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Electronic Supplementary Information

Reactions of BICAAC with hydroboranes: propensity for Lewis adduct formation and carbene insertion into B-H bond

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Contents:

1 Experimental Section

1.1 General methods

All the reactions were performed under argon/nitrogen atmosphere using glove box and standard Schlenk line techniques. Deuterated and other solvents were dried by storage over Na/K alloy, CaH_2 and molecular sieves under an argon atmosphere. All the chemicals were procured from Sigma-Aldrich and used without further purification. The bicyclic (alkyl)(amino) carbene (BICAAC) was synthesized as per the literature procedure [1]. FT-IR spectra were recorded in the range 4000-400 cm^{-1} on a Perkin-Elmer Lambda 35-spectrophotometer. The NMR spectra were recorded using Bruker 400 NMR spectrometer (^1H: 400 MHz, $^{13}C\{^1H\}$: 100 MHz, ^{11}B: 128 MHz) at room temperature with TMS as an external standard and chemical shifts are given in ppm. High-resolution mass spectrometry (HRMS) measurement were recorded on a Waters SYNAPT G2-S. Compounds **1-5** were synthesized under argon atmosphere using standard Schlenk line technique in a ventilated fume-hood. Representative reaction procedure and work-up details have been given for compound **1**. Compounds **6-8** were prepared inside a glove box and the reaction work-up and isolation of the products were done using standard Schlenk technique in a ventilated fume-hood. Representative reaction procedure and work-up details have been given for compound **6**. A standard –30 ^oC refrigerator was used to grow crystals of all compounds from their dichloromethane (DCM) solution.

1.2 Syntheses and characterization of BICAAC-borane compounds 1-8

[BICAAC·BH_3] (1)

In a Schlenk flask, BICAAC (0.31 g, 1.00 mmol) was dissolved in toluene (10 mL) and was cooled to -40 ^oC. $BH_3{\cdot}SMe_2$ (0.09 mL, 1.00 mmol) was added to it and the mixture was allowed to warm to room temperature and stirred for 2h followed by the evaporation of all volatiles under vacuum. The residue obtained was washed with hexane (15 mL) and dried under vacuum. The resulting white solid was crystallized from dichloromethane (DCM) at –30 ^oC that afforded colorless crystals of adduct **1**. Yield: 0.27 g, 82.0 %. Mp: 153-155 ^oC. FT-IR (nujol mull, cm^{-1}) ν: 2954, 2924, 2854, 2726, 2384, 2280, 2254, 1463, 1377, 1252, 1152, 848, 808, 756, 722. ^1H NMR (400 MHz, C_6D_6): δ = 7.34 (t, 1H, *p*Ar-H, $^3J_{H\text{-}H}$ = 8 Hz), 7.20 (broad d, 2H, *m*Ar-H), 2.83 (sept, 1H, C*H*$(CH_3)_2$, $^3J_{H–H}$ = 8 Hz), 2.52 (sept, 1H,

C*H*(CH_3)$_2$, $^3J_{H–H}$ = 8 Hz), 2.12-2.04 (m, 1H), 2.02-1.94 (m, 1H), 1.85-1.72 (m, 3H, BH_3), 1.59-1.50 (m, 5H), 1.29 (d, 3H, 8 Hz), 1.25-1.21 (m, 11H), 1.03-1.01 (d, 3H, $^3J_{H-H}$ = 8 Hz), 0.94 (s, 4H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, C_6D_6): δ = 144.0, 143.6, 139.0, 128.7, 124.4, 124.1, 62.3, 46.8, 43.8, 36.7, 33.1, 32.6, 29.3, 28.6, 24.7, 24.6, 24.3, 24.2, 23.5, 23.2, 19.4 ppm.* ^{11}B NMR (128 MHz, C_6D_6): δ = -26.4 (q, $^1J_{B–H}$ = 87 Hz) ppm. HRMS (ES^+): *m/z* calcd for $C_{22}H_{36}BNNa$: 348.2842; obs: 348.2865 $[M+Na]^+$.

[BICAAC·$BHCl_2$] (2)

Synthesis of **2** was carried out in a manner similar to that for **1**. The amount of reagents used were: BICAAC (0.31 g, 1.00 mmol) and $BHCl_2$·SMe_2 (0.12 mL, 1.00 mmol). Yield: 0.30 g, 76.4 %. Mp: 155-158 ^oC. FT-IR (nujol mull, cm^{-1}) ν: 2924, 2854, 2724, 2488, 1533, 1459, 1377, 1084, 1027, 934, 798, 759, 630, 605, 567. ^1H NMR (400 MHz, $CDCl_3$): δ = 7.36 (broad t, 1H, *p*Ar-H), 7.23 (broad d, 2H, *m*Ar-H), 2.68 (sept, 1H, C*H*(CH_3)$_2$, $^3J_{H–H}$ = 8 Hz), 2.50 (sept, 1H, C*H*(CH_3)$_2$, $^3J_{H–H}$ = 8 Hz), 2.17 (m, 1H), 1.99 (s, 4H), 1.87 (s, 4H), 1.52-1.47 (m, 1H, B*H*Cl_2), 1.29-1.24 (m, 13H), 1.15 (d, 3H, $^3J_{H–H}$ = 4 Hz), 0.94 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ = 143.3, 143.0, 137.4, 129.5, 124.9, 124.8, 65.7, 48.3, 43.4, 38.3, 35.6, 32.6, 28.8, 28.5, 25.8, 25.1, 24.7, 24.2, 23.8, 21.1, 20.3 ppm.* ^{11}B NMR (128 MHz, $CDCl_3$): δ = -5.41 (broad), 7.06 (s) ppm. HRMS (ES^+): *m/z* calcd for $C_{22}H_{34}NBCl_2$: 392.2087; obs: 392.2106 $[M-H]^+$.

[BICAAC·BH_2Cl] (3)

Synthesis of **3** was carried out in a manner similar to that for **1**. The amount of reagents used were: BICAAC (0.31 g, 1.00 mmol) and BH_2Cl·SMe_2 (0.10 mL, 1.00 mmol). Yield: 0.26 g, 73.5 %. Mp: 215-218 ^oC. FT-IR (nujol mull, cm^{-1}) ν: 2924, 2855, 2725, 2445, 2327, 1520, 1455, 1377, 1180, 1071, 808, 782. ^1H NMR (400 MHz, $CDCl_3$): δ = 7.36 (t, 1H, *p*Ar-H, $^3J_{H-H}$ = 8 Hz), 7.21 (d, 2H, *m*Ar-H, $^3J_{H-H}$ = 8 Hz), 2.74 (sept, 1H, C*H*(CH_3)$_2$, $^3J_{H–H}$ = 8 Hz), 2.46 (sept, 1H, C*H*(CH_3)$_2$, $^3J_{H–H}$ = 8 Hz), 2.16 (m, 1H), 1.99 (m, 2H) 1.87-1.68 (m, 6H), 1.55-1.39 (m, 2H, B*H*$_2$Cl), 1.28-1.21 (m, 13H), 1.09 (d, 3H, $^3J_{H-H}$ = 4 Hz), 0.96 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ = 143.7, 143.2 138.0, 129.2, 124.6, 124.5, 64.5, 47.9, 43.6, 37.6, 33.7, 32.7, 29.1, 28.6, 25.0, 24.7, 23.9, 23.8, 21.9, 20.1 ppm.* ^{11}B

NMR (128 MHz, $CDCl_3$): δ = -15.7 (broad) ppm. HRMS (ES^+): $C_{22}H_{34}BNCl$, [M-H] *m/z* (calc.): 358.2477, *m/z* (obs.): 358.2460.

[BICAAC·BF_3] (4)

Synthesis of **4** was carried out in a manner similar to that for **1**. The amount of reagents used were: BICAAC (0.31 g, 1.00 mmol) and $BF_3{\cdot}OEt_2$ (0.13 mL, density 1.15 gmL^{-1}, 1.00 mmol). Yield: 0.30 g, 79.3 %. Mp: 203-205 ^oC. IR (nujol mull, cm^{-1}) ν: 2953, 2923, 2853, 1619, 1588, 1560, 1475, 1466, 1455, 1446, 1435, 1377, 1366, 1345, 1317, 1258, 1230, 1217, 1182, 1090, 1048, 942, 876, 751, 741, 626, 564, 574. ^1H NMR (400 MHz, $CDCl_3$): δ = 7.39-7.36 (m, 1H, *p*Ar-H), 7.23-7.21 (m, 2H), 2.77 (sept, 1H, $CH(CH_3)_2$, $^3J_{H–H}$ = 8 Hz), 2.48 (sept, 1H, $CH(CH_3)_2$, $^3J_{H–H}$ = 8 Hz), 2.21-2.15 (m, 1H), 2.06-1.97 (m, 1H), 1.85-1.78 (m, 3H), 1.72 (s, 3H), 1.60-1.55 (m, 1H), 1.31 (d, 3H, $^3J_{H–H}$ = 4 Hz), 1.26-1.22 (m, 10H), 1.09 (d, 3H), 0.97 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ = 143.2, 142.9, 137.9, 129.4, 124.5, 124.3, 65.6, 46.7, 43.6, 38.2, 32.8, 29.4, 28.7, 24.7, 24.5, 24.4, 23.6, 23.5, 21.4, 21.4, 20.2 ppm.* ^{11}B NMR (128 MHz, $CDCl_3$): δ = -0.72 (q, $^1J_{B-F}$ = 41 Hz) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -139.7 (q, $^1J_{F-B}$= 41) ppm. HRMS (ES+): *m/z* calcd for $C_{22}H_{33}NBF_2$: 360.2678; obs: 360.2661 $[M-F]^+$.

[BICAAC·BCl_3] (5)

Synthesis of **5** was carried out in a manner similar to that for **1**. The amount of reagents used were: BICAAC (0.31 g, 1.00 mmol) and BCl_3 (1.00 mL, 1.00 mmol, 1.00 M). Yield: 0.38 g, 88.2 %. Mp: 320 ^oC (decomp). IR (nujol mull, cm^{-1}) ν: 2924, 2855, 2725, 1458, 1377, 1154, 1055, 936, 766, 720, 659. ^1H NMR (400 MHz, C_6D_6): δ= 7.09 (t, 1H, *p*Ar-H, $^3J_{H-H}$ = 8 Hz), 7.02-6.92 (m, 2H), 2.76 (sept, 1H, C*H*$(CH_3)_2$, $^3J_{H–H}$= 8 Hz), 2.55 (sept, 1H, C*H*$(CH_3)_2$, $^3J_{H–H}$= 8 Hz), 2.13-2.09 (m, 3H), 1.83-1.73 (m, 1H), 1.53-1.41 (m, 9H), 1.26-1.18 (m, 3H), 1.09-1.06 (m, 9H), 0.51 (broad signal, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, C_6D_6): δ= 143.9, 143.5, 137.8, 129.9, 124.9, 124.7, 67.6, 48.9, 42.7, 38.9, 36.1, 32.3, 29.3, 28.9, 25.5, 24.9, 24.6, 24.4, 23.9, 20.4 ppm.* ^{11}B NMR (128 MHz, C_6D_6): δ= 3.56 (broad) ppm. HRMS (ES^+): *m/z* calcd for $C_{22}H_{33}NBCl_2$: 392.2087; obs: 392.2069 $[M-Cl]^+$.

[BICAAC·BBr_3] (6)

In a glove box containing deep freezer, BICAAC (0.31 g, 1.00 mmol) was dissolved in toluene (10 mL) and this solution was cooled to -25 ^oC. To this solution, $BBr_3{\cdot}SMe_2$ (0.31 g, 1.00 mmol) was added and the mixture was allowed to warm to room temperature and stirred for 2 h. The work-up procedure similar to that of **1** was adopted to isolate **6**. Yield: 0.45 g, 81.0 %. Mp: 285 ^oC (decomp). IR (nujol mull, cm^{-1}) ν: 2921, 2854, 1456, 1377, 1261, 1153, 1098, 1020, 800, 722. ^1H NMR (400 MHz, $CDCl_3$): δ = 7.37 (t, 1H, *p*Ar-H, $^3J_{H\text{-}H}$ = 8 Hz), 7.19-7.17 (m, 2H, *m*Ar-H), 2.73 (sept, 1H, C*H*$(CH_3)_2$, $^3J_{H–H}$= 8 Hz), 2.56 (sept, 1H, C*H*$(CH_3)_2$, $^3J_{H–H}$= 8 Hz), 2.25-2.19 (m, 1H), 2.13-2.03 (m, 5H), 1.99-1.97 (m, 2H), 1.65-1.59 (m, 1H), 1.43-1.39 (m, 6H), 1.29 (t, 7H, $^3J_{H\text{-}H}$ = 8 Hz), 1.23-1.21 (m, 3H), 0.95 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ = 144.3, 143.7, 137.2, 130.0, 125.0, 124.8, 68.4, 49.5, 42.6, 39.3, 37.2, 32.5, 29.1, 28.8, 25.6, 25.4, 24.9, 24.8, 24.4, 20.7 ppm.* ^{11}B NMR (128 MHz, $CDCl_3$): δ = 34.08 (broad). HRMS (ES^+): *m/z* calcd for $C_{22}H_{33}NBBr_2$: 482.1057; obs: 482.1035 $[M\text{-}Br]^+$.

*The $^{13}C\{^1H\}$ NMR spectra of complexes **1**-**6** did not show signal for BICAAC carbon attached to boron perhaps due to quaternary nature of this carbon and the quadrupolar effect of B.

BICAAC(H)-(9-BBN) (7)

Synthesis of **7** was carried out inside a glove box in a manner described for **6**. The amount of reagents used were: BICAAC (0.31 g, 1.00 mmol) and 9-borabicyclo[3.3.1]nonane dimer $(9\text{-}BBN)_2$ (0.12 g, 0.50 mmol). Yield: 0.36 g, 83.6 %. Mp: 237–240 ^oC. FT-IR (nujol mull, cm^{-1}) ν: 2924, 2854, 1463, 1377, 1264, 1172, 1044, 1010, 898, 811, 781. ^1H NMR (400 MHz, C_6D_6): δ = 7.09 (m, 2H, *m*Ar-H, $^3J_{H\text{-}H}$ = 4 Hz), 7.03 (m, 1H, *p*Ar-H, $^3J_{H\text{-}H}$ = 4 Hz), 4.23 (s, 1H, C*H*B), 3.93 (sept, 1H, C*H*$(CH_3)_2$, $^3J_{H–H}$ = 8 Hz), 3.62 (sept, 1H, C*H*$(CH_3)_2$, $^3J_{H–H}$ = 8 Hz), 2.24 (d, 2H, $^3J_{H–H}$ = 8 Hz), 1.94-1.76 (m, 7H), 1.70-1.53 (m, 9H), 1.42 (d, 3H, $J_{H–H}$ = 4 Hz), 1.37-1.32 (m, 8H, $^3J_{H–H}$ = 8 Hz), 1.15 (t, 7H, $^3J_{H–H}$ = 8Hz), 0.92 (s, 3H), 0.80 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ = 150.9, 150.1, 146.5, 125.6, 124.8, 124.4, 62.4 (*C*HB), 52.8, 47.2, 38.4, 37.8, 36.1, 36.0, 33.5, 32.9, 31.3, 29.6, 27.8, 27.3, 27.2, 25.4, 25.3, 24.9, 23.1, 22.9, 15.9 ppm. ^{11}B NMR (128 MHz, $CDCl_3$): δ = 90 (broad) ppm. HRMS (AP^+): *m/z* calcd for $C_{30}H_{49}BN$: 434.3963; obs: 434.3940 $[M+H]^+$.

BICAAC(H)·Bcat (8)

Synthesis of **8** was carried out inside a glove box in a manner described for **6**. The amount of reagents used were: BICAAC (0.31 g, 1.00 mmol) and catecholborane (0.11 mL, 1.00 mmol). Yield: 0.35 g, 80.6 % of the diastereomeric mixture. Mp: 400 ^{o}C (decomp.). Characterization data for major diastereomeric mixture: FT-IR (nujol mull, cm^{-1}) ν: 3194, 2923, 2854, 1598, 1489, 1462, 1377, 1244, 1207, 1101, 916, 745, 731, 700. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.21-7.09 (m, 3H), 7.07-6.95 (m, 4H), 4.02-3.96 (overlapping signal from diastereomers, 1H, C*H*B), 3.57 (sept, 1H, C*H*$(CH_3)_2$), $^{3}J_{H-H}$ = 8 Hz), 2.73-2.59 (m, 1H, C*H*$(CH_3)_2$), 2.12 (broad t, 1H), 2.02-1.95 (m, 1H), 1.86-1.83 (m, 2H), 1.67-1.60 (m, 1H), 1.49-1.43 (m, 1H), 1.40 (d, 2H, *J* = 4 Hz), 1.27-1.20 (m, 8H), 1.13-1.07 (m, 3H), 1.02 (d, 2H, *J* = 4 Hz), 0.91-0.80 (m, 1H), 0.70-0.67 (m, 6H) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 152.0, 151.8 148.0, 142.6, 126.5, 124.2, 124.0 122.5, 111.5, 52.3 (*C*HB), 47.0, 36.6, 36.0, 35.7, 33.6, 29.0, 27.7, 26.4, 25.7, 25.2, 24.8, 22.8, 15.9 ppm. ^{11}B NMR (128 MHz, $CDCl_3$): δ = 33.7 (broad) ppm. HRMS (ES^{+}): *m/z* calcd for $C_{28}H_{39}BNO_2$: 432.3079; obs: 432.3060 $[M+H]^{+}$.

1.3 Heteronuclear NMR and HRMS spectra of adducts (1-6) and carbene B-H insertion products (7 and 8)

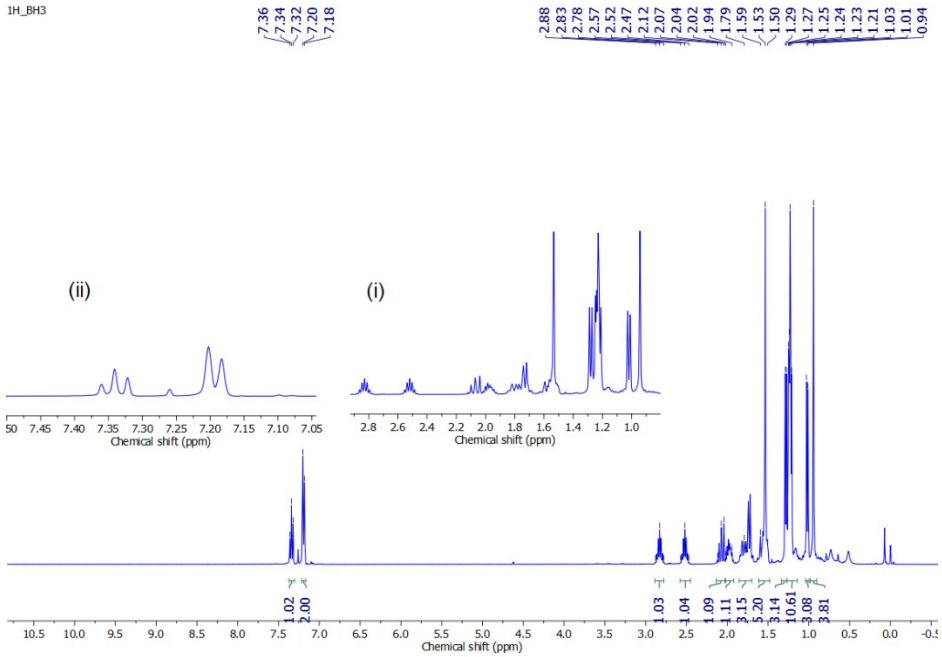


Fig. S1 ^{1}H NMR spectrum (400 MHz, C_6D_6) of [BICAAC-BH_3] adduct (**1**). Insets (i) and (ii) show expansion of selected spectral region.

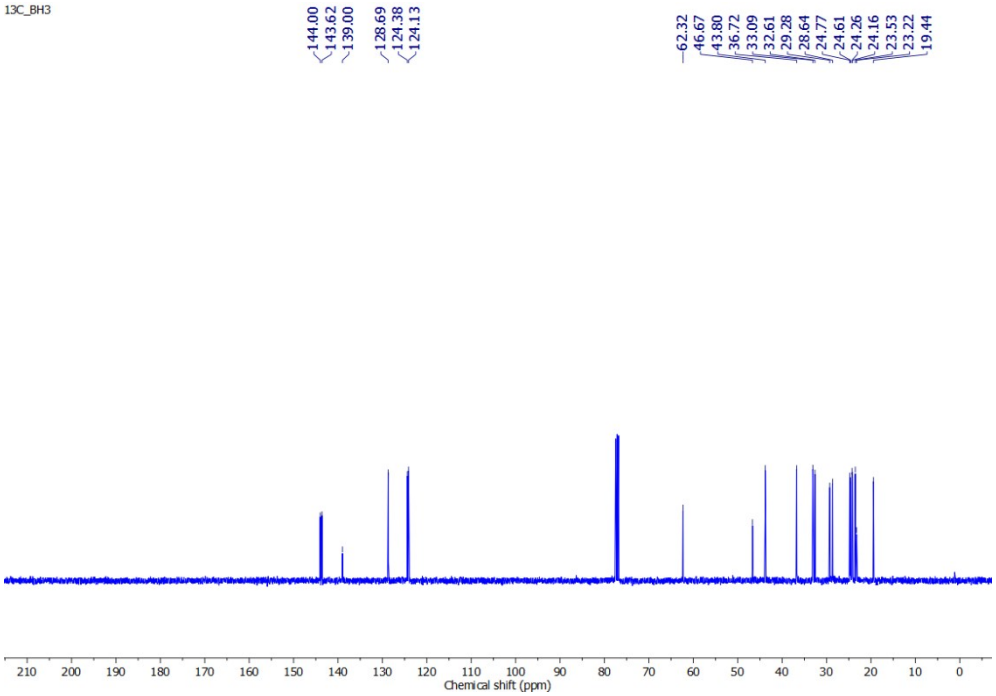


Fig. S2 $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, C_6D_6) of [BICAAC-BH_3] adduct (**1**).

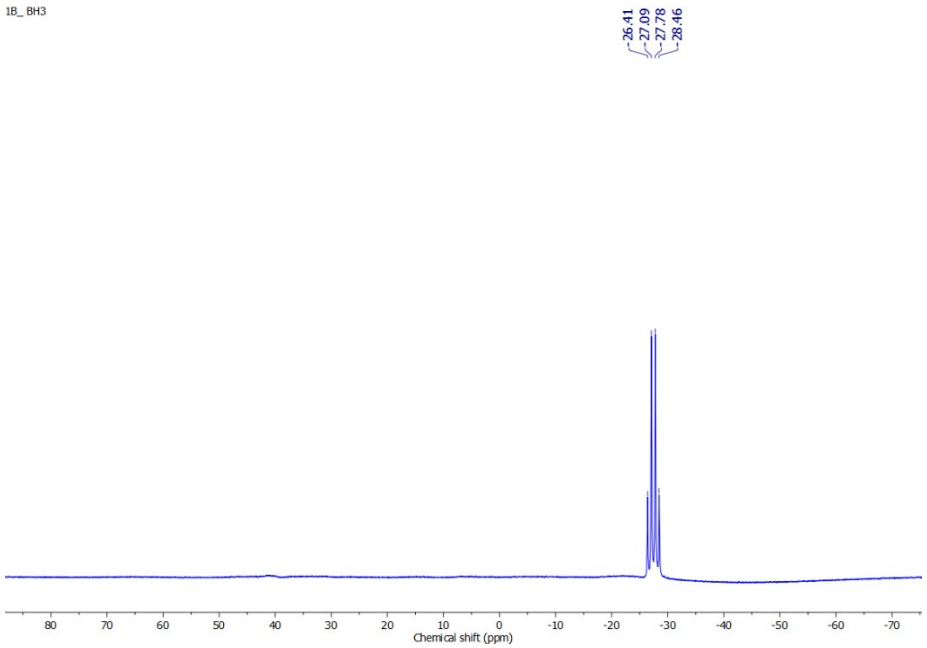


Fig. S3 ^{11}B NMR spectrum (128 MHz, C_6D_6) of [BICAAC-BH_3] adduct (**1**).

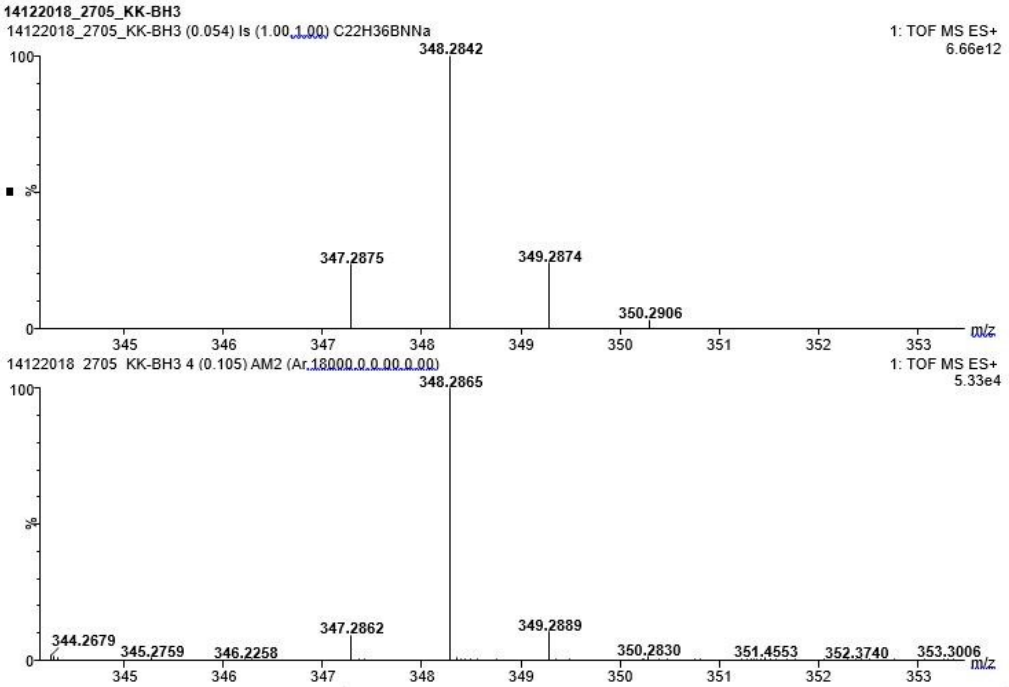


Fig. S4 HRMS spectrum of [BICAAC-BH_3] adduct (**1**).

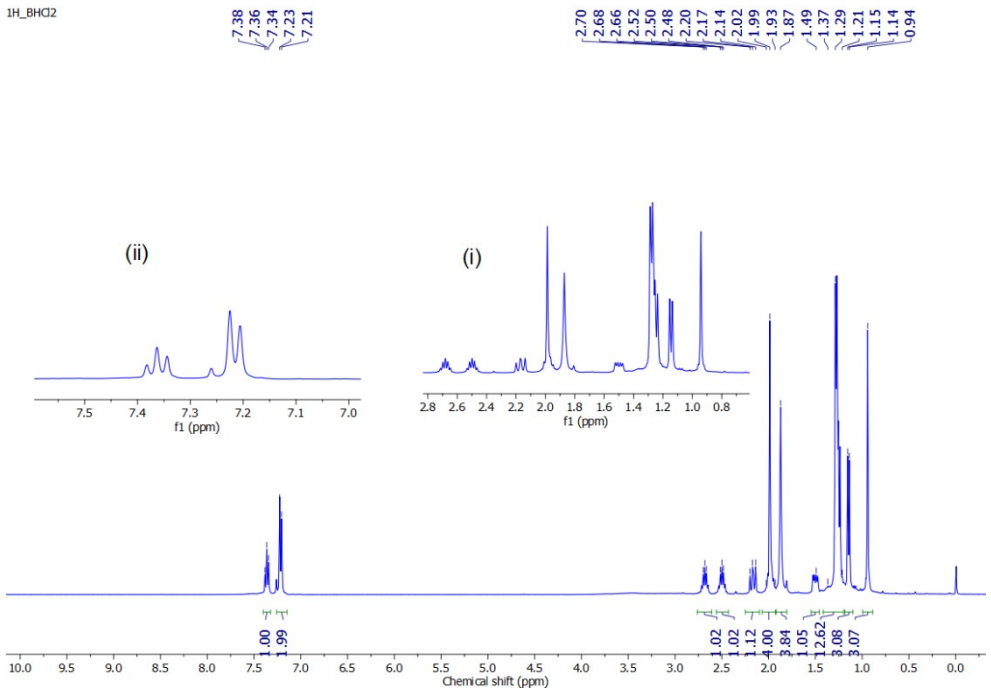


Fig. S5 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of [BICAAC-$BHCl_2$] adduct (**2**). Insets (i) and (ii) show expansion of selected spectral region.

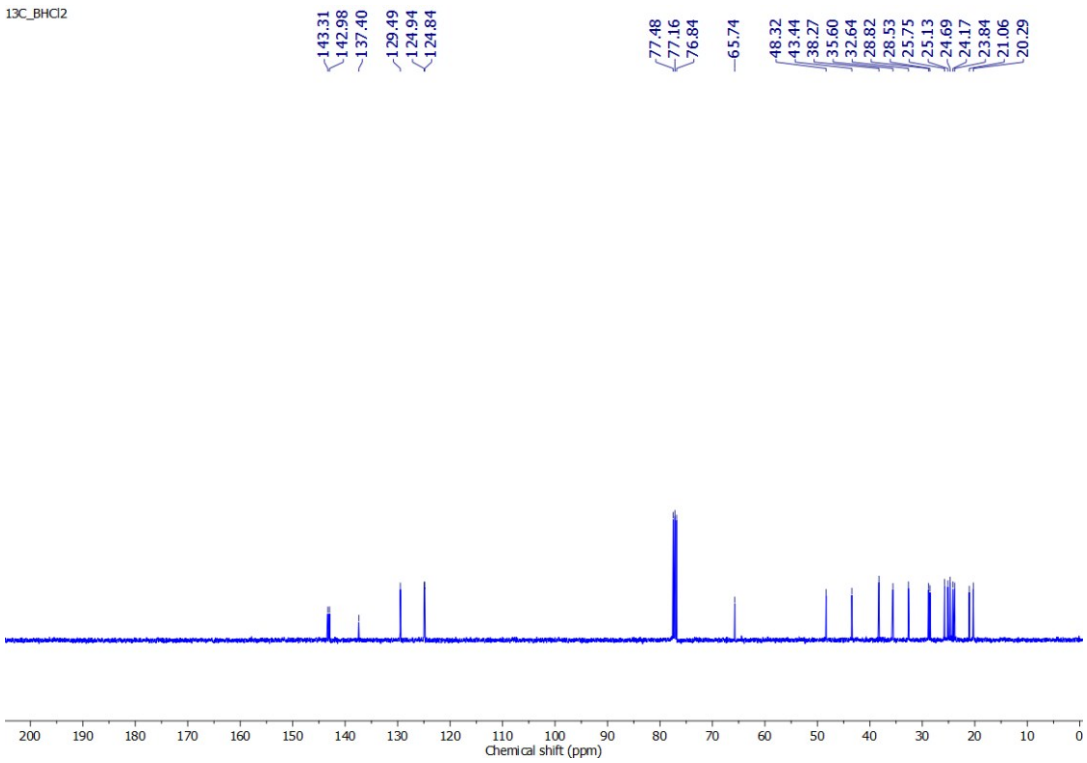


Fig. S6 $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of [BICAAC-$BHCl_2$] adduct (**2**).

