Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting information for:

Cleavage of BN Triple Bonds by Main Group Reagents

Lena Winner,[a,b]† Alexander Hermann,[a,b]† Guillaume Bélanger-Chabot,[a,b] Oscar F. González-Belman,[c]† J. Oscar C. Jiménez-Halla,[c] Hauke Kelch[a,b] and Holger Braunschweig[a,b]*

[a] *Institute for Sustainable Chemistry & Catalysis with Boron, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany.*

[b] *Institute for Inorganic Chemistry, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany.*

[c] *Departamento de Química, Universidad de Guanajuato, Noria Alta S/N 36050 Guanajuato, México.*

Methods and Materials

All manipulations were performed either under an atmosphere of dry argon or in vacuo using standard Schlenk line or glovebox techniques. Deuterated solvents were dried over molecular sieves and degassed by three freeze-pump-thaw cycles prior to use. All other solvents were distilled and degassed from appropriate drying agents. Solvents (both deuterated and non-deuterated) were stored under argon over activated 4 Å molecular sieves. NMR spectra were acquired on a Bruker Avance 500 NMR spectrometer (^{1}H: 500.1 MHz, ^{11}B{^{1}H}: 160.5 MHz, ^{13}C{^{1}H}: 125.8 MHz, ^{29}Si{^{1}H}: 99.4 MHz) or on a Bruker Avance 400 NMR spectrometer (^{1}H: 400.1 MHz, ^{11}B: 128.4 MHz). Chemical shifts (δ) are given in ppm and internally referenced to the carbon nuclei (^{13}C{^{1}H}) or residual protons (^{1}H) of the solvent. ^{29}Si{^{1}H} and ^{11}B{^{1}H} NMR spectra were referenced to external standards $SiMe_4$ and $[BF_3{\cdot}OEt_2]$ respectively. ^{1}H NMR and ^{13}C{^{1}H} NMR signals were assigned with assistance from DEPT-135 and HSQC experiments. Infrared data were acquired on a Bruker Alpha instrument in ATR mode. Elemental analysis was conducted on an Elementar vario MICRO cube elemental analyser. Mass spectrometry was performed with an Exactive Plus with Orbitrap and liquid injection field desorption ionization (LIFDI). High-resolution mass spectrometry was obtained from a Thermo Scientific Exactive Plus spectrometer.

Solvents and reagents were purchased from Sigma Aldrich. Deuterated solvents were degassed with three freeze-pump-thaw cycles and stored over molecular sieves in Young ampoules or in a glovebox. Compound **Si**,[1] *tert*-butyliminoborane **1**,[2] 1,2-dipiperidinoacetylene,[3] **3**[4] and 1,3-dimethylimidazol-2-ylidene (IMe)[5] were synthesized using literature procedures.

Isolation of silaimine **2**

Si (100 mg, 0.230 mmol) was dissolved in hexane (200 mL). *t*BuNB*t*Bu (**1**) (32.0 mg, 0.230 mmol) was added and the resulting yellow mixture was stirred for 5 minutes at room temperature. Removal of the solvent *in vacuo* yielded a yellow solid, which was recrystallized from hexane at –30 °C to give **2** as a orange solid (58 mg, 0.101 mmol, 44%).

^{1}H NMR (500.1 MHz, C_6D_6): δ = 6.97–7.29 (m, 10H, C_6H_5), 4.0 (sept, ^{3}J(^{1}H^{1}H) = 7.09 Hz, 2H, CH_3CHCH_3, 3.60 (sept, ^{3}J(^{1}H^{1}H) = 6.53 Hz, 2H, CH_3CHCH_3), 1.90 (s, 9H, *tBu*N), 1.65 (d, ^{3}J = 6.67 Hz, 6H, CH_3), 1.52 (s, 9H, *tBu*B), 1.50 (d, ^{3}J = 7.27 Hz, 6H, CH_3), 1.01 (d, ^{3}J = 6.57 Hz, 6H, CH_3), 0.83 (d, ^{3}J = 7.03 Hz, 6H, CH_3) ppm. ^{11}B NMR (160.5 MHz, C_6D_6): δ = –

1 (s) ppm. $^{13}C\{^{1}H\}$ NMR (125.8 MHz, C_6D_6): δ = 171.3 (2C, NCN), 135.5 (2C; *i*-C_6H_5), 130.1 (2C; *m*-C_6H_5), 129.0 (s, *p*-C_6H_6), 128.5 (4C; *p*-C_6H_5), 127.2 (4C; *o*-C_6H_5), 51.52 (C, $C(CH_3)_3$), 50.0 (2C, CH_3CHCH_3), 49.3 (2C, CH_3CHCH_3), 38.5 (3C, $NC(CH_3)_3$) 31.2 (3C, $BC(CH_3)_3$), 25.4 (2C, CH_3), 25.0 (2C, CH_3), 24.2 (2C, CH_3), 23.9 (2C, CH_3) ppm. ^{15}N NMR (C_6D_6, 500.1 MHz): δ = –285.1 (*N*tBu), 220.3 (*N*iPr), 205.3 (*N*iPr) ppm. $^{29}Si\{^{1}H\}$ NMR (C_6D_6, 99.4 MHz): δ = –22.3 ppm. The ^{13}C NMR resonances for the second quaternary *t*BuB-carbon can not be detected. LIFDI−MS (*m/z*) calculated for $[C_{34}H_{56}BN_5Si]$ = 575.4504; found: 575.4493.

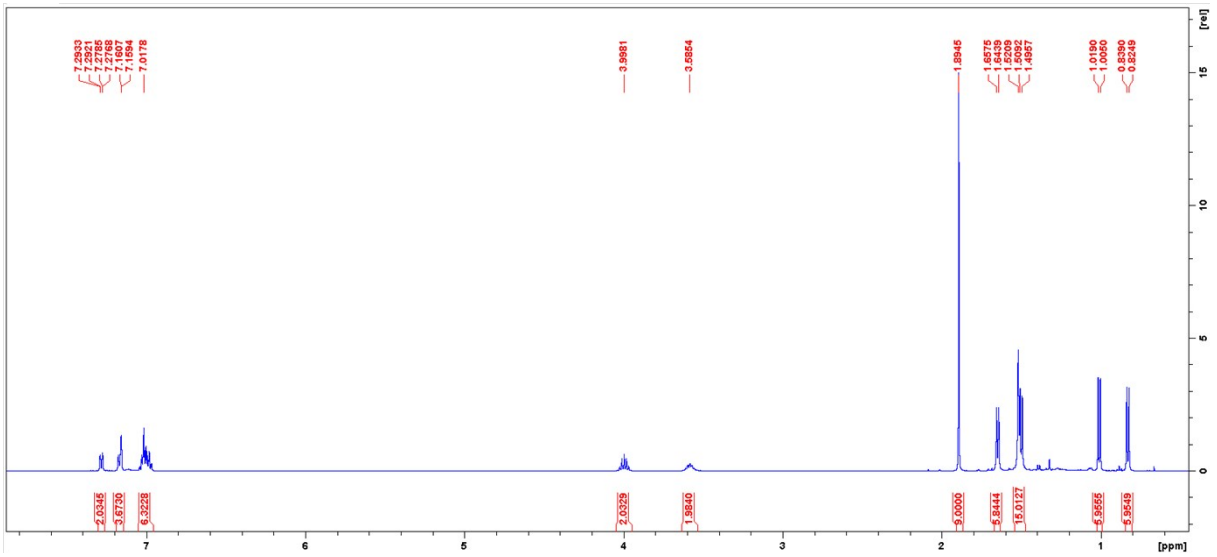


Figure S-1: ^{1}H NMR spectrum of **2** in C_6D_6.

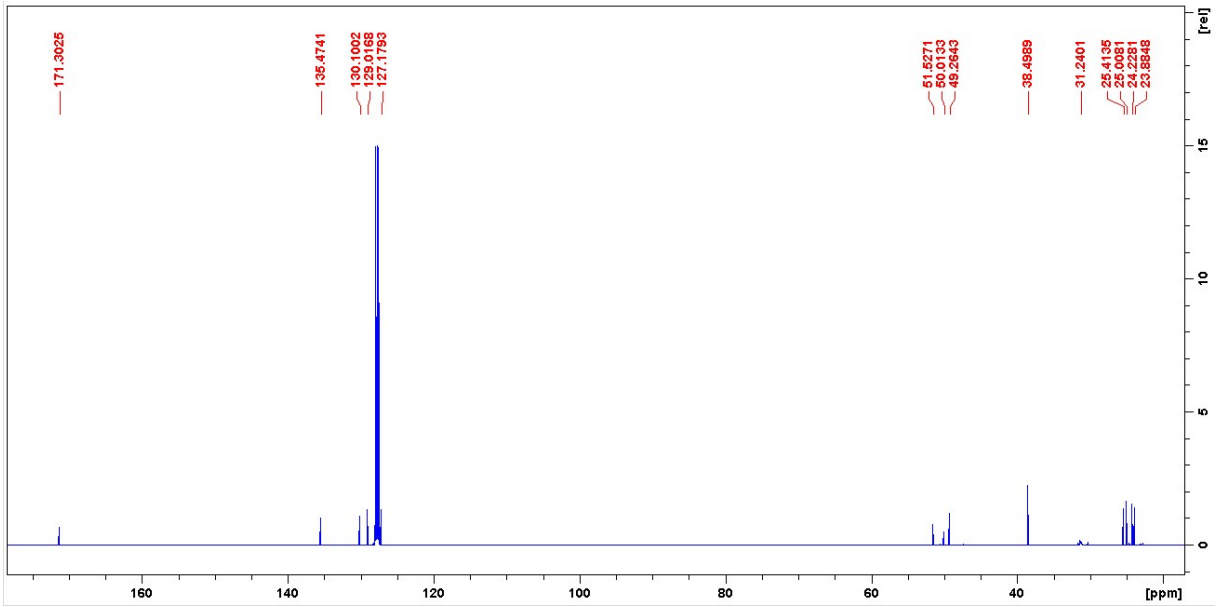


Figure S-2: ^{13}C NMR spectrum of **2** in C_6D_6.

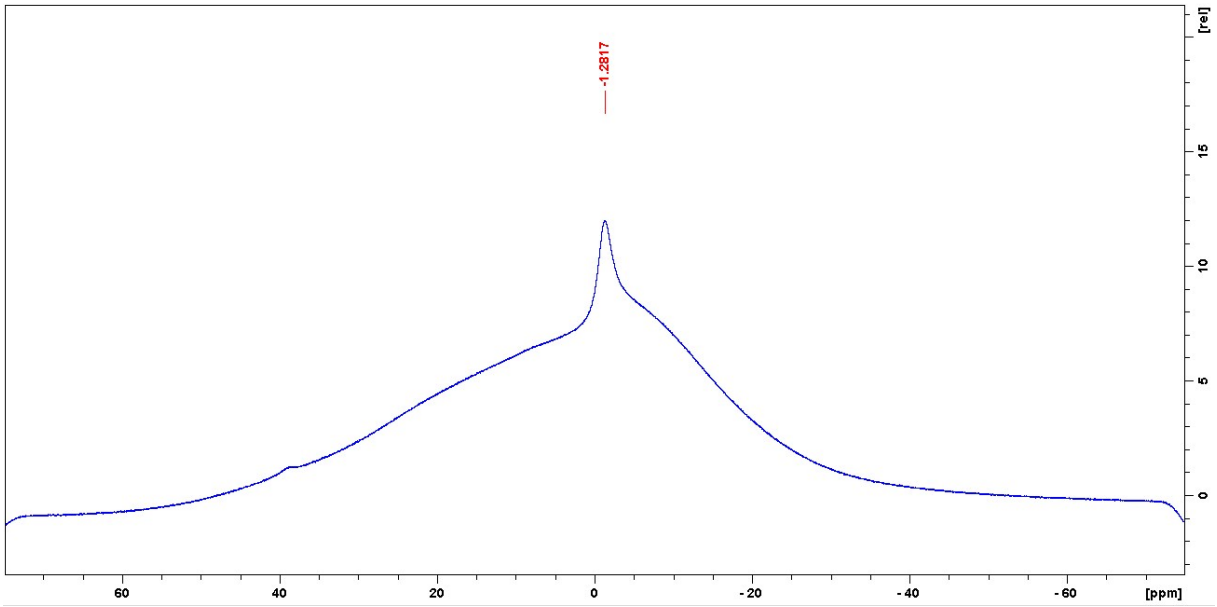


Figure S-3: ^{11}B NMR spectrum of **2** in C_6D_6.

Synthesis of Ar*NB(IMe)TMP (**4**)

To a solution of Ar*NBTMP (**3**) (0.16 g, 260 μmol) in hexane (25 mL), a solution of IMe (25.0 mg, 260 μmol) in toluene (1 mL) was added dropwise. The light yellow suspension was stirred 1.5 h and all volatiles were removed in vacuum. The residue was washed with pentane to yield pure **4** as a light yellow solid (0.15 g, 201 μmol, 77 %).

^1H NMR (500.1 MHz, 296 K, C_6D_6): δ = 7.40 (m, 4H, Ar-*H*), 7.24 (m, 4H, Ar-*H*), 7.18-7.15 (m, 6H, Ar-*H*), 7.08-6.96 (m, 8H, Ar-*H*), 6.34 (s, 2H, C*H*Ph_2), 5.07 (s, 2H, C*H*=C*H*), 2.83 (s, 6H, NCH_3), 1.81-1.76 (m, 2H, CH_2), 1.49-1.47 (m, 4H, CH_2), 1.39 (s, 12H, CH_3), 1.21 (s, 9H, C(CH_3)$_3$) ppm. $^{11}B\{^1H\}$ NMR (160.5 MHz, 296 K, C_6D_6): δ = 17 ppm. $^{13}C\{^1H\}$ NMR (125.8 MHz, 296 K, C_6D_6): δ = 149.40, 149.09, 147.05, 133.66, (Ar-C_q), 130.52, 130.09 (Ar-*C*H), 127.59 (Ar-C_q), 126.85, 125.47, 125.23 (Ar-*C*H), 119.99 (*C*H=*C*H), 53.57 (*C*(CH$_3$)$_2$), 51.63 (*C*HPh_2), 42.63 (*C*H_2), 35.69 (N*C*H_3), 34.56 (C_q, *C*(CH$_3$)$_3$), 32.36 (C(*C*H$_3$)$_2$), 32.01 (*C*H$_3$), 19.04 (CH$_2$-*C*H$_2$-CH$_2$) ppm. Elemental analysis: calculated for $C_{50}H_{60}BN_4$: C 82.51, H 8.31, N 7.70; found: C 81.90, H 8.60, N 7.64 %.

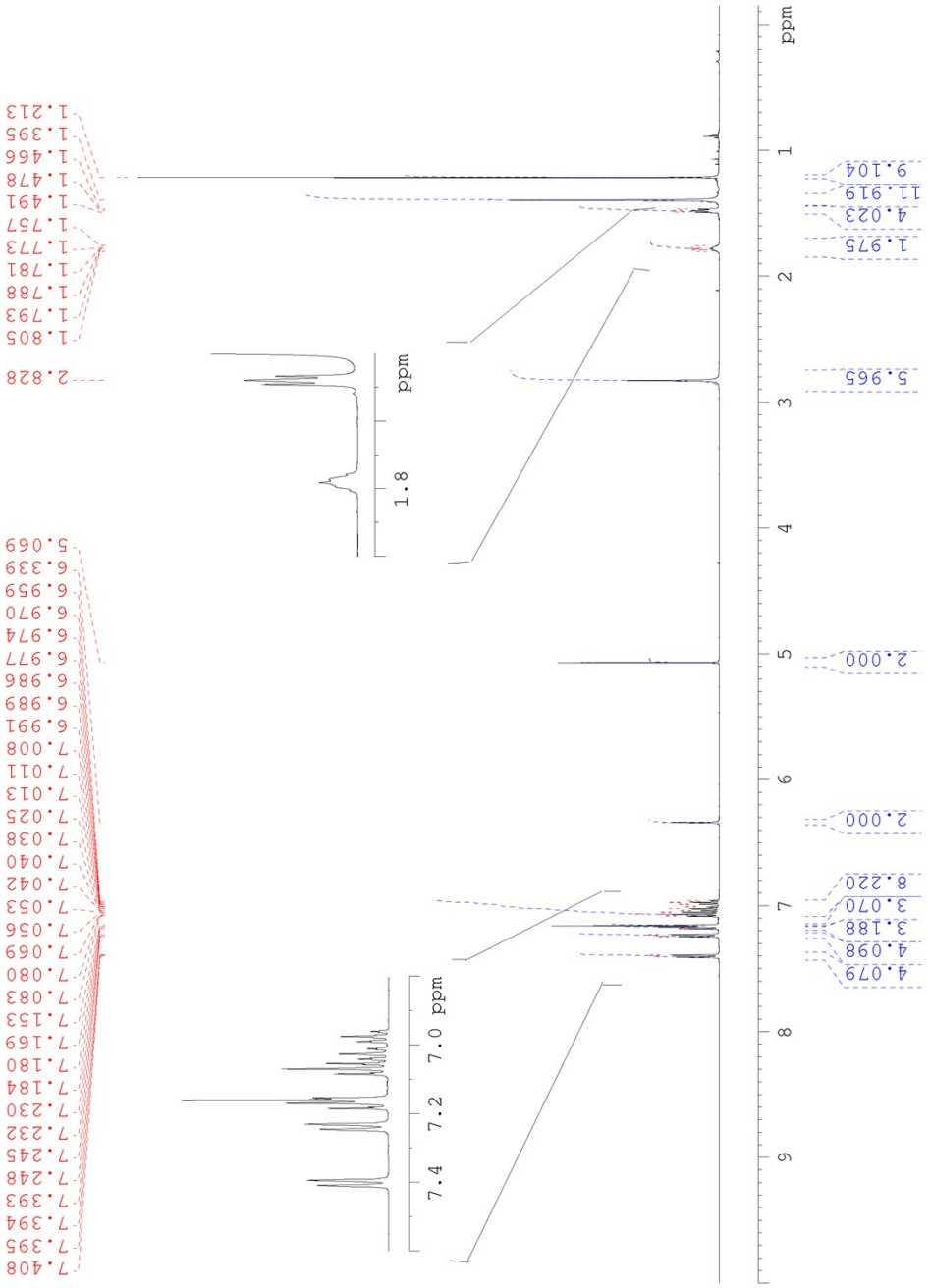


Figure S-4: ^{1}H NMR spectrum of **4** in C_6D_6. The triplet at 0.89 ppm and the corresponding multiplet at 1.24 ppm are due to residual hexane.

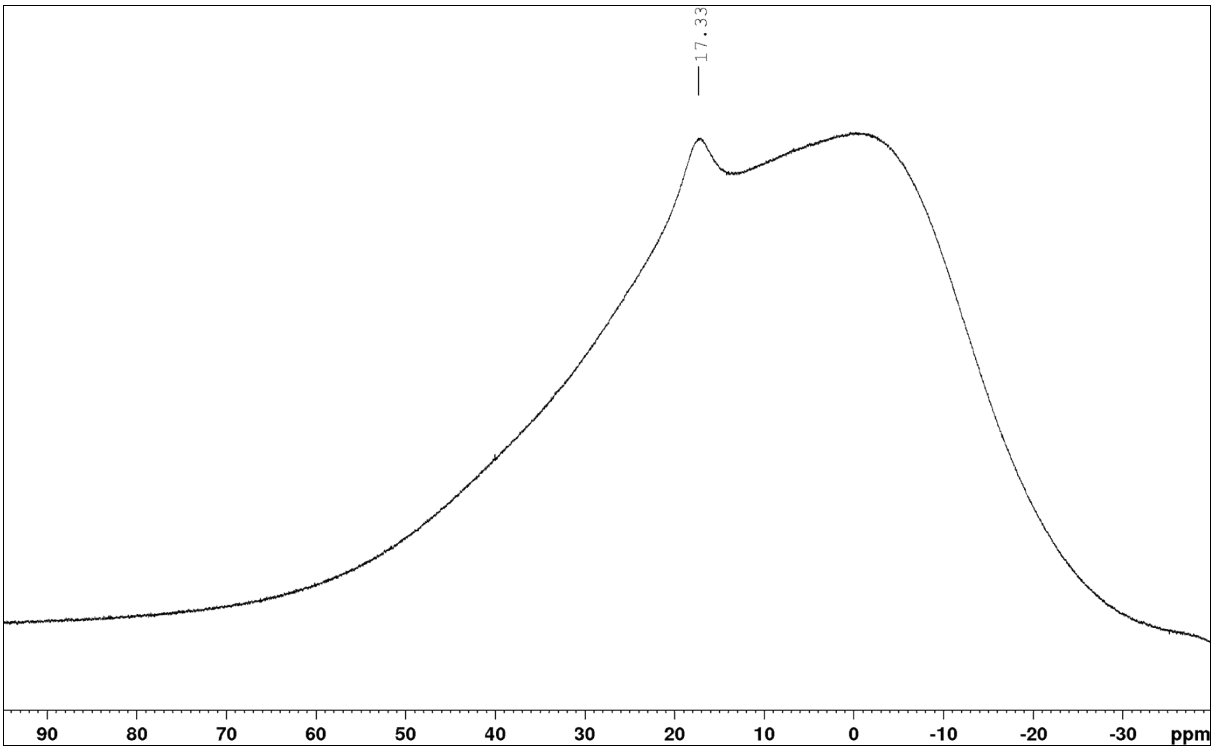


Figure S-5: ^{11}B NMR spectrum of **4** in C_6D_6.

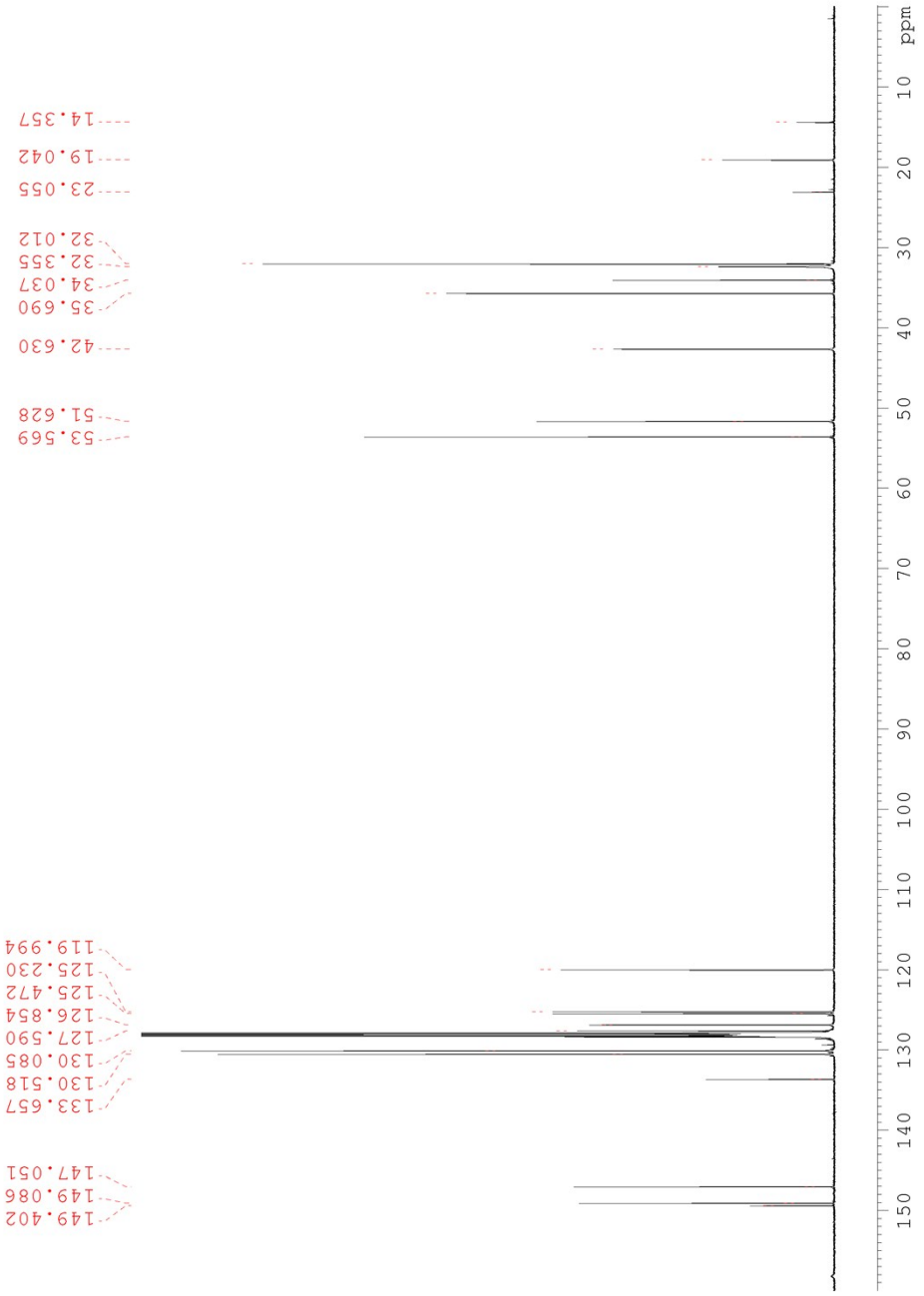


Figure S-6: $^{13}C\{^{1}H\}$ NMR spectrum of **4** in C_6D_6. The resonances at 14.36, 23.04 and 32.35 ppm correspond to residual hexane.

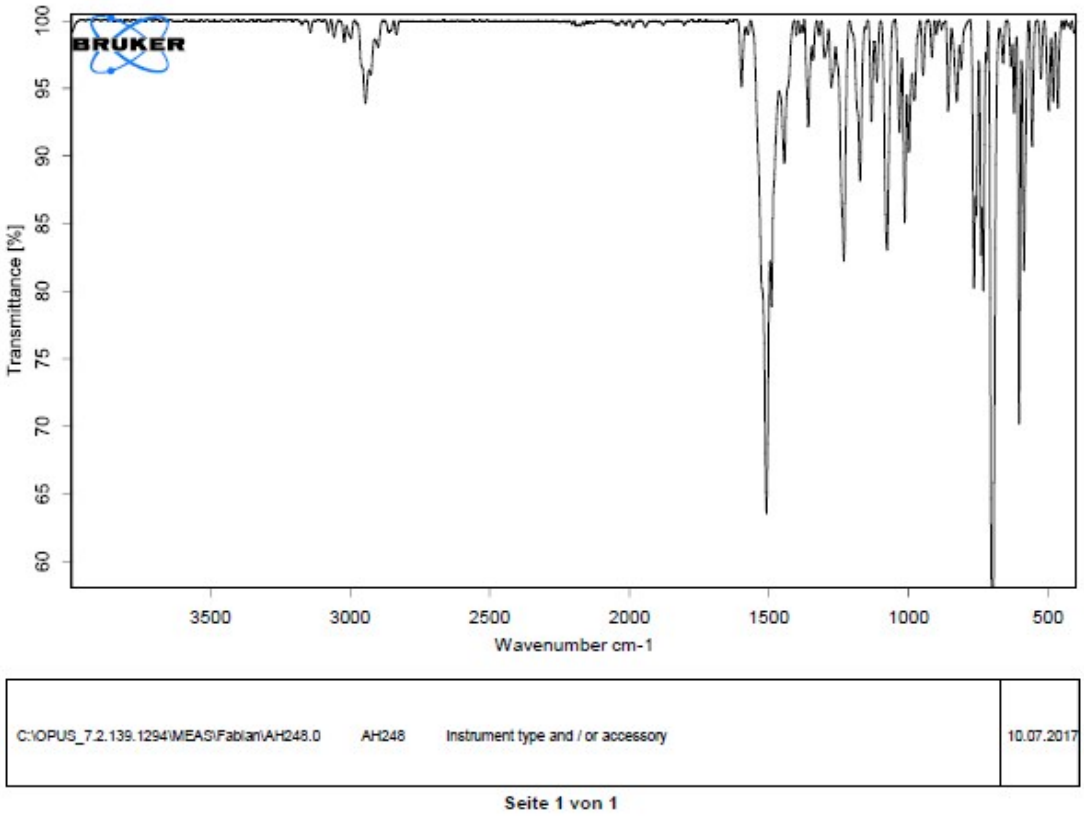


Figure S-7: ATR-IR of **4**.

Reaction of Ar*NBTMP (**3**) with 1,2-dipiperidylethyne: (synthesis of **5**)

A hexane solution (0.5 mL) of 1,2-dipiperidylethyne (20.0 mg, 104 μmol) was added to a hexane solution (0.5 mL) of Ar*NBTMP (**3**) (65.6 mg, 104 μmol). The solution was heated for 16 h at 60 °C and over the course of the reaction a color change to orange was observed. Removal of volatiles yielded pure **5** as an orange crystalline solid (73 mg, 88.7 µmol, 85%).

