40 (m, 2H, H7), 2.14 (m, 2H, H8), 2.03-1.92 (m, 3H, 2H of H8 and 1H of H9), 1.65 (m, 1H, H9).

$^{13}$C{$^1$H} NMR (126 MHz, chloroform-*d*) δ 144.1 (s, 1C, C6); 134.8 (q, 1C, C2, $J_{C\text{-}F}$ = 1.9 Hz); 129.6, 128.5, 116.9 (s, 3C, C3, C4 and C5); 57.1 (s, 2C, C7); 24.9 (s, 2C, C8); 21.3 (s, 2C, C9). The carbon linked directly to boron was not observed.

$^{19}$F{$^1$H} NMR (470 MHz): *δ* -137.6 (m).

$^{11}$B{$^1$H} NMR (160 MHz, chloroform-*d*) δ 3.1 (m).

HRMS (ESI-TOF) *m/z* Calcd for $C_{11}H_{15}BF_3N$ - H: 228.1179; Found: 228.1189.

Anal. Calcd for $C_{11}H_{15}BF_3N$: C, 57.68; H, 6.60; N, 6.12. Found: C, 57.96; H, 6.58; N, 6.29

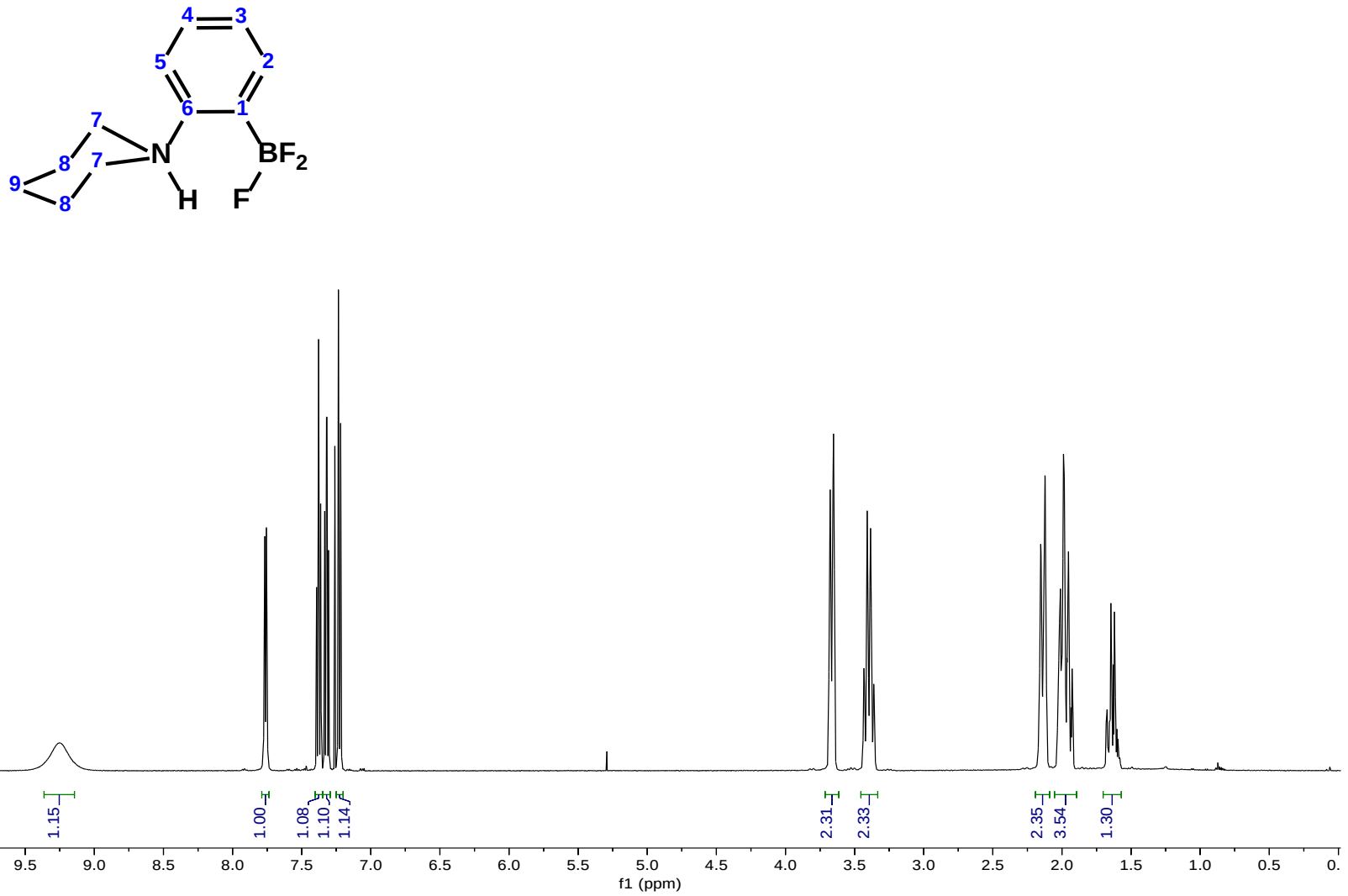



**Figure S24:** $^{1}$H NMR (500 MHz, chloroform-*d*) of 1-piperidyl(H)-2-$BF_3$-$C_6H_4$ (**2F**)

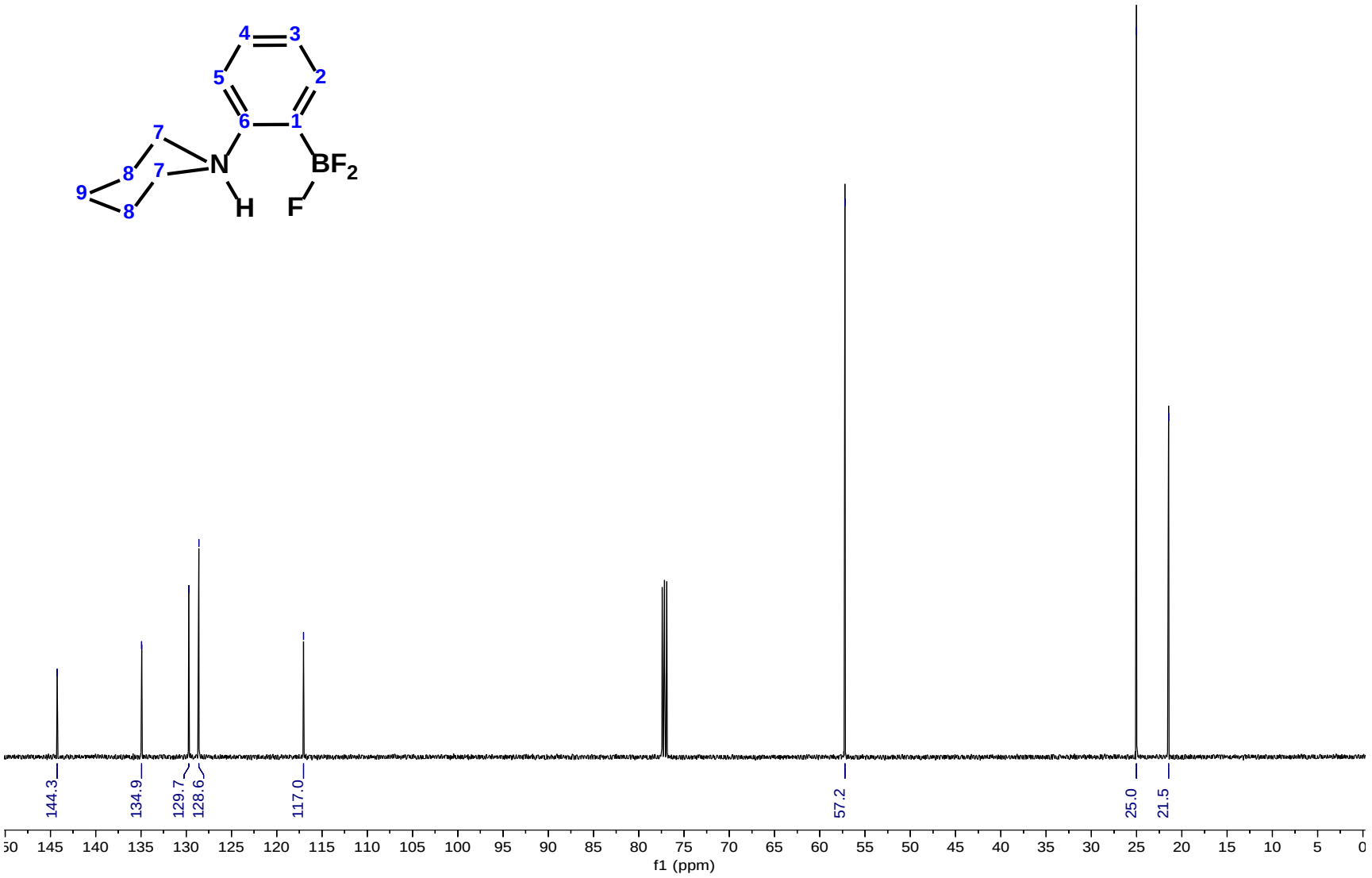



**Figure S25:** $^{13}C\{^{1}H\}$ NMR (126 MHz, chloroform-*d*) of 1-piperidyl(H)-2-$BF_3$-$C_6H_4$ (**2F**)

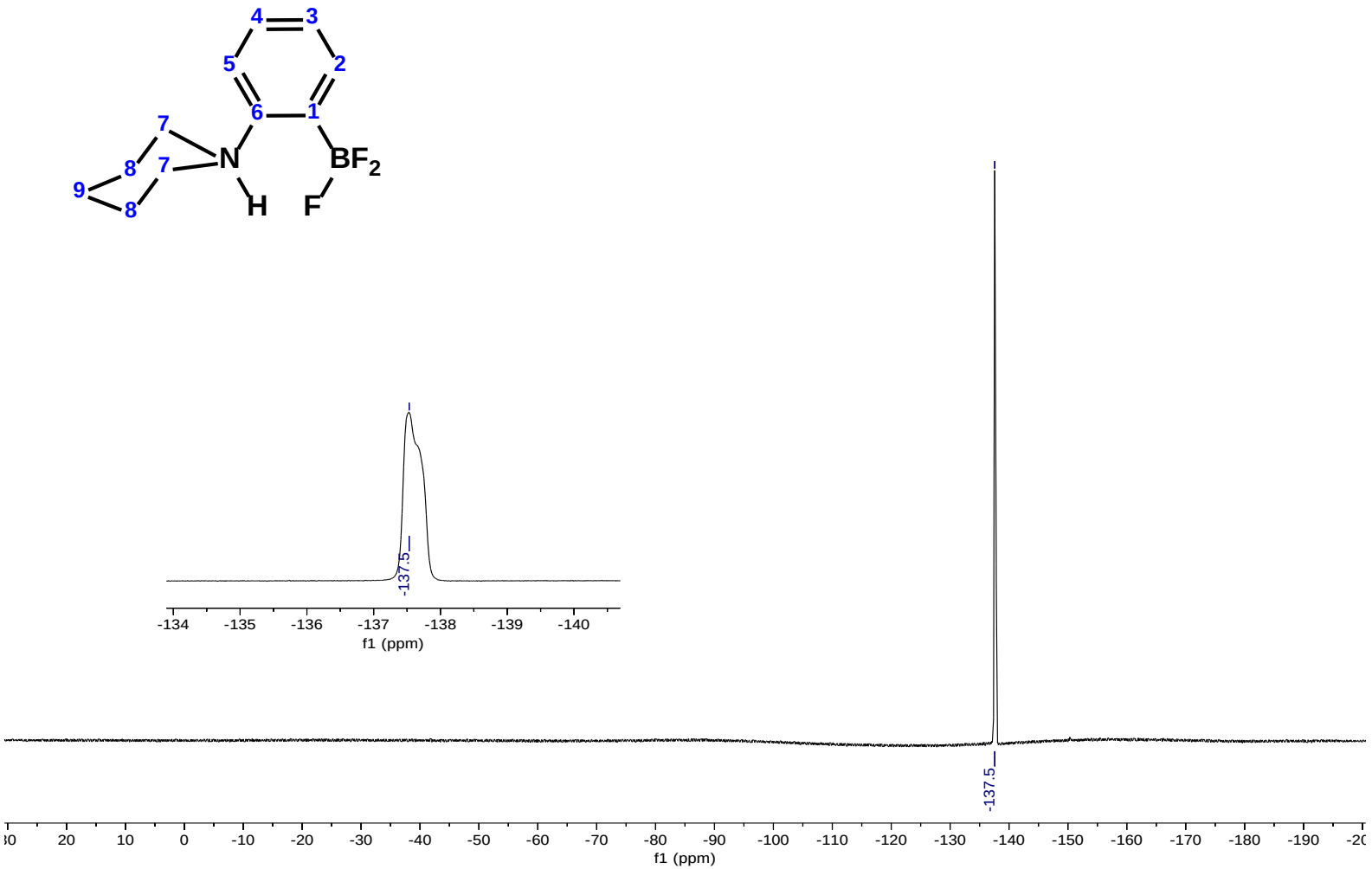



**Figure S26:** $^{19}F\{^{1}H\}$ NMR (470 MHz, chloroform-*d*) of 1-piperidyl(H)-2-$BF_3$-$C_6H_4$ (**2F**)

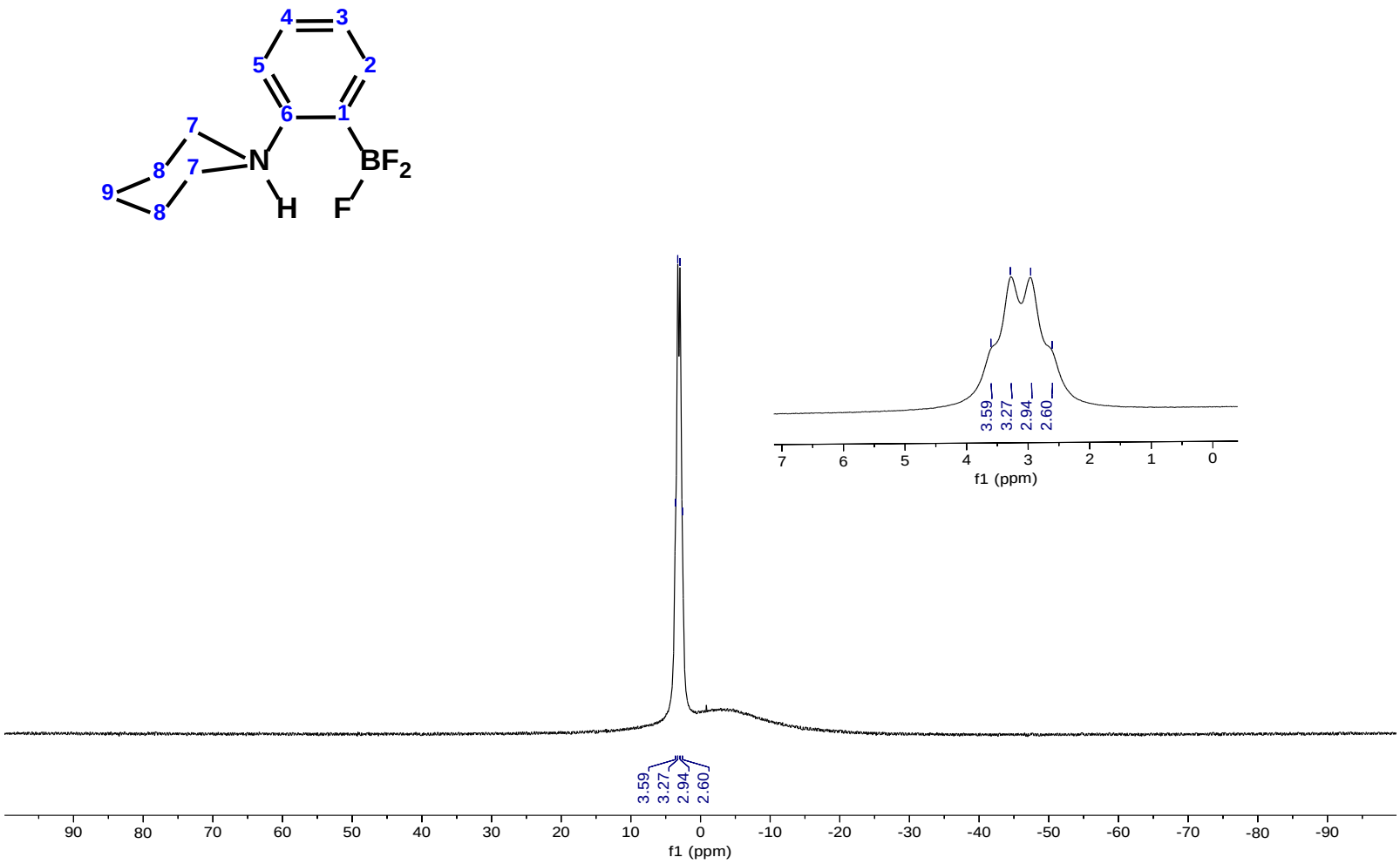



**Figure S27:** $^{11}B\{^{1}H\}$ NMR (160 MHz, chloroform-*d*) of 1-piperidyl(H)-2-$BF_3$-$C_6H_4$ (**2F**)

## 1-diethylamino(H)-2-$BF_3$-$C_6H_4$ (3F)

To a solution of 1-diethylamino-2-$B(OH)_2$-$C_6H_4$ (10.0 g, 51.8 mmol) in ethanol (500 mL) were added $KHF_2$ (24.2 g, 310.8 mmol) and 56 mL of 2M HCl solution in water. The reaction mixture was sonicated for 30 minutes and stirred at room temperature for 16 hours. After evaporation of the volatiles under reduced pressure, the residue was extracted with chloroform (3x100 mL). The combined organic fractions were dried with $MgSO_4$, followed by filtration and evaporation gave the target compound **3F** as white powder (9.55g, 85% yield).

$^1$H NMR (500 MHz, chloroform-*d*): δ 9.19 (s, br, 1H, NH); 7.82 (m, 1H, H5); 7.44 – 7.38 (m, 2H, H3 and H4); 7.16 (m, 1H, H2); 3.85 (m, 2H, H7); 3.46 (m, 2H, H7); 1.22 (t, *J* = 7.2 Hz, 6H, H8).

$^{13}$C{$^1$H} NMR (126 MHz, chloroform-*d*): δ 138.8 (s, 1C, C6); 134.8 (q, 1C, C2, $J_{C\text{-}F}$ = 1.9 Hz); 129.3, 128.9, 116.9 (s, 3C, C3, C4 and C5); 54.6 (s, 2C, C7); 10.5 (s, 2C, C8). The carbon linked directly to boron was not observed.

$^{19}$F{$^1$H} NMR (470 MHz, chloroform-*d*): δ -135.6 (m).

$^{11}$B{$^1$H} NMR (160 MHz, chloroform-*d*): δ 3.1 (m).

HRMS (ESI-TOF) *m/z* Calcd for $C_{10}H_{15}BF_3N$ - H: 216.1179; Found: 216.1187.

Anal. Calcd for $C_{10}H_{15}BF_3N$: C, 55.34; H, 6.97; N, 6.45. Found: C, 55.31; H, 7.03; N, 6.63.

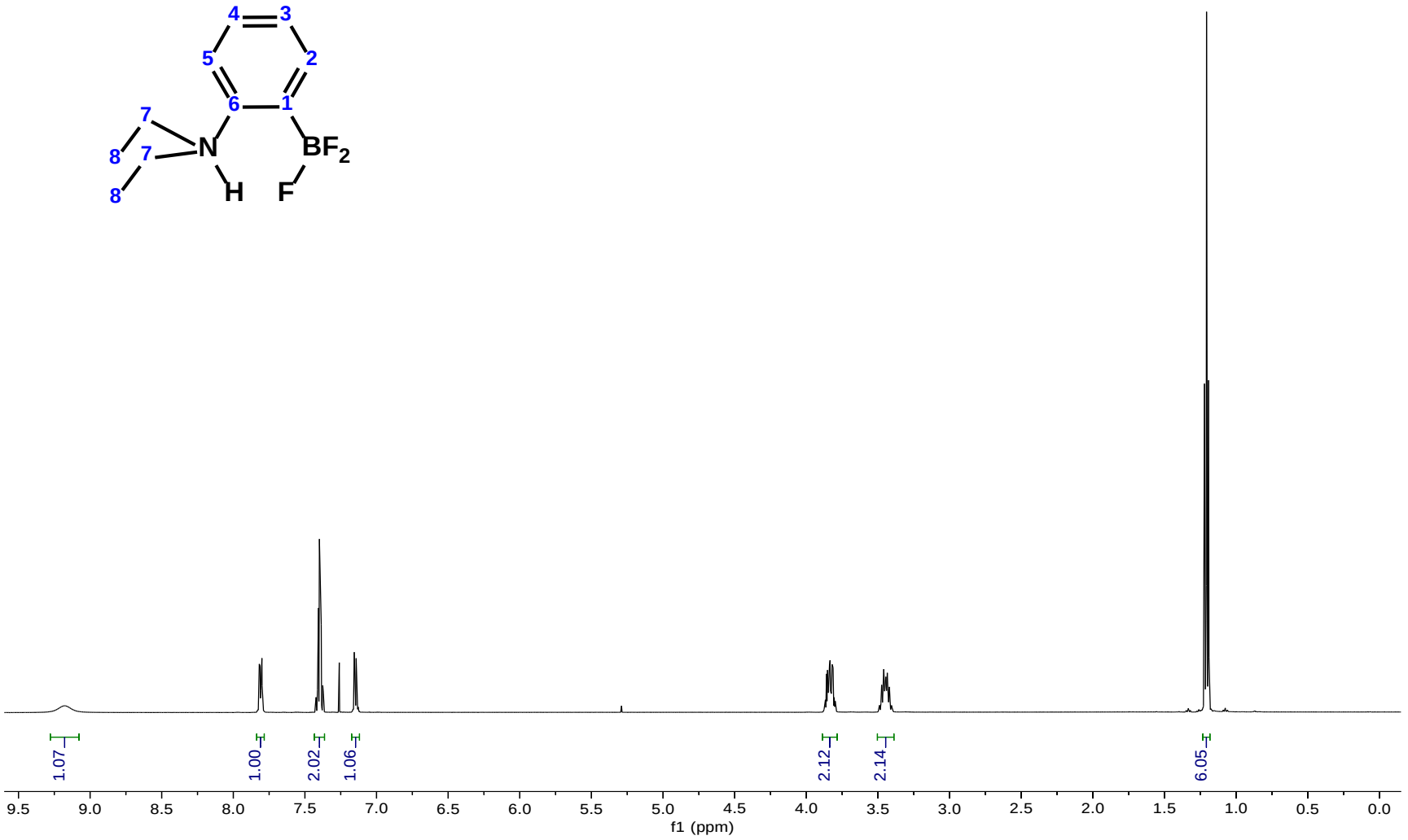



**Figure S28:** $^{1}$H NMR (500 MHz, chloroform-*d*) of 1-diethylamino(H)-2-$BF_3$-$C_6H_4$ (**3F**)

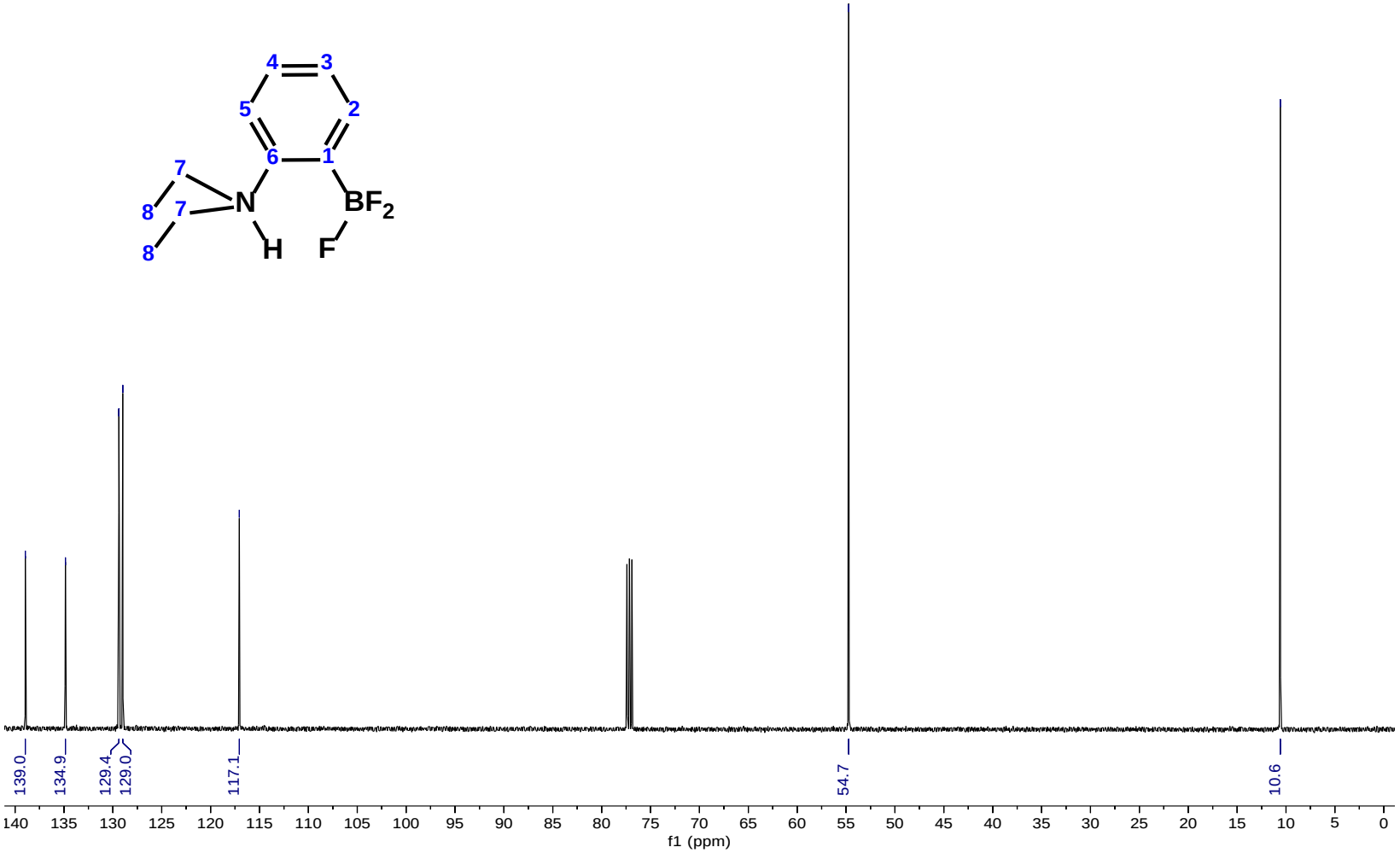



**Figure S29:** $^{13}C\{^{1}H\}$ NMR (126 MHz, chloroform-*d*) of 1-diethylamino(H)-2-$BF_3$-$C_6H_4$ (**3F**)

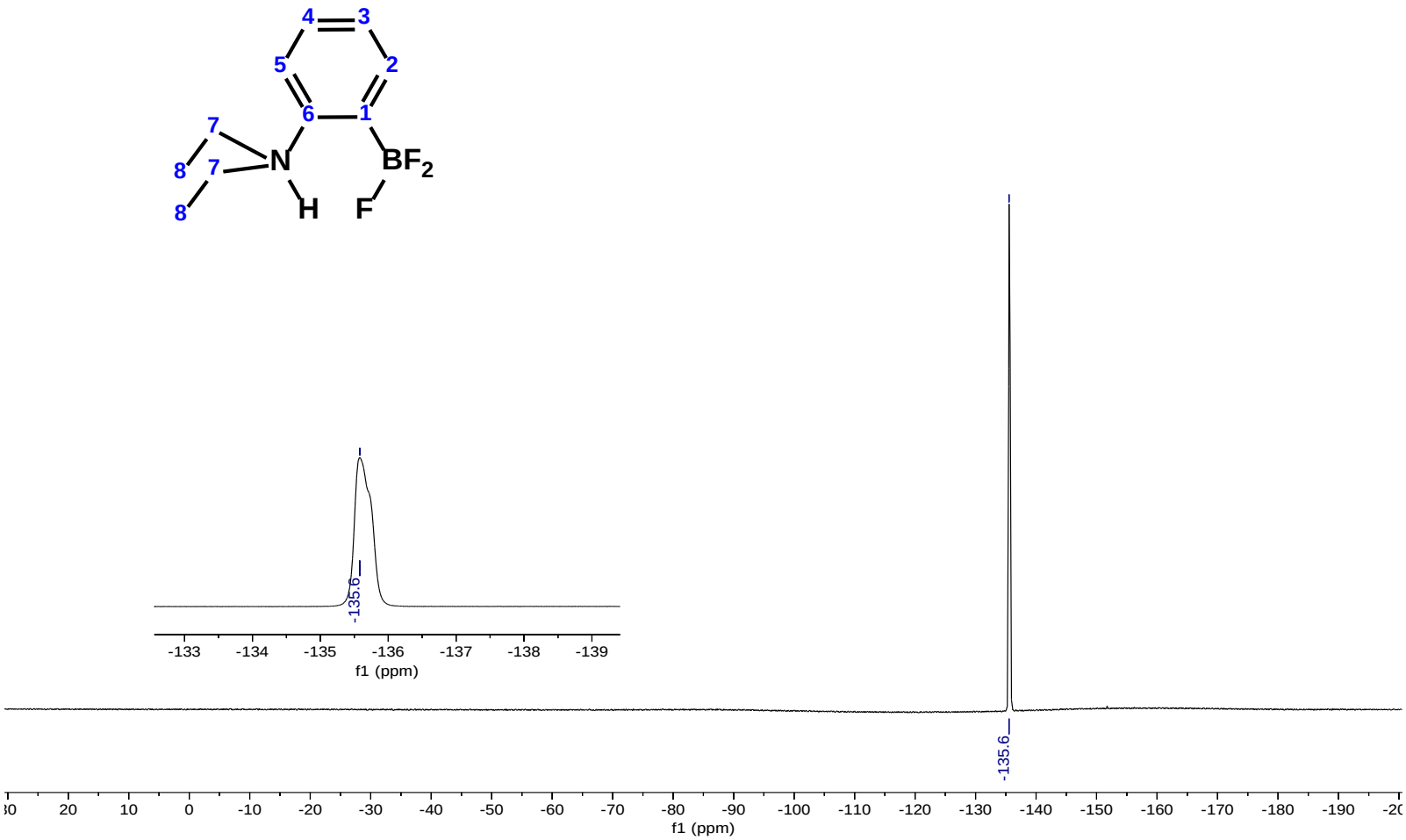



**Figure S30:** $^{19}F\{^{1}H\}$ NMR (470 MHz, chloroform-*d*) of 1-diethylamino(H)-2-$BF_3$-$C_6H_4$ (**3F**)

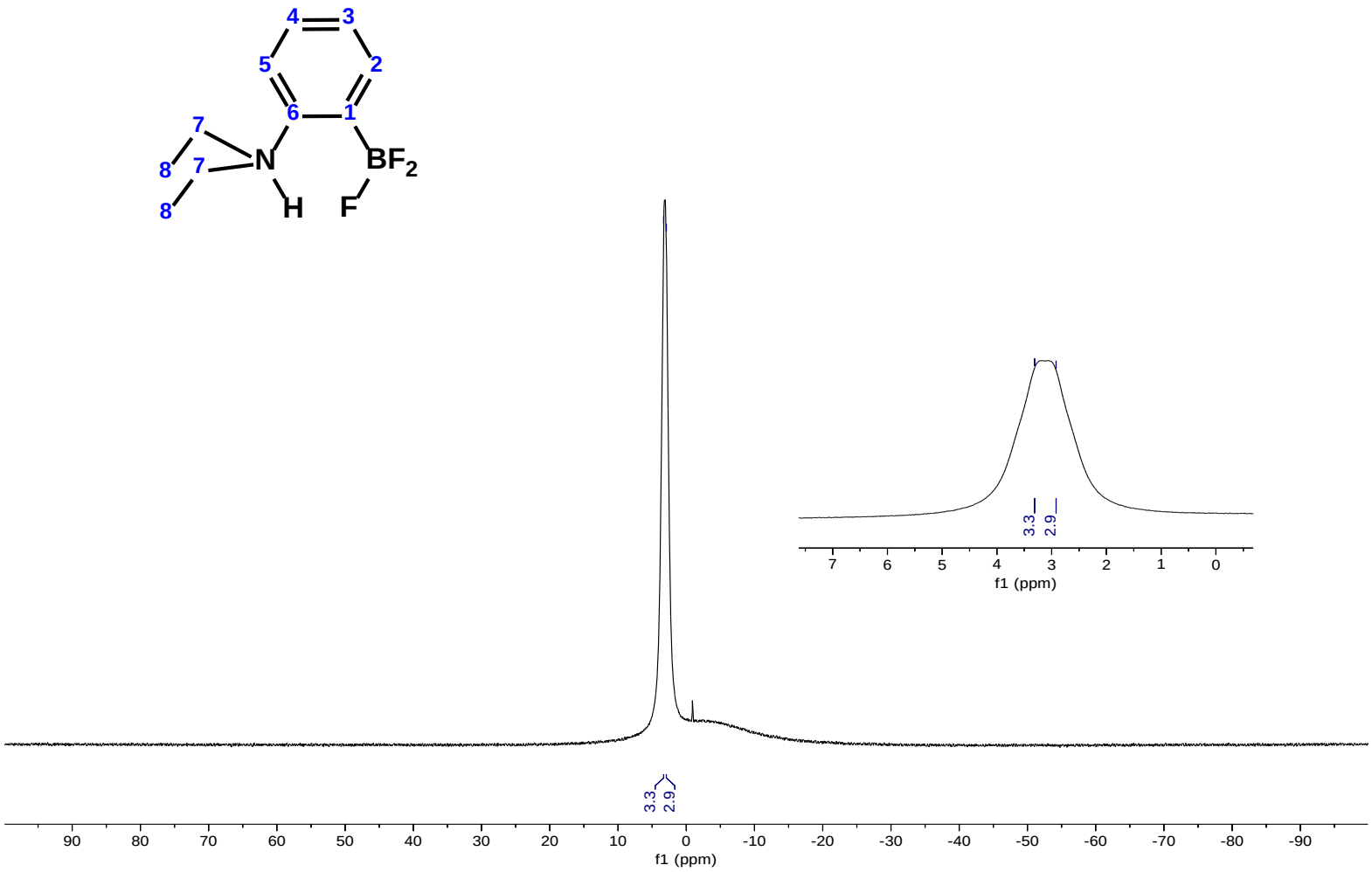
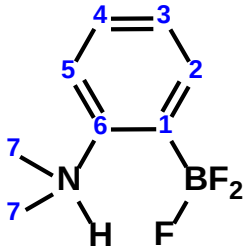



**Figure S31:** $^{11}B\{^{1}H\}$ NMR (160 MHz, chloroform-*d*) of 1-diethylamino(H)-2-$BF_3$-$C_6H_4$ (**3F**)

## 1-dimethylamino(H)-2-$BF_3$-$C_6H_4$ (4F)




To a solution of 1-dimethyl-2-$B(OH)_2$-$C_6H_4$ (1.5 g, 9.1 mmol) in ethanol (50 mL) were added $KHF_2$ (4.3g, 54.5 mmol) and 10 mL of a 2M HCl solution in water. The reaction mixture was sonicated for 30 minutes and stirred for 16 hours at room temperature. After evaporation of the volatiles under reduced pressure, the resulting white residue was extracted with chloroform (3 x 50 mL). The combined organic fractions were dried ($MgSO_4$), filtered and evaporated to yield the target compound **4F** (1.49 g, 87% yield).

$^1$H-NMR (500MHz, chloroform-*d*): δ 9.57 (s, br, 1H, NH); 7.82 (d, *J* = 6.8 Hz, 1H, H5); 7.45 – 7.39 (m, 2H, H3 and H4); 7.29 (m, 1H, H2); 3.40 (s, 3H, H7); 3.39 (s, 3H, H7).

$^{13}$C{$^1$H} NMR (126 MHz, chloroform-*d*): δ 145.1 (s, 1C, C6); 134.7 (q, 1C, C2, $J_{C\text{-}F}$ = 2.5 Hz); 129.5, 128.7, 116.3 (s, 3C, C3, C4 and C5); 47.7 (s, 2C, C7). The carbon linked directly to boron was not observed.

$^{19}$F{$^1$H} NMR (470 MHz, chloroform-*d*): δ -138.6 (m).

$^{11}$B{$^1$H} NMR (160 MHz, chloroform-*d*): δ 3.1 (m).

HRMS (ESI-TOF) *m/z* Calcd for $C_8H_{11}BF_3N$ - H: 188.0865; Found: 188.0872.

Anal. Calcd for $C_8H_{11}BF_3N$: C, 50.84; H, 5.87; N, 7.41. Found: C, 50.96; H, 5.48; N, 7.53.

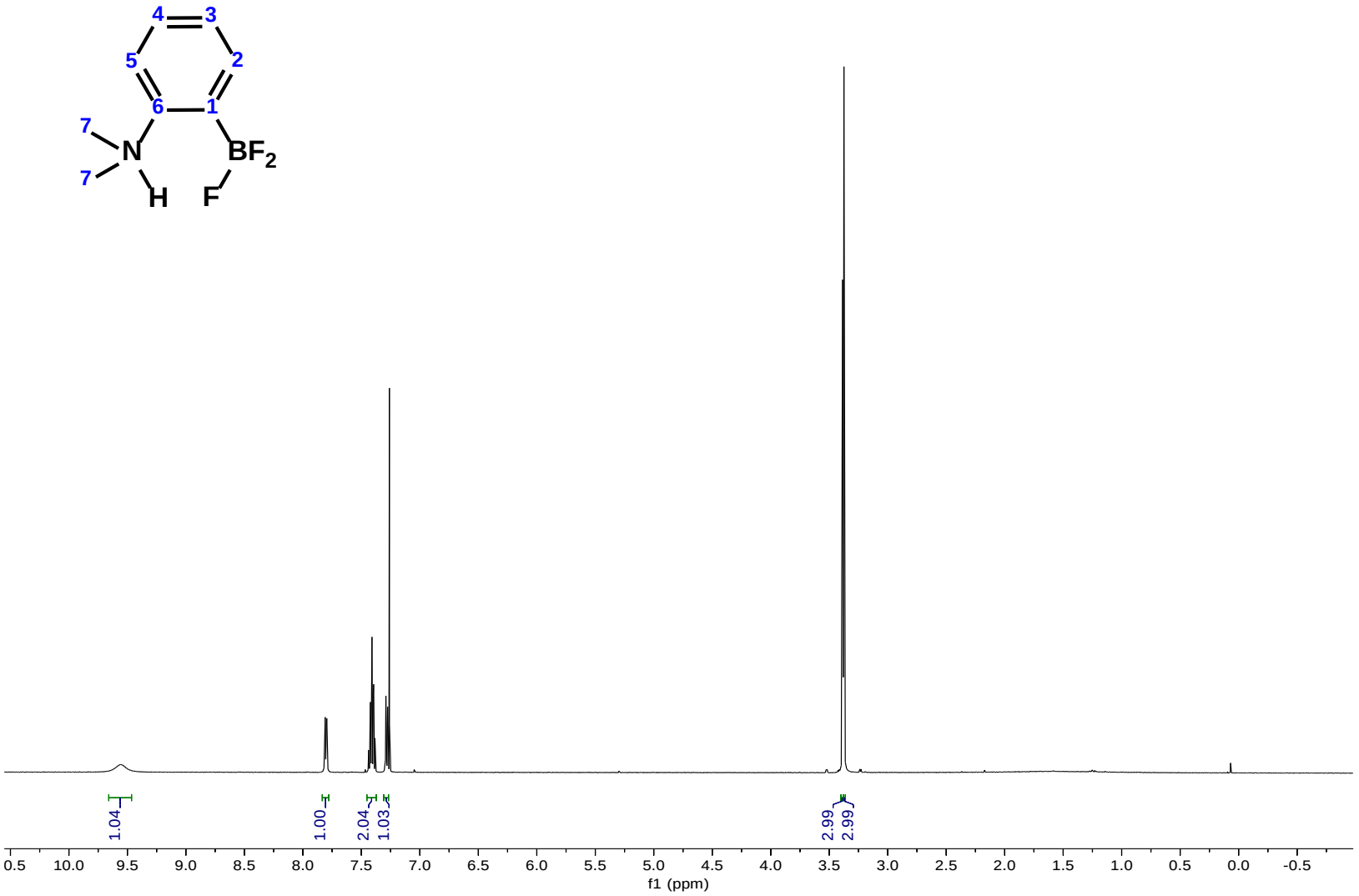



**Figure S32:** $^{1}$H NMR (500 MHz, chloroform-*d*) of 1-dimethylamino(H)-2-$BF_3$-$C_6H_4$ (**4F**)

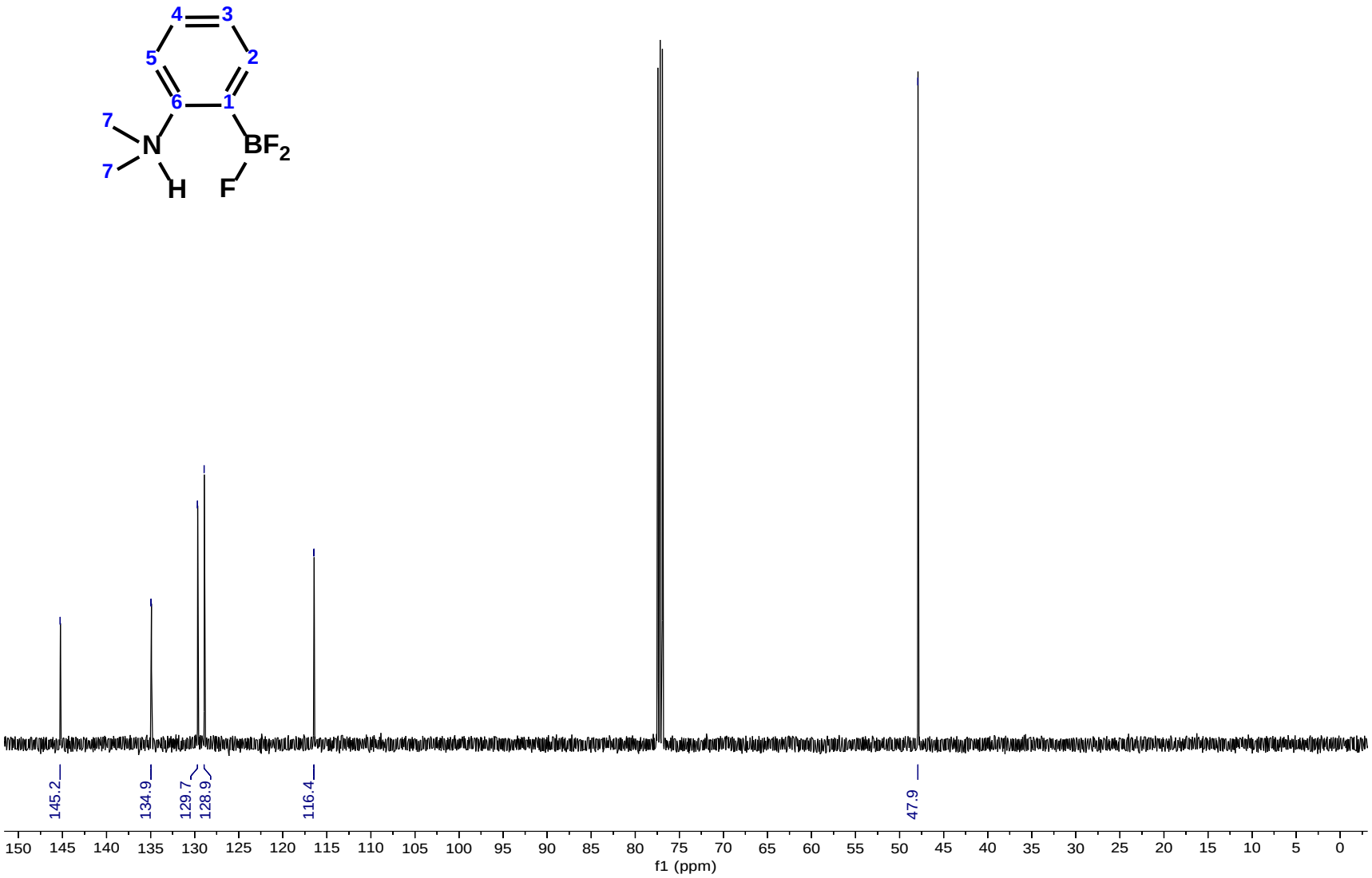



**Figure S33:** $^{13}C\{^{1}H\}$ NMR (126 MHz, chloroform-*d*) of 1-dimethylamino(H)-2-$BF_3$-$C_6H_4$ (**4F**)

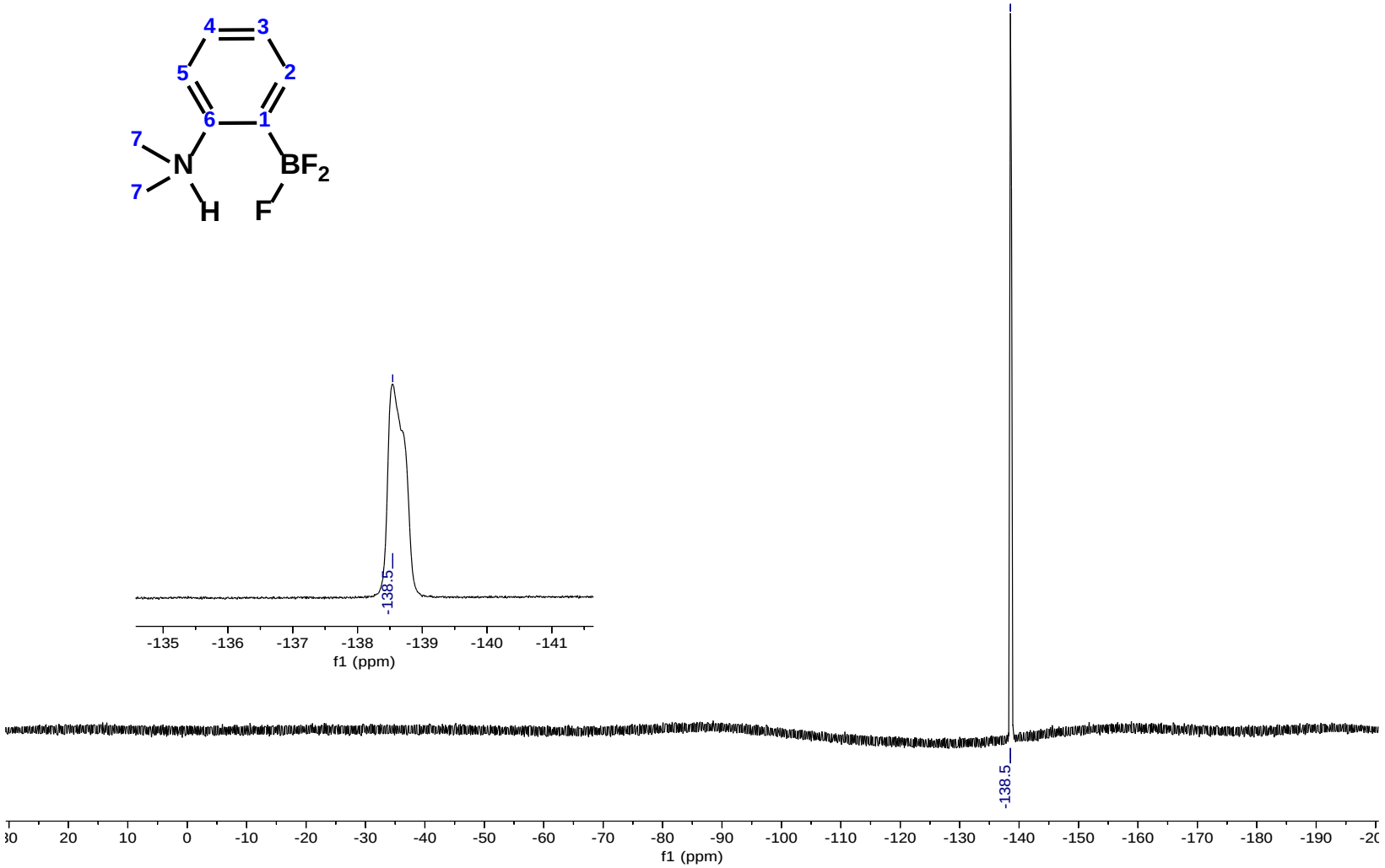



**Figure S34:** $^{19}F\{^{1}H\}$ NMR (470 MHz, chloroform-*d*) of 1-dimethylamino(H)-2-$BF_3$-$C_6H_4$ z(**4F**)

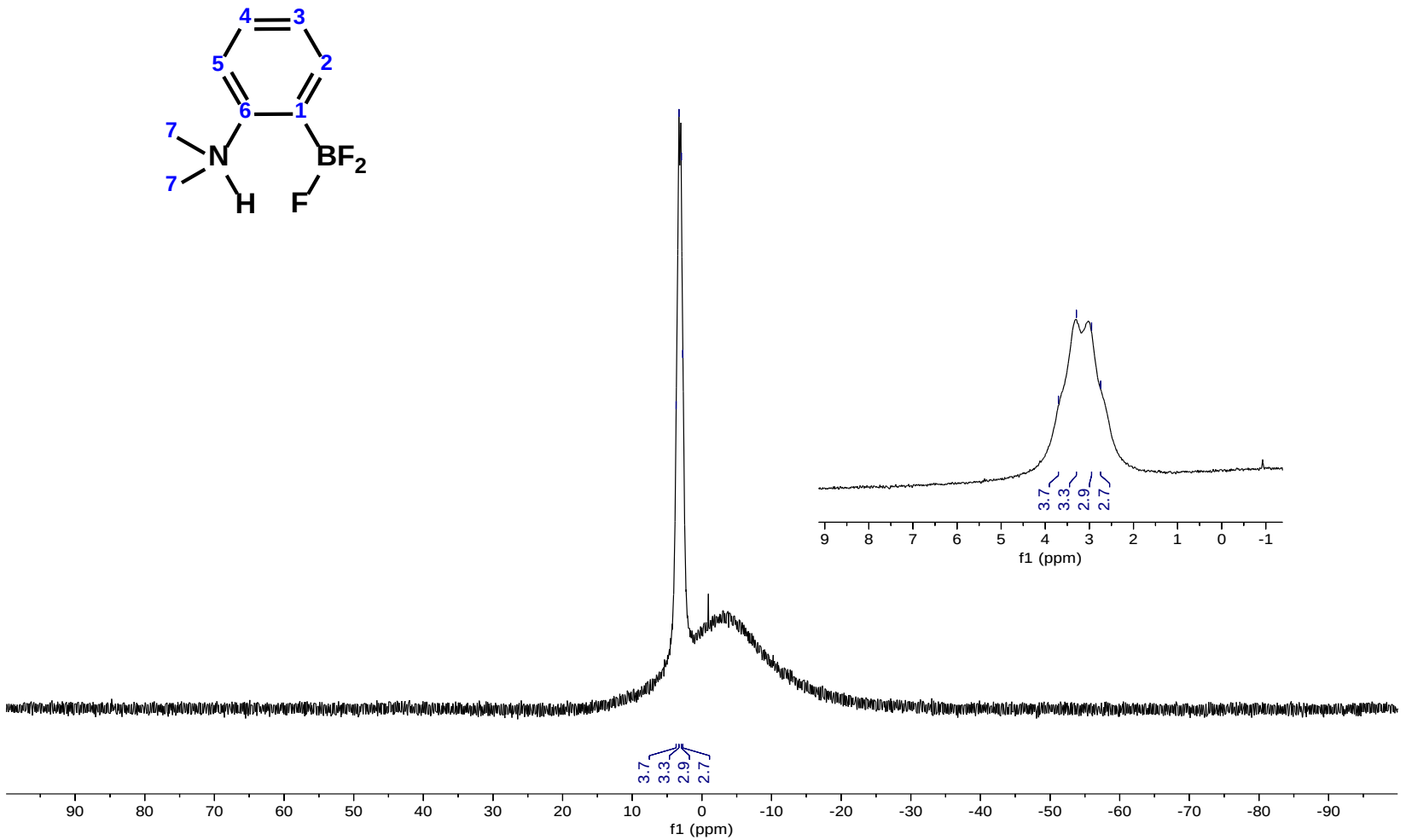
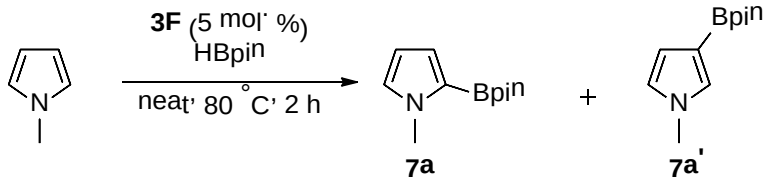



**Figure S35:** $^{11}B\{^{1}H\}$ NMR (160 MHz, chloroform-*d*) of 1-dimethylamino(H)-2-$BF_3$-$C_6H_4$ (**4F**)

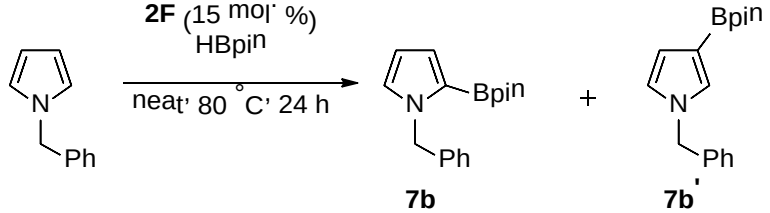
# Gram scale catalytic borylation of heteroarenes under neat conditions

## Borylation of 1-methylpyrrole



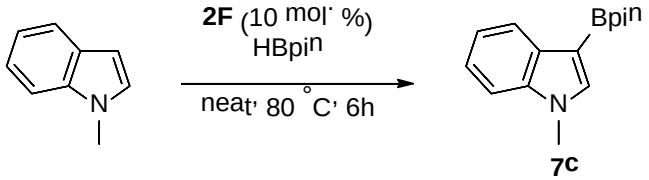

Precatalyst **3F** (133 mg, 0.58 mmol) was introduced into an oven-dried two-neck flask (100 mL) containing a magnetic stirring bar was connected to a condenser under a normal nitrogen flow. To this were added 1.1 mL (11.6 mmol) of 1-methylpyrrole (distilled before use) followed by HBpin containing stabilizer (1% $NEt_3$) (1.3 equiv, 2.4 mL) via syringe. The reaction mixture was then stirred for 2 hours at 80 °C in an oil bath. The resulting mixture was kept under reduced pressure during 30 min, and then filtered through a short pad of Celite and rinsed with ethyl ether. The resulting filtrate was evaporated to complete dryness under reduced pressure to afford 2.37g (93.3 %) of the desired 1-methyl-2-Bpin pyrrole (**7a**) as a white solid. The regioselectivity of this reaction is 98:2 (C2:C3). The obtained product was analytically similar to the one reported previously.[2,3]

## Borylation of 1-benzylpyrrole



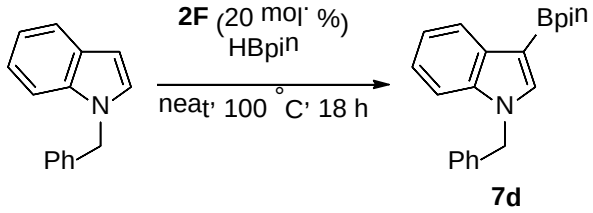

Precatalyst **2F** (437 mg, 1.91 mmol) was introduced into an oven-dried two-neck flask (100 mL) that already has a stir bar and connected to a condenser with a normal flow of nitrogen. Then, 2.0 mL (12.7 mmol) of 1-benzylpyrrole (distilled before use) followed by pinacolborane 1 % $Et_3N$ (2.3 equiv, 4.3 mL) are added via syringe. The reaction mixture was then stirred for 24 hours at 80 °C in an oil bath. The resulting mixture was kept under reduced pressure for 30 min. Crude $^1H$ NMR showed about 87% of conversion. The crude mixture was then passed through a short pad of silica gel using the ethyl ether:hexanes 80:20 solvent mixture. This was followed by performing a small flash chromatography using the silica gel as stationary phase and the petroleum ether:ethyl acetate 100:1 as mobile phase. After evaporation of the solvent to complete dryness under reduced pressure, 2.72 g (76 %) of the desired 1-benzylpyrrole-2-boronic acid pinacol ester (**7b**) was obtained as a white solid. The regioselectivity of this reaction is 100:0 (C2:C3). The obtained product was analytically similar to the one reported previously.[2,3]

## Borylation of 1-methylindole




Precatalyst **2F** (234 mg, 1.02 mmol) was introduced into an oven-dried two-neck flask (100 mL) that is already connected to a condenser with a normal flow of nitrogen. Then 1.3 mL (10.2 mmol) of 1-methylindole (distilled before use) followed by pinacolborane that contain 1 % $Et_3N$ additive (2.0 equiv, 3.0 mL) were added via syringe. The reaction mixture was then stirred for 6 hours in an oil bath kept at 80°C. The resulting mixture was kept under reduced pressure for 30 min. A small flash chromatography with silica gel as stationary phase was performed to purify the product. A mixture of petroleum ether/ethyl ether 20:1 was used as eluent to eliminate the rest of 1-methylindole, then the polarity of the eluent was increased by going to a 10:1 ratio to obtain the borylated product. After evaporation of the solvent to complete dryness under reduced pressure, a 2.10g (80%) of the desired 1-methylindole-3-boronic acid pinacol ester (**7c**) was obtained as a white solid. The obtained product was analytically similar to the one previously reported.[2,3]

## Borylation of 1-benzylindole




Precatalyst **2F** (662 mg, 2.89 mmol) was introduced into an oven-dried two-neck flask (100 mL) that is connected already to a condenser with a normal flow of nitrogen. Then 3.0 g (14.46 mmol) of 1-benzylindole (prepared according to the literature)[4] was added followed by pinacolborane that contain 1 % $Et_3N$ (2.6 equiv, 5.5 mL) via syringe. The reaction mixture was then stirred for 24 hours in an oil bath kept at 100°C. The resulting mixture was kept under reduced pressure for 30 min. The $^1H$ NMR spectrum of the crude mix showed 80% conversion. A small flash chromatography with silica gel as stationary phase and $CH_2Cl_2$ as eluent was used to purify the product. To the collected $CH_2Cl_2$ solution containing the pure product was added hexanes and the solvent was slowly evaporated until a white precipitate forms. Subsequently, the aliquot was decanted and the resulting wet residue was dried under reduced pressure to obtain the 1-benzyl-2-Bpin indole (**7d**) (3.04 g, 63 %).

$^1H$ NMR (500 MHz, chloroform-*d*): $\delta$ 8.06 (m, 1H) 7.60 (s, 1H), 7.31-7.25 (m, 4H), 7.19-7.12 (m, 4H), 5.32 (s, 2H), 1.36 (s, 12H).

$^{13}C\{^{1}H\}$ NMR (126 MHz, chloroform-*d*): $\delta$ 137.95, 137.51, 137.08, 132.08, 128.92, 127.86, 127.18, 122.88, 122.06, 120.54, 109.87, 82.94, 50.52, 25.09. The carbon linked directly to boron was not observed.

$^{11}B$ NMR (160 MHz, chloroform-*d*): $\delta$ 30.21.

HRMS (ESI-TOF) *m/z*: Calcd for $C_{21}H_{24}BNO_2$ + H: 334.1978; Found: 334.1980.

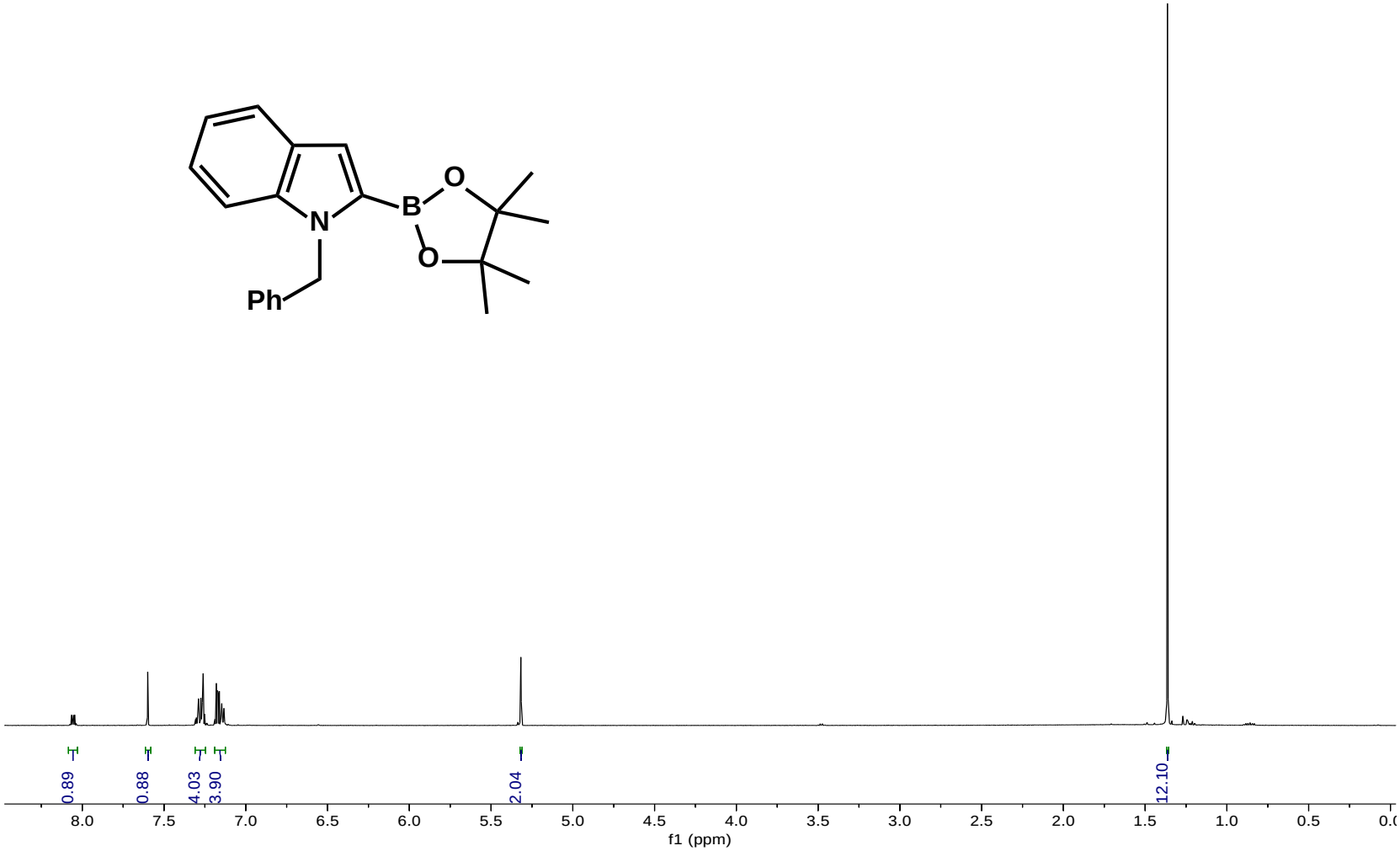



**Figure S36:** $^{1}$H NMR (500 MHz, chloroform-*d*) of 1-benzyl-2-Bpin indole (**7d**)

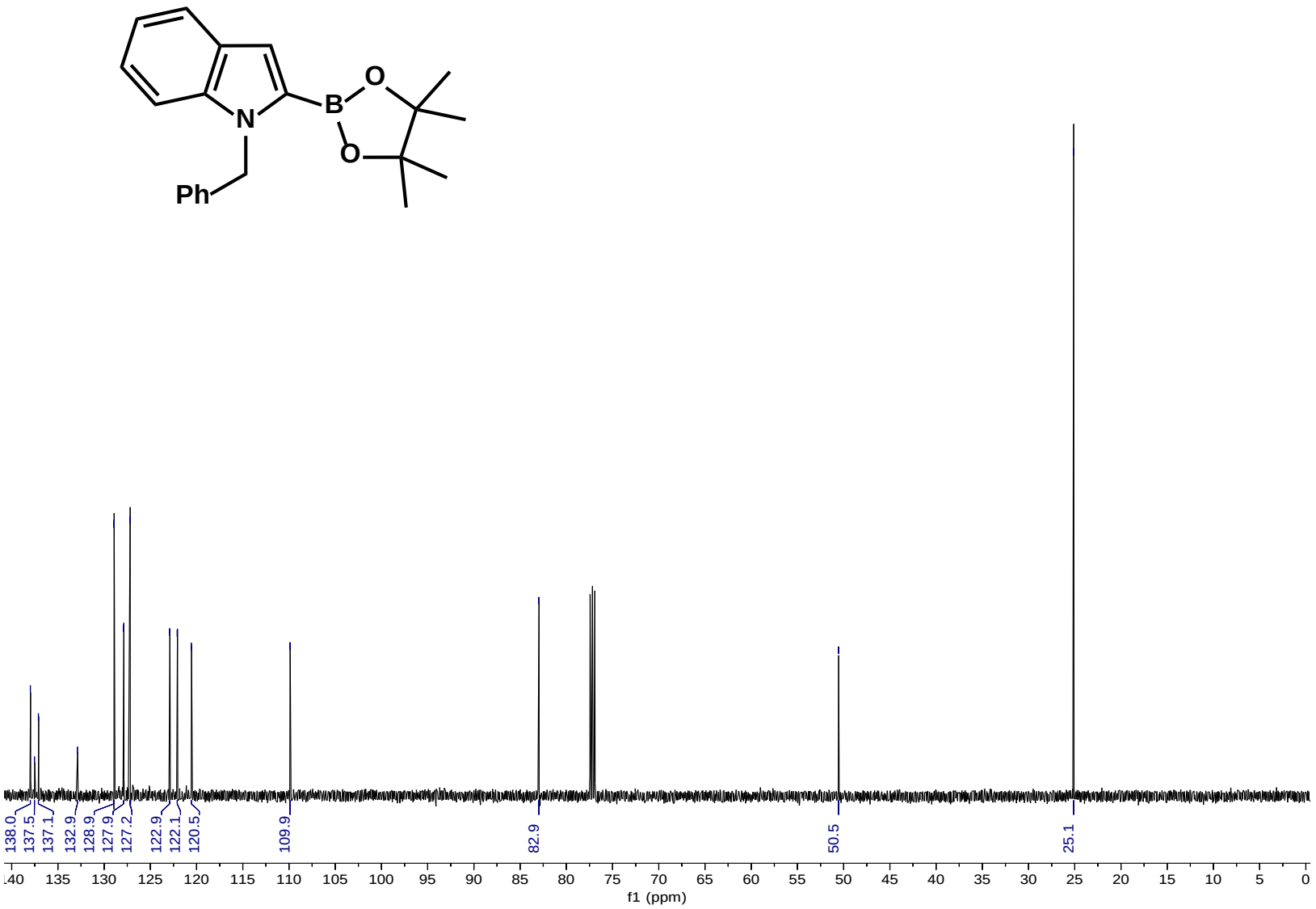
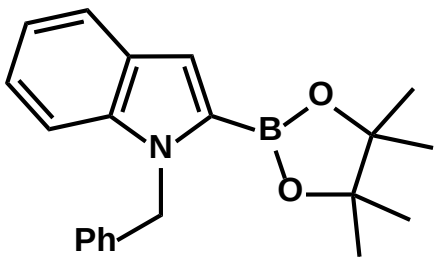



**Figure S37:** $^{13}C\{^{1}H\}$ NMR (126 MHz, chloroform-*d*) of 1-benzyl-2-Bpin indole (**7d**)



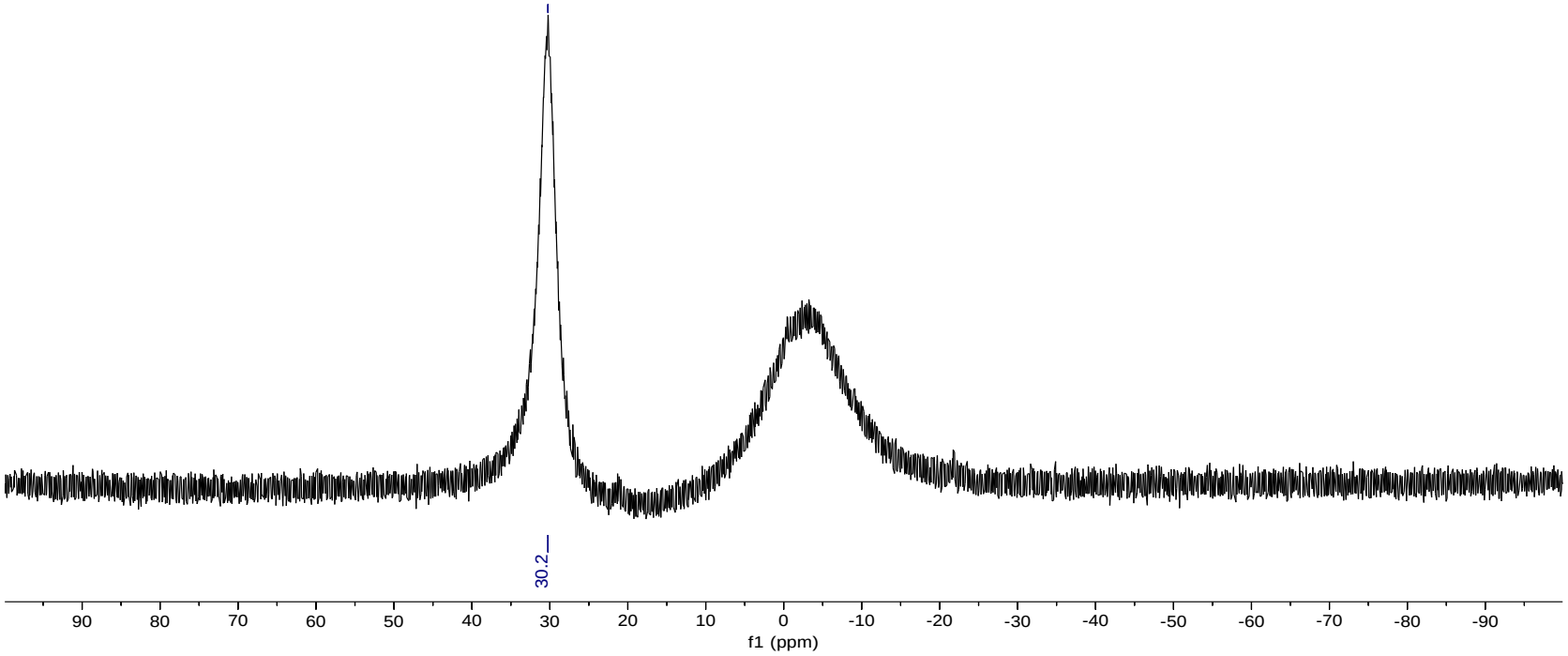
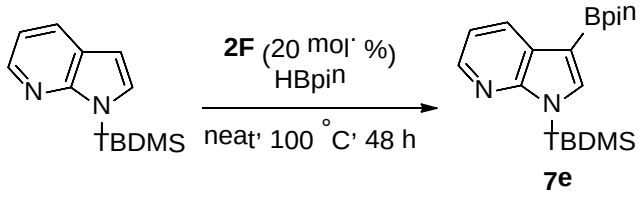




**Figure S38:** $^{11}B\{^{1}H\}$ NMR (160 MHz, chloroform-*d*) of 1-benzyl-2-Bpin indole (**7d**)

## Borylation of 1-TBDMS-7-azaindole




**7e**

Precatalyst **2F** (390 mg, 1.70 mmol) was introduced into a 100 mL oven-dried two-neck flask that is already connected to a condenser with a normal flow of nitrogen. Then 2.1 mL (8.51 mmol) of 1-(*tert*-butyldimethylsilyl)-7-azaindole followed by pinacolborane (3 equiv, 3.7 mL, 25.5 mmol) are added via syringe. The reaction mixture was then stirred at 100 °C for 48 hours in an oil bath. The resulting mixture was kept under reduced pressure for 30 min. A small flash chromatography with dry silica gel as stationary phase was performed to purify the product. Initially a 20:1 mix of petroleum ether/ethyl ether was used as eluent to eliminate the unreacted starting material, then the polarity of the eluent was increased by going to a 10:1 ratio to obtain the borylated product. After evaporation of the solvent to complete dryness under reduced pressure, the desired 1-TBDMS-2-Bpin-7-azaindole (**7e**) was obtained as a white solid. Yield: 1.89 g, 62%.

$^{1}$H NMR (500 MHz, chloroform-*d*): $\delta$ 8.27-8.32 (m, 2H), 7.74 (s, 1H), 7.11 (m, 1H), 1.39 (s, 12H), 0.98 (s, 9H), 0.68 (s, 6H).

$^{13}$C{$^{1}$H} NMR (126 MHz, chloroform-*d*): $\delta$ 155.3, 142.6, 140.7, 129.8, 126.2, 116.6, 82.9, 26.6, 24.9, 18.9, -4.2.

$^{11}$B {$^{1}$H} NMR (160 MHz, chloroform-*d*): $\delta$ 29.9 (br s).

HRMS (ESI-TOF) *m/z*: Calcd for $C_{19}H_{31}BN_2O_2Si$ + H: 359.2364; Found: 359.3906.