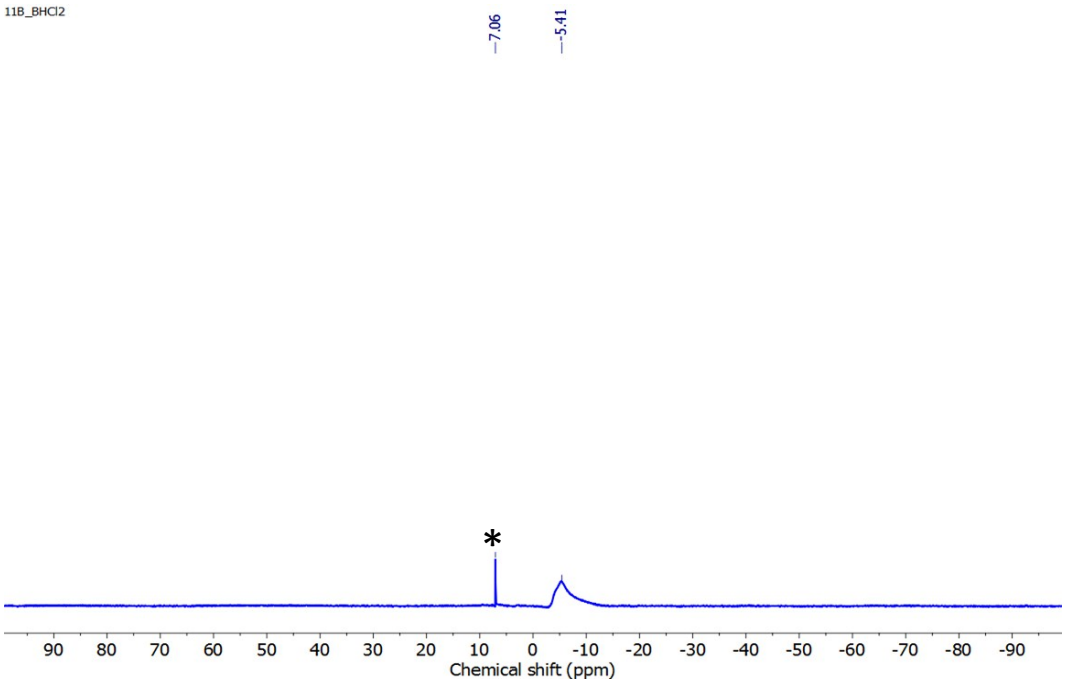

11B_BHCl2
7.06
5.41
*
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
Chemical shift (ppm)

Fig.

S7

^{11}B

NMR spectrum (128 MHz, $CDCl_3$) of [BICAAC-$BHCl_2$] adduct (**2**). *Signal for traces of $BH_2Cl{\cdot}SMe_2$/$BHCl_2{\cdot}SMe_2$ formed from exchange reaction in $BHCl_2{\cdot}SMe_2$. [2]

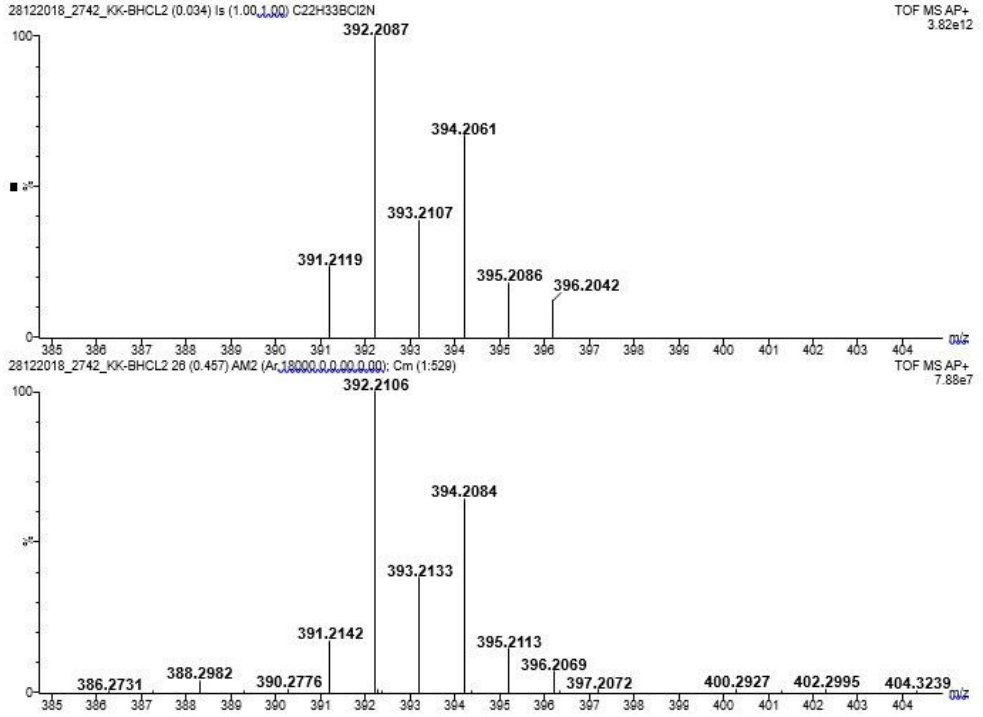


Fig. S8 HRMS spectrum of [BICAAC-$BHCl_2$] adduct (**2**).

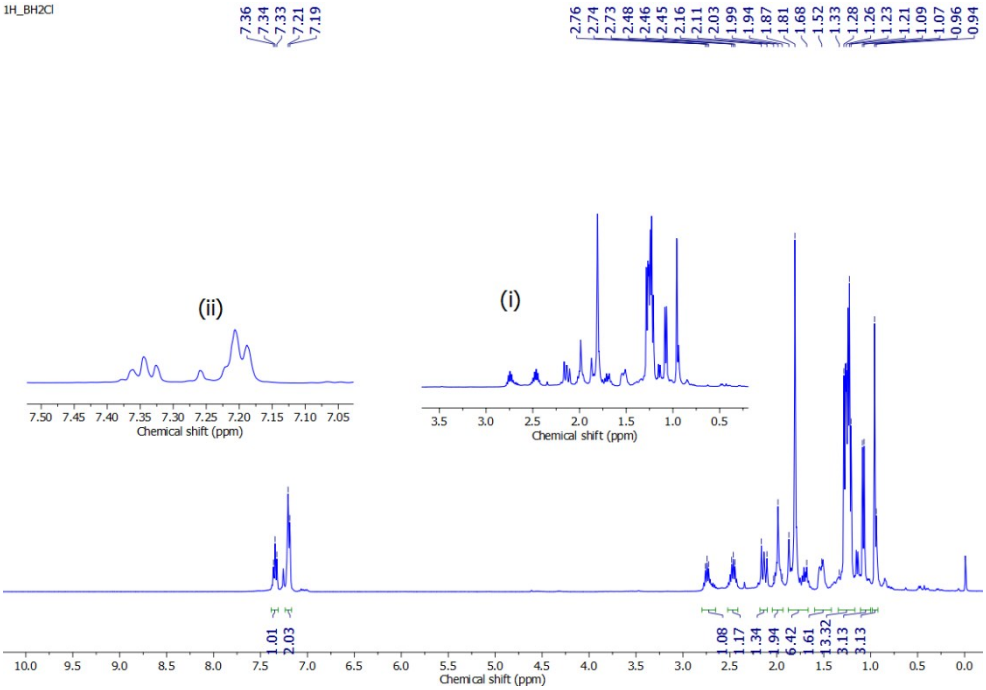


Fig. S9 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of [BICAAC-BH_2Cl] adduct (**3**). Insets (i) and (ii) show expansion of selected spectral region.

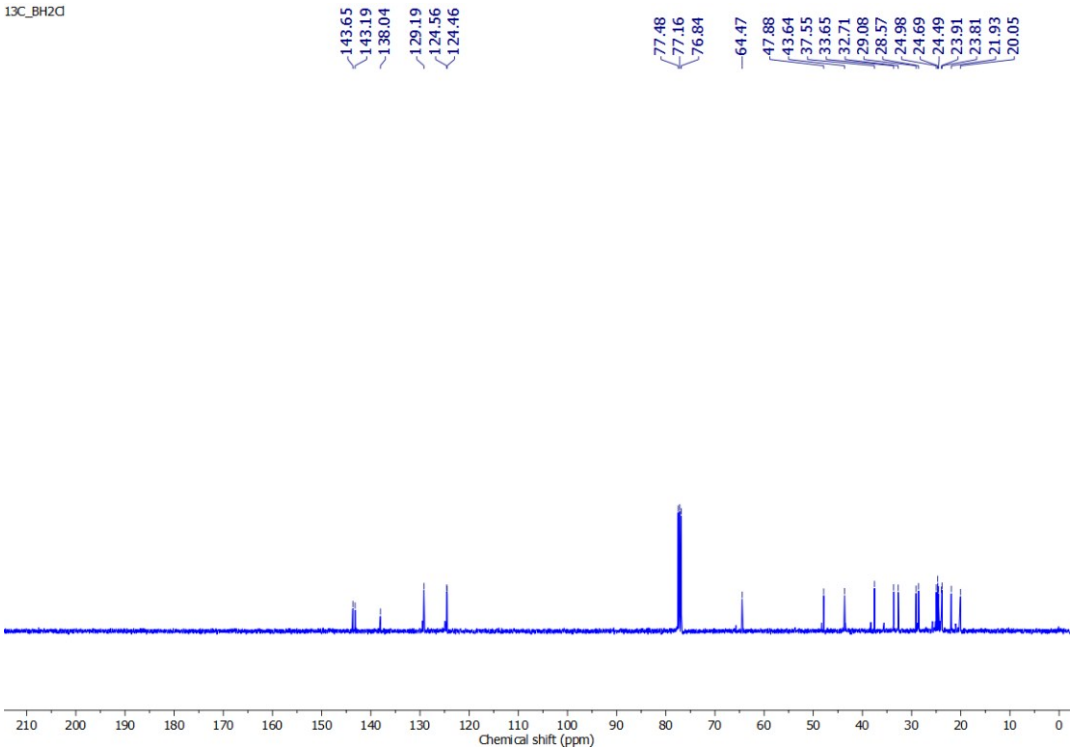


Fig. S10 $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of [BICAAC-BH_2Cl] adduct (**3**).

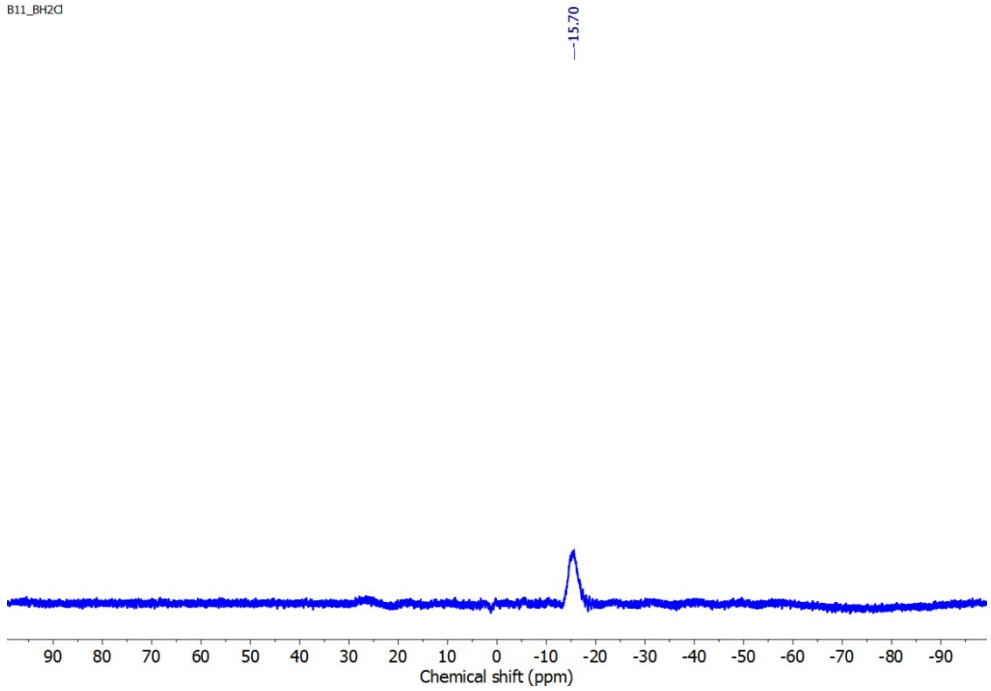


Fig. S11 ^{11}B NMR spectrum (128 MHz, $CDCl_3$) of [BICAAC-BH_2Cl] adduct (**3**).

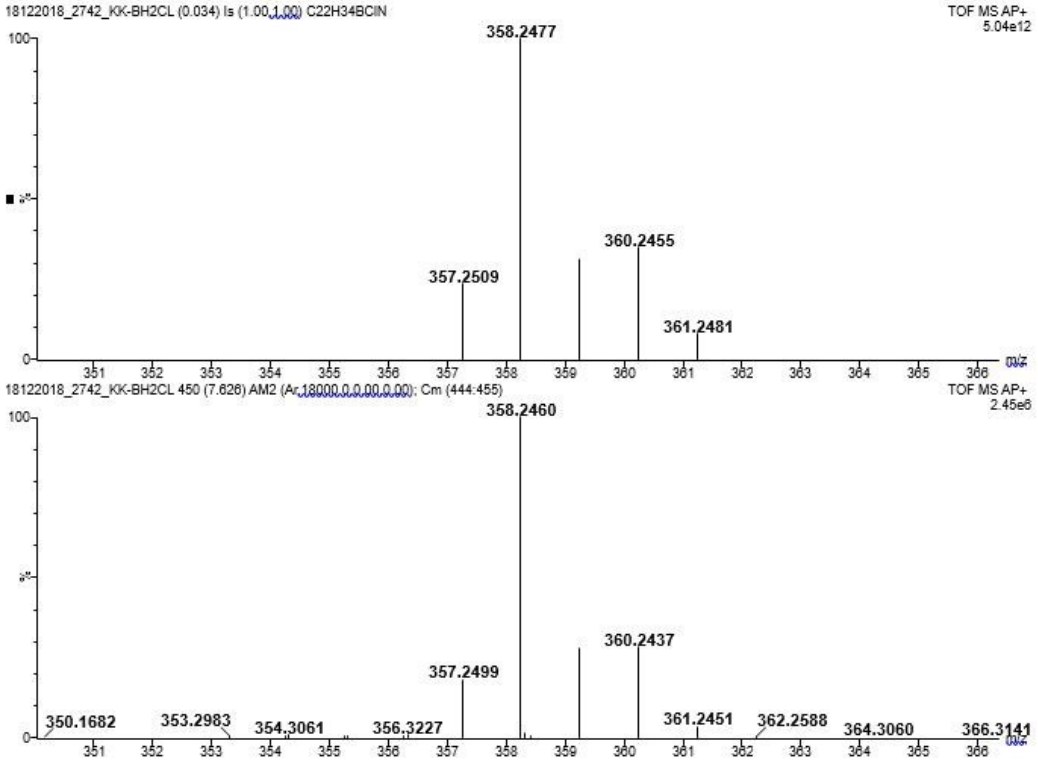


Fig. S12 HRMS spectrum of [BICAAC-BH_2Cl] adduct (**3**).

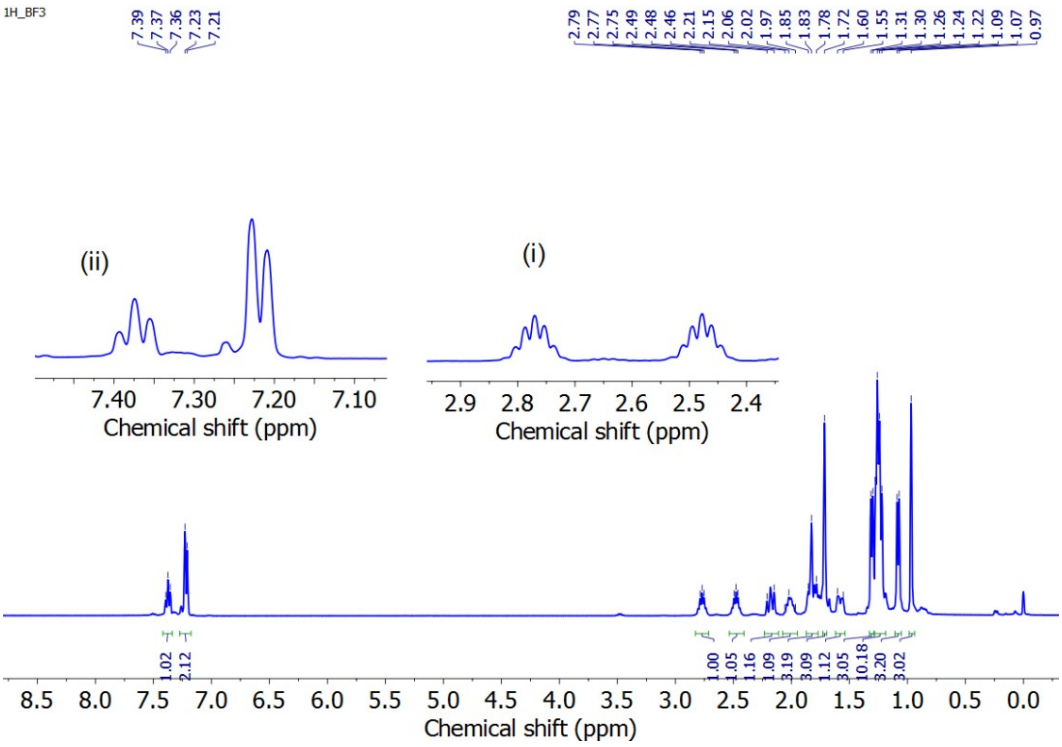


Fig. S13 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of [BICAAC-BF_3] adduct (**4**). Insets (i) and (ii) show expansion of selected spectral region.

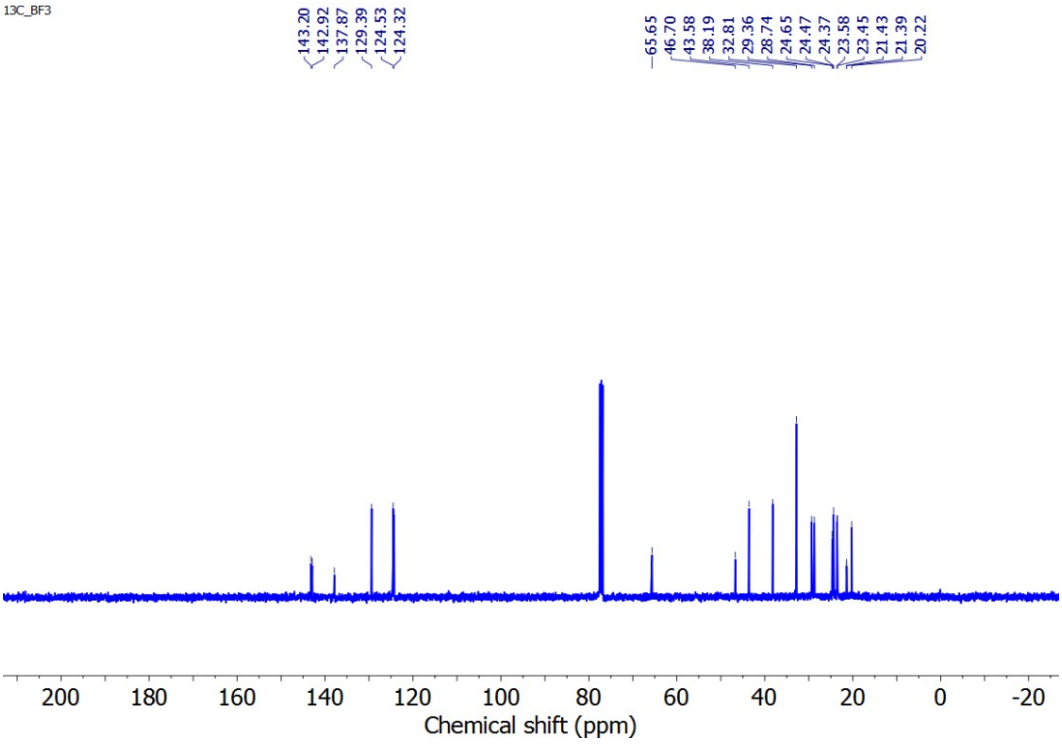


Fig. S14 $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of [BICAAC-BF_3] adduct (**4**).

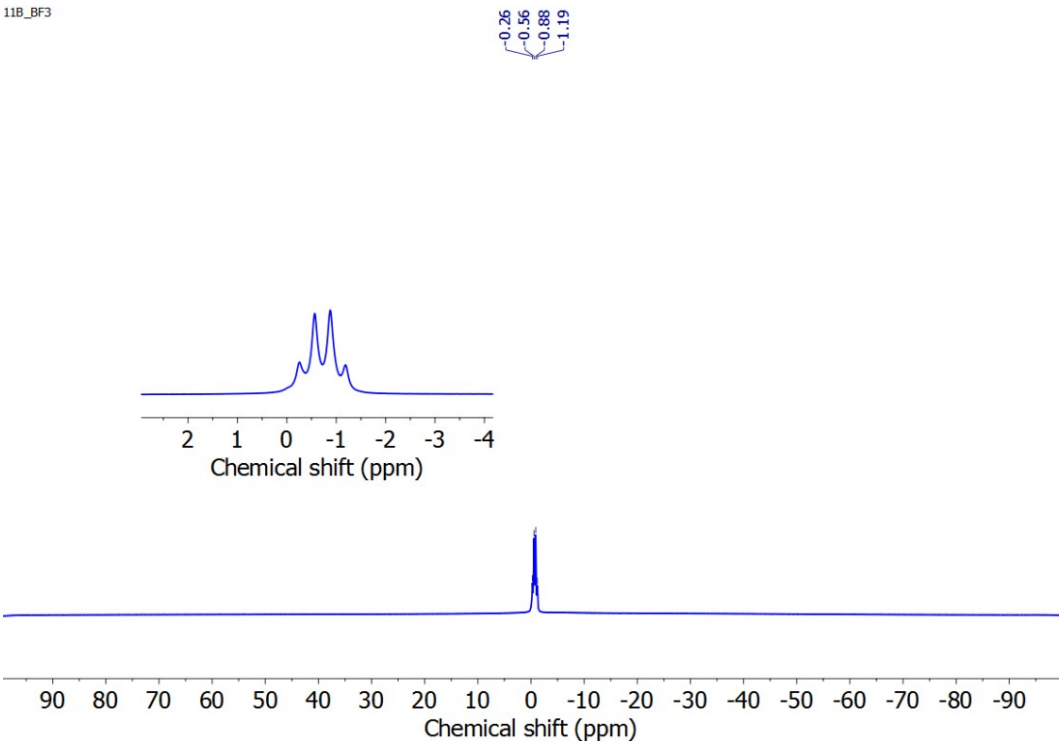


Fig. S15 ^{11}B NMR spectrum (128 MHz, $CDCl_3$) of [BICAAC-BF_3] adduct (**4**).

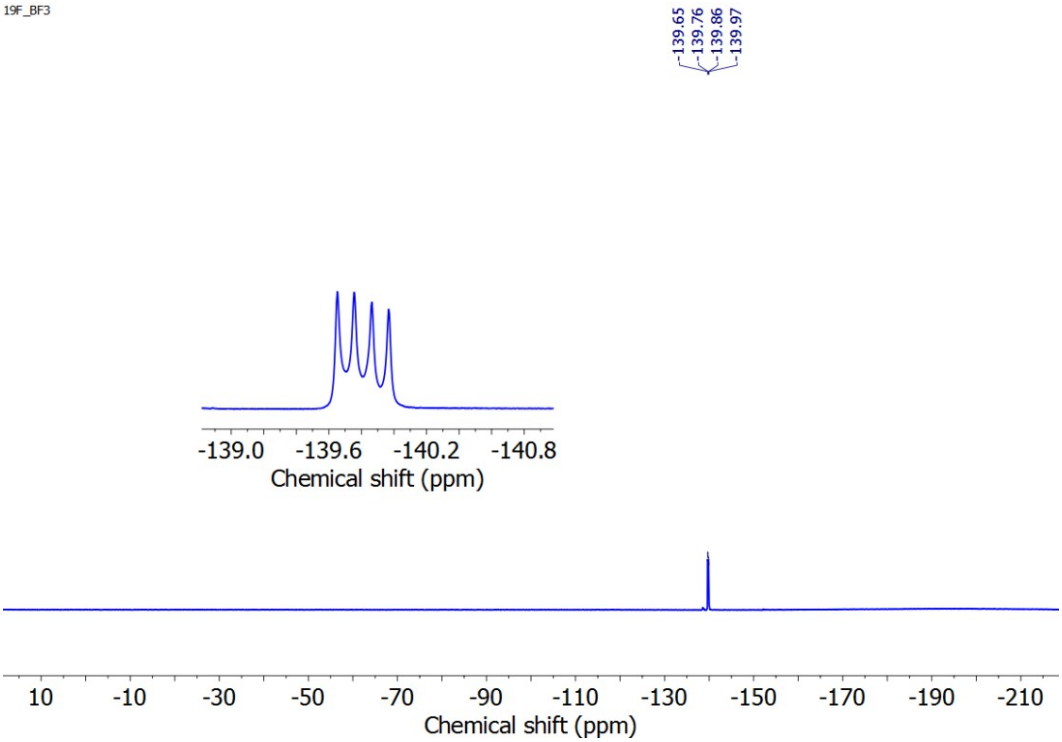


Fig. S16 ^{19}F NMR spectrum (376 MHz, $CDCl_3$) of [BICAAC-BF_3] adduct (**4**).

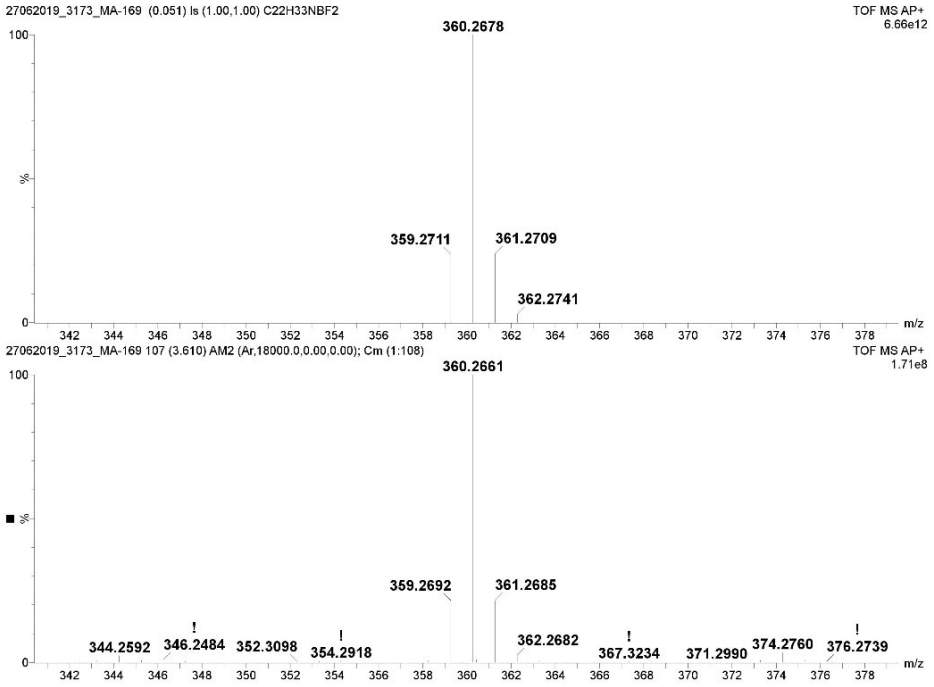


Fig. S17 HRMS spectrum of [BICAAC-BF_3] adduct (**4**).

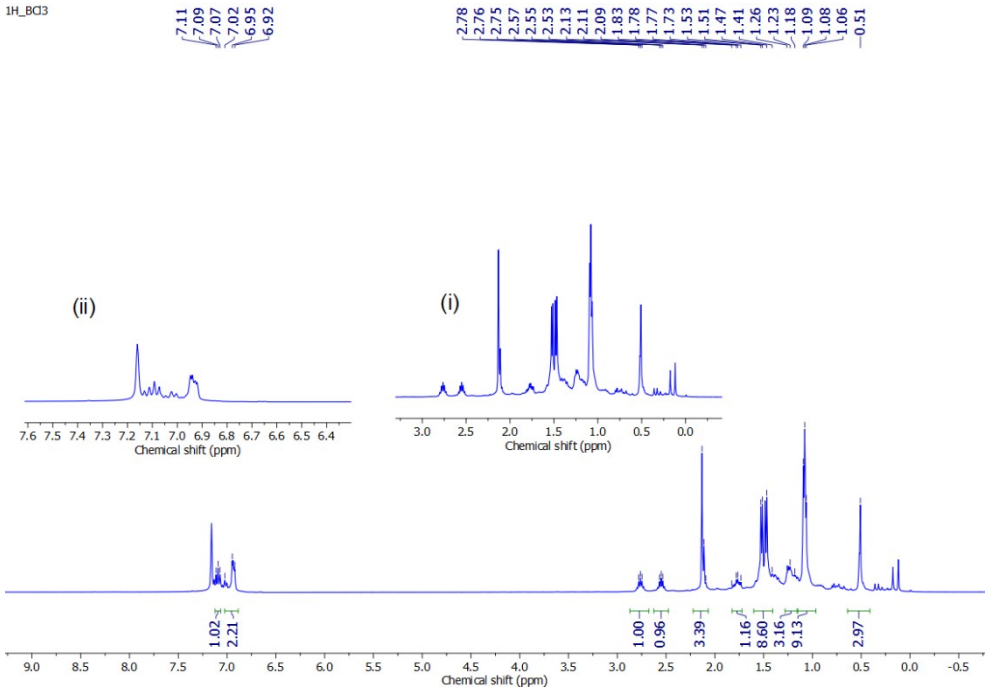


Fig. S18 ^{1}H NMR spectrum (400 MHz, C_6D_6) of [BICAAC-BCl_3] adduct (**5**). Insets (i) and (ii) show expansion of selected spectral region.

