-Supporting Information-

An Experimental and Theoretical Study into the Facile, Homogenous (N-Heterocyclic Carbene)$_2$-Pd(0) Catalyzed Diboration of Internal and Terminal Alkynes

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Table of Contents

GENERAL CONSIDERATIONS

The manipulation of air sensitive compounds and their spectroscopic measurements were undertaken using standard Schlenk line techniques under pre-dried argon (using a BASF R3-11(G) catalyst and 4 Å molecular sieves), or in a MBraun glovebox under N_2 (O_2 < 10.0 ppm). All glassware was dried in a 160 ^oC oven prior to use. All solvents used for air sensitive compounds were dried by vacuum distillation followed by distillation over potassium or stored over activated 4 Å molecular sieves under an Ar atmosphere. Dried solvents were degassed and stored over argon in ampoules containing activated 4 Å molecular sieves. Deuterated benzene, C_6D_6, was degassed and dried by refluxing over potassium for 3 days, vacuum transferred into ampoules and stored under N_2. Deuterated chloroform, $CDCl_3$, was used as purchased (open bottle). NMR spectra were recorded on a Varian VNMRS 400 (^1H 399.5 MHz; $^{13}C\{^1H\}$ 100.46 MHz; $^{29}Si\{^1H\}$ 79.4 MHz; $^{11}B\{^1H\}$) or 500 (^1H 499.91 MHz; $^{13}C\{^1H\}$ 125.71 MHz). The spectra were referenced to the corresponding protic solvent (^1H) or signals of the solvent (^{13}C). $^{29}Si\{^1H\}$ were referenced externally relative to the internal standard SiMe4. All spectra carried out on the Varian VNMRS 400 and VNMRS 500 were recorded at 303 K.

Elemental analyses were carried out at the Elemental Analysis Service, London MetropolitanUniversity. High resolution mass spectrometry was carried out by Dr. Alaa Abdul-Sada, University of Sussex.

Scaled Synthesis of Pd(ITMe)$_2$(PhC≡CPh) (1)

In a vial, isopropanol (109.0 µl, 1.42 mmol) was added to a mixture of [Pd(ITMe)(methalllyl)Cl] (0.457 g, 1.42 mmol), ^{t}-BuOK (0.161 g, 1.44 mmol) and ITMe (0.183 g, 1.48 mmol) in toluene (80 ml). The resulting reaction mixture was stirred at room temperature under a N_2 for 4 h. At this point, diphenylacetylene (0.280 g, 1.57 mmol) was added and the reaction mixture was stirred for a further 18 h. At this stage the volatiles were removed *in vacuo*. Crude **1** was dissolved in CH_3CN (100 ml) and filtered. The filtrates volatiles were removed under reduced pressure and yellow powdered solid was washed with a 1:1 toluene/hexane solution (3 x 20 ml) followed by pentane (3 x 20 ml). Yield: 0.407 g, 54 %. ^{1}H NMR (399.5 MHz, C_6D_6): δ = 7.99 (dd, $^3J_{HH}$ = 8.1, $^4J_{HH}$ = 1.3 Hz, 4H, *m*-Ph), 7.27 (m, 4H, *o*-Ph), 7.05 (tt, $^3J_{HH}$ = 7.3, $^4J_{HH}$ = 1.3 Hz, 2H, *p*-Ph), 3.49 (s, 12H, N(1,3)-C**H**$_3$), 1.54 (s, 12H, C(4,5)-CH_3). ^{13}C{^{1}H} NMR (100.46 MHz, C_6D_6): δ = 198.7 (N**C**N), 138.6 (C≡**C**), 130.1 (*o*-Ph), 128.2 (*m*-Ph), 126.3 (*i*-Ph), 124.2 (*p*-Ph), 123.1 (**C**(4,5)-CH_3), 35.2 (N(1,3)-**C**H_3), 9.0 (C(4,5)-**C**H_3).

Stock Solution of 1

Stock solutions were made in batches; in a glovebox 5 mg of **1** was dissolved in 5000 µl of C_6D_6.

Synthesis of (Z)-1,2-diphenyl-1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethane (2)

A stock solution of **1** (0.47 mg, 0.78 µmol) in C_6D_6 (471 µl) was added to a mixture of diphenylacetylene (0.032 g, 0.18 mmol) and bis(pinacolato)diboron (0.046 g, 0.18 mmol). The resulting reaction mixture was stirred at room temperature for 21 h under a N_2 atmosphere. At this point all volatiles were removed *in vacuo*. Deionized H_2O (35 ml) was added and the mixture was stirred at room temperature for 24 h. Filtration and drying under reduced pressure resulted in the collection of a white powdered solid.Yield: 0.076 g, 99%. ^{1}H NMR (399.5 MHz, $CDCl_3$): δ = 7.05 (m, 6H, Ph), 6.95 (m, 4H, Ph), 1.32 (s, 24H, Bpin).

$^{13}C\{^1H\}$ NMR (100.46 MHz, $CDCl_3$): δ = 141.4, 129.5, 127.5, 125.9, 84.2, 25.0. $^{11}B\{^1H\}$ NMR (128.2 MHz, $CDCl_3$): δ = 30.33 (spectroscopic data in agreement with the literature).

Synthesis of (*E*)-2,2'-(1-phenylethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (3)

To a stock solution of **1** (0.61 mg, 1.14 μmol) in C_6D_6 (607 μmol) was added to a mixture of phenylacetylene (25.0 μl, 0.23 mmol) and bis(pinacolato)diboron (0.058 g, 0.23 mmol). The resulting reaction mixture was stirred at room temperature for 3 h under a N_2 atmosphere. The volatiles were removed *in vacuo*, deionized H_2O (35 ml) was added to the crude material and the mixture was stirred for 24 h. Decanting the H_2O and drying under vacuum resulted in the isolation of a yellow oil. Yield: 0.074 g, 91 %. ^1H NMR (399.5 MHz, $CDCl_3$): δ = 7.43 (m, 2H, Ph), 7.28 (m, 3H, Ph), 6.28 (s, 1H, =CH), 1.37 (s, 12H, Bpin), 1.30 (s, 12H, Bpin). $^{13}C\{^1H\}$ NMR (100.46 MHz, $CDCl_3$): δ = 143.2, 128.4, 127.7, 126.7, 84.3, 83.7, 25.2, 25.0. $^{11}B\{^1H\}$ (128.2 MHz, $CDCl_3$): δ = 30.07 (spectroscopic data in agreement with the literature).

Synthesis of (*E*)-2,2'-(1-(o-tolyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (4)

A stock solution of **1** (0.42 mg, 0.79 μmol) in C_6D_6 (423 μl) was added to a mixture of 1-ethynyl-2-methylbenzene (20.0 μl, 0.16 mmol) and bis(pinacalato)diboron (0.051 g, 0.20 mmol). The resulting reaction mixture was stirred for 2 h at room temperature under a N_2 atmosphere. At this point all volatiles were removed *in vacuo*, deionized H_2O (50 ml) was then added and the mixture was stirred for 24 h. The H_2O was decanted, the resulting pale brown solid was washed with more deionized H_2O (3 x 25 ml) and dried thoroughly under a high vacuum. Yield: 0.046 g, 79 %. ^1H NMR (399.5 MHz, $CDCl_3$): δ = 7.12 (m, 4H, 3,4,5,6-Ph), 6.02 (s, 1H, =CH), 2.31 (s, 3H, $PhCH_3$), 1.33 (s, 12H, Bpin), 1.29 (s, 12H, Bpin). $^{13}C\{^1H\}$ NMR (100.46 MHz, $CDCl_3$): δ = 144.8, 134.7, 130.0, 128.1, 126.8, 125.7, 84.1, 83.7, 25.1, 25.0, 20.6, 2 C=C were not observed due to quadrapolar broadening caused by adjacent B atoms. $^{11}B\{^1H\}$ NMR (128.2 MHz, $CDCl_3$): δ = 30.03 (spectroscopic data in agreement with the literature).

Synthesis of (*E*)-2,2'-(1-(4-fluorophenyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (5)

A stock solution of **1** (0.50 mg, 0.94 µmol) in C_6D_6 (500 µl) was added to a mixture of 1-ethynyl-4-fluorobenzene (0.023 g, 0.19 mmol) and bis(pinacalato)diboron (0.048 g, 0.19 mmol). The resulting reaction mixture was stirred at room temperature for 9 h under a N_2 atmosphere. At this point the volatiles were removed *in vacuo*, deionized H_2O (35 ml) was added and the resulting mixture was stirred at room temperature for 24 h. The H_2O was then decanted and the resulting yellow oil was dried under vacuum. Yield: 0.067 g, 95 %. ^{1}H NMR (399.5 MHz, $CDCl_3$): δ = 7.41 (m, 2H, Ph), 6.98 (m, 2H, Ph), 6.24 (s, 1H, =CH), 1.37 (s, 12H, Bpin), 1.30 (s, 12H, Bpin). $^{13}C\{^1H\}$ NMR (100.46 MHz, $CDCl_3$): δ = 162.7 (d, $^1J_{CF}$ = 246.6 Hz, *p*-Ph), 139.2 (d, $^4J_{CF}$ = 3.3 Hz, *i*-Ph), 128.3 (d, $^3J_{CF}$ = 8.0 Hz, *o*-Ph), 115.3 (d, $^2J_{CF}$ = 21.4 Hz, *m*-Ph), 84.3 (Bpin), 83.7 (Bpin), 25.2 (Bpin), 25.0 (Bpin), 2 C=C were not observed due to quadrapolar broadening caused by adjacent B atoms. $^{11}B\{^1H\}$ NMR (128.2 MHz, $CDCl_3$): δ = 30.05. ^{19}F NMR (375.9 MHz, $CDCl_3$): δ = –115.10 (m) (spectroscopic data in agreement with the literature).

Synthesis of (*E*)-2,2'-(1-(4-methoxyphenyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (6)

A stock solution of **1** (0.50 mg, 0.93 µmol) in C_6D_6 (496 µl) was added to a mixture of 1-ethynyl-4-methoxybenzene (0.025 g, 0.18 mmol) and bis(pinacalato)diboron (0.055 g, 0.22 mmol). The resulting reaction mixture was stirred at room temperature for 4 h under a N_2 atmosphere. At this point all volatiles were removed *in vacuo*, deionized H_2O (35 ml) was then added and the mixture was stirred for 24 h. The H_2O was decanted, the resulting dark yellow oil was washed with more deionized H_2O (2 x 25ml) and dried thoroughly under a high vacuum. Yield: 0.063 g, 88 %. ^{1}H NMR (399.5 MHz, $CDCl_3$): δ = 7.40 (m, 2H, Ph), 6.84 (m, 2H, Ph), 6.22 (s, 1H, =CH), 3.79 (s, 3H, OMe), 1.38 (s, 12H, Bpin), 1.30 (s, 12H, Bpin). $^{13}C\{^1H\}$ NMR (100.46 MHz, $CDCl_3$): δ = 159.6, 135.6, 133.7 (**C**=C), 127.9, 114.1 (C=**C**), 113.9, 84.2, 83.6, 55.3, 25.3, 25.0. $^{11}B\{^1H\}$ NMR (128.2 MHz, $CDCl_3$): δ = 30.43 (spectroscopic data in agreement with the literature).

Synthesis of (*E*)-2,2'-(1-(4-(trifluoromethyl)phenyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane)(7)

A stock solution of **1** (0.41 mg, 0.77 μmol) in C_6D_6 (408 μl) was added to a mixture of 1-ethynyl-4-(trifluoromethyl)benzene (25.0 μl, 0.15 mmol) and bis(pinacalato)diboron (0.055 g, 0.22 mmol). The resulting reaction mixture was stirred at room temperature for 13 h under a N_2 atmosphere. At this point the volatiles were removed *in vacuo*, deionized H_2O (35 ml) was then added and the mixture was stirred for 24 h. The H_2O was then decanted and the resulting product was washed with more deionized H_2O (2 x 25 ml). The off-white solid was then dried under a high vacuum. Yield: 0.061 g, 94 %. ^{1}H NMR (399.5 MHz, $CDCl_3$): δ = 7.55 (m, 4H, *o*- and *m*-Ph), 6.35 (s, 1H, C=CH), 1.37 (s, 12H, Bpin), 1.32 (s, 12H, Bpin). ^{13}C{^{1}H} NMR (100.46 MHz, $CDCl_3$): δ = 146.9 (*i*-Ph), 129.5 (q, $^2J_{CF}$ = 32.4 Hz, *p*-Ph), 127.0 (*o*-Ph), 125.4 (q, $^3J_{CF}$ = 3.8 Hz, *m*-Ph), 124.4 (q, $^1J_{CF}$ = 272.8 Hz, **C**F_3), 84.5 (Bpin), 84.0 (Bpin), 25.1 (Bpin), 25.0 (Bpin), 2 C=C were not observed due to quadrapolar broadening caused by adjacent B atoms. ^{11}B{^{1}H} NMR (128.2 MHz, $CDCl_3$): δ = 30.28. ^{19}F NMR (375.9 MHz, $CDCl_3$): δ = –62.53 (spectroscopic data in agreement with the literature).

Synthesis of (*E*)-2,2'-(oct-1-ene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (8)

A stock solution of **1** (0.51 mg, 0.96 μl) in C_6D_6 (514 μl) was added to a mixture of 1-octyne (15.0 μl, 0.19 mmol) and bis(pinacolato)diboron (0.055 g, 0.21 mmol). The resulting reaction mixture was stirred at room temperature for 33 h under a N_2 atmosphere. At this point, the volatiles were removed *in vacuo*. The resulting crude product was stirred in deionized H_2O (30 ml) over 24 h, the H_2O was then decanted and colourless oil was dried under vacuum. Yield: 0.070 g, 87 %. ^{1}H NMR (399.5 MHz, $CDCl_3$): δ = 5.82 (s, 1H, C=CH), 2.18 (t, $^3J_{HH}$ = 7.6 Hz, 2H), 1.38 (m, 2H), 1.29 (s, 12H, Bpin), 1.27 (m, 6H), 1.24 (s, 12H, Bpin), 0.84 (t, $^3J_{HH}$ = 6.9 Hz, 3H, CH_3). ^{13}C{^{1}H} NMR (100.46 MHz, $CDCl_3$): δ = 83.5, 83.2, 39.8, 31.7, 29.1, 28.6, 24.9, 24.8, 22.5, 14.0. ^{11}B{^{1}H} NMR (128.2 MHz, $CDCl_3$): δ = 30.49 (spectroscopic data in agreement with the literature).

Synthesis of (*E*)-2,2'-(1-(3,5-bis(trifluoromethyl)phenyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (9)

A stock solution of **1** (0.38 mg, 0.71 µl) in C_6D_6 (377 µl) was added to a mixture of 1-ethynyl-3,5-bis(trifluoromethyl)benzene (25.0 µl, 0.14 mmol) and bis(pinacalato)diboron (0.049 g, 0.19 mmol). The resulting reaction mixture was stirred at room temperature for 48 h under a N_2 atmosphere. At this point all the volatiles were removed *in vacuo*. Deionized H_2O (50 ml) was added to the reaction mixture and this was allowed to stirred for 24 h. The H_2O was decanted and the product was washed with further quantities of deionized H_2O (3 x 20 ml). The yellow oil was dried under a high vacuum. Yield: 0.055 g, 79%. ^{1}H NMR (399.5 MHz, CDCl3): δ = 7.88 (s, 2H, *o*-Ph), 7.74 (s, 1H, *p*-Ph), 6.41 (s, 1H, =CH), 1.37 (s, 12H, Bpin), 1.33 (s, 12H, Bpin). ^{13}C{^{1}H} NMR (100.46 MHz, $CDCl_3$): δ = 145.3 (*i*-Ph), 131.7 (q, $^2J_{CF}$ = 32.1 Hz, *m*-Ph), 127.0 (*o*-Ph), 123.6 (q, $^1J_{CF}$ = 272.6 Hz, -**C**F_3), 121.1 (*p*-Ph), 84.8 (Bpin), 84.22 (Bpin), 25.1 (Bpin), 25.1 (Bpin), 2 C=C were not observed due to quadrapolar broadening caused by adjacent B atoms. ^{11}B{^{1}H} NMR (128.2 MHz, $CDCl_3$): δ = 30.24. ^{19}F NMR (375.9 MHz, $CDCl_3$): δ = –63.12. HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{22}H_{28}F_6O_4B_2Na$ 515.1970; Found 515.1970. Elem. Anal.: Calcd for $C_{22}H_{28}F_6O_4B_2$: C, 53.70 %; H, 5.74 %. Found: C, 53.55 %; H, 5.67 %.

Synthesis of (*E*)-2,2'-(1-mesitylethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (10)

A stock solution of **1** (0.51 mg, 0.96 µmol) in C_6D_6 (511 µl) was added to a mixture of 2-ethynl-1,3,5-trimethylbenzene (30.0 µl, 0.19 mmol) and bis(pinacolato)diboron (0.054 g, 0.21 mmol). The reaction mixture was stirred at room temperature for 1 h under a N_2 atmosphere. At this point the volatiles were removed *in vacuo*, the resulting colourless oil was washed with deionized water (3 x 30 ml) at which point a white solid precipitated. This white solid was collected by filtration and dried. Yield: 0.072 g, 94 %. ^{1}H NMR (399.5 MHz, $CDCl_3$): δ = 6.81 (s, 2H, Ph), 5.85 (s, 1H, =CH), 2.25 (s, 3H, *p*-PhCH_3), 2.18 (s, 6H, *o*-PhCH_3), 1.33 (s, 12H, *{t}*Bpin), 1.24 (s, 12H, Bpin). ^{13}C{^{1}H} NMR (100.46 MHz, $CDCl_3$): δ = 141.6 (s, *i*-Ph), 135.1 (s, *p*-Ph), 134.5 (s, *o*-Ph), 128.0 (s, *m*-Ph), 83.7 (s, Bpin), 83.4 (s, *{t}*Bpin), 25.1 (s,

*{t}*Bpin), 24.9 (s, Bpin), 21.1 (s, *p*-Ph**C**CH_3), 20.8 (s, *o*-Ph**C**CH_3), 2 C=C were not observed due to quadrapolar broadening caused by adjacent B atoms. $^{11}B\{^1H\}$ NMR (128.2 MHz, $CDCl_3$): δ = 29.71. HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{23}H_{36}O_4B_2Na$ 421.2692; Found 421.2695. Elem. Anal.: Calcd for $C_{23}H_{36}O_4B_2$: C, 69.38 %; H, 9.11 %. Found: C, 69.29 %; H, 9.16 %.

Synthesis of (*E*)-2,2'-(1-(cyclohex-1-en-1-yl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (11)

A stock solution of $Pd(ITMe)_2(PhC{\equiv}CPh)$ (0.34 mg, 0.64 μmol) in C_6D_6 (340 μl) was added to a mixture of 1-ethynylcyclohex-1-ene (15.0 μl, 0.13 mmol) and bis(pinacalato)diboron (0.039 g, 0.15 mmol). The resulting reaction mixture was stirred at room temperature for 24 h under a N_2 atmosphere. At this point all volatiles were removed *in vacuo*, deionized H_2O (35 ml) was added and the resulting mixture was stirred at room temperature for 24 h. At this point the beige solid was collected by filtration and dried under a high vacuum. Yield: 0.041 g, 89 %. ^1H NMR (399.5 MHz, C_6D_6): δ = 6.30 (m, 1H, =C**H**CH_2), 6.26 (s, 1H, =CH), 2.16 (m, 2H, {2}-CH_2), 2.05 (m, 2H, {5}-CH_2), 1.45 (m, 2H, CH_2), 1.36 (m, 2H, CH_2), 1.31 (s, 12H, cyclohexen-1-yl{**Bpin**}C=), 1.11 (s, 12H, =C{**Bpin**}H). $^{13}C\{^1H\}$ NMR (100.46 MHz, C_6D_6): δ = 140.8 ({1}cyclohexen-1-yl), 131.2 ({6}-cyclohexen-1-yl), 83.6 (cyclohexen-1-yl{**Bpin**}C=), 83.1 (=C{**Bpin**}H), 26.7 ({5}- cyclohexen-1-yl), 25.6 (cyclohexen-1-yl{**Bpin**}C=), 25.5 ({2}-cyclohexen-1-yl), 25.0 (=C{**Bpin**}H), 23.1 (cyclohexen-1-yl), 22.6 (cyclohexen-1-yl), 2 C=C were not observed due to quadrapolar broadening caused by adjacent B atoms. $^{11}B\{^1H\}$ NMR (128.2 MHz, C_6D_6): δ = 30.86. HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{34}O_4B_2Na$ 383.2535; Found 383.2526. Elem. Anal.: Calcd for $C_{20}H_{34}O_4B_2$: C, 66.71 %; H, 9.52 %. Found: C, 66.79 %; H, 9.43 %.

Synthesis of (*Z*)-2,2'-(1-(4-ethylphenyl)-2-(4-methoxyphenyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (12)

A stock solution of **1** (0.35 mg, 0.66 μmol) in C_6D_6 (354 μl) was added to a mixture of 1-ethyl-4-((4-methoxyphenyl)ethynyl)benzene (0.031 g, 0.13 mmol) and bis(pinacolato)diboron (0.043 g, 0.17 mmol).

The resulting reaction mixture was heated to 50 ˚C for 5 h under a N_2 atmosphere. Upon cooling the reaction mixture the volatiles were removed *in vacuo*. Deionized H_2O (35 ml) was added to the resulting off-white solid and this was stirred at room temperature for 24 h. The white solid was collected by filtration and dried under a high vacuum. Yield: 0.055 g, 85 %. ^{1}H NMR (399.5 MHz, $CDCl_3$): δ = 6.88 (m, 6H, *o,m*-Ph{4-Et} and *o*-Ph{4-OMe}), 6.61 (m, 2H, *m*-Ph(4-OMe}), 3.71 (s, 3H, OMe), 2.53 (q, $^3J_{HH}$ = 7.7 Hz, 2H, $\mathbf{CH_2}CH_3$), 1.32 (s, 12H, BPin), 1.32 (s, 12H, Bpin), 1.16 (t, $^3J_{HH}$ = 7.7 Hz, 3H, $CH_2\mathbf{CH_3}$). ^{1}H NMR (499.5 MHz, C_6D_6): δ = 7.30 (d, $^3J_{HH}$ = 8.2 Hz, 2H, *o*-Ph{4-Et}), 7.26 (d, $^3J_{HH}$ = 8.7 Hz, 2H, *o*-Ph{4-OMe}), 6.90 (d, $^3J_{HH}$ = 8.2 Hz, 2H, *m*-Ph{4-Et}), 6.60 (d, $^3J_{HH}$ = 8.7 Hz, *m*-Ph{4-OMe}), 3.14 (s, 3H, OMe), 2.32 (q, $^3J_{HH}$ = 7.6 Hz, 2 H, $\mathbf{CH_2}CH_3$), 1.19 (s, 12H, Bpin), 1.18 (s, 12H, Bpin), 0.95 (t, $^3J_{HH}$ = 7.6 Hz, 3H, $CH_2\mathbf{CH_3}$). ^{13}C{^{1}H} NMR (100.46 MHz, $CDCl_3$): δ = 157.8 (*p*-Ph{4-OMe}), 141.5 (*p*-Ph{4-Et}), 138.8 (*i*-Ph{4-Et}), 134.0 (*i*-Ph{4-OMe}), 130.7 (*o*-Ph{4-OMe}), 129.5 (*o*-Ph{4-Et}), 127.1 (*m*-Ph{4-Et}), 113.1 (*m*-Ph{4-OMe}), 84.1 (Bpin), 84.1 (Bpin), 55.1 (OMe), 28.6 ($\mathbf{C}H_2CH_3$), 25.1 (Bpin), 25.1 (Bpin), 15.3 ($CH_2\mathbf{C}H_3$), 2 C=C were not observed due to quadrapolar broadening caused by adjacent B atoms. ^{13}C{^{1}H} NMR (100.46 MHz, C_6D_6): δ = 158.4 (*p*-Ph{4-OMe}), 141.6 (*p*-Ph{4-Et}), 140.0 (*i*-Ph{4-Et}), 134.7 (*i*-Ph{4-OMe}), 131.1 (*o*-Ph{4-OMe}), 130.0 (*o*-Ph{4-Et}), 127.6 (*m*-Ph{4-Et}), 113.7 (*m*-Ph{4-OMe}), 83.8 (Bpin), 83.8 (Bpin), 54.5 (OMe), 28.8 ($\mathbf{C}H_2CH_3$), 25.1 (Bpin), 25.1 (Bpin), 15.3 ($CH_2\mathbf{C}H_3$), 2 C=C were not observed due to quadrapolar broadening caused by adjacent B atoms. ^{11}B{^{1}H} NMR (128.2 MHz, $CDCl_3$): 30.77. ^{11}B{^{1}H} NMR (128.2 MHz, C_6D_6): δ = 30.77. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{29}H_{40}O_5B_2H$ 491.3135; Found 491.3132. Elem. Anal.: Calcd for $C_{29}H_{40}O_5B_2$: C, 71.05 %; H, 8.22 %. Found: C, 70.94 %; H, 8.26 %.

Synthesis of (*Z*)-2,2'-(1-(naphthalen-1-yl)-2-phenylethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (13)

A stock solution of **1** (0.39 mg, 0.72 μmol) in C_6D_6 (385 μl) was added to a mixture of 1-(phenylethynyl)naphthalene (0.033 g, 0.14 mmol) and bis(pinacalato)diboron (0.049 g, 0.19 mmol). The resulting reaction mixture was heated to 50 ˚C for 24 h under a N_2 atmosphere. At this point all volatiles

were removed *in vacuo*, deionized H_2O (30 ml) was added and the reaction mixture was stirred for 24 h. The H_2O was removed and the off-white powdered solid was dried under high vacuum. Yield: 0.070 g, 94 %. ^{1}H NMR (399.5 MHz, CDCl3): δ = 7.97 (m, 1H, naphth), 7.70 (m, 1H, naphth), 7.54 (m, 1H, naphth), 7.35 (m, 1H, naphth), 7.35 (m, 1H, naphth), 7.17 (m, 1H, naphth), 6.95 (m, 1H, naphth), 6.86 (m, 5H, Ph), 1.37 (s, 6H, Bpin), 1.35 (s, 6H, Bpin), 1.21 (s, 6H, Bpin), 1.20 (s, 6H, Bpin). ^{13}C{^{1}H} NMR (100.46 MHz, $CDCl_3$): δ = 141.6, 140.1, 133.3, 132.2, 128.3, 128.1, 127.4, 126.9, 126.6, 126.3, 126.0, 125.4, 125.4, 125.1, 84.3, 84.2, 25.3, 24.9, 24.9, 24.8. ^{11}B{^{1}H} NMR (128.2 MHz, CDCl3): δ = 30.71. HRMS (ESI) m/z Calcd for $C_{30}H_{36}O_4B_2H$ 483.2872; Found 483.2871. Elem. Anal.: Calcd for $C_{30}H_{36}O_4B_2$: C, 74.72 %; H, 7.52 %. Found: C, 74.63 %; H, 7.46 %.

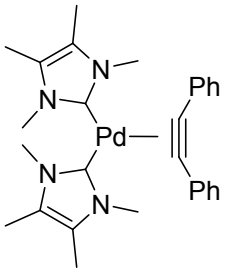
Synthesis of (*Z*)-trimethyl(2-phenyl-1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)silane (14)

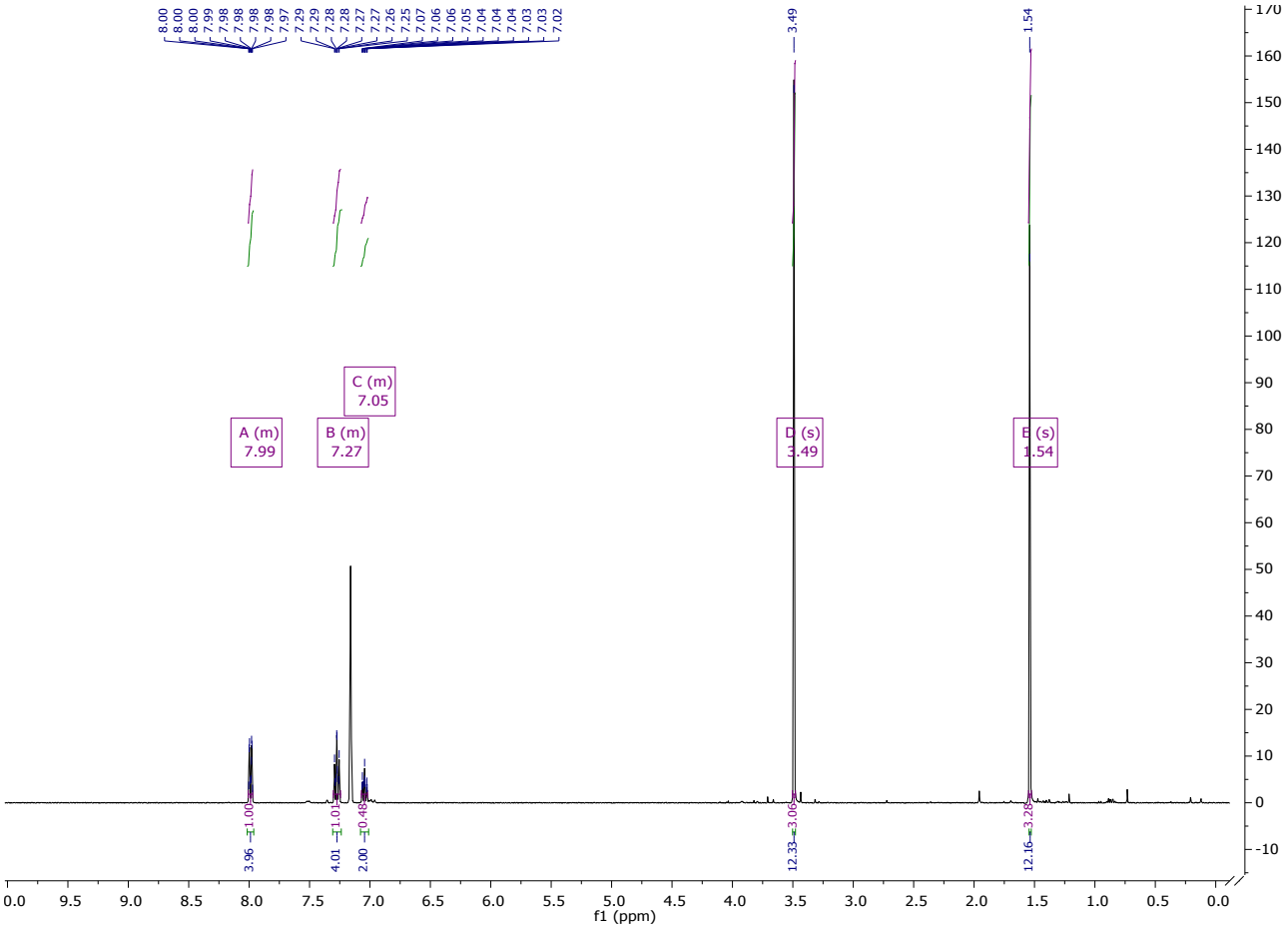
A stock solution of **1** (0.002 g, 3.06 μmol) in C_6D_6 (406 μl) was added to a mixture of trimethyl(phenylethynyl)silane (30.0 μl, 0.15 mmol) and bis(pinacolato)diboron (0.042 g, 0.17 mmol). The resulting reaction mixture was heated to 100 ˚C for 30 h under a N_2 atmosphere. Upon cooling the reaction mixture the volatiles were removed *in vacuo*. At this point all volatiles were removed *in vacuo*, deionized H_2O (30 ml) was added and the reaction mixture was stirred for 24 h. The H_2O was removed and the off-white powdered solid was dried under high vacuum. Yield: 0.056 g, 85 %. ^{1}H NMR (399.5 MHz, $CDCl_3$): δ = 7.21 (m, 3H, *m*,*p*-Ph), 7.11 (m, 2H, *o*-Ph), 1.37 (s, 12H, Bpin), 1.22 (s, 12H, Bpin), –0.18 (s, 9H, $SiMe_3$). ^{13}C{^{1}H} NMR (100.46 MHz, $CDCl_3$): δ = 146.0 (*i*-Ph), 128.0 (*o*-Ph), 127.6 (*m*-Ph), 126.3 (*p*-Ph), 84.1 (Bpin), 83.8 (Bpin), 25.7 (Bpin), 24.9 (Bpin), 1.0 ($SiMe_3$), 2 C=C were not observed due to quadrapolar broadening caused by adjacent B atoms.. ^{11}B{^{1}H} NMR (128.2 MHz, $CDCl_3$): δ = 30.80, 29.12. ^{29}Si{^{1}H} (79.4 MHz, $CDCl_3$): δ = –7.43 (spectroscopic data in agreement with the literature).

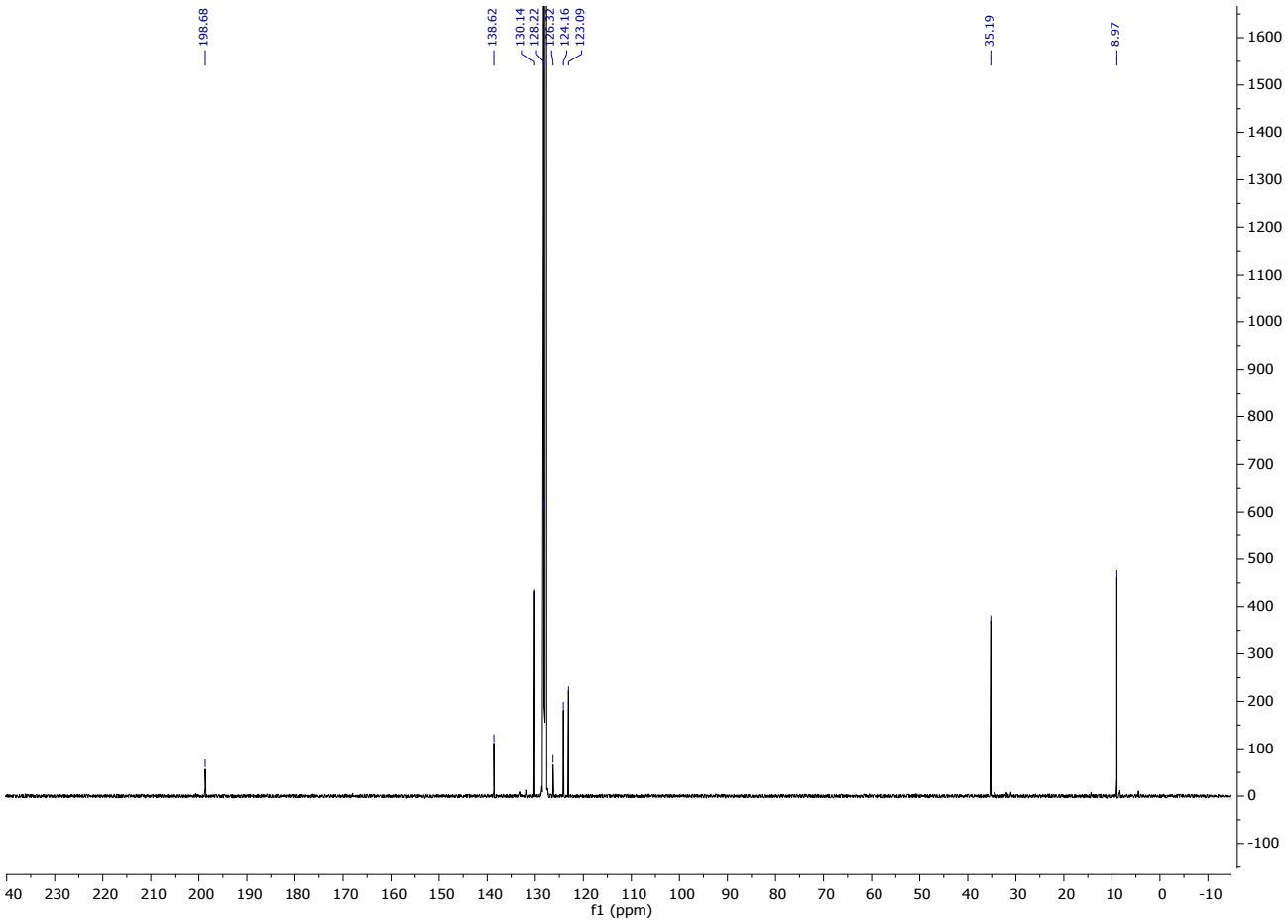
Synthesis of (*Z*)-2,2'-(oct-4-ene-4,5-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (15)

A stock solution of **1** (0.45 mg, 0.85 µl) in C_6D_6 (454 µl) was added to a mixture of 4-octyne (25.0 µl, 0.17 mmol) and bis(pinacalato)diboron (0.045 g, 0.18 mmol). The resulting reaction mixture was stirred at room temperature for 23 h under a N_2 atmosphere.At this point no further conversion was observed (39 % conversion). At this point all volatiles were removed *in vacuo*. The resulting off-white oily solid was stirred in deionized H_2O (35 ml) for 24 h. The H_2O was then decanted and the product was washed with a further quantities of deionized H_2O (3 x 25 ml). The resulting colourless oil was dried under a high vacuum. Yield: 0.012 g, 20 % (39 % conversion). ^{1}H NMR (499.5 MHz, $CDCl_3$): δ = 2.17 (m, 4H), 1.37 (m, 4H), 1.28 (s, 24H, Bpin), 0.91 (t, $^3J_{HH}$ = 7.4 Hz, 6H, CH_3). $^{13}C\{^1H\}$ (100.46 MHz, $CDCl_3$): δ = 83.4, 33.2, 25.1, 23.2, 14.7, 2 C=C were not observed due to quadrapolar broadening caused by adjacent B atoms. $^{11}B\{^1H\}$ NMR (128.2 MHz, $CDCl_3$): δ = 30.64 (spectroscopic data in agreement with the literature).

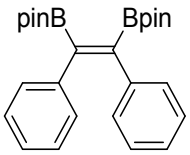
SPECTROSCOPIC DATAPd(ITMe)$_2$(PhC≡CPh) (1)

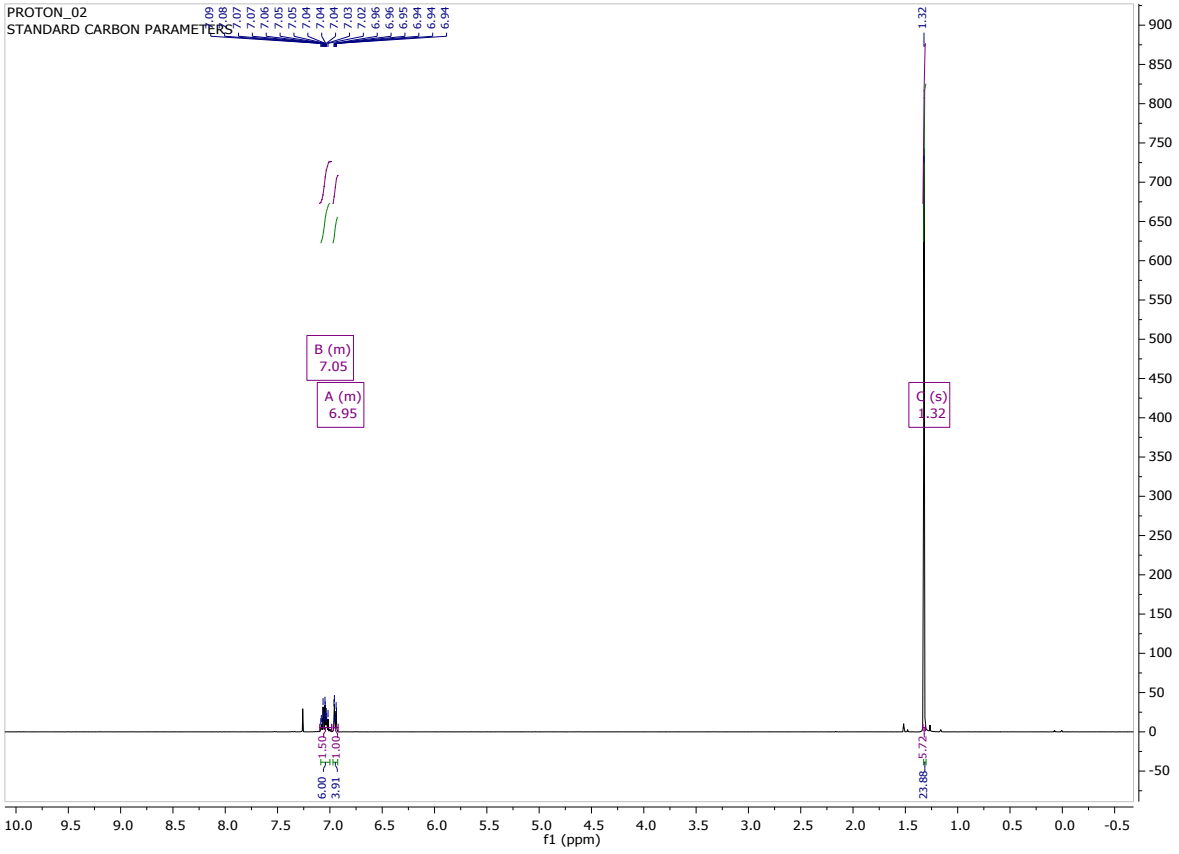


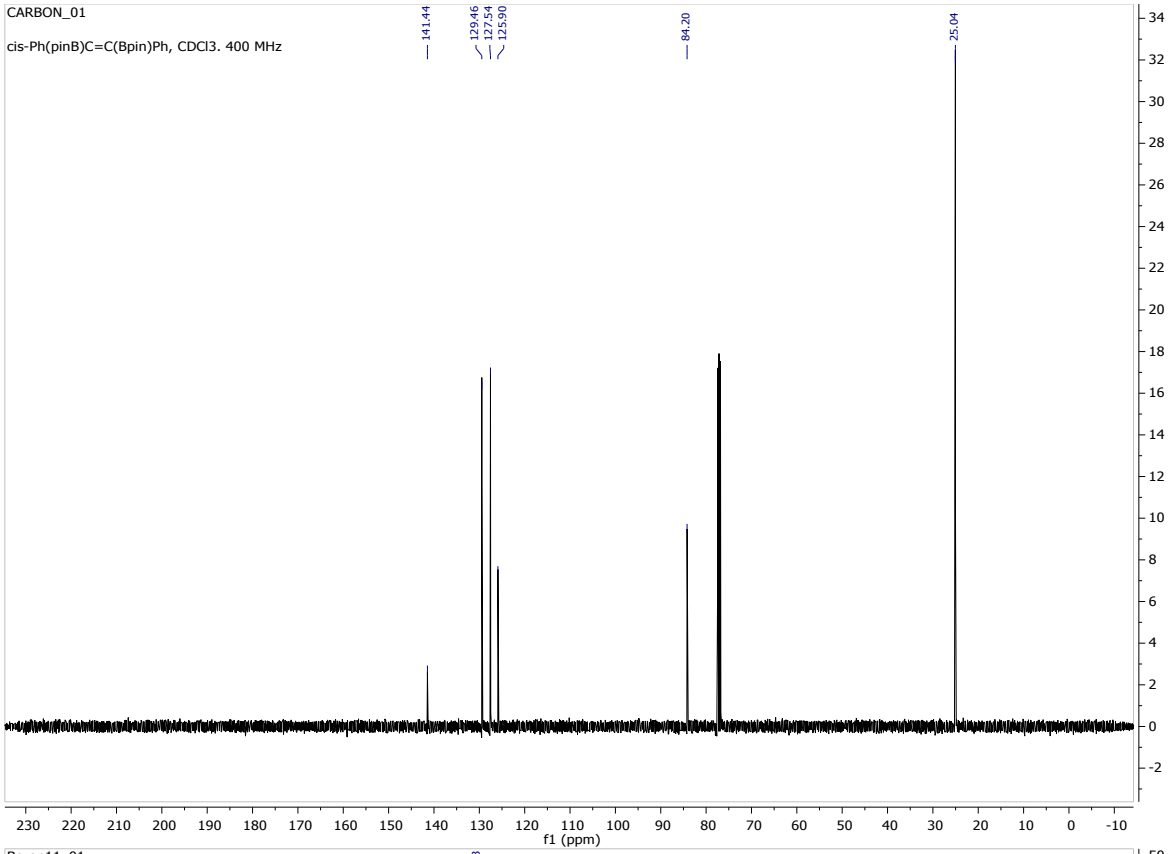

A (m)
7.99
B (m)
7.27
C (m)
7.05
D (s)
3.49
E (s)
1.54
f1 (ppm)

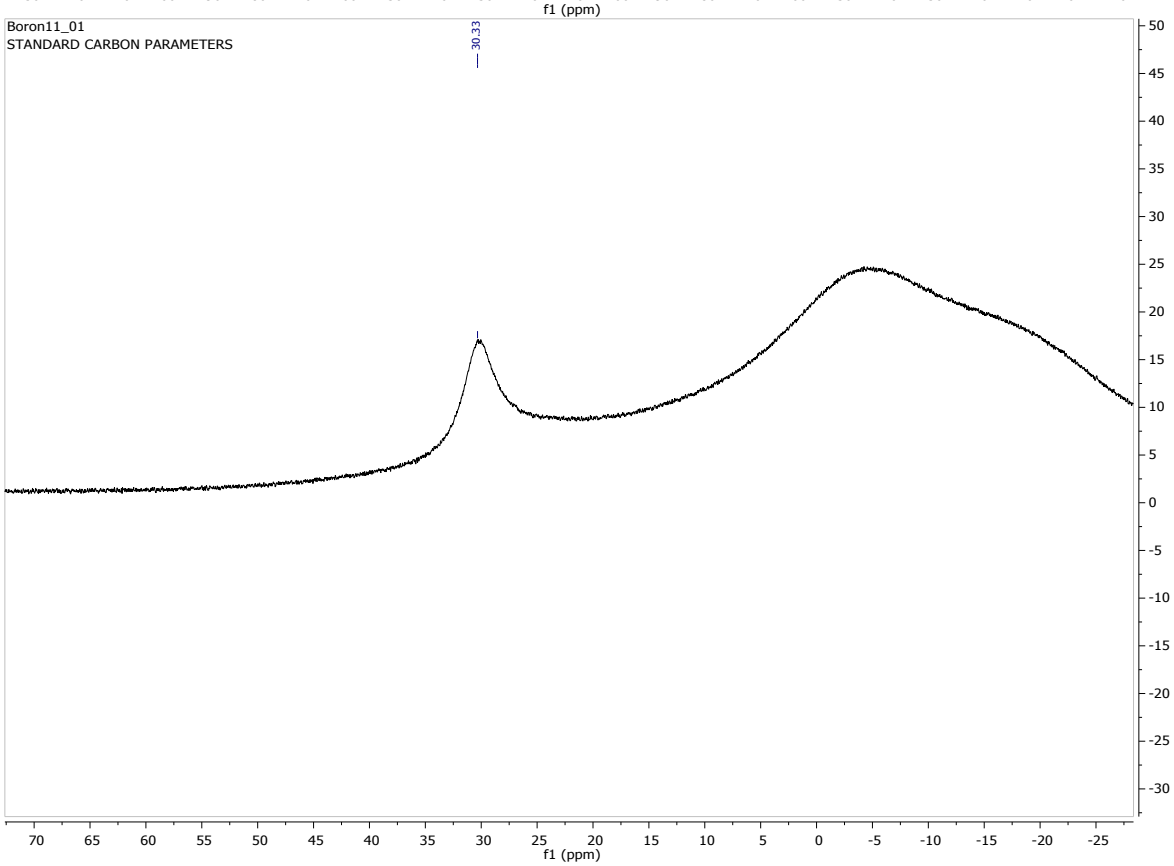

198.68
138.62
130.14
128.22
126.32
124.16
123.09
35.19
8.97
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
40 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Synthesis of (Z)-1,2-diphenyl-1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethane (2)

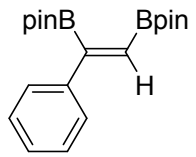


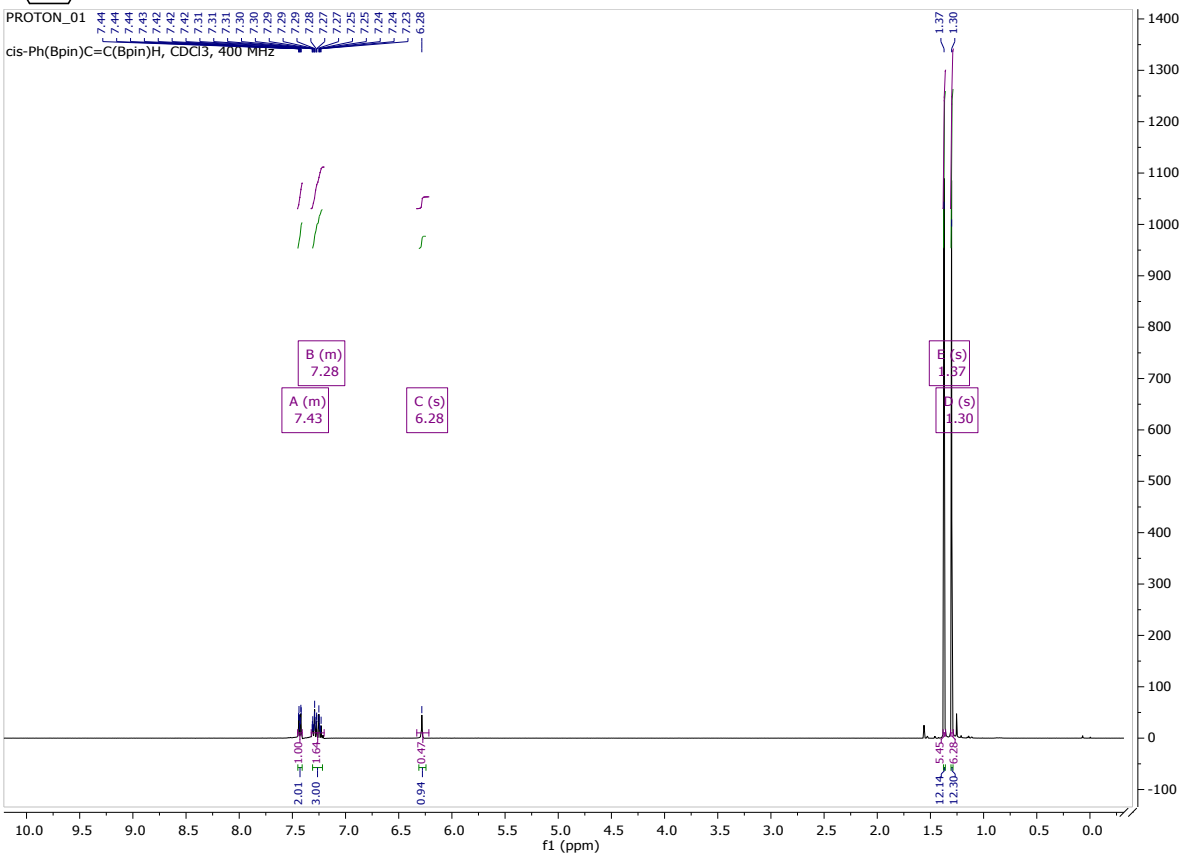


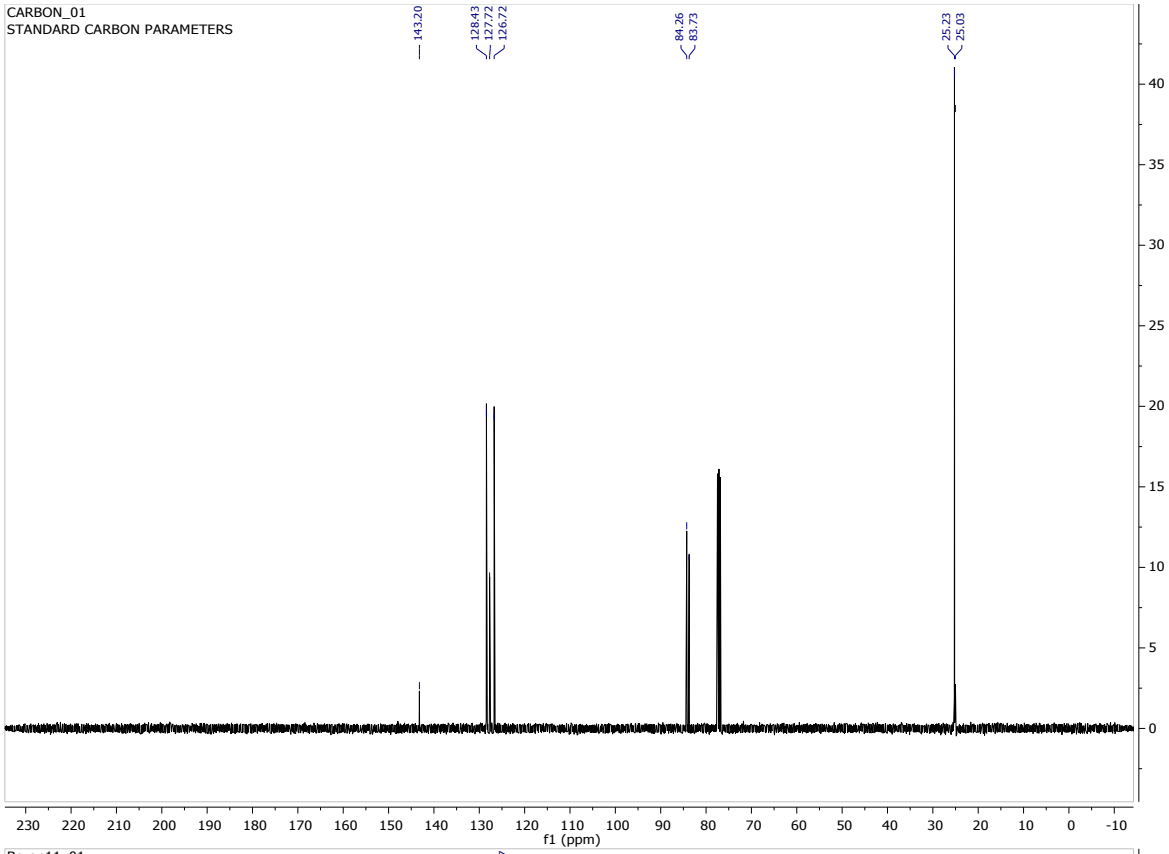

CARBON_01
cis-Ph(pinB)C=C(Bpin)Ph, CDCl3. 400 MHz
141.44
129.46
127.54
125.90
84.20
25.04
f1 (ppm)