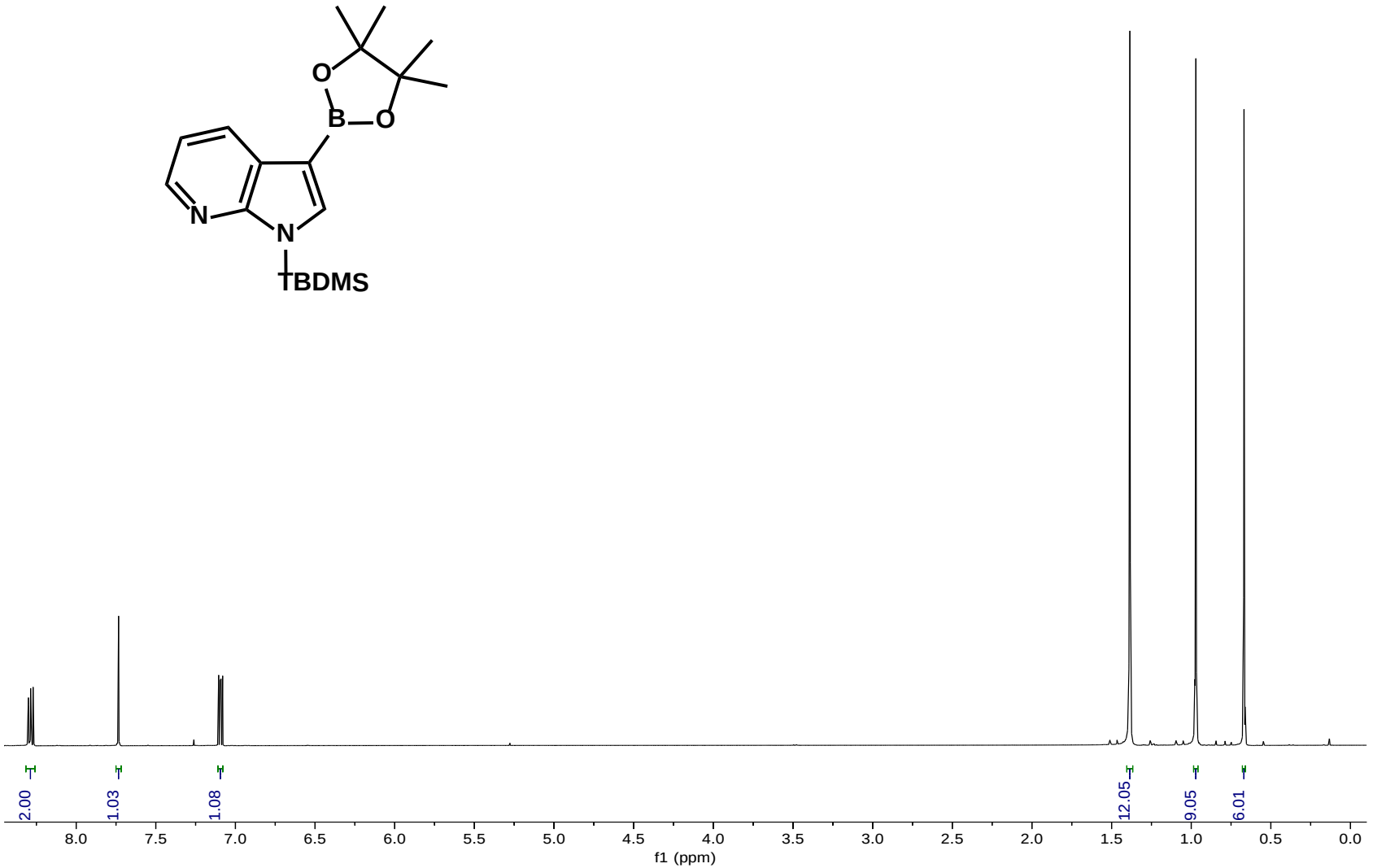



**Figure S39:** $^{1}$H NMR (500 MHz, chloroform-*d*) of 1-TBDMS-2-Bpin-7-azaindole (**7e**)

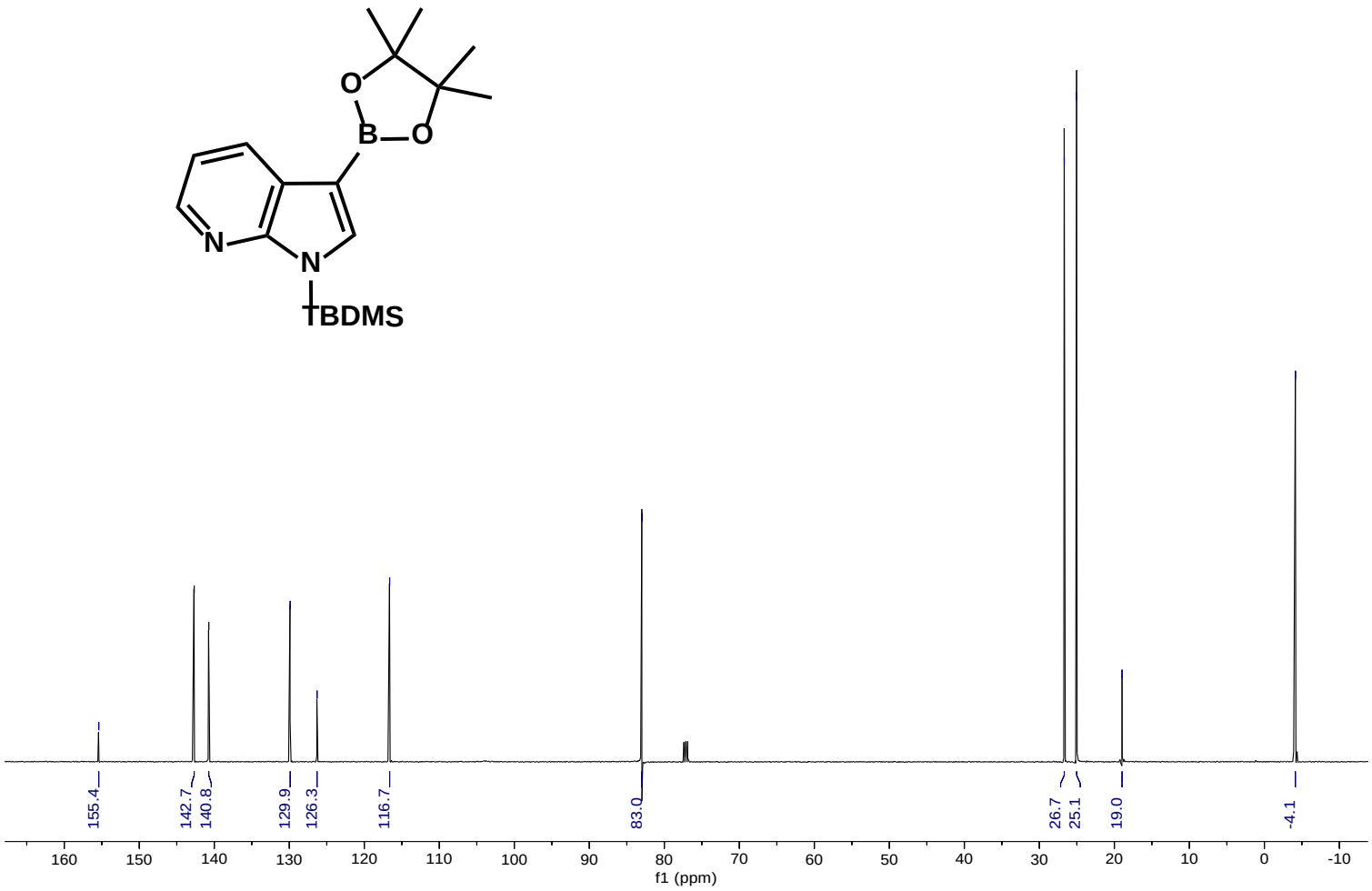



**Figure S40:** $^{13}C\{^{1}H\}$ NMR (126 MHz, chloroform-*d*) of 1-TBDMS-2-Bpin-7-azaindole (**7e**)

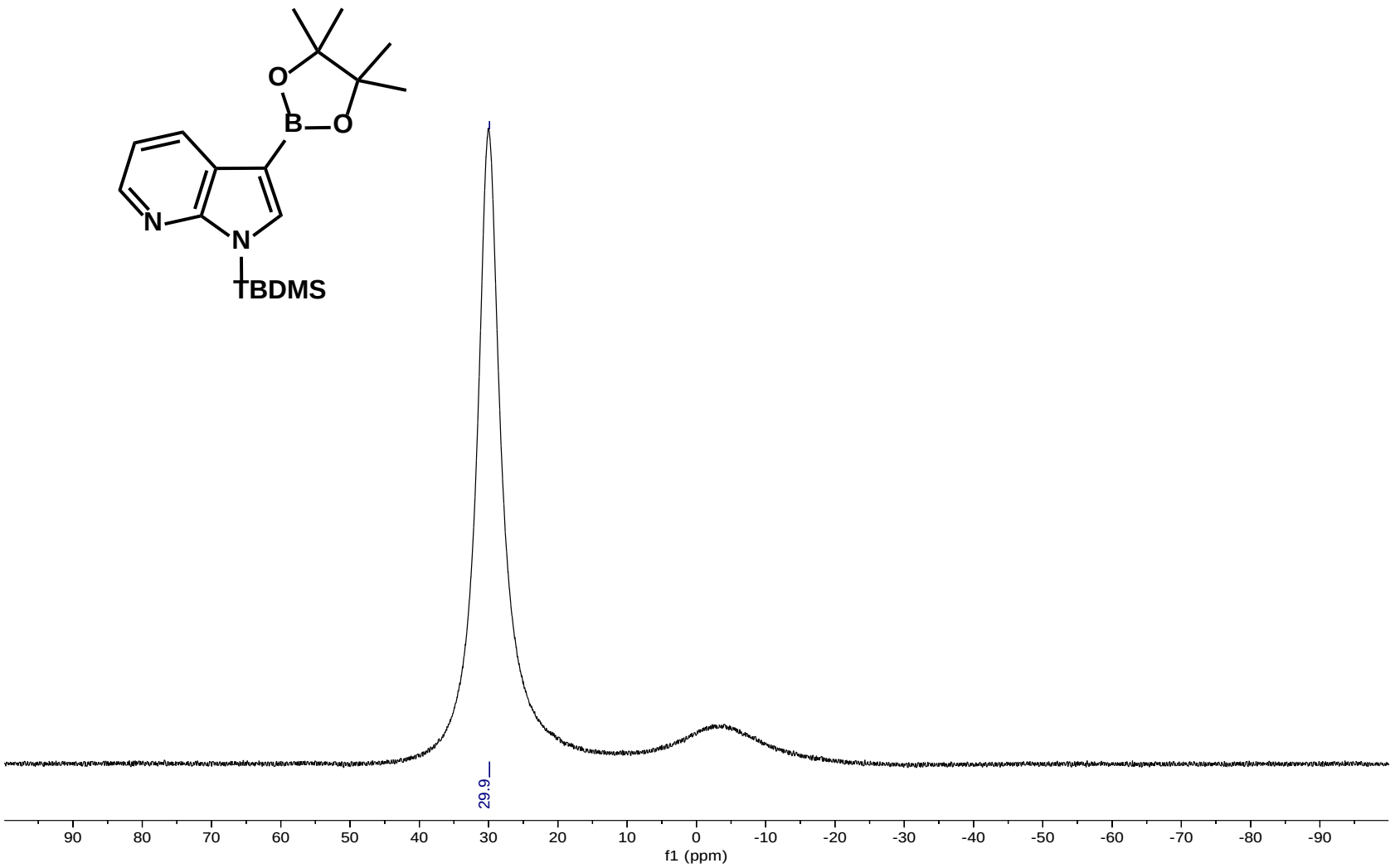
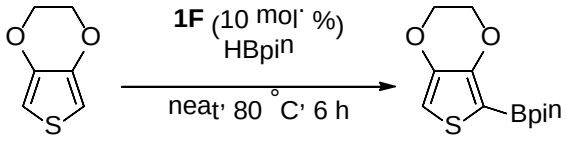



**Figure S41:** $^{11}B\{^{1}H\}$ NMR (160 MHz, chloroform-*d*) of 1-TBDMS-2-Bpin-7-azaindole (**7e**)

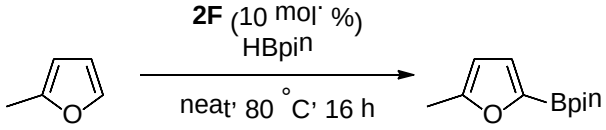
## Borylation of EDOT




**7f**

Precatalyst **1F** (260 mg, 0.9 mmol) was introduced into an oven-dried two-neck flask (100 mL) that already has a stirring bar and connected to a condenser with a normal nitrogen flow. Then, 1.5 mL of EDOT (13.5 mmol), distilled before use, followed by HBpin containing 1% $Et_3N$ stabilizer (0.87 equiv, 1.7 mL) were added via syringe. The reaction mixture was then stirred for 6 hours at 80 °C. The $^1H$ NMR of the crude solution showed the complete disappearance of HBPin (limiting reagent). The resulting mixture was kept under reduced pressure for 30 min. Subsequently, a small flash chromatography with silica gel as stationary phase was performed to purify the product. A mixture of petroleum ether/ethyl ether 20:1 was used as eluent to eliminate the excess of EDOT, and then the polarity of the eluent was increased by going to a 2:1 ratio to obtain the borylated product. After evaporation of the solvent to complete dryness under reduced pressure, 2.05 g (85% with respect to 9 mmol of HBpin available after consumption of 2.7 mmol of HBpin for the generation of active borohydride catalyst) of the desired 2-Bpin-EDOT (**7f**) was obtained as a white solid. The obtained product was analytically similar to the one reported previously.[2,3]

## Borylation of 2-methylfuran




**7g**

Precatalyst **2F** (305 mg, 1.33 mmol) was introduced into a 100 mL oven-dried two-neck flask that is already connected to a condenser with a normal nitrogen flow. Then, 1.95 mL (21.6 mmol) of 2-methylfuran (distilled before use) followed by HBpin containing 1% $Et_3N$ stabilizer (0.8 equiv, 2.5 mL) were added via syringe. The reaction mixture was then stirred at 80 °C for 16 hours in an oil bath. The resulting mixture was kept under reduced pressure for 30 min. The $^1H$ NMR spectrum of the crude solution showed 96% conversion. A small flash chromatography with dry silica gel as stationary phase and a mixture of petroleum ether/ethyl ether (20:1) was used to purify the product. Note that an UV undetectable compound that closely follows the desired product was detected by phosphomolybdic acid stain. After evaporation of the solvent to complete dryness under reduced pressure, the desired 2-Bpin-5-methyl furan (**7g**) was obtained as colorless oil. Yield: 2.13 g, 77%. The spectroscopic data obtained match the previously published data.[2,3]

# Kinetic experiments

## C-H activation

For each experiment, a quartz NMR tube containing the solution (catalysts and either 1-methylpyrrole or thiophene) with an internal capillary containing HBpin was left inside the NMR spectrometer at the selected temperature and $^{11}B\{^{1}H\}$ NMR spectra were collected every 4, 8 or 30 minutes. One $^{11}B$ resonance of the dimer (20.0 ppm for **1** and -7.7 ppm for **2**) was monitored during each experiment and its integration was normalized according to the resonance of HBpin (28 ppm). We used the same protocol for **1** and **2**.

In the first set of experiments, 31 µmol of the dimer was dissolved in 0.4 mL of chloroform-*d*, the substrate (310, 620 and 1240 µmol) was added. An NMR insert tube containing a solution of 34 µM of HBpin in 0.4 mL of chloroform-*d* was introduced inside the NMR tube as an external standard.

For the second set of experiments, a certain amount (15.5, 31 and 62 µmol) of the dimer was dissolved in 0.4 mL of chloroform-*d*, followed by 620 µmol of the substrate. An NMR insert tube containing a solution of 34 µM of HBpin in 0.4 mL of chloroform-*d* was introduced inside the NMR tube as an external standard.

The experiments with N-methylpyrrole and thiophene were done at 40 and 60 °C, respectively.

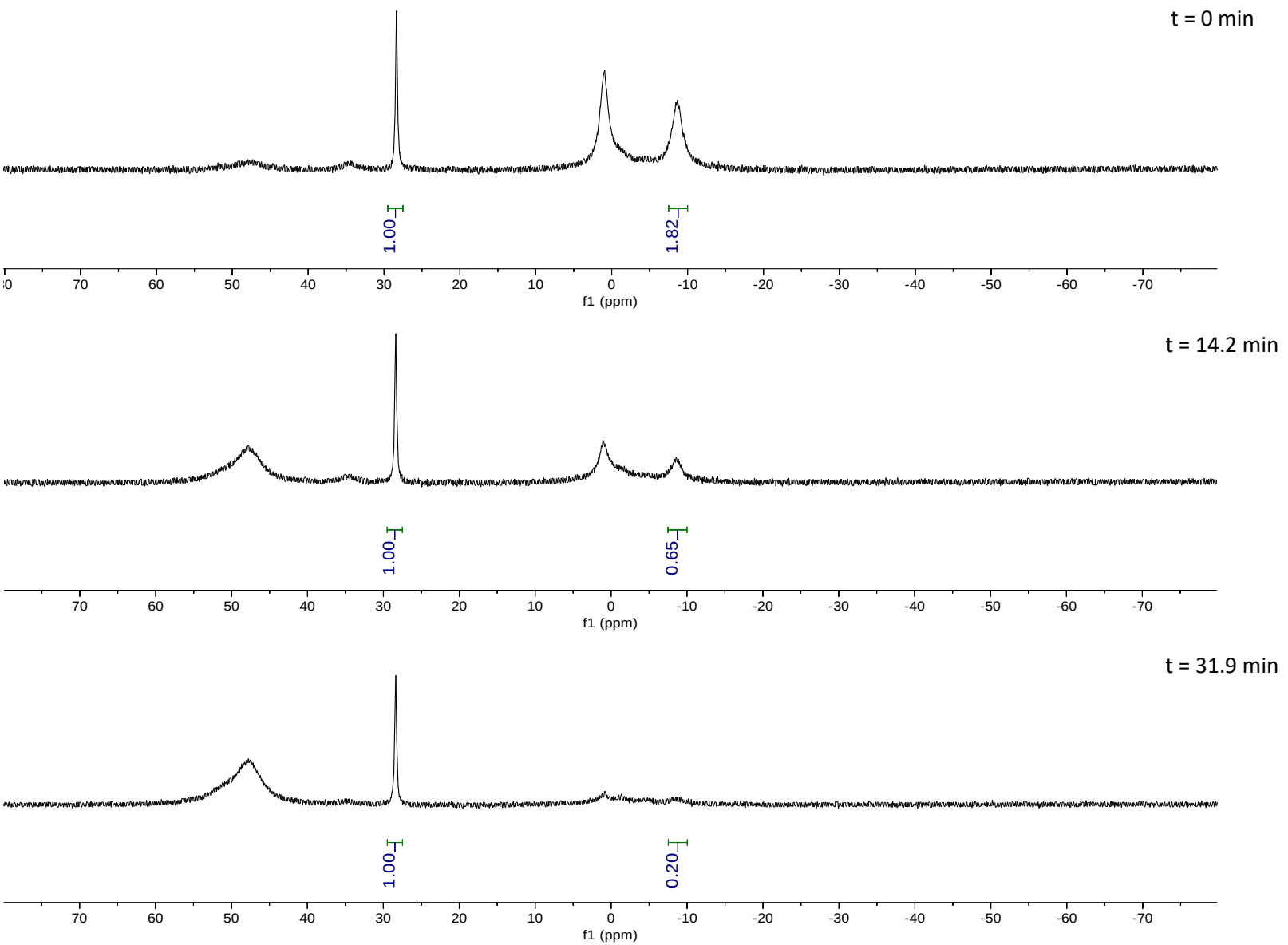



**Figure S42:** $^{11}B\{^{1}H\}$ NMR (160 MHz, chloroform-*d*) of 77.5 µM (1-piperidyl-2-$BH_2$-$C_6H_4$)$_2$ (**2**) and 1550 µM *N*-methylpyrrole at 40 °C

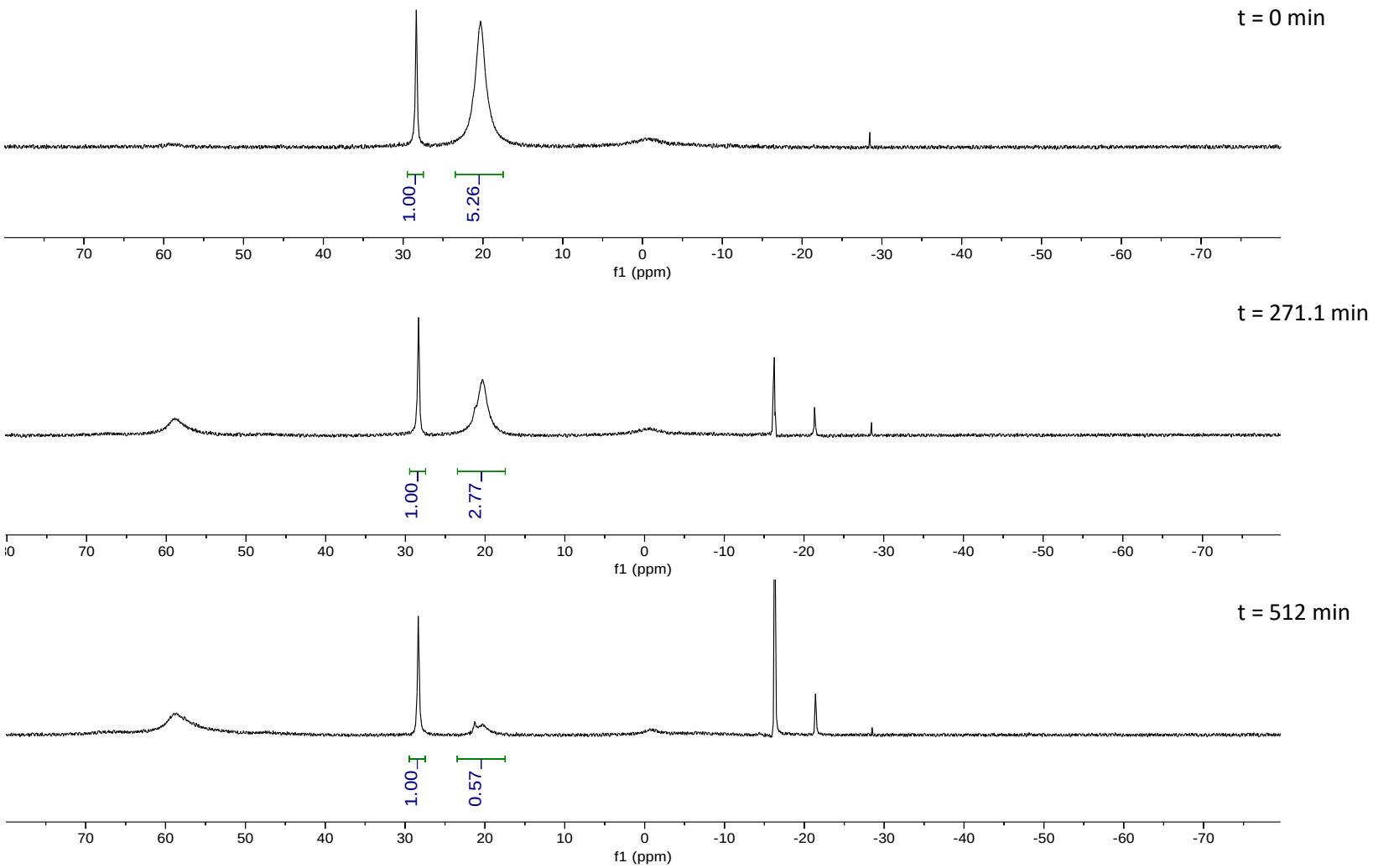



**Figure S43:** $^{11}B\{^{1}H\}$ NMR (160 MHz, chloroform-*d*) of 77.5 µM (1-tetramethylpiperidyl-2-$BH_2$-$C_6H_4$)$_2$ (**1**) and 1550 µM thiophene at 60 °C.

## Comparison of catalytic activity between 1-4.

In a glovebox, 7.75 µmol of the dimer was dissolved in 0.4 mL of chloroform-*d* solution containing 4 mg (24.7µmol) of hexamethylbenzene for 10 mL of chloroform-*d* and transferred in a J-Young NMR tube. Then, 27.5 µL (310 µmol) of N-methylpyrrole and 45.0 µL (310 µmol) of pinacolborane were added. For each experiment, the J-Young NMR tube was left inside the NMR probe at 60 °C and a spectrum was taken every 2, 5 or 15 minutes. The signal at 3.7 ppm for the $CH_3$ of *N*-methylpyrrole was followed during the course of these experiments. The integration of the methyl group was normalized with the signal of hexamethylbenzene (2.3 ppm).

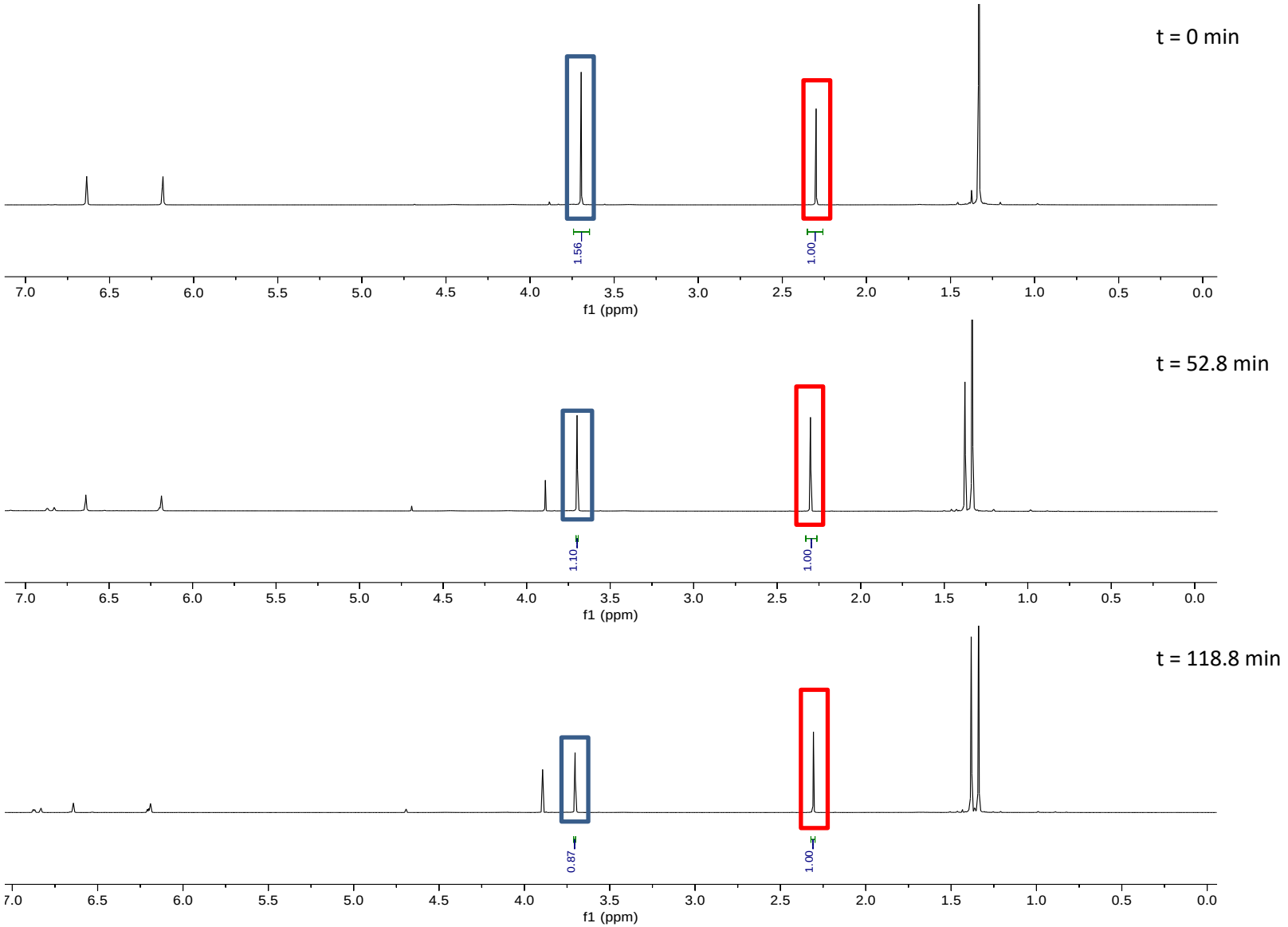



**Figure S44:** $^{1}$H NMR (500 MHz, chloroform-*d*) of the borylation catalysis of *N*-methylpyrrole with (1-tetramethylpiperidyl-2-$BH_2$-$C_6H_4$)$_2$ (**1**) as a catalyst at 60 °C

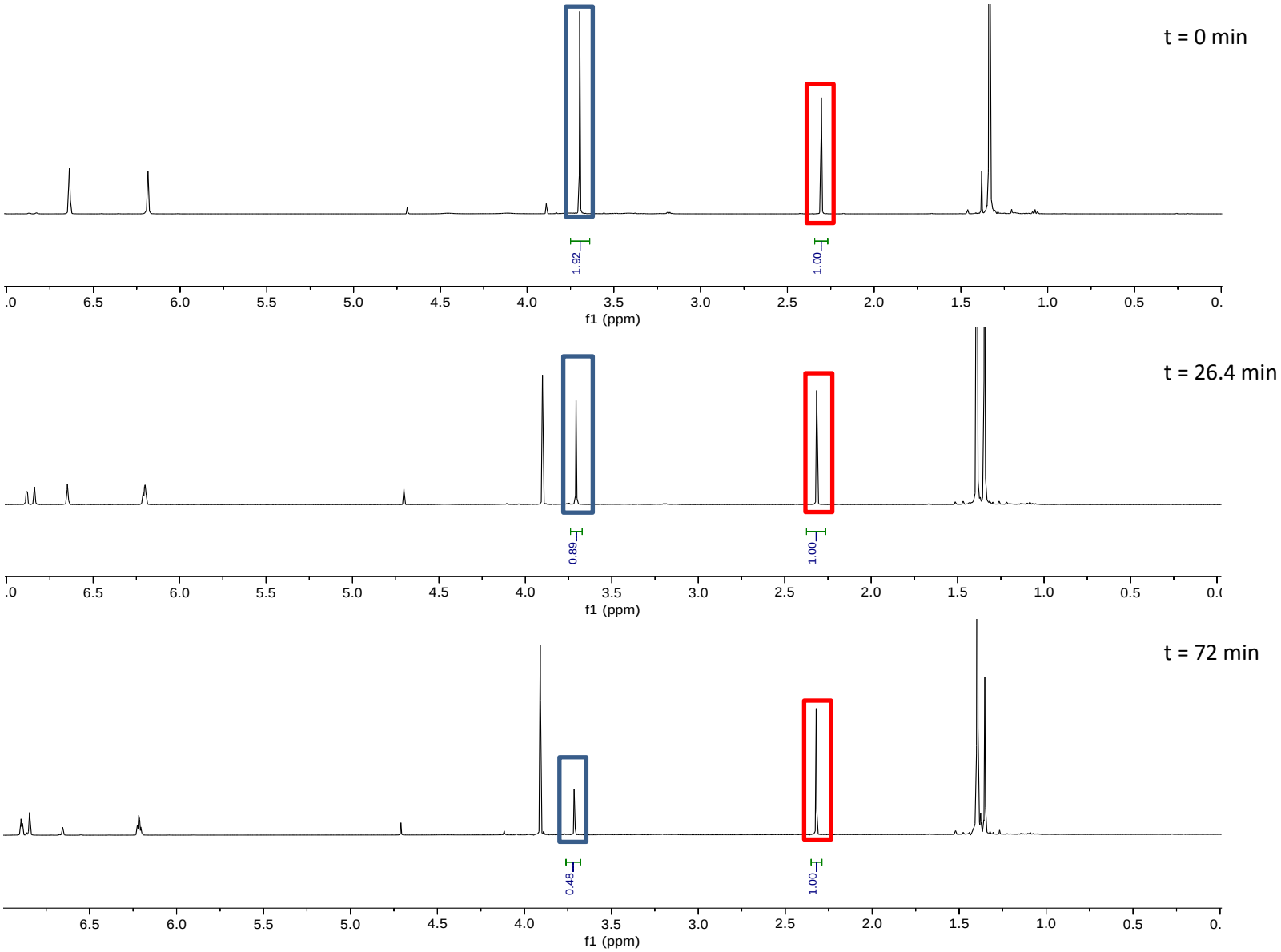



**Figure S45:** $^{1}$H NMR (500 MHz, chloroform-*d*) of the borylation catalysis of *N*-methylpyrrole with (1-diethyl-2-$BH_2$-$C_6H_4$)$_2$ (**3**) as a catalyst at 60 °C

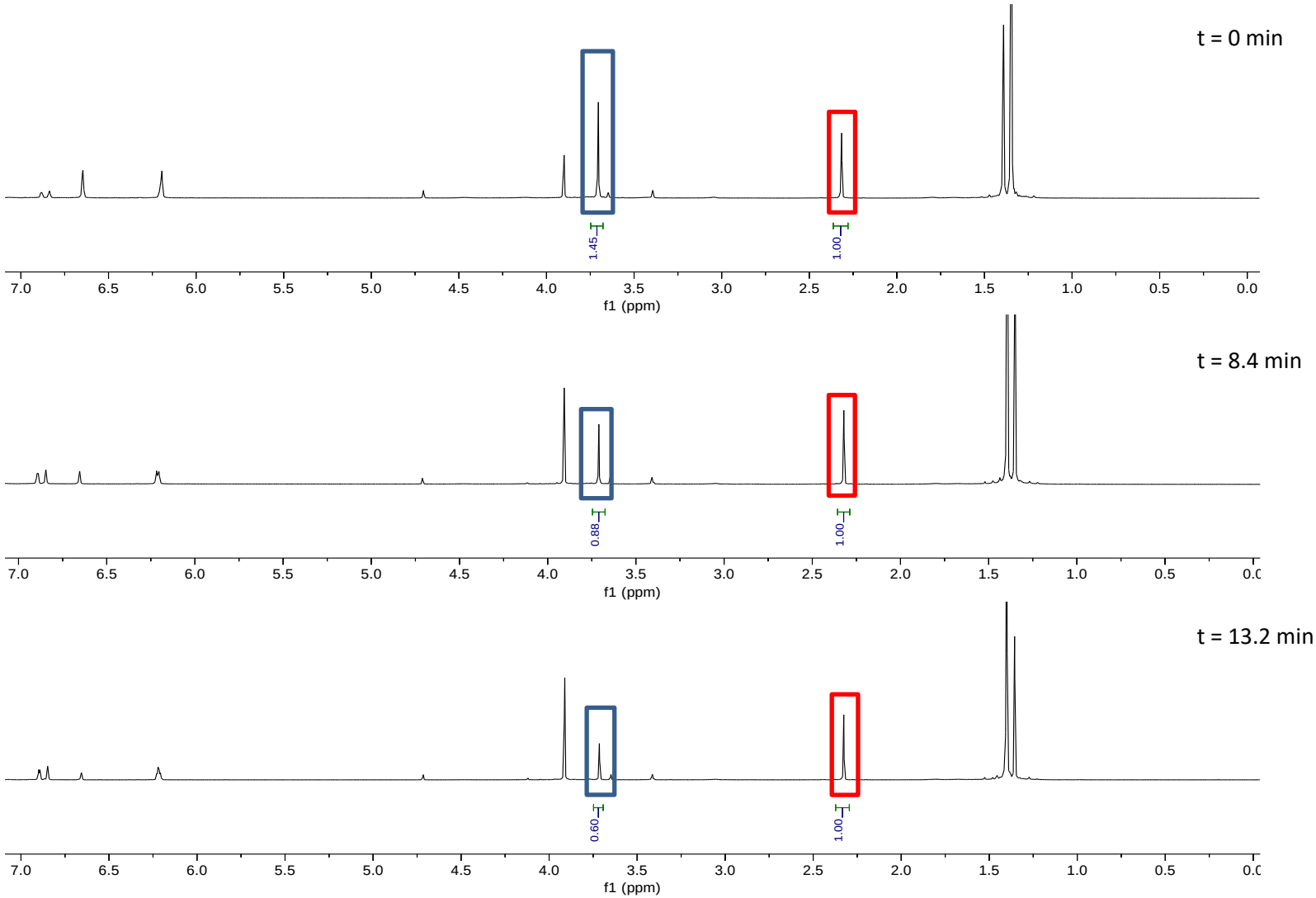



**Figure S46:** $^{1}$H NMR (500 MHz, chloroform-*d*) of the borylation catalysis of *N*-methylpyrrole with (1-piperidyl-2-$BH_2$-$C_6H_4$)$_2$ (**2**) as a catalyst at 60 °C

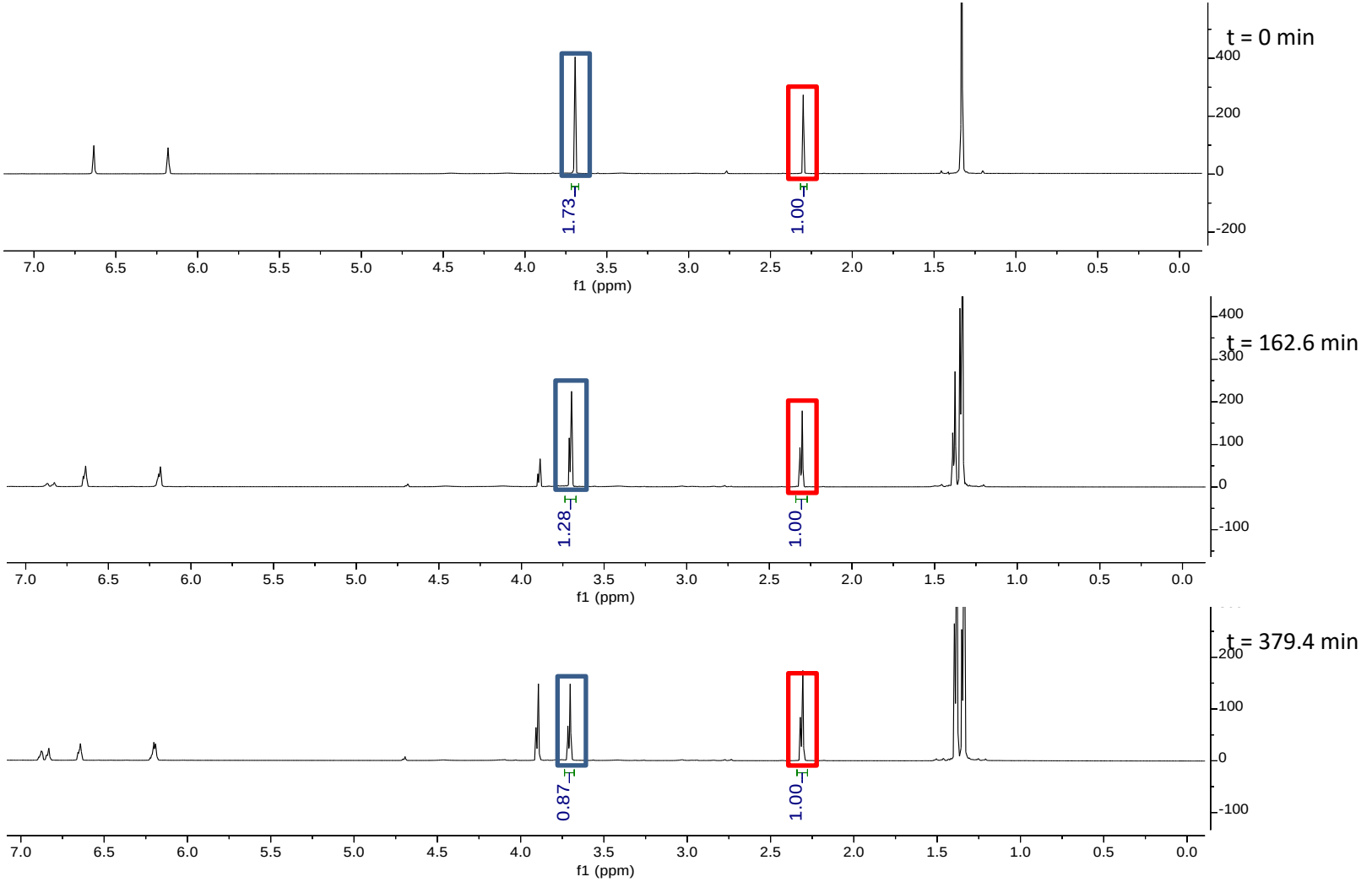



**Figure S47:** $^{1}$H NMR (500 MHz, chloroform-*d*) of the borylation catalysis of *N*-methylpyrrole with (1-dimethyl-2-$BH_2$-$C_6H_4$)$_2$ (**4**) as a catalyst at 60 °C

## Spin saturation transfer difference experiments for (2)

Spin saturation transfer experiments were used to determine the energy required to break the dimeric structure of **2** to generate the FLP opened form. The experiments was done according to the experience developed by Muñoz and al.[5]

In a glovebox apparatus, 7 mg of **2** was dissolved in 0.4 mL of chloroform-*d* in a J-Young NMR tube.

A standard 1D STD NMR pulse sequence provided by the manufacturer (Agilent Technologies) was used for the experiments. They were carried out on a Agilent Technologies NMR spectrometer (500 MHz). On-resonance frequency was selected at 7.565 ppm (one aromatic resonance on one monomeric subunit $\delta_1$), which affected a resonance at 6.866 ppm (equivalent proton on the second subunit $\delta_2$). The off-resonance frequency was set to 38 ppm. For all the SSTD NMR experiments the spectral width was between 6.0 and 8.0 ppm. Integration for signals was carried out using Mnova 11.0.4.

The difference in the integration of $\delta_2$ with and without saturation divided by the integration of $\delta_1$ without saturation ($\eta_{\mathrm{SSTD}} = \frac{\int \delta_2 - \int \delta_2^*}{\int \delta_1}$) were obtained for different saturation time (t). Plotting these values versus the saturation time (t) gave an exponential curve where a plateau was reached for longer saturation times. The exponential fit allowed us to obtain the rate constants (k) for breaking the dimer at different temperatures (**a.** to **e.**). It was also possible to calculate the longitudinal relaxation time constant ($T_{1A}$).

$$\eta_{SSTD}(\mathrm{t}) = \frac{k}{(1/T_{1A} + k)}(1 - \exp(-(1/T_{1A} + k) \cdot t))$$

$$\eta_{SSTD}(\mathrm{t}) = \mathrm{a}(1 - \exp(-b \cdot t))$$

$$a = \frac{k}{(1/T_{1A} + k)}$$

$$b = \frac{1}{T_{1A}} + k$$

$$k = a \cdot b$$

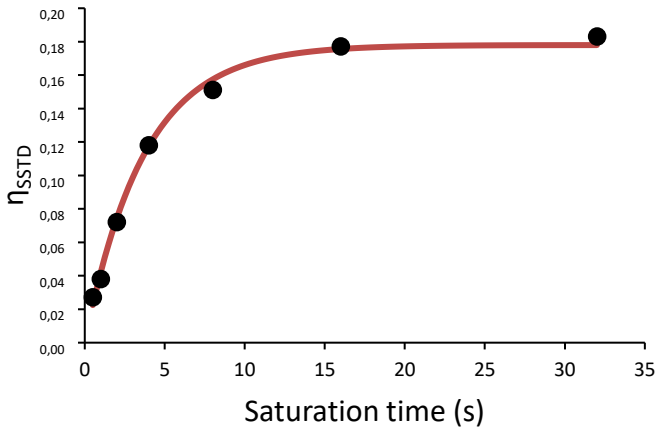
$$T_{1A} = \frac{1}{b - k}$$

**a.** (i) Values of $\eta_{SSTD}$ obtained at different saturation times for (1-piperidyl-2-$BH_2$-$C_6H_4$)$_2$ **2** at 324.15 K. (ii) Plot of $\eta_{SSTD}$ versus saturation times with the exponential fit. (iii) Values of the rate constant (*k*) and relaxation times ($T_{1A}$).

(i)

| $T_{sat}$ (s) | $\eta_{SSTD}$ |
|---|---|
| 32 | 0.183 |
| 16 | 0.177 |
| 8 | 0.151 |
| 4 | 0.118 |
| 2 | 0.072 |
| 1 | 0.038 |
| 0.5 | 0.027 |

(ii)




(iii)

$k$ = 0.048 ± 0.004 $s^{-1}$

$T_{1A}$ = 4.5 ± 0.3 s

$\eta_{SSTD}$ = a (1-exp(-b·t))

a = 0.178 ± 0.009

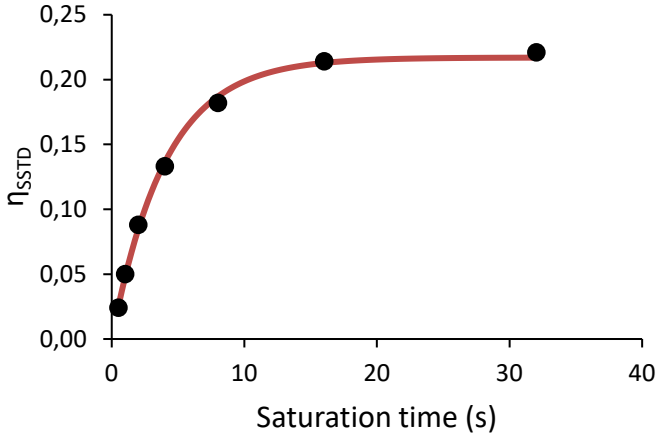
b = 0.27 ± 0.01

**b.** (i) Values of $\eta_{SSTD}$ obtained at different saturation times for (1-piperidyl-2-$BH_2$-$C_6H_4$)$_2$ **2** at 327.15 K. (ii) Plot of $\eta_{SSTD}$ versus saturation times with the exponential fit. (iii) Values of the rate constant (*k*) and relaxation times ($T_{1A}$).

(i)

| $T_{sat}$ (s) | $\eta_{SSTD}$ |
|---|---|
| 32 | 0.221 |
| 16 | 0.214 |
| 8 | 0.182 |
| 4 | 0.133 |
| 2 | 0.088 |
| 1 | 0.050 |
| 0.5 | 0.024 |

(ii)




(iii)

$k$ = 0.054 ± 0.002 $s^{-1}$

$T_{1A}$ = 5.2 ± 0.2 s

$\eta_{SSTD}$ = a (1-exp(-b·t))

a = 0.217 ± 0.005

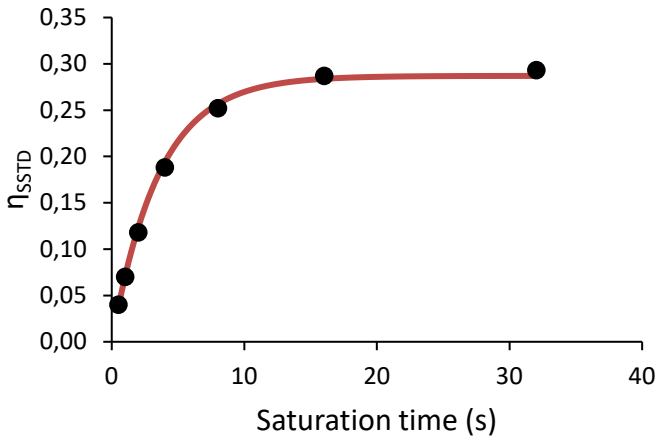
b = 0.247 ± 0.004

**c.** (i) Values of $\eta_{SSTD}$ obtained at different saturation times for (1-piperidyl-2-$BH_2$-$C_6H_4$)$_2$ **2** at 330.15 K. (ii) Plot of $\eta_{SSTD}$ versus saturation times with the exponential fit. (iii) Values of the rate constant (*k*) and relaxation times ($T_{1A}$).

(i)

| $T_{sat}$ (s) | $\eta_{SSTD}$ |
|---|---|
| 32 | 0.293 |
| 16 | 0.287 |
| 8 | 0.252 |
| 4 | 0.188 |
| 2 | 0.118 |
| 1 | 0.070 |
| 0.5 | 0.040 |

(ii)




(iii)

$k$ = 0.081 ± 0.003 $s^{-1}$

$T_{1A}$ = 5.0 ± 0.2 s

$\eta_{SSTD}$ = a (1-exp(-b·t))

a = 0.287 ± 0.007

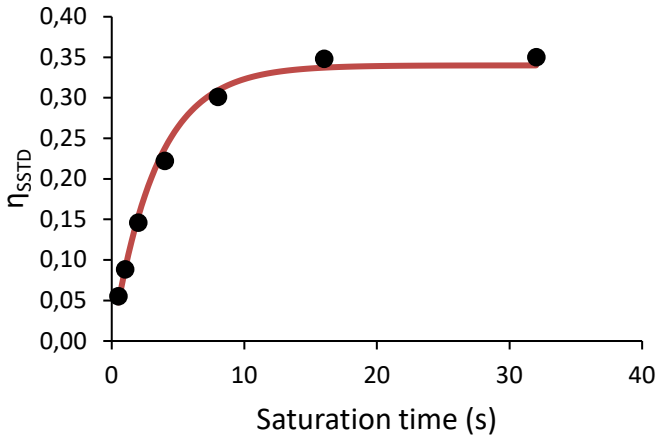
b = 0.281 ± 0.004

**d.** (i) Values of $\eta_{SSTD}$ obtained at different saturation times for (1-piperidyl-2-$BH_2$-$C_6H_4$)$_2$ **2** at 333.15 K. (ii) Plot of $\eta_{SSTD}$ versus saturation times with the exponential fit. (iii) Values of the rate constant (*k*) and relaxation times ($T_{1A}$).

(i)

| $T_{sat}$ (s) | $\eta_{SSTD}$ |
|---|---|
| 32 | 0.350 |
| 16 | 0.348 |
| 8 | 0.301 |
| 4 | 0.222 |
| 2 | 0.146 |
| 1 | 0.088 |
| 0.5 | 0.055 |

(ii)




(iii)

$k$ = 0.102 ± 0.009 $s^{-1}$

$T_{1A}$ = 4.9 ± 0.5 s

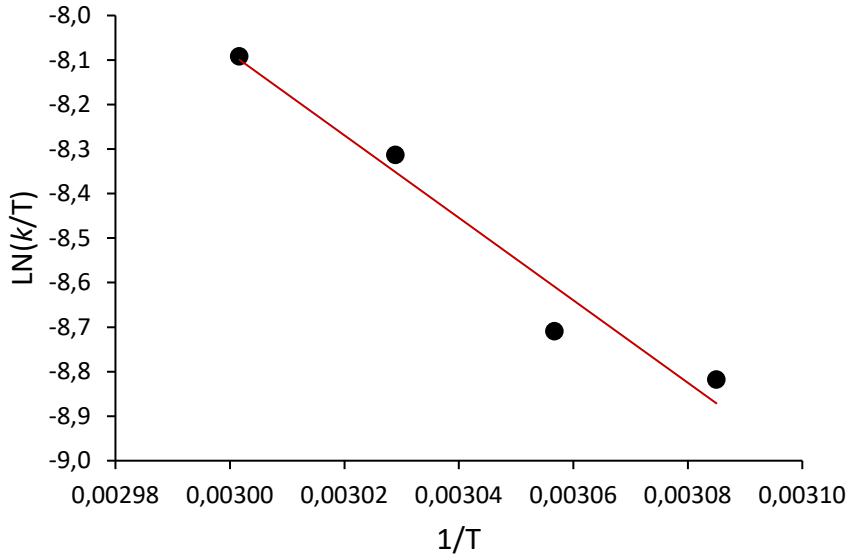
$\eta_{SSTD}$ = a (1-exp(-b·t))

a = 0.34 ± 0.02

b = 0.30 ± 0.01

**e.** Eyring plot for (1-piperidyl-2-$BH_2$-$C_6H_4$)$_2$ **2.** Slope and intercept values were used to calculate the enthalpy and entropy of activation, respectively.

| T (K) | $k$ ($s^{-1}$) | Ln($k$/T) | 1/T |
|---|---|---|---|
| 324.15 | 0.048 | -8.81776 | 0.00308 |
| 327.15 | 0.054 | -8.70919 | 0.00306 |
| 330.15 | 0.081 | -8.31285 | 0.00303 |
| 333.15 | 0.102 | -8.0913753 | 0.00300 |




Y = A + B * X  A = -9262 ± 1368  B = 19.71 ± 4.16  R = 0.9582

$$ln\left(\frac{k}{T}\right) = ln\left(\frac{k_B}{h}\right) - \frac{\Delta H^{\ddagger}}{RT} + \frac{\Delta S^{\ddagger}}{R}$$

$$\Delta S^{\ddagger} = -30 \pm 6\ Jmol^{-1}K^{-1}$$

$$\Delta H^{\ddagger} = 77 \pm 11\ kJmol^{-1}K^{-1}$$

$$E_{A(298)} = \Delta H^{\ddagger} + RT = 79 \pm 11\ kJmol^{-1}K^{-1}$$

$$\Delta G^{\ddagger}_{(298)} = \Delta H^{\ddagger} - T\Delta S^{\ddagger} = 86 \pm 13\ kJmol^{-1}K^{-1} = 20.5 \pm 3.1\ kcalmol^{-1}K^{-1}$$

## Kinetic simulations

Kinetics simulations were performed using the free simulation software ReactLab Kinsim (http://jplusconsulting.com/products/reactlab-kinsim/). The kinetics experiments of the C-H process

were simulated using the rate constants ($k_{ass}$ and $k_{diss}$) of the reactions involved and the same concentrations used experimentally. The free energies obtained by DFT and the temperature were inserted in the following Eyring equation.

$$k = \frac{k_B}{hT} \times e^{-\Delta G/RT}$$

Constants: $k_B$: Boltzmann constant, h: Planck constant, R: Gas constant

Variables: ΔG: Energy barrier, T: temperature

The rate constants were calculated for all the reactions present in the C-H activation process (1-6) for 1-methylpyrrole and thiophene. The kinetic simulations were done with those rate constants for each combination of the concentrations of the dimer and the substrate (ex: 38.8 µM and 775 µM, 38.8 µM and 1550 µM and so on) in order to compare with our experiments.

**Table S1**: Rate constants calculated for 1-methylpyrrole with **1** and **2** at 40 °C

| Reaction number | **1** | | **2** | |
|---|---|---|---|---|
| | Free energy barrier (kcal $mol^{-1}$) | k ($s^{-1}$) | Free energy barrier (kcal $mol^{-1}$) | k ($s^{-1}$) |
| 1 | 14 | 1094.5 | 20.7 | 0.02 |
| 2 | 6.9 | 99224209.2 | 11.1 | 115896.91 |
| 3 | 17.4 | 4.6 | 8.8 | 4677241.43 |
| 4 | 20.2 | 0.1 | 10.4 | 357132.59 |
| 5 | 14 | 1094.5 | 15.5 | 98.15 |
| 6 | 17 | 8.8 | 20 | 0.07 |

**Table S2**: Rate constants calculated for thiophene with **1** and **2** at 60 °C

| Reaction number | **1** | | **2** | |
|---|---|---|---|---|
| | Free energy barrier (kcal $mol^{-1}$) | k ($s^{-1}$) | Free energy barrier (kcal $mol^{-1}$) | k ($s^{-1}$) |
| 1 | 14 | 4500.02533 | 20.7 | 0.2 |
| 2 | 6.9 | 205528534.13805 | 11.1 | 360126.6 |
| 3 | 20.6 | 0.20975 | 15.2 | 734.0 |
| 4 | 26.5 | 0.00003 | 18.9 | 2.7 |
| 5 | 17 | 48.34435 | 15.4 | 542.5 |
| 6 | 16.6 | 88.48336 | 19.5 | 1.1 |

**Table S3**: Concentrations applied for the simulations

| Concentration | Dimer (μM) | Substrate (μM) |
|---|---|---|
| 1 | 38.8 | 775 |
| 2 | 77.5 | 1550 |
| 3 | 155 | 3100 |

The reactions involved in the C-H activation process:

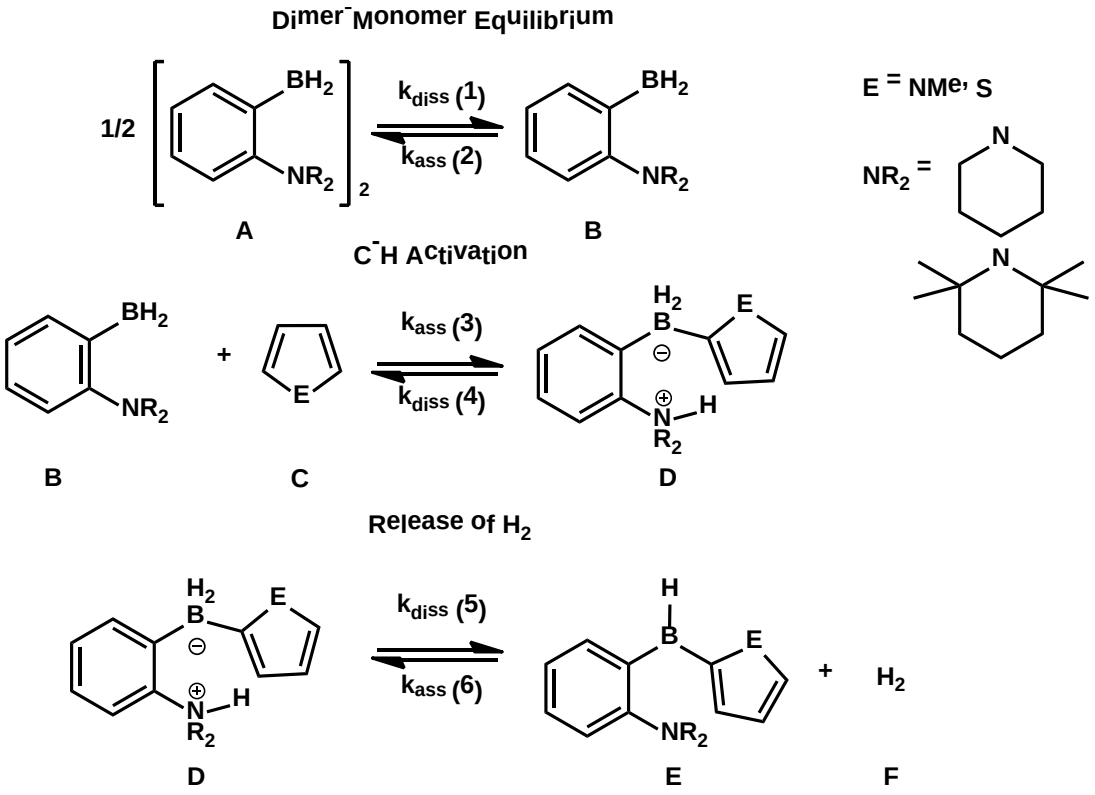
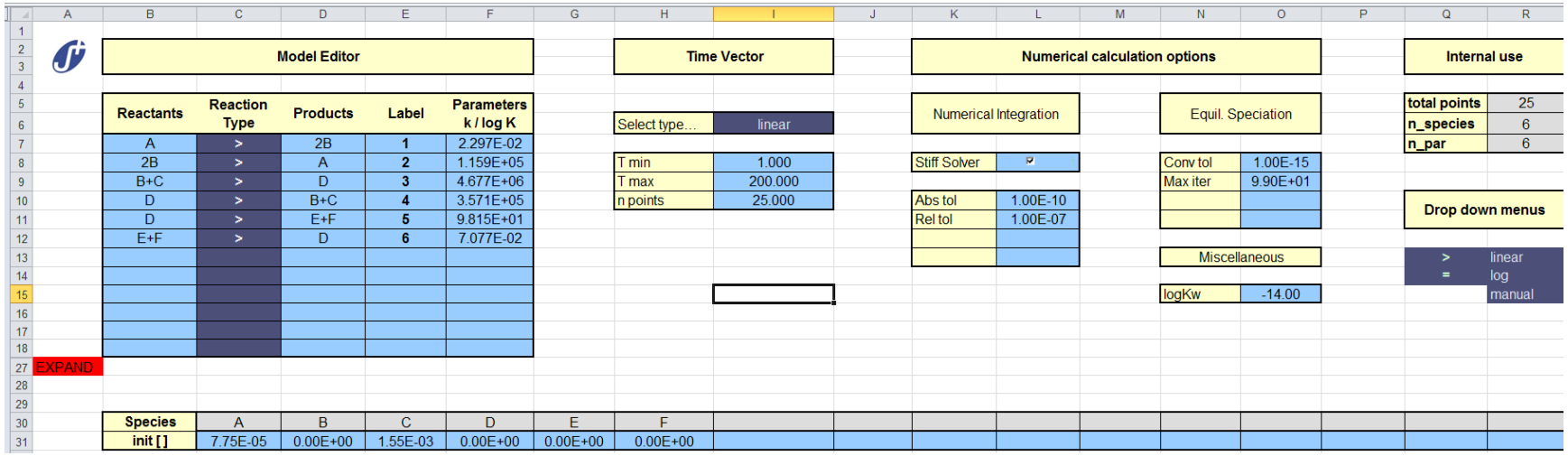



**Figure S48:** Reactions of the C-H activation process (1-6)



| Model Editor | | | | | |
|---|---|---|---|---|---|
| Reactants | Reaction Type | Products | Label | Parameters k / log K | |
| A | > | 2B | 1 | 2.297E-02 | |
| 2B | > | A | 2 | 1.159E+05 | |
| B+C | > | D | 3 | 4.677E+06 | |
| D | > | B+C | 4 | 3.571E+05 | |
| D | > | E+F | 5 | 9.815E+01 | |
| E+F | > | D | 6 | 7.077E-02 | |

EXPAND

| Time Vector | |
|---|---|
| Select type... | linear |
| T min | 1.000 |
| T max | 200.000 |
| n points | 25.000 |

| Numerical calculation options | | | | | |
|---|---|---|---|---|---|
| Numerical Integration | | Equil. Speciation | | | |
| Stiff Solver | ☑ | Conv tol | 1.00E-15 | | |
| Abs tol | 1.00E-10 | Max iter | 9.90E+01 | | |
| Rel tol | 1.00E-07 | | | | |
| | | Miscellaneous | | | |
| | | logKw | -14.00 | | |

| Internal use | |
|---|---|
| total points | 25 |
| n_species | 6 |
| n_par | 6 |

| Drop down menus | |
|---|---|
| > | linear |
| = | log |
| | manual |

| Species | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| init [ ] | 7.75E-05 | 0.00E+00 | 1.55E-03 | 0.00E+00 | 0.00E+00 | 0.00E+00 |

**Figure S49**: Example of an input file for the kinsim simulation of the reaction of **2** with 1-methylpyrrole; here with 77.5 µM of the dimer and 1550 µM of the substrate.

All simulations with 1-methylpyrrole were calculated at 40 °C and those with thiophene at 60 °C. For **1**, a transition state of 14 kcal $mol^{-1}$ for the breakage of the dimer was applied. The coefficient ($k_B$/hT) is the constant we choose to obtain an approximated simulation of the reactions. Therefore, all the reaction times shown in the kinetic simulations are not accurate predictions of what time it would really take to convert **1** and **2** since the pre-exponential factor (and the probability factor P) are not accounted for. Nonetheless, we assume that the simulations can depict the reaction trend at different concentrations of the dimer or the substrate.

## Computational details

All calculations were performed on the full structures of the reported compounds using the Gaussian 09 (Revision C.01) suite of programs.[6] The ωB97XD functional,[7] qualified as promising by Grimme[8] to describe the mechanism of FLP mediated hydrogenation of alkynes,[9] was used in combination with the 6-31+G** basis set for all atoms[10] All geometry optimizations were carried out without any symmetry constraints. The transition states were located and confirmed by frequency calculations (single imaginary frequency). Similarly, the stationary points were characterized as minima (no imaginary frequency). The energies were then refined by single point calculations to include solvent effect using the SMD solvation model[11] with the experimental solvent (chloroform) at the same level of theory.[12] All structures with their associated free enthalpy and Gibbs free energies as well as their Cartesian coordinates are fully detailed in the following section.

## Borylation mechanisms

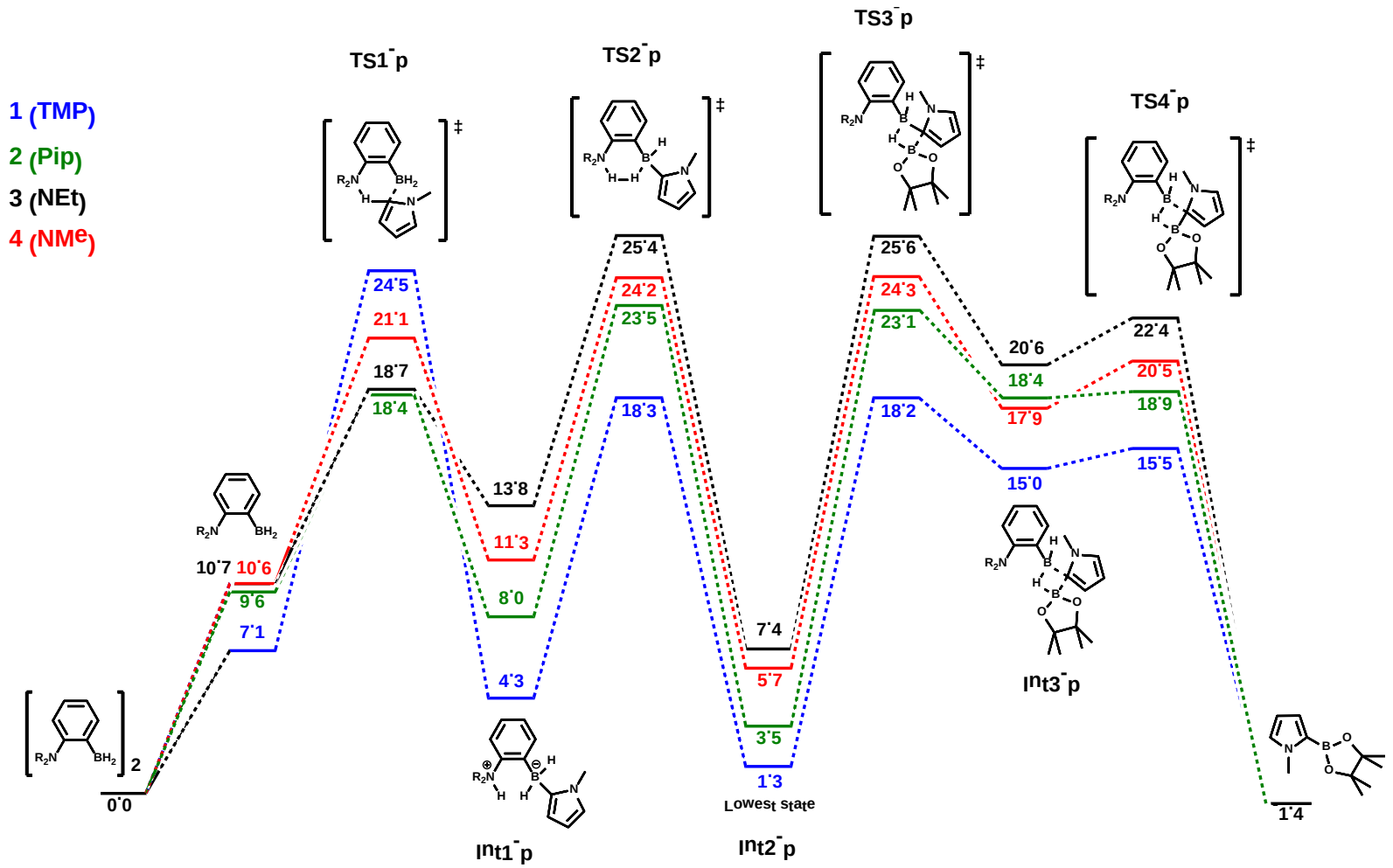



**Figure S50:** Free energies in kcal/mol of the borylation mechanism for N-methylpyrrole with different aminoboranes, calculated by DFT with theory level : ωB97XD/6-31+G** (SMD, chloroform).

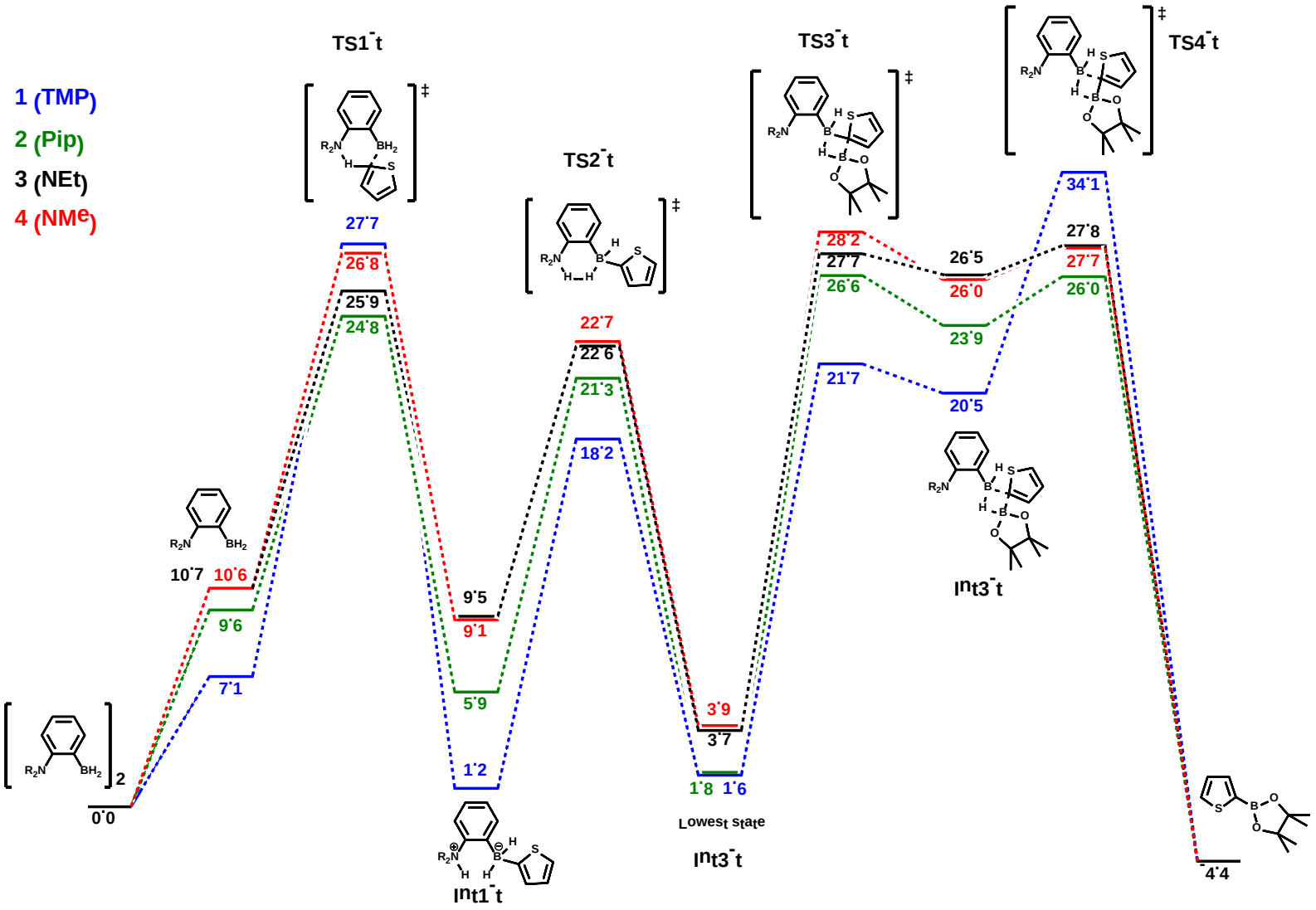



**Figure S51:** Free energies in kcal/mol of the borylation mechanism for thiophene with different aminoboranes, calculated by DFT with theory level : ωB97XD/6-31+G** (SMD, chloroform).

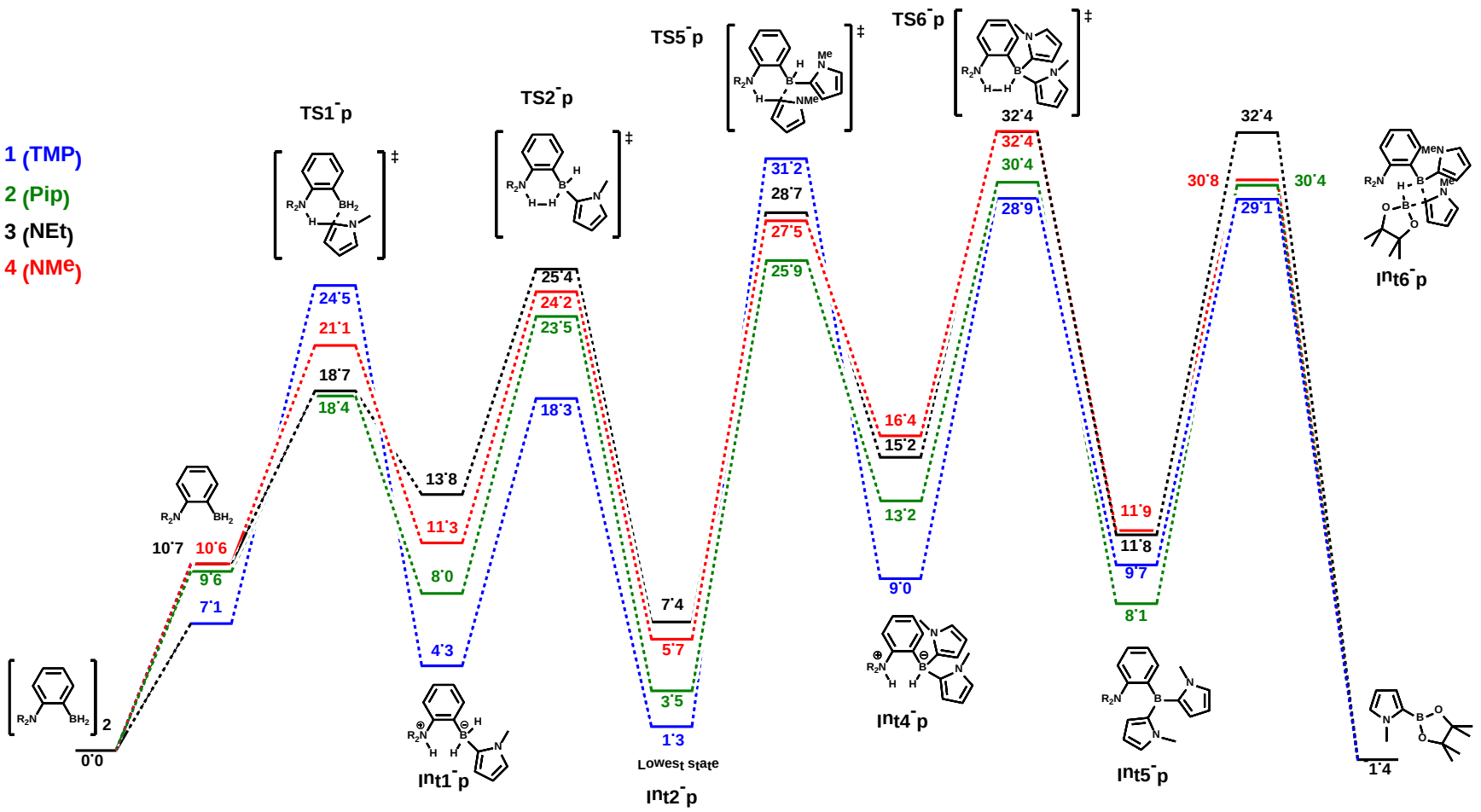



**Figure S52:** Free energies in kcal/mol of the borylation mechanism with a second activation of N-methylpyrrole with different aminoboranes, calculated by DFT with theory level : ωB97XD/6-31+G** (SMD, chloroform).

