Supporting Information

A Crystalline Dioxaborirane through Borylene Activation of Dioxygen

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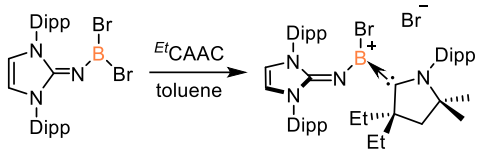
I. Preparation of Starting Materials

All manipulations were conducted within a nitrogen-filled glovebox or under a dry nitrogen atmosphere with indication, employing standard Schlenk techniques, unless otherwise specified. Toluene, *n*-hexane, and tetrahydrofuran (THF) were subjected to distillation over sodium or $LiAlH_4$ and subsequently stored using molecular sieves for purification. C_6D_6, CD_2Cl_2 were obtained by soaking the molecular sieve, which had been dried by a vacuum oil pump in pipe furnace at 300 °C for three days. NMR spectra were acquired at 298 K on a Bruker Avance 400 and Bruker Avance NEO Ascend 500 (400 (^{1}H: 400 MHz, ^{13}C{^{1}H}: 101 MHz, ^{11}B{^{1}H}: 128 MHz) 500 (^{1}H: 500 MHz, ^{13}C{^{1}H}: 126 MHz, ^{11}B{^{1}H}: 160 MHz, ^{19}F{^{1}H}: 471 MHz) NMR spectrometer. The provided data is presented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, sept = septet, m = multiplet and/or multiple resonances). High-resolution mass spectrometry (HRMS) was conducted using Thermo Fisher Scientific Q Exactive MS System and Thermo Fisher Scientific Orbitrap Exploris 120. Infrared spectra were recorded on Thermo Fisher Scientific Nicolet iS50. UV-Vis absorption spectra were measured on MAPADA UV-1800pc. Crystal data was collected on Bruker D8 QUEST Diffractometers respectively equipped with an Excillum METALJET diffractometer utilizing CuKα (λ = 1.54178), MoKα (λ = 0.71073) and GaKα (λ = 1.34138) radiation by APEX-III software suite. Commercial reagents were obtained from Energy Chemical, J&K or TCI Chemical, and were used without further purification. The abbreviations for the ligands and compounds are as follows: Dipp: 2,6-diisopropylphenyl. TMS: trimethylsilyl. ^{Dipp}NHI: (1,3-bis(2,6-diisopropylphenyl)-1,3-dihydro-2H-imidazol-2-ylidene)imino. ^{Et}CAAC: 1-(2,6-diisopropylphenyl)-3,3-diethyl-5,5-dimethylpyrrolidin-2-ylidene.

II. Experimental Details



1

Synthesis of 1:

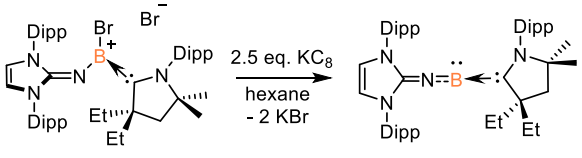
To a solution of ^{Et}CAAC (1.25 g, 4.00 mmol) in toluene (5 mL) at room temperature was slowly added a solution of ^{Dipp}NHIBBr$_2$ (2.29 g, 4.00 mmol) in toluene (6 mL) under vigorous stirring. The resulting orange-yellow suspension was stirred for 1.5 hours. The suspension was then filtered, and the collected solid was washed with toluene (3 × 3 mL). After drying under vacuum, compound **1** was obtained as an orange-yellow powder (3.23 g, 3.64 mmol) in 91.0% yield. Single crystals of **1** suitable for X-ray diffraction analysis were obtained from the THF solution at room temperature.

^{1}H NMR (500 MHz, CD_2Cl_2, 298 K, ppm): δ 7.50 (t, $^3J_{H\text{-}H}$ = 7.8 Hz, 2H, Ar-*H*), 7.43 (t, $^3J_{H\text{-}H}$ = 7.8 Hz, 1H, Ar-*H*), 7.29 (d, $^3J_{H\text{-}H}$ = 7.8 Hz, 4H, Ar-*H*), 7.14 (d, $^3J_{H\text{-}H}$ = 7.8 Hz, 1H, Ar-*H*), 6.80 (s, 2H, *H*C=C*H*), 2.89 (sept, $^3J_{H\text{-}H}$ = 6.8 Hz, 4H, C*H*(CH$_3$)$_2$), 2.28 (sept, *J* = 6.8 Hz, 2H, C*H*(CH$_3$)$_2$), 2.06 (s, 2H, ^{cyclic}C*H*$_2$), 1.78 (m, 2H, ^{Et}C*H*$_2$), 1.48-1.35 (m, 8H, ^{Et}C*H*$_2$, C*H*$_3$), 1.23 (d, $^3J_{H\text{-}H}$ = 6.8 Hz, 12H, CH(C*H*$_3$)$_2$), 1.15 (d, $^3J_{H\text{-}H}$ = 6.8 Hz, 6H, CH(C*H*$_3$)$_2$), 1.13 (d, $^3J_{H\text{-}H}$ = 6.8 Hz, 12H, CH(C*H*$_3$)$_2$), 0.73 (d, $^3J_{H\text{-}H}$ = 6.8 Hz, 6H, CH(C*H*$_3$)$_2$), 0.65 (t, $^3J_{H\text{-}H}$ = 7.4 Hz, 6H, ^{Et}C*H*$_3$).

^{13}C{^{1}H} NMR (126 MHz, CD_2Cl_2, 298 K, ppm): δ 152.36 (N=*C*), 146.93 (Ar-*C*), 144.88 (Ar-*C*), 131.84 (Ar-*C*), 131.75 (Ar-*C*), 131.55 (Ar-*C*), 131.51 (Ar-*C*), 131.47 (Ar-*C*), 126.18 (Ar-*C*), 119.64 (H*C*=*C*H), 84.70 (*C*q), 63.28 (*C*q), 40.25 (^{cyclic}*C*H$_2$), 31.28, 29.73 , 29.58 , 29.13, 25.90, 25.36, 25.22, 22.75, 10.02.

^{11}B{^{1}H} NMR (160 MHz, CD_2Cl_2, 298 K, ppm): δ 18.49 (br).

HRMS (ESI): *m/z*: [M−Br]$^+$ calcd. for $C_{49}H_{71}BN_4{}^{81}Br^+$ 805.4929, found 805.4918.



1 2

Synthesis of 2:

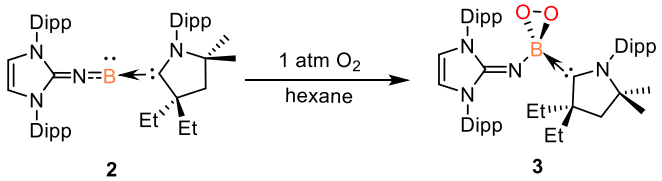
To a solid mixture of **1** (1.77 g, 2.00 mmol) and KC_8 (675 mg, 5.00 mmol) was added *n*-hexane (10 mL). The resulting mixture was stirred vigorously at room temperature for 48 hours. The mixture was then filtered, and the solid residue was washed with *n*-hexane (3 × 5 mL). The combined filtrate was concentrated under reduced pressure to approximately 3 mL. Recrystallization of the concentrated solution at −20 °C afforded compound **2** as deep red crystals (1.11 g, 1.53 mmol) in 76.5% yield.

^{1}H NMR (400 MHz, C_6D_6, 298 K, ppm): δ 7.15-7.20 (m, 3H, Ar-*H*), 7.04 (m, 6H, Ar-*H*), 5.80 (s, 2H, *H*C=C*H*), 3.68 (sept, $^3J_{H\text{-}H}$ = 6.9 Hz, 2H, C*H*(CH$_3$)$_2$), 3.02 (sept, $^3J_{H\text{-}H}$ = 6.9 Hz, 4H, C*H*(CH$_3$)$_2$), 1.88 (s, 2H, ^{cyclic}C*H*$_2$), 1.38-1.31 (m, 4H, ^{Et}C*H*$_2$), 1.31 (d, $^3J_{H\text{-}H}$ = 6.9 Hz, 6H, CH(C*H*$_3$)$_2$), 1.22 (m, 18H, CH(C*H*$_3$)$_2$, C*H*$_3$), 1.12 (d, $^3J_{H\text{-}H}$ = 6.9 Hz, 12H, CH(C*H*$_3$)$_2$), 0.91 (d, $^3J_{H\text{-}H}$ = 6.9 Hz, 6H, CH(C*H*$_3$)$_2$), 0.78 (t, $^3J_{H\text{-}H}$ = 7.4 Hz, 6H, ^{Et}C*H*$_3$).

^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K, ppm): δ 152.01 (N=*C*), 147.93 (Ar-*C*), 133.83 (Ar-*C*), 129.65 (Ar-*C*), 126.10 (Ar-*C*), 124.21 (Ar-*C*), 124.01 (Ar-*C*), 115.79 (H*C*=*C*H), 64.26 (*C*q), 52.36 (*C*q), 34.53 (^{cyclic}CH$_2$), 30.02, 28.95, 28.18, 27.33, 24.49, 24.29, 23.63, 10.98.

^{11}B{^{1}H} NMR (128 MHz, C_6D_6, 298 K, ppm): δ 57.64 (br).

HRMS (ESI): *m/z*: [M+H]$^+$ calcd. for $C_{49}H_{72}BN_4^+$ 727.5845, found 727.5851.



2 **3**

Synthesis of 3:

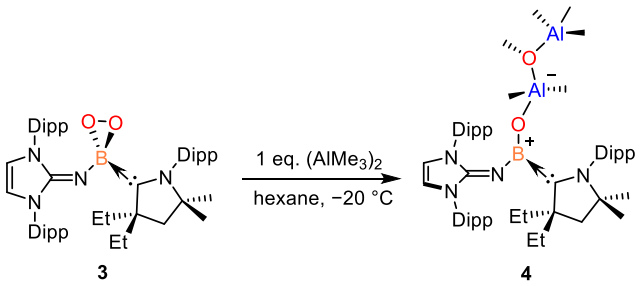
Oxygen (99.5% purity, dry) was purged through a solution of **2** (257 mg, 0.354 mmol) in *n*-hexane (10 mL), and the mixture was stirred for 10 minutes −20 °C. Upon exposure to oxygen, the deep red solution rapidly turned light yellow. The resulting mixture was soon filtered, and the residue was washed with *n*-hexane (3 × 2 mL). The combined filtrate was concentrated under reduced pressure to approximately 1 mL. Recrystallization from *n*-hexane at −20 °C afforded compound **3** as yellow crystals (117 mg, 0.154 mmol) in 43.5% yield. **Caution: 3 is unstable at room temperature.**

^{1}H NMR (500 MHz, C_6D_6, 298 K, ppm): δ 7.29 (t, $^{3}J_{H\text{-}H}$ = 7.7 Hz, 2H, Ar-*H*), 7.17 (d, $^{3}J_{H\text{-}H}$ = 7.7 Hz, 4H, Ar-*H*), 7.10 (d, $^{3}J_{H\text{-}H}$ = 7.6 Hz,1H, Ar-*H*), 7.00 (d, $^{3}J_{H\text{-}H}$ = 7.8 Hz, 2H, Ar-*H*), 5.97 (s, 2H, *H*C=C*H*), 3.35 (sept, $^{3}J_{H\text{-}H}$ = 6.9 Hz, 4H, C*H*$(CH_3)_2$), 2.60 (sept, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 2H, C*H*$(CH_3)_2$), 1.80-1.94 (m, 4H, $^{Et}CH_2$), 1.41 (d, $^{3}J_{H\text{-}H}$ = 6.9 Hz, 12H, CH(C*H*$_3)_2$), 1.40 (s, 2H, $^{cyclic}CH_2$), 1.29 (d, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 6H, CH(C*H*$_3)_2$), 1.25 (d, $^{3}J_{H\text{-}H}$ = 6.9 Hz, 12H, CH(C*H*$_3)_2$), 1.16 (d, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 6H, CH(C*H*$_3)_2$), 0.78 (s, 6H, C*H*$_3$), 0.68 (t, $^{3}J_{H\text{-}H}$ = 7.4 Hz, 6H, $^{Et}CH_3$).

^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K, ppm): δ 148.14 (N=C), 144.86 (Ar-*C*), 137.63 (Ar-*C*), 134.19 (Ar-*C*), 124.13 (Ar-*C*), 124.02 (Ar-*C*), 123.07 (Ar-*C*), 114.93 (H*C*=*C*H), 78.19 (*C*q), 61.76 (*C*q), 40.53 ($^{cyclic}CH_2$), 29.66, 29.59, 29.07, 28.92, 28.79, 26.76, 26.59, 25.61, 24.46, 23.78, 23.36, 22.59, 9.83.

^{11}B{^{1}H} NMR (128 MHz, C_6D_6, 298 K, ppm): δ −2.79 (s).

HRMS (ESI): *m/z*: [M+H]$^+$ calcd. for $C_{49}H_{72}BN_4O_2^+$ 759.5743, found 759.5739.



Synthesis of 4:

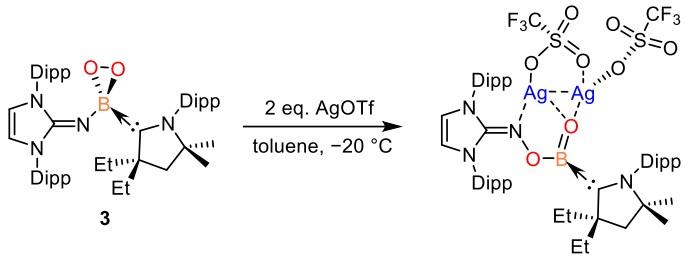
To a solution of **3** (76 mg, 0.100 mmol) in *n*-hexane (5 mL) at −20 °C was added trimethylaluminium (2 M, 100 μL, 0.20 mmol). The resulting mixture was stirred at −20 °C for 10 hours. The pale suspension was filtered, and the solid was washed with *n*-hexane (3 × 2 mL) to afford compound **4**. Single crystals of **4** suitable for X-ray diffraction analysis were obtained by cooling a saturated toluene solution to −20 °C in 71.3% yield (64 mg, 0.071 mmol).

^{1}H NMR (500 MHz, C_6D_6, 298 K, ppm): δ 7.13-7.10 (m, 5H, Ar-*H*), 7.07–6.95 (m, 2H, Ar-*H*), 6.88 (d, $^{3}J_{H\text{-}H}$ = 7.8 Hz, 2H, Ar-*H*), 5.81 (s, 2H, *H*C=C*H*), 2.85 (sept, $^{3}J_{H\text{-}H}$ = 6.7 Hz, 4H, C*H*$(CH_3)_2$), 2.72 (s, 3H, OC*H*$_3$), 2.52 (m, 2H, C*H*$(CH_3)_2$), 1.52 (d, $^{3}J_{H\text{-}H}$ = 6.7 Hz, 6H, CH(C*H*$_3)_2$), 1.40 (s, 2H, $^{cyclic}CH_2$), 1.34-1.27 (m, 4H, $^{Et}CH_2$), 1.13-1.09 (m, 9H, CH(C*H*$_3)_2$), 1.05 (d, $^{3}J_{H\text{-}H}$ = 6.6 Hz, 6H, CH(C*H*$_3)_2$), 0.97 (m, 15H, CH(C*H*$_3)_2$), 0.63 (s, 6H, C*H*$_3$), 0.60 (t, $^{3}J_{H\text{-}H}$ = 7.4 Hz, 6H, $^{Et}CH_3$), −0.03 (s, 9H, Al(C*H*$_3)_3$), −0.37 (s, 6H, Al(C*H*$_3)_2$).

$^{13}C\{^1H\}$ NMR (126 MHz, C_6D_6, 298 K, ppm): δ 148.98 (*C*=N), 146.84 (Ar-*C*), 135.29 (Ar-*C*), 131.16 (Ar-*C*), 130.65 (Ar-*C*), 129.99 (Ar-*C*), 125.54 (Ar-*C*), 125.32 (Ar-*C*), 123.84 (Ar-*C*), 116.95 (H*C*=*C*H), 81.45 (*C*q), 60.88 (*C*q), 50.48 (Al(CH_3)$_2$OCH_3), 39.73 ($^{cyclic}CH_2$), 31.45, 29.44, 28.75, 28.26, 28.12, 27.23, 26.10, 23.96, 22.96, 22.67, 15.60, 14.35, 10.90, −3.63 (Al(CH_3)$_2$OCH$_3$), −6.18 (Al(CH_3)$_3$).

$^{11}B\{^1H\}$ NMR (160 MHz, C_6D_6, 298 K, ppm): δ 18.22 (s).

HRMS (ESI): *m/z*: $[M+H]^+$ calcd. for $C_{55}H_{90}Al_2BN_4O_2^+$, 903.6782, found 903.6788.



3 5

Synthesis of 5:

To a solid mixture of **3** (76 mg, 0.100 mmol) and silver trifluoromethanesulfonate (53 mg, 0.200 mmol) at −20 °C was rapidly added toluene (10 mL). The resulting mixture was stirred at −20 °C for 12 hours. The mixture was then filtered, and the solid residue was washed with a 2:1 (V/V) mixture of *n*-hexane/toluene (3 × 6 mL) to afford compound **5** as an orange powder (88 mg, 0.0705 mmol) in 70.5% yield. Single crystals of **5** suitable for X-ray diffraction analysis were obtained by cooling a saturated toluene solution to −20 °C.

^1H NMR (500 MHz, C_6D_6, 298 K, ppm): δ 7.57 (t, $^3J_{H\text{-}H}$ = 7.8 Hz, 1H, Ar-*H*)), 7.42 (t, $^3J_{H\text{-}H}$ = 7.7 Hz, 1H, Ar-*H*), 7.28 (d, $^3J_{H\text{-}H}$ = 7.8 Hz, 2H, Ar-*H*), 7.11-7.16 (m, 3H, Ar-H) 7.03 (d, $^3J_{H\text{-}H}$ = 7.7 Hz, 2H, Ar-*H*), 5.66 (d, $^3J_{H\text{-}H}$ = 2.6 Hz, 1H, *H*C=C*H*), 5.54 (d, $^3J_{H\text{-}H}$ = 2.6 Hz, 1H, *H*C=C*H*)), 3.02 (sept, $^3J_{H\text{-}H}$ = 6.9 Hz, 2H, C*H*(CH_3)$_2$), 2.79 (sept, $^3J_{H\text{-}H}$ = 6.9 Hz, 2H, C*H*(CH_3)$_2$), 2.43 (sept, $^3J_{H\text{-}H}$ = 6.9 Hz, 2H, C*H*(CH_3)$_2$), 1.68 (s, 2H, $^{cyclic}CH_2$), 1.39 (m, 12H, CH(CH_3)$_2$, CH_2CH$_3$), 1.38 (d, $^3J_{H\text{-}H}$ = 6.9 Hz, 6H, CH(CH_3)$_2$), 1.27 (d, $^3J_{H\text{-}H}$ = 6.9 Hz, 6H, CH(CH_3)$_2$), 1.11 (m, 12H, CH(CH_3)$_2$), 1.05 (d, $^3J_{H\text{-}H}$ = 6.9 Hz, 6H, CH(CH_3)$_2$), 0.93 (s, 6H, (CH_3)$_2$), 0.80-0.65 (m, 10H, CH(CH_3)$_2$, CH$_2$CH_3).