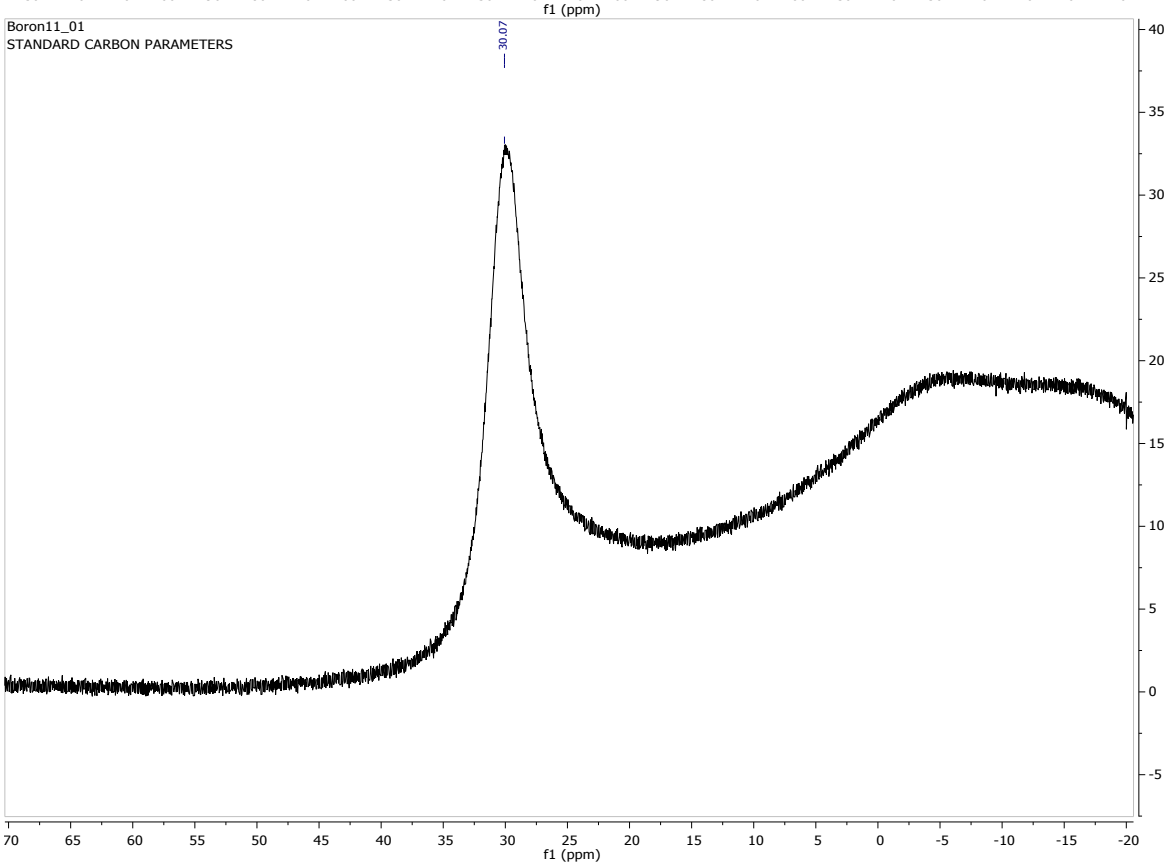

Boron11_01
STANDARD CARBON PARAMETERS
30.33
f1 (ppm)

(E)-2,2'-(1-phenylethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (3)

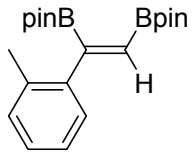


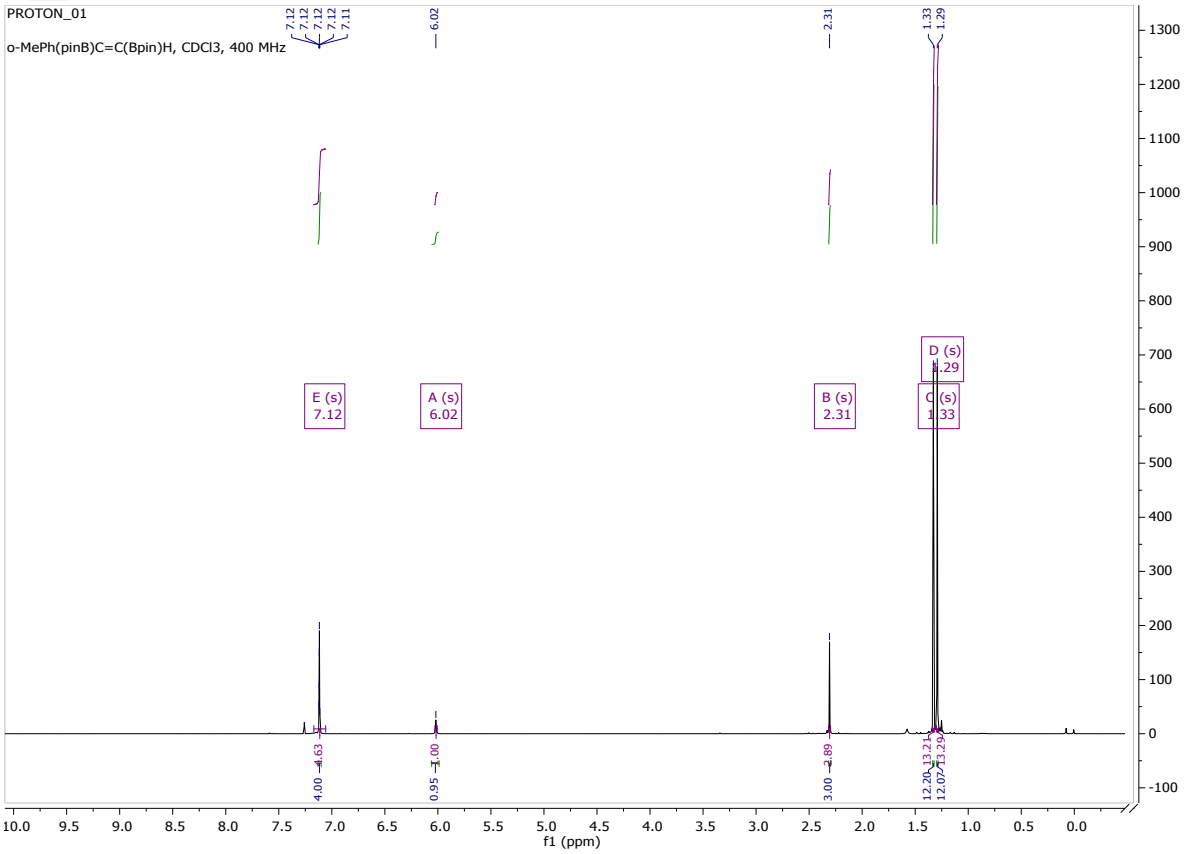


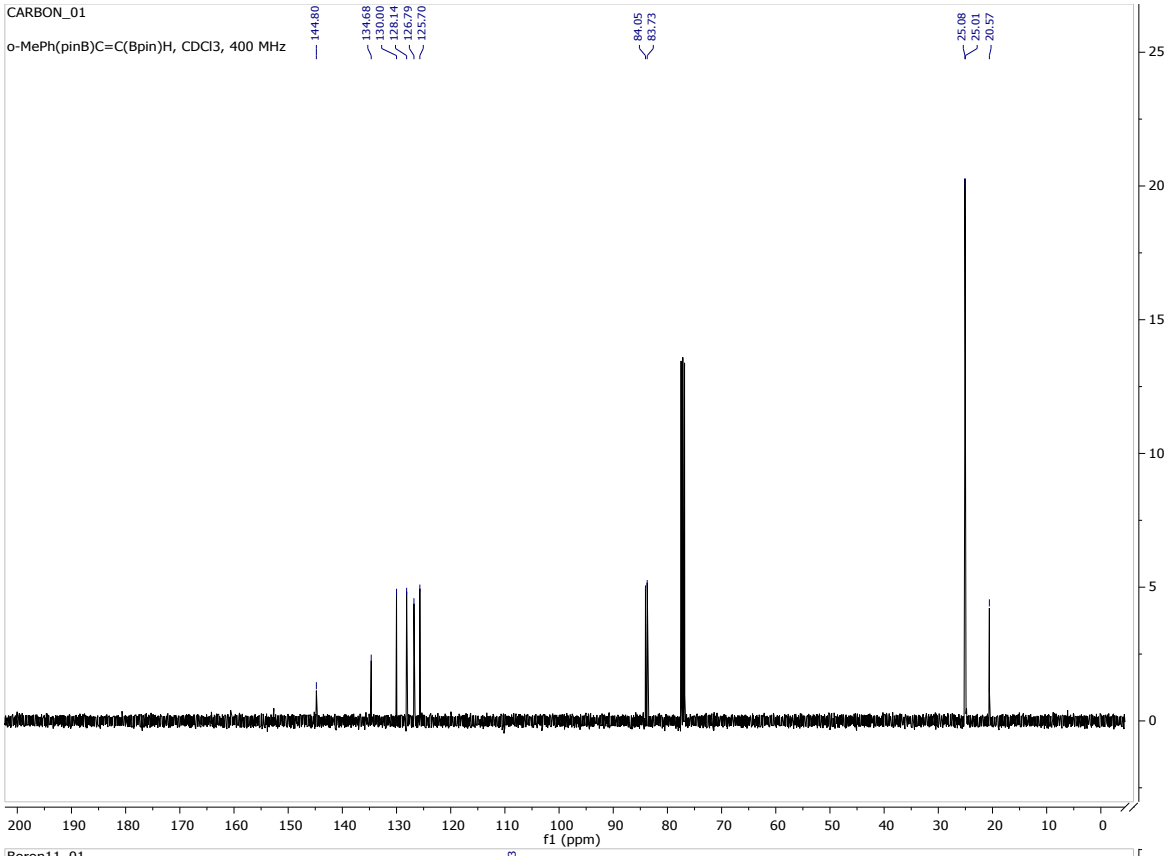

CARBON_01
STANDARD CARBON PARAMETERS
143.20
128.43
127.72
126.72
84.26
83.73
25.23
25.03
f1 (ppm)

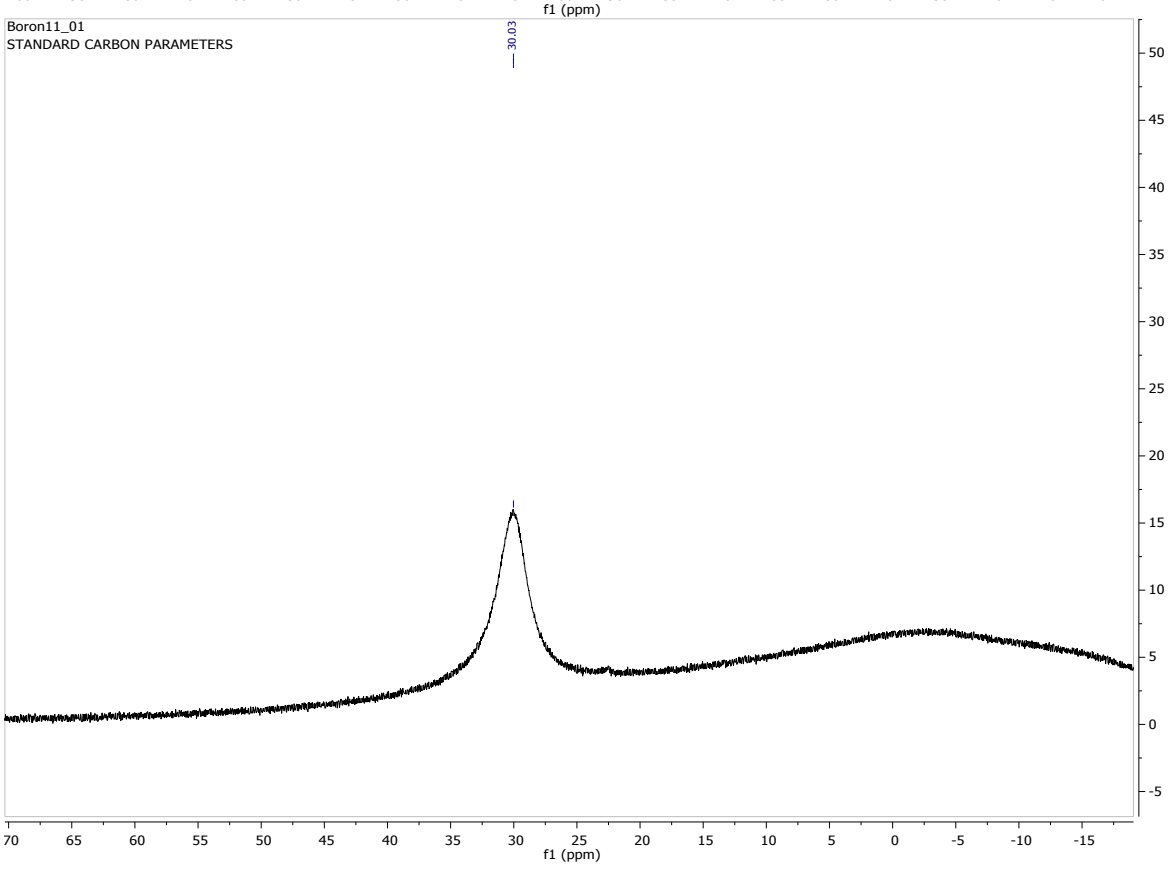

Boron11_01
STANDARD CARBON PARAMETERS
30.07
f1 (ppm)

(E)-2,2'-(1-(o-tolyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (4)

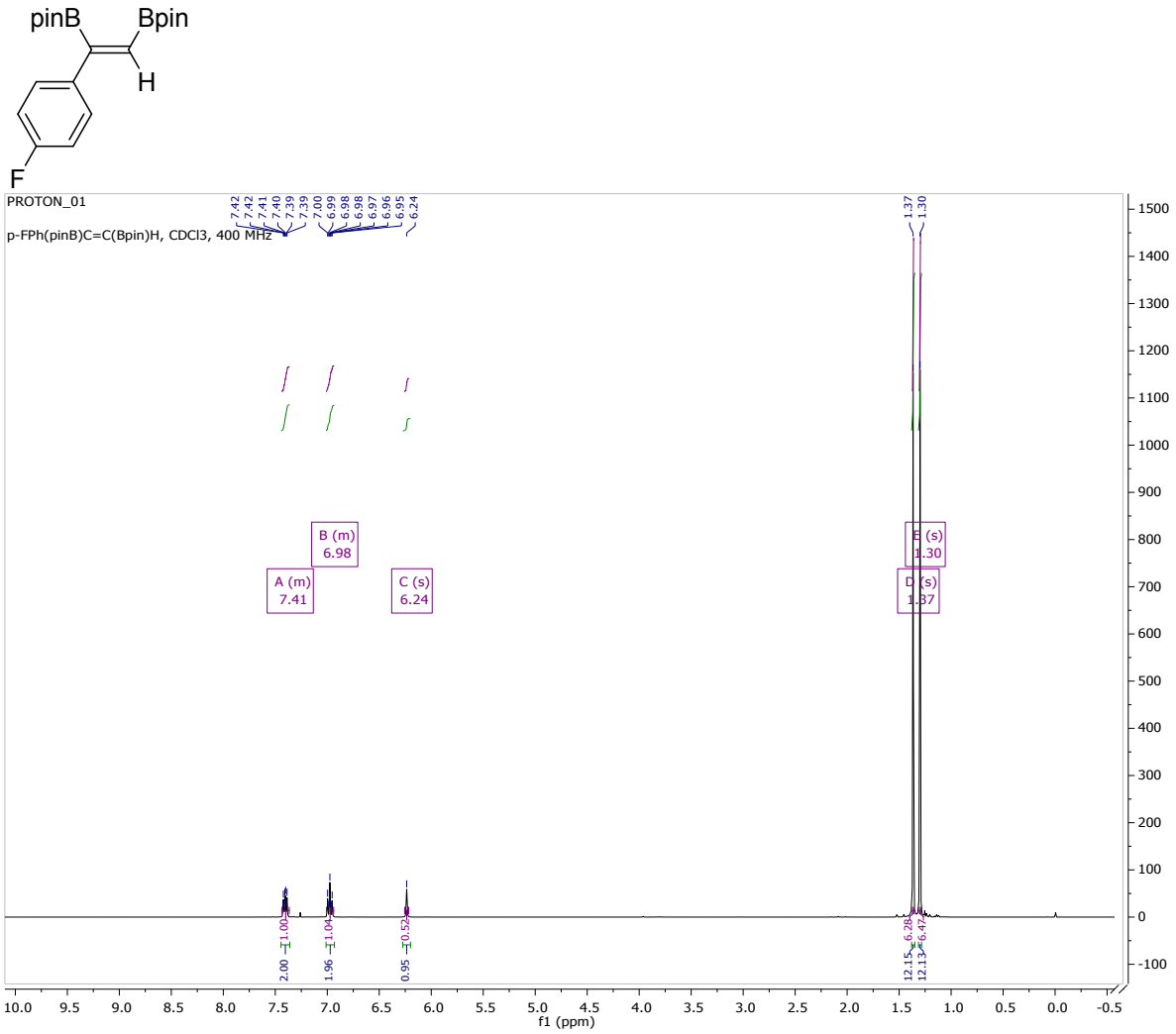


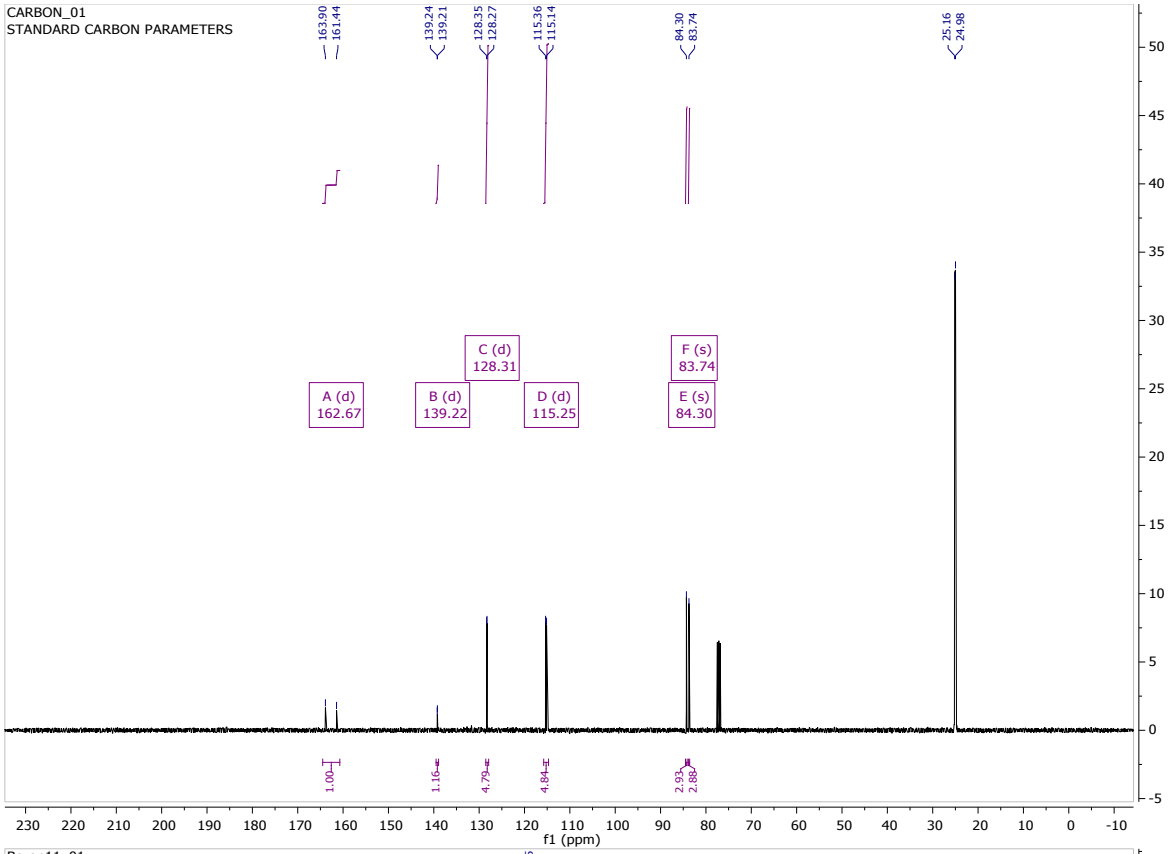


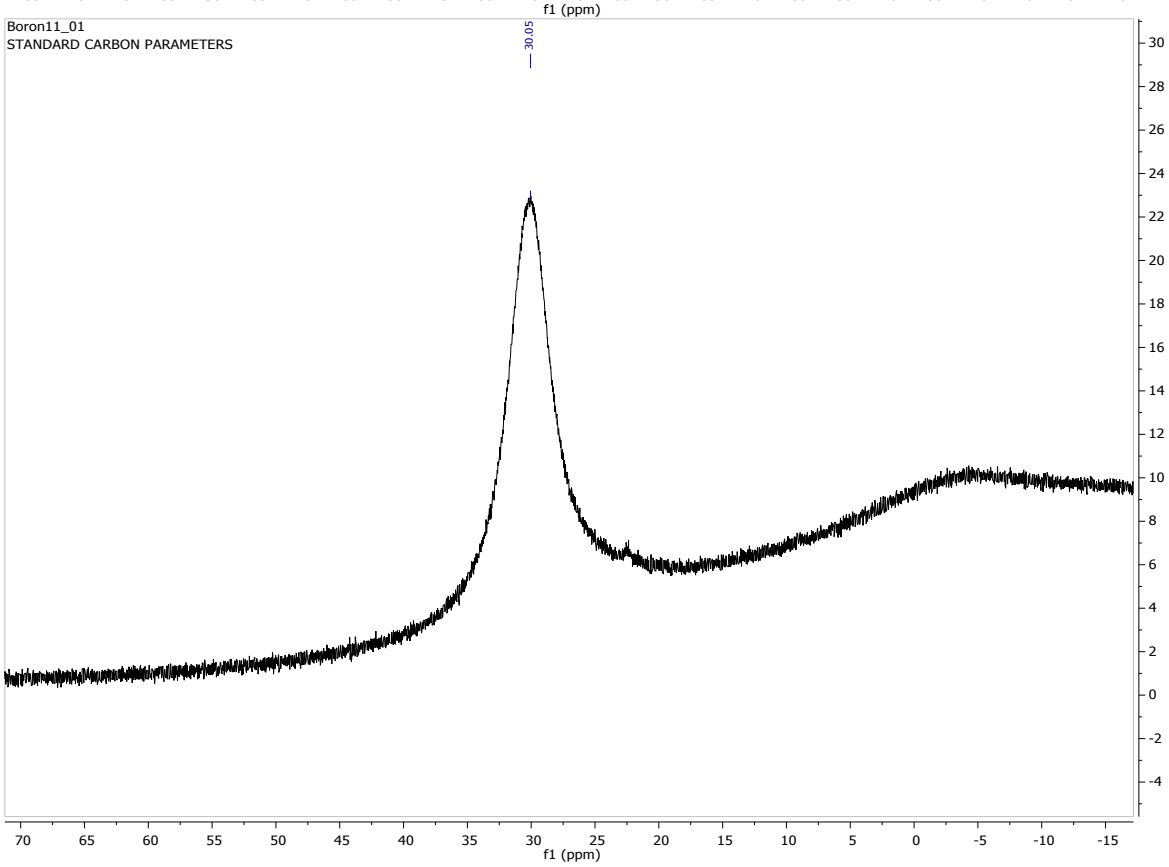

CARBON_01
o-MePh(pinB)C=C(Bpin)H, CDCl3, 400 MHz
144.80
134.68
130.00
128.14
126.79
125.70
84.05
83.73
25.08
25.01
20.57
f1 (ppm)

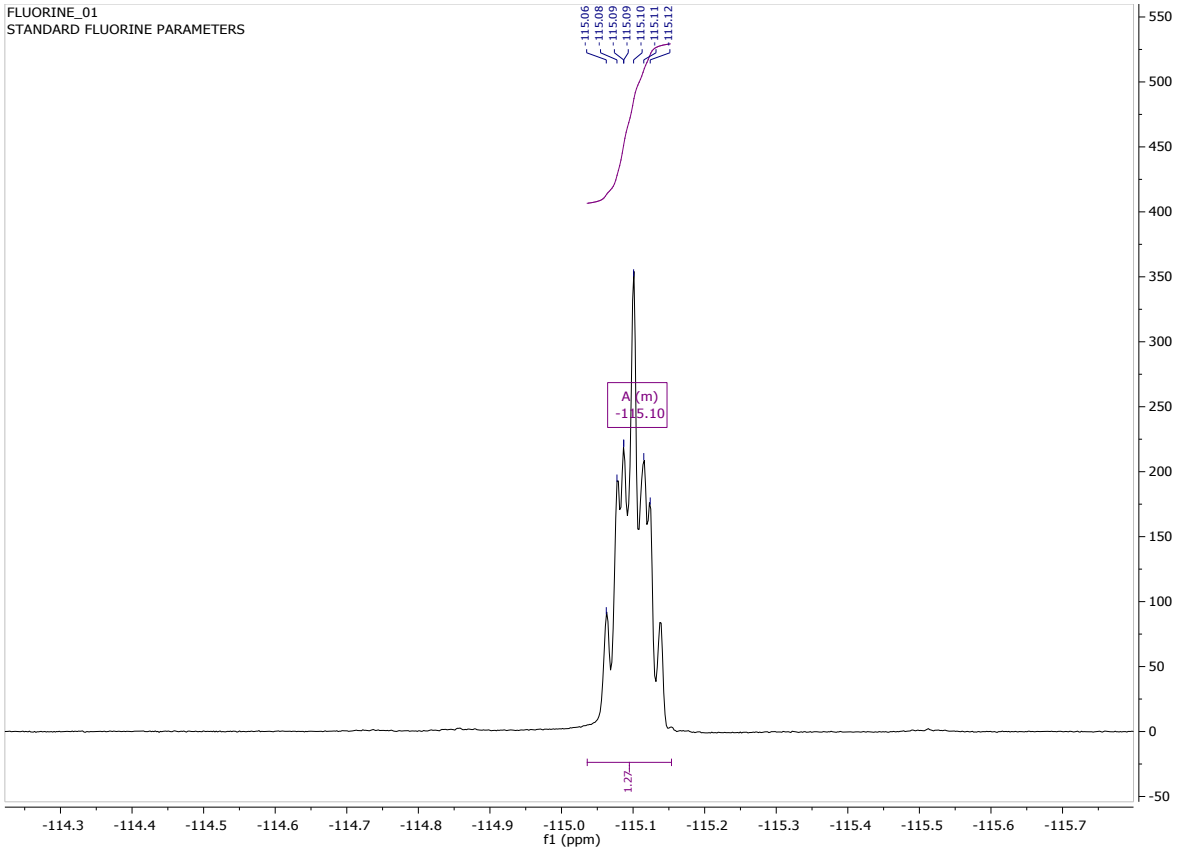

Boron11_01
STANDARD CARBON PARAMETERS
30.03
f1 (ppm)

(E)-2,2'-(1-(4-fluorophenyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (5)

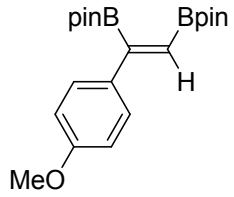


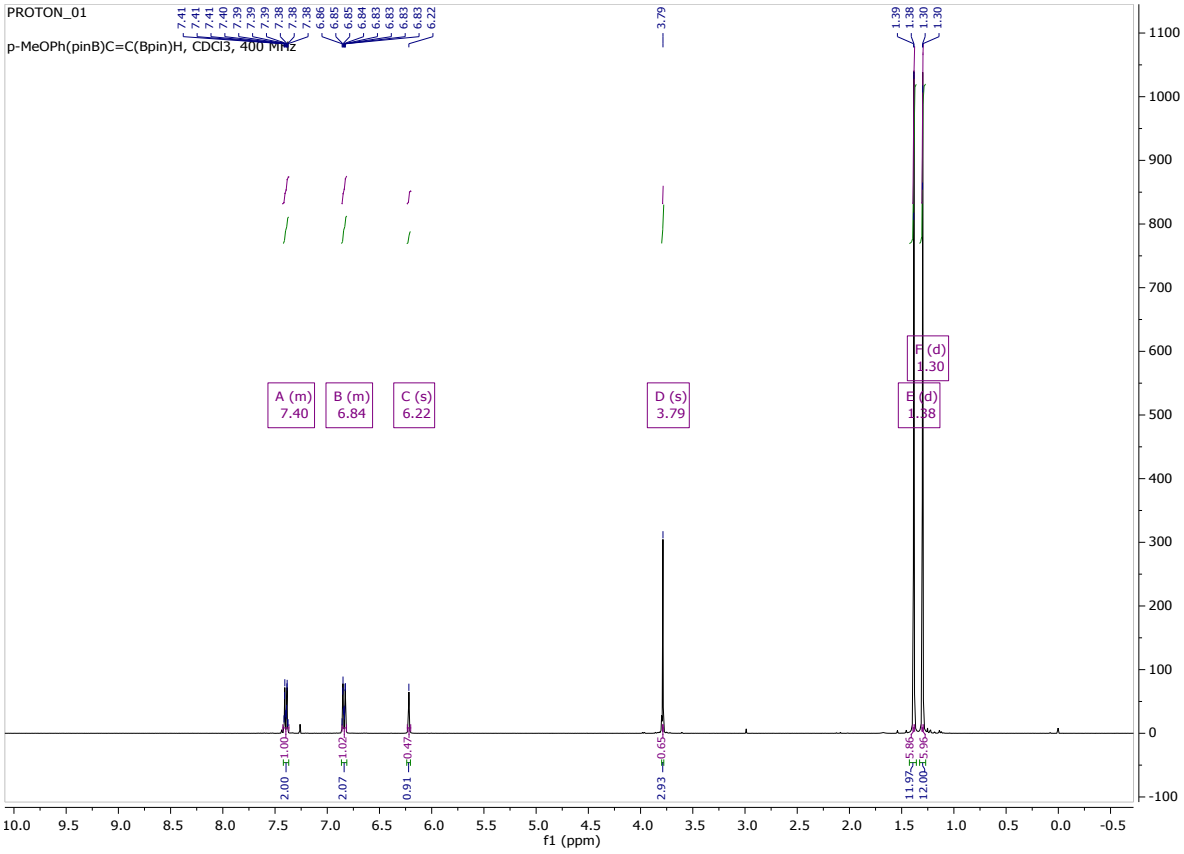

CARBON_01
STANDARD CARBON PARAMETERS
163.90
161.44
139.24
139.21
128.35
128.27
115.36
115.14
84.30
83.74
25.16
24.98
A (d)
162.67
B (d)
139.22
C (d)
128.31
D (d)
115.25
E (s)
84.30
F (s)
83.74
1.00
1.16
4.79
4.84
2.93
2.88
f1 (ppm)

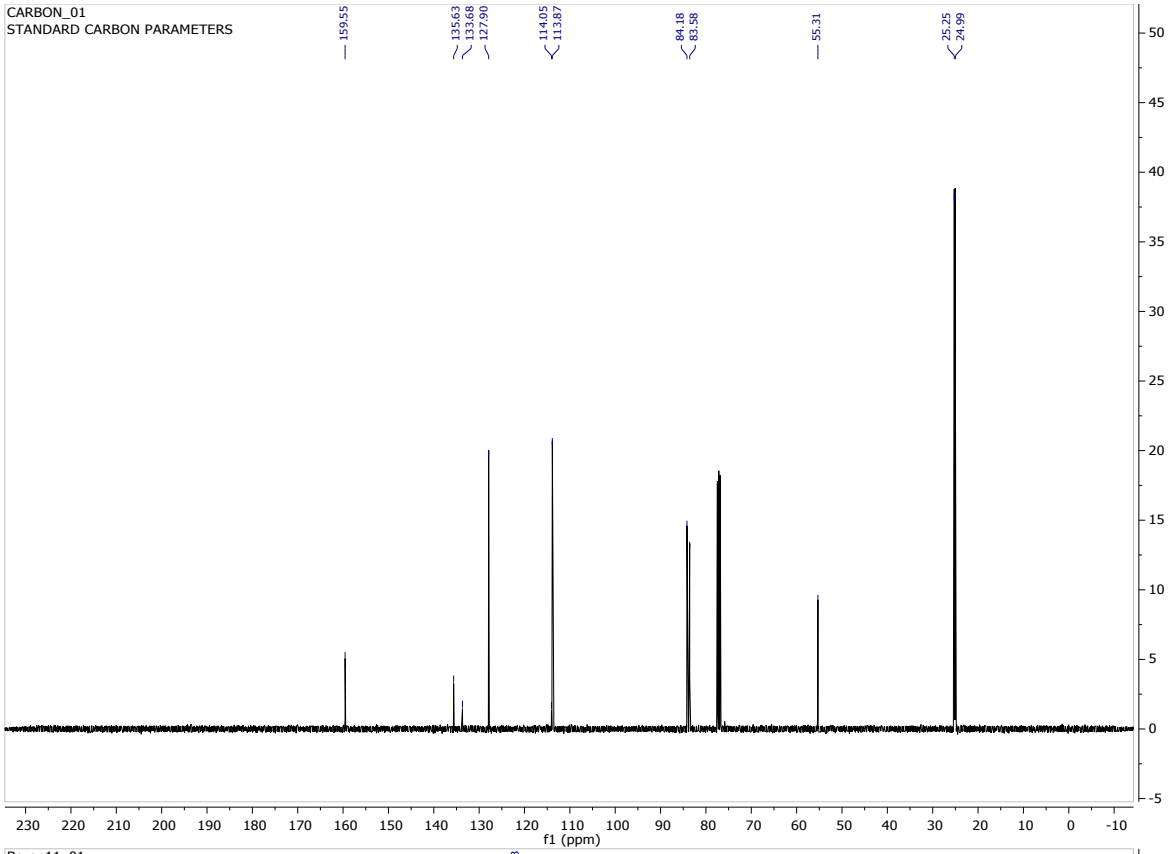

Boron11_01
STANDARD CARBON PARAMETERS
30.05
f1 (ppm)

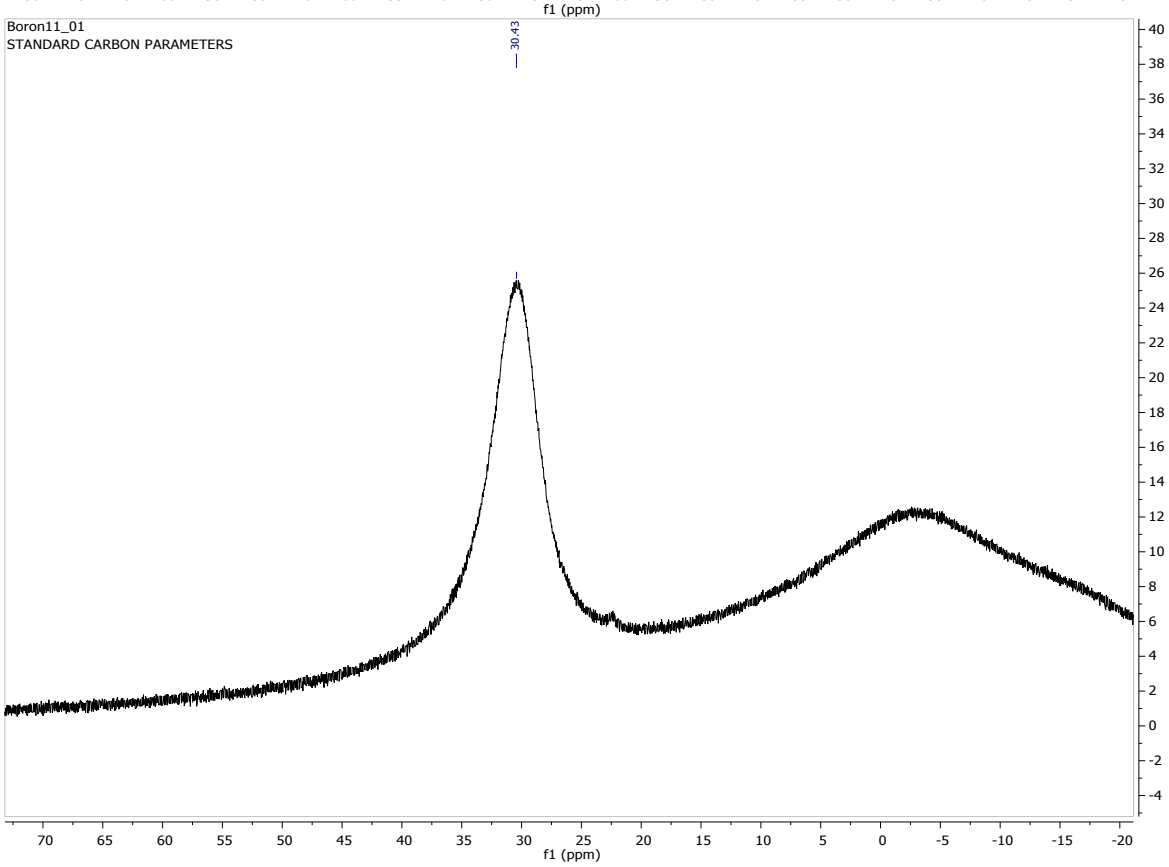

FLUORINE_01
STANDARD FLUORINE PARAMETERS
-115.06
-115.08
-115.09
-115.09
-115.10
-115.11
-115.12
A (m)
-115.10
1.27
550
500
450
400
350
300
250
200
150
100
50
0
-50
-114.3
-114.4
-114.5
-114.6
-114.7
-114.8
-114.9
-115.0
-115.1
-115.2
-115.3
-115.4
-115.5
-115.6
-115.7
f1 (ppm)

(E)-2,2'-(1-(4-methoxyphenyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (6)



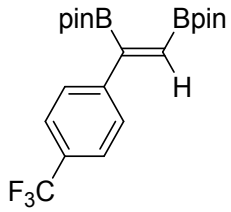


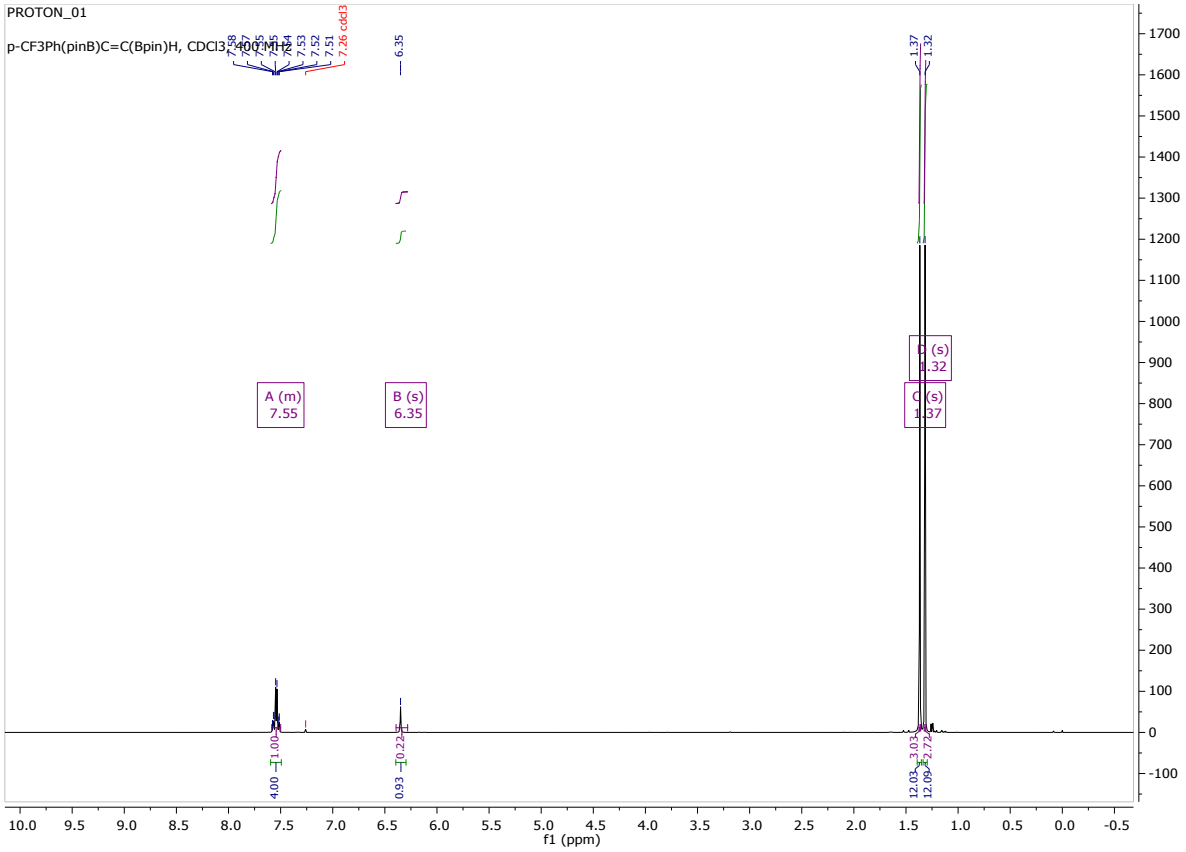

CARBON_01
STANDARD CARBON PARAMETERS
159.55
135.63
133.68
127.90
114.05
113.87
84.18
83.58
55.31
25.25
24.99
f1 (ppm)

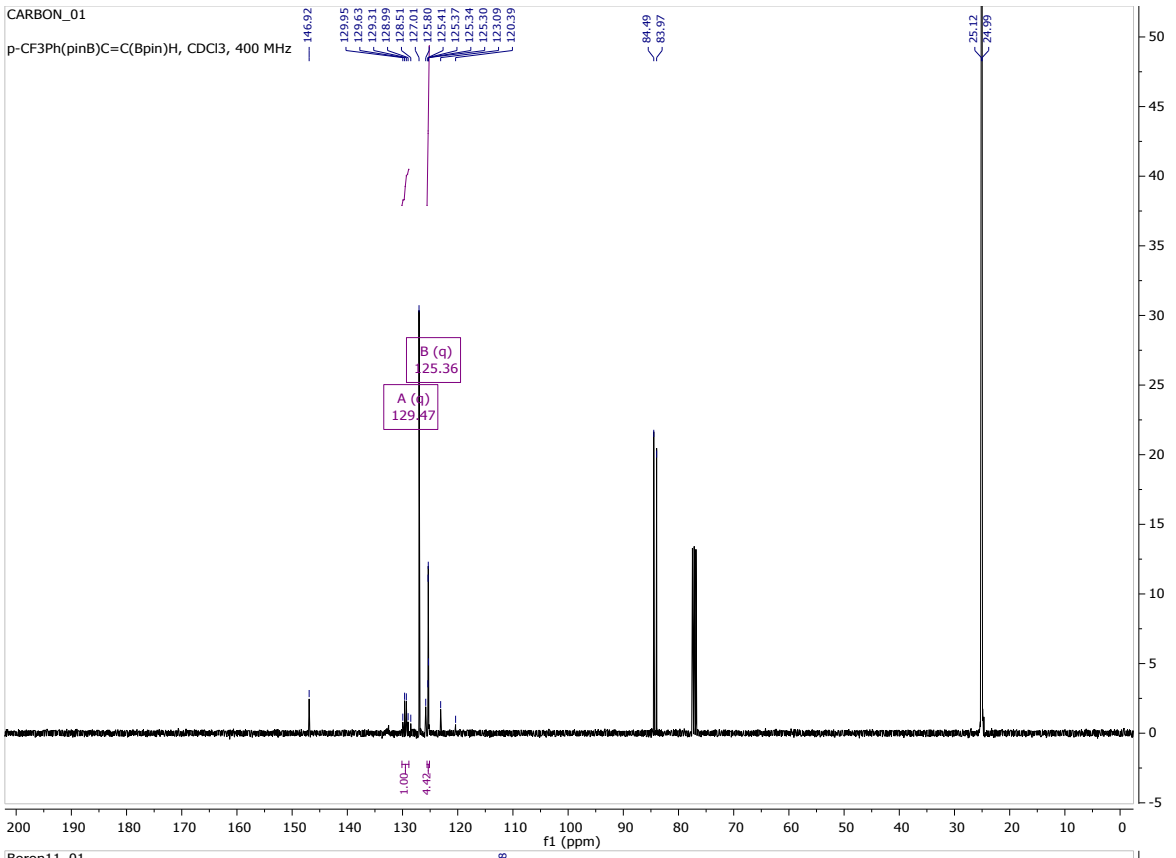

Boron11_01
STANDARD CARBON PARAMETERS
30.43
f1 (ppm)

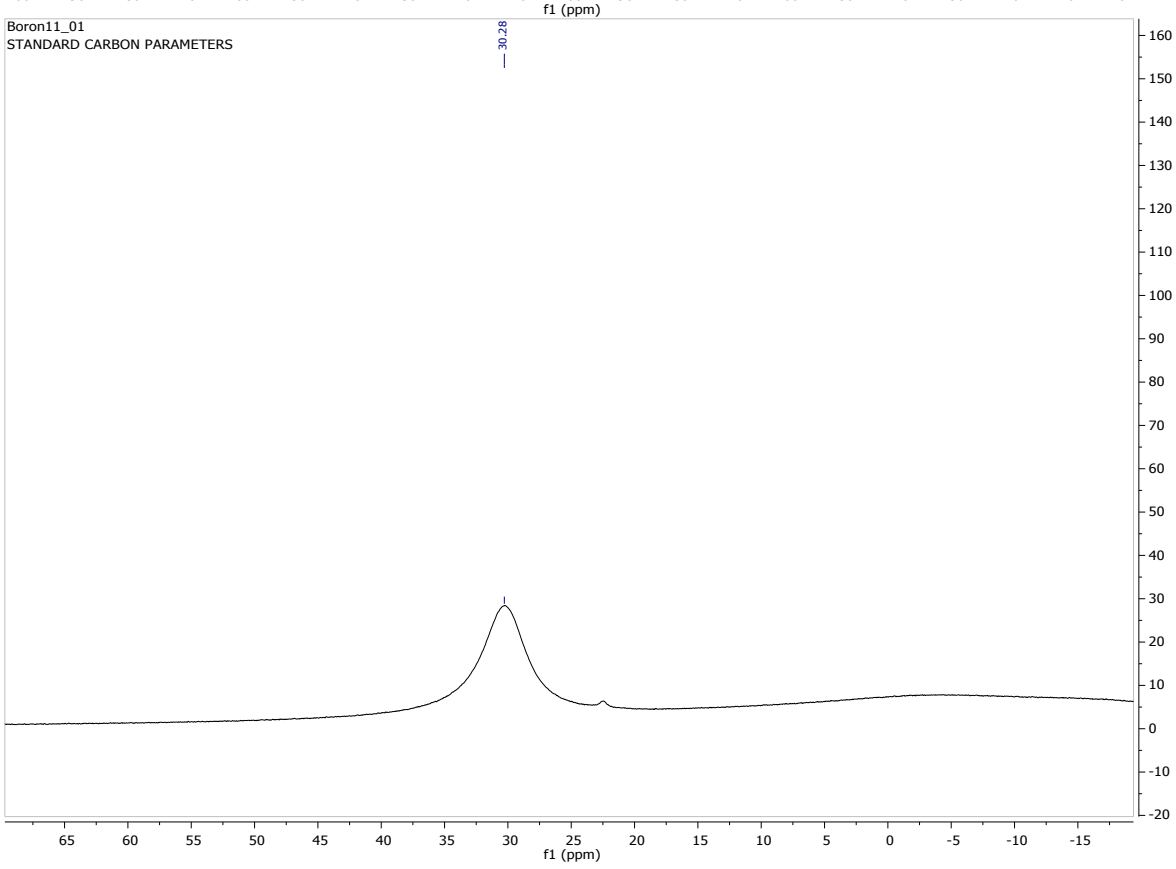
(E)-2,2'-(1-(4-(trifluoromethyl)phenyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane)

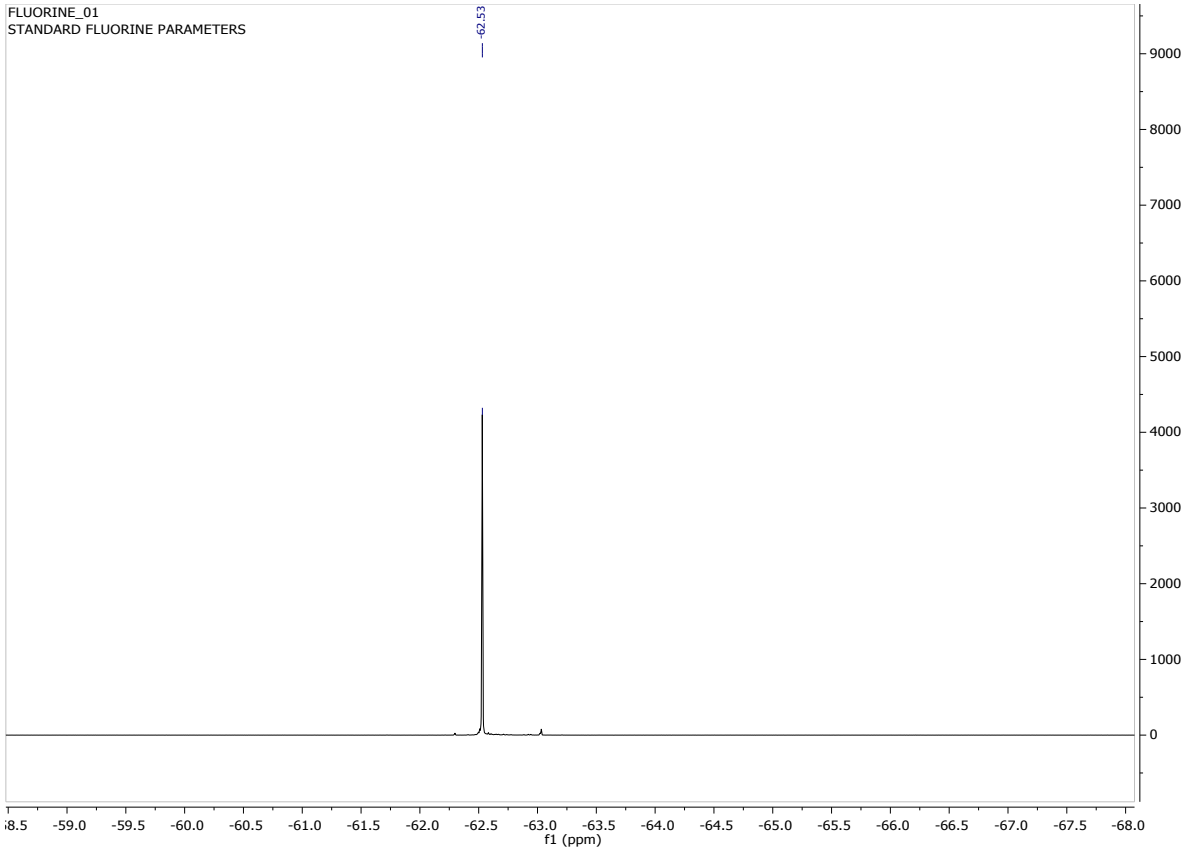
(7)



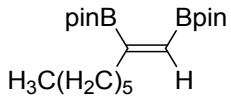


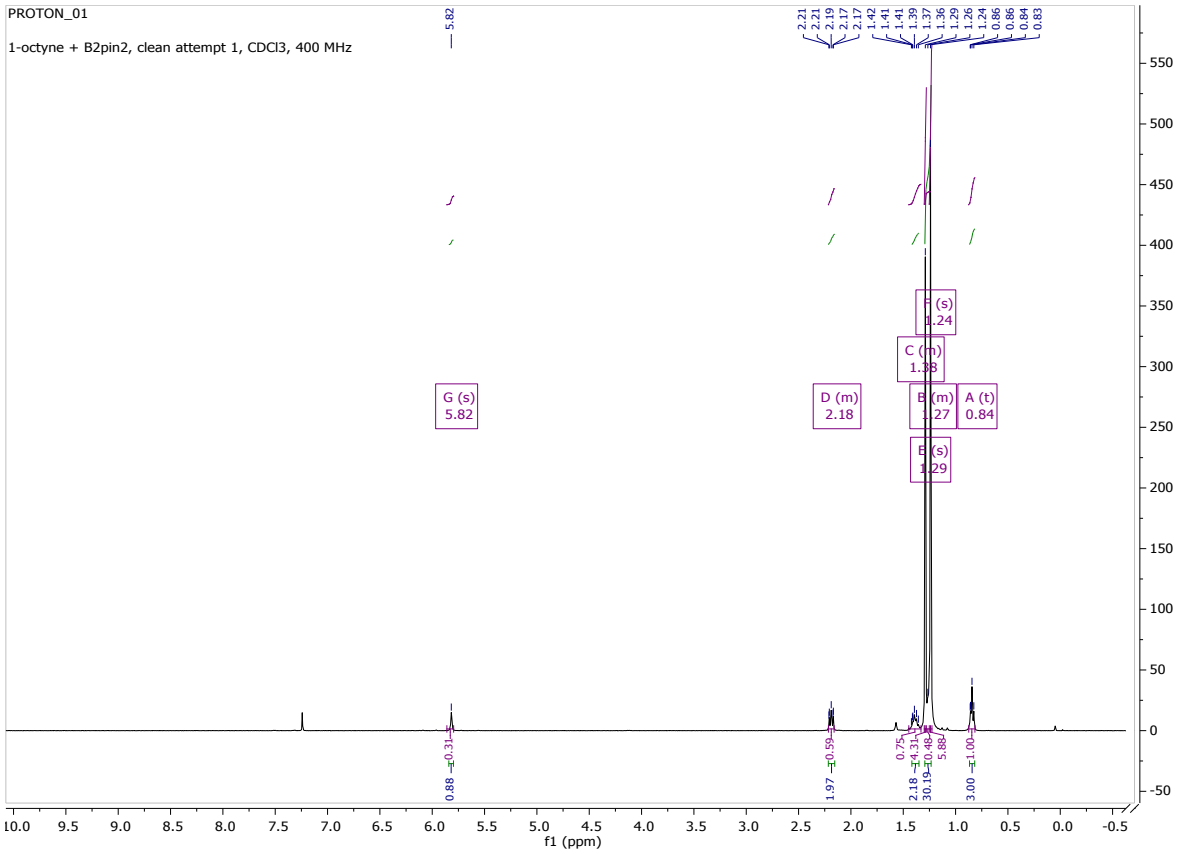

CARBON_01
p-CF3Ph(pinB)C=C(Bpin)H, CDCl3, 400 MHz
146.92
129.95
129.63
129.31
128.99
128.51
127.01
125.80
125.41
125.37
125.34
125.30
123.09
120.39
84.49
83.97
25.12
24.99
B (q)
125.36
A (q)
129.47
1.00
4.42
f1 (ppm)

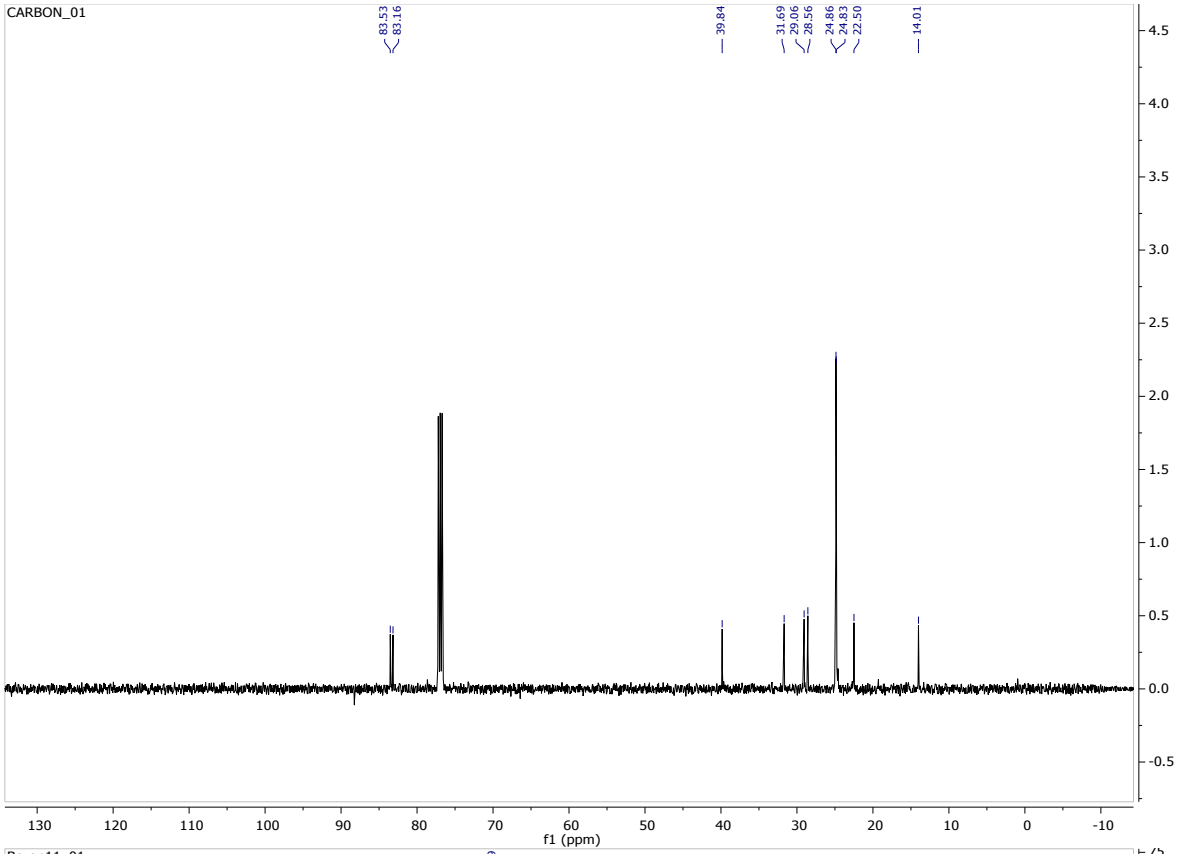

Boron11_01
STANDARD CARBON PARAMETERS
30.28
f1 (ppm)