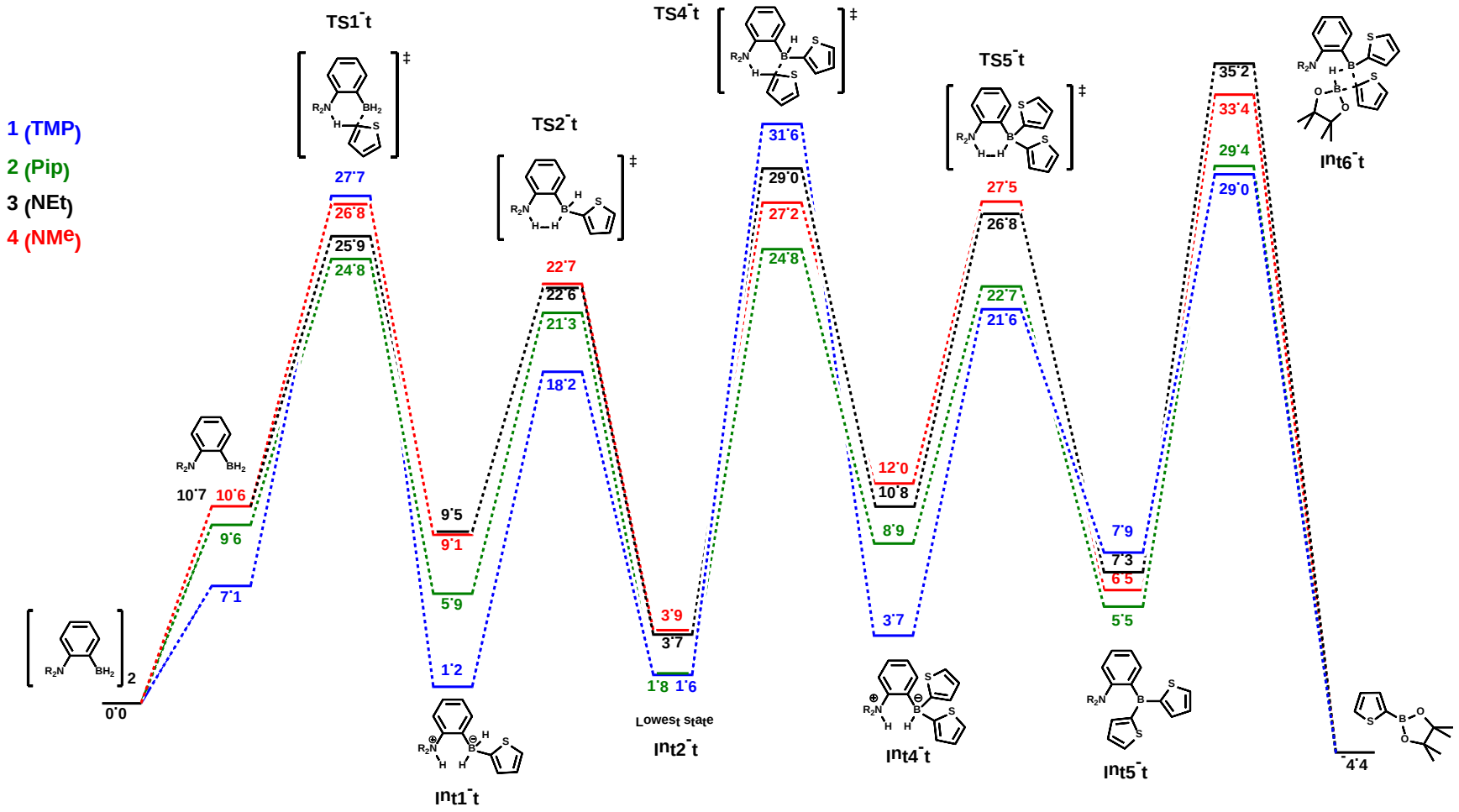
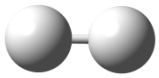



**Figure S53:** Free energies in kcal/mol of the borylation mechanism with a second activation of thiphene with different aminoboranes, calculated by DFT with theory level : ωB97XD/6-31+G** (SMD, chloroform).

## Cartesian coordinates

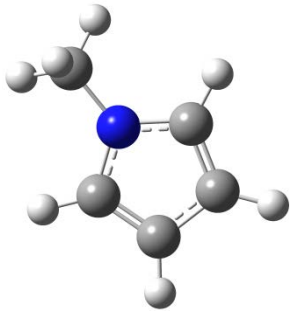
**$H_2$**



**Sum of electronic and thermal Enthalpies= -1.161269**
**Sum of electronic and thermal Free Energies= -1.176061**

| | | | |
|---|---|---|---|
| H | 1.59164900 | -0.84577100 | 0.00000000 |
| H | 0.84914700 | -0.84577100 | 0.00000000 |

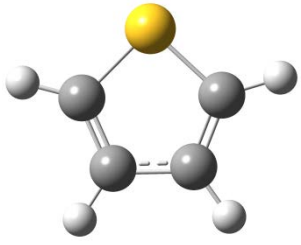
**N-methylpyrrole**



**Sum of electronic and thermal Enthalpies= -249.306345**
**Sum of electronic and thermal Free Energies= -249.341973**

| | | | |
|---|---|---|---|
| C | -4.55190900 | 0.71979400 | 0.01666400 |
| C | -3.17823200 | 0.71910200 | -0.01464000 |
| C | -2.75867800 | 2.07630300 | -0.01226700 |
| C | -3.89316300 | 2.85075400 | 0.02014700 |
| N | -4.98304400 | 2.02039700 | 0.04444600 |
| H | -5.26254000 | -0.09378700 | 0.02479100 |
| H | -2.54649000 | -0.15716000 | -0.02489400 |
| H | -1.74287500 | 2.44392900 | -0.02041000 |
| H | -4.01985300 | 3.92350700 | 0.03247400 |
| C | -6.36289800 | 2.44693100 | -0.01363600 |
| H | -6.46765200 | 3.41420800 | 0.48189800 |
| H | -6.71428100 | 2.53981600 | -1.04648200 |
| H | -6.99241000 | 1.72461000 | 0.51007600 |

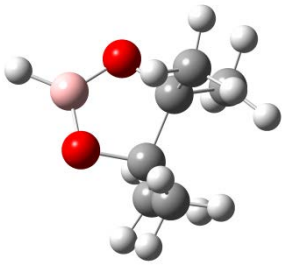
**Thiophene**



**Sum of electronic and thermal Enthalpies= -552.876021**
**Sum of electronic and thermal Free Energies= -552.908224**

| | | | |
|---|---|---|---|
| C | -2.98260600 | -1.07994300 | -0.00087200 |
| C | -1.61985600 | -1.05482000 | -0.00091500 |
| C | -1.09625300 | 0.27318800 | -0.00080500 |
| C | -2.07528400 | 1.22153700 | -0.00000500 |
| S | -3.64675500 | 0.51140500 | 0.00006600 |
| H | -3.63469700 | -1.94158900 | -0.00112300 |
| H | -1.00846700 | -1.94881000 | -0.00131400 |
| H | -0.03914400 | 0.50857800 | -0.00103200 |
| H | -1.96351500 | 2.29630200 | 0.00044100 |

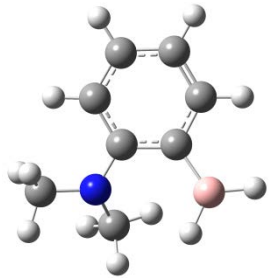
**HBpin**



**Sum of electronic and thermal Enthalpies= -411.582243**
**Sum of electronic and thermal Free Energies= -411.624133**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.68115500 | 3.95316700 | -0.07021500 | H | 1.39149900 | 5.25221200 | -1.79899900 |
| C | 0.41289300 | 3.02990100 | -0.12588400 | H | 3.08303100 | 4.95006000 | -1.35568500 |
| B | 2.28940300 | 1.77784800 | 0.01876800 | H | 2.15149800 | 3.69296100 | -2.18128700 |
| H | 2.98656700 | 0.81646900 | 0.08365500 | C | -0.57358100 | 3.36409300 | -1.23559000 |
| O | 0.98682700 | 1.72884400 | -0.38689100 | H | -1.41499000 | 2.66760900 | -1.20107400 |
| O | 2.71743700 | 3.03322100 | 0.34237700 | H | -0.96429000 | 4.37859100 | -1.10803900 |
| C | 1.60148500 | 5.08959000 | 0.93898700 | H | -0.11083700 | 3.28762900 | -2.22051400 |
| H | 2.52699200 | 5.67007700 | 0.91240700 | C | -0.31804000 | 2.92748200 | 1.21374100 |
| H | 0.77069900 | 5.75969300 | 0.69629500 | H | -0.83874400 | 3.85748200 | 1.45791800 |
| H | 1.46527500 | 4.71556900 | 1.95467600 | H | -1.05449600 | 2.12273400 | 1.15282400 |
| C | 2.09350800 | 4.49462300 | -1.43995800 | H | 0.37506400 | 2.69154500 | 2.02584700 |

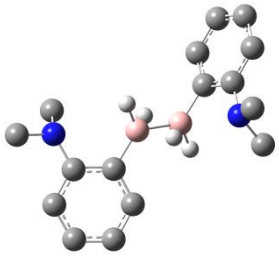
**4-open**



**Sum of electronic and thermal Enthalpies= -391.361593**
**Sum of electronic and thermal Free Energies= -391.407255**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 0.15257700 | 0.34900700 | 0.18648400 | C | 6.10121800 | 0.21037400 | -1.43375800 |
| C | 1.23081500 | 0.25431000 | 0.12035800 | H | 5.41894900 | 0.72856000 | -2.10726500 |
| C | 2.00562400 | 1.27218100 | -0.40944400 | H | 6.94492500 | 0.87488500 | -1.21985800 |
| C | 1.87491000 | -0.89338800 | 0.58012400 | H | 6.48183000 | -0.67800600 | -1.95875600 |
| C | 3.41221200 | 1.19975600 | -0.48804800 | C | 6.06955800 | -1.26822700 | 0.48335300 |
| H | 1.52718500 | 2.18844000 | -0.74494700 | H | 5.91772000 | -2.25082500 | 0.00694100 |
| C | 3.25065500 | -1.03624200 | 0.47951200 | H | 7.14415400 | -1.06740800 | 0.50232100 |
| H | 1.29338400 | -1.70791100 | 1.00291300 | H | 5.72351000 | -1.32129600 | 1.51788200 |
| C | 4.04166300 | -0.01578400 | -0.08109400 | N | 5.41071100 | -0.18796500 | -0.21764500 |
| H | 3.70286800 | -1.96602200 | 0.80321600 | H | 3.52983000 | 3.45612500 | -1.16860700 |
| B | 4.15043300 | 2.51465200 | -0.75769200 | H | 5.31238900 | 2.66074500 | -0.50976600 |

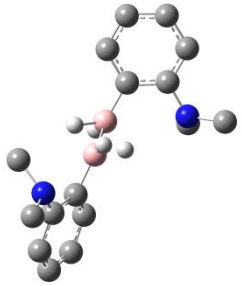
**4-*trans* dimer**



**Sum of electronic and thermal Enthalpies= -782.762429**
**Sum of electronic and thermal Free Energies= -782.828844**

| | | | |
|---|---|---|---|
| C | 0.39866200 | -2.00789900 | 0.96565000 |
| C | 1.37293100 | -1.03016300 | 1.14865700 |
| C | 0.99970900 | 0.22669800 | 1.60780900 |
| C | -0.33474600 | 0.49489100 | 1.89846500 |
| C | -1.30934800 | -0.48922500 | 1.72147700 |
| C | -0.94919300 | -1.75942200 | 1.23247400 |
| H | 0.69422700 | -2.98196800 | 0.58267800 |
| H | 2.41208800 | -1.24534600 | 0.92122100 |
| H | 1.74645100 | 1.00221700 | 1.74827900 |
| H | -0.61366700 | 1.47657600 | 2.26709100 |
| N | -2.68994400 | -0.25217600 | 2.00225100 |
| B | -2.06513000 | -2.84204800 | 0.95546600 |
| H | -2.42087900 | -3.62742600 | 1.78897800 |
| H | -3.12591800 | -2.22202700 | 0.49217700 |
| H | -1.79316200 | -3.52666800 | -0.12323900 |
| C | -3.14674200 | 1.11605100 | 1.84935100 |
| H | -4.24103100 | 1.12412600 | 1.83731000 |
| H | -2.81959000 | 1.78642800 | 2.66362700 |
| H | -2.78967300 | 1.52155400 | 0.90013700 |
| C | -3.13738600 | -0.82718100 | 3.26484800 |
| H | -2.73911600 | -0.28094300 | 4.13710100 |
| H | -4.23083100 | -0.79883600 | 3.31022300 |
| H | -2.81969000 | -1.86861900 | 3.34257700 |
| B | -2.88015300 | -2.90684100 | -0.61682000 |
| H | -2.48722100 | -2.14704600 | -1.44840700 |
| C | -4.06646100 | -3.89677700 | -0.90853800 |
| C | -4.31035600 | -4.38030400 | -2.21562600 |
| C | -4.98133100 | -4.22988400 | 0.09719700 |
| C | -5.46362800 | -5.13146100 | -2.47097400 |
| C | -6.12228100 | -4.98331900 | -0.15656600 |
| H | -4.80904600 | -3.86062600 | 1.10498400 |
| C | -6.36366500 | -5.42326200 | -1.45173500 |
| H | -5.65882200 | -5.50565700 | -3.46973200 |
| H | -6.81959400 | -5.21055300 | 0.64307100 |
| H | -7.25122900 | -6.00791700 | -1.67480100 |
| N | -3.39087400 | -4.07210000 | -3.24732900 |
| C | -3.87957600 | -4.13407400 | -4.60876900 |
| H | -3.16326200 | -3.62642600 | -5.26200700 |
| H | -4.00337500 | -5.16386800 | -4.98914600 |
| H | -4.83772900 | -3.61567500 | -4.68704100 |
| C | -2.07231300 | -4.67364900 | -3.12818700 |
| H | -2.06790900 | -5.72999700 | -3.44851900 |
| H | -1.35777300 | -4.12203200 | -3.74719300 |
| H | -1.71973900 | -4.63916100 | -2.09722700 |

**4-H-Bridged dimer**

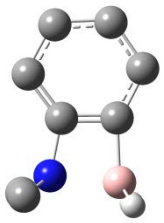


**Sum of electronic and thermal Enthalpies= -782.782335**
**Sum of electronic and thermal Free Energies= -782.848448**

| | | | |
|---|---|---|---|
| H | 0.63447700 | 1.09273400 | -2.26645000 |
| C | 1.48289000 | 0.72481200 | -1.69774800 |
| C | 2.47820500 | 1.60372800 | -1.28588100 |
| C | 1.56935100 | -0.62631100 | -1.37575800 |
| C | 3.58317700 | 1.16925200 | -0.54580900 |
| H | 2.39857300 | 2.65781100 | -1.53581600 |
| C | 2.65397700 | -1.09296700 | -0.64104800 |
| H | 0.79512600 | -1.31868500 | -1.68936700 |
| C | 3.63078400 | -0.18892800 | -0.23825300 |
| H | 2.71113400 | -2.14616000 | -0.39143400 |
| B | 4.74613500 | 2.15958300 | -0.09182600 |
| N | 4.83510500 | -0.62561100 | 0.51156700 |
| H | 5.57171900 | 2.37603500 | -0.95564700 |
| H | 4.40586100 | 3.13393600 | 0.52543600 |
| B | 5.26317300 | 0.61021500 | 1.48875100 |
| C | 6.66351700 | 0.36468700 | 2.23586100 |
| H | 5.62795600 | 1.55969300 | 0.70258300 |
| C | 6.75133000 | -0.25095400 | 3.50496600 |
| C | 7.86566800 | 0.72393600 | 1.61341900 |
| C | 8.00090800 | -0.52622800 | 4.06785400 |
| C | 9.11135900 | 0.45549800 | 2.17405700 |
| H | 8.06279000 | -1.00250200 | 5.04081800 |
| C | 9.17514300 | -0.18584700 | 3.40346300 |
| H | 10.01952400 | 0.74155500 | 1.65313300 |

| | | | |
|---|---|---|---|
| H | 10.13537700 | -0.40914200 | 3.85860200 |
| H | 4.30250600 | 0.87977100 | 2.14535700 |
| N | 5.54398600 | -0.59431900 | 4.19032700 |
| H | 7.82420000 | 1.22303800 | 0.64723600 |
| C | 5.90338700 | -0.95819800 | -0.47558900 |
| H | 5.55426300 | -1.76843800 | -1.11957900 |
| H | 6.80474800 | -1.25601100 | 0.06081700 |
| C | 4.58816500 | -1.81527100 | 1.36597000 |
| H | 3.77197100 | -1.59605100 | 2.05196800 |
| H | 4.35590400 | -2.68409600 | 0.74742300 |
| C | 5.61165800 | -1.74957700 | 5.06354300 |
| H | 4.59282000 | -2.05645300 | 5.32204600 |
| H | 6.10105000 | -2.58105200 | 4.54882000 |
| C | 4.92021100 | 0.53933100 | 4.86212800 |
| H | 3.90303100 | 0.26991800 | 5.16477500 |
| H | 5.48103500 | 0.84594900 | 5.76207200 |
| H | 4.86032700 | 1.39132100 | 4.18530800 |
| H | 6.14822600 | -1.56701700 | 6.01164700 |
| H | 6.10957200 | -0.07450800 | -1.07975400 |
| H | 5.49115500 | -2.01313900 | 1.94095800 |

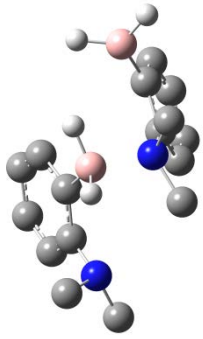
**4-close**



**Sum of electronic and thermal Enthalpies= -782.782335**
**Sum of electronic and thermal Free Energies= -782.848448**

| | | | |
|---|---|---|---|
| C | -1.26669900 | -2.38931300 | 0.65559600 |
| C | 0.08192400 | -2.12313900 | 0.81171400 |
| C | 0.91158100 | -3.18404600 | 1.16092400 |
| C | 0.33826900 | -4.44751200 | 1.33227200 |
| C | -1.03280200 | -4.66524300 | 1.16260400 |
| C | -1.88540200 | -3.61581400 | 0.81224000 |
| H | 1.98051400 | -3.05210800 | 1.30097000 |
| H | 0.96995800 | -5.28808900 | 1.60495400 |
| H | -1.43810900 | -5.66189500 | 1.30512700 |
| H | -2.95204900 | -3.76821100 | 0.67679200 |
| N | -1.78720200 | -1.06475300 | 0.30008700 |
| C | -2.34285500 | -0.98916400 | -1.06056100 |
| H | -2.50859600 | 0.05889100 | -1.31873400 |
| H | -1.62263700 | -1.41852600 | -1.75659900 |
| H | -3.28938700 | -1.53714900 | -1.12370800 |
| C | -2.71215900 | -0.50126600 | 1.29653000 |
| H | -2.88154600 | 0.55290600 | 1.06724300 |
| H | -3.66732200 | -1.03769800 | 1.28573900 |
| H | -2.25581900 | -0.58320700 | 2.28271400 |
| B | -0.13005400 | -0.56440500 | 0.45666200 |
| H | 0.24400000 | -0.16422500 | -0.62131200 |
| H | -0.06554200 | 0.24360500 | 1.35383800 |

**4-TSdimer**

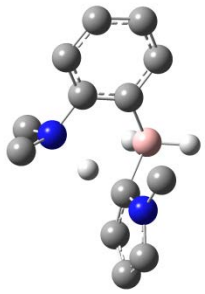


**Sum of electronic and thermal Enthalpies= -782.748383**
**Sum of electronic and thermal Free Energies= -782.811269**

| | | | |
|---|---|---|---|
| C | -2.60857900 | -0.72506900 | 0.51759400 |
| C | -1.55530200 | 0.19718600 | 0.56279400 |
| C | -1.75291000 | 1.37981200 | 1.28919500 |
| C | -2.93798900 | 1.64149900 | 1.96329100 |
| C | -3.95852700 | 0.70274400 | 1.92462500 |
| C | -3.79353000 | -0.47387400 | 1.20559300 |
| H | -0.95144000 | 2.11408400 | 1.33727100 |
| H | -3.05688400 | 2.56600100 | 2.51818700 |
| H | -4.88790000 | 0.87458200 | 2.45670100 |
| H | -4.59315200 | -1.20120900 | 1.21200300 |
| N | -2.42453900 | -2.01503000 | -0.17556600 |
| B | -0.11988800 | 0.07867900 | -0.04906500 |
| B | -1.43370800 | -3.02875300 | 0.76533400 |
| H | -1.56903200 | -4.10418100 | 0.22090600 |
| H | -0.32245900 | -2.57376100 | 0.56816100 |
| C | -1.82832200 | -2.90497400 | 2.32657200 |
| C | -1.04267200 | -2.04932600 | 3.11058700 |
| C | -2.92775200 | -3.51462100 | 2.97450800 |
| C | -1.32249300 | -1.75899200 | 4.44274300 |
| H | -0.18740400 | -1.57168700 | 2.64009000 |

| | | | |
|---|---|---|---|
| C | -3.21323700 | -3.23102400 | 4.31369800 |
| C | -2.42456000 | -2.34813200 | 5.04410900 |
| H | -0.68940700 | -1.07518400 | 5.00003400 |
| H | -4.05809000 | -3.70558900 | 4.80152100 |
| H | -2.66758600 | -2.13919700 | 6.08190700 |
| N | -3.76643000 | -4.41782200 | 2.23987600 |
| H | 0.78469600 | -0.33961000 | 0.60808100 |
| H | 0.11974300 | 0.55019500 | -1.12516600 |
| C | -3.71309600 | -2.71173500 | -0.44138300 |
| H | -4.41032500 | -2.04056600 | -0.95187600 |
| H | -3.49371700 | -3.57070800 | -1.07406900 |
| H | -4.11764300 | -3.10341100 | 0.49116800 |
| C | -1.76700300 | -1.83455700 | -1.49064400 |
| H | -2.36201400 | -1.17699300 | -2.13007400 |
| H | -0.76297000 | -1.42482700 | -1.37753100 |
| H | -1.64845200 | -2.81691200 | -1.94718400 |
| C | -3.15465200 | -5.72027500 | 2.00773900 |
| H | -3.11244700 | -6.32419000 | 2.93072500 |
| H | -3.73880100 | -6.27202500 | 1.26294800 |
| H | -2.14302700 | -5.59340500 | 1.62544100 |
| C | -5.12914200 | -4.56178100 | 2.71302000 |
| H | -5.57341000 | -3.57705300 | 2.88327400 |
| H | -5.71581700 | -5.07766400 | 1.94513800 |
| H | -5.22257600 | -5.14793200 | 3.64439000 |

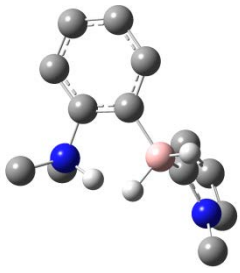
**4 -TS1-p**



**Sum of electronic and thermal Enthalpies= -640.676026**
**Sum of electronic and thermal Free Energies= -640.732409**

| | | | |
|---|---|---|---|
| C | -1.33058900 | -2.11796100 | 0.61796100 |
| C | -0.09476400 | -1.85999600 | 1.23262400 |
| C | 0.93047800 | -2.76714200 | 0.93267200 |
| C | 0.74072600 | -3.85378000 | 0.08456200 |
| C | -0.49900200 | -4.06666800 | -0.51329700 |
| C | -1.54449000 | -3.19041800 | -0.24557500 |
| H | 1.90886200 | -2.60015300 | 1.37580600 |
| H | 1.56332000 | -4.53280100 | -0.12070600 |
| H | -0.65295600 | -4.90810800 | -1.18148700 |
| H | -2.51684700 | -3.34883500 | -0.70349600 |
| H | -1.57900500 | -0.04317900 | 1.28111500 |
| B | 0.13764600 | -0.57910300 | 2.19818200 |
| N | -2.39376500 | -1.17555700 | 0.92199200 |
| C | -3.14294800 | -1.51974400 | 2.13439200 |
| C | -3.26457300 | -0.80066400 | -0.18738600 |
| H | 1.32005500 | -0.29790000 | 2.28092600 |
| C | -0.66899100 | 0.78357400 | 1.57760700 |
| C | -1.20859100 | 1.84013300 | 2.34362600 |
| C | -1.03902000 | 3.04653700 | 1.66802000 |
| H | -1.67959200 | 1.69425700 | 3.30654400 |
| H | -1.34475100 | 4.03431900 | 1.98005200 |
| H | -0.35704900 | -0.75723300 | 3.29963900 |
| C | -0.38476800 | 2.73566300 | 0.47814800 |
| H | -0.06212400 | 3.38810100 | -0.32264100 |
| H | -2.65497500 | -0.57559900 | -1.06444100 |
| H | -3.82367000 | 0.09623200 | 0.09455100 |
| H | -3.98159600 | -1.59062900 | -0.44487000 |
| H | -3.76969600 | -0.66969300 | 2.42132200 |
| H | -3.77794200 | -2.39952300 | 1.96951600 |
| H | -2.43452800 | -1.72473700 | 2.93744600 |
| N | -0.17886700 | 1.41221100 | 0.41515800 |
| C | 0.55135500 | 0.72329100 | -0.63040700 |
| H | -0.06412800 | -0.06214000 | -1.07461100 |
| H | 0.83759500 | 1.44055900 | -1.40112900 |
| H | 1.44379300 | 0.25639000 | -0.20739900 |

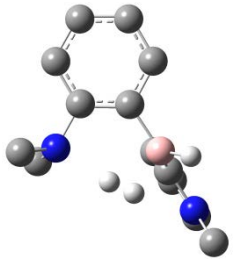
**4-Int1-p**



**Sum of electronic and thermal Enthalpies= -640.688207**
**Sum of electronic and thermal Free Energies= -640.748066**

| | | | |
|---|---|---|---|
| H | 0.89541800 | -0.59105800 | 2.56726900 |
| C | 1.75027500 | -0.32419600 | 1.95299500 |
| C | 2.29212900 | 0.95391200 | 2.03865700 |
| C | 2.29072400 | -1.26897100 | 1.08063500 |
| C | 3.39167000 | 1.35024400 | 1.26443400 |
| H | 1.85549300 | 1.67919600 | 2.71857300 |
| C | 3.38533200 | -0.92555400 | 0.29738500 |
| H | 1.86257700 | -2.26313100 | 1.00915500 |
| C | 3.89193900 | 0.36234300 | 0.41678000 |
| H | 3.81646200 | -1.64814000 | -0.39076300 |
| B | 4.00567700 | 2.85320800 | 1.23505000 |
| H | 3.82775400 | 3.42936400 | 2.29301700 |
| H | 5.23686300 | 1.73695500 | 0.00789500 |
| H | 5.25844100 | 2.78490100 | 1.10432600 |
| C | 3.39214700 | 3.62926500 | -0.03732100 |
| C | 2.38649800 | 3.28431300 | -0.92991000 |
| N | 3.86101100 | 4.85561200 | -0.45832600 |
| C | 2.25462700 | 4.31874400 | -1.89780100 |
| H | 1.78598400 | 2.38553600 | -0.86025200 |
| C | 3.18300500 | 5.27708200 | -1.57616100 |
| H | 1.55221200 | 4.36562700 | -2.71849100 |
| H | 3.41397300 | 6.22570800 | -2.04019400 |
| C | 4.92287300 | 5.58646500 | 0.19314400 |
| H | 4.71783700 | 5.68102000 | 1.26219900 |
| H | 5.88565000 | 5.07730700 | 0.07717000 |
| H | 4.99709600 | 6.58329800 | -0.24622100 |
| N | 5.06070900 | 0.77823700 | -0.39271800 |
| C | 4.76350500 | 0.91675300 | -1.84240400 |
| H | 5.64410900 | 1.32310700 | -2.34282900 |
| H | 4.51830200 | -0.06416800 | -2.25228100 |
| H | 3.92496200 | 1.60856400 | -1.94045100 |
| C | 6.27280200 | -0.02980800 | -0.11941700 |
| H | 6.11880800 | -1.05134800 | -0.46782700 |
| H | 7.12207600 | 0.41550800 | -0.63994100 |
| H | 6.44714500 | -0.02678600 | 0.95612700 |

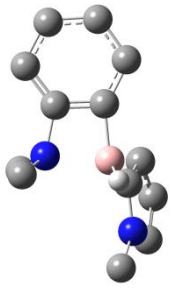
**4-TS2-p**



**Sum of electronic and thermal Enthalpies= -640.665765**
**Sum of electronic and thermal Free Energies= -640.727455**

| | | | |
|---|---|---|---|
| H | 1.51627700 | -0.31114800 | 2.95139900 |
| C | 2.25023900 | -0.17078700 | 2.16386700 |
| C | 2.87073500 | 1.06275100 | 2.00309300 |
| C | 2.57639400 | -1.22485600 | 1.31591800 |
| C | 3.81980200 | 1.28840200 | 0.99742500 |
| H | 2.61281000 | 1.87620100 | 2.67614200 |
| C | 3.51922000 | -1.03168800 | 0.31390900 |
| H | 2.09984900 | -2.19301100 | 1.43399900 |
| C | 4.13275800 | 0.21160400 | 0.15234500 |
| H | 3.77543700 | -1.85068400 | -0.35211500 |
| B | 4.41951600 | 2.75273300 | 0.83944400 |
| H | 5.71626300 | 2.00214700 | -0.14480000 |
| H | 5.93294300 | 2.64590100 | 0.26907200 |
| C | 3.70424300 | 3.70941400 | -0.16197500 |
| C | 2.54472600 | 3.49251600 | -0.89413400 |
| C | 2.22717300 | 4.67450000 | -1.60057000 |
| H | 1.97941100 | 2.56998700 | -0.88097100 |
| C | 3.20433700 | 5.59312000 | -1.28745400 |
| H | 1.38328700 | 4.84520900 | -2.25318400 |
| H | 3.34353100 | 6.61324500 | -1.61690100 |
| N | 4.08134100 | 5.01669500 | -0.41607300 |
| C | 5.27367800 | 5.65299500 | 0.09775900 |
| H | 5.35497900 | 5.49027000 | 1.17449300 |
| H | 6.17491900 | 5.25875800 | -0.38380600 |
| H | 5.21732000 | 6.72620000 | -0.09161900 |
| N | 5.11891800 | 0.42215600 | -0.88034400 |
| H | 4.94124700 | 3.22797400 | 1.81829100 |
| C | 4.52982900 | 0.67744600 | -2.19285100 |
| H | 5.31757300 | 0.98217400 | -2.88884100 |
| H | 4.02859000 | -0.21433500 | -2.60300700 |
| H | 3.80650700 | 1.49009900 | -2.11492800 |
| C | 6.16052500 | -0.59420100 | -0.93692800 |
| H | 5.80741700 | -1.55913200 | -1.33472500 |
| H | 6.96637300 | -0.24103200 | -1.58784300 |
| H | 6.56670100 | -0.75816100 | 0.06348200 |

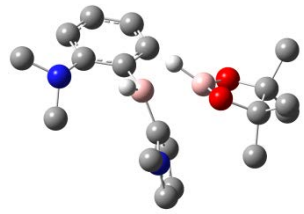
**4-N-methylpyrrole-close**



**Sum of electronic and thermal Enthalpies= -639.522845**
**Sum of electronic and thermal Free Energies= -639.580924**

| | | | |
|---|---|---|---|
| C | -2.35352800 | -3.23798900 | 1.61727800 |
| C | -0.96354900 | -3.27864700 | 1.47183300 |
| C | -0.26127400 | -2.17118700 | 0.99140200 |
| C | -1.03686500 | -1.06787100 | 0.68298300 |
| C | -2.41059400 | -0.98236800 | 0.81675900 |
| C | -3.09239900 | -2.09679200 | 1.29297400 |
| H | -2.86584600 | -4.11970200 | 1.99112100 |
| H | -0.42517000 | -4.18450000 | 1.73203200 |
| H | 0.81728900 | -2.19255400 | 0.86665000 |
| H | -4.17167000 | -2.09550600 | 1.41370500 |
| B | -2.47697100 | 0.52849500 | 0.27393100 |
| H | -2.57885800 | 1.41011000 | 1.09862500 |
| C | -3.10478400 | 0.78447200 | -1.14214800 |
| C | -3.62916000 | -0.12327500 | -2.04963600 |
| C | -4.03408100 | 0.57556000 | -3.21270500 |
| H | -3.71962200 | -1.18585500 | -1.86660700 |
| C | -3.74275500 | 1.90205500 | -2.99445700 |
| H | -4.49481300 | 0.16573600 | -4.10016400 |
| H | -3.89021600 | 2.76982400 | -3.62214200 |
| N | -3.19050100 | 2.02559100 | -1.74986800 |
| C | -2.69184700 | 3.26434300 | -1.19793700 |
| H | -2.92210800 | 3.31879600 | -0.13283500 |
| H | -1.60617500 | 3.35673300 | -1.32413200 |
| H | -3.17007000 | 4.10510600 | -1.70457800 |
| N | -0.68205400 | 0.24888700 | 0.15370900 |
| C | 0.13462700 | 1.05565200 | 1.06998500 |
| H | -0.34570300 | 1.07160900 | 2.04855000 |
| H | 1.14532400 | 0.64210400 | 1.16401600 |
| H | 0.19579100 | 2.07675800 | 0.68579100 |
| C | -0.11044500 | 0.21074100 | -1.20007800 |
| H | -0.04698300 | 1.23016700 | -1.58889400 |
| H | 0.88900500 | -0.23818600 | -1.18610800 |
| H | -0.77243200 | -0.36564500 | -1.84615100 |

**4-TS3-p**

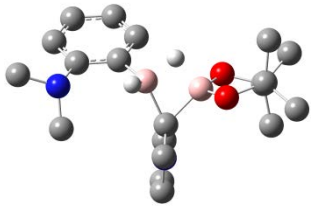


**Sum of electronic and thermal Enthalpies= -1051.097432**
**Sum of electronic and thermal Free Energies= -1051.175434**

| | | | |
|---|---|---|---|
| C | -2.08792200 | -2.04572300 | 0.90940400 |
| C | -0.74972700 | -1.66566700 | 0.97387800 |
| C | -0.32045600 | -0.38174800 | 0.62112000 |
| C | -1.30283100 | 0.55641700 | 0.22798100 |
| C | -2.64630500 | 0.17084800 | 0.15975000 |
| C | -3.03565400 | -1.12360800 | 0.48800100 |
| H | -2.38089700 | -3.05723200 | 1.17323000 |
| H | -0.01197500 | -2.40155200 | 1.28217100 |
| H | -3.40116700 | 0.88790300 | -0.14422800 |
| H | -4.08394500 | -1.40031500 | 0.42364900 |
| B | 1.21665100 | 0.03542100 | 0.62039800 |
| H | 1.74953800 | -1.15663300 | -0.09738000 |
| C | 1.93908400 | 0.23039100 | 2.01290200 |
| C | 1.52516500 | -0.16809500 | 3.28254500 |
| C | 2.33061200 | 0.47053900 | 4.24247000 |
| H | 0.70782500 | -0.85188100 | 3.46436900 |
| C | 3.22625000 | 1.25817900 | 3.54154100 |
| H | 2.26906500 | 0.38284300 | 5.31729800 |
| H | 4.01287700 | 1.90936900 | 3.89593900 |
| H | 1.58667700 | 0.77055200 | -0.25270600 |
| B | 2.58245700 | -1.61020800 | 0.69395700 |
| O | 3.90696400 | -1.39955900 | 0.43881700 |
| O | 2.30787800 | -2.73949500 | 1.40809400 |
| C | 4.63120500 | -2.29976900 | 1.31379700 |
| C | 3.56685000 | -3.42462800 | 1.60371500 |
| C | 5.87554500 | -2.77449900 | 0.57765200 |
| H | 6.54506100 | -1.92742200 | 0.40860900 |
| H | 6.41247100 | -3.51750800 | 1.17548600 |
| H | 5.63118400 | -3.21317400 | -0.39072900 |
| C | 5.02755500 | -1.50926200 | 2.55923300 |
| H | 5.59869500 | -0.62948900 | 2.25140900 |
| H | 4.15469200 | -1.16762500 | 3.11882300 |
| H | 5.65520900 | -2.11332300 | 3.22035400 |
| C | 3.59777200 | -3.97493000 | 3.02232300 |
| H | 2.82786600 | -4.74270200 | 3.13222200 |
| H | 4.56884800 | -4.43229500 | 3.23584600 |

| | | | |
|---|---|---|---|
| H | 3.40398500 | -3.19170400 | 3.75640900 |
| C | 3.60059900 | -4.56658900 | 0.58840700 |
| H | 4.50211600 | -5.17485900 | 0.70075000 |
| H | 2.72832100 | -5.20492900 | 0.74674300 |
| H | 3.55934100 | -4.18509400 | -0.43533200 |
| N | 2.99525200 | 1.11088500 | 2.21327400 |
| C | 3.74397300 | 1.77263100 | 1.16399300 |
| H | 4.17303700 | 1.02812900 | 0.49024200 |
| H | 3.09653900 | 2.44043300 | 0.59093400 |
| H | 4.54687600 | 2.35460100 | 1.61939800 |
| N | -0.90082900 | 1.87732300 | -0.10810500 |
| C | -1.78264700 | 2.63185400 | -0.97170200 |
| H | -2.69168400 | 3.00520700 | -0.46553500 |
| H | -1.24141600 | 3.50383500 | -1.35301000 |
| H | -2.08697900 | 2.02007800 | -1.82428800 |
| C | -0.42779100 | 2.68626500 | 1.00512200 |
| H | 0.14339800 | 3.53897700 | 0.62163100 |
| H | -1.26016700 | 3.07691800 | 1.61684200 |
| H | 0.22238700 | 2.10499000 | 1.65974700 |

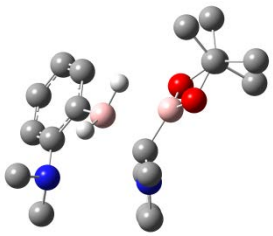
**4-Int3-p**



**Sum of electronic and thermal Enthalpies= -1051.102414**
**Sum of electronic and thermal Free Energies= -1051.185524**

| | | | |
|---|---|---|---|
| C | -1.87666500 | -2.18108000 | 0.47238900 |
| C | -0.54906000 | -1.79425100 | 0.63603800 |
| C | -0.13462400 | -0.46504700 | 0.49052900 |
| C | -1.11990500 | 0.50215600 | 0.18830500 |
| C | -2.45169700 | 0.10937400 | 0.01619000 |
| C | -2.82823900 | -1.22322300 | 0.15073900 |
| H | -2.15840500 | -3.22375300 | 0.58308600 |
| H | 0.19595300 | -2.55001300 | 0.87125100 |
| H | -3.20877800 | 0.84995800 | -0.21910500 |
| H | -3.86822200 | -1.50346600 | 0.01088600 |
| B | 1.40303200 | -0.06876600 | 0.60407900 |
| H | 2.06346300 | -1.07886100 | 0.16053900 |
| C | 1.97332200 | 0.12490500 | 2.17610500 |
| C | 1.22992500 | -0.17316700 | 3.33613500 |
| C | 1.57069100 | 0.72510200 | 4.33878700 |
| H | 0.52406300 | -0.98915800 | 3.39406300 |
| C | 2.52386300 | 1.58203500 | 3.78891800 |
| H | 1.18885500 | 0.76843500 | 5.34771500 |
| H | 3.03888300 | 2.42008500 | 4.23867000 |
| B | 2.70077700 | -1.19590900 | 1.38348900 |
| O | 4.08681500 | -1.04733900 | 1.18666200 |
| O | 2.39008500 | -2.49315900 | 1.83459500 |
| C | 4.66465000 | -2.35247100 | 1.34174100 |
| C | 3.62879200 | -3.05947700 | 2.27947800 |
| C | 4.74512700 | -2.99903400 | -0.04266900 |
| H | 5.30764400 | -2.33924700 | -0.70791700 |
| H | 5.25187200 | -3.96767900 | -0.00623700 |
| H | 3.74792600 | -3.14366700 | -0.46760700 |
| C | 6.05823500 | -2.19651400 | 1.93365400 |
| H | 6.70939800 | -1.68824300 | 1.21729000 |
| H | 6.03585000 | -1.60611000 | 2.85120500 |
| H | 6.49558100 | -3.17536500 | 2.15489600 |
| C | 3.81827600 | -2.68635400 | 3.75325000 |
| H | 2.94014700 | -3.01835500 | 4.31290700 |
| H | 4.70418300 | -3.16475100 | 4.18076000 |
| H | 3.90798400 | -1.60350700 | 3.87998100 |
| C | 3.55577000 | -4.57136100 | 2.12280500 |
| H | 4.52319000 | -5.03108800 | 2.34923500 |
| H | 2.81402700 | -4.97806100 | 2.81523100 |
| H | 3.26245900 | -4.84862700 | 1.10903600 |
| N | 2.76384200 | 1.23523500 | 2.51827500 |
| C | 3.66786900 | 1.93274200 | 1.62240500 |
| H | 4.33892800 | 1.21001900 | 1.15801900 |
| H | 3.09937100 | 2.45221500 | 0.84794000 |
| H | 4.24406700 | 2.65538900 | 2.20156200 |
| N | -0.73481300 | 1.86581400 | 0.04005700 |
| H | 1.82220500 | 0.82606000 | -0.07215500 |
| C | -1.57134600 | 2.68784700 | -0.80772500 |
| H | -2.53136900 | 2.97834800 | -0.34247900 |
| H | -1.03357500 | 3.61180100 | -1.04545000 |
| H | -1.78370300 | 2.16557200 | -1.74337500 |
| C | -0.41102700 | 2.54750200 | 1.28258400 |
| H | 0.13804100 | 3.47040600 | 1.06328700 |
| H | -1.31505300 | 2.81653400 | 1.85834300 |
| H | 0.21280000 | 1.91882600 | 1.91670500 |

**4-TS4-p**

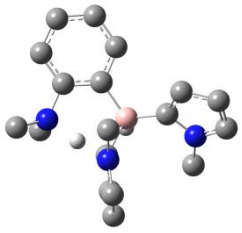


**Sum of electronic and thermal Enthalpies= -1051.102266**

**Sum of electronic and thermal Free Energies= -1051.181436**

| | | | |
|---|---|---|---|
| C | -2.14347100 | -1.47609100 | 0.97246100 |
| C | -1.04793600 | -0.65583900 | 0.62271700 |
| C | 0.02090200 | -1.26713500 | -0.03910200 |
| C | 0.04019300 | -2.62931800 | -0.33457300 |
| C | -1.03800100 | -3.42011000 | 0.03656600 |
| C | -2.12877000 | -2.84177600 | 0.68221700 |
| H | 0.88238200 | -0.65715100 | -0.29785700 |
| H | 0.89760200 | -3.06896800 | -0.83545200 |
| H | -1.04081800 | -4.48510700 | -0.17741900 |
| H | -2.97422100 | -3.46487700 | 0.95753400 |
| N | -3.24493600 | -0.88009700 | 1.66227000 |
| B | -0.96357200 | 0.89016800 | 1.01610600 |
| H | -1.92467300 | 1.59294900 | 0.83034100 |
| H | 0.00747000 | 1.42142800 | 0.49436500 |
| C | 2.55157000 | 2.73937200 | 1.79644200 |
| C | 2.99535800 | 1.27658300 | 2.16001800 |
| O | 1.19552100 | 2.77517900 | 2.28828800 |
| O | 1.75520400 | 0.54851800 | 2.12892700 |
| B | 0.74207700 | 1.47083600 | 2.27586400 |
| C | 3.34218000 | 3.83785500 | 2.49284200 |
| H | 2.96487800 | 4.81565800 | 2.18208600 |
| H | 3.25153100 | 3.76633500 | 3.57782400 |
| H | 4.40134100 | 3.77960500 | 2.22316400 |
| C | 2.50413500 | 2.99944600 | 0.29040000 |
| H | 1.99441000 | 3.94992600 | 0.11419100 |
| H | 3.50967500 | 3.06171000 | -0.13491400 |
| H | 1.94875500 | 2.21783100 | -0.23326200 |
| C | 3.95901000 | 0.64157900 | 1.16729000 |
| H | 4.89126300 | 1.21271700 | 1.11171200 |
| H | 4.19868900 | -0.37472600 | 1.48994700 |
| H | 3.52032000 | 0.58331100 | 0.17008500 |
| C | 3.54600900 | 1.15414700 | 3.58229800 |
| H | 3.65339900 | 0.09438600 | 3.82560200 |
| H | 4.52383300 | 1.63386200 | 3.68118300 |
| H | 2.86024300 | 1.60083700 | 4.30762800 |
| C | -0.69324900 | 1.07056800 | 2.79548900 |
| C | -0.84965800 | -0.09200400 | 3.59814400 |
| C | -1.73046500 | 0.17229700 | 4.62682600 |
| H | -0.34254900 | -1.02306500 | 3.38850600 |
| C | -2.12643300 | 1.50600100 | 4.46812100 |
| H | -2.07445500 | -0.50135500 | 5.39699900 |
| H | -2.81629300 | 2.09062500 | 5.06262800 |
| N | -1.51411700 | 2.04370600 | 3.41787500 |
| C | -1.70899100 | 3.39852200 | 2.93563600 |
| H | -0.74034000 | 3.88508300 | 2.82059400 |
| H | -2.20868600 | 3.36762800 | 1.96492200 |
| H | -2.32336900 | 3.94420100 | 3.65262000 |
| C | -4.16320800 | -0.15880800 | 0.79630200 |
| H | -4.79799400 | -0.83860100 | 0.19969000 |
| H | -4.81917800 | 0.47541800 | 1.40374800 |
| H | -3.60541600 | 0.48205100 | 0.11373400 |
| C | -3.95214900 | -1.72689100 | 2.59757900 |
| H | -4.56484800 | -1.09620000 | 3.25183500 |
| H | -4.62817500 | -2.46116300 | 2.12179600 |
| H | -3.23743900 | -2.27010000 | 3.22094800 |

**4-TS5-p**

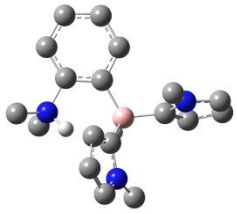


**Sum of electronic and thermal Enthalpies= -888.819625**
**Sum of electronic and thermal Free Energies= -888.887981**

| | | | |
|---|---|---|---|
| C | 1.24098400 | 0.15307200 | 1.15500100 |
| C | 2.09319400 | 1.24508700 | 1.02901400 |
| C | 1.66185700 | -1.11561300 | 0.76708300 |
| C | 3.39590500 | 1.13324400 | 0.51794500 |
| C | 2.93299000 | -1.26989300 | 0.22953900 |
| H | 1.00396500 | -1.97308800 | 0.86740300 |
| C | 3.76512300 | -0.15871500 | 0.10533600 |
| B | 4.37755800 | 2.42182100 | 0.33968400 |
| H | 5.68770100 | 0.89032100 | 0.00429500 |
| C | 6.04796500 | 1.98020800 | 0.51496700 |
| C | 7.08594100 | 2.58567200 | -0.22858700 |
| C | 8.21264900 | 2.74037300 | 0.57548400 |
| H | 6.98186500 | 2.87287200 | -1.26662600 |
| C | 7.87165200 | 2.22193900 | 1.82284500 |
| H | 9.16953900 | 3.16479800 | 0.30900800 |
| H | 8.46109600 | 2.15302800 | 2.72755300 |
| H | 0.24388000 | 0.29227000 | 1.56235700 |
| H | 3.26911100 | -2.24834600 | -0.10239600 |
| H | 1.74453100 | 2.22497700 | 1.33812300 |
| N | 6.61451100 | 1.75820700 | 1.78420400 |
| C | 5.88959100 | 1.22828700 | 2.92274600 |
| H | 5.17657600 | 0.47647700 | 2.58115400 |
| H | 6.59305500 | 0.77443200 | 3.62331500 |
| H | 5.33124900 | 2.03227500 | 3.40918900 |
| H | 4.34540500 | 2.76187100 | -0.83579500 |
| C | 4.08497100 | 3.63605800 | 1.34435900 |
| C | 3.52338800 | 3.66444000 | 2.61614600 |
| N | 4.47697600 | 4.93814100 | 1.08726100 |
| C | 3.58077100 | 4.98806800 | 3.12244200 |
| H | 3.09007000 | 2.80920800 | 3.11788000 |
| C | 4.17990100 | 5.74982800 | 2.15100800 |
| H | 3.20902000 | 5.34598600 | 4.07226700 |
| H | 4.40785400 | 6.80599000 | 2.11856700 |
| C | 5.18041100 | 5.39585200 | -0.08968700 |
| H | 5.03609700 | 6.47319400 | -0.19754900 |
| H | 6.25285000 | 5.18548300 | -0.02006500 |
| H | 4.78567000 | 4.89738100 | -0.97598100 |
| N | 5.07763900 | -0.29434200 | -0.50157900 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 5.86915800 | -1.44929700 | -0.08913600 | C | 5.06013700 | -0.10925400 | -1.95503600 |
| H | 5.52952500 | -2.38044400 | -0.56000900 | H | 6.08823500 | -0.00354400 | -2.31545700 |
| H | 6.91241200 | -1.27799400 | -0.37043900 | H | 4.58421100 | -0.96083400 | -2.45755100 |
| H | 5.80835900 | -1.55872800 | 0.99500900 | H | 4.50869200 | 0.80348900 | -2.18484100 |

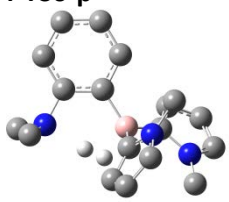
**4-Int4-p**



**Sum of electronic and thermal Enthalpies= -888.836567**
**Sum of electronic and thermal Free Energies= -888.905661**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 0.26688500 | 0.75674400 | 0.90998600 | H | 4.19824700 | 5.02500500 | 2.39041500 |
| C | 1.34115100 | 0.65082000 | 0.79290000 | H | 2.47729200 | 5.42793600 | 2.61851600 |
| C | 2.11058300 | 1.75799400 | 0.45211200 | C | 5.69697100 | 3.17231200 | 0.79196800 |
| C | 1.93682800 | -0.59416300 | 0.98092800 | C | 5.96947600 | 2.74899700 | 2.09244600 |
| C | 3.50296000 | 1.68827500 | 0.29032400 | N | 6.79086000 | 3.92731000 | 0.41754200 |
| H | 1.62914100 | 2.71867900 | 0.29108400 | C | 7.23259700 | 3.25985500 | 2.49436300 |
| C | 3.31198800 | -0.71820000 | 0.82758400 | H | 5.28114300 | 2.17563000 | 2.70306200 |
| H | 1.34019000 | -1.46167600 | 1.24246200 | C | 7.70816800 | 3.98876700 | 1.43193400 |
| C | 4.04448400 | 0.41662200 | 0.49939100 | H | 7.72463000 | 3.12753400 | 3.44752000 |
| H | 3.78779800 | -1.68455300 | 0.96474700 | H | 8.62732800 | 4.54511300 | 1.31342600 |
| B | 4.40978600 | 2.96765800 | -0.19306800 | C | 6.93677600 | 4.57584300 | -0.87074500 |
| H | 5.84390900 | 1.28679000 | 0.46816400 | H | 7.76848000 | 5.28113000 | -0.82254700 |
| H | 4.84359100 | 2.67648400 | -1.31171500 | H | 7.13389500 | 3.84192700 | -1.65835800 |
| C | 3.56032700 | 4.31969700 | -0.38332000 | H | 6.01755900 | 5.10917900 | -1.12212200 |
| C | 3.21697700 | 4.97751500 | -1.55261400 | N | 5.51188500 | 0.30289200 | 0.29939800 |
| N | 3.01658100 | 5.07273800 | 0.64375300 | C | 5.85056600 | -0.07734100 | -1.09698700 |
| C | 2.46524600 | 6.13843700 | -1.23006100 | H | 6.93238200 | -0.01908500 | -1.22913600 |
| H | 3.48152300 | 4.63136700 | -2.54338300 | H | 5.49812800 | -1.09380500 | -1.27815100 |
| C | 2.36257100 | 6.16841200 | 0.13841900 | H | 5.35315000 | 0.62703000 | -1.76204200 |
| H | 2.04402600 | 6.86177200 | -1.91437000 | C | 6.22324300 | -0.52898100 | 1.29853600 |
| H | 1.87901200 | 6.87497900 | 0.79861800 | H | 5.99706000 | -1.58290400 | 1.13725300 |
| C | 3.17950100 | 4.80835400 | 2.05626300 | H | 7.29433700 | -0.35910000 | 1.18440700 |
| H | 2.96861400 | 3.75809600 | 2.27388000 | H | 5.90822100 | -0.21873300 | 2.29314600 |

**4-TS6-p**

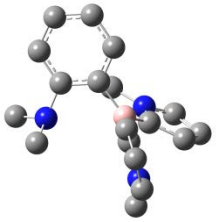


**Sum of electronic and thermal Enthalpies= -888.811023**
**Sum of electronic and thermal Free Energies= -888.879822**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 1.04968800 | 0.23124700 | 2.36293100 | H | 3.95503200 | -1.91766700 | 0.05327400 |
| C | 1.93014900 | 0.22037200 | 1.72767100 | B | 4.42724700 | 2.84825300 | 0.25234600 |
| C | 2.55081200 | 1.41594700 | 1.38151600 | H | 5.25779600 | 1.95891200 | -1.00534700 |
| C | 2.43226100 | -0.98575700 | 1.24989600 | H | 5.08975700 | 2.74358600 | -1.13507000 |
| C | 3.69024100 | 1.45391200 | 0.56580000 | C | 3.47852400 | 4.04012400 | -0.14838300 |
| H | 2.13210400 | 2.35262700 | 1.73805500 | C | 2.15898800 | 3.97164800 | -0.58148200 |
| C | 3.55517400 | -0.98099900 | 0.43181400 | C | 1.70097700 | 5.27405300 | -0.86978700 |
| H | 1.95281900 | -1.92416000 | 1.51009000 | H | 1.59724500 | 3.05336600 | -0.68183900 |
| C | 4.17820200 | 0.22194300 | 0.10210900 | C | 2.75482000 | 6.12129100 | -0.61098200 |

| | | | |
|---|---|---|---|
| H | 0.72301300 | 5.56571200 | -1.22441900 |
| H | 2.82967200 | 7.19612700 | -0.69875400 |
| C | 5.75299000 | 3.14558800 | 1.09116600 |
| C | 7.09204400 | 3.13300000 | 0.74261300 |
| C | 7.85574200 | 3.55010200 | 1.86381600 |
| H | 7.47473800 | 2.86715000 | -0.23429800 |
| C | 6.96304200 | 3.80597200 | 2.87456700 |
| H | 8.92939800 | 3.65528600 | 1.92448300 |
| H | 7.11866000 | 4.13121600 | 3.89316700 |
| N | 3.82045400 | 5.38694500 | -0.18239500 |
| N | 5.69767300 | 3.56100300 | 2.40413700 |
| C | 5.10161300 | 5.97722900 | 0.16305800 |
| H | 5.32550100 | 5.85481900 | 1.22534600 |
| H | 5.91091700 | 5.51547500 | -0.40397600 |
| H | 5.06308300 | 7.04239700 | -0.07118000 |
| C | 4.48816400 | 3.68611000 | 3.19071300 |
| H | 3.73310600 | 4.25026400 | 2.63559000 |
| H | 4.07563800 | 2.70381800 | 3.43870500 |
| H | 4.71650400 | 4.21970100 | 4.11481500 |
| N | 5.34890500 | 0.23960000 | -0.74391600 |
| C | 5.17521600 | -0.44893600 | -2.01764300 |
| H | 6.02995700 | -0.22454100 | -2.66279300 |
| H | 5.10539300 | -1.54226400 | -1.91181100 |
| H | 4.26601500 | -0.08720000 | -2.50284700 |
| C | 6.55996600 | -0.18083100 | -0.04161300 |
| H | 6.53734200 | -1.25293200 | 0.20908200 |
| H | 7.43039500 | 0.01149900 | -0.67634800 |
| H | 6.66796000 | 0.40342500 | 0.87307700 |

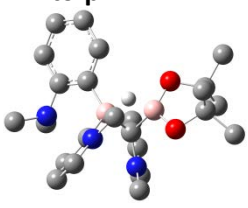
**4-Int5-p**



**Sum of electronic and thermal Enthalpies= -887.669216**
**Sum of electronic and thermal Free Energies= -887.736724**

| | | | |
|---|---|---|---|
| C | -2.73628000 | -2.70147500 | -0.37135000 |
| C | -1.40063800 | -3.07515600 | -0.44184900 |
| C | -0.40562500 | -2.10049500 | -0.45949800 |
| C | -0.73964700 | -0.74644800 | -0.41614400 |
| C | -2.08824000 | -0.35221700 | -0.36448300 |
| C | -3.06798100 | -1.34809600 | -0.33516700 |
| H | -3.51707800 | -3.45530800 | -0.35967000 |
| H | -1.12697100 | -4.12511200 | -0.48161400 |
| H | 0.63552200 | -2.40289700 | -0.51107000 |
| H | -4.11593300 | -1.05882500 | -0.30997100 |
| B | -2.51260500 | 1.17470700 | -0.39370700 |
| C | -2.64666500 | 1.88643400 | 0.97052600 |
| C | -3.01029500 | 1.26757400 | 2.16469400 |
| C | -3.15293400 | 2.25152900 | 3.16290000 |
| H | -3.18218000 | 0.20511700 | 2.27040400 |
| C | -2.84047900 | 3.45549900 | 2.56936100 |
| H | -3.44787500 | 2.10767800 | 4.19208500 |
| H | -2.77222700 | 4.44775600 | 2.99361700 |
| C | -2.98304200 | 1.84315400 | -1.69619800 |
| C | -3.94542100 | 2.85042300 | -1.80902200 |
| C | -4.24583300 | 3.04607700 | -3.16758000 |
| H | -4.39494900 | 3.35560900 | -0.96471500 |
| C | -3.45241700 | 2.15979800 | -3.87040100 |
| H | -4.95118200 | 3.74388500 | -3.59421300 |
| H | -3.35469000 | 2.00235300 | -4.93551200 |
| N | -2.55664300 | 3.24592100 | 1.25422800 |
| N | -2.71151100 | 1.43458600 | -2.99534900 |
| C | -1.90730000 | 4.25242500 | 0.43265000 |
| H | -2.39373800 | 5.21825300 | 0.58895300 |
| H | -0.84787000 | 4.34160400 | 0.69411700 |
| H | -1.99408300 | 3.98435200 | -0.61779900 |
| C | -1.74466600 | 0.42688000 | -3.38805500 |
| H | -0.79319200 | 0.61685400 | -2.88857100 |
| H | -2.09009400 | -0.57347200 | -3.11692900 |
| H | -1.60110200 | 0.48059900 | -4.46845600 |
| N | 0.25327200 | 0.28695000 | -0.47590800 |
| C | 1.45394600 | -0.04006300 | -1.22493200 |
| H | 2.13678600 | -0.72316700 | -0.68989100 |
| H | 1.18934400 | -0.49981800 | -2.18075800 |
| H | 2.00638600 | 0.88328300 | -1.42602700 |
| C | 0.59808200 | 0.84141000 | 0.83077900 |
| H | 1.21094000 | 0.14304600 | 1.42644800 |
| H | 1.16871300 | 1.76575300 | 0.69162800 |
| H | -0.30616000 | 1.07486700 | 1.39304900 |

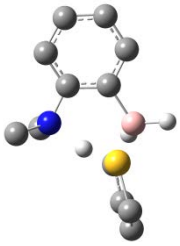
**4-Int6-p**



**Sum of electronic and thermal Enthalpies= -1299.241348**
**Sum of electronic and thermal Free Energies= -1299.330717**

| | | | |
|---|---|---|---|
| C | -1.60677600 | -2.18632700 | 0.01287500 |
| C | -0.29852100 | -1.71451800 | 0.04893600 |
| C | 0.00803700 | -0.37166200 | 0.31252700 |
| C | -1.07133200 | 0.49807500 | 0.54067100 |
| C | -2.38563300 | 0.02706000 | 0.50667200 |
| C | -2.65983100 | -1.31014000 | 0.24536300 |
| H | -1.79984500 | -3.23567400 | -0.18865400 |
| H | 0.51276000 | -2.42100200 | -0.10364300 |
| H | -3.20365800 | 0.72060000 | 0.68351200 |
| H | -3.68675700 | -1.66262900 | 0.22261100 |
| B | 1.54156100 | 0.11769700 | 0.34462200 |
| H | 2.15869500 | -0.97129000 | 0.00554700 |
| C | 2.12086300 | 0.33318500 | 1.93177400 |
| C | 1.26400400 | 0.16873500 | 3.04439700 |
| C | 1.65251000 | 1.02742400 | 4.05853900 |
| H | 0.45289100 | -0.54517100 | 3.06067800 |
| C | 2.75916600 | 1.72404900 | 3.57085400 |
| H | 1.20876100 | 1.14644300 | 5.03552400 |
| H | 3.36697800 | 2.47437700 | 4.05861600 |
| B | 2.73881000 | -1.08216500 | 1.24793600 |
| O | 4.13915900 | -1.10577400 | 1.05377800 |
| O | 2.28930500 | -2.31845400 | 1.75541400 |
| C | 4.57998200 | -2.43946000 | 1.35142100 |
| C | 3.44825600 | -2.95357300 | 2.30243400 |
| C | 4.64341000 | -3.22414500 | 0.03937800 |
| H | 5.30354000 | -2.69966700 | -0.65697100 |
| H | 5.04042800 | -4.23186700 | 0.19114900 |
| H | 3.65259000 | -3.30453000 | -0.41710100 |
| C | 5.96103600 | -2.35947900 | 1.98647600 |
| H | 6.68793200 | -2.00124500 | 1.25239100 |
| H | 5.96491700 | -1.67058900 | 2.83277900 |
| H | 6.28505500 | -3.34604500 | 2.33334300 |
| C | 3.62649800 | -2.46308300 | 3.74397900 |
| H | 2.70234700 | -2.65751600 | 4.29383300 |
| H | 4.44853200 | -2.97974400 | 4.24802300 |
| H | 3.81514600 | -1.38589100 | 3.77847800 |
| C | 3.23458300 | -4.46015900 | 2.28395900 |
| H | 4.14644600 | -4.98380100 | 2.58911400 |
| H | 2.43782200 | -4.72779800 | 2.98258400 |
| H | 2.94381600 | -4.80681900 | 1.29086700 |
| C | 2.08667600 | 1.19706100 | -0.68793000 |
| C | 1.93714700 | 2.57380000 | -0.68570200 |
| C | 2.62870300 | 3.10948000 | -1.79952000 |
| H | 1.38688400 | 3.11537800 | 0.06926700 |
| C | 3.18630400 | 2.04359200 | -2.46460700 |
| H | 2.70589800 | 4.14833000 | -2.08722400 |
| H | 3.77908100 | 2.00402900 | -3.36724900 |
| N | 3.04247200 | 1.32900600 | 2.32657900 |
| N | 2.85834000 | 0.89608300 | -1.79443200 |
| C | 3.28665600 | -0.42643200 | -2.20005400 |
| H | 2.42693100 | -1.09087300 | -2.32688400 |
| H | 3.80555600 | -0.35019000 | -3.15674700 |
| H | 3.96546700 | -0.85678300 | -1.45903100 |
| C | 4.17889300 | 1.83221400 | 1.56547800 |
| H | 4.67689900 | 0.99503400 | 1.07968600 |
| H | 3.84322000 | 2.54353700 | 0.81022500 |
| H | 4.86867800 | 2.31211000 | 2.26174800 |
| N | -0.81403300 | 1.89281100 | 0.79806700 |
| C | -1.26382700 | 2.73633400 | -0.29982700 |
| H | -0.80521400 | 2.39563200 | -1.23014800 |
| H | -2.36177600 | 2.74115700 | -0.42188500 |
| H | -0.93952800 | 3.76741500 | -0.12213900 |
| C | -1.32552000 | 2.35637700 | 2.07685600 |
| H | -0.93707000 | 3.36176100 | 2.27190800 |
| H | -2.42842900 | 2.40696700 | 2.12747600 |
| H | -0.97251800 | 1.69834200 | 2.87332400 |

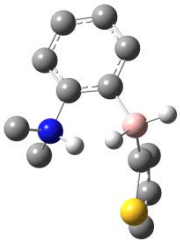
**4-TS1-t**



**Sum of electronic and thermal Enthalpies= -944.234427**
**Sum of electronic and thermal Free Energies= -944.289745**

| | | | |
|---|---|---|---|
| C | -1.30078600 | -2.13133000 | 0.64372400 |
| C | -0.08688000 | -1.84058400 | 1.28730500 |
| C | 0.98375800 | -2.69628500 | 0.99775100 |
| C | 0.85439700 | -3.77769800 | 0.13206300 |
| C | -0.36394000 | -4.02920600 | -0.49328500 |
| C | -1.44914500 | -3.19817900 | -0.23996100 |
| H | 1.94488400 | -2.49603100 | 1.46320200 |
| H | 1.70714700 | -4.42031400 | -0.06593900 |
| H | -0.47036700 | -4.86677000 | -1.17556100 |
| H | -2.40258200 | -3.38836900 | -0.72415600 |
| H | -1.56293200 | -0.03400000 | 1.32738700 |
| B | 0.06792600 | -0.58598200 | 2.28093200 |
| N | -2.40222800 | -1.23578500 | 0.93960000 |
| C | -3.18018700 | -1.64503100 | 2.11200300 |
| C | -3.24904100 | -0.87194400 | -0.19158600 |
| H | 1.21674100 | -0.25935800 | 2.46980500 |
| C | -0.71463700 | 0.82823900 | 1.51494000 |
| C | -1.06359500 | 1.92475200 | 2.29800500 |
| C | -0.77028200 | 3.17875400 | 1.72965700 |
| H | -1.50796100 | 1.79077000 | 3.27793900 |
| H | -0.95641600 | 4.13263900 | 2.20688500 |
| H | -0.56761700 | -0.69938300 | 3.31310800 |
| C | -0.20815100 | 3.05026800 | 0.48089800 |
| H | 0.11724700 | 3.85126100 | -0.17003800 |
| H | -2.61880800 | -0.58255200 | -1.03463500 |
| H | -3.86978200 | -0.01793200 | 0.09484100 |
| H | -3.91192700 | -1.68979600 | -0.50399300 |
| H | -3.84111500 | -0.82549700 | 2.41068600 |
| H | -3.78758200 | -2.53389700 | 1.89369000 |
| H | -2.49695500 | -1.86578300 | 2.93201700 |
| S | -0.03198700 | 1.42187900 | 0.01117900 |

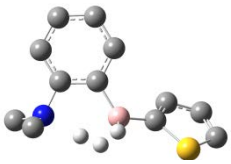
**4-Int1-t**



**Sum of electronic and thermal Enthalpies= -944.26058**
**Sum of electronic and thermal Free Energies= -944.317962**

| | | | |
|---|---|---|---|
| H | 1.30350900 | -0.38230100 | 3.00902700 |
| C | 2.06394600 | -0.14503700 | 2.27113800 |
| C | 2.58116400 | 1.14529200 | 2.19945700 |
| C | 2.51199600 | -1.13936700 | 1.40287700 |
| C | 3.56153000 | 1.50466400 | 1.26482600 |
| H | 2.22193800 | 1.90737000 | 2.88454700 |
| C | 3.48764700 | -0.83339500 | 0.46125500 |
| H | 2.10568800 | -2.14368000 | 1.45737900 |
| C | 3.97154800 | 0.46700700 | 0.42717900 |
| H | 3.84651800 | -1.59575900 | -0.22549400 |
| B | 4.17798200 | 3.00010600 | 1.07702000 |
| H | 3.92771500 | 3.70367500 | 2.03332800 |
| H | 5.20495400 | 1.83219600 | -0.29816500 |
| H | 5.41756200 | 2.90685800 | 0.98657700 |
| C | 3.60808400 | 3.61125900 | -0.31937800 |
| C | 2.37066500 | 3.48189100 | -0.89965000 |
| S | 4.63120600 | 4.51594500 | -1.40266400 |
| C | 2.23952800 | 4.10031200 | -2.18245800 |
| H | 1.56488700 | 2.94267900 | -0.41181300 |
| C | 3.39310800 | 4.69694900 | -2.59552800 |
| H | 1.32555900 | 4.10032600 | -2.76613400 |
| H | 3.57277600 | 5.24357600 | -3.51065300 |
| N | 5.01259400 | 0.84189000 | -0.56151000 |
| C | 6.28585700 | 0.10476300 | -0.36919400 |
| H | 6.12488900 | -0.95617500 | -0.56027500 |
| H | 7.03244400 | 0.50023100 | -1.05936300 |
| H | 6.60704300 | 0.25398900 | 0.66121300 |
| C | 4.52683200 | 0.81841600 | -1.96680400 |
| H | 5.30025800 | 1.23391000 | -2.61388800 |
| H | 4.30740700 | -0.21250500 | -2.24732100 |
| H | 3.62982000 | 1.43584800 | -2.01747800 |

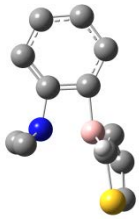
**4-TS2-t**



**Sum of electronic and thermal Enthalpies= -944.237503**
**Sum of electronic and thermal Free Energies= -944.296288**

| | | | |
|---|---|---|---|
| H | 1.20329900 | 0.55941100 | 2.47801600 |
| C | 2.00412200 | 0.45004800 | 1.75325200 |
| C | 2.68798900 | 1.57347700 | 1.29905400 |
| C | 2.33892700 | -0.81207300 | 1.27191500 |
| C | 3.72813700 | 1.47257500 | 0.36818700 |
| H | 2.40335300 | 2.55700000 | 1.66187700 |
| C | 3.36775700 | -0.94618500 | 0.34621100 |
| H | 1.80433700 | -1.69129500 | 1.61725400 |
| C | 4.05563100 | 0.18541800 | -0.08600800 |
| H | 3.63455000 | -1.92921800 | -0.03025500 |
| B | 4.52458200 | 2.75458000 | -0.15600300 |
| H | 5.04360800 | 1.70392800 | -1.40143600 |
| H | 4.93426000 | 2.52495300 | -1.54013900 |
| C | 3.68466600 | 4.06100400 | -0.45432200 |
| C | 2.35887000 | 4.19012900 | -0.78834900 |
| S | 4.41943100 | 5.63427700 | -0.40463900 |
| C | 1.93775100 | 5.53362300 | -1.00157000 |
| H | 1.70026500 | 3.33262000 | -0.87468200 |
| C | 2.95343800 | 6.42895400 | -0.82876800 |
| H | 0.92671800 | 5.81972700 | -1.26627100 |
| H | 2.91225600 | 7.50533900 | -0.92031300 |
| N | 5.13615700 | 0.10757600 | -1.03990200 |
| H | 5.62129700 | 2.93058100 | 0.31874600 |
| C | 4.92840700 | -0.80831700 | -2.15565700 |
| H | 5.68031500 | -0.60675600 | -2.92391700 |
| H | 5.01841200 | -1.86445500 | -1.86306200 |
| H | 3.93710400 | -0.64384000 | -2.58165500 |
| C | 6.44155200 | -0.08042100 | -0.40256000 |
| H | 6.53338300 | -1.08104800 | 0.04369600 |
| H | 7.23053300 | 0.04949300 | -1.14918700 |
| H | 6.57165200 | 0.66873600 | 0.38007700 |

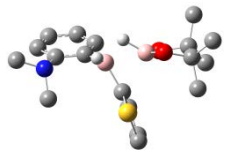
**4-Int2-t**



**Sum of electronic and thermal Enthalpies= -943.094505**
**Sum of electronic and thermal Free Energies= -943.150195**

| | | | |
|---|---|---|---|
| C | -2.33707600 | -3.24617600 | 1.59627800 |
| C | -0.94461900 | -3.29305800 | 1.47667100 |
| C | -0.22835700 | -2.19251400 | 1.00091500 |
| C | -0.99587600 | -1.09071300 | 0.66925600 |
| C | -2.37122100 | -0.99740600 | 0.77715900 |
| C | -3.06643200 | -2.10505900 | 1.25027100 |
| H | -2.85885100 | -4.12311100 | 1.96811200 |
| H | -0.41477800 | -4.19873200 | 1.75418700 |
| H | 0.85217000 | -2.21850500 | 0.89687500 |
| H | -4.14745100 | -2.09887700 | 1.35389600 |
| B | -2.39895900 | 0.51338700 | 0.22265800 |
| H | -2.52914500 | 1.40873800 | 1.02450200 |
| N | -0.63547400 | 0.22364800 | 0.13431000 |
| C | 0.16169400 | 1.04315300 | 1.06087700 |
| H | -0.33436100 | 1.06136300 | 2.03120500 |
| H | 1.17156100 | 0.63281000 | 1.17107400 |
| H | 0.22146700 | 2.06122000 | 0.67019000 |
| C | -0.02254700 | 0.17265900 | -1.20280000 |
| H | 0.03494700 | 1.18549700 | -1.60741800 |
| H | 0.98151800 | -0.26138100 | -1.14624000 |
| H | -0.65198300 | -0.42901600 | -1.85766700 |
| C | -3.01314800 | 0.77642400 | -1.21151300 |
| C | -3.48442700 | -0.12699600 | -2.13094900 |
| S | -3.12885100 | 2.37838000 | -1.87524500 |
| C | -3.92966200 | 0.45532600 | -3.35405700 |
| H | -3.51386800 | -1.19184700 | -1.92432900 |
| C | -3.78941500 | 1.81227900 | -3.36223100 |
| H | -4.33798100 | -0.10731200 | -4.18529500 |
| H | -4.05120700 | 2.50393700 | -4.15076800 |

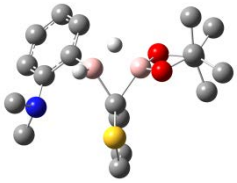
**4-TS3-t**



**Sum of electronic and thermal Enthalpies= -1354.660709**
**Sum of electronic and thermal Free Energies= -1354.735573**

| | | | |
|---|---|---|---|
| C | -2.05647800 | -2.08167000 | 0.88774500 |
| C | -0.71541700 | -1.70909900 | 0.93465100 |
| C | -0.28416500 | -0.42133200 | 0.59501700 |
| C | -1.26942000 | 0.52424300 | 0.22842000 |
| C | -2.61511000 | 0.14482000 | 0.17402200 |
| C | -3.00706900 | -1.15097000 | 0.49263400 |
| H | -2.34915900 | -3.09576000 | 1.14202500 |
| H | 0.02192400 | -2.45471600 | 1.21885300 |
| H | -3.36878200 | 0.87022100 | -0.11326600 |
| H | -4.05730300 | -1.42267800 | 0.44033700 |
| B | 1.26449900 | -0.02546100 | 0.55323800 |
| H | 1.77671400 | -1.14040800 | -0.06933200 |
| C | 1.99846100 | 0.25456400 | 1.96532400 |
| C | 1.62154400 | -0.15575600 | 3.22695000 |
| C | 2.29477100 | 0.51050600 | 4.28186900 |
| H | 0.87672200 | -0.92962200 | 3.37196900 |
| C | 3.18117500 | 1.44485800 | 3.81583600 |
| H | 2.12659900 | 0.31592000 | 5.33381600 |
| H | 3.81494600 | 2.09867900 | 4.39929800 |
| H | 1.62131100 | 0.73752700 | -0.30016300 |
| B | 2.59843600 | -1.50111200 | 0.82101700 |
| O | 3.91458800 | -1.36672900 | 0.48573300 |
| O | 2.30658900 | -2.62545900 | 1.54984300 |
| C | 4.63313800 | -2.30158900 | 1.32578900 |
| C | 3.53597100 | -3.38385200 | 1.63830500 |
| C | 5.83074700 | -2.82008000 | 0.54378100 |
| H | 6.53510700 | -2.00356700 | 0.36766400 |
| H | 6.34785200 | -3.60056500 | 1.11085300 |
| H | 5.53379600 | -3.22754400 | -0.42357200 |
| C | 5.10362000 | -1.54318600 | 2.56675900 |
| H | 5.69862800 | -0.68425300 | 2.24864800 |
| H | 4.26367600 | -1.17124400 | 3.15862600 |
| H | 5.72435900 | -2.18025300 | 3.20292000 |
| C | 3.62859600 | -3.99703200 | 3.02758200 |
| H | 2.83537300 | -4.73762700 | 3.15694000 |
| H | 4.59101500 | -4.50097500 | 3.16018600 |
| H | 3.51801500 | -3.23895800 | 3.80436100 |
| C | 3.44580100 | -4.47859400 | 0.57559700 |
| H | 4.30831000 | -5.14956000 | 0.61421600 |
| H | 2.54118900 | -5.06516300 | 0.75235900 |
| H | 3.38026500 | -4.04842400 | -0.42732600 |
| N | -0.86959100 | 1.84904700 | -0.09622200 |
| C | -1.72890400 | 2.59113700 | -0.99317300 |
| H | -2.65414400 | 2.96578200 | -0.51790000 |
| H | -1.18024500 | 3.46196100 | -1.36638100 |
| H | -2.00523900 | 1.96924900 | -1.84792500 |
| C | -0.45923500 | 2.66057700 | 1.03950500 |
| H | 0.13245900 | 3.51327900 | 0.69010500 |
| H | -1.32568600 | 3.04760200 | 1.60515900 |
| H | 0.15635300 | 2.07849500 | 1.72498600 |
| S | 3.19524800 | 1.51043600 | 2.10425400 |

