Electronic Supplementary Material (ESI) for ChemComm.

Mixed diboration of alkenes in a metal-free context

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Content:

1.Instrumentation and Chemicals

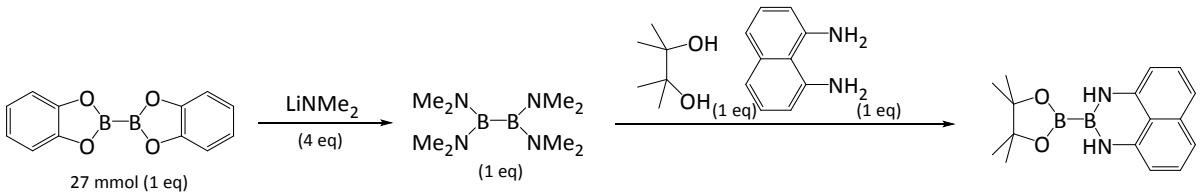
Substrates and reagents were obtained from commercial suppliers and used without further purification. All reactions were carried out under argon atmosphere using standard Schlenk-type techniques. Methanol (MeOH) was dried by calcium hydride destillation. Dichloromethane (DCM), tetrahydrofuran (THF) and n-hexane were dried and purified with a solvent purification system Pure SOLV system-4.

Deuterated chloroform ($CDCl_3$) was used as solvent for routine NMR measurements. NMR spectra were obtained on either Varian Gemini 300 or Varian Mercury 400 spectrometer. ^1H NMR chemical shifts are reported in ppm (δ) relative to tetramethylsilane, references to the chemical shifts or residual solvent resonances. ^{11}B NMR chemical shifts are reported in ppm (δ) relative to $BF_3(CH_3)_2O$. Coupling constants (*J*) are given in Hz, and the multiplicity of the NMR signals is described as singlet (s), doublet (d), triplet (t), quartet (t) and multiplet (m).

GC analyses were performed on a HP6890 gas chromatograph and an Agilent Technologies 5973 Mass selective detector (Waldbronn, Germany) equipped with an achiral capillary column HP-5 (30m, 0.25mm i. d., 0.25μm thickness) using He as the carrier gas.
ESI-TOF accurate mass analyses were carried using a 6210 Time of Flight (TOF) mass spectrometer from Agilent Technologies (Waldbronn, Germany) with an ESI interface.

2.Synthesis of the Bpin-Bdan reagent

To synthesize the mixed diboron reagent Bpin-Bdan and use it in the organocatalytic diboration reaction of alkenes, we adapted the synthetic protocol from Suginome's method.[1] Tetrakis(dimethylamino)diboron, $B_2(NMe_2)_4$, was mixed with 1,8-diaminonaphthalene and pinacol in a 1:1:1 ratio. However, since we prepared $B_2(NMe_2)_4$ from B_2cat_2 instead of BCl_3SMe_2, the global isolated yield of Bpin-Bdan resulted slightly higher (up to 75%).

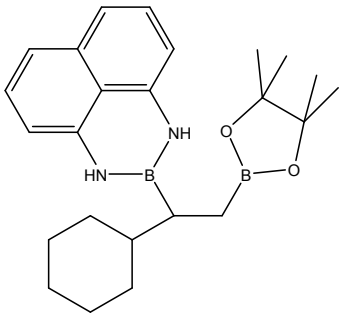


Scheme 1. Optimized synthesis of Bpin-Bdan from B_2cat_2.

3.Experimental procedure for the organocatalytic diboration of olefins

To an oven-dried Schlenk tube with a magnetic stir bar, Bpin-Bdan (0.161 g, 0.55 mmol) was added under argon. Furthermore cesiumm carbonate (48.8 mg for 30 mol% or 81.4 mg for 50 mol%), MeOH (2 mL) and substrate (0.50 mmol) were added. The vial was sealed with a teflon septum cap and heated to 70ºC in an oil bath for 16 hours. The reaction mixture was cooled to room temperature. An aliquot of 0.1 mL was diluted in dichloromethane and analysed by GC-MS to determine de conversion and selectivity. The sample was combined with the rest of the reaction mixture, all the volatiles were removed in vacuum and the crude product was purified by column chromatography.

4.Characterization of the new diborated products

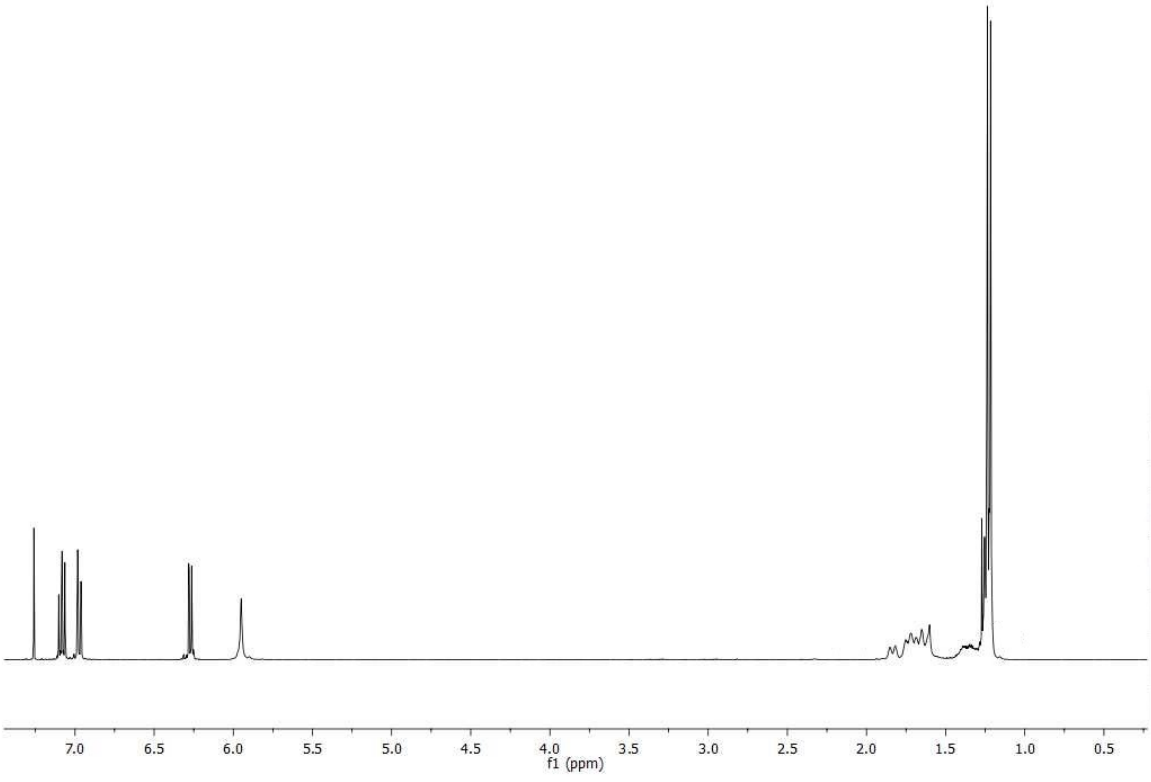


2-(1-cyclohexyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)-2,3-dihydro-1*H*-naphtho-1,8-[1,3,2]diazaborinine:

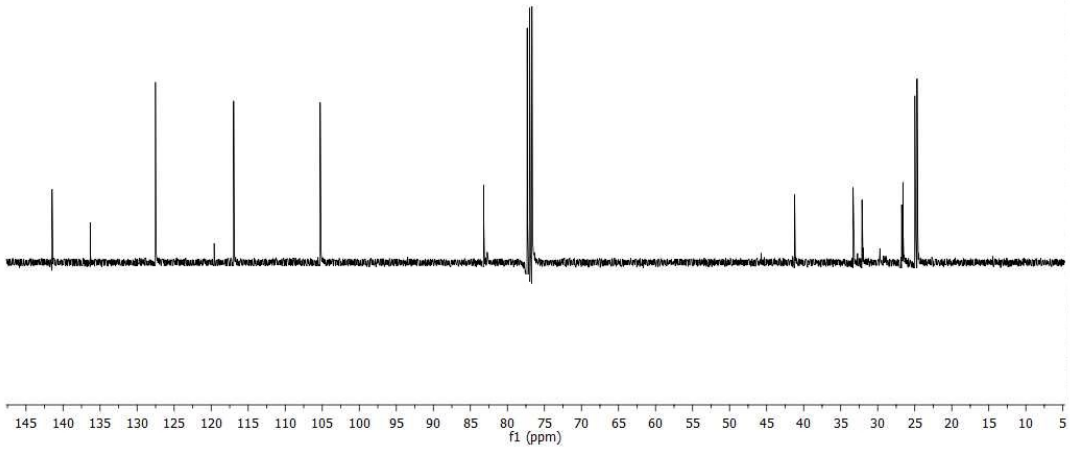
The product was purified by flash column chromatography deactivated with 10% of Et_3N (petroleum ether/EtOAc = 8:1) as a yellow oil (40 % isolated yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11 (dd, J=8.8 J=8.0 Hz, 2H), 7.02 (d, J=8.8 Hz, 2H), 6.35 (d, J=8.0 Hz, 2H), 5.95 (br s, 2H), 1.82 (m, 1H), 1.75 (m, 11H), 1.33 (m, 2H), 1.12 (s, 6H), 1.10 (s, 6H); **^{13}C NMR** (100.6 MHz, $CDCl_3$) δ 141.5, 136.5, 127.5, 117.0, 105.3, 83.3, 41.3, 33.3, 32.3, 26.8, 25.1, 24.9; **^{11}B NMR** (128.3 MHz, $CDCl_3$) δ 36.2; **MS** (70 eV) m/z: 404.6 [M^+].

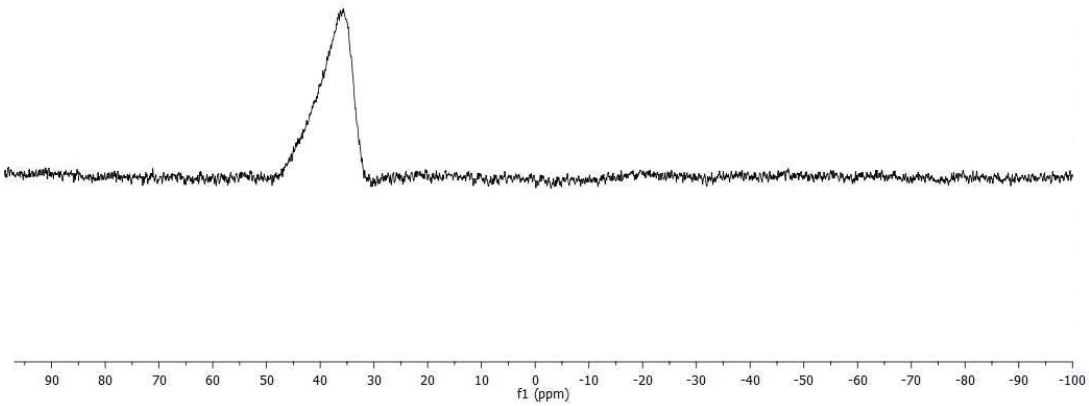
^{1}H NMR



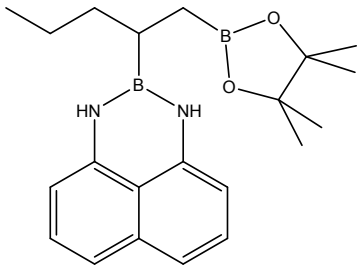
^{13}C NMR



^{11}B NMR



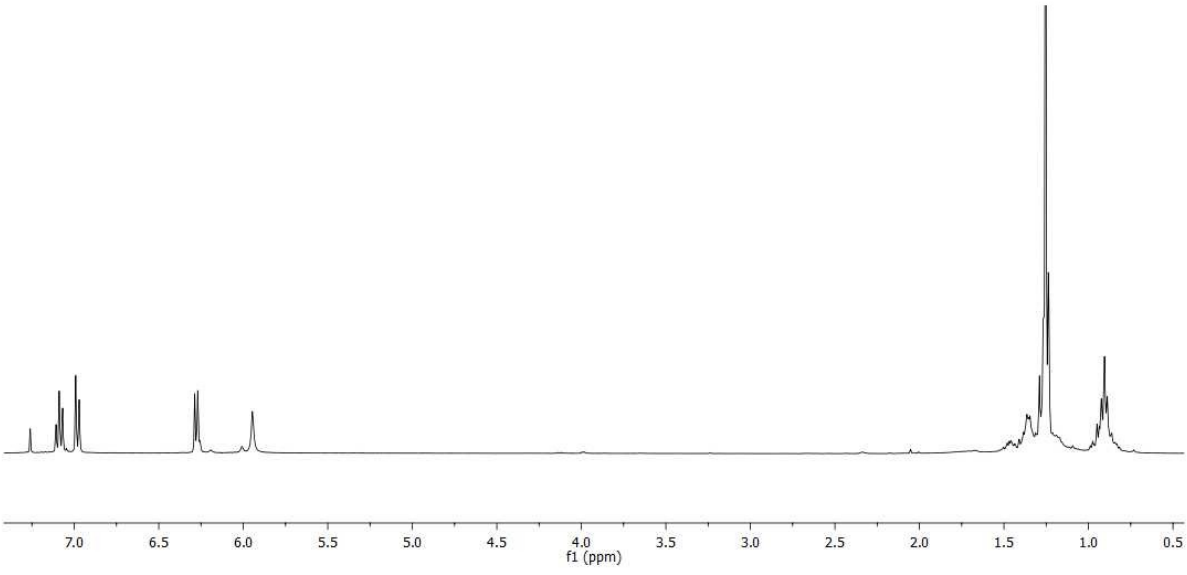
2-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pentan-2-yl)-2,3-dihydro-1*H*-naphtho-1,8-[1,3,2]diazaborinine:



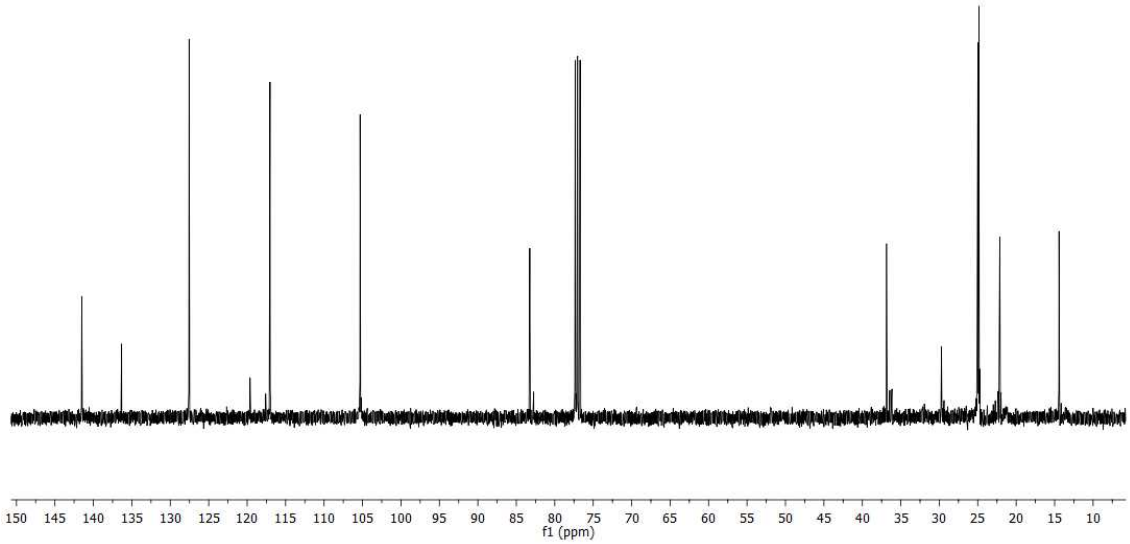
The product was purified by flash column chromatography (petroleum ether/EtOAc=15:1) as a yellow pale oil (20 % isolated yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.09 (dd, J=8.5, J=8.0 Hz, 2H), 6.97 (d, J=8.5Hz, 2H), 6.27 (d, J=8.0 Hz, 2H), 5.94 (br s, 2H), 1.46 (m, 1H), 1.36 (m, 2H), 1.25 (s, 12H) 1.24 (m, 7H); **^{13}C NMR** (100.6 MHz, $CDCl_3$) δ 141.5, 136.3, 127.6, 117.0, 105.3, 83.3, 36.9, 31.9, 29.7, 29.1, 24.9, 22.1, 14.4; **^{11}B NMR** (128.3 MHz, $CDCl_3$) δ 35.6; **MS** (70 eV) m/z: 364.3 [M^+].