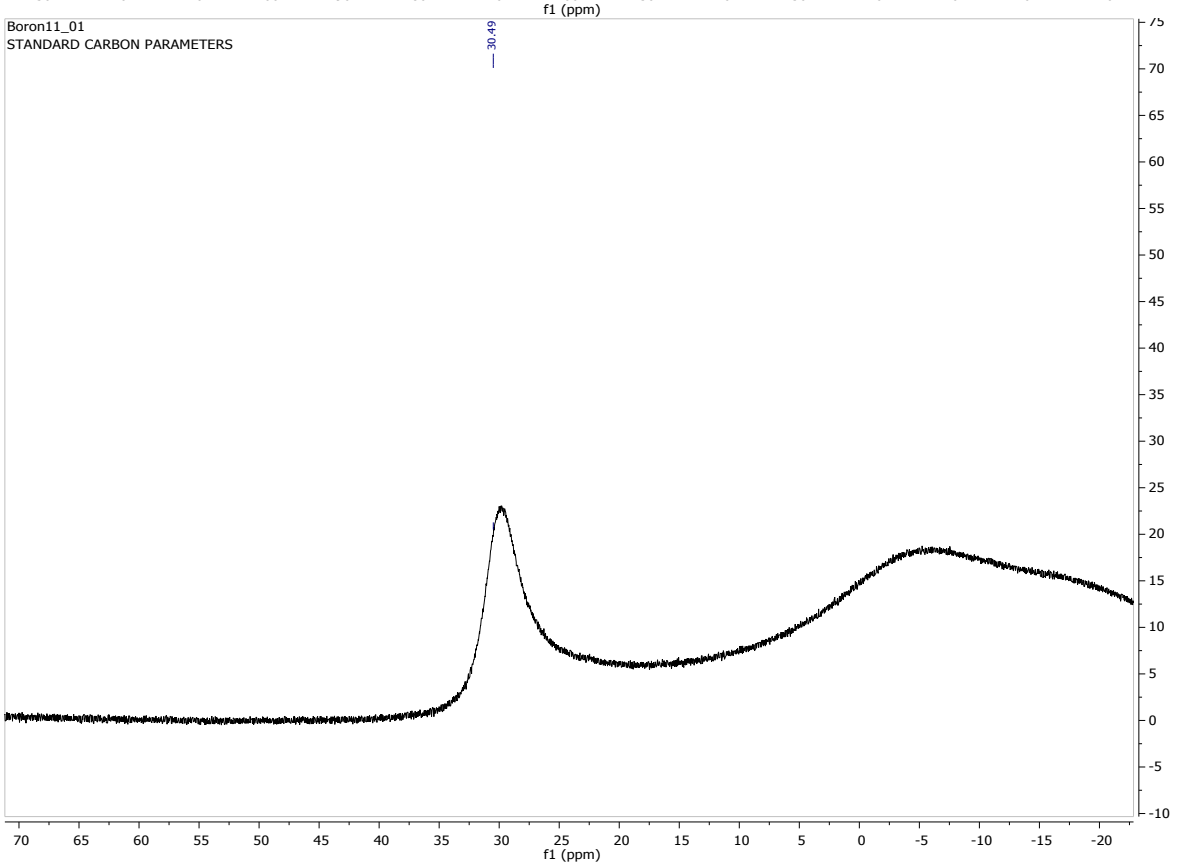

FLUORINE_01
STANDARD FLUORINE PARAMETERS
-62.53
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-59.0
-59.5
-60.0
-60.5
-61.0
-61.5
-62.0
-62.5
-63.0
-63.5
-64.0
-64.5
-65.0
-65.5
-66.0
-66.5
-67.0
-67.5
-68.0
f1 (ppm)

(E)-2,2'-(oct-1-ene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (8)

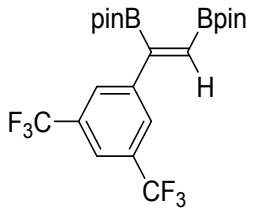


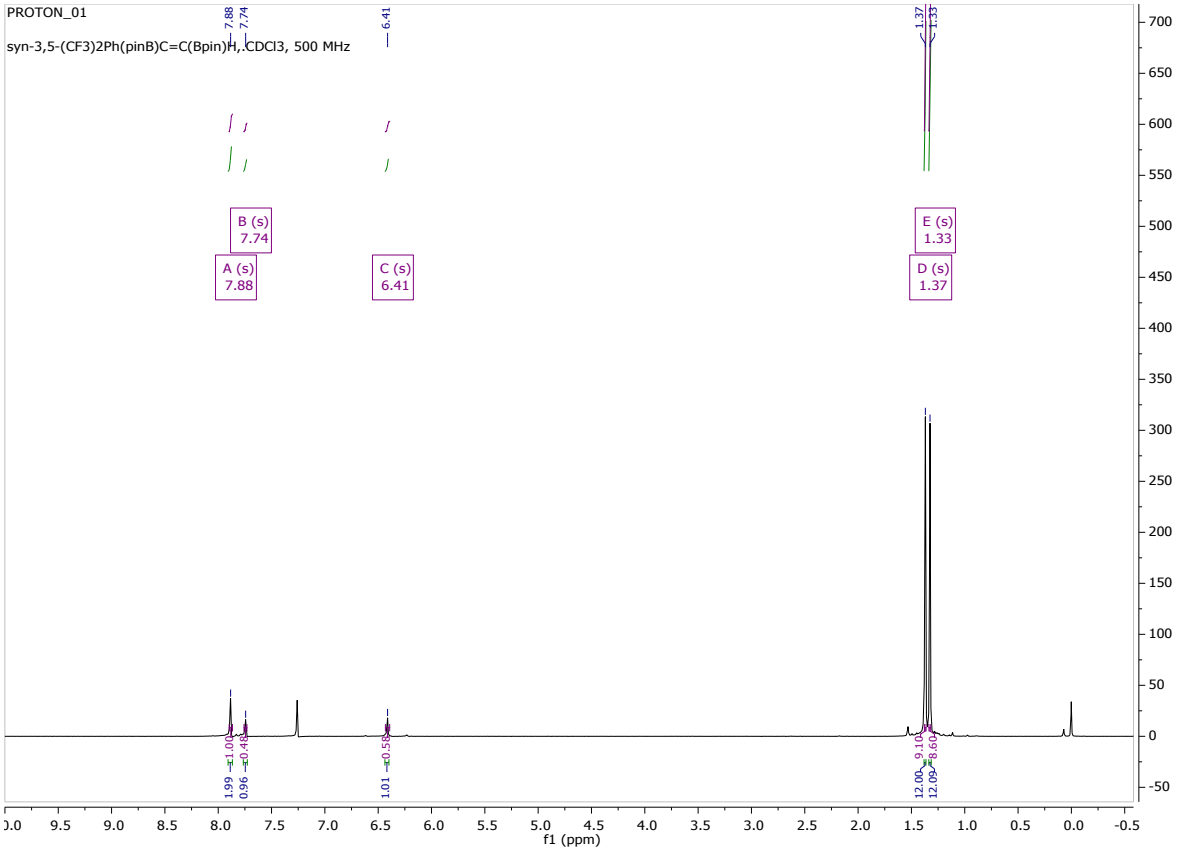


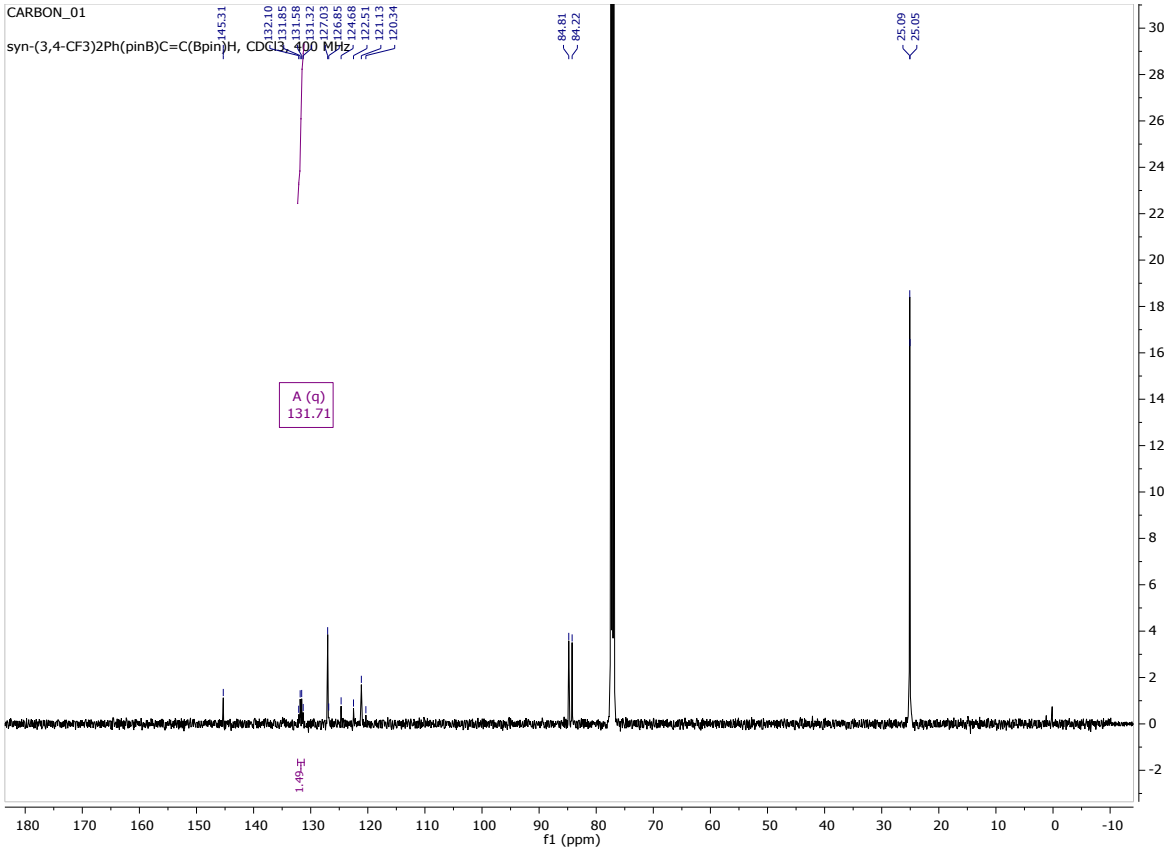

CARBON_01
83.53
83.16
39.84
31.69
29.06
28.56
24.86
24.83
22.50
14.01
f1 (ppm)

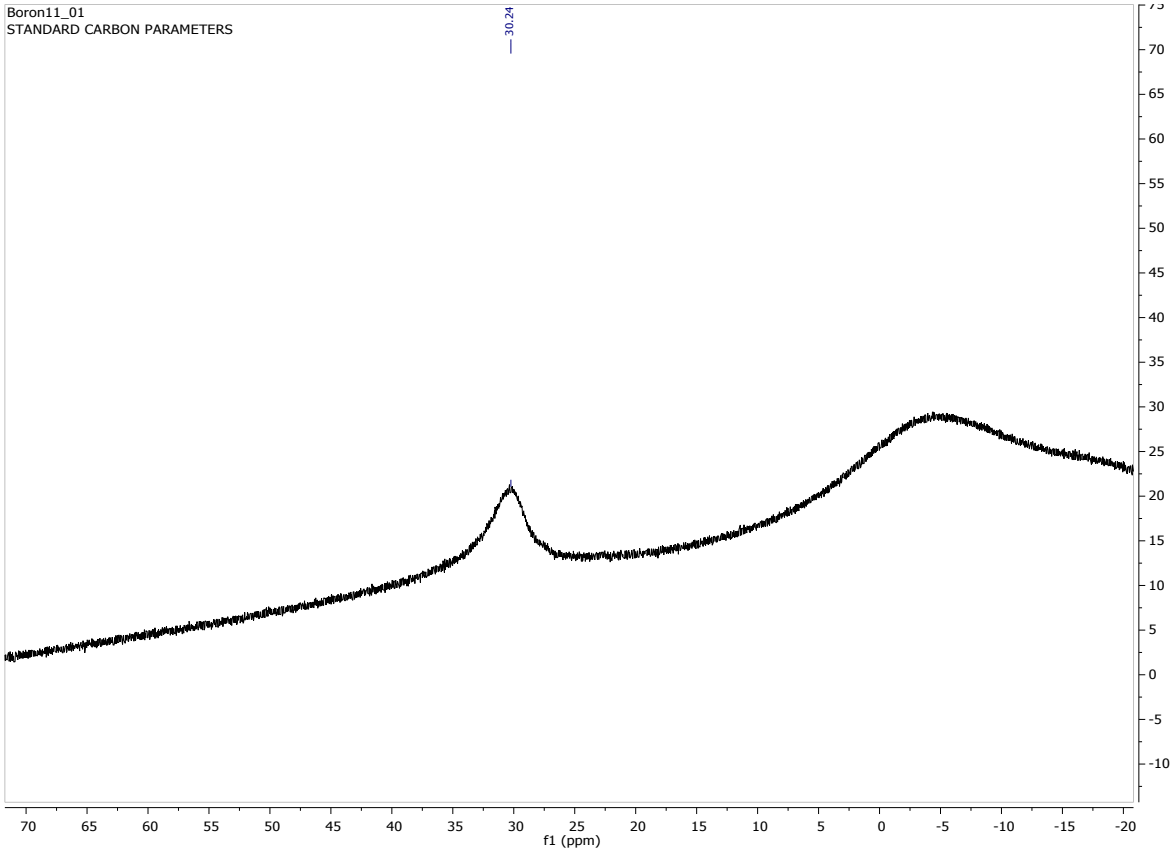

Boron11_01
STANDARD CARBON PARAMETERS
30.49
f1 (ppm)

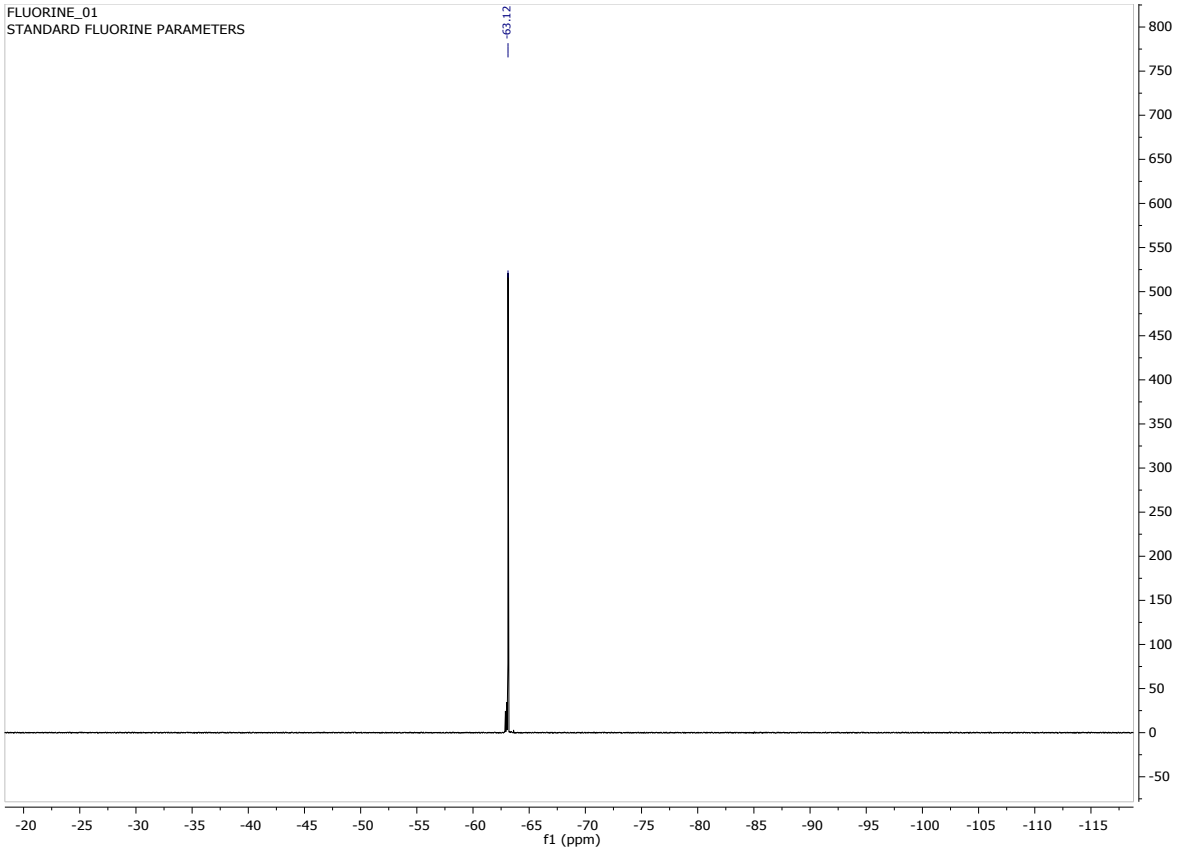
(E)-2,2'-(1-(3,5-bis(trifluoromethyl)phenyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (9)

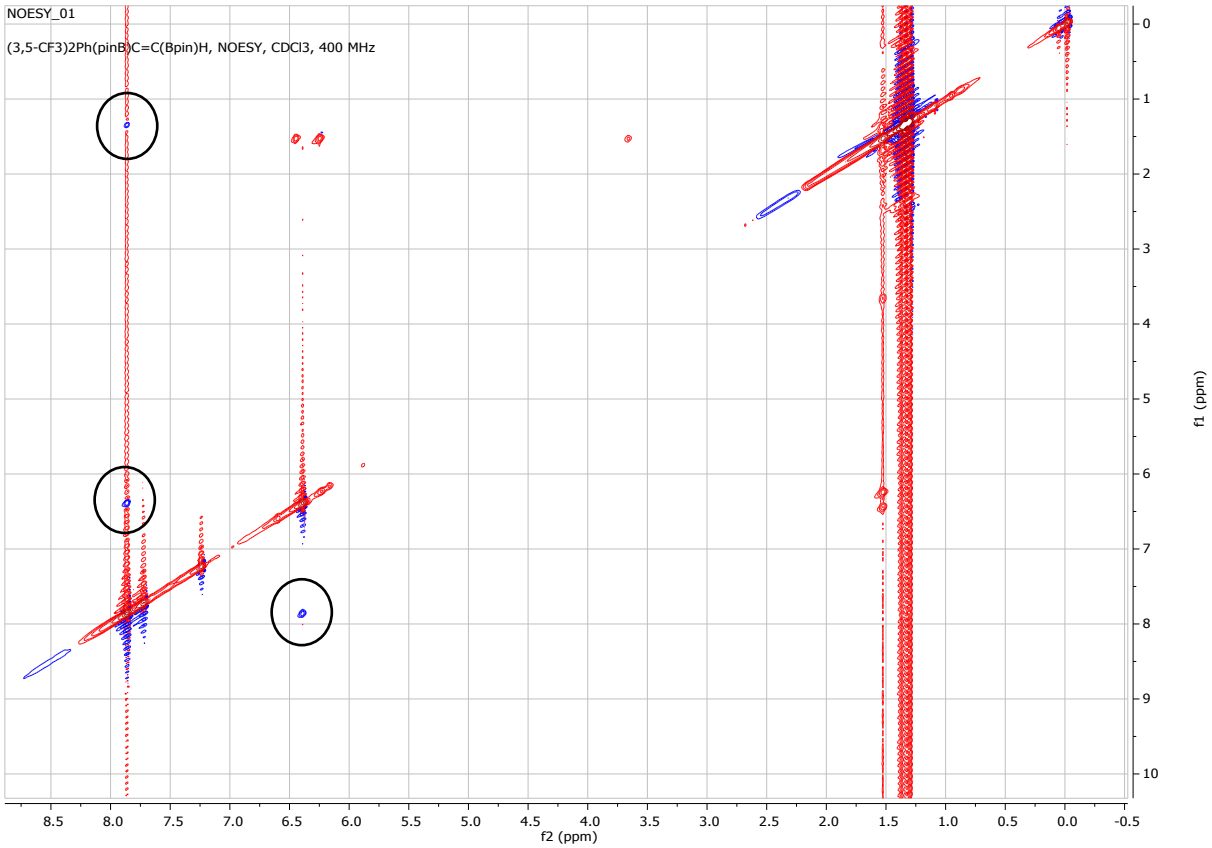




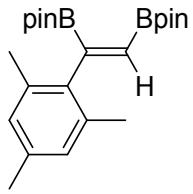

CARBON_01
syn-(3,4-CF3)2Ph(pinB)C=C(Bpin)H, CDCl3, 400 MHz
145.31
132.10
131.85
131.58
131.32
127.03
126.85
124.68
122.51
121.13
120.34
84.81
84.22
25.09
25.05
A (q)
131.71
1.49
f1 (ppm)

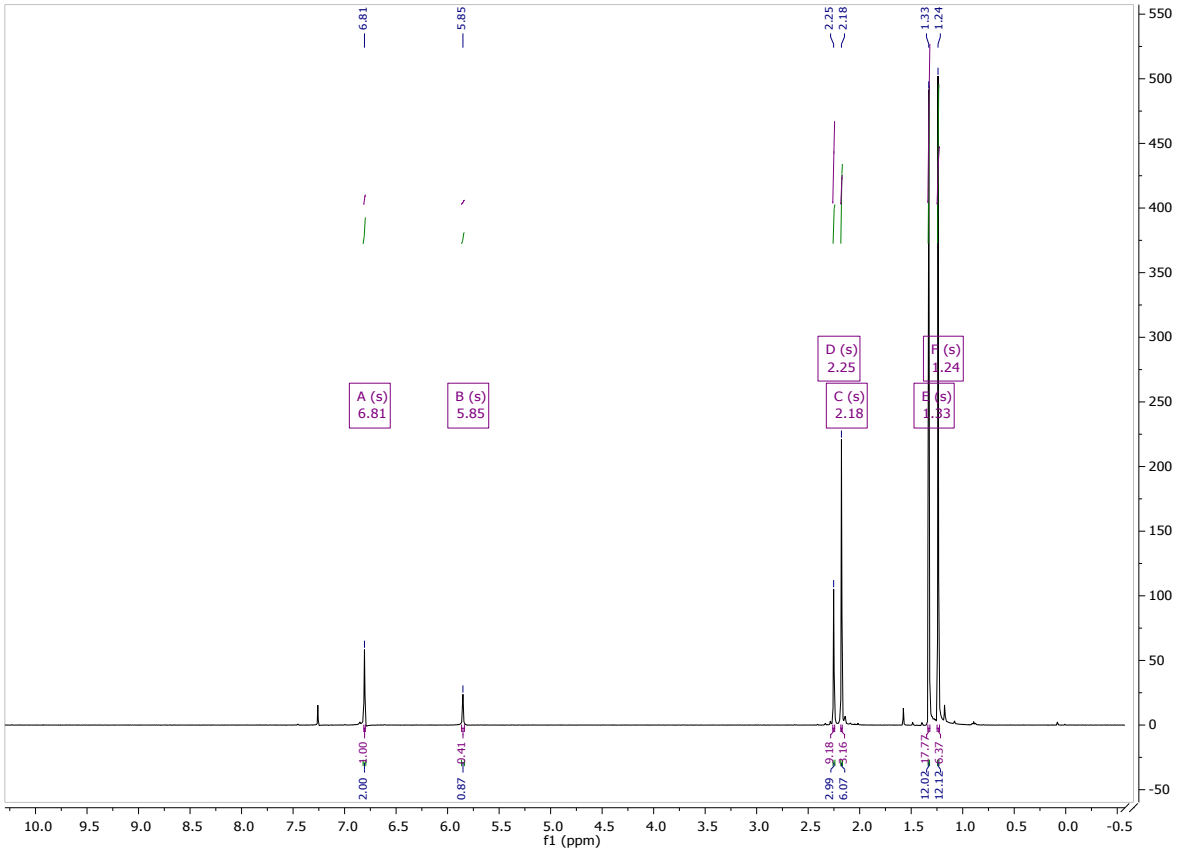

Boron11_01
STANDARD CARBON PARAMETERS
30.24
f1 (ppm)

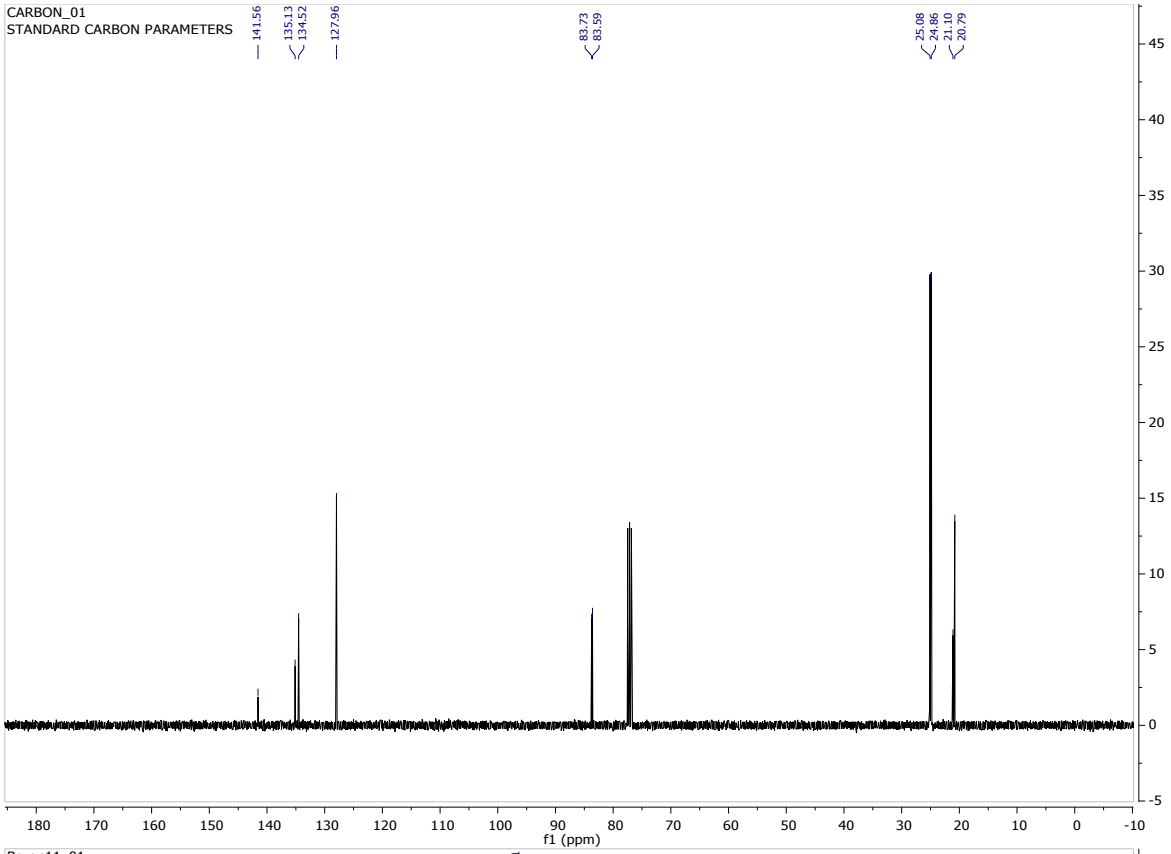

FLUORINE_01
STANDARD FLUORINE PARAMETERS
-63.12
f1 (ppm)

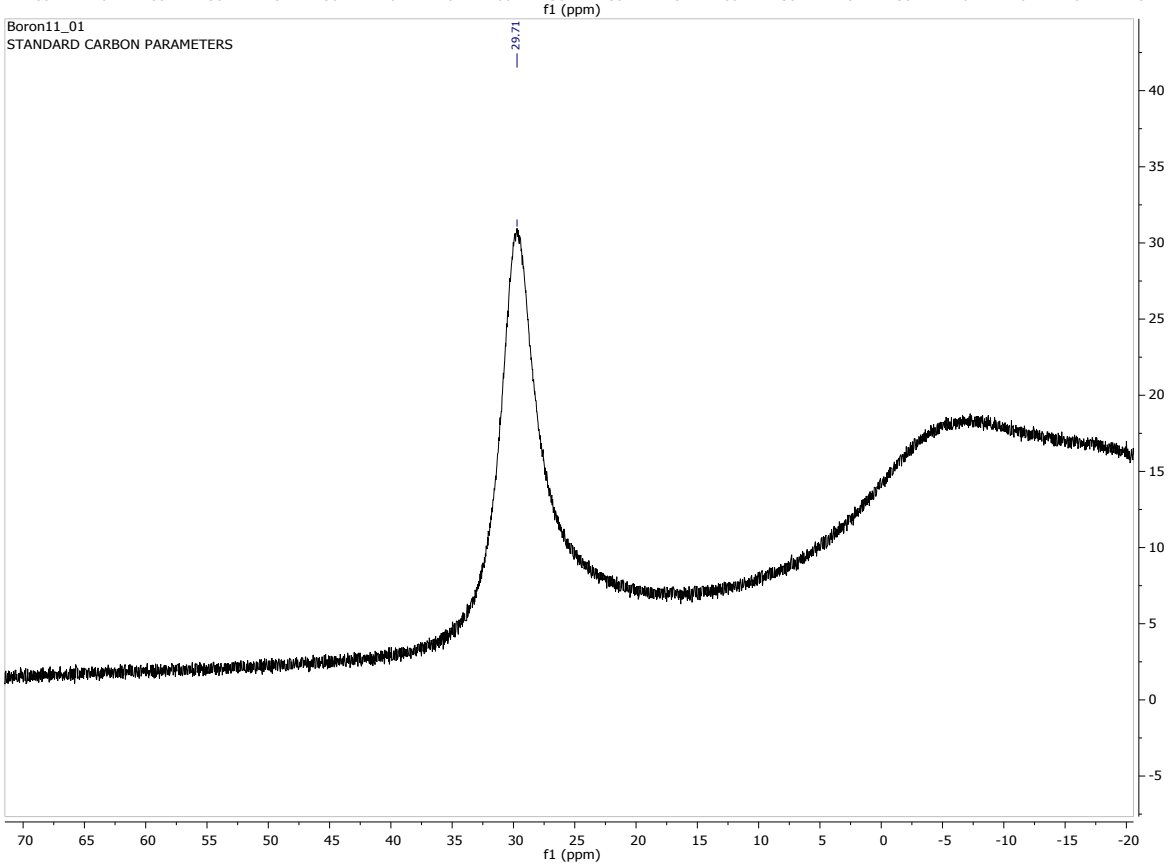

NOESY_01
(3,5-CF3)2Ph(pinB)C=C(Bpin)H, NOESY, CDCl3, 400 MHz
f2 (ppm)
f1 (ppm)

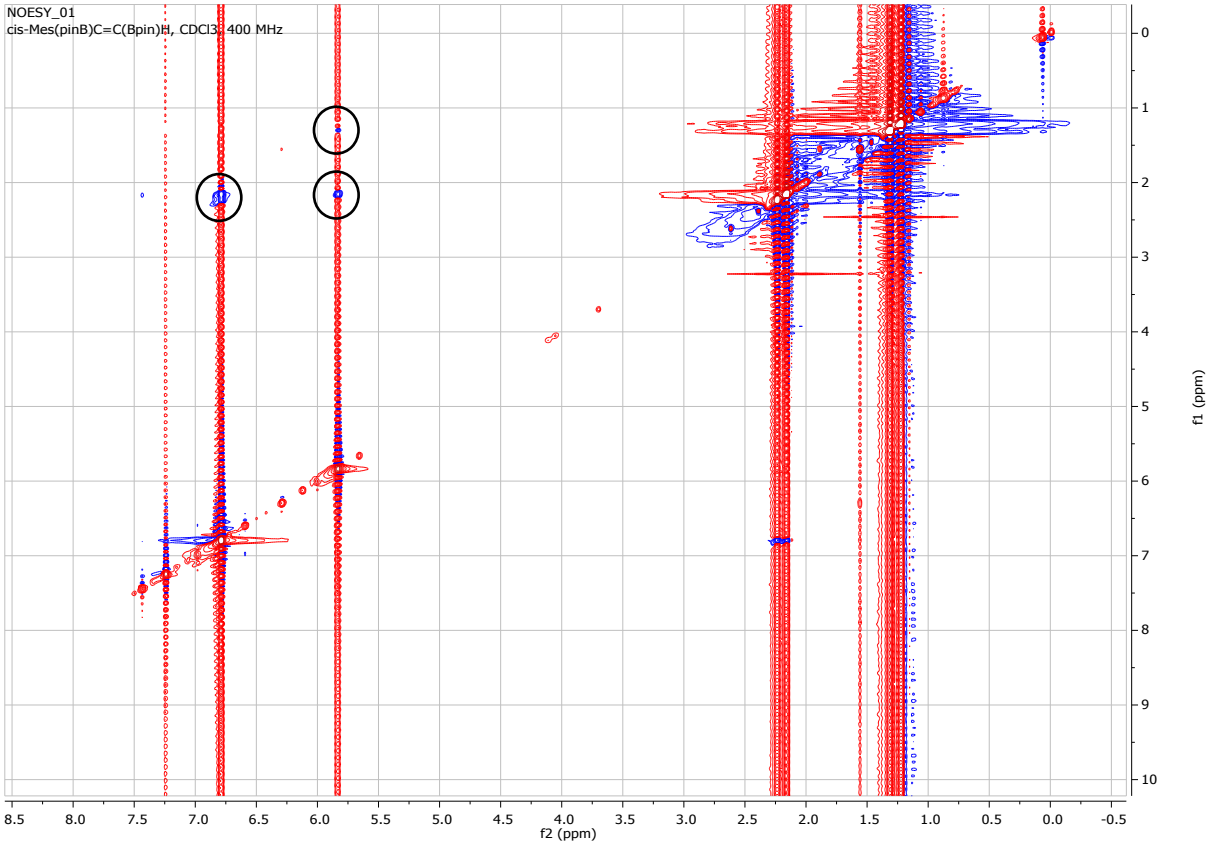
(E)-2,2'-(1-mesitylethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (10)



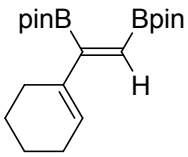


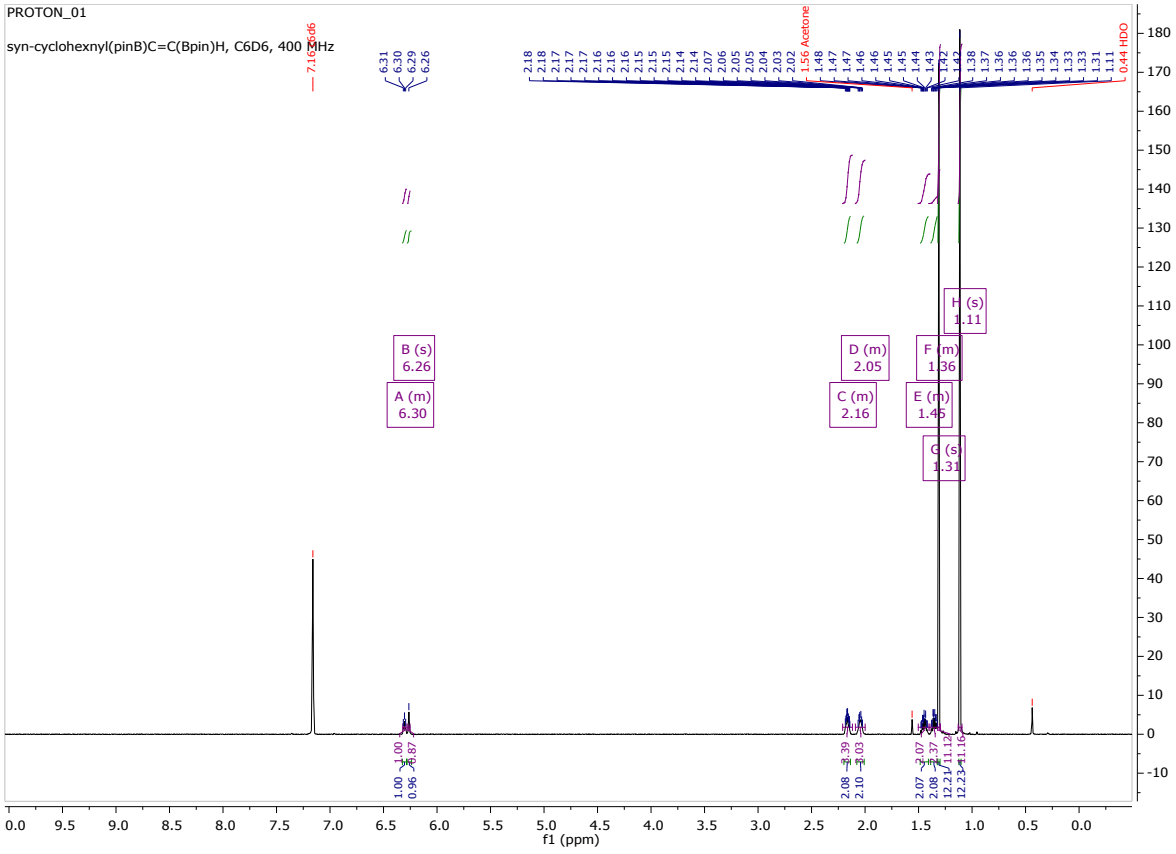

CARBON_01
STANDARD CARBON PARAMETERS
141.56
135.13
134.52
127.96
83.73
83.59
25.08
24.86
21.10
20.79
f1 (ppm)

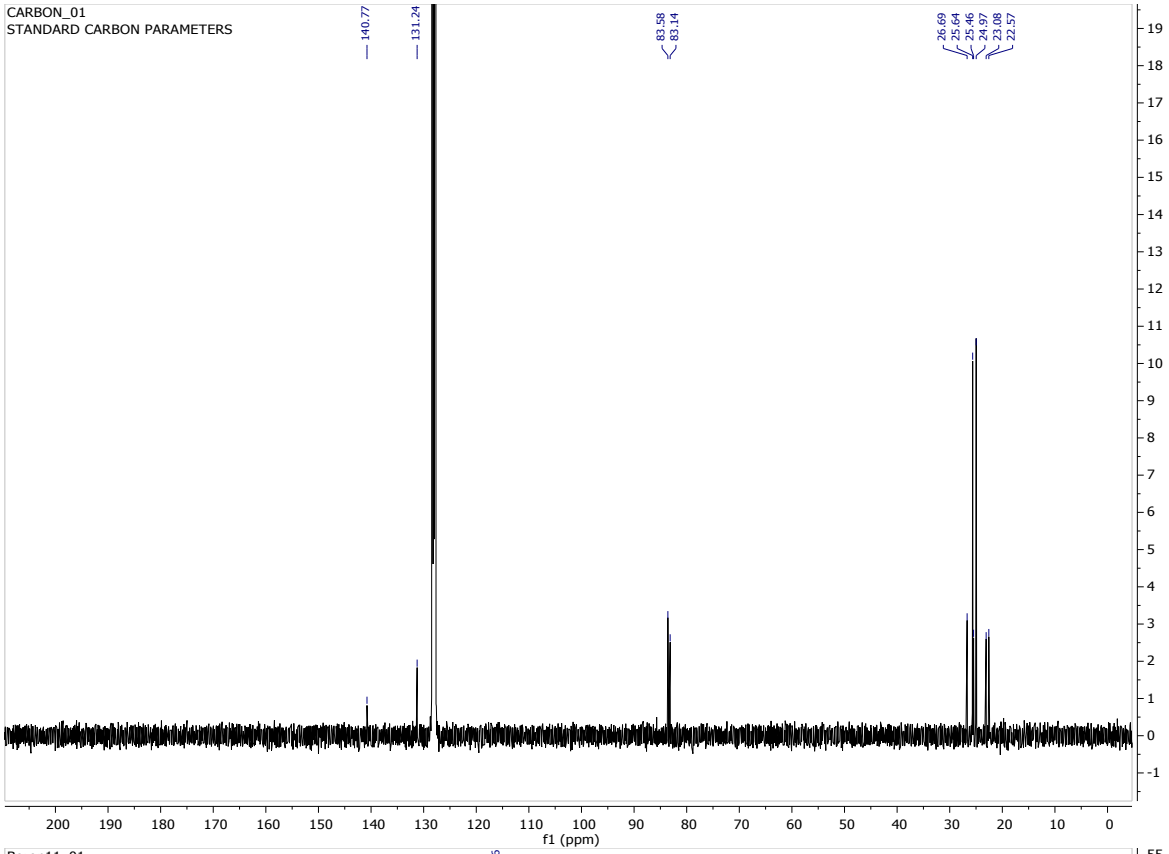

Boron11_01
STANDARD CARBON PARAMETERS
29.71
f1 (ppm)

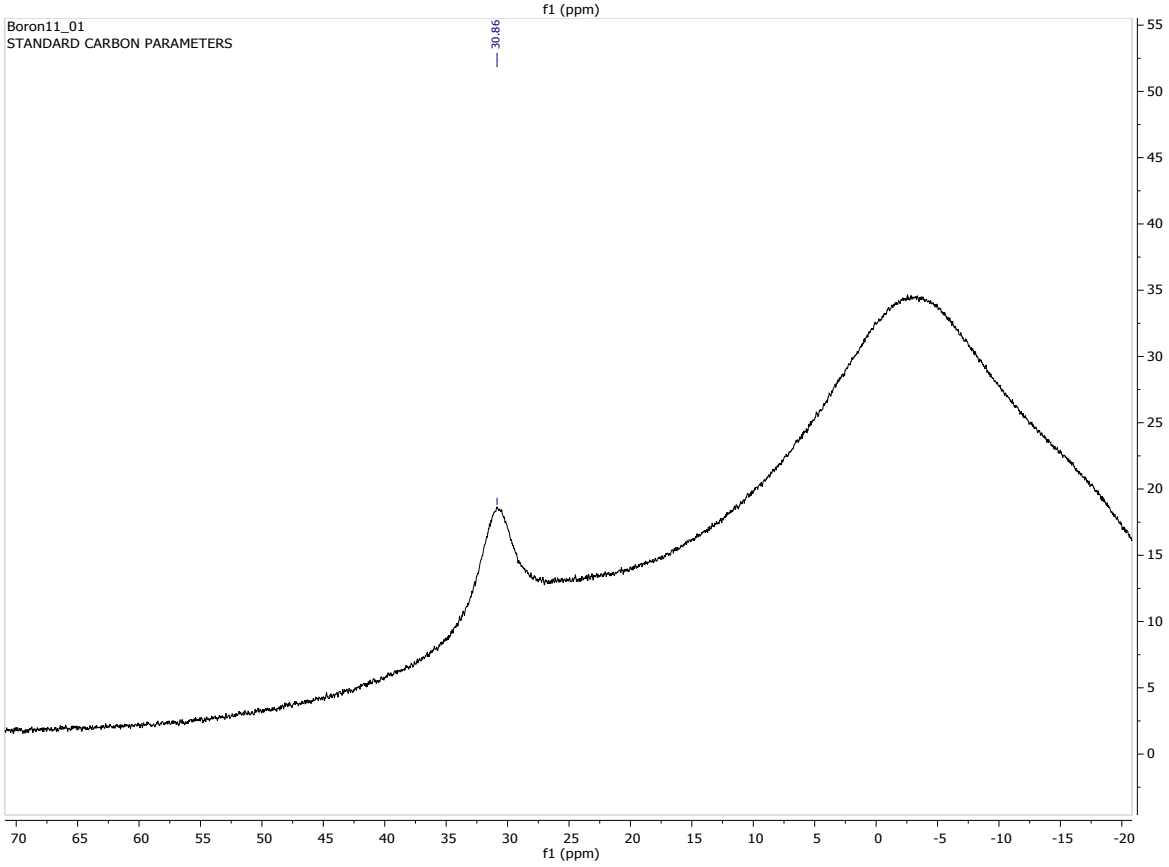

NOESY_01
cis-Mes(pinB)C=C(Bpin)H, CDCl3, 400 MHz
f2 (ppm)
f1 (ppm)

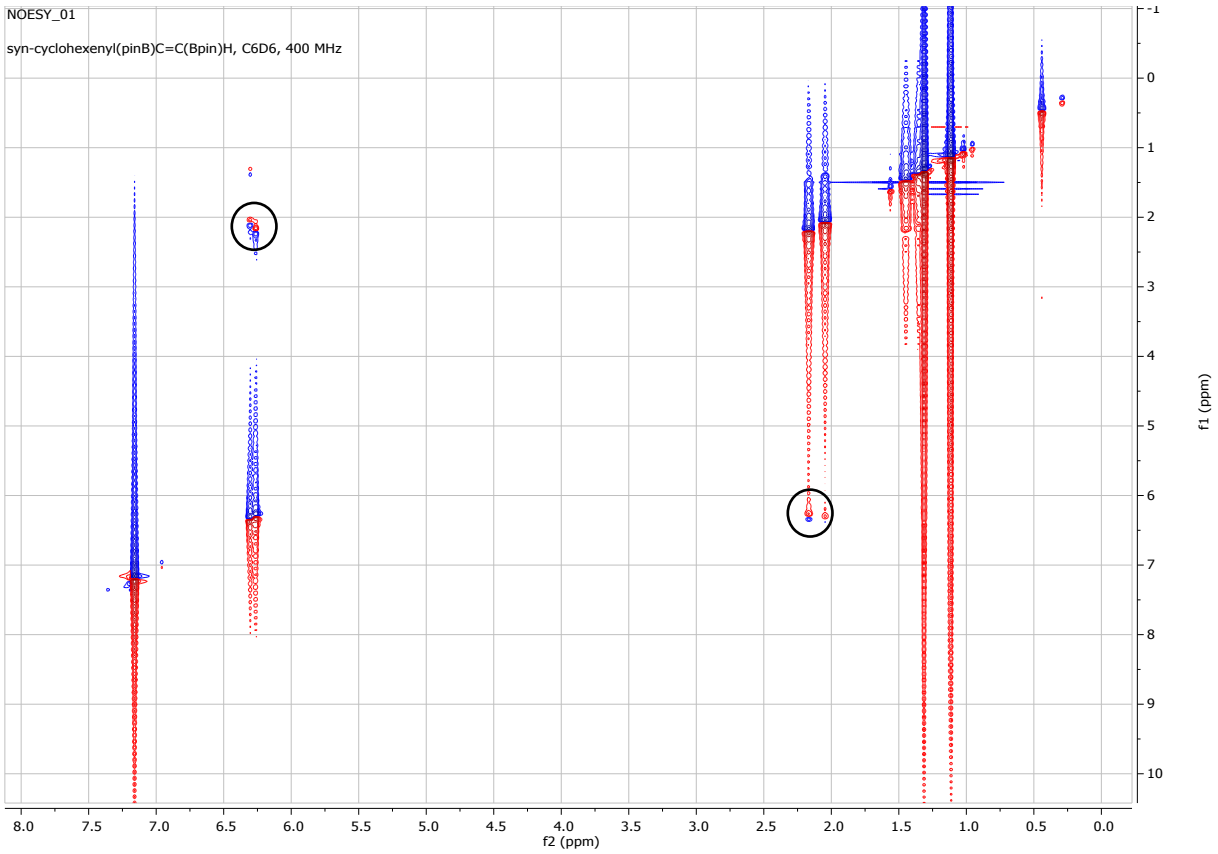
(*E*)-2,2'-(1-(cyclohex-1-en-1-yl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (11)



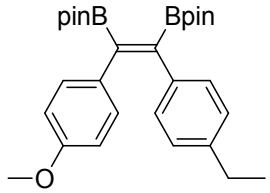


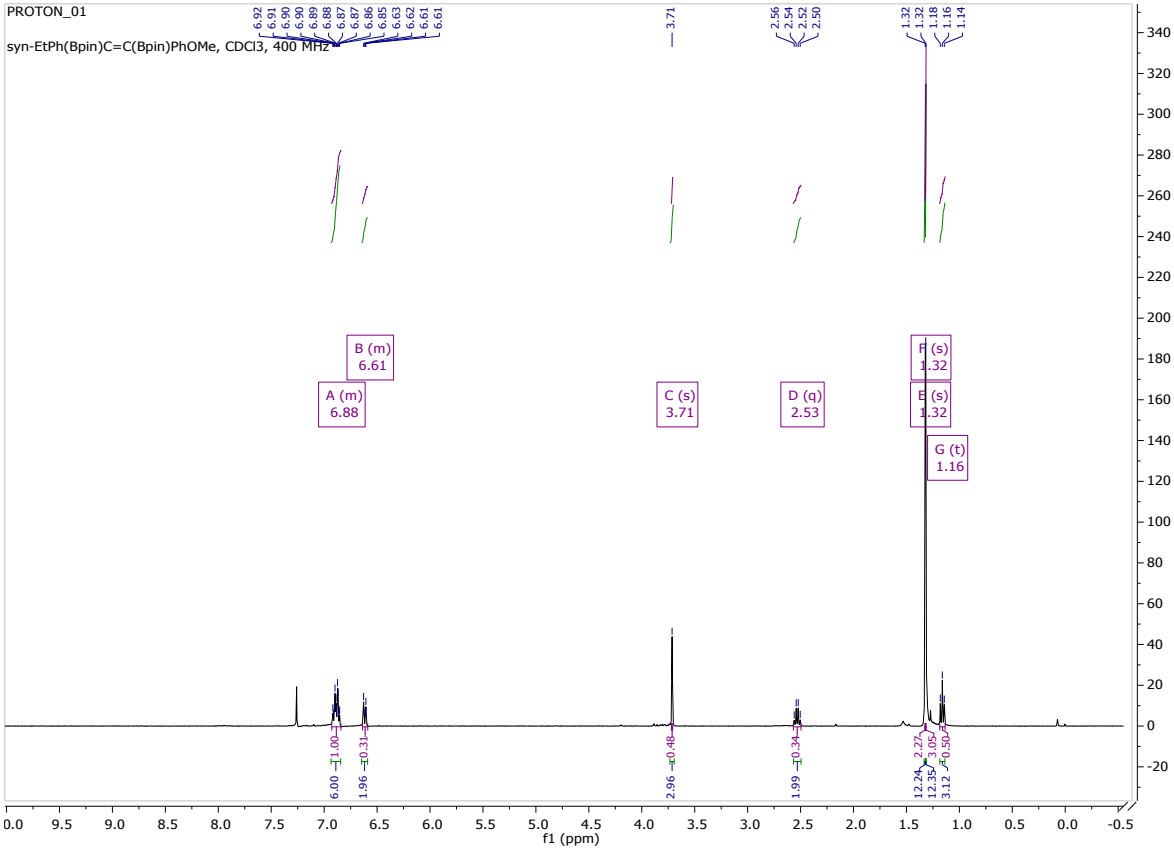

CARBON_01
STANDARD CARBON PARAMETERS
140.77
131.24
83.58
83.14
26.69
25.64
25.46
24.97
23.08
22.57
f1 (ppm)

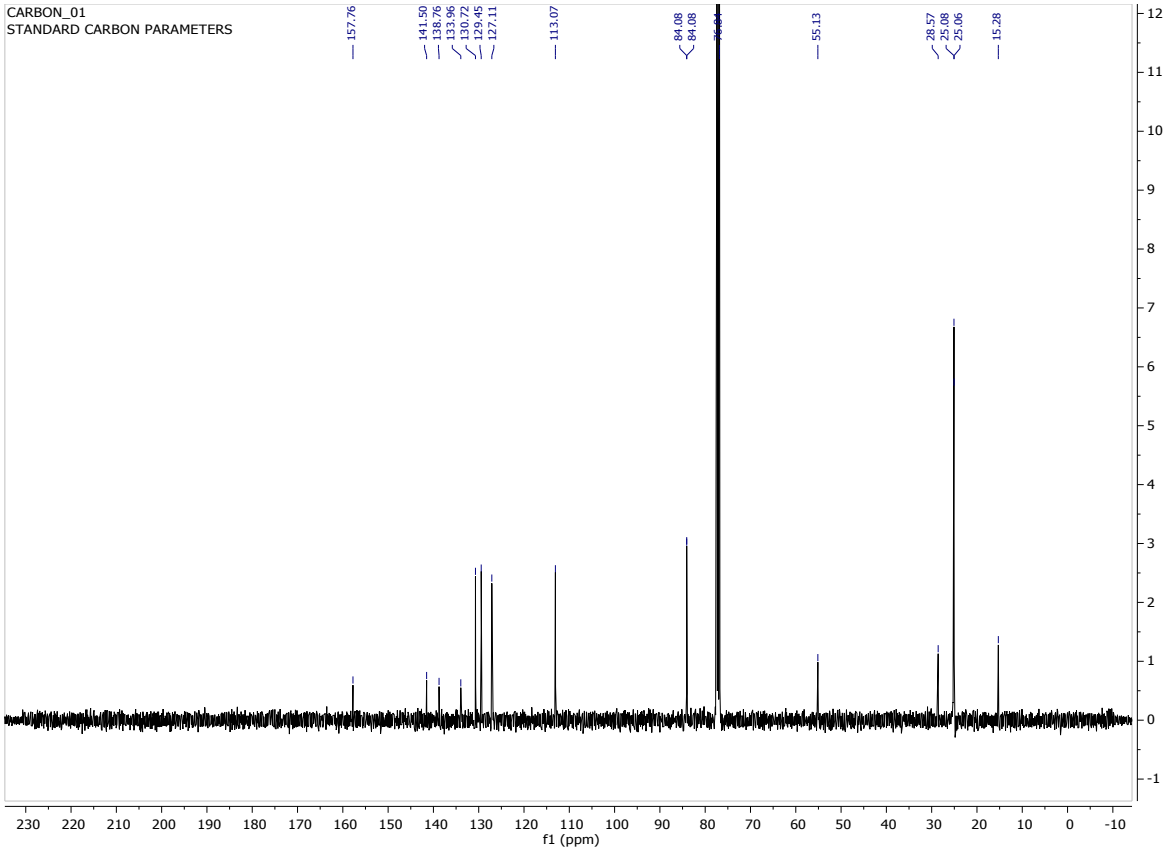

Boron11_01
STANDARD CARBON PARAMETERS
30.86
f1 (ppm)