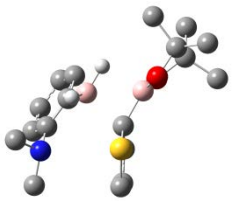
**4-Int3-t**



**Sum of electronic and thermal Enthalpies= -1354.662141**
**Sum of electronic and thermal Free Energies= -1354.739005**

| | | | |
|---|---|---|---|
| C | -1.89913500 | -2.30666200 | 0.19371400 |
| C | -0.57022000 | -1.91307000 | 0.04808200 |
| C | -0.16343900 | -0.59138600 | 0.24530500 |
| C | -1.14925400 | 0.35809800 | 0.58873300 |
| C | -2.47970500 | -0.03609300 | 0.74292800 |
| C | -2.85342900 | -1.36404000 | 0.54978200 |
| H | -2.17911700 | -3.34492600 | 0.04544500 |
| H | 0.17902600 | -2.66442800 | -0.18723300 |
| H | -3.23442900 | 0.69570300 | 1.01272400 |
| H | -3.89249400 | -1.65360900 | 0.67573800 |
| B | 1.37187400 | -0.17509100 | 0.17726500 |
| H | 2.01473800 | -1.23251900 | -0.14771200 |
| C | 1.97913700 | 0.27915800 | 1.68538700 |
| C | 1.28286400 | 0.12908100 | 2.87905400 |
| C | 1.53566000 | 1.12983100 | 3.83227400 |
| H | 0.61538800 | -0.71010600 | 3.03384800 |
| C | 2.42713900 | 2.06488500 | 3.35971500 |
| H | 1.08801500 | 1.16889800 | 4.81689700 |
| H | 2.79238100 | 2.93939100 | 3.88214800 |
| B | 2.67389900 | -1.19925400 | 1.06199700 |
| O | 4.04852200 | -1.10867600 | 0.83060500 |
| O | 2.32720500 | -2.38892100 | 1.71466100 |
| C | 4.60075400 | -2.38705700 | 1.18495100 |
| C | 3.55986600 | -2.91705700 | 2.22921500 |
| C | 4.65021900 | -3.24245900 | -0.08318400 |
| H | 5.21211100 | -2.70260700 | -0.84930500 |
| H | 5.14164700 | -4.20299300 | 0.09609700 |
| H | 3.64457400 | -3.43340600 | -0.46870300 |
| C | 6.00269200 | -2.17511100 | 1.73722500 |
| H | 6.66426100 | -1.81825100 | 0.94362300 |
| H | 6.00290000 | -1.43267400 | 2.53666900 |
| H | 6.41073900 | -3.11407200 | 2.12529400 |
| C | 3.77786500 | -2.32926100 | 3.62679000 |
| H | 2.90082900 | -2.55041200 | 4.24077000 |
| H | 4.65844000 | -2.76071000 | 4.11110500 |
| H | 3.89959500 | -1.24294900 | 3.58483700 |
| C | 3.44516900 | -4.43205500 | 2.30445500 |
| H | 4.40308700 | -4.87749200 | 2.59143500 |
| H | 2.70076600 | -4.71001700 | 3.05494700 |
| H | 3.13432300 | -4.85302600 | 1.34697900 |
| N | -0.73894800 | 1.70758200 | 0.80930500 |
| S | 2.95015200 | 1.72588500 | 1.77750000 |
| H | 1.77889900 | 0.59898500 | -0.64392800 |
| C | -1.49267900 | 2.45522800 | 1.79370600 |
| H | -1.63040000 | 1.85033900 | 2.69330200 |
| H | -0.92414300 | 3.35017100 | 2.06794600 |
| H | -2.48532800 | 2.79017400 | 1.44135200 |
| C | -0.53779400 | 2.47297000 | -0.41171800 |
| H | -1.49221700 | 2.74179400 | -0.89806200 |
| H | 0.00286700 | 3.39647700 | -0.17933700 |
| H | 0.05923900 | 1.89879900 | -1.12068200 |

**4-TS4-t**

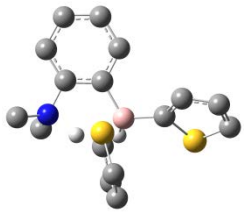


**Sum of electronic and thermal Enthalpies= -1354.659051**
**Sum of electronic and thermal Free Energies= -1354.736384**

| | | | |
|---|---|---|---|
| C | -2.23494600 | -1.44824400 | 0.97690300 |
| C | -1.07094800 | -0.72540600 | 0.63015000 |
| C | -0.02669200 | -1.43320700 | 0.02757900 |
| C | -0.09926900 | -2.80246400 | -0.22444300 |
| C | -1.24558300 | -3.49625200 | 0.13450300 |
| C | -2.30962500 | -2.82006800 | 0.72892800 |
| H | 0.88674100 | -0.89680500 | -0.21550800 |
| H | 0.73793100 | -3.32012800 | -0.68245600 |
| H | -1.32365800 | -4.56412700 | -0.04787800 |
| H | -3.20488100 | -3.37229400 | 0.99636300 |
| N | -3.30028800 | -0.75640700 | 1.62935200 |
| B | -0.87051000 | 0.81403000 | 0.96092400 |
| H | -1.74806900 | 1.61281700 | 0.80887900 |
| H | 0.17620500 | 1.24351800 | 0.51534300 |
| C | 2.54872100 | 2.78837100 | 1.74157800 |
| C | 3.07798200 | 1.37488200 | 2.17971000 |
| O | 1.18545100 | 2.76271500 | 2.21329000 |
| O | 1.88496100 | 0.56713700 | 2.15675800 |
| B | 0.81869500 | 1.43771700 | 2.25810700 |
| C | 3.26051100 | 3.96438600 | 2.39504500 |
| H | 2.83279800 | 4.90100900 | 2.02862200 |
| H | 3.15086300 | 3.94276600 | 3.48030500 |
| H | 4.32665800 | 3.95510500 | 2.14702400 |
| C | 2.51263800 | 2.97498300 | 0.22399200 |

| | | | |
|---|---|---|---|
| H | 1.94202100 | 3.87821500 | -0.00484800 |
| H | 3.52011700 | 3.08684900 | -0.18651500 |
| H | 2.02499000 | 2.13346700 | -0.27388700 |
| C | 4.10277000 | 0.76091500 | 1.23660200 |
| H | 4.99242000 | 1.39511000 | 1.16824800 |
| H | 4.40962500 | -0.21763000 | 1.61472700 |
| H | 3.69004200 | 0.62348700 | 0.23607300 |
| C | 3.60050900 | 1.35136000 | 3.61734600 |
| H | 3.75986900 | 0.31196600 | 3.91458500 |
| H | 4.54848300 | 1.88825400 | 3.71205600 |
| H | 2.87551500 | 1.79430800 | 4.30579600 |
| C | -0.56853000 | 0.98463600 | 2.87601700 |
| C | -0.69781700 | -0.22387100 | 3.56453900 |
| C | -1.63249200 | -0.20703900 | 4.60713400 |
| H | -0.11680700 | -1.09227400 | 3.27755500 |
| C | -2.22153200 | 1.03210500 | 4.73611200 |
| H | -1.87656000 | -1.05677500 | 5.23114400 |
| H | -2.98493100 | 1.31622500 | 5.44873800 |
| S | -1.64065500 | 2.15773800 | 3.60861000 |
| C | -4.12798900 | 0.04105900 | 0.73540100 |
| H | -4.79099300 | -0.58709400 | 0.11435400 |
| H | -4.75157000 | 0.72097200 | 1.32554100 |
| H | -3.50137000 | 0.63996600 | 0.07599900 |
| C | -4.11474000 | -1.54206800 | 2.53242400 |
| H | -4.69543900 | -0.86255600 | 3.16577800 |
| H | -4.83179900 | -2.21188300 | 2.02376600 |
| H | -3.47565400 | -2.14842600 | 3.17918200 |

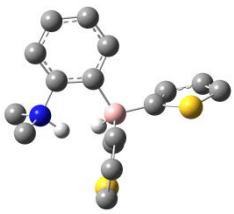
**4-TS5-t**



**Sum of electronic and thermal Enthalpies= -1495.952467**
**Sum of electronic and thermal Free Energies= -1496.021235**

| | | | |
|---|---|---|---|
| C | 1.45692100 | -0.01519900 | 1.47174000 |
| C | 2.24563500 | 1.10678300 | 1.23714400 |
| C | 1.85414700 | -1.26144500 | 0.99709000 |
| C | 3.44757100 | 1.03777100 | 0.52020900 |
| C | 3.03762000 | -1.37238500 | 0.27698100 |
| H | 1.24654600 | -2.14196900 | 1.18037400 |
| C | 3.80503200 | -0.23440500 | 0.04116700 |
| B | 4.37570900 | 2.32765400 | 0.23012500 |
| H | 5.69533600 | 0.87900600 | -0.15228100 |
| C | 6.07732000 | 1.84103200 | 0.52905700 |
| C | 7.08092200 | 2.66959500 | 0.03313500 |
| C | 8.14533600 | 2.91150000 | 0.92051700 |
| H | 7.00001200 | 3.11574600 | -0.95186800 |
| C | 7.97798600 | 2.24067800 | 2.10925700 |
| H | 8.99363700 | 3.54960900 | 0.70770500 |
| H | 8.64563600 | 2.25177800 | 2.96087400 |
| H | 0.53000300 | 0.08245700 | 2.02882300 |
| H | 3.35027500 | -2.33904100 | -0.10661100 |
| H | 1.92828500 | 2.07083100 | 1.62279100 |
| H | 4.42297500 | 2.59472800 | -0.95800700 |
| C | 4.08597200 | 3.62587200 | 1.11634400 |
| C | 3.88183600 | 3.77313600 | 2.46526900 |
| C | 3.70442800 | 5.12190500 | 2.89413400 |
| H | 3.86530600 | 2.92560900 | 3.14300700 |
| C | 3.77825900 | 6.00956200 | 1.86163700 |
| H | 3.52893900 | 5.41382700 | 3.92319300 |
| H | 3.67023800 | 7.08453800 | 1.89852100 |
| N | 5.03705600 | -0.30924900 | -0.72288800 |
| S | 4.05930100 | 5.19427900 | 0.36893500 |
| S | 6.53734300 | 1.33070200 | 2.14419600 |
| C | 4.83739200 | -0.09326100 | -2.15984200 |
| H | 5.80891100 | 0.05950200 | -2.63923200 |
| H | 4.34035400 | -0.95645500 | -2.62165100 |
| H | 4.22634200 | 0.79723000 | -2.30441200 |
| C | 5.88634900 | -1.46561300 | -0.44841700 |
| H | 5.48116000 | -2.39363700 | -0.87129500 |
| H | 6.87148100 | -1.28857500 | -0.88925600 |
| H | 5.99850700 | -1.58341700 | 0.63079600 |

**4-Int4-t**

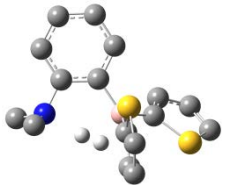


**Sum of electronic and thermal Enthalpies= -1495.979056**
**Sum of electronic and thermal Free Energies= -1496.045400**

| | | | |
|---|---|---|---|
| H | 0.71709600 | 0.52996000 | 1.93879400 |
| C | 1.68999700 | 0.47059700 | 1.46054800 |
| C | 2.26870700 | 1.61938500 | 0.92942000 |
| C | 2.34540200 | -0.75690200 | 1.38355000 |
| C | 3.52435200 | 1.59959700 | 0.30898100 |
| H | 1.74074900 | 2.56680400 | 0.98610800 |

| | | | |
|---|---|---|---|
| C | 3.58994400 | -0.82742000 | 0.76876000 |
| H | 1.89347600 | -1.65227100 | 1.79663200 |
| C | 4.13184800 | 0.34549500 | 0.26124800 |
| H | 4.11258800 | -1.77765300 | 0.69590800 |
| B | 4.29271100 | 2.90995100 | -0.31017000 |
| H | 5.59619200 | 1.29492100 | -0.68826200 |
| H | 4.67672300 | 2.59937500 | -1.45145700 |
| C | 3.32028300 | 4.18155500 | -0.45205700 |
| C | 2.42160400 | 4.46407400 | -1.44752800 |
| S | 3.19278300 | 5.39997200 | 0.78408800 |
| C | 1.63870400 | 5.63742000 | -1.22745400 |
| H | 2.32665000 | 3.83763400 | -2.32832700 |
| C | 1.94495500 | 6.25148800 | -0.05004800 |
| H | 0.88996200 | 6.00789600 | -1.91865100 |
| H | 1.52204200 | 7.15769600 | 0.36048700 |
| C | 5.60980400 | 3.18206600 | 0.61282900 |
| C | 5.75974300 | 3.07549900 | 1.97341600 |
| S | 7.14178900 | 3.63245700 | -0.08209800 |
| C | 7.07686000 | 3.35465800 | 2.45338200 |
| H | 4.93337300 | 2.79554500 | 2.61888300 |
| C | 7.94402900 | 3.66059200 | 1.44720400 |
| H | 7.36072000 | 3.32846900 | 3.49932700 |
| H | 8.99084500 | 3.91906000 | 1.52444700 |
| N | 5.45839100 | 0.30698100 | -0.40612900 |
| C | 5.44652700 | -0.48753900 | -1.66040000 |
| H | 6.41230000 | -0.38004800 | -2.15616200 |
| H | 5.25972300 | -1.53525100 | -1.42521700 |
| H | 4.65092300 | -0.09892000 | -2.29521400 |
| C | 6.57273200 | -0.05670400 | 0.50900300 |
| H | 6.43648500 | -1.08441200 | 0.84617100 |
| H | 7.51638300 | 0.04712000 | -0.02781900 |
| H | 6.54752000 | 0.63588100 | 1.35030300 |

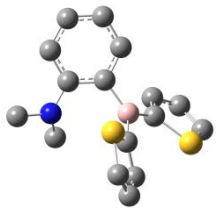
**4-TS6-t**



**Sum of electronic and thermal Enthalpies= -1495.953697**
**Sum of electronic and thermal Free Energies= -1496.020803**

| | | | |
|---|---|---|---|
| H | 0.91074600 | 0.45787900 | 2.25217900 |
| C | 1.80299200 | 0.40890800 | 1.63594800 |
| C | 2.47727900 | 1.57707900 | 1.29495100 |
| C | 2.26804500 | -0.81885700 | 1.17652400 |
| C | 3.63349100 | 1.55615000 | 0.50495800 |
| H | 2.09444400 | 2.53383300 | 1.63883200 |
| C | 3.41051300 | -0.87060000 | 0.38619900 |
| H | 1.74533300 | -1.73513000 | 1.43231900 |
| C | 4.08971600 | 0.30261500 | 0.06345300 |
| H | 3.77834500 | -1.82734200 | 0.02695900 |
| B | 4.40962800 | 2.91430400 | 0.17395400 |
| H | 5.20765500 | 1.95637100 | -1.09325300 |
| H | 5.05964200 | 2.74816800 | -1.22569000 |
| C | 3.52044100 | 4.13474600 | -0.29495400 |
| C | 2.28018900 | 4.10875500 | -0.88634900 |
| S | 4.04987200 | 5.78293100 | -0.13529300 |
| C | 1.76064600 | 5.39287300 | -1.20973900 |
| H | 1.75607900 | 3.17941400 | -1.08076500 |
| C | 2.61740000 | 6.39701900 | -0.85969600 |
| H | 0.79730700 | 5.56163300 | -1.67579400 |
| H | 2.47412800 | 7.46183800 | -0.98016600 |
| C | 5.70818300 | 3.23079000 | 1.04026700 |
| C | 6.87012300 | 3.86950000 | 0.69215000 |
| S | 5.77455600 | 2.78372500 | 2.71780100 |
| C | 7.80662100 | 4.00286900 | 1.75919400 |
| H | 7.05263700 | 4.23430400 | -0.31333300 |
| C | 7.34416700 | 3.46318100 | 2.92240200 |
| H | 8.77495600 | 4.47883700 | 1.66212500 |
| H | 7.83526400 | 3.43152100 | 3.88472900 |
| N | 5.27743800 | 0.28064000 | -0.75568000 |
| C | 5.16894500 | -0.51764200 | -1.97113700 |
| H | 6.01190000 | -0.28074800 | -2.62700100 |
| H | 5.18427700 | -1.60082700 | -1.77799900 |
| H | 4.24076100 | -0.26795400 | -2.48904700 |
| C | 6.49368300 | -0.02473000 | -0.00109100 |
| H | 6.51732400 | -1.07632000 | 0.32338000 |
| H | 7.36665400 | 0.16951200 | -0.63108000 |
| H | 6.54915400 | 0.61863500 | 0.87754500 |

**4-Int5-t**

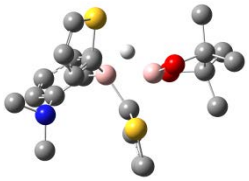


**Sum of electronic and thermal Enthalpies= -1494.809066**
**Sum of electronic and thermal Free Energies= -1494.878245**

| | | | |
|---|---|---|---|
| C | -6.63711600 | 1.40163400 | -0.11507800 |
| C | -5.29779000 | 1.78523300 | -0.38187400 |
| C | -5.05040500 | 2.99773400 | -1.04187900 |
| C | -6.09873900 | 3.83235200 | -1.41134000 |
| C | -7.41287700 | 3.49656900 | -1.10924300 |
| C | -7.66247300 | 2.29532400 | -0.45456600 |
| H | -4.03229300 | 3.30845700 | -1.24697200 |
| H | -5.87818700 | 4.76688500 | -1.91892200 |

| | | | |
|---|---|---|---|
| H | -8.22994200 | 4.15478900 | -1.38479300 |
| H | -8.68917600 | 2.01564900 | -0.23310700 |
| B | -7.03793100 | -0.02459200 | 0.40039800 |
| C | -8.03914000 | -0.12549200 | 1.57917800 |
| C | -8.33667800 | 0.87335900 | 2.48513700 |
| C | -9.28479500 | 0.50552100 | 3.47227300 |
| H | -7.87005600 | 1.85004600 | 2.42608500 |
| C | -9.72263800 | -0.78025900 | 3.30696500 |
| H | -9.63187400 | 1.16089800 | 4.26143400 |
| H | -10.45208800 | -1.31114400 | 3.90332400 |
| C | -6.48795600 | -1.29920000 | -0.29537400 |
| C | -6.28955400 | -2.56249500 | 0.22253000 |
| C | -5.73445500 | -3.48875300 | -0.69857200 |
| H | -6.51651100 | -2.80722600 | 1.25369400 |
| C | -5.52278200 | -2.92538800 | -1.92667600 |
| H | -5.51052800 | -4.52250200 | -0.46597600 |
| H | -5.13678200 | -3.40572900 | -2.81528300 |
| N | -4.24699800 | 0.94618200 | 0.00017400 |
| S | -5.97038600 | -1.27143600 | -1.95487800 |
| S | -8.97557700 | -1.54256100 | 1.96643200 |
| C | -4.18715500 | 0.40628300 | 1.34546900 |
| H | -3.43330400 | 0.93520700 | 1.95008400 |
| H | -5.14763300 | 0.51679300 | 1.85094100 |
| H | -3.93626900 | -0.66033600 | 1.32706000 |
| C | -2.94703200 | 1.12422500 | -0.60127900 |
| H | -2.37942500 | 1.97019400 | -0.17662600 |
| H | -2.36096600 | 0.21433300 | -0.44160300 |
| H | -3.04706400 | 1.27308000 | -1.67890700 |

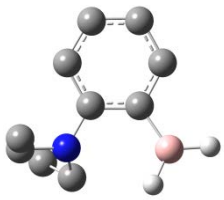
**4-Int6-t**



**Sum of electronic and thermal Enthalpies= -1906.37304**
**Sum of electronic and thermal Free Energies= -1906.459467**

| | | | |
|---|---|---|---|
| C | -1.78622000 | -2.13501100 | 0.08829700 |
| C | -0.44747500 | -1.75487800 | 0.11636800 |
| C | -0.06412300 | -0.42036000 | 0.29791100 |
| C | -1.07886000 | 0.53437500 | 0.46052900 |
| C | -2.42186900 | 0.15678100 | 0.42924200 |
| C | -2.77916100 | -1.17457900 | 0.24326100 |
| H | -2.05038700 | -3.17849600 | -0.05348900 |
| H | 0.31954700 | -2.51835100 | 0.01600800 |
| H | -3.19358000 | 0.91264200 | 0.55025500 |
| H | -3.82710600 | -1.45805000 | 0.22019700 |
| B | 1.47704100 | 0.01786400 | 0.34989200 |
| H | 2.06932700 | -1.09907500 | 0.03318300 |
| C | 1.97142400 | 0.31708000 | 1.92746600 |
| C | 1.22335300 | -0.00472800 | 3.05715300 |
| C | 1.53172900 | 0.75132600 | 4.20082600 |
| H | 0.49049000 | -0.80233800 | 3.03330400 |
| C | 2.51547800 | 1.67680700 | 3.94130500 |
| H | 1.05894300 | 0.62635900 | 5.16632800 |
| H | 2.93503300 | 2.39262400 | 4.63621600 |
| B | 2.71136000 | -1.15397200 | 1.20945900 |
| O | 4.08766500 | -1.02715000 | 1.04901900 |
| O | 2.35225600 | -2.38531000 | 1.76654100 |
| C | 4.64623800 | -2.32012300 | 1.33710700 |
| C | 3.57175200 | -2.93309300 | 2.29753500 |
| C | 4.76184600 | -3.07973600 | 0.01420500 |
| H | 5.34625200 | -2.47672100 | -0.68465000 |
| H | 5.25955200 | -4.04488300 | 0.14523900 |
| H | 3.77677900 | -3.25298800 | -0.42854600 |
| C | 6.02022100 | -2.12599700 | 1.96113000 |
| H | 6.70625300 | -1.70643600 | 1.22097300 |
| H | 5.97504600 | -1.43952300 | 2.80810700 |
| H | 6.42844400 | -3.08317900 | 2.30149100 |
| C | 3.72147200 | -2.44037500 | 3.73965800 |
| H | 2.82115200 | -2.70988100 | 4.29812000 |
| H | 4.58486000 | -2.89794900 | 4.23088800 |
| H | 3.83361700 | -1.35282000 | 3.78092700 |
| C | 3.47609100 | -4.45069400 | 2.26442000 |
| H | 4.42993900 | -4.90199300 | 2.55555400 |
| H | 2.71032500 | -4.78889000 | 2.96731600 |
| H | 3.20668700 | -4.80942200 | 1.26977600 |
| C | 2.09542400 | 1.00670500 | -0.74105900 |
| C | 2.14769800 | 2.37501700 | -0.78175400 |
| C | 2.72515500 | 2.90358900 | -1.97280600 |
| H | 1.75826900 | 2.98617000 | 0.02297200 |
| C | 3.11081800 | 1.92781200 | -2.84322100 |
| H | 2.84860100 | 3.96212800 | -2.16871400 |
| H | 3.57599000 | 2.04168100 | -3.81207000 |
| N | -0.70486300 | 1.91088600 | 0.65988700 |
| S | 2.77565500 | 0.36459900 | -2.20555200 |
| S | 3.05918000 | 1.62465800 | 2.33029700 |
| C | -1.14846900 | 2.45517900 | 1.93109200 |
| H | -2.24360000 | 2.58124400 | 2.00787000 |
| H | -0.82029300 | 1.80120900 | 2.74279200 |
| H | -0.68767100 | 3.43769900 | 2.07962100 |
| C | -1.07967200 | 2.75507300 | -0.46363700 |
| H | -2.17194200 | 2.87348000 | -0.57712500 |
| H | -0.64302600 | 3.75064300 | -0.32939400 |
| H | -0.67417700 | 2.33132500 | -1.38483500 |

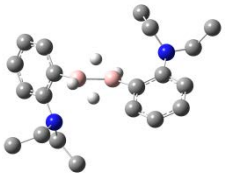
**3-open**



**Sum of electronic and thermal Enthalpies= -469.919489**
**Sum of electronic and thermal Free Energies= -469.969987**

| | | | |
|---|---|---|---|
| H | 0.15432800 | 0.18221700 | -0.37941300 |
| C | 1.23526700 | 0.13020900 | -0.30639300 |
| C | 2.02122100 | 1.24307300 | -0.56757900 |
| C | 1.86545900 | -1.05475200 | 0.06204100 |
| C | 3.42428600 | 1.21956700 | -0.45820700 |
| H | 1.54519500 | 2.18310800 | -0.83364300 |
| C | 3.25095900 | -1.13493200 | 0.13938500 |
| H | 1.27369600 | -1.94113900 | 0.27258700 |
| C | 4.05217100 | -0.01804200 | -0.13762100 |
| H | 3.70627600 | -2.08452600 | 0.39604000 |
| B | 4.15887100 | 2.56912300 | -0.48704700 |
| C | 6.15883800 | 0.19018100 | -1.35440400 |
| H | 5.69510900 | 1.05980900 | -1.82187000 |
| H | 7.18572200 | 0.48229700 | -1.10718100 |
| C | 6.07515600 | -1.14472600 | 0.69703100 |
| H | 7.15463500 | -1.05873900 | 0.53511600 |
| N | 5.45505900 | -0.09441300 | -0.10119600 |
| H | 3.56914000 | 3.54377300 | -0.86459500 |
| H | 5.28225100 | 2.68783600 | -0.09296900 |
| C | 6.15836200 | -0.97599300 | -2.34423300 |
| H | 6.67698100 | -1.85038700 | -1.93987200 |
| H | 5.13255700 | -1.27027200 | -2.58689500 |
| H | 6.66169600 | -0.68878900 | -3.27207000 |
| C | 5.79012100 | -0.98547200 | 2.18632300 |
| H | 4.72298200 | -1.07126700 | 2.40568100 |
| H | 6.31630000 | -1.75650900 | 2.75631900 |
| H | 6.12656300 | -0.00355300 | 2.52803800 |
| H | 5.80310400 | -2.15914300 | 0.36084200 |

**3-*trans* dimer**

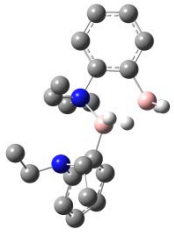


**Sum of electronic and thermal Enthalpies= -939.876189**
**Sum of electronic and thermal Free Energies= -939.955911**

| | | | |
|---|---|---|---|
| C | 0.47957500 | -2.02814000 | 0.84732600 |
| C | 1.43163300 | -1.02036000 | 0.97590600 |
| C | 1.04659700 | 0.22657300 | 1.45338100 |
| C | -0.27759300 | 0.45483100 | 1.81572600 |
| C | -1.23098400 | -0.55889500 | 1.69363000 |
| C | -0.85857300 | -1.81875800 | 1.18725600 |
| H | 0.78313500 | -2.99363800 | 0.44914600 |
| H | 2.46321400 | -1.20472800 | 0.69326500 |
| H | 1.77686900 | 1.02376900 | 1.55341500 |
| H | -0.56965300 | 1.42710300 | 2.19969700 |
| N | -2.60166900 | -0.36391300 | 2.04323100 |
| B | -1.96492500 | -2.92440300 | 0.96851000 |
| H | -2.25424800 | -3.72893600 | 1.80913300 |
| H | -3.06123200 | -2.30996400 | 0.58870900 |
| H | -1.75260600 | -3.58233500 | -0.13955800 |
| C | -3.14591100 | 0.96106000 | 1.76688200 |
| H | -2.81203600 | 1.72428400 | 2.49073500 |
| H | -2.75517900 | 1.26504100 | 0.79126100 |
| C | -2.96940800 | -0.93688600 | 3.34240000 |
| H | -4.05816400 | -1.05120400 | 3.37420800 |
| H | -2.55546400 | -1.94815800 | 3.38327600 |
| B | -2.88266300 | -2.97354100 | -0.54312700 |
| H | -2.55644100 | -2.19305900 | -1.38594300 |
| C | -4.08707500 | -3.95380500 | -0.77570900 |
| C | -4.36404300 | -4.47675700 | -2.06244300 |
| C | -5.00357300 | -4.20163100 | 0.25370700 |
| C | -5.57010700 | -5.15907900 | -2.27676500 |
| C | -6.18957400 | -4.89405400 | 0.03989700 |
| H | -4.79642000 | -3.80526600 | 1.24488200 |
| C | -6.47417300 | -5.35560800 | -1.23979300 |
| H | -5.80289900 | -5.55796600 | -3.25755000 |
| H | -6.88797700 | -5.05539100 | 0.85434700 |
| H | -7.39894600 | -5.89057300 | -1.43501900 |
| N | -3.43516500 | -4.27119200 | -3.10227000 |
| C | -3.91356100 | -4.22233800 | -4.47672200 |
| H | -3.32201800 | -3.47200400 | -5.01594800 |
| H | -4.93505100 | -3.83469900 | -4.45308200 |
| C | -2.08785600 | -4.80446100 | -2.92697000 |
| H | -2.01351200 | -5.82080700 | -3.34712800 |
| H | -1.90796000 | -4.92172800 | -1.85700400 |
| C | -3.86659600 | -5.53623300 | -5.26604100 |
| H | -4.34562400 | -5.40053200 | -6.24008000 |
| H | -2.83773500 | -5.85924900 | -5.45044800 |
| H | -4.37939300 | -6.34732500 | -4.74141600 |
| C | -1.00245800 | -3.92286400 | -3.53382500 |
| H | -0.01538400 | -4.34473100 | -3.32311500 |
| H | -1.10128500 | -3.84909100 | -4.62110900 |
| H | -1.05002300 | -2.91391400 | -3.11628700 |
| C | -2.48959600 | -0.14671200 | 4.56133900 |
| H | -2.73974900 | -0.68325200 | 5.48115000 |
| H | -1.40439500 | -0.01001600 | 4.53077000 |
| H | -2.95768300 | 0.84091200 | 4.61652600 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -4.66986400 | 0.95767800 | 1.71666000 | H | -5.03333200 | 1.92170100 | 1.35033500 |
| H | -5.11414200 | 0.79467500 | 2.70292500 | H | -5.02583400 | 0.17173000 | 1.04448800 |

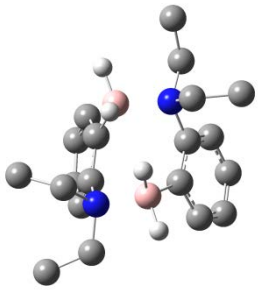
**3-H-Bridged dimer**



**Sum of electronic and thermal Enthalpies= -939.89691**
**Sum of electronic and thermal Free Energies= -939.973983**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 1.04102700 | 1.20787900 | -2.75820300 | C | 5.94069800 | -1.08785400 | -0.20286200 |
| C | 1.80139700 | 0.84290600 | -2.07463300 | H | 6.73024100 | -1.32042100 | 0.51463900 |
| C | 2.60186700 | 1.73889100 | -1.38054200 | C | 4.30135000 | -1.67336600 | 1.47957700 |
| C | 1.98185100 | -0.52880000 | -1.90302900 | H | 5.10076300 | -1.86146100 | 2.19741700 |
| C | 3.59491000 | 1.30975000 | -0.48772600 | C | 6.00582300 | -1.99679900 | 4.93350000 |
| H | 2.46628800 | 2.80568100 | -1.53419300 | H | 6.59838300 | -1.84052400 | 5.85067000 |
| C | 2.95258000 | -0.98707700 | -1.02397500 | C | 4.99336500 | 0.24936800 | 4.96532500 |
| H | 1.36864100 | -1.23821500 | -2.44886500 | H | 3.99749900 | -0.15281400 | 5.18138100 |
| C | 3.72629800 | -0.06521900 | -0.31962800 | H | 4.84223400 | 1.10456000 | 4.30548700 |
| H | 3.08885100 | -2.05524500 | -0.88911800 | H | 6.61301200 | -2.63267000 | 4.28039800 |
| B | 4.57485100 | 2.33956900 | 0.23080700 | H | 5.59537300 | -2.02539800 | -0.65066300 |
| N | 4.78671400 | -0.53893400 | 0.60418500 | H | 4.20109100 | -2.55476600 | 0.83993600 |
| H | 5.35273700 | 2.86401400 | -0.53986900 | C | 3.00153800 | -1.41792800 | 2.22155500 |
| H | 4.09363700 | 3.09915900 | 1.02813600 | H | 2.68736600 | -2.35767200 | 2.68453000 |
| B | 5.22953100 | 0.69700200 | 1.58853100 | H | 3.13156400 | -0.67760200 | 3.00943500 |
| C | 6.66438800 | 0.50723100 | 2.30313300 | H | 2.20453500 | -1.08992900 | 1.55207300 |
| H | 5.55772400 | 1.66180200 | 0.80878000 | C | 6.45262500 | -0.16922300 | -1.29789700 |
| C | 6.86879800 | -0.20973900 | 3.50634100 | H | 5.69708900 | -0.00566900 | -2.06822900 |
| C | 7.79935400 | 1.08385400 | 1.71406300 | H | 6.76155700 | 0.80283300 | -0.91580500 |
| C | 8.16280600 | -0.37736800 | 4.01280400 | H | 7.32218400 | -0.64387600 | -1.75992000 |
| C | 9.08520000 | 0.92254200 | 2.21979700 | C | 4.72895900 | -2.74041800 | 5.30803200 |
| H | 8.31089100 | -0.92710800 | 4.93593800 | H | 4.98032800 | -3.70622300 | 5.75501400 |
| C | 9.26760500 | 0.16963000 | 3.37026600 | H | 4.13103000 | -2.18813800 | 6.03827900 |
| H | 9.93143600 | 1.38144600 | 1.71853700 | H | 4.10872200 | -2.91744600 | 4.42588000 |
| H | 10.25982300 | 0.02534300 | 3.78696400 | C | 5.65750200 | 0.71832600 | 6.26107600 |
| H | 4.29471500 | 0.94486100 | 2.28272900 | H | 6.66736400 | 1.09191900 | 6.06676100 |
| N | 5.74449500 | -0.75914300 | 4.20348800 | H | 5.07564500 | 1.53178900 | 6.70360000 |
| H | 7.67449700 | 1.68649200 | 0.81787000 | H | 5.72460400 | -0.08147200 | 7.00513900 |

**3-dim8**

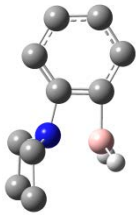


**Sum of electronic and thermal Enthalpies= -939.880008**
**Sum of electronic and thermal Free Energies= -939.952850**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| B | 1.26209200 | 14.08648700 | 5.30713500 | C | 1.50982500 | 12.54285200 | 5.72669900 |
| H | 2.29303700 | 14.52860900 | 4.85736200 | C | 2.83064900 | 12.23016300 | 6.07981900 |
| H | 0.34910800 | 14.34613100 | 4.57386300 | H | 3.58907500 | 12.98871400 | 5.90569700 |

| | | | |
|---|---|---|---|
| C | 3.21239100 | 11.02267600 | 6.65306300 |
| H | 4.24973700 | 10.84022000 | 6.91575800 |
| C | 2.23992800 | 10.06917200 | 6.89722900 |
| H | 2.48774400 | 9.12566400 | 7.37289900 |
| C | 0.92480900 | 10.31422500 | 6.51414400 |
| H | 0.19757400 | 9.54450000 | 6.72513900 |
| C | 0.56190600 | 11.51268600 | 5.90233400 |
| B | -1.55483600 | 13.06803700 | 6.28001100 |
| H | -1.61055000 | 13.93663200 | 5.45559100 |
| H | -2.67193700 | 12.70257400 | 6.56818000 |
| C | -0.72153800 | 13.34417000 | 7.64136900 |
| C | -1.17928300 | 12.62775900 | 8.75683500 |
| H | -2.10604300 | 12.07152500 | 8.64660400 |
| C | -0.51120700 | 12.57837500 | 9.97456500 |
| H | -0.91073400 | 11.99783700 | 10.80027200 |
| C | 0.68010700 | 13.26883800 | 10.10381700 |
| H | 1.24809700 | 13.23606900 | 11.02812000 |
| C | 1.15267000 | 14.03191000 | 9.04017800 |
| H | 2.08735900 | 14.55114500 | 9.18909400 |
| C | 0.45573100 | 14.10203800 | 7.83387700 |
| N | -0.84269900 | 11.71825100 | 5.45590200 |
| N | 0.95989200 | 14.98599100 | 6.73515600 |
| C | 2.24462400 | 15.67044200 | 7.11671800 |
| H | 2.12533200 | 16.11177100 | 8.10807100 |
| H | 2.99990400 | 14.88536200 | 7.18479900 |
| C | -0.08086600 | 16.03877400 | 6.44857800 |
| H | 0.27106100 | 16.59253700 | 5.57725500 |
| H | -0.97582300 | 15.50633600 | 6.14355800 |
| C | -0.90975100 | 11.98519000 | 3.96364900 |
| H | -1.93923200 | 11.76034400 | 3.67303400 |
| H | -0.76516600 | 13.05152200 | 3.82833700 |
| C | -1.75460200 | 10.56046200 | 5.77111100 |
| H | -2.76026600 | 10.94918400 | 5.61994700 |
| H | -1.66259400 | 10.37545300 | 6.84281600 |
| C | 0.09114200 | 11.24117400 | 3.08856400 |
| H | 0.10117600 | 10.16240900 | 3.24716400 |
| H | -0.17321900 | 11.42736300 | 2.04328900 |
| H | 1.10274800 | 11.61605900 | 3.25077400 |
| C | -1.62307600 | 9.26965700 | 4.96384100 |
| H | -2.30134000 | 8.53471400 | 5.40768200 |
| H | -1.93679600 | 9.41184400 | 3.92715400 |
| H | -0.62053100 | 8.84080300 | 4.95845300 |
| C | -0.39262700 | 16.96438700 | 7.61519100 |
| H | -1.21476200 | 17.62260800 | 7.32193400 |
| H | -0.71212900 | 16.39906500 | 8.49411400 |
| H | 0.45013000 | 17.60082800 | 7.89987000 |
| C | 2.71716600 | 16.77491100 | 6.18013500 |
| H | 3.73129800 | 17.05170400 | 6.48203200 |
| H | 2.74898200 | 16.45302100 | 5.13983600 |
| H | 2.10053000 | 17.67393300 | 6.25552300 |

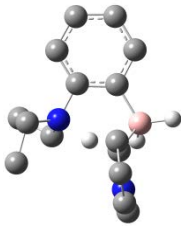
**3-close**



**Sum of electronic and thermal Enthalpies= -469.929209**
**Sum of electronic and thermal Free Energies= -469.977184**

| | | | |
|---|---|---|---|
| C | -1.23966700 | -2.38317700 | 0.62853300 |
| C | 0.10067700 | -2.15340400 | 0.87632900 |
| C | 0.87079300 | -3.22636200 | 1.31266100 |
| C | 0.24896700 | -4.46809200 | 1.47472800 |
| C | -1.11196400 | -4.65056000 | 1.21098300 |
| C | -1.90462200 | -3.58727400 | 0.77189600 |
| H | 1.93032100 | -3.12013400 | 1.52693500 |
| H | 0.83356000 | -5.31823300 | 1.81455500 |
| H | -1.55739100 | -5.63059400 | 1.34931900 |
| H | -2.96264200 | -3.71401800 | 0.56328000 |
| N | -1.69839400 | -1.05261400 | 0.20002100 |
| B | -0.03603300 | -0.60212000 | 0.46749900 |
| H | 0.44271900 | -0.24657200 | -0.58440100 |
| H | 0.00365000 | 0.22442500 | 1.34917200 |
| C | -2.68058100 | -0.49881400 | 1.17084900 |
| C | -2.89409700 | 1.00728200 | 1.10527400 |
| H | -2.28160100 | -0.75918400 | 2.15359600 |
| H | -3.62964300 | -1.03690100 | 1.04839700 |
| H | -3.37380900 | 1.33277700 | 2.03222300 |
| H | -1.93676600 | 1.52590300 | 1.01930600 |
| H | -3.53834400 | 1.31172400 | 0.28019800 |
| C | -2.13874900 | -1.08183700 | -1.22116200 |
| C | -2.20222500 | 0.26943400 | -1.91981300 |
| H | -3.10627800 | -1.59800800 | -1.27312800 |
| H | -1.40499100 | -1.71084000 | -1.72983300 |
| H | -2.23197300 | 0.10275500 | -2.99996500 |
| H | -3.08795500 | 0.84680400 | -1.65420400 |
| H | -1.31150200 | 0.85915600 | -1.69255400 |

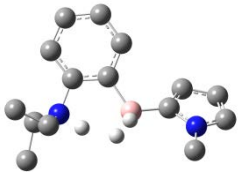
**3-TS1-p**



**Sum of electronic and thermal Enthalpies= -719.232799**
**Sum of electronic and thermal Free Energies= -719.298921**

| | | | |
|---|---|---|---|
| H | 0.26413800 | 0.24595100 | 0.02660500 |
| C | 1.33976000 | 0.13413500 | -0.07461600 |
| C | 2.13736500 | 1.25281300 | -0.29513800 |
| C | 1.92033300 | -1.12631300 | 0.03561800 |
| C | 3.52909800 | 1.16691100 | -0.43091800 |
| H | 1.67518200 | 2.23429400 | -0.35511200 |
| C | 3.29870400 | -1.25640300 | -0.08932600 |
| H | 1.30721800 | -2.00342300 | 0.21790600 |
| C | 4.07698100 | -0.12440000 | -0.32997900 |
| H | 3.76137100 | -2.23521400 | -0.00267200 |
| B | 4.45888700 | 2.47028300 | -0.64625000 |
| C | 5.97756700 | -0.35761700 | -1.85616100 |
| H | 5.42311600 | 0.38663700 | -2.43114100 |
| H | 7.03377800 | -0.06855800 | -1.89559800 |
| C | 6.18548500 | -1.07817000 | 0.52590500 |
| H | 5.72694100 | -0.84289200 | 1.49069800 |
| H | 5.99496500 | -2.14165100 | 0.33076600 |
| N | 5.52071400 | -0.21664500 | -0.46026000 |
| H | 3.87942900 | 3.50783100 | -0.39545200 |
| C | 7.68578300 | -0.82068800 | 0.59943800 |
| H | 7.88901300 | 0.24118400 | 0.77028200 |
| H | 8.11274000 | -1.38528200 | 1.43208200 |
| H | 8.20362300 | -1.13488500 | -0.31111300 |
| C | 5.78794700 | -1.74688100 | -2.45529000 |
| H | 4.73814400 | -2.04833700 | -2.40798600 |
| H | 6.09154200 | -1.73968300 | -3.50564700 |
| H | 6.39053700 | -2.50153800 | -1.94042900 |
| H | 4.94111300 | 2.49537300 | -1.76987900 |
| H | 5.81877800 | 1.16061300 | -0.01870900 |
| C | 5.78681000 | 2.31944800 | 0.42712000 |
| C | 5.67761300 | 2.28137900 | 1.83598800 |
| C | 6.76681700 | 2.93327300 | 2.40744200 |
| H | 4.85633800 | 1.80303500 | 2.35343300 |
| C | 7.55241500 | 3.37979400 | 1.34587200 |
| H | 6.98143100 | 3.08004500 | 3.45579200 |
| H | 8.48291400 | 3.93194900 | 1.36059900 |
| N | 6.98472800 | 3.01437600 | 0.18693300 |
| C | 7.49325400 | 3.33340200 | -1.13170800 |
| H | 8.48431400 | 3.77934300 | -1.03318200 |
| H | 7.56413200 | 2.42557400 | -1.73427400 |
| H | 6.82027600 | 4.02830700 | -1.63712100 |

**3-Int1-p**

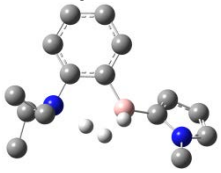


**Sum of electronic and thermal Enthalpies= -719.245846**
**Sum of electronic and thermal Free Energies= -719.306925**

| | | | |
|---|---|---|---|
| H | 0.74969400 | -0.08537100 | 1.79729400 |
| C | 1.70161700 | 0.01956300 | 1.28534800 |
| C | 2.22407600 | 1.28673300 | 1.05376200 |
| C | 2.38134300 | -1.12010300 | 0.85689000 |
| C | 3.44724100 | 1.48166500 | 0.39340100 |
| H | 1.67163300 | 2.16559900 | 1.37143500 |
| C | 3.59787700 | -0.98001600 | 0.20172000 |
| H | 1.96738500 | -2.10826000 | 1.02751800 |
| C | 4.09233800 | 0.30525000 | 0.00298200 |
| H | 4.13548600 | -1.85760700 | -0.14435400 |
| B | 4.12570300 | 2.93596200 | 0.12215100 |
| C | 5.54267900 | -0.20469500 | -1.95987200 |
| H | 4.61817100 | -0.01930700 | -2.51014300 |
| H | 5.59554300 | -1.27458400 | -1.74942600 |
| C | 6.55608900 | 0.47000100 | 0.26530700 |
| H | 7.39114800 | 0.96596700 | -0.23554400 |
| H | 6.26499600 | 1.09289100 | 1.11296300 |
| N | 5.38631100 | 0.53013300 | -0.67261800 |
| H | 4.95664600 | 3.13768300 | 1.00399500 |
| H | 5.28311300 | 1.56478000 | -0.90531800 |
| H | 4.80730400 | 2.88568400 | -0.94732800 |
| C | 6.75220600 | 0.26245900 | -2.75247400 |
| H | 7.69461100 | -0.01773400 | -2.27529600 |
| H | 6.73022300 | -0.20355900 | -3.73992600 |
| H | 6.73736700 | 1.34730500 | -2.89228300 |
| C | 6.92769200 | -0.93404800 | 0.70277200 |
| H | 7.75539200 | -0.87156700 | 1.41284000 |
| H | 6.09176300 | -1.42548500 | 1.20491500 |
| H | 7.25675500 | -1.55704100 | -0.13407400 |
| C | 3.06908500 | 4.12416400 | -0.03428200 |
| C | 1.77772700 | 4.13557700 | -0.53881200 |
| N | 3.35534600 | 5.43650600 | 0.28841600 |
| C | 1.28326500 | 5.46614700 | -0.51700700 |
| H | 1.24969400 | 3.26105800 | -0.89672600 |
| C | 2.28649700 | 6.24763900 | -0.00008900 |
| H | 0.31122200 | 5.81291500 | -0.83957300 |

| | | | |
|---|---|---|---|
| H | 2.33225900 | 7.31072100 | 0.19084000 |
| C | 4.60594800 | 5.90496900 | 0.83896300 |
| H | 4.81216100 | 5.43009000 | 1.80194000 |
| H | 5.43834300 | 5.68336100 | 0.16443000 |
| H | 4.54752500 | 6.98592600 | 0.98258600 |

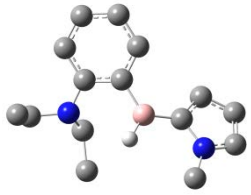
**3-TS2-p**



**Sum of electronic and thermal Enthalpies= -719.225491**
**Sum of electronic and thermal Free Energies= -719.288293**

| | | | |
|---|---|---|---|
| H | 0.75892000 | -0.15765800 | 1.90003300 |
| C | 1.70050000 | -0.03675300 | 1.37325800 |
| C | 2.26104600 | 1.22887000 | 1.23405600 |
| C | 2.33584000 | -1.14471900 | 0.82079300 |
| C | 3.47115000 | 1.42848200 | 0.55951400 |
| H | 1.74227100 | 2.09319800 | 1.63807500 |
| C | 3.54030500 | -0.98149000 | 0.14578500 |
| H | 1.89778400 | -2.13326400 | 0.91604300 |
| C | 4.10313600 | 0.28929700 | 0.03436200 |
| H | 4.03880100 | -1.84245700 | -0.28916100 |
| B | 4.10889800 | 2.88458600 | 0.38630900 |
| C | 5.48507600 | -0.17595900 | -1.94181600 |
| H | 4.53377400 | -0.04373500 | -2.46439300 |
| H | 5.62498500 | -1.25729700 | -1.80312500 |
| C | 6.52792100 | 0.46811700 | 0.23012900 |
| H | 7.34847000 | 0.99606500 | -0.26693300 |
| H | 6.27091200 | 1.05318100 | 1.11668500 |
| N | 5.34911600 | 0.52164100 | -0.65697200 |
| H | 5.03000500 | 3.13768500 | 1.12960600 |
| H | 5.07995800 | 2.07312100 | -0.82343100 |
| H | 4.87375400 | 2.90154500 | -0.86021500 |
| C | 6.62158800 | 0.38073600 | -2.78939600 |
| H | 7.60192400 | 0.17252600 | -2.35200700 |
| H | 6.59914200 | -0.08038700 | -3.77995600 |
| H | 6.52175600 | 1.46282100 | -2.91345600 |
| C | 6.96825600 | -0.93452600 | 0.63719100 |
| H | 7.80238200 | -0.86966600 | 1.34096000 |
| H | 6.15255000 | -1.47164200 | 1.12873300 |
| H | 7.30408600 | -1.52331900 | -0.22181700 |
| C | 3.12449400 | 4.06227600 | 0.05082600 |
| C | 1.85969400 | 4.03170000 | -0.51922800 |
| N | 3.41535500 | 5.39892500 | 0.26453000 |
| C | 1.38386000 | 5.35724600 | -0.64494400 |
| H | 1.34188400 | 3.12786700 | -0.81082100 |
| C | 2.37254900 | 6.17704600 | -0.15041800 |
| H | 0.43389000 | 5.68093900 | -1.04539400 |
| H | 2.41432100 | 7.25281600 | -0.05303800 |
| C | 4.63938500 | 5.91075700 | 0.84094900 |
| H | 4.80515800 | 5.49095400 | 1.83594000 |
| H | 5.50264100 | 5.66563000 | 0.21516400 |
| H | 4.56393800 | 6.99621500 | 0.92490200 |

**3-Int2-p**

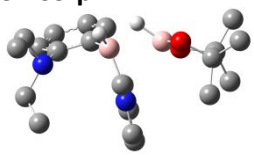


**Sum of electronic and thermal Enthalpies= -718.078296**
**Sum of electronic and thermal Free Energies= -718.141427**

| | | | |
|---|---|---|---|
| C | -2.38925000 | -2.88245400 | 1.00092300 |
| C | -1.01322600 | -2.92963900 | 1.18980700 |
| C | -0.21094700 | -1.85295700 | 0.82535800 |
| C | -0.77727300 | -0.69324800 | 0.28194300 |
| C | -2.18149600 | -0.61231200 | 0.12382200 |
| C | -2.95475400 | -1.73197900 | 0.46168800 |
| H | -3.01401500 | -3.72478700 | 1.27970800 |
| H | -0.55054400 | -3.81764900 | 1.61054200 |
| H | 0.86215300 | -1.93254600 | 0.95751900 |
| H | -4.03269400 | -1.67477800 | 0.33607400 |
| B | -2.87920300 | 0.72504200 | -0.26377000 |
| H | -2.48294100 | 1.73667700 | 0.24813300 |
| C | 1.34875500 | 0.53614300 | 0.42340400 |
| C | -0.07225800 | 0.77935700 | -1.54416200 |
| H | 1.81830300 | 1.38869200 | -0.07508900 |
| H | 1.98072700 | -0.33567400 | 0.17864500 |
| H | 0.78374700 | 0.34710300 | -2.08977000 |
| H | -0.96801000 | 0.32145700 | -1.97065300 |
| N | 0.00698000 | 0.40827300 | -0.12762600 |
| C | -4.04337700 | 0.78161100 | -1.23919700 |
| C | -4.53607100 | -0.20678100 | -2.09880500 |
| C | -5.58053800 | 0.33291100 | -2.86286400 |
| H | -4.14153700 | -1.21213900 | -2.15436700 |
| C | -5.71637900 | 1.65174100 | -2.46107200 |
| H | -6.17133500 | -0.16162100 | -3.61973900 |
| H | -6.40775400 | 2.41298800 | -2.79536100 |
| C | 1.34507300 | 0.79944200 | 1.92463100 |
| H | 0.78275900 | 1.71162000 | 2.13975300 |

| | | | |
|---|---|---|---|
| H | 0.88062600 | -0.02034300 | 2.47767200 |
| H | 2.36806600 | 0.92202800 | 2.29216500 |
| C | -0.12389700 | 2.28596400 | -1.77493200 |
| H | -1.00289800 | 2.71370700 | -1.28632400 |
| H | 0.76211700 | 2.79136400 | -1.37905500 |
| H | -0.17812800 | 2.49967600 | -2.84667600 |
| N | -4.80017300 | 1.91992700 | -1.50273400 |
| C | -4.64162100 | 3.20199100 | -0.84602700 |
| H | -4.78794200 | 3.10275800 | 0.23149600 |
| H | -3.64315100 | 3.60696000 | -1.02652500 |
| H | -5.38305500 | 3.89753200 | -1.24191100 |

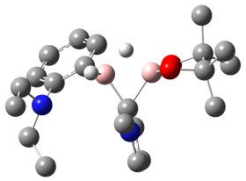
**3-TS3-p**



**Sum of electronic and thermal Enthalpies= -1129.655132**
**Sum of electronic and thermal Free Energies= -1129.735999**

| | | | |
|---|---|---|---|
| C | -2.20880100 | -1.92821100 | 0.75603400 |
| C | -0.84274900 | -1.73741000 | 0.55775700 |
| C | -0.30360400 | -0.45749000 | 0.40506300 |
| C | -1.17949900 | 0.63703000 | 0.45559200 |
| C | -2.54818800 | 0.45037300 | 0.64557600 |
| C | -3.06419000 | -0.83292800 | 0.80190500 |
| H | -2.60364900 | -2.93195500 | 0.88159000 |
| H | -0.18451900 | -2.60225200 | 0.54959200 |
| H | -3.20960500 | 1.31265900 | 0.67243700 |
| H | -4.12954800 | -0.97572600 | 0.95539600 |
| C | -0.72040900 | 2.39679000 | -1.10230600 |
| C | -0.95359300 | 2.93759900 | 1.29433600 |
| H | -1.76222800 | 2.68505800 | -1.34014500 |
| H | -0.47669700 | 1.54315600 | -1.74218200 |
| H | -1.58780800 | 3.72663200 | 0.85887700 |
| H | -1.55552400 | 2.45428300 | 2.06985600 |
| N | -0.60442200 | 1.94059700 | 0.28034000 |
| B | 1.23626800 | -0.07934800 | 0.25586300 |
| H | 1.71580300 | -1.39578500 | -0.27571400 |
| C | 1.98291100 | 0.29508000 | 1.59410700 |
| C | 1.58388500 | 0.06183500 | 2.90818400 |
| C | 2.41118300 | 0.80607600 | 3.76942300 |
| H | 0.76454100 | -0.58694500 | 3.18437400 |
| C | 3.30576500 | 1.48691200 | 2.96237000 |
| H | 2.36558300 | 0.85705700 | 4.84750500 |
| H | 4.10447100 | 2.16766800 | 3.22087300 |
| H | 1.61574000 | 0.47042000 | -0.74370200 |
| B | 2.54012300 | -1.75578600 | 0.56824500 |
| O | 3.86876200 | -1.63264200 | 0.28035500 |
| O | 2.22583700 | -2.75456700 | 1.44067600 |
| C | 4.56694700 | -2.41766000 | 1.27779000 |
| C | 3.46165300 | -3.44101300 | 1.74769300 |
| C | 5.78041000 | -3.05420200 | 0.61527400 |
| H | 6.48635500 | -2.27390000 | 0.32006000 |
| H | 6.28868300 | -3.72580500 | 1.31392100 |
| H | 5.50484200 | -3.61775300 | -0.27711000 |
| C | 5.01483700 | -1.46244300 | 2.38218000 |
| H | 5.62011800 | -0.66870800 | 1.93653700 |
| H | 4.16538100 | -0.99786700 | 2.88601200 |
| H | 5.62376500 | -1.98373100 | 3.12620100 |
| C | 3.47964500 | -3.74894500 | 3.23803500 |
| H | 2.68360200 | -4.45934600 | 3.47418100 |
| H | 4.43504000 | -4.19766700 | 3.52723300 |
| H | 3.31682700 | -2.84598300 | 3.82807600 |
| C | 3.44872400 | -4.73524700 | 0.93483800 |
| H | 4.32624200 | -5.35144900 | 1.14885600 |
| H | 2.55296400 | -5.30453500 | 1.19450400 |
| H | 3.41816700 | -4.52820000 | -0.13821100 |
| C | 0.27969000 | 3.55292300 | 1.95299300 |
| H | 0.85273700 | 2.77931800 | 2.46992500 |
| H | 0.93455300 | 4.02184600 | 1.21383300 |
| H | -0.01489400 | 4.31505300 | 2.68272300 |
| C | 0.21327400 | 3.55058900 | -1.44268600 |
| H | -0.02808400 | 4.45518900 | -0.87670100 |
| H | 1.25009300 | 3.27636800 | -1.22659100 |
| H | 0.13168800 | 3.79426400 | -2.50606900 |
| N | 3.05311400 | 1.17303100 | 1.66702400 |
| C | 3.78471800 | 1.68809200 | 0.52949000 |
| H | 4.60469500 | 2.31117900 | 0.89013700 |
| H | 4.18951300 | 0.85955300 | -0.05587100 |
| H | 3.12952400 | 2.29087800 | -0.10383000 |

**3-Int3-p**

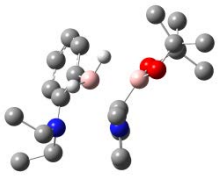


**Sum of electronic and thermal Enthalpies= -1129.658179**
**Sum of electronic and thermal Free Energies= -1129.744102**

| | | | |
|---|---|---|---|
| C | -2.11623000 | -1.90576200 | 0.98167200 |
| C | -0.75886300 | -1.68430400 | 0.76006000 |
| C | -0.25093000 | -0.40143000 | 0.53252800 |
| C | -1.15623900 | 0.67385900 | 0.52752900 |
| C | -2.51917200 | 0.45219400 | 0.73138800 |
| C | -2.99950200 | -0.83299000 | 0.96734600 |

| | | | |
|---|---|---|---|
| H | -2.48095900 | -2.91163500 | 1.16660500 |
| H | -0.06989100 | -2.52421200 | 0.79681800 |
| H | -3.21036300 | 1.29048800 | 0.70364100 |
| H | -4.06098600 | -0.99306600 | 1.13120800 |
| C | -0.63751200 | 2.30412300 | -1.14532300 |
| C | -1.13324400 | 3.05545500 | 1.14797700 |
| H | -1.66455200 | 2.50724400 | -1.50448800 |
| H | -0.29171700 | 1.41108500 | -1.67320200 |
| H | -1.77950400 | 3.74808600 | 0.58453400 |
| H | -1.76165800 | 2.61584200 | 1.92798400 |
| N | -0.63692200 | 1.98718400 | 0.28123800 |
| B | 1.30066400 | -0.10358700 | 0.33411500 |
| H | 1.82785200 | -1.24911700 | 0.03299100 |
| C | 2.06399100 | 0.36008400 | 1.73058500 |
| C | 1.51253900 | 0.33778300 | 3.02623700 |
| C | 2.14001200 | 1.30313900 | 3.80481500 |
| H | 0.75227700 | -0.36462900 | 3.33580400 |
| C | 3.06388400 | 1.93592000 | 2.97364100 |
| H | 1.96301000 | 1.53278100 | 4.84477300 |
| H | 3.74573600 | 2.74685400 | 3.19022200 |
| H | 1.68151300 | 0.56186800 | -0.58938800 |
| B | 2.59533000 | -1.19106600 | 1.16034800 |
| O | 3.93003000 | -1.24884300 | 0.71476200 |
| O | 2.29041800 | -2.27839700 | 1.99620600 |
| C | 4.59334900 | -2.13793100 | 1.62512500 |
| C | 3.44172700 | -3.13269800 | 1.99681800 |
| C | 5.77866500 | -2.77152800 | 0.91269000 |
| H | 6.52927200 | -2.00835600 | 0.68996000 |
| H | 6.24470900 | -3.53314400 | 1.54596200 |
| H | 5.47424300 | -3.23350400 | -0.02757600 |
| C | 5.07066300 | -1.31352100 | 2.82585400 |
| H | 5.70494200 | -0.50046000 | 2.46179800 |
| H | 4.22730800 | -0.87219300 | 3.36563800 |
| H | 5.65529800 | -1.91962000 | 3.52363900 |
| C | 3.57619300 | -3.76784900 | 3.37385900 |
| H | 2.74524400 | -4.45657700 | 3.54752200 |
| H | 4.51039700 | -4.33396300 | 3.44927800 |
| H | 3.55839000 | -3.01008200 | 4.15881300 |
| C | 3.22937800 | -4.20979600 | 0.93048600 |
| H | 4.03268300 | -4.95216000 | 0.93669700 |
| H | 2.28442200 | -4.72071000 | 1.13222700 |
| H | 3.17111400 | -3.76493600 | -0.06689000 |
| C | 0.00096100 | 3.82160700 | 1.82643100 |
| H | 0.59235500 | 3.13726500 | 2.43983200 |
| H | 0.67060900 | 4.28119300 | 1.09508900 |
| H | -0.39766500 | 4.61293000 | 2.47088700 |
| C | 0.26471700 | 3.47487700 | -1.51173700 |
| H | -0.08727400 | 4.41513500 | -1.07713000 |
| H | 1.28357800 | 3.29315200 | -1.15685800 |
| H | 0.29122100 | 3.60250800 | -2.59787500 |
| N | 3.01945300 | 1.38851900 | 1.75281100 |
| C | 3.81380800 | 1.81758600 | 0.61883900 |
| H | 4.54358400 | 2.55297700 | 0.95985500 |
| H | 4.32566000 | 0.95337900 | 0.19362900 |
| H | 3.16757600 | 2.26737400 | -0.13779600 |

**3-TS4-p**

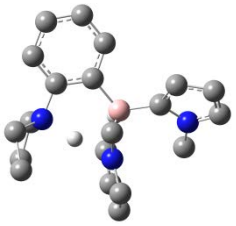


**Sum of electronic and thermal Enthalpies= -1129.659991**
**Sum of electronic and thermal Free Energies= -1129.741222**

| | | | |
|---|---|---|---|
| C | -1.98550300 | -1.64282400 | 0.98383800 |
| C | -1.11605000 | -0.62069900 | 0.51736000 |
| C | -0.08129000 | -1.01564300 | -0.34456800 |
| C | 0.13715100 | -2.32883900 | -0.73893800 |
| C | -0.70941000 | -3.31606500 | -0.25236000 |
| C | -1.75783500 | -2.97407200 | 0.58872900 |
| H | 0.60275200 | -0.24790300 | -0.69689500 |
| H | 0.95925700 | -2.57743800 | -1.40274500 |
| H | -0.56905500 | -4.35555200 | -0.53489800 |
| H | -2.42381700 | -3.75918700 | 0.92746300 |
| N | -3.03223500 | -1.36483600 | 1.88198600 |
| B | -1.14681900 | 0.92614800 | 0.91119500 |
| H | -2.10343400 | 1.59838600 | 0.61269400 |
| H | -0.16267100 | 1.48783400 | 0.43767800 |
| C | 2.42245100 | 2.60343200 | 1.74618700 |
| C | 2.73963200 | 1.13011100 | 2.18581600 |
| O | 1.05051300 | 2.75523000 | 2.16526300 |
| O | 1.45725400 | 0.48856100 | 2.09545100 |
| B | 0.50259900 | 1.48247500 | 2.15176200 |
| C | 3.25819200 | 3.66956100 | 2.43984700 |
| H | 2.97856000 | 4.65871400 | 2.06768300 |
| H | 3.10467800 | 3.65530100 | 3.52003600 |
| H | 4.32223500 | 3.51662000 | 2.23378400 |
| C | 2.47221200 | 2.80069400 | 0.23017800 |
| H | 2.03651900 | 3.77308400 | -0.01254900 |
| H | 3.50075000 | 2.77700700 | -0.14046300 |
| H | 1.89566900 | 2.03315900 | -0.29187600 |
| C | 3.71699900 | 0.39309600 | 1.28092200 |
| H | 4.68072600 | 0.91131000 | 1.24638700 |
| H | 3.88309500 | -0.61554600 | 1.66720600 |
| H | 3.32493600 | 0.30332200 | 0.26678200 |
| C | 3.18685700 | 1.02738400 | 3.64564300 |
| H | 3.18925200 | -0.02589200 | 3.93647400 |
| H | 4.19303700 | 1.43077700 | 3.79156900 |
| H | 2.49599900 | 1.56011200 | 4.30499600 |
| C | -0.96770500 | 1.19794600 | 2.67664700 |
| C | -1.19758500 | 0.11866700 | 3.57059400 |
| C | -2.05377500 | 0.53027600 | 4.57738800 |
| H | -0.73491000 | -0.84980100 | 3.45043700 |
| C | -2.36331000 | 1.86636300 | 4.30587000 |
| H | -2.42834100 | -0.04827900 | 5.40831300 |
| H | -3.01034600 | 2.54219800 | 4.84971000 |
| N | -1.72348600 | 2.27269200 | 3.21058800 |
| C | -1.84008400 | 3.58633900 | 2.60595700 |
| H | -0.84675400 | 4.01700700 | 2.47662100 |
| H | -2.31795700 | 3.49320900 | 1.62770100 |
| H | -2.44542100 | 4.22100400 | 3.25417300 |
| C | -3.94632200 | -0.25393800 | 1.65126600 |

| | | | |
|---|---|---|---|
| H | -4.74122300 | -0.33937200 | 2.39877500 |
| H | -3.45341000 | 0.70191500 | 1.84489300 |
| C | -3.53282600 | -2.40011300 | 2.76582900 |
| H | -3.78534000 | -1.92245500 | 3.72357500 |
| H | -2.71332300 | -3.09217000 | 2.97994300 |
| C | -4.75916000 | -3.17541900 | 2.26965900 |
| H | -5.05257400 | -3.93439700 | 3.00171800 |
| H | -5.61280700 | -2.50598100 | 2.12446700 |
| H | -4.56409200 | -3.67172700 | 1.31532000 |
| C | -4.55332700 | -0.22800000 | 0.25129900 |
| H | -5.25726000 | 0.60480100 | 0.15572600 |
| H | -3.77028100 | -0.10051500 | -0.50079700 |
| H | -5.08358900 | -1.16062600 | 0.03613600 |

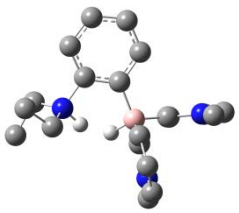
**3-TS5-p**



**Sum of electronic and thermal Enthalpies= -967.376123**
**Sum of electronic and thermal Free Energies= -967.448869**

| | | | |
|---|---|---|---|
| C | 1.34946300 | 0.04006800 | 1.09658900 |
| C | 2.15402300 | 1.16600300 | 0.96018500 |
| C | 1.85342300 | -1.22157600 | 0.79533200 |
| C | 3.48839800 | 1.09790400 | 0.52808900 |
| C | 3.15868500 | -1.33397000 | 0.33620300 |
| H | 1.23391400 | -2.10692000 | 0.89810600 |
| C | 3.94870700 | -0.19082300 | 0.20827300 |
| B | 4.40166200 | 2.43060500 | 0.33051000 |
| H | 5.82072400 | 0.96129800 | 0.11990400 |
| N | 5.29200300 | -0.30020900 | -0.34607800 |
| C | 6.09559300 | -1.43824700 | 0.14877000 |
| C | 5.22458200 | -0.19491200 | -1.82287600 |
| H | 5.60985500 | -1.82012100 | 1.04940100 |
| H | 4.63116200 | 0.69795800 | -2.03361100 |
| H | 6.07838700 | -2.25053800 | -0.59024900 |
| H | 4.66976900 | -1.06108800 | -2.21175200 |
| C | 6.07414800 | 2.08963300 | 0.61679300 |
| C | 7.12716400 | 2.73561300 | -0.07004600 |
| C | 8.19191200 | 2.95734200 | 0.79833200 |
| H | 7.07632300 | 3.00157200 | -1.11784600 |
| C | 7.79520300 | 2.44783300 | 2.03381300 |
| H | 9.14236000 | 3.42395300 | 0.58497700 |
| H | 8.32747000 | 2.42484500 | 2.97545100 |
| H | 0.32421000 | 0.14834500 | 1.43817100 |
| H | 3.55708500 | -2.30752100 | 0.06336600 |
| H | 1.73855200 | 2.14093000 | 1.19244500 |
| C | 6.57915200 | -0.08477800 | -2.50768800 |
| H | 7.16400400 | 0.74270800 | -2.09869100 |
| H | 7.16381500 | -1.00413200 | -2.41716400 |
| H | 6.42318600 | 0.10138400 | -3.57347100 |
| C | 7.53574100 | -1.06202000 | 0.49325800 |
| H | 8.07342000 | -1.95498200 | 0.82453700 |
| H | 8.07090600 | -0.63846400 | -0.35771000 |
| H | 7.56559700 | -0.32630400 | 1.30005400 |
| N | 6.56445700 | 1.92884600 | 1.92605400 |
| C | 5.80449600 | 1.35185500 | 3.01737300 |
| H | 5.28610800 | 0.45598300 | 2.67100500 |
| H | 6.48460700 | 1.08680800 | 3.82858000 |
| H | 5.06179500 | 2.07380600 | 3.36564700 |
| H | 4.41631600 | 2.71303800 | -0.86090900 |
| C | 3.99086800 | 3.67525900 | 1.25525100 |
| C | 3.35485100 | 3.73791800 | 2.49055400 |
| N | 4.33547600 | 4.98162400 | 0.95458200 |
| C | 3.32042300 | 5.08573100 | 2.93089000 |
| H | 2.92750900 | 2.88943600 | 3.00869200 |
| C | 3.93878200 | 5.82827200 | 1.95702000 |
| H | 2.87858400 | 5.47000800 | 3.83945200 |
| H | 4.11892300 | 6.89151600 | 1.88277300 |
| C | 5.08039600 | 5.41883400 | -0.20434400 |
| H | 6.15571600 | 5.26163600 | -0.06956300 |
| H | 4.75669500 | 4.86466900 | -1.08647200 |
| H | 4.89599700 | 6.48289400 | -0.36821600 |

**3-Int4-p**

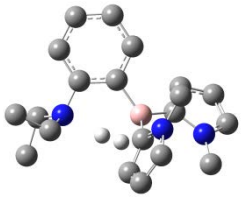


**Sum of electronic and thermal Enthalpies= -967.393709**
**Sum of electronic and thermal Free Energies= -967.470335**

| | | | |
|---|---|---|---|
| H | 0.79819600 | 0.57580900 | 2.04601600 |
| C | 1.75279900 | 0.50789300 | 1.53312500 |
| C | 2.39001400 | 1.66621300 | 1.10167200 |
| C | 2.32149200 | -0.74196200 | 1.29628900 |

| | | | |
|---|---|---|---|
| C | 3.62314400 | 1.63599800 | 0.43735400 |
| H | 1.91383100 | 2.63014100 | 1.25748200 |
| C | 3.53294900 | -0.82403600 | 0.62072400 |
| H | 1.82154300 | -1.64792100 | 1.62204900 |
| C | 4.15062600 | 0.35930400 | 0.22968700 |
| H | 3.97148000 | -1.79305800 | 0.40474800 |
| B | 4.42457100 | 2.96998500 | -0.06531700 |
| C | 5.29643700 | -0.43646500 | -1.81082300 |
| H | 4.38909800 | -0.05481300 | -2.28328700 |
| H | 5.12991600 | -1.48719400 | -1.56771000 |
| C | 6.65318300 | 0.05465200 | 0.28021600 |
| H | 7.50068800 | 0.35655400 | -0.33950900 |
| H | 6.60201300 | 0.75267500 | 1.11850300 |
| N | 5.41945900 | 0.33214900 | -0.53333300 |
| H | 5.48298700 | 1.34052900 | -0.82080700 |
| H | 4.94415100 | 2.69997300 | -1.18141800 |
| C | 6.49929900 | -0.25419400 | -2.72042600 |
| H | 7.39860600 | -0.73098700 | -2.32331500 |
| H | 6.28261900 | -0.71041800 | -3.68880100 |
| H | 6.70689700 | 0.80669200 | -2.88956700 |
| C | 6.79868800 | -1.38220100 | 0.74241400 |
| H | 7.75069800 | -1.47471500 | 1.27014900 |
| H | 6.00596600 | -1.66257100 | 1.43813000 |
| H | 6.81317800 | -2.09549300 | -0.08745200 |
| C | 3.46076100 | 4.22002500 | -0.37451900 |
| C | 2.92122000 | 4.62229800 | -1.58459600 |
| N | 2.99275100 | 5.12372900 | 0.56574200 |
| C | 2.12263400 | 5.77695600 | -1.37719800 |
| H | 3.09199800 | 4.11630400 | -2.52605200 |
| C | 2.19224700 | 6.06206000 | -0.03653300 |
| H | 1.56029500 | 6.33188500 | -2.11524600 |
| H | 1.74299800 | 6.85656600 | 0.54286200 |
| C | 3.36665200 | 5.17466800 | 1.96487000 |
| H | 3.26420500 | 4.19367700 | 2.43258600 |
| H | 4.40485700 | 5.49487100 | 2.09267100 |
| H | 2.70791500 | 5.87905700 | 2.47768700 |
| C | 5.61454500 | 3.28149900 | 0.98417100 |
| C | 5.87001600 | 2.78192000 | 2.25345500 |
| N | 6.58147500 | 4.23795100 | 0.75484000 |
| C | 7.00595000 | 3.44676900 | 2.79021100 |
| H | 5.25701800 | 2.04322300 | 2.75562600 |
| C | 7.42286500 | 4.34059100 | 1.83472700 |
| H | 7.45621000 | 3.30205200 | 3.76237600 |
| H | 8.24542700 | 5.04200900 | 1.82945300 |
| C | 6.73218200 | 4.98433800 | -0.47654100 |
| H | 7.28684000 | 5.90351900 | -0.27606100 |
| H | 7.27532000 | 4.40351200 | -1.23101100 |
| H | 5.74935300 | 5.23916000 | -0.87796000 |