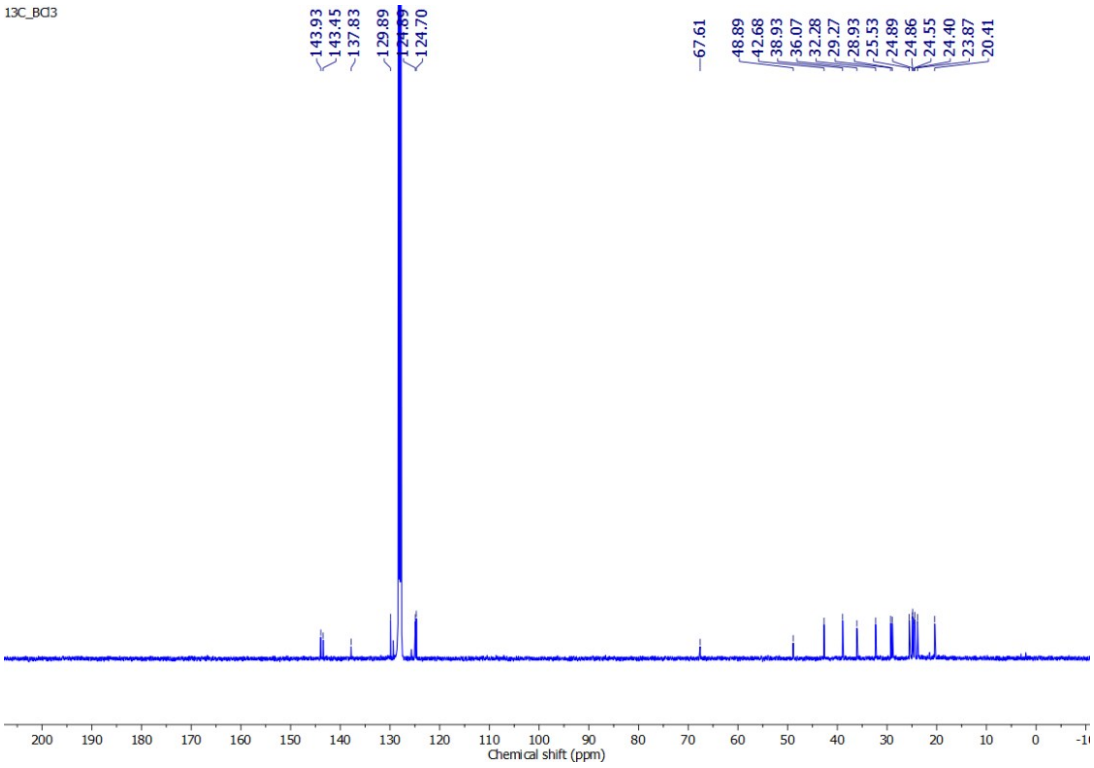


Fig. S19 $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, C_6D_6) of [BICAAC-BCl_3] adduct (**5**).

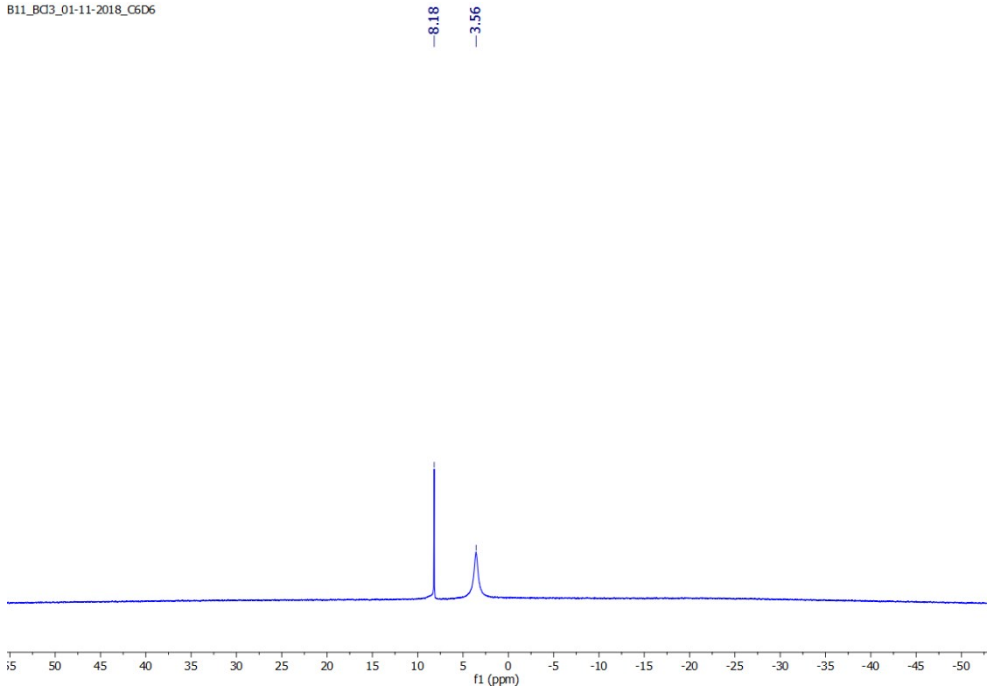


Fig. S20 ^{11}B NMR spectrum (128 MHz, C_6D_6) of [BICAAC-BCl_3] adduct (**5**).

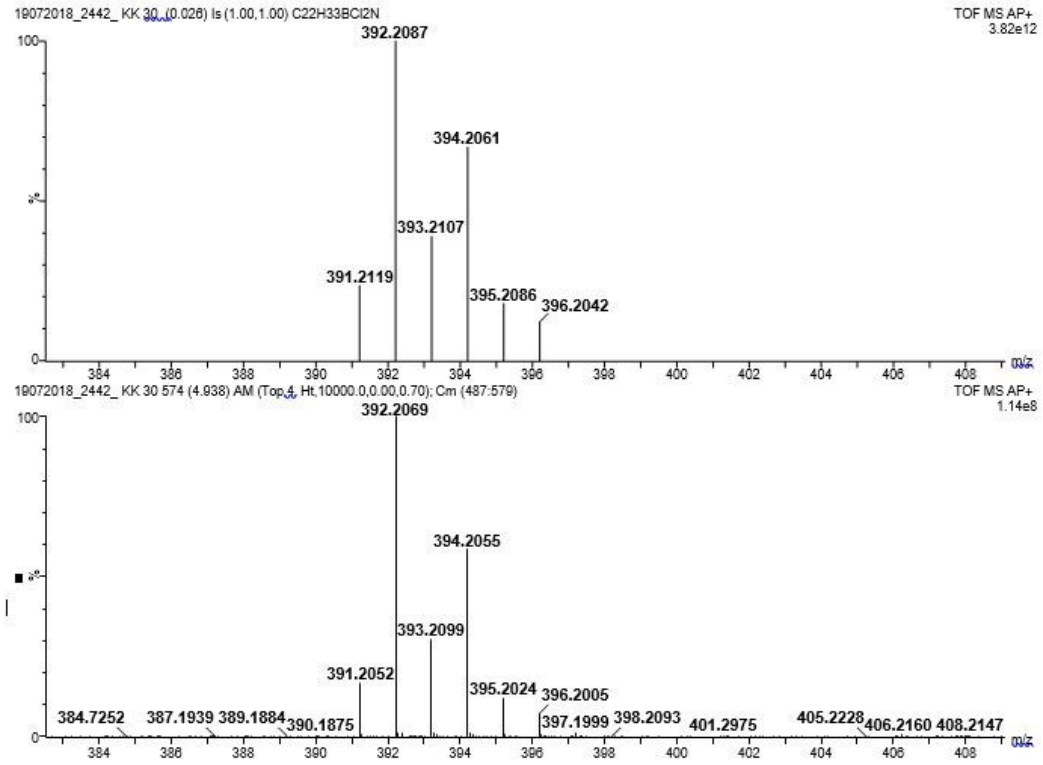


Fig. S21 HRMS spectrum of [BICAAC-BCl_3] adduct (**5**).

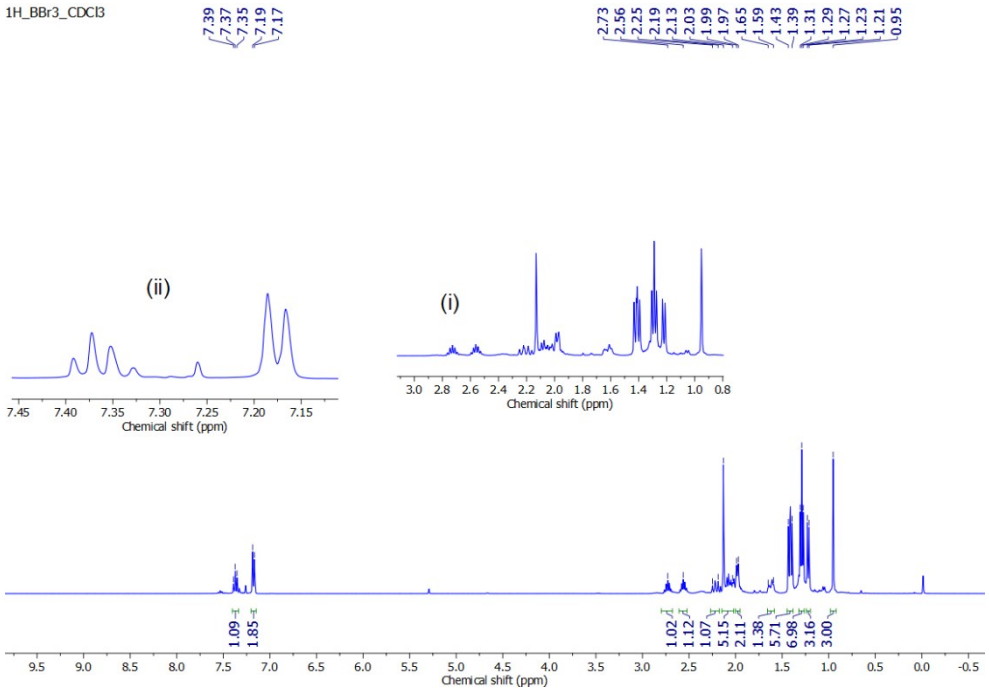


Fig. S22 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of [BICAAC-BBr_3] adduct (**6**). Insets (i) and (ii) show expansion of selected spectral region.

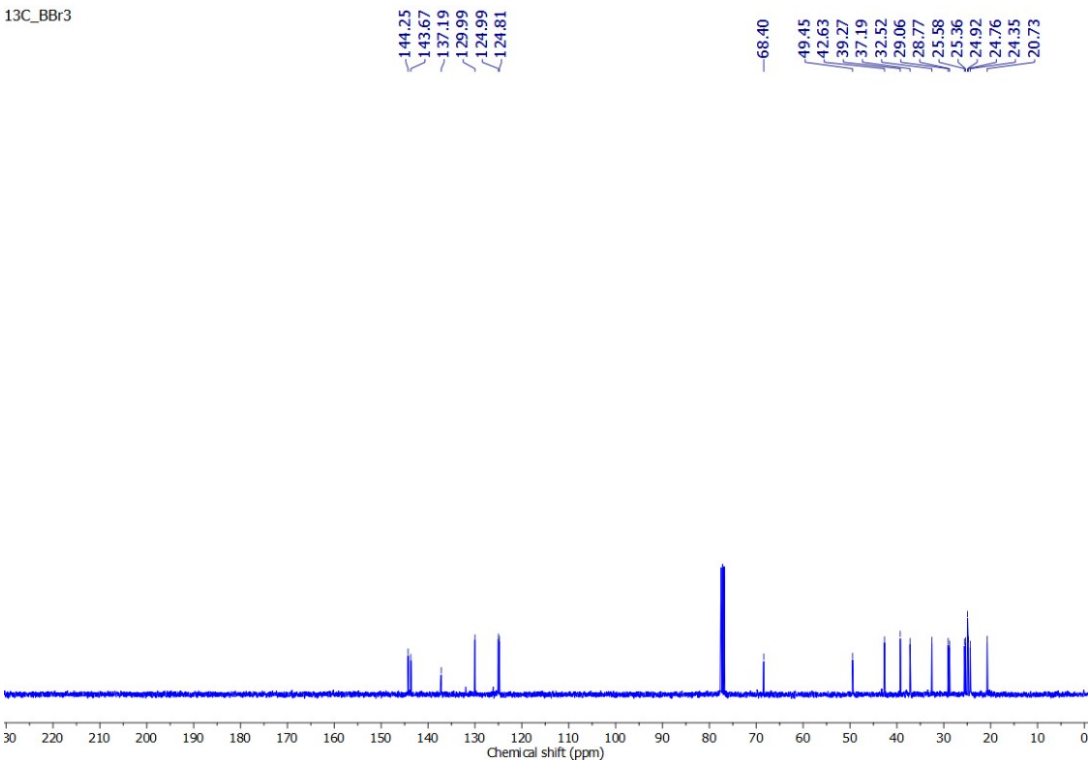


Fig. S23 $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of [BICAAC-BBr_3] adduct (**6**).

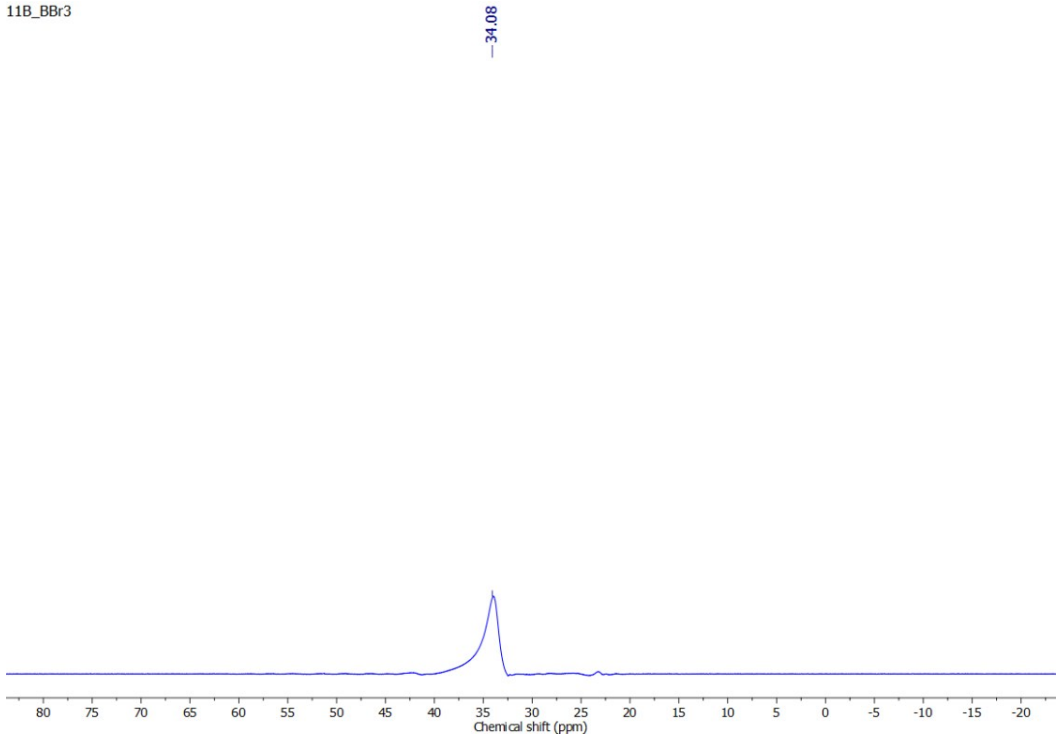


Fig. S24 ^{11}B NMR spectrum (128 MHz, $CDCl_3$) of [BICAAC-BBr_3] adduct (**6**).

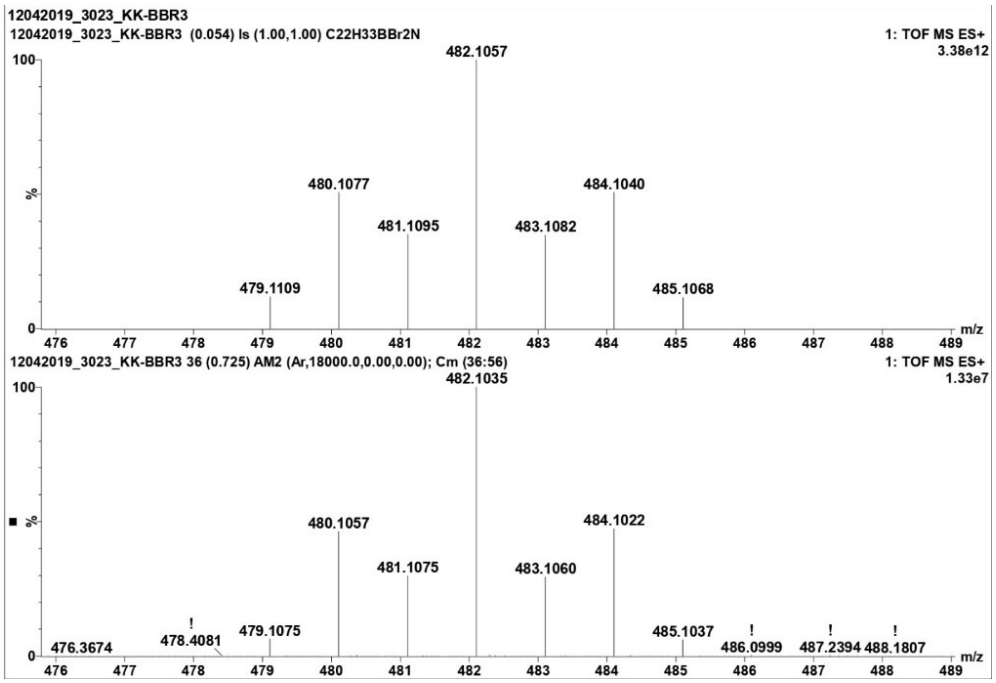


Fig. S25 HRMS spectrum of [BICAAC-BBr_3] adduct (**6**).

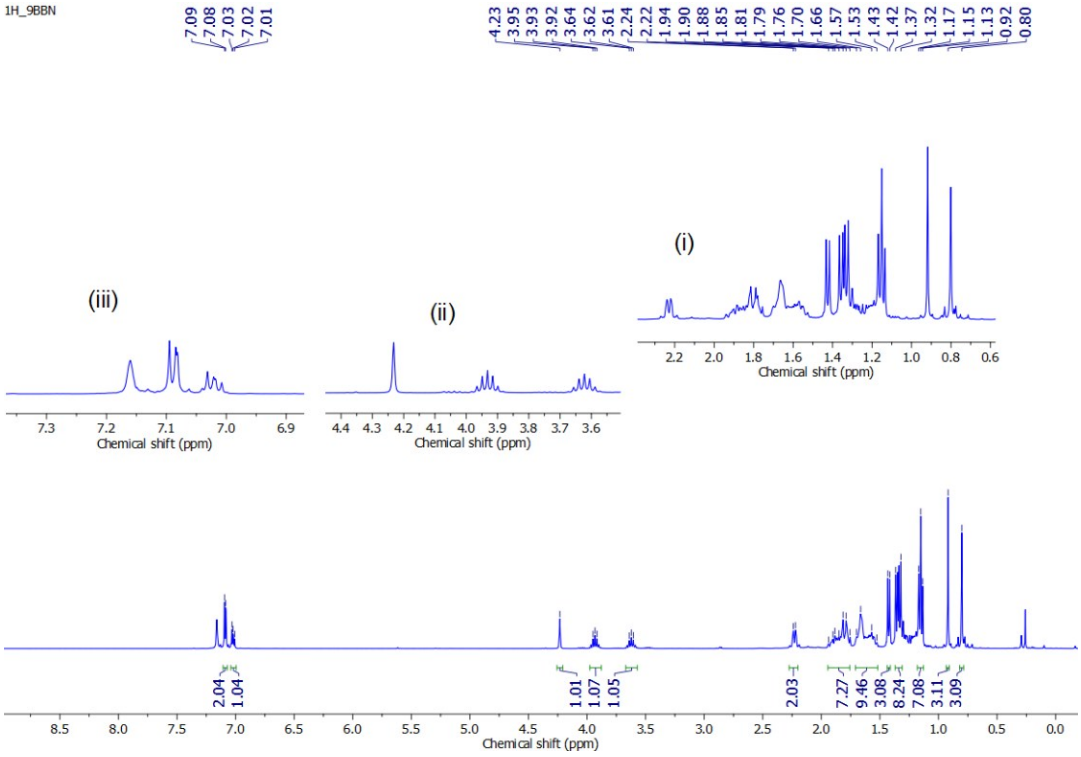


Fig. S26 ^{1}H NMR spectrum (400 MHz, C_6D_6) of carbene B-H insertion product, BICAAC(H)-(9-BBN) (**7**). Insets (i), (ii) and (iii) show expansion of selected spectral region.

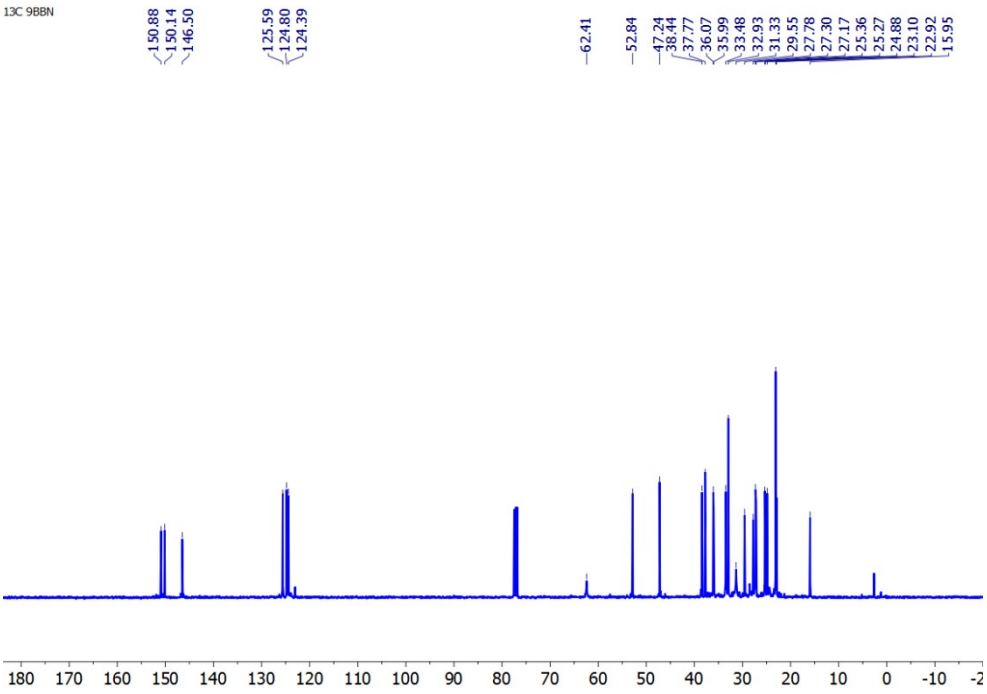


Fig. S27 $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of carbene B-H insertion product, BICAAC(H)-(9-BBN) (**7**).

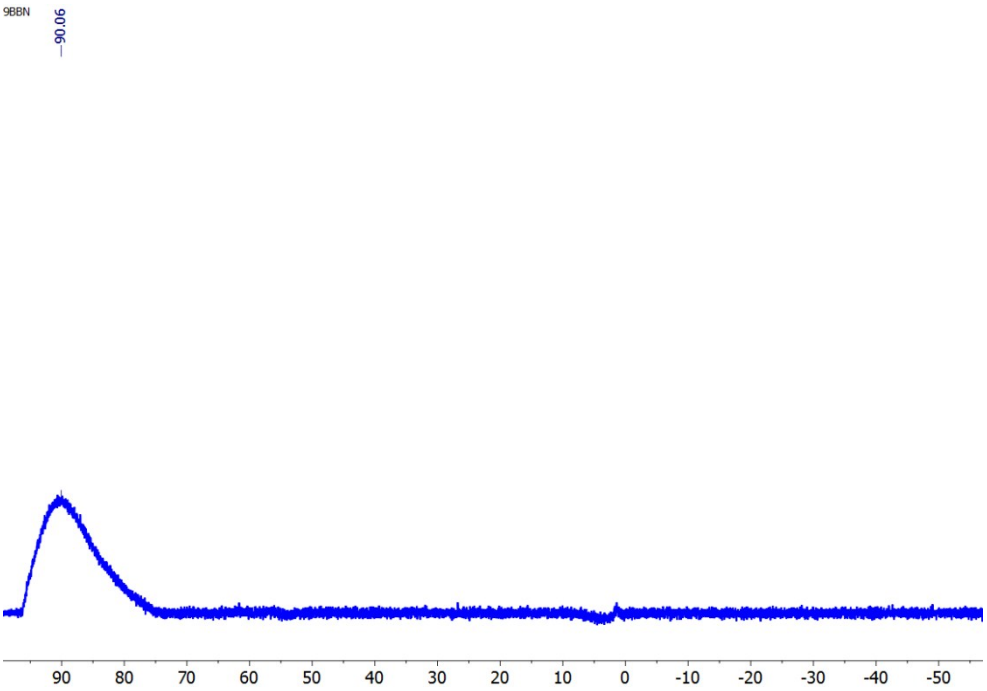


Fig. S28 ^{11}B NMR spectrum (128 MHz, $CDCl_3$) of carbene B-H insertion product, BICAAC(H)-(9-BBN) (**7**).

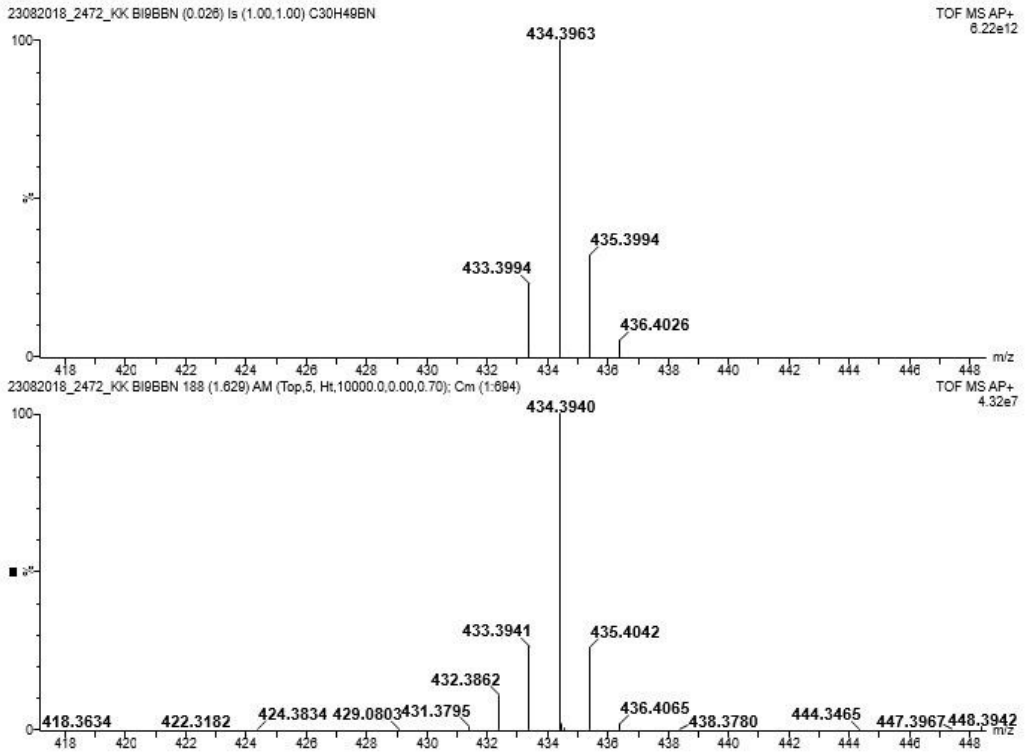


Fig. S29 HRMS spectrum of carbene B-H insertion product, BICAAC(H)-(9-BBN) (**7**).

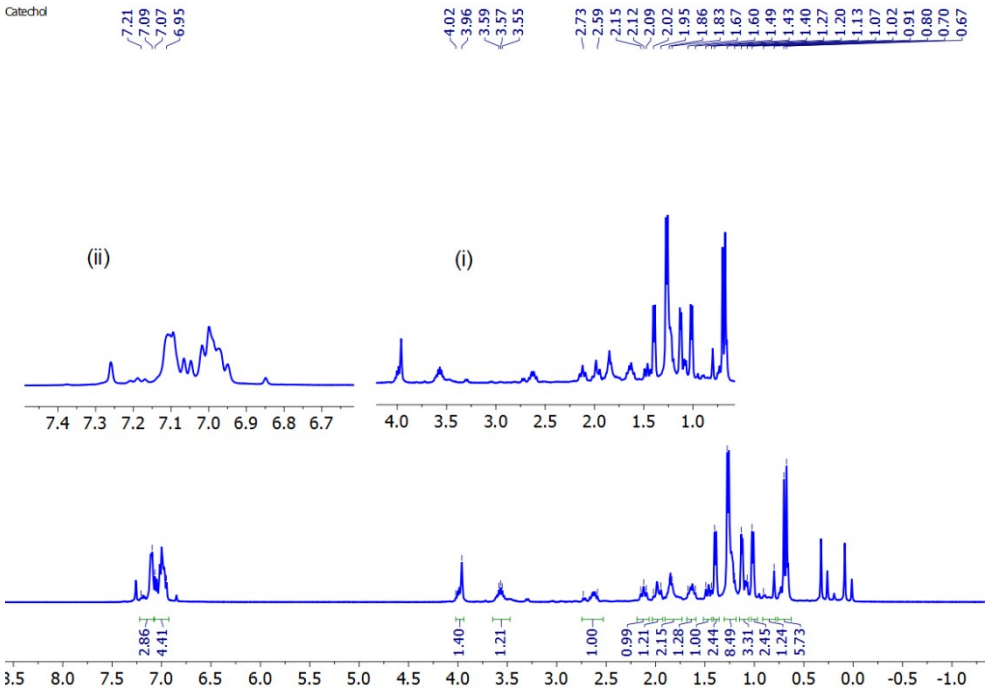


Fig. S30 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of the diastereomeric mixture, [BICAAC(H)-Bcat] (**8**). Insets (i) and (ii) show expansion of selected spectral region.

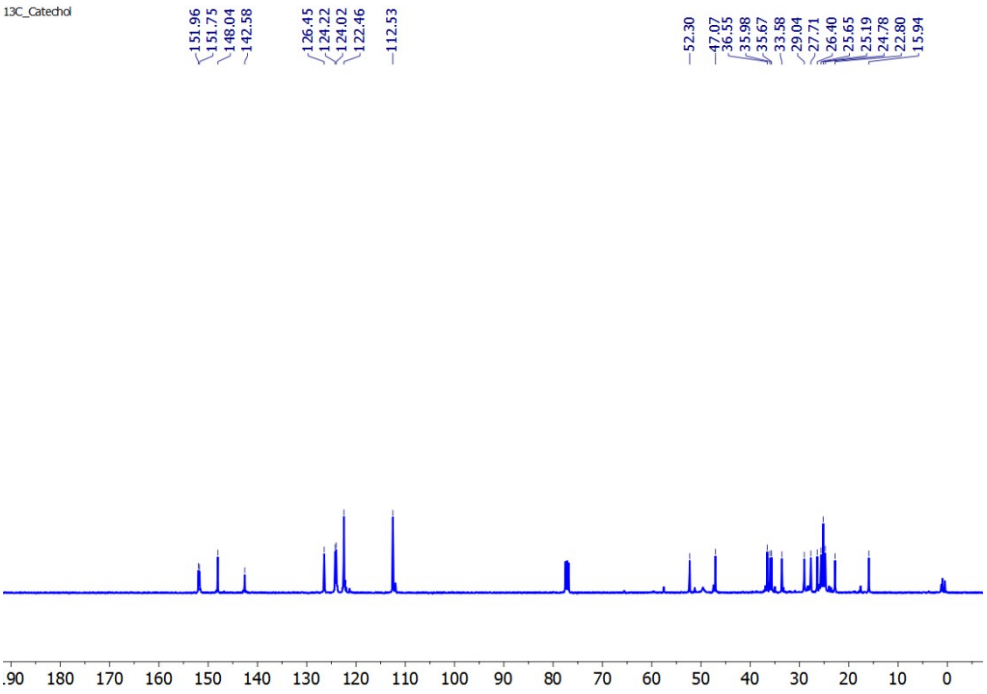


Fig. S31 $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of the diastereomeric mixture, [BICAAC(H)-Bcat] (**8**).