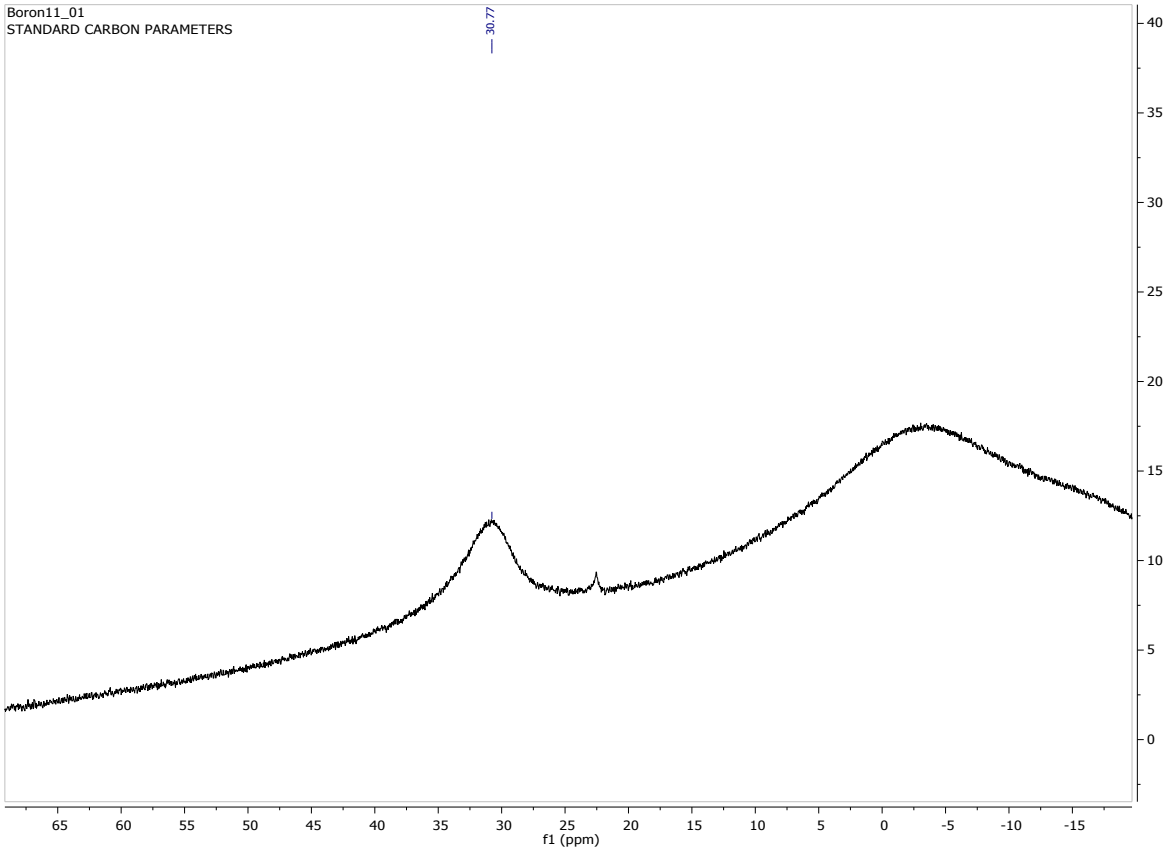

NOESY_01
syn-cyclohexenyl(pinB)C=C(Bpin)H, C6D6, 400 MHz
f2 (ppm)
f1 (ppm)

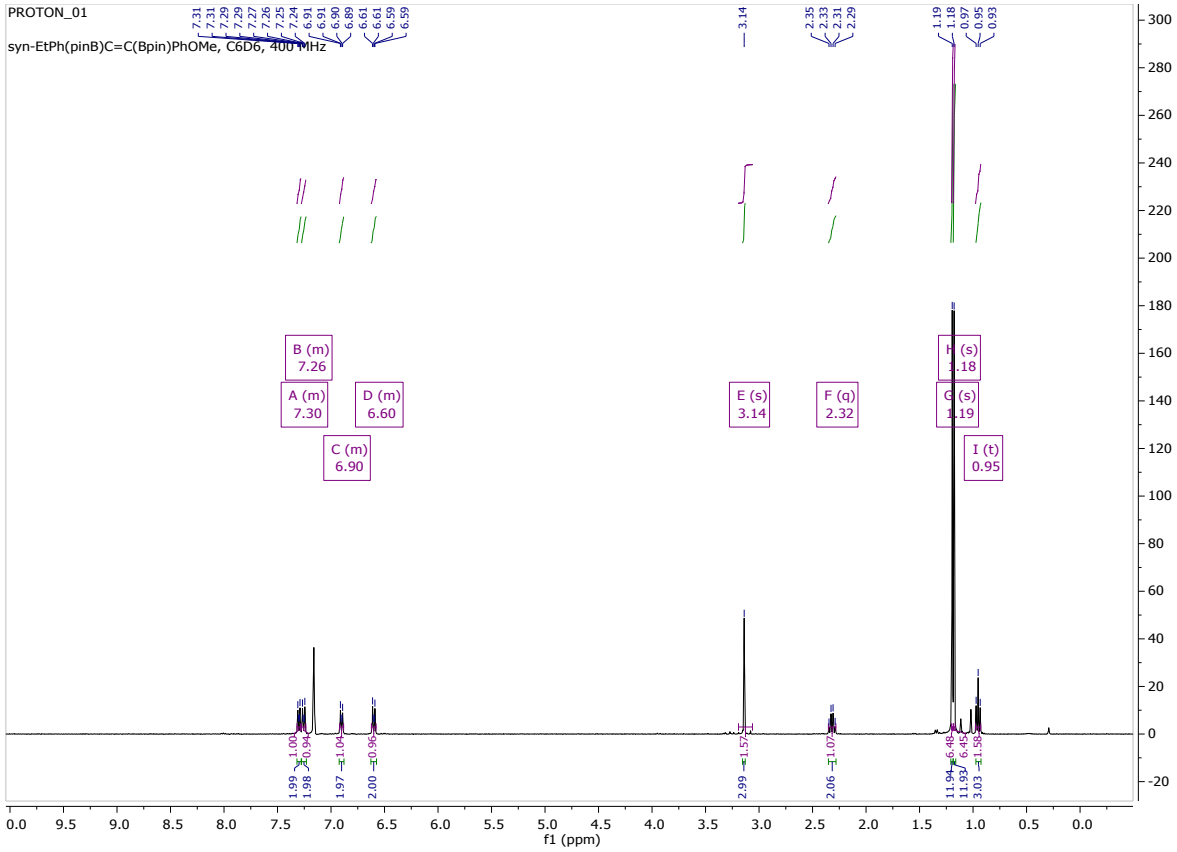
(Z)-2,2'-(1-(4-ethylphenyl)-2-(4-methoxyphenyl)ethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (12)

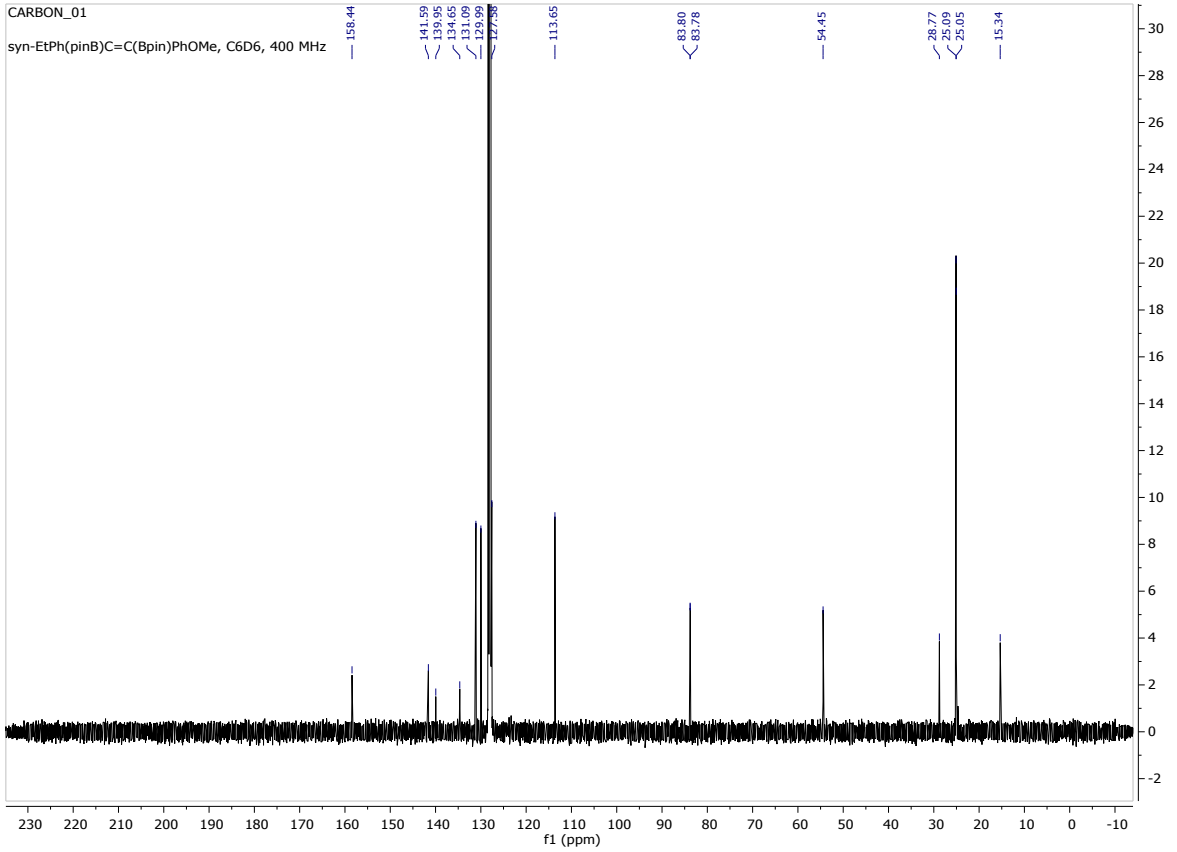


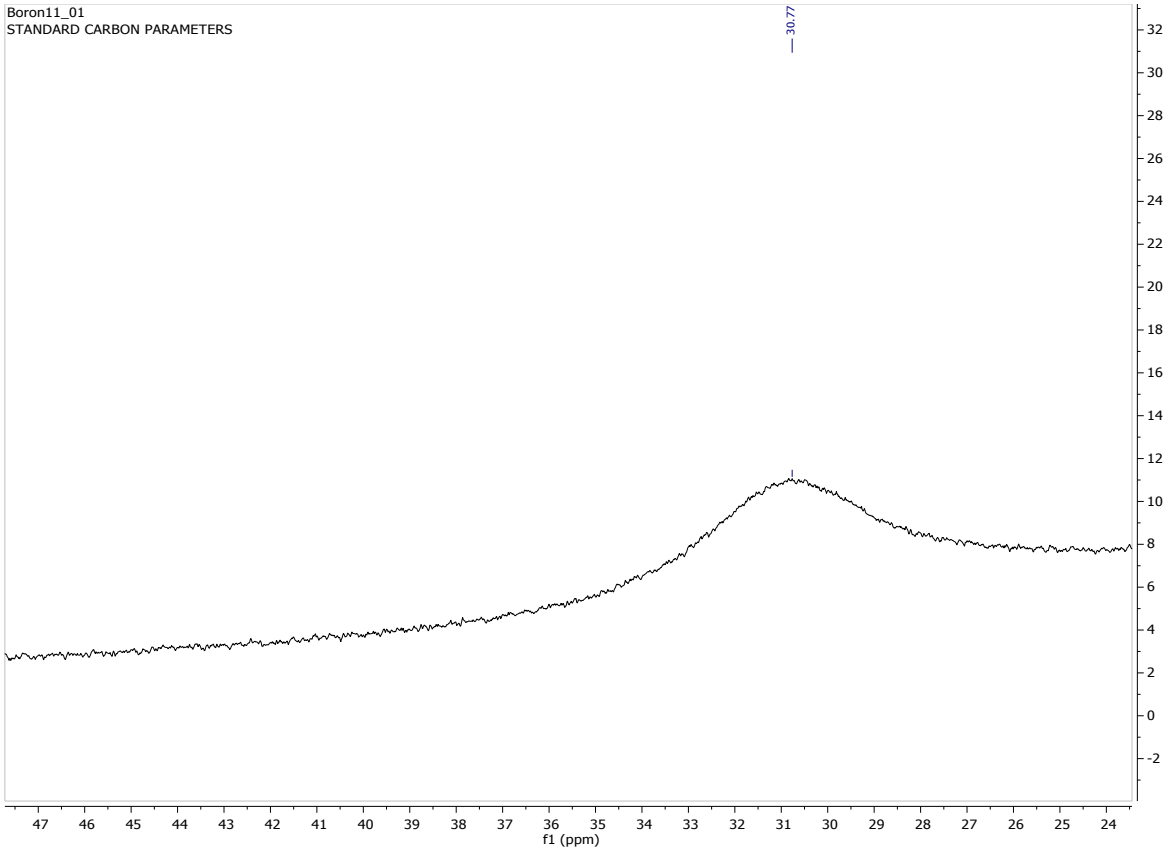


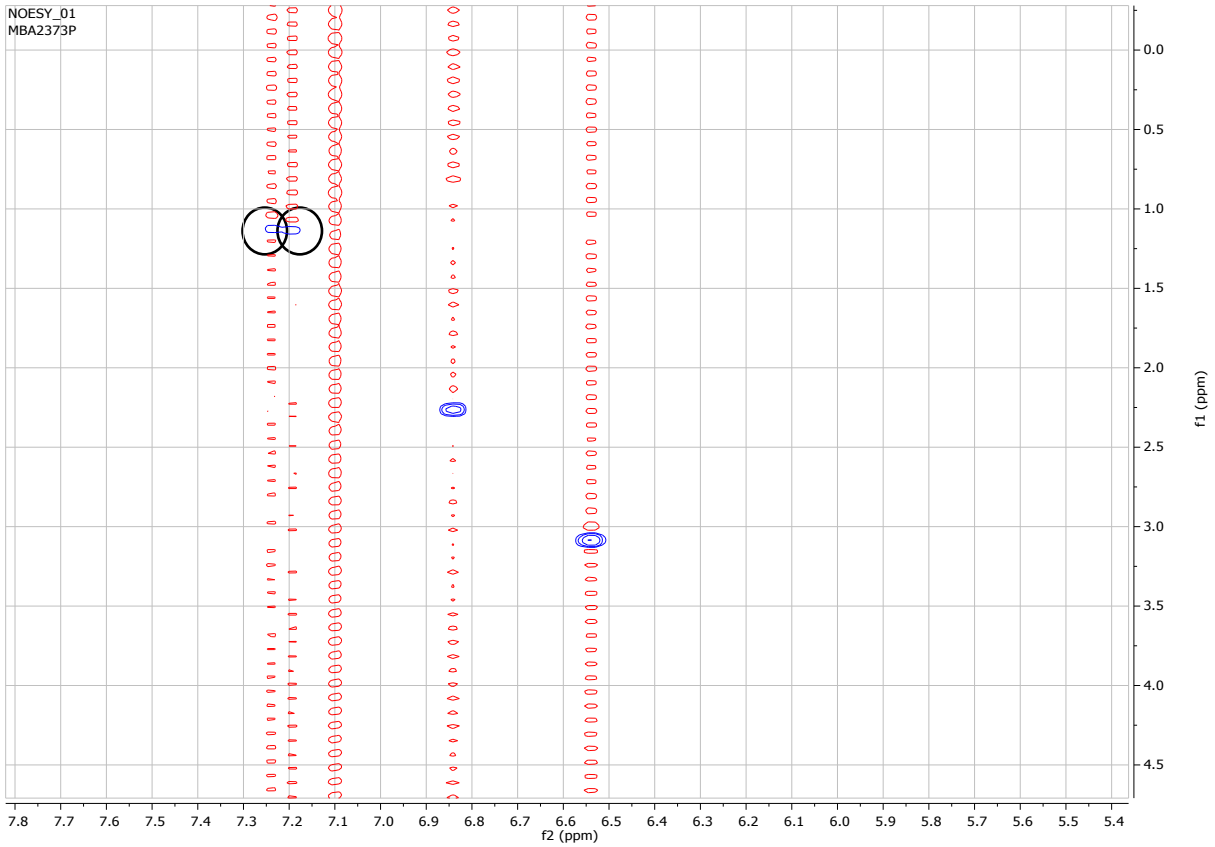

CARBON_01
STANDARD CARBON PARAMETERS
157.76
141.50
138.76
133.96
130.72
129.45
127.11
113.07
84.08
84.08
55.13
28.57
25.08
25.06
15.28
f1 (ppm)


Boron11_01
STANDARD CARBON PARAMETERS
30.77
f1 (ppm)


PROTON_01
syn-EtPh(pinB)C=C(Bpin)PhOMe, C6D6, 400 MHz
B (m) 7.26
A (m) 7.30
D (m) 6.60
C (m) 6.90
E (s) 3.14
F (q) 2.32
I (t) 0.95
f1 (ppm)

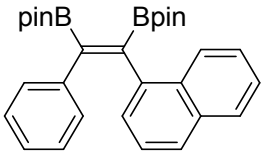

CARBON_01
syn-EtPh(pinB)C=C(Bpin)PhOMe, C6D6, 400 MHz
158.44
141.59
139.95
134.65
131.09
129.99
127.58
113.65
83.80
83.78
54.45
28.77
25.09
25.05
15.34
f1 (ppm)

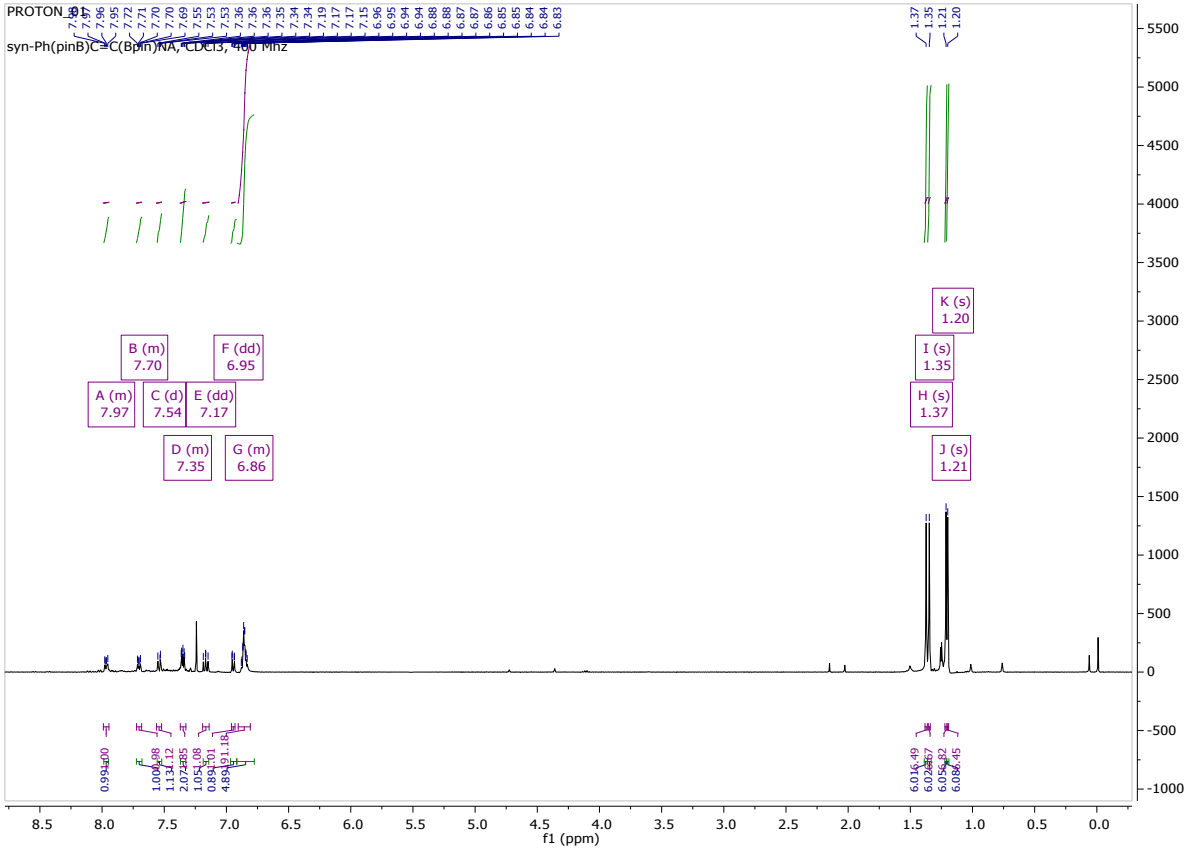

Boron11_01
STANDARD CARBON PARAMETERS
30.77
f1 (ppm)

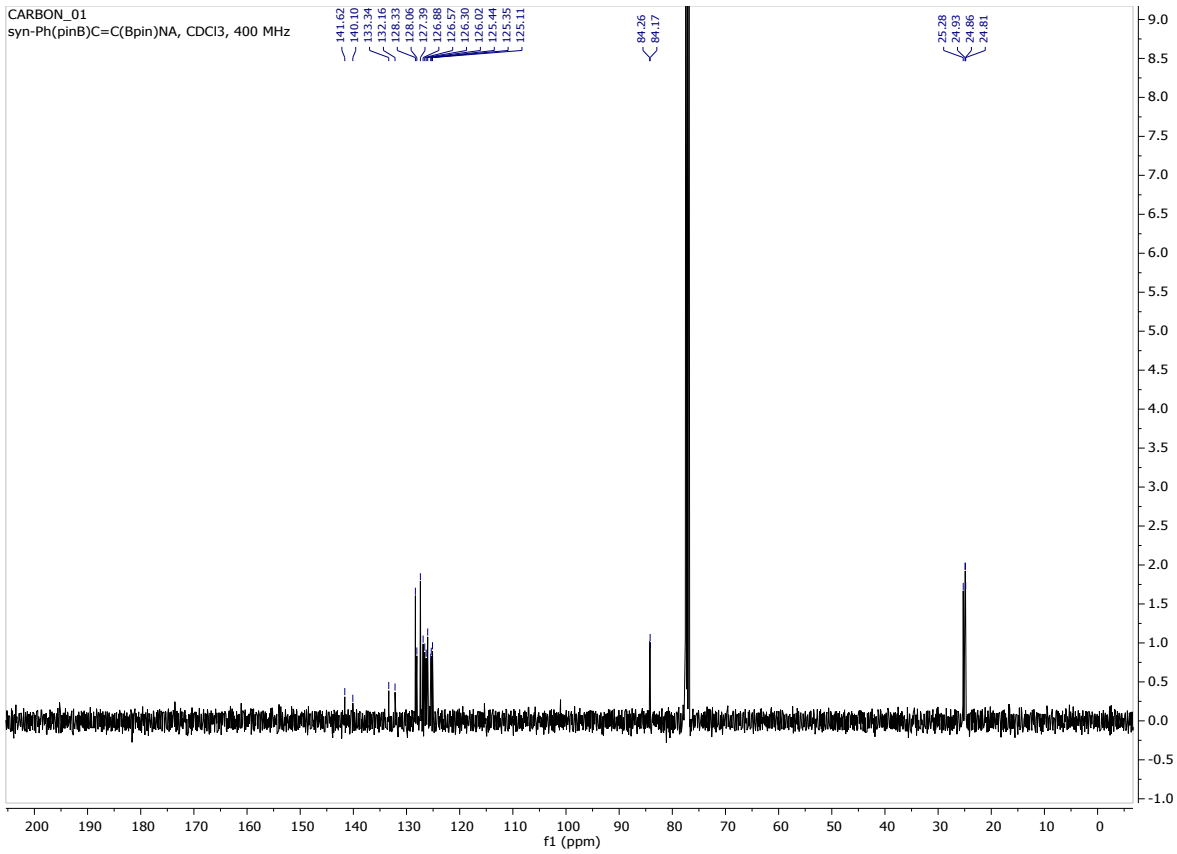

NOESY_01
MBA2373P
f2 (ppm)
f1 (ppm)

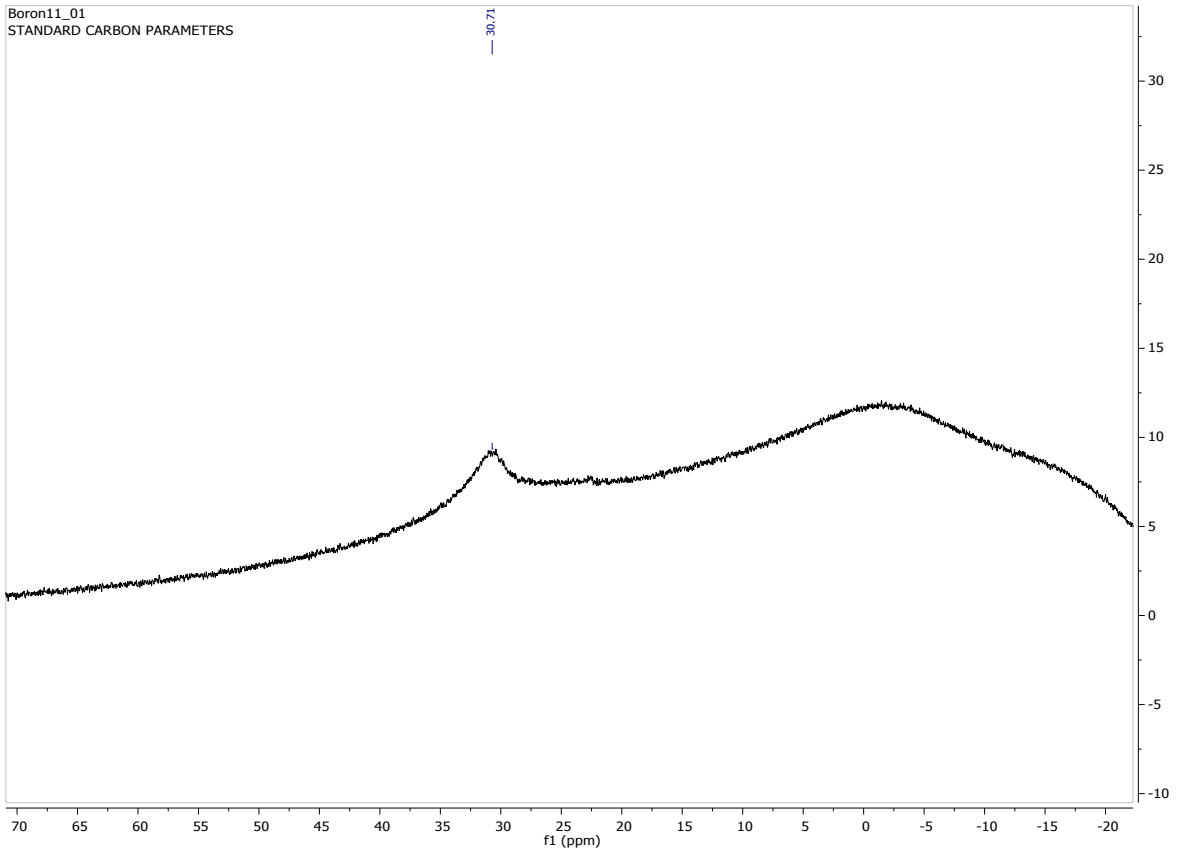
(Z)-2,2'-(1-(naphthalen-1-yl)-2-phenylethene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane)

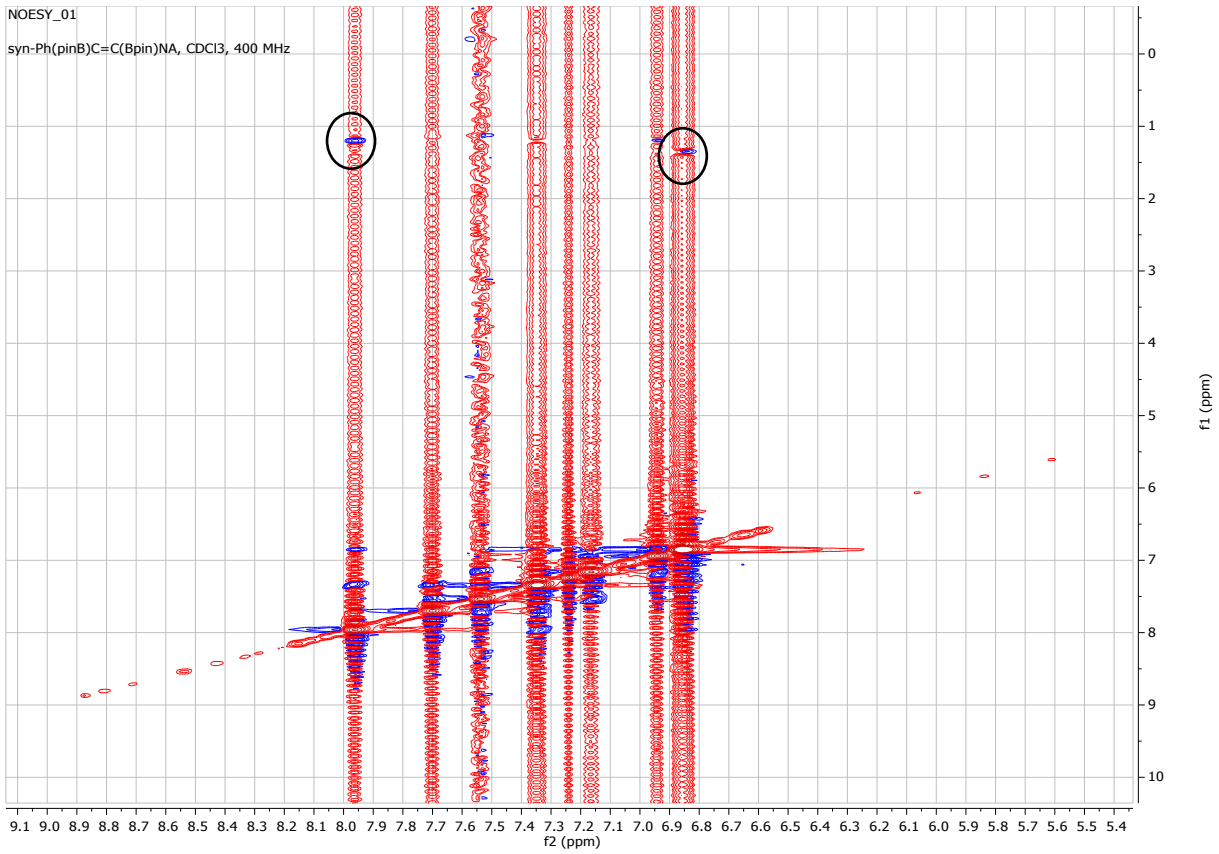
(13)



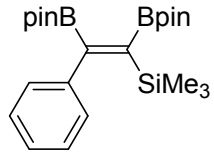


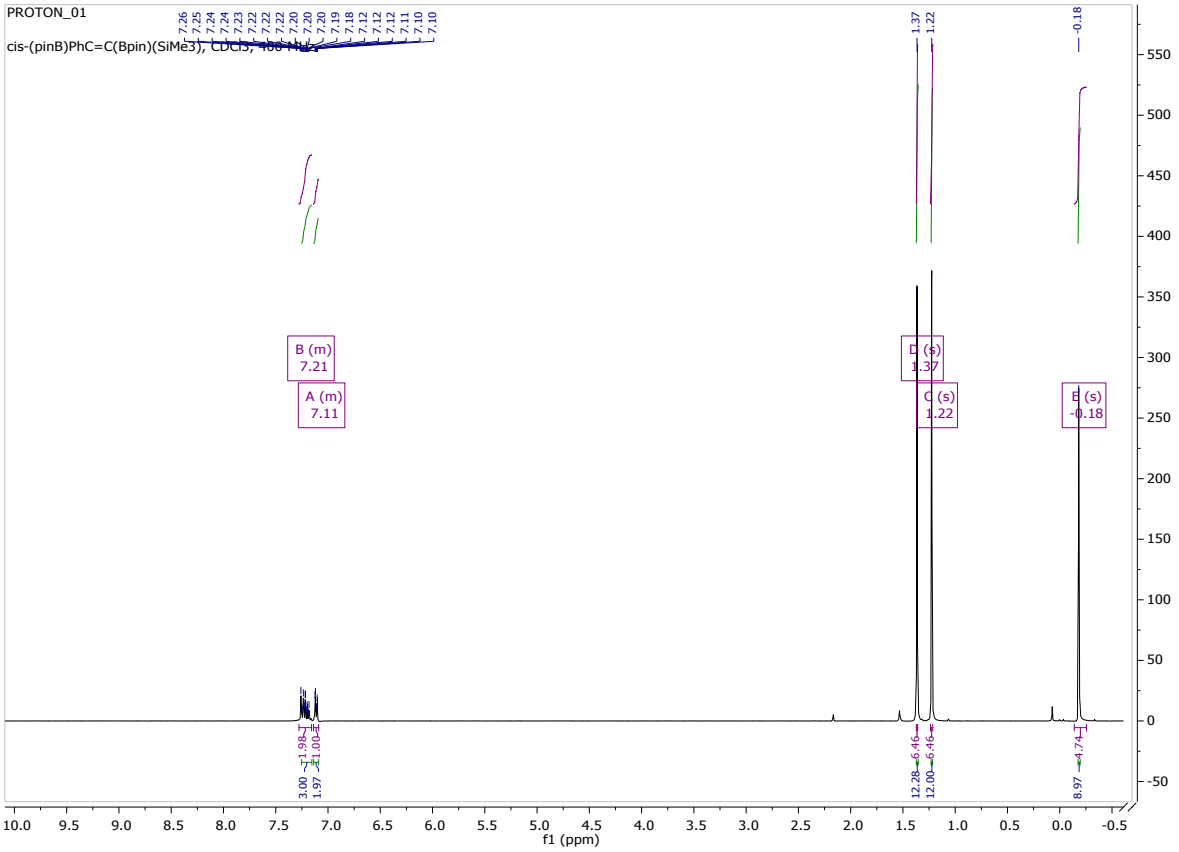

CARBON_01
syn-Ph(pinB)C=C(Bpin)NA, CDCl3, 400 MHz
141.62
140.10
133.34
132.16
128.33
128.06
127.39
126.88
126.57
126.30
126.02
125.44
125.35
125.11
84.26
84.17
25.28
24.93
24.86
24.81
f1 (ppm)

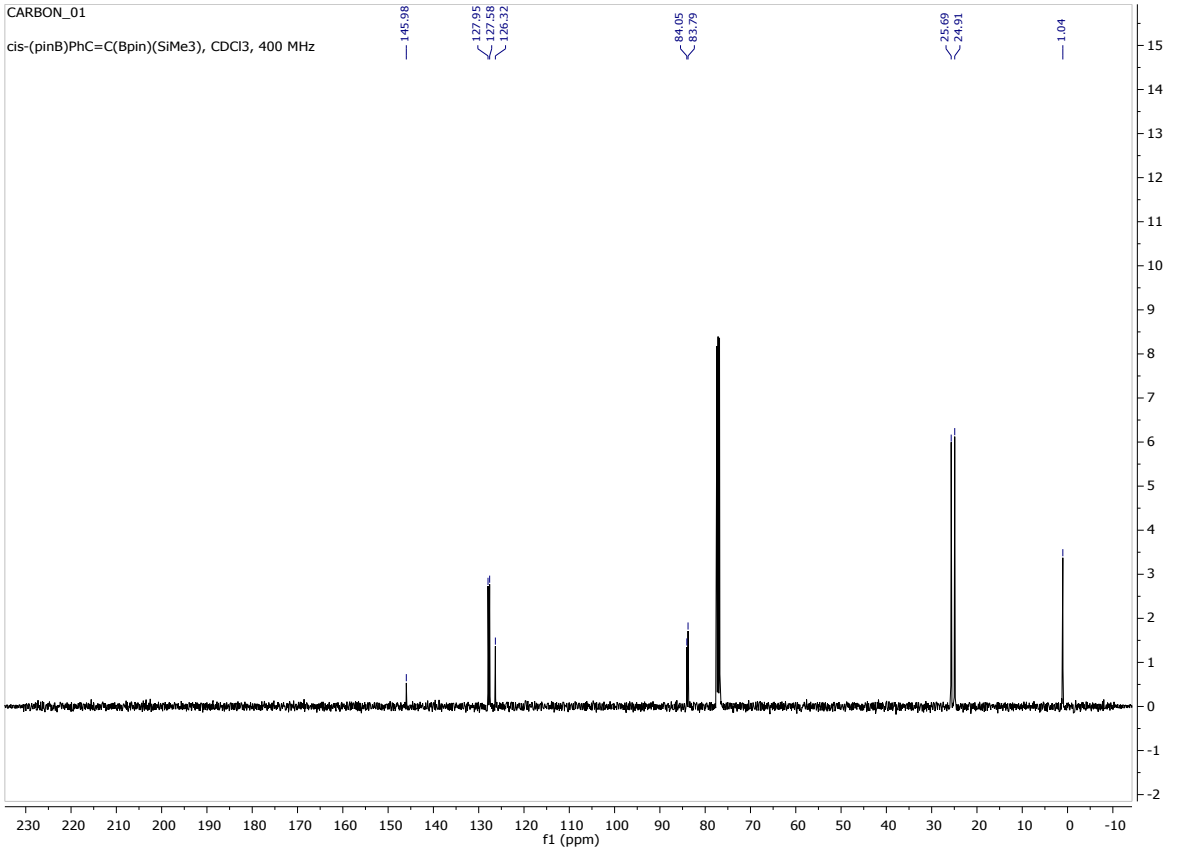

Boron11_01
STANDARD CARBON PARAMETERS
30.71
f1 (ppm)

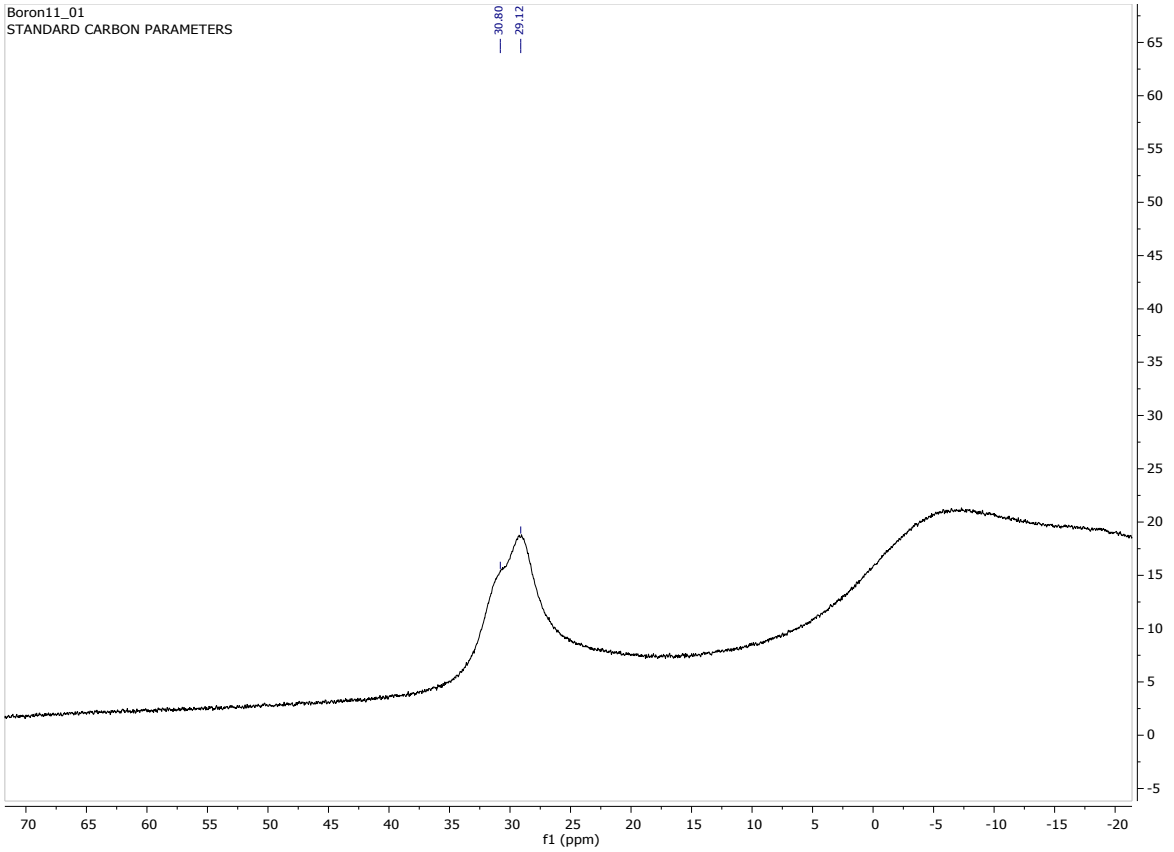


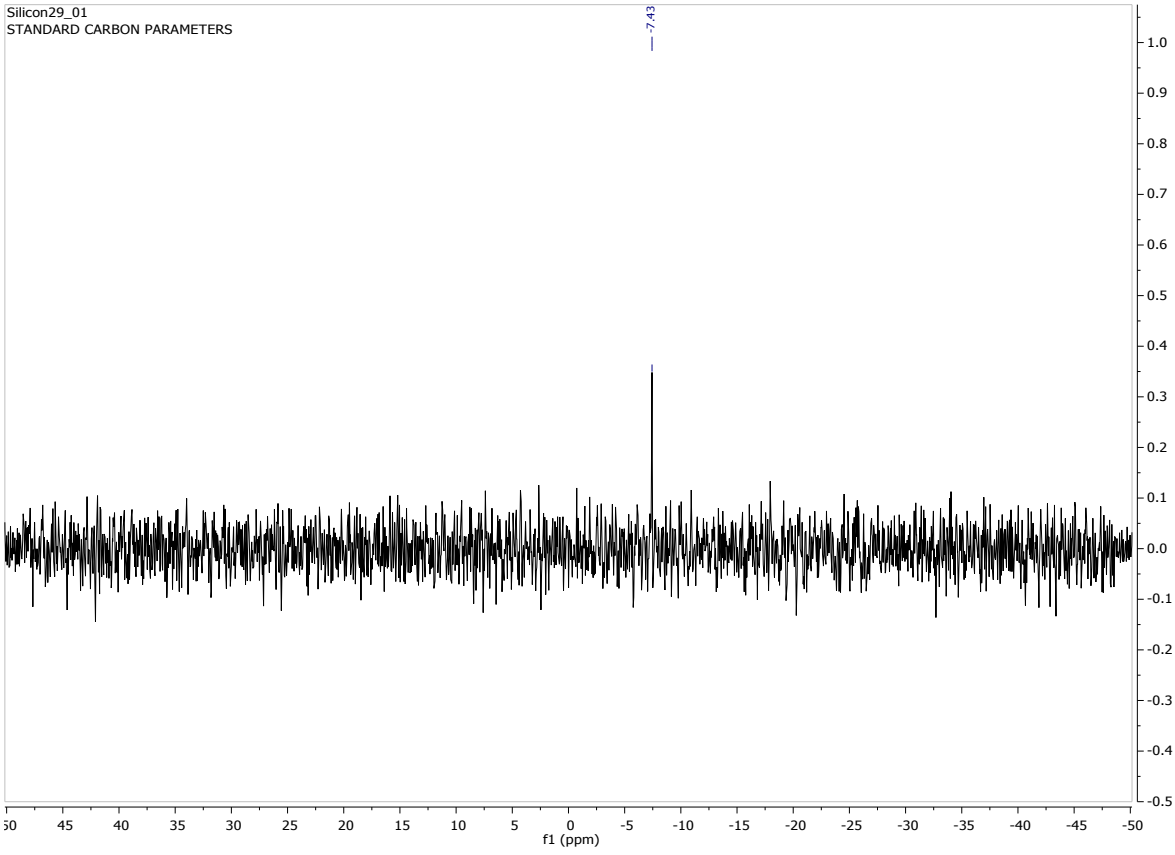
(Z)-trimethyl(2-phenyl-1,2-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)silane (14)


pinB
Bpin
SiMe3

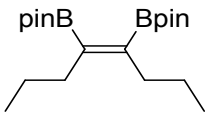

PROTON_01
cis-(pinB)PhC=C(Bpin)(SiMe3), CDCl3, 400 MHz
B (m)
7.21
A (m)
7.11
D (s)
1.37
C (s)
1.22
E (s)
-0.18
f1 (ppm)

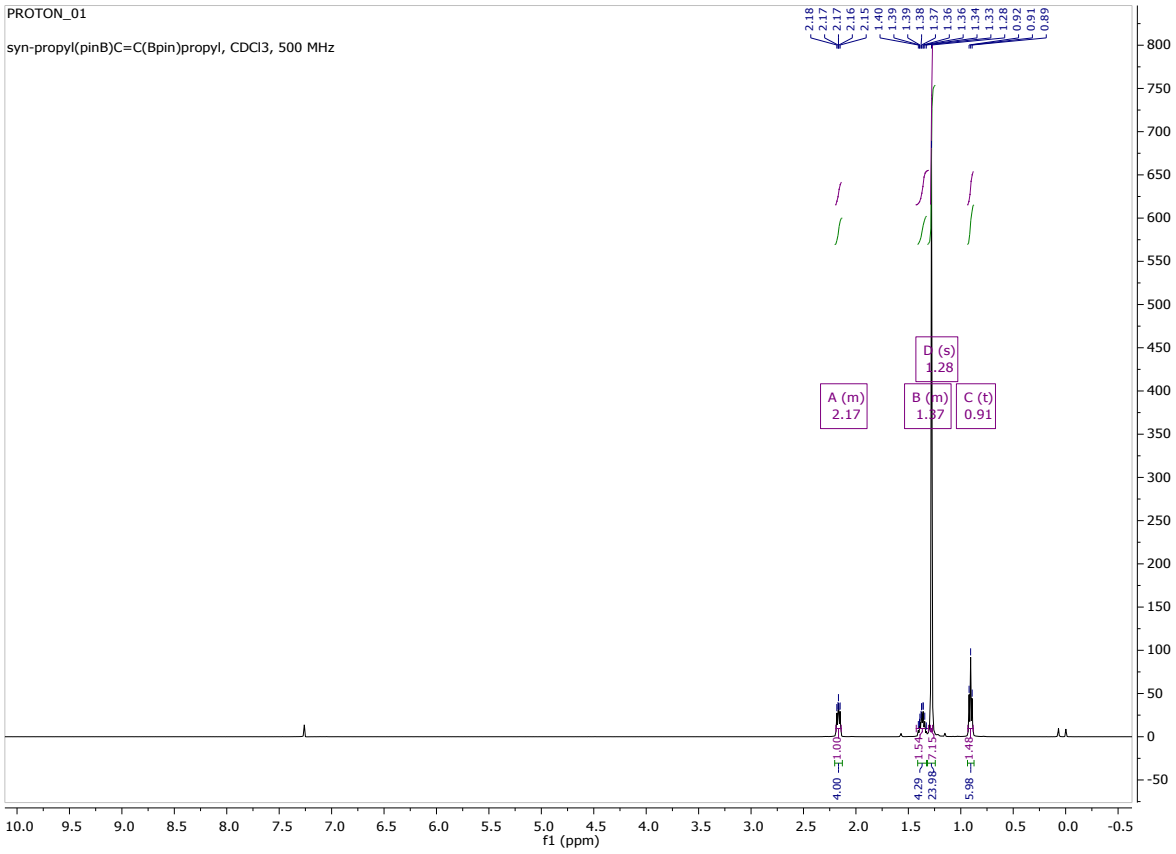

CARBON_01
cis-(pinB)PhC=C(Bpin)(SiMe3), CDCl3, 400 MHz
145.98
127.95
127.58
126.32
84.05
83.79
25.69
24.91
1.04
f1 (ppm)

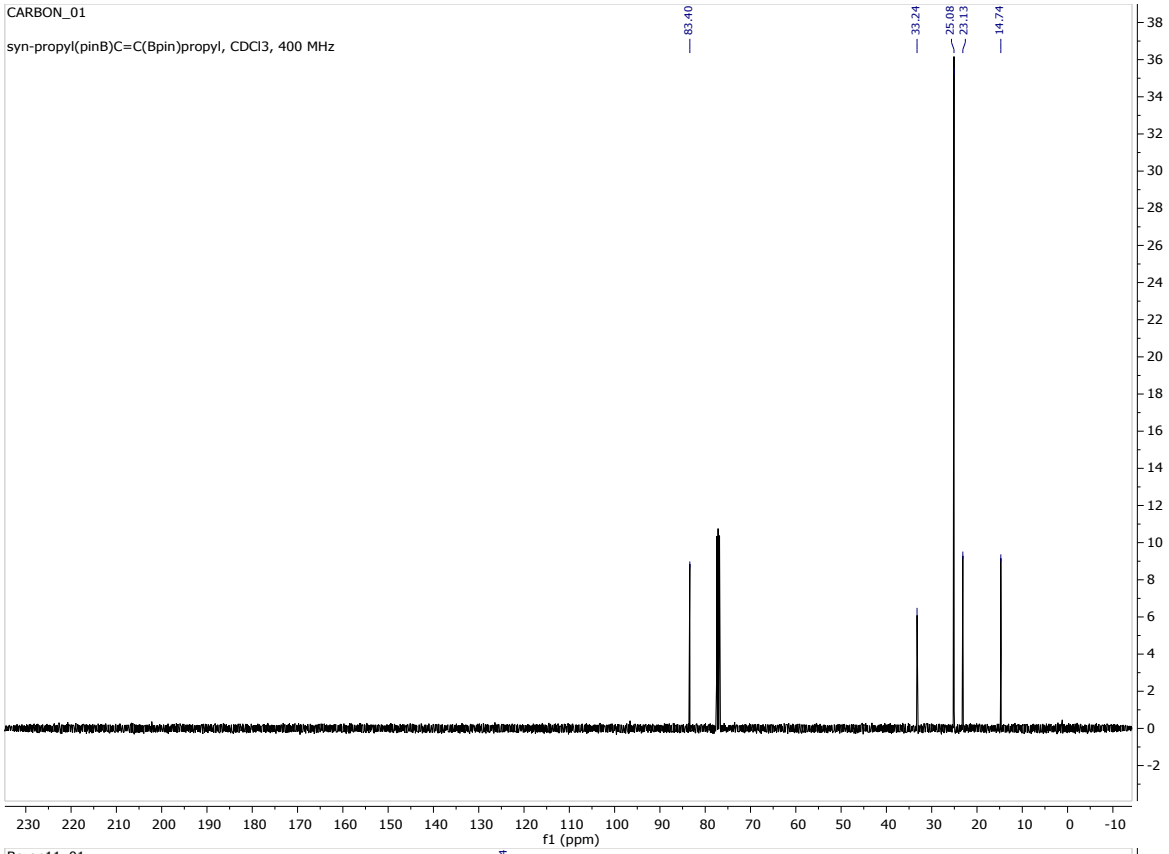

Boron11_01
STANDARD CARBON PARAMETERS
30.80
29.12
f1 (ppm)

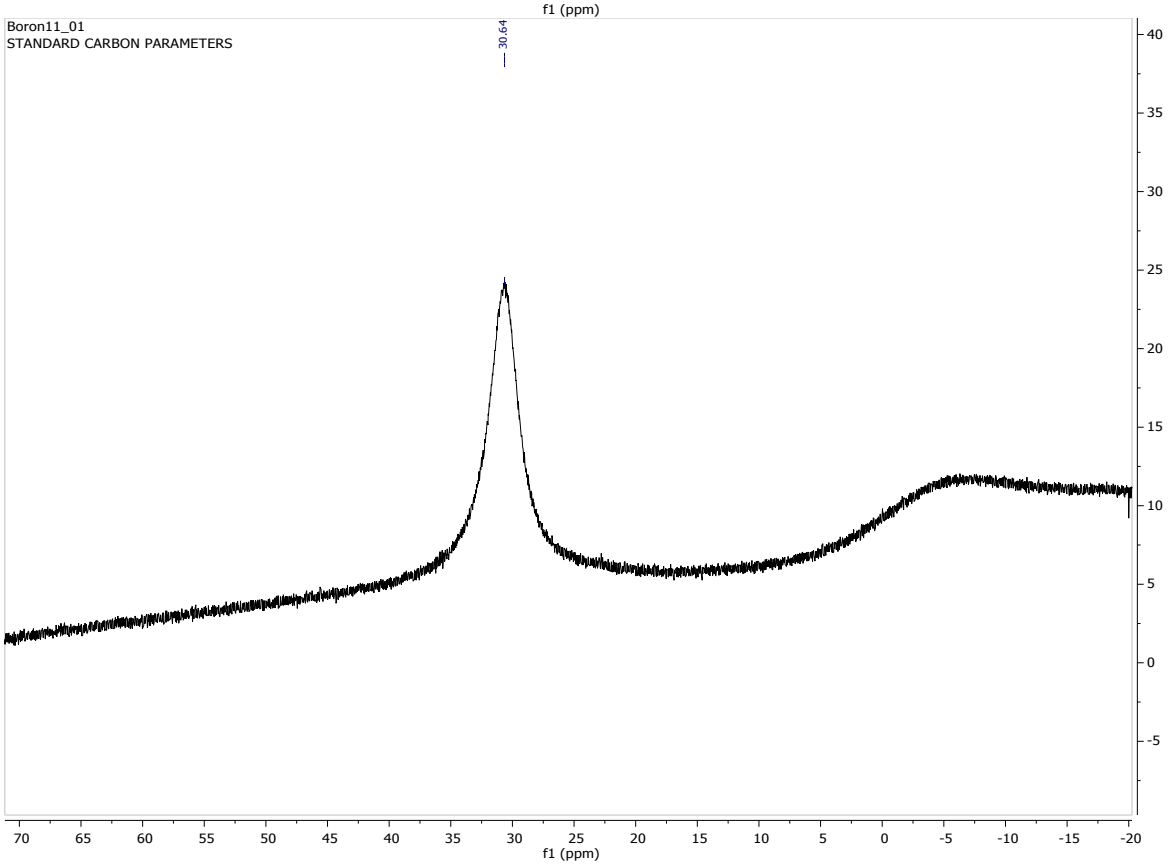

Silicon29_01
STANDARD CARBON PARAMETERS
-7.43
f1 (ppm)

(Z)-2,2'-(oct-4-ene-4,5-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (15)






CARBON_01
syn-propyl(pinB)C=C(Bpin)propyl, CDCl3, 400 MHz
83.40
33.24
25.08
23.13
14.74
f1 (ppm)


Boron11_01
STANDARD CARBON PARAMETERS
30.64
f1 (ppm)

DFT CALCULATIONS

Methods. Calculations were based on the Density Functional Theory (DFT) using Gaussian 09 suite of programs (revision D1).[1] Reactants, products, transition states and intermediates were fully optimized in the gas phase with the local functional exchange-correlation M06-L, suitable for description on thermochemical kinetics of organometallic compounds.[2] The standard 6-31G(d,p) basis set was adopted for lighter atoms, while the basis set with effective core potential SDD[3] (ECP-SDD) was used for the palladium atom (Pd).These basis set approaches are referred to as 6-31G(d,p) SDD(Pd). Frequencies calculations were also performed at the M06-L/BSI level of theory in order to verify the nature of transition states and minima along the reaction mechanism. The Intrinsic Reaction Coordinate (IRC)[4] method was also used to further authentic the transition states at the same level of theory. Solvent effects were introduced through the SMD[5] continuum solvation method by single-point calculations at geometries optimized on the gas phase using the method M06-L/BSI.[6] To refine the energetic results, the SMD single-points were performed using the Ahlrichs *et al.*[7] quadruple-ζ (def2-QZVP) basis set combined with ECP-SDD for Pd and the 6-311++G(2d,p) basis set for the remaining atoms (BSII). All quoted free energies (298,15 K) in the benzene (ε = 2.2706) solution were calculated through the SMD method by single-point calculations at the M06/BSII level on the optimized geometries in the gas phase obtained at M06-L/BSI level of theory. Analogously, Boeser et al. performed the same combination of M06 suite density functional in order to investigate the mechanism of palladium-catalyzed addition reaction of arylboronic acids to enone substrates.[8]

Results. Initially, the geometry of **1** was optimized at M06-L/BSI level of theory and compared to X-ray diffraction data [9] The optimized Pd-alkyne bond lengths Pd-C1 and Pd-C6 are longer, around 0.01 Å, than the results obtained by X-ray data. Both bond angles C6-C1-C5 and C1-C6-C25 are equal to 147.1°, in excellent agreement with the experimental values of 147.5(3)° and 146.03(3)°, respectively (Figure S1).