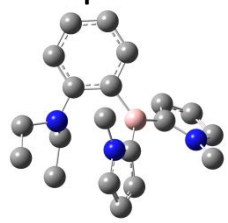
**3-TS6-p**



**Sum of electronic and thermal Enthalpies= -967.368544**
**Sum of electronic and thermal Free Energies= -967.442858**

| | | | |
|---|---|---|---|
| H | 1.16253000 | 0.07590400 | 2.31408600 |
| C | 2.03390600 | 0.12403700 | 1.66819700 |
| C | 2.62206600 | 1.35224200 | 1.38616900 |
| C | 2.55168100 | -1.03582900 | 1.10306900 |
| C | 3.74817600 | 1.46797300 | 0.55969800 |
| H | 2.18032900 | 2.25562000 | 1.79647000 |
| C | 3.66669500 | -0.95567300 | 0.27761000 |
| H | 2.09154300 | -1.99881800 | 1.30097200 |
| C | 4.27385200 | 0.27666900 | 0.02731300 |
| H | 4.07144300 | -1.85769200 | -0.17063300 |
| B | 4.39199900 | 2.91240700 | 0.26703700 |
| C | 5.29556500 | -0.27286100 | -2.11999100 |
| H | 4.33680600 | 0.06125900 | -2.52877100 |
| H | 5.23619200 | -1.36856300 | -2.03391000 |
| C | 6.70420400 | 0.12087400 | -0.10331700 |
| H | 7.51464300 | 0.56906200 | -0.68715400 |
| H | 6.65976000 | 0.68808300 | 0.82827900 |
| N | 5.43944000 | 0.37859700 | -0.81433200 |
| H | 5.23016700 | 2.09476400 | -1.05408800 |
| H | 5.00095700 | 2.86669800 | -1.16070600 |
| C | 6.41789700 | 0.09862100 | -3.08061900 |
| H | 7.37731200 | -0.32726600 | -2.77410100 |
| H | 6.19184900 | -0.28526100 | -4.07878500 |
| H | 6.53093900 | 1.18477800 | -3.14803600 |
| C | 7.01804100 | -1.34572900 | 0.18471400 |
| H | 7.97862600 | -1.41832700 | 0.70227600 |
| H | 6.25632500 | -1.79645700 | 0.82641400 |
| H | 7.09149000 | -1.93822600 | -0.73305300 |
| C | 3.35158100 | 4.04573900 | -0.07235000 |
| C | 2.04070200 | 3.88900200 | -0.51051700 |
| C | 1.47699000 | 5.16012900 | -0.74233800 |
| H | 1.55419800 | 2.93372500 | -0.65052100 |
| C | 2.45801700 | 6.07890500 | -0.44355300 |
| H | 0.47713000 | 5.38518100 | -1.08414100 |
| H | 2.44115600 | 7.15928400 | -0.47932400 |
| C | 5.73414400 | 3.28654200 | 1.04476300 |
| C | 7.04249100 | 3.43196600 | 0.61876200 |
| C | 7.83052600 | 3.86506600 | 1.71640100 |
| H | 7.38648600 | 3.25547100 | -0.39221000 |
| C | 6.98306700 | 3.97375600 | 2.79099500 |
| H | 8.89091700 | 4.07280700 | 1.72050900 |
| H | 7.16947700 | 4.25744300 | 3.81678900 |
| N | 3.58136500 | 5.41667500 | -0.04674800 |
| N | 5.72160700 | 3.62319900 | 2.38084400 |
| C | 4.80687400 | 6.09850600 | 0.33134500 |
| H | 5.04844300 | 5.93163200 | 1.38368200 |
| H | 5.65045000 | 5.74801200 | -0.26443500 |
| H | 4.66915900 | 7.16801200 | 0.16414400 |
| C | 4.55363900 | 3.59301600 | 3.23644200 |
| H | 3.71953300 | 4.11206900 | 2.75491500 |
| H | 4.24697200 | 2.56469400 | 3.44879300 |
| H | 4.78480900 | 4.09732700 | 4.17609900 |

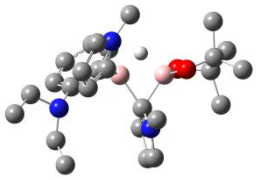
**3-Int5-p**



**Sum of electronic and thermal Enthalpies= -966.22585**
**Sum of electronic and thermal Free Energies= -966.299661**

| | | | |
|---|---|---|---|
| C | -6.69722500 | 1.36441800 | -0.11292000 |
| C | -5.31765100 | 1.62329500 | -0.28743100 |
| C | -4.90307400 | 2.89419500 | -0.70106900 |
| C | -5.83087100 | 3.89533600 | -0.97351800 |
| C | -7.18736900 | 3.66034500 | -0.79235500 |
| C | -7.60063900 | 2.41013400 | -0.34112400 |
| H | -3.84568100 | 3.11863500 | -0.79349400 |
| H | -5.48233800 | 4.87042700 | -1.30134300 |
| H | -7.91445000 | 4.44227800 | -0.98646700 |
| H | -8.65923700 | 2.22680300 | -0.17713600 |
| C | -3.12401700 | 0.56673900 | -0.72170800 |
| C | -4.28301700 | 0.27778300 | 1.42931800 |
| H | -2.29348400 | 0.83211400 | -0.04767900 |
| H | -3.14470900 | 1.33350800 | -1.49937500 |
| H | -3.67287500 | 1.05097300 | 1.93264200 |
| H | -5.28392200 | 0.34347200 | 1.86262400 |
| B | -7.26925000 | -0.05414700 | 0.27406800 |
| N | -4.39373300 | 0.58175200 | -0.00094400 |
| C | -8.24672600 | -0.09688900 | 1.46414200 |
| C | -8.23860000 | 0.79116800 | 2.54185200 |
| C | -9.18280100 | 0.36785400 | 3.49341900 |
| H | -7.58573600 | 1.65075100 | 2.60917300 |
| C | -9.77995600 | -0.76033200 | 2.96865100 |
| H | -9.41822800 | 0.82911400 | 4.44126000 |
| H | -10.58583500 | -1.36827900 | 3.35650000 |
| C | -6.83325800 | -1.34136200 | -0.45771100 |
| C | -6.63658900 | -2.59377800 | 0.12172100 |
| C | -6.02528900 | -3.44211900 | -0.82181600 |
| H | -6.87824200 | -2.83170300 | 1.14888800 |
| C | -5.88345000 | -2.69779100 | -1.97527600 |
| H | -5.73629800 | -4.47479800 | -0.69200900 |
| H | -5.49712100 | -2.97728900 | -2.94555400 |
| C | -2.83813100 | -0.77151200 | -1.40610800 |
| H | -2.83768800 | -1.60434000 | -0.70226200 |
| H | -3.60319500 | -0.98506300 | -2.15597300 |
| H | -1.86351300 | -0.73675300 | -1.90470800 |
| C | -3.71036800 | -1.09829500 | 1.74080800 |
| H | -2.65161400 | -1.17346800 | 1.47659300 |
| H | -3.79293100 | -1.28755500 | 2.81522000 |
| H | -4.26537200 | -1.87245900 | 1.20447000 |
| N | -6.35835500 | -1.44291500 | -1.75406100 |
| N | -9.21852200 | -1.04755500 | 1.76498900 |
| C | -6.35151700 | -0.38983600 | -2.74952400 |
| H | -7.28351900 | 0.17529000 | -2.70721300 |
| H | -5.52388600 | 0.30432700 | -2.58425000 |
| H | -6.25442600 | -0.83987400 | -3.73930300 |
| C | -9.71268700 | -2.10741900 | 0.90302700 |
| H | -9.49857700 | -1.86705100 | -0.13664900 |
| H | -9.24175200 | -3.06673300 | 1.13080200 |
| H | -10.79325500 | -2.19880300 | 1.03421000 |

**3-Int6-p**

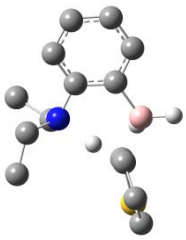


**Sum of electronic and thermal Enthalpies= -1377.795862**
**Sum of electronic and thermal Free Energies= -1377.890904**

| | | | |
|---|---|---|---|
| C | -1.61234700 | -2.12293800 | 0.04084800 |
| C | -0.28897200 | -1.69460300 | 0.03311600 |
| C | 0.06407400 | -0.33958700 | 0.12565700 |
| C | -0.98406800 | 0.59103900 | 0.21171800 |
| C | -2.31421300 | 0.16068000 | 0.22953600 |
| C | -2.63497800 | -1.18874800 | 0.14998000 |
| H | -1.83962200 | -3.18246900 | -0.02808500 |
| H | 0.49687500 | -2.44316600 | -0.01090900 |
| H | -3.10708900 | 0.90041500 | 0.30626200 |
| H | -3.67374400 | -1.50484500 | 0.16878800 |
| C | -1.22094500 | 2.65598000 | 1.46954300 |
| H | -2.21138900 | 3.11195000 | 1.29393800 |
| H | -1.37026800 | 1.87995100 | 2.22637800 |
| N | -0.69777500 | 2.00372700 | 0.26516700 |
| B | 1.61434600 | 0.09120600 | 0.18236900 |
| H | 2.19108700 | -1.05181800 | -0.05305800 |
| C | 2.11779000 | 0.39168500 | 1.77399500 |
| C | 1.20965200 | 0.30264400 | 2.85467100 |
| C | 1.60677700 | 1.16103200 | 3.86560400 |
| H | 0.36106100 | -0.36620900 | 2.85707300 |
| C | 2.76684600 | 1.78649400 | 3.40706600 |
| H | 1.13320400 | 1.32632700 | 4.82146600 |
| H | 3.39408500 | 2.51690200 | 3.90024500 |
| B | 2.72994200 | -1.09193200 | 1.19865200 |
| O | 4.13434200 | -1.14854000 | 1.04964800 |
| O | 2.24822000 | -2.27832900 | 1.78758400 |

| | | | |
|---|---|---|---|
| C | 4.54932100 | -2.45445600 | 1.47878100 |
| C | 3.37970800 | -2.87134600 | 2.43129900 |
| C | 4.64466600 | -3.35082400 | 0.24234800 |
| H | 5.33281400 | -2.89534700 | -0.47524700 |
| H | 5.02360000 | -4.34584500 | 0.49266900 |
| H | 3.66726100 | -3.46080200 | -0.23640200 |
| C | 5.91008900 | -2.33145700 | 2.14952800 |
| H | 6.66239400 | -2.03994300 | 1.41168900 |
| H | 5.89421000 | -1.57454000 | 2.93532400 |
| H | 6.21387200 | -3.28773300 | 2.58728100 |
| C | 3.51619100 | -2.25352700 | 3.82789300 |
| H | 2.56974000 | -2.38132000 | 4.35881900 |
| H | 4.31000300 | -2.73526300 | 4.40613100 |
| H | 3.72444500 | -1.18089400 | 3.77035900 |
| C | 3.14905000 | -4.37125900 | 2.54170000 |
| H | 4.04240500 | -4.87162200 | 2.92925500 |
| H | 2.32313200 | -4.56700400 | 3.23033400 |
| H | 2.89327800 | -4.80543400 | 1.57393700 |
| C | 2.25596300 | 1.05686300 | -0.90307800 |
| C | 2.22165800 | 2.43753500 | -0.98302000 |
| C | 2.93762900 | 2.84615600 | -2.13461200 |
| H | 1.71870100 | 3.06230800 | -0.26023900 |
| C | 3.39466900 | 1.69905400 | -2.73887600 |
| H | 3.09350300 | 3.85539900 | -2.48843000 |
| H | 3.96871700 | 1.55550300 | -3.64303000 |
| C | -1.10099000 | 2.61733600 | -1.00778000 |
| H | -2.17112800 | 2.42486800 | -1.20909400 |
| H | -0.53109500 | 2.10620500 | -1.79014700 |
| N | 3.07173500 | 1.35222700 | 2.17974000 |
| N | 2.98309600 | 0.62570700 | -1.99586500 |
| C | 3.29130500 | -0.75192600 | -2.31673800 |
| H | 2.37498500 | -1.34381400 | -2.40064800 |
| H | 3.81101700 | -0.78472200 | -3.27548300 |
| H | 3.93398900 | -1.19207000 | -1.54933100 |
| C | 4.25569200 | 1.78956700 | 1.45070600 |
| H | 4.72299600 | 0.92538700 | 0.98297500 |
| H | 3.98179800 | 2.51133300 | 0.68124200 |
| H | 4.94885500 | 2.23634200 | 2.16553400 |
| C | -0.25583200 | 3.69307100 | 2.03918800 |
| H | -0.09926300 | 4.53002800 | 1.35604100 |
| H | -0.64077500 | 4.09479100 | 2.98281800 |
| H | 0.71188600 | 3.22349600 | 2.23020600 |
| C | -0.86699300 | 4.11733600 | -1.12972200 |
| H | -1.14435900 | 4.43262700 | -2.13992100 |
| H | -1.48105200 | 4.69099800 | -0.42941200 |
| H | 0.18132300 | 4.37934700 | -0.97478700 |

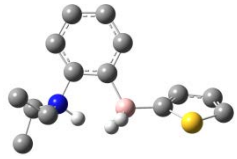
**3-TS1-t**



**Sum of electronic and thermal Enthalpies= -1022.792579**
**Sum of electronic and thermal Free Energies= -1022.85391**

| | | | |
|---|---|---|---|
| H | 0.25069900 | 0.47685400 | 0.12013900 |
| C | 1.31639000 | 0.31934200 | -0.01673300 |
| C | 2.15725200 | 1.40366900 | -0.24792800 |
| C | 1.84475200 | -0.96600900 | 0.05838100 |
| C | 3.53746700 | 1.25257700 | -0.43315200 |
| H | 1.73875700 | 2.40590700 | -0.27883700 |
| C | 3.21108200 | -1.15745600 | -0.11263200 |
| H | 1.19833400 | -1.81708300 | 0.24909300 |
| C | 4.03545500 | -0.06146900 | -0.36812600 |
| H | 3.62859500 | -2.15797100 | -0.05251500 |
| B | 4.49755700 | 2.51936400 | -0.66513200 |
| C | 5.87756800 | -0.33429700 | -1.95428200 |
| H | 5.32504900 | 0.43155200 | -2.50125800 |
| H | 6.93695800 | -0.06536900 | -2.02160900 |
| C | 6.11163000 | -1.13810000 | 0.39478900 |
| H | 5.71021500 | -0.90019300 | 1.38469600 |
| H | 5.84513100 | -2.18323600 | 0.18633900 |
| N | 5.46493700 | -0.21165100 | -0.54238100 |
| H | 4.00015400 | 3.57470200 | -0.34988400 |
| C | 7.62759700 | -0.98757300 | 0.40804700 |
| H | 7.91447200 | 0.05416300 | 0.57813600 |
| H | 8.04773900 | -1.59450200 | 1.21411100 |
| H | 8.08255800 | -1.32308000 | -0.52795100 |
| C | 5.63537400 | -1.70716100 | -2.57370400 |
| H | 6.24254000 | -2.48547400 | -2.10109500 |
| H | 4.58222400 | -1.98942500 | -2.48947100 |
| H | 5.89519600 | -1.68276100 | -3.63541200 |
| H | 5.02792500 | 2.55135700 | -1.75848100 |
| H | 5.83239700 | 1.21784900 | -0.06217600 |
| C | 5.90186900 | 2.30403300 | 0.45649500 |
| C | 5.70309700 | 2.32312400 | 1.83476500 |
| C | 6.65564900 | 3.06727600 | 2.55672500 |
| H | 4.86023700 | 1.80926500 | 2.28457900 |
| C | 7.60994900 | 3.60917600 | 1.72698200 |
| H | 6.64477000 | 3.21071800 | 3.62990400 |
| H | 8.44430000 | 4.23391700 | 2.01803200 |
| S | 7.34006100 | 3.22290300 | 0.08807600 |

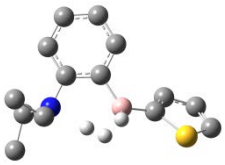
**3-Int1-t**



**Sum of electronic and thermal Enthalpies= -1022.820099**
**Sum of electronic and thermal Free Energies= -1022.88005**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 0.95101400 | 0.25786900 | 2.07963500 | H | 5.26040800 | 1.41209900 | -1.19270000 |
| C | 1.86481100 | 0.27386700 | 1.49301100 | H | 4.58767700 | 2.70441000 | -1.49726300 |
| C | 2.35992900 | 1.48432000 | 1.01978500 | C | 6.58566600 | -0.17059500 | -2.90257300 |
| C | 2.52340300 | -0.92259300 | 1.21370100 | H | 7.56651100 | -0.37375900 | -2.46576600 |
| C | 3.53420800 | 1.56042900 | 0.25805500 | H | 6.48732500 | -0.78787200 | -3.79809000 |
| H | 1.82497600 | 2.40655500 | 1.22661400 | H | 6.54964200 | 0.87796900 | -3.21284800 |
| C | 3.68942100 | -0.89912500 | 0.45768000 | C | 7.05597500 | -0.78903200 | 0.66693200 |
| H | 2.13204000 | -1.86685200 | 1.57722200 | H | 7.94646900 | -0.61602500 | 1.27536400 |
| C | 4.15725100 | 0.33368700 | 0.01672500 | H | 6.27591400 | -1.18597200 | 1.31991600 |
| H | 4.20705000 | -1.82449800 | 0.22392200 | H | 7.31256100 | -1.54278400 | -0.08310200 |
| B | 4.19380300 | 2.93122500 | -0.32292100 | C | 3.18170800 | 4.17291500 | -0.36514800 |
| C | 5.44968700 | -0.49813500 | -1.94761900 | C | 1.92782000 | 4.28212700 | -0.91245000 |
| H | 4.48142700 | -0.40537400 | -2.44318700 | S | 3.60543900 | 5.69135600 | 0.36412800 |
| H | 5.53270000 | -1.51568800 | -1.56212400 | C | 1.31766000 | 5.56306900 | -0.75415900 |
| C | 6.63711400 | 0.52875900 | 0.04419200 | H | 1.44830300 | 3.45211000 | -1.42193600 |
| H | 7.42180400 | 0.93413300 | -0.59874300 | C | 2.11447100 | 6.43889900 | -0.07799900 |
| H | 6.41258400 | 1.28053800 | 0.80201300 | H | 0.33268600 | 5.81769100 | -1.12955500 |
| N | 5.39136800 | 0.44366500 | -0.79171500 | H | 1.90789800 | 7.46882300 | 0.17719000 |
| H | 5.20395300 | 3.18903000 | 0.32480000 | | | | |

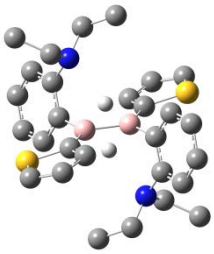
**3 –TS2-t**



**Sum of electronic and thermal Enthalpies= -1022.794546**
**Sum of electronic and thermal Free Energies= -1022.859134**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 0.97198100 | 0.17425400 | 2.20106800 | H | 5.04636200 | 2.10746900 | -1.13135700 |
| C | 1.86983000 | 0.21181500 | 1.59198700 | H | 4.83151800 | 2.88415600 | -1.25141900 |
| C | 2.45078700 | 1.43812100 | 1.28459900 | C | 6.47291800 | -0.00814600 | -2.93644400 |
| C | 2.43152000 | -0.96241600 | 1.10266400 | H | 7.48203700 | -0.18539400 | -2.55416800 |
| C | 3.60749200 | 1.53065600 | 0.50154100 | H | 6.36679900 | -0.57959500 | -3.86208800 |
| H | 1.98841500 | 2.35231000 | 1.64557000 | H | 6.37802300 | 1.05485500 | -3.17624700 |
| C | 3.58305200 | -0.90445000 | 0.32525900 | C | 7.06148700 | -0.84882000 | 0.60870300 |
| H | 1.97833800 | -1.92318200 | 1.32592300 | H | 7.95315000 | -0.69903200 | 1.22349200 |
| C | 4.17382100 | 0.32735400 | 0.04222400 | H | 6.28439700 | -1.28896700 | 1.23994100 |
| H | 4.02571100 | -1.81988600 | -0.05479500 | H | 7.31824300 | -1.56743100 | -0.17567000 |
| B | 4.24432600 | 2.94933600 | 0.14922600 | C | 3.25884400 | 4.13163600 | -0.19957200 |
| C | 5.40081700 | -0.43374400 | -1.94067700 | C | 1.98033300 | 4.08403600 | -0.70082300 |
| H | 4.41527600 | -0.36551300 | -2.41001100 | S | 3.73438300 | 5.79014900 | 0.00317800 |
| H | 5.55237200 | -1.49039700 | -1.67342700 | C | 1.39003500 | 5.36087600 | -0.91795700 |
| C | 6.60257300 | 0.48803000 | 0.03172000 | H | 1.47805800 | 3.14483300 | -0.90534600 |
| H | 7.38849500 | 0.91894500 | -0.59719300 | C | 2.22981300 | 6.38322300 | -0.57986400 |
| H | 6.42747700 | 1.20118600 | 0.84077200 | H | 0.39007300 | 5.51210000 | -1.30660300 |
| N | 5.36160100 | 0.43628400 | -0.76194600 | H | 2.03868500 | 7.44576500 | -0.63698300 |
| H | 5.26363500 | 3.25682500 | 0.71570800 | | | | |

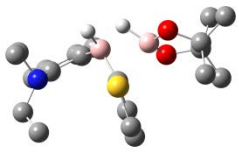
**3-Int2-t**



**Sum of electronic and thermal Enthalpies= -2043.318578**
**Sum of electronic and thermal Free Energies= -2043.426422**

| | | | |
|---|---|---|---|
| C | 0.34960300 | -2.02518500 | 0.28267700 |
| C | 1.37623400 | -1.09282600 | 0.40591700 |
| C | 1.12244000 | 0.12439700 | 1.02811300 |
| C | -0.14411900 | 0.39578900 | 1.53662000 |
| C | -1.17684700 | -0.53609100 | 1.40777600 |
| C | -0.93699900 | -1.76373500 | 0.76281500 |
| H | 0.54433600 | -2.96561600 | -0.22798000 |
| H | 2.36249300 | -1.31079000 | 0.00908200 |
| H | 1.91237300 | 0.86243000 | 1.12883400 |
| H | -0.33518400 | 1.34043900 | 2.03660200 |
| N | -2.49539500 | -0.26761800 | 1.86945400 |
| B | -2.12729100 | -2.77407500 | 0.50069800 |
| H | -3.24522700 | -2.07868300 | 0.52506100 |
| H | -2.17463200 | -3.07343700 | -0.80557100 |
| C | -2.99662700 | 1.08896200 | 1.67591300 |
| H | -2.79852500 | 1.74133300 | 2.54323000 |
| H | -2.45728400 | 1.51706900 | 0.82678000 |
| C | -2.83077300 | -0.89311100 | 3.15103300 |
| H | -3.90284900 | -0.75176700 | 3.32152000 |
| H | -2.67656600 | -1.97299300 | 3.05533700 |
| B | -3.29258500 | -2.37798100 | -0.78128000 |
| C | -4.48279200 | -3.38844700 | -1.04329900 |
| C | -4.24285200 | -4.61610300 | -1.68818000 |
| C | -5.76940000 | -3.12710700 | -0.56309200 |
| C | -5.27546900 | -5.54813500 | -1.81686700 |
| C | -6.79591300 | -4.05960700 | -0.68617500 |
| H | -5.96421100 | -2.18665500 | -0.05250700 |
| C | -6.54201300 | -5.27685900 | -1.30828300 |
| H | -5.08431000 | -6.49280200 | -2.31678400 |
| H | -7.78217100 | -3.84174500 | -0.28928200 |
| H | -7.33187200 | -6.01499000 | -1.40887700 |
| N | -2.92430600 | -4.88445200 | -2.14997600 |
| C | -2.58922700 | -4.25910200 | -3.43169700 |
| H | -1.51716800 | -4.40034700 | -3.60236300 |
| H | -2.74352900 | -3.17922300 | -3.33611800 |
| C | -2.42290100 | -6.24094600 | -1.95630700 |
| H | -2.62113100 | -6.89350800 | -2.82345500 |
| H | -2.96201000 | -6.66893300 | -1.10696800 |
| C | -3.38347600 | -4.77720600 | -4.63207800 |
| H | -3.06818600 | -4.26277700 | -5.54449900 |
| H | -3.23288200 | -5.85054900 | -4.78461800 |
| H | -4.45355200 | -4.59895900 | -4.49352900 |
| C | -0.93306900 | -6.24969700 | -1.62801700 |
| H | -0.58799400 | -7.27417200 | -1.45917300 |
| H | -0.32994200 | -5.82862200 | -2.43796500 |
| H | -0.75147500 | -5.66782000 | -0.72004800 |
| C | -2.03669400 | -0.37523800 | 4.35162300 |
| H | -2.35212000 | -0.88983600 | 5.26390300 |
| H | -0.96659700 | -0.55345200 | 4.21320500 |
| H | -2.18732800 | 0.69807500 | 4.50433300 |
| C | -4.48639100 | 1.09788000 | 1.34731200 |
| H | -5.08969300 | 0.67676900 | 2.15711000 |
| H | -4.83134300 | 2.12240200 | 1.17850800 |
| H | -4.66785500 | 0.51610600 | 0.43925100 |
| C | -2.22841900 | -4.10575400 | 1.33284200 |
| C | -3.24036900 | -5.02363400 | 1.49216100 |
| S | -0.84649400 | -4.60366800 | 2.26982900 |
| C | -2.90509600 | -6.11499700 | 2.33970100 |
| H | -4.20732000 | -4.91712200 | 1.01720700 |
| C | -1.63361000 | -6.02271400 | 2.82865900 |
| H | -3.58225000 | -6.92653300 | 2.57737100 |
| H | -1.12379400 | -6.70967900 | 3.48958500 |
| C | -3.19153000 | -1.04629300 | -1.61336600 |
| C | -2.17972900 | -0.12818900 | -1.77238100 |
| S | -4.57344200 | -0.54845800 | -2.55037600 |
| C | -2.51511500 | 0.96325900 | -2.61975900 |
| H | -1.21281300 | -0.23462200 | -1.29734100 |
| C | -3.78654100 | 0.87083600 | -3.10885900 |
| H | -1.83809000 | 1.77496400 | -2.85721900 |
| H | -4.29640400 | 1.55782000 | -3.76972900 |

**3-TS3-t**

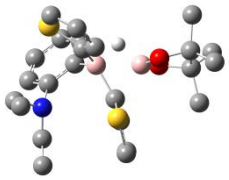


**Sum of electronic and thermal Enthalpies= -1433.218136**
**Sum of electronic and thermal Free Energies= -1433.299135**

| | | | |
|---|---|---|---|
| C | -2.13143400 | -2.01366100 | 0.71607100 |
| C | -0.77485600 | -1.78781400 | 0.49452200 |
| C | -0.25445400 | -0.49539600 | 0.37875000 |
| C | -1.14739800 | 0.58601900 | 0.48464400 |
| C | -2.50956000 | 0.36063900 | 0.69031400 |
| C | -3.00183400 | -0.93514000 | 0.81461500 |
| H | -2.50496400 | -3.02838500 | 0.81471500 |
| H | -0.10236100 | -2.63993600 | 0.44214800 |

| | | | |
|---|---|---|---|
| H | -3.19071300 | 1.20533600 | 0.74705700 |
| H | -4.06267400 | -1.09849100 | 0.97891700 |
| C | -0.58284800 | 2.35970900 | -1.03867500 |
| C | -1.08040300 | 2.90357600 | 1.31215300 |
| H | -1.58822100 | 2.68378000 | -1.36854000 |
| H | -0.31351700 | 1.49829800 | -1.65583200 |
| H | -1.69026100 | 3.67006000 | 0.80711600 |
| H | -1.73879800 | 2.41678500 | 2.03771100 |
| N | -0.61186100 | 1.90603200 | 0.35062800 |
| B | 1.29183800 | -0.15822600 | 0.16632400 |
| H | 1.75751700 | -1.35854000 | -0.28185700 |
| C | 2.08688500 | 0.33736400 | 1.48014400 |
| C | 1.75393300 | 0.15625100 | 2.80618800 |
| C | 2.48192400 | 0.97704700 | 3.70445100 |
| H | 1.00869700 | -0.56916000 | 3.10992500 |
| C | 3.36500500 | 1.79601200 | 3.05076100 |
| H | 2.35478900 | 0.96807600 | 4.77990700 |
| H | 1.63894200 | 0.43239100 | -0.82226900 |
| B | 2.56214700 | -1.59316800 | 0.67256100 |
| O | 3.87879100 | -1.60580800 | 0.30631500 |
| O | 2.20735100 | -2.56972700 | 1.56776500 |
| C | 4.55056200 | -2.42631600 | 1.29027200 |
| C | 3.39284000 | -3.36779000 | 1.79057300 |
| C | 5.70245400 | -3.14560400 | 0.60345300 |
| H | 6.45167600 | -2.41582100 | 0.28759800 |
| H | 6.17906700 | -3.84856500 | 1.29379500 |
| H | 5.36658200 | -3.69133900 | -0.27924100 |
| C | 5.08858600 | -1.49625300 | 2.37826500 |
| H | 5.73646800 | -0.74997800 | 1.91306500 |
| H | 4.28325600 | -0.96848300 | 2.89459600 |
| H | 5.67232800 | -2.05300600 | 3.11662000 |
| C | 3.46271400 | -3.72671700 | 3.26763900 |
| H | 2.62545800 | -4.37906200 | 3.52790100 |
| H | 4.39301600 | -4.25909000 | 3.48888400 |
| H | 3.40893500 | -2.83601800 | 3.89544700 |
| C | 3.23249000 | -4.62953800 | 0.94279600 |
| H | 4.05755200 | -5.32929400 | 1.10162100 |
| H | 2.29967100 | -5.12491800 | 1.22274700 |
| H | 3.18023400 | -4.38563400 | -0.12175600 |
| C | 0.06627500 | 3.56326600 | 2.07585500 |
| H | 0.62813600 | 2.80701400 | 2.62990200 |
| H | 0.76260400 | 4.06626500 | 1.40119500 |
| H | -0.31953900 | 4.30214700 | 2.78701900 |
| C | 0.42265500 | 3.47711800 | -1.28473600 |
| H | 0.14292100 | 4.39929500 | -0.76655100 |
| H | 1.41436900 | 3.17377000 | -0.93662800 |
| H | 0.47870900 | 3.70315800 | -2.35378700 |
| S | 3.30836100 | 1.56671400 | 1.35558200 |
| H | 4.03387500 | 2.52532800 | 3.48686700 |

**3-Int3-t**

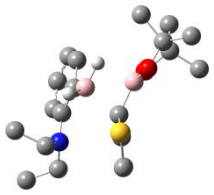


**Sum of electronic and thermal Enthalpies= -1433.216528**
**Sum of electronic and thermal Free Energies= -1433.30101**

| | | | |
|---|---|---|---|
| C | -2.09380900 | -1.97458900 | 0.93579100 |
| C | -0.74226500 | -1.73098200 | 0.70374600 |
| C | -0.24913500 | -0.43661900 | 0.51110400 |
| C | -1.16497100 | 0.63119000 | 0.54992200 |
| C | -2.52297900 | 0.38591000 | 0.76353500 |
| C | -2.98681700 | -0.91082100 | 0.96558300 |
| H | -2.44522900 | -2.98959300 | 1.09395000 |
| H | -0.04655400 | -2.56581700 | 0.70481400 |
| H | -3.22552000 | 1.21461800 | 0.76498400 |
| H | -4.04495800 | -1.08603000 | 1.13541400 |
| C | -0.59041200 | 2.29853400 | -1.07882100 |
| C | -1.20817500 | 3.00739700 | 1.19594900 |
| H | -1.59419900 | 2.54931800 | -1.47089800 |
| H | -0.26092200 | 1.40397700 | -1.61299900 |
| H | -1.83737400 | 3.69578900 | 0.60870900 |
| H | -1.86481600 | 2.55423400 | 1.94413900 |
| N | -0.66126700 | 1.95407200 | 0.34143400 |
| B | 1.29717400 | -0.12649700 | 0.28159200 |
| H | 1.81562800 | -1.27712200 | -0.02570100 |
| C | 2.08770600 | 0.41504200 | 1.63804200 |
| C | 1.61927900 | 0.38467200 | 2.94359700 |
| C | 2.20958200 | 1.33953600 | 3.79602900 |
| H | 0.88721900 | -0.34835100 | 3.25980500 |
| C | 3.11828000 | 2.12496300 | 3.12748100 |
| H | 1.97783200 | 1.45225500 | 4.84729500 |
| H | 3.70042300 | 2.94046900 | 3.53561300 |
| H | 1.66429900 | 0.50569700 | -0.66996000 |
| S | 3.25438500 | 1.70257000 | 1.48377000 |
| B | 2.58353800 | -1.25053700 | 1.06927300 |
| O | 3.90832500 | -1.34187900 | 0.65471300 |
| O | 2.23488100 | -2.26839100 | 1.96012200 |
| C | 4.54682100 | -2.22224900 | 1.59606400 |
| C | 3.36287400 | -3.15879700 | 2.01647800 |
| C | 5.69995500 | -2.92575300 | 0.89601800 |
| H | 6.47358400 | -2.19795300 | 0.63893200 |
| H | 6.14365200 | -3.68034200 | 1.55335500 |
| H | 5.36971000 | -3.40944100 | -0.02428400 |
| C | 5.07131900 | -1.37262500 | 2.75752400 |
| H | 5.73350100 | -0.60133600 | 2.35667200 |
| H | 4.25487800 | -0.87577600 | 3.29014200 |
| H | 5.63634100 | -1.97819100 | 3.47172800 |
| C | 3.46943300 | -3.72433700 | 3.42511800 |
| H | 2.61155000 | -4.36955200 | 3.63144800 |
| H | 4.38030100 | -4.32217100 | 3.53130600 |
| H | 3.48251500 | -2.92826400 | 4.17119000 |
| C | 3.11337100 | -4.28245400 | 1.00812800 |
| H | 3.89573300 | -5.04542000 | 1.05052100 |
| H | 2.15545800 | -4.75593500 | 1.23791100 |
| H | 3.06465900 | -3.88888200 | -0.01113200 |
| C | -0.11950800 | 3.78564100 | 1.93241700 |
| H | 0.45834100 | 3.10629800 | 2.56390300 |
| H | 0.57438600 | 4.26610200 | 1.23922600 |
| H | -0.56288000 | 4.56033800 | 2.56769000 |
| C | 0.37519000 | 3.43704400 | -1.37976100 |

| | | | |
|---|---|---|---|
| H | 0.03126700 | 4.38616900 | -0.95785500 |
| H | 1.36286100 | 3.21265700 | -0.96642100 |
| H | 0.46951300 | 3.57300900 | -2.46117300 |

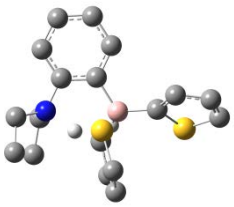
**3-TS4-t**



**Sum of electronic and thermal Enthalpies= -1433.216054**
**Sum of electronic and thermal Free Energies= -1433.299048**

| | | | |
|---|---|---|---|
| C | -1.99833500 | -1.65427400 | 1.02177300 |
| C | -1.10790100 | -0.64232700 | 0.56897200 |
| C | -0.05134600 | -1.05017400 | -0.26174300 |
| C | 0.16083400 | -2.36517100 | -0.65020500 |
| C | -0.70974300 | -3.34098700 | -0.18305100 |
| C | -1.77236000 | -2.98860400 | 0.63499900 |
| H | 0.65147100 | -0.29152900 | -0.59503500 |
| H | 0.99639600 | -2.62431600 | -1.29233800 |
| H | -0.57438400 | -4.38230900 | -0.46077100 |
| H | -2.45004900 | -3.76845100 | 0.96086400 |
| N | -3.05076900 | -1.36402100 | 1.90742300 |
| B | -1.13283200 | 0.90621400 | 0.92050800 |
| H | -2.07763000 | 1.59923300 | 0.67273200 |
| H | -0.12848000 | 1.45654700 | 0.49484500 |
| C | 2.41684500 | 2.61510900 | 1.70813600 |
| C | 2.76623000 | 1.15650000 | 2.17349700 |
| O | 1.04886500 | 2.75234600 | 2.14029000 |
| O | 1.49239700 | 0.48934900 | 2.10875200 |
| B | 0.52568100 | 1.47356300 | 2.15908000 |
| C | 3.24245800 | 3.70948100 | 2.36947900 |
| H | 2.94138700 | 4.68458300 | 1.97823200 |
| H | 3.09768900 | 3.71817700 | 3.45082200 |
| H | 4.30697300 | 3.56912500 | 2.15656500 |
| C | 2.44776000 | 2.78288700 | 0.18760400 |
| H | 1.98489700 | 3.73874700 | -0.06903800 |
| H | 3.47307500 | 2.77758000 | -0.19273400 |
| H | 1.88746900 | 1.99103900 | -0.31605300 |
| C | 3.74766000 | 0.41810000 | 1.27455100 |
| H | 4.70408900 | 0.94853100 | 1.22721200 |
| H | 3.92939500 | -0.58226000 | 1.67522600 |
| H | 3.35307400 | 0.30877800 | 0.26322400 |
| C | 3.22809300 | 1.09196800 | 3.63059600 |
| H | 3.25682700 | 0.04542200 | 3.94377800 |
| H | 4.22628500 | 1.52054500 | 3.75796400 |
| H | 2.53260100 | 1.62490000 | 4.28482000 |
| C | -0.91149500 | 1.20225900 | 2.79389900 |
| C | -1.19304800 | 0.08009900 | 3.57479300 |
| C | -2.09289300 | 0.31236200 | 4.63023100 |
| H | -0.72521000 | -0.87362400 | 3.36605700 |
| C | -2.50232300 | 1.62339300 | 4.66647200 |
| H | -2.43299100 | -0.44504000 | 5.32438900 |
| H | -3.19821500 | 2.06424800 | 5.36878100 |
| C | -3.94040900 | -0.23158000 | 1.66714200 |
| H | -4.74518100 | -0.30278200 | 2.40522700 |
| H | -3.42786700 | 0.71008600 | 1.87243000 |
| C | -3.61262800 | -2.41328900 | 2.74009600 |
| H | -3.90265100 | -1.95158100 | 3.69442700 |
| H | -2.81707200 | -3.12533000 | 2.97700900 |
| C | -4.82970200 | -3.14978600 | 2.16920900 |
| H | -5.16151300 | -3.92828600 | 2.86327100 |
| H | -5.66646500 | -2.46143900 | 2.01716000 |
| H | -4.60656500 | -3.61685800 | 1.20646700 |
| C | -4.52868300 | -0.18313400 | 0.25984700 |
| H | -5.20977400 | 0.66788000 | 0.16405800 |
| H | -3.73527500 | -0.06784600 | -0.48306800 |
| H | -5.07997300 | -1.09952500 | 0.02921800 |
| S | -1.79023100 | 2.57830500 | 3.44982200 |

**3-TS5-t**

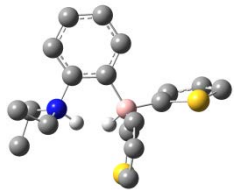


**Sum of electronic and thermal Enthalpies= -1574.507631**
**Sum of electronic and thermal Free Energies= -1574.581087**

| | | | |
|---|---|---|---|
| C | 1.54832500 | 0.10573500 | 1.30096200 |
| C | 2.39722500 | 1.19253400 | 1.11626500 |
| C | 1.96472800 | -1.17335700 | 0.94592500 |
| C | 3.68121600 | 1.05339200 | 0.57385100 |
| C | 3.23028700 | -1.35379200 | 0.40023000 |
| H | 1.30669500 | -2.02578600 | 1.08248000 |
| C | 4.06625700 | -0.25324700 | 0.22210400 |
| B | 4.68406900 | 2.29856600 | 0.34574500 |
| H | 4.95215200 | 2.46720100 | -0.83157000 |
| H | 5.99529600 | 0.81607600 | 0.27136800 |
| N | 5.38195900 | -0.40101400 | -0.37999200 |
| C | 6.13189900 | -1.60929200 | 0.02596800 |

| | | | |
|---|---|---|---|
| C | 5.28117600 | -0.21699600 | -1.84675200 |
| H | 5.68821600 | -1.97433600 | 0.95477600 |
| H | 4.59814200 | 0.61843500 | -2.00377300 |
| H | 5.99502000 | -2.39762400 | -0.72792300 |
| H | 4.81228300 | -1.11305400 | -2.28078400 |
| C | 6.26981000 | 1.77811000 | 0.98702400 |
| C | 7.41392900 | 2.50612000 | 0.67167600 |
| C | 8.30304100 | 2.70863300 | 1.74261600 |
| H | 7.56986800 | 2.89820300 | -0.32752100 |
| C | 7.84827000 | 2.11503800 | 2.89771300 |
| H | 9.23027600 | 3.26390900 | 1.68017000 |
| H | 8.33189500 | 2.12457600 | 3.86575800 |
| H | 0.55997100 | 0.25659400 | 1.72451800 |
| H | 3.55687400 | -2.34633000 | 0.10302200 |
| H | 2.06046400 | 2.18539900 | 1.39851600 |
| C | 6.60289200 | 0.07825500 | -2.53914700 |
| H | 7.11479100 | 0.91616900 | -2.05737700 |
| H | 7.27349100 | -0.78456700 | -2.55033200 |
| H | 6.40743300 | 0.35400000 | -3.57877200 |
| C | 7.62024200 | -1.36365500 | 0.26873900 |
| H | 8.09840000 | -2.30853600 | 0.54227600 |
| H | 8.13044000 | -0.97159900 | -0.61163700 |
| H | 7.77377700 | -0.65864200 | 1.08881900 |
| S | 6.35327600 | 1.32633300 | 2.67961300 |
| C | 4.29761800 | 3.67663600 | 1.05777200 |
| C | 3.88479600 | 3.95892500 | 2.33588700 |
| S | 4.43422800 | 5.16327500 | 0.16925800 |
| C | 3.67761000 | 5.34583200 | 2.59858900 |
| H | 3.73605100 | 3.18363300 | 3.08052400 |
| C | 3.94002600 | 6.12540400 | 1.51081600 |
| H | 3.34613800 | 5.74210600 | 3.55155000 |
| H | 3.85553600 | 7.19958200 | 1.42420600 |

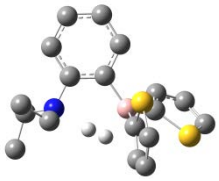
**3-Int4-t**



**Sum of electronic and thermal Enthalpies= -1574.537887**
**Sum of electronic and thermal Free Energies= -1574.610207**

| | | | |
|---|---|---|---|
| H | 0.97104200 | 0.35741200 | 2.15041400 |
| C | 1.89079200 | 0.35849800 | 1.57325100 |
| C | 2.39640400 | 1.55752700 | 1.08090600 |
| C | 2.54464800 | -0.84407200 | 1.31629300 |
| C | 3.57905500 | 1.61465400 | 0.33328300 |
| H | 1.85927400 | 2.48399800 | 1.26158500 |
| C | 3.71808200 | -0.83815600 | 0.57085200 |
| H | 2.14295700 | -1.78164200 | 1.68567600 |
| C | 4.20665500 | 0.38393300 | 0.12321400 |
| H | 4.22362600 | -1.77168900 | 0.34544100 |
| B | 4.21695000 | 2.99286100 | -0.28538000 |
| C | 5.37110800 | -0.35582600 | -1.93897100 |
| H | 4.42659200 | -0.06345100 | -2.40220400 |
| H | 5.29942300 | -1.41065000 | -1.66928200 |
| C | 6.72113300 | 0.29491700 | 0.11401500 |
| H | 7.52138100 | 0.69457500 | -0.51197700 |
| H | 6.60774500 | 0.97049200 | 0.96303100 |
| N | 5.45008900 | 0.44930000 | -0.68031700 |
| H | 5.43227800 | 1.44213500 | -0.99578800 |
| H | 4.55919600 | 2.73954600 | -1.45981900 |
| C | 6.54139600 | -0.08736400 | -2.86964200 |
| H | 7.48033100 | -0.49014300 | -2.48218600 |
| H | 6.34643700 | -0.56591800 | -3.83174100 |
| H | 6.66616900 | 0.98512100 | -3.04744500 |
| C | 7.02307200 | -1.12255700 | 0.55946700 |
| H | 7.98570300 | -1.11554900 | 1.07583600 |
| H | 6.27406000 | -1.49348400 | 1.26117600 |
| H | 7.10561500 | -1.82190100 | -0.27787400 |
| C | 3.13880600 | 4.18353200 | -0.36150000 |
| C | 2.15451100 | 4.39034400 | -1.29252000 |
| S | 3.01124500 | 5.40248400 | 0.87364000 |
| C | 1.30635700 | 5.50662000 | -1.02402200 |
| H | 2.04271800 | 3.74888900 | -2.16054300 |
| C | 1.64958400 | 6.15368800 | 0.12528300 |
| H | 0.48610500 | 5.81568000 | -1.66229000 |
| H | 1.19234800 | 7.03159400 | 0.55982600 |
| C | 5.55589000 | 3.36456700 | 0.55814600 |
| C | 5.80644800 | 3.24366600 | 1.90198300 |
| S | 6.98656500 | 3.96946500 | -0.22526600 |
| C | 7.12492200 | 3.62816400 | 2.29950800 |
| H | 5.05542300 | 2.87509200 | 2.59322200 |
| C | 7.88868300 | 4.03493800 | 1.24653900 |
| H | 7.48434100 | 3.60204900 | 3.32202100 |
| H | 8.91007800 | 4.38891600 | 1.26009600 |

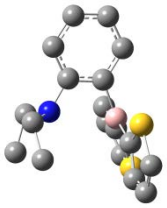
**3-TS6-t**



**Sum of electronic and thermal Enthalpies= -1574.511821**
**Sum of electronic and thermal Free Energies= -1574.584603**

| | | | |
|---|---|---|---|
| H | 1.11445900 | 0.31118500 | 2.39201800 |
| C | 1.98305600 | 0.31731300 | 1.74106400 |
| C | 2.57252700 | 1.52410400 | 1.37889400 |
| C | 2.50115700 | -0.87689200 | 1.25338200 |
| C | 3.69803600 | 1.57707600 | 0.54668300 |
| H | 2.14224900 | 2.45491700 | 1.73754500 |
| C | 3.61626000 | -0.85634800 | 0.42337100 |
| H | 2.04181800 | -1.82418400 | 1.51776700 |
| C | 4.22337600 | 0.35429500 | 0.08687500 |
| H | 4.02170400 | -1.78778000 | 0.04067000 |
| B | 4.33970700 | 2.99325000 | 0.18143100 |
| C | 5.26646000 | -0.41515600 | -1.98642000 |
| H | 4.27034900 | -0.22958400 | -2.39892600 |
| H | 5.32216100 | -1.49234300 | -1.76810400 |
| C | 6.66287400 | 0.30895400 | -0.06026500 |
| H | 7.44047800 | 0.70532800 | -0.72095000 |
| H | 6.60520900 | 0.99324300 | 0.78784800 |
| N | 5.37600200 | 0.40278900 | -0.77445700 |
| H | 5.15946300 | 2.08596300 | -1.15005900 |
| H | 4.95807800 | 2.86096900 | -1.27161400 |
| C | 6.32344600 | -0.05938900 | -3.02462200 |
| H | 7.32722400 | -0.35657500 | -2.70857000 |
| H | 6.10810100 | -0.57704400 | -3.96294900 |
| H | 6.33026300 | 1.01694100 | -3.22005800 |
| C | 7.04357000 | -1.08695900 | 0.42664000 |
| H | 7.99881000 | -1.04045000 | 0.95663200 |
| H | 6.29350400 | -1.47886900 | 1.11925300 |
| H | 7.15727400 | -1.79668800 | -0.39887500 |
| C | 3.33714100 | 4.12685400 | -0.26871800 |
| C | 2.07980200 | 3.99326000 | -0.80810900 |
| S | 3.74160400 | 5.81371700 | -0.15612300 |
| C | 1.44908400 | 5.22665600 | -1.12913900 |
| H | 1.62209600 | 3.02303500 | -0.96645700 |
| C | 2.23770700 | 6.30099700 | -0.82952200 |
| H | 0.45837100 | 5.31269500 | -1.55910300 |
| H | 2.00790800 | 7.34928500 | -0.96101300 |
| C | 5.64573200 | 3.43337500 | 0.97665100 |
| C | 6.75387700 | 4.12318400 | 0.55827300 |
| S | 5.79561800 | 3.06944900 | 2.66916800 |
| C | 7.71650400 | 4.36003600 | 1.58317000 |
| H | 6.88165800 | 4.44776500 | -0.46914200 |
| C | 7.32773200 | 3.84885700 | 2.78534900 |
| H | 8.65149900 | 4.88539700 | 1.42989200 |
| H | 7.85081300 | 3.89366200 | 3.73015400 |

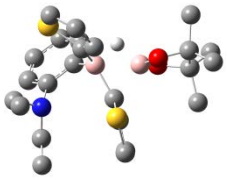
**3-Int5-t**



**Sum of electronic and thermal Enthalpies= -1573.366876**
**Sum of electronic and thermal Free Energies= -1573.439665**

| | | | |
|---|---|---|---|
| C | -6.70630100 | 1.40107700 | -0.39623400 |
| C | -5.34050800 | 1.63169000 | -0.20776200 |
| C | -4.75704600 | 2.84019800 | -0.58433600 |
| C | -5.54791500 | 3.83445000 | -1.15363300 |
| C | -6.91386900 | 3.62679200 | -1.32843700 |
| C | -7.49090100 | 2.41807800 | -0.94517200 |
| H | -3.69400700 | 3.00312700 | -0.42926800 |
| H | -5.09897100 | 4.77696700 | -1.45161000 |
| H | -7.52872300 | 4.40647500 | -1.76718100 |
| H | -8.55597700 | 2.26055500 | -1.09262200 |
| C | -3.40366200 | 0.12161200 | -0.26223000 |
| C | -4.44818500 | 0.80494000 | 1.86463700 |
| H | -2.51055700 | 0.43933900 | 0.29976700 |
| H | -3.35674700 | 0.62710200 | -1.23136900 |
| H | -3.65531400 | 1.55464000 | 2.04251900 |
| H | -5.38099300 | 1.23750000 | 2.23488900 |
| B | -7.17624600 | -0.04973900 | 0.02246400 |
| N | -4.62149600 | 0.56316200 | 0.42997400 |
| C | -7.89968500 | -0.20649900 | 1.38439200 |
| C | -8.11922200 | 0.81096700 | 2.29107100 |
| S | -8.60076600 | -1.67504300 | 2.00377700 |
| C | -8.81876800 | 0.41773600 | 3.45991800 |
| H | -7.78286300 | 1.82405900 | 2.10013700 |
| C | -9.14093200 | -0.91104600 | 3.44007600 |
| H | -9.07639300 | 1.08546400 | 4.27258000 |
| H | -9.67489500 | -1.47349700 | 4.19370600 |
| C | -6.97067300 | -1.21019300 | -0.98525800 |
| C | -6.92857200 | -2.57448800 | -0.79570100 |
| S | -6.60809000 | -0.85139200 | -2.64992000 |
| C | -6.61461800 | -3.31578100 | -1.96423100 |
| H | -7.08373200 | -3.03681000 | 0.17185600 |
| C | -6.42364500 | -2.50715700 | -3.05107400 |
| H | -6.53246400 | -4.39518900 | -1.99846300 |
| H | -6.19568300 | -2.80644900 | -4.06476200 |
| C | -3.36104800 | -1.38617400 | -0.50105200 |
| H | -3.44112500 | -1.94511200 | 0.43358200 |
| H | -4.18536000 | -1.69704200 | -1.14627700 |
| H | -2.41861100 | -1.66177100 | -0.98572500 |
| C | -4.15181400 | -0.46134000 | 2.65543000 |
| H | -3.17766600 | -0.88737000 | 2.39930100 |
| H | -4.14390600 | -0.23869600 | 3.72635700 |
| H | -4.92307800 | -1.21232600 | 2.46069700 |

**3-Int6-t**

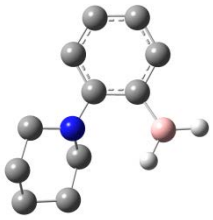


**Sum of electronic and thermal Enthalpies= -1984.928992**

**Sum of electronic and thermal Free Energies= -1985.019343**

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C | -1.52846800 | -1.94730900 | -0.84686200 | H | 4.27140900 | -3.00193400 | -0.57969300 |
| C | -0.21614000 | -1.53723800 | -0.63780500 | C | 6.27769100 | -1.41782500 | 1.75825600 |
| C | 0.09722300 | -0.25020500 | -0.18127400 | H | 6.94420800 | -0.99469200 | 1.00235600 |
| C | -0.96786100 | 0.63078400 | 0.07796700 | H | 6.12624700 | -0.66717600 | 2.53552400 |
| C | -2.28517500 | 0.22241100 | -0.14769200 | H | 6.77183300 | -2.28968100 | 2.19881300 |
| C | -2.56943700 | -1.05755300 | -0.60879900 | C | 3.97188300 | -1.84291800 | 3.49411800 |
| H | -1.73466000 | -2.95318900 | -1.19915800 | H | 3.08441200 | -2.15470900 | 4.05104000 |
| H | 0.58957400 | -2.24178600 | -0.82977900 | H | 4.85902400 | -2.17318600 | 4.04168800 |
| H | -3.09608800 | 0.92140700 | 0.03737200 | H | 3.97654500 | -0.75017900 | 3.44916600 |
| H | -3.59920300 | -1.35654700 | -0.77962000 | C | 3.98112100 | -3.97892200 | 2.18702700 |
| C | -1.35542800 | 2.16498200 | 1.87720200 | H | 4.96275100 | -4.30156500 | 2.54865900 |
| H | -2.45422600 | 2.22886500 | 1.76346600 | H | 3.22460200 | -4.33707200 | 2.89001000 |
| H | -1.15676700 | 1.28165000 | 2.49229200 | H | 3.79239300 | -4.44376400 | 1.21822600 |
| N | -0.69283400 | 1.94957500 | 0.59146500 | C | 2.22740200 | 1.12509200 | -1.21079800 |
| B | 1.61914500 | 0.22733900 | -0.04104900 | C | 3.45775000 | 1.71719700 | -1.35072300 |
| H | 2.25722500 | -0.90956100 | -0.29315400 | S | 1.31321300 | 1.34942600 | -2.67230700 |
| C | 2.04776200 | 0.61399400 | 1.51556700 | C | 3.64968500 | 2.37664300 | -2.59932900 |
| C | 1.34113400 | 0.22579000 | 2.64658300 | H | 4.22764700 | 1.65093500 | -0.59110800 |
| C | 1.58239100 | 1.00960600 | 3.79075900 | C | 2.56613000 | 2.26142400 | -3.41859700 |
| H | 0.68960300 | -0.63981700 | 2.63112000 | H | 4.55479800 | 2.90629900 | -2.87172200 |
| C | 2.47054300 | 2.02298900 | 3.52765300 | H | 2.43714800 | 2.66277100 | -4.41393900 |
| H | 1.12646300 | 0.84174100 | 4.75782100 | C | -0.92138000 | 3.02476000 | -0.38592100 |
| H | 2.82264600 | 2.77854300 | 4.21756300 | H | -1.88317100 | 3.52842200 | -0.18552900 |
| S | 2.99904000 | 2.02392100 | 1.90828600 | H | -1.01642000 | 2.56722300 | -1.37391300 |
| B | 2.91564800 | -0.88206900 | 0.84005200 | C | -0.87971400 | 3.40472900 | 2.62246800 |
| O | 4.27515500 | -0.62901000 | 0.68586600 | H | -1.31728200 | 3.41869800 | 3.62543900 |
| O | 2.66838900 | -2.09235500 | 1.48572300 | H | 0.20888200 | 3.40445200 | 2.71631300 |
| C | 4.95914500 | -1.82052700 | 1.11413300 | H | -1.18650200 | 4.32528600 | 2.11858200 |
| C | 3.91910200 | -2.46193100 | 2.09476100 | C | 0.21052700 | 4.04798300 | -0.43553500 |
| C | 5.21250400 | -2.67751500 | -0.12710400 | H | 0.01362000 | 4.78901800 | -1.21743700 |
| H | 5.75534700 | -2.07868200 | -0.86216500 | H | 0.32693500 | 4.57762900 | 0.51224400 |
| H | 5.80884800 | -3.56320700 | 0.11041000 | H | 1.15725500 | 3.55048800 | -0.65852500 |

**2-open**



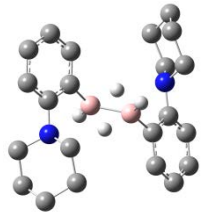
**Sum of electronic and thermal Enthalpies= -508.017222**

**Sum of electronic and thermal Free Energies= -508.066709**

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| H | 0.20669900 | 0.69833700 | 0.32162600 | H | 3.57586200 | -1.56290500 | 1.69865300 |
| C | 1.26342000 | 0.46129800 | 0.26192400 | B | 4.30534000 | 1.76407700 | -1.62999300 |
| C | 2.08139800 | 1.08416200 | -0.66935000 | H | 3.74938600 | 2.50578000 | -2.39211300 |
| C | 1.83086400 | -0.47294600 | 1.12365100 | H | 5.49725300 | 1.82142400 | -1.53559300 |
| C | 3.46112400 | 0.82053200 | -0.76056800 | C | 6.00486100 | -1.17109400 | 1.12399700 |
| H | 1.65936700 | 1.83102000 | -1.33653600 | C | 5.84044000 | -1.03195400 | -1.28579600 |
| C | 3.18003100 | -0.79727700 | 1.04154400 | C | 7.52036200 | -0.97767300 | 1.05955400 |
| H | 1.21116100 | -0.97901400 | 1.85855900 | H | 5.77407400 | -2.25355800 | 1.14102900 |
| C | 4.00985500 | -0.17588000 | 0.09755800 | H | 5.62029800 | -0.73626800 | 2.05000900 |

| | | | |
|---|---|---|---|
| C | 7.34255100 | -0.82450100 | -1.43765400 |
| H | 5.61232300 | -2.11286000 | -1.35020300 |
| H | 5.30017200 | -0.54166800 | -2.09548200 |
| H | 7.98604600 | -1.50294900 | 1.90009500 |
| H | 7.73688500 | 0.09039200 | 1.17626700 |
| H | 7.67359300 | -1.24664600 | -2.39229000 |
| H | 7.54588200 | 0.25232800 | -1.46033600 |
| N | 5.36734400 | -0.50668500 | -0.00312500 |
| C | 8.08847200 | -1.47336500 | -0.27053100 |
| H | 9.16113800 | -1.26439900 | -0.33140000 |
| H | 7.97149500 | -2.56415800 | -0.33017100 |

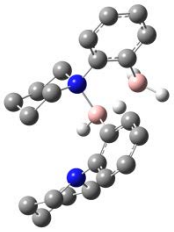
**2-*trans*-dimer**



**Sum of electronic and thermal Enthalpies= -1016.075722**
**Sum of electronic and thermal Free Energies= -1016.151440**

| | | | |
|---|---|---|---|
| C | 0.19124300 | -1.63083700 | -0.15814300 |
| C | 1.19411800 | -0.68048100 | 0.01663700 |
| C | 0.98413800 | 0.38287500 | 0.88628800 |
| C | -0.21289900 | 0.48396000 | 1.58955400 |
| C | -1.21433300 | -0.47333500 | 1.41774400 |
| C | -1.02537800 | -1.54176300 | 0.52022100 |
| H | 0.35256500 | -2.44788300 | -0.85807400 |
| H | 2.12673500 | -0.76379900 | -0.53217400 |
| H | 1.75503300 | 1.13437300 | 1.02695300 |
| H | -0.36391000 | 1.30991400 | 2.27715500 |
| B | -2.20379300 | -2.56334700 | 0.27472500 |
| H | -2.32847400 | -3.57482800 | 0.90721800 |
| H | -3.33376900 | -1.89256700 | 0.33772300 |
| H | -2.27970800 | -2.88046100 | -0.99781100 |
| B | -3.44839600 | -2.25687200 | -0.93235700 |
| H | -3.35385800 | -1.26636600 | -1.59464800 |
| C | -4.66394100 | -3.24982900 | -1.10019200 |
| C | -4.64558100 | -4.13980400 | -2.18237200 |
| C | -5.78665900 | -3.23642900 | -0.26954500 |
| C | -5.73481200 | -4.97127800 | -2.43992900 |
| C | -6.87855700 | -4.06316000 | -0.52208800 |
| H | -5.81951300 | -2.55478300 | 0.57779000 |
| C | -6.85442900 | -4.92528200 | -1.61360100 |
| H | -5.70796300 | -5.65720100 | -3.28143300 |
| H | -7.74743300 | -4.03122900 | 0.12780300 |
| H | -7.70311500 | -5.57098200 | -1.81734800 |
| C | -2.48967100 | -5.17125400 | -2.53529500 |
| C | -3.64008900 | -4.17403100 | -4.41739700 |
| C | -1.12434000 | -4.90327800 | -3.16243600 |
| H | -2.83523500 | -6.18667700 | -2.80919100 |
| H | -2.42616600 | -5.14279000 | -1.44308900 |
| C | -2.31788400 | -3.85731000 | -5.11334500 |
| H | -4.00522000 | -5.15634500 | -4.77511400 |
| H | -4.39942000 | -3.42942000 | -4.67167200 |
| H | -0.41587700 | -5.67747700 | -2.84980400 |
| H | -0.75083900 | -3.94154000 | -2.78760000 |
| H | -2.45884200 | -3.88198700 | -6.19904100 |
| H | -2.01667100 | -2.83952000 | -4.83992800 |
| C | -2.58586100 | -1.33634200 | 3.22867300 |
| C | -2.96272100 | 0.91838500 | 2.43865900 |
| C | -4.05241100 | -1.50519100 | 3.61419300 |
| H | -2.00976000 | -0.96972200 | 4.09945000 |
| H | -2.15464500 | -2.29808400 | 2.94130700 |
| C | -4.45040900 | 0.83281100 | 2.77673200 |
| H | -2.42479800 | 1.35891500 | 3.30060200 |
| H | -2.80174100 | 1.57574900 | 1.57964600 |
| H | -4.13063500 | -2.17705100 | 4.47527700 |
| H | -4.57968300 | -1.98248900 | 2.77848000 |
| H | -4.82574900 | 1.82843100 | 3.03566100 |
| H | -4.99069800 | 0.49752300 | 1.88331100 |
| N | -3.45061700 | -4.15771600 | -2.97160400 |
| N | -2.45953900 | -0.40615100 | 2.10533100 |
| C | -4.69010200 | -0.14958100 | 3.92509400 |
| H | -5.76159000 | -0.26190100 | 4.11916400 |
| H | -4.24103200 | 0.25493400 | 4.84250600 |
| C | -1.23240700 | -4.84875700 | -4.68790900 |
| H | -0.26911200 | -4.58024100 | -5.13316800 |
| H | -1.49022500 | -5.84819900 | -5.06436800 |

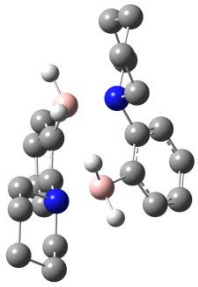
**2-H-Bridged-dimer**



**Sum of electronic and thermal Enthalpies= -1016.091971**
**Sum of electronic and thermal Free Energies= -1016.164043**

| | | | |
|---|---|---|---|
| C | -2.24202100 | -0.17239800 | 0.40246900 |
| C | -0.85582800 | -0.02562800 | 0.37490000 |
| C | -0.34605700 | 1.24183100 | 0.67402100 |
| C | -1.17910100 | 2.30932700 | 0.98927600 |
| C | -2.55660400 | 2.12449000 | 1.01979800 |
| C | -3.09742600 | 0.87744600 | 0.72246200 |
| H | 0.73090700 | 1.38377300 | 0.67444200 |
| H | -0.75454200 | 3.28065600 | 1.22304300 |
| H | -3.21782700 | 2.94412600 | 1.28095000 |
| H | -4.17201400 | 0.75510200 | 0.76333600 |
| C | -4.11731200 | -1.79538800 | 0.55316500 |
| C | -2.80684100 | -1.53768900 | -1.49715300 |
| C | -4.67337200 | -3.12603700 | 0.06693800 |
| H | -4.77459900 | -0.99679800 | 0.19762600 |
| H | -4.05297300 | -1.74533800 | 1.64068600 |
| C | -3.41534200 | -2.80731100 | -2.08350400 |
| H | -3.40554600 | -0.66432100 | -1.77944400 |
| H | -1.78899500 | -1.38258900 | -1.85747400 |
| C | -4.77149500 | -3.13689800 | -1.45834000 |
| H | -5.66355400 | -3.25148900 | 0.51772100 |
| H | -4.04386200 | -3.94490900 | 0.42774400 |
| H | -3.51755200 | -2.64458200 | -3.16147400 |
| H | -2.72668200 | -3.64439700 | -1.95123500 |
| H | -5.12361500 | -4.11006100 | -1.81386800 |
| H | -5.51249700 | -2.39289600 | -1.78150300 |
| N | -2.74076900 | -1.52045200 | 0.01694700 |
| B | 0.10301900 | -1.25555700 | 0.05630700 |
| H | 0.43697200 | -1.35908000 | -1.10382900 |
| H | 0.98792400 | -1.43401600 | 0.85385300 |
| B | -1.71086400 | -2.65567500 | 0.57720200 |
| H | -1.86969200 | -3.64383900 | -0.07207600 |
| H | -0.52888800 | -2.41566700 | 0.13693900 |
| C | -1.77258600 | -2.86395100 | 2.16594700 |
| C | -1.37822000 | -1.86411300 | 3.06633800 |
| C | -2.29480900 | -4.05699400 | 2.72498600 |
| C | -1.52845800 | -1.99014600 | 4.44420800 |
| H | -0.94828300 | -0.94709000 | 2.67985400 |
| C | -2.44922500 | -4.18149000 | 4.10938500 |
| C | -2.08143700 | -3.15053500 | 4.96618300 |
| H | -1.21667100 | -1.18395500 | 5.10073900 |
| H | -2.84949300 | -5.09880000 | 4.52770300 |
| H | -2.21205600 | -3.26828700 | 6.03778700 |
| C | -1.53724900 | -5.88607500 | 1.32186800 |
| C | -3.72499100 | -6.01878200 | 2.32988800 |
| C | -1.98026000 | -6.70621100 | 0.11486100 |
| H | -1.11725600 | -6.55722900 | 2.09544100 |
| H | -0.75049000 | -5.18470700 | 1.04138200 |
| C | -4.25923100 | -6.85359000 | 1.16568700 |
| H | -3.37360600 | -6.70798100 | 3.12244900 |
| H | -4.52578300 | -5.40867300 | 2.75912400 |
| C | -3.13193000 | -7.63910500 | 0.49292200 |
| H | -1.13139900 | -7.27650100 | -0.27626000 |
| H | -2.30433500 | -6.01323200 | -0.67201100 |
| H | -5.03636200 | -7.53306000 | 1.53194000 |
| H | -4.72859500 | -6.18396600 | 0.43456300 |
| H | -3.50679400 | -8.17182900 | -0.38698000 |
| H | -2.76023200 | -8.40028000 | 1.19251700 |
| N | -2.66835500 | -5.13258200 | 1.86457200 |

**2-dim8**



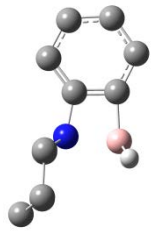
**Sum of electronic and thermal Enthalpies= -1016.082740**

**Sum of electronic and thermal Free Energies= -1016.151726**

| | | | |
|---|---|---|---|
| B | 1.32099800 | 14.00873800 | 5.20055300 |
| H | 2.34657900 | 14.41149000 | 4.70612700 |
| H | 0.40032100 | 14.22869500 | 4.46283600 |
| C | 1.56481600 | 12.48442300 | 5.69658700 |
| C | 2.89441000 | 12.18218400 | 6.02354800 |
| H | 3.64760700 | 12.93318100 | 5.80151600 |
| C | 3.29359400 | 10.99295300 | 6.62257100 |
| H | 4.33812700 | 10.81995000 | 6.86241400 |
| C | 2.33182600 | 10.04317300 | 6.91593100 |
| H | 2.59625700 | 9.11106300 | 7.40500300 |
| C | 1.00437500 | 10.27704700 | 6.56892000 |
| H | 0.28958600 | 9.50828500 | 6.82117400 |
| C | 0.62145500 | 11.46405900 | 5.94495000 |
| B | -1.46513200 | 13.05776700 | 6.24067600 |
| H | -1.49558400 | 13.88012600 | 5.36712300 |
| H | -2.59080900 | 12.76635600 | 6.56742500 |
| C | -0.62210200 | 13.39668200 | 7.58319900 |
| C | -1.07711100 | 12.74902900 | 8.74066100 |
| H | -2.00576100 | 12.18929900 | 8.66871300 |
| C | -0.40674300 | 12.77757900 | 9.95799900 |
| H | -0.80389000 | 12.24882500 | 10.81891900 |
| C | 0.78004500 | 13.48264600 | 10.04500700 |
| H | 1.34630300 | 13.51172400 | 10.97049200 |
| C | 1.25018500 | 14.17966600 | 8.93583000 |
| H | 2.18212300 | 14.71212900 | 9.05257000 |
| C | 0.55338600 | 14.16499900 | 7.72783100 |
| C | -0.80503800 | 11.73664400 | 4.01817900 |
| C | -1.65453900 | 10.47723700 | 5.90246500 |
| C | -2.20194500 | 11.83918500 | 3.42511300 |
| H | -0.30612200 | 10.82864100 | 3.65601900 |
| H | -0.20105900 | 12.59578600 | 3.74272000 |
| C | -3.06686600 | 10.49191500 | 5.32436400 |
| H | -1.15821300 | 9.57734500 | 5.52404700 |
| H | -1.68414100 | 10.43097200 | 6.99288300 |
| C | -3.04835400 | 10.62834000 | 3.80461800 |
| H | -2.09344300 | 11.92064700 | 2.33878400 |
| H | -2.67712000 | 12.76043300 | 3.77503400 |
| H | -3.54130900 | 9.55189800 | 5.62608800 |
| H | -3.64618500 | 11.30553700 | 5.76382800 |
| H | -4.06643100 | 10.72408600 | 3.41558600 |

| | | | |
|---|---|---|---|
| H | -2.61491000 | 9.72459900 | 3.35491900 |
| N | -0.80308800 | 11.65777900 | 5.52681400 |
| C | 0.00201600 | 16.04362800 | 6.32045500 |
| C | 2.32366400 | 15.70100800 | 6.91419600 |
| C | 0.40172100 | 17.03557600 | 5.23871400 |
| H | -0.15157700 | 16.56510700 | 7.27385800 |
| H | -0.91672600 | 15.52908400 | 6.05683200 |
| C | 2.77922500 | 16.73098500 | 5.88460400 |
| H | 2.16234100 | 16.23419700 | 7.85695400 |
| H | 3.09202600 | 14.94064300 | 7.06782100 |
| C | 1.68978500 | 17.76309300 | 5.61006700 |
| H | -0.42639800 | 17.74111100 | 5.11572500 |
| H | 0.52372700 | 16.50763700 | 4.28812100 |
| H | 3.67655700 | 17.20841100 | 6.29276600 |
| H | 3.06651400 | 16.23643400 | 4.95519600 |
| H | 1.99979900 | 18.44602600 | 4.81361000 |
| H | 1.51908400 | 18.37162400 | 6.50859300 |
| N | 1.04748100 | 14.98298600 | 6.57467300 |

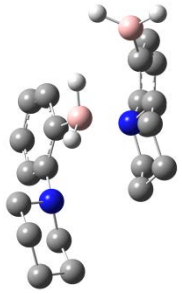
**2-close**



**Sum of electronic and thermal Enthalpies= -508.032423**
**Sum of electronic and thermal Free Energies= -508.079745**

| | | | |
|---|---|---|---|
| C | -1.34053100 | -2.42091900 | 0.68444800 |
| C | -0.02843500 | -2.05637700 | 0.92932000 |
| C | 0.85995000 | -3.05719800 | 1.30871500 |
| C | 0.37850300 | -4.36510300 | 1.41993700 |
| C | -0.95832400 | -4.68392900 | 1.16147800 |
| C | -1.86843400 | -3.69562100 | 0.77910300 |
| H | 1.90480100 | -2.84614900 | 1.51727200 |
| H | 1.05678400 | -5.16064900 | 1.71506200 |
| H | -1.29177800 | -5.71212600 | 1.25948700 |
| H | -2.90942800 | -3.92750500 | 0.57510500 |
| B | -0.34175200 | -0.51186500 | 0.59174900 |
| H | 0.07208200 | -0.05710800 | -0.45043200 |
| H | -0.38603400 | 0.27800800 | 1.50730900 |
| C | -2.42816800 | -1.08097200 | -1.07477700 |
| C | -2.97849900 | -0.67830000 | 1.27924500 |
| C | -2.85057800 | 0.33451100 | -1.44525500 |
| H | -3.27352100 | -1.77620500 | -1.17554600 |
| H | -1.61471100 | -1.43512700 | -1.71087100 |
| C | -3.41373500 | 0.74655000 | 0.96347000 |
| H | -3.83341400 | -1.36652700 | 1.21920400 |
| H | -2.54755100 | -0.75264600 | 2.27950100 |
| H | -3.22341700 | 0.33453300 | -2.47412800 |
| H | -1.96565200 | 0.97980600 | -1.41606600 |
| H | -4.19285700 | 1.04376400 | 1.67214400 |
| H | -2.55794900 | 1.41322600 | 1.11683700 |
| N | -1.94033700 | -1.13493400 | 0.32423600 |
| C | -3.91212700 | 0.86196100 | -0.47824400 |
| H | -4.15952000 | 1.90107800 | -0.71385000 |
| H | -4.83534800 | 0.27822700 | -0.59424100 |