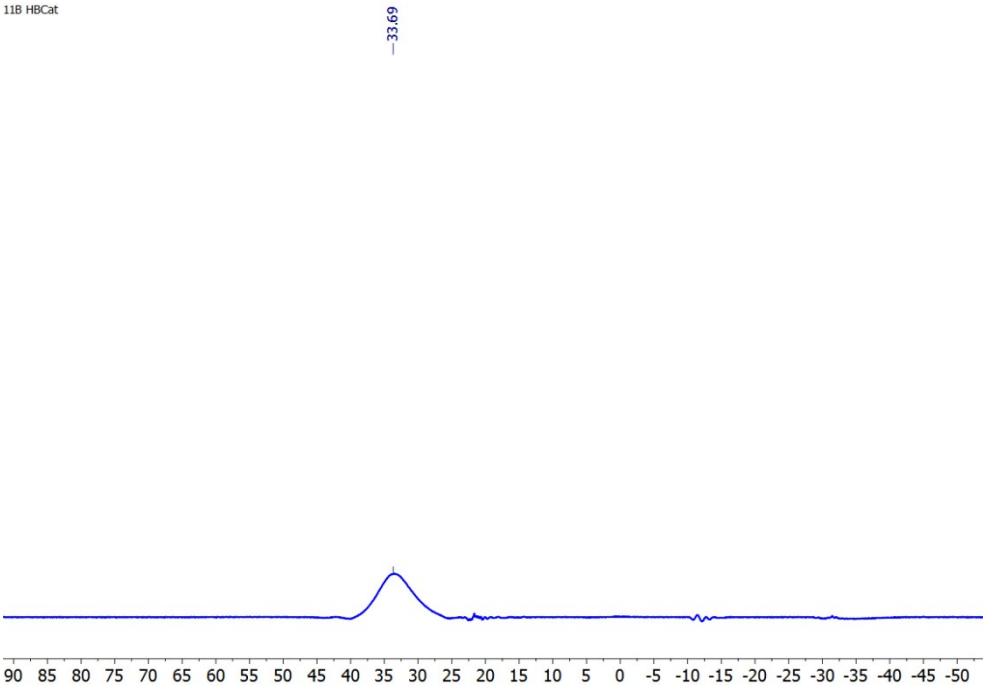


Fig. S32 ^{11}B NMR spectrum (128 MHz, $CDCl_3$) of the diastereomeric mixture, [BICAAC(H)-Bcat] (**8**).

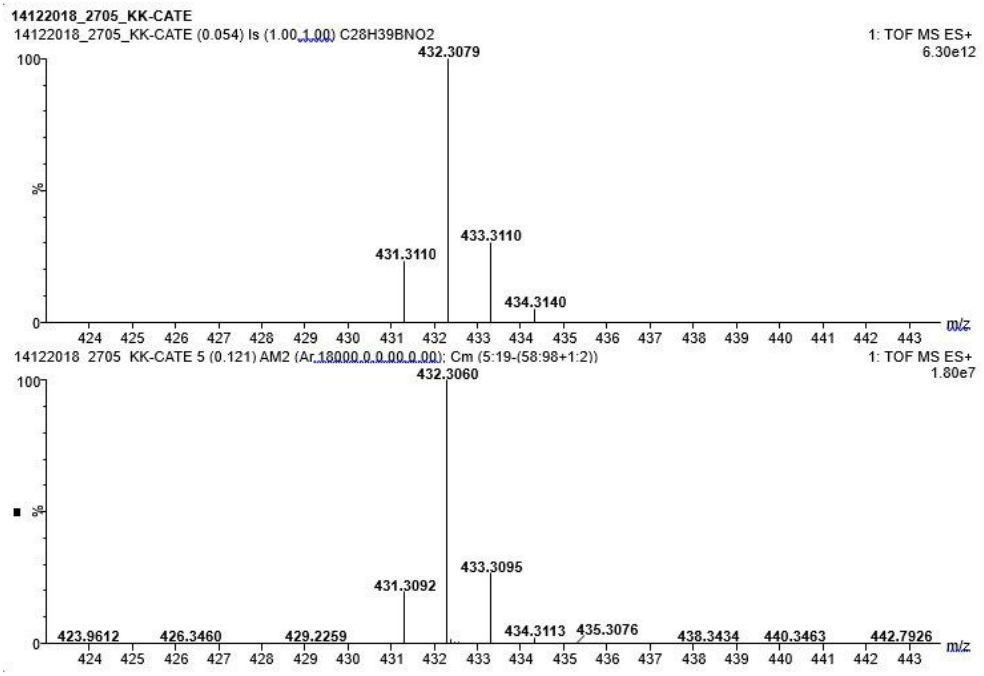


Fig. S33 HRMS spectrum of carbene B-H insertion product, [BICAAC(H)-Bcat] (**8**).

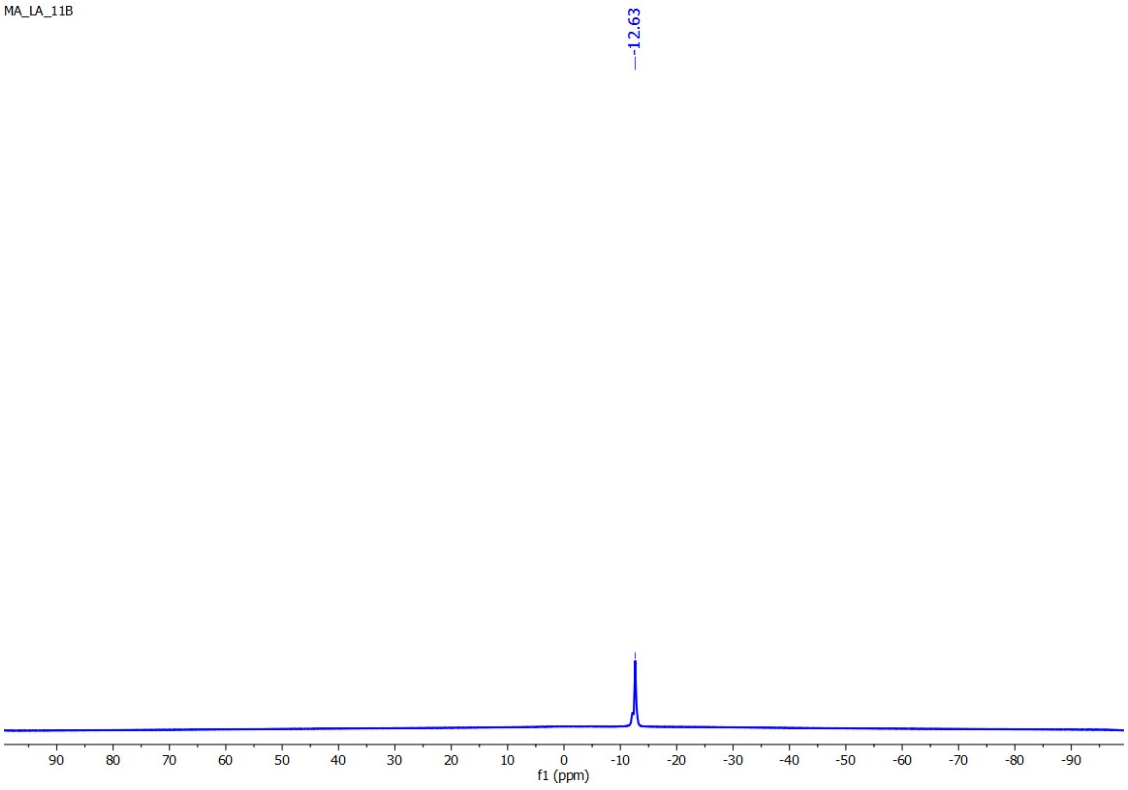


Fig. S34 ^{11}B NMR spectrum (128 MHz, $CDCl_3$) of the [BICAAC-B(C_6F_5)$_3$] adduct.

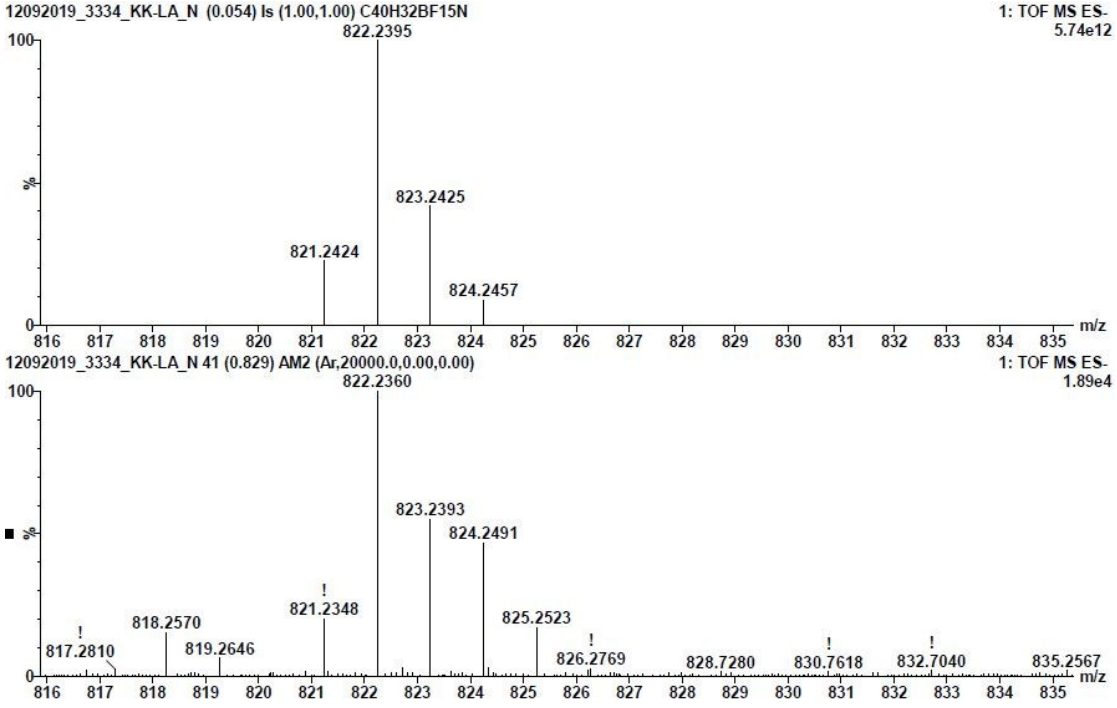


Fig. S35 HRMS spectrum of [BICAAC-B(C_6F_5)$_3$] adduct.

1.4 Single crystal X-ray characterization of compounds 1-8

The single crystal X-ray diffraction data of adduct **1-3** and complexes **7-8** were collected on a Bruker AXS KAPPA APEX-II CCD diffractometer with MoKα radiation using omega scans equipped with Oxford Cryosystem 700 plus with a sample to detector distance of 6 cm with the variable position of the detector. Unit cell determination, refinement and data collection were done using the Bruker APPEX-II suite [3], data reduction and integration were performed using SAINT v8.34A (Bruker, 2013) [4], and absorption corrections and scaling were done using SADABS-2014/5 (Bruker,2014/5) [5]. Single crystal X-ray diffraction data of **4, 5** and **6** were collected using a Rigaku XtaLAB mini diffractometer equipped with Mercury375M CCD detector. The data were collected with MoKα radiation (λ = 0.71073 Å) using omega scans. During the data collection, the detector distance was 49.9 mm (constant) and the detector was placed at 2θ = 29.85° (fixed) for all the data sets. The data collection and data reduction were done using Crystal Clear suite [6]. All the crystal structures were solved through OLEX2 [7] package using XT [8] and the structures were refined using XL [8]. All non-hydrogen atoms were refined anisotropically. All figures were generated using Mercury 3.2. Complex **2** contains two molecules A and B in the asymmetric unit, molecule A contains boron atom B1(B1A and B1B as treated as a disordered part) has disorder around the B1-C1 bond, as seen in two orientation of B1-Cl1 bond (B1A-Cl1A and B1B-Cl1B) further this molecule, BICAAC unit is found to be disordered with C9 (C9A and C9B) being located on C3 and C7 respectively. The molecule B is disordered about B2-C24 bond thereby generating two orientation of B2-Cl2 bond (B2A-Cl2A, B2B-Cl2B). All the geometric data reported here are taken from the CIF.

Table S1 Crystallographic data for complexes 1-4

Compound[a]	**1**	**2**	**3**	**4**
Chemical formula	$C_{22}H_{36}BN$	$C_{22}H_{34}BCl_2N$	$C_{22}H_{35}BClN$	$C_{22}H_{33}BF_3N$
Molar mass	325.33	394.21	359.77	379.30
Crystal system	orthorhombic	monoclinic	orthorhombic	orthorhombic
Space group	*Pbca*	$P2_1/n$	*Pbca*	$Pca2_1$
T [K]	100.0(2)	100.0(2)	100.0(2)	100.02(10)
a [Å]	15.094(3)	9.2720(2)	15.3620(11)	17.8370(5)
b [Å]	15.236(3)	15.9647(3)	18.1323(12)	23.3635(7)
c [Å]	17.615(4)	15.3820(3)	30.142(2)	15.3109(6)
α [°]	90	90	90	90
β [°]	90	106.311(1)	90	90
γ [°]	90	90	90	90
V [Å^3]	4050.8(1)	2185.27(8)	8396.0(1)	6380.6(4)
Z	8	4	8	4
D(calcd.) [g·cm^{-3}]	1.067	1.198	1.138	1.185
μ(Mo-K_α) [mm^{-1}]	0.060	0.303	0.187	0.085
Reflections collected	15760	9914	36531	31150
Independent reflections	3579	3636	7419	11255
Data/restraints/parameters	3579/0/236	3636/0/246	7419/0/490	11255/0/751
$R1$,$wR2[I>2\sigma(I)]$[a]	0.0502, 0.1151	0.0351, 0.0761	0.0862, 0.2082	0.0668, 0.1782
R1, wR2 (all data)[a]	0.0839, 0.1319	0.0503, 0.0812	0.1913, 0.2616	0.0898, 0.2029
GOF	1.044	0.962	1.045	1.036
CCDC	1935353	1935354	1935355	1954942

[a] $R1 = \Sigma||Fo| - |Fc||/\Sigma|Fo|$. $wR2 = [\Sigma w(|Fo^2| - |Fc^2|)^2/\Sigma w|Fo^2|^2]^{1/2}$

Table S2 Crystallographic data for complexes 5-8

[a] $R1 = \Sigma||Fo| - |Fc||/\Sigma|Fo|$. $wR2 = [\Sigma w(|Fo^2| - |Fc^2|)^2/\Sigma w|Fo^2|^2]^{1/2}$

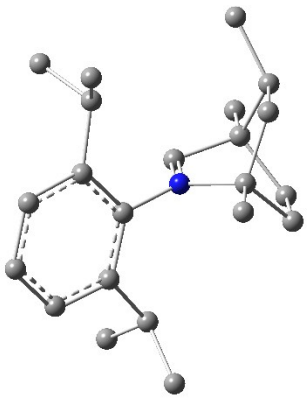
Compound[a]	**5**	**6**	**7**	**8**
Chemical formula	$C_{22}H_{33}BCl_3N$	$C_{22}H_{33}BBr_3$ N	$C_{30}H_{48}BN$	$C_{28}H_{38}BO_2$
Molar mass	428.65	528.89	433.50	431.40
Crystal system	monoclinic	monoclinic	monoclinic	triclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P\ \bar{1}$
T [K]	200.0(1)	200.0(1)	100.0(2)	100.0(2)
a [Å]	16.5507(7)	16.6037(4)	15.720(3)	10.1548(9)
b [Å]	17.6333(6)	17.7087(3)	10.4248(17)	15.6206(13)
c [Å]	17.2854(7)	17.5684(4)	16.049(3)	16.2411(14)
α [°]	90	90	90	72.926(2)
β [°]	114.292(5)	114.211(3)	98.578(4)	83.939(2)
γ [°]	90	90	90	89.112(2)
V [Å^3]	4598.0(4)	4711.27(18)	2600.7(8)	2448.6(4)
Z	4	4	4	4
D(calcd.) [g·cm^{-3}]	1.238	1.491	1.107	1.170
μ(Mo-K_α) [mm^{-1}]	0.406	5.142	0.062	0.071
Reflections collected	52223	53396	27365	34359
Independent reflections	15988	16658	4632	8661
Data/restraints/parameters	15988/0/501	16658/0/501	4625/0/296	8661/0/591
$R1$,$wR2$[$I>2\sigma(I)$][a]	0.0701/0.1727	0.0370/0.0716	0.0401/0.0937	0.0424/0.0937
R1, wR2 (all data)[a]	0.1473/0.2205	0.0738/0.0835	0.0496/0.0999	0.0651/0.1043
GOF	1.047	1.023	1.026	1.006
CCDC	1935356	1935357	1935358	1935359

2 Computational Results

To rationalize the processes involved in insertion of carbene carbon of BICAAC into the hydroboranes, we optimized the geometry and looked at the change in MOs and ESPs of all the steps involved in the process including possible adducts between BICAAC and boranes, intermediate steps during adduct formation and B-H activation, and calculated free energies in their ground states using density functional theory (DFT). The geometry optimization, frequency calculation and NBO analysis of all these structures have been carried out at B3LYP/6-31+G(d,p) level using Gaussian09 suit of the programme. The transition states were also investigated and confirmed by the IRC calculation employed in Gaussian09.[9] These calculations are in excellent agreement with the experimental observations and showed the carbene insertion into the B-H bond in case of 9-BBN and catechol borane (HBcat), and adduct formation with BH_3, BH_2Cl, and $BHCl_2$ through a series of transformations between BICAAC and boranes. The visualization of MOs and ESPs was done using Molden [10] and Chemcraft.[11]

2.1 Optimized geometry of BICAAC and molecules 1-3 and 5-8

Structure of singlet BICAAC



N	0.32210100	-0.18238100	0.02848500	H	3.23758500	-0.31182600	-2.67838900
C	1.01308300	-0.38380900	-1.07990400	C	3.15383900	0.15847600	0.19154400
C	2.41778700	-0.87351300	-0.73384500	H	4.06011600	-0.35117700	0.55184500
C	3.21207500	-1.17771800	-2.00975800	C	3.61027900	1.44232100	-0.51942800
H	2.73765500	-1.99640300	-2.56300800	H	4.08059000	2.12450900	0.20081600
H	4.24521900	-1.47291800	-1.77909100	H	2.76855100	1.97066100	-0.98200800

H	4.34590200	1.23460400	-1.30344400	H	-3.55509200	-3.07774000	0.70394500
C	2.24019600	0.47206500	1.40824400	C	-2.09976100	-2.79338200	-1.68865000
H	2.76899700	0.29378200	2.35330200	H	-3.17322600	-2.71250700	-1.89951800
H	1.94716500	1.52785200	1.41356700	H	-1.81896600	-3.85061000	-1.77926700
C	0.97438500	-0.41314500	1.38604200	H	-1.55784100	-2.22602900	-2.45253500
C	0.05042600	-0.10453300	2.56023400	C	-3.41634600	-0.36960000	-0.23920500
H	-0.25796000	0.94564900	2.57456200	H	-4.19834200	-1.12051900	-0.31489100
H	0.58378200	-0.31103900	3.49624700	C	-3.76547800	0.97756900	-0.23071900
H	-0.85352200	-0.72111700	2.54547000	H	-4.81059200	1.27296900	-0.28312900
C	1.45883000	-1.88360900	1.40245800	C	-2.76545000	1.94451900	-0.18035300
H	2.10005200	-2.01266400	2.28344300	H	-3.04094300	2.99528800	-0.21199500
H	0.60985200	-2.56249800	1.53483500	C	-1.41105700	1.59148800	-0.10607100
C	2.23138400	-2.18108300	0.09796300	C	-0.36116300	2.69762700	-0.14992600
H	1.69261200	-2.91263000	-0.51635300	H	0.60998400	2.24792200	0.05882200
H	3.21777800	-2.61535200	0.30748300	C	-0.27319300	3.29943900	-1.56843000
C	-1.07975000	0.21844600	-0.07205800	H	-0.04341700	2.52267500	-2.30536900
C	-2.07685700	-0.77774700	-0.17042200	H	0.51426800	4.06296800	-1.61226600
C	-1.76224300	-2.26758500	-0.27793300	H	-1.21900800	3.77477600	-1.85684300
H	-0.68721000	-2.39518200	-0.14885000	C	-0.59411600	3.79700700	0.90393000
C	-2.46390800	-3.10591000	0.80850100	H	-1.51636400	4.35874500	0.71417000
H	-2.21899800	-2.74965500	1.81630400	H	0.23452100	4.51573200	0.88718600
H	-2.15439500	-4.15605800	0.73614300	H	-0.66124800	3.38051500	1.91613300

Zero-point correction = 0.504158 (Hartree/Particle)

Thermal correction to Energy = 0.528125

Thermal correction to Enthalpy = 0.529069

Thermal correction to Gibbs Free Energy = 0.452678

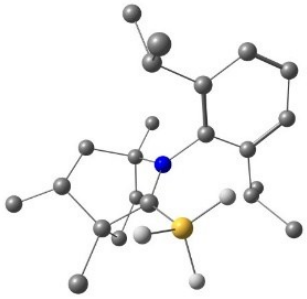
Sum of electronic and zero-point Energies = -912.435874

Sum of electronic and thermal Energies = -912.411907

Sum of electronic and thermal Enthalpies = -912.410962

Sum of electronic and thermal Free Energies = -912.487354

Structure of 1



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C	-0.94994700	-0.21210100	-1.38722300	H	1.81483100	4.18878100	-0.90075000
C	-2.94326400	0.69074500	-0.08101900	H	0.72991500	2.61164200	2.40662800
H	-2.73245200	1.54942700	0.57030800	H	1.86563500	3.78021700	1.70039500
C	-2.09696800	0.82334800	-1.37278600	H	0.13231100	4.14830600	1.74224800
H	-2.71640100	0.63536400	-2.25937700	C	1.66513400	-2.38720500	0.11264500
H	-1.69594900	1.83629500	-1.48345900	C	2.15462700	-3.00568100	1.43946600
C	-1.59868300	-1.61501100	-1.45599700	C	2.13531700	-3.23063900	-1.08943700
H	-2.18587600	-1.66757000	-2.38065700	H	0.57373000	-2.42383300	0.13689300
H	-0.82002200	-2.37959100	-1.53550100	H	1.79671500	-2.42589800	2.29512400
C	-2.48707200	-1.83129800	-0.21320800	H	1.77982800	-4.03238700	1.53739500
H	-3.52545100	-2.03442300	-0.49751300	H	3.24999800	-3.04464900	1.48151700
H	-2.15148500	-2.69817500	0.36722200	H	1.77502200	-2.82423900	-2.04197900
N	-0.25240600	-0.12198800	-0.04354000	H	3.22940100	-3.27840200	-1.14389800
C	1.18115200	0.15445000	0.01486600	H	1.76503300	-4.25938200	-0.99890200
C	1.61946600	1.49556400	0.05527400	B	-0.43455000	-0.25949300	2.53373500
C	2.09126300	-0.92438600	0.00547400	H	0.74165000	0.00626600	2.60682900
C	2.99929000	1.73544200	0.01252500	H	-1.13185300	0.54889900	3.13442500
C	3.45982900	-0.62553500	-0.03866900	H	-0.68260700	-1.35735300	3.02163200
C	3.91549400	0.68946000	-0.05151100	H	0.66802600	3.28327100	-1.89724700
H	3.36184000	2.75926000	0.04446000	C	-3.32364900	-0.83223200	1.95081800
H	4.18066300	-1.43865000	-0.04753900	H	-4.33220500	-1.13527300	1.64798300
H	4.98188300	0.89816500	-0.08740100	H	-2.89922900	-1.62783300	2.56778500
C	0.67381800	2.68376700	0.22075800	H	-3.40276000	0.06002800	2.57905000
C	0.82101900	3.72586200	-0.90581500	C	-4.44736800	0.72138100	-0.39013100
C	0.86440700	3.34256300	1.60390800	H	-5.05466700	0.75498600	0.51932300

H	-4.68470500	1.61748500	-0.97704900	H	0.44894800	1.01127000	-2.54265700
H	-4.76324700	-0.14832300	-0.98017500	H	0.79276400	-0.72286200	-2.60826900
C	-0.00933500	0.01910200	-2.56717600	H	-0.59183400	-0.06088500	-3.49226500

Zero-point correction = 0.538083 (Hartree/Particle)

Thermal correction to Energy = 0.563566

Thermal correction to Enthalpy = 0.564510

Thermal correction to Gibbs Free Energy = 0.486382

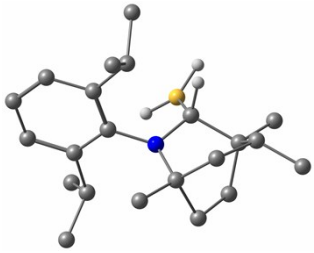
Sum of electronic and zero-point Energies = -939.107422

Sum of electronic and thermal Energies = -939.081940

Sum of electronic and thermal Enthalpie s= -939.080995

Sum of electronic and thermal Free Energies = -939.159123

Structure of 1TS



C	0.70493400	0.10656400	-1.31376000	N	0.09678900	0.17251600	-0.04818500
C	2.82272200	-0.16644300	-0.80295000	C	-1.33133300	-0.05642200	-0.03022200
C	0.94491200	0.28048100	1.17859100	C	-2.17254800	1.08988200	-0.07943500
C	3.24682300	0.97439400	0.15825600	C	-1.90638400	-1.35461600	-0.02668100
H	3.54882100	1.83627800	-0.44192300	C	-3.56182000	0.91596900	-0.04163300
C	2.02628800	1.39076000	1.03097800	C	-3.30373300	-1.47249500	0.00468900
H	2.37702700	1.64630400	2.03910800	C	-4.13001100	-0.35352100	0.01311200
H	1.55787900	2.29130500	0.62235200	H	-4.21050900	1.78750700	-0.06965200
C	1.69492400	-1.06246000	1.33920600	H	-3.75244800	-2.46255100	0.01784900
H	2.38582700	-0.97102800	2.18684000	H	-5.21068800	-0.47061300	0.04369900
H	0.99310000	-1.85752500	1.60675600	C	-1.61632600	2.50408900	-0.23122400
C	2.47190800	-1.41271400	0.04757600	C	-2.17823000	3.49255600	0.80909500
H	3.42016500	-1.90327300	0.31464700	C	-1.86055100	3.03101600	-1.66167300
H	1.93192000	-2.14692000	-0.55866100	H	-0.53504900	2.44848700	-0.08942300

H	-1.67142500	4.46122400	0.71808900	H	-2.03600900	3.13058500	1.83393900
H	-3.25087100	3.67207200	0.66727500	H	1.89373600	2.12824500	-1.67773400
H	-1.41584700	2.36633000	-2.40991900	C	3.85702900	-0.54762900	-1.86252100
H	-2.93358300	3.11400200	-1.87660500	H	3.43371000	-1.23593900	-2.60143500
H	-1.41331200	4.02542700	-1.78440800	H	4.24332300	0.32239800	-2.40150800
C	-1.08680400	-2.63879900	-0.09770400	H	4.70774700	-1.06256900	-1.38598800
C	-1.38683500	-3.43369200	-1.38623500	C	4.48854800	0.62262400	1.01586100
C	-1.28843400	-3.53075800	1.14448700	H	5.34748500	0.36376100	0.38627400
H	-0.03471800	-2.35839600	-0.13342600	H	4.77350100	1.50017300	1.60976600
H	-1.23225700	-2.81939800	-2.28058900	H	4.32253900	-0.20439100	1.71335600
H	-0.72828200	-4.30872400	-1.45589800	C	0.08106500	0.56667200	2.41070700
H	-2.42212200	-3.79459500	-1.40583100	H	-0.38083600	1.55750500	2.35745100
H	-1.07714700	-2.98606000	2.07174700	H	-0.71519200	-0.17353000	2.53533800
H	-2.31796400	-3.90304600	1.20838800	H	0.71223000	0.53670600	3.30567600
H	-0.62323300	-4.40245200	1.10244900	H	0.33031600	-0.75845300	-1.88125900
B	1.65619700	1.01049500	-2.02254900	H	1.92679800	0.69831300	-3.14782700

Zero-point correction = 0.538722 (Hartree/Particle)

Thermal correction to Energy = 0.563657

Thermal correction to Enthalpy = 0.564601

Thermal correction to Gibbs Free Energy = 0.487545

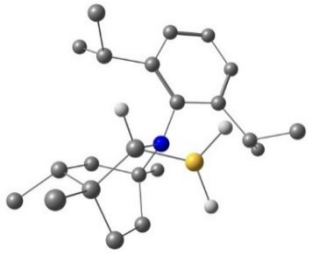
Sum of electronic and zero-point Energies = -939.034203

Sum of electronic and thermal Energies = -939.009269

Sum of electronic and thermal Enthalpies = -939.008324

Sum of electronic and thermal Free Energies = -939.085380

Structure of 1BA



C	-1.16528000	-0.27385600	1.30851700	H	-1.08729700	1.94804600	0.06652500
C	-2.57140100	-0.64768500	0.79757700	H	-1.36615300	4.03595900	-1.12742200
C	-0.73311500	-1.04510200	-1.04570600	H	0.37642100	4.32502800	-1.17513600
C	-2.89502500	0.24170800	-0.44050600	H	-0.22763100	2.79735200	2.26187000
H	-2.82968800	1.28413800	-0.10202200	H	0.50028600	4.17608800	1.42960900
C	-1.79619700	-0.01917200	-1.51262700	H	-1.26042200	3.97994700	1.43101300
H	-2.25655500	-0.43275900	-2.41976300	C	2.64126500	-1.78862700	0.20950100
H	-1.30639000	0.90884500	-1.82416100	C	3.35254800	-2.12234800	1.54057500
C	-1.47552400	-2.35678400	-0.70796600	C	3.47464600	-2.36742600	-0.95720800
H	-1.91097000	-2.72549800	-1.64501800	H	1.67860200	-2.30079300	0.22160300
H	-0.75494500	-3.11035300	-0.37695500	H	2.78950100	-1.75438800	2.40101100
C	-2.57701300	-2.12625400	0.35625100	H	3.46220800	-3.20944400	1.64350400
H	-3.56474800	-2.39039400	-0.03855500	H	4.35682800	-1.68197300	1.57254900
H	-2.40725000	-2.76422700	1.22794000	H	3.07705400	-2.09051200	-1.93848000
N	-0.06455300	-0.51745500	0.24071800	H	4.51535100	-2.02461400	-0.91792500
C	1.11828600	0.35768000	0.09939800	H	3.49276900	-3.46256500	-0.89278100
C	1.04455800	1.77398700	0.01551900	B	-0.09080700	-1.31424000	1.73751900
C	2.39759300	-0.27999000	0.06842200	H	-0.31446700	2.98277700	-2.09457400
C	2.23781100	2.50823600	-0.09771800	H	-1.12284700	0.73495400	1.71368300
C	3.54478800	0.51009400	-0.06355900	C	-3.55533800	-0.42193200	1.95489000
C	3.48023200	1.89616800	-0.14628800	H	-3.22361400	-0.96185700	2.84963100
H	2.18158700	3.59164800	-0.14961400	H	-3.63367000	0.64222500	2.21405800
H	4.51628000	0.02529400	-0.08618300	H	-4.55932400	-0.78150300	1.70190600
H	4.38685700	2.48889900	-0.23949400	C	-4.30547000	0.08106800	-1.03236300
C	-0.23264400	2.61397700	0.07173800	H	-5.08741900	0.31233500	-0.30034000
C	-0.38775000	3.53990300	-1.15360600	H	-4.43454500	0.76953000	-1.87743900
C	-0.30802700	3.43727500	1.37601600	H	-4.48474800	-0.93266500	-1.41033000