$^{13}C\{^1H\}$ NMR (126 MHz, C_6D_6, ppm): δ 149.04 (*C*=N), 146.39 (Ar-*C*), 146.07 (Ar-*C*), 144.94 (Ar-*C*), 135.73 (Ar-*C*), 132.59 (Ar-*C*), 132.08 (Ar-*C*), 130.62 (Ar-*C*), 129.91 (Ar-*C*), 129.37 (Ar-

C), 126.27 (Ar-*C*), 125.70 (Ar-*C*), 125.50 (Ar-*C*), 124.53 (Ar-*C*), 117.43 (H*C*=CH), 116.03 (HC=*C*H), 82.04 (*C*q), 59.29 (*C*q), 39.97 (^{cyclic}*C*H$_2$), 29.82, 29.58, 29.35, 29.05, 28.35, 27.12, 24.68 24.33, 24.08, 23.64, 23.47, 10.31.

^{19}F NMR (471 MHz, C_6D_6, 298 K, ppm): δ −76.68 (s).

^{11}B{^{1}H} NMR (160 MHz, C_6D_6, 298 K, ppm): δ 22.37 (br).

HRMS (ESI): *m/z*: [M+H]$^+$ calcd. for 1273.2893, found 1273.2894.

III. NMR Spectra

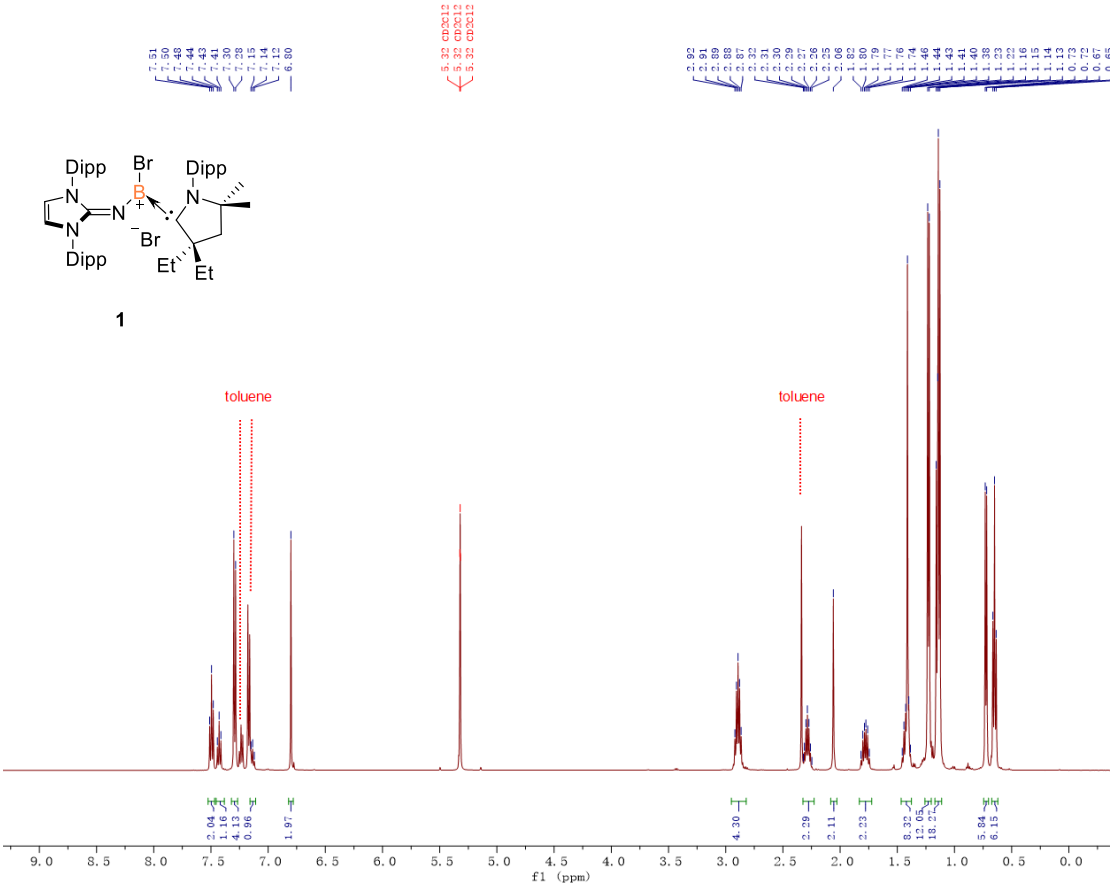


Figure S1. ^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of **1**.

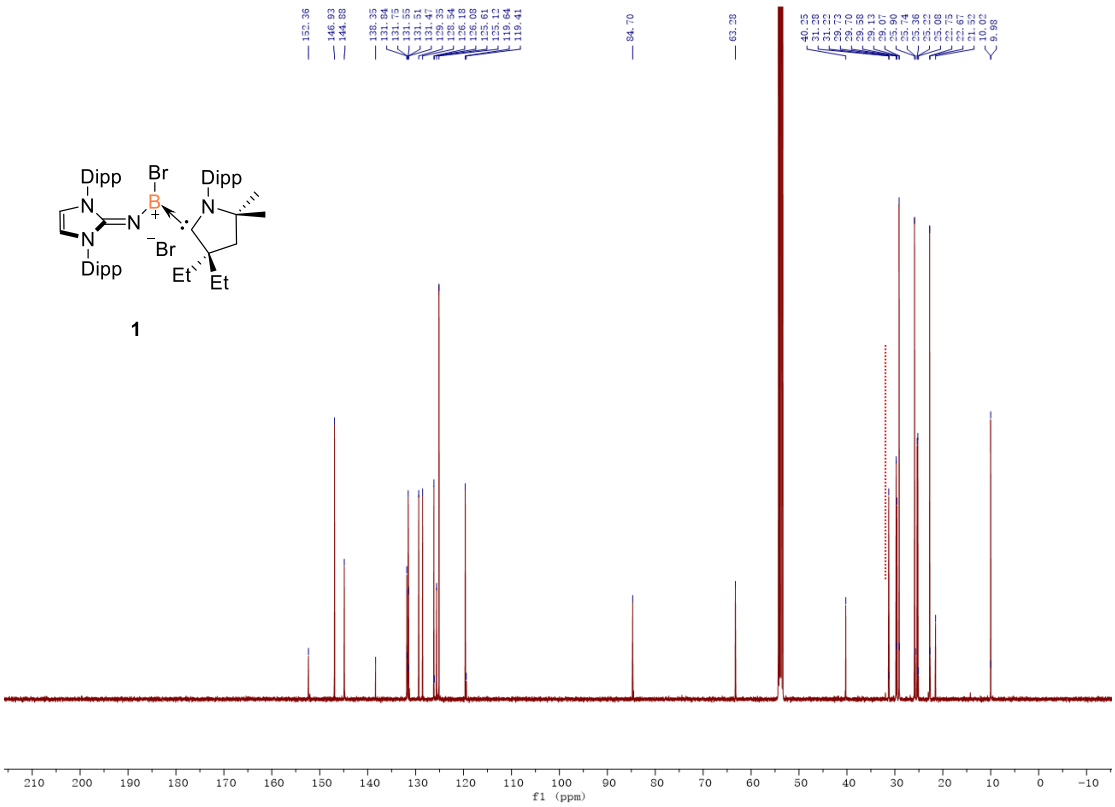


Figure S2. $^{13}C\{^{1}H\}$ NMR (126 MHz, CD_2Cl_2) spectrum of **1**.

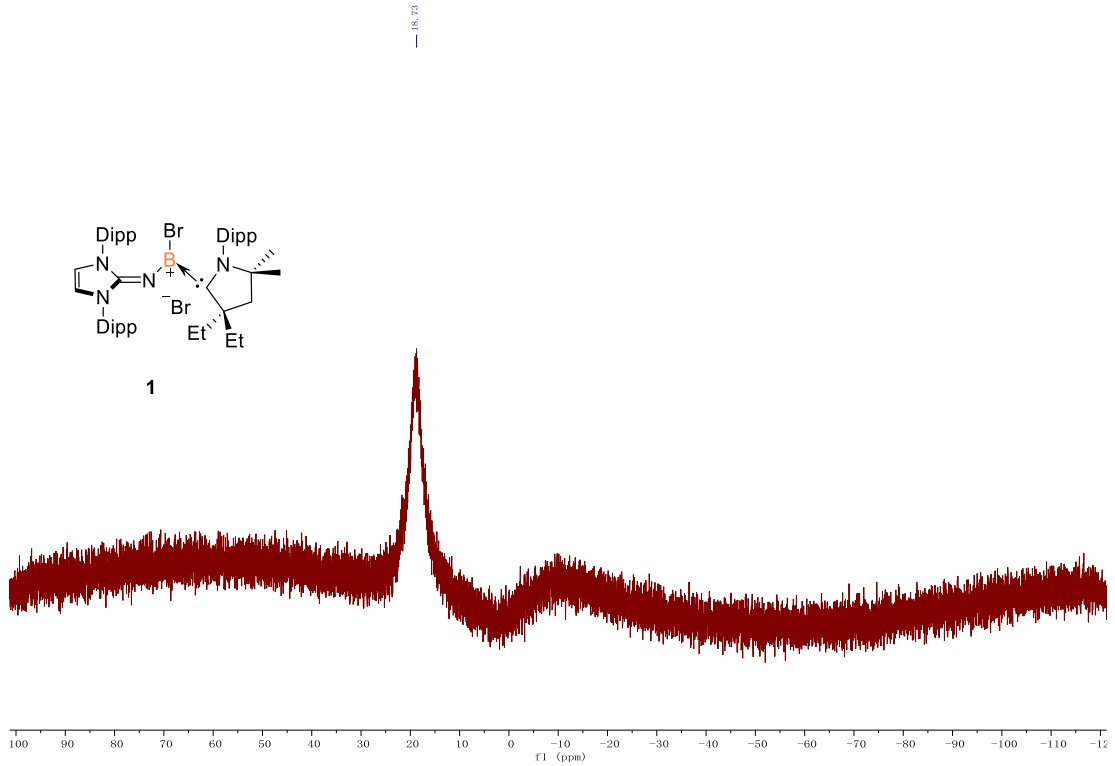


Figure S3. $^{11}B\{^{1}H\}$ NMR (160 MHz, CD_2Cl_2) spectrum of **1**.

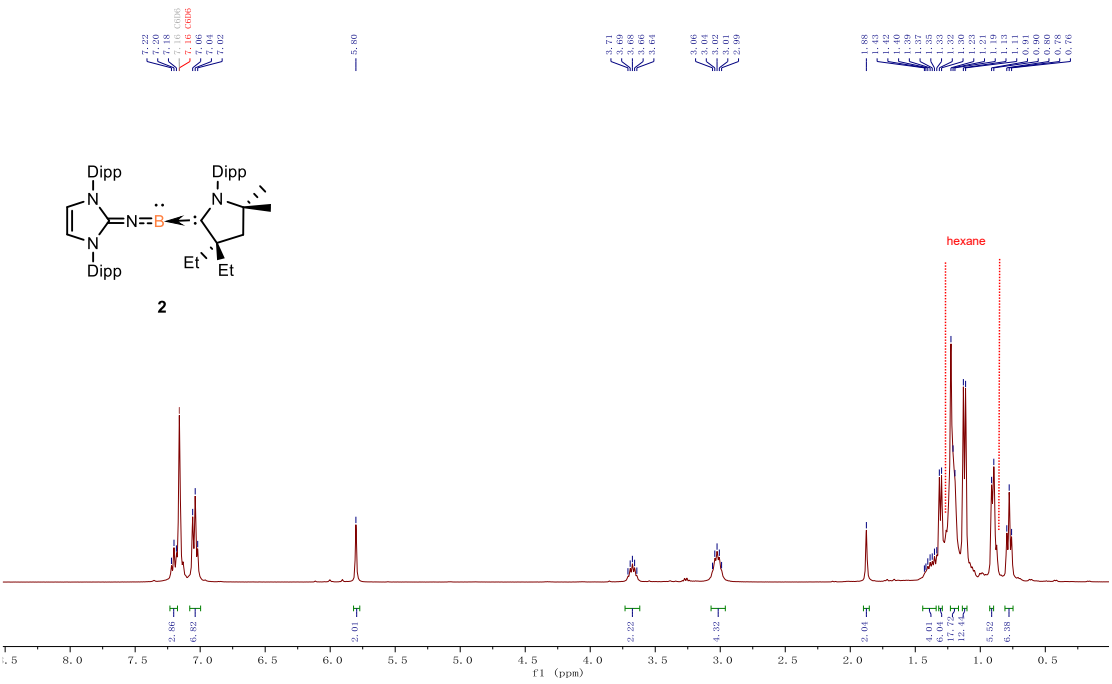


Figure S4. ^{1}H NMR (400 MHz, C_6D_6) spectrum of **2**.

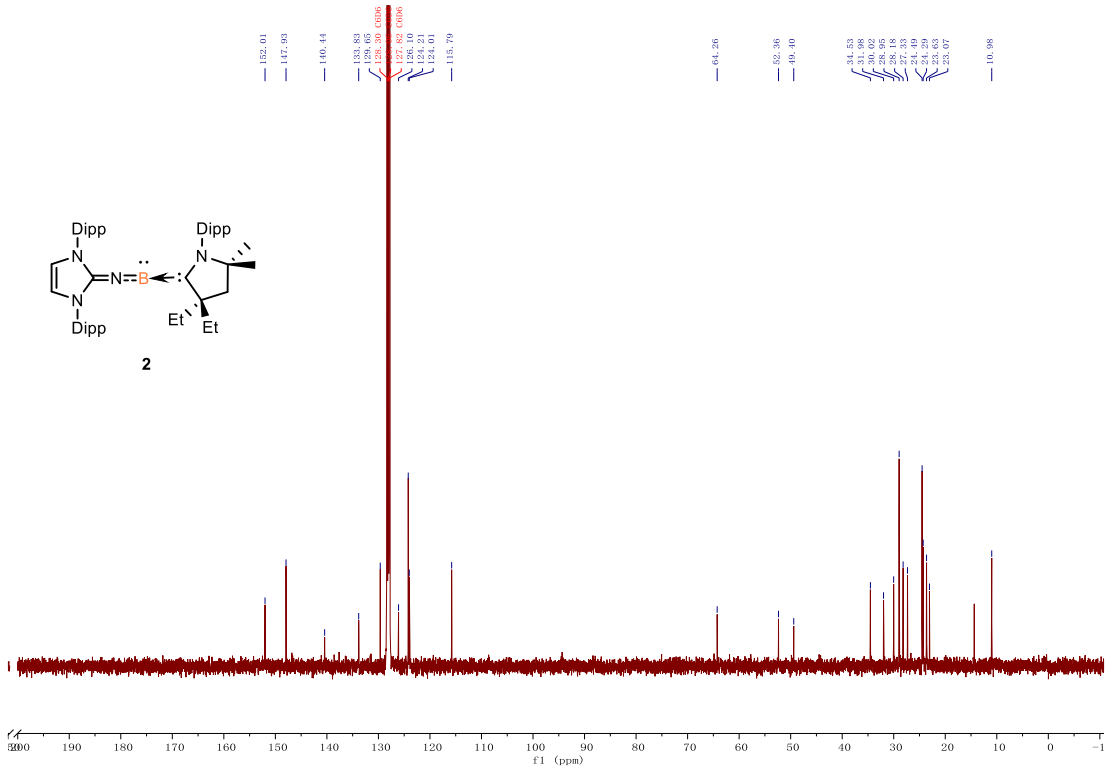


Figure S5. $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6) spectrum of **2**.

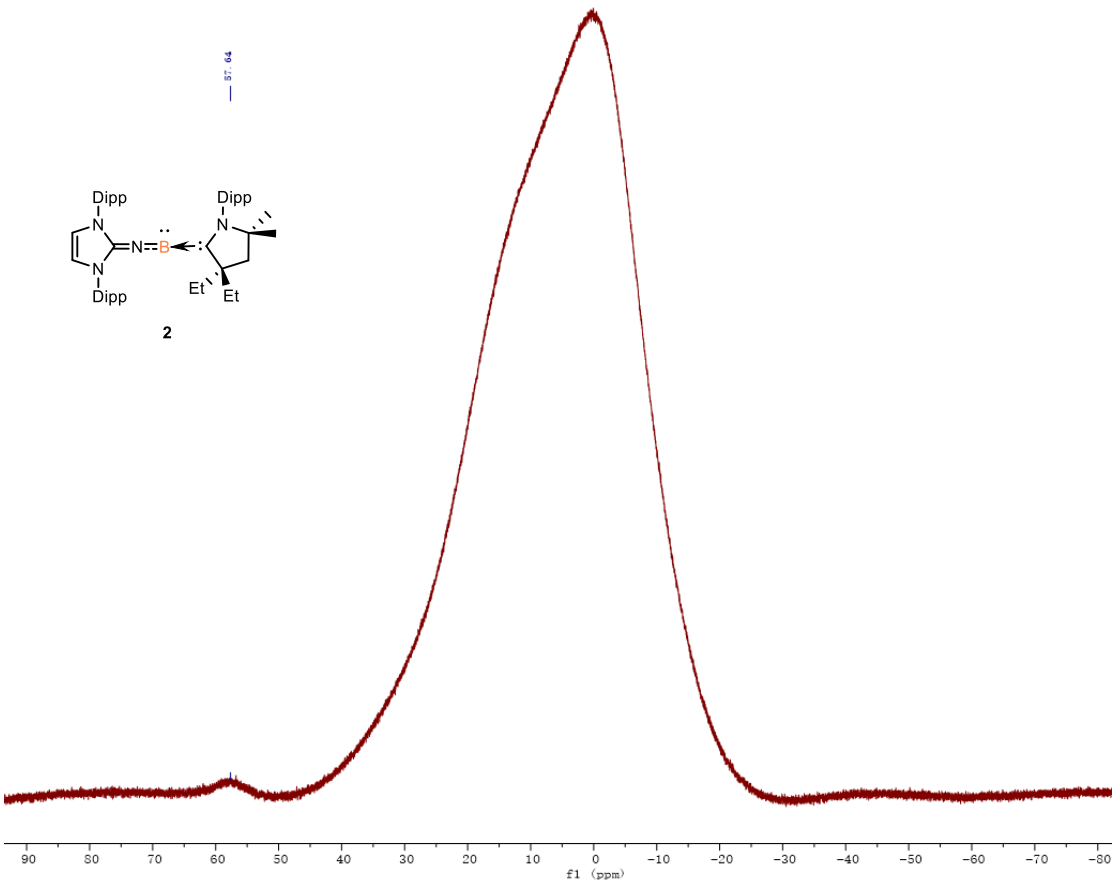


Figure S6. $^{11}B\{^{1}H\}$ NMR (128 MHz, C_6D_6) spectrum of **2**.