**2-BH-TS**

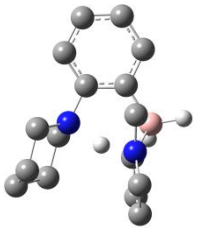


**Sum of electronic and thermal Enthalpies= -1016.057721**
**Sum of electronic and thermal Free Energies= -1016.131016**

| | | | |
|---|---|---|---|
| C | -2.58110800 | -0.66854400 | 0.52824800 |
| C | -1.46257800 | 0.17729400 | 0.51062400 |
| C | -1.52669600 | 1.36867100 | 1.24694000 |
| C | -2.64582400 | 1.72075100 | 1.98814200 |
| C | -3.73380300 | 0.86136600 | 2.00936600 |
| C | -3.70049000 | -0.32271000 | 1.28458300 |
| H | -0.66687100 | 2.03594000 | 1.25059300 |
| H | -2.65993300 | 2.64847600 | 2.55034500 |
| H | -4.61416000 | 1.09819900 | 2.59705700 |
| H | -4.55347400 | -0.98093500 | 1.35510100 |
| C | -3.90713500 | -2.55322900 | -0.33516300 |
| C | -1.93929200 | -1.77082500 | -1.53890500 |
| C | -3.97551200 | -3.78203000 | -1.22862400 |
| H | -4.55027200 | -1.76195300 | -0.74003300 |
| H | -4.25175000 | -2.83909000 | 0.65723000 |
| C | -1.95027800 | -3.00861800 | -2.42343300 |
| H | -2.48030200 | -0.94580100 | -2.01826500 |
| H | -0.89887900 | -1.46559700 | -1.41403200 |

| | | | |
|---|---|---|---|
| C | -3.36639900 | -3.54047300 | -2.60344500 |
| H | -5.03364800 | -4.05220600 | -1.31201600 |
| H | -3.47034500 | -4.60782000 | -0.72574500 |
| H | -1.50789700 | -2.72418100 | -3.38353300 |
| H | -1.30950000 | -3.77592100 | -1.98174500 |
| H | -3.36191900 | -4.46326900 | -3.19085600 |
| H | -3.96861700 | -2.80775200 | -3.15765300 |
| N | -2.52835000 | -1.97356800 | -0.17558400 |
| B | -0.07055100 | -0.03084500 | -0.17364600 |
| B | -1.52118000 | -3.00783900 | 0.74326200 |
| H | -1.63420300 | -4.10100000 | 0.24473200 |
| H | -0.41631400 | -2.54177600 | 0.52704900 |
| C | -1.92507300 | -2.88354600 | 2.29829700 |
| C | -1.24053800 | -1.94931900 | 3.08701300 |
| C | -2.97534000 | -3.58934100 | 2.92424600 |
| C | -1.59600300 | -1.65775400 | 4.39962600 |
| H | -0.41464600 | -1.40705500 | 2.63457200 |
| C | -3.34297500 | -3.29886200 | 4.24267700 |
| C | -2.66961300 | -2.32503100 | 4.97323600 |
| H | -1.04703300 | -0.90912700 | 4.96293900 |
| H | -4.15627800 | -3.84091500 | 4.71379300 |
| H | -2.97338200 | -2.11008600 | 5.99374100 |
| C | -2.86480800 | -5.86944000 | 2.17666200 |
| C | -5.03061600 | -4.88440500 | 2.56390600 |
| C | -3.43966400 | -6.87643500 | 1.18523300 |
| H | -2.84865300 | -6.31926700 | 3.18844600 |
| H | -1.83533100 | -5.62247700 | 1.91327100 |
| C | -5.68651200 | -5.81342500 | 1.54440300 |
| H | -5.11830200 | -5.35608900 | 3.56231100 |
| H | -5.55999700 | -3.92668300 | 2.61365400 |
| C | -4.92178100 | -7.13525900 | 1.45902200 |
| H | -2.86866700 | -7.80905000 | 1.24612100 |
| H | -3.31222000 | -6.48703400 | 0.16881900 |
| H | -6.73023400 | -5.98849300 | 1.82689700 |
| H | -5.68871100 | -5.32245000 | 0.56443700 |
| H | -5.35164700 | -7.78447600 | 0.68917500 |
| H | -5.02331800 | -7.66490400 | 2.41609600 |
| N | -3.64553900 | -4.62806300 | 2.19333500 |
| H | 0.85257800 | -0.44315000 | 0.46166500 |
| H | 0.13465900 | 0.38876900 | -1.27786800 |

**2-TS1-p**

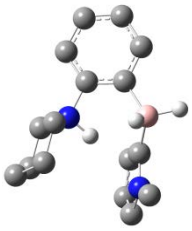


**Sum of electronic and thermal Enthalpies= -757.333392**

**Sum of electronic and thermal Free Energies= -757.394537**

| | | | |
|---|---|---|---|
| C | -1.29846200 | -2.22282100 | 0.63003700 |
| C | -0.09581200 | -1.85079700 | 1.25312100 |
| C | 1.00944500 | -2.66657800 | 0.97759800 |
| C | 0.92737800 | -3.77650600 | 0.14224200 |
| C | -0.28147300 | -4.10560900 | -0.46530400 |
| C | -1.40377300 | -3.32234100 | -0.22013900 |
| H | 1.96369000 | -2.40775500 | 1.42928200 |
| H | 1.80931300 | -4.38245400 | -0.04471200 |
| H | -0.35292100 | -4.96636200 | -1.12283300 |
| H | -2.35258000 | -3.57522500 | -0.68440500 |
| H | -1.71692600 | -0.15643900 | 1.28861600 |
| B | 0.01516000 | -0.53920300 | 2.19643500 |
| H | 1.16881000 | -0.16396200 | 2.30230800 |
| C | -0.88012100 | 0.74544300 | 1.52150900 |
| C | -1.45607900 | 1.80524700 | 2.25505200 |
| C | -1.38642900 | 2.98335400 | 1.51611100 |
| H | -1.88163100 | 1.68236600 | 3.24202600 |
| H | -1.73956500 | 3.96595600 | 1.79234600 |
| H | -0.50474400 | -0.72336700 | 3.28573100 |
| C | -0.75267800 | 2.65282500 | 0.31961900 |
| H | -0.49495300 | 3.28292300 | -0.52148800 |
| C | -3.31255800 | -1.06099400 | -0.22635000 |
| C | -3.20821100 | -1.83683800 | 2.09181300 |
| C | -4.28772000 | 0.04970700 | 0.15469400 |
| H | -3.87583100 | -1.95078700 | -0.54819400 |
| H | -2.67129300 | -0.75562600 | -1.05790700 |
| C | -4.21872200 | -0.77851700 | 2.52421500 |
| H | -2.48637800 | -2.03577600 | 2.88637700 |
| H | -3.71769200 | -2.78215700 | 1.84510200 |
| C | -5.12697500 | -0.36710700 | 1.36414100 |
| H | -4.92765200 | 0.27492200 | -0.70426700 |
| H | -3.72143900 | 0.95951300 | 0.38951800 |
| H | -4.80672000 | -1.16887700 | 3.36060000 |
| H | -3.67584900 | 0.09861900 | 2.89256300 |
| H | -5.76787900 | -1.21423600 | 1.08407500 |
| H | -5.79071600 | 0.44773800 | 1.66874300 |
| N | -2.44515000 | -1.38087700 | 0.91408100 |
| N | -0.46426600 | 1.34360700 | 0.31465900 |
| C | 0.28370900 | 0.65699000 | -0.72097400 |
| H | -0.28715100 | -0.18631100 | -1.11469100 |
| H | 0.50179600 | 1.35767200 | -1.52836200 |
| H | 1.21574400 | 0.26928300 | -0.30379400 |

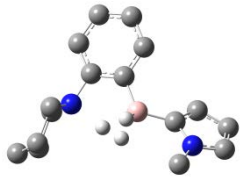
**2-Int1-p**



**Sum of electronic and thermal Enthalpies= -757.351073**
**Sum of electronic and thermal Free Energies= -757.411054**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 1.08594700 | -0.96965600 | 2.94985900 | H | 5.14959500 | 5.63710300 | -2.07805700 |
| C | 1.82757800 | -0.62542300 | 2.23501900 | C | 5.64392500 | 5.01215600 | 0.56370500 |
| C | 2.22093400 | 0.70849000 | 2.23420400 | H | 5.13603300 | 5.37849500 | 1.45794900 |
| C | 2.37829400 | -1.52489700 | 1.32485400 | H | 6.37747700 | 4.26445000 | 0.87848700 |
| C | 3.17592500 | 1.21677500 | 1.34002800 | H | 6.16122300 | 5.84184000 | 0.07789200 |
| H | 1.78413700 | 1.39692500 | 2.95151800 | C | 7.02539400 | 1.51295400 | -0.85123400 |
| C | 3.32161600 | -1.07204600 | 0.41080600 | C | 5.52057600 | 1.08553900 | -2.81375300 |
| H | 2.07754100 | -2.56731200 | 1.32278700 | C | 6.96473600 | 1.05300400 | -2.30897000 |
| C | 3.68200900 | 0.27026100 | 0.44067300 | H | 8.03955400 | 1.42942600 | -0.45036900 |
| H | 3.75802500 | -1.76251200 | -0.30441400 | H | 6.73358200 | 2.56881100 | -0.78487500 |
| B | 3.70755600 | 2.75760800 | 1.42168200 | H | 5.44975300 | 0.68040300 | -3.82741500 |
| H | 3.01362100 | 3.39350900 | 2.19759000 | H | 5.15632100 | 2.12031200 | -2.84775700 |
| H | 4.44791900 | 1.80143000 | -0.57334200 | H | 7.59410000 | 1.69254100 | -2.93381900 |
| H | 4.85240500 | 2.71958700 | 1.88002800 | H | 7.36423700 | 0.03324000 | -2.38933400 |
| C | 3.75968400 | 3.47177400 | -0.03747600 | N | 4.69365800 | 0.78032400 | -0.51011400 |
| C | 3.01196100 | 3.27628900 | -1.19663900 | C | 4.59880400 | 0.27462300 | -1.90968100 |
| N | 4.68526400 | 4.44734200 | -0.36322500 | H | 3.55262200 | 0.36880400 | -2.20522500 |
| C | 3.48962200 | 4.14532200 | -2.21576200 | H | 4.87488300 | -0.78357900 | -1.90876100 |
| H | 2.18333500 | 2.58261900 | -1.27369100 | C | 6.08720700 | 0.69670600 | 0.02766000 |
| C | 4.52452200 | 4.85938000 | -1.66217700 | H | 6.35713700 | -0.36420400 | 0.05123800 |
| H | 3.10997000 | 4.25242200 | -3.22231900 | H | 6.04250400 | 1.08403200 | 1.04603500 |

**2-TS2-p**

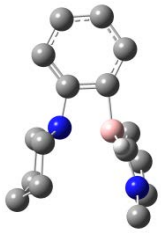


**Sum of electronic and thermal Enthalpies= -757.324861**
**Sum of electronic and thermal Free Energies= -757.386404**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 1.19622300 | 0.05856600 | 2.41993100 | H | 0.98315600 | 5.99319100 | -0.50277800 |
| C | 1.99387100 | 0.05769400 | 1.68345000 | H | 3.38134300 | 7.22078700 | -0.16780200 |
| C | 2.63273900 | 1.24892800 | 1.35184800 | N | 4.12619300 | 5.22746800 | -0.03600200 |
| C | 2.36902500 | -1.13254100 | 1.06705200 | C | 5.52710600 | 5.53167300 | 0.15427500 |
| C | 3.66608800 | 1.28899400 | 0.40945000 | H | 5.89677000 | 5.10162800 | 1.08818200 |
| H | 2.31753600 | 2.17689100 | 1.81991300 | H | 6.13103400 | 5.13783200 | -0.66868300 |
| C | 3.39318700 | -1.12787700 | 0.12631300 | H | 5.65293300 | 6.61512600 | 0.19176100 |
| H | 1.86944800 | -2.06285700 | 1.31832400 | C | 7.53382400 | 0.32573100 | -1.50725700 |
| C | 4.03213200 | 0.06993600 | -0.18269900 | C | 5.97445200 | -0.20458400 | -3.40618300 |
| H | 3.69501700 | -2.05315700 | -0.35553600 | C | 7.38513000 | -0.39988600 | -2.84601900 |
| B | 4.43025400 | 2.63896600 | 0.02019200 | H | 8.50924200 | 0.11842300 | -1.05653800 |
| H | 4.97543100 | 1.69209900 | -1.32887700 | H | 7.47382700 | 1.40989700 | -1.66333900 |
| H | 4.82566800 | 2.53974800 | -1.37004600 | H | 5.83557500 | -0.78587000 | -4.32293800 |
| C | 3.58022100 | 3.95634600 | -0.09455100 | H | 5.82134000 | 0.85024600 | -3.66436100 |
| C | 2.21948100 | 4.13304200 | -0.29975000 | H | 8.13331500 | -0.04527400 | -3.56136500 |
| C | 1.94342900 | 5.51899900 | -0.35957300 | H | 7.56849100 | -1.47260400 | -2.69757500 |
| H | 1.50365900 | 3.32786500 | -0.39647700 | N | 5.10806900 | 0.14090100 | -1.14048900 |
| C | 3.14639100 | 6.16598900 | -0.19374100 | H | 5.53691600 | 2.75088700 | 0.50137300 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 4.92141600 | -0.61879700 | -2.38118600 | C | 6.43255000 | -0.08975100 | -0.53754200 |
| H | 3.91152800 | -0.41927800 | -2.74832000 | H | 6.53514800 | -1.15467600 | -0.27157500 |
| H | 5.00188400 | -1.70159300 | -2.19103600 | H | 6.48175500 | 0.49242700 | 0.38518300 |

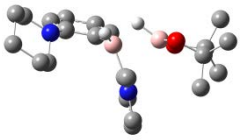
**2-Int2-p**



**Sum of electronic and thermal Enthalpies= -756.181285**
**Sum of electronic and thermal Free Energies= -756.241953**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.45995600 | -3.15092300 | 1.68346200 | C | -3.00607400 | 3.36078900 | -1.10804700 |
| C | -1.07344600 | -3.27055900 | 1.54903000 | H | -3.15998500 | 3.28549400 | -0.03155100 |
| C | -0.31007300 | -2.21895000 | 1.03741600 | H | -1.97638400 | 3.69183400 | -1.29153400 |
| C | -1.02273400 | -1.08548000 | 0.68730000 | H | -3.68875300 | 4.11263300 | -1.50960000 |
| C | -2.38991000 | -0.92343000 | 0.80983200 | C | 0.27226000 | 0.97996800 | 1.01009600 |
| C | -3.13414800 | -1.98290300 | 1.31683600 | C | 0.00308000 | 0.03992900 | -1.23564700 |
| H | -3.02119400 | -3.99148900 | 2.08117100 | C | 0.51264200 | 2.36799600 | 0.43096400 |
| H | -0.58560500 | -4.19493400 | 1.84174300 | C | 0.26971400 | 1.39792500 | -1.87172700 |
| H | 0.76590600 | -2.30434100 | 0.91939700 | C | 1.13113300 | 2.27800500 | -0.96497200 |
| H | -4.21243300 | -1.91851800 | 1.42856400 | H | 1.15901000 | 2.93207200 | 1.11044300 |
| B | -2.37967600 | 0.57318100 | 0.22566700 | H | -0.44819200 | 2.89281100 | 0.38358500 |
| H | -2.43050200 | 1.47148600 | 1.03679300 | H | 0.75659400 | 1.24110600 | -2.83905500 |
| C | -3.02754800 | 0.83604500 | -1.18151700 | H | -0.69147000 | 1.88149700 | -2.07186000 |
| C | -3.40860200 | -0.08647000 | -2.14465600 | H | 1.24663900 | 3.27619400 | -1.39866600 |
| C | -3.87994200 | 0.60686200 | -3.28466200 | H | 2.13836000 | 1.84669700 | -0.88558600 |
| H | -3.35782100 | -1.15930900 | -2.01157600 | N | -0.59439200 | 0.18609600 | 0.11173900 |
| C | -3.78349900 | 1.94773300 | -2.99416800 | H | 1.22603600 | 0.44965800 | 1.14643100 |
| H | -4.26413600 | 0.18319600 | -4.20153200 | H | -0.22964800 | 1.03395100 | 1.97849000 |
| H | -4.05030000 | 2.81748100 | -3.57823000 | H | -0.69820800 | -0.53816300 | -1.83994900 |
| N | -3.27726600 | 2.08451900 | -1.73111800 | H | 0.93768200 | -0.53115800 | -1.13907600 |

**2-TS3-p**

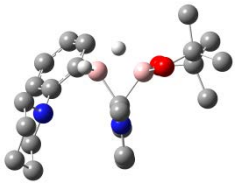


**Sum of electronic and thermal Enthalpies= -1167.754146**
**Sum of electronic and thermal Free Energies= -1167.835107**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.06201300 | -2.02358500 | 0.96227400 | H | 0.68403400 | -0.82401000 | 3.45872500 |
| C | -0.72273800 | -1.64574500 | 1.01263100 | C | 3.23172600 | 1.24776100 | 3.57228100 |
| C | -0.28883500 | -0.37609900 | 0.61530100 | H | 2.23073400 | 0.39290700 | 5.33383100 |
| C | -1.26818200 | 0.54799600 | 0.18393200 | H | 4.02204000 | 1.88806500 | 3.93819900 |
| C | -2.61414400 | 0.16697000 | 0.13713100 | H | 1.62941600 | 0.77793400 | -0.24477300 |
| C | -3.00813700 | -1.11255700 | 0.51322500 | B | 2.60665700 | -1.60315000 | 0.71603500 |
| H | -2.35805700 | -3.02407700 | 1.26231500 | O | 3.93572000 | -1.39913900 | 0.47582800 |
| H | 0.01245400 | -2.37311100 | 1.34604800 | O | 2.31989500 | -2.73690600 | 1.41935600 |
| H | -3.36617200 | 0.87836400 | -0.18679300 | C | 4.64419500 | -2.30859300 | 1.35416800 |
| H | -4.05805900 | -1.38632300 | 0.46466600 | C | 3.57320300 | -3.43314000 | 1.61296600 |
| B | 1.24913700 | 0.04057800 | 0.62283200 | C | 5.90058400 | -2.77797000 | 0.63555900 |
| H | 1.78684800 | -1.14750300 | -0.08904600 | H | 6.57796200 | -1.93218300 | 0.49346100 |
| C | 1.95655200 | 0.23373800 | 2.02442300 | H | 6.42158600 | -3.53331200 | 1.23204200 |
| C | 1.51510100 | -0.15408800 | 3.28827200 | H | 5.67328200 | -3.20001900 | -0.34426000 |
| C | 2.31262200 | 0.47599600 | 4.26002800 | C | 5.01878700 | -1.53272200 | 2.61549100 |

| | | | |
|---|---|---|---|
| H | 5.59521100 | -0.64943900 | 2.32819800 |
| H | 4.13610400 | -1.19763300 | 3.16375600 |
| H | 5.63518100 | -2.14452300 | 3.28008500 |
| C | 3.58850600 | -4.01167400 | 3.02033900 |
| H | 2.81531900 | -4.77900900 | 3.10753600 |
| H | 4.55611300 | -4.47632200 | 3.23405400 |
| H | 3.39014200 | -3.24239300 | 3.76781600 |
| C | 3.61136200 | -4.55418500 | 0.57461200 |
| H | 4.50634500 | -5.17222000 | 0.68610300 |
| H | 2.73179400 | -5.18826000 | 0.70758500 |
| H | 3.58745600 | -4.15087800 | -0.44130400 |
| N | 3.02195000 | 1.09991800 | 2.24062700 |
| C | 3.80295600 | 1.74603300 | 1.20526500 |
| H | 4.20983700 | 0.99449600 | 0.52604400 |
| H | 3.18711200 | 2.44697900 | 0.63724400 |
| H | 4.62375300 | 2.29111600 | 1.67434700 |
| C | -0.95946400 | 3.71368100 | -1.78849800 |
| C | 0.44752100 | 3.86303000 | 0.28120400 |
| C | -0.37682900 | 4.65605700 | -0.73401200 |
| H | -1.62479900 | 4.25807600 | -2.46724100 |
| H | -0.14795500 | 3.28669900 | -2.38895500 |
| H | 0.79735800 | 4.51114600 | 1.09203000 |
| H | 1.32948600 | 3.44045000 | -0.21566600 |
| H | 0.23074800 | 5.43554600 | -1.20544000 |
| H | -1.19890800 | 5.16427400 | -0.21120800 |
| N | -0.86334500 | 1.84841900 | -0.21175400 |
| C | -1.72875900 | 2.56859300 | -1.13070300 |
| H | -2.61969900 | 2.98587000 | -0.62025800 |
| H | -2.08523700 | 1.87021700 | -1.89298100 |
| C | -0.37227100 | 2.71344200 | 0.85913400 |
| H | 0.23125900 | 2.12493900 | 1.55234100 |
| H | -1.22097300 | 3.12280000 | 1.44090200 |

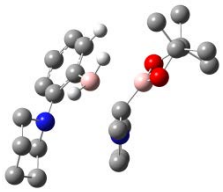
**2-Int3-p**



**Sum of electronic and thermal Enthalpies= -1167.761865**
**Sum of electronic and thermal Free Energies= -1167.842499**

| | | | |
|---|---|---|---|
| C | -1.84323900 | -2.42899700 | 0.20829000 |
| C | -0.52853700 | -1.98780600 | 0.06880300 |
| C | -0.18044700 | -0.64018500 | 0.18655800 |
| C | -1.21557000 | 0.28507300 | 0.44107700 |
| C | -2.53283200 | -0.15475600 | 0.58650600 |
| C | -2.84594700 | -1.50723500 | 0.47477300 |
| H | -2.07526400 | -3.48612000 | 0.12329100 |
| H | 0.25808700 | -2.72001200 | -0.09420200 |
| H | -3.32318400 | 0.56219100 | 0.78498300 |
| H | -3.87527000 | -1.83296300 | 0.59325100 |
| B | 1.33958900 | -0.16687900 | 0.12046700 |
| H | 2.03314100 | -1.20931700 | -0.13367800 |
| C | 1.93245100 | 0.37245800 | 1.59272000 |
| C | 1.19699700 | 0.35236600 | 2.79508000 |
| C | 1.55116200 | 1.45017300 | 3.56523400 |
| H | 0.48737300 | -0.42424900 | 3.04142700 |
| C | 2.50099800 | 2.15589100 | 2.82554300 |
| H | 1.17740800 | 1.72512500 | 4.54013100 |
| H | 3.02673500 | 3.06858900 | 3.07204200 |
| B | 2.64821600 | -1.08692600 | 1.13168700 |
| O | 4.03761300 | -1.01948700 | 0.91560000 |
| O | 2.29444400 | -2.26276500 | 1.81536300 |
| C | 4.56403800 | -2.30489800 | 1.27894600 |
| C | 3.51786800 | -2.79652600 | 2.33512900 |
| C | 4.58547600 | -3.17701200 | 0.02139800 |
| H | 5.14962700 | -2.65839300 | -0.75793900 |
| H | 5.06076100 | -4.14417000 | 0.20831200 |
| H | 3.57255800 | -3.35421100 | -0.35120400 |
| C | 5.97425200 | -2.11682700 | 1.81873300 |
| H | 6.63889900 | -1.78371400 | 1.01687200 |
| H | 5.99532700 | -1.36739300 | 2.61164100 |
| H | 6.36534800 | -3.05963700 | 2.21458800 |
| C | 3.75004100 | -2.18156900 | 3.71922700 |
| H | 2.87131000 | -2.37590800 | 4.33921300 |
| H | 4.62648700 | -2.61282500 | 4.21170700 |
| H | 3.88256000 | -1.09787800 | 3.65040600 |
| C | 3.38404400 | -4.30837500 | 2.44352300 |
| H | 4.33619400 | -4.76152100 | 2.73806800 |
| H | 2.63746000 | -4.55917500 | 3.20137200 |
| H | 3.06369900 | -4.74538800 | 1.49638600 |
| N | 2.72839400 | 1.53057100 | 1.66573800 |
| C | 3.67306300 | 1.97080200 | 0.65655200 |
| H | 4.40974500 | 1.18488900 | 0.48473100 |
| H | 3.14881000 | 2.18185200 | -0.27770300 |
| H | 4.16408900 | 2.87821100 | 1.00981200 |
| C | 0.16992700 | 3.64712500 | -0.38798200 |
| C | -0.95361400 | 3.74395600 | 1.85451000 |
| C | -0.59221900 | 4.53578000 | 0.59633600 |
| H | 0.35765000 | 4.17739400 | -1.32791700 |
| H | 1.13987800 | 3.37195100 | 0.04411300 |
| H | -1.58057600 | 4.34592900 | 2.52156400 |
| H | -0.04020600 | 3.47972000 | 2.39943100 |
| H | -0.00527000 | 5.42377900 | 0.85493100 |
| H | -1.51374700 | 4.89313300 | 0.11648600 |
| N | -0.87128100 | 1.65859500 | 0.58744700 |
| C | -0.60887900 | 2.36426600 | -0.66323000 |
| H | -1.55876700 | 2.61061200 | -1.17704300 |
| H | -0.04343900 | 1.70795000 | -1.32605000 |
| C | -1.68420200 | 2.45117700 | 1.49510200 |
| H | -1.87204300 | 1.86048700 | 2.39658800 |
| H | -2.66833800 | 2.70894200 | 1.05536300 |
| H | 1.71860600 | 0.58118700 | -0.74081800 |

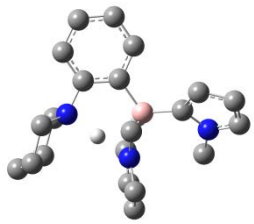
**2-TS4-p**



**Sum of electronic and thermal Enthalpies= -1167.762324**
**Sum of electronic and thermal Free Energies= -1167.841712**

| | | | |
|---|---|---|---|
| C | -2.13530100 | -1.51698100 | 1.00197600 |
| C | -1.04885300 | -0.67268100 | 0.67446200 |
| C | 0.05674300 | -1.26669700 | 0.05930000 |
| C | 0.12692400 | -2.63410700 | -0.20352700 |
| C | -0.93936100 | -3.44758400 | 0.15120000 |
| C | -2.06991300 | -2.88782800 | 0.74309500 |
| H | 0.90738400 | -0.63645300 | -0.18580100 |
| H | 1.01233000 | -3.05871600 | -0.66726300 |
| H | -0.90378700 | -4.51674400 | -0.03782000 |
| H | -2.90677400 | -3.53013000 | 0.99861000 |
| N | -3.27557400 | -0.94130100 | 1.63388800 |
| B | -1.00433700 | 0.88008400 | 1.04991100 |
| H | -2.00737400 | 1.53890700 | 0.94191100 |
| H | -0.08201900 | 1.45080400 | 0.49301900 |
| C | 2.55417700 | 2.76202600 | 1.79695500 |
| C | 3.01783700 | 1.29782900 | 2.12898100 |
| O | 1.21770400 | 2.78817100 | 2.34504700 |
| O | 1.77703800 | 0.56809000 | 2.15307100 |
| B | 0.77486400 | 1.48438700 | 2.35682700 |
| C | 3.36908400 | 3.85798900 | 2.46839000 |
| H | 2.96884100 | 4.83606600 | 2.18914700 |
| H | 3.33417400 | 3.77299100 | 3.55558900 |
| H | 4.41361600 | 3.81217500 | 2.14467300 |
| C | 2.44048700 | 3.03410600 | 0.29699600 |
| H | 1.92491200 | 3.98639400 | 0.15019900 |
| H | 3.42698500 | 3.09884100 | -0.17037400 |
| H | 1.86104300 | 2.25720000 | -0.20707400 |
| C | 3.93244700 | 0.66904500 | 1.08754300 |
| H | 4.86326200 | 1.23762500 | 0.99527500 |
| H | 4.18254700 | -0.35095600 | 1.38988300 |
| H | 3.44989300 | 0.62144100 | 0.11030900 |
| C | 3.63507100 | 1.16538100 | 3.52246700 |
| H | 3.75644900 | 0.10423400 | 3.75251800 |
| H | 4.61513100 | 1.64725700 | 3.57784800 |
| H | 2.98395600 | 1.60538800 | 4.28293600 |
| C | -0.65698300 | 1.06962100 | 2.85038900 |
| C | -0.81404900 | -0.10458300 | 3.63789000 |
| C | -1.70437200 | 0.14227300 | 4.66211800 |
| H | -0.30065900 | -1.03047900 | 3.42079500 |
| C | -2.10743000 | 1.47615100 | 4.51647600 |
| H | -2.05307400 | -0.54312000 | 5.41984200 |
| H | -2.81243800 | 2.04637000 | 5.10729400 |
| N | -1.48718300 | 2.03074600 | 3.48002200 |
| C | -1.69619700 | 3.38560900 | 3.00331400 |
| H | -0.73322600 | 3.88366500 | 2.89169200 |
| H | -2.19444700 | 3.35126600 | 2.03174700 |
| H | -2.31795000 | 3.92143500 | 3.72134800 |
| C | -4.14314900 | -0.17739000 | 0.74014100 |
| H | -3.52063900 | 0.39807500 | 0.05569500 |
| H | -4.76670700 | -0.85856300 | 0.12798300 |
| C | -4.04612700 | -1.79658700 | 2.52096100 |
| H | -4.66463300 | -2.52835600 | 1.96322500 |
| H | -3.35073700 | -2.36672200 | 3.14493600 |
| C | -5.04390200 | 0.74708800 | 1.55200000 |
| C | -4.96923200 | -0.95001800 | 3.39762300 |
| C | -5.87769900 | -0.06387600 | 2.54443500 |
| H | -4.34782000 | -0.32011500 | 4.04370000 |
| H | -5.56426300 | -1.60605300 | 4.04282500 |
| H | -4.40268300 | 1.45501000 | 2.09285900 |
| H | -5.69022100 | 1.32409300 | 0.88172600 |
| H | -6.57833000 | -0.69873800 | 1.98466800 |
| H | -6.48252700 | 0.59271100 | 3.17935900 |

**2-TS5-p**

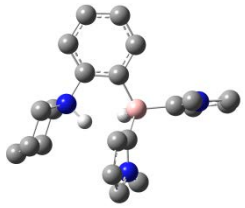


**Sum of electronic and thermal Enthalpies= -1005.476864**
**Sum of electronic and thermal Free Energies= -1005.548292**

| | | | |
|---|---|---|---|
| C | 1.26538600 | 0.17189400 | 1.14924900 |
| C | 2.12536300 | 1.25457200 | 0.99842400 |
| C | 1.68940500 | -1.11176700 | 0.81959500 |
| C | 3.43778400 | 1.11826100 | 0.51942300 |
| C | 2.97059600 | -1.29002400 | 0.31414200 |
| H | 1.02612900 | -1.96275700 | 0.93863500 |
| C | 3.81336900 | -0.18940500 | 0.16264100 |
| B | 4.42215900 | 2.40126600 | 0.32568200 |
| H | 5.74048900 | 0.89830300 | 0.03854100 |
| C | 6.08957300 | 1.95969000 | 0.56864300 |
| C | 7.15596500 | 2.58715000 | -0.11364200 |
| C | 8.24801100 | 2.71934600 | 0.73930500 |
| H | 7.09714100 | 2.90038300 | -1.14765400 |
| C | 7.85454400 | 2.17049500 | 1.95888700 |
| H | 9.21381500 | 3.15300300 | 0.52534000 |
| H | 8.40257500 | 2.08541500 | 2.88786200 |

| | | | |
|---|---|---|---|
| H | 0.26046200 | 0.33042800 | 1.52948200 |
| H | 3.30652800 | -2.28177000 | 0.02484300 |
| H | 1.77473200 | 2.24715000 | 1.26130600 |
| N | 6.60083600 | 1.70891000 | 1.85632100 |
| C | 5.82455100 | 1.17950300 | 2.96142200 |
| H | 5.10730300 | 0.44845000 | 2.58710900 |
| H | 6.49378300 | 0.70286400 | 3.68013200 |
| H | 5.26800900 | 1.99098800 | 3.43755700 |
| H | 4.43729400 | 2.70350300 | -0.86008100 |
| C | 4.11103500 | 3.64114500 | 1.29176500 |
| C | 3.53149800 | 3.69859600 | 2.55466700 |
| N | 4.50615100 | 4.93744400 | 1.01038200 |
| C | 3.58080000 | 5.03348300 | 3.03090000 |
| H | 3.08840400 | 2.85542800 | 3.06809200 |
| C | 4.19334100 | 5.77308600 | 2.05070600 |
| H | 3.19456500 | 5.41312400 | 3.96635900 |
| H | 4.41992600 | 6.82863700 | 1.99626500 |
| C | 5.22758700 | 5.37013600 | -0.16488700 |
| H | 5.06609700 | 6.44046700 | -0.31163800 |
| H | 6.30219400 | 5.18393300 | -0.06387700 |
| H | 4.86297000 | 4.83509300 | -1.04251600 |
| C | 5.93688900 | -1.46352800 | 0.11025900 |
| C | 5.10056300 | -0.33456300 | -1.89573500 |
| C | 7.37564500 | -1.34977400 | -0.38797400 |
| C | 6.51248700 | -0.23913200 | -2.46706000 |
| C | 7.41279500 | -1.34665900 | -1.91722200 |
| H | 7.95974400 | -2.18365800 | 0.01371700 |
| H | 7.81843100 | -0.42318700 | -0.00164200 |
| H | 6.45681300 | -0.28796400 | -3.55900800 |
| H | 6.93717300 | 0.73592200 | -2.20655100 |
| H | 8.43832200 | -1.21707200 | -2.27592200 |
| H | 7.06373700 | -2.31947600 | -2.28962400 |
| N | 5.13034100 | -0.35770200 | -0.42183900 |
| H | 4.49874200 | 0.52763700 | -2.19252900 |
| H | 4.59601000 | -1.24276600 | -2.26281400 |
| H | 5.51641600 | -2.43396500 | -0.19608400 |
| H | 5.89079100 | -1.41251900 | 1.20153800 |

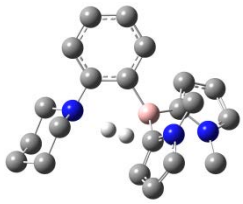
**2-Int4-p**



**Sum of electronic and thermal Enthalpies= -1005.496815**
**Sum of electronic and thermal Free Energies= -1005.568572**

| | | | |
|---|---|---|---|
| H | 0.20159200 | 0.81735800 | 1.19447400 |
| C | 1.24711000 | 0.70042500 | 0.92526700 |
| C | 1.99176400 | 1.81438500 | 0.55033900 |
| C | 1.82948800 | -0.56427300 | 0.94994400 |
| C | 3.34505500 | 1.73023400 | 0.19099800 |
| H | 1.51768100 | 2.79163900 | 0.51802200 |
| C | 3.16637500 | -0.70272800 | 0.59643800 |
| H | 1.25152000 | -1.43631800 | 1.23729100 |
| C | 3.87724300 | 0.43632400 | 0.23881800 |
| H | 3.63265300 | -1.68318500 | 0.60276700 |
| B | 4.20842200 | 3.01985000 | -0.34614700 |
| H | 5.66235300 | 1.28473000 | 0.02087700 |
| H | 4.44714500 | 2.78928000 | -1.53423800 |
| C | 3.39689700 | 4.40667100 | -0.31686500 |
| C | 2.93588000 | 5.16956500 | -1.37652900 |
| N | 3.02639300 | 5.09202900 | 0.82796000 |
| C | 2.28685100 | 6.32657100 | -0.86911000 |
| H | 3.05366500 | 4.89712500 | -2.41731500 |
| C | 2.36361400 | 6.24806900 | 0.49904500 |
| H | 1.81159000 | 7.11765900 | -1.43241200 |
| H | 2.00339500 | 6.91634900 | 1.26889100 |
| C | 3.36522100 | 4.71201600 | 2.18140600 |
| H | 3.16079000 | 3.65012900 | 2.34093000 |
| H | 4.42370600 | 4.88890700 | 2.39389200 |
| H | 2.75533800 | 5.29235000 | 2.87738300 |
| C | 5.64956600 | 3.12558400 | 0.41640500 |
| C | 6.10318900 | 2.67465700 | 1.65413100 |
| N | 6.73417700 | 3.75792400 | -0.16242100 |
| C | 7.46593700 | 3.04302000 | 1.81457500 |
| H | 5.48544300 | 2.15146000 | 2.37469600 |
| C | 7.82093400 | 3.71667600 | 0.66975100 |
| H | 8.10441400 | 2.85615600 | 2.66653000 |
| H | 8.75385100 | 4.18318200 | 0.38612100 |
| C | 6.69804500 | 4.43367600 | -1.44515100 |
| H | 7.63419800 | 4.97668800 | -1.58635000 |
| H | 6.57171300 | 3.71601700 | -2.26121200 |
| H | 5.85703600 | 5.12999600 | -1.47543600 |
| C | 7.61202000 | -0.37060800 | 0.30843900 |
| C | 6.91979300 | 0.28166900 | -2.01709700 |
| C | 7.85851000 | -0.59486200 | -1.18523400 |
| H | 8.21584700 | -1.05406900 | 0.91235800 |
| H | 7.89780200 | 0.65092600 | 0.59034900 |
| H | 7.03487600 | 0.08231400 | -3.08607100 |
| H | 7.15831300 | 1.34097600 | -1.85608000 |
| H | 8.90086900 | -0.37331300 | -1.42965900 |
| H | 7.68812700 | -1.65080200 | -1.43395300 |
| N | 5.29401900 | 0.31891600 | -0.16627500 |
| C | 6.14521200 | -0.58043400 | 0.66610500 |
| H | 5.83360600 | -1.61164000 | 0.47805000 |
| H | 5.94122500 | -0.33198100 | 1.70852900 |
| C | 5.46515900 | 0.05356900 | -1.62919300 |
| H | 4.79156200 | 0.73648100 | -2.14658200 |
| H | 5.14519400 | -0.97837000 | -1.80665000 |

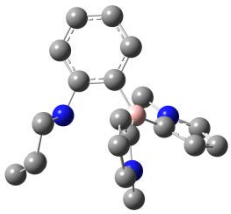
**2-TS6-p**



**Sum of electronic and thermal Enthalpies= -1005.469507**
**Sum of electronic and thermal Free Energies= -1005.541028**

| | | | |
|---|---|---|---|
| H | 1.05666300 | 0.27046600 | 2.34326100 |
| C | 1.91804500 | 0.27012900 | 1.68226100 |
| C | 2.53620500 | 1.47018600 | 1.34745200 |
| C | 2.39880900 | -0.92726400 | 1.16196200 |
| C | 3.65258800 | 1.52020800 | 0.50194500 |
| H | 2.13404800 | 2.40103300 | 1.73672400 |
| C | 3.49585500 | -0.90989300 | 0.30978700 |
| H | 1.92167000 | -1.86892800 | 1.41450900 |
| C | 4.11535900 | 0.29802900 | -0.00895800 |
| H | 3.87735600 | -1.83959800 | -0.10265800 |
| B | 4.39678200 | 2.91134500 | 0.18363900 |
| H | 5.16384100 | 2.01725400 | -1.09475900 |
| H | 4.97205400 | 2.81355800 | -1.20510900 |
| C | 3.43295700 | 4.12105800 | -0.12922700 |
| C | 2.11400800 | 4.06061300 | -0.56467800 |
| C | 1.63459400 | 5.37189000 | -0.76616200 |
| H | 1.56688900 | 3.14139200 | -0.72284800 |
| C | 2.67412600 | 6.21661300 | -0.44919600 |
| H | 0.65127700 | 5.67085800 | -1.09942600 |
| H | 2.72966800 | 7.29622500 | -0.45770400 |
| C | 5.76434300 | 3.17539500 | 0.96665400 |
| C | 7.06977700 | 3.27839900 | 0.51900700 |
| C | 7.90290500 | 3.60962900 | 1.61890200 |
| H | 7.37824100 | 3.16493700 | -0.51191300 |
| C | 7.08412400 | 3.70212500 | 2.71677900 |
| H | 8.97215400 | 3.76507700 | 1.60850800 |
| H | 7.30528900 | 3.92057900 | 3.75160700 |
| N | 3.75265700 | 5.47173900 | -0.07203200 |
| N | 5.79761900 | 3.43884500 | 2.31831800 |
| C | 5.01812300 | 6.06042500 | 0.32867800 |
| H | 5.24702600 | 5.84305300 | 1.37488500 |
| H | 5.83889300 | 5.67815600 | -0.27909700 |
| H | 4.94876100 | 7.14172100 | 0.19843600 |
| C | 4.64590300 | 3.44347600 | 3.19599400 |
| H | 3.84336300 | 4.04707900 | 2.76150600 |
| H | 4.26795200 | 2.43037400 | 3.35938400 |
| H | 4.93005300 | 3.87869500 | 4.15542800 |
| C | 7.70303200 | 0.07047400 | -1.13086000 |
| C | 6.19916900 | -0.05788900 | -3.12897700 |
| C | 7.50021900 | -0.56542700 | -2.50597500 |
| H | 8.58517000 | -0.34467700 | -0.63364300 |
| H | 7.87501700 | 1.14584700 | -1.24376600 |
| H | 6.00621300 | -0.54866100 | -4.08820000 |
| H | 6.27868100 | 1.01876400 | -3.32382600 |
| H | 8.35072400 | -0.34847200 | -3.15962900 |
| H | 7.44689000 | -1.65755200 | -2.40034400 |
| N | 5.25656400 | 0.33466200 | -0.89236200 |
| C | 6.48673400 | -0.13888100 | -0.23627800 |
| H | 6.38521300 | -1.20941700 | 0.01299200 |
| H | 6.59843100 | 0.41864000 | 0.69662600 |
| C | 5.02309800 | -0.30933300 | -2.19082200 |
| H | 4.09682300 | 0.10145700 | -2.60313400 |
| H | 4.87941800 | -1.39664300 | -2.07375600 |

**2-Int5-p**

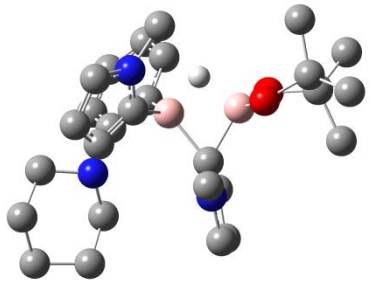


**Sum of electronic and thermal Enthalpies= -1004.326214**
**Sum of electronic and thermal Free Energies= -1004.40052**

| | | | |
|---|---|---|---|
| C | -2.61471100 | -2.71740200 | -0.68139800 |
| C | -1.26791000 | -3.02210100 | -0.50838600 |
| C | -0.34830400 | -2.00176800 | -0.28123700 |
| C | -0.77619400 | -0.67528500 | -0.23177700 |
| C | -2.12699300 | -0.35074500 | -0.41452000 |
| C | -3.03494200 | -1.38972500 | -0.64087500 |
| H | -3.33468500 | -3.51059800 | -0.85833700 |
| H | -0.93204200 | -4.05384200 | -0.55009600 |
| H | 0.70331400 | -2.23652800 | -0.14295400 |
| H | -4.08378500 | -1.15534400 | -0.80504800 |
| B | -2.55166800 | 1.17418500 | -0.41406100 |
| C | -2.62140500 | 1.89672100 | 0.94829200 |
| C | -2.93732400 | 1.29473100 | 2.16298100 |
| C | -2.97883600 | 2.28451600 | 3.16580900 |
| H | -3.13953300 | 0.23875700 | 2.28214100 |
| C | -2.66207800 | 3.47534400 | 2.54923300 |
| H | -3.21121300 | 2.15290300 | 4.21254700 |
| H | -2.53945500 | 4.46696600 | 2.96234200 |
| C | -3.06673800 | 1.83653800 | -1.70579700 |
| C | -4.03987400 | 2.83422200 | -1.79472800 |
| C | -4.37826200 | 3.02511600 | -3.14585900 |
| H | -4.46842900 | 3.33869900 | -0.93917000 |
| C | -3.59430400 | 2.14757100 | -3.86845200 |
| H | -5.10044800 | 3.71651300 | -3.55440000 |

| | | | |
|---|---|---|---|
| H | -3.52118500 | 1.99170200 | -4.93579100 |
| N | -2.46777700 | 3.25183700 | 1.21930500 |
| N | -2.82289500 | 1.42995500 | -3.01182100 |
| C | -1.89585600 | 4.25466200 | 0.33897300 |
| H | -2.42010900 | 5.20386900 | 0.47484300 |
| H | -0.83289200 | 4.40360100 | 0.55627300 |
| H | -2.00530900 | 3.94132100 | -0.69643600 |
| C | -1.85842300 | 0.43246000 | -3.43570800 |
| H | -0.90694700 | 0.59516400 | -2.92745700 |
| H | -2.20444300 | -0.57803600 | -3.20720500 |
| H | -1.70401700 | 0.52905000 | -4.51164500 |
| C | 0.47289600 | 0.60057100 | 1.39916800 |
| C | 1.31822000 | 0.43193900 | -0.85523600 |
| C | 1.13519300 | 1.95859300 | 1.60295800 |
| C | 1.99521600 | 1.79778200 | -0.75648900 |
| C | 2.35857200 | 2.11222000 | 0.69697000 |
| H | 1.41177900 | 2.07932400 | 2.65535300 |
| H | 0.39443300 | 2.73123900 | 1.36873600 |
| H | 2.88749300 | 1.81643800 | -1.39167500 |
| H | 1.29838300 | 2.55493600 | -1.13593100 |
| H | 2.78038300 | 3.11932800 | 0.78005300 |
| H | 3.13906700 | 1.41328200 | 1.02788100 |
| N | 0.12817100 | 0.41832900 | -0.01252300 |
| H | 1.02215300 | 0.22135500 | -1.88756400 |
| H | 2.04467900 | -0.35047100 | -0.56097400 |
| H | 1.15111500 | -0.20443000 | 1.74309700 |
| H | -0.44541000 | 0.53964800 | 1.98556200 |

**2-Int6-p**

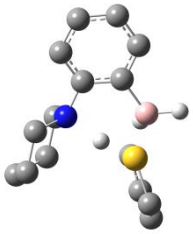


**Sum of electronic and thermal Enthalpies= -1415.898536**
**Sum of electronic and thermal Free Energies= -1415.989094**

| | | | |
|---|---|---|---|
| C | -1.47631800 | -2.18884400 | -0.37346100 |
| C | -0.17978300 | -1.71611700 | -0.20500500 |
| C | 0.10529400 | -0.36700100 | 0.05482900 |
| C | -0.98802700 | 0.51080600 | 0.15513500 |
| C | -2.29184100 | 0.03624600 | -0.01674400 |
| C | -2.54313500 | -1.30376400 | -0.28316700 |
| H | -1.65026500 | -3.24252600 | -0.56959300 |
| H | 0.64138300 | -2.42658900 | -0.25376000 |
| H | -3.12429300 | 0.73042200 | 0.05903200 |
| H | -3.56336600 | -1.65181600 | -0.41421500 |
| B | 1.64077400 | 0.10353000 | 0.14498700 |
| H | 2.25644400 | -1.01689200 | -0.05192200 |
| C | 2.16779900 | 0.48827000 | 1.71484000 |
| C | 1.26199700 | 0.47758500 | 2.79961000 |
| C | 1.61342700 | 1.46206300 | 3.70684500 |
| H | 0.44419600 | -0.22525500 | 2.87144000 |
| C | 2.75150800 | 2.07851600 | 3.18370000 |
| H | 1.12628100 | 1.71435700 | 4.63669400 |
| H | 3.34852200 | 2.87999600 | 3.59780400 |
| B | 2.77047300 | -1.00684100 | 1.22396800 |
| O | 4.17568000 | -1.09740800 | 1.09605400 |
| O | 2.25120100 | -2.16525100 | 1.83738200 |
| C | 4.54611100 | -2.41652100 | 1.52620800 |
| C | 3.36377000 | -2.79189700 | 2.48092300 |
| C | 4.60914700 | -3.31816900 | 0.29136600 |
| H | 5.31432800 | -2.89049600 | -0.42679000 |
| H | 4.95000800 | -4.32630600 | 0.54390800 |
| H | 3.62886500 | -3.39343800 | -0.18845100 |
| C | 5.91055900 | -2.34033400 | 2.19606700 |
| H | 6.67256000 | -2.07569400 | 1.45804000 |
| H | 5.92092100 | -1.58341000 | 2.98192500 |
| H | 6.18021700 | -3.30667500 | 2.63403300 |
| C | 3.51972900 | -2.17273700 | 3.87467200 |
| H | 2.57105100 | -2.27400000 | 4.40751800 |
| H | 4.30126900 | -2.67201300 | 4.45478000 |
| H | 3.75619900 | -1.10644500 | 3.80999200 |
| C | 3.08590100 | -4.28354000 | 2.59671500 |
| H | 3.96349200 | -4.81129500 | 2.98403700 |
| H | 2.25526000 | -4.45061100 | 3.28722300 |
| H | 2.81399700 | -4.71172400 | 1.63066200 |
| C | 2.22890200 | 1.04932100 | -0.98582100 |
| C | 2.11748800 | 2.42013000 | -1.12864100 |
| C | 2.79488500 | 2.81220500 | -2.30959700 |
| H | 1.60811500 | 3.05092400 | -0.41693600 |
| C | 3.30475800 | 1.66374900 | -2.86714900 |
| H | 2.89403300 | 3.81037900 | -2.71170400 |
| H | 3.87390400 | 1.50889100 | -3.77250300 |
| N | 3.08708300 | 1.51828900 | 2.01864900 |
| N | 2.96246800 | 0.60598400 | -2.06799900 |
| C | 3.34009300 | -0.76726600 | -2.32758600 |
| H | 2.45561400 | -1.40931700 | -2.37924600 |
| H | 3.85858700 | -0.81720400 | -3.28623200 |
| H | 4.00611600 | -1.13865600 | -1.54371300 |
| C | 4.28043900 | 1.88355200 | 1.26594000 |
| H | 4.81371000 | 0.97478900 | 0.99003400 |
| H | 4.00521100 | 2.43183900 | 0.36450200 |
| H | 4.91151600 | 2.50059800 | 1.90747900 |
| C | -0.90741900 | 4.24937300 | -0.35416500 |
| C | -1.01903300 | 3.72223300 | 2.09130900 |
| C | -1.47594200 | 4.68600100 | 0.99628700 |
| H | -1.32104600 | 4.85918500 | -1.16454900 |
| H | 0.17490400 | 4.41223600 | -0.35657400 |
| H | -1.47280500 | 3.98273600 | 3.05382200 |
| H | 0.07021500 | 3.77163100 | 2.21206000 |
| H | -1.17520400 | 5.71389200 | 1.22482200 |
| H | -2.57376000 | 4.67758500 | 0.95037200 |

| | | | |
|---|---|---|---|
| N | -0.77603500 | 1.90789500 | 0.45401100 |
| C | -1.20322000 | 2.77811000 | -0.64613000 |
| H | -2.28757600 | 2.67124900 | -0.84132800 |
| H | -0.67234900 | 2.45993700 | -1.54778300 |
| C | -1.40163800 | 2.29565500 | 1.71881200 |
| H | -1.07205300 | 1.59644700 | 2.49010200 |
| H | -2.50594400 | 2.22684100 | 1.66828400 |

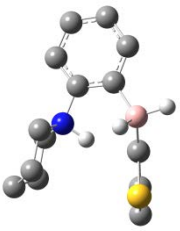
**2-TS1-t**



**Sum of electronic and thermal Enthalpies= -1060.891891**
**Sum of electronic and thermal Free Energies= -1060.950725**

| | | | |
|---|---|---|---|
| C | -1.32637400 | -2.23939400 | 0.62359400 |
| C | -0.14815000 | -1.88252200 | 1.30130200 |
| C | 0.98081600 | -2.66715800 | 1.03520200 |
| C | 0.94126100 | -3.74659600 | 0.15795000 |
| C | -0.24227900 | -4.06583700 | -0.50181200 |
| C | -1.38345000 | -3.30552000 | -0.27179000 |
| H | 1.91508500 | -2.41275000 | 1.52813500 |
| H | 1.83675500 | -4.33416600 | -0.02165500 |
| H | -0.27896000 | -4.90245600 | -1.19258900 |
| H | -2.31018700 | -3.55033500 | -0.78209100 |
| H | -1.70492400 | -0.15093400 | 1.31223000 |
| B | -0.09738500 | -0.62590500 | 2.30097100 |
| H | 1.02234200 | -0.23699200 | 2.53774200 |
| C | -0.91256300 | 0.75376600 | 1.48088300 |
| C | -1.31161900 | 1.85422300 | 2.23211400 |
| C | -1.05868900 | 3.10317200 | 1.63338400 |
| H | -1.76344000 | 1.72953700 | 3.21000700 |
| H | -1.28528800 | 4.06155100 | 2.08331200 |
| H | -0.78171400 | -0.75595900 | 3.29946000 |
| C | -0.47718900 | 2.96319500 | 0.39480800 |
| H | -0.17256900 | 3.75798000 | -0.27344900 |
| C | -3.32632400 | -1.07834300 | -0.25321500 |
| C | -3.27459500 | -1.89534200 | 2.04734500 |
| C | -4.30342100 | 0.03158900 | 0.12749500 |
| H | -3.88812200 | -1.96028000 | -0.60049200 |
| H | -2.66734500 | -0.76061100 | -1.06594500 |
| C | -4.26591700 | -0.82448100 | 2.49064200 |
| H | -2.57624200 | -2.13889900 | 2.84956800 |
| H | -3.80602600 | -2.81863300 | 1.76326100 |
| C | -5.15696400 | -0.38417500 | 1.32743800 |
| H | -4.93426700 | 0.26691900 | -0.73539700 |
| H | -3.73463700 | 0.93721500 | 0.37161100 |
| H | -4.86852900 | -1.21161600 | 3.31815500 |
| H | -3.70454800 | 0.03586100 | 2.87445400 |
| H | -5.80764400 | -1.21944600 | 1.03491100 |
| H | -5.81210200 | 0.43692500 | 1.63436600 |
| N | -2.48409100 | -1.41777800 | 0.89908000 |
| S | -0.23341300 | 1.32998800 | -0.02774600 |

**2-Int1-t**

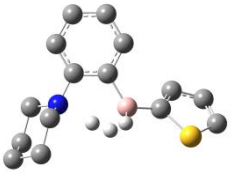


**Sum of electronic and thermal Enthalpies= -1060.920919**
**Sum of electronic and thermal Free Energies= -1060.980803**

| | | | |
|---|---|---|---|
| H | 1.34771700 | -0.39753000 | 3.27377700 |
| C | 2.07180800 | -0.19927100 | 2.48908200 |
| C | 2.60125500 | 1.07927800 | 2.34209200 |
| C | 2.46143400 | -1.23019600 | 1.63642500 |
| C | 3.53698000 | 1.39551800 | 1.34682800 |
| H | 2.28943200 | 1.86977600 | 3.01805400 |
| C | 3.38242900 | -0.96786600 | 0.62903700 |
| H | 2.05130800 | -2.22795800 | 1.75134300 |
| C | 3.87747900 | 0.32484800 | 0.51473700 |
| H | 3.69907000 | -1.75952200 | -0.04399900 |
| B | 4.22873400 | 2.86513200 | 1.19238400 |
| H | 3.75052500 | 3.63943900 | 1.99862200 |
| H | 4.82605700 | 1.68358100 | -0.57261200 |
| H | 5.43517100 | 2.74622400 | 1.41765300 |
| C | 4.04481500 | 3.44038500 | -0.32764800 |
| C | 3.03967300 | 3.24796000 | -1.24881000 |
| S | 5.25490700 | 4.46850600 | -1.04982400 |
| C | 3.22790900 | 3.91460200 | -2.49889200 |
| H | 2.16902800 | 2.64063300 | -1.01955500 |
| C | 4.39549900 | 4.61860400 | -2.54066600 |

| | | | |
|---|---|---|---|
| H | 2.52128600 | 3.87745300 | -3.32043500 |
| H | 4.77864100 | 5.22610100 | -3.34885200 |
| C | 7.25069700 | 0.88525800 | -1.14166100 |
| C | 5.46834700 | 0.81436500 | -2.91946300 |
| C | 6.92415300 | 0.48283000 | -2.58175700 |
| H | 8.26121200 | 0.57134700 | -0.86536100 |
| H | 7.21285900 | 1.97663600 | -1.04041900 |
| H | 5.20604400 | 0.44828700 | -3.91618800 |
| H | 5.31173100 | 1.90070100 | -2.92635800 |
| H | 7.59570700 | 0.99585600 | -3.27514000 |
| H | 7.09312600 | -0.59454900 | -2.70967000 |
| N | 4.86739500 | 0.64426200 | -0.53482900 |
| C | 6.26670600 | 0.27562800 | -0.15212100 |
| H | 6.31464600 | -0.81787200 | -0.13614600 |
| H | 6.41391800 | 0.65859100 | 0.85832900 |
| C | 4.51254500 | 0.18888100 | -1.91189600 |
| H | 3.47964800 | 0.49453000 | -2.08315700 |
| H | 4.57092600 | -0.90303500 | -1.92790100 |

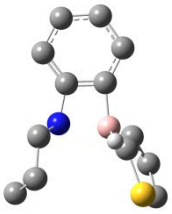
**2-TS2-t**



**Sum of electronic and thermal Enthalpies= -1060.894371**
**Sum of electronic and thermal Free Energies= -1060.956323**

| | | | |
|---|---|---|---|
| H | 1.18572300 | 0.55569900 | 2.43903000 |
| C | 1.97570300 | 0.45058100 | 1.70184800 |
| C | 2.67694100 | 1.57244000 | 1.26965000 |
| C | 2.27934600 | -0.80336000 | 1.18134100 |
| C | 3.70347500 | 1.47602800 | 0.32411800 |
| H | 2.41714400 | 2.55091900 | 1.66332700 |
| C | 3.29604500 | -0.93308800 | 0.24116600 |
| H | 1.73094100 | -1.68117800 | 1.50837300 |
| C | 4.00407600 | 0.19478700 | -0.16828500 |
| H | 3.53875400 | -1.91068900 | -0.16375100 |
| B | 4.51490000 | 2.75408300 | -0.18242500 |
| H | 4.96804900 | 1.74991700 | -1.48786400 |
| H | 4.83617500 | 2.56450700 | -1.60730400 |
| C | 3.71225300 | 4.09922900 | -0.39494800 |
| C | 2.38387500 | 4.29104100 | -0.68695300 |
| S | 4.50468300 | 5.64111000 | -0.28969000 |
| C | 2.00704200 | 5.65735400 | -0.82407800 |
| H | 1.69211400 | 3.46303000 | -0.79789900 |
| C | 3.05908300 | 6.50664800 | -0.63541300 |
| H | 1.00112600 | 5.99223100 | -1.04786100 |
| H | 3.05539700 | 7.58710600 | -0.67275000 |
| C | 7.49936900 | 0.19453300 | -1.52690300 |
| C | 5.91607700 | -0.54134300 | -3.33515600 |
| C | 7.32626300 | -0.69309600 | -2.76074700 |
| H | 8.47174200 | 0.02113900 | -1.05549300 |
| H | 7.46723600 | 1.25109100 | -1.82038900 |
| H | 5.75734600 | -1.24152500 | -4.16138700 |
| H | 5.78526200 | 0.47086400 | -3.73664200 |
| H | 8.07671100 | -0.44825400 | -3.51839600 |
| H | 7.48881900 | -1.74183000 | -2.47798100 |
| N | 5.07149000 | 0.12244600 | -1.13069000 |
| H | 5.64249000 | 2.87701900 | 0.23325600 |
| C | 4.86192200 | -0.78876000 | -2.25856000 |
| H | 3.85449000 | -0.62008400 | -2.64794200 |
| H | 4.92232600 | -1.84043800 | -1.93078200 |
| C | 6.39393800 | -0.06350100 | -0.50869000 |
| H | 6.47275500 | -1.08743700 | -0.10582800 |
| H | 6.46953400 | 0.63035800 | 0.33114200 |

**2-Int2-t**

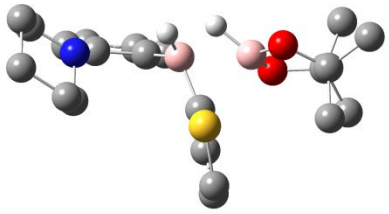


**Sum of electronic and thermal Enthalpies= -1059.751908**
**Sum of electronic and thermal Free Energies= -1059.811377**

| | | | |
|---|---|---|---|
| C | -2.52752700 | -2.97474400 | 1.75203300 |
| C | -1.15449400 | -3.20468900 | 1.62095600 |
| C | -0.31198000 | -2.23178100 | 1.07854700 |
| C | -0.93759200 | -1.05881500 | 0.69479700 |
| C | -2.28729800 | -0.78743100 | 0.81268900 |
| C | -3.11098400 | -1.76969600 | 1.35112600 |
| H | -3.15156400 | -3.75649200 | 2.17522900 |
| H | -0.73837100 | -4.15390400 | 1.94326100 |
| H | 0.75429000 | -2.40187400 | 0.96535700 |
| H | -4.18041200 | -1.61878600 | 1.46400500 |
| B | -2.14144000 | 0.68859200 | 0.19354800 |
| H | -2.13883300 | 1.61665400 | 0.96975200 |
| C | -2.79093000 | 0.99455500 | -1.21717600 |
| C | -3.21184500 | 0.12336500 | -2.19070600 |
| C | -3.73219400 | 0.75188600 | -3.35993900 |
| H | -3.15521100 | -0.95242700 | -2.05888300 |
| C | -3.71215400 | 2.11286500 | -3.26708900 |
| H | -4.11171700 | 0.21817700 | -4.22323200 |

| | | | |
|---|---|---|---|
| H | -4.05628000 | 2.83381300 | -3.99543300 |
| C | 0.49780400 | 0.91678500 | 0.97980500 |
| C | 0.19013000 | -0.06167400 | -1.24419700 |
| C | 0.86104600 | 2.26195400 | 0.36616700 |
| C | 0.59810900 | 1.24653800 | -1.90935600 |
| C | 1.51086100 | 2.07541000 | -1.00537200 |
| H | 1.53005700 | 2.79461200 | 1.04888900 |
| H | -0.05236500 | 2.85989500 | 0.26967400 |
| H | 1.09359400 | 1.01349900 | -2.85693400 |
| H | -0.30494200 | 1.81623900 | -2.14788100 |
| H | 1.71820200 | 3.04588700 | -1.46543300 |
| H | 2.47621500 | 1.56520300 | -0.88410900 |
| N | -0.41984400 | 0.16701700 | 0.08875100 |
| S | -3.06546400 | 2.62461800 | -1.75524400 |
| H | 1.06387700 | -0.71457200 | -1.10937300 |
| H | -0.54463600 | -0.59447800 | -1.85025400 |
| H | 1.40139600 | 0.31226400 | 1.14294700 |
| H | -0.01075200 | 1.03707800 | 1.93826600 |

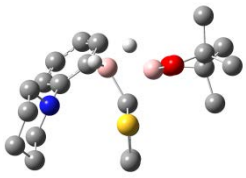
**2-TS3-t**



**Sum of electronic and thermal Enthalpies= -1471.317662**
**Sum of electronic and thermal Free Energies= -1471.395898**

| | | | |
|---|---|---|---|
| C | -2.05679900 | -2.09961300 | 0.82854000 |
| C | -0.70972800 | -1.74707800 | 0.85574800 |
| C | -0.26733900 | -0.46526500 | 0.50802300 |
| C | -1.24512100 | 0.49186500 | 0.15519900 |
| C | -2.59683400 | 0.13385000 | 0.12267800 |
| C | -3.00163900 | -1.15618200 | 0.44832200 |
| H | -2.36025600 | -3.10907200 | 1.08885900 |
| H | 0.02100700 | -2.50157200 | 1.13343300 |
| H | -3.34227200 | 0.87274700 | -0.15243500 |
| H | -4.05608900 | -1.41412100 | 0.41455900 |
| B | 1.28123000 | -0.07375100 | 0.44844400 |
| H | 1.79580000 | -1.21264100 | -0.12870700 |
| C | 2.01028700 | 0.26619600 | 1.84881100 |
| C | 1.62576200 | -0.09009500 | 3.12452900 |
| C | 2.29052000 | 0.62297400 | 4.15374500 |
| H | 0.88025400 | -0.85752900 | 3.29745900 |
| C | 3.17872100 | 1.53790200 | 3.65355600 |
| H | 2.11643400 | 0.47266800 | 5.21196200 |
| H | 3.80835000 | 2.21691600 | 4.21215600 |
| H | 1.63902900 | 0.65270000 | -0.43639200 |
| B | 2.61059300 | -1.54269400 | 0.77891000 |
| O | 3.92984600 | -1.42507100 | 0.45022200 |
| O | 2.30813900 | -2.63395800 | 1.55115400 |
| C | 4.63794400 | -2.32315900 | 1.33815300 |
| C | 3.53528500 | -3.38928800 | 1.68659100 |
| C | 5.84295800 | -2.87780300 | 0.59358000 |
| H | 6.54793700 | -2.06970900 | 0.38407700 |
| H | 6.35563700 | -3.62818100 | 1.20352300 |
| H | 5.55589100 | -3.33257300 | -0.35542600 |
| C | 5.09557900 | -1.51183000 | 2.55009500 |
| H | 5.69896400 | -0.67051800 | 2.20206900 |
| H | 4.24910500 | -1.11019700 | 3.11237900 |
| H | 5.70458500 | -2.12287700 | 3.22197100 |
| C | 3.61193500 | -3.94052800 | 3.10244500 |
| H | 2.81338300 | -4.67039900 | 3.25724500 |
| H | 4.57029000 | -4.44351100 | 3.26494400 |
| H | 3.49990300 | -3.14857700 | 3.84446200 |
| C | 3.45512000 | -4.52991800 | 0.67263000 |
| H | 4.31697600 | -5.19837000 | 0.74937800 |
| H | 2.54862500 | -5.10837700 | 0.86593500 |
| H | 3.39989500 | -4.14456800 | -0.34898600 |
| C | -0.84034100 | 3.72284900 | -1.68598100 |
| C | 0.40149100 | 3.82103800 | 0.49691100 |
| C | -0.35115800 | 4.63436500 | -0.55828900 |
| H | -1.45909500 | 4.28429700 | -2.39443300 |
| H | 0.01929600 | 3.32321200 | -2.23585200 |
| H | 0.66687900 | 4.44694700 | 1.35585500 |
| H | 1.33361500 | 3.43061200 | 0.07181700 |
| H | 0.28284600 | 5.43337800 | -0.95644900 |
| H | -1.21783500 | 5.11936500 | -0.08788000 |
| N | -0.82831800 | 1.80835500 | -0.17450400 |
| C | -1.64201100 | 2.54836800 | -1.12489600 |
| H | -2.56890700 | 2.94158500 | -0.66113200 |
| H | -1.94020600 | 1.87098400 | -1.93015900 |
| C | -0.44170300 | 2.63924700 | 0.96425600 |
| H | 0.11596500 | 2.03073900 | 1.67792800 |
| H | -1.34287000 | 3.01119300 | 1.49075000 |
| S | 3.20518000 | 1.52751900 | 1.94094300 |

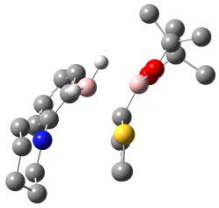
**2-Int3-t**



**Sum of electronic and thermal Enthalpies= -1471.320384**
**Sum of electronic and thermal Free Energies= -1471.400235**

| | | | |
|---|---|---|---|
| C | -1.91705700 | -2.42422300 | 0.39481000 |
| C | -0.60675000 | -2.00397300 | 0.17251900 |
| C | -0.25128200 | -0.65317400 | 0.19133500 |
| C | -1.26912500 | 0.29288700 | 0.42961900 |
| C | -2.58091000 | -0.12561700 | 0.65789800 |
| C | -2.90384300 | -1.48050000 | 0.64482700 |
| H | -2.15787700 | -3.48276300 | 0.38725400 |
| H | 0.16809700 | -2.75123300 | 0.02322200 |
| H | -3.35822800 | 0.60894200 | 0.84326100 |
| H | -3.92854700 | -1.79142200 | 0.82564600 |
| B | 1.26182800 | -0.17774300 | 0.04222600 |
| H | 1.93222200 | -1.23183200 | -0.24136800 |
| C | 1.90396900 | 0.39083900 | 1.49635200 |
| C | 1.22233900 | 0.33227900 | 2.70588000 |
| C | 1.51552900 | 1.38295700 | 3.59281200 |
| H | 0.53451500 | -0.47658100 | 2.92106800 |
| C | 2.42674900 | 2.26142000 | 3.05420000 |
| H | 1.08265800 | 1.49463800 | 4.57844100 |
| H | 2.82625400 | 3.15331400 | 3.51888800 |
| B | 2.60209700 | -1.12556800 | 0.95280100 |
| O | 3.97166800 | -1.03302400 | 0.69233800 |
| O | 2.28304600 | -2.27279700 | 1.68849800 |
| C | 4.54336200 | -2.28509200 | 1.10492400 |
| C | 3.53265400 | -2.76054600 | 2.20309300 |
| C | 4.56773800 | -3.21065700 | -0.11380800 |
| H | 5.10409500 | -2.71131600 | -0.92438800 |
| H | 5.07176400 | -4.15603400 | 0.10627500 |
| H | 3.55400000 | -3.43077000 | -0.46078400 |
| C | 5.95728100 | -2.03242100 | 1.60702800 |
| H | 6.59198200 | -1.70826200 | 0.77824400 |
| H | 5.97174100 | -1.25261600 | 2.36993400 |
| H | 6.38585000 | -2.94770700 | 2.02797400 |
| C | 3.77782800 | -2.09007300 | 3.55799300 |
| H | 2.91798700 | -2.28162600 | 4.20515800 |
| H | 4.67375500 | -2.48554100 | 4.04483300 |
| H | 3.88845900 | -1.00716200 | 3.44936000 |
| C | 3.43174300 | -4.26928000 | 2.37018500 |
| H | 4.39965000 | -4.69157000 | 2.65852900 |
| H | 2.70811500 | -4.50652100 | 3.15432200 |
| H | 3.09929000 | -4.74810300 | 1.44789500 |
| C | -0.01800100 | 3.60349500 | -0.75899400 |
| C | -0.89407100 | 3.83622100 | 1.58690500 |
| C | -0.68529200 | 4.54390500 | 0.24656900 |
| H | 0.03707100 | 4.07202100 | -1.74747900 |
| H | 1.00725900 | 3.38356000 | -0.43899800 |
| H | -1.45736600 | 4.47463800 | 2.27640600 |
| H | 0.07632200 | 3.61908600 | 2.04843700 |
| H | -0.09168400 | 5.45438000 | 0.37932700 |
| H | -1.66168400 | 4.85674500 | -0.14896300 |
| N | -0.90568600 | 1.67020800 | 0.46229900 |
| C | -0.78355700 | 2.28798500 | -0.85719200 |
| H | -1.78570600 | 2.47072700 | -1.29244600 |
| H | -0.26461800 | 1.59427600 | -1.52124700 |
| C | -1.63838200 | 2.51677000 | 1.39032400 |
| H | -1.73227000 | 1.98563900 | 2.34254100 |
| H | -2.66353700 | 2.73926800 | 1.03292600 |
| S | 2.91558000 | 1.81337800 | 1.48761900 |
| H | 1.61105900 | 0.55703100 | -0.83919500 |

**2-TS4-t**

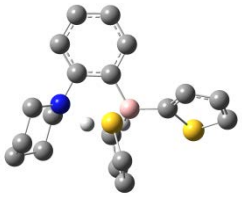


**Sum of electronic and thermal Enthalpies= -1471.318166**
**Sum of electronic and thermal Free Energies= -1471.396926**

| | | | |
|---|---|---|---|
| C | -2.16471500 | -1.50340900 | 1.01179000 |
| C | -1.04328700 | -0.70211300 | 0.69394600 |
| C | 0.05268600 | -1.33353200 | 0.09754100 |
| C | 0.07529900 | -2.70190100 | -0.16655100 |
| C | -1.02601100 | -3.47397000 | 0.17317600 |
| C | -2.14254000 | -2.87572100 | 0.75364800 |
| H | 0.93228700 | -0.73681400 | -0.12760200 |
| H | 0.95071600 | -3.15876700 | -0.61757300 |
| H | -1.02811600 | -4.54348200 | -0.01666000 |
| H | -3.00325200 | -3.48869600 | 1.00010500 |
| N | -3.28562900 | -0.88871400 | 1.63873200 |
| B | -0.94689700 | 0.84191300 | 1.05015000 |
| H | -1.88096400 | 1.58158700 | 0.94616400 |
| H | 0.05397600 | 1.35461400 | 0.58194600 |
| C | 2.52094400 | 2.77537400 | 1.73020100 |
| C | 3.03401000 | 1.34439000 | 2.12530100 |
| O | 1.17415300 | 2.76740600 | 2.24642400 |
| O | 1.82547800 | 0.56009000 | 2.11477700 |
| B | 0.77896200 | 1.44769800 | 2.26798000 |
| C | 3.27649600 | 3.92533800 | 2.38062400 |
| H | 2.85633300 | 4.87657900 | 2.04437500 |
| H | 3.20010900 | 3.88605200 | 3.46822400 |
| H | 4.33397200 | 3.89960700 | 2.09886300 |
| C | 2.44018600 | 2.98857400 | 0.21769100 |
| H | 1.87806100 | 3.90478300 | 0.02199000 |
| H | 3.43599300 | 3.09101200 | -0.22263200 |
| H | 1.92367600 | 2.16330000 | -0.27875900 |
| C | 4.02399300 | 0.73087200 | 1.14551100 |
| H | 4.92630000 | 1.34630300 | 1.07234800 |
| H | 4.31604800 | -0.26318000 | 1.49375100 |
| H | 3.58749400 | 0.62605200 | 0.15103900 |
| C | 3.59073300 | 1.28140800 | 3.54887500 |
| H | 3.73970500 | 0.23352700 | 3.82045900 |
| H | 4.54946800 | 1.80093400 | 3.63133400 |
| H | 2.88996900 | 1.72198100 | 4.26348600 |
| C | -0.58821500 | 1.02066800 | 2.95325700 |
| C | -0.74358900 | -0.18391800 | 3.63981500 |
| C | -1.62505600 | -0.12767100 | 4.72838800 |
| H | -0.22245400 | -1.07838800 | 3.32031300 |
| C | -2.14269100 | 1.13775500 | 4.89354600 |
| H | -1.88248200 | -0.96931700 | 5.35807700 |
| H | -2.85394500 | 1.45460100 | 5.64540500 |
| C | -4.12472200 | -0.10066800 | 0.73397400 |
| H | -3.48034300 | 0.47110100 | 0.06666100 |

| | | | |
|---|---|---|---|
| H | -4.74190700 | -0.77034200 | 0.10367700 |
| C | -4.09195600 | -1.73043400 | 2.50995400 |
| H | -4.71743300 | -2.44352200 | 1.93698600 |
| H | -3.42006900 | -2.32059100 | 3.14143100 |
| C | -5.03163600 | 0.83099000 | 1.53045500 |
| C | -5.01014400 | -0.86800200 | 3.37437700 |
| C | -5.89315600 | 0.02917900 | 2.50660900 |
| H | -4.38727200 | -0.24659300 | 4.02732400 |
| H | -5.62271400 | -1.51450100 | 4.01263000 |
| H | -4.39857000 | 1.53679500 | 2.08176200 |
| H | -5.65926600 | 1.41097300 | 0.84551700 |
| H | -6.59223800 | -0.59736400 | 1.93559600 |
| H | -6.49934400 | 0.69374800 | 3.13125000 |
| S | -1.56487400 | 2.24226100 | 3.74133100 |