C	0.26899900	-1.29244600	-2.17296000	H	-0.28543800	-1.57011100	-3.07640700
H	0.86352700	-0.40427800	-2.40586400	H	0.80446000	-0.91128400	2.41810600
H	0.94540900	-2.11577400	-1.93828200	H	-0.27077000	-2.49553100	1.70374800

Zero-point correction = 0.542726 (Hartree/Particle)

Thermal correction to Energy = 0.567071

Thermal correction to Enthalpy = 0.568016

Thermal correction to Gibbs Free Energy = 0.493250

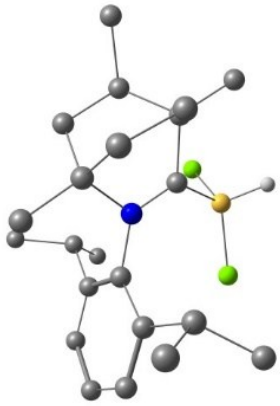
Sum of electronic and zero-point Energies = -939.090118

Sum of electronic and thermal Energies = -939.065772

Sum of electronic and thermal Enthalpies = -939.064828

Sum of electronic and thermal Free Energies = -939.139594

Structure of 2



C	-1.01049100	-0.16337300	0.71072100	H	-0.49093700	-3.11410100	-0.90449700
C	-2.41830600	-0.74444000	0.47848700	C	-2.20812000	-2.25705100	0.15642100
C	-0.79488000	-1.05239500	-1.54149700	H	-3.19020400	-2.72110900	0.01962200
C	-2.99050500	0.00403800	-0.78524800	H	-1.76147500	-2.74131600	1.03253800
H	-3.01699500	1.06465100	-0.51307500	N	-0.19911900	-0.37227100	-0.30855300
C	-2.00513300	-0.19223300	-1.96438700	C	1.22536800	-0.01527400	-0.35564100
H	-2.49540100	-0.71053700	-2.79802500	C	1.60642400	1.23985400	-0.87675900
H	-1.65656300	0.76885800	-2.35452100	C	2.17428500	-0.98735100	0.03609500
C	-1.32510500	-2.43192100	-1.08888300	C	2.97724900	1.48077000	-1.04274300
H	-1.89433600	-2.85192600	-1.92661500	C	3.52820500	-0.68334000	-0.14988900

C	3.93205600	0.53090300	-0.69665800	H	1.86752300	-3.50970800	-1.17193700
H	3.30045100	2.43996600	-1.43658200	H	3.36882500	-3.55987400	-0.24223000
H	4.28000000	-1.40778600	0.15024500	H	1.95792800	-4.46747500	0.31781600
H	4.98925800	0.74342400	-0.83415300	B	-0.71708200	0.65097300	2.09714100
C	0.62965200	2.36776700	-1.21138700	H	-1.23129000	0.07110200	3.00705700
C	0.63185500	2.73062100	-2.71152100	H	0.37095300	1.88050200	-3.35187500
C	0.93130700	3.62586500	-0.36858900	Cl	1.04550100	1.02179900	2.59012400
H	-0.37942100	2.04626700	-0.94126700	Cl	-1.67155200	2.29410100	1.79262000
H	-0.09410500	3.53001000	-2.90414600	C	-3.37721800	-0.64096400	1.67394000
H	1.61588800	3.09395000	-3.03119300	H	-2.96839200	-1.13956700	2.55633600
H	0.96095500	3.39025900	0.69756600	H	-3.59767100	0.39416700	1.94190600
H	1.89047300	4.07474200	-0.65421500	H	-4.31694900	-1.14223600	1.42112500
H	0.14859400	4.37650600	-0.52913100	C	-4.42024900	-0.40166600	-1.17632700
C	1.81763300	-2.32332700	0.69021900	H	-5.14630000	-0.16560000	-0.39303300
C	2.39870200	-2.43226900	2.11679700	H	-4.72001200	0.15063400	-2.07521300
C	2.27639800	-3.53042500	-0.15549300	H	-4.50036500	-1.47117600	-1.40883400
H	0.73032100	-2.37830100	0.78988600	C	0.19769600	-1.20548900	-2.69184400
H	2.08506000	-1.59030100	2.73900300	H	0.57470000	-0.24637800	-3.05138500
H	2.05734300	-3.36288600	2.58736500	H	1.05535800	-1.82647100	-2.42445700
H	3.49492100	-2.45337000	2.09939100	H	-0.32697700	-1.69398100	-3.52083700

Zero-point correction = 0.514248 (Hartree/Particle)

Thermal correction to Energy = 0.541639

Thermal correction to Enthalpy = 0.542583

Thermal correction to Gibbs Free Energy = 0.458508

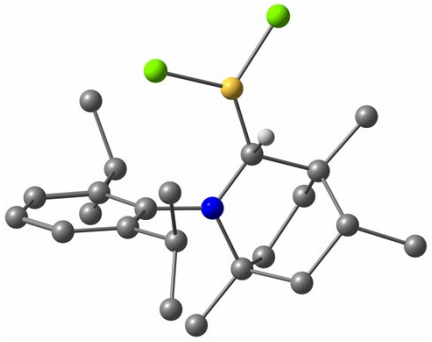
Sum of electronic and zero-point Energies = -1857.797164

Sum of electronic and thermal Energies = -1857.769774

Sum of electronic and thermal Enthalpies = -1857.768829

Sum of electronic and thermal Free Energies = -1857.852904

Structure of 2TS



C	1.10019200	-0.40573800	-0.33959400	C	-1.61550500	3.63892200	-1.15953500
C	2.54256400	-0.14008900	0.22856500	C	-1.45597600	1.91328500	-2.98231900
C	0.70939300	1.27126500	1.44786400	H	-0.15112900	2.07305400	-1.29267200
C	2.81700900	1.39678900	0.03541800	H	-1.03849100	4.33018700	-1.78649900
H	2.72165200	1.57894000	-1.04442700	H	-2.67761400	3.81767500	-1.36472700
C	1.72790700	2.21279100	0.77981200	H	-1.17196800	0.89612400	-3.26307300
H	2.18556600	2.83095800	1.56356500	H	-2.50987500	2.05334400	-3.25242500
H	1.21617200	2.90315100	0.10136500	H	-0.86462400	2.61602700	-3.58294700
C	1.47652500	0.41461900	2.48087400	C	-1.32916300	-1.80594100	1.82774500
H	1.99812500	1.08836900	3.17272700	C	-1.60890700	-3.23044200	1.30347400
H	0.76992500	-0.16469400	3.08232500	C	-1.73895200	-1.69688500	3.31098400
C	2.46994900	-0.49717000	1.73962100	H	-0.24986800	-1.64717800	1.76746500
H	3.47510800	-0.41353400	2.16738500	H	-1.31991800	-3.33490700	0.25359400
H	2.18823100	-1.55300400	1.83167300	H	-1.04631300	-3.96642200	1.89172400
N	0.15934100	0.33644400	0.39993400	H	-2.67259600	-3.48565100	1.38415900
C	-1.27816600	0.23841600	0.24203300	H	-1.53633700	-0.70046300	3.71973900
C	-1.95189700	1.16131200	-0.59833300	H	-2.80899100	-1.89650900	3.44450400
C	-2.00170100	-0.74105100	0.96418600	H	-1.18823100	-2.42972700	3.91412400
C	-3.34937700	1.10602700	-0.66624600	B	0.75364000	-1.37786400	-1.47723100
C	-3.39886300	-0.75433200	0.85763900	H	-1.43338300	3.90448600	-0.11325000
C	-4.07374600	0.16387300	0.05907800	Cl	-0.90975700	-1.63387400	-2.14111300
H	-3.88061500	1.80464500	-1.30761500	Cl	1.91475700	-2.50663300	-2.29064800
H	-3.96800300	-1.50157100	1.40471100	H	1.17666500	0.00754600	-1.61452800
H	-5.15872200	0.13767300	-0.00803400	C	3.69490500	-0.95059300	-0.37878300
C	-1.22380000	2.18024400	-1.47858900	H	3.53753300	-2.02491200	-0.27583200

H	3.86144200	-0.72987000	-1.43696900	H	4.44340200	1.65507800	1.49366800
H	4.61338800	-0.70314600	0.16254300	C	-0.37736500	2.07409100	2.16550400
C	4.22227500	1.87223100	0.44072400	H	-0.92349900	2.73894300	1.49483700
H	5.01200600	1.42834400	-0.17271500	H	-1.10446400	1.42891800	2.66592600
H	4.28566500	2.96011800	0.31454200	H	0.10735800	2.69110500	2.93096800

Zero-point correction = 0.521766 (Hartree/Particle)

Thermal correction to Energy = 0.548919

Thermal correction to Enthalpy = 0.549863

Thermal correction to Gibbs Free Energy = 0.466564

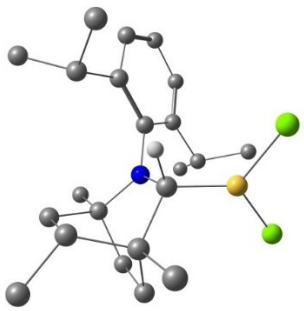
Sum of electronic and zero-point Energies = -1858.370028

Sum of electronic and thermal Energies = -1858.342875

Sum of electronic and thermal Enthalpies = -1858.341931

Sum of electronic and thermal Free Energies = -1858.425230

Structure of 2BA



C	-1.01991400	-0.33061200	0.61100100	C	-1.50663100	-0.96936600	-2.21241000
C	-2.49559700	-0.44663500	0.07268700	H	-1.98011900	-0.82759800	-3.19259600
C	-0.82153100	0.35045400	-1.78178100	H	-0.74136100	-1.74355300	-2.33345600
C	-2.88454600	0.99290500	-0.39545100	C	-2.55606900	-1.39082100	-1.15072700
H	-2.68314700	1.65727100	0.45657500	H	-3.56901700	-1.35036300	-1.56873200
C	-1.95699600	1.38806900	-1.57818700	H	-2.40247500	-2.42673000	-0.84031600
H	-2.54109700	1.43017100	-2.50892800	N	-0.10970000	0.05988800	-0.49826100
H	-1.54230200	2.39201100	-1.43831300	C	1.18856800	0.60951600	-0.17201300

C	1.34060700	1.87782300	0.46286700	H	2.79217100	-3.60521500	-0.57297500
C	2.35863300	-0.14842300	-0.47662300	H	4.02476000	-2.44579600	-0.05141700
C	2.62570600	2.34384600	0.77291300	H	2.68015800	-0.85653300	-3.17774100
C	3.62052400	0.37620900	-0.16124600	H	4.13527100	-1.41418200	-2.34861000
C	3.76429200	1.61020500	0.46092500	H	2.94322100	-2.59047800	-2.91702800
H	2.73589200	3.30931400	1.26022500	B	-0.48458900	-1.61618000	1.39027600
H	4.50905200	-0.20296900	-0.39853600	H	0.32465800	4.01382500	-0.99296500
H	4.75213800	1.99516500	0.70274700	Cl	-0.39369800	-3.24889400	0.71413800
C	0.17480400	2.79470700	0.82753300	Cl	0.05640500	-1.44526500	3.07021200
C	0.25382600	4.14925400	0.09237300	H	-1.05371800	0.46779600	1.36997400
C	0.06603700	3.01361100	2.35132500	C	-3.41669200	-0.93985500	1.19803500
H	-0.74493500	2.31438300	0.50299800	H	-3.10801800	-1.92424400	1.57162900
H	-0.64053800	4.74965800	0.30291700	H	-3.42262000	-0.24457100	2.04767600
H	1.12585000	4.73301300	0.40994400	H	-4.44767700	-1.04661700	0.84448800
H	-0.00694100	2.06175500	2.88919400	C	-4.36432500	1.20027900	-0.75692000
H	0.93884900	3.54936600	2.74344400	H	-5.02902300	1.04277800	0.09952800
H	-0.82354000	3.61074700	2.58934500	H	-4.51499700	2.23115700	-1.10159200
C	2.32839700	-1.54010600	-1.10817100	H	-4.69129800	0.53770900	-1.56770800
C	2.94442200	-2.59811000	-0.16547600	C	0.13398800	0.83991300	-2.86867300
C	3.06009700	-1.59661000	-2.46665900	H	0.66967500	1.74542400	-2.56582500
H	1.28057400	-1.80178600	-1.27400800	H	0.87161700	0.07890500	-3.13143100
H	2.50002100	-2.56885400	0.83356800	H	-0.44185400	1.07392500	-3.77154400

Zero-point correction = 0.525420 (Hartree/Particle)

Thermal correction to Energy = 0.553039

Thermal correction to Enthalpy = 0.553983

Thermal correction to Gibbs Free Energy = 0.469500

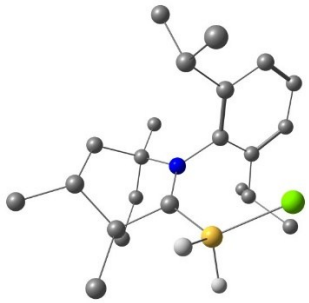
Sum of electronic and zero-point Energies = -1858.395583

Sum of electronic and thermal Energies = -1858.367964

Sum of electronic and thermal Enthalpies = -1858.367020

Sum of electronic and thermal Free Energies = -1858.451502

Structure of 3



C	-1.02049100	-0.32625000	0.91141000	H	-0.43056800	2.31184700	0.04194800
C	-2.51976900	-0.58215800	0.67699600	H	-0.13511100	4.48003700	-1.10014100
C	-1.15819200	-0.21216800	-1.51742300	H	1.55695900	4.10843800	-1.45471400
C	-3.03973500	0.70410700	-0.06930900	H	0.98326300	2.75622600	2.05697100
H	-2.76139900	1.55324000	0.56922800	H	1.95079600	3.90438900	1.11572400
C	-2.29534200	0.82755500	-1.41983800	H	0.23299500	4.23130500	1.39766100
H	-2.98195000	0.63559500	-2.25445200	C	1.56146100	-2.40220500	-0.28623400
H	-1.90208300	1.83841800	-1.56691900	C	2.23277900	-3.06751900	0.93440200
C	-1.80982000	-1.61378200	-1.54603700	C	1.85676500	-3.21159300	-1.56613100
H	-2.44844800	-1.66690600	-2.43562600	H	0.48345800	-2.44103200	-0.10977400
H	-1.03757100	-2.37846500	-1.66806200	H	2.03110100	-2.50539500	1.85019600
C	-2.62559800	-1.82561400	-0.25628700	H	1.85405300	-4.09000900	1.05768300
H	-3.68292900	-2.00342200	-0.48068700	H	3.32028800	-3.12946700	0.80601700
H	-2.27580400	-2.70479200	0.29632200	H	1.36410500	-2.78787800	-2.44901300
N	-0.36229200	-0.12934300	-0.22062900	H	2.93246500	-3.24768200	-1.77524800
C	1.07406400	0.14629700	-0.30255600	H	1.50879700	-4.24547300	-1.44912800
C	1.50940800	1.48896600	-0.32852600	B	-0.50090700	-0.35110500	2.42328400
C	1.97290000	-0.93586100	-0.41657500	H	-0.73447000	-1.48413600	2.80007700
C	2.87627200	1.72531000	-0.52101300	H	0.27145800	3.17036400	-2.22446700
C	3.32794100	-0.63701100	-0.60831000	Cl	1.29892100	0.06036100	2.84458300
C	3.77953700	0.67751900	-0.67303700	H	-1.21437500	0.41451200	3.03418400
H	3.24114500	2.74860500	-0.53510900	C	-3.33868000	-0.84659000	1.94827300
H	4.04370000	-1.45027600	-0.69050600	H	-2.90647100	-1.65563600	2.54084000
H	4.83646200	0.88495700	-0.82049900	H	-3.40229500	0.03641300	2.59017300
C	0.58719400	2.68586200	-0.09563300	H	-4.35595800	-1.14130400	1.66884200
C	0.56963700	3.66106300	-1.29073800	C	-4.56261000	0.76915700	-0.26017600
C	0.96275400	3.43576400	1.20069000	H	-5.09676000	0.81919300	0.69312900

H	-4.82224800	1.67001000	-0.82982100	H	0.15996700	1.00538400	-2.77293100
H	-4.94382000	-0.09336800	-0.82139300	H	0.48237700	-0.72954200	-2.87274200
C	-0.30694900	0.01812100	-2.76377700	H	-0.96337100	-0.05318300	-3.63871000

Zero-point correction = 0.531720 (Hartree/Particle)

Thermal correction to Energy = 0.558193

Thermal correction to Enthalpy = 0.559137

Thermal correction to Gibbs Free Energy = 0.478528

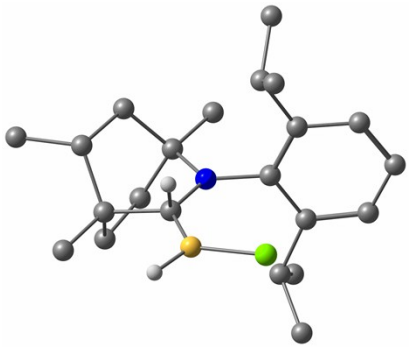
Sum of electronic and zero-point Energies = -1398.756037

Sum of electronic and thermal Energies = -1398.729564

Sum of electronic and thermal Enthalpies = -1398.728620

Sum of electronic and thermal Free Energies = -1398.809228

Structure of 3TS



C	-1.03859300	-0.16163900	0.97580600	H	-3.66277900	-1.95763000	-0.35427200
C	-2.55740900	-0.42272200	0.71497100	H	-2.13451800	-2.50558500	0.30729600
C	-1.19220600	-0.01823200	-1.47981500	N	-0.34400900	-0.03194300	-0.24115000
C	-3.11506300	0.83684000	-0.03719700	C	1.09537400	0.08035000	-0.31887000
H	-2.96124600	1.68426900	0.64619100	C	1.69881100	1.36351300	-0.31234200
C	-2.27315800	1.07241500	-1.32281000	C	1.89287600	-1.08626000	-0.42299100
H	-2.91978400	1.04411300	-2.20995100	C	3.08917300	1.45323100	-0.45697000
H	-1.80501200	2.06222300	-1.31301900	C	3.27877800	-0.94174800	-0.56915000
C	-1.92929300	-1.37849300	-1.56286000	C	3.87746400	0.31446000	-0.59554400
H	-2.66564900	-1.32818200	-2.37544400	H	3.56466900	2.43088300	-0.45214200
H	-1.22388000	-2.17134300	-1.82901200	H	3.90170100	-1.82854800	-0.65532100
C	-2.61603100	-1.66702400	-0.21054800	H	4.95507300	0.40522200	-0.70973900

C	0.90528900	2.65443800	-0.11074300	H	1.03339100	-4.25715800	-1.61644200
C	1.04947400	3.63504400	-1.29313800	B	-0.47633200	-0.24603000	2.38632900
C	1.29650100	3.36446700	1.20360200	H	-1.22318000	-0.40835800	3.29049900
H	-0.15125400	2.38390400	-0.03248100	H	0.75802600	3.18077400	-2.24618900
H	0.41728700	4.51749200	-1.13273000	Cl	1.24457700	-0.06790500	2.90194900
H	2.08335300	3.98556100	-1.39699700	H	-1.03826300	0.92491400	1.66988300
H	1.18958000	2.70174900	2.06703400	C	-3.37528800	-0.70388300	1.98174500
H	2.33780400	3.70804500	1.17457600	H	-2.98500400	-1.56748300	2.52743500
H	0.66053100	4.24497700	1.36079900	H	-3.38928100	0.15039800	2.66794400
C	1.31141500	-2.49613400	-0.35596600	H	-4.41066500	-0.92920700	1.70695700
C	1.89054500	-3.30315300	0.82507700	C	-4.61740200	0.79426100	-0.36271900
C	1.51204800	-3.27123200	-1.67465800	H	-5.24097100	0.74189200	0.53558000
H	0.23719000	-2.39774900	-0.18318700	H	-4.90043900	1.70640000	-0.90258500
H	1.75883900	-2.77352000	1.77322400	H	-4.87516500	-0.05639200	-1.00642400
H	1.38829000	-4.27622800	0.89844900	C	-0.37516700	0.21893200	-2.74994300
H	2.96264400	-3.49468000	0.69432600	H	0.11413000	1.19589100	-2.75053100
H	1.08642300	-2.73908600	-2.53271800	H	0.39627300	-0.54236000	-2.89410000
H	2.57705900	-3.43174900	-1.88202800	H	-1.05206300	0.18009900	-3.61124800

Zero-point correction = 0.529623 (Hartree/Particle)

Thermal correction to Energy = 0.555659

Thermal correction to Enthalpy = 0.556604

Thermal correction to Gibbs Free Energy = 0.476678

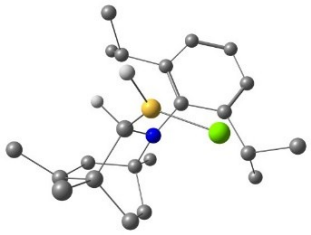
Sum of electronic and zero-point Energies = -1398.735711

Sum of electronic and thermal Energies = -1398.709675

Sum of electronic and thermal Enthalpies = -1398.708731

Sum of electronic and thermal Free Energies = -1398.788656

Structure of 3BA



C	-1.20695300	-0.13917800	0.78311500	H	-0.51781200	4.72481000	-0.37541800
C	-2.49963600	-0.86490000	0.21058100	H	1.23739500	4.65882600	-0.16745100
C	-0.84985200	-0.06103700	-1.66579300	H	-0.17097500	2.43055500	2.60385900
C	-3.22527000	0.14771800	-0.72892100	H	0.89304500	3.81110400	2.30422800
H	-3.90715700	-0.45516300	-1.34850800	H	-0.85151600	3.96954800	2.03880500
C	-2.15188400	0.78493200	-1.64565400	C	2.15570700	-1.87136600	-0.56702200
H	-2.53314600	0.87625500	-2.67101300	C	2.97226000	-2.74399000	0.41371700
H	-1.92146200	1.80412600	-1.31479600	C	2.63416800	-2.19111000	-2.00074400
C	-1.28755900	-1.51950100	-1.93777600	H	1.10560600	-2.15967000	-0.48037000
H	-1.93688600	-1.54821000	-2.82407900	H	2.78405100	-2.47737900	1.45650600
H	-0.41767600	-2.14548300	-2.16133300	H	2.71053900	-3.80097000	0.27904000
C	-2.03484500	-2.04326700	-0.68276300	H	4.05029000	-2.65183500	0.23229000
H	-2.91520000	-2.63200100	-0.97392900	H	2.02853100	-1.70626900	-2.77089100
H	-1.38966500	-2.70951100	-0.10093200	H	3.67432800	-1.87358900	-2.14660900
N	-0.21360300	-0.06868100	-0.30585100	H	2.58996600	-3.27342700	-2.17824400
C	1.10381500	0.46650300	-0.06473600	B	-0.79083200	-0.79591400	2.15737400
C	1.30693000	1.82444600	0.31829000	H	0.47523700	3.76775000	-1.49229500
C	2.24298500	-0.38276800	-0.21966500	Cl	0.15188400	-2.27497600	2.35614000
C	2.60916600	2.28987200	0.55041900	H	-1.19460400	-0.33597700	3.18110700
C	3.52449000	0.14978100	-0.01889600	H	-1.55497300	0.86890400	1.07681200
C	3.71729200	1.47048500	0.37103800	C	-3.43505400	-1.37574400	1.31777800
H	2.75819900	3.32290100	0.85488400	H	-4.37709800	-1.72989600	0.87937200
H	4.39137300	-0.49236200	-0.15002800	H	-2.99663100	-2.22259900	1.86060000
H	4.72072100	1.85595600	0.53577400	H	-3.68245400	-0.59804500	2.04866000
C	0.17433000	2.83978400	0.47381600	C	-4.08309100	1.21808900	-0.04012600
C	0.35755000	4.06632800	-0.44434500	H	-4.48857300	1.90895200	-0.79017500
C	0.00143100	3.28592400	1.94068000	H	-4.93302400	0.78604100	0.49951300
H	-0.75342900	2.36141000	0.16408300	H	-3.50129500	1.81709300	0.67234100

C	0.07327500	0.49316900	-2.75078700	H	-0.39838100	0.35134500	-3.73034800
H	1.04579000	0.00082300	-2.77138300	H	0.24871400	1.56588500	-2.61359800

Zero-point correction = 0.532724 (Hartree/Particle)

Thermal correction to Energy = 0.559147

Thermal correction to Enthalpy = 0.560092

Thermal correction to Gibbs Free Energy = 0.479205

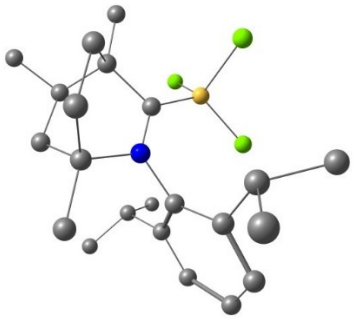
Sum of electronic and zero-point Energies = -1398.736765

Sum of electronic and thermal Energies = -1398.710342

Sum of electronic and thermal Enthalpies = -1398.709398

Sum of electronic and thermal Free Energies = -1398.790284

Structure of 5



C	1.01536100	-0.31114800	-0.07583100	H	3.17490800	-0.58565100	2.58527000
C	2.39240700	-0.14369000	0.61565100	H	2.09650400	-1.82076800	1.95908900
C	0.41828000	0.99557500	1.89847500	N	0.04604600	0.29048600	0.59037500
C	2.61821900	1.41740700	0.69602500	C	-1.36940600	0.35632300	0.19718500
H	2.53308300	1.78424300	-0.33444900	C	-1.80321200	1.46015200	-0.56967400
C	1.49864800	2.04082900	1.55477200	C	-2.25992900	-0.62861100	0.67755400
H	1.90300200	2.40401200	2.50831600	C	-3.17690800	1.57288200	-0.81766300
H	1.04649700	2.90541700	1.05933600	C	-3.62174300	-0.45530600	0.39894200
C	1.06093400	-0.08260100	2.79857900	C	-4.08299400	0.63565400	-0.33098300
H	1.39891200	0.41304700	3.71615000	H	-3.54061100	2.40443800	-1.41450600
H	0.30590400	-0.81507300	3.09562300	H	-4.33146500	-1.20008900	0.74748000
C	2.23192200	-0.73853100	2.05067800	H	-5.14488700	0.74567200	-0.53578600

C	-0.86629500	2.49992300	-1.18702500	H	-2.03185700	-2.85015300	3.36993600
C	-1.15828100	3.92830600	-0.68060600	B	0.83326600	-1.18514200	-1.47437900
C	-0.92137900	2.46546000	-2.72970800	H	-1.10710200	4.00451700	0.41153200
H	0.16057400	2.25233700	-0.90541500	Cl	-0.83613700	-1.26499900	-2.29193200
H	-0.43093200	4.63273800	-1.10232000	Cl	2.01074800	-0.43756200	-2.73592000
H	-2.15608200	4.26382800	-0.98686100	Cl	1.28175400	-2.95399700	-0.96480500
H	-0.68826600	1.46981500	-3.11440500	C	3.61841500	-0.80974800	-0.03314100
H	-1.91374600	2.75186100	-3.09832100	H	3.93467700	-0.29880500	-0.94256100
H	-0.19417000	3.17458800	-3.14365400	H	4.44462700	-0.77207800	0.68484500
C	-1.82835700	-1.89263600	1.42344500	H	3.43986300	-1.85578300	-0.27719800
C	-2.22652600	-3.16894600	0.65084000	C	4.00379200	1.84075600	1.20906500
C	-2.39793200	-1.95240700	2.85704400	H	4.04317000	2.93458100	1.28138800
H	-0.73727700	-1.89967400	1.49289300	H	4.21141400	1.43952800	2.20902000
H	-1.83024900	-3.15826300	-0.36684100	H	4.80887500	1.52716900	0.53947400
H	-1.82751400	-4.05175300	1.16459100	C	-0.76693600	1.65628900	2.59953900
H	-3.31641100	-3.27866500	0.59710100	H	-1.24408600	2.42091000	1.98388300
H	-2.11538700	-1.08220000	3.46001800	H	-1.53105900	0.93831000	2.90254400
H	-3.49313400	-2.00242900	2.84563700	H	-0.38312200	2.14258000	3.50364800

Zero-point correction = 0.517086 (Hartree/Particle)

Thermal correction to Energy = 0.545831

Thermal correction to Enthalpy = 0.546775

Thermal correction to Gibbs Free Energy = 0.461080

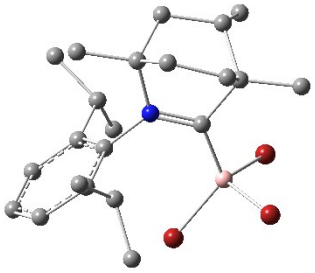
Sum of electronic and zero-point Energies = -2318.046723