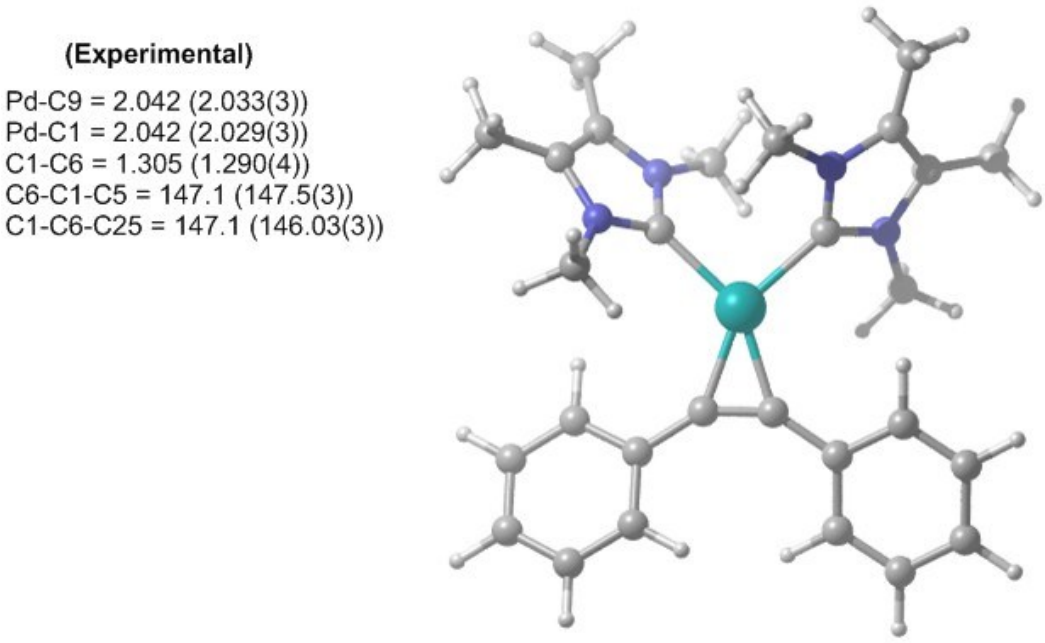


Figure S1. The optimized structure of **1** at M06-L/BSI level of theory. A comparison of theoretically and experimentally calculated bond lengths (Å).

The oxidative addition of bis(pinacolato)diboron to **1** begins with the dissociation of the alkyne from the η^2-complex, resulting in the formation the 14 electron complex **I1**. (Figure 2) This dissociation is favorable at 6.4 and 3.5 kcal·mol^{-1} for the NHC and PMe_3 complexes, respectively. The reaction continues through the incorporation of bis(pinacolato)diboron in the coordination sphere of **I1**, achieving the intermediate **I2**. The transition state **TSOA1** represents the step where the B-B bond is cleaved with

concomitant formation of two σ Pd-B bonds. This process has a free energy activation barrier relative to the separated reactants at $\Delta G^{\ddagger}$ = 9.7 kcalmol^{-1} for the NHC and 11.1 kcalmol^{-1} for the PMe_3 bis-ligand complexes. These reaction barrier weights suggest that the oxidative addition for the phosphines is kinetically less favored than with NHC ligands. Bis(boryl)palladium(II) complex (**I3)** is the product of the oxidative reaction step for both systems, and, energetically, is 8.7 kcalmol^{-1} and 6.5 kcal.mol^{-1} above the reactants with NHC and PMe_3 ligands, respectively. Alternatively, the oxidative addition step could proceed through the mono-ligand complexes as depicted in Figure S2.

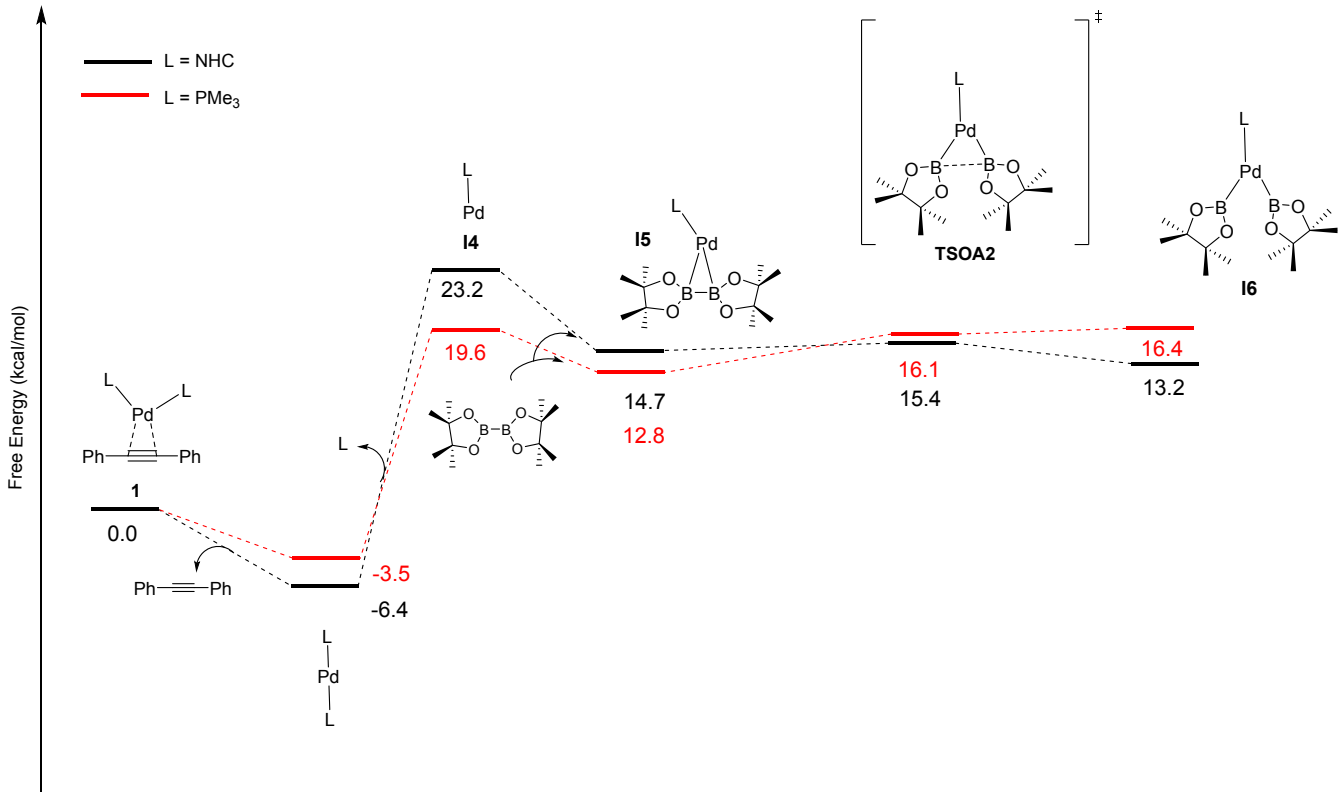
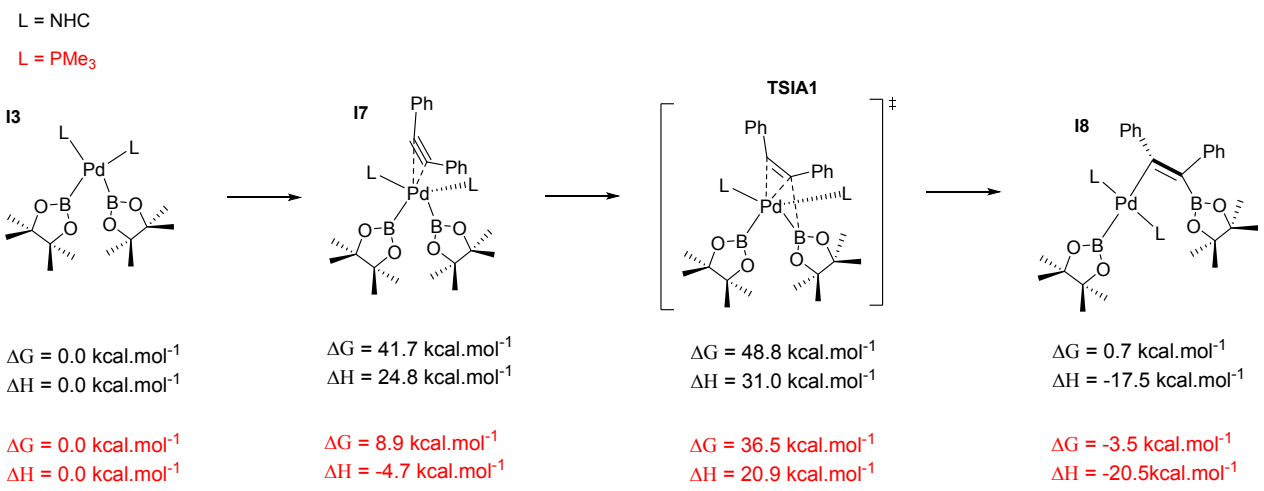


Figure S2. Free energy profile (in kcal mol^{-1}) for the oxidative addition pathways with mono-ligand pathways. Free energies in kcal•mol^{-1} at 298.15K

The next step is the alkyne insertion on the metal center. The first proposal is that the insertion of alkyne occurs directly to the bis(bory)palladium(II) complex **I3** (Scheme S1)**.** The 18-electron alkyne-palladium(II) complex **I7** is formed with a nearly square based pyramidal geometry for NHC ligand. This penta-coordinate configuration provides instability for the intermediate **I7** leading to large free energy compared to the complex **I3** (41.7 kcal·mol^{-1} for the NHC ligands). When L = PMe_3 is not observed the coordination of the alkyne to the Pd center to form the complex **I7**. This result was confirmed by Intrinsic Reaction Coordinate (IRC) calculations from **TSIA1** (see Figure S3). The complex **I7** follows the 18-electron rule, thus it was expected a more stable complex with the presence of an alkyne. However, the steric repulsion among the ligands and the entropic penalty contributed to an increase in the instability of complex **I7**. Enthalpies in solution energies were also taken in account in order to examine the impact of the entropic contribution on the energy barriers. In the sequence, the product of the alkyne insertion can be obtained through the penta-coordinate transition state **TSIA1** to form the complex **I8.** The migratory insertion of alkyne to Pd-B bond occurs by a free activation energy at $\Delta G^{\ddagger}$ = 48.8 kcal mol^{-1} for L = NHC and at $\Delta G^{\ddagger}$ = 36.5 kcal mol^{-1} for L = PMe_3 Palladium(II) complex **I8** returns to a square planar, 16-electron configuration, decreasing the free energy by *ca*. 48 kcalmol^{-1} for NHC and 39 kcalmol^{-1} for PMe_3 systems. Even though the phosphine ligands are favored in this reaction pathway, both routes have high free energy activation barriers relative to separate reactants. Another possibility for the insertion of the alkyne proceeds via a dissociate pathway. Kinect results on Pt(0)-catalyzed diboration reactions with phosphine ligands suggested that the alkyne insertion occurs from the three-coordinate species in the oxidative addition. Following this, it is a reasonable assumption that the dissociation of one L takes place from complex **I3** to generate the mono(boryl)palladium(II) complex **I6.** See Figure S4 for the overall catalytic cycle.



Scheme S1 . Associative pathway for the alkyne insertion (relative free energies and enthalpies in kcalmol^{-1}).

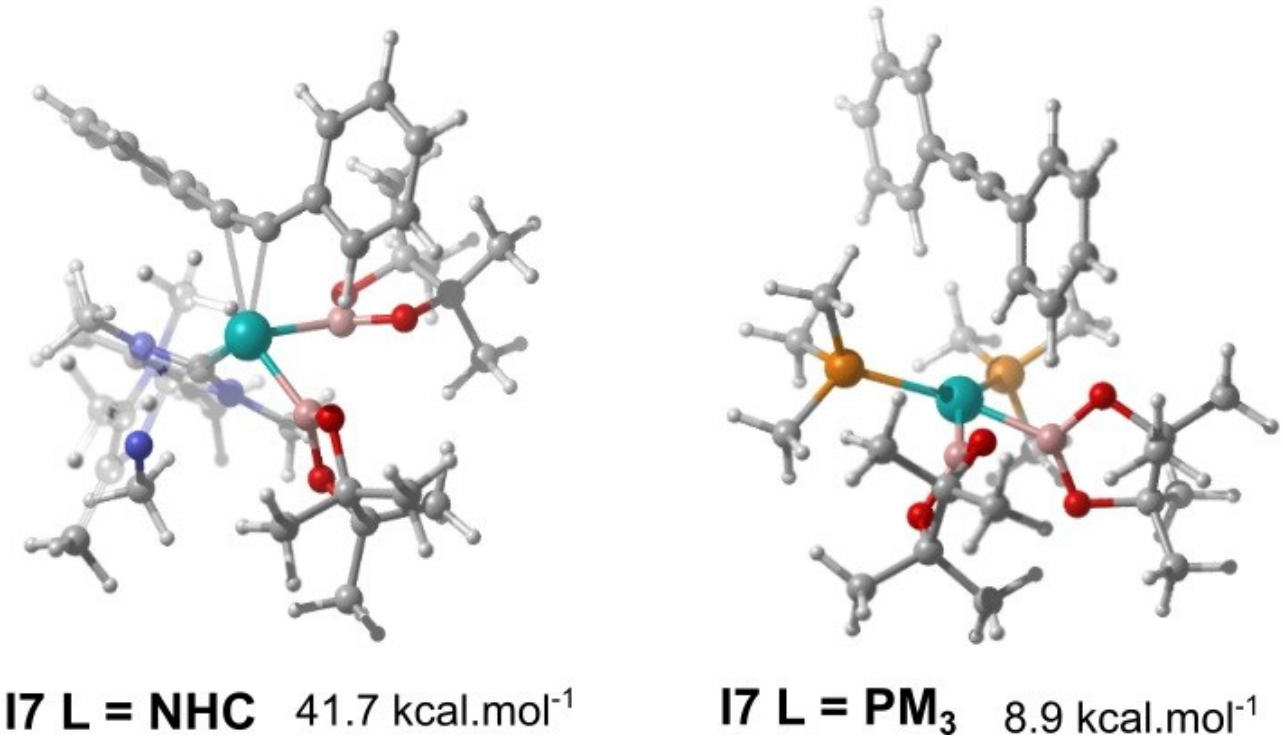


Figure S3. Optimized structure of the intermediate **I7** with L = NHC (left) and L = PM_3 (right). The stationary points were confirmed by IRC[4] calculations from TSIA1. Free energies in kcal•mol^{-1} at 298.15K.

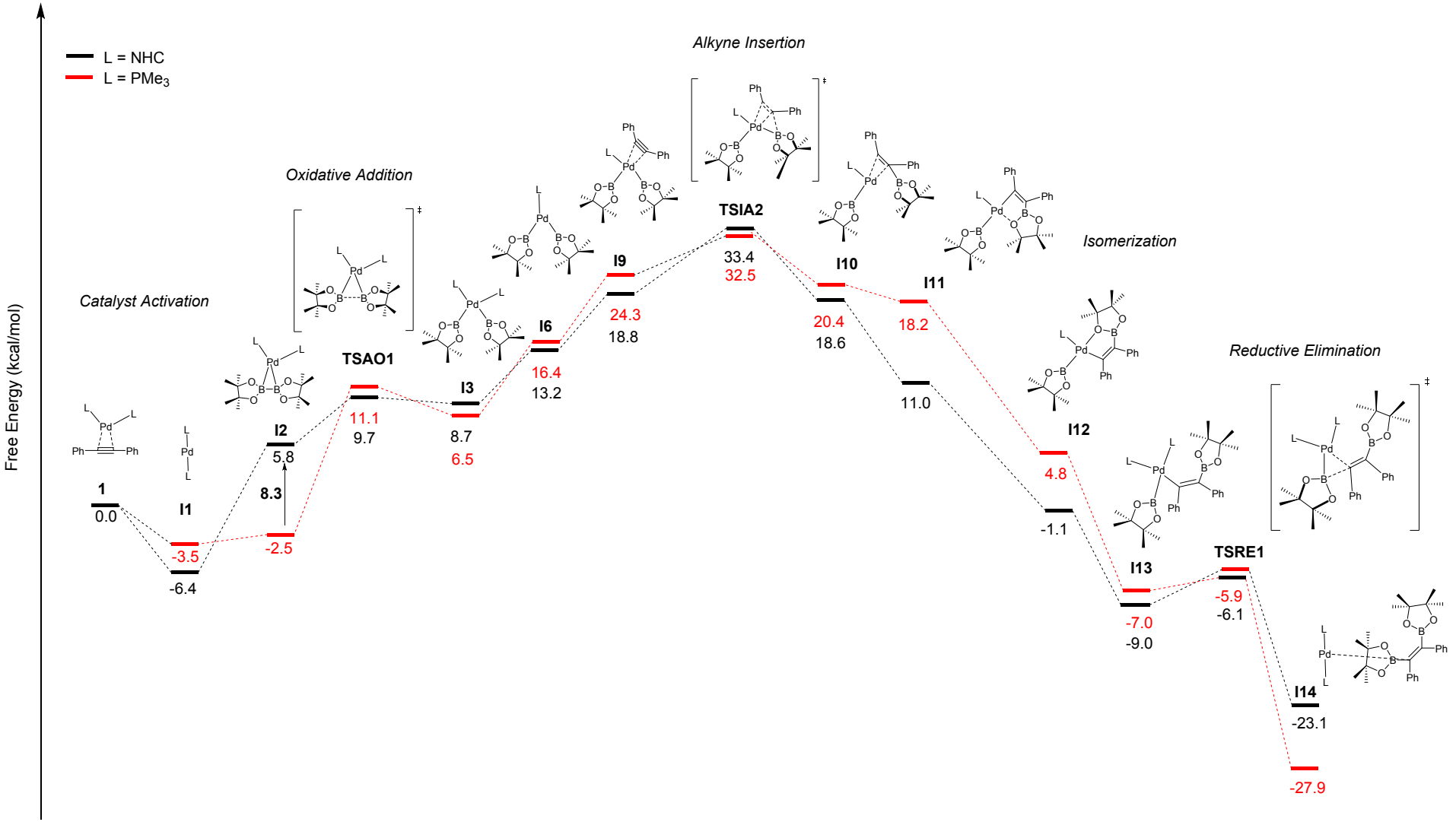


Figure S4. Free energy profile of the overall catalytic cycle for Pd(0)-catalyzed diboration of alkyne supported by NHC ligand. All free energies are given in kcal•mol^{-1} at 298.15 K and relative to separate reactants.

The insertion step itself begins with the formation of the η^2-alkyne complex **I9** for both systems, NHC and PMe_3 ligands. The free energy activation barrier of the migratory insertion of alkyne is estimated at $\Delta G^{\ddagger}$ = 33.4 kcalmol^{-1} for NHC and $\Delta G^{\ddagger}$ = 32.5 kcalmol^{-1} for the PMe_3 ligands (Figure S4). The transition state **TSIA2** is associated to the migratory insertion of alkyne with one ligand attached on metal center. The alkyne triple bond and the Pd-B bonds are broken forming a new C-B bond in the intermediate **I10**. The 14-electron palladium(II) complex **I10** has a vacant site that can interact with an oxygen atom, allowing the Bpin group to rotate around the B-C bond. The coordination of the oxygen in the ligand contributes to the stabilization of the positive cen tral palladium(II) in **I11**. The intermediate **I11** is stabilized by $\Delta\Delta G$ = 7.6 kcalmol^{-1} for the NHC and $\Delta\Delta G$ = 2.2 kcalmol^{-1} for PMe_3 systems, compared to **I10**. Complex **I11** has a nearly planar structure in relation to the metal center, with the pinacolato and the allyl ligands in a *trans* orientation. However, a *cis* orientation between these two ligands is necessary in order to allow the reductive elimination step, and therefore a *cis*-*trans* isomerization process involving intermediates **I11** and **I12** should occur. One could assume that the isomerization process would take place through a tetrahedral transition state although we were unable to find the transition state corresponding to this *cis*-*trans* isomerization. Nevertheless, it is well known that tetrahedral arrangements involving d^8 palladium(II) are usually very unstable. Probably, the planar isomerization occurs through a rotation around the Pd-B bond, similarly to that suggested by Cui and co-workers in mechanistic studies on the Pt(0)-catalyzed diboration alkyne reaction.[10b] The profile energy of the alkyne insertion pathway with a ligand attached on metal is analogous for NHC and PMe_3 systems. The results discussed so far suggest that the reductive elimination should occur from the *cis* complex **I12**. The re-coordination of other ligand is reasonable, since the 16-electron configuration is achieved forming the palladium(II) complex **I13** with a square planar geometry. The free energy barrier from **I13** is computed at $\Delta G^{\ddagger}$ = -6.1 kcal mol^{-1} for NHC and -5.9 kcal mol^{-1} for PMe_3 via transition state **TSRE1** (Figure S4). The second C-B bond is formed in complex **I14** and the 1,2-diborated product is ready to be released.

Diborations of unsaturated compounds catalyzed by transition-metal complexes play an important role in the synthesis of organoboron compounds[11-13] and density Functional Theory (DFT) has been used with success for the description of these reaction mechanisms. Several examples recently reported in the literature shown free energy barriers above 20 kcal.mol^{-1}. Nagashima et al.[14] studied a trans-diboration of alkynes by designing a pseudo-intramolecular reaction. Using an anionic strategy, the activation barrier of the addition of boryl anion was significantly lowered comparing to other approach (23.2 kcal/mol against 51.9 kcal/mol). Liu et al.[15] detailed the mechanism for the Pt diimine catalyzed diboration of acyclic α,β-unsaturated carbonyl compounds. The oxidative addition step in such reaction has energy barriers of approximately 25.0 kcal/mol. For the insertion step, barriers from 24.4 kcal/mol to 38.3 kcal/mol were observed depending on the studied pathway. Xie et al.[16] elucidate the mechanisms for the Ni- and Pd- catalyzed cycloaddition of anhydride to alkyne using phosphines as ligands. The most favorable pathway for the addition and decarboxylation steps catalyzed by Pd presented barriers equal 28.6 and 21.7 kcal/mol, respectively. In summary, the results reported in the present work have shown to be in agreement with many other analogous studies reported recently.

CARTESIAN COORDINATES, IMAGINARY FREQUENCIES, SCF ENERGIES, ENTALPHIES AND FREE ENERGIES (AT 298.15 K AND 1 ATM) FOR THE REACTANTS, PRODUCTS, INTERMEDIATES AND TRANSITION STATES.

(Imaginary frequencies for the transition states at M06-L/BS1 level of theory).

Bpin

M06-L/BSI SCF energy in gas: -822.460971 a.u.

M06/BSII SCF energy in benzene: -822.2648766 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -821.945549 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -821.879960 a.u.

B	0.842953000	-0.001068000	-0.000060000
B	-0.842971000	-0.001062000	-0.000033000
O	-1.605018000	-1.108113000	0.290439000
O	-1.603870000	1.106821000	-0.290560000
O	1.605026000	-1.108100000	-0.290539000
O	1.603831000	1.106827000	0.290487000
C	-2.980136000	-0.656704000	0.419570000
C	-2.979464000	0.656860000	-0.419674000
C	2.980155000	-0.656716000	-0.419538000
C	2.979421000	0.656887000	0.419654000
C	-3.897867000	-1.746004000	-0.096143000
H	-3.813230000	-2.634486000	0.534870000
H	-4.942458000	-1.416603000	-0.074646000
H	-3.647706000	-2.034755000	-1.118570000

C	-3.221923000	-0.412469000	1.902467000
H	-2.997811000	-1.325671000	2.459214000
H	-2.573272000	0.382458000	2.282231000
H	-4.261076000	-0.134018000	2.102853000
C	-3.896090000	1.747073000	0.096072000
H	-3.810547000	2.635455000	-0.534951000
H	-4.941019000	1.418735000	0.074596000
H	-3.645611000	2.035570000	1.118490000
C	-3.221557000	0.412903000	-1.902581000
H	-4.261000000	0.135539000	-2.102962000
H	-2.996488000	1.325876000	-2.459316000
H	-2.573742000	-0.382689000	-2.282371000
C	3.896047000	1.747110000	-0.096114000
H	3.810502000	2.635529000	0.534863000
H	4.940981000	1.418795000	-0.074641000
H	3.645556000	2.035562000	-1.118541000
C	3.221473000	0.413013000	1.902578000
H	2.573703000	-0.382598000	2.282395000
H	4.260933000	0.135728000	2.102997000
H	2.996341000	1.326002000	2.459256000
C	3.222124000	-0.412578000	-1.902425000
H	2.573564000	0.382366000	-2.282310000
H	4.261319000	-0.134212000	-2.102718000
H	2.998008000	-1.325808000	-2.459121000
C	3.897841000	-1.746002000	0.096334000

H	3.647554000	-2.034699000	1.118744000
H	3.813245000	-2.634506000	-0.534649000
H	4.942447000	-1.416630000	0.074949000

Alkyne

M06-L/BSI SCF energy in gas: -539.400743 a.u.

M06/BSII SCF energy in benzene: -539.183729 a.u.

M06/BSII//M06-L/BSI free energy in benzene:: -539.032244 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -538.981251 a.u.

C	-0.609530000	-0.042546000	-0.002798000
C	0.609592000	-0.046871000	0.003104000
C	2.026320000	-0.025302000	0.002877000
C	2.769642000	-1.220064000	-0.000112000
H	2.241278000	-2.169009000	-0.000702000
H	4.718148000	-2.114927000	-0.005965000
C	4.157275000	-1.184381000	-0.003030000
H	5.916791000	0.059128000	-0.005457000
C	4.830818000	0.035601000	-0.002622000
H	4.625000000	2.179808000	0.001917000
C	4.105278000	1.225562000	0.001339000
C	2.717860000	1.200610000	0.004172000
H	2.147951000	2.125071000	0.006935000
H	-2.152189000	2.127608000	-0.004673000
C	-2.720167000	1.201934000	-0.002694000
C	-2.026257000	-0.022626000	-0.000755000
C	-2.767284000	-1.218842000	0.001530000

H	-2.236916000	-2.166674000	0.002773000
C	-4.154953000	-1.185867000	0.002045000
H	-4.713971000	-2.117526000	0.003760000
C	-4.830891000	0.032801000	0.000036000
H	-5.916917000	0.054180000	0.000106000
C	-4.107679000	1.224157000	-0.002221000
H	-4.629319000	2.177345000	-0.003923000

***Syn*-1,2-diborated product**

M06-L/BSI SCF energy in gas: -1361.946540 a.u.

M06/BSII SCF energy in benzene: -1361.521093 a.u.

M06/BSII//M06-L/BSI free energy in benzene:: -1361.02093 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1360.92932 a.u.

B	0.001369000	1.678322000	-0.059342000
B	-0.788109000	-1.167263000	-0.076404000
O	0.180959000	2.969799000	0.373713000
O	-1.289245000	1.432057000	-0.485081000
O	-1.392791000	-1.773785000	-1.150652000
O	-1.542132000	-1.222487000	1.074056000
C	1.104586000	0.590970000	-0.074547000
C	0.714120000	-0.716414000	-0.087888000
C	-1.026005000	3.699475000	0.038610000
C	-2.089875000	2.562590000	-0.043279000
C	-2.740488000	-2.120071000	-0.736491000
C	-2.601888000	-2.180715000	0.816229000
C	1.645375000	-1.867345000	0.014472000

C	1.429142000	-3.024343000	-0.753173000
C	2.714999000	-1.871415000	0.925794000
H	0.597218000	-3.044817000	-1.452785000
H	2.884848000	-0.995098000	1.545264000
C	2.271945000	-4.125784000	-0.640146000
C	3.544958000	-2.977559000	1.047308000
H	2.094084000	-5.003543000	-1.256293000
H	4.362580000	-2.958264000	1.763208000
C	3.332315000	-4.108854000	0.260488000
H	3.985618000	-4.971992000	0.355213000
C	2.521736000	1.023151000	-0.115520000
C	3.411705000	0.492247000	-1.061224000
C	3.002534000	1.999922000	0.768424000
H	3.048773000	-0.256241000	-1.761768000
H	2.322628000	2.437389000	1.493482000
C	4.736784000	0.906582000	-1.108824000
C	4.333246000	2.404553000	0.729731000
H	5.406801000	0.483328000	-1.852687000
H	4.688211000	3.152741000	1.434045000
C	5.206614000	1.860550000	-0.207822000
H	6.244171000	2.181620000	-0.241618000
C	-3.121082000	-3.431826000	-1.392497000
H	-3.186726000	-3.303775000	-2.476157000
H	-2.383950000	-4.211634000	-1.189010000
H	-4.097376000	-3.777679000	-1.035466000

C	-3.648951000	-0.995303000	-1.203855000
H	-3.373684000	-0.057772000	-0.714477000
H	-3.529095000	-0.855937000	-2.281208000
H	-4.701519000	-1.211609000	-0.995614000
C	-2.092421000	-3.528266000	1.308636000
H	-2.849318000	-4.311822000	1.206161000
H	-1.198734000	-3.835100000	0.755395000
H	-1.820274000	-3.447332000	2.363828000
C	-3.840114000	-1.765783000	1.583108000
H	-3.638744000	-1.786121000	2.657306000
H	-4.162609000	-0.756669000	1.318054000
H	-4.668720000	-2.453584000	1.382277000
C	-3.194540000	2.821202000	-1.047298000
H	-3.705051000	3.763121000	-0.817986000
H	-2.806337000	2.877799000	-2.065865000
H	-3.942274000	2.024482000	-1.013638000
C	-2.667034000	2.187922000	1.313514000
H	-3.222639000	1.250616000	1.219705000
H	-1.876306000	2.026264000	2.052096000
H	-3.346520000	2.958276000	1.690975000
C	-0.775214000	4.371759000	-1.303932000
H	-1.614162000	5.008291000	-1.600939000
H	0.119979000	4.993873000	-1.232516000
H	-0.609405000	3.630433000	-2.090896000
C	-1.287285000	4.732593000	1.114873000

H	-1.315667000	4.281143000	2.108489000
H	-0.496948000	5.487491000	1.108659000
H	-2.240440000	5.243141000	0.939074000

L = NHC

1

M06-L/BSI SCF energy in gas: -1434.30308 a.u.

M06/BSII SCF energy in benzene: -1433.779393 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1433.287460 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1433.181866 a.u.

H	-4.922992000	-5.155982000	0.386025000
C	-4.344380000	-4.238144000	0.324551000
H	-5.983429000	-3.063958000	-0.435296000
C	-4.938418000	-3.062267000	-0.134629000
C	-4.204176000	-1.886206000	-0.208792000
H	-4.666287000	-0.972359000	-0.576266000
C	-2.845453000	-1.853499000	0.166614000
C	-2.261235000	-3.053150000	0.615068000
C	-3.001389000	-4.225139000	0.700203000
H	-2.530393000	-5.137422000	1.060155000
H	-1.210289000	-3.028495000	0.900790000
C	-2.064817000	-0.648130000	0.075536000
C	-2.064709000	0.648446000	-0.075169000
C	-2.845137000	1.853931000	-0.166485000
H	-4.666267000	0.973142000	0.576089000
C	-4.203937000	1.886882000	0.208627000

C	-4.937983000	3.063047000	0.134175000
H	-5.983059000	3.064930000	0.434612000
C	-4.343666000	4.238784000	-0.325003000
H	-4.922129000	5.156700000	-0.386710000
C	-3.000594000	4.225538000	-0.700355000
H	-2.529380000	5.137711000	-1.060301000
C	-2.260638000	3.053446000	-0.614931000
Pd	-0.130418000	0.000012000	0.000315000
C	1.297639000	-1.548966000	0.140854000
N	2.419328000	-1.629942000	0.921756000
H	3.018011000	-1.119139000	2.865079000
N	1.397822000	-2.670108000	-0.638062000
C	0.421572000	-3.019716000	-1.644629000
H	0.004047000	-4.014091000	-1.457350000
H	-0.380171000	-2.277803000	-1.592276000
H	0.867125000	-3.005250000	-2.645422000
H	2.098410000	-5.439297000	-0.926970000
C	2.868833000	-4.672491000	-1.069952000
C	2.542042000	-3.414248000	-0.362875000
H	3.812062000	-5.084655000	-0.703746000
H	2.971859000	-4.525477000	-2.151684000
C	3.194967000	-2.750829000	0.632443000
C	4.451952000	-3.065821000	1.347398000
H	4.289546000	-3.231850000	2.419375000
H	4.903887000	-3.974900000	0.943455000

H	5.193851000	-2.262962000	1.259869000
H	1.892979000	-0.006492000	-2.051063000
C	2.763049000	0.639663000	-1.914864000
H	3.613519000	0.025398000	-1.591598000
H	3.017506000	1.118379000	-2.865146000
N	2.419325000	1.629460000	-0.921752000
C	1.297889000	1.548706000	-0.140449000
C	2.763489000	-0.640302000	1.914873000
H	3.614046000	-0.026224000	1.591482000
H	0.868249000	3.004940000	2.645791000
C	0.422532000	3.019787000	1.645076000
H	-0.379533000	2.278219000	1.592734000
H	0.005411000	4.014378000	1.458059000
N	1.398441000	2.669954000	0.638259000
C	2.542648000	3.413938000	0.362586000
H	2.972957000	4.525396000	2.151122000
C	2.869772000	4.672248000	1.069384000
H	3.813004000	5.084200000	0.702947000
H	2.099451000	5.439159000	0.926406000
C	3.195168000	2.750309000	-0.632858000
C	4.451942000	3.065112000	-1.348270000
H	5.193744000	2.262132000	-1.261026000
H	4.289179000	3.231198000	-2.420185000
H	4.904167000	3.974109000	-0.944465000
H	-1.209632000	3.028601000	-0.900420000

H	1.893603000	0.006058000	2.051280000

1_alkyne

M06-L/BSI SCF energy in gas: -1050.855299 a.u.

M06/BSII SCF energy in benzene: -1050.477534 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1050.158931 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1050.07639 a.u.

Pd	1.523782000	-0.712015000	-0.515703000
B	1.582567000	1.156795000	0.357593000
B	-2.789262000	0.054854000	0.412230000
O	1.606558000	1.434490000	1.726531000
O	2.002432000	2.264537000	-0.371783000
O	-3.547354000	-0.591759000	-0.538990000
O	-3.549341000	0.823437000	1.264012000
C	-0.306733000	0.390867000	-0.224396000
C	-1.250878000	-0.195008000	0.580296000
C	2.243824000	2.717603000	1.916857000
C	2.053835000	3.399323000	0.525003000
C	-4.902944000	-0.083697000	-0.443828000
C	-4.942163000	0.522342000	1.000330000
C	-0.941992000	-1.281673000	1.537259000
C	0.261473000	-1.369691000	2.264545000
C	-1.883368000	-2.311605000	1.729129000
H	0.988852000	-0.569769000	2.184731000
H	-2.815736000	-2.286009000	1.165830000
C	0.507654000	-2.439608000	3.116916000

C	-1.634162000	-3.384827000	2.580569000
H	1.440638000	-2.469899000	3.676023000
H	-2.381414000	-4.166399000	2.693810000
C	-0.432540000	-3.457782000	3.278790000
H	-0.233762000	-4.290797000	3.947898000
C	-0.733216000	1.354912000	-1.260520000
C	-1.728569000	2.324113000	-1.049245000
C	-0.103745000	1.341002000	-2.517765000
H	-2.191509000	2.408055000	-0.067644000
H	0.705014000	0.624273000	-2.672175000
C	-2.097021000	3.212622000	-2.055920000
C	-0.479976000	2.215111000	-3.528001000
H	-2.863265000	3.959440000	-1.857345000
H	0.020341000	2.172241000	-4.492529000
C	-1.482298000	3.159169000	-3.303597000
H	-1.767535000	3.855499000	-4.087751000
C	-5.860493000	-1.237071000	-0.671164000
H	-5.751386000	-1.614969000	-1.691155000
H	-5.669830000	-2.063314000	0.017160000
H	-6.898777000	-0.912567000	-0.541527000
C	-5.061029000	0.958962000	-1.538674000
H	-4.366643000	1.790570000	-1.396717000
H	-4.831655000	0.503544000	-2.505563000
H	-6.081021000	1.354124000	-1.575076000
C	-5.376932000	-0.477098000	2.062920000

H	-6.436273000	-0.735466000	1.969057000
H	-4.789776000	-1.398746000	2.008582000
H	-5.214352000	-0.041461000	3.051733000
C	-5.743682000	1.803323000	1.123874000
H	-5.704163000	2.170682000	2.152654000
H	-5.352909000	2.586362000	0.470310000
H	-6.794797000	1.631976000	0.867097000
C	3.196274000	4.298039000	0.095260000
H	3.324672000	5.131184000	0.795365000
H	4.140280000	3.750826000	0.035445000
H	2.987660000	4.718111000	-0.892316000
C	0.727316000	4.133909000	0.406750000
H	0.538240000	4.372148000	-0.643820000
H	-0.100073000	3.508820000	0.753738000
H	0.726260000	5.063961000	0.984897000
C	3.704477000	2.453949000	2.258526000
H	4.246837000	3.379738000	2.475647000
H	3.757551000	1.813919000	3.144091000
H	4.219329000	1.940900000	1.439969000
C	1.563553000	3.430398000	3.070056000
H	0.484881000	3.497002000	2.919714000
H	1.739528000	2.887426000	4.002828000
H	1.961098000	4.444315000	3.191583000
P	0.576445000	-2.712556000	-1.524199000
C	-1.198720000	-2.639681000	-1.966643000

H	-1.382413000	-1.803456000	-2.646862000
H	-1.540461000	-3.569657000	-2.434482000
H	0.171208000	-5.080283000	-0.967466000
H	-1.794322000	-2.452500000	-1.069808000
C	0.614407000	-4.211898000	-0.466779000
H	1.645172000	-4.450532000	-0.189438000
H	0.060548000	-4.011116000	0.455624000
H	2.353353000	-3.598452000	-2.941233000
C	1.298061000	-3.353725000	-3.088818000
H	1.238968000	-2.583655000	-3.862877000
H	0.776491000	-4.249344000	-3.444512000
P	3.788665000	-1.055034000	-0.345613000
C	4.862031000	0.303443000	-0.951352000
H	4.468425000	1.262139000	-0.604358000
H	5.903171000	0.185424000	-0.631370000
H	5.708165000	-2.520884000	-0.863561000
H	4.829204000	0.324437000	-2.043821000
C	4.640098000	-2.498256000	-1.107442000
H	4.182663000	-3.428273000	-0.758551000
H	4.533631000	-2.458621000	-2.194915000
H	3.874326000	-2.154362000	1.809024000
C	4.315434000	-1.239685000	1.401957000
H	3.927596000	-0.400856000	1.986580000
H	5.404613000	-1.289764000	1.510358000

I1

M06-L/BSI SCF energy in gas: -894,868570 a.u.

M06/BSII SCF energy in benzene: -894,868570 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -894,265389 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -894,187894 a.u.

Pd	-0.000002000	0.000026000	-0.000138000
C	2.038096000	-0.000033000	-0.000138000
N	2.898258000	0.755188000	-0.755241000
H	2.790339000	2.729489000	-1.470306000
N	2.898063000	-0.755268000	0.755194000
C	2.440531000	-1.722768000	1.722734000
H	2.790882000	-1.470531000	2.729424000
H	1.345932000	-1.698868000	1.699503000
H	2.790131000	-2.729619000	1.470095000
H	5.328834000	-1.009252000	2.254795000
C	5.348769000	-1.169924000	1.169956000
C	4.233451000	-0.481960000	0.482074000
H	6.310654000	-0.803677000	0.802974000
H	5.328158000	-2.254845000	1.009956000
C	4.233583000	0.481871000	-0.481790000
C	5.349062000	1.169862000	-1.169378000
H	5.328956000	2.254686000	-1.008633000
H	6.310864000	0.802956000	-0.802837000
H	5.328847000	1.009936000	-2.254319000
H	-1.346188000	-1.699625000	-1.698887000
C	-2.440788000	-1.723730000	-1.721770000

H	-2.791593000	-1.472272000	-2.728493000
H	-2.790057000	-2.730494000	-1.468309000
N	-2.898187000	-0.755670000	-0.754721000
C	-2.038095000	0.000118000	-0.000091000
C	2.440938000	1.722577000	-1.722998000
H	2.791669000	1.470326000	-2.729548000
H	-2.790288000	2.730606000	1.468346000
C	-2.440677000	1.723927000	1.721652000
H	-1.346077000	1.700052000	1.698485000
H	-2.791065000	1.472337000	2.728490000
N	-2.898133000	0.755788000	0.754716000
C	-4.233497000	0.482251000	0.481700000
H	-5.328311000	2.255450000	1.008321000
C	-5.348880000	1.170636000	1.169053000
H	-6.310729000	0.804098000	0.802266000
H	-5.329001000	1.010699000	2.254002000
C	-4.233534000	-0.482241000	-0.481503000
C	-5.348948000	-1.170740000	-1.168691000
H	-5.328683000	-1.011521000	-2.253735000
H	-5.328795000	-2.255458000	-1.007238000
H	-6.310788000	-0.803643000	-0.802440000
H	1.346337000	1.698628000	-1.700054000

I2

M06-L/BSI SCF energy in gas: -1717.352147 a.u.

M06/BSII SCF energy in benzene: -1716.848478 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1716.191515 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1716.070986 a.u.

Pd	-0.009808000	-1.062230000	-0.003069000
C	-2.012497000	-1.543494000	-0.032519000
N	-2.782804000	-1.903403000	-1.105650000
H	-2.486539000	-2.821393000	-2.971063000
N	-2.890261000	-1.634802000	1.013166000
C	-2.513937000	-1.354471000	2.378748000
H	-2.618726000	-2.248317000	3.003188000
H	-1.471202000	-1.028075000	2.363957000
H	-3.124109000	-0.548124000	2.796507000
H	-5.062582000	-2.990583000	2.312695000
C	-5.279546000	-2.227778000	1.555364000
C	-4.156553000	-2.044634000	0.609089000
H	-6.180951000	-2.542138000	1.023814000
H	-5.521448000	-1.304414000	2.095690000
C	-4.089405000	-2.210683000	-0.743196000
C	-5.126523000	-2.587850000	-1.728290000
H	-4.868525000	-3.500332000	-2.278857000
H	-6.082320000	-2.765964000	-1.229464000
H	-5.287790000	-1.799814000	-2.474812000
H	1.171015000	-1.734125000	2.408985000
C	2.261969000	-1.798845000	2.470356000
H	2.637056000	-0.895533000	2.965150000

H	2.553458000	-2.678201000	3.051974000
N	2.755220000	-1.891503000	1.117695000
C	1.991595000	-1.547130000	0.035358000
C	-2.288913000	-1.873567000	-2.460500000
H	-2.746372000	-1.056636000	-3.029052000
H	3.117648000	-0.598456000	-2.798754000
C	2.502596000	-1.398464000	-2.375774000
H	1.461228000	-1.067124000	-2.368317000
H	2.606316000	-2.299051000	-2.990510000
N	2.871430000	-1.664979000	-1.005509000
C	4.133102000	-2.077340000	-0.589433000
H	5.505028000	-1.379259000	-2.089157000
C	5.256659000	-2.289034000	-1.529057000
H	6.155158000	-2.597085000	-0.989020000
H	5.036342000	-3.067071000	-2.269756000
C	4.060653000	-2.215435000	0.765948000
C	5.091869000	-2.582432000	1.761121000
H	5.252371000	-1.784619000	2.497198000
H	4.828519000	-3.486690000	2.322785000
H	6.049156000	-2.770907000	1.268968000
H	-1.209175000	-1.702844000	-2.401593000
O	-1.610297000	1.405026000	1.162220000
C	-2.570065000	2.427683000	0.854668000
C	-1.926805000	3.757133000	1.239815000
H	-1.643036000	3.722420000	2.294780000

H	-2.600173000	4.607256000	1.087243000
H	-1.013847000	3.927546000	0.660404000
C	-3.823119000	2.202059000	1.680461000
H	-4.242499000	1.206246000	1.514347000
H	-3.589150000	2.298176000	2.745116000
H	-4.593386000	2.943023000	1.437972000
H	-2.128182000	4.255540000	-1.309026000
C	-2.980096000	3.582890000	-1.431229000
H	-3.881805000	4.095983000	-1.077310000
H	-3.102306000	3.388858000	-2.500686000
C	-2.767872000	2.274280000	-0.689680000
C	-3.874518000	1.293321000	-1.048358000
H	-3.773468000	0.360782000	-0.490856000
H	-3.819305000	1.062604000	-2.116825000
H	-4.866063000	1.711685000	-0.841790000
O	-1.509326000	1.720462000	-1.116025000
B	-0.844285000	1.199175000	0.001165000
B	0.865540000	1.185437000	-0.011745000
O	1.631597000	1.385050000	-1.174315000
O	1.540362000	1.695096000	1.105559000
C	2.598124000	2.401319000	-0.867616000
C	2.800565000	2.242798000	0.675826000
C	3.904259000	1.255554000	1.026191000
H	3.799963000	0.327032000	0.462849000
H	3.852129000	1.017965000	2.093562000

H	4.261558000	1.172455000	-1.538600000
H	4.896710000	1.671994000	0.820049000
C	3.846715000	2.171135000	-1.699070000
H	3.608822000	2.272133000	-2.762382000
H	4.622133000	2.907004000	-1.457429000
H	3.925604000	4.057505000	1.064341000
H	3.148813000	3.349778000	2.488819000
C	3.022771000	3.547994000	1.420536000
H	2.173838000	4.225521000	1.304613000
H	2.640689000	4.581327000	-1.093829000
C	1.961503000	3.735839000	-1.246423000
H	1.673459000	3.706064000	-2.300358000
H	1.051905000	3.910023000	-0.662945000

TSOA1

Imaginary Frequency: -53.68

M06-L/BSI SCF energy in gas: -1717.351074 a.u.

M06/BSII SCF energy in benzene: -1716.845759 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1716.185297 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1716.069042 a.u.

Pd	-0.002372000	-0.892519000	-0.060103000
C	-1.937247000	-1.712902000	-0.060412000
N	-2.736989000	-2.009204000	-1.133171000
H	-2.548301000	-2.875092000	-3.037196000
N	-2.816046000	-1.770389000	0.989494000
C	-2.425377000	-1.496607000	2.351507000

H	-2.515432000	-2.391668000	2.977456000
H	-1.386752000	-1.156973000	2.329139000
H	-3.034388000	-0.694410000	2.779457000
H	-5.067658000	-2.989674000	2.290613000
C	-5.237237000	-2.210877000	1.537365000
C	-4.109085000	-2.093118000	0.587142000
H	-6.159589000	-2.462327000	1.008065000
H	-5.416282000	-1.276045000	2.083279000
C	-4.060548000	-2.240484000	-0.766813000
C	-5.123101000	-2.543442000	-1.750432000
H	-4.925274000	-3.465202000	-2.310907000
H	-6.085842000	-2.667480000	-1.248511000
H	-5.239667000	-1.740531000	-2.489616000
H	0.989757000	-2.178400000	2.302477000
C	2.068635000	-2.037187000	2.414709000
H	2.238153000	-1.072522000	2.907485000
H	2.485385000	-2.837489000	3.032803000
N	2.646446000	-2.059636000	1.093315000
C	1.918150000	-1.737938000	-0.021563000
C	-2.253504000	-1.973582000	-2.490776000
H	-2.630655000	-1.093854000	-3.024233000
H	3.149610000	-0.632949000	-2.753284000
C	2.559234000	-1.481154000	-2.393486000
H	1.503691000	-1.204150000	-2.441619000
H	2.747913000	-2.349865000	-3.034000000

N	2.861888000	-1.777077000	-1.014307000
C	4.126248000	-2.111653000	-0.535855000
H	5.519728000	-1.255339000	-1.926199000
C	5.312999000	-2.204182000	-1.414736000
H	6.201600000	-2.463198000	-0.834213000
H	5.196813000	-2.965869000	-2.195180000
C	3.990268000	-2.285716000	0.809482000
C	4.987945000	-2.615954000	1.850866000
H	5.045755000	-1.840172000	2.624758000
H	4.764177000	-3.560294000	2.362309000
H	5.983076000	-2.713440000	1.410157000
H	-1.162989000	-1.908793000	-2.444010000
O	-1.631302000	1.342866000	1.180165000
C	-2.506372000	2.451222000	0.902231000
C	-1.756931000	3.718300000	1.296111000
H	-1.446679000	3.640790000	2.341426000
H	-2.372182000	4.616855000	1.178977000
H	-0.851341000	3.834829000	0.692303000
C	-3.764654000	2.300153000	1.736309000
H	-4.236115000	1.327352000	1.572835000
H	-3.520016000	2.382202000	2.799670000
H	-4.495164000	3.081765000	1.498268000
H	-2.026313000	4.293182000	-1.232070000
C	-2.900417000	3.650643000	-1.360568000
H	-3.782372000	4.187686000	-0.992778000

H	-3.035248000	3.477274000	-2.431915000
C	-2.725655000	2.329184000	-0.637363000
C	-3.854157000	1.368963000	-0.993351000
H	-3.735251000	0.417035000	-0.466927000
H	-3.827616000	1.165254000	-2.068386000
H	-4.838417000	1.783430000	-0.748466000
O	-1.494308000	1.721595000	-1.079316000
B	-0.941242000	1.028492000	0.002097000
B	0.961830000	1.015666000	-0.045971000
O	1.668979000	1.375099000	-1.200076000
O	1.507338000	1.655291000	1.072424000
C	2.544541000	2.467676000	-0.864903000
C	2.741534000	2.284887000	0.672036000
C	3.869531000	1.317500000	1.007825000
H	3.763262000	0.385199000	0.445343000
H	3.829278000	1.074380000	2.074109000
H	4.284718000	1.367241000	-1.547592000
H	4.855160000	1.744994000	0.792840000
C	3.814714000	2.344574000	-1.685398000
H	3.585247000	2.462422000	-2.748705000
H	4.541109000	3.118026000	-1.410603000
H	3.785742000	4.131556000	1.119409000
H	3.019537000	3.359558000	2.515865000
C	2.900115000	3.576994000	1.450662000
H	2.025905000	4.222214000	1.336527000

H	2.421620000	4.643227000	-1.058220000
C	1.805778000	3.752160000	-1.220547000
H	1.512301000	3.717219000	-2.272802000
H	0.891023000	3.847713000	-0.627158000

I3

M06-L/BSI SCF energy in gas: -1717.351659 a.u.

M06/BSII SCF energy in benzene: -1716.847826 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1716.187282 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1716.069433 a.u.

Pd	-0.000440000	-0.852576000	-0.046242000
C	-1.887872000	-1.833964000	-0.093352000
N	-2.667326000	-2.037104000	-1.200025000
H	-2.559415000	-2.644435000	-3.205532000
N	-2.789861000	-1.938403000	0.930448000
C	-2.430094000	-1.719570000	2.310582000
H	-2.500159000	-2.643470000	2.895699000
H	-1.404191000	-1.342889000	2.321485000
H	-3.071362000	-0.956212000	2.760877000
H	-5.112611000	-3.182069000	2.080547000
C	-5.237464000	-2.335961000	1.393750000
C	-4.084843000	-2.179962000	0.479110000
H	-6.155523000	-2.507740000	0.826681000
H	-5.397809000	-1.445690000	2.014182000
C	-4.008705000	-2.235487000	-0.880484000
C	-5.055993000	-2.436695000	-1.906305000

H	-4.879828000	-3.331603000	-2.515583000
H	-6.036032000	-2.550242000	-1.436585000
H	-5.119734000	-1.587066000	-2.597750000
H	0.958937000	-2.044090000	2.386496000
C	2.042794000	-1.944956000	2.483975000
H	2.259501000	-0.959991000	2.913554000
H	2.426182000	-2.723152000	3.150485000
N	2.612888000	-2.072044000	1.164833000
C	1.882231000	-1.843318000	0.029827000
C	-2.155284000	-1.876806000	-2.539099000
H	-2.398441000	-0.885307000	-2.938000000
H	3.112096000	-0.823281000	-2.716268000
C	2.534264000	-1.675133000	-2.344608000
H	1.475572000	-1.413838000	-2.409082000
H	2.743172000	-2.554974000	-2.962946000
N	2.828550000	-1.928510000	-0.955158000
C	4.102766000	-2.180630000	-0.452023000
H	5.475772000	-1.400398000	-1.907975000
C	5.293431000	-2.309122000	-1.320920000
H	6.187864000	-2.496241000	-0.722005000
H	5.199314000	-3.134518000	-2.037201000
C	3.966133000	-2.266360000	0.901335000
C	4.965637000	-2.492640000	1.968650000
H	4.995187000	-1.660815000	2.683582000
H	4.763424000	-3.402656000	2.546753000

H	5.966508000	-2.593206000	1.542197000
H	-1.067513000	-1.965828000	-2.489993000
O	-1.749591000	1.214668000	1.237189000
C	-2.480822000	2.439222000	1.026507000
C	-1.585515000	3.581457000	1.489056000
H	-1.299281000	3.413275000	2.530669000
H	-2.083680000	4.554187000	1.415507000
H	-0.663925000	3.609508000	0.899257000
C	-3.753752000	2.391154000	1.849070000
H	-4.336367000	1.492872000	1.628466000
H	-3.509176000	2.380606000	2.915317000
H	-4.384058000	3.267097000	1.657552000
H	-1.825283000	4.356186000	-0.988655000
C	-2.747537000	3.797240000	-1.162461000
H	-3.586784000	4.384864000	-0.772681000
H	-2.880151000	3.697627000	-2.243522000
C	-2.696623000	2.428123000	-0.515225000
C	-3.903705000	1.592330000	-0.929285000
H	-3.875371000	0.604493000	-0.454837000
H	-3.884600000	1.447669000	-2.013715000
H	-4.850104000	2.077760000	-0.666296000
O	-1.521094000	1.731673000	-0.984512000
B	-1.084214000	0.896752000	0.048624000
B	1.085415000	0.896914000	-0.091364000
O	1.758127000	1.265651000	-1.260656000

O	1.518872000	1.683793000	0.980981000
C	2.495891000	2.474533000	-0.988821000
C	2.703861000	2.388476000	0.551298000
C	3.898844000	1.520060000	0.931902000
H	3.865243000	0.557794000	0.408200000
H	3.867140000	1.318335000	2.007045000
H	4.349952000	1.547386000	-1.622346000
H	4.852864000	2.008005000	0.703343000
C	3.773157000	2.457752000	-1.805843000
H	3.534783000	2.495951000	-2.872841000
H	4.406462000	3.321103000	-1.571689000
H	3.611918000	4.322378000	0.904233000
H	2.890612000	3.574978000	2.338152000
C	2.765133000	3.725294000	1.262081000
H	1.848690000	4.299451000	1.108314000
H	2.112613000	4.608395000	-1.275308000
C	1.610113000	3.643263000	-1.400757000
H	1.331431000	3.528906000	-2.451726000
H	0.683885000	3.647400000	-0.817677000

I4

M06-L/BSI SCF energy in gas: -511.397141 a.u.