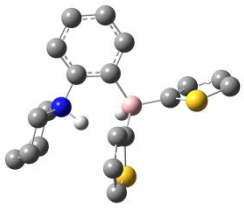
**2-TS5-t**



**Sum of electronic and thermal Enthalpies= -1612.610508**
**Sum of electronic and thermal Free Energies= -1612.682816**

| | | | |
|---|---|---|---|
| C | 1.44444800 | 0.03254800 | 1.46460200 |
| C | 2.26315000 | 1.12490000 | 1.19439100 |
| C | 1.85044700 | -1.25010600 | 1.11027500 |
| C | 3.50383800 | 0.98692300 | 0.55938300 |
| C | 3.07242100 | -1.42919300 | 0.47211300 |
| H | 1.21921400 | -2.10719700 | 1.32294600 |
| C | 3.87109300 | -0.32177700 | 0.19656400 |
| B | 4.47695800 | 2.23573500 | 0.24611700 |
| H | 5.78947900 | 0.76680000 | 0.07953600 |
| C | 6.13780900 | 1.73595600 | 0.74896000 |
| C | 7.20917300 | 2.51617500 | 0.32384900 |
| C | 8.18332000 | 2.77160700 | 1.30633500 |
| H | 7.24615400 | 2.91695800 | -0.68328600 |
| C | 7.87438600 | 2.16049200 | 2.49896200 |
| H | 9.06772400 | 3.37767200 | 1.15619200 |
| H | 8.44721100 | 2.19679100 | 3.41631600 |
| H | 0.48843700 | 0.18173500 | 1.95738100 |
| H | 3.39169100 | -2.42573200 | 0.18246800 |
| H | 1.93847800 | 2.11921100 | 1.48569300 |
| H | 4.65013300 | 2.40277500 | -0.94868600 |
| C | 4.14903200 | 3.60797800 | 0.99414200 |
| C | 3.85076600 | 3.87900000 | 2.30608200 |
| C | 3.66207500 | 5.26304900 | 2.59596400 |
| H | 3.77292400 | 3.09693900 | 3.05436600 |
| C | 3.82253400 | 6.05116000 | 1.49449200 |
| H | 3.41780200 | 5.65171000 | 3.57793100 |
| H | 3.72618700 | 7.12547700 | 1.42331400 |
| C | 5.96466600 | -1.61377300 | -0.08798000 |
| C | 5.03193000 | -0.33503200 | -1.94816700 |
| C | 7.37696800 | -1.45609600 | -0.64680400 |
| C | 6.41358700 | -0.15102000 | -2.56636900 |
| C | 7.34693800 | -1.29602300 | -2.16832000 |
| H | 7.97474300 | -2.32659200 | -0.35898500 |
| H | 7.84403000 | -0.57540000 | -0.18951000 |
| H | 6.31485900 | -0.08644700 | -3.65427500 |
| H | 6.82822800 | 0.80398800 | -2.22174500 |
| H | 8.35568300 | -1.12227700 | -2.55502200 |
| H | 6.98728500 | -2.22898600 | -2.62299100 |
| N | 5.14128900 | -0.46304200 | -0.48227000 |
| S | 4.20013800 | 5.10075900 | 0.10739700 |
| S | 6.41083000 | 1.29026200 | 2.42204800 |
| H | 5.52282600 | -2.55145100 | -0.45954600 |
| H | 4.54499600 | -1.23703900 | -2.35258700 |
| H | 5.97589100 | -1.65791400 | 1.00449100 |
| H | 4.38911100 | 0.52073300 | -2.15842800 |

**2-Int4-t**

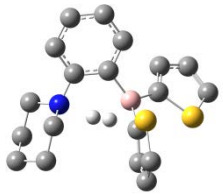


**Sum of electronic and thermal Enthalpies= -1612.641014**
**Sum of electronic and thermal Free Energies= -1612.708225**

| | | | |
|---|---|---|---|
| H | 0.54677300 | 0.49886300 | 1.74618900 |
| C | 1.53002800 | 0.44437400 | 1.28886100 |
| C | 2.11384100 | 1.59622900 | 0.77098300 |
| C | 2.19302300 | -0.77870100 | 1.22242600 |
| C | 3.38214300 | 1.59029100 | 0.17380800 |
| H | 1.57608800 | 2.53856800 | 0.81616200 |
| C | 3.45340800 | -0.83699800 | 0.64030300 |
| H | 1.73663900 | -1.67923700 | 1.61937900 |
| C | 4.00527900 | 0.33947000 | 0.14903600 |
| H | 3.98123200 | -1.78383700 | 0.57442300 |
| B | 4.07087100 | 2.91183000 | -0.52229700 |
| H | 5.61566600 | 1.31100700 | -0.49047600 |

| | | | |
|---|---|---|---|
| H | 4.18254900 | 2.66094300 | -1.72441400 |
| C | 3.15024100 | 4.22369100 | -0.37125400 |
| C | 2.15820700 | 4.67325400 | -1.20279200 |
| S | 3.22505400 | 5.26059500 | 1.02582400 |
| C | 1.46276200 | 5.82860200 | -0.73174000 |
| H | 1.93413600 | 4.17899400 | -2.14211600 |
| C | 1.93191100 | 6.26168500 | 0.47208500 |
| H | 0.65691900 | 6.31618200 | -1.26895500 |
| H | 1.60462700 | 7.11581800 | 1.04828900 |
| C | 5.57436400 | 3.14823100 | 0.08611900 |
| C | 6.07941500 | 2.90133100 | 1.34263000 |
| S | 6.83704600 | 3.84776500 | -0.88867400 |
| C | 7.44878700 | 3.26577000 | 1.52200800 |
| H | 5.46400900 | 2.47270100 | 2.12794700 |
| C | 7.99637300 | 3.79044100 | 0.38792900 |
| H | 7.99201600 | 3.15039600 | 2.45286400 |
| H | 9.00189900 | 4.16124900 | 0.24471600 |
| C | 7.76608900 | -0.11361900 | -0.32250900 |
| C | 6.65177400 | 0.10376100 | -2.57006200 |
| C | 7.79200300 | -0.55332900 | -1.78855100 |
| H | 8.52389500 | -0.64611600 | 0.25915800 |
| H | 7.99129300 | 0.95703900 | -0.23634500 |
| H | 6.61037100 | -0.27420200 | -3.59545100 |
| H | 6.81384000 | 1.18653100 | -2.63187500 |
| H | 8.75350700 | -0.29764100 | -2.24114000 |
| H | 7.69165000 | -1.64536500 | -1.84491500 |
| N | 5.34051100 | 0.30763400 | -0.48449300 |
| C | 6.40523100 | -0.37906000 | 0.30761300 |
| H | 6.17300600 | -1.44729600 | 0.32444800 |
| H | 6.33909600 | 0.01716600 | 1.32172500 |
| C | 5.30344300 | -0.14990700 | -1.90953300 |
| H | 4.49873500 | 0.40954900 | -2.38790300 |
| H | 5.04299100 | -1.21301500 | -1.89347100 |

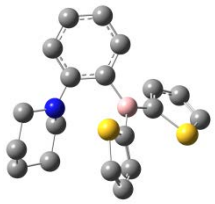
**2-TS6-t**



**Sum of electronic and thermal Enthalpies= -1612.610854**
**Sum of electronic and thermal Free Energies= -1612.686247**

| | | | |
|---|---|---|---|
| H | 0.88175400 | 0.46840300 | 2.27025200 |
| C | 1.74850700 | 0.41776600 | 1.61874000 |
| C | 2.43280500 | 1.58126400 | 1.27998900 |
| C | 2.17244600 | -0.80647300 | 1.11362400 |
| C | 3.55919300 | 1.55744600 | 0.44863900 |
| H | 2.08159100 | 2.53606700 | 1.66114400 |
| C | 3.28570800 | -0.86075000 | 0.28219600 |
| H | 1.64197300 | -1.71889800 | 1.36747900 |
| C | 3.97854300 | 0.30550000 | -0.03706600 |
| H | 3.62345200 | -1.81502200 | -0.11102500 |
| B | 4.34745500 | 2.90640900 | 0.11716000 |
| H | 5.05596300 | 1.99533200 | -1.24125300 |
| H | 4.87668200 | 2.77322200 | -1.36753200 |
| C | 3.47690700 | 4.17205800 | -0.24701700 |
| C | 2.19944300 | 4.21544100 | -0.75261500 |
| S | 4.08584100 | 5.79129700 | -0.07371000 |
| C | 1.71435100 | 5.52915300 | -0.99922200 |
| H | 1.62598600 | 3.31465400 | -0.94196300 |
| C | 2.63459100 | 6.48567400 | -0.67726900 |
| H | 0.73048700 | 5.75195700 | -1.39426000 |
| H | 2.52763700 | 7.55875700 | -0.75490200 |
| C | 5.73022500 | 3.14594200 | 0.86927600 |
| C | 6.90697900 | 3.68147300 | 0.41284900 |
| S | 5.89638900 | 2.72979500 | 2.54718800 |
| C | 7.93598900 | 3.75710600 | 1.39754600 |
| H | 7.03482800 | 4.01096800 | -0.61326500 |
| C | 7.52833400 | 3.28032700 | 2.60737200 |
| H | 8.92770200 | 4.15173300 | 1.21214300 |
| H | 8.09065400 | 3.22937600 | 3.52904700 |
| C | 7.58754100 | 0.25627800 | -1.05188000 |
| C | 6.14843400 | -0.15793200 | -3.07299900 |
| C | 7.49116900 | -0.45556600 | -2.40266200 |
| H | 8.50200800 | -0.03163000 | -0.52396900 |
| H | 7.62748500 | 1.34247500 | -1.19748800 |
| H | 6.03848300 | -0.73470300 | -3.99693600 |
| H | 6.09888100 | 0.90363600 | -3.34464900 |
| H | 8.31762400 | -0.15836000 | -3.05574500 |
| H | 7.58283600 | -1.53910000 | -2.24685200 |
| N | 5.13704300 | 0.27833600 | -0.88845400 |
| C | 4.98782500 | -0.47826000 | -2.13369700 |
| H | 4.03112900 | -0.20261200 | -2.58602900 |
| H | 4.96428800 | -1.56532300 | -1.94263600 |
| C | 6.37918800 | -0.06622200 | -0.18029800 |
| H | 6.37420500 | -1.13926200 | 0.08217600 |
| H | 6.41070500 | 0.50359300 | 0.74980000 |

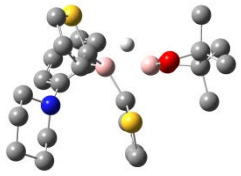
**2-Int5-t**



**Sum of electronic and thermal Enthalpies= -1611.468017**
**Sum of electronic and thermal Free Energies= -1611.537514**

| | | | |
|---|---|---|---|
| C | -6.66435300 | 1.37217900 | -0.15372900 |
| C | -5.32470700 | 1.72829100 | -0.43946300 |
| C | -5.05272900 | 2.95173500 | -1.06121600 |
| C | -6.08473200 | 3.82488200 | -1.39013300 |
| C | -7.40107300 | 3.50896300 | -1.07754000 |
| C | -7.67401600 | 2.29686200 | -0.45085700 |
| H | -4.02793200 | 3.23550800 | -1.27428300 |
| H | -5.85113000 | 4.76824600 | -1.87479300 |
| H | -8.20548800 | 4.19473400 | -1.32223100 |
| H | -8.70386200 | 2.03961400 | -0.21699300 |
| B | -7.06470500 | -0.05241600 | 0.37205300 |
| C | -8.01411300 | -0.14192400 | 1.59251100 |
| C | -8.26431000 | 0.85852600 | 2.51104200 |
| C | -9.17467100 | 0.49799300 | 3.53570000 |
| H | -7.79037100 | 1.83047600 | 2.43501800 |
| C | -9.63231600 | -0.78302500 | 3.38651500 |
| H | -9.48293300 | 1.15521200 | 4.33930100 |
| H | -10.34249300 | -1.30742000 | 4.01118300 |
| C | -6.55626600 | -1.33117800 | -0.34473700 |
| C | -6.33646500 | -2.58949000 | 0.17699100 |
| C | -5.77129800 | -3.51045500 | -0.74372400 |
| H | -6.54619800 | -2.83095700 | 1.21259000 |
| C | -5.58011500 | -2.94947700 | -1.97659000 |
| H | -5.52763000 | -4.53897000 | -0.50800200 |
| H | -5.19776100 | -3.42897000 | -2.86724200 |
| C | -3.04448100 | 0.90905600 | -0.82226400 |
| C | -4.10545400 | 0.55657700 | 1.33126900 |
| C | -2.27679600 | -0.40634100 | -0.69271000 |
| C | -3.35935000 | -0.75801000 | 1.53834600 |
| C | -2.03386100 | -0.75197800 | 0.77617300 |
| H | -1.32806900 | -0.32623000 | -1.23416900 |
| H | -2.86704800 | -1.20056800 | -1.16505300 |
| H | -3.19253400 | -0.91529400 | 2.60925400 |
| H | -3.99015600 | -1.57572600 | 1.17213500 |
| H | -1.53344200 | -1.72128400 | 0.86706900 |
| H | -1.36216600 | -0.00250700 | 1.21772900 |
| N | -4.29692300 | 0.82934300 | -0.09127300 |
| S | -6.05966000 | -1.30448800 | -2.00894000 |
| S | -8.94832000 | -1.55016000 | 2.01561900 |
| H | -2.40648200 | 1.73796900 | -0.45748800 |
| H | -3.27026800 | 1.10378800 | -1.87429700 |
| H | -3.54019000 | 1.38231100 | 1.80527300 |
| H | -5.08007900 | 0.51714900 | 1.82413800 |

**2-Int6-t**

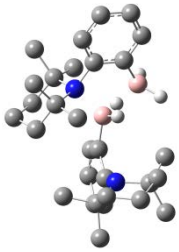


**Sum of electronic and thermal Enthalpies= -2023.029584**
**Sum of electronic and thermal Free Energies= -2023.123573**

| | | | |
|---|---|---|---|
| C | -1.70376100 | -2.26426600 | -0.20877300 |
| C | -0.37945900 | -1.83761800 | -0.14362600 |
| C | -0.04972400 | -0.49452500 | 0.06459400 |
| C | -1.10136000 | 0.42603500 | 0.21202600 |
| C | -2.42816500 | 0.00110300 | 0.14321100 |
| C | -2.73199500 | -1.34072600 | -0.06705400 |
| H | -1.92794900 | -3.31464600 | -0.36681300 |
| H | 0.41541700 | -2.57344800 | -0.23387400 |
| H | -3.22852400 | 0.72767800 | 0.25180600 |
| H | -3.76834000 | -1.66065700 | -0.12005600 |
| B | 1.46748700 | 0.02384100 | 0.11577800 |
| H | 2.12089600 | -1.10078500 | -0.11889000 |
| C | 1.92821700 | 0.46584300 | 1.65519500 |
| C | 1.10389300 | 0.25765900 | 2.75576800 |
| C | 1.36527300 | 1.08961900 | 3.85861200 |
| H | 0.33857700 | -0.50868100 | 2.74114300 |
| C | 2.40204300 | 1.95381200 | 3.60346500 |
| H | 0.82599700 | 1.05473600 | 4.79626400 |
| H | 2.81320900 | 2.69821200 | 4.27257800 |
| B | 2.70463500 | -1.09177200 | 1.06210400 |
| O | 4.08530500 | -0.96153400 | 0.95629300 |
| O | 2.32632600 | -2.25568400 | 1.73082500 |
| C | 4.64379900 | -2.19309100 | 1.44719600 |
| C | 3.51484200 | -2.70986900 | 2.40279800 |
| C | 4.86592000 | -3.10975700 | 0.24256400 |
| H | 5.48808000 | -2.58522300 | -0.48641000 |
| H | 5.37023800 | -4.03726000 | 0.52827300 |
| H | 3.91689600 | -3.36182400 | -0.23880400 |
| C | 5.96772500 | -1.88837200 | 2.13246000 |
| H | 6.69185700 | -1.53473400 | 1.39419300 |
| H | 5.85233400 | -1.11357100 | 2.89210300 |
| H | 6.37280200 | -2.78944000 | 2.60408000 |
| C | 3.56134000 | -2.04676200 | 3.78241400 |
| H | 2.62427200 | -2.25654600 | 4.30460300 |
| H | 4.38894300 | -2.43340200 | 4.38366300 |
| H | 3.66831400 | -0.96107900 | 3.70138800 |
| C | 3.44017000 | -4.22224000 | 2.54615700 |
| H | 4.37603100 | -4.61624700 | 2.95522200 |
| H | 2.63048700 | -4.48932900 | 3.23013600 |
| H | 3.24615000 | -4.70212100 | 1.58582000 |
| C | 1.98385800 | 0.89791800 | -1.11642600 |
| C | 2.61077400 | 2.10966900 | -1.22698700 |
| C | 2.84144000 | 2.53506800 | -2.56953000 |
| H | 2.89190600 | 2.70818700 | -0.37040700 |
| C | 2.38949000 | 1.63454200 | -3.48489800 |
| H | 3.32128900 | 3.47013700 | -2.83246000 |
| H | 2.43420300 | 1.69843000 | -4.56296100 |
| C | -0.31064000 | 4.02198000 | -0.48455500 |
| C | -0.77009600 | 3.71860800 | 1.96428900 |
| C | -0.88673800 | 4.67274900 | 0.77407200 |
| H | -0.47207400 | 4.65781800 | -1.36140400 |
| H | 0.76971000 | 3.88815700 | -0.36794200 |

| | | | |
|---|---|---|---|
| H | -1.24844600 | 4.14458800 | 2.85315400 |
| H | 0.28638900 | 3.54652100 | 2.20297000 |
| H | -0.38008100 | 5.62035500 | 0.98516400 |
| H | -1.94731700 | 4.90811300 | 0.60825900 |
| N | -0.77271700 | 1.80185200 | 0.44987700 |
| C | -0.93387600 | 2.65084000 | -0.72957600 |
| H | -2.00482000 | 2.77124500 | -0.98788800 |
| H | -0.44474800 | 2.16052400 | -1.57503900 |
| C | -1.41104900 | 2.37541800 | 1.62870500 |
| H | -1.29109800 | 1.67327000 | 2.45932600 |
| H | -2.49885700 | 2.52697500 | 1.48250300 |
| S | 1.67388500 | 0.27098400 | -2.71366000 |
| S | 3.05185600 | 1.74848200 | 2.04405300 |

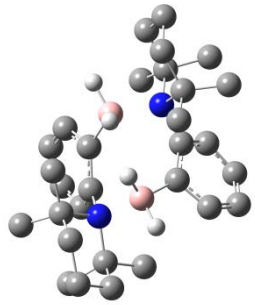
**1-H-Bridged dimer**



**Sum of electronic and thermal Enthalpies= -1330.242959**
**Sum of electronic and thermal Free Energies= -1330.333200**

| | | | |
|---|---|---|---|
| H | 0.54493900 | 1.65317100 | -1.57857200 |
| C | 1.44312600 | 1.14533200 | -1.24106800 |
| C | 2.41258300 | 1.82931300 | -0.52555100 |
| C | 1.64754800 | -0.19745400 | -1.53552800 |
| C | 3.58009200 | 1.20801700 | -0.06338800 |
| H | 2.27484600 | 2.88487100 | -0.30802400 |
| C | 2.79803700 | -0.83809600 | -1.09452300 |
| H | 0.92096400 | -0.75518600 | -2.11750300 |
| C | 3.75209400 | -0.15494900 | -0.33328400 |
| H | 2.93603700 | -1.86340800 | -1.38703400 |
| B | 4.65803400 | 2.07834600 | 0.70628100 |
| H | 5.30273000 | 2.80509400 | -0.01905300 |
| H | 4.28908700 | 2.62773800 | 1.70653800 |
| B | 5.44364000 | 0.22670300 | 1.51066700 |
| C | 6.79547200 | 0.15537500 | 2.42979800 |
| H | 5.72734400 | 1.33858100 | 0.94220500 |
| C | 6.86536900 | -0.11046200 | 3.83227400 |
| C | 7.98559300 | 0.62300900 | 1.84017500 |
| C | 8.09641700 | 0.04863600 | 4.49025900 |
| C | 9.20046100 | 0.74973700 | 2.49693400 |
| H | 8.13614400 | -0.12368700 | 5.55592800 |
| C | 9.25919400 | 0.44364000 | 3.84648900 |
| H | 10.07544000 | 1.10754400 | 1.96347700 |
| H | 10.18399200 | 0.54430000 | 4.40611000 |
| H | 4.44937400 | 0.22560800 | 2.13651200 |
| H | 7.96260200 | 0.93157000 | 0.80133400 |
| C | 4.77923500 | -2.24044600 | 0.80016300 |
| C | 6.05051600 | -0.84993500 | -1.04796900 |
| C | 6.16123700 | -2.80764300 | 1.16511100 |
| C | 7.33109600 | -1.59125000 | -0.62913800 |
| C | 7.08497400 | -2.96626900 | -0.03068100 |
| H | 5.99818400 | -3.77050400 | 1.65752800 |
| H | 6.64616300 | -2.15984200 | 1.89478000 |
| H | 7.96358200 | -1.66009400 | -1.52038900 |
| H | 7.88253700 | -0.99688000 | 0.09881000 |
| H | 6.66540700 | -3.65872600 | -0.76959000 |
| H | 8.03630500 | -3.39879500 | 0.29369700 |
| C | 5.82187700 | -1.77405400 | 5.40535600 |
| C | 5.03651900 | 0.66525200 | 5.32681600 |
| C | 4.39177700 | -2.16733000 | 5.82905600 |
| C | 3.64966700 | 0.18996600 | 5.79609400 |
| C | 3.69109600 | -1.08185400 | 6.63076500 |
| H | 4.43879100 | -3.10542000 | 6.39344500 |
| H | 3.80622900 | -2.36677900 | 4.92409800 |
| H | 3.17323400 | 1.00611700 | 6.35100300 |
| H | 3.03829500 | 0.00549600 | 4.90381600 |
| H | 4.21173700 | -0.91000400 | 7.58075600 |
| H | 2.67439700 | -1.39704800 | 6.88853000 |
| N | 5.71993000 | -0.48733200 | 4.63365900 |
| N | 5.01763500 | -0.81294000 | 0.15612000 |
| C | 4.79936100 | 1.81604300 | 4.34556500 |
| H | 5.73070200 | 2.23350100 | 3.95577300 |
| H | 4.18891400 | 1.50118000 | 3.50421100 |
| H | 4.26694600 | 2.61822700 | 4.86481900 |
| C | 5.80455600 | 1.28506300 | 6.52132100 |
| H | 6.84171800 | 1.50468600 | 6.25810800 |
| H | 5.33118600 | 2.23463900 | 6.78788800 |
| H | 5.79427700 | 0.66989300 | 7.42094700 |
| C | 6.74014300 | -1.81226000 | 6.66143700 |
| H | 6.63539900 | -0.95625700 | 7.32233500 |
| H | 6.49549600 | -2.70653700 | 7.24378000 |
| H | 7.79257900 | -1.90043200 | 6.38317400 |
| C | 6.34508800 | -2.89725000 | 4.50405400 |
| H | 5.64938900 | -3.11880700 | 3.69931500 |
| H | 7.32033200 | -2.65485300 | 4.07419700 |
| H | 6.46180300 | -3.80571900 | 5.10299000 |
| C | 3.90539900 | -2.10307600 | 2.05611500 |
| H | 3.64022700 | -3.11344000 | 2.38456400 |
| H | 4.39897400 | -1.59179400 | 2.88032600 |
| H | 2.97690900 | -1.57479100 | 1.82238400 |
| C | 4.05071900 | -3.32091300 | -0.04139900 |
| H | 2.96869900 | -3.20363500 | 0.00119100 |
| H | 4.35423200 | -3.40966300 | -1.07878100 |
| H | 4.27764300 | -4.27896600 | 0.43431600 |
| C | 6.41726900 | 0.57483200 | -1.48388900 |
| H | 7.14843500 | 0.49207900 | -2.29222100 |
| H | 5.55146700 | 1.11692600 | -1.86620200 |
| H | 6.86878900 | 1.17709100 | -0.70219800 |
| C | 5.50914000 | -1.51096800 | -2.33306400 |
| H | 6.26911800 | -1.36130400 | -3.10394800 |
| H | 5.35715400 | -2.58453600 | -2.26048200 |
| H | 4.59399200 | -1.04123000 | -2.69014000 |

**1-dim8**

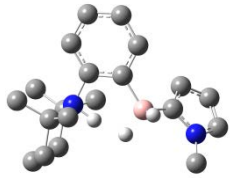


**Sum of electronic and thermal Enthalpies= -1330.147074**

**Sum of electronic and thermal Free Energies= -1330.233579**

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| B | 1.22949700 | 14.26806900 | 5.25374300 | C | 3.01521400 | 16.64535500 | 6.26476900 |
| H | 2.20416400 | 14.75682600 | 4.74748700 | C | 2.12901000 | 17.81770500 | 5.87880500 |
| H | 0.28744200 | 14.55339200 | 4.60536800 | H | 0.10193200 | 18.15431400 | 5.23452900 |
| C | 1.55406600 | 12.66515500 | 5.43020100 | H | 0.87086800 | 16.75664000 | 4.49520400 |
| C | 2.92623400 | 12.37760000 | 5.27527200 | H | 3.94491900 | 16.99784600 | 6.72647600 |
| H | 3.54311600 | 13.16394700 | 4.85422300 | H | 3.29686700 | 16.10173100 | 5.36463400 |
| C | 3.54750100 | 11.20093400 | 5.66208800 | H | 2.59814300 | 18.37687500 | 5.06295100 |
| H | 4.61524100 | 11.06483400 | 5.52358100 | H | 2.01996300 | 18.52812100 | 6.70596100 |
| C | 2.77176900 | 10.25069100 | 6.30134300 | N | 0.98375100 | 15.13653300 | 6.75041300 |
| H | 3.20736400 | 9.35995700 | 6.74253800 | C | -0.33972900 | 17.18616500 | 7.72077900 |
| C | 1.39387100 | 10.41752800 | 6.32056500 | H | -1.18905300 | 17.82581300 | 7.47181700 |
| H | 0.83109900 | 9.63205200 | 6.78881300 | H | -0.66679500 | 16.51462600 | 8.51845400 |
| C | 0.75768600 | 11.53143900 | 5.75374400 | H | 0.43950800 | 17.84195200 | 8.09739600 |
| B | -1.49326200 | 12.92429500 | 5.97542500 | C | 2.34271200 | 16.49196500 | 8.63441800 |
| H | -1.46413300 | 13.63478100 | 5.03544500 | H | 3.15229600 | 16.14469200 | 9.28061000 |
| H | -2.63733900 | 12.62225400 | 6.18754100 | H | 2.52682700 | 17.55172900 | 8.45151200 |
| C | -0.90637300 | 13.53087600 | 7.38709000 | H | 1.42994800 | 16.42261800 | 9.21021000 |
| C | -1.73454000 | 13.22716400 | 8.48761700 | C | 3.36328100 | 14.50315700 | 7.43805200 |
| H | -2.72646600 | 12.85141400 | 8.26109600 | H | 2.91282900 | 13.59044300 | 7.82631100 |
| C | -1.36417500 | 13.32039000 | 9.81983100 | H | 3.81576200 | 14.25948800 | 6.48256200 |
| H | -2.05780800 | 13.04715800 | 10.60854900 | H | 4.17083200 | 14.80082700 | 8.11105100 |
| C | -0.05915000 | 13.68821600 | 10.09435200 | C | -1.31669400 | 16.06608300 | 5.80461800 |
| H | 0.34321500 | 13.66164000 | 11.10194700 | H | -1.22676200 | 15.55435200 | 4.85418700 |
| C | 0.73251100 | 14.16055100 | 9.05651700 | H | -1.95876300 | 15.48570600 | 6.46445900 |
| H | 1.72385600 | 14.47533400 | 9.32338500 | H | -1.81007000 | 17.02456800 | 5.62094800 |
| C | 0.27679500 | 14.24106600 | 7.73248700 | C | -0.31021400 | 12.60723900 | 3.05567900 |
| C | -0.86450500 | 11.39318000 | 3.81807800 | H | 0.76828200 | 12.71064900 | 3.15890300 |
| C | -1.43792100 | 10.19668800 | 6.04377000 | H | -0.52539900 | 12.42437600 | 1.99914900 |
| C | -2.36792000 | 11.33843200 | 3.48810100 | H | -0.78534100 | 13.54109000 | 3.33123800 |
| C | -2.92052300 | 10.15670200 | 5.60623200 | C | -0.11378300 | 10.19419400 | 3.20104500 |
| C | -3.12572100 | 10.17212800 | 4.10073300 | H | -0.02196300 | 10.37951800 | 2.12890900 |
| H | -2.44745100 | 11.29837500 | 2.39644800 | H | 0.90041900 | 10.10980300 | 3.59925700 |
| H | -2.82082200 | 12.28125800 | 3.80609200 | H | -0.62180300 | 9.24043600 | 3.30766700 |
| H | -3.33634000 | 9.24229800 | 6.04529900 | C | -0.86918200 | 8.78691800 | 5.64191200 |
| H | -3.46055300 | 10.99242300 | 6.04757600 | H | -0.79684100 | 8.16735200 | 6.53896800 |
| H | -4.19312500 | 10.26859900 | 3.87814000 | H | -1.55385600 | 8.27184600 | 4.96619000 |
| H | -2.80649100 | 9.22874200 | 3.64305900 | H | 0.10559700 | 8.77774400 | 5.17391700 |
| N | -0.70886600 | 11.46531300 | 5.41926200 | C | -1.44777900 | 10.31639800 | 7.57888400 |
| C | 0.03935500 | 16.40366600 | 6.44511500 | H | -0.52780400 | 10.71760900 | 8.00234500 |
| C | 2.37822900 | 15.67798400 | 7.28923000 | H | -2.25906800 | 10.95751100 | 7.90682800 |
| C | 0.76834900 | 17.30831800 | 5.43355800 | H | -1.62255700 | 9.32896400 | 8.01262600 |

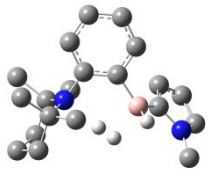
**1-Int1-p**



**Sum of electronic and thermal Enthalpies= -914.456694**
**Sum of electronic and thermal Free Energies= -914.526715**

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| H | 0.67872700 | -0.05581500 | 2.18142600 | | C | 5.18827900 | 0.16654500 | -1.98144300 |
| C | 1.62149500 | -0.00898600 | 1.64466200 | | C | 7.74644300 | 0.34640900 | -0.41973100 |
| C | 2.27562900 | 1.20604200 | 1.49602200 | | C | 6.49719500 | 0.74618500 | -2.54167000 |
| C | 2.16966700 | -1.17186100 | 1.10546500 | | C | 7.75356900 | 0.13594900 | -1.93000900 |
| C | 3.49480400 | 1.32622400 | 0.80952800 | | H | 8.64199000 | -0.08285000 | 0.04015200 |
| H | 1.83470300 | 2.10763800 | 1.91060000 | | H | 7.76862000 | 1.42346600 | -0.20951100 |
| C | 3.37172800 | -1.10373900 | 0.41541000 | | H | 6.48321000 | 0.60771700 | -3.62709200 |
| H | 1.66654600 | -2.12629800 | 1.21987500 | | H | 6.49964400 | 1.82887100 | -2.36175900 |
| C | 4.00112600 | 0.13359000 | 0.28097300 | | H | 8.63954100 | 0.61044500 | -2.36175000 |
| H | 3.79946800 | -2.00485700 | -0.00621600 | | H | 7.82744200 | -0.93024600 | -2.17313300 |
| B | 4.21760000 | 2.77809900 | 0.67248300 | | N | 5.27949600 | 0.28456000 | -0.44529400 |
| H | 4.51499100 | 3.17639600 | 1.79166300 | | C | 4.01647000 | 1.04604000 | -2.43223100 |
| H | 5.39650400 | 1.32771800 | -0.31575200 | | H | 3.05620700 | 0.60963400 | -2.15105700 |
| H | 5.32488800 | 2.70081400 | 0.07244100 | | H | 4.05861100 | 2.05474900 | -2.01292900 |
| C | 3.29442700 | 3.80899600 | -0.13508000 | | H | 4.05114000 | 1.12579000 | -3.52236500 |
| C | 2.10377600 | 3.64659100 | -0.82654700 | | C | 4.94912600 | -1.25731600 | -2.48387800 |
| N | 3.63376600 | 5.13935100 | -0.28037600 | | H | 5.78124200 | -1.93729500 | -2.30513100 |
| C | 1.72470100 | 4.89432600 | -1.39168000 | | H | 4.04082200 | -1.68587300 | -2.05939700 |
| H | 1.55978600 | 2.71372500 | -0.90150700 | | H | 4.80235000 | -1.19876500 | -3.56578000 |
| C | 2.69536500 | 5.79729100 | -1.03609900 | | C | 6.59911700 | -1.78520500 | 0.33151100 |
| H | 0.84332600 | 5.10960800 | -1.97984500 | | H | 6.73380100 | -2.24957300 | -0.64425800 |
| H | 2.79827400 | 6.85223900 | -1.24892300 | | H | 7.46632400 | -2.05187000 | 0.94208600 |
| C | 4.82907500 | 5.74062300 | 0.26038900 | | H | 5.72106000 | -2.21713100 | 0.81245900 |
| H | 4.90025700 | 5.55360800 | 1.33495800 | | C | 6.46472000 | 0.26827900 | 1.72617900 |
| H | 5.72718100 | 5.33123200 | -0.21479700 | | H | 6.30995600 | 1.34958900 | 1.75924300 |
| H | 4.79973000 | 6.81851800 | 0.08764500 | | H | 5.66423900 | -0.20718500 | 2.29583600 |
| C | 6.52241000 | -0.25919000 | 0.28661300 | | H | 7.41771900 | 0.03888000 | 2.21105500 |

**1-TS2-p**

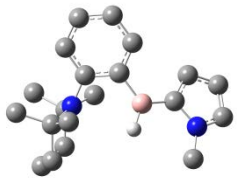


**Sum of electronic and thermal Enthalpies= -914.429973**
**Sum of electronic and thermal Free Energies= -914.504492**

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| H | 1.31467300 | 0.11213300 | 2.67179500 | | C | 1.98688600 | 5.09781200 | -1.06410000 |
| C | 2.10352400 | 0.08548400 | 1.92659100 | | H | 1.77446900 | 2.89025200 | -0.78204600 |
| C | 2.78823000 | 1.24806400 | 1.59503300 | | C | 3.04661400 | 5.91967500 | -0.74257700 |
| C | 2.43479000 | -1.10557800 | 1.29320000 | | H | 1.05775100 | 5.41109800 | -1.51737600 |
| C | 3.81886800 | 1.26670400 | 0.64291600 | | H | 3.17178900 | 6.98594000 | -0.86887500 |
| H | 2.51166400 | 2.17875200 | 2.08350500 | | N | 4.03246900 | 5.16517000 | -0.18449900 |
| C | 3.44245400 | -1.11325300 | 0.33667300 | | C | 5.30375900 | 5.67847800 | 0.27785400 |
| H | 1.91263700 | -2.02584700 | 1.53584700 | | H | 5.43711700 | 5.48470300 | 1.34486300 |
| C | 4.13980100 | 0.05355200 | 0.00161100 | | H | 6.13343600 | 5.21494500 | -0.26378000 |
| H | 3.69293400 | -2.04309200 | -0.15911000 | | H | 5.33568400 | 6.75572600 | 0.10762500 |
| B | 4.50562100 | 2.68757200 | 0.44199300 | | C | 6.47998200 | -0.55189600 | -0.58639700 |
| H | 5.52964600 | 1.87819600 | -0.90718600 | | C | 4.70048700 | -0.07776200 | -2.41872100 |
| H | 5.64204400 | 2.65108000 | -0.82017600 | | C | 7.55417800 | -0.10761500 | -1.59662600 |
| C | 3.63864500 | 3.83672100 | -0.13411400 | | C | 5.85463600 | 0.35048200 | -3.34447600 |
| C | 2.36244500 | 3.79262100 | -0.68430500 | | C | 7.16376100 | -0.36793300 | -3.04535000 |

| | | | |
|---|---|---|---|
| H | 8.49465700 | -0.61144300 | -1.34813400 |
| H | 7.72659200 | 0.96854600 | -1.46734500 |
| H | 5.54695400 | 0.18669000 | -4.38282700 |
| H | 6.01147000 | 1.43019900 | -3.22578500 |
| H | 7.95051500 | -0.00973600 | -3.71730100 |
| H | 7.06515200 | -1.44393900 | -3.23145400 |
| N | 5.17325900 | 0.04177700 | -1.00370400 |
| C | 6.86572600 | 0.02025200 | 0.78708300 |
| H | 7.87275900 | -0.32109600 | 1.04518200 |
| H | 6.86815700 | 1.11276700 | 0.78257600 |
| H | 6.18254700 | -0.31446000 | 1.57101700 |
| C | 6.49288100 | -2.08913000 | -0.45281400 |
| H | 5.75656200 | -2.42622300 | 0.27949000 |
| H | 6.30263200 | -2.60223400 | -1.39579000 |
| H | 7.47691200 | -2.41088500 | -0.09670700 |
| C | 4.19034600 | -1.47290700 | -2.83763000 |
| H | 3.84518900 | -1.42908100 | -3.87567200 |
| H | 4.95549900 | -2.24770100 | -2.78061800 |
| H | 3.33953200 | -1.78197400 | -2.22726300 |
| C | 3.53913000 | 0.90610100 | -2.63318000 |
| H | 2.65294300 | 0.61231300 | -2.06510200 |
| H | 3.80241000 | 1.92587300 | -2.34217100 |
| H | 3.27188500 | 0.91587700 | -3.69426500 |
| H | 5.41698100 | 2.96609400 | 1.17991200 |

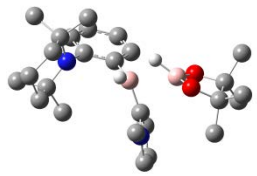
**1-Int2-p**



**Sum of electronic and thermal Enthalpies= -913.282531**
**Sum of electronic and thermal Free Energies= -913.355462**

| | | | |
|---|---|---|---|
| C | -2.60297300 | -2.87692200 | 1.21213500 |
| C | -1.24328200 | -3.09243000 | 1.40209300 |
| C | -0.32737400 | -2.10166500 | 1.05858700 |
| C | -0.75630100 | -0.87811300 | 0.53576200 |
| C | -2.13310900 | -0.65218800 | 0.32982000 |
| C | -3.03464100 | -1.67181400 | 0.66766700 |
| H | -3.32242500 | -3.64462500 | 1.47939800 |
| H | -0.88955500 | -4.03377100 | 1.81194100 |
| H | 0.73265200 | -2.28403500 | 1.19299000 |
| H | -4.09752500 | -1.50799600 | 0.51257600 |
| B | -2.63735000 | 0.71246400 | -0.24930300 |
| H | -2.20712400 | 1.74264800 | 0.18693700 |
| C | -3.69733100 | 0.76999400 | -1.33788300 |
| C | -4.25865200 | -0.25847700 | -2.10390100 |
| C | -5.16099700 | 0.29630100 | -3.02163500 |
| H | -4.00527600 | -1.30388200 | -1.99400300 |
| C | -5.13997200 | 1.66548900 | -2.80989900 |
| H | -5.75879600 | -0.22088500 | -3.75754200 |
| H | -5.68859800 | 2.45493500 | -3.30506200 |
| N | -4.26848800 | 1.94732500 | -1.81526800 |
| C | -3.97099700 | 3.28208200 | -1.33429700 |
| H | -4.20222900 | 3.37168500 | -0.27089700 |
| H | -2.91422700 | 3.51557900 | -1.48201900 |
| H | -4.57531400 | 3.99976700 | -1.89080100 |
| C | 0.82242600 | 0.88006500 | 1.29628800 |
| C | 0.82553600 | 0.03877600 | -1.14438300 |
| C | 1.27991800 | 2.25294800 | 0.77009900 |
| C | 1.31409200 | 1.43438100 | -1.57552300 |
| C | 2.11557800 | 2.15623000 | -0.49996100 |
| H | 1.83285500 | 2.76955400 | 1.56297100 |
| H | 0.38192600 | 2.84658300 | 0.55703300 |
| H | 1.89749300 | 1.33391600 | -2.49781600 |
| H | 0.42959700 | 2.03851700 | -1.81553100 |
| H | 2.38956100 | 3.15818400 | -0.84734800 |
| H | 3.05840800 | 1.63192300 | -0.30262000 |
| N | 0.15905800 | 0.16393400 | 0.17637800 |
| C | -0.19077700 | -0.42987200 | -2.19650400 |
| H | -0.55448100 | -1.44094300 | -1.99644800 |
| H | -1.05530700 | 0.23754800 | -2.24637100 |
| H | 0.29042100 | -0.43177700 | -3.17925000 |
| C | 1.99580800 | -0.97044700 | -1.17697400 |
| H | 2.84551900 | -0.65695900 | -0.56945700 |
| H | 1.66718900 | -1.95225300 | -0.82603600 |
| H | 2.35544700 | -1.09064000 | -2.20421000 |
| C | 2.01966800 | 0.15138200 | 1.95063400 |
| H | 2.38434300 | 0.74247900 | 2.79735900 |
| H | 1.72241800 | -0.82416600 | 2.34151400 |
| H | 2.85882800 | 0.00604900 | 1.26990800 |
| C | -0.20567400 | 1.12934400 | 2.41135000 |
| H | 0.24036300 | 1.77730200 | 3.17232700 |
| H | -1.09774400 | 1.62054200 | 2.01905200 |
| H | -0.51054600 | 0.19948200 | 2.89791800 |

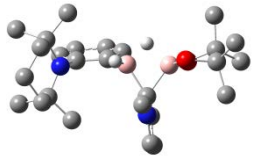
**1-TS3-p**



**Sum of electronic and thermal Enthalpies= -1324.859996**
**Sum of electronic and thermal Free Energies= -1324.952727**

| | | | |
|---|---|---|---|
| C | -2.12133100 | -1.92648200 | 1.30252400 |
| C | -0.77669400 | -1.57857300 | 1.23349400 |
| C | -0.35758000 | -0.31297500 | 0.80016200 |
| C | -1.34619800 | 0.61994800 | 0.42196300 |
| C | -2.69789700 | 0.26332600 | 0.50313100 |
| C | -3.08869100 | -0.99757700 | 0.93985700 |
| H | -2.41028000 | -2.91747000 | 1.63985400 |
| H | -0.02997700 | -2.31531800 | 1.51794200 |
| H | -3.45283000 | 0.98728900 | 0.21840300 |
| H | -4.14372100 | -1.24876500 | 0.99519600 |
| B | 1.18114300 | 0.10317200 | 0.78874800 |
| H | 1.68697600 | -1.04296200 | -0.03528700 |
| C | 1.93636500 | 0.17494200 | 2.17443400 |
| C | 1.56091500 | -0.31885400 | 3.42233100 |
| C | 2.37651100 | 0.26732300 | 4.40580300 |
| H | 0.75787400 | -1.02478100 | 3.57941400 |
| C | 3.24074300 | 1.11958000 | 3.74224900 |
| H | 2.34139800 | 0.10513600 | 5.47316000 |
| H | 4.02386300 | 1.75955800 | 4.12366000 |
| H | 1.56090300 | 0.89747100 | -0.02163200 |
| B | 2.54806600 | -1.54548600 | 0.69254300 |
| O | 3.86356900 | -1.30275900 | 0.41757100 |
| O | 2.30268600 | -2.72939100 | 1.32534600 |
| C | 4.61856100 | -2.25511100 | 1.20696200 |
| C | 3.57346800 | -3.41143800 | 1.43741900 |
| C | 5.85039000 | -2.65920900 | 0.40989300 |
| H | 6.51355300 | -1.79744900 | 0.30064300 |
| H | 6.40099500 | -3.44775000 | 0.93220600 |
| H | 5.58808600 | -3.01534500 | -0.58726000 |
| C | 5.03575800 | -1.55288100 | 2.49764000 |
| H | 5.58855200 | -0.64519400 | 2.24158800 |
| H | 4.17295000 | -1.26447900 | 3.10113000 |
| H | 5.68634800 | -2.19412900 | 3.09894200 |
| C | 3.64760700 | -4.06530900 | 2.80958000 |
| H | 2.88750500 | -4.84705200 | 2.88274400 |
| H | 4.62808900 | -4.52639100 | 2.96419000 |
| H | 3.46677600 | -3.33891000 | 3.60314600 |
| C | 3.59304000 | -4.47230600 | 0.33733500 |
| H | 4.50353100 | -5.07635000 | 0.37940000 |
| H | 2.73235700 | -5.13245800 | 0.46760900 |
| H | 3.52110000 | -4.01429800 | -0.65276300 |
| N | 2.98236600 | 1.05924800 | 2.41250200 |
| C | 3.69355600 | 1.81144500 | 1.39846600 |
| H | 4.10563000 | 1.12788000 | 0.65346200 |
| H | 3.02488200 | 2.52026800 | 0.90351200 |
| H | 4.50697900 | 2.36011500 | 1.87595000 |
| C | -1.02709200 | 2.13685500 | -1.50991700 |
| C | -1.07991700 | 3.04541300 | 0.90638600 |
| C | -0.08603200 | 3.30008300 | -1.87368900 |
| C | -0.14848400 | 4.18151300 | 0.44364200 |
| C | -0.31904700 | 4.54312300 | -1.02555200 |
| H | -0.20109600 | 3.52630900 | -2.93987700 |
| H | 0.94622000 | 2.95939500 | -1.72176800 |
| H | -0.31226700 | 5.05558800 | 1.08420200 |
| H | 0.88667400 | 3.85250800 | 0.60365100 |
| H | 0.39171700 | 5.32831500 | -1.30503200 |
| H | -1.31928500 | 4.95440200 | -1.20782900 |
| N | -0.94951900 | 1.91615300 | -0.04503800 |
| C | -0.51501300 | 0.88612500 | -2.24304200 |
| H | 0.48064600 | 0.60736500 | -1.89267900 |
| H | -1.18232300 | 0.03196700 | -2.10431600 |
| H | -0.45619700 | 1.09829100 | -3.31522800 |
| C | -2.44355500 | 2.42372800 | -2.06189000 |
| H | -2.40163700 | 2.50913900 | -3.15310200 |
| H | -3.12882300 | 1.60688500 | -1.82377800 |
| H | -2.87214300 | 3.35079200 | -1.67897200 |
| C | -2.51793500 | 3.58661500 | 1.08384500 |
| H | -3.19122900 | 2.79437200 | 1.42037800 |
| H | -2.52631200 | 4.37003000 | 1.84893100 |
| H | -2.92849300 | 4.01790100 | 0.16992700 |
| C | -0.59678700 | 2.60399500 | 2.29557300 |
| H | 0.42980600 | 2.23407900 | 2.26043200 |
| H | -0.62724900 | 3.46070500 | 2.97610500 |
| H | -1.22508800 | 1.81580700 | 2.71753700 |

**1-Int3-p**

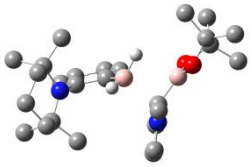


**Sum of electronic and thermal Enthalpies= -1324.866045**
**Sum of electronic and thermal Free Energies= -1324.957706**

| | | | |
|---|---|---|---|
| C | -2.09993100 | -1.87615600 | 1.44614300 |
| C | -0.76183700 | -1.51659600 | 1.32932500 |
| C | -0.36596400 | -0.25336400 | 0.86518400 |
| C | -1.37438500 | 0.65895800 | 0.48837000 |
| C | -2.71956800 | 0.28598500 | 0.60819200 |
| C | -3.08657900 | -0.96642100 | 1.08721500 |
| H | -2.36842400 | -2.86256000 | 1.81282100 |
| H | 0.00368200 | -2.23679000 | 1.60762500 |
| H | -3.48977100 | 0.99094800 | 0.31695100 |
| H | -4.13726000 | -1.22702400 | 1.17349400 |
| B | 1.18014000 | 0.13202000 | 0.78102000 |
| H | 1.76571400 | -0.89605900 | 0.26251700 |
| C | 1.94291600 | 0.32719300 | 2.25863700 |
| C | 1.38451000 | 0.04081000 | 3.52052400 |
| C | 1.90347200 | 0.92154600 | 4.46016900 |
| H | 0.67887600 | -0.75896700 | 3.69253200 |
| C | 2.77498300 | 1.76212500 | 3.76921400 |
| H | 1.68909000 | 0.96560200 | 5.51731400 |
| H | 3.37413000 | 2.58519000 | 4.13417300 |
| H | 1.53799000 | 1.01046600 | 0.05351500 |
| B | 2.55975600 | -1.00692800 | 1.37996600 |
| O | 3.88270800 | -0.88211900 | 0.90790100 |
| O | 2.35291900 | -2.26623900 | 1.97463000 |
| C | 4.62167200 | -1.91841400 | 1.57058900 |
| C | 3.53735300 | -3.03498200 | 1.72410200 |
| C | 5.81351200 | -2.30162700 | 0.70626800 |
| H | 6.52759800 | -1.47458900 | 0.66770300 |
| H | 6.32534100 | -3.17359300 | 1.12576600 |
| H | 5.50446000 | -2.53175100 | -0.31455000 |
| C | 5.09643900 | -1.36873000 | 2.92034400 |
| H | 5.66793100 | -0.45344000 | 2.74299500 |
| H | 4.24918400 | -1.12043200 | 3.56720800 |

| | | | |
|---|---|---|---|
| H | 5.74009100 | -2.08105700 | 3.44425400 |
| C | 3.76110800 | -3.98180600 | 2.89454800 |
| H | 2.96866200 | -4.73425900 | 2.91883100 |
| H | 4.72028800 | -4.49982800 | 2.79293700 |
| H | 3.74855200 | -3.44481500 | 3.84452300 |
| C | 3.32233600 | -3.82588700 | 0.43108900 |
| H | 4.14867900 | -4.51495200 | 0.23336800 |
| H | 2.40177000 | -4.40708700 | 0.52597700 |
| H | 3.21543300 | -3.15429900 | -0.42526900 |
| N | 2.80232400 | 1.41995700 | 2.47553100 |
| C | 3.56482700 | 2.10983100 | 1.45190400 |
| H | 4.25568100 | 2.79991800 | 1.93805100 |
| H | 4.12066800 | 1.37699100 | 0.86642200 |
| H | 2.89323400 | 2.66818200 | 0.79537200 |
| C | -1.11467500 | 2.11046500 | -1.50083200 |
| C | -1.16673500 | 3.10395800 | 0.88196100 |
| C | -0.22848100 | 3.29781000 | -1.91980800 |
| C | -0.29266200 | 4.26062900 | 0.36116400 |
| C | -0.50421600 | 4.56103100 | -1.11597100 |
| H | -0.36494000 | 3.47871400 | -2.99197300 |
| H | 0.81938200 | 3.00811700 | -1.76880700 |
| H | -0.48227400 | 5.14958400 | 0.97364400 |
| H | 0.75894400 | 3.98285600 | 0.51191200 |
| H | 0.16599800 | 5.36614500 | -1.43632700 |
| H | -1.52480500 | 4.92008700 | -1.29546000 |
| N | -1.01283700 | 1.94669800 | -0.02985900 |
| C | -0.55548300 | 0.85751400 | -2.19411800 |
| H | 0.45790700 | 0.64086500 | -1.85064300 |
| H | -1.17686200 | -0.02217600 | -2.00993000 |
| H | -0.52522500 | 1.02984400 | -3.27469000 |
| C | -2.54894100 | 2.31724700 | -2.04253100 |
| H | -2.52393000 | 2.38391700 | -3.13556000 |
| H | -3.18972000 | 1.47179100 | -1.78103600 |
| H | -3.01812700 | 3.22904800 | -1.67011800 |
| C | -0.62869700 | 2.72777900 | 2.26970600 |
| H | 0.40970900 | 2.39986700 | 2.20325400 |
| H | -0.67185700 | 3.60262300 | 2.92633100 |
| H | -1.20964400 | 1.92750800 | 2.73430000 |
| C | -2.61880600 | 3.59896100 | 1.08005600 |
| H | -3.25109200 | 2.80030500 | 1.47491500 |
| H | -2.63424700 | 4.41733800 | 1.80775600 |
| H | -3.07206200 | 3.97011000 | 0.15975100 |

**1-TS4-p**

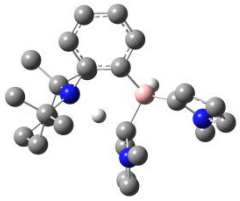


**Sum of electronic and thermal Enthalpies= -1324.862923**
**Sum of electronic and thermal Free Energies= -1324.956953**

| | | | |
|---|---|---|---|
| C | -2.08868800 | -1.92215700 | 0.86086500 |
| C | -0.93189500 | -1.17755800 | 1.18330900 |
| C | 0.29841200 | -1.66800200 | 0.71579100 |
| C | 0.41044600 | -2.86040000 | 0.01075900 |
| C | -0.73309000 | -3.59706600 | -0.27613900 |
| C | -1.96923500 | -3.11850700 | 0.13944200 |
| H | 1.19885300 | -1.09346600 | 0.91720300 |
| H | 1.38451000 | -3.20757900 | -0.32266700 |
| H | -0.66774300 | -4.52930000 | -0.82958200 |
| H | -2.86706100 | -3.67534900 | -0.10504400 |
| B | -1.01303400 | 0.20816000 | 1.97516000 |
| H | -2.06178100 | 0.49264200 | 2.48529600 |
| H | -0.52006600 | 1.14161900 | 1.37477800 |
| C | 2.08497600 | 3.02999400 | 2.09020400 |
| C | 3.01413900 | 1.78725900 | 1.85619900 |
| O | 1.12202600 | 2.51377000 | 3.03753000 |
| O | 2.11865800 | 0.68060700 | 2.08946600 |
| B | 1.08546200 | 1.15233700 | 2.85995300 |
| C | 2.77448700 | 4.23598900 | 2.71070500 |
| H | 2.04991500 | 5.04365900 | 2.84279300 |
| H | 3.20254500 | 3.99922800 | 3.68591500 |
| H | 3.57224100 | 4.59857800 | 2.05496300 |
| C | 1.31281200 | 3.44781200 | 0.83909100 |
| H | 0.54456500 | 4.17040500 | 1.12452100 |
| H | 1.97389500 | 3.91538300 | 0.10415400 |
| H | 0.81555400 | 2.59300700 | 0.37486200 |
| C | 3.57962800 | 1.66834700 | 0.44911800 |
| H | 4.20062700 | 2.53733500 | 0.20949000 |
| H | 4.20316800 | 0.77346400 | 0.37910000 |
| H | 2.78474300 | 1.58709400 | -0.29345600 |
| C | 4.13323500 | 1.67168400 | 2.89196400 |
| H | 4.60562100 | 0.69162700 | 2.79204700 |
| H | 4.89636900 | 2.44157500 | 2.74766400 |
| H | 3.73772300 | 1.75696800 | 3.90789700 |
| C | 0.09775300 | 0.20613500 | 3.60632600 |
| C | 0.44923000 | -1.11649300 | 3.98284300 |
| C | -0.12944100 | -1.41662600 | 5.20274900 |
| H | 1.05857400 | -1.76598400 | 3.37138100 |
| C | -0.82664100 | -0.27060700 | 5.59724600 |
| H | -0.08812600 | -2.34890100 | 5.74509800 |
| H | -1.43196000 | -0.10562300 | 6.47856900 |
| N | -0.67822700 | 0.68942600 | 4.68464000 |
| C | -1.30897300 | 1.99610500 | 4.73491500 |
| H | -1.81156000 | 2.10754100 | 5.69618600 |
| H | -0.55546700 | 2.77331900 | 4.61066000 |
| H | -2.03730700 | 2.07282900 | 3.92410400 |
| C | -4.15767000 | -0.72905500 | 0.20210200 |
| C | -4.04927800 | -2.11548600 | 2.37667500 |
| C | -5.21059000 | 0.16479500 | 0.88491400 |
| C | -5.09145800 | -1.15329900 | 2.97668600 |
| C | -6.03406500 | -0.56943400 | 1.93415300 |
| H | -5.85748800 | 0.59822500 | 0.11346200 |
| H | -4.68375700 | 0.99481100 | 1.37265700 |
| H | -5.64946700 | -1.67963500 | 3.76009400 |
| H | -4.55006500 | -0.32861700 | 3.45807900 |
| H | -6.74323300 | 0.11909400 | 2.40675100 |
| H | -6.63500300 | -1.36134200 | 1.47065400 |
| N | -3.38332700 | -1.43938100 | 1.24386900 |
| C | -3.22263400 | 0.20007300 | -0.58867700 |
| H | -2.66685100 | 0.85873900 | 0.08345600 |
| H | -2.50367400 | -0.36149000 | -1.19030100 |
| H | -3.82173800 | 0.81853500 | -1.26497700 |
| C | -4.84789000 | -1.65626500 | -0.82584100 |
| H | -5.32847400 | -1.05738600 | -1.60728500 |

| | | | |
|---|---|---|---|
| H | -4.11518200 | -2.30497400 | -1.31219800 |
| H | -5.61681900 | -2.28683000 | -0.37581200 |
| C | -4.72253900 | -3.46702500 | 2.04005500 |
| H | -3.98917600 | -4.18026400 | 1.65609000 |
| H | -5.15745800 | -3.90115900 | 2.94719700 |
| H | -5.52329000 | -3.37242600 | 1.30441900 |
| C | -3.00633000 | -2.38359300 | 3.46932500 |
| H | -2.48847600 | -1.45902000 | 3.72672100 |
| H | -3.50280100 | -2.77151700 | 4.36514700 |
| H | -2.25828800 | -3.11441700 | 3.15201200 |

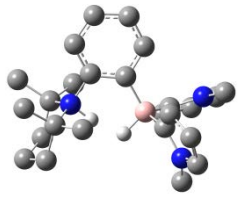
**1-TS5-p**



**Sum of electronic and thermal Enthalpies= -1162.567383**
**Sum of electronic and thermal Free Energies= -1162.649627**

| | | | |
|---|---|---|---|
| C | -1.69171000 | -2.12373500 | 0.71862200 |
| C | -0.40134200 | -1.61238900 | 0.66367300 |
| C | -0.11298500 | -0.24249200 | 0.50752600 |
| C | -1.22131700 | 0.62691000 | 0.34780700 |
| C | -2.51898300 | 0.09600500 | 0.42147600 |
| C | -2.76723400 | -1.25611800 | 0.61113800 |
| H | -1.84729300 | -3.19067700 | 0.84685400 |
| H | 0.41736600 | -2.31640600 | 0.76776600 |
| H | -3.35886600 | 0.76973000 | 0.31574300 |
| H | -3.78866700 | -1.62151600 | 0.66023900 |
| B | 1.45917700 | 0.16647800 | 0.57152700 |
| H | 1.99817000 | -0.94710300 | 0.14809000 |
| C | 2.06158100 | 0.17743400 | 2.17731200 |
| C | 1.20993100 | -0.15226800 | 3.25837700 |
| C | 1.60029000 | 0.54179600 | 4.39002100 |
| H | 0.38855000 | -0.84880900 | 3.17232800 |
| C | 2.70558300 | 1.30195600 | 4.01211300 |
| H | 1.15397500 | 0.51366600 | 5.37246600 |
| H | 3.32098500 | 1.96221400 | 4.60873300 |
| B | 2.70052300 | -1.13036500 | 1.30352800 |
| O | 4.07707500 | -1.04355000 | 0.99674000 |
| O | 2.38417900 | -2.43604400 | 1.74223800 |
| C | 4.64692000 | -2.34401500 | 1.20323400 |
| C | 3.62071200 | -3.00268100 | 2.18423900 |
| C | 4.70787200 | -3.05732200 | -0.14848400 |
| H | 5.27977500 | -2.44141200 | -0.84804900 |
| H | 5.19986800 | -4.03093500 | -0.06908100 |
| H | 3.70421400 | -3.20679800 | -0.55693500 |
| C | 6.05009300 | -2.17063800 | 1.76865800 |
| H | 6.69457400 | -1.69984300 | 1.02133100 |
| H | 6.04304500 | -1.53721800 | 2.65739600 |
| H | 6.48533600 | -3.14036800 | 2.03053400 |
| C | 3.84610200 | -2.58192000 | 3.64110300 |
| H | 2.97183900 | -2.87459400 | 4.22772200 |
| H | 4.73060600 | -3.06376600 | 4.06754800 |
| H | 3.96072900 | -1.49750800 | 3.73254500 |
| C | 3.52348400 | -4.51836200 | 2.08687800 |
| H | 4.49012200 | -4.98360400 | 2.30497600 |
| H | 2.79532500 | -4.88736000 | 2.81380800 |
| H | 3.19763300 | -4.83094300 | 1.09345200 |
| C | 2.14398800 | 1.26585000 | -0.34870800 |
| C | 2.26245300 | 2.63270000 | -0.18603900 |
| C | 2.93382800 | 3.17484200 | -1.30802000 |
| H | 1.88309100 | 3.18124900 | 0.66278800 |
| C | 3.20955100 | 2.11968400 | -2.14453500 |
| H | 3.17598600 | 4.21210800 | -1.48970800 |
| H | 3.70101900 | 2.08707000 | -3.10599400 |
| N | 2.98645900 | 1.10415400 | 2.71933300 |
| N | 2.73821200 | 0.97435000 | -1.56275700 |
| C | 2.82766700 | -0.33752100 | -2.16692600 |
| H | 1.83534800 | -0.79001300 | -2.25494400 |
| H | 3.25201400 | -0.23690600 | -3.16687000 |
| H | 3.47251300 | -0.99011400 | -1.57337200 |
| C | 4.16557000 | 1.68684100 | 2.08514800 |
| H | 4.48852400 | 1.04671300 | 1.27012500 |
| H | 3.94333300 | 2.67883300 | 1.69354800 |
| H | 4.95994100 | 1.74380700 | 2.83233300 |
| C | -1.37838700 | 2.41740900 | -1.34349100 |
| C | -1.36746900 | 2.96257700 | 1.18189300 |
| C | -0.83599100 | 3.83617900 | -1.59194900 |
| C | -0.87534900 | 4.37687100 | 0.81608600 |
| C | -1.32401700 | 4.84300200 | -0.56090500 |
| H | -1.11945800 | 4.14454800 | -2.60477100 |
| H | 0.25752900 | 3.79191800 | -1.55824700 |
| H | -1.20988100 | 5.07073100 | 1.59561600 |
| H | 0.21911200 | 4.37961300 | 0.83558500 |
| H | -0.90790900 | 5.83414600 | -0.77193400 |
| H | -2.41509600 | 4.94980800 | -0.60203500 |
| C | -0.63949000 | 1.47352000 | -2.30307600 |
| H | -0.81505100 | 1.80074100 | -3.33294700 |
| H | 0.43267400 | 1.49459600 | -2.10987500 |
| H | -0.99672100 | 0.44400900 | -2.21251300 |
| C | -2.87401700 | 2.37318400 | -1.74428300 |
| H | -2.98102100 | 2.74512500 | -2.76869400 |
| H | -3.26165200 | 1.35249000 | -1.73081600 |
| H | -3.50969500 | 2.98959600 | -1.10691800 |
| C | -0.58077500 | 2.51042700 | 2.41766000 |
| H | -0.93789800 | 1.54725400 | 2.79027000 |
| H | 0.48249500 | 2.41074400 | 2.19015500 |
| H | -0.69674300 | 3.24501300 | 3.22121400 |
| C | -2.85265700 | 3.04910000 | 1.61383300 |
| H | -3.21633100 | 2.08764000 | 1.98278200 |
| H | -2.94754100 | 3.76736200 | 2.43517100 |
| H | -3.51352600 | 3.38238600 | 0.81214600 |
| N | -1.06258200 | 2.03004900 | 0.06417300 |

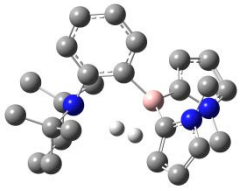
**1-Int4-p**



**Sum of electronic and thermal Enthalpies= -1162.598646**
**Sum of electronic and thermal Free Energies= -1162.685051**

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| H | 1.05282000 | 0.85007700 | 2.57418000 | | C | 6.97263900 | 4.93341200 | 0.16375300 |
| C | 1.90766000 | 0.65373500 | 1.93423800 | | H | 7.55985300 | 5.81962100 | 0.41359300 |
| C | 2.68108700 | 1.70862700 | 1.46884100 | | H | 7.58568200 | 4.26914500 | -0.45578400 |
| C | 2.22567200 | -0.65491800 | 1.58128500 | | H | 6.09941400 | 5.23235600 | -0.42018400 |
| C | 3.80157200 | 1.52577900 | 0.64398600 | | C | 6.45389200 | -0.63752300 | -0.14945900 |
| H | 2.40463900 | 2.72080000 | 1.74383100 | | C | 4.69958900 | -0.32793100 | -2.12365400 |
| C | 3.30364200 | -0.88815000 | 0.73876900 | | C | 7.54776200 | -0.30405100 | -1.17817800 |
| H | 1.63398100 | -1.48802300 | 1.94570800 | | C | 5.89305000 | 0.01130300 | -3.03101000 |
| C | 4.05569500 | 0.19429000 | 0.28538000 | | C | 7.19116100 | -0.67516700 | -2.61415100 |
| H | 3.54146900 | -1.90303100 | 0.44586900 | | H | 8.46695400 | -0.80667800 | -0.86209800 |
| B | 4.73878200 | 2.80577100 | 0.20275000 | | H | 7.74531600 | 0.77447500 | -1.12560200 |
| H | 5.44046500 | 1.01605900 | -0.78187500 | | H | 5.62227700 | -0.25873800 | -4.05649500 |
| H | 5.54092700 | 2.45590200 | -0.70178100 | | H | 6.03814700 | 1.09950600 | -3.01948600 |
| C | 3.90639100 | 4.01017400 | -0.48782900 | | H | 7.99898900 | -0.36406100 | -3.28279200 |
| C | 3.70933000 | 4.25963400 | -1.83713700 | | H | 7.10514200 | -1.76217500 | -2.72365500 |
| N | 3.26116800 | 5.04175200 | 0.17797900 | | N | 5.15727600 | 0.00688900 | -0.68362700 |
| C | 2.93765900 | 5.44078500 | -1.99057500 | | C | 3.52116600 | 0.59338200 | -2.45667500 |
| H | 4.11360900 | 3.65626900 | -2.64017900 | | H | 2.61245500 | 0.28749400 | -1.93496400 |
| C | 2.68521200 | 5.90220100 | -0.72464900 | | H | 3.71654000 | 1.63600000 | -2.20294500 |
| H | 2.60281500 | 5.89547400 | -2.91242600 | | H | 3.33735900 | 0.53109300 | -3.53290200 |
| H | 2.14841800 | 6.77642100 | -0.38367200 | | C | 4.24023700 | -1.77316300 | -2.32495900 |
| C | 3.37468200 | 5.37369200 | 1.58617700 | | H | 3.47454000 | -2.05963300 | -1.60405100 |
| H | 3.34045400 | 4.48044200 | 2.20710200 | | H | 3.78380100 | -1.82984900 | -3.31686100 |
| H | 4.32280900 | 5.87774600 | 1.80082800 | | H | 5.04541800 | -2.50522900 | -2.29923400 |
| H | 2.54787700 | 6.03308400 | 1.86064000 | | C | 6.34437200 | -2.14211100 | 0.09712700 |
| C | 5.61882200 | 3.27098700 | 1.47186400 | | H | 7.27707800 | -2.46213700 | 0.56918600 |
| C | 5.59387200 | 2.88903300 | 2.80434600 | | H | 5.53764600 | -2.37752600 | 0.79229000 |
| N | 6.56249500 | 4.27726400 | 1.38663000 | | H | 6.21948400 | -2.73370300 | -0.80765500 |
| C | 6.52755800 | 3.67665600 | 3.52803100 | | C | 6.79116600 | 0.04684000 | 1.17624100 |
| H | 4.94501300 | 2.12437100 | 3.21152100 | | H | 6.81693400 | 1.13499800 | 1.09184900 |
| C | 7.11229300 | 4.52424700 | 2.61977900 | | H | 6.06862300 | -0.20430200 | 1.95502500 |
| H | 6.74318800 | 3.63286900 | 4.58654700 | | H | 7.77764900 | -0.29809700 | 1.49820700 |
| H | 7.87717700 | 5.27833800 | 2.74216400 | | | | | |

**1-TS6-p**

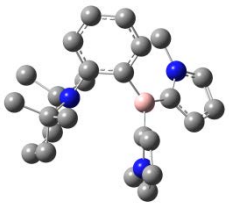


**Sum of electronic and thermal Enthalpies= -1162.571333**
**Sum of electronic and thermal Free Energies= -1162.65323**

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| H | 1.35447200 | 0.18991100 | 2.71385300 | | H | 1.88954300 | -1.94955600 | 1.54123400 |
| C | 2.14336600 | 0.14838800 | 1.96935500 | | C | 4.17942100 | 0.09391800 | 0.04148400 |
| C | 2.86011400 | 1.29462500 | 1.65049600 | | H | 3.65898900 | -1.97856000 | -0.16312900 |
| C | 2.43787800 | -1.04015700 | 1.31625700 | | B | 4.58445000 | 2.74966500 | 0.51389800 |
| C | 3.89716300 | 1.30951300 | 0.70284400 | | H | 5.64579000 | 1.91164200 | -0.86190800 |
| H | 2.58559200 | 2.22303000 | 2.14117100 | | H | 5.70121100 | 2.68702100 | -0.86440100 |
| C | 3.44110500 | -1.05393100 | 0.35657000 | | C | 3.65190500 | 3.83870800 | -0.09914600 |

| | | | |
|---|---|---|---|
| C | 2.33768000 | 3.68614900 | -0.53620800 |
| C | 1.85291700 | 4.93014800 | -0.98002200 |
| H | 1.79871500 | 2.74930700 | -0.51979000 |
| C | 2.88579700 | 5.82900600 | -0.81539100 |
| H | 0.87377400 | 5.15237100 | -1.37817700 |
| H | 2.93661800 | 6.88562400 | -1.03885700 |
| C | 5.79011900 | 3.22065800 | 1.44660100 |
| C | 7.15935300 | 3.24992400 | 1.23944900 |
| C | 7.77343600 | 3.91263300 | 2.33096400 |
| H | 7.66261400 | 2.85717700 | 0.36616700 |
| C | 6.76498300 | 4.27683400 | 3.18652400 |
| H | 8.82771600 | 4.10064200 | 2.47301000 |
| H | 6.79214100 | 4.78045500 | 4.14210300 |
| N | 3.95957700 | 5.18375000 | -0.28668100 |
| N | 5.57181300 | 3.86625800 | 2.64809300 |
| C | 5.22695300 | 5.84074500 | -0.01709700 |
| H | 5.43132700 | 5.89551300 | 1.05477000 |
| H | 6.05057600 | 5.30381900 | -0.48950100 |
| H | 5.18248000 | 6.85156300 | -0.42583400 |
| C | 4.29043100 | 4.05789300 | 3.29495400 |
| H | 3.54183200 | 4.36591100 | 2.56043900 |
| H | 3.95205100 | 3.14126700 | 3.78724800 |
| H | 4.38478700 | 4.84519800 | 4.04496500 |
| C | 6.46544100 | -0.68089800 | -0.56893200 |
| C | 4.75434900 | 0.00701300 | -2.38331600 |
| C | 7.58575100 | -0.18825300 | -1.50239700 |
| C | 5.93942400 | 0.44088600 | -3.26881000 |
| C | 7.22877900 | -0.31915800 | -2.97866800 |
| H | 8.50448600 | -0.74014800 | -1.27486700 |
| H | 7.78383000 | 0.86738900 | -1.27589500 |
| H | 5.65071200 | 0.32400600 | -4.31925500 |
| H | 6.11763800 | 1.51110200 | -3.10671400 |
| H | 8.04048500 | 0.07635700 | -3.59816100 |
| H | 7.12176100 | -1.37535500 | -3.25275700 |
| N | 5.21434200 | 0.04026000 | -0.95916700 |
| C | 6.83183300 | -0.29904700 | 0.87139400 |
| H | 7.82307300 | -0.70027600 | 1.10352400 |
| H | 6.85999400 | 0.78102800 | 1.01626800 |
| H | 6.12278100 | -0.71663200 | 1.59069700 |
| C | 6.40208300 | -2.22463500 | -0.60650100 |
| H | 5.61995200 | -2.60479500 | 0.05342300 |
| H | 6.24237100 | -2.63620900 | -1.60251700 |
| H | 7.35317000 | -2.62374100 | -0.23919500 |
| C | 4.20081900 | -1.34694800 | -2.87894800 |
| H | 3.79427900 | -1.21621200 | -3.88695600 |
| H | 4.95567100 | -2.13095100 | -2.93286700 |
| H | 3.38380600 | -1.69572700 | -2.24384500 |
| C | 3.62551400 | 1.03266000 | -2.57221300 |
| H | 2.71501800 | 0.72977200 | -2.04894400 |
| H | 3.89941100 | 2.02767100 | -2.21836000 |
| H | 3.39131900 | 1.10847800 | -3.63825400 |

**1-Int5-p**

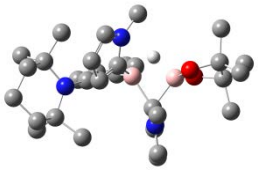


**Sum of electronic and thermal Enthalpies= -1161.425654**
**Sum of electronic and thermal Free Energies= -1161.507807**

| | | | |
|---|---|---|---|
| C | -2.47369400 | -2.73654100 | -0.72589200 |
| C | -1.14178300 | -3.07929000 | -0.52704500 |
| C | -0.20356900 | -2.08414800 | -0.27426100 |
| C | -0.56817500 | -0.73392200 | -0.19917500 |
| C | -1.91016400 | -0.37365300 | -0.45530300 |
| C | -2.83724800 | -1.39494000 | -0.70843100 |
| H | -3.21937900 | -3.50402000 | -0.90894300 |
| H | -0.83015500 | -4.11873400 | -0.56469900 |
| H | 0.83211500 | -2.36038600 | -0.11445300 |
| H | -3.87355200 | -1.12645400 | -0.90294400 |
| B | -2.43491200 | 1.11994100 | -0.49531800 |
| C | -2.56839500 | 1.91808400 | 0.83446200 |
| C | -3.22667000 | 1.45438600 | 1.96550200 |
| C | -3.33414500 | 2.51475500 | 2.89406400 |
| H | -3.60295200 | 0.44728400 | 2.08462400 |
| C | -2.72029300 | 3.60246200 | 2.31902700 |
| H | -3.79923500 | 2.48836900 | 3.86870900 |
| H | -2.54000500 | 4.59575200 | 2.70524200 |
| C | -3.04236000 | 1.75033600 | -1.76389400 |
| C | -3.77523500 | 2.94347000 | -1.79417200 |
| C | -4.22733100 | 3.18085500 | -3.09892600 |
| H | -3.96494700 | 3.55551200 | -0.92355000 |
| C | -3.77081300 | 2.12262100 | -3.86077600 |
| H | -4.81463500 | 4.01418800 | -3.45527900 |
| H | -3.90438400 | 1.91473300 | -4.91360200 |
| N | -2.28251000 | 3.25169100 | 1.07203100 |
| N | -3.06803000 | 1.26988900 | -3.07638600 |
| C | -1.45906300 | 4.11703400 | 0.25173000 |
| H | -1.93497100 | 5.09540000 | 0.14312100 |
| H | -0.46849100 | 4.25017800 | 0.69852200 |
| H | -1.34776100 | 3.67968300 | -0.73940800 |
| C | -2.57260300 | 0.00124800 | -3.58024200 |
| H | -1.68932700 | -0.30710700 | -3.03043600 |
| H | -3.32817300 | -0.78270700 | -3.47989800 |
| H | -2.31448300 | 0.11939600 | -4.63461800 |
| C | 0.88117000 | 0.25139500 | 1.57191100 |
| C | 1.29517100 | 0.79235600 | -0.89417400 |
| C | 1.27674600 | 1.69631700 | 1.92760900 |
| C | 1.75697600 | 2.20173700 | -0.47737000 |
| C | 2.28706600 | 2.28626800 | 0.94923100 |
| H | 1.67770800 | 1.71755500 | 2.94761800 |
| H | 0.36036600 | 2.29963100 | 1.92378700 |
| H | 2.51406700 | 2.55011600 | -1.18993100 |
| H | 0.89459100 | 2.87033200 | -0.57223400 |
| H | 2.49281100 | 3.33202200 | 1.20361600 |
| H | 3.24634900 | 1.76133000 | 1.03066700 |
| C | 2.06591500 | -0.69956300 | 1.87266700 |
| H | 2.22231200 | -0.73310100 | 2.95566300 |
| H | 1.85300900 | -1.71996100 | 1.54708300 |
| H | 3.00858000 | -0.38891600 | 1.42422600 |

| | | | |
|---|---|---|---|
| C | -0.25252100 | -0.17230100 | 2.51270900 |
| H | -1.14338300 | 0.43147200 | 2.35247000 |
| H | -0.51372700 | -1.22611100 | 2.38409500 |
| H | 0.07663000 | -0.03139200 | 3.54678300 |
| C | 2.51911100 | -0.10033800 | -1.21358100 |
| H | 2.99401400 | 0.24945700 | -2.13599800 |
| H | 3.28000600 | -0.08418000 | -0.43443800 |
| H | 2.21339100 | -1.13779200 | -1.37348100 |
| C | 0.53282100 | 0.94372300 | -2.21443300 |
| H | 0.30864300 | -0.03099500 | -2.65519700 |
| H | -0.39810800 | 1.50068500 | -2.08589800 |
| H | 1.15612200 | 1.49212900 | -2.92690700 |
| N | 0.38760800 | 0.27720400 | 0.16172500 |