^{1}H NMR (500.1 MHz, 296 K, C_6D_6): δ = 7.33-7.30 (m, 10H, Ar-*H*), 7.17-7.11 (m, 8H, Ar-*H*), 7.05-7.02 (m, 4 H, Ar-*H*), 6.88 (s, 2H, C*H*Ph$_2$), 3.19 (m, 4H, C*H*$_2$), 3.00-2.98 (m, 1H, C*H*$_2$), 2.57 (m, 4H, C*H*$_2$), 2.02-1.91 (m, 1H, C*H*$_2$), 1.62-1.58 (m, 1H, C*H*$_2$), 1.53 (s, 6H, C*H*$_3$), 1.50 (m, 1H, C*H*$_2$), 1.45-1.34 (m, 10H, C*H*$_2$), 1.23 (s, 6H, C*H*$_3$), 1.13-1.09 (m, 3H, C*H*$_2$), 1.02 (s, 9H, C(C*H*$_3$)$_3$), 0.93 (s, 1H, C*H*$_2$) ppm. ^{11}B{^{1}H} NMR (128.4 MHz, 296 K, C_6D_6): δ = 34 ppm. ^{13}C{^{1}H} NMR (125.8 MHz, 296 K, C_6D_6): δ = 192.62 (C_q, C=*C*=N), 147.78, 145.26, 137.29, 136.68 (Ar-C_q), 130.31, 128.55, 127.39, 126.52 (Ar-*C*H), 55.63 (CH$_2$-*C*H$_2$-CH$_2$), 55.42 (*C*H$_2$), 52.20 (*C*(CH$_3$)$_2$), 51.51 (*C*HPh$_2$), 49.29, 49.00, 41.64 (*C*H$_2$), 34.61 (C_q, *C*(CH$_3$)$_3$), 33.91 (C(*C*H$_3$)$_2$), 31.65 (C=*C*BN), 31.12 (C(*C*H$_3$)), 29.18 (C(*C*H$_3$)$_2$), 27.91, 27.26, 26.72,

25.87, 25.74, 24.24, (CH$_2$), 19.35 (CH$_2$-CH$_2$-CH$_2$) ppm. Elemental analysis: calculated for $C_{57}H_{71}BN_4$: C 83.18, H 8.70, N 6.81; found: C 83.02, H 8.80, N 6.86 %.

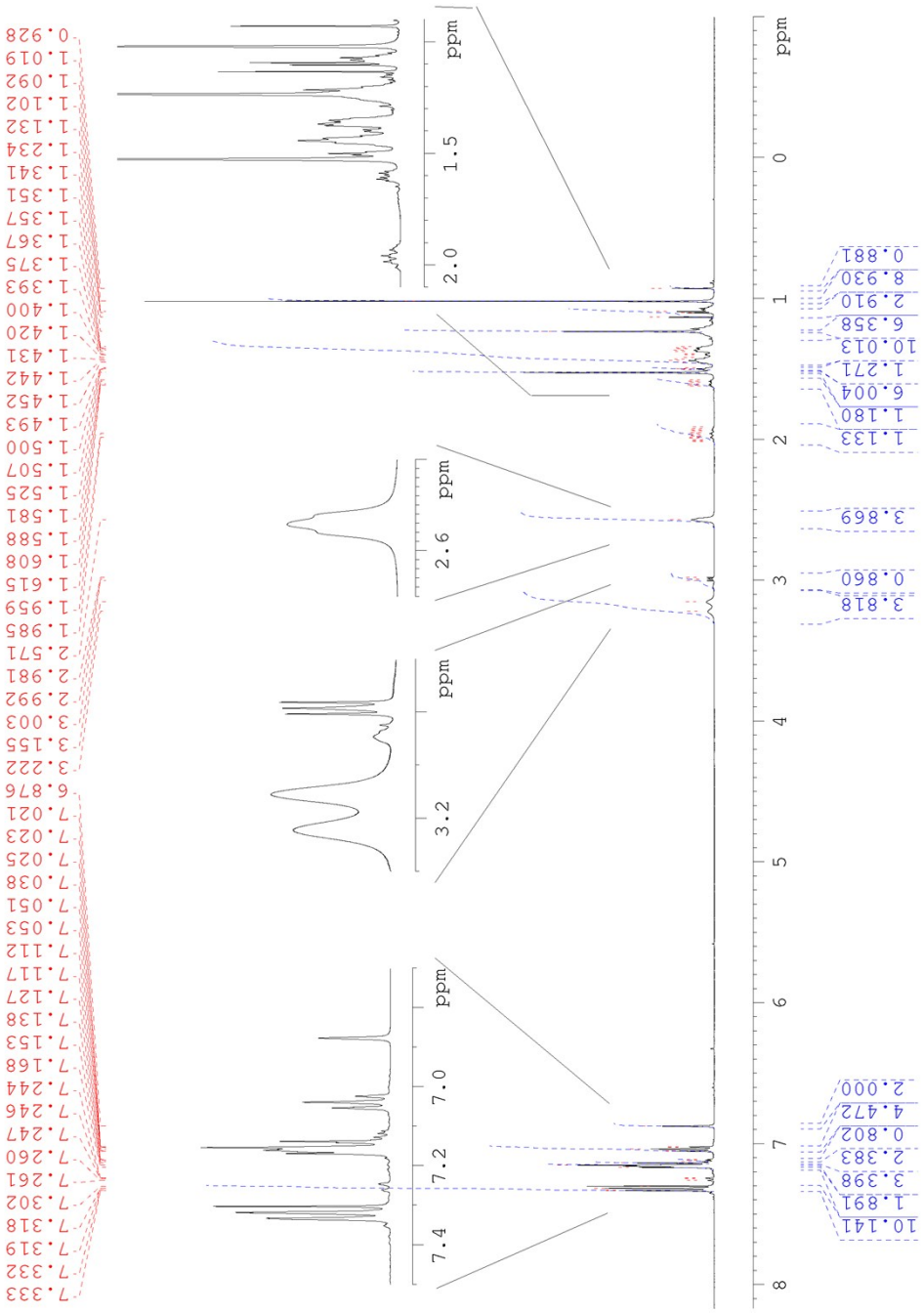


Figure S-8: ^{1}H NMR spectrum of **5** in C_6D_6.

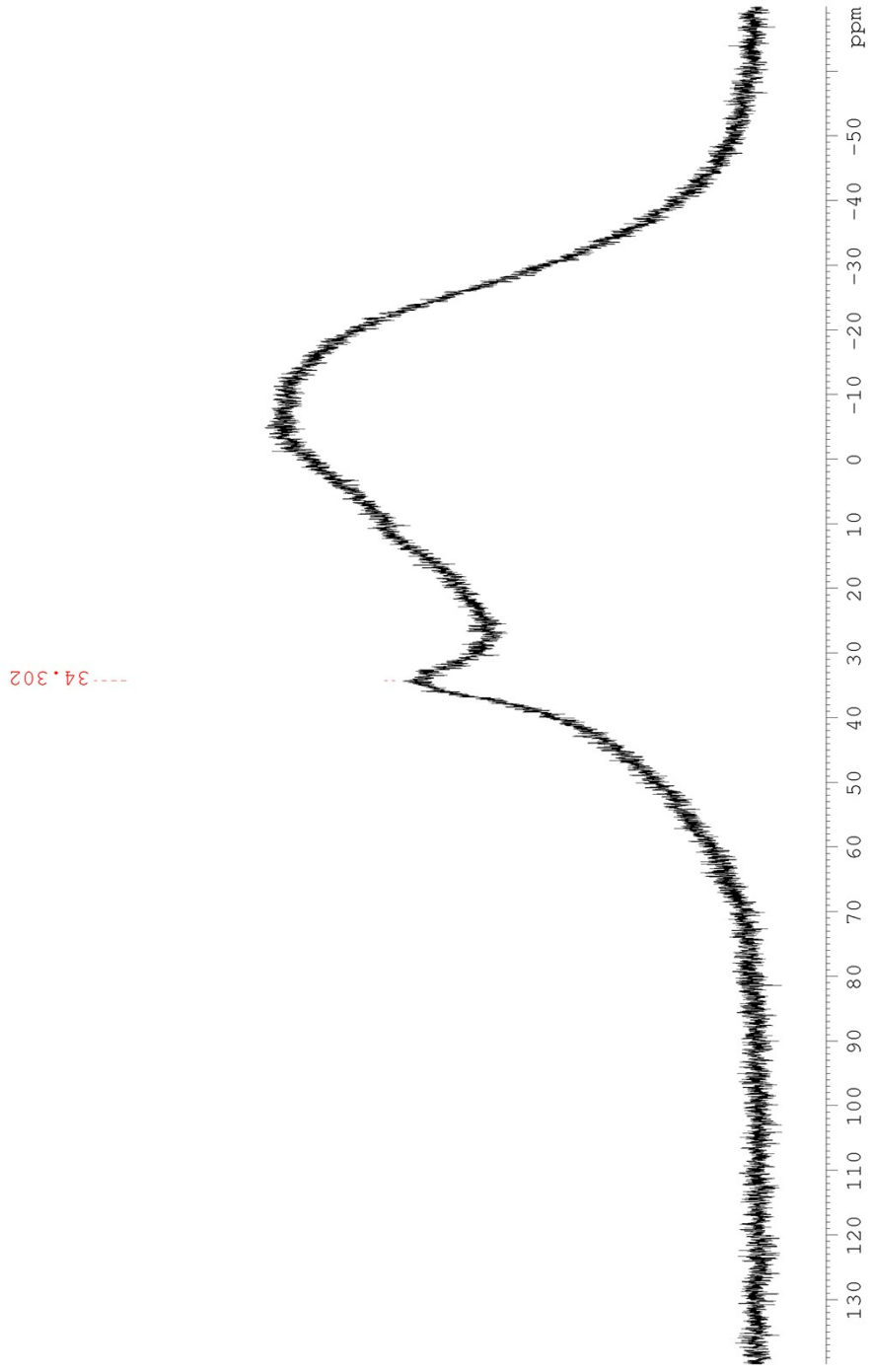


Figure S-9: ^{11}B NMR spectrum of **5** in C_6D_6.

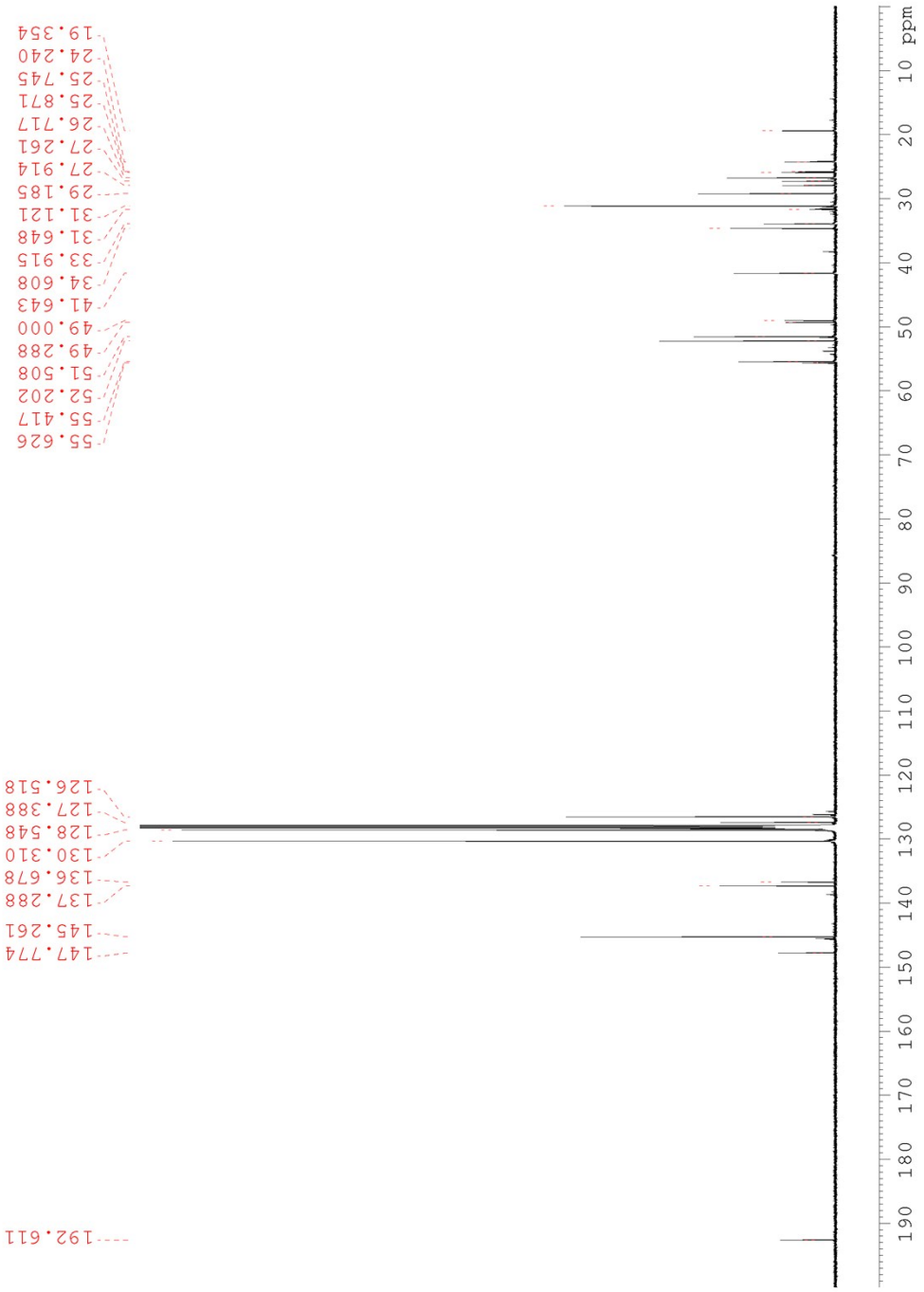


Figure S-10: $^{13}C\{^{1}H\}$ NMR spectrum of **5** in C_6D_6.

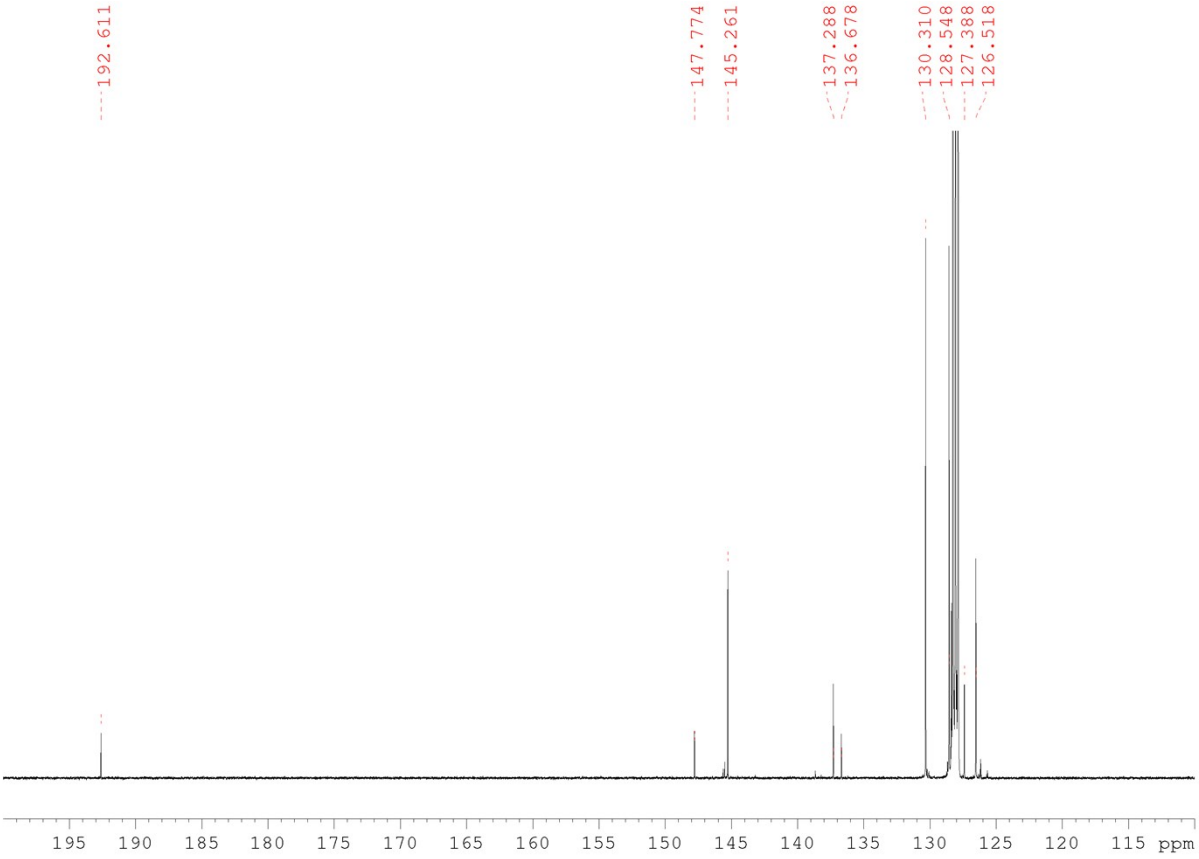


Figure S-11: $^{13}C\{^{1}H\}$ NMR spectrum of **5** in C_6D_6 (110 to 200 ppm region).

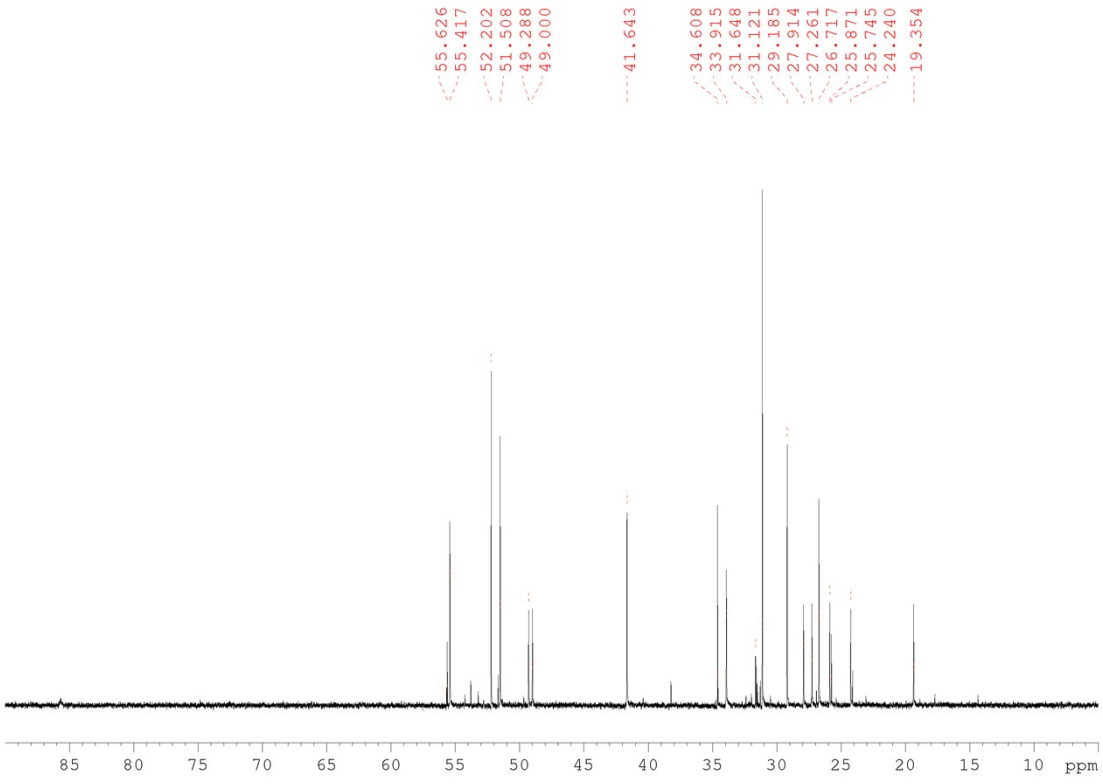


Figure S-12: $^{13}C\{^{1}H\}$ NMR spectrum of **5** in C_6D_6 (aliphatic region).

X-ray crystallographic details

The crystal data of **2**, **4**, and **5** were collected on a BRUKER SMART-APEX diffractometer with a CCD area detector and graphite monochromated $Mo_{K\alpha}$ radiation (**2**), BRUKER X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation or on a BRUKER D8 QUEST diffractometer (**4** and **5**). The structures were solved using the intrinsic phasing method (SHELXT),[6] refined with the SHELXLprogram[7] and expanded using Fourier techniques. Unless otherwise stated, all non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealised geometric positions. Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication nos. CCDC-1830914 (**2**), 1830913 (**4**), 1830912 (**5**). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/.

Crystal data of **2**

One isopropyl group is disordered over two orientations related by a rotation about the N-C axis. It was modelled as a two-part disorder with a refined ratio of 0.8:0.2. The displacement parameters of atoms C10 and C102 of the 7 were restrained to the same value with similarity restraint SIMU.

Table S-1: Crystal structure determination parameters for **2**.

Data	**test_a**
Empirical formula	$C_{34}H_{56}BN_5Si$
Formula weight ($g \cdot mol^{-1}$)	573.73
Temperature (K)	100(2)
Radiation, λ (Å)	$Mo_{K\alpha}$ 0.71073
Crystal system	Monoclinic
Space group	*P*21/*n*
Unit cell dimensions	
a (Å)	19.1168(9)
b (Å)	17.0388(8)
c (Å)	21.9556(8)
α (°)	90
β (°)	105.534(2)
γ (°)	90
Volume ($Å^3$)	6890.3(5)
Z	8
Calculated density ($Mg \cdot m^{-3}$)	1.106

Absorbtion coefficient (mm^{-1})	0.098
$F(000)$	2512
Theta range for collection	2.037 to 26.371°
Reflections collected	91458
Independent reflections	14074
Minimum/maximum transmission	0.6860/0.7454
Refinement method	Full-matrix least-squares on F^2
Data / parameters / restrains	14074 / 797 / 66
Goodness-of-fit on F^2	0.906
Final R indices [I>2σ(I)]	R_1 = 0.0384, wR^2 = 0.0918
R indices (all data)	R_1 = 0.0572, wR^2 = 0.1018
Maximum/minimum residual electron density ($e \cdot Å^{-3}$)	0.338 / –0.338

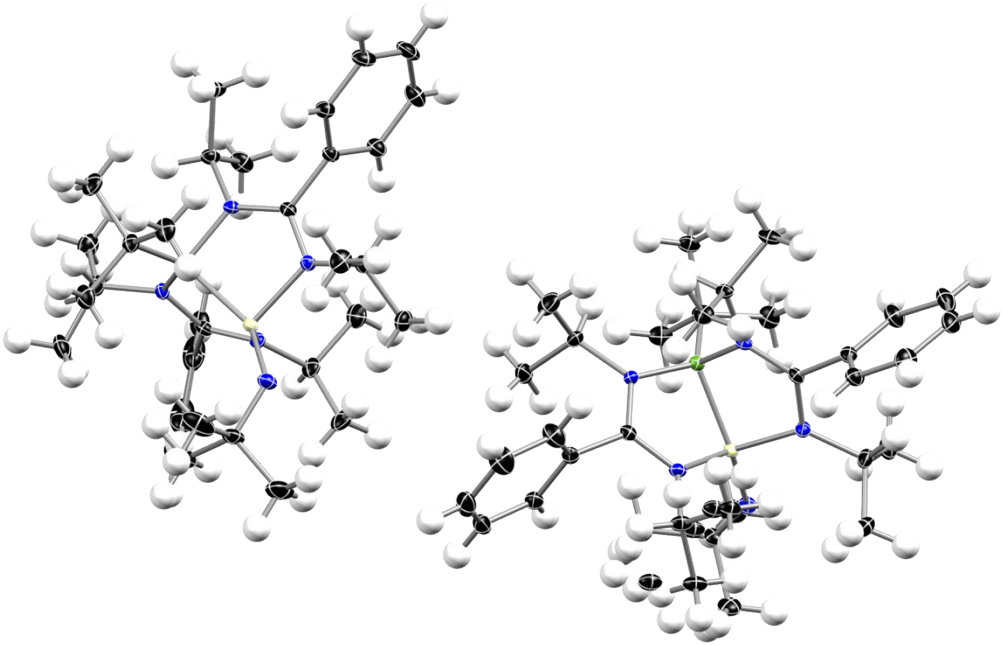


Figure S-13: Solid-state structure of **2** showing the two crystallographically independent molecules making the asymmetric unit. One isopropyl group is disordered over two positions related by a rotation about the N-C axis.

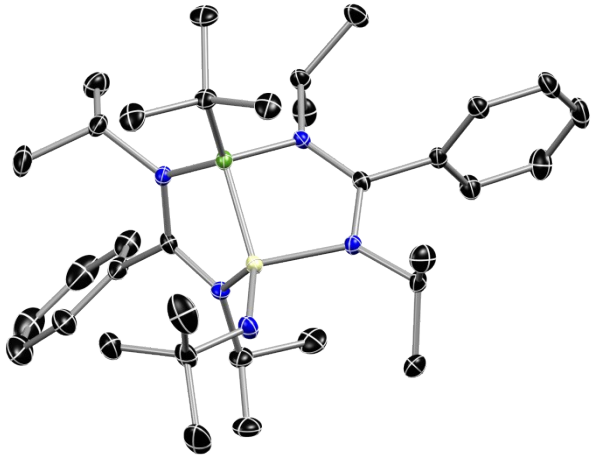


Figure S-14: Solid-state structure of **2** showing one of the two crystallographically independent molecules making the asymmetric unit. Hydrogen atoms were omitted for clarity.

Crystal data of **4**

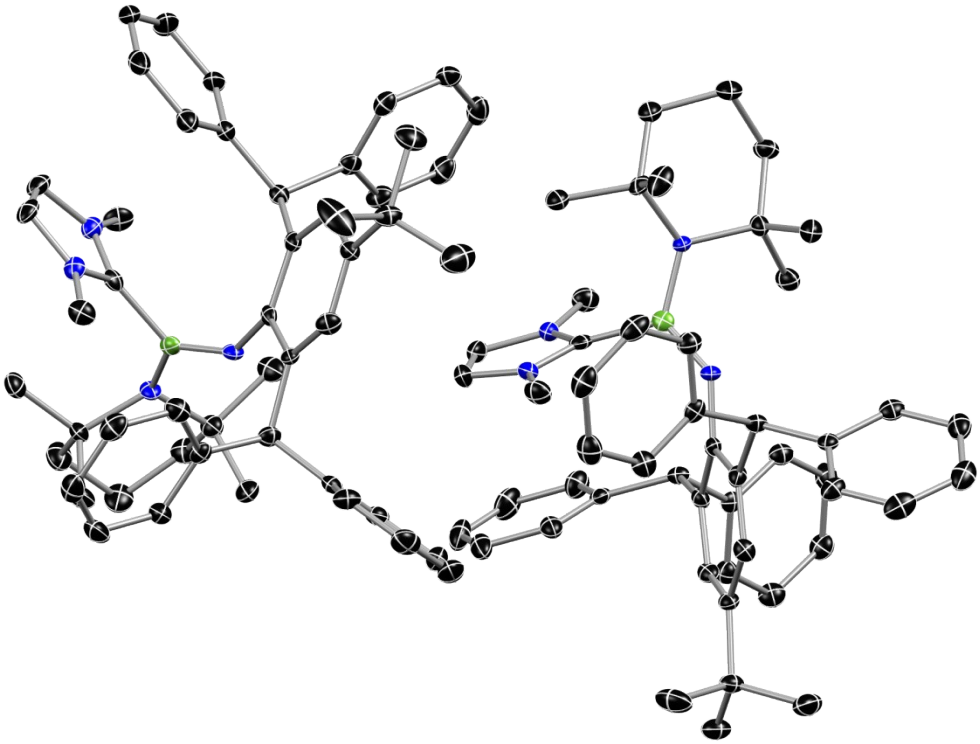


Figure S-15: Solid-state structure of **4** showing the two crystallographically independent molecules making the asymmetric unit. Hydrogen atoms were omitted for clarity.

Table S-2: Crystal structure determination parameters for **4**.

Data	**test_a**
Empirical formula	$C_{50}H_{59}BN_4$
Formula weight ($g \cdot mol^{-1}$)	726.82
Temperature (K)	100(2)
Radiation, λ (Å)	$Mo_{K\alpha}$ 0.71073
Crystal system	Triclinic
Space group	$P\ \bar{1}$
Unit cell dimensions	
a (Å)	13.134(5)
b (Å)	16.944(3)
c (Å)	19.889(5)
α (°)	79.28(3)
β (°)	81.864(15)
γ (°)	73.209(15)
Volume ($Å^3$)	4146(2)
Z	4
Calculated density ($Mg \cdot m^{-3}$)	1.165
Absorbtion coefficient (mm^{-1})	0.067
F(000)	1568
Theta range for collection	2.228 to 26.020°
Reflections collected	37771
Independent reflections	16157
Minimum/maximum transmission	0.6131/0.7453
Refinement method	Full-matrix least-squares on F^2
Data / parameters / restrains	16157 / 1009 / 0
Goodness-of-fit on F^2	0.980
Final R indices [I>2σ(I)]	R_1 = 0.0735, wR^2 = 0.1467
R indices (all data)	R_1 = 0.1821, wR^2 = 0.1909
Maximum/minimum residual electron density ($e \cdot Å^{-3}$)	0.390 / –0.334

Crystal data of **5**

The displacement parameters of atoms C1>C3 of residues 1 and 2 were restrained to the same value with similarity restraint SIMU. The atomic displacement parameters of atoms C1_1>C3_1 and C1_2>C3_2 were restraint with RIGU keyword in ShelXL input ('enhanced rigid bond' restraint for all bonds in the connectivity list. The *tert*-butyl group (residues 1 and 2) is disordered over two orientations related by a rotation about the Ph-$C_{(Me)3}$ axis. This was modelled as a two-part disorder with a refined ratio of 0.7 : 0.3.

Table S-3: Crystal structure determination parameters for **5**.