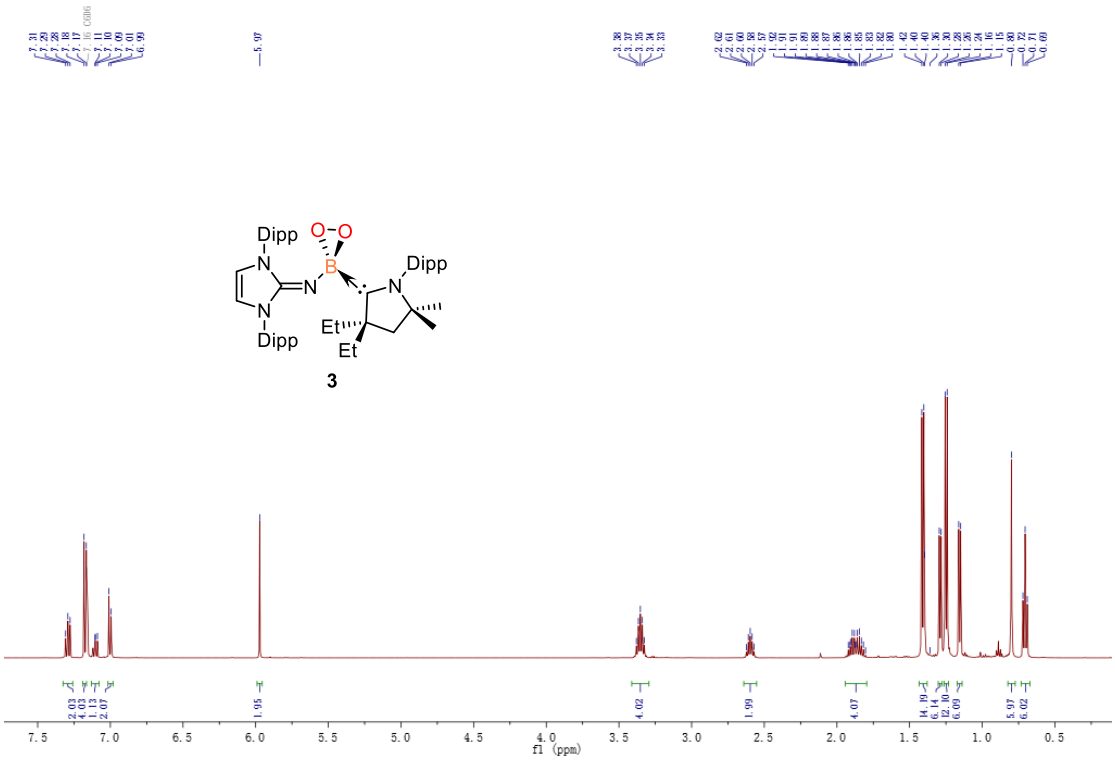


Figure S7. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **3**.

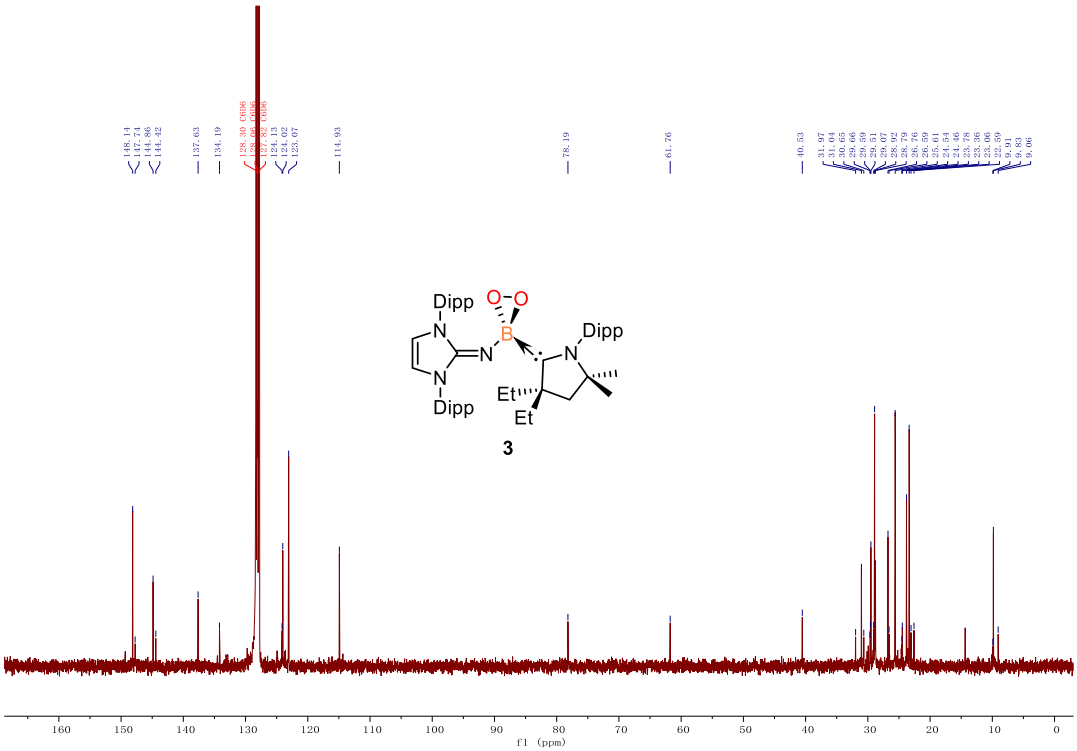


Figure S8. $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6) spectrum of **3**.

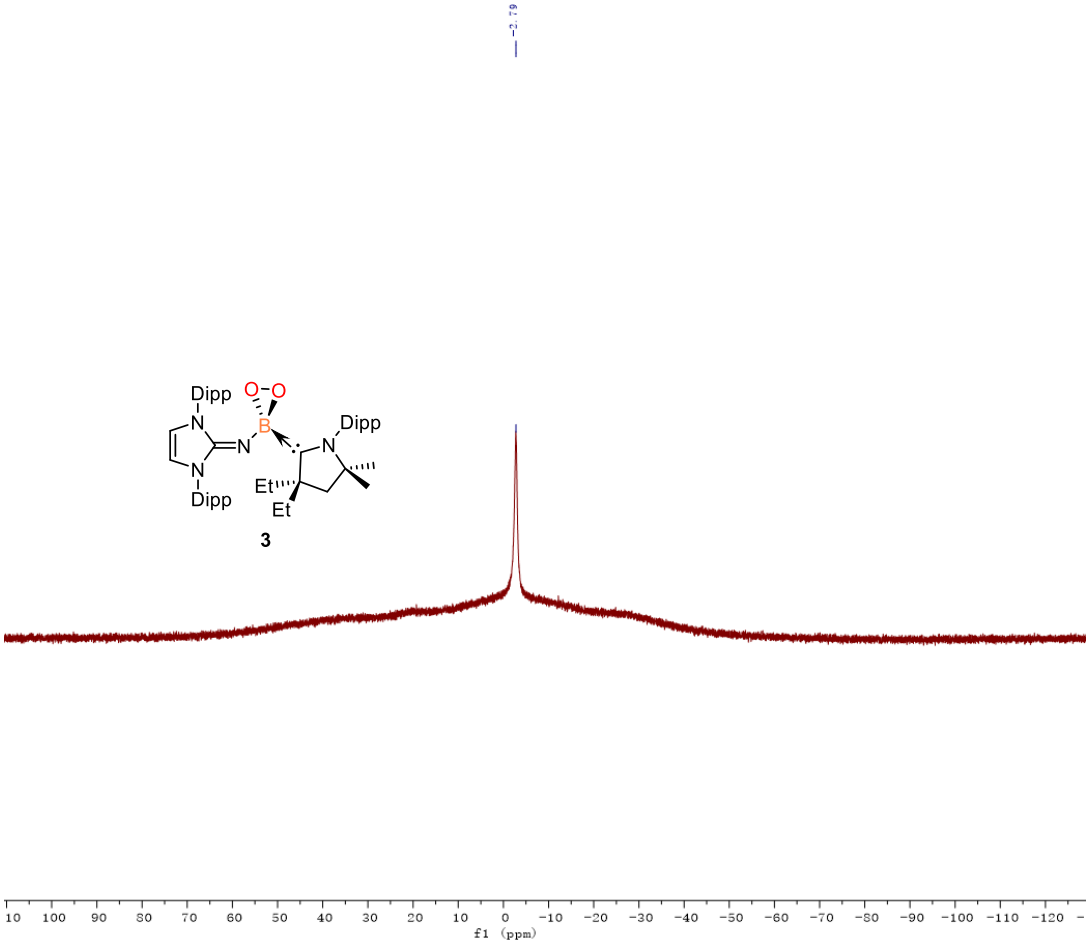


Figure S9. $^{11}B\{^{1}H\}$ NMR (128 MHz, C_6D_6) spectrum of **3**.

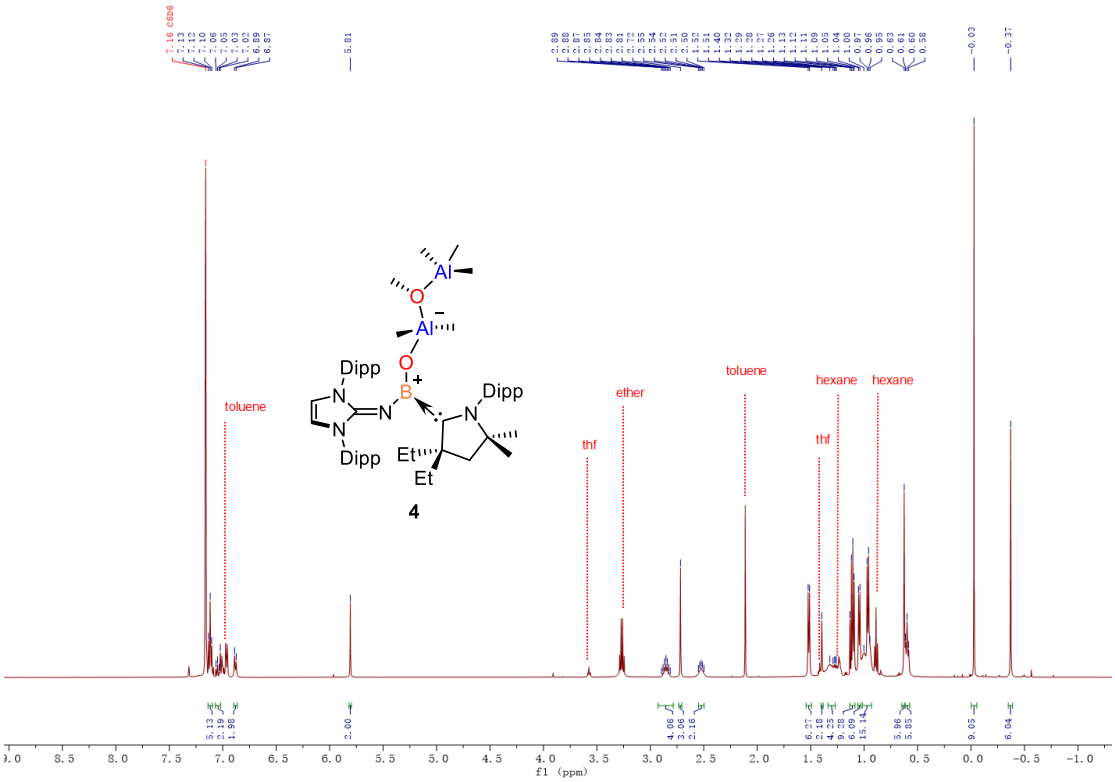


Figure S10. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **4**.

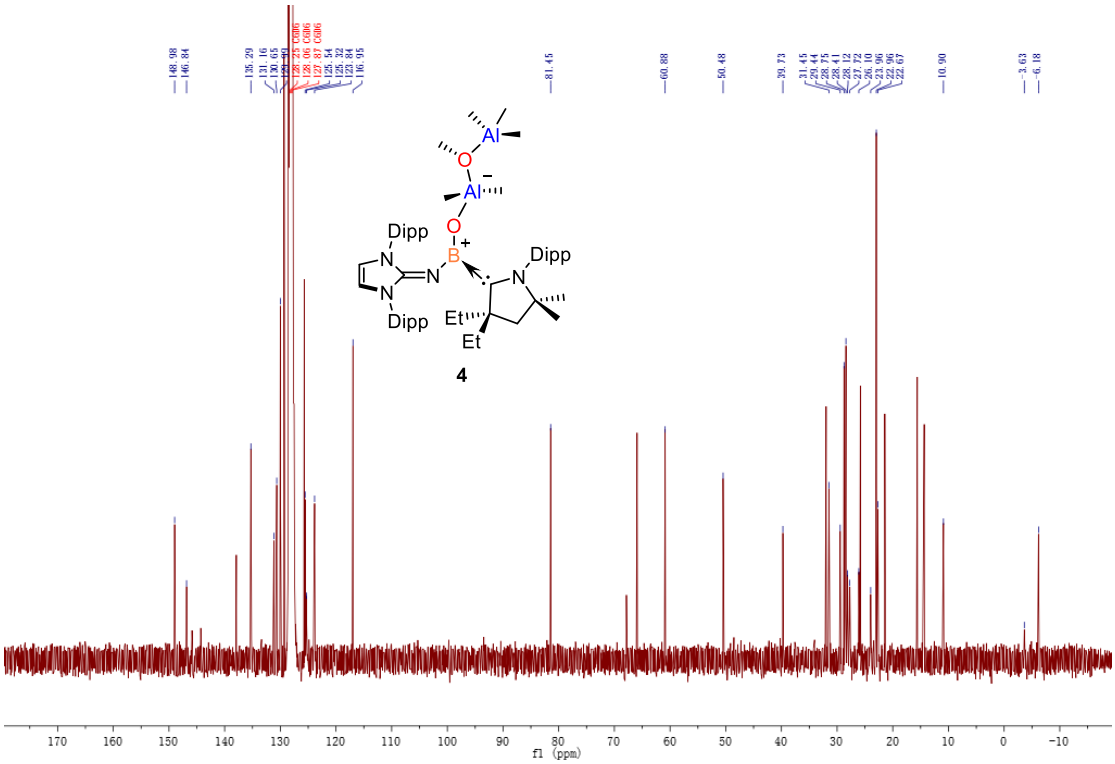


Figure S11. ^{13}C{^{1}H} NMR (126 MHz, C_6D_6) spectrum of **4**.

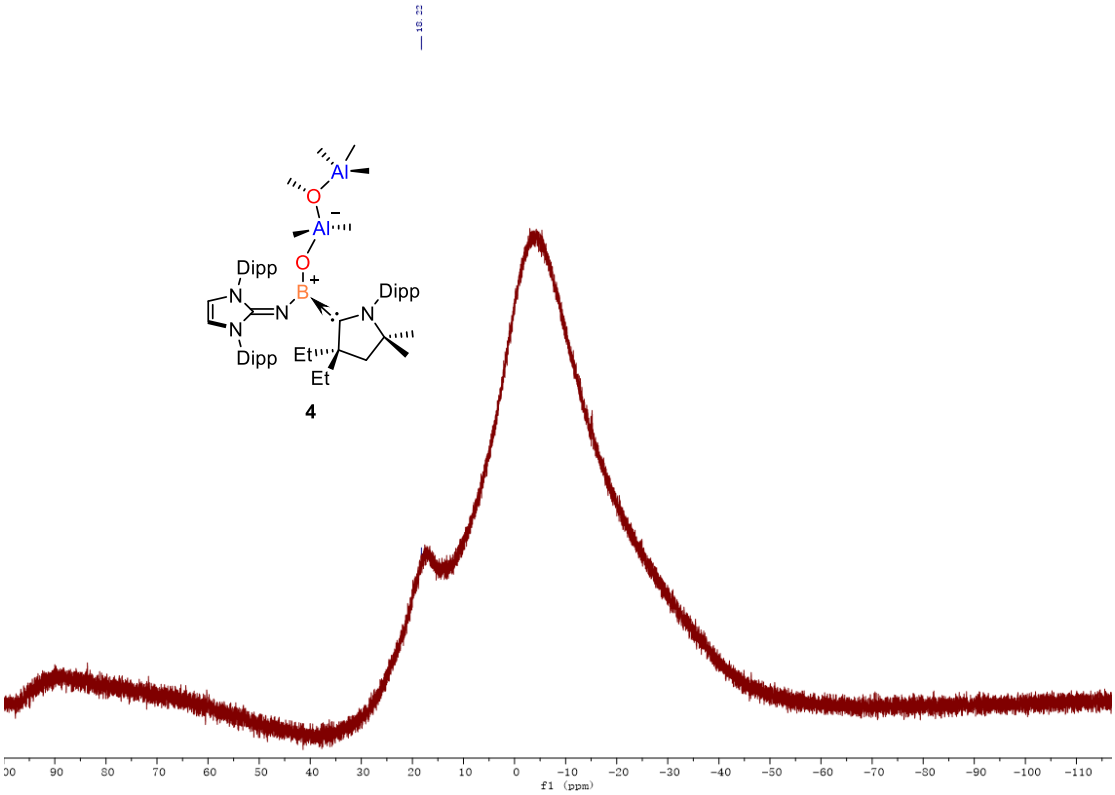


Figure S12. $^{11}B\{^{1}H\}$ NMR (160 MHz, C_6D_6) spectrum of **4**.