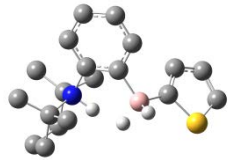
**1-Int6-p**



**Sum of electronic and thermal Enthalpies= -1572.996371**
**Sum of electronic and thermal Free Energies= -1573.10103**

| | | | |
|---|---|---|---|
| C | -1.69171000 | -2.12373500 | 0.71862200 |
| C | -0.40134200 | -1.61238900 | 0.66367300 |
| C | -0.11298500 | -0.24249200 | 0.50752600 |
| C | -1.22131700 | 0.62691000 | 0.34780700 |
| C | -2.51898300 | 0.09600500 | 0.42147600 |
| C | -2.76723400 | -1.25611800 | 0.61113800 |
| H | -1.84729300 | -3.19067700 | 0.84685400 |
| H | 0.41736600 | -2.31640600 | 0.76776600 |
| H | -3.35886600 | 0.76973000 | 0.31574300 |
| H | -3.78866700 | -1.62151600 | 0.66023900 |
| B | 1.45917700 | 0.16647800 | 0.57152700 |
| H | 1.99817000 | -0.94710300 | 0.14809000 |
| C | 2.06158100 | 0.17743400 | 2.17731200 |
| C | 1.20993100 | -0.15226800 | 3.25837700 |
| C | 1.60029000 | 0.54179600 | 4.39002100 |
| H | 0.38855000 | -0.84880900 | 3.17232800 |
| C | 2.70558300 | 1.30195600 | 4.01211300 |
| H | 1.15397500 | 0.51366600 | 5.37246600 |
| H | 3.32098500 | 1.96221400 | 4.60873300 |
| B | 2.70052300 | -1.13036500 | 1.30352800 |
| O | 4.07707500 | -1.04355000 | 0.99674000 |
| O | 2.38417900 | -2.43604400 | 1.74223800 |
| C | 4.64692000 | -2.34401500 | 1.20323400 |
| C | 3.62071200 | -3.00268100 | 2.18423900 |
| C | 4.70787200 | -3.05732200 | -0.14848400 |
| H | 5.27977500 | -2.44141200 | -0.84804900 |
| H | 5.19986800 | -4.03093500 | -0.06908100 |
| H | 3.70421400 | -3.20679800 | -0.55693500 |
| C | 6.05009300 | -2.17063800 | 1.76865800 |
| H | 6.69457400 | -1.69984300 | 1.02133100 |
| H | 6.04304500 | -1.53721800 | 2.65739600 |
| H | 6.48533600 | -3.14036800 | 2.03053400 |
| C | 3.84610200 | -2.58192000 | 3.64110300 |
| H | 2.97183900 | -2.87459400 | 4.22772200 |
| H | 4.73060600 | -3.06376600 | 4.06754800 |
| H | 3.96072900 | -1.49750800 | 3.73254500 |
| C | 3.52348400 | -4.51836200 | 2.08687800 |
| H | 4.49012200 | -4.98360400 | 2.30497600 |
| H | 2.79532500 | -4.88736000 | 2.81380800 |
| H | 3.19763300 | -4.83094300 | 1.09345200 |
| C | 2.14398800 | 1.26585000 | -0.34870800 |
| C | 2.26245300 | 2.63270000 | -0.18603900 |
| C | 2.93382800 | 3.17484200 | -1.30802000 |
| H | 1.88309100 | 3.18124900 | 0.66278800 |
| C | 3.20955100 | 2.11968400 | -2.14453500 |
| H | 3.17598600 | 4.21210800 | -1.48970800 |
| H | 3.70101900 | 2.08707000 | -3.10599400 |
| N | 2.98645900 | 1.10415400 | 2.71933300 |
| N | 2.73821200 | 0.97435000 | -1.56275700 |
| C | 2.82766700 | -0.33752100 | -2.16692600 |
| H | 1.83534800 | -0.79001300 | -2.25494400 |
| H | 3.25201400 | -0.23690600 | -3.16687000 |
| H | 3.47251300 | -0.99011400 | -1.57337200 |
| C | 4.16557000 | 1.68684100 | 2.08514800 |
| H | 4.48852400 | 1.04671300 | 1.27012500 |
| H | 3.94333300 | 2.67883300 | 1.69354800 |
| H | 4.95994100 | 1.74380700 | 2.83233300 |
| C | -1.37838700 | 2.41740900 | -1.34349100 |
| C | -1.36746900 | 2.96257700 | 1.18189300 |
| C | -0.83599100 | 3.83617900 | -1.59194900 |
| C | -0.87534900 | 4.37687100 | 0.81608600 |
| C | -1.32401700 | 4.84300200 | -0.56090500 |
| H | -1.11945800 | 4.14454800 | -2.60477100 |
| H | 0.25752900 | 3.79191800 | -1.55824700 |
| H | -1.20988100 | 5.07073100 | 1.59561600 |
| H | 0.21911200 | 4.37961300 | 0.83558500 |
| H | -0.90790900 | 5.83414600 | -0.77193400 |
| H | -2.41509600 | 4.94980800 | -0.60203500 |
| C | -0.63949000 | 1.47352000 | -2.30307600 |
| H | -0.81505100 | 1.80074100 | -3.33294700 |
| H | 0.43267400 | 1.49459600 | -2.10987500 |
| H | -0.99672100 | 0.44400900 | -2.21251300 |
| C | -2.87401700 | 2.37318400 | -1.74428300 |
| H | -2.98102100 | 2.74512500 | -2.76869400 |
| H | -3.26165200 | 1.35249000 | -1.73081600 |
| H | -3.50969500 | 2.98959600 | -1.10691800 |
| C | -0.58077500 | 2.51042700 | 2.41766000 |
| H | -0.93789800 | 1.54725400 | 2.79027000 |
| H | 0.48249500 | 2.41074400 | 2.19015500 |
| H | -0.69674300 | 3.24501300 | 3.22121400 |
| C | -2.85265700 | 3.04910000 | 1.61383300 |
| H | -3.21633100 | 2.08764000 | 1.98278200 |
| H | -2.94754100 | 3.76736200 | 2.43517100 |
| H | -3.51352600 | 3.38238600 | 0.81214600 |
| N | -1.06258200 | 2.03004900 | 0.06417300 |

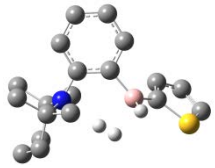
**1-Int1-t**



**Sum of electronic and thermal Enthalpies= -1218.029832**
**Sum of electronic and thermal Free Energies= -1218.098155**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 1.00558300 | 0.36168900 | 2.55301800 | C | 6.32698400 | 0.35420900 | -2.79716200 |
| C | 1.88560500 | 0.31325100 | 1.91871700 | C | 7.61783500 | -0.23042800 | -2.23524900 |
| C | 2.54318600 | 1.48005100 | 1.55341000 | H | 8.69880600 | -0.21504900 | -0.35063800 |
| C | 2.35236400 | -0.92282400 | 1.47429500 | H | 7.85583600 | 1.28131500 | -0.72682400 |
| C | 3.68426800 | 1.47820900 | 0.73473000 | H | 6.19502200 | 0.08152600 | -3.84858700 |
| H | 2.16641400 | 2.43787700 | 1.90032900 | H | 6.38703600 | 1.44962800 | -2.76169100 |
| C | 3.47783900 | -0.97665600 | 0.66411400 | H | 8.46981200 | 0.13627400 | -2.81483300 |
| H | 1.84559700 | -1.84008800 | 1.75529100 | H | 7.62625800 | -1.32218300 | -2.33222000 |
| C | 4.11306200 | 0.21405500 | 0.31323100 | N | 5.31377400 | 0.22977000 | -0.54867100 |
| H | 3.84315900 | -1.93504600 | 0.31668600 | C | 3.88363400 | 0.78097800 | -2.49076200 |
| B | 4.41998400 | 2.87720700 | 0.34028400 | H | 2.94908000 | 0.45942900 | -2.02734700 |
| H | 4.85059500 | 3.39991100 | 1.35510600 | H | 4.02878800 | 1.83878500 | -2.25734400 |
| H | 5.46346000 | 1.27539100 | -0.57322100 | H | 3.78160800 | 0.67909000 | -3.57460900 |
| H | 5.43404300 | 2.68882000 | -0.37551100 | C | 4.72731000 | -1.55087100 | -2.31497500 |
| C | 3.43307600 | 3.84779100 | -0.48446700 | H | 5.53131000 | -2.24395800 | -2.07184300 |
| C | 2.20014800 | 3.61349700 | -1.04008700 | H | 3.82172200 | -1.85964800 | -1.79193100 |
| S | 3.90123900 | 5.48474900 | -0.84592700 | H | 4.52942900 | -1.64534300 | -3.38616700 |
| C | 1.63863000 | 4.72287100 | -1.74525100 | C | 6.72089800 | 0.47607300 | 1.47104200 |
| H | 1.69630000 | 2.65755600 | -0.93772400 | H | 6.59751000 | 1.55594200 | 1.35812200 |
| C | 2.45314100 | 5.81380100 | -1.72965400 | H | 5.97410800 | 0.12155600 | 2.18380700 |
| H | 0.67277400 | 4.70397600 | -2.23767700 | H | 7.71356100 | 0.28189000 | 1.88648800 |
| H | 2.28182200 | 6.78313900 | -2.17652700 | C | 6.65441800 | -1.76126400 | 0.38810200 |
| C | 6.61353600 | -0.25551200 | 0.12694000 | H | 6.66532300 | -2.36572500 | -0.51787200 |
| C | 5.06426800 | -0.08574800 | -2.03890800 | H | 7.57964700 | -1.97241700 | 0.93120800 |
| C | 7.77518500 | 0.18784200 | -0.77762000 | H | 5.82765600 | -2.08269600 | 1.02208000 |

**1-TS2-t**

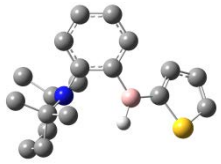


**Sum of electronic and thermal Enthalpies= -1217.999145**
**Sum of electronic and thermal Free Energies= -1218.070984**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 1.27846400 | 0.58185300 | 2.69362200 | H | 1.90662900 | 2.98916600 | -1.03376600 |
| C | 2.06531400 | 0.46649300 | 1.95479500 | C | 2.83043500 | 6.19257400 | -1.22387500 |
| C | 2.77942500 | 1.57558400 | 1.51834300 | H | 0.99676100 | 5.29587200 | -1.93836200 |
| C | 2.36597300 | -0.78490500 | 1.43344500 | H | 2.70774400 | 7.23530700 | -1.48230500 |
| C | 3.81147000 | 1.47943300 | 0.57080000 | C | 6.42427400 | -0.50915400 | -0.48308800 |
| H | 2.52831400 | 2.55219800 | 1.92451000 | C | 4.64875000 | -0.18688400 | -2.34978300 |
| C | 3.37356900 | -0.90545300 | 0.48420400 | C | 7.50418600 | -0.20824600 | -1.53884000 |
| H | 1.82103200 | -1.66557700 | 1.75867400 | C | 5.80772500 | 0.11127700 | -3.31957900 |
| C | 4.10330100 | 0.20523400 | 0.04269200 | C | 7.09788800 | -0.60879000 | -2.95054500 |
| H | 3.60174000 | -1.88297500 | 0.07797800 | H | 8.43101200 | -0.71013900 | -1.24066900 |
| B | 4.52792200 | 2.86412800 | 0.27681900 | H | 7.70847400 | 0.86998500 | -1.52652100 |
| H | 5.56864600 | 1.97816100 | -1.10847200 | H | 5.48905400 | -0.15167300 | -4.33410000 |
| H | 5.68071700 | 2.74281000 | -1.12829800 | H | 5.99483700 | 1.19243000 | -3.31656500 |
| C | 3.68755000 | 4.00512600 | -0.37170200 | H | 7.89019800 | -0.34397700 | -3.65817000 |
| C | 2.44659600 | 3.92667600 | -0.96262500 | H | 6.96840200 | -1.69512100 | -3.02438100 |
| S | 4.24598400 | 5.65038700 | -0.41851600 | N | 5.13006500 | 0.06653800 | -0.95734300 |
| C | 1.95423100 | 5.16736800 | -1.44868700 | C | 6.83373200 | 0.20242700 | 0.81590700 |

| | | | |
|---|---|---|---|
| H | 6.87285700 | 1.28591400 | 0.68310100 |
| H | 6.14380700 | -0.01740100 | 1.63405500 |
| H | 7.82984500 | -0.13959600 | 1.11273900 |
| C | 6.40035800 | -2.02271100 | -0.18002700 |
| H | 5.66036100 | -2.25994100 | 0.58711100 |
| H | 6.19195800 | -2.63246700 | -1.06008300 |
| H | 7.37795000 | -2.32857100 | 0.20638700 |
| C | 4.10140600 | -1.60483200 | -2.62367400 |
| H | 3.77398700 | -1.66728100 | -3.66655800 |
| H | 4.84328400 | -2.38870800 | -2.46762900 |
| H | 3.23277300 | -1.82262700 | -1.99935600 |
| C | 3.51155000 | 0.79847100 | -2.66501700 |
| H | 2.61960100 | 0.58832800 | -2.06904600 |
| H | 3.80754200 | 1.83440600 | -2.48302200 |
| H | 3.24042100 | 0.70410500 | -3.72085100 |
| H | 5.48647800 | 3.16823500 | 0.93341700 |

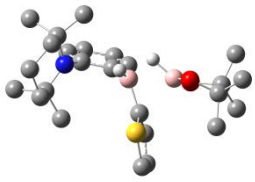
**1-Int2-t**



**Sum of electronic and thermal Enthalpies= -1216.848376**
**Sum of electronic and thermal Free Energies= -1216.921431**

| | | | |
|---|---|---|---|
| C | -2.65831200 | -2.74788800 | 1.21237000 |
| C | -1.31158900 | -2.99819600 | 1.44811200 |
| C | -0.35435800 | -2.04866600 | 1.10118200 |
| C | -0.72781500 | -0.82893300 | 0.52944100 |
| C | -2.09118200 | -0.56854100 | 0.27836700 |
| C | -3.03550900 | -1.54870800 | 0.61753500 |
| H | -3.40805600 | -3.48471700 | 1.48253300 |
| H | -1.00021500 | -3.93718200 | 1.89573400 |
| H | 0.69495500 | -2.26098500 | 1.26937900 |
| H | -4.08829500 | -1.35685400 | 0.42825700 |
| B | -2.53260100 | 0.79345700 | -0.34750800 |
| H | -2.07804200 | 1.82661600 | 0.04996100 |
| C | -3.59826300 | 0.85525800 | -1.45471600 |
| C | -4.14349400 | -0.16448800 | -2.21241800 |
| C | -5.07495300 | 0.26979700 | -3.18579900 |
| H | -3.85771600 | -1.20016600 | -2.06715900 |
| C | -5.23714900 | 1.63090500 | -3.17155300 |
| H | -5.60181100 | -0.38732700 | -3.86647500 |
| H | -5.88788400 | 2.22195500 | -3.80139000 |
| C | 0.90204700 | 0.88756500 | 1.27609000 |
| C | 0.90779400 | -0.01215900 | -1.14712900 |
| C | 1.43440200 | 2.22272800 | 0.72440200 |
| C | 1.47776800 | 1.34573000 | -1.59741900 |
| C | 2.29325600 | 2.05051300 | -0.52158700 |
| H | 1.99296600 | 2.73367000 | 1.51677900 |
| H | 0.57211700 | 2.85307800 | 0.47388800 |
| H | 2.07380300 | 1.19238400 | -2.50410700 |
| H | 0.63329200 | 1.99092500 | -1.87082200 |
| H | 2.62728300 | 3.02727500 | -0.88721000 |
| H | 3.20260600 | 1.48313400 | -0.28906000 |
| N | 0.22746600 | 0.17177400 | 0.16072600 |
| C | -0.11573500 | -0.44303000 | -2.20842400 |
| H | -0.54412100 | -1.42598000 | -1.99634500 |
| H | -0.93505800 | 0.27722200 | -2.28883700 |
| H | 0.38068500 | -0.49380200 | -3.18213600 |
| C | 2.02012500 | -1.08465500 | -1.13912100 |
| H | 2.86775500 | -0.81197300 | -0.50938300 |
| H | 1.62847900 | -2.04388900 | -0.79008400 |
| H | 2.40188600 | -1.23358200 | -2.15448700 |
| C | 2.05100200 | 0.12330700 | 1.97444500 |
| H | 2.43841600 | 0.72981300 | 2.79974800 |
| H | 1.69756400 | -0.81675900 | 2.40360300 |
| H | 2.88753900 | -0.09585900 | 1.31040500 |
| C | -0.13734400 | 1.21415800 | 2.35982600 |
| H | 0.32252800 | 1.85686900 | 3.11682000 |
| H | -0.99404100 | 1.74078500 | 1.93532600 |
| H | -0.50045200 | 0.31279700 | 2.86017900 |
| S | -4.25393200 | 2.37693300 | -1.98717400 |

**1-TS3-t**

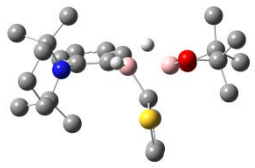


**Sum of electronic and thermal Enthalpies= -1628.423409**
**Sum of electronic and thermal Free Energies= -1628.51348**

| | | | |
|---|---|---|---|
| C | -2.08410300 | -1.98101300 | 1.26054200 |
| C | -0.74171500 | -1.62530600 | 1.18097500 |
| C | -0.33005300 | -0.35423800 | 0.75479200 |
| C | -1.32920600 | 0.57741800 | 0.39816700 |
| C | -2.67753800 | 0.20827500 | 0.47833100 |
| C | -3.05952100 | -1.05781400 | 0.90724600 |
| H | -2.36350200 | -2.97614500 | 1.59378400 |
| H | 0.00813600 | -2.36357400 | 1.45170000 |
| H | -3.43720500 | 0.92991600 | 0.20019100 |
| H | -4.11257900 | -1.31676100 | 0.96397700 |
| B | 1.22042100 | 0.04372700 | 0.69459300 |
| H | 1.70538500 | -1.04419100 | -0.01764200 |

| | | | |
|---|---|---|---|
| C | 1.99319300 | 0.22039000 | 2.09800100 |
| C | 1.66925300 | -0.26817600 | 3.34555400 |
| C | 2.36827600 | 0.35081300 | 4.41244800 |
| H | 0.93733400 | -1.05656900 | 3.47598100 |
| C | 3.22270400 | 1.32572000 | 3.97048800 |
| H | 2.23814600 | 0.09661500 | 5.45708300 |
| H | 3.86510600 | 1.95797500 | 4.56797300 |
| H | 1.58930200 | 0.85212300 | -0.10734900 |
| B | 2.56407300 | -1.46421600 | 0.80468700 |
| O | 3.86837300 | -1.29415200 | 0.44466100 |
| O | 2.30116900 | -2.63119900 | 1.47255600 |
| C | 4.62033200 | -2.26598700 | 1.21082700 |
| C | 3.54241400 | -3.37507500 | 1.50077300 |
| C | 5.79638200 | -2.73086800 | 0.36432000 |
| H | 6.48988200 | -1.90030100 | 0.21289900 |
| H | 6.33513000 | -3.53774800 | 0.87103100 |
| H | 5.47174600 | -3.08616900 | -0.61471700 |
| C | 5.12760400 | -1.56941600 | 2.47327200 |
| H | 5.70852100 | -0.69205700 | 2.18030700 |
| H | 4.30695100 | -1.23224500 | 3.11111100 |
| H | 5.77134400 | -2.23425800 | 3.05585700 |
| C | 3.67250700 | -4.04383300 | 2.86124700 |
| H | 2.89015700 | -4.79820200 | 2.97648900 |
| H | 4.64281900 | -4.54143100 | 2.95364900 |
| H | 3.56980200 | -3.31889600 | 3.67003100 |
| C | 3.44171100 | -4.42602000 | 0.39576600 |
| H | 4.31538400 | -5.08347500 | 0.38625400 |
| H | 2.55108400 | -5.03433200 | 0.56980800 |
| H | 3.34477500 | -3.95665000 | -0.58680100 |
| C | -1.00584700 | 2.14886000 | -1.49694000 |
| C | -1.11333900 | 2.99578000 | 0.93447800 |
| C | -0.03490700 | 3.30277300 | -1.81020700 |
| C | -0.13380100 | 4.11662100 | 0.54035500 |
| C | -0.24881000 | 4.52368900 | -0.92366400 |
| H | -0.13177800 | 3.56892400 | -2.86927900 |
| H | 0.98641900 | 2.93218900 | -1.65776900 |
| H | -0.29687100 | 4.97883300 | 1.19742400 |
| H | 0.88416400 | 3.75152400 | 0.72644200 |
| H | 0.49563400 | 5.29176600 | -1.15916400 |
| H | -1.22873700 | 4.97575600 | -1.12012300 |
| N | -0.95100600 | 1.88761200 | -0.03754500 |
| C | -0.51498300 | 0.90964500 | -2.26318200 |
| H | 0.47004200 | 0.59376000 | -1.91624900 |
| H | -1.20573800 | 0.06895000 | -2.15950700 |
| H | -0.44010400 | 1.15535900 | -3.32703500 |
| C | -2.41061100 | 2.47600500 | -2.05696900 |
| H | -2.36184800 | 2.54496000 | -3.14896600 |
| H | -3.12274700 | 1.68487500 | -1.80956000 |
| H | -2.81101800 | 3.42175800 | -1.69079900 |
| C | -2.54695600 | 3.56551400 | 1.05482700 |
| H | -3.25732700 | 2.77857100 | 1.32044000 |
| H | -2.57638500 | 4.31590300 | 1.85187900 |
| H | -2.89763300 | 4.04798400 | 0.14230900 |
| C | -0.72058600 | 2.51222400 | 2.33787000 |
| H | 0.28668600 | 2.09533700 | 2.34771800 |
| H | -0.74500000 | 3.36089700 | 3.02842100 |
| H | -1.40957300 | 1.75121700 | 2.71355000 |
| S | 3.17545800 | 1.48577800 | 2.26617000 |

**1-Int3-t**

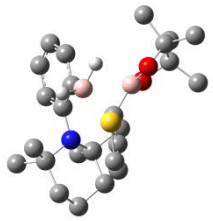


**Sum of electronic and thermal Enthalpies= -1628.4229**
**Sum of electronic and thermal Free Energies= -1628.515363**

| | | | |
|---|---|---|---|
| C | -2.05399500 | -1.91103600 | 1.35145500 |
| C | -0.72203400 | -1.51630500 | 1.28886500 |
| C | -0.34085300 | -0.23364800 | 0.86581100 |
| C | -1.35945800 | 0.66295100 | 0.47611500 |
| C | -2.69765400 | 0.25242700 | 0.53756600 |
| C | -3.04986300 | -1.01889100 | 0.97552100 |
| H | -2.30915300 | -2.91229800 | 1.68578000 |
| H | 0.04883900 | -2.22690300 | 1.57529300 |
| H | -3.47411200 | 0.94465900 | 0.23295300 |
| H | -4.09586100 | -1.30789900 | 1.01621600 |
| B | 1.20220500 | 0.17962900 | 0.81599100 |
| H | 1.79663600 | -0.83470600 | 0.28373900 |
| C | 1.93891900 | 0.38434300 | 2.32289700 |
| C | 1.35568600 | 0.06737500 | 3.54326400 |
| C | 1.76629400 | 0.87971000 | 4.61614600 |
| H | 0.64826800 | -0.74787600 | 3.63387600 |
| C | 2.66616300 | 1.83748100 | 4.21197100 |
| H | 1.41733700 | 0.77300200 | 5.63506600 |
| H | 3.13653300 | 2.59142400 | 4.82937600 |
| H | 1.57168200 | 1.07080100 | 0.11197500 |
| B | 2.56871800 | -0.98306400 | 1.38730500 |
| O | 3.89204400 | -0.85677000 | 0.95857900 |
| O | 2.33337000 | -2.22742200 | 1.99059200 |
| C | 4.61441100 | -1.91298400 | 1.61224700 |
| C | 3.51358300 | -3.01515700 | 1.75987600 |
| C | 5.79714500 | -2.30851300 | 0.74072100 |
| H | 6.52107100 | -1.49053700 | 0.70470400 |
| H | 6.29783400 | -3.19018600 | 1.15350200 |
| H | 5.48168500 | -2.52776100 | -0.28046900 |
| C | 5.10550600 | -1.38503500 | 2.96379600 |
| H | 5.68932400 | -0.47728900 | 2.79256400 |
| H | 4.26759900 | -1.13039600 | 3.62021700 |
| H | 5.73909100 | -2.11547800 | 3.47487200 |
| C | 3.70873000 | -3.95849200 | 2.93765800 |
| H | 2.90532500 | -4.69937100 | 2.95665400 |
| H | 4.66118500 | -4.49069600 | 2.84847500 |
| H | 3.69544200 | -3.41721600 | 3.88510400 |
| C | 3.29698900 | -3.81024400 | 0.47013700 |
| H | 4.11719700 | -4.50907700 | 0.28250900 |
| H | 2.36957500 | -4.38103400 | 0.56170300 |
| H | 3.20396800 | -3.14339700 | -0.39155200 |
| C | -1.05684800 | 2.18018100 | -1.45943600 |
| C | -1.25083900 | 3.10071800 | 0.94316000 |
| C | -0.17094600 | 3.39279700 | -1.80019100 |
| C | -0.35772500 | 4.27852700 | 0.51115800 |
| C | -0.49587500 | 4.62494400 | -0.96575000 |
| H | -0.26675800 | 3.60926500 | -2.87032600 |
| H | 0.87327000 | 3.11111200 | -1.61602600 |

| | | | |
|---|---|---|---|
| H | -0.58920600 | 5.14675700 | 1.13913200 |
| H | 0.68548500 | 4.00112000 | 0.70922200 |
| H | 0.18456800 | 5.44320200 | -1.22489500 |
| H | -1.50826700 | 4.98565100 | -1.18503100 |
| N | -1.01594500 | 1.97334400 | 0.00993800 |
| C | -0.45110700 | 0.95737600 | -2.16708400 |
| H | 0.55217800 | 0.74539600 | -1.79358500 |
| H | -1.06553100 | 0.06345000 | -2.03428100 |
| H | -0.38188700 | 1.16341800 | -3.23974500 |
| C | -2.46972100 | 2.38170300 | -2.05677600 |
| H | -2.39920900 | 2.45841800 | -3.14705200 |
| H | -3.11503800 | 1.52965500 | -1.82965400 |
| H | -2.96017300 | 3.28726800 | -1.69792400 |
| C | -0.80953400 | 2.68814100 | 2.35457000 |
| H | 0.23157400 | 2.36359500 | 2.35291300 |
| H | -0.90002800 | 3.54588100 | 3.02836200 |
| H | -1.42398800 | 1.87713300 | 2.75384400 |
| C | -2.71949900 | 3.57364400 | 1.05814400 |
| H | -2.79192600 | 4.36189200 | 1.81509100 |
| H | -3.11376400 | 3.98026300 | 0.12623300 |
| H | -3.36955200 | 2.75543900 | 1.37700800 |
| S | 3.01022300 | 1.74785700 | 2.54786300 |

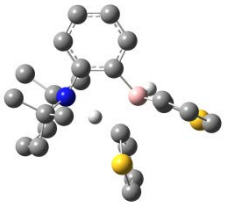
**1-TS4-t**



**Sum of electronic and thermal Enthalpies= -1628.403204**
**Sum of electronic and thermal Free Energies= -1628.493771**

| | | | |
|---|---|---|---|
| C | -1.91016500 | -1.50557300 | 0.60458400 |
| C | -1.07076100 | -0.42679500 | 0.23815800 |
| C | -0.15557700 | -0.67991600 | -0.80508800 |
| C | -0.07970100 | -1.87733400 | -1.50153100 |
| C | -0.96532500 | -2.89488600 | -1.18128000 |
| C | -1.86410000 | -2.69320800 | -0.14431900 |
| H | 0.51938100 | 0.11841500 | -1.10194300 |
| H | 0.65330500 | -2.00251800 | -2.29281700 |
| H | -0.96056300 | -3.83594200 | -1.72278800 |
| H | -2.55944700 | -3.48490400 | 0.09770500 |
| B | -1.06644700 | 1.14937200 | 0.56793200 |
| H | -1.87495000 | 1.79345100 | -0.03966900 |
| H | 0.04641600 | 1.59015200 | 0.29791200 |
| C | 2.54806000 | 2.00436400 | 2.03333700 |
| C | 2.25271200 | 0.64743600 | 2.76385700 |
| O | 1.25401400 | 2.64189300 | 2.04432000 |
| O | 0.88115400 | 0.39800600 | 2.40812500 |
| B | 0.33096600 | 1.61222000 | 2.05010500 |
| C | 3.53713200 | 2.91252700 | 2.74826600 |
| H | 3.67715200 | 3.83093500 | 2.17260300 |
| H | 3.17822400 | 3.18651000 | 3.74151600 |
| H | 4.50917600 | 2.41914400 | 2.84768900 |
| C | 2.96524800 | 1.81260700 | 0.57414700 |
| H | 2.93432200 | 2.78072000 | 0.06848100 |
| H | 3.97951000 | 1.41065800 | 0.50000400 |
| H | 2.28644500 | 1.13346500 | 0.05212200 |
| C | 3.09319400 | -0.53116000 | 2.29456500 |
| H | 4.15797800 | -0.33827600 | 2.45990300 |
| H | 2.81536600 | -1.42595800 | 2.85766500 |
| H | 2.92740700 | -0.73651300 | 1.23603800 |
| C | 2.30255500 | 0.76706200 | 4.28767400 |
| H | 1.88191200 | -0.14219600 | 4.72473000 |
| H | 3.32731600 | 0.88458400 | 4.65112400 |
| H | 1.70870000 | 1.61812000 | 4.63273800 |
| C | -1.22888800 | 1.89821300 | 2.25799000 |
| C | -1.98882800 | 1.23431300 | 3.21623900 |
| C | -2.94392400 | 2.03237900 | 3.86575700 |
| H | -1.84302600 | 0.18259600 | 3.39625900 |
| C | -2.91054900 | 3.32985800 | 3.40813400 |
| H | -3.62422800 | 1.67987500 | 4.63018600 |
| H | -3.53728700 | 4.14830800 | 3.73871800 |
| S | -1.73404400 | 3.58382800 | 2.21070400 |
| C | -4.21981700 | -1.14219700 | 1.43979200 |
| C | -2.46214400 | -2.42386900 | 2.83979900 |
| C | -4.97419100 | -0.85800500 | 2.75205900 |
| C | -3.26211800 | -2.03474500 | 4.10042900 |
| C | -4.75512400 | -1.90910200 | 3.83026600 |
| H | -6.03991800 | -0.74987200 | 2.52222400 |
| H | -4.63527000 | 0.11050100 | 3.13550500 |
| H | -3.06729400 | -2.78137700 | 4.87756800 |
| H | -2.89400500 | -1.08078800 | 4.49589900 |
| H | -5.28393000 | -1.62500400 | 4.74672500 |
| H | -5.17156000 | -2.87507700 | 3.52147500 |
| N | -2.79272100 | -1.45004400 | 1.74932400 |
| C | -0.96099700 | -2.32016100 | 3.16011600 |
| H | -0.74117400 | -2.92424500 | 4.04669900 |
| H | -0.35350100 | -2.69740000 | 2.33410300 |
| H | -0.62957900 | -1.29754100 | 3.34569300 |
| C | -2.73168800 | -3.92993400 | 2.56987500 |
| H | -3.74372900 | -4.13621800 | 2.22109900 |
| H | -2.02772500 | -4.33969900 | 1.84494200 |
| H | -2.58714300 | -4.48510500 | 3.50244300 |
| C | -4.27852900 | 0.14243600 | 0.60165700 |
| H | -3.78695200 | 0.96938100 | 1.11727700 |
| H | -3.79807200 | 0.01535800 | -0.37103700 |
| H | -5.32490700 | 0.41462900 | 0.43055500 |
| C | -4.97136100 | -2.23024100 | 0.63843900 |
| H | -5.06264500 | -3.17626100 | 1.17447400 |
| H | -5.98583500 | -1.88176300 | 0.41894600 |
| H | -4.47860300 | -2.42219200 | -0.31714300 |

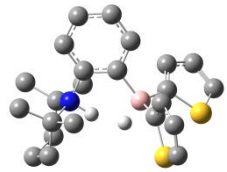
**1-TS5-t**



**Sum of electronic and thermal Enthalpies= -1769.704985**
**Sum of electronic and thermal Free Energies= -1769.781852**

| | | | |
|---|---|---|---|
| C | 1.01544000 | 0.51292600 | 0.52061700 |
| C | 2.01595100 | 1.46943600 | 0.60121600 |
| C | 1.32972200 | -0.77702000 | 0.10517000 |
| C | 3.35802800 | 1.19836300 | 0.28129600 |
| C | 2.64284900 | -1.08363700 | -0.21897400 |
| H | 0.56180000 | -1.54046900 | 0.03157700 |
| C | 3.64723800 | -0.11141300 | -0.12980900 |
| B | 4.36337400 | 2.46658500 | 0.31068700 |
| H | 5.64222200 | 0.91635500 | -0.14261100 |
| C | 6.11240000 | 2.07354500 | 0.14097900 |
| C | 6.81352900 | 2.73001600 | -0.87565500 |
| C | 8.09592600 | 3.19718900 | -0.54159900 |
| H | 6.37099000 | 2.88764200 | -1.85211200 |
| C | 8.40950300 | 2.90680300 | 0.76487500 |
| H | 8.75126500 | 3.73487800 | -1.21465900 |
| H | 9.32271300 | 3.15674600 | 1.28899200 |
| H | -0.00768900 | 0.77121000 | 0.77670100 |
| H | 2.87818300 | -2.08710200 | -0.54657100 |
| H | 1.76103600 | 2.47401000 | 0.92598600 |
| H | 4.17612700 | 3.12967500 | -0.68980400 |
| C | 4.23969500 | 3.32538700 | 1.65524300 |
| C | 3.88957200 | 2.92777600 | 2.92041900 |
| C | 4.00152300 | 3.94813000 | 3.91232200 |
| H | 3.55507300 | 1.91741900 | 3.13238000 |
| C | 4.44028500 | 5.12996400 | 3.39387900 |
| H | 3.76351700 | 3.80660600 | 4.96029900 |
| H | 4.59802300 | 6.06714800 | 3.90913400 |
| C | 5.71855300 | -1.37806000 | 0.50237800 |
| C | 5.30524000 | -0.60059100 | -1.94429100 |
| C | 7.23172000 | -1.30628600 | 0.21849800 |
| C | 6.83246800 | -0.56610800 | -2.14132700 |
| C | 7.57897100 | -1.55203600 | -1.24722100 |
| H | 7.73465100 | -2.03743900 | 0.86025100 |
| H | 7.60857500 | -0.32246100 | 0.51098500 |
| H | 7.04408400 | -0.76733300 | -3.19700600 |
| H | 7.19783500 | 0.44402700 | -1.93220300 |
| H | 8.65725100 | -1.43370500 | -1.39305800 |
| H | 7.34499700 | -2.58435600 | -1.53184600 |
| C | 5.41863900 | -0.90161200 | 1.93326000 |
| H | 4.39347300 | -1.14660200 | 2.22008600 |
| H | 6.09907600 | -1.40449100 | 2.62614900 |
| H | 5.54176300 | 0.17244000 | 2.06309400 |
| C | 5.27492200 | -2.85434700 | 0.45392300 |
| H | 4.20744400 | -2.96843900 | 0.64023700 |
| H | 5.52586300 | -3.36410200 | -0.47437400 |
| H | 5.79625000 | -3.37933000 | 1.26042500 |
| C | 4.73545900 | -1.87754400 | -2.59169000 |
| H | 4.89916400 | -1.80208700 | -3.67105100 |
| H | 5.21478000 | -2.79624400 | -2.25829100 |
| H | 3.65992900 | -1.96515500 | -2.43666400 |
| C | 4.65609800 | 0.57443400 | -2.69200600 |
| H | 3.57109100 | 0.45844700 | -2.74086100 |
| H | 4.85476600 | 1.53678500 | -2.22431300 |
| H | 5.04416000 | 0.59937000 | -3.71460900 |
| N | 5.03566700 | -0.42578400 | -0.46172700 |
| S | 4.70576300 | 4.99834200 | 1.69346400 |
| S | 7.15273300 | 2.08922300 | 1.56292300 |

**1-Int4-t**

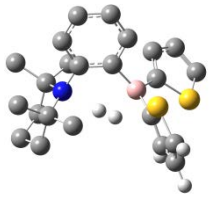


**Sum of electronic and thermal Enthalpies= -1769.746554**
**Sum of electronic and thermal Free Energies= -1769.826321**

| | | | |
|---|---|---|---|
| H | 1.31023100 | 0.67066600 | 2.67196500 |
| C | 2.10903000 | 0.54171000 | 1.94810600 |
| C | 2.82487200 | 1.64425200 | 1.50024700 |
| C | 2.41004500 | -0.72923300 | 1.46505200 |
| C | 3.87227400 | 1.53717000 | 0.57161200 |
| H | 2.56540800 | 2.63428500 | 1.86384700 |
| C | 3.42869400 | -0.88375100 | 0.53444100 |
| H | 1.85477900 | -1.59703100 | 1.80500600 |
| C | 4.13580400 | 0.24089800 | 0.11241100 |
| H | 3.65803000 | -1.87058300 | 0.15299700 |
| B | 4.69806200 | 2.86904500 | 0.10083800 |
| H | 5.48649000 | 1.15684400 | -0.92707100 |
| H | 5.47325700 | 2.59514500 | -0.84693200 |
| C | 3.67124100 | 3.97492600 | -0.48505900 |
| C | 2.38739600 | 3.81715100 | -0.94608800 |
| S | 4.14497500 | 5.63353300 | -0.71318400 |
| C | 1.79222700 | 5.00187500 | -1.47675200 |
| H | 1.86985500 | 2.86458100 | -0.89643800 |
| C | 2.63283300 | 6.07185800 | -1.42016700 |
| H | 0.78525300 | 5.05158100 | -1.87569900 |
| H | 2.44425300 | 7.08796700 | -1.73759600 |
| C | 5.66036000 | 3.39093700 | 1.29734200 |

| | | | |
|---|---|---|---|
| C | 5.55985600 | 3.26135500 | 2.65817000 |
| S | 7.13697100 | 4.23923500 | 0.92689400 |
| C | 6.63787900 | 3.84143700 | 3.39500200 |
| H | 4.72973800 | 2.74752800 | 3.13072000 |
| C | 7.57544000 | 4.41065400 | 2.58776700 |
| H | 6.70934300 | 3.83010800 | 4.47678200 |
| H | 8.48431100 | 4.92120200 | 2.87374100 |
| C | 6.53636300 | -0.50511500 | -0.36803900 |
| C | 4.77643000 | -0.11841600 | -2.33812400 |
| C | 7.62626500 | -0.13080200 | -1.38534500 |
| C | 5.98105800 | 0.23119000 | -3.22718900 |
| C | 7.27088200 | -0.47750200 | -2.82691700 |
| H | 8.55118600 | -0.62881800 | -1.07921000 |
| H | 7.81127400 | 0.94861000 | -1.30906000 |
| H | 5.71041800 | -0.00292800 | -4.26140400 |
| H | 6.13966100 | 1.31630600 | -3.18159000 |
| H | 8.08102300 | -0.16156600 | -3.49021600 |
| H | 7.17405500 | -1.56172800 | -2.95435100 |
| N | 5.22707000 | 0.13845100 | -0.87972100 |
| C | 3.63251300 | 0.85691500 | -2.63926300 |
| H | 2.72435700 | 0.59219200 | -2.09409700 |
| H | 3.88607200 | 1.89156300 | -2.39646500 |
| H | 3.41694300 | 0.80189400 | -3.70978800 |
| C | 4.27893200 | -1.54023400 | -2.59771600 |
| H | 3.46746100 | -1.81355900 | -1.92275600 |
| H | 3.87347900 | -1.56189600 | -3.61283100 |
| H | 5.05776500 | -2.29938100 | -2.54531500 |
| C | 6.86726200 | 0.14287500 | 0.97932100 |
| H | 7.85572900 | -0.20649800 | 1.28982400 |
| H | 6.89578300 | 1.23280100 | 0.91964000 |
| H | 6.14657400 | -0.13433600 | 1.75062900 |
| C | 6.44590300 | -2.01811300 | -0.16997900 |
| H | 7.39992000 | -2.34822800 | 0.24973600 |
| H | 5.67124500 | -2.28478000 | 0.54946200 |
| H | 6.28587000 | -2.57670300 | -1.09029600 |

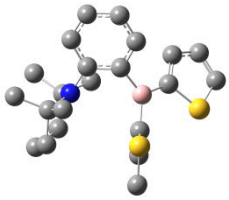
**1-TS6-t**



**Sum of electronic and thermal Enthalpies= -1769.716003**
**Sum of electronic and thermal Free Energies= -1769.797816**

| | | | |
|---|---|---|---|
| H | 1.29228000 | 0.59447900 | 2.72239900 |
| C | 2.08055400 | 0.48301900 | 1.98471500 |
| C | 2.79570500 | 1.59423900 | 1.55543400 |
| C | 2.38337800 | -0.76503400 | 1.45769500 |
| C | 3.83122100 | 1.50354200 | 0.61191400 |
| H | 2.54211500 | 2.56949400 | 1.96346900 |
| C | 3.39072000 | -0.88083100 | 0.50749900 |
| H | 1.83846500 | -1.64774400 | 1.77723000 |
| C | 4.12142800 | 0.23151200 | 0.07334800 |
| H | 3.61533800 | -1.85611900 | 0.09460500 |
| B | 4.56383700 | 2.89160700 | 0.32086000 |
| H | 5.54358400 | 1.91241000 | -0.98255400 |
| H | 5.63800500 | 2.69247700 | -1.00154800 |
| C | 3.70683800 | 3.99413200 | -0.40363600 |
| C | 2.48017400 | 3.84602800 | -1.00885400 |
| S | 4.19603400 | 5.66162800 | -0.50095700 |
| C | 1.94897200 | 5.04442800 | -1.55791100 |
| H | 1.97111900 | 2.88999100 | -1.04426100 |
| C | 2.78061500 | 6.11019300 | -1.36370600 |
| H | 0.99477800 | 5.11307600 | -2.06588000 |
| H | 2.62543100 | 7.13585200 | -1.66883100 |
| C | 5.69741300 | 3.36134700 | 1.32364600 |
| C | 6.78972300 | 4.16268600 | 1.10052500 |
| S | 5.65952700 | 2.89218100 | 2.99578600 |
| C | 7.58522600 | 4.40250200 | 2.25715800 |
| H | 7.02605300 | 4.56474100 | 0.12070400 |
| C | 7.08487200 | 3.78208200 | 3.36361600 |
| H | 8.48314000 | 5.00849000 | 2.26315500 |
| H | 7.47487800 | 3.80306100 | 4.37156900 |
| C | 6.43069600 | -0.53105400 | -0.48644500 |
| C | 4.65115400 | -0.12695200 | -2.33230600 |
| C | 7.50793300 | -0.22079900 | -1.54188100 |
| C | 5.80939800 | 0.17016600 | -3.30293700 |
| C | 7.08908600 | -0.58030000 | -2.96031800 |
| H | 8.42944000 | -0.74149200 | -1.26034800 |
| H | 7.72616000 | 0.85424900 | -1.50246100 |
| H | 5.47763300 | -0.06344000 | -4.32038200 |
| H | 6.01555800 | 1.24776100 | -3.27611100 |
| H | 7.88139000 | -0.31054300 | -3.66604200 |
| H | 6.94201400 | -1.66228700 | -3.06003400 |
| N | 5.14619600 | 0.09759600 | -0.93434000 |
| C | 6.87351100 | 0.12463500 | 0.82799300 |
| H | 6.98690400 | 1.20531600 | 0.72066800 |
| H | 6.16584400 | -0.06553100 | 1.63824400 |
| H | 7.84257600 | -0.28838600 | 1.12315000 |
| C | 6.36941500 | -2.05178200 | -0.23151700 |
| H | 5.64995200 | -2.29220700 | 0.55373700 |
| H | 6.11627400 | -2.62962200 | -1.12052600 |
| H | 7.34996600 | -2.39512600 | 0.11323900 |
| C | 4.07843700 | -1.53016900 | -2.62525800 |
| H | 3.71432500 | -1.55565200 | -3.65732800 |
| H | 4.81436500 | -2.32759900 | -2.52152600 |
| H | 3.22892300 | -1.75658600 | -1.97835800 |
| C | 3.52917300 | 0.87919400 | -2.62814900 |
| H | 2.63930100 | 0.67902200 | -2.02586600 |
| H | 3.84358000 | 1.90871100 | -2.44443000 |
| H | 3.24686900 | 0.79656600 | -3.68191300 |

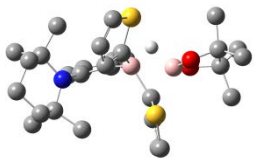
**1-Int5-t**



**Sum of electronic and thermal Enthalpies= -1768.563873**
**Sum of electronic and thermal Free Energies= -1768.643551**

| | | | |
|---|---|---|---|
| C | -6.59518700 | 1.38556400 | -0.21336200 |
| C | -5.26687700 | 1.87454500 | -0.21331700 |
| C | -5.04641100 | 3.23133700 | -0.47895500 |
| C | -6.08628500 | 4.08852200 | -0.82104500 |
| C | -7.38761600 | 3.60611700 | -0.87204200 |
| C | -7.62967600 | 2.27897500 | -0.53916600 |
| H | -4.03730400 | 3.62077800 | -0.42192300 |
| H | -5.87738300 | 5.13171300 | -1.03793800 |
| H | -8.20928300 | 4.26110700 | -1.14384900 |
| H | -8.65446200 | 1.91773700 | -0.53265700 |
| B | -7.00855900 | -0.06488100 | 0.24926700 |
| C | -8.07951000 | -0.15450200 | 1.36732800 |
| C | -8.53451900 | 0.85311000 | 2.19724900 |
| C | -9.51788900 | 0.44411500 | 3.12848300 |
| H | -8.14754700 | 1.86330300 | 2.13161000 |
| C | -9.82057000 | -0.88594400 | 3.00142200 |
| H | -9.98041400 | 1.09831100 | 3.85715800 |
| H | -10.53890400 | -1.45450100 | 3.57635000 |
| C | -6.47846000 | -1.41480600 | -0.33367700 |
| C | -5.99737500 | -2.49025100 | 0.37770800 |
| C | -5.59192800 | -3.58906800 | -0.42992200 |
| H | -5.91942300 | -2.48214100 | 1.45913300 |
| C | -5.80563500 | -3.35912400 | -1.75776300 |
| H | -5.17630800 | -4.50953700 | -0.03899400 |
| H | -5.63000500 | -4.02961500 | -2.58715100 |
| C | -3.20932900 | 0.77190500 | -1.07448800 |
| C | -3.68837400 | 0.86626400 | 1.44389700 |
| C | -2.60701300 | -0.63099100 | -0.87434700 |
| C | -2.98365700 | -0.49718300 | 1.59017600 |
| C | -1.96263200 | -0.79370600 | 0.49848400 |
| H | -1.87326800 | -0.82123000 | -1.66644900 |
| H | -3.41229700 | -1.36780900 | -0.98471700 |
| H | -2.51716200 | -0.54941100 | 2.58097700 |
| H | -3.75707800 | -1.27232600 | 1.55103700 |
| H | -1.58497100 | -1.81495300 | 0.61724200 |
| H | -1.09073200 | -0.13551400 | 0.59507200 |
| N | -4.17220200 | 0.98860900 | 0.04442400 |
| C | -3.96542700 | 0.79006700 | -2.40971900 |
| H | -4.85055900 | 0.15869000 | -2.37104100 |
| H | -4.27326400 | 1.80069300 | -2.68957600 |
| H | -3.30728100 | 0.40862400 | -3.19630400 |
| C | -2.05896500 | 1.79935400 | -1.22633000 |
| H | -2.43458600 | 2.82215800 | -1.28973800 |
| H | -1.31936200 | 1.75781300 | -0.42786300 |
| H | -1.52996200 | 1.59298200 | -2.16266400 |
| C | -2.76484800 | 2.02082400 | 1.89642700 |
| H | -2.59669200 | 1.95976800 | 2.97649300 |
| H | -1.78729700 | 2.00158300 | 1.41659800 |
| H | -3.23135800 | 2.98806200 | 1.68769900 |
| C | -4.87158300 | 0.85721600 | 2.41890700 |
| H | -5.42867500 | 1.79769200 | 2.40465000 |
| H | -5.56643000 | 0.04346800 | 2.20357600 |
| H | -4.49369100 | 0.70333200 | 3.43381500 |
| S | -6.46852000 | -1.79594400 | -2.02525100 |
| S | -8.90712500 | -1.63703700 | 1.76560100 |

**1-Int6-t**



**Sum of electronic and thermal Enthalpies= -2180.128938**
**Sum of electronic and thermal Free Energies= -2180.234083**

| | | | |
|---|---|---|---|
| C | -1.75658800 | -2.11448800 | 0.73671900 |
| C | -0.45927900 | -1.61947000 | 0.70319900 |
| C | -0.15415000 | -0.25366500 | 0.54450000 |
| C | -1.24707400 | 0.63267800 | 0.37562100 |
| C | -2.55162400 | 0.11584900 | 0.41882800 |
| C | -2.81837900 | -1.23369400 | 0.60233300 |
| H | -1.92795700 | -3.17880700 | 0.86532400 |
| H | 0.35076700 | -2.33229700 | 0.82110200 |
| H | -3.38212200 | 0.79819800 | 0.29593800 |
| H | -3.84480800 | -1.58704600 | 0.62821200 |
| B | 1.42032400 | 0.12249000 | 0.63895500 |
| H | 1.96133000 | -0.99385300 | 0.25313800 |
| C | 1.93493800 | 0.21232100 | 2.27033700 |
| C | 1.15712600 | -0.19339500 | 3.35486900 |
| C | 1.45359000 | 0.44906500 | 4.56607700 |
| H | 0.40097900 | -0.96164800 | 3.24493400 |
| C | 2.46393000 | 1.37049400 | 4.41127700 |
| H | 0.95281200 | 0.25423400 | 5.50534200 |
| H | 2.88171600 | 2.01113300 | 5.17722200 |
| B | 2.66317300 | -1.13138100 | 1.41628000 |
| O | 4.03068400 | -0.96033000 | 1.20717000 |
| O | 2.36326400 | -2.43172000 | 1.85096900 |
| C | 4.62442300 | -2.26431100 | 1.29578900 |
| C | 3.61997700 | -3.01535800 | 2.23341900 |

| | | | |
|---|---|---|---|
| C | 4.67233000 | -2.85233800 | -0.11580800 |
| H | 5.20497900 | -2.15534200 | -0.76704500 |
| H | 5.19057300 | -3.81537800 | -0.13482900 |
| H | 3.66560100 | -2.99097600 | -0.52074400 |
| C | 6.03111300 | -2.11580900 | 1.85655400 |
| H | 6.65454000 | -1.56955200 | 1.14429800 |
| H | 6.02655300 | -1.56105600 | 2.79615500 |
| H | 6.48448000 | -3.09765600 | 2.02671600 |
| C | 3.84584400 | -2.70238200 | 3.71503200 |
| H | 2.98483300 | -3.06198300 | 4.28427300 |
| H | 4.74512900 | -3.19245000 | 4.09850800 |
| H | 3.93837700 | -1.62504200 | 3.88247600 |
| C | 3.54277800 | -4.51848800 | 2.01381200 |
| H | 4.51632800 | -4.98429500 | 2.19662400 |
| H | 2.81874200 | -4.95714700 | 2.70548400 |
| H | 3.22691900 | -4.75227300 | 0.99594200 |
| C | 2.19240400 | 1.16842100 | -0.28773100 |
| C | 2.29582300 | 2.53072000 | -0.20698800 |
| C | 3.03386400 | 3.13016700 | -1.26805400 |
| H | 1.82868000 | 3.09741000 | 0.58722700 |
| C | 3.49805300 | 2.20984600 | -2.16073400 |
| H | 3.20586300 | 4.19574500 | -1.36222700 |
| H | 4.08349500 | 2.38099200 | -3.05291500 |
| C | -1.36166800 | 2.46445800 | -1.28022800 |
| C | -1.40263100 | 2.95202300 | 1.25343600 |
| C | -0.78990400 | 3.87830700 | -1.48728900 |
| C | -0.87186300 | 4.36422700 | 0.93583500 |
| C | -1.27409300 | 4.87149300 | -0.44103600 |
| H | -1.05125000 | 4.21578300 | -2.49647500 |
| H | 0.30240800 | 3.81349300 | -1.44150700 |
| H | -1.21380900 | 5.04756200 | 1.72132100 |
| H | 0.22240700 | 4.34424800 | 0.99021700 |
| H | -0.83133600 | 5.85742700 | -0.61946800 |
| H | -2.36102400 | 5.00452100 | -0.50393200 |
| C | -0.63532400 | 1.52832700 | -2.25456600 |
| H | -0.78827700 | 1.88818900 | -3.27691400 |
| H | 0.43414400 | 1.51018000 | -2.05167000 |
| H | -1.01845800 | 0.50623800 | -2.19779600 |
| C | -2.85259400 | 2.45796200 | -1.70064700 |
| H | -2.93463300 | 2.84695200 | -2.72083800 |
| H | -3.26071600 | 1.44529900 | -1.71097700 |
| H | -3.48777700 | 3.07723500 | -1.06657000 |
| C | -0.66982200 | 2.46405200 | 2.50726900 |
| H | -1.03968800 | 1.48895600 | 2.83439100 |
| H | 0.40141700 | 2.38015000 | 2.31777100 |
| H | -0.82164800 | 3.17502700 | 3.32549100 |
| C | -2.89993500 | 3.05572700 | 1.63674600 |
| H | -3.29302600 | 2.09309200 | 1.97015400 |
| H | -3.00715100 | 3.75505200 | 2.47260600 |
| H | -3.52936000 | 3.42206200 | 0.82509700 |
| N | -1.06442000 | 2.04085500 | 0.12381600 |
| S | 3.04738200 | 1.45078500 | 2.81778100 |
| S | 3.04922200 | 0.61657600 | -1.69593500 |

## Crystallographic data

Crystals were mounted on CryoLoops with Paratone-N and optically aligned on a Bruker SMART APEX-II X-ray diffractometer with 1K CCD detector using a digital camera. Initial intensity measurements were performed using a fine-focused sealed tube, graphite-monochromated, X-ray source (Mo $K\alpha$, $\lambda$ = 0.71073 Å) at 50 kV and 30 mA. Standard APEX-II[13] software package was used for determining the unit cells, generating the data collection strategy, and controlling data collection. SAINT was used for data integration including Lorentz and polarization corrections. Semi-empirical absorption corrections were applied using SCALE (SADABS).[14] The structure was solved by direct methods using XT[15] and the refinement was carried out using SHELX2014/7.[16] All the calculations have been performed within the APEX-II or OLEX2 GUI software.[17] All of the H atoms on C atoms were generated geometrically and refined in riding model. In the case of **3 (NEt)**, the SQUEEZE subroutine of the PLATON[18] software suit was used to remove the scattering contributions from the highly disordered solvent molecules.

Atomic coordinates and additional structural information are provided in the .cif files of the Supporting Information. Crystallographic data have been deposited with CCDC (CCDC 1565313-1565317) These data can be obtained upon request from the Cambridge Crystallographic Data

Centre, 12 Union Road, Cambridge CB2 1EZ, UK, E-mail: deposit@ccdc.cam.ac.uk, or via the Internet at www.ccdc.cam.ac.uk.

| Compound | **3** | **2** | **4F** | **3F** | **2F** |
|---|---|---|---|---|---|
| Empirical formula | C20H32B2N2 | C22H32B2N2 | C8H11B1F3N1 | C10H15B1F3N1 | C11H15B1F3N3 |
| Formula weight | 322.09 | 346.12 | 188.99 | 217.04 | 229.05 |
| Temperature | 150 K | 150 K | 150 K | 150 K | 150 K |
| Wavelength | 0.71073 Å | 0.71073 Å | 0.71073 Å | 0.71073 Å | 0.71073 Å |
| Crystal system | Monoclinic | Monoclinic | Monoclinic | Monoclinic | Monoclinic |
| Space group | P 21/n | P 21/n | P 21/c | P 21/n | P 21/c |
| Unit cell dimensions | a=10.9852(12) Å<br>b=12.8546(14) Å<br>c=16.2845(18) Å<br>$\alpha=\gamma=$ 90°.<br>$\beta=$ 107.721(2)° | a=20.3173(17) Å<br>b=10.2417(9) Å<br>c=21.1401(18) Å<br>$\alpha=\gamma=$ 90°.<br>$\beta=$ 112.303(1)° | a=7.8345(9) Å<br>b=11.0250(12) Å<br>c=10.4161(12) Å<br>$\alpha=\gamma=$ 90°.<br>$\beta=$ 99.184(2)° | a=7.546(5) Å<br>b=12.600(8) Å<br>c=11.855(8) Å<br>$\alpha=\gamma=$ 90°.<br>$\beta=$ 105.288(6)° | a=13.0093(5) Å<br>b=8.6076(3) Å<br>c=20.1758(8) Å<br>$\alpha=\gamma=$ 90°.<br>$\beta=$ 104.532(1)° |
| Volume | 2190.4(4) $Å^3$ | 4069.8(6) $Å^3$ | 888.16(17) $Å^3$ | 1087.3(12) $Å^3$ | 2186.98(14) $Å^3$ |
| Z | 4 | 8 | 4 | 4 | 8 |
| Density (calculated) | 0.980 $Mg/m^3$ | 1.130 $Mg/m^3$ | 1.413 $Mg/m^3$ | 1.326 $Mg/m^3$ | 1.391 $Mg/m^3$ |
| Absorption coefficient | 0.055 $mm^{-1}$ | 0.064 $mm^{-1}$ | 0.126 $mm^{-1}$ | 0.112 $mm^{-1}$ | 0.116 $mm^{-1}$ |
| F(000) | 708 | 1504 | 392 | 456 | 960 |
| Crystal size | 0.30 x 0.15 x 0.15 $mm^3$ | 0.35 x 0.5 x 0.15 $mm^3$ | 0.5 x 0.3 x 0.3 $mm^3$ | 0.5 x 0.45 x 0.3 $mm^3$ | 0.4 x 0.35 x 0.3 $mm^3$ |
| Reflections collected | 19795 | 51110 | 12353 | 4251 | 30343 |
| Ind. reflections | 5515<br>[R(int) = 0.0326] | 9994<br>[R(int) = 0.0417] | 3219<br>[R(int) = 0.0352] | 1704<br>[R(int) = 0.0343] | 7914<br>[R(int) = 0.0301] |
| Comp. $\Theta$ = 25.242° | 0.999 | 0.999 | 0.949 | 0.984 | 0.973 |
| Refinement method | Full-matrix least-squares on $F^2$ | Full-matrix least-squares on $F^2$ | Full-matrix least-squares on $F^2$ | Full-matrix least-squares on $F^2$ | Full-matrix least-squares on $F^2$ |
| Data / rest. / para. | 4230/0/345 | 12405/0/501 | 3219/0/120 | 1704/0/175 | 7914/0/289 |
| Goodness-of-fit on $F^2$ | 1.039 | 1.015 | 1.062 | 1.066 | 1.041 |
| Final R indices [I>2sigma(I)] | R1 = 0.0355 | R1 = 0.0478 | R1 = 0.0380 | R1 = 0.0479 | R1 = 0.0416 |
| R indices (all data) | R1 = 0.0457 ,<br>wR2 = 0.0831 | R1 = 0.0673 ,<br>wR2 = 0.1285 | R1 = 0.0464 ,<br>wR2 = 0.1083 | R1 = 0.0705 ,<br>wR2 = 0.1323 | R1 =0.0592<br>wR2 = 0.1152 |
| Largest diff. peak and hole | 0.2 and -0.2 $e.Å^{-3}$ | 0.3 and -0.2 $e.Å^{-3}$ | 0.4 and -0.3 $e.Å^{-3}$ | 0.3 and -0.3 $e.Å^{-3}$ | 0.4 and -0.3 $e.Å^{-3}$ |

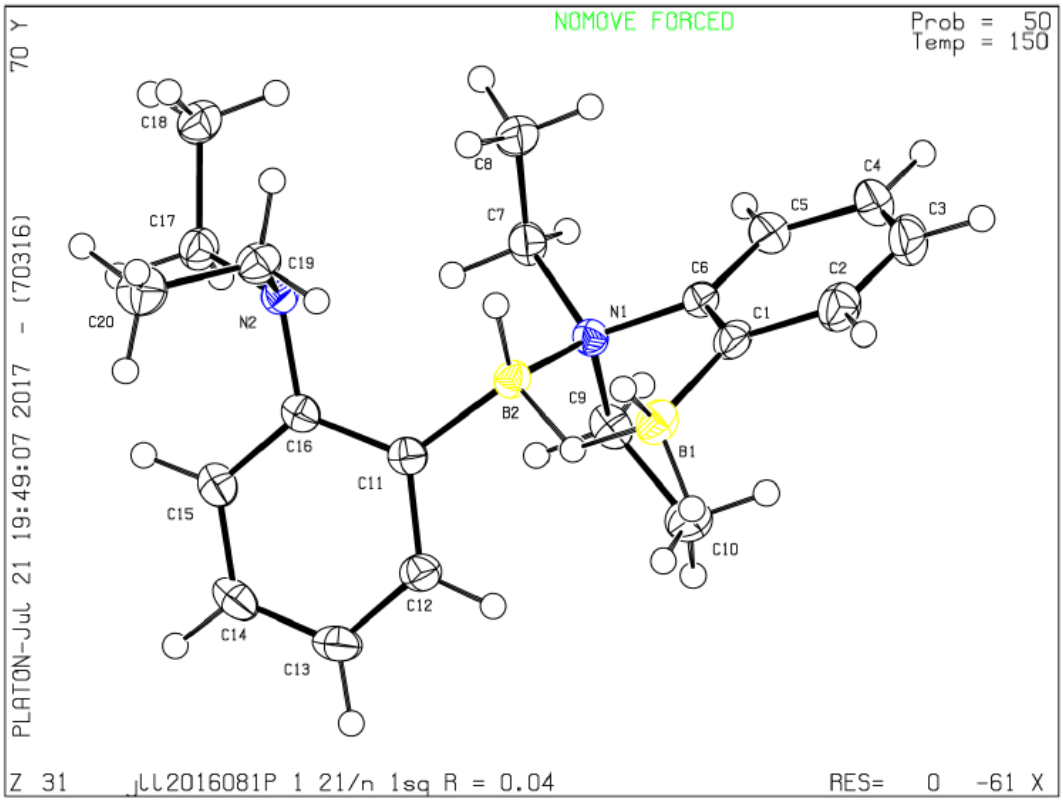



**Figure S54**: Crystal structure of compound **3**

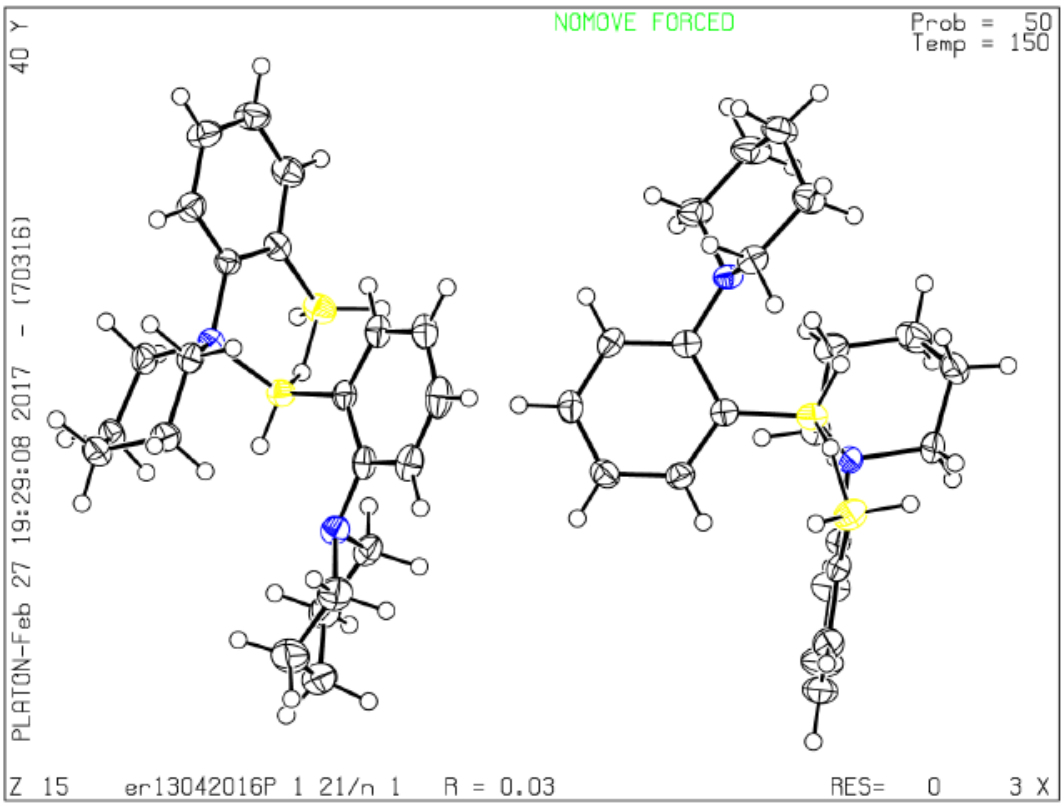



**Figure S55**: Crystal structure of compound **2**

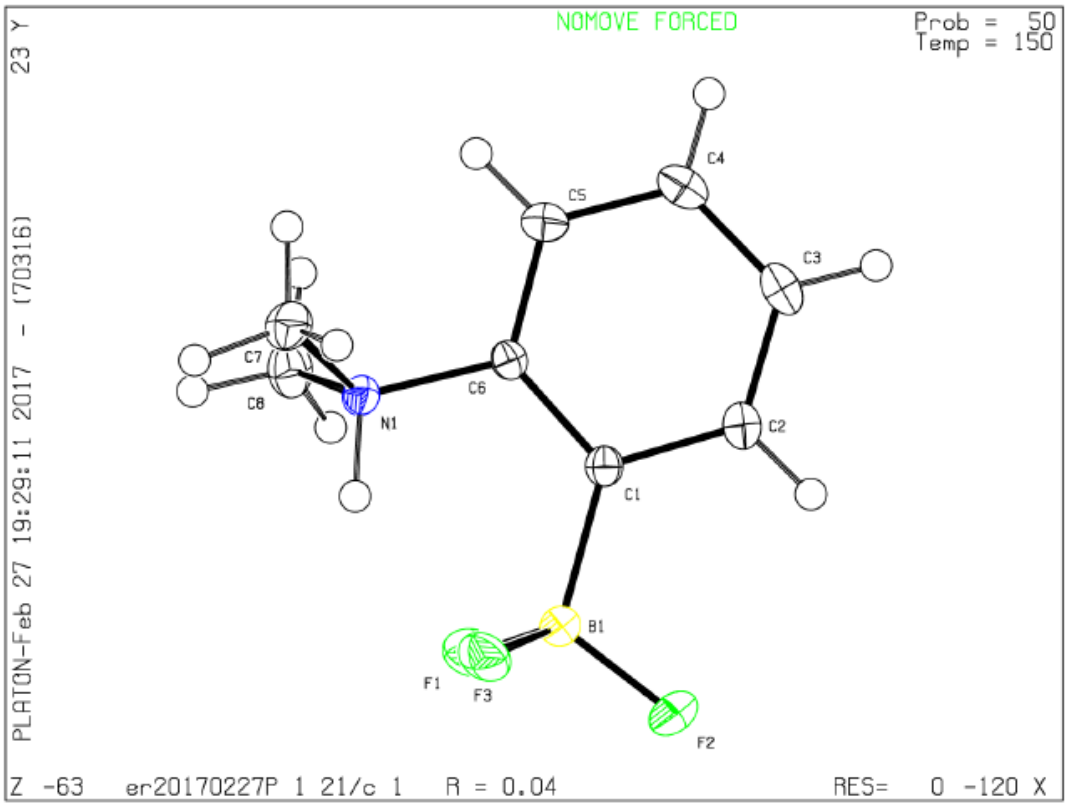



**Figure S56**: Crystal structure of compound **4F**

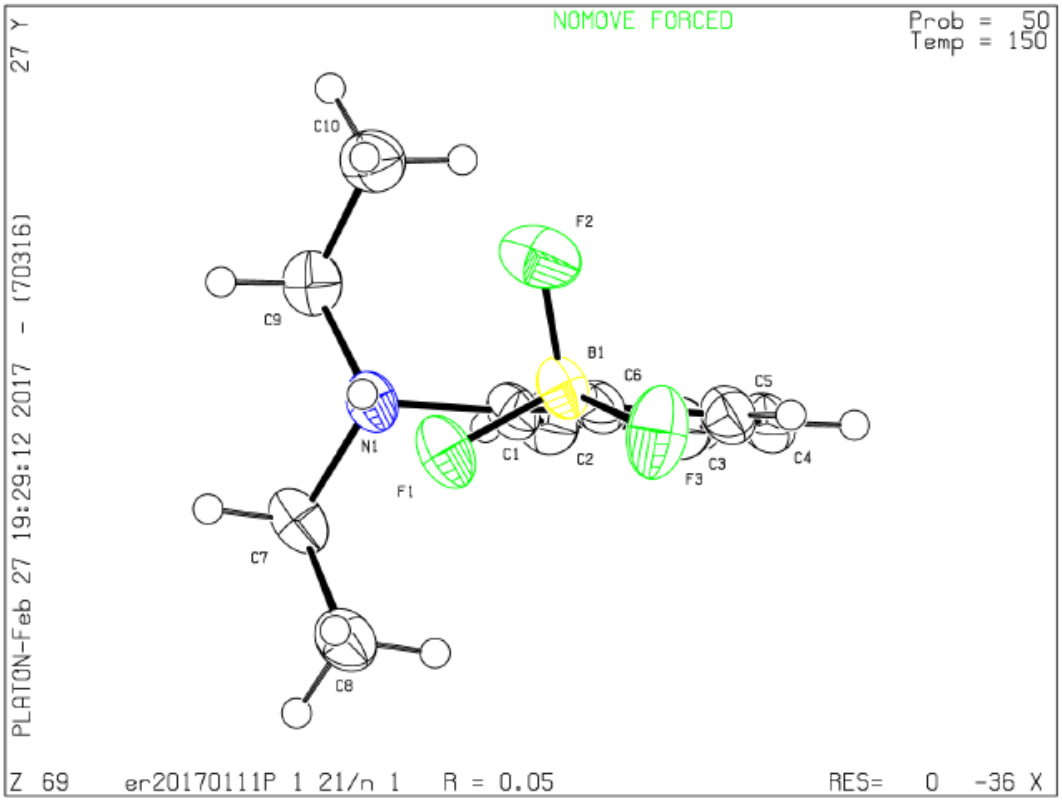



**Figure S57**: Crystal structure of compound **3F**

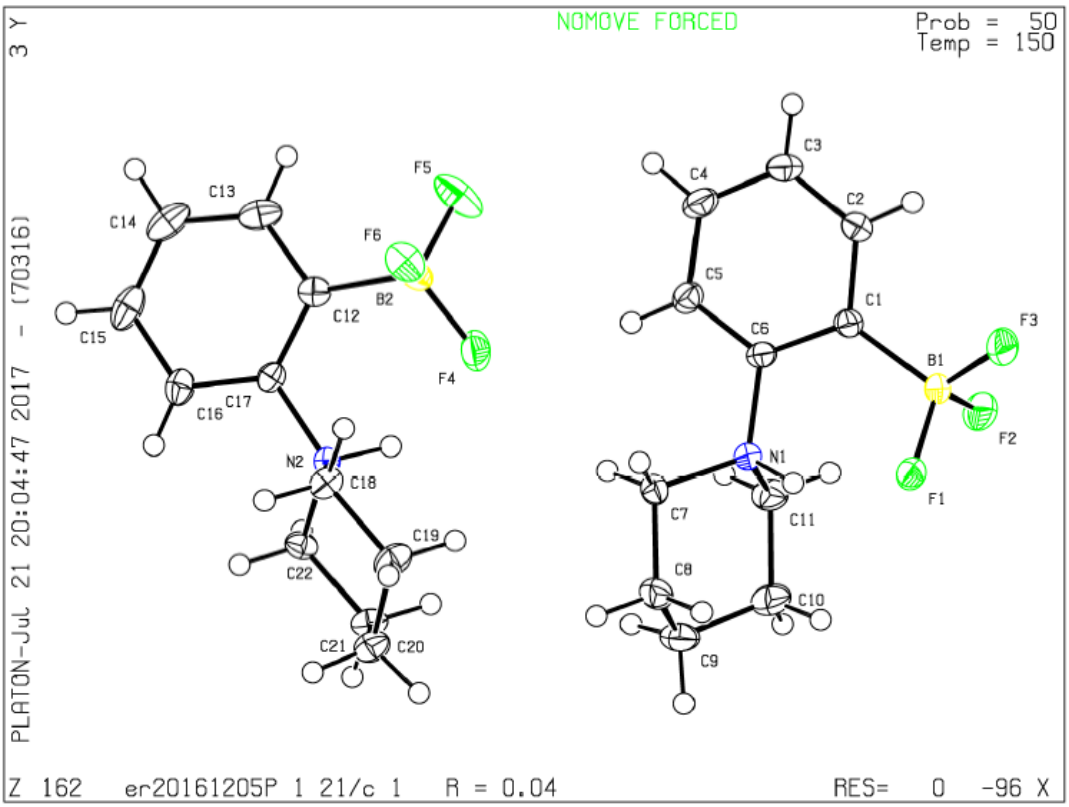



**Figure S58**: Crystal structure of compound **2F**

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