Data	**test_a**
Empirical formula	$C_{57}H_{71}BN_4$
Formula weight ($g \cdot mol^{-1}$)	822.98
Temperature (K)	100(2)
Radiation, λ (Å)	$Mo_{K\alpha}$ 0.71073
Crystal system	Triclinic

Space group	$P\ \bar{1}$
Unit cell dimensions	
a (Å)	10.344(8)
b (Å)	15.310(9)
c (Å)	15.375(10)
α (°)	96.097(14)
β (°)	93.50(2)
γ (°)	101.648(17)
Volume (Å^3)	2363(3)
Z	2
Calculated density (Mg·m^{-3})	1.157
Absorbtion coefficient (mm^{-1})	0.066
F(000)	892
Theta range for collection	2.026 to 26.021°
Reflections collected	125549
Independent reflections	9301
Minimum/maximum transmission	0.6800/0.7454
Refinement method	Full-matrix least-squares on F^2
Data / parameters / restrains	9301 / 597 / 36
Goodness-of-fit on F^2	0.993
Final R indices [I>2σ(I)]	R_1 = 0.0451, wR^2 = 0.0950
R indices (all data)	R_1 = 0.0896, wR^2 = 0.1117
Maximum/minimum residual electron density (e·Å^{-3})	0.212 / –0.254

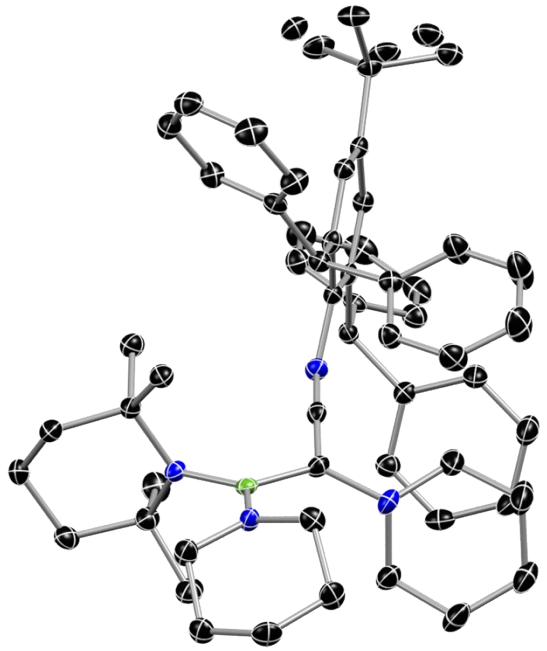


Figure S-16: Solid-state structure of **5** showing the asymmetric unit. One *tert*-butyl group is disordered over two positions related by a rotation about the C_{Ar}-C_{tBu} axis. Hydrogen atoms were omitted for clarity.

Computational Details

We have performed gas-phase geometry optimizations using the Gaussian16 rev. A.03 program.[8] This reaction mechanism was developed exploring the potential energy surface of the new global hybrid meta density-functional M08-HX developed by Truhlar and coworkers,[9] which has shown a broad accuracy for main group chemistry in terms of energy barriers. The electronic configurations of the molecules belonging to this mechanism were described with a split-valence basis set of triple-ζ quality with one polarization function, cep-121g*,[10-12] for all the atoms. Geometry optimizations were carried out without symmetry constraints, and the stationary points were characterized by analytical frequency calculations. That is, minimum points (reactants, intermediates and products) must have all-positive harmonic frequencies whereas maximum points (transition state) exhibit one and only one negative frequency. The reported Gibbs free energies in this work include zero-point energy, thermal and entropic corrections evaluated at 298 K and 1354 atm. This change in pressure was incorporated because the entropic contribution calculated within the ideal gas approximation at P =1 atm likely exaggerates the expected values for the association or dissociation of molecules in the condensed phase,[13-21] as suggested by Martin and coworkers.[22] Also, we performed calculations for including the solvent effect through the PCM model[23-26] using the SMD parameters[27] according to the Truhlar's model using hexane as solvent. And, for improving the numerical results, we carried out single-point calculations on the gas-phase optimized geometries using a complete basis set, def2-SVPD, for all of the atoms. These energies were added to the gas-phase calculations reported as our final energy values. That way, our composed level of theory can be named (SMD:hexane)M08-HX/def2-SVPD//M08-HX/cep-121G*.

Regarding the reaction mechanism for the formation of species **2**, we have performed DFT calculations at the M08-HX/def2-SVPD//M08-HX/cep-121G* level for proposing a plausible reaction route. The reaction starts from the η^2-coordination of the iminoborane (**1**) moiety to the silylene **Si**. Then, a 1,2-cycloaddition to one of the Si-N bonds via transition state **2-TS1**, where the boron atom inserts into the vicinal nitrogen, occurs through a low energy barrier of 19.7 kcal·mol^{-1}. This leads to six-membered non-planar heterocycle **2-Int1**, which is an endergonic reaction step of 4.9 kcal·mol^{-1} with respect to the reactants. Later, as a second reaction step and because of the steric hindrance between the *tert*-butyl groups, the boron atom is transferred to the silicon center, releasing the *t*-butyl-imine fragment through **2-TS2**

overcoming an energy barrier of 15.1 kcal·mol^{-1} with respect to **2-Int1**. The formation of **2-Int2** is an endothermic reaction step of 9.4 kcal·mol^{-1} with respect to the reactants. Finally, one of the nitrogen atoms of the other ligand undergoes a sigmatropic rearrangement from the silicon center to the boron atom, generating the reaction product **2** in a very fast reaction step (**2-TS3**; energy barrier of 2.8 kcal·mol^{-1} with respect to **2-Int2**) and a very exergonic reaction energy of –28.4 kcal·mol^{-1} with respect to the reactants and an overall enthalpy change of –35.0 kcal·mol^{-1} with respect to the reactants.

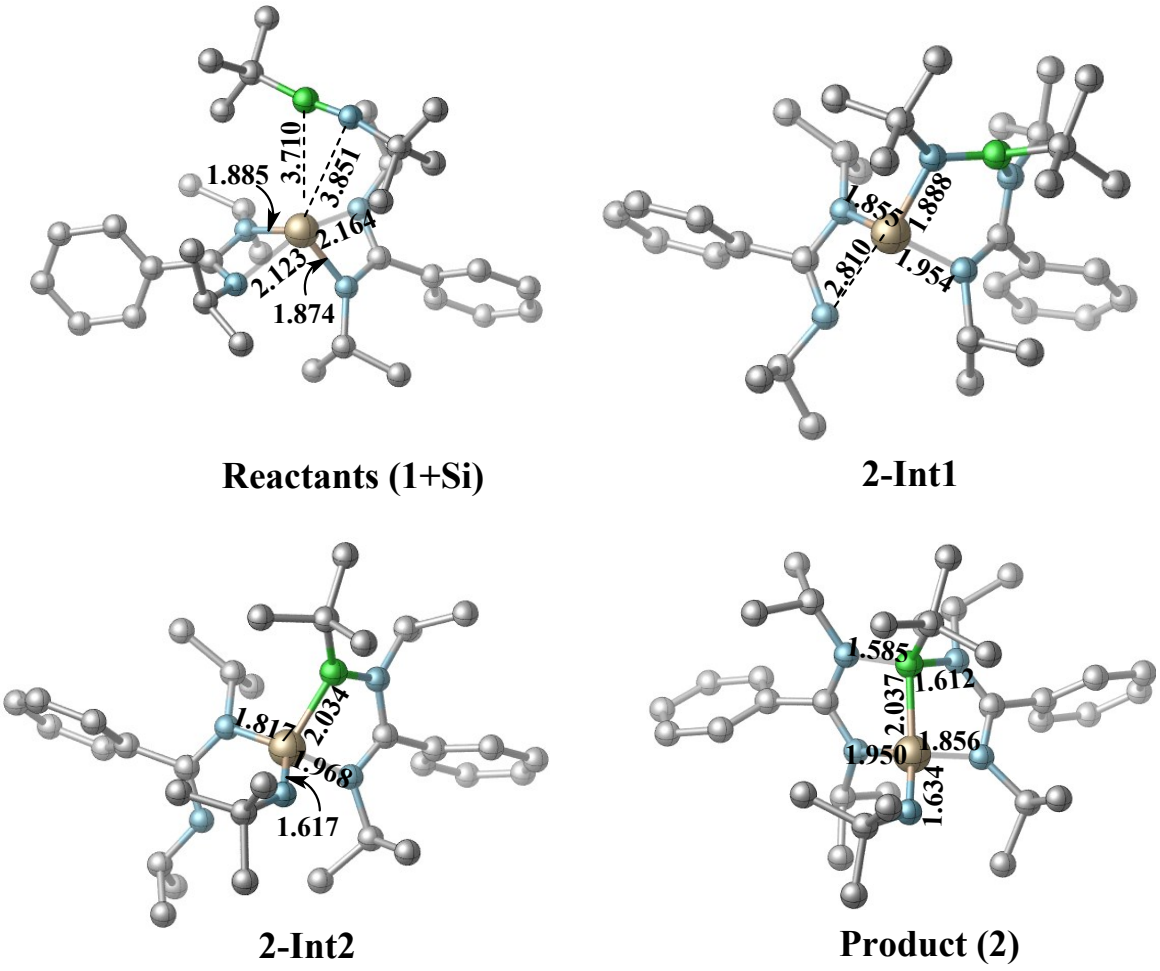
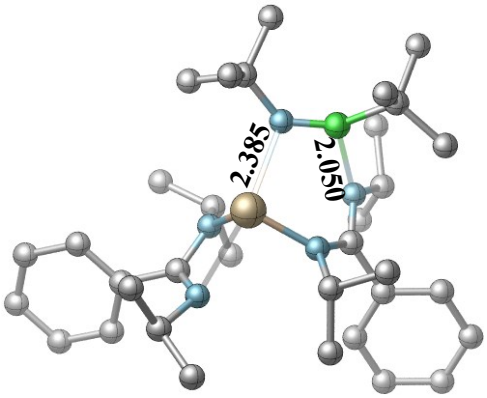
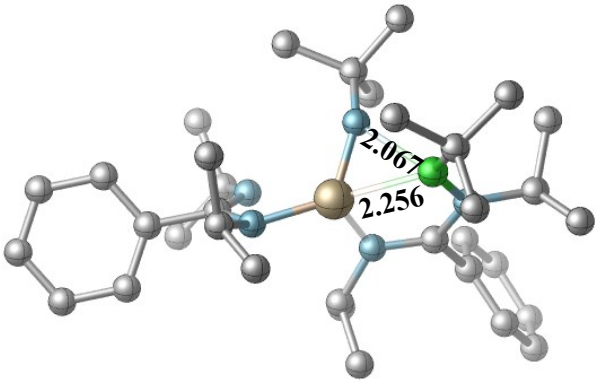


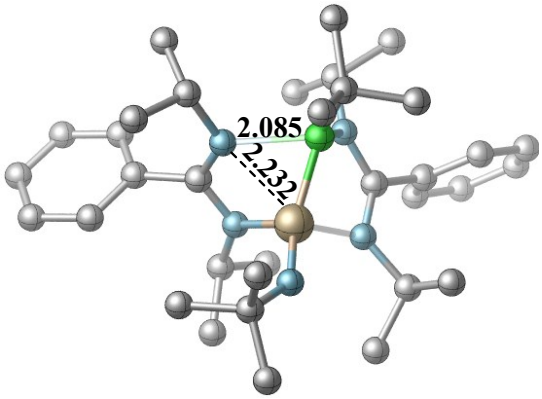
Figure S-17: Optimized geometries of reactants, intermediates and product of the proposed reaction mechanism. Selected bond distances are shown in Å. Color code: green for boron, light blue for nitrogen, brown for silicon and grey for carbon atoms. Hydrogen atoms are not shown for clarity.



2-TS1



2-TS2



2-TS3

Figure S-18: Optimized geometries of the transition states involved in the proposed reaction mechanism. Key bond distances are shown in Å. Color code: green for boron, light blue for nitrogen, brown for silicon and grey for carbon atoms. Hydrogen atoms are not shown for clarity.

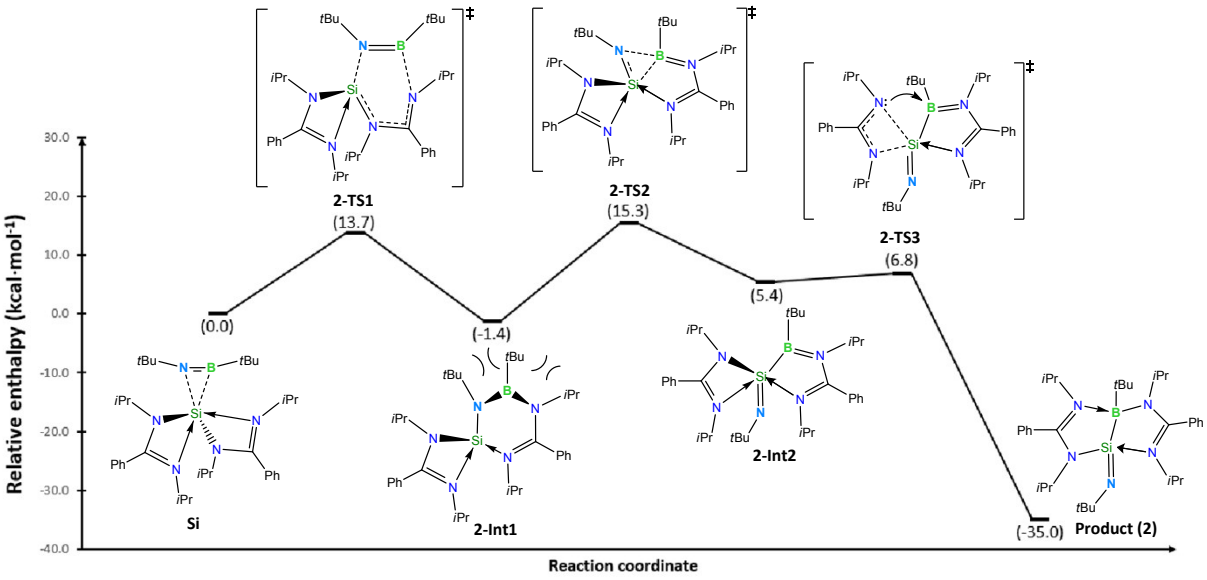


Figure S-19: Energy profile for the proposed reaction mechanism for the formation of **2** calculated at the (SMD:hexane)M08-HX/def2-SVPD//M08-HX/cep-121G* level.

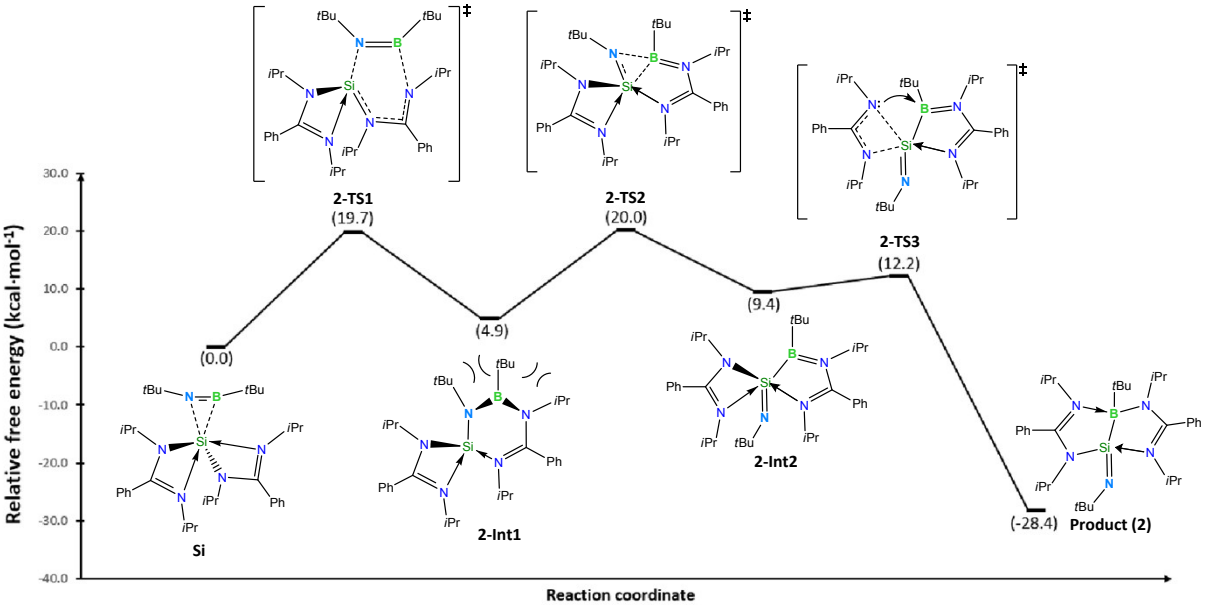


Figure S-20: Energy profile for the proposed reaction mechanism for the formation of **2** calculated at the (SMD:hexane)M08-HX/def2-SVPD//M08-HX/cep-121G* level. Gibbs free energies are given in kcal·mol^{-1}.

Table S1. Cartesian coordinates (xyz) of the optimized geometries of all the compounds involved in the reaction mechanism.

Silylene (Si)

E(scf) = –213.471010942 a.u.

Si	0.023839	-0.125582	-1.565782
N	-1.147110	-0.964999	-0.351163
N	-1.669660	1.068341	-0.944118
C	-2.099168	-0.015004	-0.331076
C	-3.488423	-0.194773	0.214186
C	-3.785697	0.205031	1.526249
C	-4.492185	-0.758077	-0.589923
C	-5.076160	0.019819	2.042099
H	-3.000624	0.654069	2.141667
C	-5.783672	-0.934703	-0.076952
H	-4.251762	-1.066960	-1.610208
C	-6.074843	-0.552264	1.241365
H	-5.300902	0.323010	3.066459
H	-6.561722	-1.375001	-0.703571
H	-7.079893	-0.696843	1.642418
C	-1.040797	-2.165521	0.474795
H	-0.256894	-2.764352	-0.008400
C	-2.550234	2.156536	-1.362894
H	-3.554914	1.764500	-1.612021
C	-0.545885	-1.793708	1.885081
H	0.388295	-1.217060	1.811808
H	-1.296805	-1.172099	2.400826
H	-0.366817	-2.691805	2.496363
C	-2.314947	-3.029467	0.541350
H	-2.737242	-3.188806	-0.461237
H	-2.061565	-4.011084	0.969259
H	-3.093419	-2.581289	1.175348
C	-2.707415	3.194492	-0.234780
H	-1.724139	3.596183	0.055985
H	-3.339233	4.034335	-0.561745
H	-3.167993	2.743001	0.655822
C	-1.943281	2.804032	-2.617231
H	-2.568448	3.635573	-2.973994
H	-0.940481	3.198671	-2.386354
H	-1.829794	2.066251	-3.423273
N	1.143886	0.858005	-0.414861
N	1.708716	-1.235315	-0.722567
C	2.095513	-0.073624	-0.231299
C	3.448790	0.179348	0.373917
C	3.691424	-0.208925	1.700580
C	4.471208	0.778530	-0.378512

Si + Iminoborane (1)

E(scf) = –282.315913680 a.u.

Si	-0.028660	0.143810	0.311387
N	1.211039	-1.165407	0.823867
N	1.518789	-0.273751	-1.143168
C	2.064451	-1.026906	-0.209326
C	3.475209	-1.542474	-0.236024
C	3.762039	-2.784018	-0.824549
C	4.508434	-0.777808	0.328064
C	5.075801	-3.272492	-0.826678
H	2.951204	-3.364491	-1.274379
C	5.822913	-1.262814	0.317100
H	4.272186	0.189143	0.780293
C	6.106044	-2.513108	-0.253004
H	5.294640	-4.242919	-1.276287
H	6.625404	-0.667580	0.757067
H	7.129490	-2.893203	-0.254382
C	1.213574	-2.163118	1.890990
H	0.506676	-1.771674	2.636337
C	2.286311	0.368515	-2.208496
H	3.283104	0.674663	-1.833491
C	0.650331	-3.495905	1.364089
H	-0.340490	-3.330421	0.914497
H	1.316625	-3.910572	0.589117
H	0.559008	-4.239156	2.171070
C	2.569889	-2.364425	2.592709
H	3.022003	-1.399078	2.861843
H	2.415068	-2.943490	3.515464
H	3.286948	-2.916969	1.968928
C	2.476316	-0.593944	-3.396185
H	1.494403	-0.954496	-3.743293
H	2.976274	-0.088033	-4.236033
H	3.079347	-1.467173	-3.109885
C	1.521391	1.626300	-2.652318
H	2.086454	2.184230	-3.413682
H	0.550851	1.338492	-3.091106
H	1.322708	2.287607	-1.795239
N	-1.271228	-0.826538	-0.722226
N	-1.592717	-0.754854	1.430388
C	-2.145104	-1.067499	0.266615
C	-3.565458	-1.530577	0.108912
C	-3.897075	-2.845575	0.470747
C	-4.563230	-0.659426	-0.357728

C	4.945770	0.024166	2.282340
H	2.891675	-0.689009	2.271651
C	5.726877	1.002642	0.200093
H	4.272932	1.079549	-1.410252
C	5.963097	0.631527	1.532819
H	5.128451	-0.270185	3.317625
H	6.520164	1.469952	-0.386585
H	6.940355	0.812334	1.984689
C	2.680482	-2.260859	-1.101462
H	3.558811	-2.199320	-0.431990
C	0.961841	2.131707	0.279495
H	0.230754	2.677882	-0.335609
C	2.221481	3.010975	0.390202
H	1.923431	4.020838	0.709950
H	2.937246	2.625390	1.130046
H	2.736208	3.094039	-0.577581
C	0.335016	1.895410	1.666017
H	1.032907	1.325818	2.303108
H	0.108095	2.848319	2.169517
H	-0.594331	1.315677	1.565030
C	3.149979	-2.026052	-2.550298
H	2.284777	-2.035034	-3.229603
H	3.641766	-1.046039	-2.645681
H	3.861405	-2.803567	-2.868054
C	2.048793	-3.652790	-0.960147
H	2.758203	-4.436546	-1.263676
H	1.743959	-3.844998	0.079137
H	1.157598	-3.730164	-1.603055
C	-5.218572	-3.296881	0.344266
H	-3.112726	-3.508668	0.846292
C	-5.884839	-1.107710	-0.473237
H	-4.294352	0.362030	-0.640647
C	-6.212456	-2.427964	-0.127361
H	-5.471544	-4.323251	0.616867
H	-6.658929	-0.428781	-0.836037
H	-7.242304	-2.777472	-0.223237
C	-2.397464	-0.361841	2.587887
H	-3.288915	-1.013337	2.655632
C	-1.244367	-1.323424	-2.095274
H	-0.537729	-0.657611	-2.616073
C	-2.586794	-1.253075	-2.843248
H	-2.413083	-1.452091	-3.911296
H	-3.308667	-1.996646	-2.476791
H	-3.038785	-0.254221	-2.747728
C	-0.659971	-2.747288	-2.124703
H	-1.323489	-3.437949	-1.576913
H	-0.554175	-3.114776	-3.157265
H	0.327502	-2.756930	-1.639096
C	-2.863725	1.101566	2.439283
H	-1.990378	1.756915	2.287687
H	-3.528309	1.211597	1.567980
H	-3.412330	1.438360	3.332127
C	-1.552284	-0.523885	3.858728
H	-2.103056	-0.180223	4.746191
H	-1.264601	-1.573897	4.013544
H	-0.632634	0.078076	3.769995
C	-1.618885	3.836819	-1.103191
C	-2.703197	4.677067	-0.388416
H	-2.355685	5.700772	-0.184128
H	-3.604869	4.742907	-1.020992
H	-2.993180	4.219219	0.570017
C	-1.265349	4.487949	-2.461384
H	-0.499411	3.903123	-2.994725
H	-2.163108	4.537157	-3.100902
H	-0.881774	5.511126	-2.333010
C	-2.172084	2.416628	-1.355431
H	-1.445522	1.782631	-1.887001
H	-2.411329	1.904921	-0.410137
H	-3.090669	2.480010	-1.967412
C	1.864694	3.769432	1.309944
C	2.540427	5.140763	1.521135
H	1.838490	5.842605	1.994413
H	3.426241	5.040131	2.167485
H	2.855033	5.565024	0.556447
C	2.862507	2.796525	0.639266

H	3.749354	2.654908	1.278531
H	2.374562	1.822658	0.472521
H	3.191227	3.191052	-0.334928
C	1.422180	3.186240	2.670656
H	0.714451	3.869383	3.163078
H	0.922311	2.218877	2.509951
H	2.290012	3.039729	3.333212
B	-0.322451	3.805322	-0.206383
N	0.717547	3.918257	0.473850

2-TS1

E(scf) = –282.293948872 a.u.

ν_{min} = –216.08 cm^{-1}

Si	0.407861	-0.761413	1.071137
N	-0.819256	0.678581	0.982177
N	-2.050944	0.077215	-0.881020
C	-1.603522	1.010572	-0.077402
C	-1.933955	2.464122	-0.332246
C	-0.910266	3.357912	-0.689859
C	-3.258326	2.919255	-0.256138
C	-1.210683	4.693285	-0.977975
H	0.121496	2.999099	-0.720444
C	-3.557534	4.263845	-0.521979
H	-4.053027	2.221525	0.021420
C	-2.535625	5.149753	-0.889437
H	-0.411757	5.381485	-1.260337
H	-4.588002	4.616102	-0.446052
H	-2.769260	6.194299	-1.104641
C	-0.821737	1.444943	2.256746
H	-0.116910	0.878162	2.893394
C	-2.763996	0.345686	-2.146510
H	-3.696169	0.902186	-1.936324
C	-0.296377	2.893532	2.225265
H	0.604237	2.966700	1.602407
H	-1.051364	3.607746	1.868915
H	-0.023826	3.187147	3.251017
C	-2.197569	1.398627	2.942449
H	-2.541331	0.362962	3.074311
H	-2.146925	1.877338	3.932043
H	-2.947839	1.945026	2.347917
C	-1.965126	1.136605	-3.197444
H	-1.100494	0.545688	-3.528033
H	-2.608515	1.310530	-4.072991
H	-1.613083	2.111436	-2.840179
C	-3.121213	-1.012090	-2.769966
H	-3.636836	-0.874368	-3.731244

2-Int1

E(scf) = –282.338079024 a.u.