Sum of electronic and thermal Energies = -2318.017979

Sum of electronic and thermal Enthalpies = -2318.017035

Sum of electronic and thermal Free Energies = -2318.102729

Structure of 6



Br	2.55077300	0.37412600	-1.66007000	H	3.29778200	-0.19980900	2.07624300
Br	0.01984500	-1.62286900	-1.83652500	H	3.54908200	1.53491700	2.29564500
Br	2.06395100	-2.16307500	0.62185100	H	3.53360900	0.83286100	0.66958000
N	-0.61811500	0.67705900	0.77030200	C	-1.73377300	0.15266900	-0.02799300
C	0.65673300	0.36862300	0.59950000	C	-2.15612900	0.87475200	-1.16514500
C	1.56139400	1.06321700	1.64563200	C	-3.27232100	0.39244400	-1.85890000
C	1.33453000	2.62337800	1.57906400	H	-3.60770400	0.91548000	-2.74979600
H	1.80631700	2.99365600	2.49903100	C	-3.94598800	-0.75198500	-1.44528900
C	-0.17559600	2.92794800	1.64531000	H	-4.80727100	-1.11018700	-2.00350100
H	-0.40146300	3.63557100	2.45192100	C	-3.50177900	-1.44761800	-0.32525600
H	-0.52546600	3.39287800	0.71868400	H	-4.01528700	-2.35636300	-0.02520600
C	-0.97729300	1.64013600	1.90490100	C	-2.39079900	-1.01841300	0.41017100
C	-0.45942000	1.00260800	3.21434100	C	-1.93297000	-1.87181600	1.59553000
H	-0.57135200	1.75279900	4.00603200	H	-0.99873200	-1.45598400	1.98253000
H	-1.08854200	0.15464700	3.49624900	C	-1.62485300	-3.32576100	1.17716900
C	1.00811900	0.58953200	3.03195000	H	-2.53489400	-3.85251700	0.86543700
H	1.13247400	-0.49542300	3.09865500	H	-1.20048300	-3.87146900	2.02832600
H	1.64530200	1.03354600	3.80521000	H	-0.90708400	-3.36370800	0.35567400
C	-2.47130300	1.94314100	1.99680500	C	-2.96827800	-1.87862600	2.74106200
H	-3.07452200	1.04906000	2.16065800	H	-3.20627100	-0.87368600	3.10589200
H	-2.85147300	2.44956300	1.10768100	H	-2.58736300	-2.46241200	3.58810700
H	-2.61858400	2.61128700	2.85290000	H	-3.90812100	-2.34132700	2.41760400
C	2.00298900	3.34407100	0.40139200	C	-1.44638800	2.11457600	-1.71090000
H	3.08538700	3.18845600	0.38341900	H	-0.58911000	2.33103800	-1.07034000
H	1.82071700	4.42302000	0.48800800	C	-0.88913600	1.88434200	-3.13186500
H	1.60688600	3.00849200	-0.56168400	H	-0.19260500	1.04354400	-3.15817300
C	3.07575800	0.78056700	1.65448200	H	-0.35611300	2.78171200	-3.46930400

H	-1.69499500	1.68638800	-3.84873600	H	-1.80269100	4.23712800	-2.04942700
C	-2.36065700	3.35839000	-1.70376700	H	-2.75745600	3.58264500	-0.70740800
H	-3.21592100	3.22552400	-2.37641300	B	1.23115400	-0.68084000	-0.51574200

Zero-point correction = 0.515289 (Hartree/Particle)

Thermal correction to Energy = 0.544970

Thermal correction to Enthalpy = 0.545914

Thermal correction to Gibbs Free Energy = 0.456860

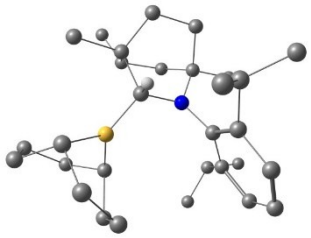
Sum of electronic and zero-point Energies = -8652.651602

Sum of electronic and thermal Energies = -8652.621921

Sum of electronic and thermal Enthalpies = -8652.620977

Sum of electronic and thermal Free Energies = -8652.710031

Structure of 7



C	0.68759400	-3.14192400	-1.04533400	H	3.81359600	-2.92293700	-1.06192200
C	1.55313800	-2.43870500	-2.12109100	H	4.61407100	-1.52584700	-1.74081800
C	3.12197400	-1.63113200	1.44789800	C	1.34073500	-3.12882900	0.34742700
C	2.44190100	-1.27420800	-1.54755200	H	2.26224900	-3.72421300	0.31878100
C	4.20822300	-1.35827500	0.37625100	H	0.68130100	-3.64189300	1.05831900
C	3.82247200	-1.82581200	-1.04084000	C	1.66636700	-1.67927100	0.87430800
H	0.47760200	-4.17503200	-1.35302700	H	0.97757400	-1.42124800	1.68167900
H	3.32452500	-2.58455400	1.95630500	H	2.61946100	-0.57061500	-2.36883600
H	5.15480300	-1.82809600	0.67518100	B	1.58170100	-0.68370500	-0.35006400
H	-0.28925600	-2.64396900	-0.97689000	C	0.71459800	0.66232000	-0.51143200
H	0.89671600	-2.05056000	-2.90928500	C	1.55593400	1.98938700	-0.32527700
H	3.18869600	-0.85897600	2.22550200	C	-0.75244500	2.13394400	0.90953400
H	4.41489900	-0.27978200	0.34471300	C	0.71029800	3.16218100	-0.88040400

H	1.26866100	4.09928800	-0.76078400	C	-1.77374400	-0.97906700	2.48977400
H	0.58875500	3.02110800	-1.96247600	C	-1.23147300	-2.30309200	3.06933100
C	-0.65490000	3.24439000	-0.16861700	C	-3.01988000	-0.58958900	3.32583900
H	-0.77082100	4.21578900	0.32981800	H	-1.00083300	-0.21683200	2.62135200
H	-1.49197400	3.16426000	-0.86878300	H	-0.34783500	-2.66193900	2.54122900
C	0.41074800	2.37863100	1.89677200	H	-0.96045300	-2.16159700	4.12343500
H	0.33007700	3.40385800	2.28578000	H	-1.98687400	-3.09711700	3.03274100
H	0.31180200	1.70550900	2.75635400	H	-3.55568900	0.27039700	2.91704800
C	1.79015600	2.17870100	1.20519900	H	-3.73056400	-1.42399300	3.36476600
H	2.22643600	1.24023500	1.57193400	H	-2.72964300	-0.35662300	4.35865600
N	-0.53309900	0.76881900	0.32766800	H	0.44623500	0.67567600	-1.58202300
C	-1.61766100	-0.13308600	0.00590500	H	2.21541900	-3.16701500	-2.61041800
C	-2.17991300	-0.20046000	-1.30800000	H	-3.01743000	2.45391600	-3.40173000
C	-2.11933200	-1.03957800	0.99747800	H	-4.00951200	1.01524300	-3.10796500
C	-3.08668700	-1.22207200	-1.62699600	H	-3.61670500	2.10069800	-1.76783300
C	-3.04545800	-2.02392200	0.62396800	C	2.87074300	1.95870800	-1.11809400
C	-3.50959300	-2.14608300	-0.68039100	H	3.59765500	1.24792300	-0.71629100
H	-3.48910200	-1.27761600	-2.63545300	H	2.68913900	1.69562700	-2.16610800
H	-3.40891300	-2.71804100	1.37700700	H	3.33897100	2.94944300	-1.10806400
H	-4.21116300	-2.93268000	-0.94758700	C	2.76862100	3.30045000	1.58687500
C	-1.93414900	0.84046500	-2.40399100	H	2.83896800	3.37510800	2.67950400
C	-3.22088800	1.64833200	-2.68422300	H	3.77950000	3.11965300	1.20497800
C	-1.39024600	0.23775000	-3.71458900	H	2.43649000	4.27870100	1.21659900
H	-1.19504200	1.55222700	-2.04496500	C	-2.09399300	2.28133000	1.62646600
H	-0.46998800	-0.33135300	-3.54546200	H	-2.13457700	1.69804100	2.54526300
H	-2.11553800	-0.43639900	-4.18512800	H	-2.23575400	3.33284400	1.90156700
H	-1.16740600	1.03441500	-4.43565900	H	-2.93419100	1.98685500	0.98847600

Zero-point correction = 0.730721 (Hartree/Particle)

Thermal correction to Energy = 0.762823

Thermal correction to Enthalpy = 0.763767

Thermal correction to Gibbs Free Energy = 0.671683

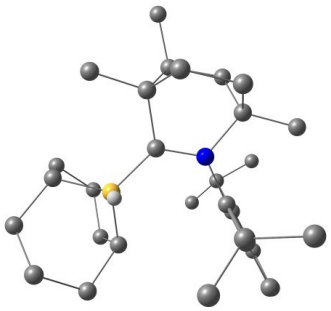
Sum of electronic and zero-point Energies = -1250.981269

Sum of electronic and thermal Energies = -1250.949167

Sum of electronic and thermal Enthalpies = -1250.948223

Sum of electronic and thermal Free Energies = -1251.040307

Structure of 7A



C	3.74901600	-1.88575800	-1.36460100	C	0.45942200	0.88409600	-0.38776800
C	4.34462200	-0.69289000	-0.60427000	C	0.51661100	2.38407900	-0.80299000
C	2.46401100	-1.48204800	1.72967300	C	-1.92284100	1.55650000	-0.46065600
C	3.30432200	0.41870800	-0.18991100	C	-0.32289800	2.55360700	-2.10566300
C	2.59701800	-0.04100800	2.23973500	H	-0.29644300	3.60858400	-2.40039400
C	3.48393400	0.80583900	1.30449800	H	0.17759000	1.99693500	-2.90569700
H	4.54250200	-2.60218400	-1.62308500	C	-1.76298500	2.07285900	-1.90540100
H	3.46827900	-1.92588400	1.70953600	C	-1.63713100	2.73341000	0.49285100
H	2.99419500	-0.02629300	3.26537600	H	-2.29561600	3.56207100	0.20139500
H	3.34104400	-1.52499800	-2.31827500	H	-1.90494300	2.46920700	1.52029900
H	5.13111000	-0.23620100	-1.22299400	C	-0.15471600	3.16130300	0.39324000
H	1.90854500	-2.09264900	2.45482300	H	0.37095300	2.83274500	1.29980400
H	1.59771000	0.41354200	2.29656100	N	-0.82567400	0.51991800	-0.21322600
H	4.54024000	0.69504600	1.59854800	C	-1.28113200	-0.82782700	0.12946700
H	3.24439600	1.86938000	1.45872200	C	-1.52643800	-1.74854300	-0.91969800
C	2.63564400	-2.58786200	-0.56090100	C	-1.57244500	-1.15143800	1.47946700
H	3.08068000	-3.35913700	0.08816100	C	-2.03891400	-3.00828300	-0.58282400
H	1.98458300	-3.13522800	-1.25431500	C	-2.09406200	-2.42468000	1.74740000
C	1.79750100	-1.60463000	0.30950800	C	-2.32404200	-3.35010900	0.73469200
H	0.82414100	-2.07654700	0.45923000	H	-2.22134300	-3.73344400	-1.37085600
H	3.58434500	1.28705500	-0.78348700	H	-2.31927000	-2.69868200	2.77401900
B	1.75466600	-0.13000300	-0.45292400	H	-2.72259600	-4.33331500	0.97193100

C	-1.28632300	-1.45030700	-2.40326400	H	1.57024800	-0.25467300	-1.68528900
C	-2.60545300	-1.44761900	-3.20873600	H	4.86415000	-1.07167800	0.28713800
C	-0.30118300	-2.43724200	-3.05964600	H	-3.34844000	-0.75131800	-2.80682900
H	-2.40871000	-1.16453300	-4.25027700	H	-2.03688000	1.28946100	-2.61628900
H	-3.06241900	-2.44434700	-3.21909600	H	-2.48217700	2.88869200	-2.04751200
H	0.66992100	-2.41452600	-2.56415300	H	-0.83232500	-0.46057500	-2.48325800
H	-0.67932200	-3.46643500	-3.03560300	C	1.89702000	2.96957500	-1.11278300
H	-0.15165200	-2.16503100	-4.11189700	H	2.55051000	3.00479800	-0.23966100
C	-1.34626900	-0.21445800	2.67332900	H	2.39521500	2.40681000	-1.90373100
C	-0.52757100	-0.88472800	3.79852300	H	1.76934900	3.99541600	-1.47516600
C	-2.66410400	0.29606800	3.30108800	C	-0.02575400	4.69156900	0.33688700
H	-0.77345500	0.64906100	2.32249500	H	-0.58287500	5.13441000	1.17185500
H	0.37510200	-1.36417800	3.42117300	H	1.01213900	5.02571700	0.42307700
H	-0.23094600	-0.13194600	4.53854400	H	-0.44350500	5.10525100	-0.58995500
H	-1.11982800	-1.64270500	4.32507700	C	-3.34340900	1.02170600	-0.27509400
H	-3.26523800	0.90448800	2.62106500	H	-4.03427200	1.85660600	-0.44154100
H	-3.28655900	-0.54357400	3.63331600	H	-3.58745300	0.23906200	-0.99552300
H	-2.44059400	0.91088200	4.18186400	H	-3.53239600	0.62611100	0.72116700

Zero-point correction = 0.729774 (Hartree/Particle)

Thermal correction to Energy = 0.761345

Thermal correction to Enthalpy = 0.762289

Thermal correction to Gibbs Free Energy = 0.672318

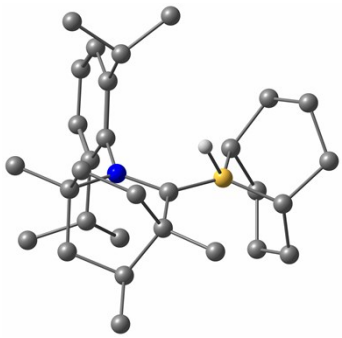
Sum of electronic and zero-point Energies = -1250.967710

Sum of electronic and thermal Energie s= -1250.936138

Sum of electronic and thermal Enthalpies = -1250.935194

Sum of electronic and thermal Free Energies = -1251.025165

Structure of 7TS



C	3.16841400	-2.20507500	-1.60953400	H	0.02613000	3.64245900	-2.38998200
C	4.08385400	-1.16770600	-0.94692200	H	0.36640700	2.01061000	-2.93479300
C	2.50922700	-1.73251000	1.70029900	C	-1.56207800	2.22087400	-1.92399200
C	3.31976600	0.06977000	-0.34079800	C	-1.36598100	2.89162500	0.45775200
C	2.95628400	-0.34265200	2.17629400	H	-1.91212300	3.79057300	0.14019400
C	3.80742800	0.37551200	1.10815800	H	-1.68021800	2.68292300	1.48552500
H	3.76498800	-3.00852300	-2.06457300	C	0.15873200	3.13721400	0.38343500
H	3.40755000	-2.34060200	1.53079200	H	0.62961000	2.72093800	1.28436200
H	3.51301000	-0.42146900	3.12091300	N	-0.80763000	0.59112300	-0.19655500
H	2.62960300	-1.71864900	-2.43671700	C	-1.37196100	-0.68825100	0.18603700
H	4.81865600	-0.81047600	-1.68236500	C	-1.73061600	-1.61943600	-0.82571300
H	1.96787800	-2.24768200	2.50497600	C	-1.63063500	-0.97554400	1.55286700
H	2.06693500	0.26489800	2.39653900	C	-2.30869100	-2.83672700	-0.44088800
H	4.86304100	0.08085400	1.21295900	C	-2.22714600	-2.20204100	1.87573200
H	3.77733800	1.45811500	1.29916700	C	-2.55797600	-3.13275800	0.89531800
C	2.15708300	-2.78856500	-0.60642600	H	-2.57824400	-3.56243300	-1.20411400
H	2.63144600	-3.60725700	-0.04389900	H	-2.43067800	-2.43687800	2.91703100
H	1.32552600	-3.25344500	-1.14802100	H	-3.01158100	-4.08158400	1.17139500
C	1.62076100	-1.72140600	0.39410300	C	-1.56059100	-1.35259000	-2.32544700
H	0.61987200	-2.03224900	0.69048600	C	-2.92307300	-1.28480600	-3.05242100
H	3.60801800	0.91161600	-0.96250300	C	-0.67490700	-2.39170600	-3.04112200
B	1.71161000	-0.22458700	-0.25208500	H	-2.77630000	-1.01138400	-4.10485200
C	0.56320800	0.82319300	-0.39086200	H	-3.42728600	-2.25842100	-3.03182800
C	0.74679500	2.31883500	-0.82790400	H	0.34274100	-2.39189000	-2.64903900
C	-1.76561400	1.73067100	-0.47690000	H	-1.07840900	-3.40679900	-2.94433600
C	-0.08242800	2.58625400	-2.11621900	H	-0.62266700	-2.15834700	-4.11200200

C	-1.28693500	-0.02335900	2.70222100	H	-2.21082100	3.09091100	-2.08643700
C	-0.42574100	-0.69843600	3.79043200	H	-1.06580300	-0.38556400	-2.43642900
C	-2.54329100	0.56540100	3.38278400	C	2.17067400	2.79117400	-1.13549300
H	-0.70246400	0.80188600	2.28559200	H	2.83987200	2.72068900	-0.27551500
H	0.45441400	-1.18703500	3.37114500	H	2.60380600	2.23530400	-1.96994700
H	-0.08650200	0.05113600	4.51599600	H	2.13201000	3.84143500	-1.44232400
H	-0.99737000	-1.45284200	4.34482700	C	0.46498000	4.64358200	0.37775300
H	-3.17435300	1.13693700	2.69684000	H	-0.05893200	5.12348700	1.21392700
H	-3.16160100	-0.23068800	3.81523900	H	1.53177100	4.85707900	0.49602800
H	-2.24798200	1.23620000	4.19953800	H	0.11899900	5.12935300	-0.54394300
H	1.11049000	-0.01290300	-1.47668000	C	-3.23490900	1.36196200	-0.26515100
H	4.67200200	-1.66964400	-0.16659200	H	-3.83595500	2.26389700	-0.43068900
H	-3.60463000	-0.55364000	-2.60817000	H	-3.57938500	0.59968900	-0.96564500
H	-1.88951900	1.45603900	-2.63314100	H	-3.44173100	1.00346900	0.74303400

Zero-point correction = 0.727793 (Hartree/Particle)

Thermal correction to Energy = 0.759076

Thermal correction to Enthalpy = 0.760020

Thermal correction to Gibbs Free Energy = 0.670591

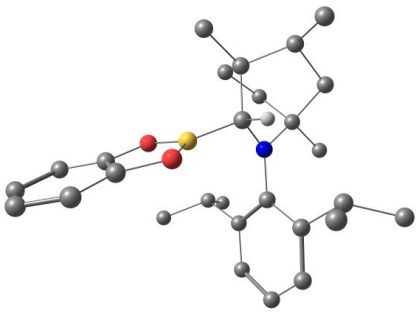
Sum of electronic and zero-point Energies = -1250.962393

Sum of electronic and thermal Energies = -1250.931110

Sum of electronic and thermal Enthalpies = -1250.930166

Sum of electronic and thermal Free Energies = -1251.019595

Structure of 8



O	2.06221800	-0.60510500	-0.83427500	N	-1.17683900	-0.09454800	-0.40326700
O	1.88597600	-0.82835900	1.43780400	C	3.31255200	-0.44485700	-0.26912400

C	-0.34920000	-1.18980300	0.14858200	H	4.20435000	-0.56844400	3.02943500
H	-0.63365900	-1.42526900	1.19154200	C	0.40768300	-3.57520800	-0.44385600
C	3.20420500	-0.57860500	1.11529300	H	1.37005400	-3.30506300	-0.89489500
C	-2.07818700	0.59473400	2.39582900	H	0.09272200	-4.52375200	-0.89757800
H	-2.19619800	-0.35303000	1.87129000	H	0.57461800	-3.75846500	0.62440600
C	-0.64748700	-2.48686400	-0.68815400	C	-3.42097200	0.52836100	-1.34832200
C	4.52430500	-0.19419400	-0.89137800	H	-3.84787800	0.86402900	-0.39727700
H	4.59802200	-0.09301100	-1.96948000	H	-4.23858200	0.14250100	-1.96848600
C	-2.08179600	-2.98079500	-0.31693900	H	-3.00085500	1.40187700	-1.85128900
H	-2.37103600	-3.68782800	-1.10957500	C	-1.88204000	-1.16163700	-2.48166200
C	-1.27253000	2.90717100	1.87611500	H	-1.58925900	-0.35669800	-3.16426400
H	-1.58487800	3.16991900	2.88377500	H	-2.70180300	-1.70805900	-2.96886900
C	-0.43832800	2.24363300	-0.71780300	C	1.57977800	2.38087700	-2.26422900
C	5.64598000	-0.07831000	-0.05430300	H	1.69358300	3.47165700	-2.23927400
H	6.61824200	0.11873000	-0.49715800	H	1.97567900	2.03205900	-3.22652200
C	-1.03070700	1.24193400	0.10851100	H	2.20183700	1.95941600	-1.47037300
C	-1.44334700	1.59036400	1.42670900	C	-2.21331000	-3.73266700	1.01526800
C	0.10251000	1.95801100	-2.11895100	H	-1.64183800	-4.66728700	1.02282900
H	0.05137500	0.87712300	-2.26690000	H	-3.26504600	-3.98968800	1.19484700
C	-0.31709000	3.55194800	-0.22803200	H	-1.87715000	-3.12556300	1.86529500
H	0.12198100	4.31814500	-0.86203400	C	-1.17619900	0.33650200	3.62120800
C	-0.72702000	3.89019200	1.05724500	H	-0.18030600	-0.00636900	3.32095600
H	-0.61632700	4.90949500	1.41997100	H	-1.62182900	-0.42872700	4.26984200
C	-2.38603500	-0.57624500	-1.13970800	H	-1.04947800	1.24661900	4.22052700
C	-3.03514300	-1.75736700	-0.37084600	C	-3.48739000	1.03279000	2.84597500
H	-3.97854400	-2.03045500	-0.86181300	H	-3.45754900	1.95656300	3.43573400
H	-3.29997100	-1.43294300	0.64192800	H	-3.94410200	0.25587200	3.47227500
C	5.53657000	-0.20977900	1.33691300	H	-4.14709600	1.20799000	1.98849400
H	6.42558500	-0.11252200	1.95373600	C	-0.72670400	2.64051000	-3.22762700
C	-0.68408400	-2.10287700	-2.18950300	H	-1.77395300	2.32313800	-3.22110700
H	-0.75570900	-3.01943200	-2.79050900	H	-0.31070000	2.40012200	-4.21457900
H	0.26179100	-1.62237800	-2.46175500	H	-0.71117700	3.73226400	-3.11816500
C	4.30091700	-0.46505500	1.95325100	B	1.19116600	-0.84391500	0.22737600

Zero-point correction = 0.612140 (Hartree/Particle)

Thermal correction to Energy = 0.642735

Thermal correction to Enthalpy = 0.643679

Thermal correction to Gibbs Free Energy = 0.552725

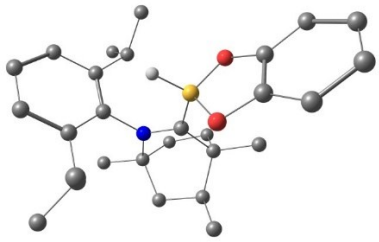
Sum of electronic and zero-point Energies = -1319.441531

Sum of electronic and thermal Energies = -1319.410936

Sum of electronic and thermal Enthalpies = -1319.409992

Sum of electronic and thermal Free Energies = -1319.500947

Structure of 8A



O	2.08225000	1.42098700	-0.29894500	C	-2.15850000	-0.12487900	1.73521900
O	2.12521200	-0.46593800	1.15316500	C	-1.70871800	2.49767500	-1.10380200
N	-1.08246000	-0.34408600	-0.49444200	H	-1.13908700	1.79137700	-1.71165700
C	3.34825800	1.17204100	0.13749800	C	-2.95370600	2.49312900	1.08432100
C	0.22980400	-0.36414200	-0.59182700	H	-3.24323100	3.51492000	0.85562000
C	3.37412700	0.05612400	0.99654200	C	-3.34775500	1.92741200	2.29303500
C	-1.66618500	-1.49532000	2.19539700	H	-3.95344600	2.49874000	2.99188100
H	-1.11880600	-1.95793800	1.37154600	C	-1.87382500	-1.17325000	-1.49867500
C	0.72782300	-1.20614900	-1.75721200	C	-1.34662300	-2.61881700	-1.36434800
C	4.50975700	1.85769200	-0.18411300	H	-1.88301600	-3.24368800	-2.08835500
H	4.47907000	2.71792100	-0.84748800	H	-1.59981600	-3.00501000	-0.37151100
C	0.18192000	-2.67362100	-1.60470800	C	5.74610100	0.30011700	1.23207900
H	0.37094000	-3.14692400	-2.57841100	H	6.68910900	-0.03108000	1.65996300
C	-2.93888000	0.63659900	2.61492500	C	0.04730200	-0.59590400	-3.02697700
H	-3.21573000	0.21526600	3.57717900	H	0.40567200	-1.15442300	-3.89967800
C	-2.17382400	1.78133000	0.16310000	H	0.39441800	0.43576700	-3.14889700
C	5.72066100	1.40506400	0.38040800	C	4.56152500	-0.39597900	1.55188200
H	6.64410400	1.92978100	0.14809200	H	4.57037100	-1.25719000	2.21464500
C	-1.81071400	0.45940200	0.49876400	C	2.24744500	-1.20017900	-1.95948000

H	2.60756600	-0.20093400	-2.21426800	H	0.41736700	-4.49327400	-0.44809300
H	2.49816800	-1.87600700	-2.78725400	H	0.86874400	-3.02809000	0.44893200
H	2.78773300	-1.53229900	-1.07279800	C	-0.66828000	-1.35626200	3.36565600
C	-3.38206900	-1.10387300	-1.27671100	H	0.18623100	-0.73248200	3.08891000
H	-3.67749800	-1.50635500	-0.30453400	H	-0.28806500	-2.34445600	3.65293400
H	-3.86711000	-1.70638400	-2.05292100	H	-1.15020400	-0.91357800	4.24586100
H	-3.76525700	-0.08310300	-1.35310400	C	-2.81977000	-2.44563200	2.57494200
C	-1.48639300	-0.66195400	-2.90792900	H	-3.37710800	-2.07630600	3.44362100
H	-1.95207300	0.30956100	-3.09830100	H	-2.42201200	-3.43362000	2.83655300
H	-1.91433000	-1.36238300	-3.63474900	H	-3.53494000	-2.57564900	1.75404100
C	-0.74671400	3.65581900	-0.76233600	C	-2.88742600	2.99969200	-1.96247400
H	-1.24687800	4.42394000	-0.16026400	H	-3.57700500	2.18996600	-2.23007400
H	-0.39245900	4.13134700	-1.68535200	H	-2.51367600	3.44708000	-2.89149800
H	0.12645600	3.29623100	-0.21065600	H	-3.46861400	3.76789800	-1.43909800
C	0.89823600	-3.51060200	-0.53439800	B	1.19569600	0.49162000	0.47073700
H	1.94956800	-3.67840800	-0.78587600	H	0.50244300	1.08667600	1.26605500

Zero-point correction = 0.610091 (Hartree/Particle)

Thermal correction to Energy = 0.641003

Thermal correction to Enthalpy = 0.641947

Thermal correction to Gibbs Free Energy = 0.550024

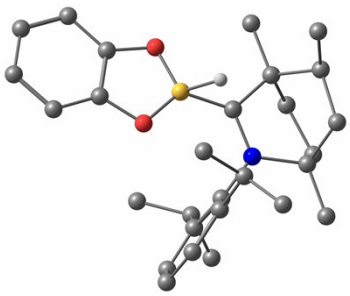
Sum of electronic and zero-point Energies = -1319.413606

Sum of electronic and thermal Energies = -1319.382695

Sum of electronic and thermal Enthalpies = -1319.381751

Sum of electronic and thermal Free Energies = -1319.473673

Structure of 8TS



O	1.75429300	-0.40036900	-0.35151100
O	2.24688600	1.79480400	0.27454000
N	-1.28479600	0.18747900	0.09431800
C	3.11248900	-0.22738200	-0.28357800
C	-0.30991700	1.15021800	0.17338500
H	0.43654500	1.37099500	-1.16983000
C	3.40681500	1.08982100	0.08909100
C	-1.06063700	-1.10971000	-2.56674800
H	-1.22884800	-0.05543600	-2.33153300
C	-0.89524100	2.54151100	0.48662800
C	4.11009900	-1.15897500	-0.51749700
H	3.86857300	-2.17863100	-0.80259400
C	-1.93528300	2.96765500	-0.61234400
H	-2.51855100	3.77698700	-0.14907100
C	-0.74976800	-3.25410300	-1.28864200
H	-0.72357300	-3.75854600	-2.25101900
C	-0.75255700	-1.96648500	1.20595700
C	5.44122600	-0.72495100	-0.36733200
H	6.25115000	-1.42761500	-0.54450900
C	-0.98864100	-1.23321800	0.01959300
C	-0.95471200	-1.86953500	-1.24511400
C	-0.66625400	-1.32024500	2.58584700
H	-0.85934300	-0.25268500	2.46825700
C	-0.54658900	-3.34921600	1.10541000
H	-0.36696300	-3.92802400	2.00768500
C	-0.55922000	-3.99597600	-0.12641500
H	-0.40340000	-5.07071000	-0.18217000
C	-2.70957700	0.67994600	0.17678900
C	-2.88212100	1.77477600	-0.89513700
H	-3.92895400	2.10383500	-0.90681000
H	-2.67770900	1.34796900	-1.88352900
C	5.73559200	0.59030000	0.00385700
H	6.77203000	0.89894500	0.11201100
C	-1.71298100	2.33597400	1.79727700
H	-2.08056900	3.31526100	2.12716400
H	-1.04142500	1.97462400	2.58495600
C	4.71196500	1.52780900	0.24057400
H	4.93014500	2.55131100	0.53092700
C	0.13924600	3.64857500	0.71766800
H	0.76424600	3.43542000	1.58898000
H	-0.38996400	4.59320100	0.89729700
H	0.80750100	3.78812600	-0.13391600
C	-3.73155300	-0.44069700	-0.00086900
H	-3.69212100	-0.88352900	-0.99850600
H	-4.73387500	-0.02120300	0.14277600
H	-3.59348900	-1.24195500	0.73084500
C	-2.88117800	1.35500400	1.56120500
H	-2.93097300	0.59404400	2.34622600
H	-3.84557900	1.87865600	1.57026100
C	0.75166100	-1.45680400	3.17945000
H	1.00557700	-2.50583000	3.37421800
H	0.81866500	-0.91560200	4.13171400
H	1.50697000	-1.05184500	2.49868000
C	-1.33771900	3.52950300	-1.90843500
H	-0.78366100	4.45855600	-1.73920000
H	-2.14132300	3.75005800	-2.62250800
H	-0.65748600	2.81259300	-2.38480400
C	0.26109300	-1.19079500	-3.36200500
H	1.10773800	-0.86009100	-2.75534800
H	0.20231300	-0.55866800	-4.25712300
H	0.46192600	-2.21723400	-3.69347200
C	-2.22988300	-1.59077600	-3.45033600
H	-2.08655800	-2.62928300	-3.77198600
H	-2.29737400	-0.97376200	-4.35502400
H	-3.19401900	-1.53639400	-2.93357400
C	-1.71996100	-1.87848400	3.56357300
H	-2.73742700	-1.77341200	3.16875700
H	-1.67093000	-1.34608400	4.52180400
H	-1.55408600	-2.94279400	3.76880400
B	1.18212100	0.89369600	-0.08808100

Zero-point correction = 0.607304 (Hartree/Particle)

Thermal correction to Energy = 0.637643

Thermal correction to Enthalpy = 0.638587

Thermal correction to Gibbs Free Energy = 0.548850

Sum of electronic and zero-point Energies = -1319.404363

Sum of electronic and thermal Energies = -1319.374024

Sum of electronic and thermal Enthalpies = -1319.373079

Sum of electronic and thermal Free Energies = -1319.462816

2.2 Calculation of free energy for the interaction of BICAAC with various boranes

Table S3. Calculation of ΔG for the interaction of BICAAC and BH_3

Properties/Molecules	BICAAC	BH_3	1	1TS	1BA
Zero-point correction (Hartree/Particle)	0.504158	0.026394	0.538083	0.538722	0.542726
Thermal correction to Energy (Hartree/Particle)	0.528125	0.029280	0.563566	0.563657	0.567071
Thermal correction to Enthalpy (Hartree/Particle)	0.529069	0.030224	0.564510	0.564601	0.568016
Thermal correction to Gibbs Free Energy (Hartree/Particle)	0.452678	0.008838	0.486382	0.487545	0.493250
Sum of electronic and thermal Free Energies (Hartree/Particle)G_{tot}	-912.487354	-26.606098	-939.159123	-939.085380	-939.139594
Relative Free Energy (Hartree/Particle)	0.000000	0.000000	-0.065671	0.008072	-0.046142
Relative Free Energy ΔG (kcal/mole)	0.000000	0.000000	-41.209209	5.065261	-28.954566