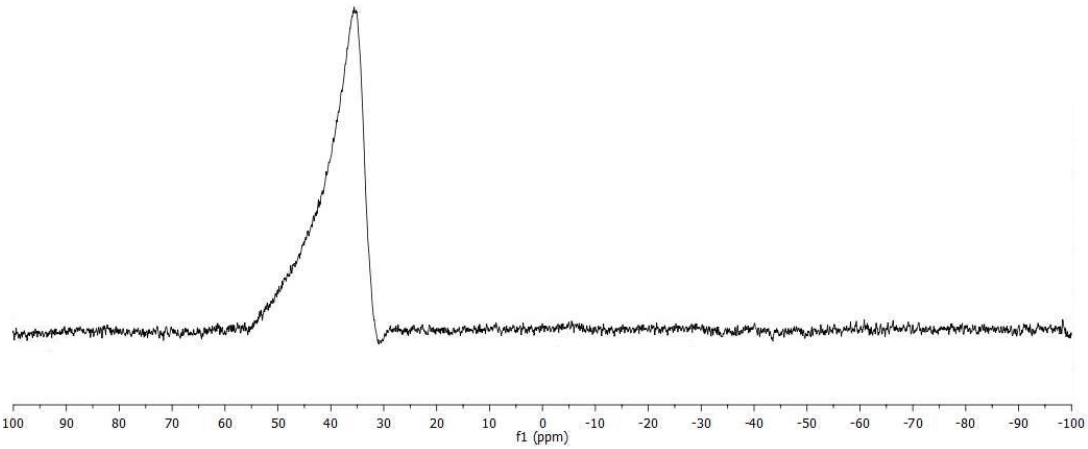
^{1}H NMR



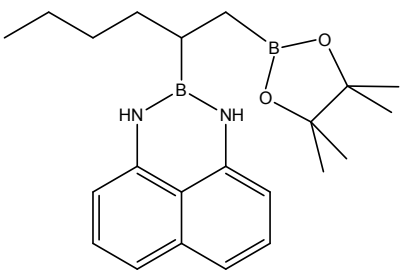
^{13}C NMR



^{11}B NMR

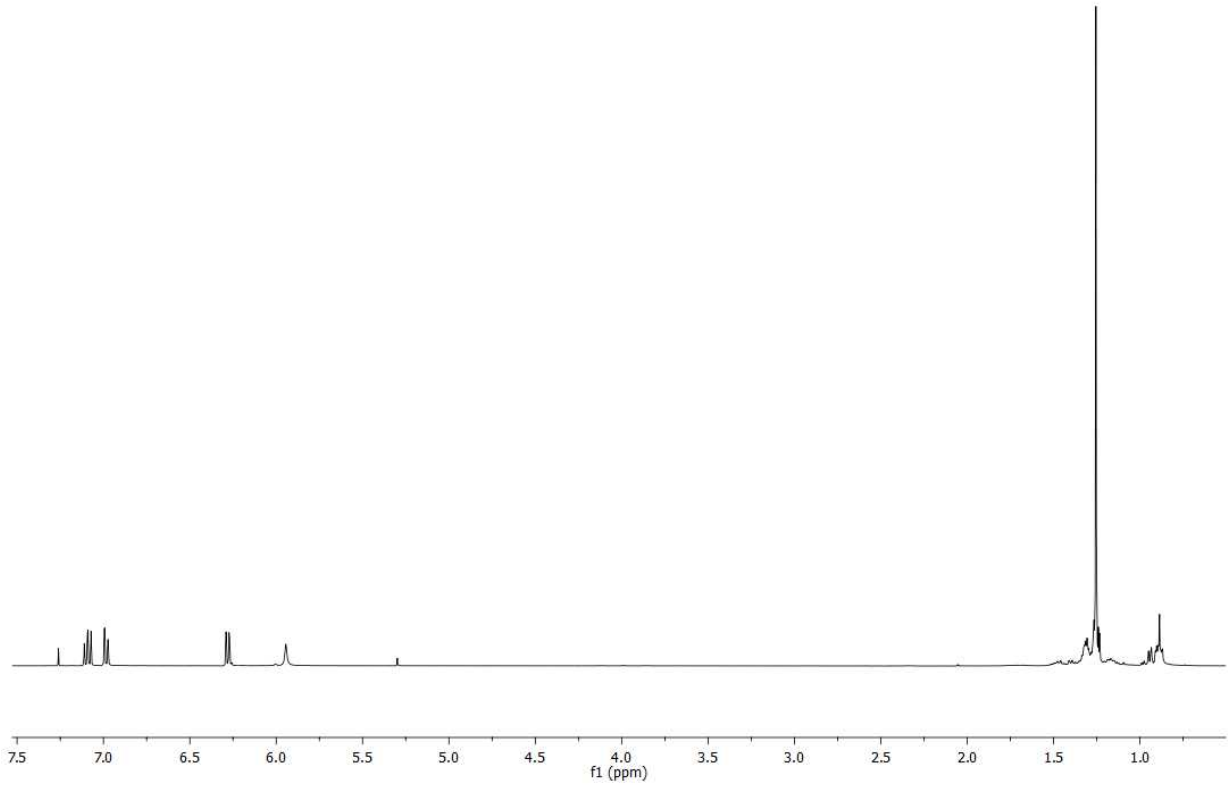


2-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexan-2-yl)-2,3-dihydro-1*H*-naphtho-1,8-[1,3,2]diazaborinine:

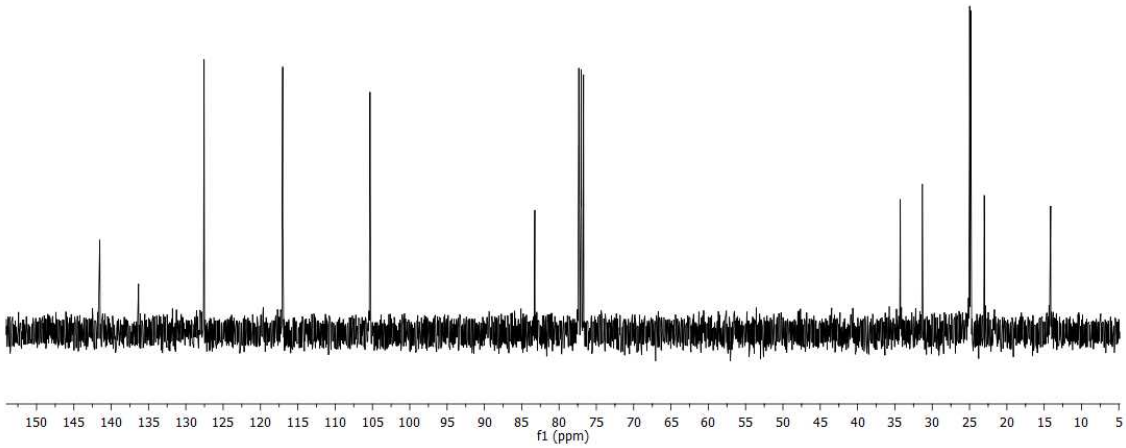


The product was purified by flash column chromatography (petroleum ether/EtOAc=15:1) as a yellow pale oil (17% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.08 (dd, J=8.0, J=7.6 Hz, 2H), 6.98 (d, J=8.0 Hz, 2H), 6.27 (d, J=7.6 Hz, 2H), 5.94 (br s, 2H), 1.31 (m, 3H), 1.25 (s, 12H), 0.87 (m, 9H).**^{13}C NMR** (100.6 MHz, $CDCl_3$) δ 141.7, 136.3, 127.7, 117.0, 106.3, 105.2, 83.2, 34.3, 31.4, 24.9, 24.9, 23.1, 14.1; **^{11}B NMR** (128.3 MHz, $CDCl_3$) δ 36.5; **MS** (70 eV) m/z: 378.3 [M^+].

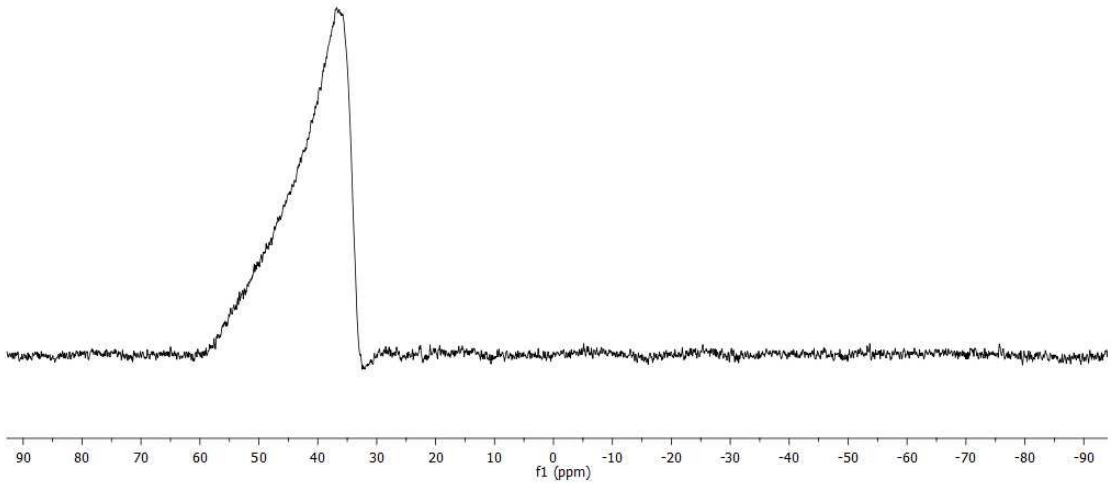
^{1}H NMR



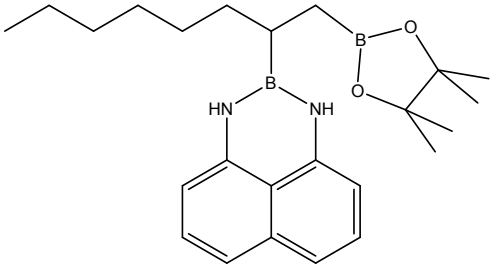
^{13}C NMR



^{11}B NMR

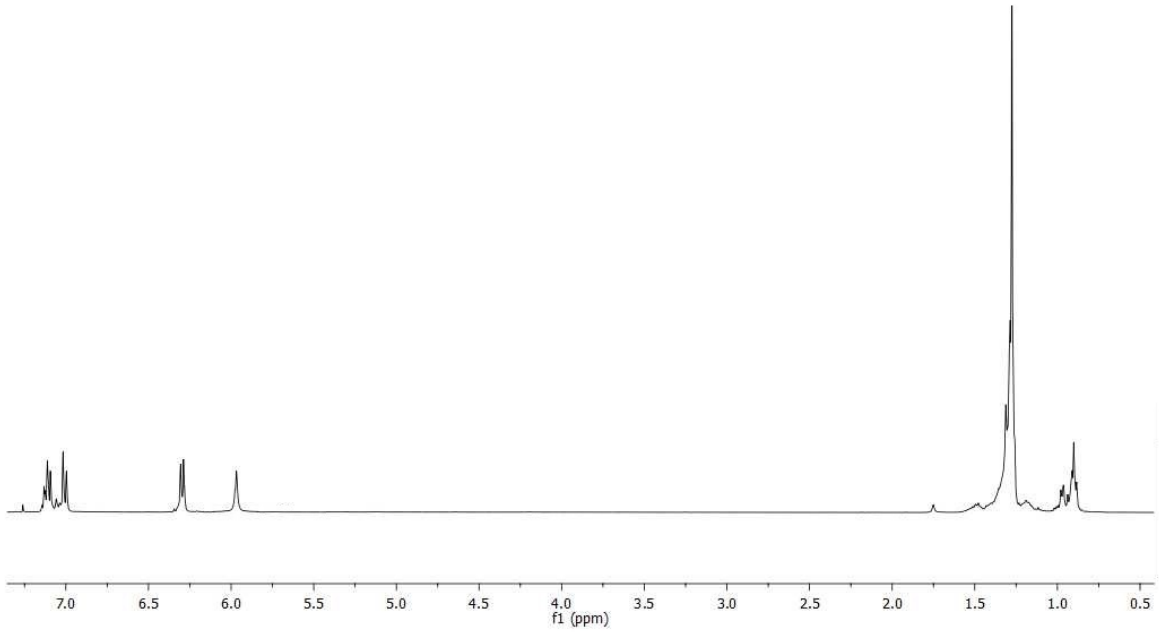


2-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)octan-2-yl)-2,3-dihydro-1*H*-naphtho-1,8-[1,3,2]diazaborinine:



The product was purified by flash column chromatography (petroleum ether/EtOAc=15:1) as a yellow pale oil (25% isolated yield**). ^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.11 (dd, J=8.0, J=7.9 Hz, 2H), 7.01 (d, J=8.0 Hz, 2H), 6.31 (d, J=7.9 Hz, 2H), 5.97 (br s, 2H), 1.36 (m, 5H), 1.26 (s, 12H), 0.86 (m, 11H); **^{13}C NMR** (100.6 MHz, $CDCl_3$) δ 141.5, 136.3, 127.6, 117.0, 105.3, 105.2, 83.3, 34.6, 31.9, 29.7, 29.1, 25.0, 24.9, 22.7, 14.2; **^{11}B NMR** (128.3 MHz, $CDCl_3$) δ 34.5; **MS** (70 eV) m/z: 406.3 [M^+].

^{1}H NMR



^{13}C NMR

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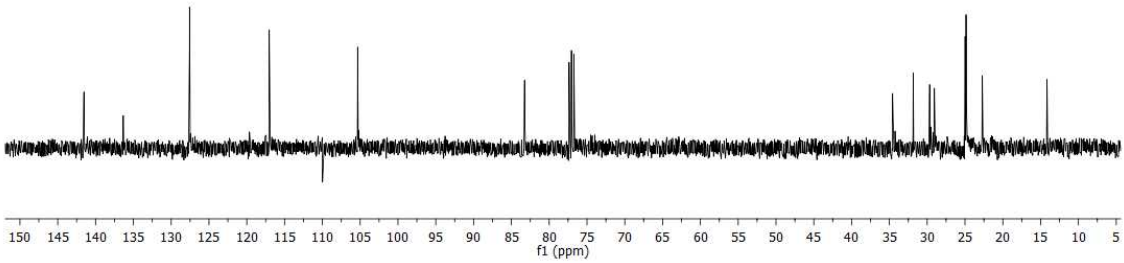

^{11}B NMR

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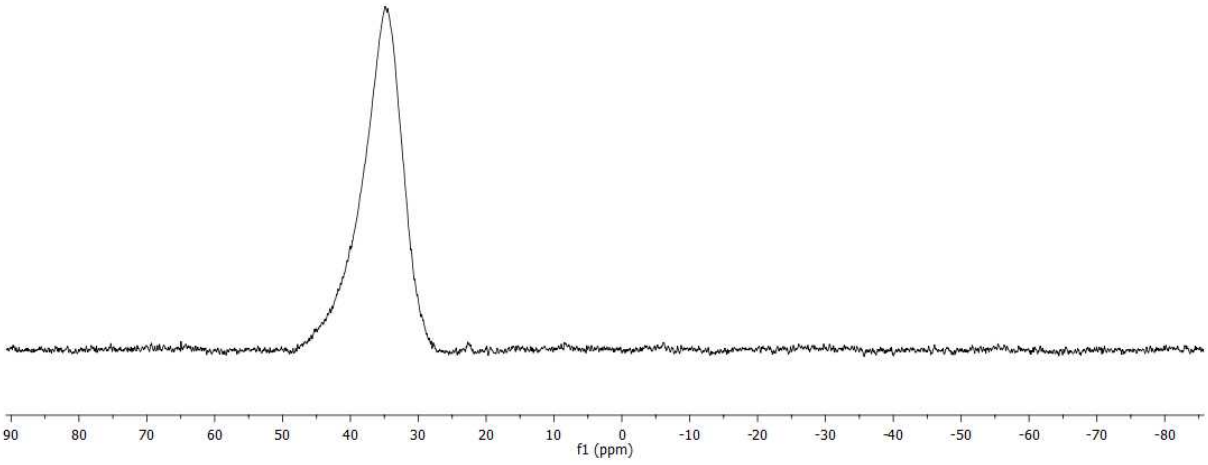
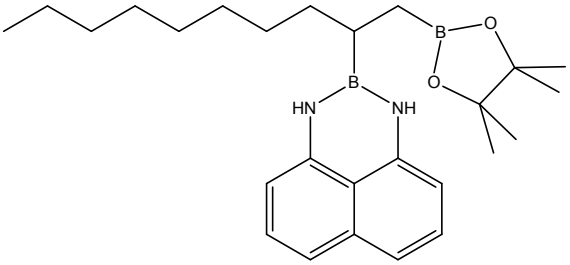
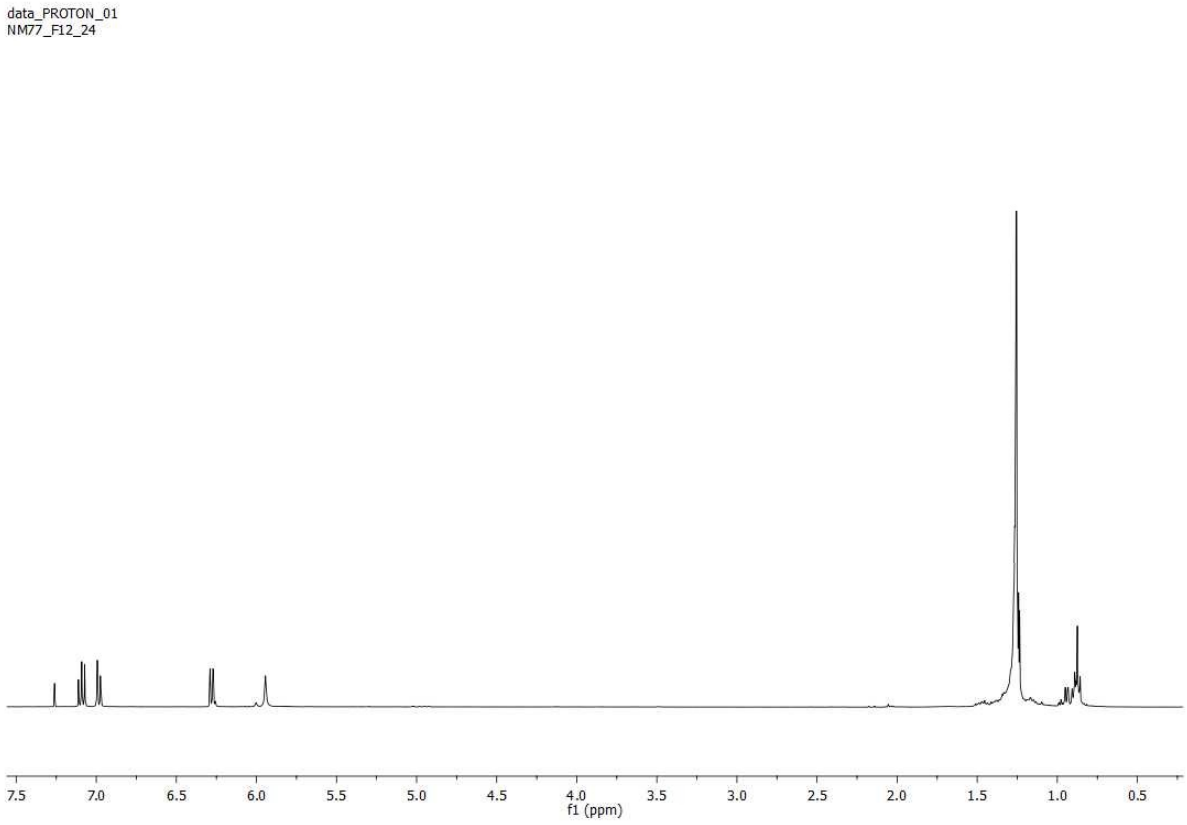