Si	-0.336522	0.823687	1.052923
N	0.886511	-0.698633	0.983163
N	2.158517	0.130533	-0.738729
C	1.675047	-0.923068	-0.058273
C	2.058532	-2.319805	-0.477175
C	1.070083	-3.190561	-0.964987
C	3.385170	-2.761165	-0.362315
C	1.409584	-4.493104	-1.345237
H	0.033758	-2.846618	-1.010903
C	3.720412	-4.074704	-0.721472
H	4.149870	-2.081371	0.022093
C	2.734727	-4.938672	-1.218344
H	0.638664	-5.165757	-1.725283
H	4.750205	-4.420403	-0.614464
H	2.997050	-5.959474	-1.502993
C	0.787924	-1.592290	2.167617
H	-0.037829	-1.146526	2.746154
C	2.827051	-0.030579	-2.059243
H	3.668438	-0.736407	-1.951919
C	0.425361	-3.072784	1.958067
H	-0.431301	-3.175044	1.281079
H	1.269258	-3.674770	1.592380
H	0.131708	-3.483201	2.936894
C	2.084331	-1.480632	2.989500
H	2.315775	-0.432229	3.226082
H	1.991986	-2.038757	3.933086
H	2.932185	-1.908227	2.427667
C	1.880550	-0.563429	-3.145740
H	1.073770	0.159765	-3.329135
H	2.445707	-0.691558	-4.080804
H	1.435879	-1.530879	-2.888874
C	3.376945	1.320550	-2.540456
H	3.678033	1.233732	-3.593406
H	2.598864	2.101184	-2.480563

H	-2.199551	-1.589959	-2.943580	H	4.248238	1.652163	-1.970161
H	-3.768565	-1.606839	-2.116403	N	-1.477475	0.425553	-0.353994
N	1.461464	-0.459369	-0.435510	N	-2.309115	-1.177795	1.070183
N	2.221025	0.723224	1.298451	C	-2.536515	-0.340751	0.111080
C	2.510770	0.198983	0.133637	C	-3.924574	0.003367	-0.385882
C	3.908177	0.112321	-0.426699	C	-4.698733	-0.890665	-1.141611
C	4.573808	1.248494	-0.912148	C	-4.449706	1.261659	-0.050768
C	4.568710	-1.126920	-0.408815	C	-5.973593	-0.515998	-1.588974
C	5.883238	1.141712	-1.401278	H	-4.296416	-1.878953	-1.381170
H	4.060063	2.213511	-0.906261	C	-5.729427	1.632379	-0.482153
C	5.881404	-1.232303	-0.885106	H	-3.835005	1.947806	0.540800
H	4.038669	-2.005476	-0.029058	C	-6.488845	0.747194	-1.262727
C	6.537474	-0.098624	-1.388584	H	-6.565613	-1.210233	-2.188976
H	6.393171	2.026156	-1.788213	H	-6.131721	2.612605	-0.218137
H	6.390713	-2.197820	-0.868423	H	-7.481706	1.038745	-1.611275
H	7.558147	-0.181329	-1.767302	C	-3.427968	-1.678247	1.873052
C	3.287455	0.969308	2.275240	H	-4.368599	-1.714242	1.293818
H	4.229501	1.227521	1.757799	C	-1.358050	0.730507	-1.791921
C	1.278871	-0.621897	-1.886288	H	-0.365743	1.206374	-1.887791
H	0.277089	-1.073375	-1.987845	C	-2.400608	1.699455	-2.406125
C	2.299997	-1.535469	-2.602124	H	-1.997113	2.101223	-3.349658
H	1.890006	-1.830136	-3.580686	H	-3.346513	1.190059	-2.642170
H	3.251764	-1.015605	-2.784651	H	-2.631569	2.544599	-1.747062
H	2.511853	-2.448914	-2.033426	C	-1.377452	-0.574204	-2.610831
C	1.300739	0.761274	-2.563315	H	-2.370153	-1.045374	-2.541237
H	2.288998	1.228108	-2.426918	H	-1.171855	-0.388442	-3.676886
H	1.120583	0.681585	-3.646409	H	-0.633348	-1.283089	-2.228644
H	0.538406	1.420559	-2.129873	C	-3.626916	-0.719877	3.063089
C	3.520800	-0.310805	3.101211	H	-2.681114	-0.618106	3.617045
H	2.589095	-0.603990	3.607409	H	-3.913141	0.282424	2.710334
H	3.823446	-1.145223	2.450001	H	-4.406463	-1.090902	3.746436
H	4.305733	-0.154834	3.857054	C	-3.102728	-3.091248	2.375482
C	2.894450	2.131682	3.195513	H	-3.941137	-3.502769	2.957140
H	3.675321	2.311486	3.949159	H	-2.890329	-3.772823	1.538171
H	2.738037	3.059113	2.626512	H	-2.213634	-3.062281	3.023396
H	1.957006	1.892781	3.721704	C	3.652606	1.936065	0.597101
C	-3.741637	-1.907234	0.555782	C	4.517352	3.051709	-0.081129
C	-4.684010	-2.909408	-0.163983	H	4.008338	3.596910	-0.885681
H	-4.185222	-3.841574	-0.458347	H	4.834430	3.798804	0.664500
H	-5.510283	-3.173410	0.518114	H	5.440542	2.630428	-0.510742
H	-5.146893	-2.478112	-1.063750	C	3.421346	2.342333	2.080581
C	-3.548812	-2.420191	2.010245	H	2.713756	1.665840	2.586533
H	-2.776823	-1.849196	2.550797	H	4.377498	2.311410	2.630547
H	-4.497465	-2.339079	2.567980	H	3.026444	3.360713	2.177644
H	-3.245917	-3.477274	2.025155	C	4.531903	0.658116	0.678302
C	-4.489377	-0.559858	0.634531	H	4.033442	-0.131559	1.264650
H	-3.920983	0.186623	1.207231	H	4.781181	0.245989	-0.312739

H	-4.693376	-0.148105	-0.366023
H	-5.460384	-0.706156	1.137875
C	-0.573330	-3.711645	0.221010
C	-1.616454	-4.722975	-0.294587
H	-1.939751	-4.460337	-1.314489
H	-1.192661	-5.739530	-0.312743
H	-2.499943	-4.744750	0.360315
C	-0.288187	-4.019609	1.710013
H	-0.045632	-5.089184	1.821461
H	0.555578	-3.427712	2.086324
H	-1.159455	-3.794622	2.340116
C	0.735587	-3.913702	-0.566759
H	0.566357	-3.735250	-1.640421
H	1.494112	-3.196500	-0.214985
H	1.128120	-4.934210	-0.431901
B	-2.235052	-1.780933	-0.034918
N	-1.023220	-2.328598	-0.016072

2-TS2

E(scf) = –282.283050416 a.u.

ν_{min} = –159.73 cm^{-1}

Si	-0.084517	0.849733	0.403455
N	0.701232	-0.818124	0.569786
N	2.718624	0.351825	0.194272
C	2.022826	-0.804685	0.384860
C	2.754002	-2.121600	0.307894
C	2.684626	-2.842826	-0.895509
C	3.512509	-2.618811	1.378550
C	3.348988	-4.069641	-1.017452
H	2.095383	-2.440047	-1.723559
C	4.163599	-3.854590	1.261231
H	3.595107	-2.035932	2.299224
C	4.079196	-4.582421	0.065020
H	3.290206	-4.628330	-1.953299
H	4.741872	-4.244830	2.100768
H	4.588720	-5.543589	-0.025587
C	-0.019518	-1.935004	1.245417
H	-1.060582	-1.594132	1.245411
C	4.165979	0.231141	-0.157508
H	4.389185	-0.834872	-0.262413
C	-0.019019	-3.294012	0.522850
H	-0.111014	-3.153868	-0.563490
H	0.878452	-3.893645	0.729574
H	-0.892227	-3.870608	0.866078
C	0.401407	-2.058016	2.719817
H	0.363436	-1.074550	3.211447
H	5.483275	0.892593	1.184338
C	0.538043	3.457688	0.550224
C	1.594439	4.420491	-0.019233
H	1.839123	4.148856	-1.059436
H	1.189044	5.443908	-0.024152
H	2.521936	4.437985	0.563545
C	0.276042	3.790800	2.041590
H	0.198204	4.884373	2.156864
H	-0.661899	3.338466	2.388815
H	1.072786	3.426460	2.700138
C	-0.771622	3.743922	-0.215072
H	-0.625219	3.598434	-1.296597
H	-1.574648	3.067795	0.118393
H	-1.100804	4.779980	-0.037487
B	2.166483	1.507618	-0.008039
N	0.894149	2.028051	0.279800

2-Int2

E(scf) = -282.299643189 a.u.

B	1.241823	1.775247	0.133688
Si	-0.086929	0.424359	0.874021
N	2.331522	1.006525	-0.468346
N	-0.474701	0.238860	2.433252
N	1.366614	-0.863012	0.555976
N	-1.261853	0.362243	-0.510831
N	-2.142457	-1.725938	0.012687
C	-4.012767	-0.876234	-2.411033
H	-3.443194	-1.737658	-2.770693
C	-0.354117	3.745361	0.461070
H	-0.854179	3.685746	-0.518688
H	-0.458624	4.781222	0.827255
H	-0.895935	3.085605	1.158864
C	1.139540	3.355206	0.362967
C	1.737838	3.461005	1.800225
H	1.597868	4.487243	2.181198
H	2.818308	3.241816	1.813959
H	1.238488	2.767058	2.496290
C	1.842329	4.379918	-0.550801
H	1.470129	4.331760	-1.588050
H	2.936325	4.262748	-0.571001
H	1.636008	5.399342	-0.182802
C	-3.562934	-0.178376	-1.278351
C	-4.299428	0.917820	-0.803500
H	-3.940213	1.455324	0.077120
C	-5.467244	1.320793	-1.464121

H	-0.285564	-2.738126	3.245929	H	-6.037684	2.172546	-1.088024
H	1.415525	-2.467418	2.823534	C	-5.898125	0.638810	-2.612263
C	4.458278	0.865164	-1.524185	H	-6.801292	0.961740	-3.134044
H	4.181290	1.924285	-1.554725	C	-5.170623	-0.463900	-3.084027
H	5.532260	0.782928	-1.748781	H	-5.505596	-1.002560	-3.972782
H	3.899400	0.345230	-2.315934	C	-0.848683	0.981452	-1.794367
C	5.079963	0.753913	0.959206	H	0.002440	1.643468	-1.545014
H	6.123791	0.496338	0.726809	C	-1.859945	1.913846	-2.499043
H	5.020661	1.841084	1.073119	H	-2.628500	1.367640	-3.062591
H	4.816393	0.293219	1.923121	H	-1.311396	2.548332	-3.213335
N	-1.978867	-0.815150	-0.858057	H	-2.368104	2.565937	-1.776369
N	-1.806178	0.668848	0.881024	C	-0.321702	-0.087765	-2.768910
C	-2.587313	-0.136904	0.046202	H	-1.136404	-0.769897	-3.061433
C	-4.066144	-0.192982	0.342913	H	0.463368	-0.694101	-2.288536
C	-4.523065	-0.887899	1.475498	H	0.084484	0.367765	-3.685658
C	-4.987141	0.421642	-0.516340	C	-2.293727	-0.595073	-0.567228
C	-5.895292	-1.004847	1.721888	C	-2.877605	-3.941655	-0.693673
H	-3.793987	-1.345838	2.150249	H	-3.677367	-4.693967	-0.623500
C	-6.363447	0.312423	-0.265006	H	-1.949433	-4.387181	-0.304849
H	-4.622638	0.983810	-1.380187	H	-2.718521	-3.701541	-1.755667
C	-6.818436	-0.408841	0.846907	C	-3.241435	-2.685330	0.118919
H	-6.247141	-1.558851	2.594414	H	-4.194364	-2.277971	-0.265058
H	-7.077821	0.789756	-0.938541	C	-3.433118	-3.055606	1.599517
H	-7.889394	-0.500684	1.037743	H	-3.730173	-2.178291	2.190795
C	-2.445035	1.783880	1.622017	H	-2.491584	-3.443606	2.017081
H	-3.444427	1.443656	1.931477	H	-4.210353	-3.827389	1.707951
C	-2.562086	-1.858590	-1.705294	C	-1.764750	-0.647738	4.295019
H	-1.696590	-2.484837	-1.991236	H	-2.544023	-0.445901	5.049650
C	-3.116186	-1.280830	-3.021416	H	-0.827567	-0.901185	4.815358
H	-3.422124	-2.098372	-3.691832	H	-2.066748	-1.523829	3.700368
H	-3.996204	-0.648010	-2.834182	C	-1.525978	0.561976	3.359328
H	-2.354216	-0.676779	-3.533076	C	-2.857349	0.906019	2.649396
C	-3.581688	-2.806426	-1.040327	H	-3.165868	0.066902	2.005361
H	-4.579527	-2.356436	-0.941234	H	-2.718320	1.795144	2.009070
H	-3.682092	-3.714301	-1.654251	H	-3.669822	1.119758	3.364702
H	-3.240968	-3.108756	-0.037113	C	-1.119173	1.775211	4.232751
C	-2.606711	3.013801	0.710053	H	-1.875224	2.003477	5.003616
H	-1.627966	3.343697	0.328078	H	-0.988123	2.669362	3.600112
H	-3.229703	2.762203	-0.163096	H	-0.158799	1.568202	4.729851
H	-3.080328	3.849516	1.247050	C	3.550678	0.785481	-2.716231
C	-1.655563	2.111881	2.899086	H	2.652358	0.246520	-3.052997
H	-2.193587	2.869689	3.487120	H	4.361338	0.059882	-2.571178
H	-1.529319	1.210481	3.517163	H	3.857417	1.467463	-3.522673
H	-0.654113	2.504624	2.669107	C	3.264494	1.625503	-1.456338
C	2.471662	3.193774	0.693561	H	2.696761	2.497690	-1.804263
C	3.584836	3.876484	-0.140087	C	4.567069	2.151353	-0.826592
H	3.309086	3.910010	-1.207127	H	5.013810	2.911656	-1.485065

H	3.707696	4.919848	0.198322
H	4.572252	3.399898	-0.059375
C	1.238523	4.119806	0.551505
H	0.405045	3.759980	1.172236
H	1.500241	5.139629	0.885312
H	0.880783	4.157024	-0.486333
C	2.849377	3.218327	2.198890
H	1.991818	2.885821	2.805106
H	3.699514	2.569299	2.453831
H	3.110373	4.245836	2.508544
C	0.334402	1.435452	-2.448406
C	1.333984	2.387453	-3.132548
H	2.359449	2.153556	-2.809168
H	1.287368	2.306393	-4.230987
H	1.117702	3.428459	-2.845345
C	-1.093105	1.813932	-2.905407
H	-1.234540	1.647747	-3.987758
H	-1.834502	1.215189	-2.356401
H	-1.278605	2.876610	-2.684239
C	0.660957	-0.021337	-2.852827
H	1.694768	-0.258158	-2.547877
H	-0.019896	-0.715513	-2.335285
H	0.580053	-0.177148	-3.942377
B	2.005007	1.694204	0.296567
N	0.401939	1.639411	-1.007523
H	5.306415	1.349925	-0.696672
H	4.375726	2.617434	0.150548
C	2.355104	-0.342978	-0.119613
C	3.554858	-1.172380	-0.481438
C	3.418910	-2.181319	-1.450915
H	2.445854	-2.341872	-1.923337
C	4.525168	-2.956599	-1.810027
H	4.421786	-3.731088	-2.571848
C	5.765129	-2.740988	-1.185695
H	6.628504	-3.347735	-1.464747
C	5.890798	-1.758971	-0.194720
H	6.847725	-1.605084	0.307013
C	4.783665	-0.972562	0.159560
H	4.870807	-0.211495	0.938219
C	2.207884	-1.740459	2.680737
H	1.510219	-1.074480	3.207766
H	3.172479	-1.224198	2.550268
H	2.381698	-2.646187	3.280325
C	1.593642	-2.126395	1.321883
H	2.311009	-2.744077	0.762054
C	0.305931	-2.924498	1.520965
H	-0.422162	-2.323606	2.080633
H	0.546798	-3.837109	2.087448
H	-0.150536	-3.200270	0.563371

2-TS3

E(scf) = –282.294964970 a.u.

ν_{min} = –264.15 cm^{-1}

B	-0.469111	0.128862	1.524967
Si	0.226283	1.200779	0.060035
N	-1.443057	-0.769832	0.792053
N	0.744916	2.708235	-0.226033
N	-1.577477	0.943244	-0.768853
N	1.489080	-0.447467	1.099371
N	0.992198	-0.132601	-1.037928
C	2.850967	-3.001623	-0.655459
H	1.970038	-3.501664	-0.246742
C	0.264050	1.609970	3.525345
H	1.334281	1.358711	3.472517
H	0.047291	1.917250	4.563885
H	0.117930	2.482428	2.869109
C	-0.675784	0.462242	3.089544
C	-2.110412	1.063017	3.117943
H	-2.328144	1.492470	4.111009
H	-2.872334	0.294924	2.909157

Product (2)

E(scf) = –282.363061595 a.u.

B	-0.027923	-0.107084	1.392659
Si	0.019064	1.398249	0.021055
N	-1.267104	-0.891383	0.722416
N	0.278771	2.991021	-0.235332
N	-1.678563	0.966960	-0.591296
N	1.298150	-0.899361	1.035640
N	1.091216	0.142370	-1.015533
C	2.983236	-2.682598	-1.237144
H	2.072932	-3.283599	-1.176735
C	0.820035	1.003242	3.635810
H	1.640706	0.327530	3.922877
H	0.490035	1.513123	4.558573
H	1.237779	1.772138	2.966173
C	-0.366279	0.273220	2.965839
C	-1.529906	1.296689	2.900297
H	-1.853512	1.590398	3.915055
H	-2.410143	0.871155	2.385966
H	-1.238090	2.215128	2.361651

H	-2.220420	1.869069	2.371601	C	-0.855423	-0.856901	3.904997
C	-0.660017	-0.704600	4.105601	H	-0.134584	-1.680296	4.042683
H	0.271242	-1.292577	4.092688	H	-1.794420	-1.301267	3.539128
H	-1.490634	-1.405740	3.919667	H	-1.065031	-0.448996	4.910020
H	-0.791100	-0.318804	5.131709	C	2.990989	-1.371070	-0.741383
C	2.928932	-1.601291	-0.638733	C	4.156674	-0.592770	-0.847426
C	4.054233	-0.957726	-1.181788	H	4.142261	0.437315	-0.480090
H	4.091712	0.135130	-1.188483	C	5.318004	-1.137646	-1.407230
C	5.113275	-1.713605	-1.699606	H	6.223104	-0.531466	-1.475259
H	5.990796	-1.208241	-2.106998	C	5.313247	-2.456537	-1.887709
C	5.040409	-3.114709	-1.702484	H	6.216570	-2.880294	-2.330534
H	5.863052	-3.704222	-2.111698	C	4.144352	-3.225038	-1.807542
C	3.906181	-3.756727	-1.186689	H	4.132372	-4.246892	-2.191197
H	3.840608	-4.846316	-1.196662	C	2.080202	-1.615203	2.072128
C	2.333088	-0.849920	2.240437	H	1.465951	-1.490038	2.969142
H	1.807115	-0.452302	3.114517	C	3.450571	-0.973412	2.370114
C	3.718558	-0.180657	2.237364	H	4.217281	-1.293109	1.651792
H	4.337083	-0.515691	1.392530	H	3.789001	-1.273038	3.373633
H	4.255638	-0.426480	3.166089	H	3.383073	0.124358	2.345314
H	3.613161	0.913225	2.180286	C	2.222052	-3.137285	1.857754
C	2.426976	-2.373275	2.465867	H	3.026770	-3.383488	1.153606
H	3.184134	-2.845425	1.826313	H	1.286575	-3.583448	1.488822
H	1.453343	-2.852924	2.271006	H	2.468370	-3.612528	2.819323
H	2.701409	-2.576489	3.512505	C	1.742708	-0.704658	-0.215242
C	1.778753	-0.749777	-0.157250	C	0.147204	-0.569233	-3.153613
C	-0.273120	-0.898409	-3.040097	H	0.284864	-0.609284	-4.244441
H	-0.140547	-1.218880	-4.084296	H	-0.791151	-0.038402	-2.937036
H	-1.058221	-0.132980	-3.011655	H	0.053728	-1.599995	-2.772683
H	-0.610896	-1.763871	-2.449908	C	1.328896	0.148240	-2.473929
C	1.061072	-0.366081	-2.486782	H	2.242530	-0.422675	-2.696766
H	1.806438	-1.159688	-2.653449	C	1.516914	1.569798	-3.019763
C	1.524866	0.897583	-3.233771	H	2.415375	2.036019	-2.590138
H	2.610276	1.034023	-3.120943	H	0.667483	2.217132	-2.768286
H	1.034763	1.791929	-2.824441	H	1.633915	1.530624	-4.113283
H	1.299474	0.817629	-4.308078	C	1.711483	4.849328	-0.902336
C	1.777807	4.741929	-1.049175	H	2.540999	5.517751	-0.614755
H	2.651039	5.414007	-0.997732	H	0.815968	5.460249	-1.091970
H	0.875754	5.312685	-0.780277	H	1.978432	4.342068	-1.843246
H	1.661029	4.394760	-2.089298	C	1.399502	3.803860	0.194873
C	1.921974	3.522745	-0.107795	C	2.689888	2.978294	0.447549
C	3.209187	2.755199	-0.502837	H	3.002013	2.484304	-0.487455
H	3.146672	2.429273	-1.552019	H	2.504678	2.189859	1.201283
H	3.310382	1.860083	0.135043	H	3.526418	3.601463	0.806461
H	4.116912	3.370813	-0.381362	C	1.039034	4.565831	1.493507
C	2.113459	4.036976	1.340299	H	1.846407	5.245450	1.817163
H	2.967043	4.731407	1.426100	H	0.831577	3.854743	2.309326
H	2.289332	3.183743	2.017037	H	0.125665	5.156850	1.326639

H	1.201014	4.552616	1.677383
C	-1.171292	-3.109841	0.015204
H	-0.172968	-2.807698	-0.333615
H	-1.867221	-3.052625	-0.836192
H	-1.134421	-4.157965	0.348103
C	-1.629890	-2.192065	1.159997
H	-0.917301	-2.328074	1.988426
C	-3.019037	-2.612080	1.681121
H	-2.919212	-3.568941	2.215887
H	-3.745478	-2.757369	0.869363
H	-3.428288	-1.871811	2.383788
C	-2.103528	-0.133312	-0.233782
C	-3.485261	-0.600090	-0.617686
C	-3.727098	-1.320530	-1.796360
H	-2.899121	-1.557631	-2.467457
C	-5.030664	-1.733086	-2.108289
H	-5.213698	-2.304195	-3.020337
C	-6.095272	-1.406074	-1.256931
H	-7.109539	-1.725664	-1.503440
C	-5.857475	-0.658604	-0.093576
H	-6.685076	-0.391306	0.565929
C	-4.554538	-0.259237	0.226843
H	-4.355502	0.309905	1.138647
C	-2.882348	2.975867	-0.465471
H	-2.002080	3.441336	0.004731
H	-3.498705	2.505913	0.317055
H	-3.481351	3.757398	-0.955926
C	-2.406085	1.930469	-1.493136
H	-3.281041	1.417682	-1.927104
C	-1.612337	2.625146	-2.609074
H	-0.723703	3.109254	-2.178303
H	-2.247448	3.390034	-3.079698
H	-1.294293	1.924648	-3.394320
C	-0.887571	-3.165594	-0.204554
H	0.084953	-2.790190	-0.547739
H	-1.600264	-3.099241	-1.039866
H	-0.784245	-4.227892	0.066871
C	-1.381063	-2.343286	0.999373
H	-0.667451	-2.495346	1.824544
C	-2.744588	-2.879630	1.485848
H	-2.573136	-3.828654	2.016159
H	-3.436766	-3.081609	0.656671
H	-3.235795	-2.185918	2.181692
C	-2.053011	-0.231677	-0.132177
C	-3.382953	-0.793717	-0.561588
C	-3.518451	-1.442941	-1.796838
H	-2.648558	-1.543501	-2.451301
C	-4.765509	-1.954682	-2.182901
H	-4.867961	-2.471171	-3.139035
C	-5.879169	-1.793652	-1.346323
H	-6.850150	-2.190587	-1.648405
C	-5.749528	-1.109150	-0.127983
H	-6.618810	-0.967608	0.516660
C	-4.502373	-0.608102	0.263935
H	-4.387364	-0.080208	1.214727
C	-3.130742	2.901338	-0.126324
H	-2.265636	3.474724	0.237849
H	-3.592365	2.374514	0.724193
H	-3.872840	3.594883	-0.549565
C	-2.659119	1.902449	-1.197944
H	-3.521575	1.309461	-1.537792
C	-2.069582	2.638408	-2.409064
H	-1.213623	3.248566	-2.090000
H	-2.840487	3.293088	-2.842217
H	-1.746755	1.935048	-3.191568

Iminoborane (1)

E(scf) = –68.8314197092 a.u.

C	0.000000	0.000000	-2.145787
C	-1.261217	0.728164	-2.667306
H	-1.293779	1.774290	-2.328579
H	-1.262132	0.728692	-3.770198
H	-2.183470	0.233300	-2.328579
C	1.261217	0.728164	-2.667306
H	2.183470	0.233300	-2.328579
H	1.262132	0.728692	-3.770198
H	1.293779	1.774290	-2.328579
C	0.000000	-1.456328	-2.667306

H	0.889691	-2.007590	-2.328579
H	-0.889691	-2.007590	-2.328579
H	0.000000	-1.457384	-3.770198
C	0.000000	0.000000	2.100915
C	0.000000	1.456482	2.614127
H	-0.891588	1.988884	2.252783
H	0.000000	1.477220	3.714677
H	0.891588	1.988884	2.252783
C	1.261350	-0.728241	2.614127
H	1.279310	-0.738610	3.714677
H	1.276630	-1.766580	2.252783
H	2.168219	-0.222304	2.252783
C	-1.261350	-0.728241	2.614127
H	-2.168219	-0.222304	2.252783
H	-1.276630	-1.766580	2.252783
H	-1.279310	-0.738610	3.714677
B	0.000000	0.000000	-0.572717
N	0.000000	0.000000	0.673055

Formation of 5. Geometry optimizations were performed in gas phase using the Gaussian09 computational package[8] without any symmetry restriction. We chose the DFT formalism for our calculations carried out with the PBE0 hybrid density-functional which mixes 25% of HF exchange in its formulation.[28] Grimme's D3 method[29] for incorporating dispersion effects was explicitly included in the geometry optimizations. The electronic configurations of hydrogen, carbon, nitrogen, and boron atoms were described with Pople's double-ζ 6-31G* basis set containing one polarization function.[30, 31] Later, harmonic frequency calculations were performed for two reasons: 1) to verify the nature of the stationary points on the potential energy surface (reaction intermediates and products must have zero negative eigenvalues in the Hessian and transition states one and only one negative eigenvalue which corresponds to the reaction coordinate); and 2) for incorporating the zero–point energy as well as thermal corrections to our reported energy values at 298.15 K and 1354 atm. Single-point calculations on the PBE0-optimized geometries were performed using the M06 functional[30] with the same basis set for all the atoms. Moreover, in these single-point calculations, the solvent effect was also added by utilizing the Truhlar and coworkers' SMD solvation model[27] using *n*-hexane as the solvent of reaction.

In this part, we discuss in further detail a proposed reaction mechanism when PipCCPip (**Pip**) and iminoborane **3** react, producing iminoketene **5**. In the following, **Figure S-19** and **Figure S-20** show the energy profile in the enthalpy and Gibbs free energy scales, respectively. The reaction starts when an alkyne carbon atom attacks at the boron atom with an energy barrier of 16.9 kcal·mol^{-1} (through transition state **5-TS1**). Because of a partial stabilization of the generated carbocation by donation of the nearby piperidine nitrogen (**Figure S-23**), this produces intermediate **5-Int1** (stepwise cycloaddition) which is 11.5 kcal·mol^{-1} higher in energy than the reactants. Then, the formation of the N–C bond occurs in the second transition state, **5-TS2** (energy barrier = 12.9 kcal·mol^{-1} with respect to **5-Int1**) leading to the product of cycloaddition, **5-Int2**, which is an exergonic reaction (–3.2 kcal·mol^{-1} in total, from reactants). In the third step, the cleavage of the single N-B bond takes place with an energy barrier of 10.7 kcal·mol^{-1} (**5-TS3**) to obtain intermediate **5-Int3** for an endergonic step of 0.1 kcal·mol^{-1}, followed by a rotation of the central C-C bond 1.2 kcal·mol^{-1} uphill (intermediate **5-Int4**). As suggested by one of our reviewers, we tried to locate a transition state connecting from **5-Int3** to **5-Int4**. However, despite of many attempts (like performing a

relaxed scan varying the appropriate dihedral angle by steps of 20° from one minimum to the other) we were not able to catch a transition state or even just provide a rough estimation of the energy barrier necessary for this process because some frequency calculations tests over some calculated points only deliver positive eigenvalues, even when the calculations were constrained to a certain dihedral value. We also looked for other reaction steps that could help to understand the rotation as a step-wise mechanism and other variants but, unfortunately, it was not possible to find a plausible route despite our best efforts. Even so, because of these rotamers are only 1.2 (1.8 in enthalpy scale) kcal·mol^{-1} of energy difference, we believe this rotational barrier would not change the kinetic view of our energy profile, which is governed by the cycloaddition of the alkyne to the iminoborane **3**.

From this last step, intermediate **5-Int5** can be reached through the formation of a new N-B bond via **5-TS4** (energy barrier = 3.1 kcal·mol^{-1} with respect to **5-Int4**), which is more stable than **5-Int2** by −1.6 kcal·mol^{-1}. Finally, there is a ligand transfer of the piperidine that was attached to boron in the previous step to be completely exchanged to boron. This is achieved with only 6.2 kcal·mol^{-1} (**5-TS5**) and the reaction reaches the product **5** which is −16.5 kcal·mol^{-1} lower in energy. In summary, this is an exergonic reaction with a total reaction energy of ΔG_R = −21.3 kcal·mol^{-1}.

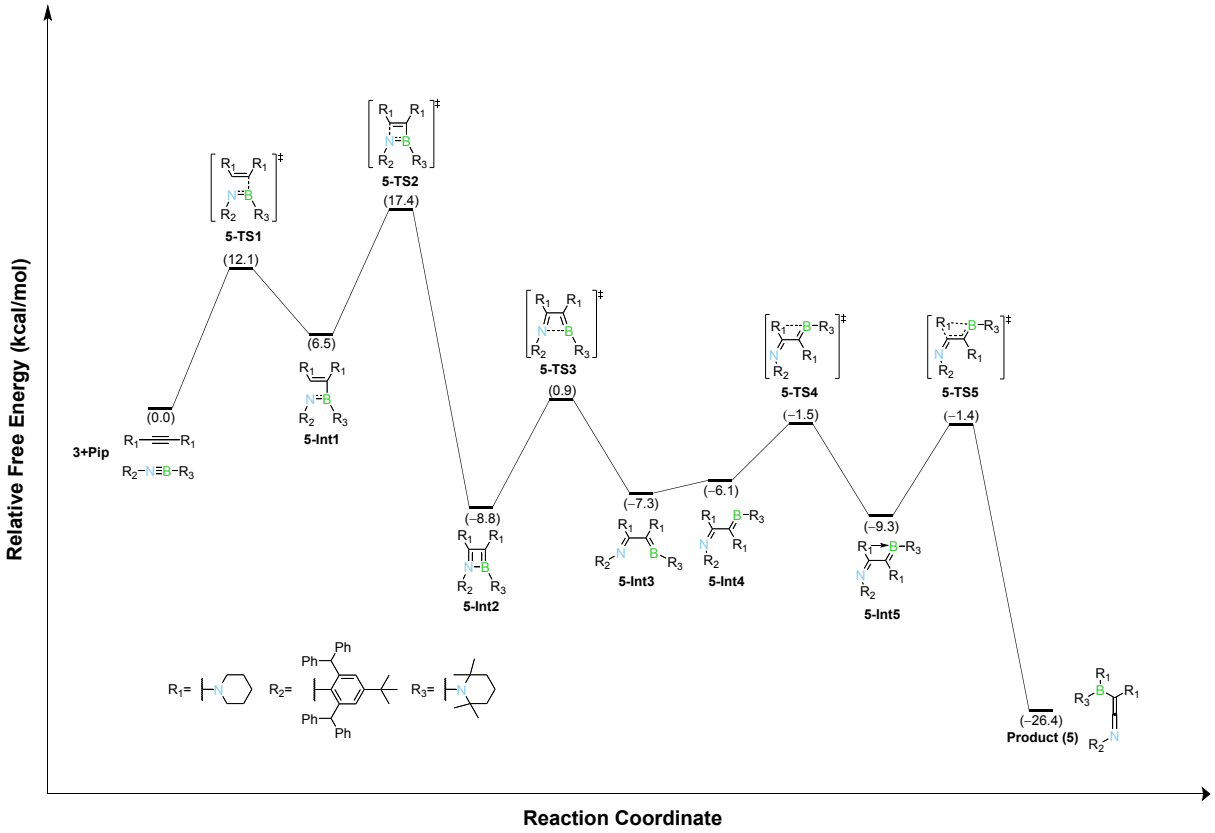


Figure S-21: Energy profile for the proposed reaction mechanism between PipCCPip (**Pip**) and iminoborane **3** calculated at (SMD:n-hexane)M06/6–31G(d)//PBE0/6–31G(d) level. Enthalpies are given in kcal·mol^{-1}.