Table S4. Calculation of ΔG for the interaction of BICAAC and $BHCl_2$

Properties/Molecules	BICAAC	$BHCl_2$	2	2TS	2BA
Zero-point correction (Hartree/Particle)	0.504158	0.014919	0.525218	0.521766	0.525420
Thermal correction to Energy (Hartree/Particle)	0.528125	0.018442	0.552706	0.548919	0.553039
Thermal correction to Enthalpy (Hartree/Particle)	0.529069	0.019386	0.553650	0.549863	0.553983
Thermal correction to Gibbs Free Energy (Hartree/Particle)	0.452678	-0.011035	0.470937	0.466564	0.469500
Sum of electronic and thermal Free Energies (Hartree/Particle)G_{tot}	-912.487354	-945.934562	-1858.458082	-1858.425230	-1858.451502
Relative Free Energy (Hartree/Particle)	0.000000	0.000000	-0.036166	-0.003314	-0.029586
Relative Free Energy ΔG (kcal/mole)	0.000000	0.000000	-22.694527	-2.079568	-18.565511

Table S5. Calculation of ΔG for the interaction of BICAAC and BH_2Cl

Properties/Molecules	BICAAC	BH_2Cl	3	3TS	3BA
Zero-point correction (Hartree/Particle)	0.504158	0.021300	0.531720	0.529623	0.532724
Thermal correction to Energy (Hartree/Particle)	0.528125	0.024316	0.558193	0.555659	0.559147
Thermal correction to Enthalpy (Hartree/Particle)	0.529069	0.025260	0.559137	0.556604	0.560092
Thermal correction to Gibbs Free Energy (Hartree/Particle)	0.452678	-0.001350	0.478528	0.476678	0.479205
Sum of electronic and thermal Free Energies (Hartree/Particle)G_{tot}	-912.487354	-486.273423	-1398.809228	-1398.788656	-1398.790284
Relative Free Energy (Hartree/Particle)	0.000000	0.000000	-0.048451	-0.027879	-0.029507
Relative Free Energy ΔG (kcal/mole)	0.000000	0.000000	-30.403487	-17.494351	-18.515938

Table S6. Calculation of ΔG for the interaction of BICAAC and 9-BBN

Properties/Molecules	BICAAC	9-BBN	7A	7TS	7
Zero-point correction (Hartree/Particle)	0.504158	0.218716	0.729774	0.727793	0.730721
Thermal correction to Energy (Hartree/Particle)	0.528125	0.227070	0.761345	0.759076	0.762823
Thermal correction to Enthalpy (Hartree/Particle)	0.529069	0.228014	0.762289	0.760020	0.763767
Thermal correction to Gibbs Free Energy (Hartree/Particle)	0.452678	0.186315	0.672318	0.670591	0.671683
Sum of electronic and thermal Free Energies (Hartree/Particle)G_{tot}	-912.487354	-338.539607	-1251.025165	-1251.019595	-1251.040307
Relative Free Energy (Hartree/Particle)	0.000000	0.000000	0.001796	0.007366	-0.013346
Relative Free Energy ΔG (kcal/mole)	0.000000	0.000000	1.127008	4.622239	-8.374748

Table S7. Calculation of ΔG for the interaction of BICAAC and catechol borane

Properties/Molecules	BICAAC	Catechol borane	8A	8TS	8
Zero-point correction (Hartree/Particle)	0.504158	0.102512	0.610091	0.607304	0.612140
Thermal correction to Energy (Hartree/Particle)	0.528125	0.108527	0.641003	0.637643	0.642735
Thermal correction to Enthalpy (Hartree/Particle)	0.529069	0.109472	0.641947	0.638587	0.643679
Thermal correction to Gibbs Free Energy (Hartree/Particle)	0.452678	0.072309	0.550024	0.548850	0.552725
Sum of electronic and thermal Free Energies (Hartree/Particle)G_{tot}	-912.487354	-406.978500	-1319.473673	-1319.462816	-1319.500947
Relative Free Energy (Hartree/Particle)	0.000000	0.000000	-0.007819	0.003038	-0.035093
Relative Free Energy ΔG (kcal/mole)	0.000000	0.000000	-4.906501	1.906375	-22.021208

2.3 Results of IRC calculations for the transition states (1TS-3TS, 7TS and 8TS)

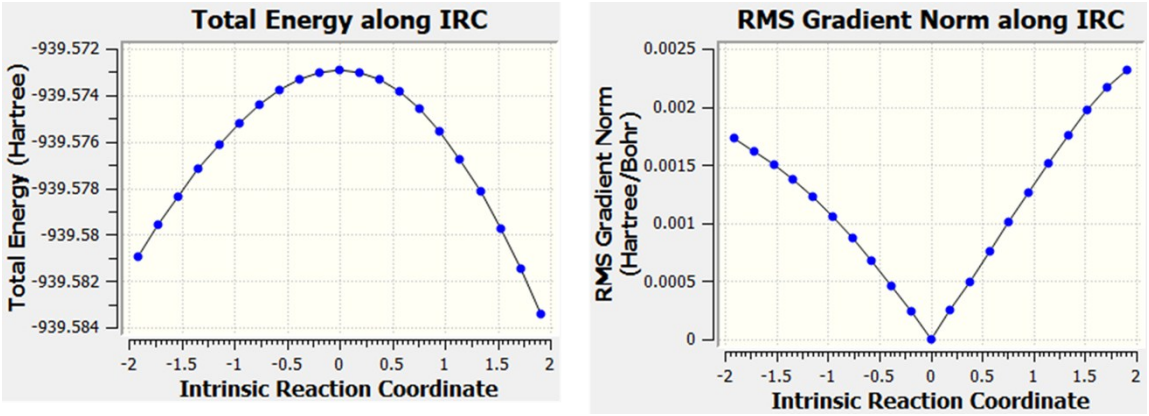


Fig. S36 Results of IRC calculation for **1TS**.

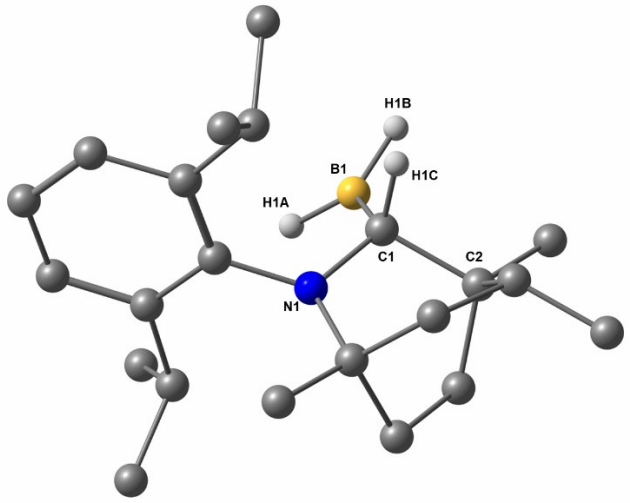


Fig. S37 Optimized structure of **1TS**.

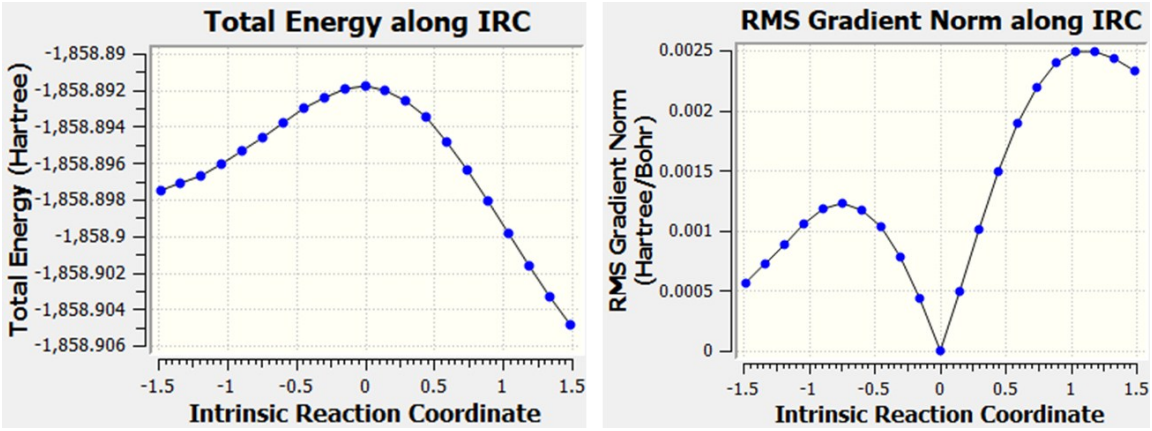


Fig. S38 Results of IRC calculation for **2TS**.

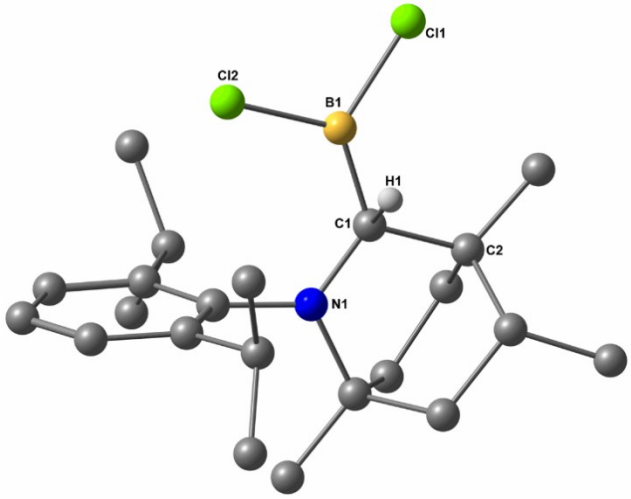


Fig. S39 Optimized structure of **2TS**.

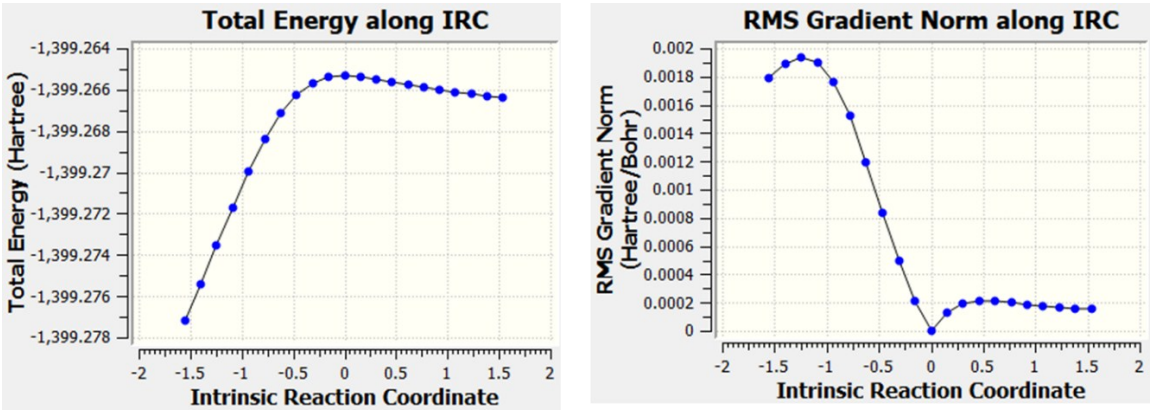


Fig. S40 Results of IRC calculation for **3TS**.

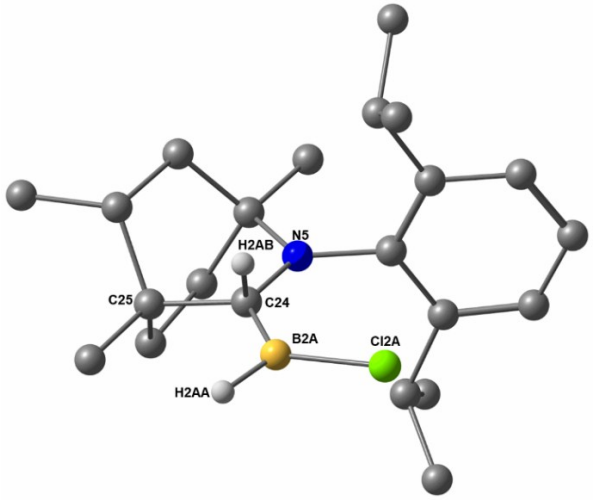


Fig. S41 Optimized structure of **3TS**.

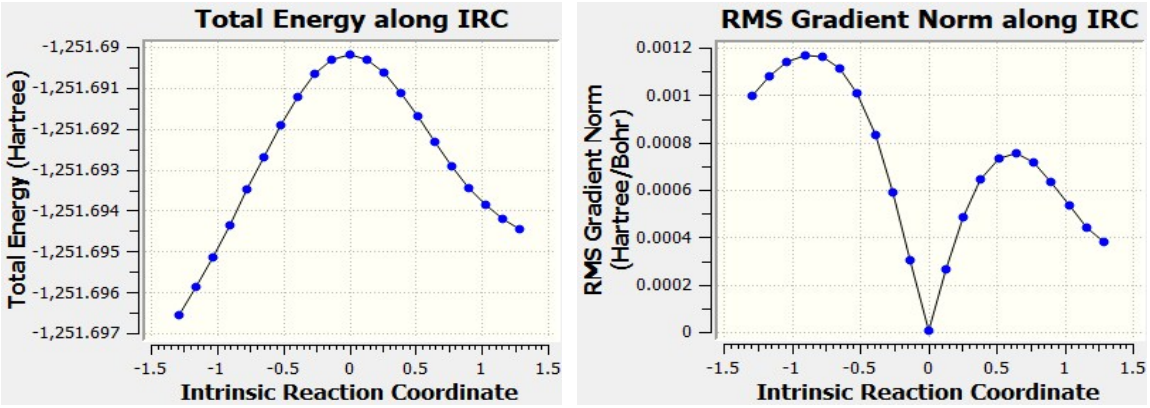


Fig. S42 Results of IRC calculation for **7TS**.

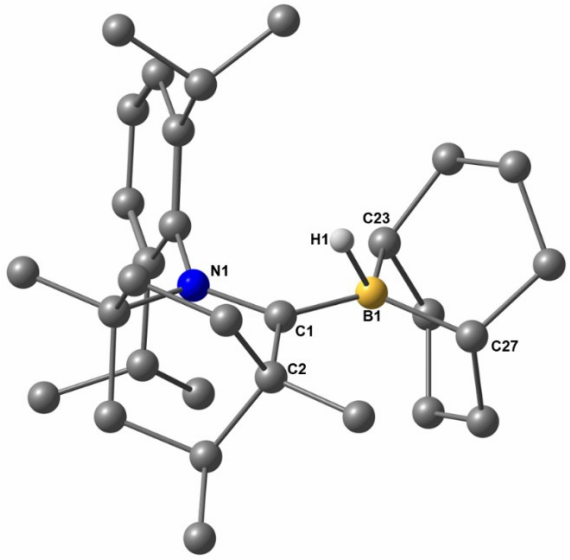


Fig. S43 Optimized structure of **7TS**.

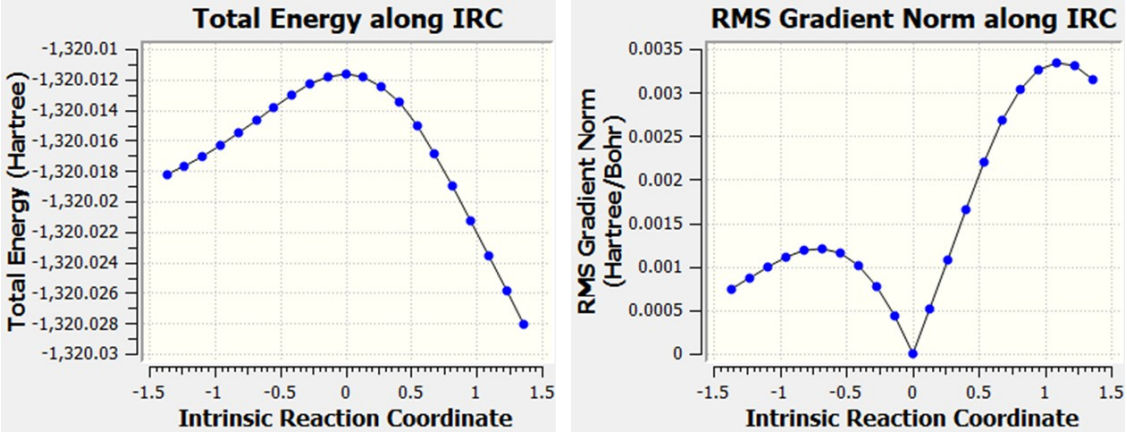


Fig. S44 Results of IRC calculation for **8TS**.

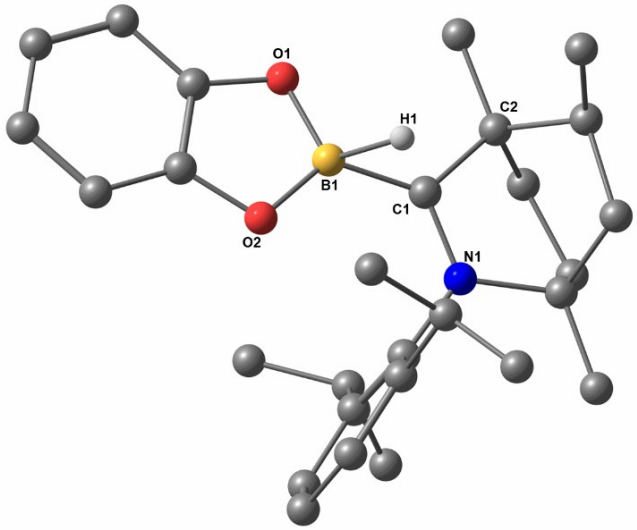


Fig. S45 Optimized structure of **8TS**.

2.4 Plausible mechanism for Lewis adduct formation and B-H bond activation

The shape of monomeric boranes is usually trigonal-planar where a non-bonding *p*-orbital (as LUMO) on B stays perpendicular to the molecular plane. During our studies of MOs, it was found that the filled sp^2 hybrid orbital of BICAAC gave away its electrons to the empty non-bonding *p*-orbital of borane and formed an adduct (Fig. S44 (i)). The LUMO of BICAAC having *p*-character interacts (Fig. S44 (ii)) with the B-H hydrogen and the molecule performs a bond rotation to form a transition state (Fig. S44 (iii)) where the orbital lobes of BICAAC and borane overlap well. In the end, the hydrogen migrates and forms a σ-bond with $C_{carbene}$ leaving the boron (Fig. S44 (iv)).

The migration of hydrogen was made possible via generation of hydride. Fig. S44 (v) shows the relative charges of each atom in the case of **7**.

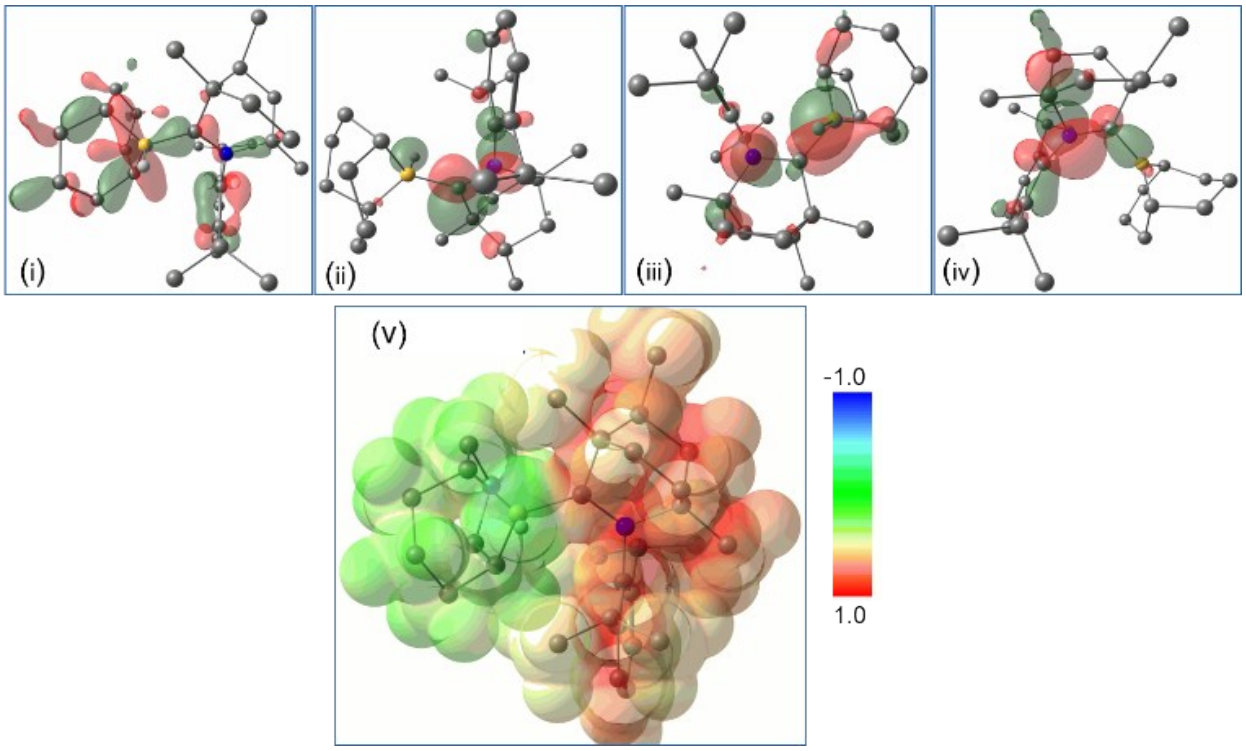


Fig. S46 MOs and ESP during the interaction of BICAAC and 9-BBN. (i) HOMO-2 of **7A**, (ii) LUMO of **7A**, (iii) HOMO of **7TS**, (iv) HOMO of **7**, (v) ESP plot of **7A**.

Table S8 Hydride formation from adducts and B-H activated products. H in the parenthesis in each compound was removed to calculate the values of ΔG_{FBD}. The values of ΔG_{FBD} are expressed in kcal/mol.

Entry	Lewis adducts	ΔG_{FBD}	B-H activation product	ΔG_{FBD}
1	BICAAC-BH_2(H) (**1**)	0	BICAAC(H)-BH_2 (**1BA**)	-12.3
2	BICAAC-BH(H)Cl (**2**)	0	BICAAC(H)-BHCl (**2BA**)	-12.0
3	BICAAC-B(H)Cl2 (**3**)	0	BICAAC(H)-BCl_2 (**3BA**)	-4.1
4	BICAAC-9-BBN(H) (**7A**)	0	BICAAC(H)-9-BBN (**7BA**)	9.5
5	BICAAC-(H)Bcat (**8A**)	0	BICAAC(H)-Bcat (**8BA**)	17.1

In Table S8, the possibility of hydride formation (C-H bond) was judged by comparing the calculated free energy of bond dissociation (ΔG_{FBD}) of B-H and C-H bonds between the Lewis adducts and their corresponding B-H activated products. In the case of **1**, the hydride removal from **1BA** is thermodynamically feasible (ΔG_{FBD} = -12.3 kcal/mol) when compared to adduct **1** and indicate the adduct formation is preferred over B-H activation in line with the experimental observation. The similar results were observed in the case of **2BA** (ΔG_{FBD} = -12.0 kcal/mol) and **3BA** (ΔG_{FBD} = -4.1 kcal/mol). On the other hand, hydride removal from B-H activated products **7** (ΔG_{FBD} = 9.5 kcal/mol) and **8** (ΔG_{FBD} = 17.1 kcal/mol) were thermodynamically not feasible with respect to their adducts implying the B-H activation leading to the C-H bond formation as the preferred reaction pathway again supporting the experimental observations. Hence, it can be concluded that the bond activation of B-H bond involved hydride formation after carbene lone pair donation into the non-bonding orbital of boranes.

2.5 Molecular orbitals during Lewis adduct formation and B-H bond activation

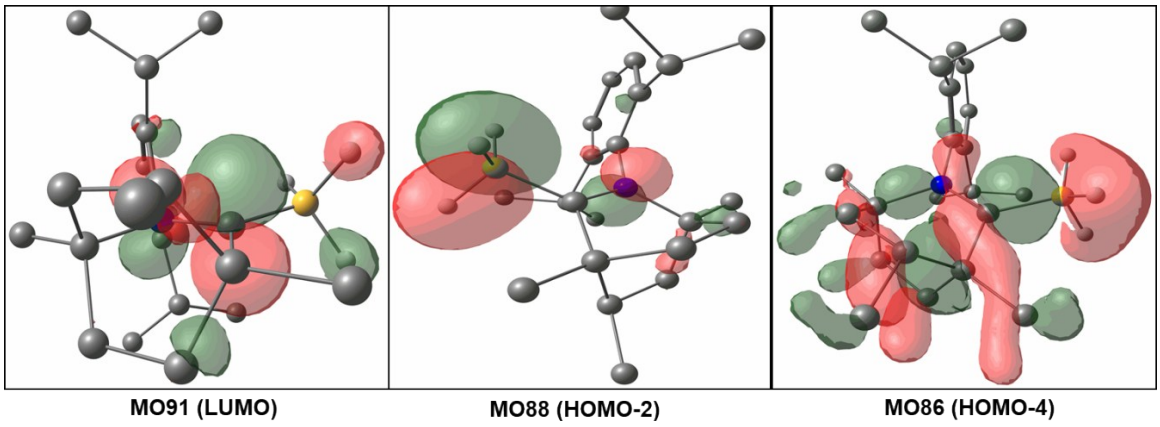


Fig. S47 Important molecular orbitals for **1**.

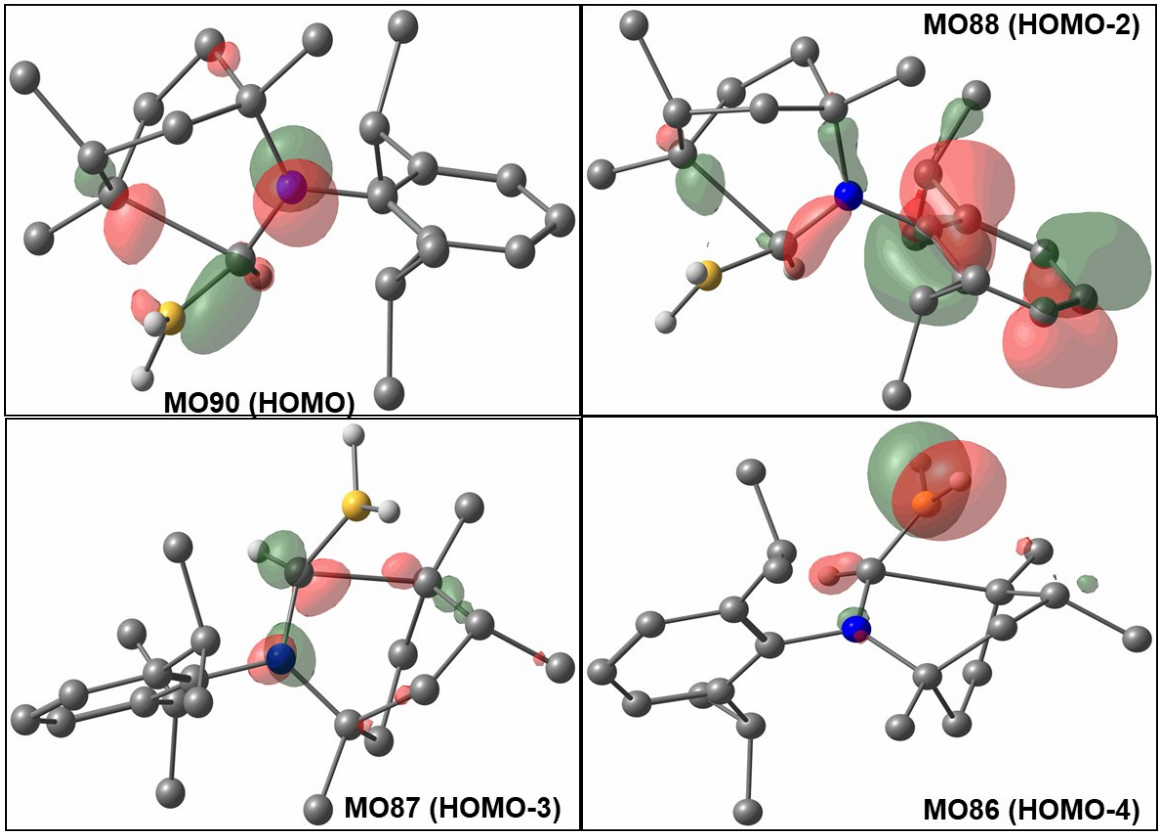


Fig. S48 Important molecular orbitals for **1TS**.

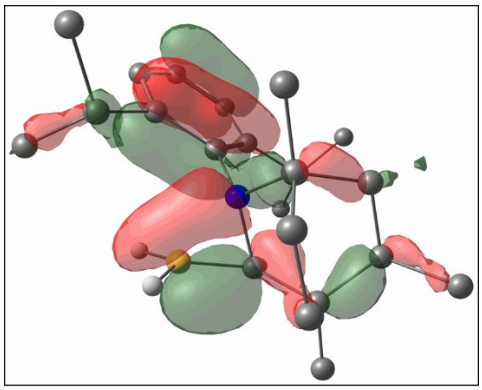


Fig. S49 Important molecular orbitals for **1BA**.

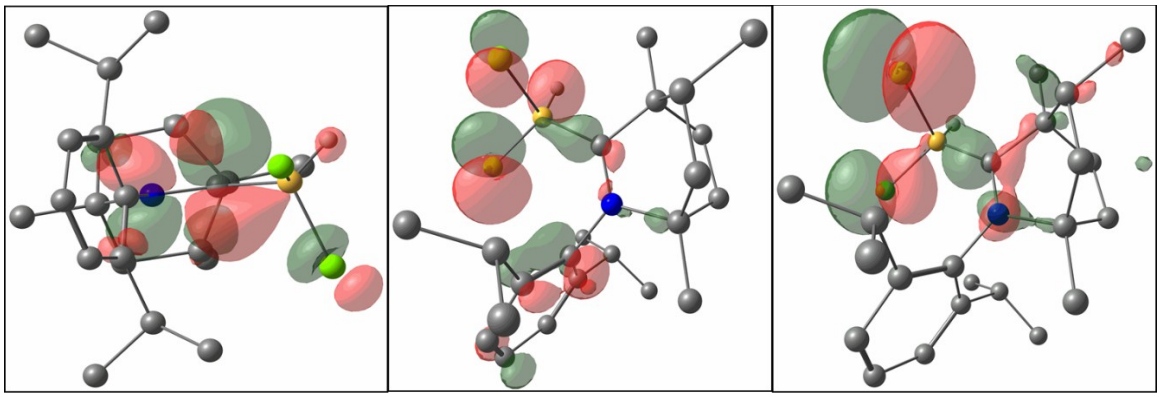


Fig. S50 Important molecular orbitals for **2**.