2-(1-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)decan-2-yl)-2,3-dihydro1*H*-naphtho-1,8-[1,3,2]diazaborinine:

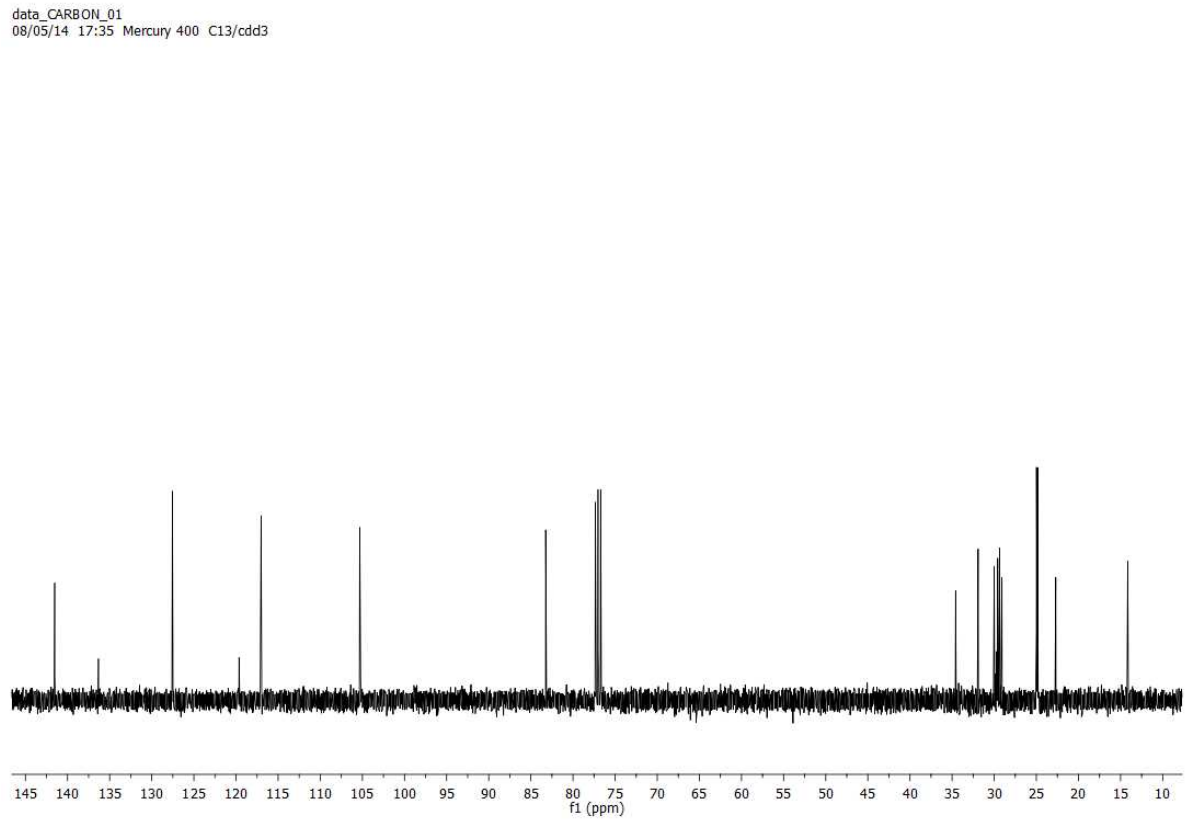


The product was purified by flash column chromatography (petroleum ether/EtOAc=15:1) as a yellow oil (70% isolated yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.09 (dd, J=8.6, J=8.0 Hz, 2H), 6.98 (d, J=8.6 Hz, 2H), 6.28 (d, J=8.0 Hz, 2H), 5.94 (br s, 2H),1.40 (m, 5H), 1.27 (s, 12H), 0.92 (m, 15H); **^{13}C NMR** (100.6 MHz, $CDCl_3$) δ 141.6, 136.4, 127.7, 119.7, 117.2, 105.6, 83.5, 34.9, 32.2, 30.0, 29.6, 29.4, 29.1, 24.9, 24.8, 22.7 14.1; **^{11}B NMR** (128,3 MHz, $CDCl_3$) δ 32.3; **MS** (70 eV) m/z: 434.4 [M^+]. **HRMS** (ESI-TOF) m/z: [M+H] $^+$Calcd for $C_{26}H_{40}B_2O_2N_2$ 435.3354; Found 435.3338.

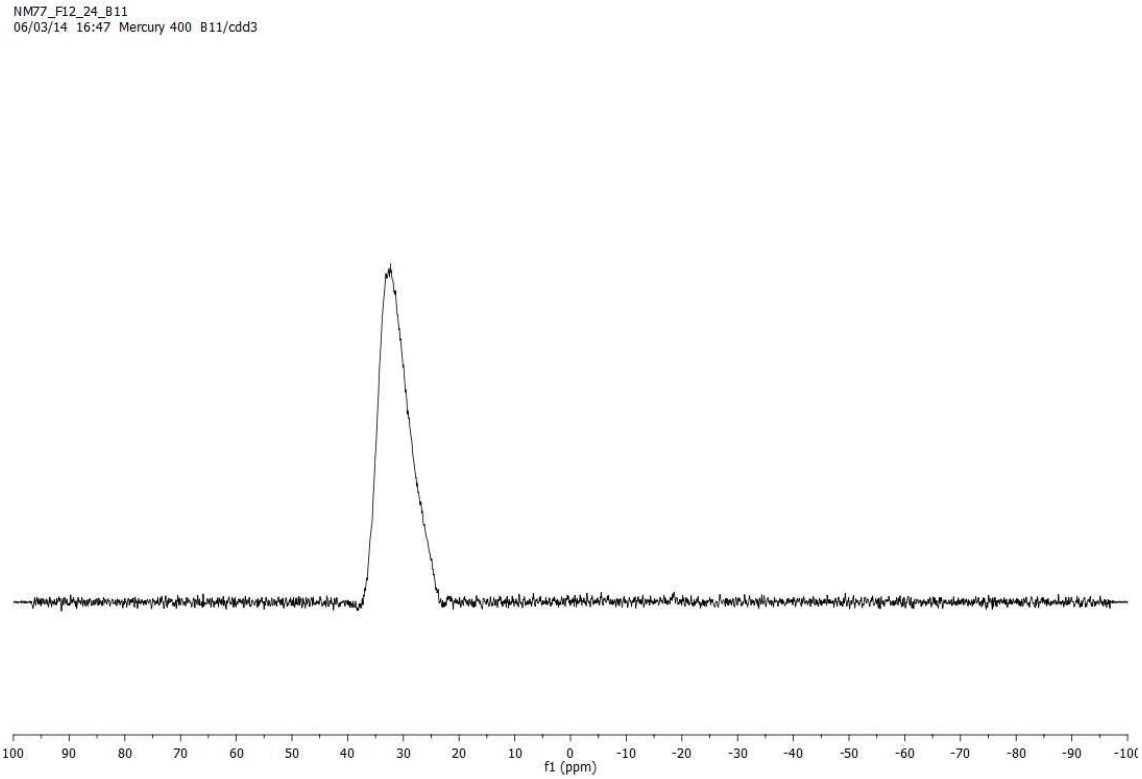
^{1}H NMR



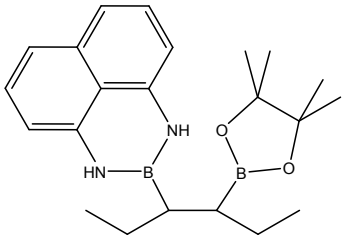
^{13}C NMR



^{11}B NMR

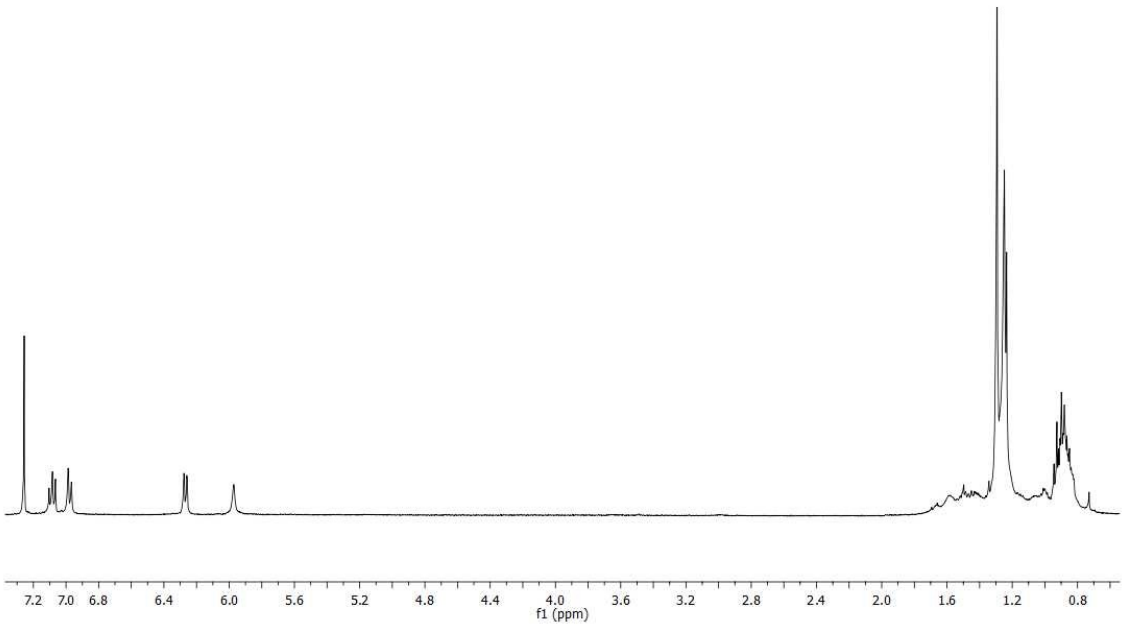


2-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexan-3-yl)-2,3-dihydro-1*H*-naphtho-1,8-[1,3,2]diazaborinine:

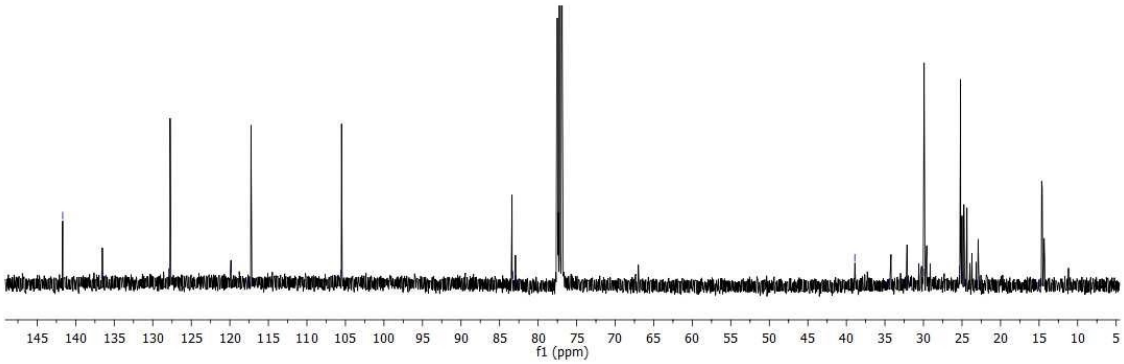


The product was purified by flash column chromatography (petroleum ether/EtOAc=15:1) as a yellow oil (24% isolated yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.09 (dd, J=8.2, J=8.0 Hz, 2H), 6.98 (d, J=8.2 Hz, 2H), 6.27 (d, J=8.0 Hz, 2H), 5.93 (br s, 2H), 1.33 (m, 2H), 1.25 (s, 12H), 1.21 (m, 6H), 0.84 (m, 4H); **^{13}C NMR** (100.6 MHz, $CDCl_3$) δ 141.7, 136.6, 127.9, 119.8, 117.4, 105.6, 83.2, 82.8, 38.9, 34.4, 32.1, 30.1, 25.3, 24.8, 24.4, 22.7, 14.9; **^{11}B NMR** (128,3 MHz, $CDCl_3$) δ 38.1; **MS** (70 eV) m/z: 378.3 [M^+].

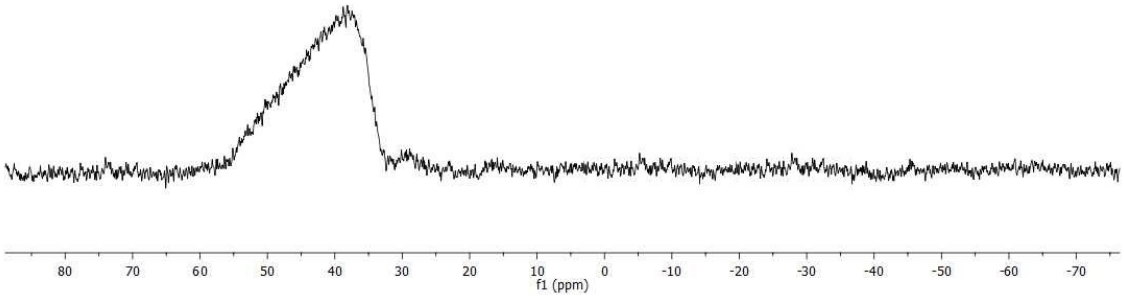
^{1}H NMR



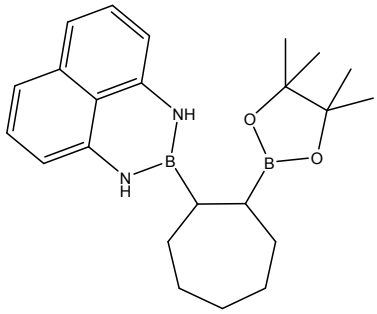
^{13}C NMR



^{11}B NMR



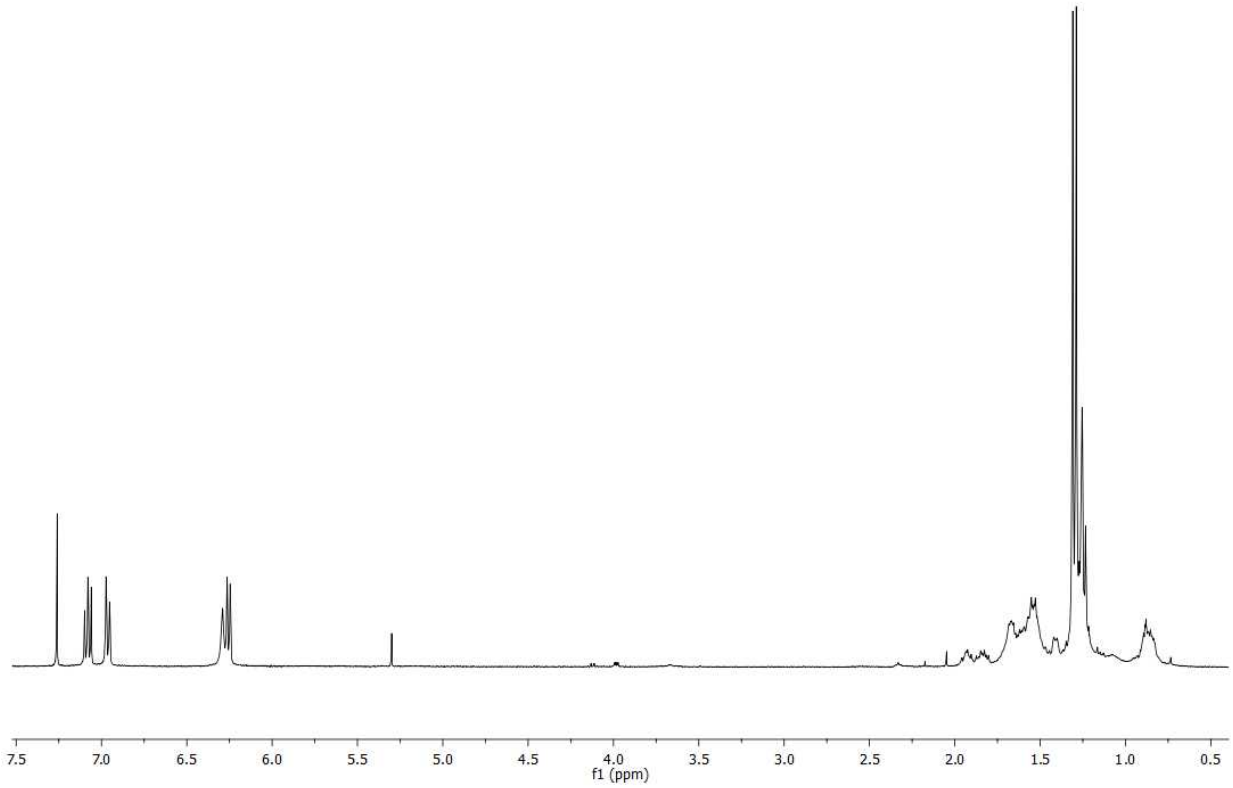
2-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)heptyl)-2,3-dihydro-1*H*-naphtho-1,8-[1,3,2]diazaborinine:



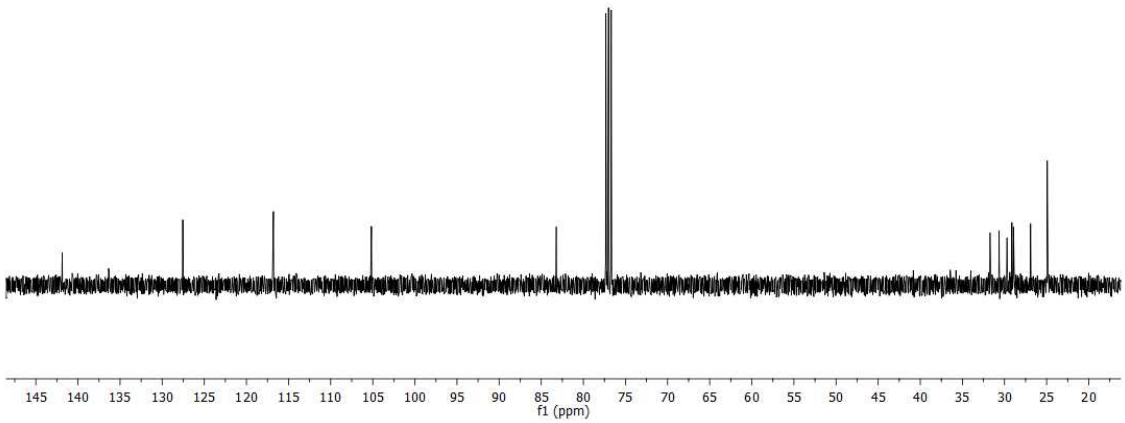
The product was purified by flash column chromatography (petroleum ether/EtOAc=15:1) as a colourless oil (42% isolated yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.08 (dd, J=8.4, J=8.0 Hz, 2H), 6.96 (d, J=8.4 Hz, 2H), 6.29 (br s, 2H), 6.25 (d, *J*=8.0 Hz, 2H), 1.93 (m, 1H), 1.85 (m, 1H), 1.55 (m, 6H), 1.29 (s, 12H), 0.88 (m, 4H); **^{13}C NMR** (100.6 MHz, $CDCl_3$) δ 141.8, 136.2, 127.5, 116.7, 105.1, 83.3; 31.8, 30.6, 29.7, 29.6, 28.8, 27.6, 25.1; **^{11}B NMR** (128,3 MHz, $CDCl_3$) δ 39.7; **MS**(70 eV) m/z : 390.3 [M^+].

HRMS (ESI-TOF) m/z: [M+H] $^+$ Calcd for $C_{23}H_{32}B_2O_2N_2$ 391.2728; Found 391.2752.

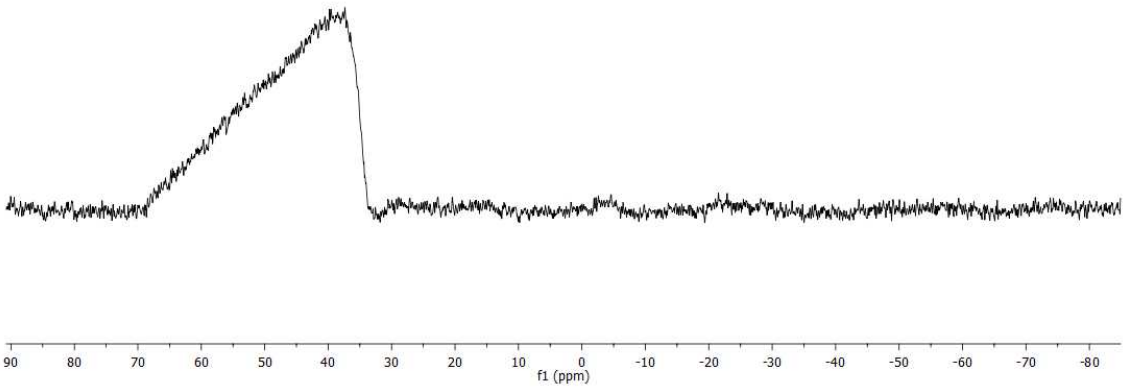
^{1}H NMR



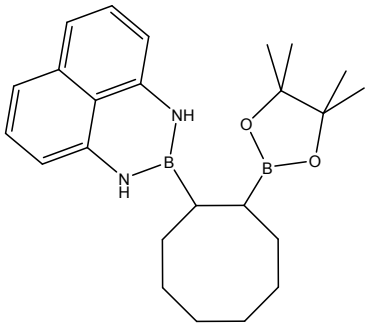
^{13}C NMR



^{11}B NMR

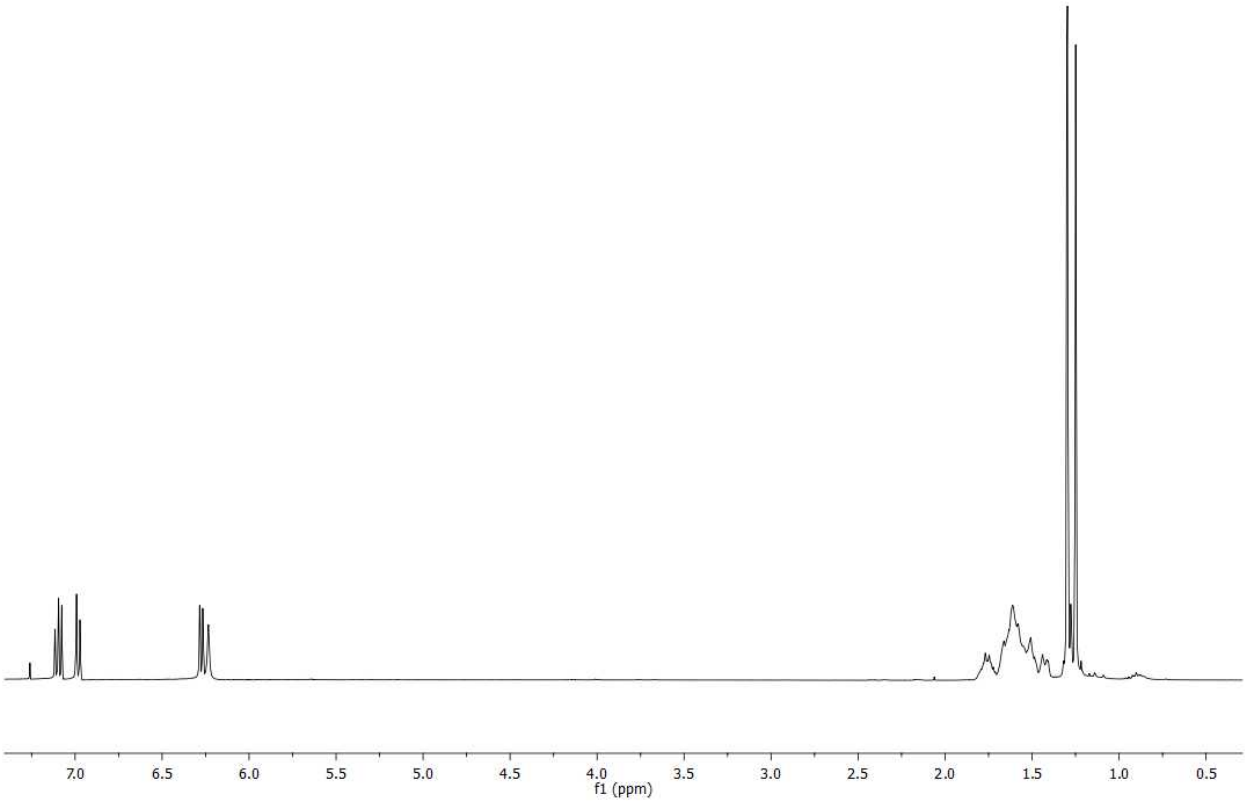


2-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)cyclooctyl)-2,3-dihydro-1*H*-naphtho-1,8-[1,3,2]diazaborinine:

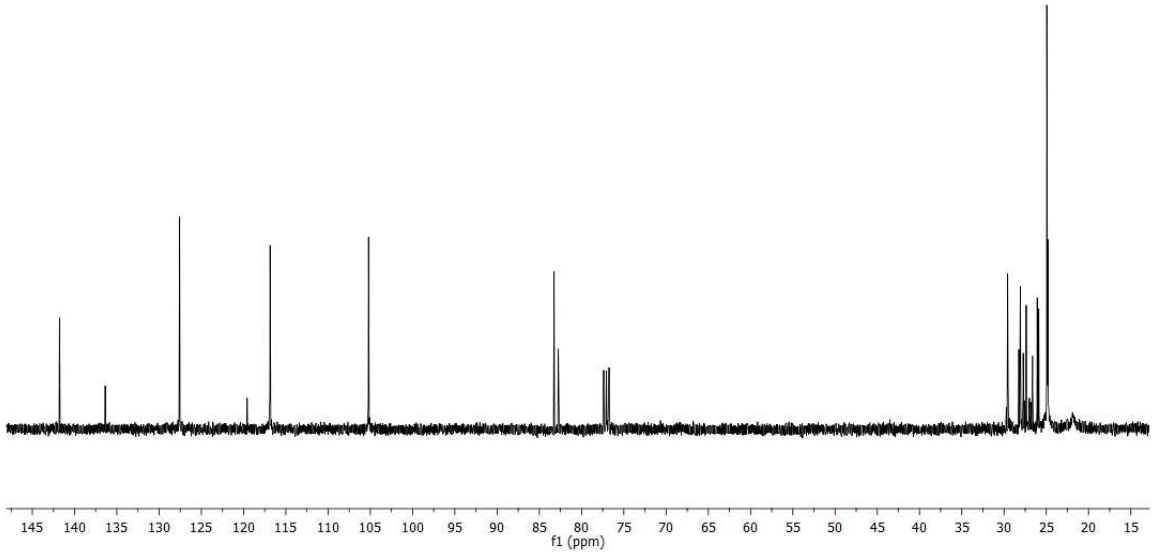


The product was purified by flash column chromatography (petroleum ether/EtOAc=15:1) as a colourless oil (32% isolated yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.09 (dd, J=7.6, J=7.2 Hz, 2H), 7.01 (d, J=7.6 Hz, 2H), 6.27 (d, J=7.2 Hz, 2H), 6.23 (br s, 2H), 1.80-1.45 (m, 14H), 1.30 (s, 6H), 1.25 (s, 6H); **^{13}C NMR** (100.6 MHz, $CDCl_3$) δ 141.8, 136.9, 127.8, 119.5, 116.8, 105.2, 83.6, 82.6, 28.8, 27.6, 26.5, 26.0, 25., 25.0; **^{11}B NMR** (128,3 MHz, $CDCl_3$) δ 34.9; **MS** (70 eV) m/z : 404.3 [M^+].

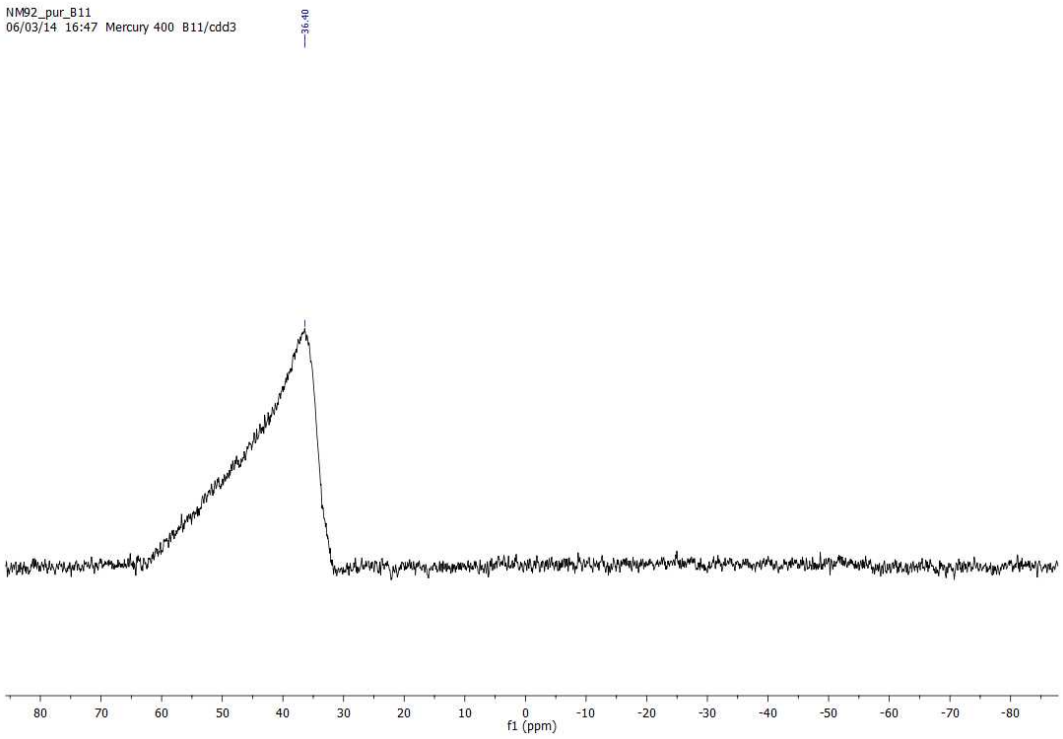
^{1}H NMR



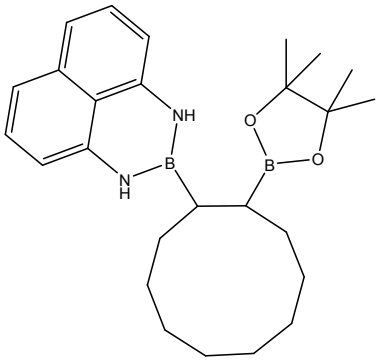
^{13}C NMR



^{11}B NMR

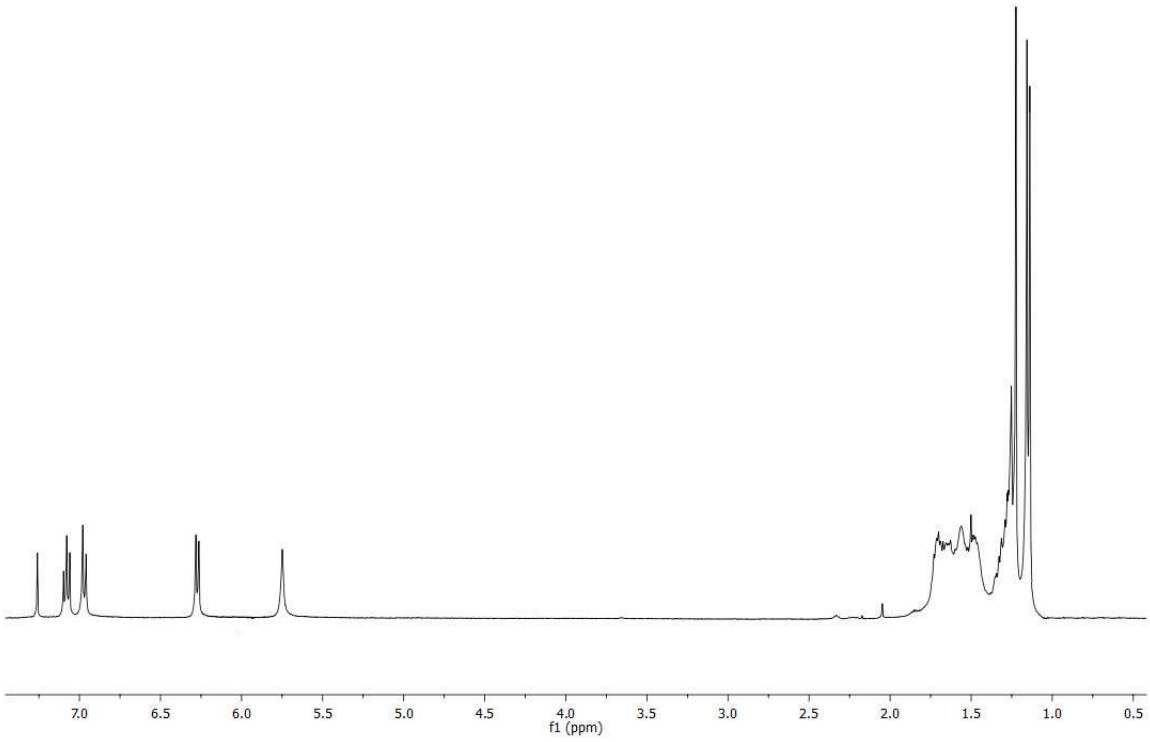


2-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)cyclodecyl)-2,3-dihydro-1*H*-naphtho-1,8-[1,3,2]diazaborinine:

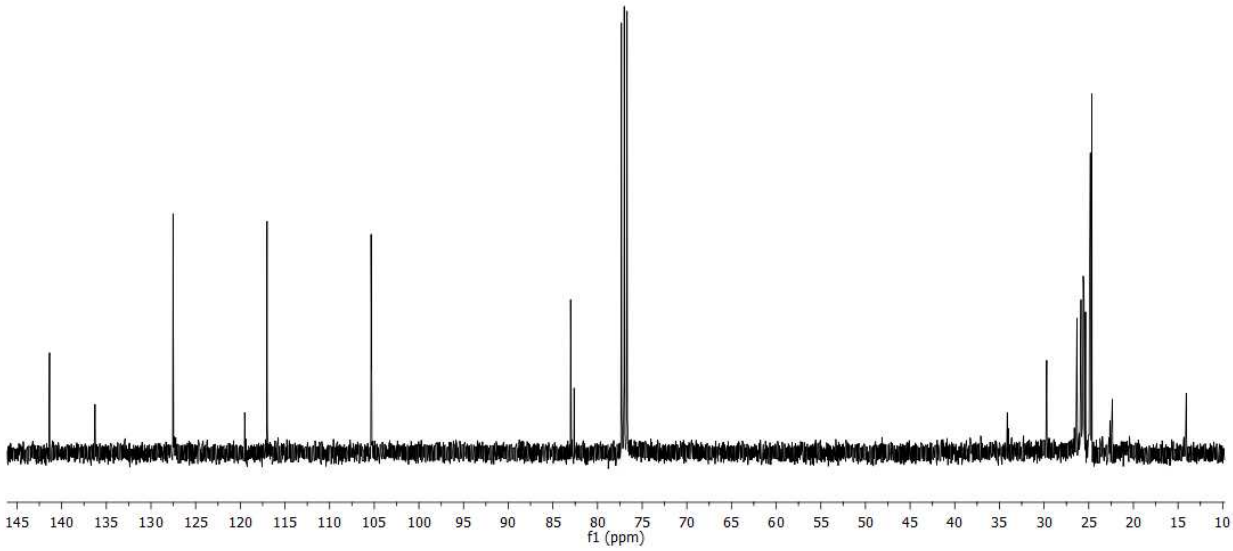


The product was purified by flash column chromatography (petroleum ether/EtOAc=15:1) as a colourless oil (21% isolated yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.09 (dd, J=7.8, J=7.2 Hz, 2H), 7.02 (d, J=7.2 Hz, 2H), 6.41 (d, J=7.8 Hz, 2H), 5.62 (br s, 2H), 1.77-1.49 (m, 14H), 1.28 (s, 6H), 1.22 (s, 6H), 1.21 (m, 4H); **^{13}C NMR** (100.6 MHz, $CDCl_3$) δ 141.4, 136.32, 127.54, 119.49, 117.01, 105.36, 83.09, 82.72, 34.34, 29.82, 26.38, 25.64, 25.46, 24.77, 22.39, 14.06; **^{11}B NMR** (128,3 MHz, $CDCl_3$) δ 38.4; **MS**(70 eV) m/z : 432.3 [M^+].

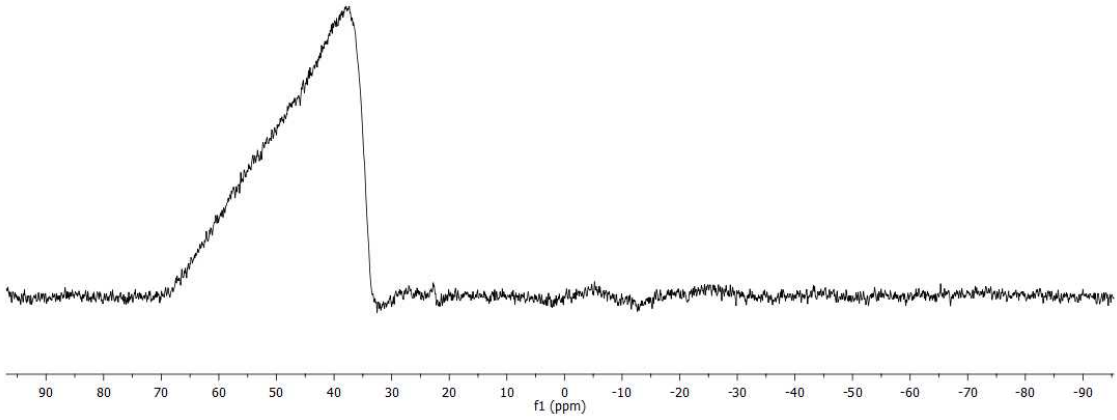
^{1}H NMR



^{13}C NMR

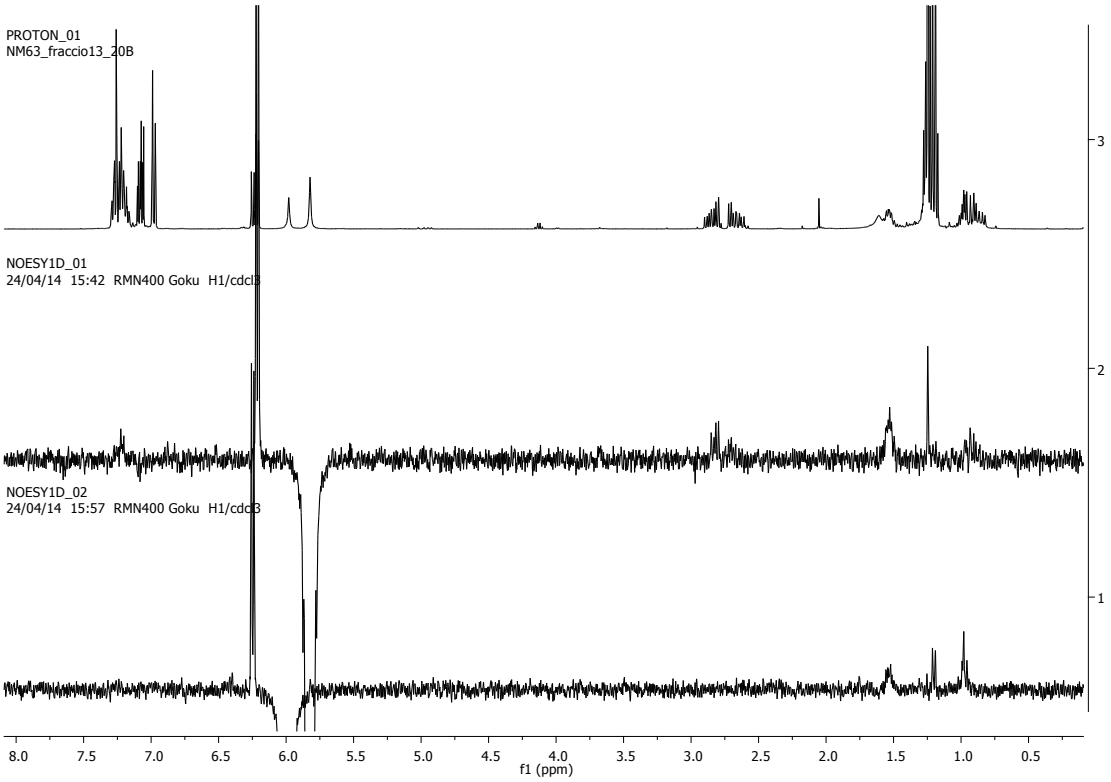


^{11}B NMR



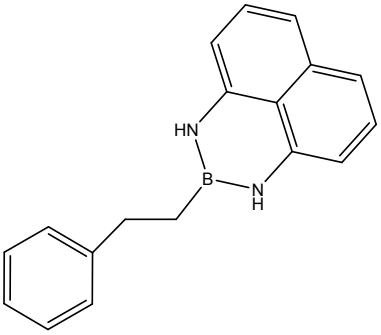
5. Polarization transfer NMR experiments

Based on the 1D selective NOE NMR experiments the regiochemistry of the major diborated isomer was confirmed.



6.Characterization of the hydroborated products

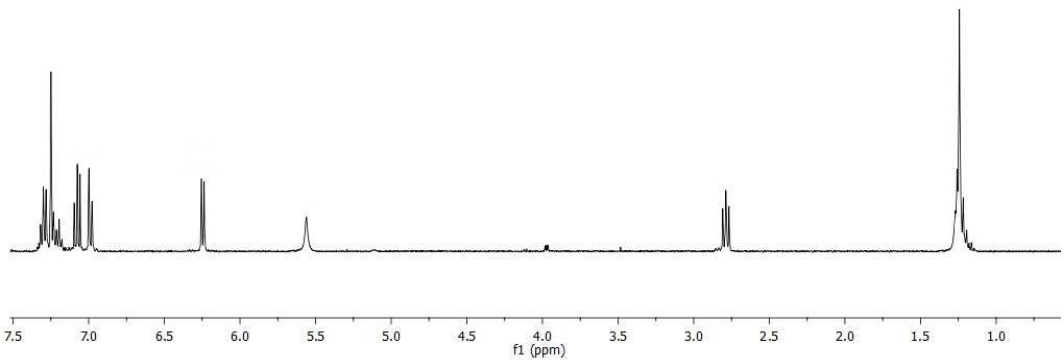
2-phenethyl-2,3-dihydro-1H-naphtho-1,8-[1,3,2]diazaborinine:



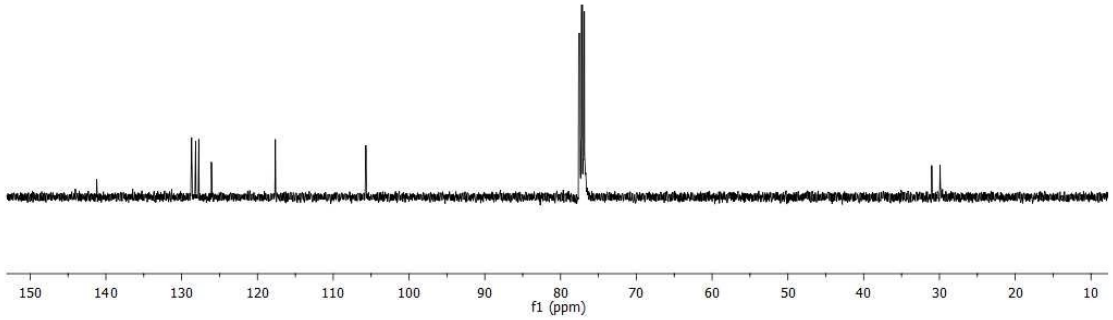
The product was purified by flash column chromatography deactivated with 10% of Et_3N (petroleum ether/EtOAc = 20:1) as a yellow oil (30% isolated yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.17 (m, 5H), 7.05 (dd, J =8.8, 8.0 Hz, 2H), 6.97 (d, J=8.8 Hz, 2H), 6.22 (d, J=8.0 Hz, 2H), 5.54 (br s, 2H), 2.76 (t, J=8.0 Hz, 2H), 1.22 (t, J=8.0 Hz, 2H); **^{13}C NMR** (100.6 MHz, $CDCl_3$) δ 141.2, 128.7, 128.2, 127.8, 126.1, 117.6, 105.7, 31.0, 29.9; **^{11}B NMR** (128.3 MHz, $CDCl_3$) δ 32.6; **MS** (70 eV) m/z: 272.3 [M^+].

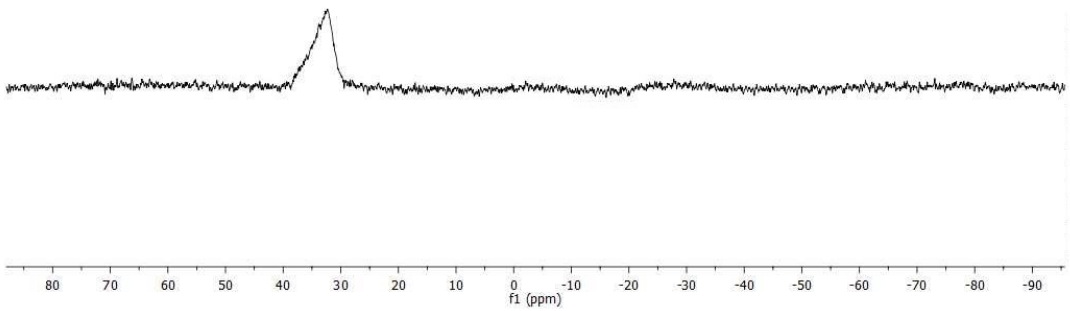
^{1}H NMR



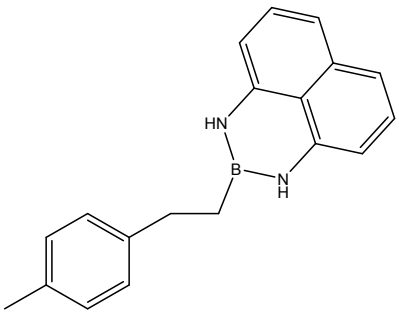
^{13}C NMR



^{11}B NMR



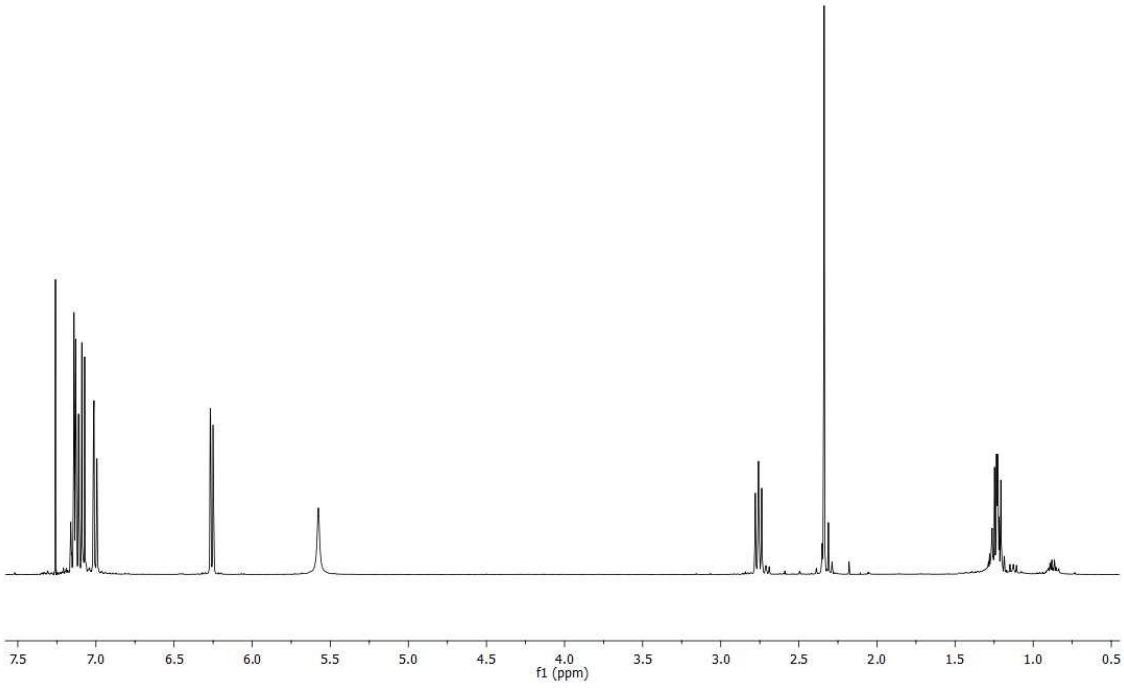
2-(4-methylphenethyl)-2,3-dihydro-1H-naphtho-1,8-[1,3,2]diazaborinine:



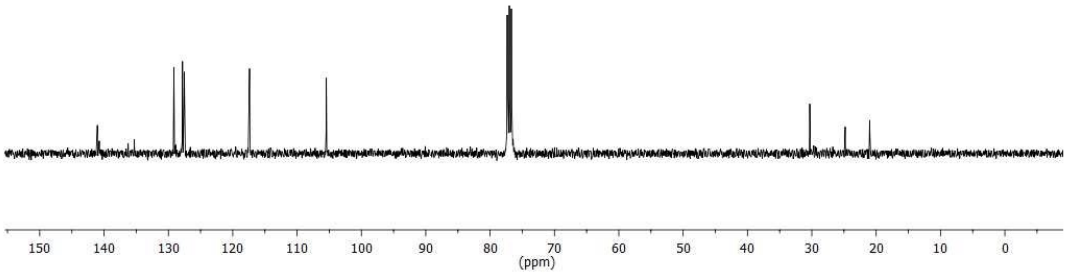
The product was purified by flash column chromatography deactivated with 10% of Et_3N (petroleum ether/EtOAc = 20:1) as a yellow oil (36.6% isolated yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15-7.07 (m, 6H), 7.01 (d, J=8.4 Hz, 2H), 6.25 (d, J=8.0 Hz, 2H), 5.56 (br s, 2H), 2.76 (t, J=8.0 Hz, 2H), 2.35 (s, 3H), 1.23 (t, J=8.0 Hz, 2H); **^{13}C NMR** (100.6 MHz, $CDCl_3$) δ 141.5, 136.3, 135.3, 129.2, 127.8, 127.5, 117.4, 110.0, 105.5, 30.3, 24.8, 21.0; **^{11}B NMR** (128.3 MHz, $CDCl_3$) δ 31.7; **MS** (70 eV) m/z: 286.3 [M^+].