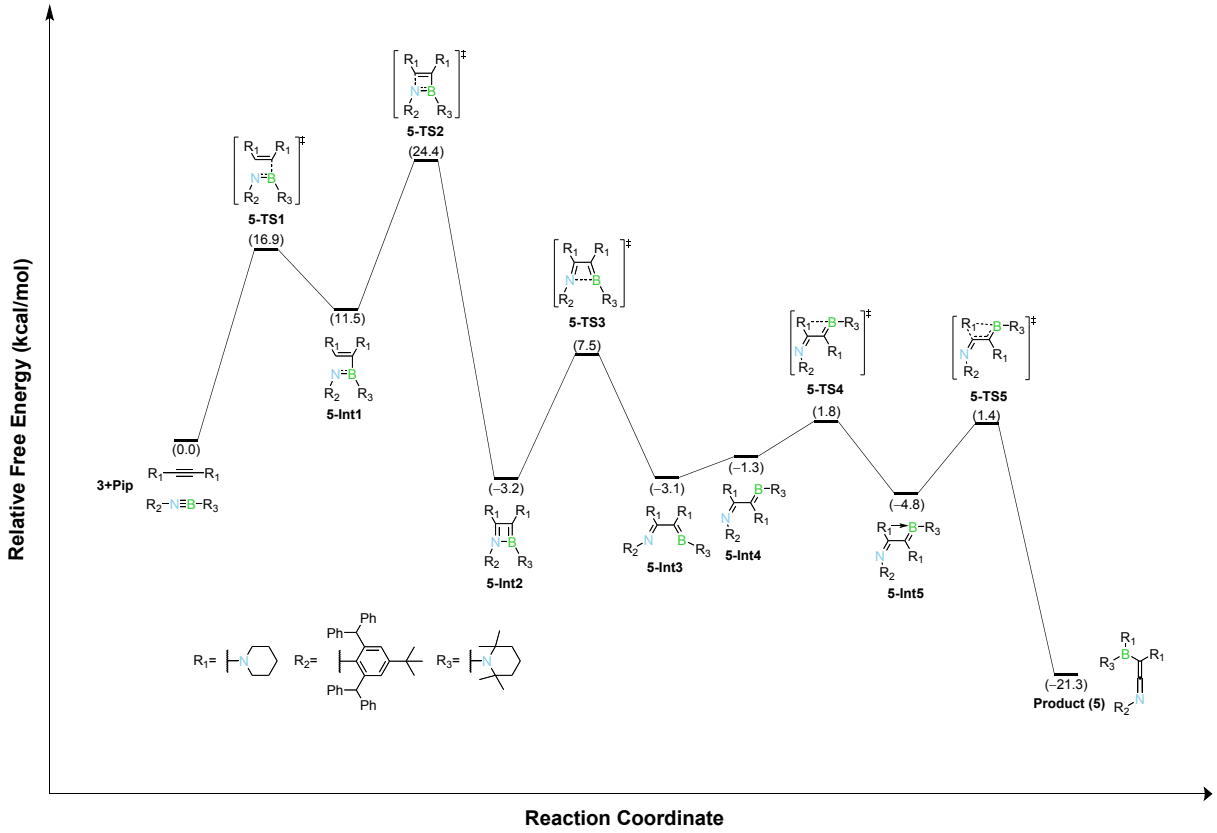


Figure S-22: Energy profile for the proposed reaction mechanism between **Pip** and iminoborane **3** calculated at (SMD:n-hexane)M06/6–31G(d)//PBE0/6–31G(d) level. Gibbs free energies are given in kcal·mol^{-1}.

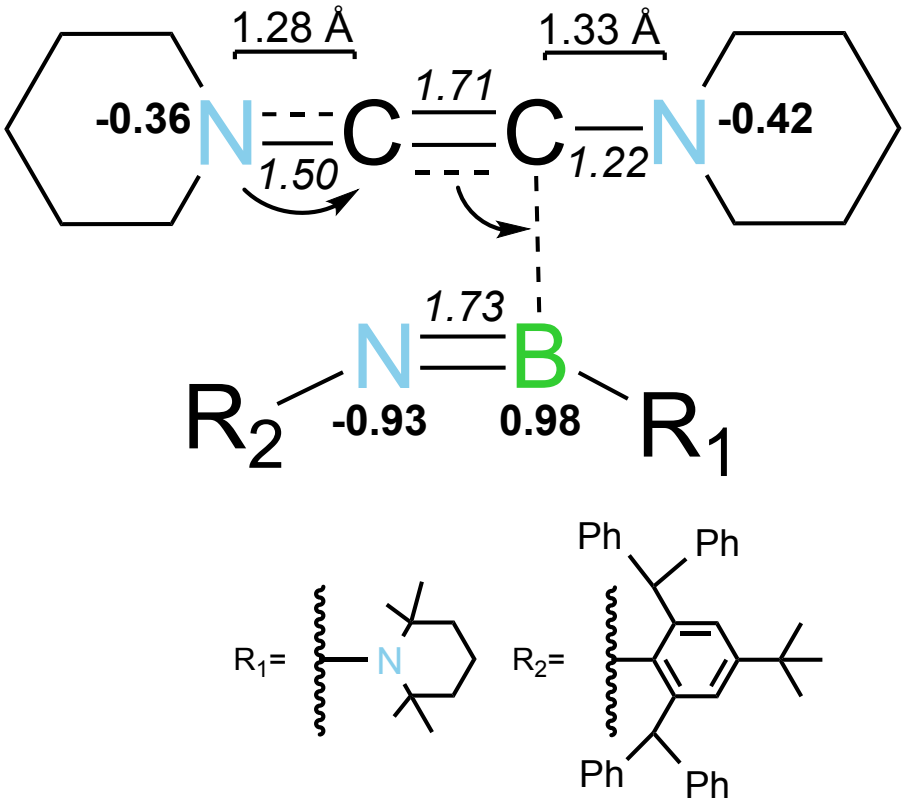


Figure S-23: NBO analysis of transition state **5-TS1** showing natural charges (in bold) and Mayer bond indices (in italics) calculated at the same level of theory.

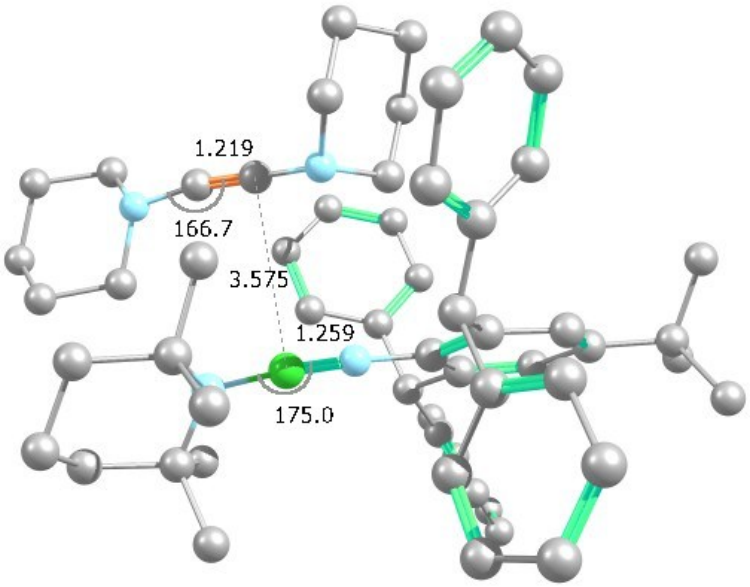


Figure S-24: Optimized structure of adduct (PipCCPip–-iminoborane) **3+Pip**. Distances are given in Å and angles in º. Hydrogens were omitted for clarity.

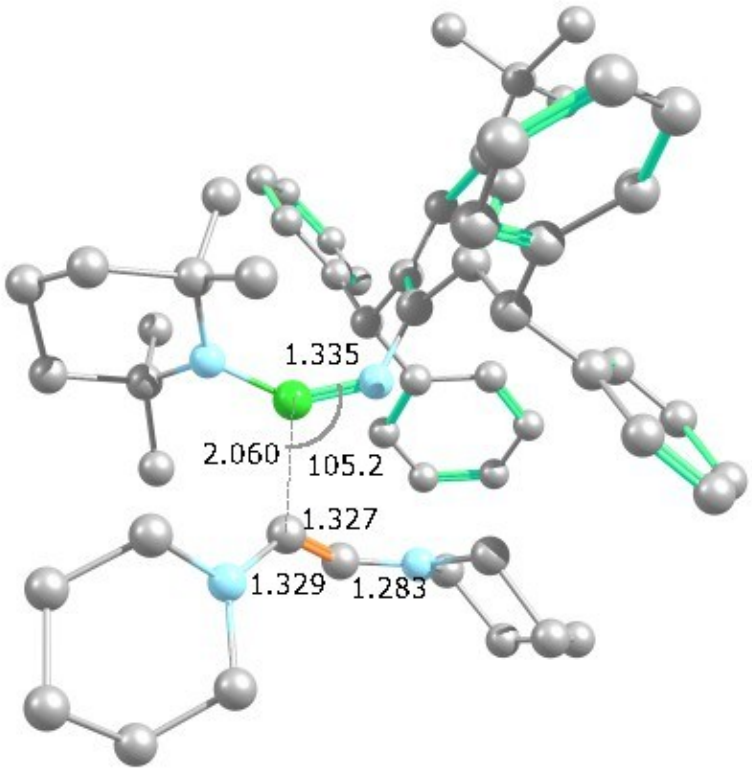


Figure S-25: Optimized structure of transition state **5-TS1**. Distances are given in Å and º in º. Hydrogens are omitted for clarity.

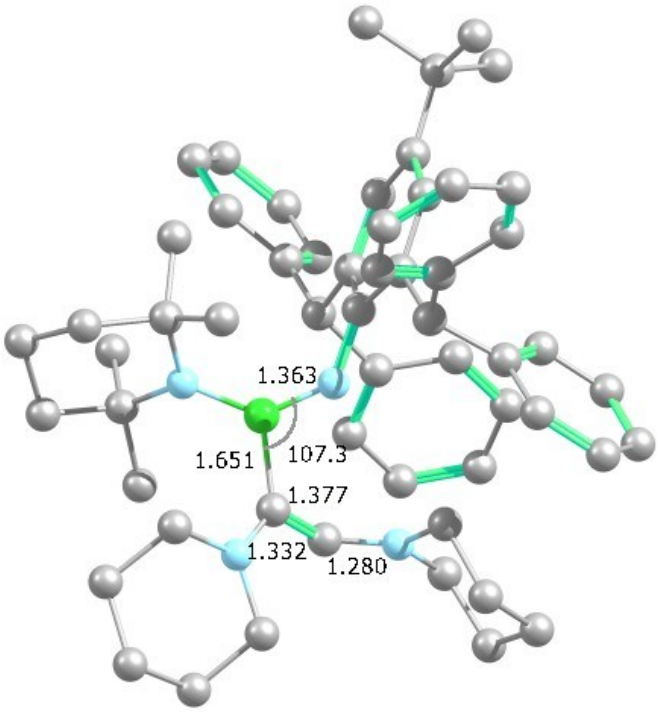


Figure S-26: Optimized structure of intermediate **5-Int1**. Distances are given in Å and angles in º. Hydrogens are omitted for clarity.

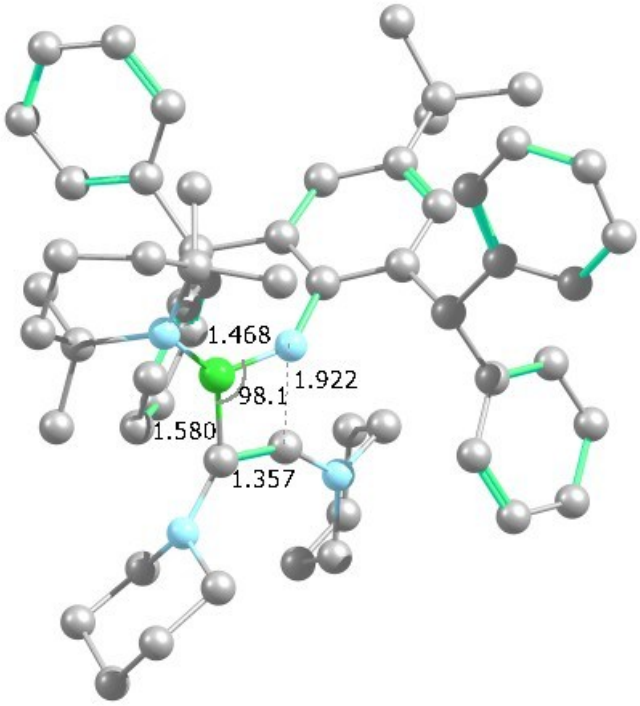


Figure S-27: Optimized structure of transition state **5-TS2**. Distances are given in Å and angles in º. Hydrogens were omitted for clarity.

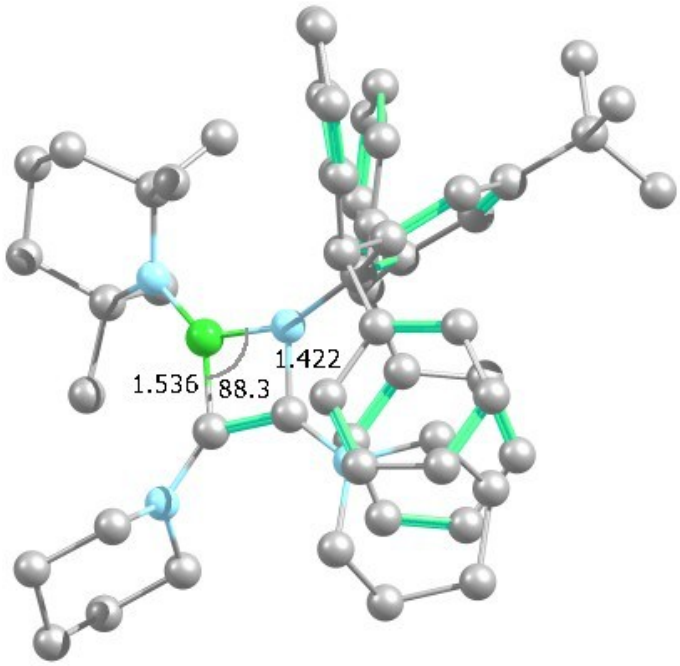


Figure S-28: Optimized structure of intermediate **5-Int2**. Distances are given in Å and angles in º. Hydrogens were omitted for clarity.

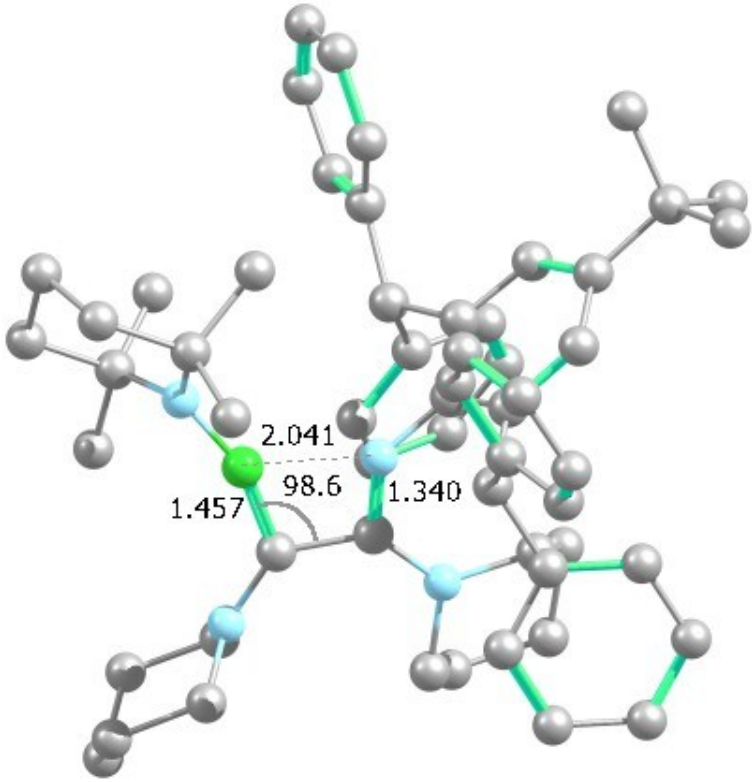


Figure S-29: Optimized structure of transition state **5-TS3**. Distances are given in Å and angles in º. Hydrogens were omitted for clarity.

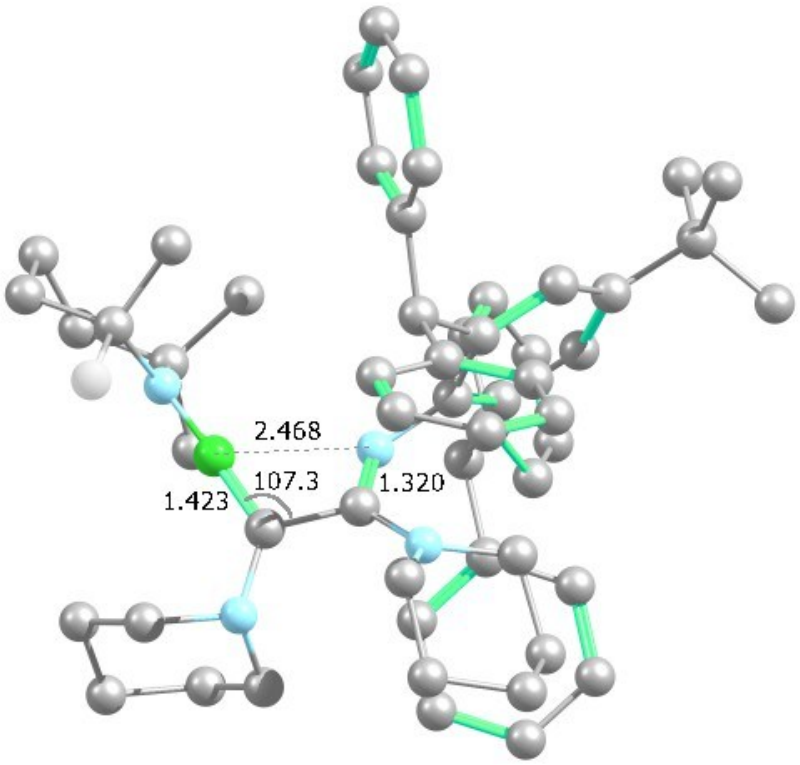


Figure S-30: Optimized structure of intermediate **5-Int3**. Distances are given in Å and angles in º. Hydrogens were omitted for clarity.

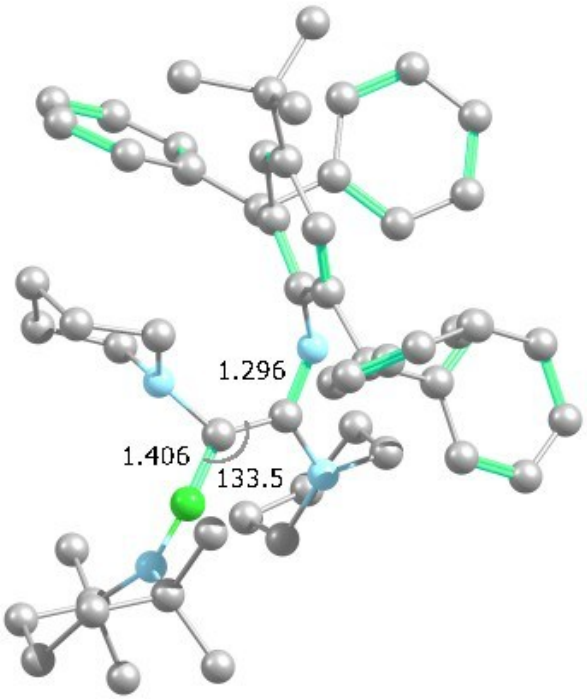


Figure S-31: Optimized structure of intermediate **5-Int4**. Distances are given in Å and angles in º. Hydrogens were omitted for clarity.

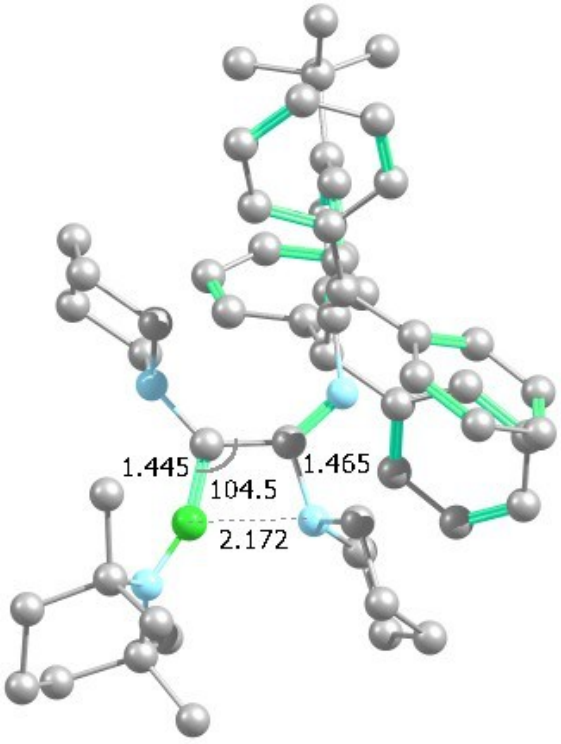


Figure S-32: Optimized structure of transition state **5-TS4**. Distances are given in Å and angles in º. Hydrogens were omitted for clarity.

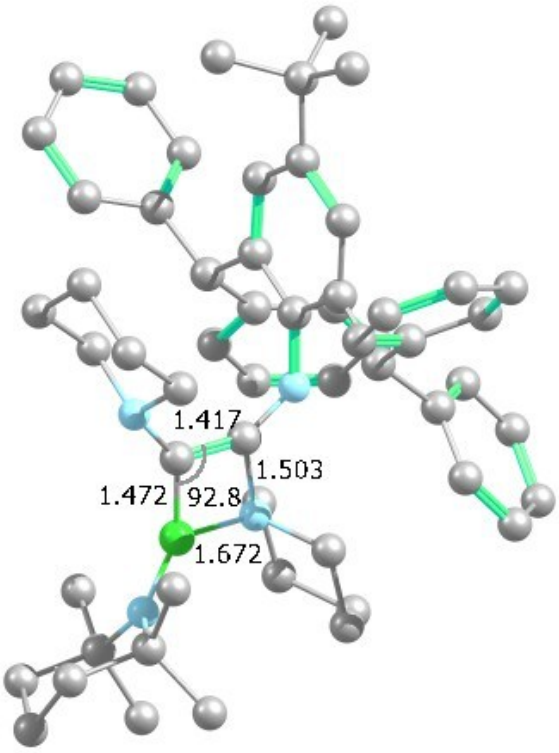


Figure S-33: Optimized structure of intermediate **5-Int5**. Distances are given in Å and angles in º. Hydrogens were omitted for clarity.

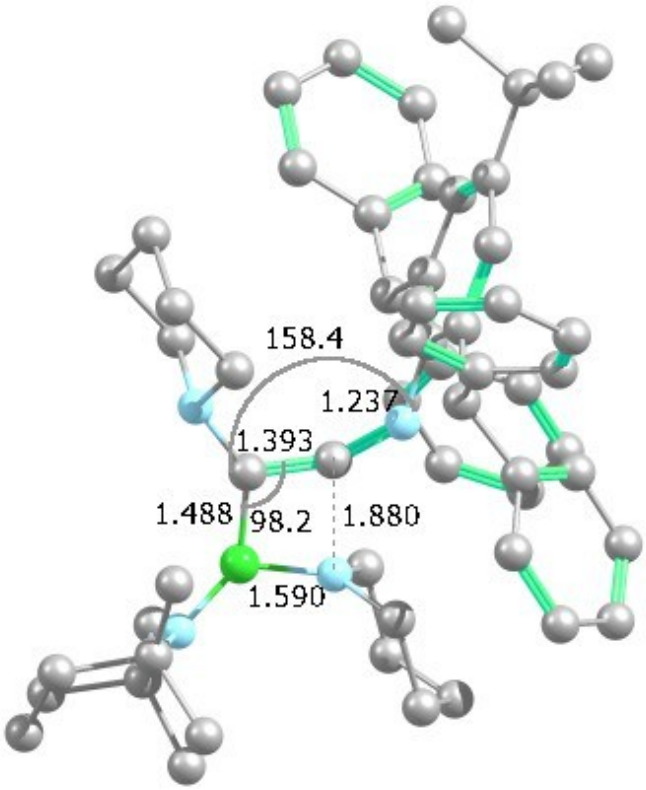


Figure S-34: Optimized structure of transition state **5-TS5**. Distances are given in Å and angles in º. Hydrogens were omitted for clarity.

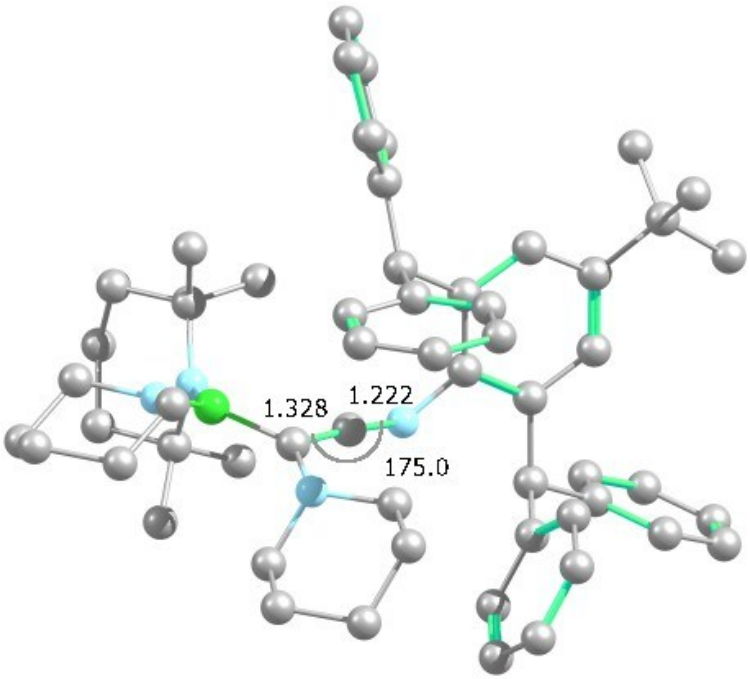


Figure S-35: Optimized structure of product **5**. Distances are given in Å and angles in º. Hydrogens were omitted for clarity.

Table S2. Cartesian coordinates (xyz) of the optimized geometries for all the species involved in the reaction mechanism calculated at the D3-PBE0/6-31G(d) level. Coordinates are given in Å.

3 + Pip

E(scf) = -2456.00521480 a.u.

6	1.285950000	0.331492000	-0.437776000
5	-1.036144000	-0.379033000	-1.348564000
7	0.011395000	0.106863000	-0.847030000
6	2.147918000	-0.745616000	-0.133371000
7	-2.162088000	-0.860403000	-2.006457000
6	3.463148000	-0.483988000	0.227152000
1	4.122021000	-1.333327000	0.394730000
6	3.960180000	0.812984000	0.367925000
6	1.780575000	1.646171000	-0.339215000
6	3.091456000	1.863746000	0.078217000
1	3.437671000	2.890135000	0.142893000
6	0.837955000	2.799859000	-0.628264000
1	0.165834000	2.464933000	-1.430554000
6	0.565975000	3.390522000	1.811640000
1	1.640432000	3.552919000	1.847391000
6	-0.021428000	3.016433000	0.597977000
6	-0.207684000	3.526653000	2.958465000
1	0.260716000	3.809893000	3.897633000
6	-1.580514000	3.279373000	2.908655000
1	-2.184095000	3.363640000	3.808405000
6	-2.168601000	2.900108000	1.706950000
1	-3.228178000	2.671140000	1.666125000
6	-1.392009000	2.773032000	0.557170000
1	-1.844007000	2.444730000	-0.374543000
6	1.543630000	4.044007000	-1.139071000
6	2.458031000	3.912236000	-2.192260000
1	2.672502000	2.918742000	-2.579032000
6	3.102259000	5.022936000	-2.724425000
1	3.810886000	4.896988000	-3.539302000
6	2.841658000	6.294771000	-2.212331000
1	3.346287000	7.165131000	-2.623708000
6	1.286697000	5.320180000	-0.637656000
1	0.577533000	5.442457000	0.175569000
6	1.931207000	6.437555000	-1.170221000
1	1.718122000	7.423061000	-0.763611000
6	1.672014000	-2.170370000	-0.286302000
1	0.612569000	-2.119045000	-0.556367000
6	1.720281000	-3.032222000	0.959456000
6	1.036791000	-4.254256000	0.911056000
1	0.534129000	-4.534466000	-0.012534000
6	0.983145000	-5.093167000	2.017691000
1	0.436482000	-6.030879000	1.960059000
6	1.620810000	-4.725390000	3.203590000
1	1.575838000	-5.374103000	4.074241000
6	2.309141000	-3.517759000	3.261570000
1	2.802619000	-3.214906000	4.181566000
6	2.359185000	-2.677591000	2.147881000
1	2.874615000	-1.725444000	2.219867000
6	2.372942000	-2.790785000	-1.482579000
6	3.346149000	-3.781683000	-1.368663000

5-TS1

E(scf) = −2456.00178311 a.u.