M06/BSII SCF energy in benzene: -511.2447256 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -511.0991431 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -511.0484411 a.u.

Pd	-2.095901000	0.000000000	-0.000016000
H	-0.829681000	-2.419425000	-0.000003000
C	0.264381000	-2.443708000	-0.000073000
H	0.618843000	-2.973271000	0.890285000
H	0.618645000	-2.972957000	-0.890704000
N	0.711911000	-1.072354000	0.000113000
C	-0.142997000	0.000017000	0.000066000
H	0.617982000	2.972751000	0.891197000
C	0.264404000	2.443731000	0.000160000
H	-0.829660000	2.419481000	-0.000816000
H	0.619580000	2.973496000	-0.889791000
N	0.711928000	1.072365000	-0.000046000
C	2.046483000	0.681048000	-0.000095000
H	3.141614000	2.306980000	0.879969000
C	3.161883000	1.653300000	-0.000149000
H	4.123007000	1.133634000	0.000547000
H	3.142416000	2.306064000	-0.880969000
C	2.046471000	-0.681063000	-0.000035000
C	3.161857000	-1.653333000	0.000124000
H	3.141858000	-2.306497000	0.880634000
H	3.142104000	-2.306615000	-0.880304000
H	4.122988000	-1.133682000	0.000211000

I5

M06-L/BSI SCF energy in gas: -1333.913396 a.u.

M06/BSII SCF energy in benzene: -1333.544822 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1333.05814 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1332.962189 a.u.

Pd	-0.406866000	-0.886570000	-0.786564000
B	-0.471680000	1.425411000	0.009352000
B	-1.893133000	0.538937000	0.164689000
O	0.429354000	1.619132000	1.060032000
O	-0.159808000	2.243537000	-1.076612000
O	-2.602687000	0.258846000	1.324123000
O	-2.559646000	0.012622000	-0.974692000
C	1.304239000	2.705270000	0.699397000
C	1.166311000	2.768351000	-0.856538000
C	-3.907304000	-0.228613000	0.941521000
C	-3.676520000	-0.803901000	-0.491170000
C	-3.215059000	-2.250574000	-0.488774000
H	-2.883164000	-2.525449000	-1.495222000
H	-2.364423000	-2.390894000	0.189502000
H	-4.021730000	-2.930559000	-0.194688000
C	-4.358781000	-1.255211000	1.961875000
H	-5.315859000	-1.702101000	1.670834000
H	-3.624050000	-2.054091000	2.080257000
H	-4.494288000	-0.775757000	2.934945000

C	-4.843322000	0.973976000	0.950724000
H	-4.811886000	1.442247000	1.937497000
H	-4.531938000	1.720630000	0.214371000
H	-5.878208000	0.688231000	0.737745000
C	-4.836699000	-0.617100000	-1.447581000
H	-5.083344000	0.437377000	-1.584304000
H	-4.584538000	-1.034855000	-2.425878000
H	-5.729045000	-1.136223000	-1.080336000
C	0.768322000	3.952976000	1.391158000
H	0.707888000	3.768755000	2.466965000
H	1.411693000	4.823676000	1.226922000
H	-0.237560000	4.193563000	1.035316000
C	2.701890000	2.386303000	1.201072000
H	3.052540000	1.415573000	0.838545000
H	3.419303000	3.152770000	0.886256000
H	2.705657000	2.358493000	2.295514000
C	2.141760000	1.845803000	-1.574669000
H	1.869685000	1.791714000	-2.632874000
H	3.176007000	2.199572000	-1.497529000
H	2.075121000	0.836344000	-1.160661000
C	1.237827000	4.165259000	-1.443503000
H	2.208812000	4.628294000	-1.233713000
H	1.116509000	4.117759000	-2.529129000
H	0.453429000	4.812753000	-1.046797000
H	1.554399000	-1.551244000	-2.656472000

C	1.401452000	-1.446537000	-0.142967000
N	2.541904000	-1.692121000	-0.861987000
C	2.571078000	-1.747923000	-2.303529000
H	2.897225000	-2.731694000	-2.656210000
H	3.242667000	-0.984696000	-2.710892000
C	3.661550000	-1.818798000	-0.046540000
C	5.017193000	-2.066973000	-0.585226000
H	5.353246000	-1.257906000	-1.245204000
H	5.068858000	-2.995049000	-1.166763000
H	5.743471000	-2.148811000	0.226631000
C	3.217681000	-1.661597000	1.232957000
C	3.942691000	-1.678744000	2.522486000
H	5.009480000	-1.850067000	2.361269000
H	3.579839000	-2.466951000	3.192657000
H	3.838266000	-0.729778000	3.062266000
N	1.846889000	-1.446411000	1.149543000
C	0.995109000	-1.199822000	2.292123000
H	1.075667000	-2.019980000	3.012613000
H	-0.033101000	-1.122223000	1.930346000
H	1.257522000	-0.255170000	2.775349000

TSOA2

Imaginary Frequency: -29.48

M06-L/BSI SCF energy in gas: -1333.903224 a.u.

M06/BSII SCF energy in benzene: -1333.542456 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1333.057094 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1332.961012 a.u.

Pd	-0.415471000	0.317894000	-0.453184000
B	1.197421000	-1.030423000	-0.159549000
B	1.682629000	0.691941000	0.029709000
O	1.095424000	-1.864596000	0.954966000
O	1.560239000	-1.747415000	-1.298351000
O	2.119001000	1.124585000	1.270133000
O	2.135798000	1.514196000	-0.995498000
C	1.554681000	-3.175715000	0.552368000
C	1.345024000	-3.144222000	-0.991996000
C	3.038953000	2.220344000	1.043521000
C	2.612186000	2.730397000	-0.364592000
C	1.428956000	3.688808000	-0.310940000
H	1.047646000	3.841214000	-1.324593000
H	0.617843000	3.264926000	0.292129000
H	1.710998000	4.662185000	0.104108000
C	2.873672000	3.231644000	2.159504000
H	3.495482000	4.115476000	1.977681000
H	1.834650000	3.552047000	2.256825000
H	3.182540000	2.793113000	3.112099000
C	4.441688000	1.627859000	1.056983000

H	4.598527000	1.099267000	2.000660000
H	4.572412000	0.910465000	0.241265000
H	5.210127000	2.401951000	0.963487000
C	3.734858000	3.308207000	-1.200886000
H	4.524175000	2.574764000	-1.376380000
H	3.350938000	3.628644000	-2.173083000
H	4.176705000	4.181986000	-0.708559000
C	3.022982000	-3.270225000	0.944775000
H	3.122499000	-3.067457000	2.014051000
H	3.436785000	-4.263236000	0.741121000
H	3.618935000	-2.528749000	0.403922000
C	0.737384000	-4.223030000	1.281731000
H	-0.333498000	-4.082734000	1.115531000
H	1.007817000	-5.231428000	0.948685000
H	0.924000000	-4.162611000	2.357518000
C	-0.086584000	-3.468921000	-1.399945000
H	-0.218515000	-3.231398000	-2.458590000
H	-0.328502000	-4.526387000	-1.249118000
H	-0.795548000	-2.853161000	-0.834757000
C	2.330681000	-3.978617000	-1.784470000
H	2.253042000	-5.037165000	-1.511669000
H	2.121387000	-3.891054000	-2.853943000
H	3.359014000	-3.653239000	-1.615118000
H	-1.969242000	2.398676000	-1.586962000
C	-2.440756000	0.405691000	-0.123609000

N	-3.362775000	1.332945000	-0.516217000
C	-3.028052000	2.481076000	-1.325691000
H	-3.191189000	3.413064000	-0.774890000
H	-3.626666000	2.502534000	-2.241413000
C	-4.635935000	1.050583000	-0.033743000
C	-5.807500000	1.909137000	-0.316951000
H	-6.013276000	1.988351000	-1.391019000
H	-5.671571000	2.930543000	0.057817000
H	-6.704004000	1.504004000	0.158002000
C	-4.519426000	-0.100774000	0.688481000
C	-5.528698000	-0.886297000	1.432920000
H	-6.518834000	-0.437150000	1.327178000
H	-5.304807000	-0.937777000	2.504968000
H	-5.595416000	-1.918966000	1.071492000
N	-3.180861000	-0.468577000	0.621021000
C	-2.618631000	-1.632509000	1.269499000
H	-2.855483000	-1.629449000	2.337471000
H	-1.531848000	-1.591843000	1.140202000
H	-3.006819000	-2.555472000	0.824172000

I6

M06-L/BSI SCF energy in gas: -1333.905412 a.u.

M06/BSII SCF energy in benzene: -1333.545573 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1333.06066 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1332.963003 a.u.

Pd	0.661499000	-0.218754000	-0.071969000
B	-1.030291000	0.952663000	-0.139178000
B	-1.299659000	-0.938735000	0.061478000
O	-1.119511000	1.862763000	0.911116000
O	-1.747447000	1.390626000	-1.247995000
O	-2.075826000	-1.173954000	1.189360000
O	-1.633060000	-1.806748000	-0.972458000
C	-2.093849000	2.864194000	0.540217000
C	-2.085578000	2.778565000	-1.015994000
C	-3.086014000	-2.147236000	0.822395000
C	-2.425408000	-2.866354000	-0.389113000
C	-1.460978000	-3.967122000	0.036172000
H	-0.877340000	-4.286334000	-0.831607000
H	-0.762881000	-3.602085000	0.796352000
H	-1.988003000	-4.839933000	0.435624000
C	-3.365007000	-3.034064000	2.018283000
H	-4.061473000	-3.837749000	1.753354000
H	-2.448548000	-3.483636000	2.405234000
H	-3.817861000	-2.448153000	2.822652000
C	-4.330406000	-1.364081000	0.427387000
H	-4.627260000	-0.717044000	1.257354000
H	-4.129918000	-0.734161000	-0.446119000
H	-5.169998000	-2.026088000	0.192201000

C	-3.395314000	-3.381128000	-1.433564000
H	-3.990795000	-2.572121000	-1.861370000
H	-2.846288000	-3.860067000	-2.248717000
H	-4.075489000	-4.125075000	-1.003559000
C	-3.422623000	2.435463000	1.146652000
H	-3.300008000	2.304237000	2.224743000
H	-4.208405000	3.178285000	0.973156000
H	-3.749720000	1.479022000	0.729278000
C	-1.656400000	4.200501000	1.106117000
H	-0.636996000	4.449776000	0.802301000
H	-2.323149000	5.005119000	0.775821000
H	-1.683909000	4.169545000	2.198787000
C	-0.979313000	3.615176000	-1.645461000
H	-0.885710000	3.351613000	-2.701918000
H	-1.189252000	4.687431000	-1.572818000
H	-0.017375000	3.414346000	-1.162792000
C	-3.417474000	3.069096000	-1.678008000
H	-3.753278000	4.087435000	-1.451902000
H	-3.324214000	2.978572000	-2.763537000
H	-4.188228000	2.369589000	-1.347349000
H	2.162551000	-2.468448000	-0.932760000
C	2.751697000	-0.204971000	-0.001507000
N	3.647716000	-1.174247000	-0.335567000
C	3.252272000	-2.470539000	-0.838152000
H	3.554337000	-3.267322000	-0.151404000

H	3.698857000	-2.660563000	-1.818669000
C	4.962388000	-0.769120000	-0.133322000
C	6.121984000	-1.643722000	-0.416200000
H	6.162552000	-1.949062000	-1.468284000
H	6.102864000	-2.562057000	0.182196000
H	7.056922000	-1.126018000	-0.190026000
C	4.895046000	0.508248000	0.342301000
C	5.960937000	1.457229000	0.732790000
H	6.945959000	1.009985000	0.582129000
H	5.890637000	1.747733000	1.787536000
H	5.926219000	2.381258000	0.144253000
N	3.543079000	0.822439000	0.416607000
C	3.014446000	2.087980000	0.877966000
H	3.387684000	2.319960000	1.879745000
H	1.923921000	1.997364000	0.909227000
H	3.293129000	2.900167000	0.198738000

I7

M06-L/BSI SCF energy in gas: -2256.749816 a.u.

M06/BSII SCF energy in benzene: -2256.005574 a.u.

M06/BSII//M06-L/BSI free energy in benzene:: -2255.166538 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -2255.02227 a.u.

Pd	-0.032765000	0.288287000	-0.169863000
H	0.152377000	2.792831000	1.334068000
C	0.883864000	3.557714000	1.066147000
H	0.416684000	4.548698000	1.084276000

H	1.694703000	3.539473000	1.803980000
N	1.389257000	3.248100000	-0.251473000
C	1.013224000	2.152784000	-0.986043000
H	1.965913000	1.749664000	-4.114031000
C	1.860077000	1.267471000	-3.138433000
H	0.935765000	0.692432000	-3.115058000
H	2.700375000	0.581117000	-2.984556000
N	1.810740000	2.260756000	-2.089556000
C	2.663259000	3.360323000	-2.040577000
H	3.162830000	3.853519000	-4.074832000
C	3.642433000	3.668254000	-3.106157000
H	4.217751000	4.561334000	-2.850732000
H	4.356041000	2.849054000	-3.256653000
C	2.389651000	3.994769000	-0.868189000
C	2.978146000	5.207981000	-0.259268000
H	2.232992000	5.993986000	-0.087677000
H	3.445508000	4.996260000	0.710835000
H	3.750470000	5.625801000	-0.909508000
O	2.905484000	-0.298440000	0.270793000
C	3.968542000	0.072545000	1.172436000
C	4.355093000	1.507402000	0.834380000
H	4.607079000	1.568544000	-0.229086000
H	5.216016000	1.853877000	1.416456000
H	3.513611000	2.184257000	1.012464000
C	5.141599000	-0.862120000	0.952828000

H	4.833020000	-1.907423000	1.019368000
H	5.566932000	-0.700728000	-0.042054000
H	5.934044000	-0.684081000	1.688932000
H	3.648660000	1.945663000	3.313374000
C	3.781896000	0.904609000	3.617247000
H	4.845934000	0.738137000	3.820788000
H	3.235715000	0.755063000	4.553103000
C	3.277009000	-0.055798000	2.559986000
C	3.284916000	-1.486610000	3.076373000
H	2.908918000	-2.166275000	2.305675000
H	2.623003000	-1.561931000	3.944305000
H	4.287098000	-1.807576000	3.379551000
O	1.901198000	0.272402000	2.245573000
B	1.686131000	-0.026709000	0.895495000
C	-1.518448000	-0.384021000	-1.906842000
C	-0.393267000	-0.957570000	-1.949869000
C	0.405870000	-2.012658000	-2.532128000
C	-0.171014000	-2.889504000	-3.470430000
C	1.745558000	-2.204376000	-2.165367000
H	-1.213042000	-2.746761000	-3.749487000
H	2.176664000	-1.541823000	-1.419420000
C	0.571717000	-3.929490000	-4.014421000
C	2.485288000	-3.241521000	-2.721203000
H	0.109601000	-4.604251000	-4.730795000
H	3.521490000	-3.379413000	-2.420453000

C	1.904656000	-4.109515000	-3.643779000
H	2.483604000	-4.924424000	-4.070898000
C	-2.862309000	0.042818000	-2.032549000
C	-3.783983000	-0.188873000	-0.986086000
C	-3.312825000	0.739304000	-3.174919000
H	-3.430003000	-0.704036000	-0.094201000
H	-2.614551000	0.918883000	-3.988458000
C	-5.088299000	0.270921000	-1.081623000
C	-4.619499000	1.203985000	-3.253076000
H	-5.779114000	0.088614000	-0.260632000
H	-4.941847000	1.746233000	-4.138802000
C	-5.515711000	0.981255000	-2.207775000
H	-6.536659000	1.347947000	-2.271416000
H	-4.629281000	4.153353000	1.227697000
C	-4.861264000	3.088108000	1.347653000
H	-5.351807000	2.761093000	0.421536000
C	-3.656255000	2.277067000	1.631245000
C	-3.313148000	1.508503000	2.703534000
C	-4.022461000	1.247771000	3.976111000
H	-3.462781000	1.608821000	4.847670000
H	-4.992831000	1.750361000	3.981972000
H	-4.202847000	0.178307000	4.136413000
H	-5.587275000	3.000117000	2.159850000
N	-2.610134000	2.153864000	0.724670000
N	-2.073594000	0.952818000	2.399250000

H	-1.278602000	0.625034000	4.302544000
C	-1.333748000	0.127102000	3.328653000
H	-1.810075000	-0.850368000	3.446161000
H	-0.322655000	-0.012377000	2.941876000
C	-1.621502000	1.318156000	1.163778000
H	-3.458390000	2.648604000	-1.130912000
C	-2.567566000	2.865841000	-0.532246000
H	-1.676889000	2.534468000	-1.072521000
H	-2.508606000	3.946916000	-0.358014000
B	-0.131069000	-1.555951000	0.718016000
O	-1.400932000	-1.945302000	1.157648000
O	0.734787000	-2.643124000	0.736170000
C	0.045467000	-3.779258000	1.313957000
C	-1.454125000	-3.390407000	1.136422000
H	-1.367402000	-3.460439000	-1.032427000
C	-2.016490000	-3.798190000	-0.219132000
H	-2.136590000	-4.883682000	-0.298933000
H	-2.995806000	-3.331627000	-0.360275000
H	-2.058975000	-3.481343000	3.223691000
C	-2.374812000	-3.856820000	2.247565000
H	-2.410784000	-4.950928000	2.296681000
H	-3.390952000	-3.497286000	2.058778000
H	0.188177000	-2.948758000	3.313466000
C	0.461801000	-3.863123000	2.775645000
H	1.546943000	-3.977457000	2.841479000

H	-0.000748000	-4.716309000	3.282672000
H	1.539474000	-5.212441000	0.731116000
C	0.475335000	-5.023676000	0.561871000
H	0.324186000	-4.911462000	-0.514136000
H	-0.081412000	-5.903138000	0.905321000

TSIA1

Imaginary Frequency: -169.66

M06-L/BSI SCF energy in gas: -2256.737028 a.u.

M06/BSII SCF energy in benzene: -2255.994992 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -2255.155282 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -2255.012389 a.u.

Pd	0.044414000	-0.347734000	0.018153000
H	2.251221000	-2.149439000	-0.934361000
C	3.094449000	-2.430487000	-0.302533000
H	3.154975000	-3.521455000	-0.217028000
H	4.014838000	-2.062220000	-0.766667000
N	2.905125000	-1.815548000	0.991338000
C	1.773739000	-1.137595000	1.359184000
H	1.070639000	-0.279850000	4.395787000
C	1.232840000	0.153759000	3.404196000
H	0.279488000	0.248780000	2.886040000
H	1.668627000	1.152114000	3.517960000
N	2.095375000	-0.691916000	2.609262000
C	3.372767000	-1.070672000	3.007315000
H	3.362525000	-1.046575000	5.157280000

C	3.953922000	-0.679487000	4.310317000
H	4.964266000	-1.081268000	4.417621000
H	4.019955000	0.409982000	4.417883000
C	3.890522000	-1.791897000	1.974382000
C	5.217470000	-2.422428000	1.795374000
H	5.145415000	-3.494966000	1.579918000
H	5.778867000	-1.968889000	0.967993000
H	5.820941000	-2.308086000	2.698871000
O	2.068633000	1.946274000	0.166336000
C	3.389910000	2.284160000	-0.314214000
C	4.385809000	1.565146000	0.587530000
H	4.187041000	1.840056000	1.628029000
H	5.422855000	1.828692000	0.353056000
H	4.271333000	0.479200000	0.505556000
C	3.572385000	3.785719000	-0.223656000
H	2.763548000	4.317128000	-0.728586000
H	3.574028000	4.099130000	0.824124000
H	4.525299000	4.095794000	-0.667739000
H	5.129974000	0.453737000	-1.641442000
C	4.704213000	1.230612000	-2.281398000
H	5.421934000	2.056520000	-2.343606000
H	4.586824000	0.813295000	-3.285593000
C	3.365941000	1.710509000	-1.758636000
C	2.701947000	2.658187000	-2.748513000
H	1.742762000	3.007855000	-2.352876000

H	2.508200000	2.125990000	-3.684964000
H	3.328462000	3.528328000	-2.970948000
O	2.483311000	0.570587000	-1.615586000
B	1.620183000	0.840328000	-0.549015000
C	-1.782498000	-0.677921000	1.253753000
C	-1.490319000	0.593263000	1.176989000
C	-1.738307000	1.791375000	1.967857000
C	-2.942112000	1.925696000	2.681759000
C	-0.791109000	2.824718000	2.038494000
H	-3.678101000	1.125545000	2.624215000
H	0.132927000	2.717641000	1.472772000
C	-3.190776000	3.062113000	3.441391000
C	-1.041925000	3.953293000	2.810962000
H	-4.128851000	3.153019000	3.983995000
H	-0.298097000	4.745388000	2.861388000
C	-2.241929000	4.082038000	3.509820000
H	-2.438418000	4.971545000	4.102787000
C	-2.639597000	-1.656202000	1.836840000
C	-4.025991000	-1.662690000	1.567740000
C	-2.125159000	-2.678388000	2.664311000
H	-4.432579000	-0.886436000	0.923101000
H	-1.055701000	-2.691655000	2.869608000
C	-4.849503000	-2.646548000	2.098236000
C	-2.961784000	-3.638610000	3.214936000
H	-5.912746000	-2.634147000	1.869995000

H	-2.544531000	-4.403489000	3.866098000
C	-4.327930000	-3.637732000	2.929193000
H	-4.977467000	-4.400610000	3.349024000
H	-0.067667000	-5.914172000	-2.295869000
C	-0.893497000	-5.284956000	-2.649784000
H	-1.771484000	-5.543119000	-2.046601000
C	-0.573580000	-3.842129000	-2.573636000
C	-0.471849000	-2.893162000	-3.545867000
C	-0.648454000	-2.979751000	-5.012473000
H	0.272192000	-2.741762000	-5.559043000
H	-0.948943000	-3.989157000	-5.303150000
H	-1.419941000	-2.289542000	-5.373079000
H	-1.106074000	-5.576132000	-3.681163000
N	-0.306839000	-3.191045000	-1.373857000
N	-0.145618000	-1.705925000	-2.896858000
H	0.695336000	-0.541963000	-4.421378000
C	0.000287000	-0.442476000	-3.581650000
H	-0.970707000	-0.092788000	-3.949417000
H	0.398536000	0.280793000	-2.870118000
C	-0.050232000	-1.860040000	-1.545582000
H	-1.388195000	-4.068591000	0.203701000
C	-0.357734000	-3.830068000	-0.078783000
H	0.046827000	-3.126119000	0.652923000
H	0.235597000	-4.750370000	-0.081850000
B	-1.197524000	1.070164000	-0.806941000

O	-2.293036000	0.676653000	-1.582671000
O	-0.966390000	2.437098000	-0.946967000
C	-1.922036000	2.979785000	-1.878925000
C	-3.023599000	1.867603000	-1.939214000
H	-3.696817000	2.192794000	0.102274000
C	-4.118720000	2.059067000	-0.898097000
H	-4.749837000	2.924460000	-1.124923000
H	-4.752040000	1.167707000	-0.880328000
H	-2.891348000	1.402302000	-4.059464000
C	-3.642192000	1.664671000	-3.309718000
H	-4.158667000	2.570958000	-3.645584000
H	-4.376353000	0.855094000	-3.269832000
H	-0.815014000	2.228640000	-3.590831000
C	-1.201373000	3.177506000	-3.206315000
H	-0.352377000	3.851068000	-3.059878000
H	-1.856691000	3.617503000	-3.965260000
H	-1.566165000	5.023964000	-1.314087000
C	-2.400563000	4.317193000	-1.343012000
H	-2.792240000	4.225746000	-0.327457000
H	-3.181742000	4.742432000	-1.983664000

I8

M06-L/BSI SCF energy in gas: -2256.813570 a.u.

M06/BSII SCF energy in benzene: -2256.075216 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -2255.231849 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -2255.089796 a.u.

Pd	0.607848000	0.262981000	-0.603407000
H	2.545449000	-1.039745000	-2.212988000
C	3.106597000	-1.868201000	-1.776812000
H	2.925742000	-2.777311000	-2.357292000
H	4.171449000	-1.616318000	-1.794010000
N	2.645206000	-2.045479000	-0.417903000
C	1.734040000	-1.239755000	0.187160000
H	-0.195831000	-1.879096000	2.503532000
C	0.685356000	-1.233792000	2.416841000
H	0.347247000	-0.253630000	2.074834000
H	1.170827000	-1.140347000	3.393070000
N	1.615962000	-1.752000000	1.439020000
C	2.414347000	-2.877274000	1.610126000
H	1.437111000	-4.078138000	3.091718000
C	2.425749000	-3.660101000	2.864446000
H	3.125805000	-4.494903000	2.786848000
H	2.727068000	-3.056324000	3.728984000
C	3.072279000	-3.062426000	0.430825000
C	4.022823000	-4.107070000	-0.006235000
H	3.609053000	-4.707942000	-0.825362000
H	4.971254000	-3.685073000	-0.359463000
H	4.251311000	-4.786772000	0.817699000
O	2.713073000	1.660650000	1.078384000
C	4.150042000	1.650162000	1.251459000

C	4.506915000	0.322907000	1.911826000
H	3.927666000	0.213268000	2.833674000
H	5.570979000	0.263955000	2.164505000
H	4.257380000	-0.519451000	1.257865000
C	4.547752000	2.810239000	2.141497000
H	4.152207000	3.757061000	1.767323000
H	4.155997000	2.659778000	3.151447000
H	5.637942000	2.895432000	2.214436000
H	5.903368000	-0.035714000	-0.235289000
C	5.965669000	1.026575000	-0.484084000
H	6.782410000	1.468214000	0.098391000
H	6.226471000	1.109466000	-1.543094000
C	4.656519000	1.742549000	-0.215332000
C	4.721769000	3.175592000	-0.727004000
H	3.786098000	3.704963000	-0.521816000
H	4.871597000	3.165942000	-1.809614000
H	5.543203000	3.737357000	-0.270110000
O	3.603108000	1.072914000	-0.946982000
B	2.431144000	1.143006000	-0.196228000
C	-1.048098000	-1.233517000	-0.585176000
C	-2.217328000	-1.078195000	0.097441000
C	-3.312818000	-2.075585000	0.185416000
C	-3.696821000	-2.863182000	-0.914108000
C	-4.051886000	-2.221061000	1.373842000
H	-3.154895000	-2.753615000	-1.851070000

H	-3.775499000	-1.621018000	2.239867000
C	-4.747034000	-3.767712000	-0.822231000
C	-5.101019000	-3.130012000	1.467926000
H	-5.021050000	-4.362303000	-1.690568000
H	-5.645570000	-3.229522000	2.404539000
C	-5.454792000	-3.910815000	0.370560000
H	-6.276953000	-4.618284000	0.440576000
C	-0.630946000	-2.538134000	-1.124846000
C	-0.079476000	-2.680608000	-2.412108000
C	-0.604277000	-3.681476000	-0.297201000
H	-0.032779000	-1.807740000	-3.063360000
H	-1.016346000	-3.600157000	0.707780000
C	0.433595000	-3.893412000	-2.859992000
C	-0.057376000	-4.883720000	-0.728078000
H	0.837601000	-3.965559000	-3.868262000
H	-0.038721000	-5.737200000	-0.052709000
C	0.460836000	-5.004301000	-2.017757000
H	0.878468000	-5.947414000	-2.360814000
H	-2.966182000	2.952351000	-4.522500000
C	-3.172434000	3.255564000	-3.489331000
H	-4.039182000	2.675602000	-3.151000000
C	-2.009648000	3.064177000	-2.595668000
C	-1.310193000	3.956709000	-1.846054000
C	-1.442110000	5.424104000	-1.709158000
H	-0.539939000	5.957712000	-2.031288000

H	-2.272973000	5.788740000	-2.317848000
H	-1.638667000	5.727305000	-0.672820000
H	-3.466737000	4.307385000	-3.510767000
N	-1.451365000	1.819853000	-2.341864000
N	-0.361757000	3.216186000	-1.147096000
H	1.251109000	4.515936000	-0.825893000
C	0.584483000	3.854059000	-0.261801000
H	0.057826000	4.454922000	0.488942000
H	1.175371000	3.093923000	0.247261000
C	-0.439110000	1.874078000	-1.423908000
H	-2.886972000	0.290796000	-2.445725000
C	-1.969090000	0.613157000	-2.947852000
H	-1.227073000	-0.174160000	-2.838101000
H	-2.169375000	0.791341000	-4.008030000
B	-2.445121000	0.240062000	0.883575000
O	-2.971347000	1.407041000	0.358881000
O	-2.216534000	0.345308000	2.247720000
C	-2.370498000	1.739460000	2.600960000
C	-3.322481000	2.254225000	1.478375000
H	-4.947679000	0.941399000	2.070413000
C	-4.790273000	1.986462000	1.784431000
H	-5.163044000	2.626485000	2.590392000
H	-5.385590000	2.179854000	0.888414000
H	-2.089572000	3.871343000	0.751034000
C	-3.114822000	3.701321000	1.084871000

H	-3.327511000	4.370301000	1.926316000
H	-3.783683000	3.967058000	0.259806000
H	-0.552059000	2.215965000	1.530214000
C	-0.980003000	2.354372000	2.530608000
H	-0.320148000	1.846079000	3.239966000
H	-0.983478000	3.421702000	2.776465000
H	-2.215764000	1.437092000	4.724696000
C	-2.935659000	1.833249000	4.003511000
H	-3.861188000	1.262270000	4.102853000
H	-3.140840000	2.875344000	4.272481000

I9

M06-L/BSI SCF energy in gas: -1873.346616 a.u.

M06/BSII SCF energy in benzene: -1872.751229 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1872.083904 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1871.962799 a.u.

Pd	-0.062620000	0.487148000	0.008207000
H	-1.280808000	0.213289000	2.486561000
C	-2.366013000	0.302001000	2.578074000
H	-2.744142000	-0.514336000	3.200074000
H	-2.611714000	1.259102000	3.049705000
N	-2.923182000	0.228021000	1.245823000
C	-2.157630000	0.255886000	0.123221000
H	-3.072387000	-0.637994000	-2.821686000
C	-2.689055000	0.234268000	-2.284892000
H	-1.599115000	0.227011000	-2.335501000

H	-3.073036000	1.148280000	-2.749668000
N	-3.062235000	0.183541000	-0.887825000
C	-4.368802000	0.127951000	-0.413586000
H	-5.522861000	-0.865720000	-1.927780000
C	-5.540134000	0.042464000	-1.313724000
H	-6.467202000	0.030786000	-0.736705000
H	-5.591865000	0.892779000	-2.003230000
C	-4.280420000	0.155973000	0.948786000
C	-5.322398000	0.085220000	1.996542000
H	-5.226752000	-0.819578000	2.609479000
H	-5.280032000	0.940709000	2.679975000
H	-6.318165000	0.071529000	1.547931000
O	2.245634000	-1.122323000	1.150992000
C	3.316100000	-2.064100000	0.888461000
C	2.842575000	-3.407197000	1.427549000
H	2.598563000	-3.302493000	2.487882000
H	3.604403000	-4.185722000	1.318675000
H	1.931288000	-3.729807000	0.914099000
C	4.565483000	-1.609533000	1.613960000
H	4.847355000	-0.594661000	1.326655000
H	4.396728000	-1.624693000	2.694719000
H	5.405308000	-2.278682000	1.395256000
H	3.064619000	-4.148053000	-1.044779000
C	3.779935000	-3.364348000	-1.304240000
H	4.776933000	-3.691110000	-0.987832000

H	3.788935000	-3.264900000	-2.393123000
C	3.422309000	-2.034456000	-0.668453000
C	4.337857000	-0.938262000	-1.192203000
H	4.088975000	0.031857000	-0.755088000
H	4.220029000	-0.860370000	-2.276099000
H	5.389199000	-1.154837000	-0.975687000
O	2.070575000	-1.686674000	-1.063260000
B	1.461077000	-1.053949000	0.010611000
B	-0.377378000	-1.628880000	-0.081825000
O	-0.905784000	-2.126545000	-1.271116000
O	-0.619756000	-2.503394000	0.974198000
C	-1.260034000	-3.507054000	-1.049171000
C	-1.498674000	-3.549393000	0.493807000
C	-2.920071000	-3.162679000	0.878332000
H	-3.233339000	-2.248290000	0.367103000
H	-2.965345000	-2.984295000	1.956943000
H	-3.303656000	-3.145599000	-1.686754000
H	-3.634074000	-3.955904000	0.632950000
C	-2.479398000	-3.834911000	-1.889190000
H	-2.229448000	-3.759966000	-2.951340000
H	-2.828780000	-4.855479000	-1.697447000
H	-1.694584000	-5.687574000	0.769973000
H	-1.294825000	-4.788037000	2.241234000
C	-1.107928000	-4.850879000	1.165595000
H	-0.048907000	-5.074774000	1.023113000

H	-0.265383000	-5.420479000	-1.395290000
C	-0.068796000	-4.347355000	-1.487779000
H	0.165778000	-4.121722000	-2.531203000
H	0.817759000	-4.094980000	-0.898631000
C	0.145493000	2.545591000	-0.087425000
C	1.331523000	2.047923000	-0.028954000
C	2.750472000	2.295624000	0.008127000
C	3.369451000	3.028836000	-1.020786000
C	3.544837000	1.834286000	1.071993000
H	2.761793000	3.382154000	-1.850519000
H	3.077484000	1.240361000	1.852511000
C	4.734531000	3.287005000	-0.986486000
C	4.905431000	2.119067000	1.111069000
H	5.196026000	3.846050000	-1.796628000
H	5.501426000	1.765510000	1.949696000
C	5.509647000	2.838360000	0.081234000
H	6.575520000	3.047025000	0.110225000
C	-0.660373000	3.739321000	-0.112807000
C	-2.060509000	3.699212000	-0.008598000
C	-0.042696000	4.999216000	-0.243506000
H	-2.544371000	2.731579000	0.092748000
H	1.040931000	5.044924000	-0.321712000
C	-2.813488000	4.867075000	-0.029270000
C	-0.798759000	6.163068000	-0.264442000
H	-3.896172000	4.811054000	0.054799000

H	-0.301553000	7.124739000	-0.363949000
C	-2.188526000	6.105048000	-0.157925000
H	-2.777586000	7.017817000	-0.175500000

TSIA2

Imaginary Frequency: -45.23

M06-L/BSI SCF energy in gas: -1873.319628 a.u.

M06/BSII SCF energy in benzene: -1872.72818 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1872.060578 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1871.941355 a.u.

Pd	-0.135330000	0.479764000	-0.010617000
H	-1.183499000	0.934500000	2.470189000
C	-2.097203000	1.526631000	2.559072000
H	-2.838097000	0.954966000	3.125110000
H	-1.877552000	2.457901000	3.090342000
N	-2.575757000	1.793023000	1.221992000
C	-1.883694000	1.453632000	0.099444000
H	-3.065872000	0.938125000	-2.772521000
C	-2.370721000	1.648025000	-2.315303000
H	-1.367307000	1.219584000	-2.360913000
H	-2.394840000	2.596740000	-2.859872000
N	-2.691631000	1.853362000	-0.920935000
C	-3.867946000	2.429561000	-0.447840000
H	-5.340929000	2.120725000	-1.977484000
C	-4.927201000	2.923520000	-1.354672000

H	-5.752248000	3.353166000	-0.782411000
H	-4.560276000	3.698985000	-2.037120000
C	-3.792127000	2.395872000	0.912955000
C	-4.741984000	2.843528000	1.954633000
H	-5.096588000	2.009982000	2.573116000
H	-4.295357000	3.578626000	2.633879000
H	-5.618927000	3.308132000	1.498540000
O	1.641529000	-1.719916000	1.339369000
C	1.783972000	-3.142080000	1.104991000
C	0.451772000	-3.784586000	1.464300000
H	0.212581000	-3.562800000	2.507719000
H	0.479272000	-4.872106000	1.337393000
H	-0.358853000	-3.371737000	0.858325000
C	2.884428000	-3.660646000	2.010988000
H	3.816239000	-3.108215000	1.867627000
H	2.584320000	-3.554240000	3.057095000
H	3.077888000	-4.722505000	1.822420000
H	0.366992000	-4.332696000	-1.087677000
C	1.455005000	-4.378995000	-1.153599000
H	1.789044000	-5.337683000	-0.741504000
H	1.727964000	-4.354263000	-2.211900000
C	2.114325000	-3.221262000	-0.427294000
C	3.606453000	-3.222083000	-0.733049000
H	4.136708000	-2.419092000	-0.217550000
H	3.748686000	-3.077795000	-1.807472000

H	4.065823000	-4.175454000	-0.451197000
O	1.558947000	-1.987508000	-0.943814000
B	1.382774000	-1.119745000	0.119679000
B	-1.580075000	-1.024621000	-0.153809000
O	-2.255519000	-1.297545000	-1.342472000
O	-2.189284000	-1.689142000	0.909239000
C	-3.219697000	-2.344396000	-1.089281000
C	-3.454624000	-2.215631000	0.445138000
C	-4.519802000	-1.180158000	0.787265000
H	-4.329804000	-0.235165000	0.266284000
H	-4.499863000	-0.983707000	1.863714000
H	-4.839927000	-1.080647000	-1.792086000
H	-5.525452000	-1.524583000	0.522936000
C	-4.442880000	-2.087587000	-1.948726000
H	-4.182301000	-2.184347000	-3.006797000
H	-5.238809000	-2.809104000	-1.732096000
H	-4.648166000	-3.991186000	0.784808000
H	-3.873415000	-3.334525000	2.233925000
C	-3.734618000	-3.519948000	1.165065000
H	-2.909271000	-4.226870000	1.054239000
H	-3.262876000	-4.506823000	-1.381123000
C	-2.568783000	-3.664788000	-1.472707000
H	-2.218664000	-3.611746000	-2.506651000
H	-1.701780000	-3.863559000	-0.835186000
C	1.495286000	1.741734000	0.032929000

C	2.039224000	0.533695000	-0.013386000
C	3.476345000	0.184264000	-0.170234000
C	4.074671000	0.178851000	-1.434626000
C	4.259751000	-0.083277000	0.959528000
H	3.458757000	0.368347000	-2.309704000
H	3.782063000	-0.107460000	1.935561000
C	5.437724000	-0.070170000	-1.562881000
C	5.622986000	-0.328566000	0.825479000
H	5.893024000	-0.070723000	-2.550091000
H	6.222728000	-0.530556000	1.709470000
C	6.216166000	-0.324749000	-0.435961000
H	7.279685000	-0.521677000	-0.540143000
C	1.947653000	3.114198000	0.011219000
C	1.006301000	4.136256000	-0.205668000
C	3.293872000	3.484928000	0.201303000
H	-0.034774000	3.845635000	-0.341440000
H	4.039124000	2.713647000	0.376856000
C	1.388926000	5.470686000	-0.247648000
C	3.672222000	4.820982000	0.166018000
H	0.643958000	6.243320000	-0.420423000
H	4.715644000	5.087676000	0.315738000
C	2.725111000	5.819141000	-0.060951000
H	3.027503000	6.862572000	-0.087850000

I9

M06-L/BSI SCF energy in gas: -1873.34594 a.u.

M06/BSII SCF energy in benzene: -1872.754578 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1872.084285 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1871.965419 a.u.

Pd	0.138085000	0.606451000	-0.909030000
H	2.024606000	-0.761870000	-2.671774000
C	3.049321000	-0.703184000	-2.299702000
H	3.251807000	-1.595309000	-1.696649000
H	3.742965000	-0.664597000	-3.143344000
N	3.159166000	0.495371000	-1.504212000
C	2.079903000	1.109334000	-0.933595000
H	2.048854000	2.839351000	1.665744000
C	1.871875000	3.049000000	0.606223000
H	0.810789000	2.888663000	0.396219000
H	2.134174000	4.087191000	0.384469000
N	2.634099000	2.146030000	-0.227740000
C	4.017329000	2.169179000	-0.353332000
H	4.724465000	3.164394000	1.409013000
C	4.855375000	3.184962000	0.320313000
H	5.912741000	3.008338000	0.112090000
H	4.620940000	4.203416000	-0.010641000
C	4.351509000	1.121107000	-1.159678000
C	5.667730000	0.645613000	-1.638230000
H	5.856951000	-0.394831000	-1.348408000
H	5.757924000	0.696558000	-2.729691000
H	6.469340000	1.255667000	-1.216316000

O	-1.541556000	-1.839665000	-2.247083000
C	-1.024581000	-3.187011000	-2.188403000
C	0.490273000	-3.088609000	-2.293205000
H	0.745489000	-2.570130000	-3.222303000
H	0.964080000	-4.076177000	-2.311323000
H	0.900483000	-2.519200000	-1.451491000
C	-1.589187000	-3.974714000	-3.353454000
H	-2.679838000	-3.936515000	-3.375714000
H	-1.220178000	-3.561681000	-4.295992000
H	-1.279680000	-5.024466000	-3.300564000
H	0.440823000	-4.144634000	0.062690000
C	-0.535612000	-4.613662000	-0.078084000
H	-0.403880000	-5.539771000	-0.648820000
H	-0.929780000	-4.880050000	0.907531000
C	-1.494749000	-3.671655000	-0.778138000
C	-2.904112000	-4.248664000	-0.791332000
H	-3.598972000	-3.573074000	-1.300083000
H	-3.250510000	-4.376851000	0.237868000
H	-2.942673000	-5.221622000	-1.291388000
O	-1.550166000	-2.441066000	-0.029289000
B	-1.686999000	-1.405696000	-0.942933000
B	1.067396000	-0.225013000	0.682736000
O	1.016081000	0.341512000	1.937247000
O	1.704996000	-1.452793000	0.674031000
C	1.337560000	-0.729574000	2.871570000

C	2.266903000	-1.630375000	2.007215000
C	3.699124000	-1.115038000	1.947223000
H	3.724029000	-0.044039000	1.714909000
H	4.241783000	-1.644394000	1.157649000
H	2.851184000	0.501557000	3.822171000
H	4.229205000	-1.275578000	2.891621000
C	1.993412000	-0.119891000	4.091657000
H	1.274822000	0.507516000	4.625717000
H	2.333767000	-0.899984000	4.781515000
H	2.609323000	-3.260396000	3.379888000
H	2.872592000	-3.668886000	1.678719000
C	2.235003000	-3.100582000	2.362634000
H	1.223330000	-3.505382000	2.300054000
H	0.165829000	-2.178330000	3.998403000
C	0.024488000	-1.411149000	3.229970000
H	-0.677731000	-0.663993000	3.609446000
H	-0.434759000	-1.873859000	2.349160000
C	-1.819754000	1.130408000	-1.323329000
C	-2.062048000	0.031036000	-0.495449000
C	-2.672601000	0.174323000	0.864750000
C	-2.268932000	1.202303000	1.729699000
C	-3.659680000	-0.710142000	1.319188000
H	-1.483501000	1.881593000	1.401414000
H	-3.974692000	-1.526750000	0.672638000
C	-2.838646000	1.352093000	2.988118000

C	-4.234709000	-0.562904000	2.578348000
H	-2.505020000	2.157460000	3.638500000
H	-5.003194000	-1.259748000	2.904771000
C	-3.828408000	0.470172000	3.419120000
H	-4.275507000	0.584531000	4.403167000
C	-2.424968000	2.434783000	-1.167066000
C	-1.656362000	3.597859000	-1.380229000
C	-3.797369000	2.602709000	-0.880941000
H	-0.609583000	3.470759000	-1.658487000
H	-4.409384000	1.718221000	-0.717796000
C	-2.210579000	4.863332000	-1.245712000
C	-4.360067000	3.867620000	-0.796005000
H	-1.591938000	5.745414000	-1.395180000
H	-5.420898000	3.972608000	-0.580739000
C	-3.569103000	5.005779000	-0.962060000
H	-4.012237000	5.995216000	-0.886379000

I10

M06-L/BSI SCF energy in gas: -1873.364839 a.u.

M06/BSII SCF energy in benzene: -1872.767956 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1872.096405 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1871.978369 a.u.

Pd	-0.225969000	-0.254616000	-0.274176000
B	-2.122732000	-1.058938000	0.005028000
B	2.448280000	-1.595568000	-0.145033000
O	-3.066748000	-1.365276000	-0.970643000

O	-2.681400000	-1.173631000	1.277725000
O	1.116442000	-1.971434000	-0.422735000
O	3.198792000	-2.703891000	0.154755000
C	1.721764000	0.721970000	-0.248486000
C	2.817091000	-0.108511000	-0.176312000
C	-4.249313000	-1.877354000	-0.303590000
C	-4.119030000	-1.251456000	1.112697000
C	0.932381000	-3.347124000	0.025636000
C	2.391844000	-3.882919000	-0.105769000
C	4.230347000	0.333749000	-0.114493000
C	4.688866000	1.436146000	-0.854594000
C	5.167882000	-0.354519000	0.672889000
H	3.986019000	1.972134000	-1.487519000
H	4.843668000	-1.222586000	1.241111000
C	6.015231000	1.844398000	-0.794385000
C	6.495578000	0.056315000	0.737596000
H	6.340867000	2.699799000	-1.381468000
H	7.197593000	-0.491136000	1.362528000
C	6.927489000	1.159608000	0.006353000
H	7.965537000	1.478307000	0.052787000
C	1.778696000	2.173093000	-0.053285000
C	1.074440000	3.053468000	-0.897085000
C	2.405097000	2.733072000	1.078559000
H	0.568802000	2.638809000	-1.768482000
H	2.960990000	2.075253000	1.743675000

C	1.000078000	4.414669000	-0.629571000
C	2.310759000	4.091209000	1.360252000
H	0.447517000	5.065825000	-1.304418000
H	2.796330000	4.489922000	2.248464000
C	1.607167000	4.943904000	0.509736000
H	1.535952000	6.006013000	0.729487000
C	-1.420044000	1.290786000	-0.240651000
N	-2.198902000	1.780765000	-1.246324000
H	-3.321769000	0.939733000	-2.806691000
C	-2.284765000	1.185722000	-2.560420000
H	-1.880372000	1.864915000	-3.318017000
C	-2.865525000	2.938165000	-0.853636000
H	-4.635986000	3.037552000	-2.062730000
C	-3.786361000	3.661215000	-1.757221000
H	-4.190961000	4.546543000	-1.262239000
H	-3.288987000	3.995880000	-2.675012000
C	-2.499570000	3.172884000	0.438075000
C	-2.866417000	4.255207000	1.375950000
H	-1.994717000	4.853656000	1.667118000
H	-3.591753000	4.930954000	0.917817000
H	-3.314187000	3.865628000	2.298087000
N	-1.623308000	2.152513000	0.790920000
C	-0.972805000	2.032070000	2.076335000
H	-0.394416000	2.934195000	2.296588000
H	-1.710389000	1.857443000	2.866304000

H	-0.294015000	1.177218000	2.023464000
H	-1.701132000	0.263240000	-2.545024000
C	-0.091725000	-4.004121000	-0.872617000
H	-1.049163000	-3.481721000	-0.772260000
H	0.199444000	-3.962221000	-1.923527000
H	-0.239899000	-5.051914000	-0.590196000
C	0.437206000	-3.292297000	1.461036000
H	1.167592000	-2.804221000	2.114141000
H	-0.493010000	-2.714010000	1.498610000
H	0.240229000	-4.295120000	1.852675000
C	2.727943000	-4.345870000	-1.515652000
H	2.449370000	-3.592600000	-2.258013000
H	3.805316000	-4.511015000	-1.590544000
H	2.217750000	-5.281575000	-1.764573000
C	2.758437000	-4.947450000	0.907423000
H	3.792902000	-5.265909000	0.755223000
H	2.664994000	-4.578178000	1.930296000
H	2.114432000	-5.826227000	0.794999000
C	-4.704371000	-2.080060000	2.236699000
H	-5.781110000	-2.227874000	2.095812000
H	-4.227467000	-3.060017000	2.302357000
H	-4.559010000	-1.571396000	3.193670000
C	-4.640210000	0.180885000	1.168065000
H	-4.307760000	0.648617000	2.099796000
H	-4.240501000	0.773380000	0.336999000

H	-5.733913000	0.223907000	1.132226000
C	-4.136030000	-3.395473000	-0.285415000
H	-5.033964000	-3.867197000	0.127160000
H	-3.993364000	-3.760093000	-1.306314000
H	-3.274850000	-3.715155000	0.310756000
C	-5.469968000	-1.440065000	-1.088075000
H	-5.482947000	-0.357223000	-1.237580000
H	-5.473237000	-1.915591000	-2.072974000
H	-6.393787000	-1.728075000	-0.573709000

I11

M06-L/BSI SCF energy in gas: -1873,379953 a.u.

M06/BSII SCF energy in benzene: -1872,785985 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1872,115628 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1871,996723 a.u.

Pd	-0.225969000	-0.254616000	-0.274176000
B	-2.122732000	-1.058938000	0.005028000
B	2.448280000	-1.595568000	-0.145033000
O	-3.066748000	-1.365276000	-0.970643000
O	-2.681400000	-1.173631000	1.277725000
O	1.116442000	-1.971434000	-0.422735000
O	3.198792000	-2.703891000	0.154755000
C	1.721764000	0.721970000	-0.248486000
C	2.817091000	-0.108511000	-0.176312000
C	-4.249313000	-1.877354000	-0.303590000
C	-4.119030000	-1.251456000	1.112697000

C	0.932381000	-3.347124000	0.025636000
C	2.391844000	-3.882919000	-0.105769000
C	4.230347000	0.333749000	-0.114493000
C	4.688866000	1.436146000	-0.854594000
C	5.167882000	-0.354519000	0.672889000
H	3.986019000	1.972134000	-1.487519000
H	4.843668000	-1.222586000	1.241111000
C	6.015231000	1.844398000	-0.794385000
C	6.495578000	0.056315000	0.737596000
H	6.340867000	2.699799000	-1.381468000
H	7.197593000	-0.491136000	1.362528000
C	6.927489000	1.159608000	0.006353000
H	7.965537000	1.478307000	0.052787000
C	1.778696000	2.173093000	-0.053285000
C	1.074440000	3.053468000	-0.897085000
C	2.405097000	2.733072000	1.078559000
H	0.568802000	2.638809000	-1.768482000
H	2.960990000	2.075253000	1.743675000
C	1.000078000	4.414669000	-0.629571000
C	2.310759000	4.091209000	1.360252000
H	0.447517000	5.065825000	-1.304418000
H	2.796330000	4.489922000	2.248464000
C	1.607167000	4.943904000	0.509736000
H	1.535952000	6.006013000	0.729487000
C	-1.420044000	1.290786000	-0.240651000

N	-2.198902000	1.780765000	-1.246324000
H	-3.321769000	0.939733000	-2.806691000
C	-2.284765000	1.185722000	-2.560420000
H	-1.880372000	1.864915000	-3.318017000
C	-2.865525000	2.938165000	-0.853636000
H	-4.635986000	3.037552000	-2.062730000
C	-3.786361000	3.661215000	-1.757221000
H	-4.190961000	4.546543000	-1.262239000
H	-3.288987000	3.995880000	-2.675012000
C	-2.499570000	3.172884000	0.438075000
C	-2.866417000	4.255207000	1.375950000
H	-1.994717000	4.853656000	1.667118000
H	-3.591753000	4.930954000	0.917817000
H	-3.314187000	3.865628000	2.298087000
N	-1.623308000	2.152513000	0.790920000
C	-0.972805000	2.032070000	2.076335000
H	-0.394416000	2.934195000	2.296588000
H	-1.710389000	1.857443000	2.866304000
H	-0.294015000	1.177218000	2.023464000
H	-1.701132000	0.263240000	-2.545024000
C	-0.091725000	-4.004121000	-0.872617000
H	-1.049163000	-3.481721000	-0.772260000
H	0.199444000	-3.962221000	-1.923527000
H	-0.239899000	-5.051914000	-0.590196000
C	0.437206000	-3.292297000	1.461036000

H	1.167592000	-2.804221000	2.114141000
H	-0.493010000	-2.714010000	1.498610000
H	0.240229000	-4.295120000	1.852675000
C	2.727943000	-4.345870000	-1.515652000
H	2.449370000	-3.592600000	-2.258013000
H	3.805316000	-4.511015000	-1.590544000
H	2.217750000	-5.281575000	-1.764573000
C	2.758437000	-4.947450000	0.907423000
H	3.792902000	-5.265909000	0.755223000
H	2.664994000	-4.578178000	1.930296000
H	2.114432000	-5.826227000	0.794999000
C	-4.704371000	-2.080060000	2.236699000
H	-5.781110000	-2.227874000	2.095812000
H	-4.227467000	-3.060017000	2.302357000
H	-4.559010000	-1.571396000	3.193670000
C	-4.640210000	0.180885000	1.168065000
H	-4.307760000	0.648617000	2.099796000
H	-4.240501000	0.773380000	0.336999000
H	-5.733913000	0.223907000	1.132226000
C	-4.136030000	-3.395473000	-0.285415000
H	-5.033964000	-3.867197000	0.127160000
H	-3.993364000	-3.760093000	-1.306314000
H	-3.274850000	-3.715155000	0.310756000
C	-5.469968000	-1.440065000	-1.088075000
H	-5.482947000	-0.357223000	-1.237580000

H	-5.473237000	-1.915591000	-2.072974000
H	-6.393787000	-1.728075000	-0.573709000

I12

M06-L/BSI SCF energy in gas: -1873,379953 a.u.

M06/BSII SCF energy in benzene: -1872,785985 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1872,115628 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1871,996723 a.u.