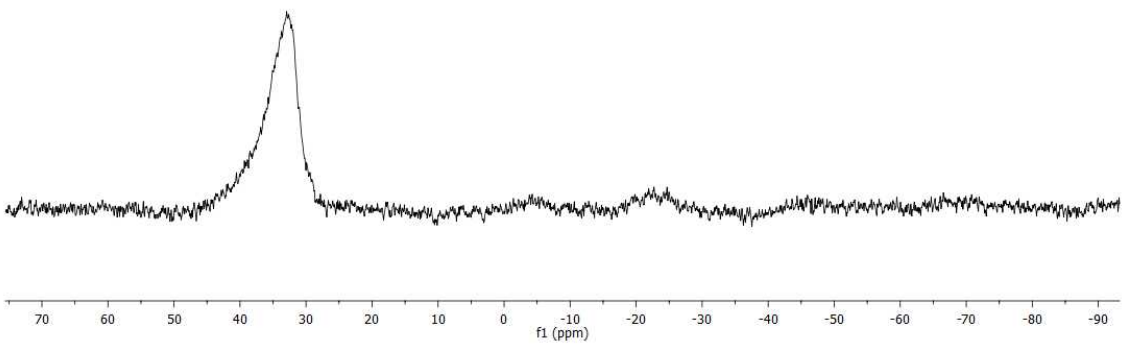
^{1}H NMR



^{13}C NMR



^{11}B NMR



7. Computational details

All calculations were performed using the Gaussian09 series of programs.[2] Calculations were performed within the framework of density functional theory (DFT)[3] using the B3LYP functional.[4] All the atoms were represented by means of the 6-31G(d,p) basis set.[5] All geometry optimizations were full, with no restrictions. All stationary points located in the potential energy hypersurface were characterized as minima or transition states by vibrational analysis. Transition states had one and only one imaginary frequency, whose normal mode corresponded to the expected motion. Solvent effects of the methanol (ε = 32.613) were introduced to the optimized vacuum geometries using the self consistent field approach, by means of the integral equation formalism polarizable continuum model (IEFPCM).[6] Free energies corrections were computed by employing the following equation.

$$\Delta GMeOH = \Delta EMeOH + (\Delta GGAS - \Delta EGAS)$$

8. Computational-determined mechanism for attack of boryl moiety to the terminal and the internal carbons of the alkene

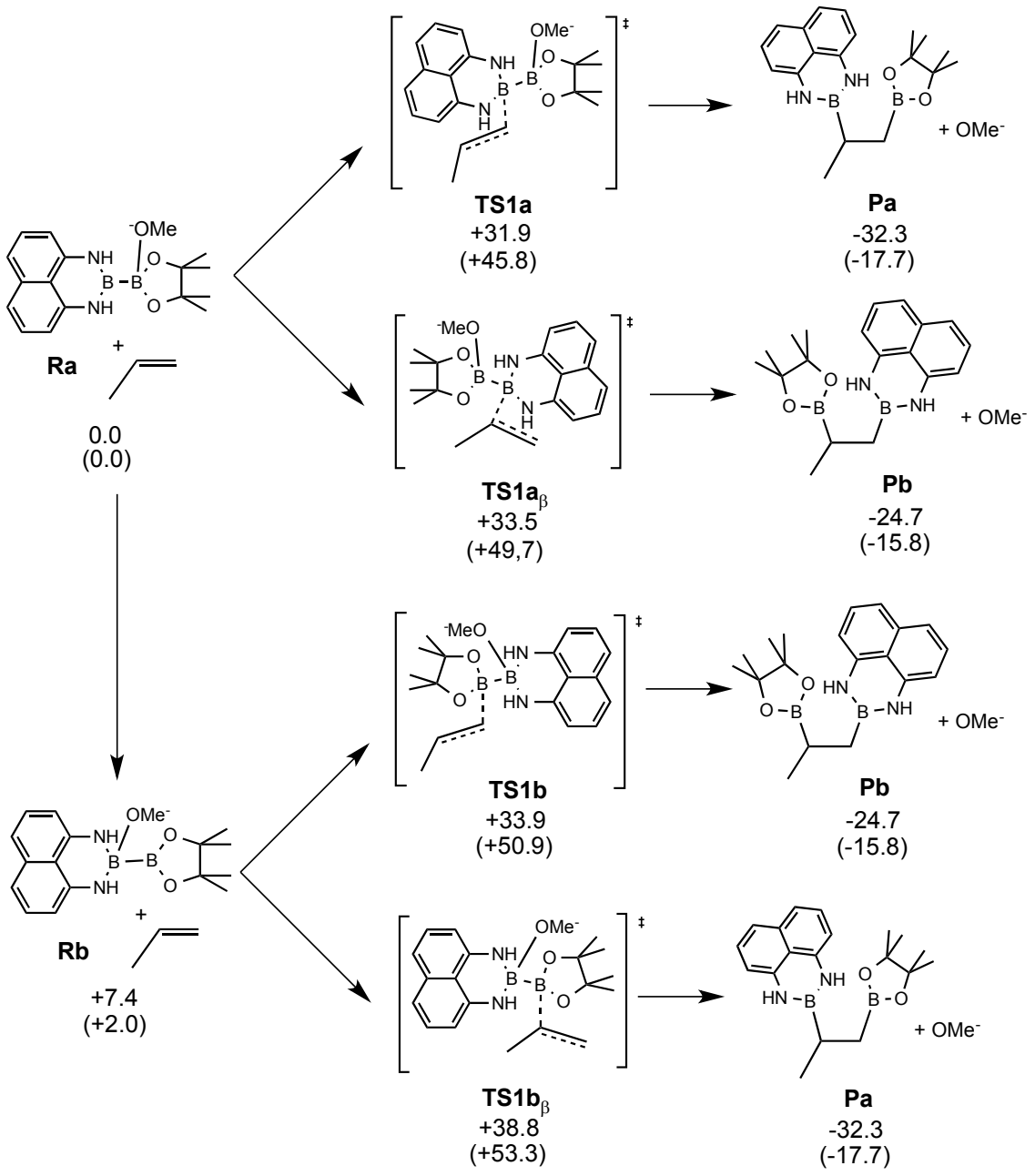


Figure S1. Possible mechanisms for the nucleophilic attack of the Bdan and Bpin moieties to the terminal and to the internal carbon of the alkene. Electronic energies and Gibbs free energies in MeOH (in parenthesis) in kcal.mol^{-1}.

9. Geometries, absolute energies, and imaginary frequencies and their corresponding Normal Mode of Vibration (MNV)

Ra. E_{elec} = -1046,8218142 a.u. (ΔG_{sol} = -1046,55558825 a.u)

C	-4.149961000	-2.198927000	-1.138759000
C	-4.855194000	-1.019059000	-0.990829000
C	-4.200368000	0.141872000	-0.491596000
C	-2.817137000	0.060118000	-0.128978000
C	-2.102535000	-1.182192000	-0.277912000
C	-2.793523000	-2.293335000	-0.795176000
H	-5.931675000	1.445166000	-0.624978000
H	-4.655205000	-3.082513000	-1.528635000
H	-5.907013000	-0.957763000	-1.260963000
C	-4.879223000	1.385222000	-0.357042000
C	-2.120098000	1.231451000	0.339979000
H	-2.260911000	-3.235463000	-0.913373000
C	-2.837312000	2.437952000	0.441084000
C	-4.195653000	2.497546000	0.098260000
H	-2.321097000	3.327689000	0.797184000
H	-4.719861000	3.448137000	0.196120000
N	-0.782529000	-1.231218000	0.052532000
N	-0.793045000	1.146622000	0.630518000
B	-0.020935000	-0.158872000	0.863675000
C	3.565928000	0.983218000	-0.477538000
C	3.718649000	-0.582021000	-0.528628000
B	1.615397000	-0.017162000	0.278310000
O	2.360899000	-1.028558000	-0.342028000
O	2.385964000	1.150166000	0.331980000
C	4.545864000	-1.148002000	0.638132000
H	4.428973000	-2.235706000	0.655755000
H	5.612600000	-0.915452000	0.541114000
H	4.185828000	-0.758443000	1.593986000
C	4.242495000	-1.147120000	-1.850902000
H	5.260585000	-0.796828000	-2.059348000
H	4.265554000	-2.240237000	-1.796409000
H	3.598678000	-0.869288000	-2.687507000
C	4.724248000	1.733583000	0.183838000
H	5.659853000	1.593754000	-0.370973000
H	4.500032000	2.804837000	0.204162000
H	4.876546000	1.406181000	1.214236000
C	3.261902000	1.607805000	-1.849626000
H	2.959163000	2.648462000	-1.700962000
H	4.132214000	1.591256000	-2.515597000
H	2.433560000	1.088419000	-2.338698000
O	-0.053038000	-0.423163000	2.342050000
C	0.548068000	-1.584953000	2.805304000
H	0.475527000	-1.626857000	3.904019000
H	0.075311000	-2.508014000	2.415594000

H	1.625504000	-1.660711000	2.547675000
H	-0.336602000	-2.118518000	-0.133056000
H	-0.388368000	1.997717000	0.995685000

TSa-b E_{elec} = -1046,7947686 a.u. (ΔG_{sol} = -1046,53078577 a.u)

C	4.420340000	2.473581000	-0.013499000
C	5.124488000	1.284320000	-0.028522000
C	4.429410000	0.045753000	-0.116343000
C	2.997144000	0.056479000	-0.176206000
C	2.286019000	1.305848000	-0.157042000
C	3.015845000	2.498417000	-0.078383000
H	6.196245000	-1.214466000	-0.103020000
H	4.958381000	3.417059000	0.050735000
H	6.210114000	1.278601000	0.020764000
C	5.110693000	-1.203214000	-0.153247000
C	2.273503000	-1.180494000	-0.282880000
H	2.483235000	3.446411000	-0.065178000
C	2.989286000	-2.382968000	-0.325828000
C	4.394017000	-2.380200000	-0.258180000
H	2.446352000	-3.321553000	-0.408044000
H	4.921696000	-3.331180000	-0.288662000
N	0.914651000	1.286233000	-0.237486000
N	0.900989000	-1.138851000	-0.359285000
B	0.075146000	0.070966000	-0.165425000
C	-3.775146000	-0.656718000	-0.504121000
C	-3.770067000	0.835971000	0.000939000
B	-1.587568000	0.074523000	-0.155368000
O	-2.406974000	1.233889000	-0.244592000
O	-2.417916000	-1.079662000	-0.272260000
C	-4.048947000	0.960683000	1.508705000
H	-3.856493000	1.993094000	1.818456000
H	-5.088324000	0.720576000	1.755902000
H	-3.385129000	0.310156000	2.081394000
C	-4.699066000	1.781104000	-0.765712000
H	-5.746387000	1.474373000	-0.668358000
H	-4.609006000	2.794757000	-0.361031000
H	-4.447255000	1.820393000	-1.827799000
C	-4.724200000	-1.591450000	0.250784000
H	-5.766841000	-1.272950000	0.140580000
H	-4.640745000	-2.606688000	-0.151353000
H	-4.485148000	-1.630540000	1.315671000
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H	-3.830412000	-1.799546000	-2.333517000
H	-5.075461000	-0.538714000	-2.275679000
H	-3.379313000	-0.105146000	-2.578359000
O	-0.741218000	0.047564000	1.526189000
C	-0.708780000	-1.151520000	2.250200000
H	0.313009000	-1.558587000	2.348955000

H	-1.093266000	-0.998170000	3.274343000
H	-1.328333000	-1.941411000	1.792605000
H	0.452356000	-2.040780000	-0.435560000
H	0.472929000	2.194384000	-0.206122000

Imaginary frequency= -311.6 cm^{-1}

NMV:

C	-0.02	0.00	-0.01
C	-0.01	0.00	-0.01
C	-0.02	0.00	0.00
C	-0.02	0.00	0.02
C	-0.04	-0.01	0.03
C	-0.02	0.00	0.00
H	-0.01	0.01	-0.01
H	-0.02	0.00	-0.02
H	-0.01	0.00	-0.01
C	-0.01	0.00	-0.01
C	-0.04	0.00	0.03
H	-0.01	0.00	0.01
C	-0.01	0.00	0.00
C	-0.01	0.00	-0.01
H	-0.01	-0.01	0.01
H	-0.01	0.00	-0.02
N	-0.04	0.00	0.09
N	-0.03	-0.02	0.07
B	-0.12	-0.04	0.51
C	-0.06	0.01	-0.02
C	-0.05	0.00	-0.03
B	-0.12	0.04	-0.45
O	-0.05	0.00	-0.09
O	-0.03	0.04	-0.08
C	0.03	0.00	-0.01
H	0.03	0.01	-0.02
H	0.05	-0.01	0.03
H	0.06	0.01	-0.04
C	-0.05	0.01	0.00
H	-0.05	0.02	0.01
H	-0.02	0.00	0.00
H	-0.06	0.00	-0.01
C	-0.01	-0.01	0.01
H	-0.01	-0.03	0.03
H	0.00	-0.01	0.00
H	0.02	0.00	0.00
C	-0.05	0.00	-0.02
H	-0.04	0.00	-0.01
H	-0.05	-0.01	-0.02
H	-0.05	0.00	-0.02
O	0.50	0.00	0.00
C	0.14	-0.01	0.00
H	0.04	-0.21	0.20

H	-0.03	0.10	-0.09
H	0.07	0.10	-0.11
H	0.01	-0.04	0.08
H	-0.01	0.01	0.10

Rb E_{elec} = -1046,810090 a.u. (ΔG_{sol} = -1046,55245419 a.u)

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C	-5.162689000	-0.741235000	-0.606093000
C	-4.301162000	0.319075000	-0.211518000
C	-2.903335000	0.048740000	-0.053314000
C	-2.398528000	-1.272858000	-0.288741000
C	-3.282892000	-2.282099000	-0.675572000
H	-5.834442000	1.846812000	-0.085534000
H	-5.320268000	-2.809209000	-1.132078000
H	-6.224125000	-0.540019000	-0.727632000
C	-4.774246000	1.637411000	0.032918000
C	-2.010680000	1.100110000	0.341871000
H	-2.900291000	-3.284039000	-0.854985000
C	-2.521556000	2.379425000	0.572205000
C	-3.895261000	2.631980000	0.414917000
H	-1.844344000	3.174904000	0.872339000
H	-4.268595000	3.637605000	0.599662000
N	-1.045522000	-1.496137000	-0.118603000
N	-0.674619000	0.793004000	0.478426000
B	-0.071986000	-0.499761000	0.268035000
C	3.171683000	1.058804000	-0.141177000
C	3.521907000	-0.281606000	-0.904038000
B	1.648758000	-0.693033000	0.449847000
O	2.305137000	-1.001574000	-0.842565000
O	2.242047000	0.649254000	0.842302000
C	4.635610000	-1.088366000	-0.197973000
H	4.695040000	-2.075147000	-0.669944000
H	5.620571000	-0.609047000	-0.276071000
H	4.378490000	-1.242575000	0.851310000
C	3.904987000	-0.100045000	-2.380484000
H	4.798218000	0.527430000	-2.497038000
H	4.120911000	-1.078909000	-2.823483000
H	3.086190000	0.346553000	-2.949496000
C	4.365836000	1.735807000	0.549418000
H	5.145412000	2.025502000	-0.167668000
H	4.026775000	2.642884000	1.063545000
H	4.806661000	1.074711000	1.298584000
C	2.483616000	2.086148000	-1.068008000
H	2.086377000	2.901278000	-0.452051000
H	3.165443000	2.523241000	-1.808607000
H	1.646727000	1.619578000	-1.594501000
O	2.028035000	-1.736044000	1.442319000
C	1.603565000	-1.522395000	2.749623000

H	1.899511000	-2.376785000	3.380243000
H	2.037346000	-0.610406000	3.197968000
H	0.502237000	-1.420086000	2.838837000
H	-0.041983000	1.534754000	0.754212000
H	-0.732720000	-2.441981000	-0.287745000

TS1a E_{elec} = -1164,6849746 a.u. (ΔG_{sol} = -1164,33958227 a.u)