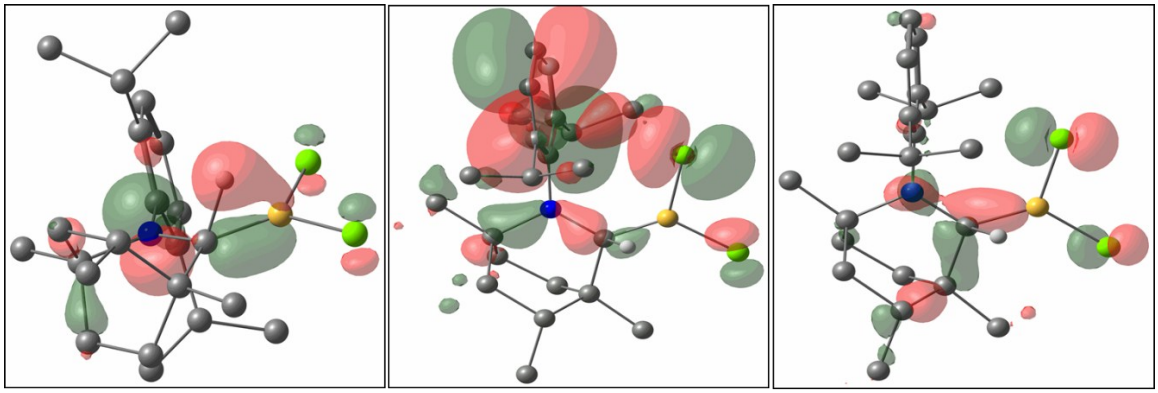


Fig. S51 Important molecular orbitals for **2TS**.

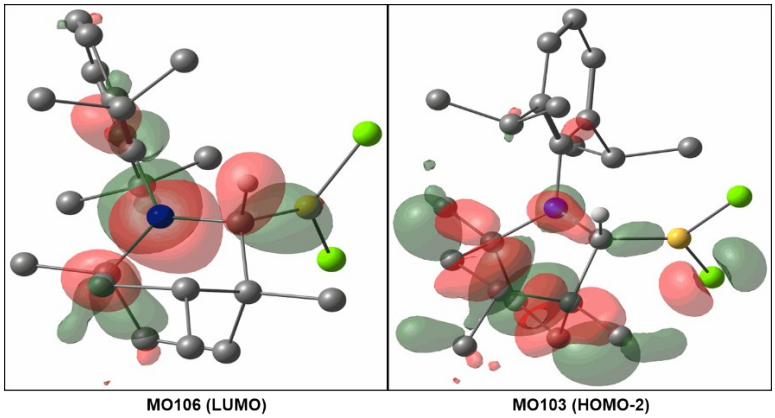


Fig. S52 Important molecular orbitals for **2BA**.

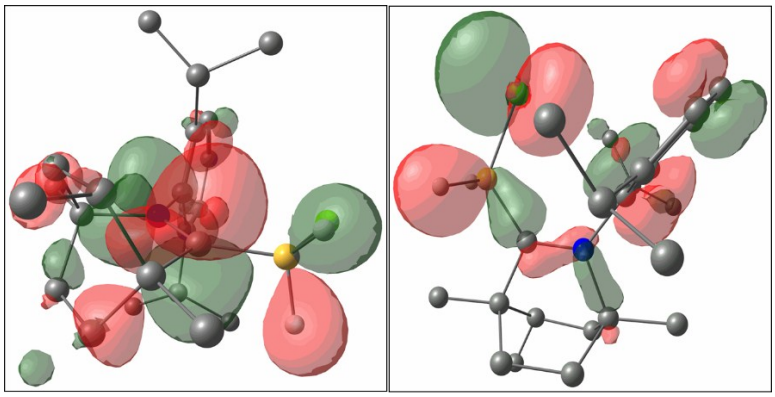


Fig. S53 Important molecular orbitals for **3**.

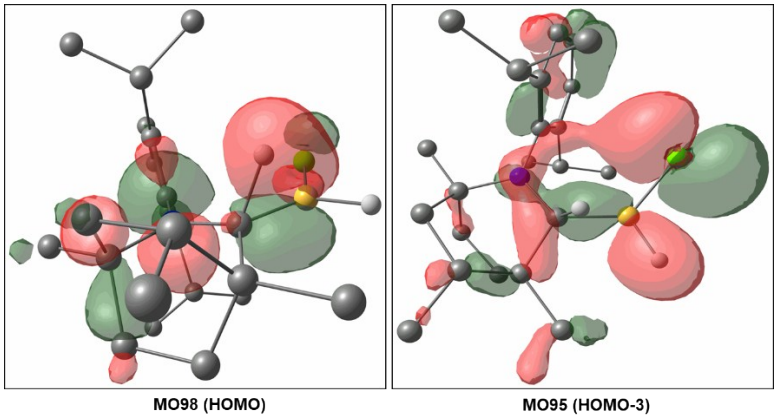


Fig. S54 Important molecular orbitals for **3TS**.

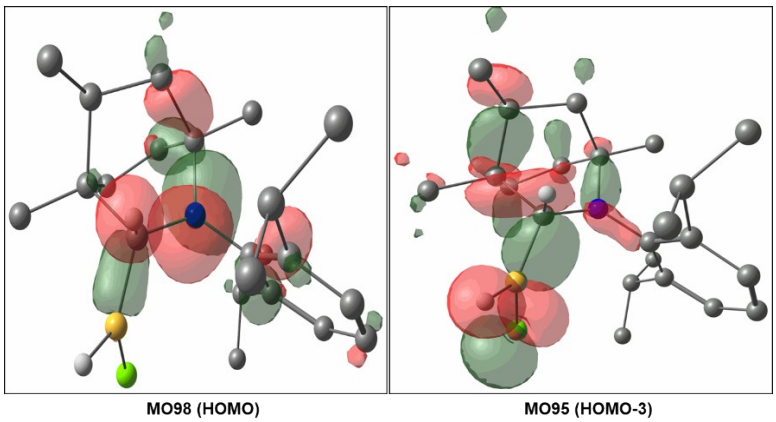


Fig. S55 Important molecular orbitals for **3BA**.

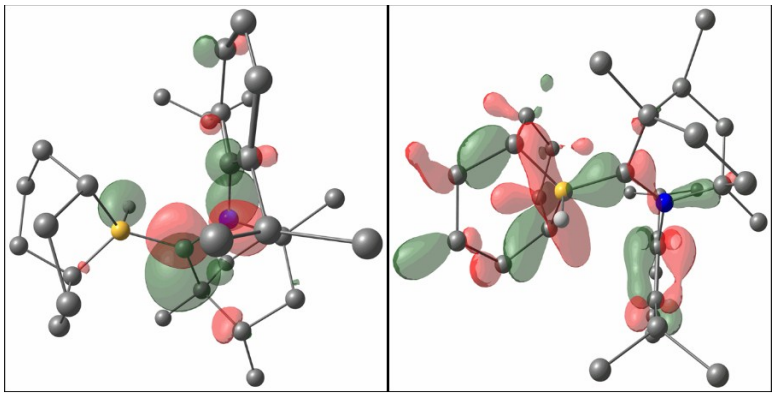


Fig. S56 Important molecular orbitals for **7A**.

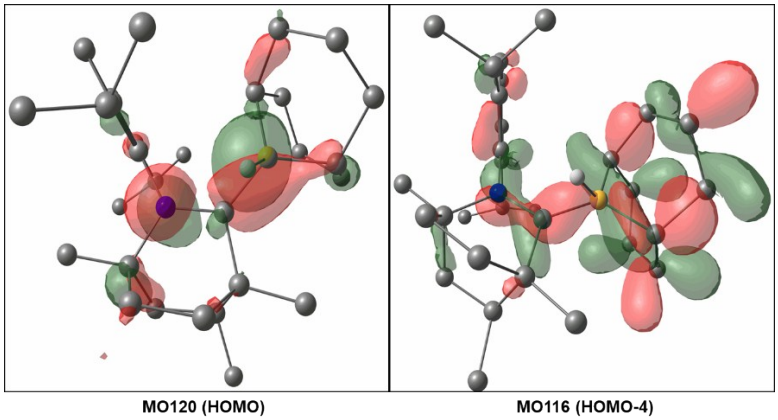


Fig. S57 Important molecular orbitals for **7TS**.

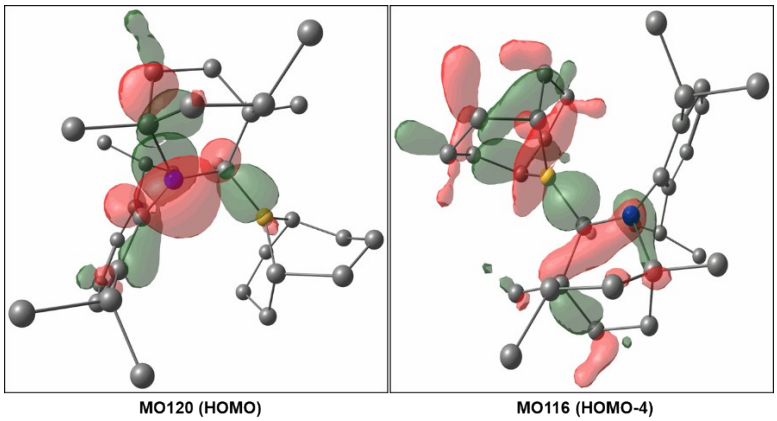


Fig. S58 Important molecular orbitals for **7**.

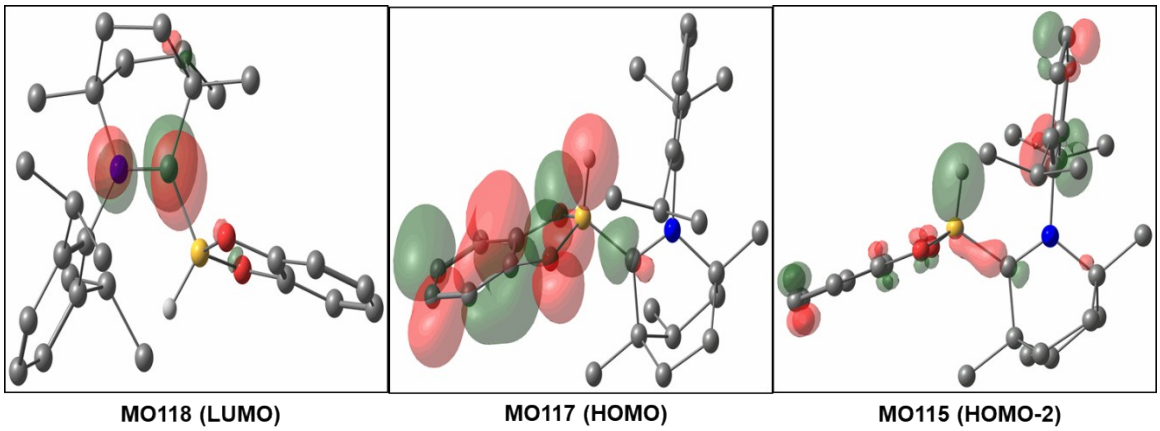


Fig. S59 Important molecular orbitals for **8A**.

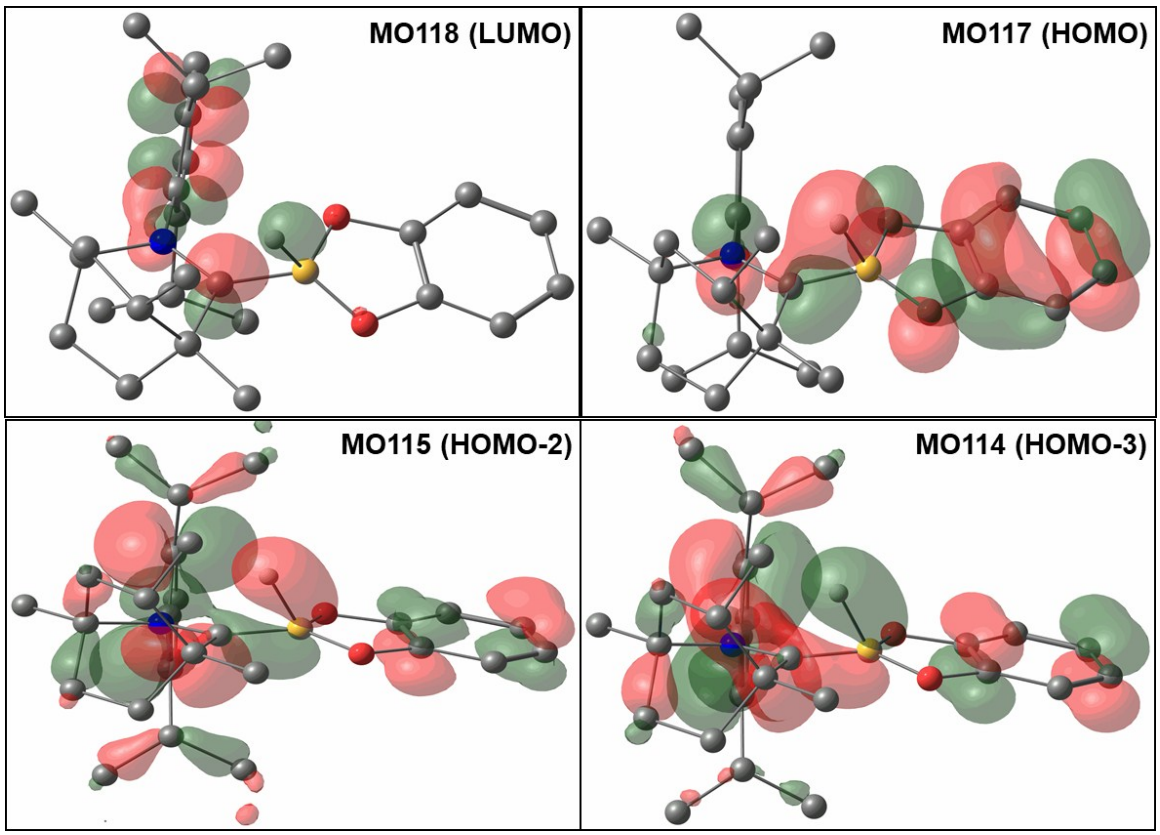


Fig. S60 Important molecular orbitals for **8TS**.

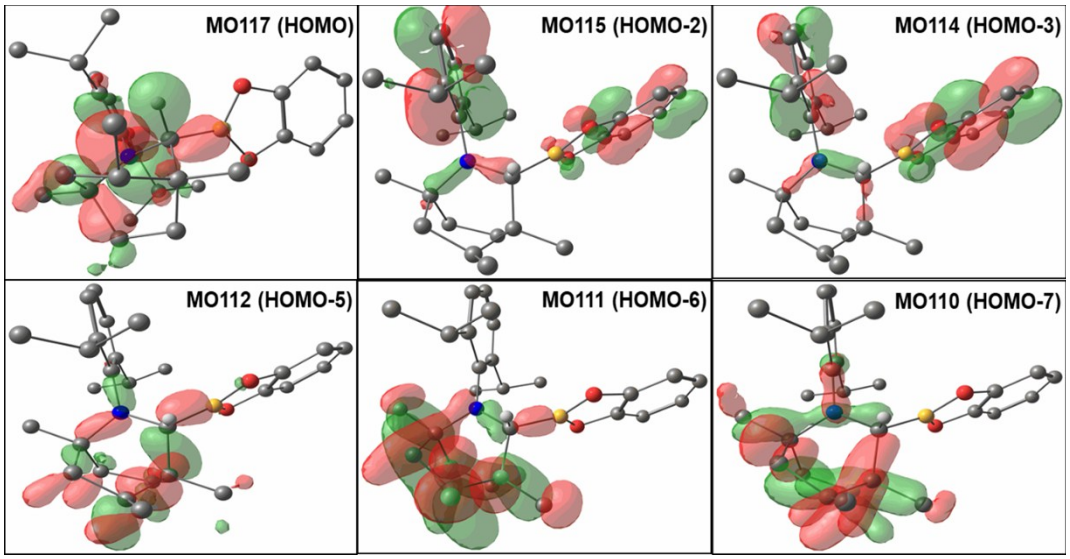


Fig. S61 Important molecular orbitals for **8**.

2.6 Electrostatic potentials (ESPs) during Lewis adduct formation and B-H bond activation

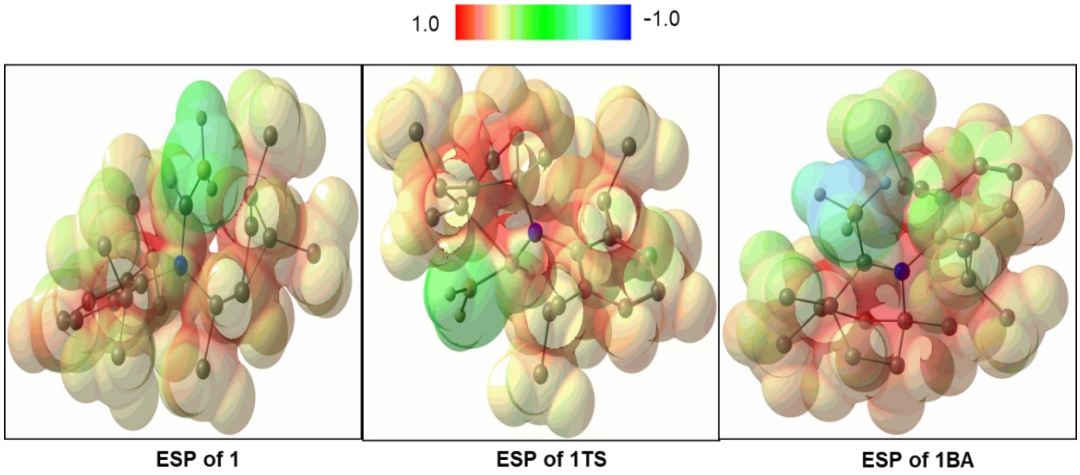


Fig. S62 ESPs for the interaction of BICAAC and BH_3.

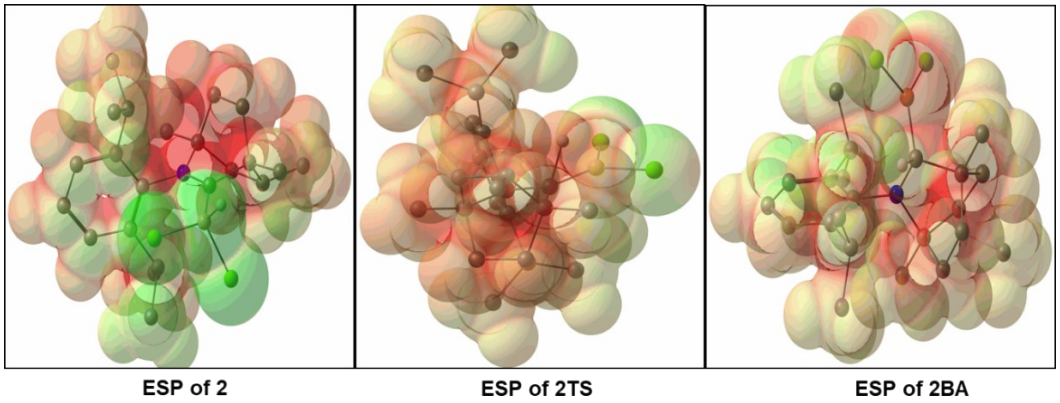


Fig. S63 ESPs for the interaction of BICAAC and $BHCl_2$.

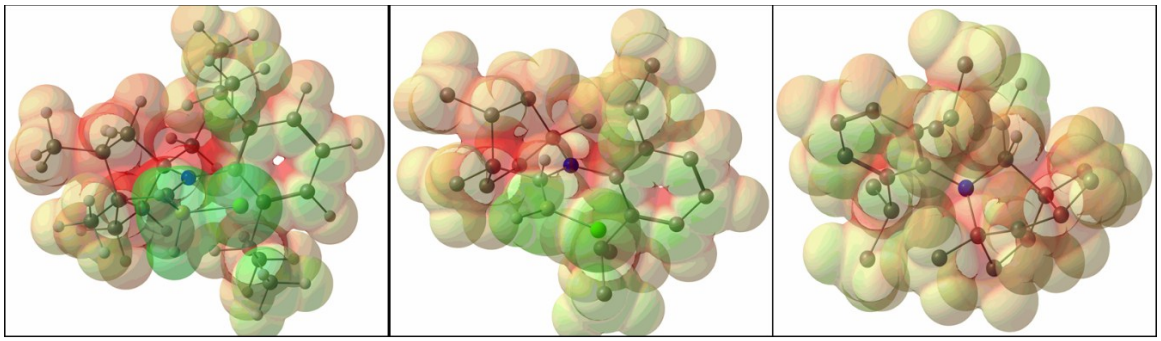


Fig. S64 ESPs for the interaction of BICAAC and BH_2Cl.

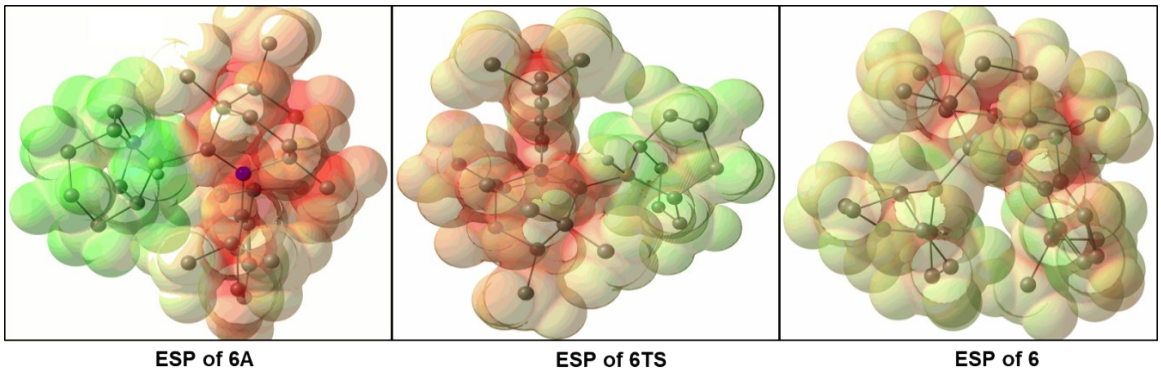


Fig. S65 ESPs for the interaction of BICAAC and 9-BBN.

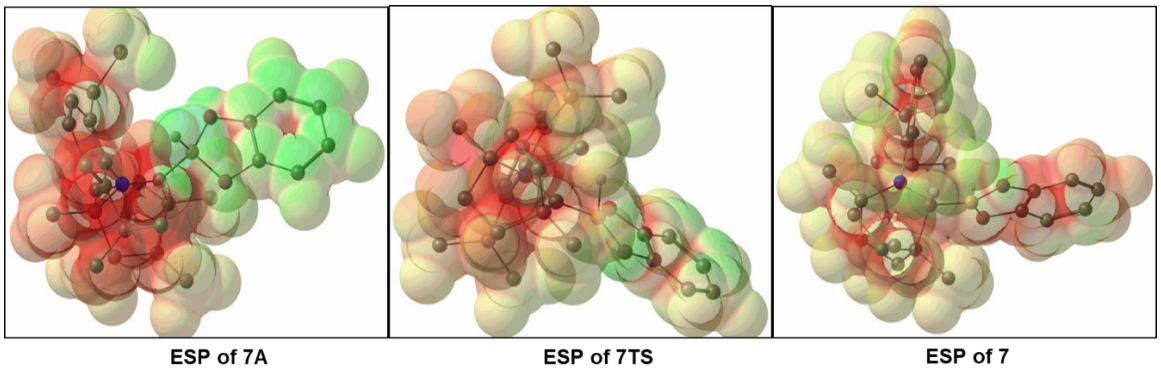


Fig. S66 ESPs for the interaction of BICAAC and HBcat.

2.7 Calculation of free energy of bond dissociation (ΔG_{FBD})

Free energy of bond dissociation was calculated to further verify the adduct formation and B-H activation in the compounds. To achieve this we needed to investigate the free energy change (ΔG_{eqn}) in the following equations: **eqn. 1** and **eqn. 2**. The difference in the free energy change ($\Delta G_{FBD} = \Delta G_{eqn2} - \Delta G_{eqn1}$) would signify the feasibility of occurrence of **eqn. 2** over **eqn. 1** which has been listed in the **Table S8**.

$$BICAAC - B(H)H_2 \rightarrow BICAAC - BH_2^+ + H^- \quad \textbf{..... (eqn. 1)}$$

$$BICAAC(H) - BH_2 \rightarrow BICAAC - BH_2^+ + H^- \quad \textbf{..... (eqn. 2)}$$

$$\Delta G_{eqn1} = \Delta G[BICAAC - BH_2^+] + \Delta G[H^-] - \Delta G[BICAAC - B(H)H_2]$$

$$\Delta G_{eqn2} = \Delta G[BICAAC - BH_2^+] + \Delta G[H^-] - \Delta G[BICAAC(H) - BH_2]$$

Table S9 Calculation of ΔG_{FBD} for the interaction of BICAAC and BH_3

Properties/Molecules	hydride	BICAAC-BH_2^+	BICAAC-BH_2^+	BICAAC-BH_2(H) (1)	BICAAC(H)-BH_2 (1BA)
Zero-point correction (Hartree/Particle)	0.000000	0.529084		0.538083	0.542726
Thermal correction to Energy (Hartree/Particle)	0.001416	0.554890		0.563566	0.567071
Thermal correction to Enthalpy (Hartree/Particle)	0.002360	0.555834		0.564510	0.568016
Thermal correction to Gibbs Free Energy (Hartree/Particle)	-0.010000	0.476552		0.486382	0.493250
Sum of electronic and zero-point Energies (Hartree/Particle) E_{zpe}	-0.461817	-938.299226		-939.107422	-939.090118
Sum of electronic and thermal Free Energies (Hartree/Particle) G_{tot}	-0.471816	-938.351758		-939.159123	-939.139594
BDE (Hartree/Particle)		0.335549	0.316020	0.000000	0.000000
BDE (kcal/mole)		210.560353	198.305710	0.000000	0.000000
		ΔG_{eqn1}	ΔG_{eqn2}		

Table S10 Calculation of ΔG_{FBD} for the interaction of BICAAC and $BHCl_2$

Properties/Molecules	**hydride**	**BICAAC-BCl_2^+**	**BICAAC-BCl_2^+**	**BICAAC-$BHCl_2$ (2)**	**BICAAC(H)-BCl_2 (2BA)**
Zero-point correction (Hartree/Particle)	0.000000	0.515808		0.525218	0.525420
Thermal correction to Energy (Hartree/Particle)	0.001416	0.543361		0.552706	0.553039
Thermal correction to Enthalpy (Hartree/Particle)	0.002360	0.544306		0.553650	0.553983
Thermal correction to Gibbs Free Energy (Hartree/Particle)	-0.010000	0.460280		0.470937	0.469500
Sum of electronic and zero-point Energies (Hartree/Particle) E_{zpe}	-0.461817	-1857.600231		-1858.403801	-1858.395583
Sum of electronic and thermal Free Energies (Hartree/Particle) G_{tot}	-0.471816	-1857.655758		-1858.458082	-1858.451502
BDE (Hartree/Particle)		0.330508	0.323928	0.000000	0.000000
BDE (kcal/mole)		207.397075	203.268059	0.000000	0.000000
		ΔG_{eqn1}	**ΔG_{eqn2}**		

Table S11 Calculation of ΔG_{FBD} for the interaction of BICAAC and BH_2Cl

Properties/Molecules	hydride	BICAAC-$BHCl^+$	BICAAC-$BHCl^+$	BICAAC-BH(H)Cl (3)	BICAAC(H)-BHCl (3BA)
Zero-point correction (Hartree/Particle)	0.000000	0.522895		0.531720	0.532724
Thermal correction to Energy (Hartree/Particle)	0.001416	0.549574		0.558193	0.559147
Thermal correction to Enthalpy (Hartree/Particle)	0.002360	0.550518		0.559137	0.560092
Thermal correction to Gibbs Free Energy (Hartree/Particle)	-0.010000	0.468315		0.478528	0.479205
Sum of electronic and zero-point Energies (Hartree/Particle) E_{zpe}	-0.461817	-1397.950851		-1398.756037	-1398.736765
Sum of electronic and thermal Free Energies (Hartree/Particle) G_{tot}	-0.471816	-1398.005431		-1398.809228	-1398.790284
BDE (Hartree/Particle)		0.331981	0.313037	0.000000	0.000000
BDE (kcal/mole)		208.321397	196.433848	0.000000	0.000000
		ΔG_{eqn1}	ΔG_{eqn2}		

Table S12 Calculation of ΔG_{FBD} for the interaction of BICAAC and 9-BBN

Properties/Molecules	**hydride**	**BICAAC-9-BBN$^+$**	**BICAAC-9-BBN$^+$**	**BICAAC-9-BBN(H) (7A)**	**BICAAC(H)-(9-BBN) (7)**
Zero-point correction (Hartree/Particle)	0.000000	0.721704		0.729774	0.730721
Thermal correction to Energy (Hartree/Particle)	0.001416	0.753829		0.761345	0.762823
Thermal correction to Enthalpy (Hartree/Particle)	0.002360	0.754773		0.762289	0.763767
Thermal correction to Gibbs Free Energy (Hartree/Particle)	-0.010000	0.662689		0.672318	0.671683
Sum of electronic and zero-point Energies (Hartree/Particle) E_{zpe}	-0.461817	-1250.203890		-1250.967710	-1250.981269
Sum of electronic and thermal Free Energies (Hartree/Particle) G_{tot}	-0.471816	-1250.262905		-1251.025165	-1251.040307
BDE (Hartree/Particle)		0.290444	0.305586	0.000000	0.000000
BDE (kcal/mole)		182.256514	191.758271	0.000000	0.000000
		ΔG_{eqn1}	**ΔG_{eqn2}**		

Table S13 Calculation of ΔG_{FBD} for the interaction of BICAAC and HBcat

Properties/Molecules	hydride	BICAAC-Bcat$^+$	BICAAC- Bcat$^+$	BICAAC-(H)Bcat (8A)	BICAAC(H)-Bcat (8)
Zero-point correction (Hartree/Particle)	0.000000	0.602860		0.610091	0.612140
Thermal correction to Energy (Hartree/Particle)	0.001416	0.633474		0.641003	0.642735
Thermal correction to Enthalpy (Hartree/Particle)	0.002360	0.634418		0.641947	0.643679
Thermal correction to Gibbs Free Energy (Hartree/Particle)	-0.010000	0.542999		0.550024	0.552725
Sum of electronic and zero-point Energies (Hartree/Particle) E_{zpe}	-0.461817	-1318.653629		-1319.413606	-1319.441531
Sum of electronic and thermal Free Energies (Hartree/Particle) G_{tot}	-0.471816	-1318.713490		-1319.473673	-1319.500947
BDE (Hartree/Particle)		0.288367	0.315641	0.000000	0.000000
BDE (kcal/mole)		180.953176	198.067884	0.000000	0.000000
		ΔG_{eqn1}	ΔG_{eqn2}		

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