Pd	0.224399000	0.430461000	-0.209020000
B	1.530249000	-1.044287000	0.016140000
B	-2.607064000	1.376012000	-0.050885000
O	2.035731000	-1.421782000	1.249839000
O	2.167439000	-1.697525000	-1.025214000
O	-1.435320000	2.035184000	-0.459855000
O	-3.560271000	2.287308000	0.341666000
C	-1.456540000	-0.796212000	-0.216627000
C	-2.670076000	-0.155603000	-0.084731000
C	2.881461000	-2.580029000	1.033570000
C	3.294005000	-2.414293000	-0.462609000
C	-1.519931000	3.402010000	0.017698000
C	-3.064648000	3.613287000	0.026781000
C	-3.991481000	-0.829743000	-0.004584000
C	-4.345565000	-1.902677000	-0.838823000
C	-4.952182000	-0.378872000	0.915086000
H	-3.626686000	-2.262340000	-1.570475000
H	-4.708838000	0.460212000	1.561474000

C	-5.593222000	-2.507829000	-0.742870000
C	-6.199652000	-0.985796000	1.014534000
H	-5.838872000	-3.337065000	-1.402032000
H	-6.919857000	-0.618620000	1.742058000
C	-6.527507000	-2.056399000	0.187646000
H	-7.502183000	-2.531612000	0.262910000
C	-1.354767000	-2.265696000	-0.232210000
C	-0.722934000	-2.920450000	-1.303378000
C	-1.861990000	-3.057879000	0.811397000
H	-0.284658000	-2.316161000	-2.094392000
H	-2.353551000	-2.568308000	1.648812000
C	-0.656588000	-4.308720000	-1.358633000
C	-1.759670000	-4.444440000	0.774636000
H	-0.184701000	-4.790467000	-2.212559000
H	-2.155965000	-5.034012000	1.598180000
C	-1.172108000	-5.080519000	-0.317709000
H	-1.106981000	-6.164826000	-0.352515000
C	2.029915000	1.464625000	-0.088659000
N	2.785595000	1.701548000	1.021126000
H	2.962832000	0.675208000	2.841847000
C	2.329442000	1.429597000	2.367254000
H	2.329391000	2.343759000	2.969780000
C	4.057879000	2.161920000	0.699750000
H	5.340209000	1.571064000	2.313847000
C	5.078236000	2.460892000	1.728287000

H	5.995720000	2.828902000	1.264109000
H	4.739644000	3.222598000	2.439902000
C	4.108075000	2.223444000	-0.662765000
C	5.200333000	2.612533000	-1.581457000
H	4.913742000	3.440055000	-2.240508000
H	6.080306000	2.931043000	-1.018472000
H	5.507387000	1.780887000	-2.227253000
N	2.864406000	1.795851000	-1.114224000
C	2.497155000	1.638484000	-2.503547000
H	2.494897000	2.602297000	-3.022543000
H	3.188644000	0.959227000	-3.010501000
H	1.494684000	1.202556000	-2.527203000
H	1.316260000	1.026378000	2.297993000
C	-0.741763000	4.287960000	-0.931440000
H	0.321402000	4.028632000	-0.884616000
H	-1.075376000	4.163595000	-1.963501000
H	-0.845420000	5.342921000	-0.655784000
C	-0.908318000	3.436236000	1.410488000
H	-1.460040000	2.787759000	2.098662000
H	0.121323000	3.068650000	1.351545000
H	-0.892760000	4.450074000	1.822608000
C	-3.613682000	3.984553000	-1.342817000
H	-3.240409000	3.304873000	-2.114107000
H	-4.703413000	3.909930000	-1.325695000
H	-3.342512000	5.007597000	-1.622407000

C	-3.561296000	4.576775000	1.084677000
H	-4.649578000	4.661471000	1.031581000
H	-3.297983000	4.240420000	2.089440000
H	-3.137657000	5.575032000	0.930312000
C	3.466323000	-3.714315000	-1.221614000
H	4.252096000	-4.331160000	-0.770962000
H	2.537867000	-4.289764000	-1.237106000
H	3.753039000	-3.508697000	-2.256858000
C	4.512516000	-1.516305000	-0.640977000
H	4.623338000	-1.267062000	-1.700930000
H	4.392828000	-0.578674000	-0.085533000
H	5.434713000	-2.002301000	-0.305309000
C	2.023909000	-3.810825000	1.280677000
H	2.606053000	-4.734836000	1.198857000
H	1.600657000	-3.758435000	2.287319000
H	1.190426000	-3.860527000	0.573731000
C	4.030956000	-2.514640000	2.020406000
H	4.564425000	-1.561951000	1.952550000
H	3.650491000	-2.617395000	3.040669000
H	4.748441000	-3.324499000	1.847306000

I13

M06-L/BSI SCF energy in gas: -2256.825485 a.u.

M06/BSII SCF energy in benzene: - 2256.088614 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -2255.247331 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -2255.103653 a.u.

Pd	-0.929235000	0.525867000	0.079620000
B	-0.752936000	-1.022971000	1.385466000
B	1.389752000	-1.656003000	-0.974176000
O	-0.984347000	-0.920435000	2.761779000
O	-0.302894000	-2.305394000	1.077520000
O	0.362855000	-1.518125000	-1.900208000
O	1.956423000	-2.916251000	-1.034782000
C	1.119155000	0.418520000	0.451900000
C	1.963110000	-0.503043000	-0.104349000
C	-0.835626000	-2.241565000	3.340915000
C	0.099828000	-2.940409000	2.314387000
C	0.107362000	-2.814657000	-2.488595000
C	1.449156000	-3.573762000	-2.211599000
C	3.435020000	-0.497525000	0.089304000
C	4.283473000	-0.801361000	-0.989042000
C	4.044198000	-0.216684000	1.323901000
H	3.838867000	-1.036194000	-1.955812000
H	3.416022000	0.009676000	2.181842000
C	5.666846000	-0.803467000	-0.852945000
C	5.426811000	-0.221579000	1.465879000
H	6.293300000	-1.037317000	-1.710778000
H	5.867019000	-0.003853000	2.436243000
C	6.248424000	-0.511443000	0.378305000
H	7.329411000	-0.516142000	0.491129000
C	1.564635000	1.596207000	1.218599000

C	2.476865000	2.519781000	0.677497000
C	0.984984000	1.905323000	2.463157000
H	2.944482000	2.290203000	-0.278939000
H	0.263712000	1.205388000	2.883461000
C	2.770877000	3.711150000	1.332203000
C	1.313433000	3.076170000	3.137710000
H	3.458613000	4.419877000	0.873398000
H	0.863184000	3.282605000	4.106622000
C	2.195437000	3.997155000	2.569637000
H	2.435296000	4.922733000	3.087528000
C	-2.966230000	0.346636000	-0.210465000
N	-3.564819000	0.088895000	-1.409668000
H	-3.255257000	-0.812236000	-3.272992000
C	-2.814668000	-0.036653000	-2.639219000
H	-2.798321000	0.909132000	-3.193826000
C	-4.951919000	0.022772000	-1.303431000
H	-5.647101000	-1.230721000	-2.905432000
C	-5.833738000	-0.245574000	-2.460887000
H	-6.882276000	-0.221593000	-2.155435000
H	-5.706348000	0.494473000	-3.259593000
C	-5.241141000	0.236146000	0.010983000
C	-6.533759000	0.271458000	0.730408000
H	-6.687617000	1.221656000	1.255392000
H	-7.364540000	0.144595000	0.032363000
H	-6.613636000	-0.523219000	1.481870000

N	-4.018964000	0.425602000	0.652698000
C	-3.870693000	0.680241000	2.067839000
H	-4.277288000	1.662041000	2.335164000
H	-4.391962000	-0.084797000	2.651562000
H	-2.805907000	0.640072000	2.309940000
H	-1.786888000	-0.314305000	-2.380872000
C	-0.207962000	-2.613605000	-3.960574000
H	-1.157901000	-2.080874000	-4.069202000
H	0.564511000	-2.031231000	-4.468221000
H	-0.308496000	-3.576188000	-4.474226000
C	-1.090731000	-3.424461000	-1.775849000
H	-0.887518000	-3.565189000	-0.713113000
H	-1.940008000	-2.737421000	-1.852426000
H	-1.376993000	-4.380123000	-2.228078000
C	2.486900000	-3.360581000	-3.307756000
H	2.230473000	-3.891930000	-4.229953000
H	2.592986000	-2.295999000	-3.542854000
H	3.456582000	-3.722602000	-2.955981000
C	1.288265000	-5.052591000	-1.920618000
H	2.263283000	-5.497442000	-1.703788000
H	0.638017000	-5.222341000	-1.060082000
H	0.862505000	-5.577501000	-2.783139000
C	-0.094902000	-4.435358000	2.166272000
H	0.124813000	-4.958716000	3.103649000
H	-1.115264000	-4.681835000	1.861610000

H	0.590808000	-4.813668000	1.401627000
C	1.568435000	-2.611054000	2.541161000
H	2.148006000	-2.911783000	1.663875000
H	1.708271000	-1.533262000	2.673332000
H	1.966896000	-3.127766000	3.420781000
C	-2.222972000	-2.867886000	3.392544000
H	-2.209172000	-3.852739000	3.871499000
H	-2.890898000	-2.219865000	3.967521000
H	-2.637257000	-2.977693000	2.384750000
C	-0.259741000	-2.098541000	4.735097000
H	0.657072000	-1.505513000	4.728513000
H	-0.978856000	-1.599678000	5.391495000
H	-0.035128000	-3.079287000	5.169833000
C	-0.487633000	2.402582000	-1.003356000
N	-0.593582000	3.634322000	-0.428680000
H	-2.159052000	4.682897000	0.505499000
C	-1.421084000	3.903849000	0.725079000
H	-1.930419000	2.972953000	0.988070000
H	-0.806617000	4.217230000	1.574902000
C	0.252508000	4.570963000	-1.012595000
C	0.905825000	3.914942000	-2.012315000
N	0.432366000	2.606258000	-1.987939000
C	0.921828000	1.551017000	-2.845413000
H	2.000567000	1.409776000	-2.708680000
H	0.726073000	1.780773000	-3.898980000

H	0.424337000	0.621060000	-2.563266000
H	2.150337000	5.437653000	-2.815842000
H	2.906616000	3.843494000	-2.781207000
C	1.958024000	4.370033000	-2.946905000
H	1.683896000	4.210882000	-3.996517000
H	1.100823000	6.517145000	-1.106431000
H	-0.566963000	6.501922000	-0.525325000
H	0.743254000	5.961278000	0.531078000
C	0.382579000	5.953957000	-0.505513000

TSRE1

Imaginary Frequency: -80.57

M06-L/BSI SCF energy in gas: -2256.822705 a.u.

M06/BSII SCF energy in benzene: -2256.085285 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -2255.242756 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -2255.103388 a.u.

Pd	-0.936815000	0.651606000	0.004821000
B	-0.489859000	-0.821574000	1.349954000
B	1.283724000	-1.820207000	-0.845281000
O	-0.656959000	-0.694446000	2.744397000
O	-0.422418000	-2.192147000	1.021141000
O	0.300786000	-1.592472000	-1.796240000
O	1.819344000	-3.087578000	-0.956002000
C	1.039128000	0.208818000	0.667291000
C	1.878623000	-0.706773000	0.074566000
C	-0.893215000	-2.013178000	3.283825000

C	-0.178758000	-2.919938000	2.243103000
C	0.011998000	-2.855432000	-2.444427000
C	1.323973000	-3.666010000	-2.181096000
C	3.344150000	-0.727893000	0.267946000
C	4.195285000	-1.055733000	-0.801276000
C	3.944821000	-0.456529000	1.509960000
H	3.757468000	-1.286044000	-1.771316000
H	3.310002000	-0.213042000	2.358788000
C	5.576819000	-1.080986000	-0.650353000
C	5.324294000	-0.491756000	1.666423000
H	6.207497000	-1.328352000	-1.500997000
H	5.758941000	-0.282641000	2.640885000
C	6.150761000	-0.797818000	0.586304000
H	7.230128000	-0.822891000	0.710095000
C	1.539862000	1.429359000	1.339999000
C	2.473822000	2.243211000	0.668660000
C	1.033956000	1.903333000	2.564476000
H	2.874756000	1.898928000	-0.282817000
H	0.313650000	1.292003000	3.100790000
C	2.862351000	3.475144000	1.174537000
C	1.449424000	3.125858000	3.085995000
H	3.566097000	4.088097000	0.612678000
H	1.051422000	3.460568000	4.041807000
C	2.355377000	3.927795000	2.393340000
H	2.667289000	4.887415000	2.798662000

C	-2.968883000	0.476014000	-0.225648000
N	-3.631424000	0.156968000	-1.378620000
H	-3.403204000	-0.883181000	-3.182154000
C	-2.943137000	-0.057754000	-2.629858000
H	-2.961872000	0.842495000	-3.255607000
C	-5.013751000	0.147286000	-1.211633000
H	-5.815354000	-1.191721000	-2.690625000
C	-5.951189000	-0.171376000	-2.311363000
H	-6.985559000	-0.087460000	-1.969726000
H	-5.831078000	0.504554000	-3.166314000
C	-5.239711000	0.458432000	0.095640000
C	-6.499277000	0.579070000	0.862829000
H	-6.604423000	1.563742000	1.333486000
H	-7.362065000	0.434778000	0.208071000
H	-6.570568000	-0.165578000	1.665200000
N	-3.985016000	0.645712000	0.673241000
C	-3.759146000	1.007676000	2.053061000
H	-3.986905000	2.065300000	2.231119000
H	-4.386039000	0.401798000	2.714003000
H	-2.704751000	0.819830000	2.280616000
H	-1.901548000	-0.305500000	-2.399525000
C	-0.274009000	-2.582611000	-3.910193000
H	-1.204763000	-2.015975000	-4.009909000
H	0.524341000	-2.004077000	-4.381064000
H	-0.395266000	-3.519113000	-4.465914000

C	-1.213221000	-3.457059000	-1.772636000
H	-1.025959000	-3.661891000	-0.717839000
H	-2.035094000	-2.735712000	-1.816604000
H	-1.528339000	-4.377351000	-2.275877000
C	2.391469000	-3.419073000	-3.240572000
H	2.145305000	-3.898133000	-4.193707000
H	2.521479000	-2.346158000	-3.420460000
H	3.346221000	-3.817757000	-2.887489000
C	1.119398000	-5.153063000	-1.973833000
H	2.078744000	-5.636482000	-1.770539000
H	0.454350000	-5.350381000	-1.130508000
H	0.690413000	-5.617482000	-2.868670000
C	-0.760489000	-4.312189000	2.100350000
H	-0.703562000	-4.860467000	3.047596000
H	-1.804448000	-4.281033000	1.778761000
H	-0.191446000	-4.879147000	1.356068000
C	1.325565000	-2.991516000	2.472966000
H	1.811008000	-3.415800000	1.589527000
H	1.746914000	-1.994840000	2.635828000
H	1.569111000	-3.614926000	3.339671000
C	-2.401706000	-2.231395000	3.306364000
H	-2.667717000	-3.199914000	3.743068000
H	-2.869591000	-1.447804000	3.909793000
H	-2.814885000	-2.175785000	2.293442000
C	-0.323177000	-2.080734000	4.686371000

H	0.726235000	-1.780203000	4.705424000
H	-0.877324000	-1.412895000	5.352396000
H	-0.400497000	-3.096389000	5.091264000
C	-0.311922000	2.447200000	-1.130715000
N	-0.335360000	3.707425000	-0.605522000
H	-1.778884000	4.963042000	0.266188000
C	-1.175767000	4.081439000	0.508107000
H	-1.828938000	3.231970000	0.723647000
H	-0.568350000	4.290742000	1.395094000
C	0.618072000	4.544794000	-1.173847000
C	1.260929000	3.798105000	-2.114540000
N	0.672387000	2.537309000	-2.073109000
C	1.115257000	1.408109000	-2.856942000
H	2.163489000	1.169296000	-2.636695000
H	1.021003000	1.610714000	-3.929758000
H	0.507848000	0.543067000	-2.582510000
H	2.702506000	5.165920000	-2.867490000
H	3.277732000	3.499954000	-2.776993000
C	2.401696000	4.123372000	-2.998315000
H	2.167757000	3.978926000	-4.059875000
H	1.648793000	6.400919000	-1.276585000
H	-0.047144000	6.561721000	-0.813059000
H	1.132820000	5.948022000	0.350754000
C	0.843036000	5.930230000	-0.707788000

I14

M06-L/BSI SCF energy in gas: -2256.841866 a.u.

M06/BSII SCF energy in benzene: -2256.113692 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -2255.269635 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -2255.12637 a.u.

Pd	1.563445000	-1.652858000	-0.902529000
B	0.012139000	0.492498000	1.684603000
B	-1.485124000	2.351108000	-0.065165000
O	0.565635000	0.098563000	2.882077000
O	0.767377000	1.459497000	1.044346000
O	-1.173138000	2.498960000	-1.398451000
O	-1.480630000	3.543334000	0.624612000
C	-1.429298000	0.104635000	1.242549000
C	-2.111992000	1.034866000	0.509180000
C	1.878851000	0.699318000	2.979270000
C	1.760927000	1.912873000	2.003549000
C	-0.766020000	3.879276000	-1.589080000
C	-1.428863000	4.595322000	-0.370104000
C	-3.578049000	1.005380000	0.264376000
C	-4.116009000	1.336720000	-0.991130000
C	-4.477435000	0.738141000	1.310732000
H	-3.440577000	1.582582000	-1.808278000
H	-4.081073000	0.504582000	2.295429000
C	-5.492965000	1.349967000	-1.202440000
C	-5.849113000	0.767419000	1.103122000
H	-5.882695000	1.594381000	-2.187711000

H	-6.521513000	0.559653000	1.931479000
C	-6.366017000	1.063432000	-0.158148000
H	-7.440395000	1.081787000	-0.319844000
C	-2.045606000	-1.162042000	1.707083000
C	-2.917149000	-1.879035000	0.872524000
C	-1.779985000	-1.700270000	2.977570000
H	-3.120038000	-1.497083000	-0.123456000
H	-1.100060000	-1.179874000	3.642609000
C	-3.517113000	-3.059545000	1.287343000
C	-2.383023000	-2.883134000	3.396346000
H	-4.187191000	-3.583938000	0.608196000
H	-2.167182000	-3.269207000	4.389730000
C	-3.257070000	-3.570238000	2.558023000
H	-3.727368000	-4.493428000	2.888066000
C	3.456051000	-0.897134000	-0.885669000
N	3.927101000	0.254129000	-1.465798000
H	3.192657000	2.192622000	-1.762251000
C	3.068142000	1.180372000	-2.162190000
H	3.279340000	1.194099000	-3.237192000
C	5.286012000	0.451667000	-1.245429000
H	5.620807000	2.572765000	-1.312465000
C	6.012231000	1.641317000	-1.742073000
H	7.071849000	1.582787000	-1.481652000
H	5.946372000	1.742487000	-2.831684000
C	5.707443000	-0.611990000	-0.503109000

C	7.037939000	-0.946433000	0.051194000
H	7.416460000	-1.904747000	-0.324118000
H	7.769487000	-0.179039000	-0.213074000
H	7.019935000	-1.019715000	1.145747000
N	4.589303000	-1.413391000	-0.306704000
C	4.585026000	-2.636067000	0.458918000
H	5.243775000	-3.387159000	0.010725000
H	4.904752000	-2.455304000	1.491426000
H	3.553194000	-3.005049000	0.454692000
H	2.036638000	0.848570000	-1.994208000
C	-1.262594000	4.340798000	-2.944494000
H	-0.769249000	3.770707000	-3.736300000
H	-2.340494000	4.199649000	-3.049424000
H	-1.036005000	5.400903000	-3.103061000
C	0.752226000	3.900998000	-1.537414000
H	1.108234000	3.504594000	-0.581288000
H	1.143055000	3.259659000	-2.331266000
H	1.150570000	4.910371000	-1.682195000
C	-2.870504000	5.006077000	-0.637232000
H	-2.933584000	5.838847000	-1.344521000
H	-3.450981000	4.166870000	-1.034479000
H	-3.335486000	5.314976000	0.302232000
C	-0.641441000	5.763265000	0.188019000
H	-1.144965000	6.162604000	1.072567000
H	0.370252000	5.471295000	0.478077000

H	-0.566299000	6.569118000	-0.550337000
C	3.048026000	2.239545000	1.275137000
H	3.840039000	2.485272000	1.991948000
H	3.378774000	1.397019000	0.665838000
H	2.910540000	3.109942000	0.624504000
C	1.188511000	3.155328000	2.670143000
H	0.949397000	3.897065000	1.903795000
H	0.259027000	2.929884000	3.201319000
H	1.897799000	3.596808000	3.377257000
C	2.872474000	-0.355232000	2.522067000
H	3.906683000	0.007523000	2.559526000
H	2.789344000	-1.228562000	3.175754000
H	2.640909000	-0.676561000	1.498683000
C	2.126937000	1.083365000	4.425149000
H	1.333994000	1.721380000	4.820871000
H	2.178715000	0.183958000	5.044326000
H	3.080226000	1.613907000	4.525354000
C	-0.248666000	-2.547465000	-1.191222000
N	-0.654706000	-3.807070000	-0.837414000
H	0.262470000	-5.631017000	-0.339670000
C	0.083100000	-4.637046000	0.082868000
H	1.039249000	-4.135463000	0.264375000
H	-0.458282000	-4.742315000	1.030572000
C	-1.887575000	-4.143520000	-1.379046000
C	-2.292108000	-3.060793000	-2.103660000

N	-1.284952000	-2.112630000	-1.974121000
C	-1.333592000	-0.787088000	-2.542126000
H	-2.190762000	-0.227582000	-2.150439000
H	-1.401996000	-0.826535000	-3.634520000
H	-0.412330000	-0.274829000	-2.247800000
H	-4.212511000	-3.660432000	-2.793811000
H	-4.093417000	-1.939171000	-2.412578000
C	-3.548509000	-2.793312000	-2.838424000
H	-3.376663000	-2.564238000	-3.896880000
H	-3.530131000	-5.475867000	-1.596554000
H	-1.968612000	-6.291576000	-1.484468000
H	-2.706745000	-5.599459000	-0.038306000
C	-2.550309000	-5.439263000	-1.112928000

TSRE2

Imaginary Frequency: -141.74

M06-L/BSI SCF energy in gas: -2256.815845 a.u.

M06/BSII SCF energy in benzene: -2256.077022 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -2255.230936 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -2255.092964 a.u.

Pd	1.099999000	-0.613077000	-0.626200000
B	1.501468000	1.124388000	0.345216000
B	-2.980742000	0.772988000	0.574788000
O	1.668010000	1.311563000	1.729088000
O	2.145519000	2.157735000	-0.349637000
O	-3.865520000	0.409906000	-0.423145000

O	-3.601622000	1.458428000	1.595431000
C	-0.470671000	0.836214000	-0.122420000
C	-1.489436000	0.296063000	0.622801000
C	2.647389000	2.351297000	1.926011000
C	2.555337000	3.162989000	0.596577000
C	-5.131932000	1.063014000	-0.151381000
C	-5.030793000	1.369407000	1.380038000
C	-1.344979000	-0.924406000	1.448412000
C	-0.246351000	-1.176472000	2.292026000
C	-2.365582000	-1.890259000	1.406360000
H	0.539732000	-0.430386000	2.367241000
H	-3.214948000	-1.730215000	0.742571000
C	-0.184035000	-2.342755000	3.047945000
C	-2.291712000	-3.065734000	2.148352000
H	0.667176000	-2.505448000	3.707623000
H	-3.092164000	-3.799640000	2.074318000
C	-1.199486000	-3.299752000	2.977730000
H	-1.142561000	-4.208715000	3.571940000
C	-0.781611000	2.014168000	-0.961358000
C	-1.620885000	3.053961000	-0.524104000
C	-0.200349000	2.151898000	-2.234847000
H	-2.021234000	3.024620000	0.487707000
H	0.507050000	1.385054000	-2.554112000
C	-1.907907000	4.146367000	-1.338814000
C	-0.498721000	3.230613000	-3.056515000

H	-2.555688000	4.937904000	-0.966576000
H	-0.045075000	3.299069000	-4.042608000
C	-1.360753000	4.235531000	-2.615373000
H	-1.584024000	5.087523000	-3.251962000
C	-0.212048000	-2.239384000	-1.351985000
N	-1.447475000	-2.131074000	-1.921648000
H	-2.194189000	-1.250477000	-3.671731000
C	-1.883474000	-0.967271000	-2.660270000
H	-2.708125000	-0.460011000	-2.150092000
C	-2.235655000	-3.256686000	-1.715784000
H	-3.722765000	-3.300696000	-3.273022000
C	-3.638126000	-3.340506000	-2.180138000
H	-4.098788000	-4.274841000	-1.849223000
H	-4.239303000	-2.511620000	-1.784256000
C	-1.467605000	-4.131371000	-1.006237000
C	-1.762001000	-5.474740000	-0.462083000
H	-1.594707000	-5.511112000	0.621997000
H	-2.805590000	-5.743445000	-0.644953000
H	-1.138973000	-6.258059000	-0.911379000
N	-0.246607000	-3.496070000	-0.813012000
C	0.852807000	-4.072683000	-0.076358000
H	0.643504000	-4.085508000	1.000331000
H	1.045450000	-5.096210000	-0.413989000
H	1.732012000	-3.451641000	-0.262781000
H	-1.037861000	-0.281544000	-2.720699000

C	-6.248372000	0.112470000	-0.536626000
H	-6.230524000	-0.063654000	-1.616160000
H	-6.150062000	-0.853017000	-0.034827000
H	-7.226520000	0.535377000	-0.282887000
C	-5.178684000	2.315366000	-1.012024000
H	-4.368777000	3.002132000	-0.752840000
H	-5.049149000	2.037627000	-2.061614000
H	-6.133262000	2.840583000	-0.908298000
C	-5.528820000	0.228078000	2.255143000
H	-6.614683000	0.107559000	2.190316000
H	-5.055569000	-0.718833000	1.976897000
H	-5.265877000	0.434000000	3.295502000
C	-5.664816000	2.679915000	1.801774000
H	-5.536518000	2.827454000	2.877162000
H	-5.208522000	3.528573000	1.287437000
H	-6.738984000	2.681440000	1.586533000
C	3.870313000	3.751356000	0.118944000
H	4.281709000	4.456474000	0.850107000
H	4.613830000	2.970642000	-0.065342000
H	3.714025000	4.294159000	-0.818033000
C	1.477341000	4.236373000	0.635074000
H	1.315397000	4.621578000	-0.375522000
H	0.527322000	3.824633000	0.986759000
H	1.757363000	5.073093000	1.284303000
C	4.003305000	1.677802000	2.107858000

H	4.792940000	2.405481000	2.324328000
H	3.946483000	0.980113000	2.949623000
H	4.288763000	1.114461000	1.214013000
C	2.284396000	3.133729000	3.173690000
H	1.257834000	3.501830000	3.130879000
H	2.375853000	2.495777000	4.057522000
H	2.955470000	3.990082000	3.306586000
H	4.423355000	-0.033763000	-3.436139000
H	2.712417000	-0.097565000	-2.917732000
C	3.722066000	0.208466000	-2.632461000
H	3.714603000	1.290516000	-2.459821000
H	6.494459000	0.944282000	-1.846974000
H	6.694875000	-0.635908000	-2.599557000
C	6.553321000	-0.130515000	-1.636391000
H	7.455227000	-0.299899000	-1.043391000
C	5.358770000	-0.620491000	-0.913672000
N	4.068503000	-0.504071000	-1.424627000
C	3.122314000	-1.007505000	-0.575163000
N	3.873475000	-1.469264000	0.475213000
H	3.510619000	-1.363447000	2.541288000
C	3.288770000	-2.004492000	1.680537000
H	3.653596000	-3.017173000	1.887165000
H	2.204605000	-2.023879000	1.540892000
C	5.235970000	-1.241074000	0.293163000
C	6.248734000	-1.620316000	1.302404000

H	6.082671000	-1.109218000	2.259399000
H	6.248463000	-2.696833000	1.511341000
H	7.251489000	-1.354339000	0.959525000

L = PM_3

1

M06-L/BSI SCF energy in gas: -1589.184936 a.u.

M06/BSII SCF energy in benzene: -1589.283781 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1589.344204 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1589.254433 a.u.

H	-3.975194000	5.240777000	-0.002153000
C	-3.403635000	4.316892000	-0.010537000
H	-4.929936000	3.173301000	0.991163000
C	-3.938216000	3.155124000	0.545969000
C	-3.212669000	1.971420000	0.533756000
H	-3.628121000	1.064671000	0.967435000
C	-1.922108000	1.922348000	-0.028232000
C	-1.398881000	3.102676000	-0.581689000
C	-2.131838000	4.283239000	-0.579216000
H	-1.709319000	5.182670000	-1.020322000
H	-0.405985000	3.061312000	-1.026040000
C	-1.176562000	0.690668000	-0.031855000
C	-1.226924000	-0.600310000	0.038383000
C	-2.066664000	-1.769336000	0.031178000
H	-3.700842000	-0.777288000	-0.961258000

C	-3.356993000	-1.715126000	-0.531019000
C	-4.172487000	-2.838803000	-0.547463000
H	-5.162600000	-2.777601000	-0.992262000
C	-3.729851000	-4.041044000	0.004327000
H	-4.371207000	-4.917723000	-0.008020000
C	-2.459488000	-4.108886000	0.573131000
H	-2.107909000	-5.040086000	1.010312000
C	-1.637043000	-2.989069000	0.579802000
Pd	0.758122000	-0.030152000	0.004269000
H	-0.643502000	-3.028294000	1.022937000
P	2.101620000	-1.946851000	-0.116776000
P	2.243230000	1.779244000	0.115858000
C	3.840179000	-1.816807000	-0.710541000
H	4.283974000	-2.803229000	-0.885137000
H	3.875195000	-1.245331000	-1.642499000
H	4.448226000	-1.291262000	0.030367000
C	1.474721000	-3.225441000	-1.276379000
H	1.437152000	-2.809250000	-2.286250000
H	2.110683000	-4.117639000	-1.283951000
H	0.455904000	-3.511675000	-1.002575000
C	2.383006000	-2.950232000	1.398874000
H	2.989821000	-3.838882000	1.191605000
H	2.893572000	-2.342152000	2.150556000
H	1.428743000	-3.267369000	1.826843000
C	3.970094000	1.522124000	0.702078000

H	3.969518000	0.959327000	1.639950000
H	4.530424000	0.945554000	-0.038147000
H	4.488048000	2.473941000	0.863922000
C	2.592662000	2.754870000	-1.404128000
H	3.266865000	3.594842000	-1.202322000
H	3.050742000	2.107442000	-2.156784000
H	1.663146000	3.143312000	-1.827479000
C	1.720881000	3.104658000	1.275097000
H	1.654108000	2.694014000	2.285697000
H	2.426039000	3.943392000	1.278733000
H	0.726975000	3.470530000	1.003859000

1_alkyne

M06-L/BSI SCF energy in gas: -1128.502476 a.u.

M06/BSII SCF energy in benzene: -1128.222198 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1127.966264 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1127.894693 a.u.

H	0.394915000	6.334704000	-0.114865000
C	0.479218000	5.252031000	-0.086534000
H	2.630355000	5.262987000	0.033862000
C	1.733971000	4.649951000	-0.002234000
C	1.847135000	3.267089000	0.033452000
H	2.824296000	2.795926000	0.096345000
C	0.697669000	2.456130000	-0.014655000
C	-0.561000000	3.075107000	-0.097371000
C	-0.665874000	4.458346000	-0.133647000

H	-1.646241000	4.922432000	-0.200336000
H	-1.442663000	2.437996000	-0.133475000
C	0.828860000	1.031347000	0.014034000
C	1.371562000	-0.108762000	-0.006296000
C	2.375917000	-1.127395000	-0.016771000
H	3.963539000	0.215177000	0.554193000
C	3.710605000	-0.809564000	0.296935000
C	4.689085000	-1.794298000	0.284860000
H	5.715083000	-1.534341000	0.530671000
C	4.361148000	-3.109827000	-0.039785000
H	5.130429000	-3.876989000	-0.049136000
C	3.042322000	-3.436269000	-0.352224000
H	2.781241000	-4.459768000	-0.606847000
C	2.057834000	-2.458169000	-0.339476000
Pd	-0.722873000	-0.407774000	0.040281000
H	1.023168000	-2.695055000	-0.581091000
P	-2.893912000	-1.182283000	0.051582000
C	-3.892030000	-1.110938000	1.592449000
H	-4.891027000	-1.537466000	1.447272000
H	-3.383369000	-1.659790000	2.388082000
H	-3.994993000	-0.073795000	1.920018000
C	-4.064713000	-0.422412000	-1.141421000
H	-3.679020000	-0.531617000	-2.157419000
H	-5.056513000	-0.884841000	-1.082726000
H	-4.162207000	0.646552000	-0.936397000

C	-3.060388000	-2.959589000	-0.379185000
H	-2.638089000	-3.141820000	-1.369979000
H	-2.506562000	-3.569863000	0.338212000
H	-4.109416000	-3.275241000	-0.375820000

I1

M06-L/BSI SCF energy in gas: -1050.173195 a.u.

M06/BSII SCF energy in benzene: -1050.079132 a.u.

M06/BSII//M06-L/BSI free energy in benzene:: -1049.894013 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1049.832381 a.u.

Pd	0.000176000	0.018329000	-0.024973000
P	-2.288722000	-0.000771000	0.002236000
P	2.288781000	-0.000026000	0.002521000
C	-3.184543000	1.118613000	-1.149478000
H	-2.896686000	2.154879000	-0.957985000
H	-2.911860000	0.884481000	-2.180977000
H	-4.271146000	1.025590000	-1.039145000
C	-3.125775000	-1.593394000	-0.377774000
H	-4.216621000	-1.498378000	-0.327510000
H	-2.844858000	-1.929949000	-1.378394000
H	-2.803391000	-2.358609000	0.332161000
C	-3.118594000	0.432776000	1.584979000
H	-2.830424000	1.441812000	1.889039000
H	-4.210130000	0.386656000	1.494777000
H	-2.798218000	-0.254588000	2.371166000

C	3.184514000	1.116652000	-1.151817000
H	4.271101000	1.017439000	-1.046979000
H	2.905590000	0.886002000	-2.182421000
H	2.903243000	2.154137000	-0.957367000
C	3.121476000	0.433471000	1.583616000
H	2.803093000	-0.255233000	2.369497000
H	4.212825000	0.387892000	1.491508000
H	2.833349000	1.441804000	1.889849000
C	3.122010000	-1.595012000	-0.376394000
H	2.801091000	-2.357539000	0.337056000
H	2.836266000	-1.933965000	-1.374826000
H	4.213286000	-1.502230000	-0.330819000

I2

M06-L/BSI SCF energy in gas: -1872.677405 a.u.

M06/BSII SCF energy in benzene: -1872.370043 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1871.837973 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1871.736469 a.u.

Pd	0.000024000	0.000655000	-1.181215000
O	1.752033000	0.972276000	1.222406000
C	2.994406000	0.407354000	1.701492000
C	2.965083000	0.489486000	3.222505000
H	2.811500000	1.528343000	3.525745000
H	3.901514000	0.135735000	3.665876000

H	2.143161000	-0.107634000	3.627955000
C	4.155573000	1.212105000	1.154541000
H	4.159720000	1.232617000	0.062727000
H	4.099294000	2.243803000	1.514556000
H	5.110433000	0.792108000	1.489446000
H	3.228129000	-2.100957000	3.059175000
C	3.624993000	-2.081504000	2.042199000
H	4.699156000	-1.870645000	2.091540000
H	3.500349000	-3.080697000	1.614387000
C	2.909632000	-1.057510000	1.183634000
C	3.338492000	-1.187003000	-0.273120000
H	2.811754000	-0.456613000	-0.901507000
H	3.077860000	-2.185500000	-0.637937000
H	4.418508000	-1.051728000	-0.393874000
O	1.490277000	-1.313357000	1.247394000
B	0.841499000	-0.087598000	1.086849000
B	-0.841628000	0.086056000	1.086862000
O	-1.752230000	-0.973866000	1.221460000
O	-1.490326000	1.311760000	1.248267000
C	-2.994513000	-0.409252000	1.701153000
C	-2.909708000	1.056026000	1.184439000
C	-3.338679000	1.186709000	-0.272159000
H	-2.811961000	0.456867000	-0.901188000
H	-3.078118000	2.185526000	-0.636131000
H	-4.160121000	-1.233240000	0.061917000

H	-4.418698000	1.051496000	-0.392941000
C	-4.155799000	-1.213526000	1.153745000
H	-4.099509000	-2.245496000	1.512970000
H	-5.110596000	-0.793754000	1.489101000
H	-4.699107000	1.868633000	2.093113000
H	-3.500159000	3.078915000	1.616912000
C	-3.624916000	2.079382000	2.043894000
H	-3.227985000	2.097926000	3.060864000
H	-3.901323000	-0.139209000	3.665907000
C	-2.964960000	-0.492588000	3.222091000
H	-2.811307000	-1.531683000	3.524474000
H	-2.142978000	0.104225000	3.627869000
P	-0.429829000	-2.257415000	-1.568184000
C	0.411275000	-3.009476000	-3.020921000
H	1.495343000	-2.943634000	-2.897321000
H	0.134165000	-4.062149000	-3.150301000
H	-2.314409000	-3.714237000	-2.186456000
H	0.147317000	-2.459896000	-3.927820000
C	-2.182060000	-2.653731000	-1.943906000
H	-2.783186000	-2.416451000	-1.062514000
H	-2.541974000	-2.047861000	-2.779197000
H	-0.644207000	-3.242544000	0.623736000
C	-0.092610000	-3.514283000	-0.278851000
H	0.967710000	-3.514731000	-0.021186000
H	-0.394521000	-4.512690000	-0.615283000

P	0.429994000	2.259281000	-1.565776000
C	-0.411118000	3.012924000	-3.017699000
H	-1.495191000	2.946887000	-2.894283000
H	-0.134058000	4.065762000	-3.145819000
H	2.314186000	3.717142000	-2.182602000
H	-0.147036000	2.464410000	-3.925209000
C	2.182138000	2.656351000	-1.941140000
H	2.783456000	2.418297000	-1.060099000
H	2.542107000	2.051465000	-2.777121000
H	0.644291000	3.241878000	0.627231000
C	0.092596000	3.514605000	-0.275002000
H	-0.967721000	3.514507000	-0.017318000
H	0.394313000	4.513471000	-0.610252000

TSOA1

Imaginary Frequency: -27.95

M06-L/BSI SCF energy in gas: -1872.652767 a.u.

M06/BSII SCF energy in benzene: -1872.346353 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1871.816433 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1871.714744 a.u.

Pd	0.278952000	1.173647000	0.032573000
O	1.603524000	-1.546203000	0.696422000
C	2.108311000	-2.737527000	0.050466000
C	1.217049000	-3.890118000	0.494803000
H	1.211950000	-3.940098000	1.586624000

H	1.563728000	-4.851723000	0.102458000
H	0.185540000	-3.734596000	0.164562000
C	3.536511000	-2.978954000	0.497681000
H	4.175839000	-2.115214000	0.300535000
H	3.563935000	-3.182792000	1.571711000
H	3.964599000	-3.844908000	-0.019789000
H	0.696144000	-4.052766000	-2.070403000
C	1.636731000	-3.575197000	-2.354447000
H	2.435205000	-4.324096000	-2.305840000
H	1.546253000	-3.247849000	-3.393698000
C	1.948570000	-2.390896000	-1.461243000
C	3.123581000	-1.595739000	-2.013118000
H	3.350306000	-0.740392000	-1.369042000
H	2.862945000	-1.210795000	-3.002403000
H	4.024945000	-2.210009000	-2.108651000
O	0.804857000	-1.506336000	-1.455455000
B	0.715964000	-0.930852000	-0.190427000
B	-1.054205000	-0.515544000	0.239694000
O	-2.123509000	-0.640929000	-0.654072000
O	-1.392816000	-1.032027000	1.486373000
C	-3.097069000	-1.519563000	-0.043082000
C	-2.806114000	-1.333713000	1.477540000
C	-3.521094000	-0.131732000	2.078052000
H	-3.349981000	0.763500000	1.472407000
H	-3.122316000	0.059108000	3.077548000

H	-4.706646000	-0.066315000	-0.225363000
H	-4.600027000	-0.296771000	2.163842000
C	-4.488671000	-1.106724000	-0.478330000
H	-4.591151000	-1.220374000	-1.561080000
H	-5.247045000	-1.737631000	-0.001298000
H	-4.082968000	-2.895062000	2.266505000
H	-2.806750000	-2.358655000	3.369189000
C	-3.037480000	-2.571354000	2.321989000
H	-2.400812000	-3.398510000	1.999982000
H	-3.503462000	-3.663823000	-0.175722000
C	-2.784981000	-2.924331000	-0.543668000
H	-2.809300000	-2.928859000	-1.636450000
H	-1.781131000	-3.232432000	-0.235134000
P	-1.241230000	2.622517000	-1.020029000
C	-0.896820000	4.420223000	-1.232464000
H	0.121417000	4.554474000	-1.607893000
H	-1.596465000	4.897350000	-1.928853000
H	-3.590854000	3.287644000	-1.355649000
H	-0.962882000	4.928582000	-0.266556000
C	-3.036475000	2.678120000	-0.633033000
H	-3.419139000	1.653849000	-0.663498000
H	-3.202879000	3.080310000	0.369772000
H	-1.660680000	1.032369000	-2.783972000
C	-1.316752000	2.069904000	-2.768691000
H	-0.318381000	2.097907000	-3.212045000

H	-1.992161000	2.691374000	-3.367975000
P	2.284038000	1.919916000	0.985946000
C	2.834182000	3.675335000	0.877999000
H	2.011265000	4.334544000	1.167935000
H	3.695616000	3.880127000	1.524516000
H	4.660745000	1.432130000	1.428903000
H	3.104396000	3.918457000	-0.153198000
C	3.891501000	1.063408000	0.740974000
H	3.735749000	-0.005563000	0.912936000
H	4.244749000	1.199184000	-0.284940000
H	1.919742000	0.680861000	3.036869000
C	2.105998000	1.732665000	2.804846000
H	1.246444000	2.308176000	3.156749000
H	3.002513000	2.068088000	3.339178000

I3

M06-L/BSI SCF energy in gas: -1872.65783 a.u.

M06/BSII SCF energy in benzene: -1872.352225 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1871.823689 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1871.719447 a.u.

Pd	-1.170064000	-0.000034000	0.000131000
O	0.815345000	-2.146510000	-0.786367000
C	2.130896000	-2.689094000	-0.509147000
C	3.108714000	-1.957693000	-1.417009000
H	2.804795000	-2.097022000	-2.457709000
H	4.131353000	-2.332298000	-1.302109000

H	3.092119000	-0.883813000	-1.210726000
C	2.116529000	-4.172311000	-0.820716000
H	1.326262000	-4.693295000	-0.274618000
H	1.946766000	-4.327422000	-1.889844000
H	3.074957000	-4.636987000	-0.562946000
H	4.159571000	-1.189559000	0.816562000
C	3.750507000	-2.018962000	1.398374000
H	4.401769000	-2.889192000	1.259173000
H	3.785402000	-1.737305000	2.454613000
C	2.323381000	-2.338297000	0.996097000
C	1.736207000	-3.381789000	1.936953000
H	0.703069000	-3.619528000	1.666692000
H	1.730413000	-2.983676000	2.954939000
H	2.317272000	-4.309833000	1.933781000
O	1.524421000	-1.140088000	1.142391000
B	0.571878000	-1.117759000	0.125385000
B	0.571654000	1.117979000	-0.125394000
O	0.815007000	2.146778000	0.786338000
O	1.524199000	1.140350000	-1.142385000
C	2.130531000	2.689448000	0.509139000
C	2.323097000	2.338617000	-0.996090000
C	1.735924000	3.382043000	-1.937013000
H	0.702762000	3.619762000	-1.666839000
H	1.730215000	2.983910000	-2.954991000
H	1.325731000	4.693566000	0.274542000

H	2.316956000	4.310110000	-1.933818000
C	2.116047000	4.172680000	0.820662000
H	1.946271000	4.327810000	1.889784000
H	3.074437000	4.637423000	0.562872000
H	4.401472000	2.889593000	-1.259090000
H	3.785221000	1.737643000	-2.454526000
C	3.750253000	2.019330000	-1.398299000
H	4.159325000	1.189970000	-0.816433000
H	4.130974000	2.332844000	1.302208000
C	3.108361000	1.958160000	1.417082000
H	2.804381000	2.097516000	2.457761000
H	3.091866000	0.884263000	1.210870000
P	-2.562227000	1.917269000	0.246078000
C	-4.388821000	1.936630000	0.013782000
H	-4.843207000	1.148047000	0.620033000
H	-4.830554000	2.897658000	0.300537000
H	-2.733410000	4.309214000	-0.323292000
H	-4.636428000	1.737195000	-1.032520000
C	-2.087568000	3.470718000	-0.605981000
H	-1.057126000	3.699479000	-0.319197000
H	-2.120510000	3.343313000	-1.690854000
H	-1.357785000	2.613623000	2.207966000
C	-2.417672000	2.455701000	1.992696000
H	-2.786787000	1.673970000	2.660962000
H	-2.975054000	3.379953000	2.181980000

P	-2.561733000	-1.917777000	-0.246074000
C	-4.388287000	-1.937576000	-0.013515000
H	-4.842912000	-1.148900000	-0.619465000
H	-4.829900000	-2.898600000	-0.300467000
H	-2.732431000	-4.309932000	0.322496000
H	-4.635745000	-1.738452000	1.032881000
C	-2.086601000	-3.471463000	0.605286000
H	-1.056226000	-3.699997000	0.318068000
H	-2.119225000	-3.344458000	1.690215000
H	-1.357360000	-2.612914000	-2.208411000
C	-2.417274000	-2.455510000	-1.992911000
H	-2.786847000	-1.673702000	-2.660838000
H	-2.974277000	-3.379942000	-2.182434000

I4

M06-L/BSI SCF energy in gas: -589.053808 a.u.

M06/BSII SCF energy in benzene: -588.9986361 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -588.9170132 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -588.8752732 a.u.

Pd	1.319568000	-0.000216000	0.000069000
P	-0.859616000	0.000091000	0.000155000
C	-1.713339000	1.624557000	0.113566000
H	-2.803284000	1.504178000	0.108687000
H	-1.417676000	2.136171000	1.032147000
H	-1.422758000	2.256245000	-0.728685000

C	-1.714566000	-0.713322000	-1.463175000
H	-1.422008000	-1.757653000	-1.592252000
H	-2.804358000	-0.660232000	-1.353521000
H	-1.422735000	-0.170737000	-2.364964000
C	-1.715512000	-0.910410000	1.349101000
H	-1.425312000	-1.963161000	1.329057000
H	-1.422041000	-0.501315000	2.318335000
H	-2.805205000	-0.839851000	1.248742000

I5

M06-L/BSI SCF energy in gas: -1411.565926 a.u.

M06/BSII SCF energy in benzene: -1411.296669 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1410.873338 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1410.786743 a.u.

Pd	0.375833000	-0.778616000	-0.866024000
O	1.638292000	1.170757000	-0.879419000
C	3.056216000	1.219123000	-0.536155000
C	3.468968000	2.672445000	-0.705791000
H	3.264481000	2.989113000	-1.731288000
H	4.536015000	2.812036000	-0.507024000
H	2.904289000	3.323112000	-0.032693000
C	3.805351000	0.324356000	-1.500257000
H	3.380062000	-0.684437000	-1.510636000
H	3.741409000	0.728387000	-2.514145000
H	4.864265000	0.254013000	-1.229097000

H	3.875606000	2.550028000	1.863233000
C	4.077862000	1.478049000	1.829429000
H	5.099340000	1.328515000	1.462691000
H	4.028153000	1.094179000	2.851699000
C	3.079528000	0.741512000	0.956478000
C	3.270627000	-0.762140000	1.104802000
H	2.533448000	-1.305883000	0.498771000
H	3.120937000	-1.039370000	2.152145000
H	4.275850000	-1.074417000	0.804096000
O	1.745415000	1.053456000	1.427322000
B	0.904796000	1.116679000	0.334123000
B	-0.771030000	1.193410000	0.250225000
O	-1.664714000	0.775062000	1.229573000
O	-1.426333000	1.794586000	-0.818261000
C	-2.971673000	1.278063000	0.866123000
C	-2.837190000	1.509498000	-0.671496000
C	-3.121509000	0.259622000	-1.492655000
H	-2.502250000	-0.574477000	-1.143770000
H	-2.854008000	0.448122000	-2.535822000
H	-3.785131000	-0.732189000	0.840698000
H	-4.176731000	-0.030670000	-1.453760000
C	-4.010048000	0.248915000	1.266976000
H	-4.033872000	0.144544000	2.355514000
H	-5.010708000	0.547234000	0.935343000
H	-4.704691000	2.537996000	-1.036677000

H	-3.474450000	2.779735000	-2.284720000
C	-3.632134000	2.683815000	-1.207256000
H	-3.332400000	3.623365000	-0.739705000
H	-4.175847000	2.990261000	1.481296000
C	-3.177051000	2.572199000	1.642416000
H	-3.054557000	2.374819000	2.710303000
H	-2.437444000	3.323766000	1.351755000
P	-0.489057000	-2.588335000	0.112726000
C	-2.114181000	-3.309313000	-0.359035000
H	-2.103576000	-3.613374000	-1.408422000
H	-2.355158000	-4.179858000	0.261265000
H	-1.133017000	-3.244625000	2.393714000
H	-2.905881000	-2.565250000	-0.236495000
C	-0.727683000	-2.346903000	1.912886000
H	0.232550000	-2.095614000	2.371656000
H	-1.394880000	-1.497324000	2.076682000
H	1.536449000	-3.877845000	0.507547000
C	0.548939000	-4.106418000	0.098192000
H	0.685163000	-4.462670000	-0.925666000
H	0.097883000	-4.908111000	0.694337000

TSOA2

Imaginary Frequency: -24.16

M06-L/BSI SCF energy in gas: -1411.551301 a.u.

M06/BSII SCF energy in benzene: -1411.288794 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1410.868186 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1410.780572 a.u.

Pd	-0.762761000	-1.077348000	-0.357098000
O	2.019880000	-0.734583000	-1.152304000
C	3.403409000	-0.842603000	-0.716296000
C	4.073882000	0.468556000	-1.101711000
H	3.970890000	0.623367000	-2.178286000
H	5.139652000	0.466784000	-0.852055000
H	3.600384000	1.314495000	-0.594168000
C	4.054960000	-2.008280000	-1.430026000
H	3.490866000	-2.932376000	-1.290703000
H	4.111407000	-1.806294000	-2.502782000
H	5.075130000	-2.166265000	-1.063053000
H	4.427675000	0.679115000	1.491204000
C	4.364756000	-0.399485000	1.647455000
H	5.332971000	-0.844851000	1.393181000
H	4.183944000	-0.574049000	2.711342000
C	3.253296000	-1.017865000	0.824587000
C	3.020459000	-2.465457000	1.235942000
H	2.226779000	-2.920387000	0.635247000
H	2.708923000	-2.494554000	2.282743000
H	3.928156000	-3.068032000	1.128890000
O	2.019636000	-0.304090000	1.101495000
B	1.282964000	-0.303015000	-0.065375000
B	-0.097928000	0.900039000	-0.093451000
O	-0.491724000	1.520283000	1.088966000

O	-0.083442000	1.794329000	-1.160536000
C	-0.527885000	2.941908000	0.828958000
C	-0.760575000	2.992651000	-0.711124000
C	-2.228416000	2.843037000	-1.087867000
H	-2.673289000	1.987526000	-0.569425000
H	-2.307949000	2.664988000	-2.163303000
H	-2.590582000	3.074323000	1.486161000
H	-2.805210000	3.740546000	-0.842140000
C	-1.630913000	3.566806000	1.658538000
H	-1.393984000	3.481010000	2.722456000
H	-1.741451000	4.631432000	1.423266000
H	-0.569132000	5.123612000	-1.024402000
H	-0.351913000	4.143637000	-2.482225000
C	-0.146689000	4.188667000	-1.409286000
H	0.936492000	4.217490000	-1.275433000
H	0.885091000	4.580158000	1.133220000
C	0.832907000	3.491644000	1.237816000
H	1.024222000	3.233146000	2.282191000
H	1.627925000	3.043872000	0.633131000
P	-2.874325000	-1.855345000	0.071190000
C	-3.977791000	-2.587057000	-1.204780000
H	-3.531165000	-3.499304000	-1.607121000
H	-4.963676000	-2.829691000	-0.791962000
H	-4.916721000	-0.937179000	1.094051000
H	-4.103982000	-1.884927000	-2.032033000

C	-3.961032000	-0.534986000	0.738513000
H	-3.450872000	-0.025328000	1.559651000
H	-4.158961000	0.204844000	-0.041188000
H	-2.531922000	-2.751527000	2.306063000
C	-3.012923000	-3.119072000	1.396822000
H	-2.502095000	-4.036821000	1.096342000
H	-4.060338000	-3.354027000	1.617689000

I6

M06-L/BSI SCF energy in gas: -1411.551763 a.u.

M06/BSII SCF energy in benzene: -1411.288179 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1410.86764 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1410.778559 a.u.

Pd	-1.051609000	-1.033186000	-0.165997000
O	1.731291000	-1.318973000	-1.090953000
C	3.145581000	-1.357987000	-0.761468000
C	3.747512000	-0.084009000	-1.338073000
H	3.543202000	-0.046263000	-2.410777000
H	4.830923000	-0.038485000	-1.188519000
H	3.290556000	0.801997000	-0.885673000
C	3.766964000	-2.583322000	-1.398187000
H	3.239811000	-3.495761000	-1.113023000
H	3.729876000	-2.498646000	-2.487351000
H	4.817643000	-2.683733000	-1.103847000
H	4.337750000	0.391255000	1.159660000
C	4.284993000	-0.658103000	1.457201000

H	5.234380000	-1.139307000	1.196819000
H	4.176531000	-0.694977000	2.544394000
C	3.122290000	-1.369319000	0.795829000
C	2.945302000	-2.766028000	1.373998000
H	2.110434000	-3.285326000	0.894205000
H	2.725973000	-2.689655000	2.441759000
H	3.848631000	-3.371730000	1.250011000
O	1.903699000	-0.635952000	1.091190000
B	1.079477000	-0.748600000	-0.013157000
B	-0.077615000	0.775251000	-0.058828000
O	-0.347265000	1.538385000	1.072177000
O	0.333479000	1.571806000	-1.124340000
C	0.133579000	2.877609000	0.807761000
C	0.081855000	2.948063000	-0.746984000
C	-1.300323000	3.307505000	-1.275813000
H	-2.069910000	2.687013000	-0.806327000
H	-1.332050000	3.126708000	-2.353213000
H	-1.814326000	3.716526000	1.257633000
H	-1.544711000	4.359421000	-1.095757000
C	-0.764623000	3.869125000	1.518715000
H	-0.666596000	3.753996000	2.601436000
H	-0.490717000	4.899012000	1.263838000
H	1.033867000	4.865648000	-1.052973000
H	1.043949000	3.805167000	-2.469913000
C	1.141474000	3.825717000	-1.381176000

H	2.148050000	3.486814000	-1.127400000
H	1.982278000	3.949445000	1.257846000
C	1.553654000	2.946359000	1.353073000
H	1.546212000	2.667175000	2.409477000
H	2.201146000	2.235545000	0.830928000
P	-3.355908000	-1.260422000	0.025748000
C	-4.428492000	-2.118214000	-1.195651000
H	-4.161686000	-3.176226000	-1.250919000
H	-5.487853000	-2.037125000	-0.928042000
H	-5.218517000	0.321739000	0.317535000
H	-4.280827000	-1.685392000	-2.187626000
C	-4.149403000	0.392263000	0.086595000
H	-3.652834000	1.001874000	0.846652000
H	-4.025950000	0.893246000	-0.876622000
H	-3.516958000	-1.475475000	2.439831000
C	-3.966079000	-1.997716000	1.592244000
H	-3.673340000	-3.048364000	1.654090000
H	-5.056969000	-1.930251000	1.668445000

I7

M06-L/BSI SCF energy in gas: -2412.080668 a.u.

M06/BSII SCF energy in benzene: -2411.55787392 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -2410.852175 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -2410.718364 a.u.