ν_{min} = −119.2 cm^{-1}

6	0.905181000	0.046001000	-0.247377000
5	-1.441561000	-0.601124000	-0.532652000
7	-0.438395000	0.106351000	-0.009165000
6	1.713663000	-1.037118000	0.188023000
7	-1.744196000	-1.560233000	-1.571451000
6	3.070583000	-1.065871000	-0.110054000
1	3.650945000	-1.919174000	0.231809000
6	3.700945000	-0.065533000	-0.852200000
6	1.572907000	1.126103000	-0.881669000
6	2.925286000	1.036058000	-1.203116000
1	3.380559000	1.869985000	-1.726343000
6	0.852028000	2.456864000	-0.982377000
1	-0.220015000	2.236659000	-1.067263000
6	1.798465000	2.776759000	1.381328000
1	2.332834000	1.837670000	1.280229000
6	1.021686000	3.238677000	0.316996000
6	1.861929000	3.490977000	2.578493000
1	2.458662000	3.104375000	3.401515000
6	1.165374000	4.687134000	2.723048000
1	1.212257000	5.241894000	3.656607000
6	0.409759000	5.171476000	1.653487000
1	-0.131842000	6.109612000	1.750268000
6	0.339205000	4.450969000	0.466481000
1	-0.250432000	4.825573000	-0.367621000
6	1.250716000	3.295996000	-2.177019000
6	0.479496000	3.279163000	-3.340912000
1	-0.424926000	2.677930000	-3.366581000
6	0.854167000	4.022529000	-4.458055000
1	0.238720000	3.997331000	-5.354100000
6	2.009771000	4.800072000	-4.425812000
1	2.304292000	5.380554000	-5.296299000
6	2.396122000	4.098952000	-2.147750000
1	2.981295000	4.146264000	-1.232465000
6	2.778732000	4.838053000	-3.263558000
1	3.675516000	5.451289000	-3.222758000
6	1.105563000	-2.104955000	1.069962000
1	0.072609000	-2.242575000	0.728521000
6	1.005790000	-1.666364000	2.520120000
6	0.132146000	-2.348371000	3.373233000
1	-0.497836000	-3.132554000	2.957885000
6	0.083859000	-2.057043000	4.733108000
1	-0.596188000	-2.605001000	5.380806000
6	0.900675000	-1.056977000	5.262092000
1	0.863487000	-0.823179000	6.323029000
6	1.760506000	-0.357400000	4.417179000
1	2.397290000	0.427930000	4.817438000
6	1.816075000	-0.665008000	3.057332000
1	2.498996000	-0.134119000	2.400780000
6	1.818512000	-3.442307000	0.921972000
6	2.425330000	-4.113671000	1.983624000

1	3.597728000	-4.171926000	-0.385943000	1	2.387044000	-3.688150000	2.981751000
6	3.981929000	-4.278406000	-2.507244000	6	3.085712000	-5.326413000	1.776175000
1	4.740287000	-5.050811000	-2.405680000	1	3.553730000	-5.831138000	2.617799000
6	3.646938000	-3.792710000	-3.768113000	6	3.152049000	-5.884140000	0.504074000
1	4.139852000	-4.184765000	-4.653865000	1	3.667170000	-6.827843000	0.344075000
6	2.674245000	-2.798467000	-3.888129000	6	2.557336000	-5.215088000	-0.567121000
1	2.406935000	-2.411545000	-4.868386000	1	2.608199000	-5.633341000	-1.569456000
6	2.047880000	-2.299875000	-2.752400000	6	1.904253000	-4.007320000	-0.357388000
1	1.301769000	-1.510161000	-2.829634000	1	1.464356000	-3.473689000	-1.193581000
6	5.400814000	1.019804000	0.810764000	6	5.167793000	-0.214932000	-1.222743000
6	5.765248000	2.498733000	0.919464000	6	5.689214000	0.986187000	-2.008341000
1	5.654734000	3.007744000	-0.045973000	1	5.124635000	1.127591000	-2.938098000
1	6.808955000	2.596114000	1.241716000	1	6.743730000	0.827054000	-2.265059000
1	5.130037000	3.010763000	1.652897000	1	5.614298000	1.908281000	-1.418248000
6	5.601069000	0.367291000	2.184442000	6	6.012174000	-0.364284000	0.048341000
1	5.379761000	-0.706272000	2.147151000	1	5.698840000	-1.237004000	0.633072000
1	4.939482000	0.828307000	2.928216000	1	5.912869000	0.526236000	0.681440000
1	6.640522000	0.492062000	2.515313000	1	7.071081000	-0.490438000	-0.214202000
6	6.345707000	0.359806000	-0.200821000	6	5.335889000	-1.472626000	-2.085285000
1	6.138577000	-0.712221000	-0.297220000	1	4.984798000	-2.364196000	-1.551922000
1	7.387900000	0.481829000	0.122810000	1	6.392956000	-1.617004000	-2.347226000
1	6.230139000	0.818789000	-1.189957000	1	4.754815000	-1.379512000	-3.011025000
6	-2.543365000	-0.121927000	-3.239380000	6	-1.129469000	-1.317712000	-2.900788000
6	-3.985194000	-0.465467000	-3.618475000	6	-2.056987000	-1.822813000	-4.016264000
1	-4.198162000	-0.002502000	-4.590260000	1	-1.520707000	-1.723543000	-4.968752000
1	-4.656029000	-0.008242000	-2.879559000	1	-2.933547000	-1.158764000	-4.066529000
6	-4.246863000	-1.963608000	-3.646625000	6	-2.541999000	-3.244797000	-3.799904000
1	-3.624555000	-2.449143000	-4.409723000	1	-1.694228000	-3.942400000	-3.798614000
1	-5.291664000	-2.157375000	-3.917026000	1	-3.207380000	-3.550981000	-4.616748000
6	-3.944345000	-2.534652000	-2.269491000	6	-3.271629000	-3.293393000	-2.468796000
1	-4.604729000	-2.053068000	-1.533556000	1	-4.132809000	-2.613131000	-2.516132000
1	-4.138768000	-3.613611000	-2.231765000	1	-3.658792000	-4.298943000	-2.259867000
6	-2.495586000	-2.300537000	-1.835999000	6	-2.374133000	-2.871843000	-1.297297000
6	-1.588248000	-0.420814000	-4.400858000	6	0.266739000	-1.936825000	-3.055827000
1	-1.701009000	-1.437147000	-4.785060000	1	0.238753000	-3.027317000	-3.131149000
1	-0.550774000	-0.287200000	-4.070144000	1	0.898630000	-1.648804000	-2.209615000
1	-1.781287000	0.275122000	-5.226506000	1	0.732717000	-1.555760000	-3.973786000
6	-2.469271000	1.376882000	-2.947062000	6	-0.965097000	0.187099000	-3.123061000
1	-1.439794000	1.693637000	-2.737832000	1	-0.145967000	0.590454000	-2.526331000
1	-3.096665000	1.632390000	-2.087688000	1	-1.890577000	0.724124000	-2.878930000
1	-2.823378000	1.933638000	-3.822037000	1	-0.725220000	0.364435000	-4.178776000
6	-1.536415000	-3.203651000	-2.619408000	6	-1.349438000	-3.985344000	-1.037761000
1	-1.727593000	-4.251553000	-2.356838000	1	-1.880635000	-4.919998000	-0.815890000
1	-0.495677000	-2.970351000	-2.364389000	1	-0.718905000	-3.746700000	-0.179419000
1	-1.649918000	-3.105659000	-3.701799000	1	-0.695691000	-4.171626000	-1.890316000
6	-2.381723000	-2.656263000	-0.357088000	6	-3.257781000	-2.807098000	-0.052684000
1	-2.625118000	-3.717506000	-0.227534000	1	-3.669829000	-3.807543000	0.126741000
1	-3.070471000	-2.051176000	0.238946000	1	-4.088426000	-2.108678000	-0.184325000
1	-1.372919000	-2.486301000	0.038868000	1	-2.694975000	-2.497890000	0.835091000
6	-3.495466000	0.002314000	1.781476000	6	-3.149840000	0.168571000	0.323474000
6	-2.371694000	-0.433484000	1.966706000	6	-2.848892000	0.208766000	1.615384000
7	-1.163229000	-0.970333000	2.167350000	7	-2.139888000	0.933079000	2.402751000
6	-0.088463000	-0.051741000	2.554483000	6	-1.627507000	2.263961000	2.047852000
6	-1.131207000	-2.232840000	2.910156000	6	-1.684553000	0.468796000	3.711159000
1	-0.177598000	0.852130000	1.951513000	1	-1.956771000	2.491101000	1.032944000
1	0.861070000	-0.538755000	2.302185000	1	-0.536475000	2.205709000	2.049414000
6	-0.149460000	0.254424000	4.046794000	6	-2.096076000	3.276830000	3.084029000
1	-0.181758000	-2.727607000	2.688225000	1	-0.594966000	0.372522000	3.648318000

1	-1.945362000	-2.864543000	2.540709000	1	-2.106963000	-0.521841000	3.882476000
6	-1.235932000	-1.984739000	4.412088000	6	-2.062789000	1.459057000	4.806141000
1	-2.213281000	-1.529016000	4.626699000	1	-3.155887000	1.466642000	4.921828000
1	-1.180340000	-2.938731000	4.952610000	1	-1.628353000	1.113735000	5.752257000
6	-0.115291000	-1.042438000	4.857144000	6	-1.577364000	2.866417000	4.460552000
1	0.848912000	-1.545522000	4.688407000	1	-0.478386000	2.877915000	4.430322000
1	-0.192803000	-0.831370000	5.931472000	1	-1.896435000	3.581197000	5.228873000
1	0.679103000	0.918760000	4.323631000	1	-1.718831000	4.265039000	2.805230000
1	-1.084932000	0.796218000	4.243470000	1	-3.195495000	3.314145000	3.092281000
7	-4.678450000	0.404947000	1.279838000	7	-4.291573000	0.412178000	-0.312153000
6	-4.673220000	0.839478000	-0.112509000	6	-4.466398000	0.141433000	-1.730690000
6	-5.567821000	1.175506000	2.139693000	6	-5.380692000	1.143377000	0.325168000
1	-3.984284000	0.191699000	-0.663816000	1	-3.619219000	-0.466634000	-2.055572000
1	-4.289319000	1.876632000	-0.183369000	1	-4.448970000	1.097838000	-2.280035000
6	-6.078229000	0.787629000	-0.697114000	6	-5.794229000	-0.560665000	-1.992523000
1	-5.248523000	2.235026000	2.184581000	1	-5.418482000	2.162217000	-0.093844000
1	-5.499335000	0.762230000	3.150164000	1	-5.155409000	1.222853000	1.393400000
6	-6.995011000	1.110748000	1.609719000	6	-6.717797000	0.448088000	0.092690000
1	-7.340206000	0.069447000	1.659060000	1	-6.702303000	-0.524020000	0.603760000
1	-7.650644000	1.716378000	2.247518000	1	-7.520069000	1.049227000	0.537933000
6	-7.046330000	1.596871000	0.162934000	6	-6.954556000	0.234719000	-1.400472000
1	-6.750892000	2.656518000	0.130582000	1	-7.017155000	1.213065000	-1.900395000
1	-8.066772000	1.530511000	-0.233386000	1	-7.906971000	-0.281153000	-1.570290000
1	-6.060664000	1.172674000	-1.724869000	1	-5.918340000	-0.699875000	-3.073820000
1	-6.404522000	-0.261084000	-0.735307000	1	-5.765922000	-1.556961000	-1.531138000

5-Int1

E(scf) = −2456.02169149 a.u.

6	0.947039000	0.109010000	-0.176980000
5	-1.361723000	-0.707116000	-0.651954000
7	-0.407911000	0.084561000	-0.084891000
6	1.753165000	-0.932624000	0.359744000
7	-1.327245000	-1.738162000	-1.715582000
6	3.136490000	-0.874174000	0.266380000
1	3.714283000	-1.695404000	0.683050000
6	3.805397000	0.180224000	-0.361600000
6	1.633198000	1.233775000	-0.704553000
6	3.022074000	1.236876000	-0.817446000
1	3.494911000	2.107885000	-1.259556000
6	0.843652000	2.510463000	-0.913460000
1	-0.175479000	2.216412000	-1.198184000
6	1.329548000	2.837893000	1.582816000
1	1.954061000	1.950838000	1.561778000
6	0.712325000	3.264940000	0.405380000
6	1.117139000	3.514668000	2.784420000
1	1.590895000	3.151677000	3.693413000
6	0.294697000	4.638007000	2.824520000
1	0.126471000	5.164642000	3.760562000
6	-0.300309000	5.091400000	1.645649000
1	-0.933158000	5.975800000	1.660801000
6	-0.090895000	4.409652000	0.451466000
1	-0.556658000	4.759577000	-0.467614000
6	1.391543000	3.395870000	-2.010604000
6	0.910628000	3.272054000	-3.316000000
1	0.117692000	2.557504000	-3.520201000
6	1.437502000	4.046265000	-4.346803000

5-TS2

E(scf) = −2456.01356770 a.u.

ν_{min} = −145.8 cm^{-1}

6	0.972091000	0.212323000	0.087326000
5	-1.426936000	-0.062963000	1.288812000
7	-0.112263000	-0.371958000	0.713034000
6	0.885694000	1.341389000	-0.767485000
7	-1.710923000	0.969850000	2.252265000
6	2.017674000	1.775250000	-1.444061000
1	1.926090000	2.647917000	-2.085671000
6	3.268481000	1.172451000	-1.287998000
6	2.240111000	-0.383220000	0.278226000
6	3.356246000	0.103470000	-0.401349000
1	4.316676000	-0.359315000	-0.198274000
6	2.380721000	-1.586681000	1.191652000
1	1.498317000	-1.579714000	1.842258000
6	3.256639000	-3.198907000	-0.565544000
1	4.074904000	-2.508422000	-0.750362000
6	2.297546000	-2.875570000	0.399318000
6	3.171783000	-4.387532000	-1.283149000
1	3.926577000	-4.625225000	-2.028418000
6	2.116331000	-5.271436000	-1.049703000
1	2.046891000	-6.199798000	-1.610886000
6	1.154692000	-4.956282000	-0.092040000
1	0.327244000	-5.635800000	0.096606000
6	1.249237000	-3.765689000	0.627318000
1	0.489032000	-3.503978000	1.358764000
6	3.608983000	-1.492172000	2.083682000
6	3.932493000	-0.263095000	2.673385000
1	3.333571000	0.611278000	2.432710000
6	5.009501000	-0.148710000	3.545189000

1	1.049175000	3.937565000	-5.356614000	1	5.241833000	0.815711000	3.990166000
6	2.457416000	4.959579000	-4.085290000	6	5.790363000	-1.264950000	3.845129000
1	2.870319000	5.564163000	-4.888702000	1	6.635606000	-1.177200000	4.522812000
6	2.404660000	4.325214000	-1.756018000	6	4.395152000	-2.603533000	2.393629000
1	2.766819000	4.440766000	-0.737397000	1	4.159587000	-3.565659000	1.948409000
6	2.938835000	5.097283000	-2.784588000	6	5.477413000	-2.491142000	3.266305000
1	3.729743000	5.811287000	-2.568596000	1	6.077449000	-3.369413000	3.491323000
6	1.065465000	-2.040569000	1.123038000	6	-0.432328000	2.053665000	-0.958099000
1	0.156400000	-2.284007000	0.562386000	1	-1.050270000	1.785038000	-0.094000000
6	0.611544000	-1.588427000	2.497272000	6	-1.152968000	1.543531000	-2.192332000
6	-0.433302000	-2.270159000	3.127499000	6	-2.369055000	0.874322000	-2.069311000
1	-0.964133000	-3.042512000	2.574309000	1	-2.754900000	0.673840000	-1.074805000
6	-0.766589000	-2.001680000	4.451892000	6	-3.060745000	0.437035000	-3.198603000
1	-1.571251000	-2.555199000	4.930403000	1	-4.006730000	-0.086551000	-3.081625000
6	-0.069517000	-1.024711000	5.163684000	6	-2.539851000	0.668821000	-4.468935000
1	-0.325586000	-0.813918000	6.199094000	1	-3.074721000	0.327957000	-5.351449000
6	0.949692000	-0.314434000	4.532123000	6	-1.324050000	1.342596000	-4.601118000
1	1.495611000	0.453941000	5.075006000	1	-0.908792000	1.526491000	-5.588582000
6	1.289770000	-0.599044000	3.209706000	6	-0.638303000	1.776111000	-3.471126000
1	2.103432000	-0.067890000	2.723095000	1	0.306285000	2.302577000	-3.575237000
6	1.903414000	-3.306884000	1.198753000	6	-0.355149000	3.576230000	-0.947621000
6	2.358025000	-3.853647000	2.399051000	6	-1.413000000	4.316887000	-1.487291000
1	2.097699000	-3.375928000	3.338845000	1	-2.229391000	3.794638000	-1.978248000
6	3.143921000	-5.007541000	2.404042000	6	-1.435326000	5.706005000	-1.403790000
1	3.488429000	-5.416481000	3.350776000	1	-2.270593000	6.255788000	-1.830116000
6	3.489131000	-5.629426000	1.208822000	6	-0.392905000	6.388171000	-0.780303000
1	4.101555000	-6.527513000	1.213791000	1	-0.405566000	7.473168000	-0.717812000
6	3.046273000	-5.085416000	0.001854000	6	0.666374000	5.663881000	-0.239644000
1	3.313532000	-5.556886000	-0.940757000	1	1.487528000	6.180185000	0.251289000
6	2.265599000	-3.936180000	0.000535000	6	0.683188000	4.273218000	-0.320976000
1	1.937632000	-3.500086000	-0.937725000	1	1.513472000	3.724352000	0.110706000
6	5.319452000	0.133868000	-0.495042000	6	4.462871000	1.727906000	-2.047459000
6	5.874296000	1.371047000	-1.197371000	6	5.740389000	0.936983000	-1.775508000
1	5.453767000	1.476031000	-2.204956000	1	6.011425000	0.971605000	-0.713237000
1	6.964674000	1.286631000	-1.284125000	1	6.566757000	1.366732000	-2.354222000
1	5.644033000	2.283624000	-0.633350000	1	5.625591000	-0.113997000	-2.069019000
6	5.959134000	0.039022000	0.895568000	6	4.172142000	1.680250000	-3.552403000
1	5.613712000	-0.853977000	1.429464000	1	3.279378000	2.264943000	-3.803230000
1	5.700963000	0.919539000	1.497075000	1	4.007366000	0.646735000	-3.880505000
1	7.052606000	-0.015511000	0.806828000	1	5.021243000	2.094427000	-4.111455000
6	5.712240000	-1.105517000	-1.309619000	6	4.692329000	3.184595000	-1.624354000
1	5.343796000	-2.021779000	-0.832967000	1	3.804898000	3.798956000	-1.817511000
1	6.805288000	-1.173880000	-1.395937000	1	5.535581000	3.610375000	-2.183780000
1	5.283299000	-1.050433000	-2.317683000	1	4.920517000	3.240358000	-0.552960000
6	-0.549742000	-1.467124000	-2.948160000	6	-0.608706000	1.492993000	3.113710000
6	-1.281434000	-2.027560000	-4.182368000	6	-1.149904000	1.965892000	4.472759000
1	-0.618679000	-1.903842000	-5.048722000	1	-0.311194000	2.419948000	5.015357000
1	-2.173394000	-1.409222000	-4.369321000	1	-1.470574000	1.081826000	5.043552000
6	-1.725326000	-3.469962000	-4.028858000	6	-2.322354000	2.916260000	4.361194000
1	-0.855925000	-4.127710000	-3.901120000	1	-2.040685000	3.817970000	3.801217000
1	-2.253188000	-3.807230000	-4.929855000	1	-2.655248000	3.240449000	5.355010000
6	-2.628818000	-3.550989000	-2.811587000	6	-3.421219000	2.165771000	3.639877000
1	-3.504494000	-2.908625000	-2.978126000	1	-3.686788000	1.274799000	4.227572000
1	-2.996502000	-4.572880000	-2.651657000	1	-4.327504000	2.775382000	3.535819000
6	-1.909493000	-3.086583000	-1.535899000	6	-3.002207000	1.711393000	2.235306000
6	0.891429000	-1.998543000	-2.922318000	6	0.188216000	2.628819000	2.466560000
1	0.943502000	-3.086010000	-3.030668000	1	-0.387164000	3.547402000	2.333552000
1	1.381075000	-1.702587000	-1.990433000	1	0.562387000	2.310688000	1.492991000

1	1.455774000	-1.562467000	-3.757015000	1	1.053907000	2.868569000	3.099200000
6	-0.447677000	0.043436000	-3.187443000	6	0.396480000	0.384217000	3.454532000
1	0.267090000	0.512093000	-2.511855000	1	1.105679000	0.214216000	2.646542000
1	-1.424352000	0.531275000	-3.077289000	1	-0.120506000	-0.555526000	3.679262000
1	-0.092818000	0.210233000	-4.212613000	1	0.972311000	0.688521000	4.337441000
6	-0.868086000	-4.155118000	-1.158148000	6	-2.944602000	2.934906000	1.303667000
1	-1.365750000	-5.131188000	-1.082961000	1	-3.880660000	3.501509000	1.391833000
1	-0.411087000	-3.941979000	-0.189688000	1	-2.851808000	2.616520000	0.260020000
1	-0.065605000	-4.249411000	-1.889383000	1	-2.117101000	3.611754000	1.518490000
6	-2.941233000	-3.109854000	-0.407846000	6	-4.148392000	0.846691000	1.725056000
1	-3.302201000	-4.139326000	-0.295811000	1	-5.082463000	1.408833000	1.849796000
1	-3.801348000	-2.470661000	-0.626981000	1	-4.213086000	-0.097415000	2.269533000
1	-2.511756000	-2.789735000	0.548395000	1	-4.037881000	0.610636000	0.663812000
6	-2.822613000	-0.212222000	-0.064273000	6	-2.253209000	-1.212391000	0.586919000
6	-2.826682000	-0.143262000	1.310890000	6	-1.238772000	-1.621252000	-0.216513000
7	-2.465929000	0.813023000	2.081622000	7	-0.804699000	-2.482838000	-1.120948000
6	-2.063536000	2.150162000	1.616803000	6	-1.699456000	-3.521991000	-1.614242000
6	-2.458566000	0.691347000	3.538904000	6	0.320656000	-2.210007000	-2.009587000
1	-1.978499000	2.116533000	0.530937000	1	-2.480476000	-3.701491000	-0.872363000
1	-1.071692000	2.351441000	2.026479000	1	-1.093615000	-4.436071000	-1.706802000
6	-3.062019000	3.173878000	2.139358000	6	-2.271821000	-3.124393000	-2.971378000
1	-1.428287000	0.865332000	3.871657000	1	0.908200000	-3.134418000	-2.067879000
1	-2.730583000	-0.334360000	3.788514000	1	0.946555000	-1.439828000	-1.566020000
6	-3.410393000	1.716166000	4.149214000	6	-0.181686000	-1.793679000	-3.385558000
1	-4.438233000	1.455201000	3.858150000	1	-0.696865000	-0.834588000	-3.294228000
1	-3.350896000	1.650808000	5.242315000	1	0.677652000	-1.648119000	-4.052140000
6	-3.085689000	3.129538000	3.665689000	6	-1.138477000	-2.837771000	-3.957085000
1	-2.091241000	3.422758000	4.031852000	1	-0.588705000	-3.771258000	-4.151580000
1	-3.811682000	3.846523000	4.067715000	1	-1.548080000	-2.490995000	-4.913625000
1	-2.764971000	4.164925000	1.782390000	1	-2.928583000	-3.921212000	-3.344176000
1	-4.062700000	2.951650000	1.738921000	1	-2.876471000	-2.218761000	-2.839143000
7	-3.908231000	0.064357000	-0.785520000	7	-3.520968000	-1.828951000	0.713769000
6	-3.995641000	-0.176874000	-2.220279000	6	-3.604915000	-3.014922000	1.534745000
6	-5.063676000	0.739447000	-0.204893000	6	-4.441458000	-1.802458000	-0.398402000
1	-3.114864000	-0.753300000	-2.508363000	1	-2.879833000	-2.913465000	2.349471000
1	-3.973219000	0.796848000	-2.734555000	1	-3.339264000	-3.937757000	0.972591000
6	-5.282204000	-0.910245000	-2.582930000	6	-5.019046000	-3.177730000	2.086520000
1	-5.103944000	1.763103000	-0.608874000	1	-4.262602000	-2.627906000	-1.118739000
1	-4.918926000	0.811125000	0.876879000	1	-4.292947000	-0.864568000	-0.944098000
6	-6.357829000	0.003509000	-0.533564000	6	-5.877800000	-1.912810000	0.104044000
1	-6.333845000	-0.980623000	-0.046516000	1	-6.099102000	-1.029917000	0.718403000
1	-7.203031000	0.563755000	-0.115888000	1	-6.571795000	-1.922470000	-0.746551000
6	-6.504077000	-0.175004000	-2.041862000	6	-6.035174000	-3.177104000	0.946558000
1	-6.577281000	0.813799000	-2.519000000	1	-5.854920000	-4.055582000	0.307440000
1	-7.424223000	-0.721863000	-2.278558000	1	-7.057150000	-3.262194000	1.336105000
1	-5.330037000	-1.015216000	-3.673761000	1	-5.087416000	-4.105166000	2.669621000
1	-5.248978000	-1.921431000	-2.156759000	1	-5.227917000	-2.335846000	2.760333000

5-Int2

E(scf) = −2456.06530881 a.u.

5-TS3

E(scf) = −2455.73280242 a.u.