C	-4.716269000	-1.169150000	1.463724000
C	-5.113019000	0.024495000	0.888693000
C	-4.176574000	0.807760000	0.157369000
C	-2.837972000	0.318895000	-0.007127000
C	-2.450618000	-0.932352000	0.591918000
C	-3.402260000	-1.649507000	1.331910000
H	-5.536116000	2.443855000	-0.272318000
H	-5.433644000	-1.756817000	2.033121000
H	-6.130574000	0.388254000	1.004748000
C	-4.519594000	2.076818000	-0.387345000
C	-1.859902000	1.121593000	-0.696870000
H	-3.112742000	-2.589616000	1.795773000
C	-2.238972000	2.381968000	-1.181157000
C	-3.559081000	2.838248000	-1.028572000
H	-1.501636000	2.995737000	-1.693261000
H	-3.825863000	3.814004000	-1.429744000
N	-1.159213000	-1.367261000	0.441624000
N	-0.590593000	0.633482000	-0.842235000
B	-0.150043000	-0.726948000	-0.439627000
C	3.316682000	1.141501000	-0.163170000
C	3.968903000	-0.262007000	0.170020000
B	1.717588000	-0.344056000	0.701928000
O	2.831506000	-1.132751000	0.273660000
O	2.009612000	1.038440000	0.425726000
C	4.696448000	-0.276328000	1.527697000
H	4.964824000	-1.309562000	1.769738000
H	5.614929000	0.319522000	1.514924000
H	4.048896000	0.096547000	2.325508000
C	4.908677000	-0.804474000	-0.909676000
H	5.762771000	-0.136447000	-1.064135000
H	5.297793000	-1.780765000	-0.602227000
H	4.391388000	-0.933537000	-1.862775000
C	4.032038000	2.344121000	0.465845000
H	5.060624000	2.432413000	0.099042000
H	3.502701000	3.265413000	0.200903000
H	4.057064000	2.273673000	1.555051000
C	3.161368000	1.402556000	-1.671105000
H	2.545870000	2.297045000	-1.813562000
H	4.127260000	1.578155000	-2.155763000
H	2.669268000	0.569465000	-2.177456000
O	1.239103000	-0.667390000	2.005283000

C	0.462759000	0.271273000	2.718234000
H	0.325183000	-0.101306000	3.740588000
H	0.954455000	1.252189000	2.770168000
H	-0.528874000	0.410379000	2.269834000
H	0.107085000	1.303475000	-1.136314000
H	-0.914714000	-2.185402000	0.980858000
C	0.739260000	-1.685172000	-1.523076000
C	-0.414727000	-1.963260000	-2.323291000
H	-0.766021000	-1.197574000	-3.010760000
C	-1.317731000	-3.131081000	-2.081265000
H	-1.862636000	-3.407181000	-2.993858000
H	-0.756512000	-4.019472000	-1.754327000
H	-2.080434000	-2.951568000	-1.299589000
H	1.522715000	-1.078677000	-1.976100000
H	1.189588000	-2.542500000	-1.019163000

Imaginary frequency= -333.8 cm^{-1}
NMV:

C	0.01	-0.01	-0.01
C	0.01	-0.01	0.00
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	0.01	0.01	0.00
C	0.01	0.00	-0.02
H	0.00	0.00	0.00
H	0.01	-0.01	-0.01
H	0.01	-0.01	0.00
C	0.00	0.00	0.00
C	0.00	-0.01	0.00
H	0.02	0.00	-0.01
C	0.00	-0.01	-0.01
C	0.00	-0.01	-0.01
H	0.00	-0.01	0.00
H	0.00	0.00	0.00
N	0.04	0.03	0.03
N	0.02	0.02	0.04
B	0.33	0.26	0.50
C	-0.04	-0.01	0.02
C	-0.07	-0.02	0.01
B	-0.35	-0.09	-0.28
O	-0.06	-0.01	-0.07
O	-0.02	0.03	-0.04
C	-0.05	-0.02	0.01
H	-0.04	-0.02	0.01
H	-0.04	-0.02	0.00
H	-0.05	-0.02	0.01
C	-0.02	0.01	0.02
H	-0.01	0.01	0.05
H	-0.02	0.00	0.01
H	0.01	0.02	0.00

C	0.00	-0.01	0.00
H	0.00	-0.02	0.00
H	0.01	0.00	0.00
H	0.00	0.00	0.01
C	0.01	0.00	0.00
H	0.02	0.00	-0.01
H	0.02	-0.01	0.01
H	0.02	0.00	-0.01
O	0.07	0.02	0.08
C	0.03	-0.01	0.02
H	-0.01	0.04	0.04
H	-0.03	0.03	0.03
H	0.01	-0.01	0.02
H	0.02	0.09	0.17
H	0.06	0.14	0.18
C	-0.01	-0.12	-0.22
C	0.08	-0.09	-0.07
H	-0.01	-0.04	0.02
C	0.01	-0.01	-0.01
H	0.01	-0.03	0.01
H	-0.06	0.02	0.12
H	0.05	0.24	-0.05
H	-0.13	0.12	-0.08
H	0.04	0.00	-0.09

TS1b E_{elec} = -1164,681879 a.u. (ΔG_{sol} = -1164,33274694 a.u)

C	-4.798170000	1.362244000	1.388063000
C	-5.203521000	0.219284000	0.725828000
C	-4.295342000	-0.471045000	-0.125714000
C	-2.968995000	0.045016000	-0.290587000
C	-2.568248000	1.233235000	0.412459000
C	-3.495448000	1.872496000	1.244469000
H	-5.668094000	-2.056075000	-0.687047000
H	-5.495567000	1.883462000	2.040463000
H	-6.211069000	-0.168820000	0.849151000
C	-4.662303000	-1.663557000	-0.810396000
C	-2.030412000	-0.636367000	-1.143754000
H	-3.197254000	2.770449000	1.780580000
C	-2.436743000	-1.814957000	-1.784919000
C	-3.740992000	-2.310385000	-1.612874000
H	-1.731898000	-2.338418000	-2.426369000
H	-4.025095000	-3.225246000	-2.128850000
N	-1.292358000	1.713817000	0.239053000
N	-0.779138000	-0.107122000	-1.316595000
B	-0.226929000	1.056284000	-0.569625000
C	3.235657000	-0.959757000	-0.458639000
C	3.670290000	0.485640000	0.026817000
B	1.397657000	0.126884000	0.526681000
O	2.541843000	0.934317000	0.799148000

O	1.796674000	-0.926736000	-0.350642000
C	3.881827000	1.475581000	-1.130992000
H	4.059696000	2.473121000	-0.716615000
H	4.748447000	1.205900000	-1.743752000
H	2.992824000	1.527064000	-1.761194000
C	4.907639000	0.512671000	0.933373000
H	5.798327000	0.149953000	0.408593000
H	5.102081000	1.543091000	1.248647000
H	4.765138000	-0.091963000	1.831685000
C	3.588780000	-1.287050000	-1.913941000
H	4.672918000	-1.299955000	-2.070297000
H	3.203385000	-2.280764000	-2.164636000
H	3.146668000	-0.570117000	-2.608673000
C	3.768095000	-2.086198000	0.442595000
H	3.361806000	-3.042143000	0.098751000
H	4.860392000	-2.150566000	0.407366000
H	3.458955000	-1.938728000	1.479781000
O	0.591498000	1.913741000	-1.384570000
C	0.909307000	3.202972000	-0.910423000
H	1.562642000	3.691860000	-1.641547000
H	0.010847000	3.828560000	-0.790263000
H	1.443140000	3.167020000	0.048147000
H	-1.074055000	2.524150000	0.801848000
H	-0.107919000	-0.716153000	-1.766117000
C	0.352763000	-0.116164000	1.905766000
C	1.048323000	-1.143780000	2.611022000
C	0.791366000	-2.591268000	2.319187000
H	1.233941000	-3.243707000	3.083090000
H	-0.287301000	-2.812028000	2.284864000
H	1.197612000	-2.923283000	1.346075000
H	1.977642000	-0.894604000	3.121042000
H	0.338020000	0.872740000	2.372443000
H	-0.652755000	-0.389760000	1.584820000

Imaginary frequency= -349.7 cm^{-1}

NMV

C	-0.01	-0.01	0.01
C	0.00	0.00	0.00
C	0.00	0.00	0.00
C	-0.01	0.00	0.01
C	-0.04	0.00	0.01
C	-0.01	-0.01	0.01
H	0.00	0.00	0.00
H	-0.01	-0.01	0.01
H	0.00	0.00	0.00
C	0.00	0.00	0.00
C	-0.02	-0.01	0.01
H	-0.01	0.00	-0.01
C	0.01	0.00	0.01
C	0.00	0.00	0.00

H	0.01	0.01	0.00
H	0.00	0.00	0.00
N	-0.04	0.05	-0.06
N	-0.01	0.03	-0.01
B	-0.36	0.22	-0.32
C	0.00	0.00	-0.01
C	0.01	0.00	-0.01
B	0.19	-0.31	0.46
O	0.04	-0.01	0.04
O	0.00	-0.01	0.05
C	0.00	0.01	0.00
H	-0.02	0.01	0.00
H	0.01	0.02	0.01
H	0.01	-0.01	-0.02
C	0.02	0.00	-0.01
H	0.02	0.00	-0.01
H	0.01	-0.01	-0.01
H	0.01	-0.01	-0.02
C	-0.02	0.01	-0.01
H	-0.02	0.01	-0.01
H	-0.02	0.00	-0.01
H	-0.02	0.01	-0.01
C	0.00	0.00	-0.01
H	0.04	0.00	-0.04
H	0.01	0.03	0.03
H	-0.08	0.00	-0.03
O	0.05	-0.05	0.09
C	0.01	0.01	0.02
H	0.02	-0.06	-0.01
H	-0.01	-0.02	-0.06
H	-0.02	0.04	0.02
H	-0.03	0.11	-0.16
H	0.04	0.13	-0.06
C	0.12	0.09	-0.31
C	0.02	0.00	0.10
C	0.03	0.01	-0.02
H	0.02	-0.03	-0.05
H	0.01	-0.02	0.03
H	-0.05	-0.10	-0.05
H	0.14	-0.03	-0.10
H	-0.21	0.01	-0.08
H	0.08	-0.04	-0.13

TS2a E_{elec} = -1164,7219758 a.u. (ΔG_{sol} = -1164,38000097 a.u)

C	-3.672159000	-0.394595000	-0.481529000
C	-2.765709000	-1.477015000	0.236686000
B	-1.410175000	0.097968000	-0.754386000
O	-1.479612000	-0.834109000	0.307356000
O	-2.716239000	0.360625000	-1.248731000

C	-2.592394000	-2.760146000	-0.595938000
H	-1.823554000	-3.381666000	-0.126960000
H	-3.516012000	-3.344604000	-0.655286000
H	-2.261612000	-2.527876000	-1.612026000
C	-3.207442000	-1.849245000	1.653897000
H	-4.207012000	-2.296942000	1.652772000
H	-2.511852000	-2.582582000	2.074508000
H	-3.218162000	-0.978755000	2.313187000
C	-4.707780000	-0.972683000	-1.453757000
H	-5.420275000	-1.622489000	-0.934409000
H	-5.273492000	-0.155839000	-1.913681000
H	-4.234967000	-1.545150000	-2.254427000
C	-4.397517000	0.547390000	0.494462000
H	-4.821792000	1.382907000	-0.070994000
H	-5.216662000	0.035095000	1.009440000
H	-3.724607000	0.961042000	1.247660000
O	-0.363216000	-0.036338000	-1.668137000
C	-0.355467000	0.783445000	-2.815340000
H	0.451450000	0.447742000	-3.475315000
H	-1.305260000	0.726983000	-3.364440000
H	-0.172168000	1.834067000	-2.555634000
C	-1.114667000	2.151214000	0.214472000
C	-0.174796000	3.101563000	1.037501000
H	0.073060000	4.011912000	0.479653000
C	-0.615908000	3.423264000	2.457321000
H	0.153743000	3.979477000	3.010184000
H	-1.538200000	4.023405000	2.487005000
H	-0.820297000	2.511351000	3.033824000
H	-1.488912000	2.631803000	-0.692523000
H	-1.948349000	1.842421000	0.844235000
C	1.839287000	-0.267866000	1.370291000
C	2.604549000	0.935294000	-0.671725000
C	2.708366000	-0.184483000	0.226263000
C	1.966279000	-1.366757000	2.232470000
C	3.482557000	1.007245000	-1.763000000
C	3.688329000	-1.202804000	-0.006827000
C	2.925049000	-2.364397000	1.985804000
H	1.310631000	-1.440146000	3.097197000
C	4.439364000	0.000090000	-1.980012000
H	3.414777000	1.853764000	-2.442685000
C	3.774564000	-2.299384000	0.896922000
C	4.550683000	-1.087417000	-1.134031000
H	2.994083000	-3.205395000	2.673119000
H	5.103058000	0.085111000	-2.838329000
H	4.513865000	-3.075848000	0.718431000
H	5.293424000	-1.860355000	-1.313435000
B	0.633213000	1.840648000	0.646145000
N	0.937377000	0.735363000	1.599720000
N	1.680753000	1.909021000	-0.412397000
H	1.668720000	2.670676000	-1.076138000

H 0.305679000 0.558427000 2.367526000

Imaginary frequency= -343.5 cm^{-1}
NMV:

C	0.02	0.01	-0.01
C	0.04	0.03	-0.01
B	0.07	0.37	0.21
O	0.00	0.06	0.05
O	-0.02	0.03	0.01
C	0.03	0.03	-0.01
H	0.03	0.02	-0.01
H	0.03	0.03	-0.01
H	0.04	0.03	0.00
C	0.00	0.00	-0.02
H	0.01	-0.01	-0.03
H	0.00	0.00	-0.01
H	-0.01	-0.01	0.00
C	0.01	0.00	0.00
H	0.01	-0.01	0.00
H	0.00	-0.01	0.00
H	0.01	0.00	-0.01
C	-0.02	-0.02	0.01
H	-0.02	-0.01	0.01
H	-0.03	-0.03	-0.02
H	-0.04	-0.03	0.03
O	-0.02	0.01	0.01
C	0.00	0.00	0.02
H	0.00	0.00	0.01
H	0.01	0.02	0.00
H	0.00	0.02	-0.01
C	-0.32	-0.15	-0.12
C	-0.09	-0.21	-0.13
H	-0.12	-0.23	-0.17
C	-0.01	-0.08	-0.10
H	0.03	-0.05	-0.21
H	0.01	-0.05	-0.14
H	-0.02	-0.02	-0.01
H	-0.34	0.13	0.03
H	-0.35	0.20	0.01
C	0.03	-0.02	0.00
C	0.02	-0.02	0.00
C	0.01	-0.01	0.00
C	0.00	-0.01	0.00
C	0.00	-0.01	0.00
C	0.01	-0.01	0.00
C	0.00	-0.01	0.00
H	0.01	0.00	0.00
C	0.00	-0.01	0.00
H	0.00	0.00	0.01
C	0.00	-0.01	0.00

C	0.00	0.00	0.00
H	0.01	-0.01	0.00
H	0.00	-0.01	0.00
H	0.00	-0.01	0.00
H	0.00	0.00	0.00
B	0.25	0.02	0.11
N	0.04	0.01	0.00
N	0.02	-0.01	0.03
H	0.01	0.03	0.07
H	0.05	0.07	0.02

TS2b E_{elec} = -1164,716438 a.u. (ΔG_{sol} = -1164,37609239 a.u)

C	-2.365209000	2.973654000	-0.687297000
C	-3.653022000	2.696628000	-0.269879000
C	-4.055877000	1.351226000	-0.048711000
C	-3.110757000	0.298148000	-0.276929000
C	-1.784950000	0.609681000	-0.732879000
C	-1.430283000	1.948420000	-0.918918000
H	-6.083888000	1.812213000	0.567926000
H	-2.060261000	4.005612000	-0.845352000
H	-4.367844000	3.496843000	-0.098628000
C	-5.364631000	1.015316000	0.399579000
C	-3.492466000	-1.062182000	-0.031752000
H	-0.420676000	2.185363000	-1.240360000
C	-4.783311000	-1.346233000	0.411395000
C	-5.707355000	-0.303336000	0.619334000
H	-5.069858000	-2.378271000	0.596099000
H	-6.708671000	-0.551222000	0.963438000
N	-0.895482000	-0.419916000	-0.985416000
N	-2.554097000	-2.053039000	-0.253194000
B	-1.205718000	-1.806662000	-0.715552000
C	4.169883000	0.048158000	0.159180000
C	3.243639000	0.935134000	-0.760427000
B	2.029523000	0.115496000	1.034394000
O	1.914160000	0.614954000	-0.269910000
O	3.363115000	-0.105745000	1.354583000
C	3.314512000	0.613863000	-2.252695000
H	2.618967000	1.256111000	-2.801890000
H	4.320664000	0.799216000	-2.642762000
H	3.049807000	-0.425334000	-2.456618000
C	3.442194000	2.443187000	-0.544719000
H	4.406173000	2.786439000	-0.931689000
H	2.650948000	2.985018000	-1.071258000
H	3.381415000	2.703234000	0.515998000
C	4.429786000	-1.356409000	-0.402919000
H	5.089605000	-1.327489000	-1.275234000
H	4.912024000	-1.962603000	0.369801000
H	3.497782000	-1.850599000	-0.686115000
C	5.498694000	0.695649000	0.552063000

H	6.054360000	0.020964000	1.210612000
H	6.116737000	0.886974000	-0.331188000
H	5.349271000	1.637916000	1.082722000
O	-0.537009000	-2.903282000	-1.215500000
C	0.845875000	-2.820065000	-1.517246000
H	1.185282000	-3.812055000	-1.833167000
H	1.038751000	-2.112948000	-2.336940000
H	1.368836000	-2.491377000	-0.606985000
H	0.076411000	-0.131868000	-1.048733000
H	-2.866901000	-3.002404000	-0.103799000
C	0.542733000	-1.625648000	1.698595000
C	0.844824000	-0.143596000	2.015790000
C	1.105839000	0.224255000	3.495390000
H	1.281721000	1.300935000	3.659008000
H	0.254319000	-0.069775000	4.126068000
H	1.986858000	-0.306794000	3.878568000
H	-0.006683000	0.461001000	1.666399000
H	-0.411376000	-1.918914000	2.178151000
H	1.321435000	-2.252182000	2.176875000