Pd	-0.140557000	-1.087923000	0.382132000
O	1.344623000	0.147461000	-1.953232000

C	2.569963000	0.123675000	-2.723899000
C	3.493972000	1.180868000	-2.136497000
H	2.999193000	2.155088000	-2.177290000
H	4.437324000	1.245725000	-2.688737000
H	3.709652000	0.965418000	-1.085653000
C	2.238026000	0.459893000	-4.164604000
H	1.475331000	-0.207372000	-4.572454000
H	1.855884000	1.482477000	-4.225363000
H	3.128826000	0.393671000	-4.799478000
H	5.024084000	-0.851925000	-1.631450000
C	4.593473000	-1.469450000	-2.422745000
H	5.055251000	-1.180543000	-3.373624000
H	4.862279000	-2.509758000	-2.219395000
C	3.085472000	-1.328156000	-2.487935000
C	2.511030000	-2.325821000	-3.484344000
H	1.422638000	-2.232158000	-3.556862000
H	2.742179000	-3.343572000	-3.156748000
H	2.931937000	-2.185062000	-4.485095000
O	2.536084000	-1.649692000	-1.184294000
B	1.440093000	-0.817470000	-0.955439000
B	1.625311000	-0.287611000	1.137274000
O	2.282847000	-1.032482000	2.112669000
O	2.214493000	0.972632000	1.015502000
C	3.493657000	-0.326644000	2.475408000
C	3.131797000	1.145068000	2.123653000

C	2.357471000	1.856750000	3.224966000
H	1.526299000	1.239430000	3.580752000
H	1.936057000	2.783763000	2.824733000
H	2.935916000	-0.305747000	4.573287000
H	2.993413000	2.104937000	4.080815000
C	3.784194000	-0.578056000	3.940801000
H	3.996535000	-1.638278000	4.102770000
H	4.658324000	-0.006453000	4.272633000
H	5.053142000	2.074084000	2.465419000
H	3.965631000	3.009550000	1.432007000
C	4.302056000	1.996080000	1.671468000
H	4.785329000	1.581180000	0.783949000
H	5.578158000	-0.431573000	1.833447000
C	4.607167000	-0.879484000	1.597223000
H	4.677703000	-1.960278000	1.742573000
H	4.380597000	-0.707898000	0.540024000
P	-1.376513000	-0.869551000	2.405497000
P	-1.306111000	-2.433690000	-1.199240000
C	-1.970876000	0.833744000	2.733151000
H	-2.446861000	0.922099000	3.715928000
H	-1.127144000	1.528143000	2.676716000
H	-2.685435000	1.132180000	1.960581000
C	-0.431556000	-1.231048000	3.936624000
H	0.465577000	-0.610042000	3.976046000
H	-1.037893000	-1.062194000	4.833228000

H	-0.091364000	-2.269466000	3.920982000
C	-2.891359000	-1.854307000	2.762646000
H	-3.305884000	-1.614293000	3.748359000
H	-3.659803000	-1.664397000	2.009383000
H	-2.647839000	-2.920149000	2.738131000
C	-2.926095000	-3.289175000	-0.993348000
H	-2.930536000	-3.872367000	-0.068349000
H	-3.738255000	-2.559923000	-0.942928000
H	-3.126866000	-3.965701000	-1.831853000
C	-1.570195000	-1.628097000	-2.824654000
H	-0.657802000	-1.104373000	-3.122765000
H	-1.863895000	-2.343857000	-3.600601000
H	-2.354564000	-0.872002000	-2.724660000
C	-0.263716000	-3.883699000	-1.623916000
H	-0.630462000	-4.407979000	-2.513828000
H	0.767928000	-3.562094000	-1.780190000
H	-0.262456000	-4.580474000	-0.781314000
C	-2.400446000	2.667465000	-0.695792000
C	-3.436693000	2.034483000	-0.585868000
C	-4.603129000	1.252802000	-0.409401000
C	-5.890252000	1.802026000	-0.550468000
H	-5.989330000	2.850107000	-0.817368000
H	-8.003707000	1.455359000	-0.455269000
C	-7.016253000	1.016064000	-0.344537000
H	-7.770332000	-0.936836000	0.169169000

C	-6.886685000	-0.326970000	0.004921000
H	-5.508230000	-1.930741000	0.419181000
C	-5.615936000	-0.883118000	0.144353000
C	-4.483421000	-0.106533000	-0.062659000
H	-3.482889000	-0.527436000	0.043735000
H	0.050938000	1.818224000	-0.038144000
C	0.022502000	2.843978000	-0.403495000
C	-1.200618000	3.412248000	-0.802385000
C	-1.217052000	4.729243000	-1.298297000
H	-2.162509000	5.165926000	-1.607739000
C	-0.038543000	5.455850000	-1.392453000
H	-0.061981000	6.471256000	-1.778984000
C	1.169765000	4.886883000	-0.990216000
H	2.090612000	5.460103000	-1.062934000
C	1.193990000	3.584264000	-0.495881000
H	2.122594000	3.116389000	-0.181969000

TSIA1

Imaginary Frequency: -181.06

M06-L/BSI SCF energy in gas: -2412.056635 a.u.

M06/BSII SCF energy in benzene: -2411.51424835 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -2410.808063 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -2410.677707 a.u.

Pd	-0.015563000	-0.798404000	-0.023504000
O	2.626475000	0.421767000	1.027521000
C	4.063449000	0.264807000	0.954465000

C	4.473779000	-0.660184000	2.092013000
H	4.137415000	-0.233344000	3.041165000
H	5.559478000	-0.791551000	2.143353000
H	4.012790000	-1.648073000	1.986223000
C	4.700080000	1.630136000	1.127803000
H	4.288847000	2.351603000	0.418476000
H	4.506574000	2.006168000	2.136156000
H	5.786273000	1.581776000	0.989547000
H	5.277233000	-2.192050000	0.142554000
C	5.401766000	-1.360921000	-0.555377000
H	6.360721000	-0.874483000	-0.343894000
H	5.452457000	-1.773573000	-1.566886000
C	4.258697000	-0.372146000	-0.454215000
C	4.346316000	0.669169000	-1.561602000
H	3.511222000	1.373319000	-1.493116000
H	4.288488000	0.170834000	-2.533702000
H	5.283151000	1.234529000	-1.523284000
O	3.008229000	-1.080418000	-0.651476000
B	2.031840000	-0.439699000	0.114949000
C	-2.126437000	-0.322626000	0.358283000
C	-1.384566000	0.652880000	0.812383000
C	-1.365623000	1.655150000	1.866140000
C	-2.564272000	2.211016000	2.346338000
C	-0.150551000	2.089450000	2.421016000
H	-3.509505000	1.872033000	1.928588000

H	0.776206000	1.665461000	2.039850000
C	-2.546861000	3.175043000	3.347095000
C	-0.141818000	3.048321000	3.426136000
H	-3.483094000	3.595110000	3.705897000
H	0.805960000	3.374684000	3.847278000
C	-1.335456000	3.600636000	3.889570000
H	-1.322498000	4.357684000	4.669296000
C	-3.422940000	-0.883369000	0.176510000
C	-4.581423000	-0.077645000	0.114832000
C	-3.580954000	-2.276311000	0.013696000
H	-4.474289000	1.001116000	0.197899000
H	-2.681387000	-2.891365000	0.012433000
C	-5.833842000	-0.645812000	-0.072636000
C	-4.837401000	-2.841085000	-0.147407000
H	-6.712012000	-0.007247000	-0.121410000
H	-4.936532000	-3.918091000	-0.255761000
C	-5.971224000	-2.028728000	-0.193005000
H	-6.953672000	-2.469738000	-0.335059000
B	-0.186943000	1.150717000	-0.739991000
O	-0.923631000	1.316143000	-1.920513000
O	0.528234000	2.300470000	-0.441660000
C	0.279353000	3.276667000	-1.477057000
C	-1.021473000	2.737542000	-2.154481000
H	-2.241262000	3.054898000	-0.382824000
C	-2.290736000	3.221825000	-1.463990000

H	-2.470476000	4.287309000	-1.640131000
H	-3.144202000	2.658985000	-1.852986000
H	-0.281777000	2.507912000	-4.184383000
C	-1.111046000	2.975981000	-3.648968000
H	-1.108418000	4.047317000	-3.878270000
H	-2.042729000	2.554048000	-4.036874000
H	1.608988000	2.279581000	-2.875046000
C	1.483739000	3.262000000	-2.407565000
H	2.386556000	3.478060000	-1.828804000
H	1.398002000	4.014628000	-3.197941000
H	1.081246000	4.931965000	-0.360781000
C	0.131474000	4.632659000	-0.812859000
H	-0.619311000	4.601067000	-0.019467000
H	-0.154416000	5.401227000	-1.539968000
P	-0.019318000	-1.878075000	-2.134837000
C	0.516497000	-3.629908000	-2.235550000
H	-0.137065000	-4.247035000	-1.610554000
H	0.491809000	-4.016577000	-3.260510000
H	1.004799000	-1.594485000	-4.355470000
H	1.535591000	-3.713665000	-1.847412000
C	1.053043000	-1.084677000	-3.386948000
H	0.716039000	-0.050562000	-3.505345000
H	2.082866000	-1.075803000	-3.022099000
H	-1.966290000	-0.879875000	-3.135390000
C	-1.620709000	-1.911388000	-3.024561000

H	-2.371003000	-2.449884000	-2.439111000
H	-1.531575000	-2.376098000	-4.013159000
P	0.373406000	-2.500786000	1.708831000
C	-0.960182000	-3.616494000	2.312211000
H	-1.257790000	-4.305587000	1.516050000
H	-0.647514000	-4.201296000	3.184657000
H	1.163660000	-2.426999000	4.049249000
H	-1.837202000	-3.020689000	2.580294000
C	0.877990000	-1.701767000	3.278677000
H	1.710238000	-1.021304000	3.078792000
H	0.046695000	-1.094462000	3.648545000
H	2.599991000	-3.181117000	1.019224000
C	1.733669000	-3.704121000	1.435374000
H	1.419231000	-4.447191000	0.697009000
H	2.023100000	-4.225052000	2.354680000

I8

M06-L/BSI SCF energy in gas: -2412.115261 a.u.

M06/BSII SCF energy in benzene: -2411.58287027 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -2410.871916 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -2410.743673 a.u.

Pd	0.599198000	0.508166000	0.103949000
O	3.358717000	-0.948493000	0.017385000
C	4.774477000	-0.650481000	-0.080474000
C	5.095453000	-0.490105000	-1.560592000
H	4.821611000	-1.407043000	-2.090565000

H	6.160729000	-0.305277000	-1.731186000
H	4.529171000	0.334967000	-2.004938000
C	5.559539000	-1.815239000	0.491436000
H	5.244706000	-2.057857000	1.508301000
H	5.409424000	-2.705064000	-0.126110000
H	6.633011000	-1.595486000	0.505527000
H	5.637872000	1.967068000	-0.872397000
C	5.895166000	1.675771000	0.148397000
H	6.907377000	1.255686000	0.141000000
H	5.912618000	2.581621000	0.760196000
C	4.900012000	0.683812000	0.719750000
C	5.178839000	0.464125000	2.199880000
H	4.501872000	-0.281416000	2.625283000
H	5.031126000	1.405006000	2.737399000
H	6.206188000	0.128398000	2.374512000
O	3.569929000	1.248801000	0.606594000
B	2.669565000	0.235962000	0.286631000
C	-1.532862000	0.895371000	-0.126335000
C	-2.415293000	-0.154813000	-0.077690000
C	-3.863117000	-0.049094000	0.227236000
C	-4.343765000	0.852405000	1.192978000
C	-4.801356000	-0.894233000	-0.387532000
H	-3.633039000	1.506107000	1.696145000
H	-4.454958000	-1.618434000	-1.123304000
C	-5.694828000	0.926442000	1.506104000

C	-6.155544000	-0.820708000	-0.079754000
H	-6.035709000	1.634079000	2.258086000
H	-6.858724000	-1.482667000	-0.579845000
C	-6.611533000	0.092827000	0.867489000
H	-7.668509000	0.147714000	1.113651000
C	-1.924861000	2.304014000	-0.266586000
C	-1.076119000	3.336337000	0.183019000
C	-3.051053000	2.694442000	-1.025004000
H	-0.162532000	3.057383000	0.709072000
H	-3.706618000	1.924568000	-1.424586000
C	-1.355641000	4.676229000	-0.064239000
C	-3.319615000	4.029915000	-1.291230000
H	-0.680413000	5.444345000	0.305903000
H	-4.189545000	4.293045000	-1.888324000
C	-2.480829000	5.033169000	-0.804448000
H	-2.693243000	6.077917000	-1.014762000
B	-1.837476000	-1.576091000	-0.279477000
O	-2.328161000	-2.714565000	0.331808000
O	-0.777151000	-1.866276000	-1.128869000
C	-0.373526000	-3.231002000	-0.849975000
C	-1.693824000	-3.850845000	-0.298150000
H	-2.751138000	-3.551284000	-2.170134000
C	-2.630388000	-4.322414000	-1.402692000
H	-2.265306000	-5.234138000	-1.885848000
H	-3.614729000	-4.529357000	-0.974647000

H	-0.948776000	-4.573436000	1.607069000
C	-1.499880000	-4.939256000	0.737603000
H	-0.950416000	-5.786756000	0.313289000
H	-2.470086000	-5.306016000	1.082836000
H	0.374147000	-2.726349000	1.120835000
C	0.737939000	-3.168723000	0.186825000
H	1.554741000	-2.538473000	-0.177716000
H	1.136479000	-4.163957000	0.411394000
H	1.088306000	-3.422604000	-2.420675000
C	0.135757000	-3.872047000	-2.126092000
H	-0.570546000	-3.750358000	-2.950578000
H	0.308998000	-4.943534000	-1.976794000
P	0.283311000	0.197868000	2.378535000
C	-0.101906000	1.760675000	3.251762000
H	-1.030406000	2.180146000	2.855147000
H	-0.215628000	1.594467000	4.328405000
H	1.389130000	-0.580410000	4.435007000
H	0.696482000	2.488017000	3.084408000
C	1.672536000	-0.439522000	3.386552000
H	2.028841000	-1.389924000	2.977973000
H	2.495203000	0.278552000	3.333664000
H	-1.013876000	-1.878001000	2.560823000
C	-1.105387000	-0.856981000	2.939415000
H	-2.049570000	-0.460325000	2.557634000
H	-1.138566000	-0.885130000	4.033532000

P	1.016329000	0.954796000	-2.112831000
C	-0.387666000	1.481335000	-3.158579000
H	-0.786871000	2.433022000	-2.797855000
H	-0.083588000	1.590253000	-4.205212000
H	2.000106000	-0.187817000	-4.050514000
H	-1.187401000	0.739546000	-3.084088000
C	1.663744000	-0.474032000	-3.048360000
H	2.486753000	-0.932015000	-2.494152000
H	0.860114000	-1.209947000	-3.131315000
H	3.156932000	2.089381000	-1.893636000
C	2.227049000	2.288743000	-2.431503000
H	1.823508000	3.227015000	-2.040684000
H	2.430829000	2.407397000	-3.500818000

I9

M06-L/BSI SCF energy in gas: -1950.98436 a.u.

M06/BSII SCF energy in benzene: -1950.489256 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1949.887233 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1949.774168 a.u.

Pd	0.556857000	-0.414628000	0.077827000
O	-1.444397000	1.585143000	-1.048017000
C	-2.626844000	2.392255000	-0.811116000
C	-3.792397000	1.644380000	-1.443417000
H	-3.580094000	1.479935000	-2.503176000
H	-4.731026000	2.200998000	-1.356075000

H	-3.918836000	0.660396000	-0.984854000
C	-2.458976000	3.743890000	-1.473515000
H	-1.577002000	4.271093000	-1.108146000
H	-2.357140000	3.616545000	-2.555285000
H	-3.338993000	4.370830000	-1.291545000
H	-4.685149000	1.598655000	0.998502000
C	-4.095392000	2.459410000	1.321975000
H	-4.621505000	3.370487000	1.016012000
H	-4.051153000	2.447243000	2.414317000
C	-2.693421000	2.433212000	0.746427000
C	-1.847591000	3.543658000	1.349138000
H	-0.842405000	3.551083000	0.920047000
H	-1.755671000	3.383412000	2.426568000
H	-2.298693000	4.527842000	1.185195000
O	-2.070117000	1.172577000	1.116831000
B	-1.271388000	0.771059000	0.059720000
B	-1.463505000	-1.143208000	-0.036394000
O	-1.982163000	-1.907682000	1.002933000
O	-2.159511000	-1.377685000	-1.218654000
C	-3.229838000	-2.484540000	0.549823000
C	-3.043030000	-2.502185000	-0.998520000
C	-2.309677000	-3.739923000	-1.498258000
H	-1.396613000	-3.914449000	-0.919222000
H	-2.019647000	-3.588450000	-2.541199000
H	-2.606292000	-4.539008000	0.942248000

H	-2.932026000	-4.638517000	-1.438928000
C	-3.417282000	-3.849316000	1.183500000
H	-3.462730000	-3.751094000	2.271609000
H	-4.356500000	-4.302290000	0.847593000
H	-5.031223000	-3.093313000	-1.610854000
H	-4.086231000	-2.276779000	-2.866151000
C	-4.313375000	-2.286746000	-1.796804000
H	-4.791676000	-1.337195000	-1.546740000
H	-5.330784000	-1.930666000	0.751104000
C	-4.338130000	-1.547781000	1.008973000
H	-4.279925000	-1.428151000	2.093823000
H	-4.216296000	-0.555934000	0.566555000
C	2.507587000	0.402987000	-0.166889000
C	1.722231000	1.395073000	-0.048874000
C	1.541144000	2.819929000	0.026726000
C	1.896831000	3.502884000	1.203487000
C	1.054902000	3.559472000	-1.062504000
H	2.262184000	2.930926000	2.052525000
H	0.749518000	3.031757000	-1.960869000
C	1.774846000	4.884475000	1.283290000
C	0.954944000	4.943975000	-0.979452000
H	2.049565000	5.395784000	2.202249000
H	0.587245000	5.504232000	-1.835918000
C	1.306592000	5.612859000	0.191431000
H	1.215796000	6.693586000	0.252769000

C	3.826689000	-0.128647000	-0.378023000
C	4.084774000	-1.013718000	-1.438540000
C	4.884598000	0.215138000	0.481340000
H	3.269991000	-1.268975000	-2.112499000
H	4.693113000	0.901435000	1.302432000
C	5.355371000	-1.543959000	-1.626840000
C	6.150961000	-0.325803000	0.292862000
H	5.537048000	-2.223411000	-2.455727000
H	6.956213000	-0.054957000	0.970802000
C	6.392096000	-1.210302000	-0.757111000
H	7.382419000	-1.633208000	-0.898784000
P	1.323732000	-2.626173000	0.620830000
C	0.276412000	-3.748739000	1.621096000
H	-0.567124000	-4.110318000	1.032555000
H	0.866272000	-4.604403000	1.966656000
H	3.091807000	-3.606050000	2.002253000
H	-0.139346000	-3.215505000	2.477748000
C	2.813221000	-2.592671000	1.694252000
H	3.657117000	-2.138121000	1.172070000
H	2.608161000	-1.996343000	2.587022000
H	2.733930000	-3.344567000	-1.225148000
C	1.876302000	-3.773817000	-0.701423000
H	1.074687000	-3.926392000	-1.428383000
H	2.170273000	-4.743449000	-0.285234000

TSIA2

Imaginary Frequency: -192.22

M06-L/BSI SCF energy in gas: -1950.969619 a.u.

M06/BSII SCF energy in benzene: -1950.4728289 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1949.874199 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1949.758606 a.u.

Pd	-0.357732000	-0.986538000	-0.300248000
O	-0.171603000	0.596411000	2.077203000
C	0.730191000	1.454321000	2.826752000
C	1.925277000	0.603603000	3.233316000
H	1.574188000	-0.252354000	3.816037000
H	2.631657000	1.169242000	3.849818000
H	2.449102000	0.217822000	2.352137000
C	-0.001518000	1.981552000	4.042956000
H	-0.937329000	2.473037000	3.769132000
H	-0.238146000	1.159848000	4.724305000
H	0.621541000	2.699702000	4.587866000
H	3.254635000	2.366679000	1.877839000
C	2.477438000	3.134093000	1.922581000
H	2.567147000	3.657475000	2.880689000
H	2.665818000	3.857676000	1.124308000
C	1.096180000	2.534128000	1.767079000
C	0.040051000	3.621096000	1.638670000
H	-0.962424000	3.187210000	1.573015000
H	0.213858000	4.188141000	0.719818000
H	0.066397000	4.311629000	2.487633000

O	1.064611000	1.763550000	0.535726000
B	0.188407000	0.717219000	0.741671000
B	1.696157000	-0.749784000	-0.604078000
O	2.157382000	-0.251231000	-1.810360000
O	2.751362000	-1.095861000	0.232023000
C	3.582348000	-0.003849000	-1.690066000
C	3.991555000	-0.943882000	-0.510796000
C	4.404418000	-2.333360000	-0.974952000
H	3.666181000	-2.755476000	-1.663483000
H	4.483067000	-2.996361000	-0.108083000
H	4.021616000	-1.342274000	-3.349654000
H	5.373619000	-2.320716000	-1.483880000
C	4.243829000	-0.326861000	-3.016007000
H	3.886104000	0.363696000	-3.784117000
H	5.331631000	-0.215314000	-2.945342000
H	5.978123000	-0.181916000	-0.102149000
H	5.243228000	-1.082868000	1.232991000
C	5.037641000	-0.373196000	0.426477000
H	4.701726000	0.562585000	0.879237000
H	4.809207000	1.755274000	-1.308140000
C	3.752381000	1.474825000	-1.370421000
H	3.287322000	2.066652000	-2.164406000
H	3.254021000	1.737172000	-0.434903000
C	-2.366791000	-0.230241000	-0.293792000
C	-1.522073000	0.762720000	-0.427668000

C	-1.468202000	2.062793000	-1.089910000
C	-0.371638000	2.400677000	-1.898279000
C	-2.525208000	2.976215000	-0.963679000
H	0.447406000	1.689932000	-1.990276000
H	-3.378536000	2.718381000	-0.341007000
C	-0.340268000	3.617454000	-2.565485000
C	-2.482683000	4.197549000	-1.627557000
H	0.512178000	3.862230000	-3.194528000
H	-3.307210000	4.897372000	-1.517789000
C	-1.390686000	4.524885000	-2.428596000
H	-1.359907000	5.480496000	-2.945252000
C	-3.758449000	-0.562228000	-0.261340000
C	-4.244756000	-1.713378000	-0.911073000
C	-4.678499000	0.236377000	0.448944000
H	-3.536386000	-2.340744000	-1.447828000
H	-4.310000000	1.109189000	0.982790000
C	-5.596248000	-2.026161000	-0.888647000
C	-6.024996000	-0.099639000	0.494146000
H	-5.953749000	-2.907429000	-1.415128000
H	-6.715896000	0.524628000	1.055021000
C	-6.493260000	-1.225398000	-0.181197000
H	-7.548386000	-1.481902000	-0.151205000
P	-0.100351000	-3.198980000	0.323674000
C	1.079969000	-4.287239000	-0.553301000
H	2.068409000	-3.822623000	-0.523403000

H	1.137865000	-5.275323000	-0.085048000
H	-1.305335000	-5.233375000	0.999480000
H	0.789620000	-4.406589000	-1.599635000
C	-1.561174000	-4.293711000	0.497488000
H	-2.338362000	-3.780495000	1.069159000
H	-1.974181000	-4.523769000	-0.488010000
H	-0.077529000	-2.642146000	2.682171000
C	0.590399000	-3.194446000	2.016808000
H	1.550225000	-2.670780000	1.994832000
H	0.730179000	-4.210489000	2.401894000

I10

M06-L/BSI SCF energy in gas: -1950.969619 a.u.

M06/BSII SCF energy in benzene: -1950.4728289 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1949.874199 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1949.758606 a.u.

Pd	-0.285413000	1.109740000	-0.250267000
O	0.120498000	-0.518025000	-2.821458000
C	1.500222000	-0.715744000	-3.206413000
C	2.261689000	0.536818000	-2.790073000
H	1.773779000	1.408499000	-3.238973000
H	3.304072000	0.510855000	-3.125774000
H	2.248983000	0.655104000	-1.700512000
C	1.562771000	-0.904094000	-4.708577000
H	0.903473000	-1.708007000	-5.041724000

H	1.253962000	0.015088000	-5.213522000
H	2.584137000	-1.137639000	-5.028942000
H	3.560511000	-1.125732000	-1.265512000
C	3.350797000	-1.981155000	-1.912127000
H	4.034094000	-1.957491000	-2.768406000
H	3.557932000	-2.893935000	-1.345062000
C	1.906860000	-1.973586000	-2.371720000
C	1.545350000	-3.282343000	-3.059968000
H	0.505567000	-3.271598000	-3.401811000
H	1.659001000	-4.105208000	-2.348994000
H	2.189112000	-3.481930000	-3.922338000
O	1.055824000	-1.863914000	-1.207823000
B	-0.019954000	-1.067185000	-1.559477000
B	1.214668000	0.650721000	1.075638000
O	0.911502000	0.340347000	2.384963000
O	2.535968000	0.377754000	0.763237000
C	1.980654000	-0.533072000	2.852852000
C	3.188005000	-0.047649000	1.997940000
C	3.875338000	1.179340000	2.578402000
H	3.145941000	1.955392000	2.832858000
H	4.568971000	1.591090000	1.839692000
H	2.290388000	0.706336000	4.607262000
H	4.445773000	0.937363000	3.480634000
C	2.140940000	-0.343583000	4.346020000
H	1.245876000	-0.697051000	4.864243000

H	2.994798000	-0.918800000	4.721052000
H	4.645228000	-1.530419000	2.581643000
H	5.006974000	-0.711615000	1.055501000
C	4.198939000	-1.124473000	1.666955000
H	3.738726000	-1.944478000	1.112691000
H	2.290764000	-2.685885000	2.902826000
C	1.564779000	-1.959928000	2.522100000
H	0.593670000	-2.170908000	2.977906000
H	1.459246000	-2.103664000	1.440861000
C	-2.067327000	0.243962000	-0.808474000
C	-1.276884000	-0.894962000	-0.651323000
C	-1.559918000	-1.955579000	0.359012000
C	-2.045741000	-1.626993000	1.633610000
C	-1.347840000	-3.309617000	0.066440000
H	-2.184173000	-0.577767000	1.887027000
H	-0.960132000	-3.587098000	-0.911341000
C	-2.322265000	-2.613384000	2.572510000
C	-1.622513000	-4.299206000	1.005585000
H	-2.692618000	-2.331761000	3.555318000
H	-1.451767000	-5.343039000	0.753637000
C	-2.112124000	-3.956401000	2.262982000
H	-2.321955000	-4.728268000	2.998757000
C	-3.449766000	0.410275000	-0.432222000
C	-3.906722000	1.654987000	0.045035000
C	-4.398921000	-0.620909000	-0.597729000

H	-3.177753000	2.459256000	0.144351000
H	-4.060885000	-1.587039000	-0.965357000
C	-5.237037000	1.848592000	0.386439000
C	-5.737384000	-0.411278000	-0.298702000
H	-5.565480000	2.810505000	0.771989000
H	-6.456053000	-1.214086000	-0.442692000
C	-6.161261000	0.818875000	0.205590000
H	-7.208686000	0.977349000	0.448129000
P	0.482921000	3.224532000	-0.158995000
C	2.255599000	3.523168000	-0.491301000
H	2.492178000	3.230142000	-1.517177000
H	2.509200000	4.579794000	-0.356952000
H	0.596816000	5.056164000	1.463894000
H	2.861885000	2.906216000	0.175827000
C	0.238419000	4.021679000	1.468043000
H	-0.823659000	4.013205000	1.724209000
H	0.767376000	3.455832000	2.238731000
H	-1.391760000	4.432898000	-1.120594000
C	-0.314965000	4.413559000	-1.303834000
H	-0.161427000	4.080763000	-2.333250000
H	0.091060000	5.424792000	-1.187389000

I11

M06-L/BSI SCF energy in gas: -1951.002073 a.u.

M06/BSII SCF energy in benzene: -1950.50340909 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1949.896962 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1949.785702 a.u.

Pd	0.450711000	-0.455871000	0.077682000
B	2.533285000	-0.277960000	-0.049585000
B	-1.455588000	1.889180000	0.044317000
O	3.299196000	-0.940215000	-1.004495000
O	3.331824000	0.564638000	0.713330000
O	-0.072986000	1.727710000	-0.183256000
O	-1.759542000	3.191522000	0.335673000
C	-1.735127000	-0.535811000	-0.044379000
C	-2.378574000	0.676776000	-0.065151000
C	4.600488000	-0.299819000	-1.072306000
C	4.722037000	0.387458000	0.325291000
C	0.582181000	2.952867000	0.290156000
C	-0.569792000	3.987545000	0.114079000
C	-3.842530000	0.868490000	-0.227705000
C	-4.584988000	0.135212000	-1.167146000
C	-4.528928000	1.818094000	0.545242000
H	-4.073892000	-0.591607000	-1.793097000
H	-3.973850000	2.411239000	1.267637000
C	-5.953475000	0.327192000	-1.313039000
C	-5.900462000	2.006008000	0.405284000
H	-6.501222000	-0.252693000	-2.052030000
H	-6.407991000	2.741880000	1.024786000
C	-6.621502000	1.260398000	-0.523644000
H	-7.692206000	1.409381000	-0.636104000

C	-2.484286000	-1.794398000	-0.070064000
C	-2.245648000	-2.764349000	-1.058708000
C	-3.412373000	-2.111182000	0.939854000
H	-1.549431000	-2.521577000	-1.860867000
H	-3.626562000	-1.363828000	1.700978000
C	-2.898511000	-3.992131000	-1.040360000
C	-4.043408000	-3.349036000	0.974505000
H	-2.706509000	-4.716725000	-1.829096000
H	-4.747508000	-3.570653000	1.773210000
C	-3.790285000	-4.300008000	-0.013017000
H	-4.288916000	-5.265086000	0.011341000
C	1.799016000	3.229826000	-0.563327000
H	2.568850000	2.485474000	-0.353562000
H	1.559275000	3.204751000	-1.628568000
H	2.208625000	4.217625000	-0.324133000
C	0.966356000	2.717072000	1.739880000
H	0.080827000	2.537609000	2.357843000
H	1.620120000	1.841893000	1.796882000
H	1.507133000	3.575132000	2.151379000
C	-0.663355000	4.536428000	-1.302425000
H	-0.654286000	3.730378000	-2.041693000
H	-1.602424000	5.083911000	-1.411787000
H	0.161566000	5.219392000	-1.526427000
C	-0.550724000	5.116772000	1.123877000
H	-1.388820000	5.793758000	0.940035000

H	-0.634888000	4.743293000	2.146071000
H	0.375201000	5.695985000	1.040767000
C	5.393145000	1.748072000	0.307352000
H	6.430676000	1.666094000	-0.035182000
H	4.873823000	2.454658000	-0.343275000
H	5.406083000	2.168835000	1.316597000
C	5.376335000	-0.488753000	1.383158000
H	5.253568000	-0.020469000	2.363051000
H	4.919005000	-1.479694000	1.429015000
H	6.447400000	-0.615102000	1.195952000
C	4.538503000	0.691936000	-2.226205000
H	5.497369000	1.196394000	-2.382064000
H	4.277385000	0.158588000	-3.143509000
H	3.771336000	1.453581000	-2.056136000
C	5.647957000	-1.360145000	-1.349286000
H	5.618813000	-2.162403000	-0.608192000
H	5.479910000	-1.803866000	-2.334154000
H	6.654039000	-0.926290000	-1.344200000
P	0.961036000	-2.575131000	0.521899000
C	2.513833000	-2.947074000	1.424183000
H	2.589259000	-2.341340000	2.330645000
H	2.548300000	-4.007061000	1.696744000
H	1.520187000	-4.612716000	-0.681846000
H	3.361930000	-2.716514000	0.776625000
C	1.207136000	-3.603116000	-0.968211000

H	0.280312000	-3.669379000	-1.540409000
H	1.980434000	-3.141306000	-1.586354000
H	-1.139363000	-2.938650000	1.748166000
C	-0.243005000	-3.522695000	1.542653000
H	0.224679000	-3.796604000	2.491430000
H	-0.553023000	-4.434389000	1.024767000

I12

M06-L/BSI SCF energy in gas: -1951.018427 a.u.

M06/BSII SCF energy in benzene: -1950.52071352 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -1949.918322 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -1949.803991 a.u.

Pd	-0.299682000	-0.926026000	-0.343517000
B	-2.077387000	-0.135760000	0.131841000
B	2.616312000	-0.332923000	0.083674000
O	-2.278620000	0.726909000	1.181482000
O	-3.269856000	-0.499720000	-0.478539000
O	2.066471000	-1.535345000	-0.388248000
O	3.822759000	-0.540768000	0.704936000
C	0.538574000	0.979637000	-0.286376000
C	1.899772000	1.008899000	-0.107856000
C	-3.702250000	0.852528000	1.412715000
C	-4.335618000	0.315501000	0.080870000
C	2.825046000	-2.611631000	0.239591000
C	4.199600000	-1.919766000	0.491438000
C	2.723395000	2.249149000	-0.123009000

C	2.586833000	3.210593000	-1.136522000
C	3.693198000	2.474978000	0.865455000
H	1.847568000	3.051494000	-1.917775000
H	3.825811000	1.738388000	1.652798000
C	3.375502000	4.354662000	-1.153223000
C	4.478626000	3.623501000	0.853255000
H	3.249814000	5.082088000	-1.951454000
H	5.216508000	3.778122000	1.636928000
C	4.324892000	4.569869000	-0.156003000
H	4.941012000	5.464988000	-0.168585000
C	-0.230801000	2.231926000	-0.393376000
C	-1.104713000	2.462910000	-1.465012000
C	-0.119443000	3.229628000	0.589145000
H	-1.226571000	1.683422000	-2.217107000
H	0.548230000	3.061575000	1.430644000
C	-1.800158000	3.664141000	-1.577532000
C	-0.842547000	4.411437000	0.498312000
H	-2.453113000	3.829263000	-2.432121000
H	-0.745111000	5.162953000	1.278012000
C	-1.678511000	4.643478000	-0.593149000
H	-2.233230000	5.574659000	-0.673752000
C	2.903352000	-3.792094000	-0.703215000
H	1.924383000	-4.258994000	-0.818886000
H	3.257833000	-3.493045000	-1.691164000
H	3.587872000	-4.549378000	-0.305988000

C	2.095867000	-2.973913000	1.523854000
H	2.071699000	-2.125974000	2.215085000
H	1.057798000	-3.232863000	1.287504000
H	2.560221000	-3.825591000	2.030487000
C	5.109354000	-1.946431000	-0.728519000
H	4.578890000	-1.613570000	-1.625188000
H	5.946873000	-1.265337000	-0.561460000
H	5.511760000	-2.946752000	-0.914879000
C	4.936203000	-2.418020000	1.718315000
H	5.881706000	-1.880948000	1.828383000
H	4.353526000	-2.263590000	2.628571000
H	5.164590000	-3.485622000	1.628322000
C	-4.638591000	1.405506000	-0.933936000
H	-5.463145000	2.045595000	-0.604132000
H	-3.763252000	2.034931000	-1.110136000
H	-4.923387000	0.942945000	-1.883127000
C	-5.555182000	-0.567747000	0.268471000
H	-5.903148000	-0.931164000	-0.702844000
H	-5.344570000	-1.435722000	0.898317000
H	-6.375863000	-0.006508000	0.728271000
C	-4.004296000	2.309396000	1.707220000
H	-5.079189000	2.464470000	1.853978000
H	-3.488728000	2.614721000	2.621705000
H	-3.660519000	2.960674000	0.900486000
C	-4.021675000	-0.009303000	2.626413000

H	-3.764188000	-1.058604000	2.449907000
H	-3.428528000	0.337056000	3.476224000
H	-5.080267000	0.044352000	2.899855000
P	-1.486218000	-2.965156000	-0.601684000
C	-2.600820000	-3.423423000	0.781740000
H	-3.325502000	-2.618366000	0.922677000
H	-3.137214000	-4.355355000	0.575014000
H	-1.394512000	-5.376692000	-1.016567000
H	-2.027428000	-3.538803000	1.705727000
C	-0.652843000	-4.584966000	-0.866260000
H	-0.011007000	-4.539801000	-1.749166000
H	-0.035667000	-4.851612000	-0.004178000
H	-2.561353000	-1.996159000	-2.572072000
C	-2.633404000	-2.948405000	-2.047223000
H	-3.666632000	-3.063330000	-1.711424000
H	-2.392154000	-3.760807000	-2.737980000

I13

M06-L/BSI SCF energy in gas: -2412.122988 a.u.

M06/BSII SCF energy in benzene: -2411.587004 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -2410.877515 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -2410.747082 a.u.

Pd	-1.302386000	0.683590000	-0.164695000
B	-0.907191000	-0.281799000	1.622002000
B	1.155167000	-1.347489000	-0.928043000

O	-0.775549000	0.284464000	2.877042000
O	-0.647671000	-1.644756000	1.656671000
O	-0.006009000	-1.441384000	-1.680609000
O	1.834474000	-2.549586000	-0.887568000
C	0.790693000	0.959057000	0.009561000
C	1.681940000	-0.024066000	-0.324362000
C	-0.507394000	-0.774551000	3.834022000
C	-0.002978000	-1.939796000	2.925293000
C	-0.227791000	-2.838586000	-1.976184000
C	1.212229000	-3.432808000	-1.846826000
C	3.151170000	0.110077000	-0.161494000
C	4.021165000	-0.308777000	-1.180355000
C	3.725844000	0.640472000	1.004692000
H	3.598378000	-0.729136000	-2.092115000
H	3.070775000	0.967568000	1.810646000
C	5.400334000	-0.182708000	-1.053124000
C	5.103918000	0.761297000	1.138756000
H	6.049154000	-0.505862000	-1.863871000
H	5.521048000	1.173707000	2.054228000
C	5.949628000	0.354157000	0.108584000
H	7.027102000	0.449402000	0.213076000
C	1.159133000	2.335390000	0.379818000
C	2.134192000	3.051611000	-0.343257000
C	0.448185000	3.032766000	1.374981000
H	2.702405000	2.538028000	-1.115871000

H	-0.319499000	2.496323000	1.928926000
C	2.380562000	4.396215000	-0.087308000
C	0.716314000	4.369051000	1.648370000
H	3.130758000	4.924698000	-0.670873000
H	0.160612000	4.878098000	2.432343000
C	1.677211000	5.063094000	0.913851000
H	1.872944000	6.112723000	1.116400000
C	-0.840491000	-2.935154000	-3.360560000
H	-1.830252000	-2.466695000	-3.358222000
H	-0.231907000	-2.428244000	-4.113059000
H	-0.966062000	-3.980160000	-3.664390000
C	-1.190907000	-3.384017000	-0.932777000
H	-0.757239000	-3.350064000	0.067788000
H	-2.080691000	-2.745797000	-0.908022000
H	-1.497517000	-4.409207000	-1.165819000
C	2.017116000	-3.313481000	-3.134937000
H	1.662370000	-4.005370000	-3.905517000
H	1.965063000	-2.295769000	-3.536676000
H	3.066156000	-3.537398000	-2.924890000
C	1.269998000	-4.849913000	-1.312556000
H	2.309281000	-5.182963000	-1.248679000
H	0.832782000	-4.917865000	-0.313877000
H	0.734185000	-5.540075000	-1.973575000
C	-0.430684000	-3.325331000	3.367880000
H	-0.041020000	-3.555526000	4.365717000

H	-1.518116000	-3.429591000	3.389183000
H	-0.033734000	-4.074539000	2.676220000
C	1.496756000	-1.902772000	2.676525000
H	1.748748000	-2.596257000	1.868314000
H	1.820439000	-0.907811000	2.358710000
H	2.064016000	-2.185097000	3.569452000
C	-1.820046000	-1.089024000	4.536904000
H	-1.686904000	-1.825897000	5.335586000
H	-2.220225000	-0.172760000	4.979749000
H	-2.562265000	-1.478953000	3.834624000
C	0.513699000	-0.260333000	4.829937000
H	1.407484000	0.113292000	4.325498000
H	0.086705000	0.561041000	5.411834000
H	0.813153000	-1.049354000	5.528931000
P	-1.186766000	1.861616000	-2.303388000
P	-3.555713000	0.235061000	0.025014000
C	-1.090500000	3.686726000	-2.163341000
H	-0.945423000	4.163709000	-3.138792000
H	-2.006455000	4.075676000	-1.710045000
H	-0.254989000	3.951580000	-1.508433000
C	0.327982000	1.479623000	-3.257513000
H	0.383636000	0.400048000	-3.420436000
H	0.345621000	2.005815000	-4.217784000
H	1.203874000	1.768269000	-2.670587000
C	-2.461979000	1.669261000	-3.615803000

H	-3.441203000	1.993820000	-3.251160000
H	-2.216377000	2.254877000	-4.508457000
H	-2.539220000	0.616478000	-3.904036000
C	-4.355999000	-0.641430000	-1.377767000
H	-4.239910000	-0.063017000	-2.297375000
H	-3.872732000	-1.610118000	-1.530869000
H	-5.423388000	-0.807123000	-1.194743000
C	-4.660132000	1.688224000	0.211913000
H	-4.552491000	2.350829000	-0.651131000
H	-5.711037000	1.392515000	0.301542000
H	-4.371678000	2.253216000	1.101211000
C	-4.104943000	-0.806284000	1.428418000
H	-3.554018000	-1.751973000	1.413746000
H	-3.861553000	-0.296927000	2.365298000
H	-5.181072000	-1.008868000	1.399715000

TSRE1

Imaginary Frequency:

M06-L/BSI SCF energy in gas: -2412.126798 a.u.

M06/BSII SCF energy in benzene: -2411.587901a.u.

M06/BSII//M06-L/BSI free energy in benzene: -2410.875717 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -2410.748654 a.u.

Pd	-1.494354000	0.300556000	-0.321512000
B	-0.566191000	-0.336810000	1.411184000
B	1.546700000	-1.043581000	-0.785304000
O	-0.612155000	0.215008000	2.688989000

O	-0.064349000	-1.639336000	1.459304000
O	0.511792000	-1.433695000	-1.615430000
O	2.539983000	-1.998691000	-0.711158000
C	0.451302000	1.021354000	0.140555000
C	1.625826000	0.375134000	-0.160491000
C	-0.266605000	-0.820556000	3.642063000
C	0.527810000	-1.839265000	2.766979000
C	0.726386000	-2.821412000	-1.963680000
C	2.264108000	-2.983245000	-1.733353000
C	2.966771000	0.961353000	0.049542000
C	3.987222000	0.770174000	-0.895933000
C	3.277949000	1.703813000	1.201611000
H	3.773104000	0.185797000	-1.789306000
H	2.505486000	1.850884000	1.954932000
C	5.251309000	1.321209000	-0.717168000
C	4.542719000	2.247578000	1.386616000
H	6.018553000	1.166853000	-1.471859000
H	4.757351000	2.815550000	2.288441000
C	5.535973000	2.064768000	0.425247000
H	6.524491000	2.491988000	0.570003000
C	0.337107000	2.470228000	0.409438000
C	1.094940000	3.399038000	-0.332387000
C	-0.644377000	2.987378000	1.276852000
H	1.853633000	3.032305000	-1.019965000
H	-1.252495000	2.290362000	1.846130000

C	0.886902000	4.768168000	-0.207479000
C	-0.838537000	4.356974000	1.413370000
H	1.483284000	5.456176000	-0.801862000
H	-1.597853000	4.723909000	2.099862000
C	-0.078057000	5.258190000	0.670677000
H	-0.238374000	6.328455000	0.769951000
C	0.270015000	-3.024859000	-3.395887000
H	-0.808948000	-2.853650000	-3.463398000
H	0.764427000	-2.337247000	-4.085859000
H	0.468873000	-4.049182000	-3.729534000
C	-0.113288000	-3.669308000	-1.021348000
H	0.188678000	-3.524307000	0.017611000
H	-1.157109000	-3.351580000	-1.100720000
H	-0.050559000	-4.732287000	-1.276722000
C	3.087954000	-2.584049000	-2.950744000
H	2.997733000	-3.311164000	-3.763824000
H	2.774115000	-1.605080000	-3.329521000
H	4.140656000	-2.513028000	-2.664719000
C	2.688126000	-4.345691000	-1.224325000
H	3.770247000	-4.368743000	-1.070489000
H	2.205751000	-4.582317000	-0.273363000
H	2.432656000	-5.129406000	-1.945971000
C	0.339922000	-3.293420000	3.154736000
H	0.674528000	-3.472848000	4.182535000
H	-0.704574000	-3.604708000	3.072276000

H	0.935604000	-3.933650000	2.496943000
C	2.008388000	-1.509241000	2.660515000
H	2.460416000	-2.116330000	1.870640000
H	2.166818000	-0.461064000	2.392646000
H	2.533951000	-1.708987000	3.600022000
C	-1.573656000	-1.390830000	4.176399000
H	-1.404149000	-2.146019000	4.950378000
H	-2.168573000	-0.583584000	4.613474000
H	-2.161489000	-1.848998000	3.373878000
C	0.532131000	-0.192855000	4.766839000
H	1.401095000	0.347241000	4.385654000
H	-0.090759000	0.515139000	5.320438000
H	0.880818000	-0.956913000	5.470656000
P	-1.616221000	1.371365000	-2.494085000
P	-3.508079000	-0.647932000	0.233172000
C	-1.992269000	3.166381000	-2.441764000
H	-1.942227000	3.623880000	-3.436086000
H	-2.990702000	3.327158000	-2.026168000
H	-1.272929000	3.663084000	-1.783139000
C	-0.002321000	1.368862000	-3.363862000
H	0.285395000	0.338713000	-3.588429000
H	-0.031273000	1.955409000	-4.288473000
H	0.759990000	1.782586000	-2.695926000
C	-2.736180000	0.808412000	-3.839639000
H	-3.778344000	0.900725000	-3.521738000

H	-2.597975000	1.388493000	-4.758967000
H	-2.546234000	-0.246019000	-4.059377000
C	-4.982512000	-0.585627000	-0.867075000
H	-5.862379000	-1.047112000	-0.404374000
H	-5.218491000	0.455218000	-1.106711000
H	-4.765982000	-1.104558000	-1.805065000
C	-4.205312000	0.074507000	1.768116000
H	-4.435154000	1.130012000	1.599788000
H	-5.115799000	-0.441164000	2.093550000
H	-3.452705000	0.026945000	2.559464000
C	-3.477112000	-2.438376000	0.639411000
H	-3.376784000	-3.016740000	-0.283105000
H	-2.602370000	-2.660937000	1.257885000
H	-4.389153000	-2.759393000	1.154728000

14

M06-L/BSI SCF energy in gas: -2412.160878 a.u.

M06/BSII SCF energy in benzene: -2411.625614 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -2410.912677 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -2410.784624 a.u.

Pd	2.531919000	-0.403467000	-1.253250000
B	-0.838078000	-1.054724000	1.450930000
B	-1.330386000	1.734524000	0.538646000
O	-0.550032000	-2.294893000	1.967087000
O	0.126583000	-0.115265000	1.747034000

O	-0.529622000	2.147313000	-0.498781000
O	-1.271071000	2.550666000	1.637662000
C	-2.139681000	-0.719092000	0.675472000
C	-2.375935000	0.581052000	0.330130000
C	0.787518000	-2.221391000	2.530309000
C	0.949250000	-0.693161000	2.795635000
C	0.304655000	3.222778000	0.009011000
C	-0.513572000	3.724188000	1.245731000
C	-3.638314000	1.059547000	-0.282549000
C	-3.613241000	2.004737000	-1.321934000
C	-4.889380000	0.640219000	0.199173000
H	-2.652593000	2.345877000	-1.702951000
H	-4.926738000	-0.076122000	1.015583000
C	-4.794495000	2.484306000	-1.880146000
C	-6.066153000	1.132620000	-0.348158000
H	-4.750904000	3.202386000	-2.695070000
H	-7.022223000	0.798115000	0.045631000
C	-6.025274000	2.051846000	-1.395828000
H	-6.947836000	2.432972000	-1.825049000
C	-3.052982000	-1.836021000	0.331134000
C	-3.567797000	-1.979034000	-0.967213000
C	-3.381944000	-2.814793000	1.279551000
H	-3.310913000	-1.237033000	-1.720686000
H	-2.975380000	-2.734936000	2.283585000
C	-4.389403000	-3.049136000	-1.299226000

C	-4.214242000	-3.880114000	0.951199000
H	-4.771273000	-3.140044000	-2.312955000
H	-4.461923000	-4.621346000	1.706840000
C	-4.721658000	-4.002948000	-0.339099000
H	-5.364801000	-4.839685000	-0.598103000
C	0.483912000	4.243058000	-1.096648000
H	1.034395000	3.789406000	-1.925862000
H	-0.473480000	4.601945000	-1.481154000
H	1.058757000	5.105210000	-0.741061000
C	1.636451000	2.597972000	0.383565000
H	1.493050000	1.828582000	1.145222000
H	2.063593000	2.094771000	-0.494723000
H	2.349398000	3.345342000	0.748825000
C	-1.535332000	4.795181000	0.890332000
H	-1.055710000	5.741743000	0.622067000
H	-2.164972000	4.477538000	0.052976000
H	-2.188017000	4.970289000	1.749188000
C	0.332516000	4.162356000	2.424107000
H	-0.311072000	4.478010000	3.249615000
H	0.969422000	3.349759000	2.781898000
H	0.972608000	5.008560000	2.151915000
C	2.369405000	-0.187236000	2.657487000
H	3.044345000	-0.756421000	3.307461000
H	2.708476000	-0.276546000	1.617958000
H	2.434400000	0.864996000	2.953274000

C	0.336154000	-0.243316000	4.114691000
H	0.256587000	0.847385000	4.114464000
H	-0.671620000	-0.650007000	4.243212000
H	0.943730000	-0.550552000	4.971601000
C	1.750614000	-2.743576000	1.475544000
H	2.769778000	-2.817984000	1.869791000
H	1.433566000	-3.741680000	1.160808000
H	1.781519000	-2.092300000	0.587774000
C	0.833675000	-3.082844000	3.775684000
H	0.046399000	-2.815270000	4.483386000
H	0.705354000	-4.134912000	3.508063000
H	1.800945000	-2.980143000	4.279305000
P	0.740548000	-1.190188000	-2.476523000
P	4.664731000	-0.004554000	-0.527493000
C	5.949237000	0.116943000	-1.836798000
H	6.946988000	0.279582000	-1.412467000
H	5.958683000	-0.800985000	-2.428689000
H	5.711162000	0.943102000	-2.510760000
C	5.436226000	-1.268218000	0.567090000
H	6.480423000	-1.025559000	0.795753000
H	4.878119000	-1.333606000	1.505622000
H	5.394853000	-2.249348000	0.087660000
C	5.056126000	1.515427000	0.438478000
H	6.122344000	1.578564000	0.685420000
H	4.771645000	2.402058000	-0.134185000

H	4.479126000	1.523284000	1.367781000
C	1.214098000	-1.738311000	-4.167474000
H	2.003451000	-2.490850000	-4.104019000
H	0.358834000	-2.161263000	-4.707825000
H	1.607144000	-0.891282000	-4.734714000
C	-0.082229000	-2.717007000	-1.866878000
H	-0.509231000	-2.557652000	-0.872525000
H	-0.884472000	-3.042943000	-2.539134000
H	0.659055000	-3.516386000	-1.781605000
C	-0.716502000	-0.145324000	-2.872127000
H	-0.390945000	0.790788000	-3.333381000
H	-1.405100000	-0.664380000	-3.549635000
H	-1.241196000	0.113775000	-1.949754000

TSER2

Imaginary Frequency: -103.33

M06-L/BSI SCF energy in gas: -2412.117684 a.u.

M06/BSII SCF energy in benzene: -2411.58070 a.u.

M06/BSII//M06-L/BSI free energy in benzene: -2410.870923 a.u.

M06/BSII//M06-L/BSI entalphy in benzene: -2410.742032 a.u.

Pd	1.523782000	-0.712015000	-0.515703000
B	1.582567000	1.156795000	0.357593000
B	-2.789262000	0.054854000	0.412230000
O	1.606558000	1.434490000	1.726531000
O	2.002432000	2.264537000	-0.371783000
O	-3.547354000	-0.591759000	-0.538990000

O	-3.549341000	0.823437000	1.264012000
C	-0.306733000	0.390867000	-0.224396000
C	-1.250878000	-0.195008000	0.580296000
C	2.243824000	2.717603000	1.916857000
C	2.053835000	3.399323000	0.525003000
C	-4.902944000	-0.083697000	-0.443828000
C	-4.942163000	0.522342000	1.000330000
C	-0.941992000	-1.281673000	1.537259000
C	0.261473000	-1.369691000	2.264545000
C	-1.883368000	-2.311605000	1.729129000
H	0.988852000	-0.569769000	2.184731000
H	-2.815736000	-2.286009000	1.165830000
C	0.507654000	-2.439608000	3.116916000
C	-1.634162000	-3.384827000	2.580569000
H	1.440638000	-2.469899000	3.676023000
H	-2.381414000	-4.166399000	2.693810000
C	-0.432540000	-3.457782000	3.278790000
H	-0.233762000	-4.290797000	3.947898000
C	-0.733216000	1.354912000	-1.260520000
C	-1.728569000	2.324113000	-1.049245000
C	-0.103745000	1.341002000	-2.517765000
H	-2.191509000	2.408055000	-0.067644000
H	0.705014000	0.624273000	-2.672175000
C	-2.097021000	3.212622000	-2.055920000
C	-0.479976000	2.215111000	-3.528001000

H	-2.863265000	3.959440000	-1.857345000
H	0.020341000	2.172241000	-4.492529000
C	-1.482298000	3.159169000	-3.303597000
H	-1.767535000	3.855499000	-4.087751000
C	-5.860493000	-1.237071000	-0.671164000
H	-5.751386000	-1.614969000	-1.691155000
H	-5.669830000	-2.063314000	0.017160000
H	-6.898777000	-0.912567000	-0.541527000
C	-5.061029000	0.958962000	-1.538674000
H	-4.366643000	1.790570000	-1.396717000
H	-4.831655000	0.503544000	-2.505563000
H	-6.081021000	1.354124000	-1.575076000
C	-5.376932000	-0.477098000	2.062920000
H	-6.436273000	-0.735466000	1.969057000
H	-4.789776000	-1.398746000	2.008582000
H	-5.214352000	-0.041461000	3.051733000
C	-5.743682000	1.803323000	1.123874000
H	-5.704163000	2.170682000	2.152654000
H	-5.352909000	2.586362000	0.470310000
H	-6.794797000	1.631976000	0.867097000
C	3.196274000	4.298039000	0.095260000
H	3.324672000	5.131184000	0.795365000
H	4.140280000	3.750826000	0.035445000
H	2.987660000	4.718111000	-0.892316000
C	0.727316000	4.133909000	0.406750000

H	0.538240000	4.372148000	-0.643820000
H	-0.100073000	3.508820000	0.753738000
H	0.726260000	5.063961000	0.984897000
C	3.704477000	2.453949000	2.258526000
H	4.246837000	3.379738000	2.475647000
H	3.757551000	1.813919000	3.144091000
H	4.219329000	1.940900000	1.439969000
C	1.563553000	3.430398000	3.070056000
H	0.484881000	3.497002000	2.919714000
H	1.739528000	2.887426000	4.002828000
H	1.961098000	4.444315000	3.191583000
P	0.576445000	-2.712556000	-1.524199000
C	-1.198720000	-2.639681000	-1.966643000
H	-1.382413000	-1.803456000	-2.646862000
H	-1.540461000	-3.569657000	-2.434482000
H	0.171208000	-5.080283000	-0.967466000
H	-1.794322000	-2.452500000	-1.069808000
C	0.614407000	-4.211898000	-0.466779000
H	1.645172000	-4.450532000	-0.189438000
H	0.060548000	-4.011116000	0.455624000
H	2.353353000	-3.598452000	-2.941233000
C	1.298061000	-3.353725000	-3.088818000
H	1.238968000	-2.583655000	-3.862877000
H	0.776491000	-4.249344000	-3.444512000
P	3.788665000	-1.055034000	-0.345613000

C	4.862031000	0.303443000	-0.951352000
H	4.468425000	1.262139000	-0.604358000
H	5.903171000	0.185424000	-0.631370000
H	5.708165000	-2.520884000	-0.863561000
H	4.829204000	0.324437000	-2.043821000
C	4.640098000	-2.498256000	-1.107442000
H	4.182663000	-3.428273000	-0.758551000
H	4.533631000	-2.458621000	-2.194915000
H	3.874326000	-2.154362000	1.809024000
C	4.315434000	-1.239685000	1.401957000
H	3.927596000	-0.400856000	1.986580000
H	5.404613000	-1.289764000	1.510358000

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