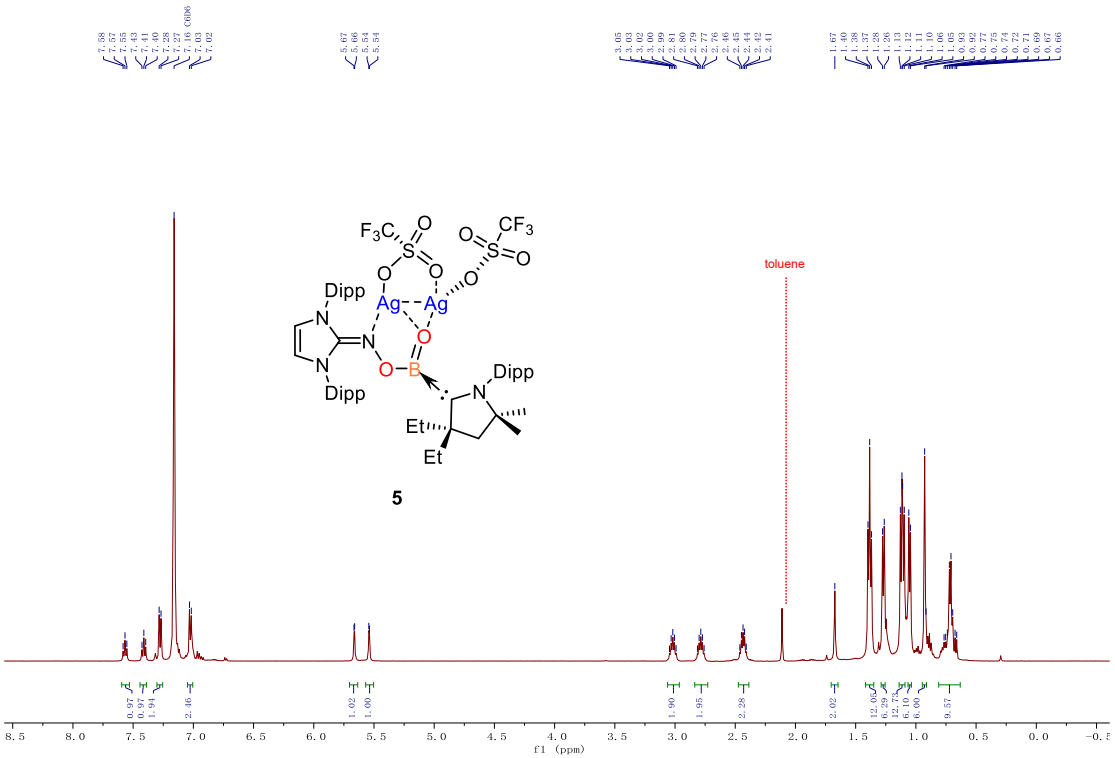


Figure S13. ^{1}H NMR (500 MHz, C_6D_6) spectrum of **5**.

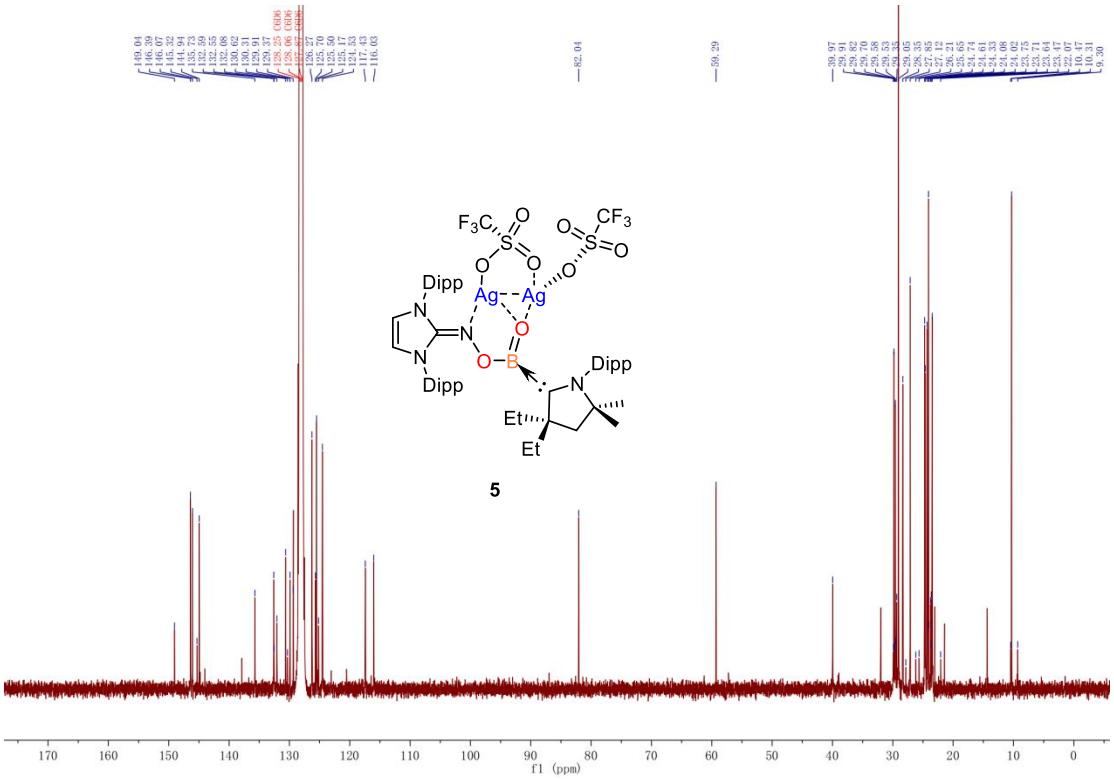


Figure S14. $^{13}C\{^{1}H\}$ NMR (126 MHz, C_6D_6) spectrum of **5**.

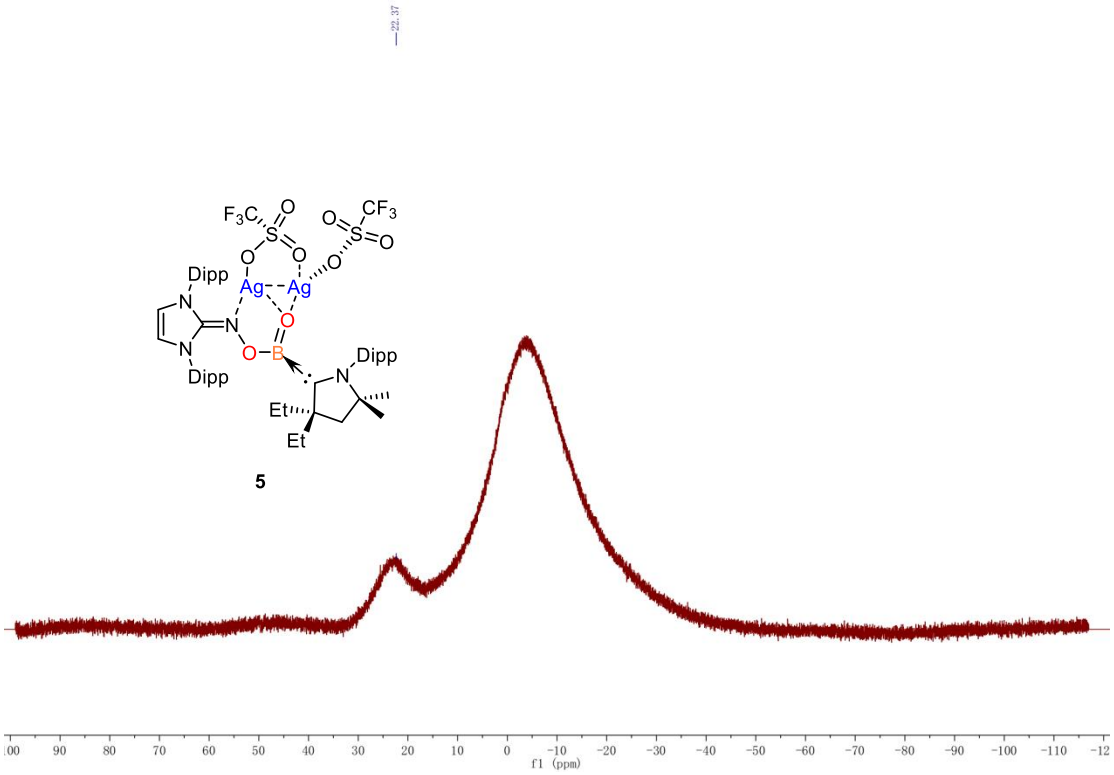


Figure S15. $^{11}B\{^{1}H\}$ NMR (160 MHz, C_6D_6) spectrum of **5**.

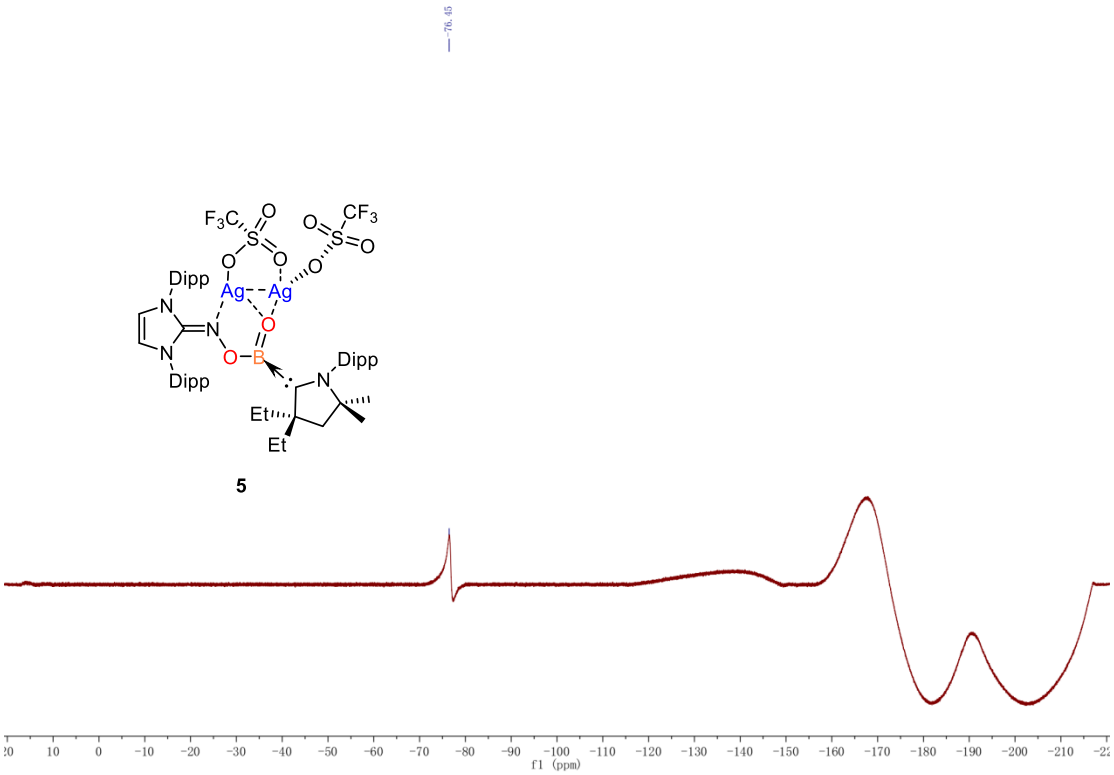


Figure S16. ^{19}F NMR (471 MHz, C_6D_6) spectrum of **5**.

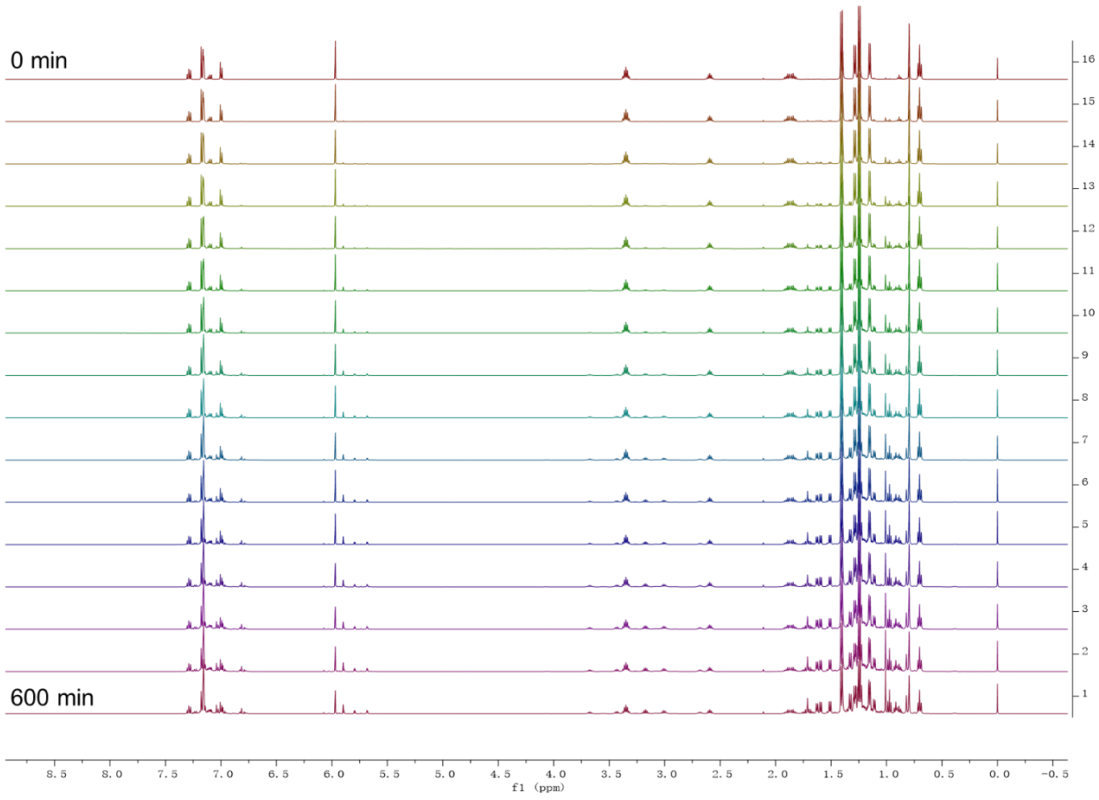


Figure S17. The decomposition of **3** was monitored by ^1H NMR in C_6D_6 at 298 K using $Si(CH_3)_4$ as an internal standard within 40-minute intervals.

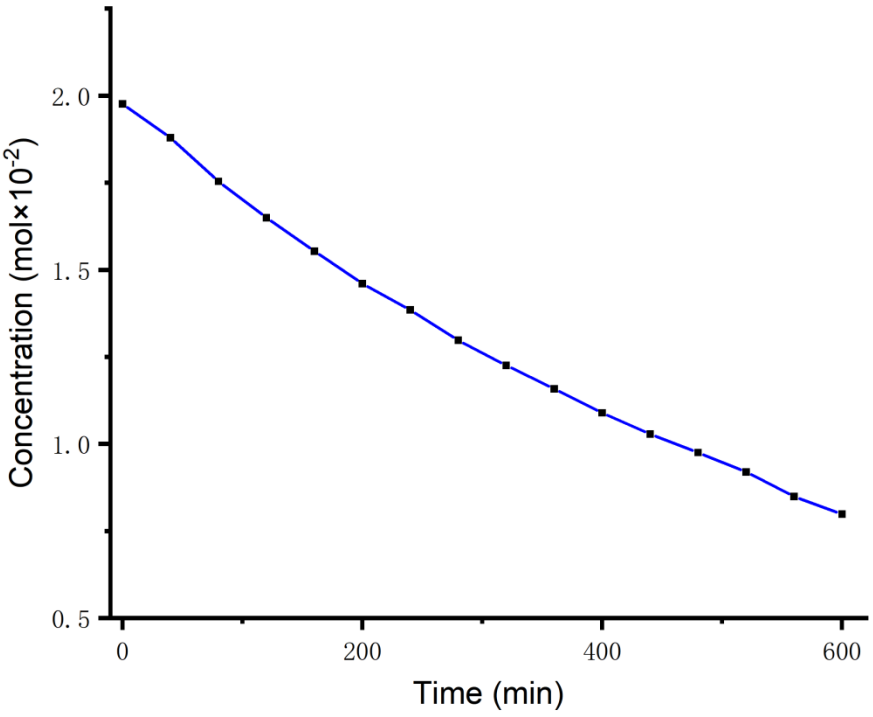


Figure S18. The relationship between concentration (10^{-2} M) and time (min) for the decomposition of **3** in C_6D_6.

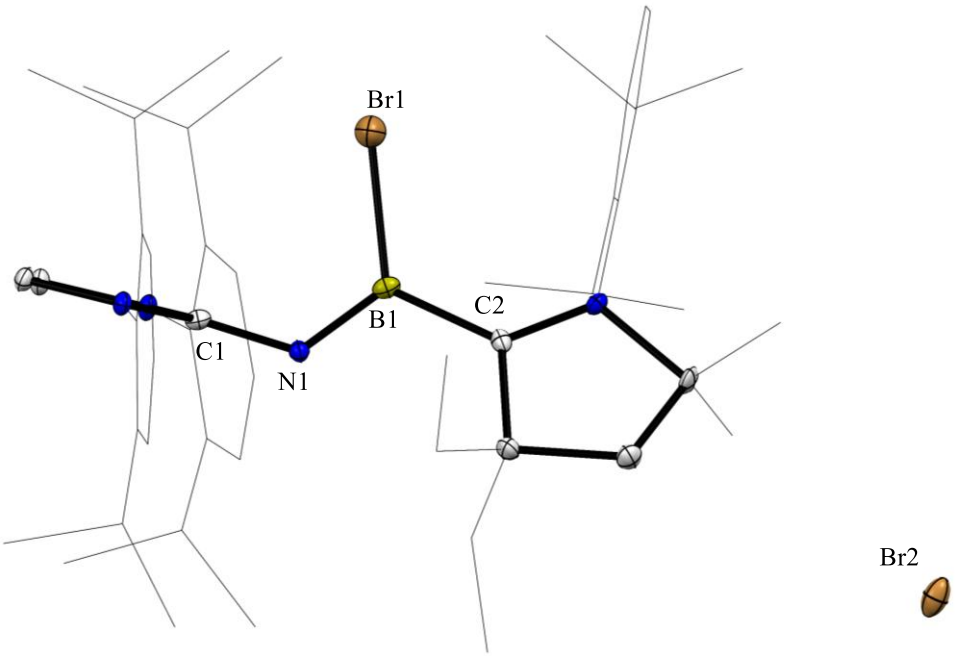


Figure S19. Solid-state structure of **1**. Anisotropic displacement ellipsoids are shown at the 30% probability level. Hydrogen atoms are omitted for clarity.

IV.X-ray Crystallography

Table S1. Crystal data and structure refinement for 1.

Identification code	**1** / 2552624
Empirical formula	$C_{49}H_{71}BBr_2N_4$
Formula weight	886.72
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.6053(12)
b/Å	25.104(2)
c/Å	15.4687(13)
α/°	90
β/°	110.476(3)
γ/°	90
Volume/Å^3	4949.4(7)
Z	4
ρ_{calc}g/cm^3	1.190
μ/mm^{-1}	1.534
F(000)	1872.0
Crystal size/mm^3	0.201 × 0.12 × 0.081
Radiation	GaKα (λ = 1.34138)
2Θ range for data collection/°	6.126 to 114.262
Index ranges	$-16 \le h \le 16$, $-31 \le k \le 31$, $-18 \le l \le 19$
Reflections collected	45424
Independent reflections	10036 [R_{int} = 0.0843, R_{sigma} = 0.0869]
Data/restraints/parameters	10036/0/521
Goodness-of-fit on F^2	1.072
Final R indexes [I>=2σ (I)]	R_1= 0.0588, wR_2= 0.1538
Final R indexes [all data]	R_1= 0.0973, wR_2= 0.1696
Largest diff. peak/hole / e Å^{-3}	0.83/−1.52

Table S2. Crystal data and structure refinement for 2.