ν_{min} = −151.4 cm^{-1}

6	0.922592000	0.187426000	0.004709000	6	1.036950000	0.099736000	-0.121564000
5	-1.476842000	-0.153038000	1.318123000	5	-1.859783000	-0.044403000	1.377245000
7	-0.196566000	-0.489177000	0.528979000	7	-0.135688000	-0.452233000	0.363808000
6	0.817670000	1.361008000	-0.772501000	6	1.020239000	1.296628000	-0.871689000
7	-1.717707000	0.869995000	2.277057000	7	-2.063772000	1.079891000	2.167683000
6	1.953301000	1.864993000	-1.393813000	6	2.211845000	1.816231000	-1.358230000
1	1.850160000	2.758208000	-2.004173000	1	2.173026000	2.734905000	-1.938579000
6	3.219130000	1.300963000	-1.217124000	6	3.451963000	1.240261000	-1.064829000
6	2.197433000	-0.356836000	0.245484000	6	2.280182000	-0.448814000	0.243846000
6	3.319988000	0.206456000	-0.364590000	6	3.459795000	0.121105000	-0.235178000
1	4.290633000	-0.222782000	-0.138840000	1	4.400897000	-0.313806000	0.087692000
6	2.351676000	-1.589323000	1.118132000	6	2.312290000	-1.660245000	1.154046000
1	1.446387000	-1.642655000	1.735246000	1	1.361099000	-1.648034000	1.701093000
6	3.357059000	-3.094883000	-0.659923000	6	3.306878000	-3.203276000	-0.593471000
1	4.157408000	-2.369794000	-0.779916000	1	4.086445000	-2.463544000	-0.756347000
6	2.349885000	-2.848618000	0.276959000	6	2.316070000	-2.945373000	0.357883000
6	3.338482000	-4.248372000	-1.437307000	6	3.286561000	-4.376851000	-1.340832000
1	4.127424000	-4.424431000	-2.163990000	1	4.061926000	-4.561623000	-2.079920000
6	2.305125000	-5.174337000	-1.288278000	6	2.264872000	-5.308100000	-1.151758000
1	2.286148000	-6.074672000	-1.896852000	1	2.242142000	-6.221609000	-1.740200000
6	1.300198000	-4.939896000	-0.351680000	6	1.272318000	-5.058783000	-0.205322000
1	0.492491000	-5.656380000	-0.225466000	1	0.470642000	-5.776990000	-0.052348000
6	1.325706000	-3.782857000	0.425518000	6	1.301682000	-3.884299000	0.544494000
1	0.529780000	-3.583821000	1.139210000	1	0.515063000	-3.674614000	1.265645000
6	3.541723000	-1.489855000	2.061680000	6	3.421951000	-1.545254000	2.184200000
6	3.846383000	-0.265954000	2.671221000	6	3.455467000	-0.390065000	2.976883000
1	3.266389000	0.614462000	2.409464000	1	2.708266000	0.382524000	2.807639000
6	4.883845000	-0.163234000	3.591866000	6	4.429659000	-0.222292000	3.952717000
1	5.102352000	0.797853000	4.050793000	1	4.438698000	0.680501000	4.558619000
6	5.642087000	-1.285824000	3.922401000	6	5.396760000	-1.209514000	4.151985000
1	6.455829000	-1.207033000	4.638593000	1	6.162943000	-1.079994000	4.911998000
6	4.306479000	-2.607935000	2.402052000	6	4.388016000	-2.528043000	2.393036000
1	4.085898000	-3.566042000	1.940672000	1	4.372209000	-3.432717000	1.792145000
6	5.347823000	-2.507428000	3.323783000	6	5.371110000	-2.359588000	3.370263000
1	5.931002000	-3.390819000	3.571614000	1	6.118175000	-3.135509000	3.518101000
6	-0.519491000	2.046298000	-0.939350000	6	-0.309163000	1.982952000	-1.090242000
1	-1.131956000	1.722465000	-0.090049000	1	-0.923685000	1.694456000	-0.226613000
6	-1.222739000	1.573525000	-2.195948000	6	-1.019152000	1.447922000	-2.315487000
6	-2.390041000	0.819652000	-2.102527000	6	-2.223436000	0.758285000	-2.187004000
1	-2.737138000	0.515210000	-1.117477000	1	-2.593715000	0.531184000	-1.189406000
6	-3.071120000	0.422926000	-3.252813000	6	-2.923850000	0.336507000	-3.316573000
1	-3.982049000	-0.164187000	-3.161834000	1	-3.863680000	-0.197936000	-3.198323000
6	-2.582566000	0.769582000	-4.509429000	6	-2.419317000	0.594426000	-4.588654000
1	-3.109326000	0.457841000	-5.407430000	1	-2.962940000	0.266576000	-5.470717000
6	-1.410066000	1.521704000	-4.609274000	6	-1.203759000	1.268876000	-4.723933000
1	-1.020439000	1.794500000	-5.586570000	1	-0.797188000	1.463494000	-5.713008000
6	-0.738785000	1.924038000	-3.459561000	6	-0.509501000	1.690339000	-3.594286000
1	0.167275000	2.519661000	-3.535154000	1	0.433362000	2.222814000	-3.693690000
6	-0.493382000	3.569793000	-0.861894000	6	-0.255695000	3.504046000	-1.067539000
6	-1.604488000	4.282674000	-1.328556000	6	-1.200996000	4.260143000	-1.767993000
1	-2.416893000	3.742092000	-1.806231000	1	-1.920635000	3.755342000	-2.405674000
6	-1.684714000	5.664774000	-1.189557000	6	-1.238044000	5.648295000	-1.655290000
1	-2.561071000	6.191176000	-1.558977000	1	-1.984509000	6.210888000	-2.210349000
6	-0.647251000	6.370047000	-0.583145000	6	-0.326280000	6.311966000	-0.838893000
1	-0.704473000	7.450261000	-0.477815000	1	-0.351424000	7.395167000	-0.753037000
6	0.463619000	5.674402000	-0.114086000	6	0.620775000	5.570875000	-0.134618000
1	1.281028000	6.207960000	0.364450000	1	1.340397000	6.072622000	0.507592000
6	0.537492000	4.289419000	-0.249443000	6	0.653339000	4.183666000	-0.247406000

1	1.406234000	3.765321000	0.134313000	1	1.393731000	3.617887000	0.308397000
6	4.416262000	1.929463000	-1.913242000	6	4.719897000	1.894507000	-1.593166000
6	5.714162000	1.179538000	-1.622263000	6	5.978079000	1.129254000	-1.189059000
1	5.947277000	1.187384000	-0.550507000	1	6.089666000	1.093734000	-0.098531000
1	6.541913000	1.661039000	-2.156335000	1	6.860174000	1.628648000	-1.607391000
1	5.651643000	0.135954000	-1.955219000	1	5.954079000	0.099519000	-1.567409000
6	4.178691000	1.922727000	-3.428107000	6	4.660339000	1.958661000	-3.123833000
1	3.271770000	2.479791000	-3.690590000	1	3.786503000	2.527309000	-3.462802000
1	4.066662000	0.895584000	-3.795916000	1	4.598163000	0.949762000	-3.549508000
1	5.028697000	2.388801000	-3.942918000	1	5.561287000	2.449357000	-3.514800000
6	4.572270000	3.378189000	-1.432739000	6	4.817618000	3.319728000	-1.033071000
1	3.670560000	3.966333000	-1.640911000	1	3.942382000	3.917841000	-1.313423000
1	5.419698000	3.853978000	-1.943212000	1	5.715664000	3.817414000	-1.422298000
1	4.756696000	3.405661000	-0.351768000	1	4.878520000	3.295602000	0.061870000
6	-0.611713000	1.416000000	3.110539000	6	-0.984966000	1.490318000	3.102019000
6	-1.121346000	1.830982000	4.498271000	6	-1.571046000	2.171194000	4.342564000
1	-0.284567000	2.310650000	5.021391000	1	-0.735673000	2.585778000	4.920834000
1	-1.381368000	0.921222000	5.059192000	1	-2.055884000	1.406407000	4.966454000
6	-2.339769000	2.728744000	4.444058000	6	-2.600475000	3.234131000	3.998753000
1	-2.118469000	3.647843000	3.885122000	1	-2.151044000	4.022228000	3.380306000
1	-2.647966000	3.026967000	5.453675000	1	-2.977392000	3.712155000	4.910889000
6	-3.434282000	1.938017000	3.757073000	6	-3.731230000	2.552869000	3.247029000
1	-3.635210000	1.029587000	4.343734000	1	-4.150156000	1.759857000	3.883291000
1	-4.370770000	2.506550000	3.699475000	1	-4.542158000	3.253653000	3.013141000
6	-3.057829000	1.518897000	2.331129000	6	-3.262939000	1.924556000	1.931166000
6	0.106104000	2.595142000	2.454229000	6	0.024043000	2.413605000	2.419152000
1	-0.531572000	3.469997000	2.313196000	1	-0.416870000	3.361570000	2.102181000
1	0.493519000	2.290738000	1.481459000	1	0.446381000	1.917663000	1.541793000
1	0.958031000	2.896926000	3.078531000	1	0.843964000	2.637238000	3.114647000
6	0.439284000	0.332933000	3.364718000	6	-0.239403000	0.239281000	3.567598000
1	1.064968000	0.173767000	2.489875000	1	0.274159000	-0.242045000	2.729548000
1	-0.037922000	-0.613104000	3.645983000	1	-0.937909000	-0.475534000	4.018222000
1	1.095954000	0.652405000	4.182992000	1	0.510369000	0.522391000	4.316313000
6	-3.113211000	2.741942000	1.403730000	6	-2.998271000	3.016385000	0.889140000
1	-4.099490000	3.216958000	1.485502000	1	-3.893906000	3.641118000	0.780349000
1	-2.980788000	2.429011000	0.362697000	1	-2.785510000	2.567127000	-0.085664000
1	-2.355363000	3.494963000	1.627865000	1	-2.160188000	3.667051000	1.149001000
6	-4.155165000	0.568282000	1.861905000	6	-4.393165000	1.041039000	1.406982000
1	-5.126454000	1.034359000	2.070438000	1	-5.318928000	1.627628000	1.365327000
1	-4.095606000	-0.395782000	2.373102000	1	-4.538536000	0.171278000	2.056297000
1	-4.090466000	0.375078000	0.788334000	1	-4.172674000	0.670011000	0.401476000
6	-2.182657000	-1.292156000	0.567218000	6	-2.187950000	-1.261896000	0.647680000
6	-0.998762000	-1.436121000	-0.165045000	6	-0.953798000	-1.394116000	-0.124363000
7	-0.620294000	-2.208213000	-1.192137000	7	-0.690318000	-2.241281000	-1.133720000
6	-1.486838000	-3.286715000	-1.638835000	6	-1.569715000	-3.348498000	-1.468192000
6	0.490890000	-1.988431000	-2.110925000	6	0.426030000	-2.146122000	-2.068126000
1	-2.248105000	-3.472501000	-0.884391000	1	-2.325792000	-3.460242000	-0.697870000
1	-0.853323000	-4.184227000	-1.712990000	1	-0.947665000	-4.257412000	-1.467021000
6	-2.094265000	-2.976275000	-3.001474000	6	-2.180789000	-3.153174000	-2.850994000
1	1.070123000	-2.920368000	-2.153018000	1	0.983459000	-3.090543000	-2.016843000
1	1.142398000	-1.204060000	-1.740642000	1	1.094635000	-1.341859000	-1.776180000
6	-0.039417000	-1.629765000	-3.495730000	6	-0.093623000	-1.917420000	-3.483049000
1	-0.566523000	-0.674573000	-3.433080000	1	-0.588973000	-0.944750000	-3.520594000
1	0.811668000	-1.498562000	-4.176247000	1	0.760681000	-1.884583000	-4.171160000
6	-0.986456000	-2.706535000	-4.018022000	6	-1.074240000	-3.013523000	-3.893625000
1	-0.421724000	-3.636410000	-4.185463000	1	-0.536082000	-3.970636000	-3.970745000
1	-1.414549000	-2.402008000	-4.981099000	1	-1.499702000	-2.794423000	-4.880918000
1	-2.728638000	-3.813334000	-3.320740000	1	-2.839928000	-3.998942000	-3.086138000

1	-2.727836000	-2.088467000	-2.903091000	1	-2.789461000	-2.241963000	-2.834316000
7	-3.368722000	-2.039489000	0.613378000	7	-3.379333000	-2.008799000	0.689687000
6	-3.424497000	-3.241574000	1.411048000	6	-3.483752000	-3.183004000	1.524371000
6	-4.334365000	-1.976407000	-0.457188000	6	-4.345181000	-1.940505000	-0.383303000
1	-2.676766000	-3.150270000	2.205859000	1	-2.724875000	-3.103639000	2.309253000
1	-3.166358000	-4.150151000	0.820027000	1	-3.279701000	-4.120228000	0.958694000
6	-4.820430000	-3.440567000	1.998528000	6	-4.884135000	-3.291691000	2.124295000
1	-4.174904000	-2.769260000	-1.219449000	1	-4.221356000	-2.771026000	-1.109717000
1	-4.215623000	-1.015352000	-0.968181000	1	-4.178314000	-1.009270000	-0.934753000
6	-5.753645000	-2.125137000	0.085709000	6	-5.770190000	-2.010245000	0.160261000
1	-5.969026000	-1.268470000	0.738281000	1	-5.960133000	-1.118762000	0.771693000
1	-6.474200000	-2.116038000	-0.742942000	1	-6.486490000	-2.012820000	-0.672087000
6	-5.867998000	-3.419467000	0.887919000	6	-5.935185000	-3.264807000	1.016358000
1	-5.691156000	-4.272602000	0.214208000	1	-5.800261000	-4.151329000	0.377070000
1	-6.877535000	-3.535381000	1.301755000	1	-6.946808000	-3.319147000	1.437510000
1	-4.861467000	-4.386126000	2.555074000	1	-4.968215000	-4.212332000	2.716515000
1	-5.022117000	-2.621734000	2.702734000	1	-5.040923000	-2.437585000	2.797452000

5-Int3

E(scf) = −2456.04906479 a.u.

6	0.979842000	0.162442000	0.127020000
5	-2.500724000	-0.471349000	-0.994276000
7	-0.215689000	-0.512211000	-0.063166000
6	2.177548000	-0.506512000	-0.212601000
7	-2.616196000	0.033806000	-2.256089000
6	3.399229000	0.121861000	-0.027461000
1	4.304901000	-0.418497000	-0.292608000
6	3.493567000	1.439420000	0.436731000
6	1.054915000	1.516613000	0.495754000
6	2.302510000	2.125069000	0.655918000
1	2.318402000	3.180364000	0.913260000
6	-0.209661000	2.344270000	0.567124000
1	-0.981323000	1.759075000	0.045719000
6	0.078154000	2.698804000	3.074233000
1	1.141656000	2.505636000	2.963970000
6	-0.746719000	2.606616000	1.954066000
6	-0.454460000	3.024357000	4.321805000
1	0.200079000	3.083124000	5.187806000
6	-1.818089000	3.275189000	4.459894000
1	-2.232152000	3.529027000	5.432064000
6	-2.649490000	3.190389000	3.342669000
1	-3.716106000	3.375585000	3.440829000
6	-2.114063000	2.855977000	2.103150000
1	-2.757386000	2.783767000	1.227815000
6	-0.030204000	3.631870000	-0.231103000
6	0.384835000	3.523020000	-1.564777000
1	0.577326000	2.533289000	-1.971507000
6	0.553713000	4.652042000	-2.354940000
1	0.872840000	4.545810000	-3.389059000
6	0.321062000	5.920872000	-1.819777000
1	0.457125000	6.807547000	-2.433602000
6	-0.258638000	4.901855000	0.295945000
1	-0.578486000	5.004803000	1.328675000
6	-0.081288000	6.040038000	-0.493989000
1	-0.259472000	7.022892000	-0.064775000
6	2.061497000	-1.912812000	-0.768758000
1	1.158250000	-1.904897000	-1.391907000
6	1.799594000	-2.905325000	0.340854000

5-Int4

E(scf) = −2456.03812347 a.u.

6	1.153952000	0.301466000	0.143905000
5	-3.036308000	-0.709077000	0.037386000
7	0.523417000	-0.233988000	1.247515000
6	2.269271000	-0.360625000	-0.406123000
7	-4.370450000	-0.814509000	-0.221780000
6	2.958047000	0.214376000	-1.466296000
1	3.812760000	-0.321182000	-1.872948000
6	2.585762000	1.441383000	-2.016463000
6	0.838476000	1.597629000	-0.322579000
6	1.544722000	2.133042000	-1.396590000
1	1.264749000	3.116124000	-1.757164000
6	-0.239606000	2.387343000	0.401417000
1	-1.171004000	1.806220000	0.346135000
6	1.393414000	2.550673000	2.354826000
1	2.209302000	2.356178000	1.663893000
6	0.081429000	2.560863000	1.876569000
6	1.654771000	2.731571000	3.711190000
1	2.682544000	2.702651000	4.064829000
6	0.606091000	2.931930000	4.607703000
1	0.808586000	3.068869000	5.666906000
6	-0.706191000	2.943952000	4.137029000
1	-1.532257000	3.089362000	4.828913000
6	-0.962193000	2.758101000	2.781314000
1	-1.985633000	2.752522000	2.412427000
6	-0.524594000	3.714431000	-0.268970000
6	-1.437023000	3.763901000	-1.325524000
1	-1.961413000	2.854914000	-1.609944000
6	-1.665557000	4.949518000	-2.018475000
1	-2.380440000	4.969582000	-2.837549000
6	-0.977021000	6.107910000	-1.661308000
1	-1.152060000	7.036279000	-2.198791000
6	0.161781000	4.878380000	0.080535000
1	0.872379000	4.844660000	0.902203000
6	-0.062795000	6.067386000	-0.609972000
1	0.478694000	6.966111000	-0.325376000
6	2.788082000	-1.609438000	0.279942000
1	1.962706000	-1.983978000	0.900689000
6	3.872820000	-1.129260000	1.234141000

6	0.634607000	-3.671812000	0.342038000	6	3.487412000	-0.514652000	2.431654000
1	-0.095674000	-3.522387000	-0.448503000	1	2.427820000	-0.440485000	2.661870000
6	0.400798000	-4.609592000	1.346076000	6	4.442064000	0.031898000	3.283467000
1	-0.514058000	-5.196877000	1.329573000	1	4.123832000	0.506913000	4.208890000
6	1.331934000	-4.785433000	2.367526000	6	5.796198000	-0.027856000	2.953436000
1	1.151268000	-5.514118000	3.153439000	1	6.543172000	0.395914000	3.619999000
6	2.484758000	-4.000409000	2.391724000	6	6.184425000	-0.632896000	1.760060000
1	3.205399000	-4.116640000	3.197288000	1	7.236793000	-0.680239000	1.490514000
6	2.712404000	-3.063307000	1.387770000	6	5.227880000	-1.176550000	0.904048000
1	3.602827000	-2.438425000	1.406234000	1	5.532616000	-1.649347000	-0.026131000
6	3.218103000	-2.270302000	-1.684771000	6	3.199533000	-2.759337000	-0.619518000
6	4.021183000	-3.397603000	-1.520298000	6	3.880367000	-3.846736000	-0.057816000
1	3.834452000	-4.071682000	-0.689946000	1	4.170312000	-3.799718000	0.988932000
6	5.058124000	-3.668152000	-2.415682000	6	4.191377000	-4.970462000	-0.816487000
1	5.673953000	-4.552258000	-2.270247000	1	4.721264000	-5.800754000	-0.356170000
6	5.305028000	-2.815424000	-3.486271000	6	3.823219000	-5.034510000	-2.160454000
1	6.114762000	-3.025919000	-4.180129000	1	4.064960000	-5.912076000	-2.754498000
6	4.502523000	-1.686365000	-3.662740000	6	3.144814000	-3.961798000	-2.731519000
1	4.683493000	-1.012787000	-4.496795000	1	2.848143000	-3.993296000	-3.777278000
6	3.470895000	-1.421196000	-2.770999000	6	2.841014000	-2.835774000	-1.967800000
1	2.851847000	-0.534931000	-2.893799000	1	2.309216000	-2.007097000	-2.422295000
6	4.865222000	2.077160000	0.595925000	6	3.310612000	1.959884000	-3.248882000
6	4.781543000	3.506123000	1.128068000	6	2.766529000	3.307851000	-3.716930000
1	4.233033000	4.156868000	0.436179000	1	1.699090000	3.242070000	-3.961327000
1	5.793492000	3.911162000	1.249452000	1	3.308337000	3.628514000	-4.615060000
1	4.278433000	3.536727000	2.102723000	1	2.893015000	4.077181000	-2.945417000
6	5.704387000	1.243940000	1.571968000	6	4.805736000	2.116171000	-2.949281000
1	5.818755000	0.214112000	1.214074000	1	5.248795000	1.164729000	-2.633413000
1	5.228772000	1.212766000	2.559958000	1	4.961249000	2.846770000	-2.146506000
1	6.704971000	1.683239000	1.678938000	1	5.336672000	2.462025000	-3.846255000
6	5.565752000	2.107988000	-0.768858000	6	3.127440000	0.942099000	-4.382901000
1	5.665435000	1.099265000	-1.186625000	1	3.542924000	-0.034153000	-4.104813000
1	6.569285000	2.542851000	-0.668826000	1	3.636475000	1.287785000	-5.292590000
1	4.990212000	2.715296000	-1.478054000	1	2.061125000	0.807958000	-4.606104000
6	-3.452517000	1.234069000	-2.529805000	6	-5.012819000	-2.152300000	-0.117196000
6	-4.076749000	1.118383000	-3.923102000	6	-5.876312000	-2.392151000	-1.360138000
1	-4.602376000	2.057797000	-4.134751000	1	-6.426804000	-3.330193000	-1.215287000
1	-4.827676000	0.315265000	-3.902959000	1	-5.205562000	-2.530301000	-2.220214000
6	-3.049446000	0.798635000	-4.997950000	6	-6.820178000	-1.235974000	-1.655656000
1	-2.290293000	1.589996000	-5.048264000	1	-7.533097000	-1.101984000	-0.831475000
1	-3.530287000	0.751892000	-5.982161000	1	-7.410622000	-1.452472000	-2.553506000
6	-2.405580000	-0.537201000	-4.661785000	6	-6.001914000	0.030606000	-1.860723000
1	-3.186743000	-1.311157000	-4.653662000	1	-5.332559000	-0.116225000	-2.720479000
1	-1.663365000	-0.826855000	-5.416032000	1	-6.645851000	0.890229000	-2.084697000
6	-1.710408000	-0.534727000	-3.298915000	6	-5.142993000	0.381639000	-0.642733000
6	-2.644125000	2.523320000	-2.405216000	6	-5.845148000	-2.282718000	1.160697000
1	-1.851698000	2.606633000	-3.150875000	1	-6.771964000	-1.705312000	1.124185000
1	-2.179460000	2.587142000	-1.418203000	1	-5.262986000	-1.951509000	2.027519000
1	-3.310755000	3.385943000	-2.526397000	1	-6.115579000	-3.335549000	1.306184000
6	-4.580734000	1.282756000	-1.502534000	6	-3.916825000	-3.218541000	-0.084420000
1	-4.185524000	1.409570000	-0.487322000	1	-3.336534000	-3.179305000	0.844143000
1	-5.168676000	0.357668000	-1.534422000	1	-3.229308000	-3.091407000	-0.929349000
1	-5.237182000	2.129954000	-1.732426000	1	-4.387651000	-4.206500000	-0.153303000
6	-0.394808000	0.247601000	-3.349508000	6	-6.003462000	0.912520000	0.505485000
1	0.326399000	-0.297134000	-3.972102000	1	-6.418396000	1.888186000	0.225622000
1	0.007537000	0.332592000	-2.335401000	1	-5.387687000	1.038991000	1.402928000
1	-0.519250000	1.246900000	-3.775922000	1	-6.838950000	0.251614000	0.746031000
6	-1.385710000	-1.977130000	-2.916372000	6	-4.164200000	1.481809000	-1.045144000

1	-0.759911000	-2.420806000	-3.700146000	1	-4.729894000	2.339506000	-1.427210000
1	-2.306374000	-2.566249000	-2.822377000	1	-3.487995000	1.125719000	-1.831783000
1	-0.841672000	-2.003526000	-1.964985000	1	-3.559757000	1.822394000	-0.196039000
6	-2.455383000	-0.956593000	0.343182000	6	-1.638074000	-0.659080000	0.179686000
6	-1.136285000	-0.643070000	0.874069000	6	-0.751746000	-0.455034000	1.320177000
7	-0.925526000	-0.555871000	2.215225000	7	-1.298250000	-0.509348000	2.590639000
6	-1.972679000	-0.186871000	3.160291000	6	-2.378070000	-1.429147000	2.915682000
6	0.365751000	-0.765342000	2.845564000	6	-0.363243000	-0.400256000	3.708048000
1	-2.891800000	0.020410000	2.616641000	1	-3.146425000	-1.412421000	2.141619000
1	-1.645883000	0.735701000	3.657615000	1	-2.845661000	-1.068245000	3.842221000
6	-2.168063000	-1.265649000	4.215025000	6	-1.826363000	-2.837128000	3.125404000
1	0.707685000	0.185296000	3.282206000	1	-0.942419000	-0.075842000	4.583348000
1	1.092892000	-1.082944000	2.101367000	1	0.372266000	0.372288000	3.482352000
6	0.247325000	-1.838803000	3.925426000	6	0.292015000	-1.754517000	3.975409000
1	0.017358000	-2.789427000	3.430686000	1	0.883665000	-2.020357000	3.090434000
1	1.221809000	-1.956240000	4.415973000	1	0.981794000	-1.681844000	4.825858000
6	-0.844012000	-1.504114000	4.938254000	6	-0.772808000	-2.822107000	4.236609000
1	-0.567713000	-0.585586000	5.478643000	1	-1.277658000	-2.598009000	5.188950000
1	-0.938384000	-2.305490000	5.682115000	1	-0.311540000	-3.811971000	4.341294000
1	-2.945618000	-0.945089000	4.920379000	1	-2.639047000	-3.535987000	3.366140000
1	-2.511296000	-2.185438000	3.726968000	1	-1.372310000	-3.162422000	2.177408000
7	-3.364610000	-1.746816000	1.100430000	7	-1.198237000	-1.114766000	-1.109077000
6	-4.728600000	-1.746890000	0.601163000	6	-0.501435000	-2.384148000	-1.152735000
6	-2.875516000	-3.113840000	1.282170000	6	-0.819188000	-0.210860000	-2.180830000
1	-5.049419000	-0.704991000	0.486676000	1	-0.877686000	-3.006490000	-0.332018000
1	-5.360548000	-2.215997000	1.370824000	1	0.576995000	-2.235840000	-0.990178000
6	-4.904176000	-2.523435000	-0.709398000	6	-0.724137000	-3.084412000	-2.491700000
1	-3.505659000	-3.593736000	2.047160000	1	0.265734000	-0.022538000	-2.194061000
1	-1.852806000	-3.063295000	1.672102000	1	-1.315665000	0.749382000	-2.012283000
6	-2.932379000	-3.921068000	-0.013114000	6	-1.201204000	-0.835381000	-3.517358000
1	-2.276755000	-3.432691000	-0.745025000	1	-2.285936000	-1.017391000	-3.539471000
1	-2.556715000	-4.939915000	0.150047000	1	-0.948385000	-0.149972000	-4.336989000
6	-4.364238000	-3.946376000	-0.550583000	6	-0.444485000	-2.153914000	-3.672153000
1	-5.002854000	-4.489473000	0.163249000	1	0.630685000	-1.927677000	-3.709336000
1	-4.414049000	-4.487336000	-1.504223000	1	-0.702069000	-2.650970000	-4.615983000
1	-5.965225000	-2.538834000	-0.992665000	1	-0.081360000	-3.972417000	-2.544080000
1	-4.362977000	-2.011910000	-1.517940000	1	-1.770324000	-3.419133000	-2.545627000

5-TS4

E(scf) = −2456.03247272 a.u.

ν_{min} = −94.0 cm^{-1}

5-Int5

E(scf) = −2456.05153345 a.u.