Imaginary frequency= -174.3 cm^{-1}
NMV:

C	-0.01	0.01	-0.01
C	-0.01	0.00	-0.01
C	0.00	0.00	0.00
C	0.01	0.00	0.01
C	0.01	0.01	0.00
C	-0.01	0.02	-0.01
H	-0.01	-0.02	-0.02
H	-0.02	0.01	-0.01
H	-0.02	-0.01	-0.01
C	0.00	-0.01	-0.01
C	0.04	0.00	0.03
H	-0.01	0.03	-0.02
C	0.02	-0.01	0.01
C	0.01	-0.02	-0.01
H	0.03	-0.01	0.02
H	0.01	-0.02	-0.02
N	0.02	0.03	0.00
N	0.06	0.02	0.09
B	0.13	0.02	0.22
C	0.01	0.01	0.00
C	0.02	0.01	-0.01
B	0.01	0.04	-0.02
O	0.02	0.02	-0.01
O	-0.02	0.00	-0.01
C	0.01	0.00	-0.01
H	0.01	0.01	0.00
H	0.01	0.00	-0.01
H	0.00	0.01	0.00

C	0.02	0.01	-0.01
H	0.02	0.01	-0.01
H	0.02	0.01	-0.01
H	0.02	0.01	-0.01
C	0.01	0.01	0.00
H	0.02	0.01	0.01
H	0.00	0.01	0.01
H	0.01	0.01	-0.01
C	0.00	0.00	0.01
H	0.00	0.00	0.02
H	0.01	0.00	0.02
H	0.00	0.00	0.01
O	0.03	0.01	0.03
C	0.01	-0.02	0.00
H	0.00	-0.01	-0.04
H	0.02	0.01	0.02
H	0.06	-0.06	-0.02
H	0.01	0.06	0.01
H	0.08	0.02	0.14
C	-0.39	0.02	-0.11
C	-0.05	-0.04	-0.10
C	0.02	-0.12	-0.07
H	0.14	-0.15	-0.05
H	-0.01	-0.04	-0.08
H	-0.04	-0.23	-0.09
H	0.04	0.13	-0.03
H	-0.19	0.14	0.37
H	-0.26	-0.13	-0.50

Pa E_{elec} = -1049,610266 a.u. (ΔG_{sol} = -1049,23805971 a.u)

C	-3.787431000	-0.619350000	0.946237000
C	-3.478970000	-0.736623000	-0.595105000
B	-2.357660000	1.057519000	0.306150000
O	-2.332655000	0.163855000	-0.746213000
O	-3.281656000	0.714956000	1.262503000
C	-4.592257000	-0.173221000	-1.486881000
H	-4.225492000	-0.106418000	-2.514913000
H	-5.474790000	-0.818835000	-1.479654000
H	-4.892938000	0.828621000	-1.167374000
C	-3.073460000	-2.127885000	-1.074098000
H	-3.893843000	-2.837895000	-0.930452000
H	-2.840000000	-2.096002000	-2.142350000
H	-2.196580000	-2.501844000	-0.542316000
C	-5.267482000	-0.677100000	1.316343000
H	-5.698387000	-1.643312000	1.036075000
H	-5.379779000	-0.559849000	2.398102000
H	-5.839025000	0.114067000	0.827814000
C	-2.987628000	-1.606091000	1.805878000
H	-3.098234000	-1.330271000	2.858238000

H	-3.349047000	-2.630592000	1.680874000
H	-1.922603000	-1.580064000	1.558362000
C	-1.476920000	2.357947000	0.395707000
C	-0.352905000	2.545866000	-0.662651000
H	-0.795470000	2.326947000	-1.646257000
C	0.125316000	4.009712000	-0.686801000
H	0.897226000	4.177641000	-1.446583000
H	-0.704493000	4.693009000	-0.902236000
H	0.540723000	4.312378000	0.283301000
H	-2.183691000	3.201544000	0.319021000
H	-1.064608000	2.443658000	1.411358000
C	3.184184000	0.991790000	0.196126000
C	1.663227000	-0.842687000	-0.518199000
C	2.944772000	-0.395437000	-0.062171000
C	4.434249000	1.407703000	0.638817000
C	1.454016000	-2.194884000	-0.767411000
C	3.998411000	-1.344892000	0.137926000
C	5.464922000	0.465231000	0.832823000
H	4.611911000	2.461736000	0.833974000
C	2.497220000	-3.121645000	-0.566884000
H	0.483427000	-2.531079000	-1.120901000
C	5.263107000	-0.878015000	0.591966000
C	3.740687000	-2.718810000	-0.125197000
H	6.434628000	0.812627000	1.179453000
H	2.309738000	-4.173311000	-0.767323000
H	6.064495000	-1.595300000	0.744853000
H	4.537065000	-3.441948000	0.026076000
B	0.834012000	1.504619000	-0.456265000
N	2.135436000	1.887642000	-0.010324000
N	0.662435000	0.107701000	-0.698844000
H	-0.244430000	-0.239942000	-0.990583000
H	2.353489000	2.856189000	0.179314000

Pb E_{elec} = -1049,60988 a.u. (ΔG_{sol} = -1049,23805971 a.u)

C	-5.552510000	0.835026000	0.531346000
C	-5.405393000	-0.535950000	0.574763000
C	-4.152069000	-1.134701000	0.267452000
C	-3.051878000	-0.288379000	-0.085909000
C	-3.235621000	1.130849000	-0.123894000
C	-4.476270000	1.676873000	0.183595000
H	-4.782725000	-3.187463000	0.564819000
H	-6.513816000	1.283415000	0.768035000
H	-6.241564000	-1.175256000	0.843455000
C	-3.950574000	-2.542447000	0.297329000
C	-1.780574000	-0.869799000	-0.397623000
H	-4.610557000	2.754713000	0.153964000
C	-1.626620000	-2.251426000	-0.358753000
C	-2.715878000	-3.075782000	-0.010283000
H	-0.663345000	-2.690960000	-0.601906000

H	-2.571521000	-4.152774000	0.013617000
N	-2.143364000	1.922843000	-0.474743000
N	-0.733972000	-0.016301000	-0.734932000
B	-0.850981000	1.405244000	-0.795263000
C	3.834469000	-0.443498000	0.846109000
C	3.406194000	-0.886404000	-0.605365000
B	2.383432000	1.096666000	-0.045156000
O	2.265349000	-0.004557000	-0.869570000
O	3.370365000	0.940943000	0.897026000
C	2.943746000	-2.335275000	-0.734289000
H	2.628726000	-2.530545000	-1.763536000
H	3.762338000	-3.022269000	-0.497881000
H	2.105305000	-2.556731000	-0.071258000
C	4.455948000	-0.569265000	-1.677214000
H	5.327258000	-1.223835000	-1.587623000
H	4.013338000	-0.721596000	-2.665533000
H	4.794102000	0.468831000	-1.612254000
C	3.092142000	-1.195507000	1.957728000
H	3.427619000	-2.233633000	2.032057000
H	3.289807000	-0.702335000	2.913498000
H	2.011286000	-1.190439000	1.790337000
C	5.338003000	-0.459676000	1.111063000
H	5.534423000	-0.107824000	2.127992000
H	5.735133000	-1.475711000	1.023498000
H	5.878690000	0.186839000	0.417551000
H	-2.317634000	2.918634000	-0.491304000
H	0.161119000	-0.448915000	-0.933983000
C	0.360780000	2.343348000	-1.201025000
C	1.533578000	2.420682000	-0.181005000
C	1.075895000	2.957770000	1.191564000
H	1.922606000	3.079082000	1.873860000
H	0.581470000	3.931112000	1.089222000
H	0.361883000	2.277790000	1.671212000
H	2.256948000	3.154351000	-0.577475000
H	0.757015000	1.999192000	-2.166404000
H	-0.014719000	3.361270000	-1.377335000

TS1a (Ph) E_{elec} = -1356,444250 a.u. (ΔG_{sol} = -1356,04915501 a.u)

C	4.190389000	-1.259256000	1.949982000
C	4.376976000	-2.259175000	1.014105000
C	3.368961000	-2.527172000	0.046676000
C	2.177149000	-1.731004000	0.049157000
C	2.005441000	-0.696659000	1.032797000
C	3.019113000	-0.481313000	1.973241000
H	4.401400000	-4.170909000	-0.922835000
H	4.963656000	-1.063370000	2.689604000
H	5.284928000	-2.856192000	1.010680000
C	3.496442000	-3.569315000	-0.914210000
C	1.134692000	-2.000941000	-0.902003000

H	2.894771000	0.299801000	2.719022000
C	1.296303000	-3.048845000	-1.814111000
C	2.475084000	-3.816329000	-1.811942000
H	0.505967000	-3.256628000	-2.531041000
H	2.579182000	-4.619649000	-2.537985000
N	0.841656000	0.036811000	1.024965000
N	0.007699000	-1.215224000	-0.873609000
B	-0.210955000	-0.057256000	0.000541000
C	-4.051458000	-0.386477000	-0.671667000
C	-4.196851000	0.803320000	0.369975000
B	-2.104135000	-0.160756000	0.655661000
O	-2.841580000	1.076371000	0.747262000
O	-2.809556000	-1.004156000	-0.303676000
C	-4.980672000	0.400390000	1.635071000
H	-4.917919000	1.218013000	2.360808000
H	-6.038773000	0.212598000	1.424938000
H	-4.547404000	-0.489139000	2.097353000
C	-4.811595000	2.084070000	-0.203901000
H	-5.833792000	1.912588000	-0.558621000
H	-4.852676000	2.851871000	0.575890000
H	-4.218401000	2.478286000	-1.031408000
C	-5.160139000	-1.445494000	-0.585520000
H	-6.143582000	-1.017308000	-0.809869000
H	-4.966714000	-2.238023000	-1.316367000
H	-5.200587000	-1.905372000	0.403974000
C	-3.952866000	0.087761000	-2.132153000
H	-3.656726000	-0.759409000	-2.759487000
H	-4.910741000	0.466241000	-2.504270000
H	-3.206051000	0.875060000	-2.253899000
O	-1.889301000	-0.751458000	1.963446000
C	-1.524876000	-2.106076000	2.075300000
H	-1.642171000	-2.413779000	3.122468000
H	-2.156799000	-2.754265000	1.452112000
H	-0.477997000	-2.279159000	1.788164000
H	-0.754449000	-1.501778000	-1.474520000
H	0.769148000	0.724444000	1.760400000
C	-0.576692000	1.521315000	-0.918486000
C	0.679482000	1.813417000	-1.491411000
H	0.949193000	1.292802000	-2.409245000
H	-1.342539000	1.182827000	-1.610185000
H	-0.992162000	2.206569000	-0.185146000
C	1.718974000	2.615418000	-0.908274000
C	2.948855000	2.798653000	-1.597548000
C	1.590390000	3.275767000	0.344460000
C	3.966965000	3.592642000	-1.082488000
H	3.086296000	2.303844000	-2.556851000
C	2.616194000	4.064773000	0.857694000
H	0.670969000	3.170063000	0.912264000
C	3.814515000	4.235020000	0.154040000
H	4.890884000	3.709779000	-1.644140000

H	2.480605000	4.554248000	1.819546000
H	4.611309000	4.851896000	0.559178000

Imaginary frequency= -360.8 cm^{-1}
NMV:

C	0.00	-0.01	0.00
C	0.00	0.00	0.00
C	-0.01	-0.01	0.01
C	-0.01	-0.01	0.02
C	0.00	-0.01	0.02
C	0.00	-0.01	0.01
H	0.00	0.00	0.00
H	0.01	0.00	0.00
H	0.00	0.00	-0.01
C	0.00	0.00	0.00
C	-0.01	-0.01	0.01
H	0.01	0.00	0.00
C	-0.01	-0.01	0.01
C	-0.01	0.00	0.01
H	0.00	0.00	0.00
H	0.00	0.01	0.00
N	0.04	0.04	-0.02
N	0.02	0.05	-0.03
B	0.33	0.35	-0.35
C	-0.03	0.02	-0.02
C	-0.06	0.01	-0.02
B	-0.34	-0.07	0.14
O	-0.05	-0.02	0.05
O	-0.01	0.01	0.04
C	-0.03	0.00	-0.01
H	-0.02	0.00	-0.01
H	-0.03	0.00	0.00
H	-0.04	0.00	-0.01
C	-0.01	0.02	-0.01
H	0.00	0.03	-0.03
H	-0.01	0.01	0.00
H	0.01	0.01	0.00
C	0.00	-0.01	-0.01
H	0.00	-0.01	-0.01
H	0.01	0.00	-0.01
H	0.01	0.00	-0.01
C	0.01	0.00	-0.01
H	0.01	-0.01	0.00
H	0.01	-0.01	-0.01
H	0.01	-0.01	0.00
O	0.11	0.04	-0.07
C	0.03	0.00	-0.03
H	0.02	0.07	-0.02
H	-0.02	0.05	-0.02
H	0.01	0.00	-0.05

H	0.10	0.18	-0.19
H	0.17	0.26	-0.21
C	-0.02	-0.33	0.27
C	0.03	-0.06	0.03
H	-0.01	-0.05	0.02
H	-0.08	0.12	0.09
H	0.01	-0.04	0.04
C	-0.04	-0.06	-0.02
C	0.01	0.00	0.00
C	0.00	-0.01	0.01
C	-0.01	0.00	0.00
H	0.03	0.00	0.00
C	0.00	0.00	-0.01
H	0.00	0.00	0.02
C	0.01	0.02	0.01
H	-0.01	0.00	-0.01
H	-0.01	0.00	-0.01
H	0.01	0.01	0.01

I1a (Ph) E_{elec} = -830,0294179 a.u. (ΔG_{sol} = -829,84531567 a.u)

C	1.523254000	-2.040192000	-1.658752000
C	1.864931000	-1.664465000	-0.201839000
H	1.784011000	-2.482632000	0.515592000
H	1.433878000	-3.115152000	-1.834124000
H	2.143480000	-1.570908000	-2.426057000
C	-1.017055000	0.870400000	-0.760791000
C	-1.983243000	-1.295600000	0.018214000
C	-2.076163000	0.136956000	-0.114522000
C	-1.145733000	2.261836000	-0.888856000
C	-3.044247000	-1.985299000	0.624691000
C	-3.234937000	0.826963000	0.369471000
C	-2.283572000	2.925918000	-0.399803000
H	-0.350263000	2.824004000	-1.372831000
C	-4.171745000	-1.293153000	1.098666000
H	-2.982109000	-3.066302000	0.728238000
C	-3.312740000	2.240366000	0.218309000
C	-4.279308000	0.080559000	0.985232000
H	-2.348071000	4.006287000	-0.513771000
H	-4.974129000	-1.859399000	1.567612000
H	-4.189085000	2.764748000	0.590114000
H	-5.156111000	0.604630000	1.356340000
B	0.371019000	-1.248979000	-0.948277000
N	0.064935000	0.191927000	-1.252610000
N	-0.876578000	-1.936141000	-0.463975000
H	-0.865683000	-2.935517000	-0.311798000
H	0.799394000	0.784644000	-1.614351000
C	2.857344000	-0.664839000	0.159592000
C	3.314277000	-0.558772000	1.501758000
C	3.392390000	0.285096000	-0.750601000

C	4.217318000	0.419195000	1.903448000
H	2.940459000	-1.272256000	2.234319000
C	4.297272000	1.267517000	-0.343465000
H	3.111862000	0.238299000	-1.799613000
C	4.720929000	1.352624000	0.985292000
H	4.538066000	0.454276000	2.942845000
H	4.680710000	1.971702000	-1.079536000
H	5.426156000	2.117304000	1.298248000

I1a (Me) E_{elec} = -638,2740673 a.u. (ΔG_{sol} = -638,14183586 a.u)

C	3.361577000	-0.523578000	-1.066000000
C	3.346452000	-0.456240000	0.484488000
H	3.571893000	-1.417746000	0.960506000
C	4.069461000	0.699170000	1.154974000
H	3.841715000	0.762001000	2.229042000
H	5.167802000	0.645622000	1.064151000
H	3.771234000	1.663683000	0.720619000
H	3.665426000	-1.474141000	-1.514220000
H	3.848793000	0.321441000	-1.563021000
C	-0.134841000	1.164416000	-0.228851000
C	-0.410603000	-1.314844000	-0.093325000
C	-0.985235000	0.009868000	-0.059353000
C	-0.729333000	2.439690000	-0.211512000
C	-1.270643000	-2.418765000	0.056012000
C	-2.396609000	0.177028000	0.119486000
C	-2.113949000	2.585680000	-0.030031000
H	-0.098613000	3.317177000	-0.338491000
C	-2.651068000	-2.236373000	0.236507000
H	-0.849846000	-3.421881000	0.032767000
C	-2.944281000	1.491733000	0.135259000
C	-3.219293000	-0.975527000	0.271897000
H	-2.536831000	3.588817000	-0.020021000
H	-3.283579000	-3.115009000	0.351287000
H	-4.015005000	1.618096000	0.273177000
H	-4.289821000	-0.847953000	0.410220000
B	1.955633000	-0.331056000	-0.320472000
N	1.201954000	0.991012000	-0.414417000
N	0.929292000	-1.458559000	-0.278083000
H	1.255442000	-2.415411000	-0.255834000
H	1.724693000	1.849874000	-0.517616000

10.References

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