Identification code	**2** / 2552625
Empirical formula	$C_{52}H_{78}BN_4$
Formula weight	769.99
Temperature/K	100.0
Crystal system	triclinic
Space group	P−1
a/Å	9.4498(4)
b/Å	12.2199(5)
c/Å	21.1498(9)
α/°	84.786(3)
β/°	80.996(3)
γ/°	77.371(3)
Volume/Å^3	2349.76(17)
Z	2
ρ_{calc}g/cm^3	1.088
μ/mm^{-1}	0.465
F(000)	846.0
Crystal size/mm^3	0.152 × 0.086 × 0.046
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	7.426 to 136.886
Index ranges	−11 ≤ h ≤ 11, −14 ≤ k ≤ 14, −22 ≤ l ≤ 25
Reflections collected	36115
Independent reflections	8595 [R_{int}= 0.0785, R_{sigma}= 0.0707]
Data/restraints/parameters	8595/0/532
Goodness-of-fit on F^2	1.082
Final R indexes [I>=2σ (I)]	R_1= 0.0736, wR_2= 0.2026
Final R indexes [all data]	R_1= 0.1068, wR_2= 0.2238
Largest diff. peak/hole / e Å^{-3}	0.58/−0.39

Table S3. Crystal data and structure refinement for 3.

Identification code	**3** / 2552626
Empirical formula	$C_{49}H_{71}BN_4O_2$
Formula weight	758.90
Temperature/K	100.00
Crystal system	triclinic
Space group	P−1
a/Å	9.4460(8)
b/Å	12.0085(9)
c/Å	19.9587(15)
α/°	95.716(5)
β/°	91.330(5)
γ/°	96.723(6)
Volume/Å^3	2235.8(3)
Z	2
ρ_{calc}g/cm^3	1.127
μ/mm^{-1}	0.518
F(000)	828.0
Crystal size/mm^3	0.07 × 0.06 × 0.04
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	4.452 to 137.738
Index ranges	−11 ≤ h ≤ 11, −14 ≤ k ≤ 14, −23 ≤ l ≤ 24
Reflections collected	24543
Independent reflections	8111 [R_{int}= 0.0650, R_{sigma}= 0.0565]
Data/restraints/parameters	8111/0/522
Goodness-of-fit on F^2	1.041
Final R indexes [I>=2σ (I)]	R_1= 0.1098, wR_2= 0.2645
Final R indexes [all data]	R_1= 0.1600, wR_2= 0.3108
Largest diff. peak/hole / e Å^{-3}	0.48/−0.33

Table S4. Crystal data and structure refinement for 4.

Identification code	**4** / 2552627
Empirical formula	$C_{55}H_{89}Al_2BN_4O_2$
Formula weight	903.07
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.1957(4)
b/Å	21.9001(7)
c/Å	21.6388(8)
α/°	90
β/°	103.7620(10)
γ/°	90
Volume/Å^3	6073.8(4)
Z	4
ρ_{calc}g/cm^3	0.988
μ/mm^{-1}	0.085
F(000)	1976.0
Crystal size/mm^3	0.171 × 0.083 × 0.043
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.096 to 54.984
Index ranges	−17 ≤ h ≤ 17, −28 ≤ k ≤ 28, −28 ≤ l ≤ 28
Reflections collected	166360
Independent reflections	13925 [R_{int}= 0.0764, R_{sigma}= 0.0298]
Data/restraints/parameters	13925/0/630
Goodness−of−fit on F^2	1.138
Final R indexes [I>=2σ (I)]	R_1= 0.0570, wR_2= 0.1279
Final R indexes [all data]	R_1= 0.0663, wR_2= 0.1320
Largest diff. peak/hole / e Å^{-3}	0.35/−0.30

Table S5. Crystal data and structure refinement for 5.

Identification code	**5** / 2552628
Empirical formula	$C_{51}H_{71}Ag_2BF_6N_4O_8S_2$
Formula weight	1272.78
Temperature/K	100.0
Crystal system	triclinic
Space group	P−1
a/Å	13.1275(8)
b/Å	21.4522(11)
c/Å	22.9324(15)
α/°	74.241(2)
β/°	82.040(2)
γ/°	88.240(2)
Volume/Å^3	6155.3(6)
Z	4
ρ_{calc}g/cm^3	1.373
μ/mm^{-1}	0.771
F(000)	2616.0
Crystal size/mm^3	0.178 × 0.016 × 0.015
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	3.714 to 52.73
Index ranges	−16 ≤ h ≤ 16, −26 ≤ k ≤ 26, −28 ≤ l ≤ 28
Reflections collected	95710
Independent reflections	25059 [R_{int}= 0.0636, R_{sigma}= 0.0517]
Data/restraints/parameters	25059/12/1365
Goodness-of-fit on F^2	1.129
Final R indexes [I>=2σ (I)]	R_1= 0.0798, wR_2= 0.1508
Final R indexes [all data]	R_1= 0.1113, wR_2= 0.1718
Largest diff. peak/hole / e Å^{-3}	2.21/−1.36

V. Fourier Transform Infrared Spectrum

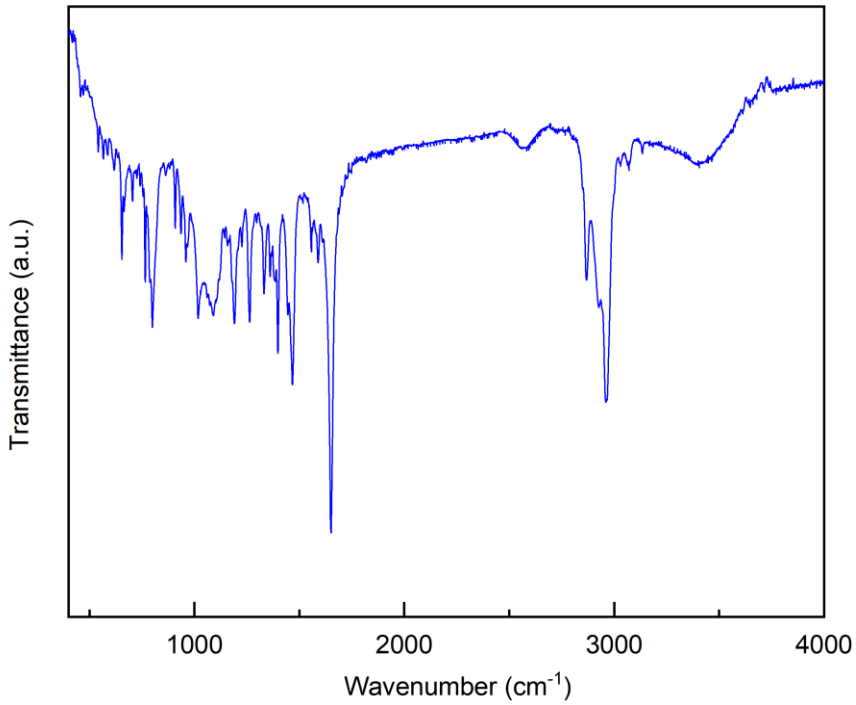


Figure S20. Fourier transform infrared spectroscopy spectrum of **3**.

VI. Computational Details

Geometry optimizations were performed using the Gaussian 16 package with the M06-2X density functional.[错误!不能识别的开关参数。] The def2-SVP basis set was employed for all the atoms. Frequency calculations at the same level of theory were performed were performed to identify the number of imaginary frequencies (zero for local minimum and one for transition states) and provide the thermal corrections of Gibbs free energy and electron energy. Natural bond orbital (NBO) calculations were carried out using NBO 7.0 program at the M06-2X/def2-SVP level of theory.[错误!不能识别的开关参数。] Intrinsic bond orbital (IBOs) computations at B3LYP-D3/def2-TZVP/def2-J level of theory were performed with ORCA programs and visualized by IBOView program.[错误!不能识别的开关参数。] The minimum energy crossing point (MECP) calculations were performed based on Gaussian 16 program at the M06-2X/def2-SVP level of theory from Tian Lu, sobMECP program method.[错误!不能识别的开关参数。] The AIM and ETS-NOCV analyses were carried out using the free software Multiwfn.[错误!不能识别的开关参数。]

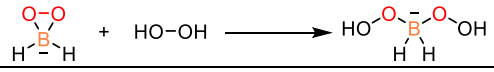
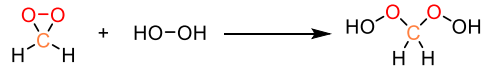
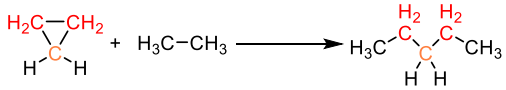
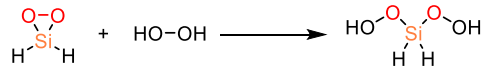
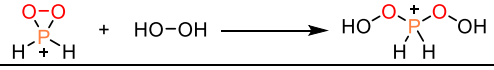
Compounds	Equations	ΔH
$BO_2H_2^-$		−28.98
CO_2H_2		−31.80
C_3H_6		−26.58
SiO_2H_2		−67.57
$PO_2H_2^+$		−61.95

Figure S21. Ring strain energies calculated for simplified $BO_2H_2^-$, CO_2H_2, C_3H_6, SiO_2H_2 and $PO_2H_2^+$, which based on the designed isodesmotic equations. The relative enthalpy changes are given in kcal/mol.

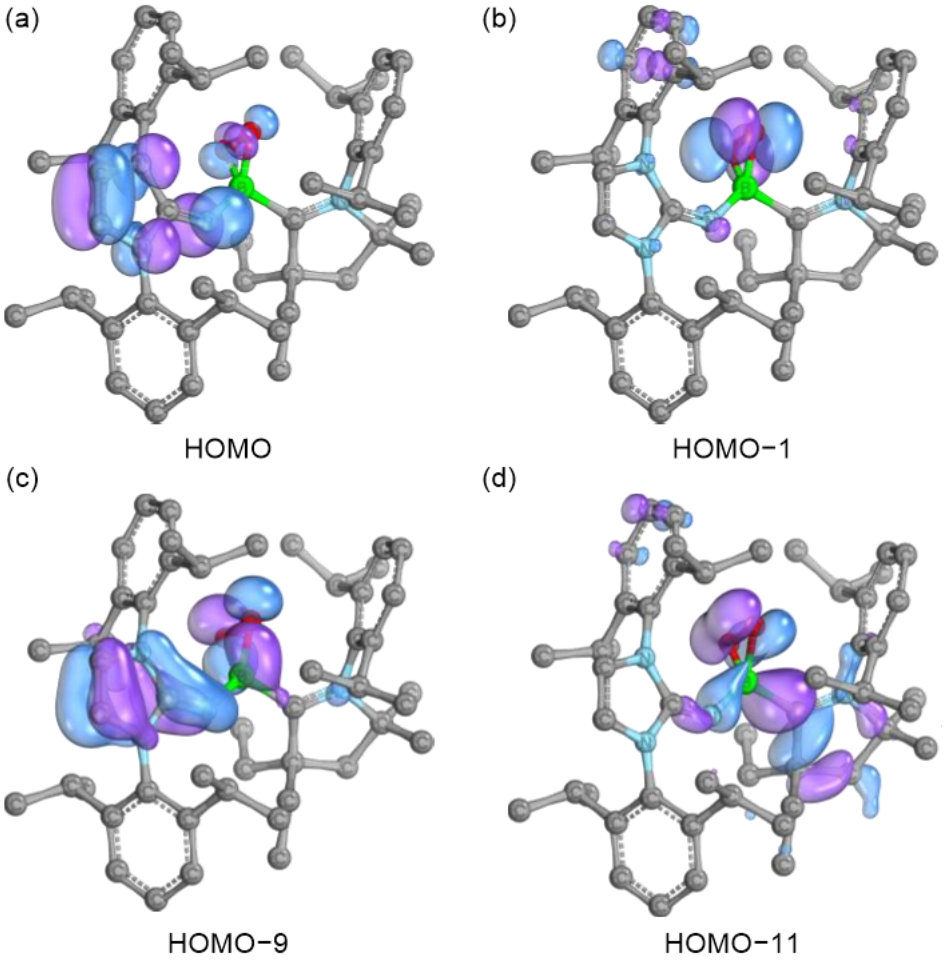


Figure S22. Molecule orbitals of **3**: (a) HOMO orbital. (b) HOMO−1 orbital. (c) HOMO−9 orbital. (d) HOMO−11 orbital.

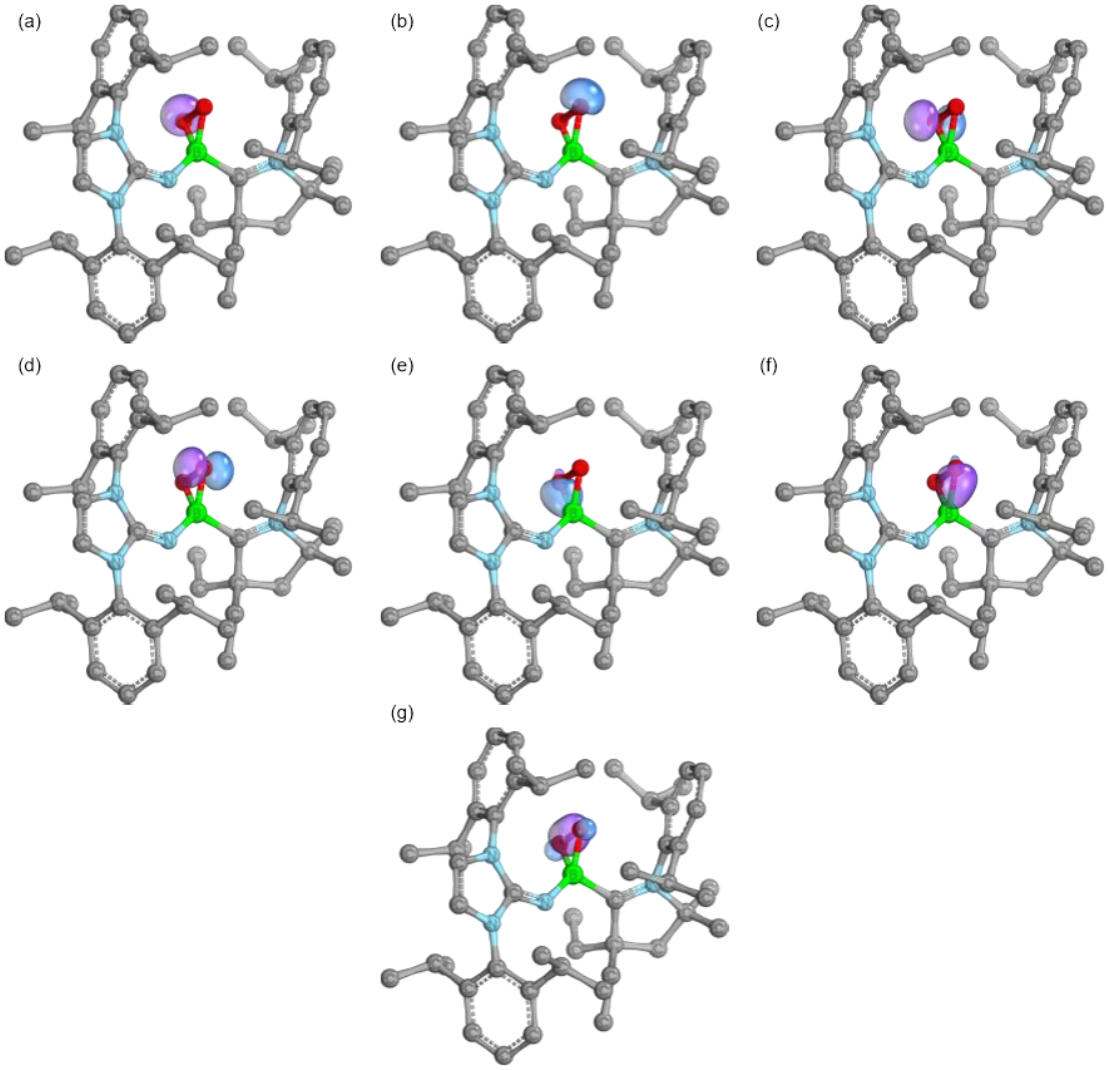


Figure S23. Depiction of selected IBOs of **3**. (a) lone-pair orbital at O1 atom in the B1−O1−O2 plane. (b) lone-pair orbital at O2 atom in the B1−O1−O2 plane. (c) lone-pair orbital at O1 atom out of the B1−O1−O2 plane. (d) lone-pair orbital at O2 atom out of the B1−O1−O2 plane. (e) B1−O2 σ-bonding orbital. (f) B1−O1 σ-bonding orbital. (g) O1−O2 σ-bonding orbital.

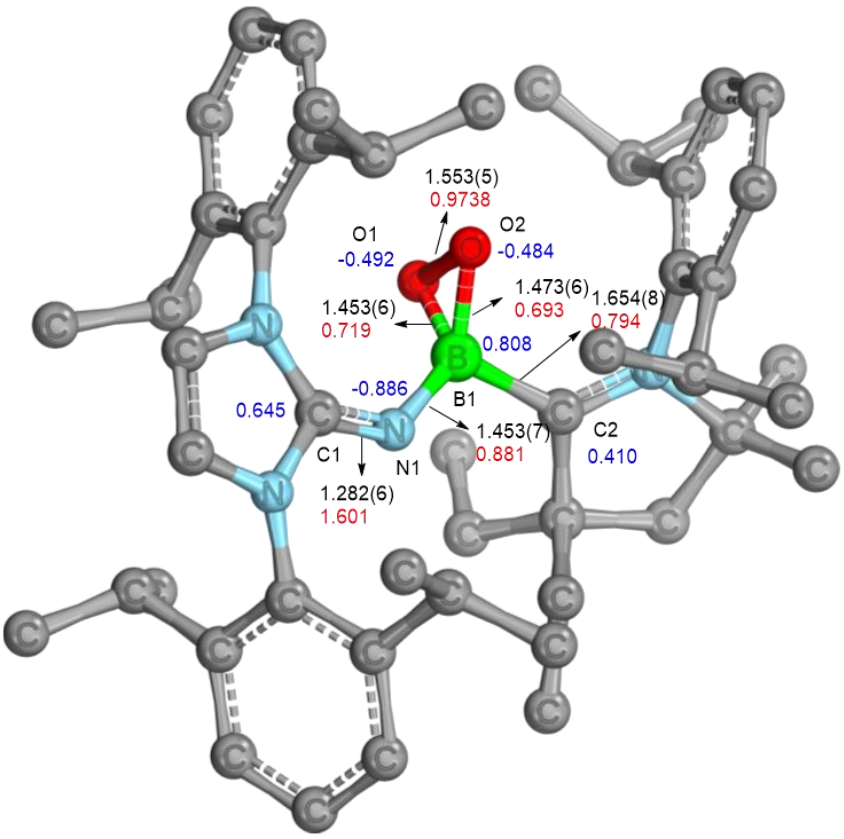


Figure S24. The NBO calculation of **3**. All hydrogens are omitted for clarity. Red: WBIs. Black: crystal bond lengths. Blue: natural charges.