6	1.346092000	0.001439000	0.425582000	6	1.377265000	0.005315000	0.463207000
5	-2.906143000	-0.165694000	-0.988919000	5	-2.835913000	-0.219990000	-0.755381000
7	0.075997000	-0.139658000	0.936437000	7	0.074495000	-0.123504000	0.899283000
6	2.107844000	-1.144212000	0.120150000	6	2.140214000	-1.147008000	0.193472000
7	-4.223007000	-0.047278000	-1.379396000	7	-4.178850000	-0.069969000	-1.217498000
6	3.415908000	-0.983928000	-0.319000000	6	3.472548000	-0.997879000	-0.171080000
1	3.986002000	-1.867695000	-0.589772000	1	4.050119000	-1.885789000	-0.410936000
6	4.008133000	0.276086000	-0.446148000	6	4.081807000	0.257608000	-0.260751000
6	1.937353000	1.275187000	0.360862000	6	1.975119000	1.275434000	0.417194000
6	3.255318000	1.391057000	-0.082596000	6	3.317367000	1.380752000	0.050420000
1	3.686017000	2.383056000	-0.159839000	1	3.757641000	2.369641000	-0.011715000
6	1.074159000	2.479836000	0.700075000	6	1.090886000	2.486599000	0.667758000
1	0.166038000	2.378142000	0.087476000	1	0.232581000	2.365224000	-0.009628000
6	1.008353000	1.634911000	3.121502000	6	0.802260000	1.685589000	3.089388000
1	1.767118000	0.899751000	2.873106000	1	1.574108000	0.940319000	2.925182000
6	0.573777000	2.518634000	2.136002000	6	0.473199000	2.559672000	2.055286000
6	0.441512000	1.656956000	4.394672000	6	0.111929000	1.725511000	4.299921000
1	0.775539000	0.942188000	5.142867000	1	0.365350000	1.017140000	5.084913000
6	-0.560060000	2.574939000	4.702746000	6	-0.908216000	2.653904000	4.498445000
1	-1.007874000	2.585913000	5.693163000	1	-1.451443000	2.678958000	5.439627000
6	-0.979985000	3.484385000	3.731177000	6	-1.221289000	3.556378000	3.481125000
1	-1.753594000	4.212544000	3.962322000	1	-2.006739000	4.293833000	3.627320000
6	-0.412735000	3.453759000	2.461476000	6	-0.532564000	3.506380000	2.273308000
1	-0.743393000	4.153902000	1.696667000	1	-0.783393000	4.198449000	1.471615000
6	1.734382000	3.778183000	0.292962000	6	1.776148000	3.774829000	0.272557000
6	1.579682000	4.256565000	-1.009795000	6	1.735578000	4.193609000	-1.059133000
1	0.935356000	3.715299000	-1.698543000	1	1.161591000	3.612494000	-1.777602000
6	2.248794000	5.403227000	-1.430172000	6	2.430258000	5.328712000	-1.468035000
1	2.116362000	5.764927000	-2.446862000	1	2.387496000	5.644605000	-2.507423000
6	3.086403000	6.084826000	-0.548696000	6	3.179451000	6.057695000	-0.545311000
1	3.610604000	6.979591000	-0.874198000	1	3.723381000	6.943941000	-0.861573000
6	2.572253000	4.468367000	1.170935000	6	2.527051000	4.510065000	1.190861000
1	2.688598000	4.098363000	2.186503000	1	2.555909000	4.184902000	2.227804000
6	3.245293000	5.614167000	0.753898000	6	3.225382000	5.645250000	0.785425000
1	3.895191000	6.141418000	1.447765000	1	3.806808000	6.209355000	1.510339000
6	1.433647000	-2.501094000	0.234758000	6	1.445798000	-2.497063000	0.265374000
1	0.503468000	-2.429448000	-0.348058000	1	0.558269000	-2.418332000	-0.379447000
6	0.994394000	-2.855859000	1.646697000	6	0.903325000	-2.845524000	1.642793000
6	0.118382000	-3.930913000	1.815034000	6	0.003713000	-3.909361000	1.746752000
1	-0.184587000	-4.502430000	0.939664000	1	-0.238022000	-4.480232000	0.852097000
6	-0.378904000	-4.259214000	3.072031000	6	-0.593329000	-4.226900000	2.962956000
1	-1.069175000	-5.092109000	3.181351000	1	-1.299709000	-5.051395000	3.021255000
6	0.003980000	-3.514864000	4.188277000	6	-0.288278000	-3.483032000	4.103245000
1	-0.389490000	-3.760234000	5.171363000	1	-0.757864000	-3.720798000	5.054310000
6	0.900872000	-2.459980000	4.033471000	6	0.632211000	-2.440337000	4.014881000
1	1.209324000	-1.875286000	4.896829000	1	0.882437000	-1.857823000	4.898352000
6	1.396093000	-2.137974000	2.771355000	6	1.227444000	-2.129325000	2.793858000
1	2.075170000	-1.299833000	2.646820000	1	1.923230000	-1.298851000	2.719487000
6	2.268847000	-3.595305000	-0.392026000	6	2.309008000	-3.600002000	-0.304456000
6	3.228880000	-4.284471000	0.351624000	6	3.202216000	-4.307791000	0.501664000
1	3.316680000	-4.078179000	1.415388000	1	3.216756000	-4.109506000	1.570472000
6	4.059275000	-5.221407000	-0.258706000	6	4.060398000	-5.253780000	-0.054165000
1	4.802716000	-5.750286000	0.332390000	1	4.751243000	-5.797868000	0.584940000
6	3.937875000	-5.481381000	-1.623038000	6	4.033837000	-5.502880000	-1.425605000
1	4.584901000	-6.213128000	-2.099739000	1	4.702342000	-6.241609000	-1.859976000
6	2.979760000	-4.799473000	-2.371569000	6	3.143391000	-4.800757000	-2.236655000
1	2.876112000	-4.997713000	-3.435497000	1	3.114864000	-4.990111000	-3.306811000
6	2.153127000	-3.861750000	-1.757820000	6	2.288618000	-3.854372000	-1.677292000

1	1.414068000	-3.319225000	-2.342011000	1	1.603293000	-3.293231000	-2.308545000
6	5.420889000	0.376193000	-1.003390000	6	5.526572000	0.344631000	-0.732323000
6	5.917696000	1.819066000	-1.067181000	6	6.042068000	1.782177000	-0.758223000
1	5.277965000	2.431516000	-1.714484000	1	5.451247000	2.404640000	-1.441455000
1	6.936164000	1.836772000	-1.473762000	1	7.084140000	1.790315000	-1.100052000
1	5.936274000	2.277943000	-0.070942000	1	6.003561000	2.236883000	0.239431000
6	6.383542000	-0.431353000	-0.124624000	6	6.426411000	-0.477928000	0.197579000
1	6.085223000	-1.485050000	-0.074296000	1	6.114485000	-1.528518000	0.224635000
1	6.399934000	-0.030382000	0.896158000	1	6.387483000	-0.081986000	1.219710000
1	7.400427000	-0.381699000	-0.536045000	1	7.466127000	-0.437740000	-0.153172000
6	5.433754000	-0.203950000	-2.424166000	6	5.616827000	-0.228593000	-2.152927000
1	5.110722000	-1.251697000	-2.424998000	1	5.284758000	-1.273210000	-2.179056000
1	6.447099000	-0.153405000	-2.844706000	1	6.653361000	-0.185656000	-2.513181000
1	4.755872000	0.362352000	-3.075505000	1	4.983383000	0.348071000	-2.838624000
6	-5.148559000	-1.191440000	-1.249226000	6	-5.135974000	-1.189723000	-1.160208000
6	-5.958803000	-1.339561000	-2.540488000	6	-5.854567000	-1.347079000	-2.509200000
1	-6.706097000	-2.129825000	-2.392129000	1	-6.616710000	-2.130399000	-2.401803000
1	-5.277062000	-1.668894000	-3.337258000	1	-5.119872000	-1.695408000	-3.249045000
6	-6.614687000	-0.032382000	-2.964369000	6	-6.460705000	-0.046270000	-3.007328000
1	-7.343945000	0.293088000	-2.211103000	1	-7.224420000	0.319638000	-2.308105000
1	-7.169491000	-0.174711000	-3.899354000	1	-6.962015000	-0.203752000	-3.970115000
6	-5.540725000	1.029428000	-3.151441000	6	-5.342861000	0.971329000	-3.152419000
1	-4.863448000	0.709879000	-3.955913000	1	-4.626322000	0.602087000	-3.899724000
1	-5.981100000	1.989330000	-3.449952000	1	-5.726492000	1.936296000	-3.508394000
6	-4.699317000	1.260048000	-1.890298000	6	-4.578535000	1.210090000	-1.843185000
6	-6.083890000	-1.041514000	-0.043834000	6	-6.187541000	-1.050458000	-0.049488000
1	-6.902910000	-0.341694000	-0.227359000	1	-6.954236000	-0.310892000	-0.295416000
1	-5.518490000	-0.693316000	0.824170000	1	-5.721076000	-0.752665000	0.891811000
1	-6.530462000	-2.014537000	0.195371000	1	-6.695564000	-2.011563000	0.101694000
6	-4.316104000	-2.455788000	-1.044580000	6	-4.359081000	-2.487565000	-0.932685000
1	-3.770011000	-2.418655000	-0.094857000	1	-3.898606000	-2.524733000	0.056948000
1	-3.596588000	-2.583258000	-1.861909000	1	-3.574539000	-2.597175000	-1.690797000
1	-4.984129000	-3.324829000	-1.022648000	1	-5.045901000	-3.338970000	-1.010002000
6	-5.493358000	2.021297000	-0.824864000	6	-5.426732000	2.044940000	-0.874421000
1	-6.469117000	1.573142000	-0.624317000	1	-5.617117000	3.037787000	-1.302159000
1	-5.660674000	3.052269000	-1.160407000	1	-4.885024000	2.170066000	0.070229000
1	-4.922981000	2.045200000	0.111266000	1	-6.392964000	1.582839000	-0.657296000
6	-3.494780000	2.117981000	-2.278905000	6	-3.350477000	2.044433000	-2.204733000
1	-3.856322000	3.016966000	-2.792290000	1	-3.689976000	2.948864000	-2.724288000
1	-2.818069000	1.565730000	-2.942798000	1	-2.677457000	1.478286000	-2.857723000
1	-2.927675000	2.429331000	-1.393982000	1	-2.791871000	2.351378000	-1.312453000
6	-1.465677000	-0.102893000	-1.080789000	6	-1.432261000	-0.133386000	-1.191790000
6	-1.016950000	-0.176852000	0.277945000	6	-0.944757000	-0.176087000	0.137609000
7	-2.238941000	-0.321540000	1.072087000	7	-2.279033000	-0.300684000	0.819169000
6	-2.427182000	0.857577000	1.928892000	6	-2.526405000	0.923843000	1.630125000
6	-2.184555000	-1.556000000	1.866210000	6	-2.265592000	-1.501019000	1.696754000
1	-2.433016000	1.738760000	1.276972000	1	-2.530396000	1.769433000	0.934653000
1	-1.572051000	0.950132000	2.612811000	1	-1.674419000	1.039402000	2.308196000
6	-3.715526000	0.747163000	2.724724000	6	-3.813432000	0.834413000	2.423851000
1	-1.307507000	-1.514391000	2.528890000	1	-1.385607000	-1.397762000	2.343039000
1	-2.026346000	-2.391094000	1.175653000	1	-2.094582000	-2.367865000	1.054082000
6	-3.447059000	-1.745018000	2.689491000	6	-3.509969000	-1.643078000	2.553808000
1	-4.305894000	-1.905409000	2.025083000	1	-4.387029000	-1.868175000	1.937691000
1	-3.327015000	-2.648345000	3.300106000	1	-3.348655000	-2.500187000	3.218852000
6	-3.695750000	-0.523400000	3.572011000	6	-3.761189000	-0.370386000	3.358340000
1	-2.877447000	-0.441647000	4.302112000	1	-2.935374000	-0.224597000	4.069687000
1	-4.631423000	-0.633936000	4.133908000	1	-4.688505000	-0.458008000	3.936891000
1	-3.812111000	1.636313000	3.359708000	1	-3.921181000	1.765038000	2.994087000

1	-4.572217000	0.731154000	2.037392000	1	-4.667691000	0.759273000	1.740913000
7	-0.725836000	0.077133000	-2.278763000	7	-0.732375000	0.048851000	-2.408917000
6	0.132208000	-1.035662000	-2.656560000	6	0.127553000	-1.080193000	-2.746978000
6	-0.033268000	1.352886000	-2.391446000	6	0.024064000	1.296634000	-2.463515000
1	-0.442104000	-1.961736000	-2.527736000	1	-0.462898000	-1.999287000	-2.645793000
1	1.023097000	-1.092671000	-2.007868000	1	0.982187000	-1.143083000	-2.047804000
6	0.610446000	-0.885906000	-4.095257000	6	0.682422000	-0.938375000	-4.158255000
1	0.854649000	1.387224000	-1.738393000	1	0.880909000	1.271979000	-1.768050000
1	-0.723376000	2.141548000	-2.069475000	1	-0.640541000	2.111735000	-2.155013000
6	0.432935000	1.589268000	-3.821978000	6	0.563697000	1.538272000	-3.866663000
1	-0.442190000	1.642150000	-4.484608000	1	-0.279559000	1.627977000	-4.564991000
1	0.963071000	2.549530000	-3.877952000	1	1.124529000	2.482404000	-3.885639000
6	1.343236000	0.443789000	-4.259828000	6	1.457502000	0.371677000	-4.281206000
1	2.237975000	0.437629000	-3.617990000	1	2.326452000	0.334426000	-3.606093000
1	1.678784000	0.581493000	-5.295246000	1	1.836299000	0.509089000	-5.301605000
1	1.270111000	-1.726479000	-4.348798000	1	1.330831000	-1.795637000	-4.383605000
1	-0.257340000	-0.915501000	-4.768252000	1	-0.152191000	-0.944380000	-4.872071000

5-TS5

E(scf) = −2456.02783845 a.u.

ν_{min} = −190.1 cm^{-1}

6	1.491955000	0.018067000	0.315754000	7	-0.568445000	-0.508441000	0.772724000
5	-2.950639000	-0.284538000	-0.666921000	6	-1.614862000	0.286517000	0.296373000
7	0.163030000	-0.247586000	0.604222000	5	2.994713000	-0.152144000	0.676146000
6	2.355617000	-1.057063000	0.048733000	6	-2.904810000	-0.189276000	0.587605000
7	-4.312894000	-0.110189000	-1.090451000	7	1.979309000	-1.955977000	-0.995286000
6	3.703213000	-0.793555000	-0.159285000	7	4.265445000	-0.075373000	0.051932000
1	4.366454000	-1.624574000	-0.380945000	6	-4.014731000	0.551464000	0.194560000
6	4.221304000	0.504673000	-0.106653000	1	-5.000142000	0.161604000	0.423292000
6	1.982285000	1.328639000	0.388081000	6	-3.877704000	1.770646000	-0.471179000
6	3.343090000	1.550652000	0.172668000	7	2.776055000	0.468499000	1.992392000
1	3.707369000	2.571104000	0.214388000	6	-2.586760000	2.209351000	-0.768221000
6	0.993925000	2.446653000	0.665887000	1	-2.447713000	3.141343000	-1.309358000
1	0.159591000	2.289589000	-0.032700000	6	-1.450014000	1.487172000	-0.415967000
6	0.766531000	1.488852000	3.034154000	6	-0.332622000	4.217701000	0.045838000
1	1.594550000	0.816507000	2.832061000	1	-0.844846000	3.753509000	0.883539000
6	0.363943000	2.388399000	2.048616000	6	0.091213000	3.413649000	-1.019641000
6	0.086285000	1.415024000	4.249224000	6	-0.091585000	1.907326000	-0.923834000
1	0.400617000	0.690936000	4.996879000	1	0.650685000	1.568492000	-0.191074000
6	-0.998100000	2.252323000	4.499859000	6	-0.109666000	5.589819000	0.038824000
1	-1.533550000	2.188638000	5.443583000	1	-0.446156000	6.194651000	0.877207000
6	-1.390737000	3.175363000	3.529476000	6	0.542485000	6.187089000	-1.040503000
1	-2.232312000	3.838026000	3.715153000	1	0.718560000	7.259539000	-1.049035000
6	-0.712108000	3.239815000	2.317253000	6	0.733677000	4.021075000	-2.098288000
1	-1.021806000	3.949620000	1.552897000	1	1.063840000	3.414309000	-2.935956000
6	1.576727000	3.803834000	0.342815000	6	0.241170000	1.167133000	-2.207938000
6	1.568264000	4.250541000	-0.980707000	6	-0.740930000	0.791175000	-3.126110000
1	1.095360000	3.633901000	-1.742472000	1	-1.782762000	1.019609000	-2.919565000
6	2.168171000	5.458229000	-1.325460000	6	-0.397296000	0.098622000	-4.286088000
1	2.150934000	5.796086000	-2.358616000	1	-1.174913000	-0.200266000	-4.984386000
6	2.789976000	6.232593000	-0.346354000	6	0.933583000	-0.217494000	-4.546082000
1	3.259099000	7.176071000	-0.612843000	1	1.199669000	-0.769360000	-5.443735000
6	2.200900000	4.583298000	1.317308000	6	1.920927000	0.164881000	-3.639536000
1	2.204997000	4.235924000	2.347319000	1	2.961366000	-0.090705000	-3.820032000
6	2.804790000	5.791721000	0.975597000	6	1.574736000	0.850471000	-2.480994000
1	3.287561000	6.390361000	1.743879000	1	2.341704000	1.110758000	-1.756774000
6	1.757115000	-2.450253000	-0.013185000	6	0.959367000	5.397923000	-2.107695000

Product (5)

E(scf) = −2456.07563798 a.u.

1	0.900272000	-2.382143000	-0.699910000	1	1.462510000	5.851972000	-2.957611000
6	1.172055000	-2.917277000	1.310037000	6	-4.423456000	-1.813563000	1.764446000
6	0.311733000	-4.018261000	1.302345000	6	-3.030262000	-1.562372000	1.223821000
1	0.120980000	-4.529086000	0.360619000	1	-2.336620000	-1.580432000	2.075345000
6	-0.310362000	-4.447893000	2.470111000	6	-7.023813000	-2.092432000	2.777672000
1	-0.986814000	-5.298544000	2.442230000	1	-8.031127000	-2.203001000	3.170529000
6	-0.075883000	-3.778810000	3.671781000	6	-6.670704000	-2.695515000	1.573392000
1	-0.569919000	-4.102587000	4.584205000	1	-7.402967000	-3.279673000	1.021756000
6	0.800647000	-2.696124000	3.693275000	6	-5.377888000	-2.556338000	1.069021000
1	0.993741000	-2.169437000	4.624684000	1	-5.103161000	-3.031400000	0.131328000
6	1.425638000	-2.274727000	2.520891000	6	-2.564474000	-2.645152000	0.265942000
1	2.091254000	-1.416229000	2.534118000	6	-2.792480000	-2.551877000	-1.109044000
6	2.721107000	-3.447202000	-0.615265000	1	-3.264087000	-1.656985000	-1.507448000
6	3.558994000	-4.230914000	0.178506000	6	-2.407045000	-3.582429000	-1.964022000
1	3.463081000	-4.177421000	1.259988000	1	-2.585487000	-3.491090000	-3.032415000
6	4.502051000	-5.073221000	-0.407828000	6	-1.779506000	-4.717489000	-1.455755000
1	5.148544000	-5.680067000	0.221078000	1	-1.462759000	-5.513762000	-2.124004000
6	4.616890000	-5.138294000	-1.795031000	6	-1.533036000	-4.810907000	-0.086575000
1	5.351463000	-5.796083000	-2.252158000	1	-1.026824000	-5.683846000	0.317617000
6	3.782533000	-4.356922000	-2.594514000	6	-1.925663000	-3.781352000	0.765158000
1	3.864761000	-4.403429000	-3.677474000	1	-1.731195000	-3.850177000	1.833083000
6	2.842800000	-3.516688000	-2.005161000	6	0.589172000	-0.668969000	0.416322000
1	2.197610000	-2.892596000	-2.621698000	6	1.822056000	-0.954450000	0.015331000
6	5.704207000	0.719951000	-0.376119000	6	2.693408000	-3.115906000	-0.478413000
6	6.103268000	2.191034000	-0.282936000	1	2.066873000	-3.656689000	0.259724000
1	5.556684000	2.798871000	-1.014373000	1	3.582973000	-2.755845000	0.049369000
1	7.176364000	2.291061000	-0.485928000	6	3.065350000	-4.061334000	-1.611411000
1	5.903080000	2.594578000	0.717214000	1	3.740656000	-3.533534000	-2.299248000
6	6.529351000	-0.073750000	0.644085000	1	3.605904000	-4.925744000	-1.205170000
1	6.298731000	-1.144262000	0.593443000	6	1.808034000	-4.498381000	-2.359215000
1	6.319793000	0.274678000	1.662769000	1	1.164046000	-5.068751000	-1.672887000
1	7.600882000	0.056871000	0.443468000	1	2.061821000	-5.156712000	-3.199835000
6	6.034593000	0.216327000	-1.787337000	6	1.045499000	-3.267615000	-2.836731000
1	5.792727000	-0.847429000	-1.895852000	1	1.645104000	-2.718000000	-3.573839000
1	7.104988000	0.350027000	-1.992764000	1	0.099791000	-3.550640000	-3.313627000
1	5.461948000	0.775227000	-2.537642000	6	0.744774000	-2.338696000	-1.672290000
6	-5.280047000	-1.216302000	-0.983087000	1	0.258766000	-1.428683000	-2.035194000
6	-6.157082000	-1.270371000	-2.242898000	1	0.052161000	-2.838182000	-0.972736000
1	-6.914550000	-2.052350000	-2.098189000	6	6.559783000	-0.639843000	0.730240000
1	-5.521611000	-1.573185000	-3.087481000	1	6.210237000	-1.545954000	1.245515000
6	-6.796522000	0.066975000	-2.573172000	1	7.430270000	-0.257237000	1.278373000
1	-7.463152000	0.385275000	-1.760525000	6	5.442953000	0.400563000	0.755149000
1	-7.413911000	-0.016808000	-3.476050000	1	5.152905000	0.648550000	1.779099000
6	-5.688165000	1.084386000	-2.780477000	1	5.817469000	1.320609000	0.272013000
1	-5.074100000	0.768527000	-3.635803000	6	6.926086000	-0.978498000	-0.711923000
1	-6.096801000	2.076501000	-3.012899000	1	7.327750000	-0.075134000	-1.195852000
6	-4.767532000	1.214838000	-1.559530000	1	7.710205000	-1.744943000	-0.750574000
6	-6.177757000	-1.154716000	0.260162000	6	5.679509000	-1.437828000	-1.461744000
1	-6.922045000	-0.356363000	0.204522000	1	5.898683000	-1.601234000	-2.525096000
1	-5.569682000	-0.998174000	1.153720000	1	5.339639000	-2.395780000	-1.048462000
1	-6.719578000	-2.103201000	0.371500000	6	4.550189000	-0.415815000	-1.334710000
6	-4.514095000	-2.540071000	-0.936778000	1	4.850777000	0.506619000	-1.864288000
1	-3.992973000	-2.673826000	0.012700000	1	3.639585000	-0.806977000	-1.791186000
1	-3.786081000	-2.586938000	-1.755630000	6	2.721090000	-0.401633000	3.179100000
1	-5.220600000	-3.372027000	-1.044879000	6	3.647552000	0.164348000	4.268098000
6	-5.492085000	1.971421000	-0.434350000	1	3.542991000	-0.450753000	5.172038000
1	-6.458394000	1.527147000	-0.184190000	1	4.686024000	0.062608000	3.918408000
1	-5.670378000	3.011769000	-0.736209000	6	3.374878000	1.629742000	4.570615000

1	-4.870871000	1.969331000	0.469067000	1	4.069665000	1.997239000	5.336304000
6	-3.583753000	2.080201000	-1.990447000	1	2.363410000	1.746121000	4.981483000
1	-3.976322000	3.013756000	-2.412126000	6	3.523962000	2.440999000	3.291454000
1	-2.978844000	1.562430000	-2.742277000	1	4.569717000	2.383181000	2.956780000
1	-2.938536000	2.332836000	-1.140394000	1	3.294622000	3.500686000	3.467110000
6	-1.605811000	-0.091736000	-1.273658000	6	2.623552000	1.920415000	2.159607000
6	-0.843487000	-0.228688000	-0.115363000	6	3.261673000	-1.788293000	2.818867000
7	-2.443665000	-0.557421000	0.815102000	1	3.352323000	-2.386418000	3.733747000
6	-2.589307000	0.548775000	1.771730000	1	4.253208000	-1.710762000	2.354876000
6	-2.195448000	-1.828524000	1.498821000	1	2.589159000	-2.310738000	2.131094000
1	-2.790724000	1.463172000	1.204615000	6	1.311026000	-0.608731000	3.754856000
1	-1.617318000	0.668133000	2.267774000	1	1.346941000	-1.379657000	4.536327000
6	-3.650288000	0.298531000	2.830890000	1	0.623122000	-0.937098000	2.970673000
1	-1.222639000	-1.730490000	2.003528000	1	0.906033000	0.298665000	4.208517000
1	-2.085991000	-2.609509000	0.741974000	6	1.164271000	2.320636000	2.463573000
6	-3.250262000	-2.162499000	2.544877000	1	1.021501000	3.388194000	2.259695000
1	-4.224140000	-2.341470000	2.072509000	1	0.894829000	2.147223000	3.508722000
1	-2.945427000	-3.089324000	3.046094000	1	0.467458000	1.747454000	1.844876000
6	-3.363415000	-1.017639000	3.550104000	6	3.036871000	2.654986000	0.881675000
1	-2.405004000	-0.921873000	4.081739000	1	2.867942000	3.728922000	1.019551000
1	-4.137941000	-1.231173000	4.296825000	1	2.447700000	2.345594000	0.013684000
1	-3.623242000	1.137607000	3.537020000	1	4.092871000	2.493685000	0.653998000
1	-4.646424000	0.282315000	2.372807000	6	-4.786672000	-1.211511000	2.972771000
7	-1.045350000	0.185831000	-2.552357000	1	-4.046469000	-0.621508000	3.509538000
6	-0.287636000	-0.951720000	-3.064697000	6	-6.074891000	-1.348307000	3.479134000
6	-0.216172000	1.388345000	-2.536231000	1	-6.339543000	-0.876245000	4.421903000
1	-0.934306000	-1.835513000	-3.021481000	6	-5.067101000	2.618108000	-0.897504000
1	0.596561000	-1.148428000	-2.421806000	6	-5.046494000	2.787363000	-2.421818000
6	0.195202000	-0.691598000	-4.485667000	6	-6.400335000	1.989914000	-0.496993000
1	0.670532000	1.246654000	-1.886990000	6	-4.960344000	3.998405000	-0.236823000
1	-0.815790000	2.203109000	-2.113730000	1	-4.120830000	3.270717000	-2.754924000
6	0.265209000	1.740805000	-3.936611000	1	-5.892607000	3.409256000	-2.741495000
1	-0.606980000	1.956478000	-4.568415000	1	-5.123582000	1.812384000	-2.918776000
1	0.885695000	2.645980000	-3.894376000	1	-6.468837000	1.859122000	0.589851000
6	1.051474000	0.571922000	-4.524431000	1	-6.538337000	1.009757000	-0.969881000
1	1.954755000	0.409748000	-3.916991000	1	-7.220732000	2.643073000	-0.817304000
1	1.377399000	0.793162000	-5.548261000	1	-4.988346000	3.904361000	0.855458000
1	0.761601000	-1.560116000	-4.846573000	1	-5.799838000	4.630419000	-0.554408000
1	-0.680597000	-0.563311000	-5.135592000	1	-4.025911000	4.500529000	-0.513730000

References

1. K. Junold, J. A. Baus, C. Burschka and R. Tacke, *Angew. Chem. Int. Ed.*, 2012, **51**, 7020-7023.
2. P. Paetzold, C. von Plotho, G. Schmid, R. Boese, B. Schrader, D. Bougeard, U. Pfeiffer, R. Gleiter and W. Schüfer, *Chem. Ber.*, 1984, **117**, 1089-1102.
3. A. R. Petrov, C. G. Daniliuc, P. G. Jones and M. Tamm, *Chem. - Eur. J.*, 2010, **16**, 11804-11808.
4. J. Bohnke, T. Bruckner, A. Hermann, O. F. Gonzalez-Belman, M. Arrowsmith, J. O. C. Jimenez-Halla and H. Braunschweig, *Chem. Sci.*, 2018, **9**, 5354-5359.
5. A. J. Arduengo, H. V. R. Dias, R. L. Harlow and M. Kline, *J. Am. Chem. Soc.*, 1992, **114**, 5530-5534.
6. G. Sheldrick, *Acta Crystallogr. Sect. A: Found. Crystallogr.*, 2015, **71**, 3-8.
7. G. Sheldrick, *Acta Crystallogr. Sect. A: Found. Crystallogr.*, 2008, **64**, 112-122.
8. Gaussian 09, Revision E.01, M. J. Frisch; G. W. Trucks; H. B. Schlegel; G. E. Scuseria; M. A. Robb; J. R. Cheeseman; G. Scalmani; V. Barone; B. Mennucci; G. A. Petersson; H. Nakatsuji; M. Caricato; X. Li; H. P. Hratchian; A. F. Izmaylov; J. Bloino; G. Zheng; J. L. Sonnenberg; M. Hada; M. Ehara; K. Toyota; R. Fukuda; J. Hasegawa; M. Ishida; T. Nakajima; Y. Honda; O. Kitao; H. Nakai; T. Vreven; J. A. Montgomery Jr; J. E. Peralta; F. Ogliaro; M. Bearpark; J. J. Heyd; E. Brothers; K. N. Kudin; V. N. Staroverov; R. Kobayashi; J. Normand; K. Raghavachari; A. Rendell; J. C. Burant; S. S. Iyengar; J. Tomasi; M. Cossi; N. Rega; J. M. Millam; M. Klene; J. E. Knox; J. B. Cross; V. Bakken; C. Adamo; J. Jaramillo; R. Gomperts; R. E. Stratmann; O. Yazyev; A. J. Austin; R. Cammi; C. Pomelli; J. W. Ochterski; R. L. Martin; K. Morokuma; V. G. Zakrzewski; G. A. Voth; P. Salvador; J. J. Dannenberg; S. Dapprich; A. D. Daniels; Ö. Farkas; J. B. Foresman; J. V. Ortiz; J. Cioslowski; D. J. Fox. Gaussian, Inc., Wallingford CT, 2009.
9. Y. Zhao and D. G. Truhlar, *J. Chem. Theory Comput.*, 2008, **4**, 1849-1868.
10. T. R. Cundari and W. J. Stevens, *J. Chem. Phys.*, 1993, **98**, 5555-5565.
11. W. J. Stevens, M. Krauss, H. Basch and P. G. Jasien, *Can. J. Chem.*, 1992, **70**, 612-630.
12. W. J. Stevens, H. Basch and M. Krauss, *J. Chem. Phys.*, 1984, **81**, 6026-6033.
13. N. Riache, A. Dery, E. Callens, A. Poater, M. Samantaray, R. Dey, J. Hong, K. Li, L. Cavallo and J.-M. Basset, *Organometallics*, 2015, **34**, 690-695.
14. E. Pump, C. Slugovc, L. Cavallo and A. Poater, *Organometallics*, 2015, **34**, 3107-3111.
15. A. Poater, E. Pump, S. V. C. Vummaleti and L. Cavallo, *J. Chem. Theory Comput.*, 2014, **10**, 4442-4448.
16. S. Manzini, A. Poater, D. J. Nelson, L. Cavallo, A. M. Z. Slawin and S. P. Nolan, *Angew. Chem. Int. Ed.*, 2014, **53**, 8995-8999.
17. S. Manzini, A. Poater, D. J. Nelson, L. Cavallo and S. P. Nolan, *Chem. Sci.*, 2014, **5**, 180-188.
18. C. A. Urbina-Blanco, A. Poater, T. Lebl, S. Manzini, A. M. Z. Slawin, L. Cavallo and S. P. Nolan, *J. Am. Chem. Soc.*, 2013, **135**, 7073-7079.
19. X. Solans-Monfort, C. Copéret and O. Eisenstein, *Organometallics*, 2012, **31**, 6812-6822.
20. M. García-Melchor, M. C. Pacheco, C. Nájera, A. Lledós and G. Ujaque, *ACS Catalysis*, 2012, **2**, 135-144.
21. F. P. Rotzinger, *Chem. Rev.*, 2005, **105**, 2003-2038.
22. R. L. Martin, P. J. Hay and L. R. Pratt, *J. Phys. Chem. A*, 1998, **102**, 3565-3573.
23. M. Cossi, V. Barone, B. Mennucci and J. Tomasi, *Chem. Phys. Lett.*, 1998, **286**, 253-260.
24. V. Barone, M. Cossi and J. Tomasi, *J. Comput. Chem.*, 1998, **19**, 404-417.
25. V. Barone and M. Cossi, *J. Phys. Chem. A*, 1998, **102**, 1995-2001.
26. J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.*, 2005, **105**, 2999-3094.
27. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378-6396.
28. C. Adamo and V. Barone, *J. Chem. Phys.*, 1999, **110**, 6158-6170.
29. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
30. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.
31. Dunning, T. H. Jr.; Hay, P. J. in Methods of Electronic Structure Theory, Vol. 2, H. F. Schaefer III, ed., Plenum Press, 1977.