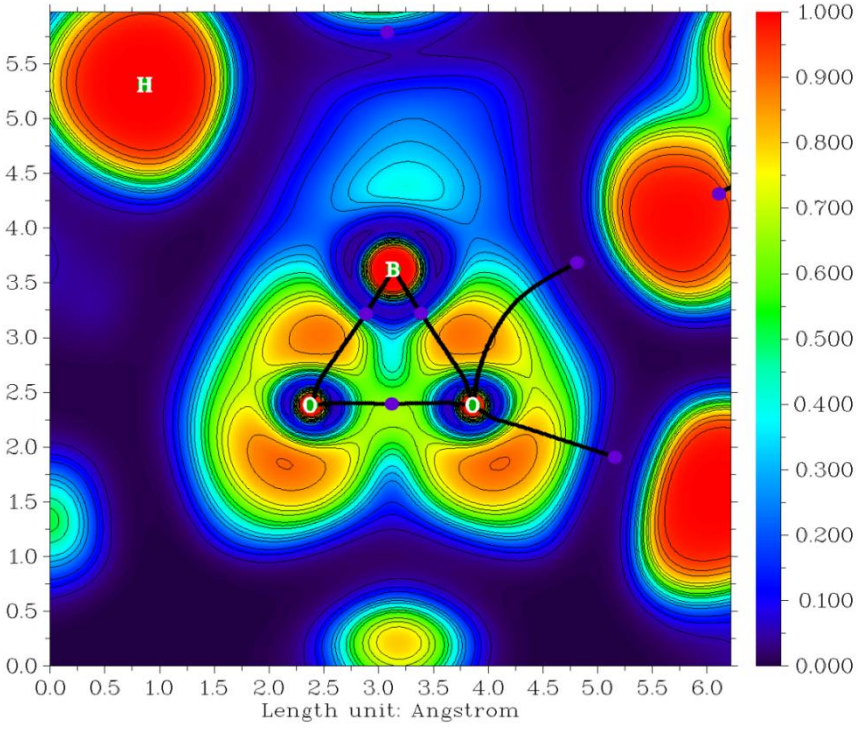


Figure S25. ELF plot of **3** in the B(1)−O(1)−O2 plane.

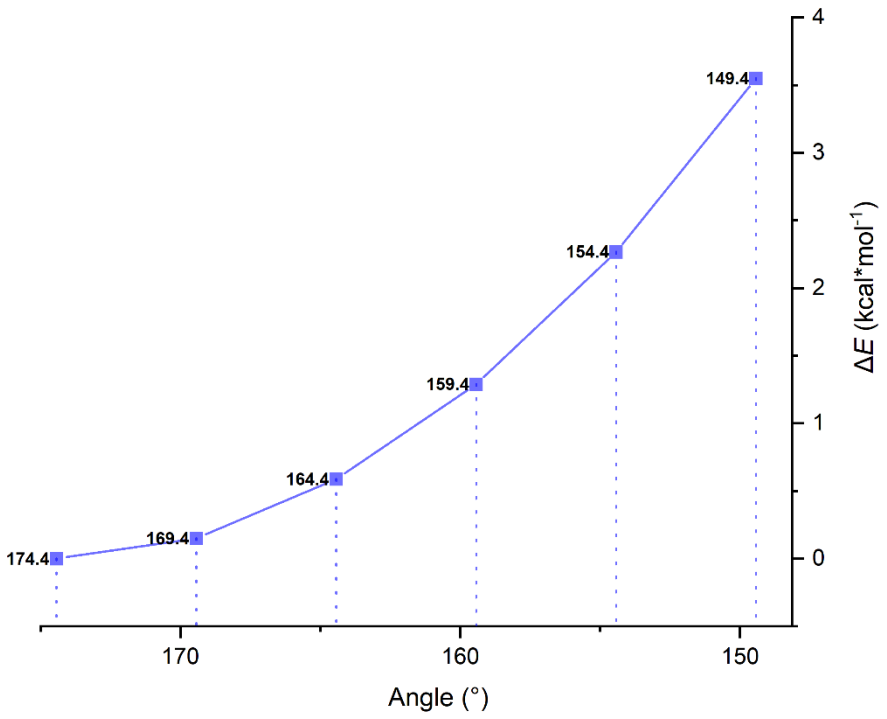


Figure S26. The relationship between N1−B1−C2 angles (°) and relative single-point energy Δ*E* (kcal/mol) of **2**.

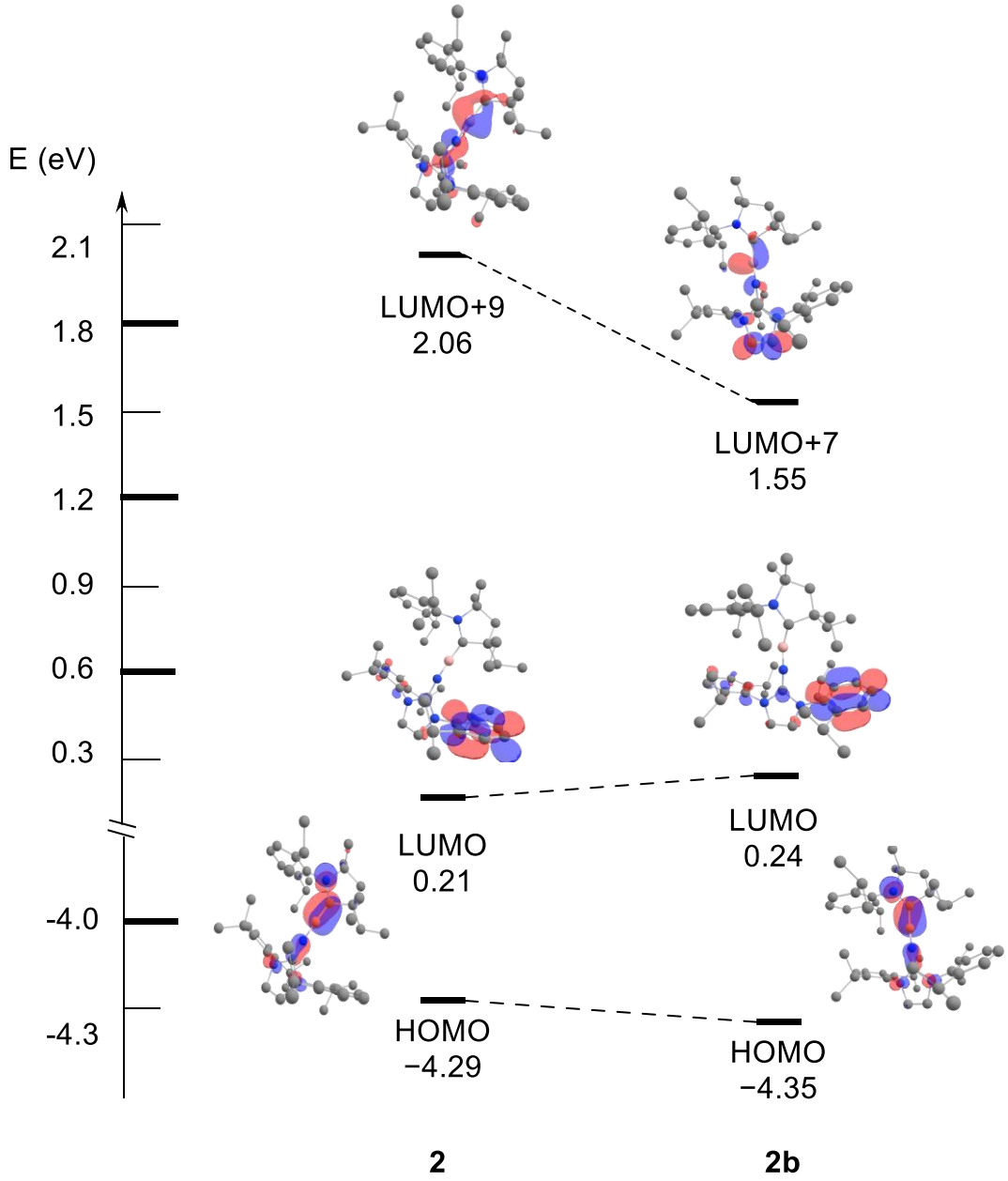


Figure S27. The molecule orbitals of **2** and **2b**.

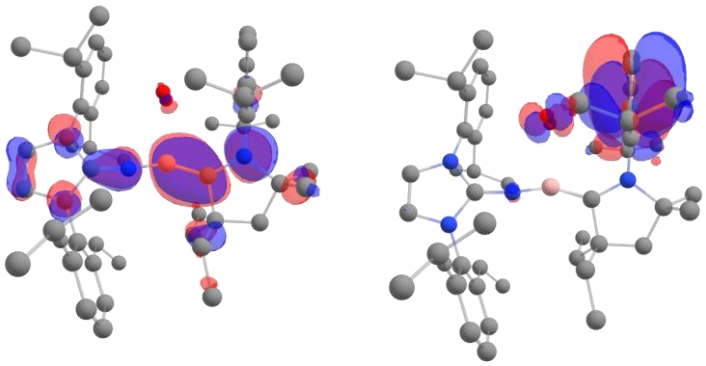


Figure S28. Calculated frontier molecular orbitals of **^{3}TS1**.

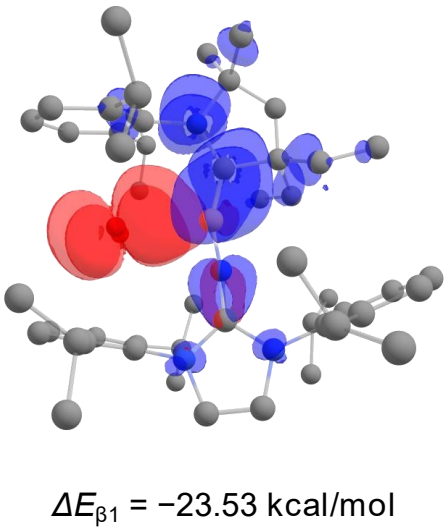


Figure S29. Plot of deformation density of the orbital interaction between borylene **2** and $^3O_2$ in **^{3}TS1** with the corresponding interaction energy.

VII. Calculated Cartesian Coordinates

2

N	2.75371500	−1.44449000	0.00557500
N	−0.74869200	0.21075100	0.01663500
N	−2.31336800	1.98926900	0.32631900
O	1.52570800	2.44603800	0.28088400
N	−3.10258500	−0.07125000	0.31011300
O	1.51998300	2.50890600	−0.90119300
C	−1.92401500	0.65928000	0.20329300
C	1.34943200	−1.57380600	−0.10148400
C	3.38097600	−0.19332900	0.24434000
C	−1.54262900	3.10330000	−0.13479500
C	−0.92677100	3.94985700	0.80313600
C	3.38390700	0.40750200	1.52661300
C	3.42617700	−2.73854000	0.21253900
C	−3.22005400	−1.49435100	0.26680000
C	3.99385400	0.47244200	−0.84604100
C	1.03443200	−3.04144200	−0.43625300
C	−3.35035300	−2.18872200	1.48352000
C	−0.97418300	3.63436900	2.28856500
H	−0.99750000	2.53604900	2.37759300
C	−1.46032400	3.32708700	−1.52053100
C	4.07286400	1.61273400	1.70765400
H	4.08909100	2.07364200	2.69831700
C	−0.17013600	5.32586600	−1.04709900
H	0.37085400	6.20292200	−1.40574700
C	4.65896800	1.68155400	−0.62121800
H	5.13608900	2.19402900	−1.45979100
C	−3.69608800	2.05469700	0.50431800
H	−4.20651200	3.00829100	0.58709000
C	4.71672500	2.24323800	0.64969000
H	5.24865400	3.18245400	0.81164300
C	−0.25168700	5.07398900	0.31931600

H	0.23875100	5.75121200	1.01883200
C	−3.24431800	−2.14463800	−0.98369400
C	−3.53465600	−3.57351500	1.42854200
H	−3.64254200	−4.14248000	2.35238400
C	2.43603400	−3.70289800	−0.46467500
H	2.43896100	−4.68529300	0.02951400
H	2.75216300	−3.86663700	−1.50515400
C	−4.17534500	0.79635300	0.51308400
H	−5.18552800	0.41944500	0.63770800
C	−0.75653100	4.45362900	−1.95742800
H	−0.66479100	4.64797300	−3.02761500
C	3.90749500	−0.07097500	−2.26264400
H	3.45901400	−1.06974000	−2.19181100
C	3.61306900	−3.10383100	1.69357900
H	4.26473900	−2.37178500	2.19012900
H	4.08575900	−4.09391200	1.77912900
H	2.65264100	−3.13819200	2.22602200
C	0.11596700	−3.65331200	0.64559500
H	0.60339800	−3.52117700	1.62481800
H	−0.80305500	−3.04227100	0.68519900
C	2.60902300	−0.16389700	2.70426200
H	2.18570600	−1.12407400	2.38926400
C	4.80021900	−2.76992200	−0.45757300
H	4.71955900	−2.62066100	−1.54253500
H	5.27841700	−3.74440200	−0.28046500
H	5.45656500	−1.98817900	−0.04431300
C	−2.06358700	2.36695100	−2.53248500
H	−2.73122200	1.67581400	−1.99568000
C	−3.20768300	−1.46230300	2.81060000
H	−3.61623100	−0.44802200	2.68431000
C	−3.56933700	−4.23685500	0.20683900
H	−3.70452300	−5.31943500	0.18112800
B	0.30991400	−0.60163900	−0.01726000
C	−3.41412600	−3.53275000	−0.98410400

H	−3.42587700	−4.07535200	−1.92921600
C	−2.24750200	4.19099300	2.93718800
H	−2.28845400	5.28480700	2.81907500
H	−2.26213500	3.96185100	4.01300900
H	−3.15486200	3.76416600	2.48987900
C	2.96500700	0.78166400	−3.11837500
H	3.33055300	1.81806600	−3.20185200
H	1.96052300	0.81342700	−2.67521500
H	2.88438500	0.36225700	−4.13339800
C	0.33661700	−3.17183900	−1.80784500
H	0.23110300	−4.24315400	−2.05433200
H	−0.68656000	−2.78129200	−1.67717500
C	5.28184000	−0.19115700	−2.92627100
H	5.19308300	−0.69294400	−3.90175100
H	5.98230800	−0.76653400	−2.30429500
H	5.72807800	0.79909600	−3.10638000
C	−0.27022300	−5.11796100	0.45509900
H	−0.87044900	−5.46834800	1.30789900
H	0.61207800	−5.77213100	0.38071800
H	−0.87748400	−5.26525000	−0.44930300
C	−0.96115300	1.52900400	−3.19279000
H	−1.39687200	0.81818300	−3.91285900
H	−0.39474400	0.96035300	−2.43997400
H	−0.25481300	2.17516900	−3.73766900
C	0.26067200	4.14057500	3.03517900
H	1.18768300	3.84196900	2.52530500
H	0.27668600	3.72774400	4.05412100
H	0.25241500	5.23751600	3.12768200
C	1.43016700	0.74862100	3.06245600
H	0.84057900	0.30800600	3.88142200
H	0.76626600	0.89543000	2.19799700
H	1.78851600	1.73508200	3.39529000
C	−3.09727900	−1.35870700	−2.28091300
H	−2.25354300	−0.66169600	−2.13248400

C	−3.97450900	−2.12761400	3.95277800
H	−3.52373100	−3.09091500	4.23447900
H	−5.02716300	−2.30517000	3.68885700
H	−3.94645500	−1.48554000	4.84448900
C	−1.72028400	−1.32272800	3.16487500
H	−1.59965700	−0.74013800	4.09074300
H	−1.14775500	−0.83108600	2.36409400
H	−1.27488100	−2.31772300	3.32251200
C	−2.91529900	3.09228400	−3.57722000
H	−2.30369700	3.75366800	−4.20887600
H	−3.69738800	3.70189700	−3.10217600
H	−3.40210700	2.36356500	−4.24185400
C	3.48850800	−0.37833500	3.94071300
H	3.81770200	0.58360700	4.36296200
H	4.38903600	−0.96542300	3.71483500
H	2.92295800	−0.90406600	4.72484400
C	−4.35688800	−0.53828300	−2.59632400
H	−5.21813400	−1.20970600	−2.73582800
H	−4.21166700	0.02437300	−3.53132100
H	−4.60762500	0.18290600	−1.80902400
C	1.00333400	−2.45159800	−2.97352200
H	1.08530800	−1.37526300	−2.76654300
H	0.42077300	−2.58305500	−3.89772600
H	2.01570100	−2.83581600	−3.17330000
C	−2.77708100	−2.23248500	−3.49472300
H	−1.92210000	−2.89862100	−3.32291200
H	−2.53989200	−1.59187400	−4.35623600
H	−3.64422000	−2.85011400	−3.77560500

^{3}TS1

N	2.62218500	−1.62388500	−0.12741100
N	−0.89203500	0.18797700	−0.01506200
N	−2.11729700	2.20241700	0.39352800
O	1.50196200	1.59768500	0.67767100

N	−3.22943000	0.30224200	0.38798800
O	1.59891500	1.80328800	−0.51738300
C	−1.95873000	0.83405000	0.23338900
C	1.24681800	−1.47389300	−0.23863100
C	3.47623300	−0.52085200	0.15421300
C	−1.15290600	3.16563800	−0.04301300
C	−0.34207200	3.80825600	0.90812500
C	3.66933300	−0.08292400	1.48379200
C	3.07465900	−3.03082100	−0.20059700
C	−3.53019900	−1.09316200	0.35813900
C	4.04417200	0.19145600	−0.92677400
C	0.63607100	−2.82950300	−0.64650900
C	−3.63686100	−1.77943100	1.58049700
C	−0.43179400	3.44211200	2.38012400
H	−0.66808100	2.36542500	2.41839600
C	−1.04101100	3.40719000	−1.42221500
C	4.47417600	1.03894300	1.70889800
H	4.63125400	1.38611900	2.73291300
C	0.69284200	5.02354900	−0.91840600
H	1.42608300	5.75459100	−1.26265700
C	4.83725000	1.30938700	−0.65194900
H	5.27854700	1.86826500	−1.48032600
C	−3.45936900	2.49003900	0.63510500
H	−3.80286800	3.51226200	0.75278100
C	5.05799000	1.73057400	0.65426000
H	5.67687400	2.60793400	0.85001400
C	0.57274400	4.75458900	0.44232900
H	1.22652300	5.26625500	1.14858200
C	−3.69547100	−1.72842300	−0.88855600
C	−3.95121600	−3.14158200	1.53664800
H	−4.04468300	−3.70540100	2.46548500
C	1.89038700	−3.69083600	−0.92334500
H	1.75979700	−4.73528000	−0.60810700
H	2.09869700	−3.70365100	−2.00254000

C	−4.13833800	1.32459800	0.65103400
H	−5.18965800	1.11458700	0.81979900
C	−0.09823700	4.35007300	−1.84185400
H	0.02269000	4.55246000	−2.90787400
C	3.79770900	−0.18944000	−2.37903700
H	3.19407000	−1.10684000	−2.37879100
C	3.29378400	−3.66107300	1.18339100
H	4.09547300	−3.14136100	1.72455400
H	3.59070100	−4.71363000	1.06416400
H	2.38192700	−3.63219100	1.79422400
C	−0.24266400	−3.38371200	0.50229300
H	0.33359300	−3.33665400	1.43997300
H	−1.08354700	−2.68093800	0.63554400
C	3.00535800	−0.74821400	2.68009400
H	2.42027400	−1.59542500	2.30428800
C	4.37688500	−3.17163100	−0.98830200
H	4.25554800	−2.85492500	−2.03165400
H	4.69319200	−4.22473500	−0.98669300
H	5.17928900	−2.57333100	−0.53000700
C	−1.86167700	2.64101300	−2.44714300
H	−2.64000200	2.07322900	−1.91351700
C	−3.32783500	−1.08290400	2.89564300
H	−3.59614900	−0.02124400	2.78495300
C	−4.13308000	−3.78909200	0.31972400
H	−4.36936000	−4.85443300	0.30235000
B	0.30639600	−0.38632900	−0.03490500
C	−3.99691000	−3.09351200	−0.87919100
H	−4.12449600	−3.62636600	−1.82121400
C	−1.56265600	4.20669900	3.07894700
H	−1.38235500	5.29104800	3.01796200
H	−1.61595500	3.92828400	4.14196000
H	−2.54132000	3.99798300	2.62667200
C	2.98757100	0.87694400	−3.12506400
H	3.50688500	1.84831100	−3.11778900

H	2.00282300	1.01727800	−2.66311500
H	2.84532500	0.57437200	−4.17437200
C	−0.23916100	−2.69095500	−1.91167200
H	−0.60130300	−3.69310300	−2.20043700
H	−1.12999100	−2.11218300	−1.61836800
C	5.11336300	−0.46405600	−3.11666300
H	4.91403800	−0.86007200	−4.12407000
H	5.74185600	−1.18661600	−2.57770000
H	5.69706800	0.46174100	−3.23603400
C	−0.79951200	−4.79280400	0.31542000
H	−1.41243000	−5.07313700	1.18464900
H	−0.00383600	−5.54654600	0.21795600
H	−1.44736100	−4.86361200	−0.57000200
C	−0.97525500	1.63037200	−3.18538000
H	−1.57546400	1.02779600	−3.88581700
H	−0.47818300	0.95372000	−2.47411100
H	−0.19458300	2.14777100	−3.76494500
C	0.88652000	3.65439500	3.12422200
H	1.72160400	3.18349700	2.58691800
H	0.82279600	3.21026500	4.12834700
H	1.10598100	4.72551000	3.25443400
C	2.02428200	0.18762100	3.39616500
H	1.57282300	−0.33224000	4.25555600
H	1.21938400	0.51044600	2.72287700
H	2.53771600	1.08361800	3.77841100
C	−3.53677900	−0.95118000	−2.18945700
H	−2.62213400	−0.34181500	−2.08062000
C	−4.12571200	−1.63799600	4.07535700
H	−3.80307000	−2.65642800	4.33842700
H	−5.20401500	−1.66416600	3.86153700
H	−3.96523100	−1.00984000	4.96299800
C	−1.81974400	−1.15341400	3.17827100
H	−1.57338400	−0.59904600	4.09637700
H	−1.22532800	−0.73999600	2.34993500

H	−1.51024900	−2.20180000	3.31545700
C	−2.57973500	3.57469900	−3.42457400
H	−1.86408300	4.13929100	−4.04073600
H	−3.21463900	4.29776700	−2.89267200
H	−3.21622600	2.99319200	−4.10791200
C	4.04714200	−1.26193500	3.68212800
H	4.55137200	−0.42108900	4.18314000
H	4.82573700	−1.86881200	3.19943900
H	3.56591600	−1.87117200	4.46219300
C	−4.71794700	−0.00361800	−2.44177200
H	−5.65126100	−0.57890000	−2.54171500
H	−4.55910100	0.55106800	−3.37926600
H	−4.85085900	0.73156800	−1.63855900
C	0.41301500	−2.02230600	−3.11758600
H	0.81218400	−1.03390400	−2.84800600
H	−0.32308100	−1.88235300	−3.92339800
H	1.23796000	−2.61900300	−3.53538200
C	−3.35440700	−1.84950600	−3.41300500
H	−2.55709500	−2.59096100	−3.26981700
H	−3.09625000	−1.23476300	−4.28738600
H	−4.28549200	−2.38562000	−3.65380100

^{3}INT1

N	2.50612600	−1.64521700	−0.35095000
N	−0.97166800	0.00650000	−0.11637400
N	−1.90245600	2.14852600	0.62670300
O	1.15092200	0.86331300	0.82054000
N	−3.15987900	0.35675200	0.65800700
O	1.78225300	1.75725000	0.10890500
C	−1.87929200	0.78904100	0.34779600
C	1.16896600	−1.37651800	−0.47533700
C	3.47045400	−0.65834400	0.03813200
C	−0.95349600	3.11216800	0.15460700
C	−0.03808000	3.67927000	1.05584900

C	3.80836200	−0.47959700	1.39590900
C	2.88720500	−3.03629600	−0.72209800
C	−3.57981200	−1.00389100	0.53866500
C	4.01194200	0.18033400	−0.96148800
C	0.47520300	−2.59183900	−1.09366400
C	−3.61743500	−1.79840000	1.69639400
C	0.02676100	3.22741700	2.50433600
H	−0.37617500	2.20335700	2.53649700
C	−1.01476300	3.48403600	−1.19991800
C	4.72997400	0.51954400	1.72567400
H	4.99842500	0.67119500	2.77351800
C	0.80239800	5.03181500	−0.77373100
H	1.50203700	5.78429800	−1.14110000
C	4.92770400	1.16457500	−0.58056600
H	5.34939700	1.82381700	−1.34217000
C	−3.16151600	2.51760200	1.09332300
H	−3.39025500	3.55057800	1.33333900
C	5.29181100	1.33349500	0.74994400
H	6.00405800	2.11173500	1.02884800
C	0.82717700	4.66018000	0.56634700
H	1.55748100	5.11389300	1.23699900
C	−3.91344500	−1.50118100	−0.73662800
C	−4.03983700	−3.12557100	1.56160500
H	−4.08602200	−3.77006700	2.44005700
C	1.66308500	−3.47451900	−1.53827900
H	1.46306200	−4.54776900	−1.41579600
H	1.87082100	−3.30452900	−2.60470500
C	−3.93277800	1.40998900	1.12598700
H	−4.96393000	1.26738000	1.43333200
C	−0.10399400	4.44348000	−1.65015300
H	−0.11090200	4.74015500	−2.70081500
C	3.60424300	0.09555900	−2.42574800
H	2.95433600	−0.78206200	−2.54381700
C	3.08084500	−3.92160700	0.51539500

H	3.92888200	−3.57174500	1.11766300
H	3.29557100	−4.95074500	0.19250800
H	2.18401700	−3.94179700	1.14786500
C	−0.41022200	−3.26784800	−0.01301500
H	0.19704500	−3.42984900	0.89225600
H	−1.18448400	−2.53608200	0.26814200
C	3.18379800	−1.28622100	2.52460400
H	2.47832100	−1.99733000	2.07569700
C	4.17442600	−3.08435900	−1.54311400
H	4.06929100	−2.54852300	−2.49416700
H	4.41311500	−4.13333900	−1.77026500
H	5.01977000	−2.65323000	−0.98607500
C	−2.01545300	2.86646100	−2.16406700
H	−2.75655100	2.30250800	−1.57595700
C	−3.12449900	−1.25931800	3.02955600
H	−3.33615400	−0.17968100	3.05531300
C	−4.38946900	−3.63664000	0.31711000
H	−4.70889100	−4.67637200	0.22753700
B	0.42253900	−0.13091000	0.00841100
C	−4.31746700	−2.83616000	−0.82065400
H	−4.57723800	−3.26286300	−1.78930000
C	−0.84715700	4.11868600	3.39515300
H	−0.49615900	5.16154400	3.35491200
H	−0.80011600	3.78249300	4.44168300
H	−1.90036100	4.10436900	3.08132600
C	2.78650500	1.31932600	−2.85819400
H	3.37835100	2.24229900	−2.75116100
H	1.88447500	1.43639200	−2.24356600
H	2.49461400	1.22119800	−3.91559800
C	−0.41926700	−2.22404200	−2.29667700
H	−0.79503000	−3.16248500	−2.73934900
H	−1.28874100	−1.68320000	−1.89519900
C	4.82034900	−0.07532200	−3.34370000
H	4.49453000	−0.26982900	−4.37666700

H	5.46636600	−0.90378800	−3.02057800
H	5.43376700	0.83827000	−3.35989000
C	−1.08027100	−4.57874800	−0.41597700
H	−1.65790300	−4.97992500	0.42944400
H	−0.35353000	−5.34972900	−0.71426100
H	−1.78725300	−4.43624300	−1.24586800
C	−1.31937200	1.87293500	−3.09891100
H	−2.04934500	1.40084400	−3.77595800
H	−0.82201300	1.08312000	−2.51875100
H	−0.55993300	2.38023900	−3.71476600
C	1.46094600	3.17374100	3.03557200
H	2.11261200	2.61621100	2.34795600
H	1.47479400	2.68024600	4.01857300
H	1.87544300	4.18448900	3.17423000
C	2.38401900	−0.40097400	3.48866700
H	1.92058800	−1.02184000	4.27080600
H	1.60009700	0.15541600	2.96028400
H	3.04096700	0.32911400	3.98732800
C	−3.83095700	−0.61066700	−1.96859700
H	−2.88013700	−0.05793900	−1.88924000
C	−3.82105500	−1.89246600	4.23376600
H	−3.53447200	−2.94747600	4.35785200
H	−4.91585300	−1.84286700	4.14351700
H	−3.52660600	−1.36807400	5.15387900
C	−1.60194900	−1.43460100	3.12963100
H	−1.22276200	−0.99459000	4.06407400
H	−1.08102300	−0.96457800	2.28249600
H	−1.34498200	−2.50582900	3.12215600
C	−2.78532600	3.93015500	−2.95087300
H	−2.12188100	4.49167200	−3.62548900
H	−3.27376400	4.64942900	−2.27788900
H	−3.56039200	3.45596100	−3.57106100
C	4.24734600	−2.06452400	3.31023500
H	4.88009100	−1.37400200	3.88884900

H	4.91262600	−2.64430300	2.65554400
H	3.77306200	−2.75525300	4.02364500
C	−4.97924000	0.40664800	−2.01375200
H	−5.94706800	−0.11302700	−2.08707000
H	−4.87326700	1.05491100	−2.89738400
H	−5.00238000	1.05270400	−1.12655100
C	0.23359000	−1.38487400	−3.38964200
H	0.66093800	−0.46005300	−2.97767200
H	−0.50992000	−1.10061300	−4.14949700
H	1.03988500	−1.92303300	−3.91174300
C	−3.79749700	−1.39353300	−3.28098200
H	−3.02056100	−2.17045800	−3.27660700
H	−3.58962100	−0.70777000	−4.11522000
H	−4.76689100	−1.87323300	−3.48718900

^{3}INT2

N	2.65133300	−1.14840600	−0.83649200
N	−0.98936500	0.02409000	−0.28218900
N	−2.06696100	1.78274000	0.98948600
O	0.99526300	0.39368300	1.14658700
N	−2.90252700	−0.23492800	1.07782000
O	0.28399700	0.20200800	2.21890600
C	−1.87335500	0.49577000	0.53427900
C	1.28378200	−1.03211600	−0.94545400
C	3.45655300	−0.18780100	−0.13905100
C	−1.44325400	2.92866900	0.39838500
C	−0.42532200	3.61665300	1.08034000
C	4.01391500	−0.48666800	1.12293000
C	3.23770900	−2.17099800	−1.74760000
C	−3.04802700	−1.64250400	0.85945100
C	3.65526000	1.08660300	−0.72053100
C	0.76190100	−2.01946600	−1.98036600
C	−2.58633500	−2.53070000	1.83975700
C	0.01239500	3.24436700	2.48421700

H	−0.41051000	2.25889500	2.71659000
C	−1.91130700	3.33515600	−0.86655100
C	4.81762900	0.47293000	1.74826700
H	5.25529400	0.24476500	2.72244200
C	−0.26426500	5.11545100	−0.82640200
H	0.20942200	5.96987500	−1.31279400
C	4.45176700	2.01798100	−0.04869700
H	4.60676200	3.00359300	−0.49262800
C	−3.17971100	1.82448300	1.82474500
H	−3.50880700	2.75145100	2.28252700
C	5.04561800	1.71467800	1.17071200
H	5.67042100	2.45173800	1.67772000
C	0.15022400	4.71989400	0.44015100
H	0.94398400	5.27245900	0.94632700
C	−3.59945800	−2.08318500	−0.36312800
C	−2.74930000	−3.90302700	1.60669700
H	−2.40526900	−4.61674100	2.35805500
C	2.05620000	−2.47568000	−2.68929900
H	2.02993000	−3.54042200	−2.96265800
H	2.18703600	−1.90765700	−3.62215100
C	−3.68771300	0.57293700	1.89132200
H	−4.53757600	0.17652900	2.43759300
C	−1.28915700	4.42962900	−1.47180000
H	−1.62175700	4.75701200	−2.45916000
C	3.00022300	1.51251600	−2.02438300
H	2.53003500	0.62812500	−2.47120300
C	3.67621300	−3.43358800	−0.99727000
H	4.50921400	−3.22124700	−0.31694900
H	4.01679300	−4.18582700	−1.72398200
H	2.84995000	−3.86601300	−0.41729500
C	0.05189900	−3.17417700	−1.22264500
H	0.76733000	−3.61543800	−0.51014800
H	−0.74570700	−2.71923800	−0.61055300
C	3.72893000	−1.77351200	1.87900400

H	3.05512000	−2.38066800	1.25962400
C	4.44035600	−1.61421900	−2.50848200
H	4.16342700	−0.72672400	−3.09319600
H	4.81615600	−2.37940300	−3.20322900
H	5.25544600	−1.34035400	−1.82212600
C	−3.07315500	2.64526200	−1.56472900
H	−3.48775500	1.88778400	−0.88237800
C	−1.88449600	−2.05652100	3.09864400
H	−1.77349800	−0.96584800	3.03720900
C	−3.32037400	−4.36247300	0.42878800
H	−3.43420700	−5.43458800	0.25932300
B	0.37095600	−0.18480900	−0.07042400
C	−3.72842500	−3.45938100	−0.55327000
H	−4.14390500	−3.84003000	−1.48605600
C	−0.54794700	4.25337800	3.49427700
H	−0.15388600	5.26299000	3.29887500
H	−0.26332400	3.96932600	4.51807200
H	−1.64563400	4.30858300	3.44562800
C	1.89449700	2.54076000	−1.75629000
H	2.31281300	3.44774800	−1.29208500
H	1.12172500	2.14844200	−1.07569600
H	1.40152600	2.83888400	−2.69501000
C	−0.23555900	−1.41107400	−2.99007400
H	−0.42190100	−2.16631700	−3.77268600
H	−1.18973500	−1.24899700	−2.46304900
C	4.01097800	2.07170000	−3.03131100
H	3.52146800	2.24550700	−4.00147700
H	4.85545600	1.38487000	−3.18654200
H	4.42249000	3.03522300	−2.69483100
C	−0.55032200	−4.27477200	−2.09129800
H	−0.93371100	−5.08929200	−1.45993900
H	0.18617900	−4.70970200	−2.78512900
H	−1.39636500	−3.90358000	−2.68802700
C	−2.60591500	1.91545600	−2.82516400

H	−3.45383600	1.40925700	−3.31295800
H	−1.84737500	1.16392200	−2.56812900
H	−2.16733600	2.61861400	−3.55100100
C	1.53432000	3.12883900	2.60882700
H	1.94810500	2.45054100	1.84952800
H	1.79699800	2.72819800	3.59888700
H	2.02240500	4.11127900	2.50797800
C	3.01022600	−1.48736700	3.20377500
H	2.73676100	−2.43329700	3.69642600
H	2.10020300	−0.89355500	3.05344500
H	3.66754800	−0.93278800	3.89141400
C	−4.01437200	−1.08672400	−1.43479600
H	−3.20933600	−0.33697300	−1.48268000
C	−2.69982100	−2.39005000	4.35130300
H	−2.83075400	−3.47782300	4.46102000
H	−3.70032000	−1.93464500	4.31191400
H	−2.18865700	−2.01963100	5.25184900
C	−0.47067400	−2.63995600	3.17823100
H	0.07139400	−2.20362500	4.02983600
H	0.09725500	−2.41105000	2.26358700
H	−0.49374800	−3.73304300	3.31158800
C	−4.20171500	3.63462700	−1.87100700
H	−3.88098000	4.39739800	−2.59647400
H	−4.53611400	4.15216300	−0.96035200
H	−5.06370400	3.10551800	−2.30381600
C	5.01316200	−2.56514900	2.15887800
H	5.63067500	−2.04197100	2.90516000
H	5.63269000	−2.69621400	1.26098500
H	4.77489000	−3.55945800	2.56580200
C	−5.32322500	−0.37242100	−1.07437700
H	−6.15267100	−1.09465500	−1.02420800
H	−5.56988400	0.37707000	−1.84265400
H	−5.26171100	0.14615100	−0.10794700
C	0.19382000	−0.10416900	−3.64465900

H	0.29329800	0.69165000	−2.89331900
H	−0.55254700	0.22052900	−4.38428300
H	1.15549600	−0.19557300	−4.17376200
C	−4.13017300	−1.70993000	−2.82494900
H	−3.21980300	−2.26127700	−3.10077800
H	−4.28806900	−0.92057600	−3.57400700
H	−4.98670900	−2.39846000	−2.89066200

MECP

N	2.68392200	−1.03666200	−0.83517500
N	−0.91870400	0.12100800	−0.24232400
N	−2.18138600	1.72353600	1.02357300
O	0.15274100	0.08676900	2.33492400
N	−2.80422500	−0.36812600	1.12351500
O	0.95158900	−0.24763300	1.36138100
C	−1.85383700	0.46440900	0.58512500
C	1.31273100	−1.04706300	−0.95095500
C	3.37621000	0.05196200	−0.20478000
C	−1.61931700	2.92255500	0.47715400
C	−0.58539300	3.59158300	1.15129900
C	3.98023500	−0.10817900	1.06314800
C	3.35170300	−2.02268300	−1.73014900
C	−2.87558600	−1.77023100	0.83554100
C	3.41446700	1.31008300	−0.85545300
C	0.87658300	−2.09976300	−1.95283900
C	−2.39677400	−2.68787800	1.78160900
C	−0.02216500	3.10459800	2.47135500
H	−0.51495600	2.15573900	2.71561700
C	−2.14408400	3.38703700	−0.74392600
C	4.66796000	0.97398000	1.62306800
H	5.14142800	0.85230600	2.59946100

C	−0.56293500	5.22510600	−0.64652800
H	−0.14210900	6.12845900	−1.09124200
C	4.10389700	2.36412300	−0.24739800
H	4.13529400	3.33569900	−0.74530700
C	−3.28206300	1.65631200	1.87133100
H	−3.69282900	2.54576600	2.33749700
C	4.74163400	2.20063100	0.97596400
H	5.27919700	3.03336600	1.43296900
C	−0.07278400	4.75448100	0.56571800
H	0.73256800	5.29156700	1.07097600
C	−3.40220600	−2.17588900	−0.41271300
C	−2.50011600	−4.05311300	1.48041600
H	−2.14114400	−4.78740200	2.20439900
C	2.20054800	−2.40857700	−2.68434000
H	2.27736200	−3.45865800	−3.00115700
H	2.26871600	−1.78842100	−3.59163400
C	−3.66116700	0.36005000	1.94318500
H	−4.46646700	−0.11801200	2.49159400
C	−1.58899600	4.54405100	−1.29546000
H	−1.96727900	4.91805900	−2.24884800
C	2.70824500	1.59091900	−2.17316200
H	2.33845300	0.63717600	−2.57028900
C	3.86223400	−3.24673900	−0.95851200
H	4.67891600	−2.97425500	−0.27984300
H	4.24914900	−3.99211900	−1.66919000
H	3.06532700	−3.71744600	−0.36881400
C	0.31324200	−3.30996800	−1.15521700
H	1.06179500	−3.63027100	−0.41488700
H	−0.54339600	−2.93415100	−0.56828200
C	3.89933600	−1.39299600	1.87000400

H	3.25421100	−2.08760700	1.31474100
C	4.52484200	−1.39492300	−2.47970600
H	4.19997400	−0.52644200	−3.06787600
H	4.95433500	−2.13655500	−3.16880200
H	5.31463700	−1.07042100	−1.78554400
C	−3.26210500	2.66135300	−1.47313500
H	−3.63287800	1.85572200	−0.82121900
C	−1.75584800	−2.25373800	3.08654700
H	−1.67351700	−1.15939400	3.07541200
C	−3.03501500	−4.47832600	0.27364200
H	−3.10322900	−5.54467200	0.05181300
B	0.36124900	−0.33798700	0.01701700
C	−3.47017300	−3.54624300	−0.66871000
H	−3.86607200	−3.90038600	−1.62018400
C	−0.32412700	4.10174700	3.59464100
H	0.15226500	5.07486000	3.39930400
H	0.06036600	3.72583900	4.55416300
H	−1.40564400	4.27312300	3.69983400
C	1.49704800	2.50618800	−1.94628500
H	1.81651300	3.46861400	−1.51635500
H	0.76458100	2.05599300	−1.25696900
H	0.98525800	2.71674000	−2.89892200
C	−0.23106700	−1.62160200	−2.91353600
H	−0.39140000	−2.40788500	−3.67044200
H	−1.15910000	−1.55026700	−2.32257500
C	3.64442300	2.20593000	−3.21979100
H	3.13442300	2.26238100	−4.19349000
H	4.56583400	1.61858200	−3.34392500
H	3.93678700	3.23036000	−2.94453800
C	−0.13900100	−4.51227400	−1.97879300

H	−0.45176900	−5.33084300	−1.31434200
H	0.66456300	−4.90003500	−2.62424000
H	−0.99925800	−4.26724800	−2.61860800
C	−2.72595600	2.00733500	−2.74922900
H	−3.52074000	1.43765800	−3.25623700
H	−1.90064000	1.32326500	−2.50766700
H	−2.35185100	2.76698200	−3.45403300
C	1.48061800	2.82757500	2.36155500
H	1.70963100	2.14389200	1.53023200
H	1.85009400	2.36091700	3.28678700
H	2.04742800	3.75852800	2.19935800
C	3.26500800	−1.16842800	3.24936900
H	3.16231800	−2.13240900	3.77171100
H	2.27336800	−0.70547200	3.17419700
H	3.90377200	−0.52524600	3.87491600
C	−3.87299900	−1.15564100	−1.44077500
H	−3.10047800	−0.37070800	−1.47699100
C	−2.61248200	−2.66028400	4.28948400
H	−2.72316800	−3.75421700	4.34563500
H	−3.62060400	−2.22371600	4.23277200
H	−2.14330600	−2.32084900	5.22438800
C	−0.33263800	−2.80877400	3.20680200
H	0.16386200	−2.38406900	4.09122200
H	0.27145500	−2.54647300	2.32579000
H	−0.33752100	−3.90502300	3.31218900
C	−4.44513500	3.58870500	−1.76339600
H	−4.16292100	4.39664600	−2.45536400
H	−4.82428700	4.05017100	−0.84015800
H	−5.26569700	3.02397300	−2.23043200
C	5.29033100	−2.01834500	2.05022700

H	5.89671900	−1.40912600	2.73852100
H	5.84721400	−2.08645300	1.10527600
H	5.21150800	−3.02777100	2.48179900
C	−5.20552200	−0.50874100	−1.03855900
H	−6.00211300	−1.26748100	−0.99544100
H	−5.49610900	0.24657300	−1.78548900
H	−5.15363200	−0.00974700	−0.06174300
C	0.00444700	−0.28712800	−3.60516100
H	0.09219200	0.51357100	−2.85956000
H	−0.83863700	−0.04436300	−4.26906000
H	0.91703100	−0.28556100	−4.22188900
C	−3.99797600	−1.73210800	−2.85136400
H	−3.07942500	−2.24511200	−3.16987500
H	−4.19934000	−0.92010900	−3.56501100
H	−4.83480600	−2.44404200	−2.92262200

^{1}INT3

N	2.54744400	−1.12900800	−0.93133000
N	−0.82628500	0.26458400	−0.37368000
N	−2.00258500	1.88056500	0.95733800
O	−0.08490900	−0.15566300	2.37741500
N	−2.76860400	−0.15676800	0.96942600
O	0.68944800	−0.73327000	1.32742400
C	−1.75053200	0.62446600	0.48228800
C	1.25959300	−1.25789300	−0.91978400
C	3.28133500	−0.12055100	−0.17858200
C	−1.31198600	3.05772400	0.53124300
C	−0.26281700	3.56961400	1.31037900
C	3.79221000	−0.40326100	1.10755200
C	3.26753100	−2.08816100	−1.85791300

C	−2.96507600	−1.53197200	0.62866600
C	3.45917100	1.13598100	−0.79591800
C	0.79937300	−2.38957200	−1.79574000
C	−2.70500100	−2.52491700	1.58655200
C	0.21895300	2.87731900	2.56911400
H	−0.38002900	1.97007800	2.71853400
C	−1.73503000	3.67008600	−0.66393200
C	4.58384800	0.58358900	1.70641200
H	4.99506900	0.39191900	2.69875100
C	−0.04423300	5.37249200	−0.30603800
H	0.45434600	6.28640500	−0.63434100
C	4.24806100	2.08348200	−0.13854500
H	4.39229700	3.06363600	−0.59589700
C	−3.08954400	1.85461500	1.82073100
H	−3.42310800	2.74759400	2.33848000
C	4.82954300	1.80338400	1.09094900
H	5.44688900	2.55245000	1.58906300
C	0.35557900	4.74572000	0.86879500
H	1.17295700	5.16693900	1.45822100
C	−3.43789200	−1.83903100	−0.67022200
C	−2.94497200	−3.85894500	1.22296300
H	−2.75708900	−4.64721100	1.95480600
C	2.09116400	−2.84196200	−2.51299900
H	2.23602700	−3.92730300	−2.42660300
H	2.04312800	−2.60645600	−3.58539000
C	−3.55954800	0.58668800	1.83610900
H	−4.39081800	0.14005700	2.37169100
C	−1.07607600	4.83280500	−1.07047600
H	−1.37829400	5.32560400	−1.99696500
C	2.76659600	1.54269500	−2.08816400

H	2.33101400	0.64788100	−2.54690000
C	4.17063900	−3.00592600	−1.04384800
H	4.96977600	−2.42788700	−0.56264100
H	4.63505400	−3.73532700	−1.72212000
H	3.60946700	−3.55317100	−0.27416600
C	0.23242800	−3.46862000	−0.83672900
H	1.02382500	−3.75573000	−0.12309500
H	−0.57128400	−3.01108400	−0.23480600
C	3.50295100	−1.65739700	1.92514400
H	2.80747100	−2.28770700	1.35288700
C	4.11336800	−1.33207900	−2.87903600
H	3.49715300	−0.72295600	−3.55319900
H	4.65500600	−2.06903000	−3.48875800
H	4.85219600	−0.68451000	−2.38534400
C	−2.84366600	3.07983800	−1.51918900
H	−3.32796500	2.27962100	−0.94011000
C	−2.18954400	−2.21089600	2.97827100
H	−1.92179500	−1.14794400	3.00756200
C	−3.40265700	−4.18733200	−0.04391200
H	−3.57681500	−5.23169200	−0.30994100
B	0.27147300	−0.46468200	0.07974000
C	−3.63870000	−3.18401000	−0.98474400
H	−3.99561400	−3.45987500	−1.97698400
C	0.09147800	3.78757800	3.79271200
H	0.73120500	4.68056900	3.70598600
H	0.39724500	3.24411200	4.69848500
H	−0.94484100	4.13019500	3.93342200
C	1.60488300	2.49843300	−1.78548000
H	1.97122300	3.41934800	−1.30587500
H	0.86293400	2.03801000	−1.11466400

H	1.09160600	2.78126900	−2.71839400
C	−0.29988400	−1.90441400	−2.75801400
H	−0.50940000	−2.71961800	−3.46952400
H	−1.20967400	−1.74209900	−2.16110800
C	3.72838400	2.16382100	−3.10509100
H	3.20786700	2.33054300	−4.05969300
H	4.60141500	1.52279400	−3.29442300
H	4.09648500	3.14162000	−2.76124700
C	−0.30836500	−4.70642500	−1.54244800
H	−0.63111900	−5.44799100	−0.79880900
H	0.44717200	−5.18249100	−2.18648700
H	−1.18454700	−4.46341000	−2.15934000
C	−2.25427600	2.43910000	−2.78007400
H	−3.04543000	1.95137600	−3.37218500
H	−1.50307400	1.68528900	−2.50416400
H	−1.77406000	3.20026300	−3.41602000
C	1.65185200	2.37522900	2.38156500
H	1.70821300	1.67878600	1.53068800
H	1.97172900	1.81572700	3.27273500
H	2.35708300	3.20684000	2.21245800
C	2.80971100	−1.30701400	3.25343100
H	2.56771500	−2.24175600	3.78308400
H	1.87620700	−0.74227100	3.11746600
H	3.49549300	−0.73807400	3.90188200
C	−3.74235600	−0.73956800	−1.68124600
H	−2.88491200	−0.04730400	−1.66506800
C	−3.25356300	−2.52557800	4.03417600
H	−3.50517800	−3.59842300	4.04502700
H	−4.18577200	−1.96904600	3.85280900
H	−2.88558200	−2.25658200	5.03512500

C	−0.87939100	−2.95048400	3.25981100
H	−0.48827800	−2.64117600	4.23983100
H	−0.12597000	−2.67303900	2.50973100
H	−1.01676000	−4.04478900	3.27393100
C	−3.92181200	4.10946800	−1.86388900
H	−3.52338300	4.91337200	−2.50124000
H	−4.33833500	4.57023000	−0.95678400
H	−4.74386800	3.62866900	−2.41502100
C	4.78119200	−2.44683400	2.24653500
H	5.43173400	−1.86192900	2.91436000
H	5.37340900	−2.71515600	1.36318200
H	4.52100100	−3.37392300	2.77825600
C	−5.00848400	0.04003100	−1.29812000
H	−5.88482600	−0.62637400	−1.31332700
H	−5.18536800	0.85152300	−2.02151500
H	−4.93763500	0.49029400	−0.29931200
C	0.03906800	−0.62034000	−3.50426200
H	0.14699200	0.21372600	−2.79400800
H	−0.76689300	−0.35327900	−4.20292300
H	0.96776800	−0.71132900	−4.09193100
C	−3.88669300	−1.25043400	−3.11519200
H	−3.02544300	−1.85674900	−3.43028900
H	−3.97126000	−0.39701700	−3.80348600
H	−4.79612500	−1.85902400	−3.23690700

TS2

N	2.41014600	−1.47733900	−0.85683600
N	−0.90392400	0.20671300	−0.48355500
N	−1.66407200	2.06490600	0.88008000
O	−0.13708700	−0.46323300	2.07919500

N	−2.90285800	0.28109000	0.79649200
O	0.93510300	0.08549700	1.21223900
C	−1.72311500	0.80824200	0.34466100
C	1.12062500	−1.35901100	−0.84371000
C	3.31278800	−0.55599000	−0.18590300
C	−0.71541400	3.06701300	0.50552000
C	0.36932700	3.34268800	1.35555100
C	3.78521300	−0.84972200	1.11044400
C	2.94085100	−2.61447900	−1.70526600
C	−3.34508100	−1.04682500	0.50686000
C	3.65666500	0.62973000	−0.86133200
C	0.45598500	−2.49504200	−1.57703700
C	−3.27227700	−2.02018000	1.51534800
C	0.54733100	2.62484900	2.68091400
H	0.01144500	1.66465600	2.62536900
C	−0.94335000	3.76233800	−0.69609800
C	4.70700500	0.04059100	1.66810800
H	5.09234600	−0.16114600	2.66905700
C	1.04891900	5.06100700	−0.22593400
H	1.74826500	5.84826800	−0.51419200
C	4.56738500	1.49301100	−0.24271500
H	4.84524400	2.42136200	−0.74465300
C	−2.77147600	2.29322500	1.68594500
H	−2.91718100	3.23982100	2.19468300
C	5.10810400	1.19189900	0.99999900
H	5.82118700	1.87323100	1.46645200
C	1.24741400	4.35788700	0.95863900
H	2.10115100	4.59925100	1.59377300
C	−3.84025900	−1.32223600	−0.78645900
C	−3.75700300	−3.30039600	1.21173400

H	−3.72533100	−4.07601900	1.97941300
C	1.63813800	−3.26098600	−2.21802200
H	1.60873200	−4.32592800	−1.95000700
H	1.59326500	−3.20322600	−3.31456700
C	−3.53607000	1.17910500	1.64359800
H	−4.47871400	0.94046900	2.12459600
C	−0.03334400	4.76290500	−1.04910500
H	−0.17635600	5.31768400	−1.97875200
C	3.02714300	1.05469900	−2.17915600
H	2.45001000	0.21316800	−2.57894200
C	3.78038500	−3.57066000	−0.86709400
H	4.65616700	−3.05661000	−0.45000400
H	4.13626900	−4.37996200	−1.51990500
H	3.20149100	−4.01895400	−0.04934200
C	−0.26273200	−3.32494200	−0.48127800
H	0.48801500	−3.65181600	0.25964500
H	−0.95591200	−2.65556200	0.05509200
C	3.31889600	−2.02253200	1.96296000
H	2.59591600	−2.60770300	1.37728400
C	3.80420100	−2.06432800	−2.83915600
H	3.22490400	−1.43683800	−3.52917300
H	4.20687900	−2.91307400	−3.40954700
H	4.64937900	−1.48034000	−2.44714000
C	−2.12127500	3.43894900	−1.60280800
H	−2.80258000	2.77250100	−1.05200000
C	−2.71197400	−1.72832800	2.89735900
H	−2.20730900	−0.75347700	2.86042000
C	−4.26245900	−3.59661000	−0.04641000
H	−4.62843600	−4.60168900	−0.26441400
B	0.30789100	−0.24744400	0.04576100

C	−4.29169900	−2.61856200	−1.04084900
H	−4.67757100	−2.87346000	−2.02794500
C	−0.04746600	3.47026100	3.81497800
H	0.47114200	4.43908000	3.89892100
H	0.05538600	2.94236500	4.77456000
H	−1.11629100	3.67597100	3.65721800
C	2.03881100	2.20156400	−1.94264400
H	2.55883200	3.09059000	−1.55627500
H	1.26176100	1.92895900	−1.21101600
H	1.54018200	2.48039800	−2.88417300
C	−0.55915900	−1.98717100	−2.61785800
H	−0.86538400	−2.85094300	−3.23061100
H	−1.44323100	−1.62596800	−2.07429600
C	4.06721800	1.44587900	−3.23245500
H	3.57073000	1.65656500	−4.19115500
H	4.80903400	0.65106700	−3.39536500
H	4.60909300	2.35682800	−2.93827800
C	−1.02257800	−4.53277700	−1.01669900
H	−1.45533200	−5.10100500	−0.18166900
H	−0.37249000	−5.21438100	−1.58742100
H	−1.85504700	−4.22455700	−1.66387800
C	−1.65305100	2.67986300	−2.84871100
H	−2.51487700	2.39889600	−3.47507900
H	−1.11806800	1.76490800	−2.55696300
H	−0.98067800	3.30645700	−3.45681100
C	2.01073800	2.29198700	2.97129600
H	2.45084500	1.73985700	2.13060900
H	2.06514800	1.64459800	3.85914600
H	2.61201300	3.19274300	3.17963500
C	2.58839300	−1.55030400	3.22965100

H	2.36204300	−2.42842800	3.85516000
H	1.64273900	−1.03945000	2.99581300
H	3.23795200	−0.88557100	3.82109200
C	−3.89076300	−0.23479400	−1.85203900
H	−2.92342100	0.29066800	−1.80912600
C	−3.84228600	−1.68312400	3.93221200
H	−4.34380100	−2.66095900	4.01143800
H	−4.60906400	−0.93864100	3.67077900
H	−3.44177900	−1.42692400	4.92394900
C	−1.63830000	−2.74318700	3.29932700
H	−1.22950000	−2.47232600	4.28381800
H	−0.80808200	−2.70185700	2.58246700
H	−2.04090000	−3.76655000	3.37066100
C	−2.91859400	4.69030300	−1.97821700
H	−2.32344000	5.37682700	−2.59908100
H	−3.24586100	5.23881500	−1.08342700
H	−3.81107300	4.41136000	−2.55789500
C	4.49071400	−2.92769000	2.37193100
H	5.13616500	−2.40905000	3.09703800
H	5.12336200	−3.23664500	1.52958500
H	4.11028900	−3.83291400	2.86765000
C	−5.00894500	0.77751000	−1.56763300
H	−5.99252900	0.28470300	−1.61344400
H	−4.99471700	1.58061100	−2.32102500
H	−4.90548100	1.24297700	−0.57804300
C	−0.02784600	−0.87044100	−3.50729200
H	0.20561200	0.01885300	−2.90215300
H	−0.77952200	−0.57112700	−4.25196100
H	0.87902700	−1.17124900	−4.05844200
C	−4.04230800	−0.78216300	−3.27090100

H	−3.28437300	−1.54596500	−3.49848100
H	−3.93017700	0.03630100	−3.99686300
H	−5.03670200	−1.22713300	−3.43089300

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