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Supporting Information

Carbodiimide and Isocyanate Hydroboration by a Cyclic Carbodiphosphorane Catalyst

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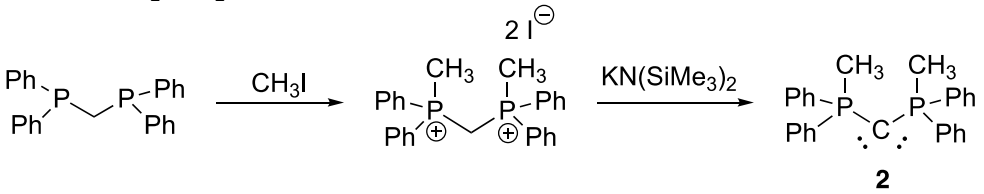
General Considerations

All experiments were conducted using standard Schlenk techniques or in a nitrogen atmosphere glovebox. Solvents were dried by passage through solvent purification columns and stored over activated 3Å molecular sieves. Deuterated solvents were purchased from Cambridge Isotope Laboratory and were degassed and stored over activated 3Å molecular sieves.

Bis(diphenylphosphino)methane (Combi-Blocks), pinacolborane (Oakwood), and solid carbodiimide or isocyanate substrates (Aldrich or Matrix Scientific) were used as received. 1,3-diiodopropane (Combi-Blocks), methyl iodide (Aldrich) and liquid carbodiimide and isocyanate substrates (Aldrich) were degassed and stored over activated 3Å molecular sieves prior to use. Compounds **1**,[1] **3**,[2,3] **4**,[4] and **5**,[5] methylenetriphenylphosphorane,[6] isopropylenetriphenylphosphorane,[7] 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene (IPr),[8,9] $IPrCH_2$,[10] *N*,*N*′-di-*p*-tolylcarbodiimide,[11] and *N*,*N*′-di-*p*-methoxycarbodiimide[11] were prepared according to literature procedures.

Solution NMR spectroscopy was performed using a Bruker AVANCE III 400 MHz NMR spectrometer at 25 °C. ^{1}H NMR spectra were calibrated internally to resonances for the residual proteo solvent relative to tetramethylsilane. ^{13}C, ^{31}P, and ^{11}B NMR spectra were referenced using the absolute reference function of MestReNova version 14.2.0 software.

Synthesis of Carbodiphosphorane 2

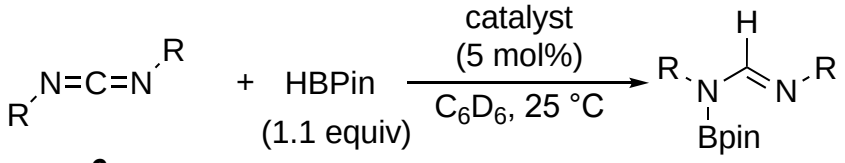


This synthesis was adapted from a procedure reported by Schmidbaur and co-workers.[12]

Bis(diphenylphosphino)methane (4.000 g, 10.41 mmol) was added to an oven-dried 100 mL Teflon-stoppered flask equipped with a magnetic stir bar in the glovebox. Toluene (40 mL) was added, followed by addition of methyl iodide (1.3 mL, 20.88 mmol). The flask was sealed, removed from the glovebox, and stirred at 80 °C for 72 hours. After 72 hours, the reaction flask was cooled to room temperature and was cycled into the glovebox. The reaction mixture was filtered on a fine-fritted funnel. The white solid was washed with diethyl ether (2 x 10 mL) and pentane (1 x 20 mL) and dried under vacuum (4.75 g, 68 % yield).

In a glovebox, the bis(phosphonium) precursor (0.570 g, 0.853 mmol) was suspended in THF (8 mL) in a scintillation vial equipped with a magnetic stir-bar. In a separate scintillation vial, potassium bis(trimethylsilyl)amide (0.340 g, 1.706 mmol) was dissolved in THF (8 mL). Both vials were cooled in the glovebox freezer (–35 °C) for 20 minutes. After removing the vials from the glovebox freezer, the potassium bis(trimethylsilyl)amide solution was added dropwise to the stirred suspension of bis(phosphonium) salt in THF. The reaction mixture stirred for 3 hours at room temperature. The resulting yellow solution was filtered through a fine-fritted funnel and the filtrate was concentrated under vacuum. The resulting oil was washed with diethyl ether (2 × 5 mL) and pentane (2 × 5 mL) and dried under vacuum to afford a pale-yellow powder of carbodiphosphorane **2** (0.28 g, 80 % yield). ^{1}H NMR (400 MHz, C_6D_6) δ 7.83 (m, 8H), 7.04–7.12 (overlapping signals, 12H), 1.67 (m, 6H). ^{13}C NMR (101 Mz, C_6D_6) δ 140.1 (m), 130.9 (t, J = 5.2 Hz), 128.9, 127.6 (m) , 20.1 (m), 12.6 (t, J = 93 Hz). ^{31}P NMR (162 MHz, C_6D_6) δ –13.4.

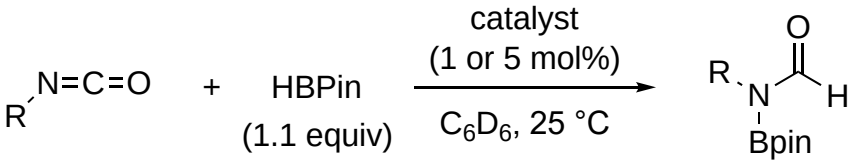
General Procedure for Carbodiimide Hydroboration Catalysis



6 **7**

In a glovebox, a J. Young NMR tube was charged with 0.50 mL of benzene-d_6, carbodiimide (0.24 mmol), pinacolborane (0.27 mmol, 1.1 equiv), and catalyst (0.012 mmol). The reaction progress was monitored by ^{1}H NMR spectroscopy. At the specified time, 1,3,5-tris(trifluoromethyl)benzene (0.24 mmol) was added to the NMR tube as an internal standard to determine the reaction yield.

General Procedure for Isocyanate Hydroboration Catalysis



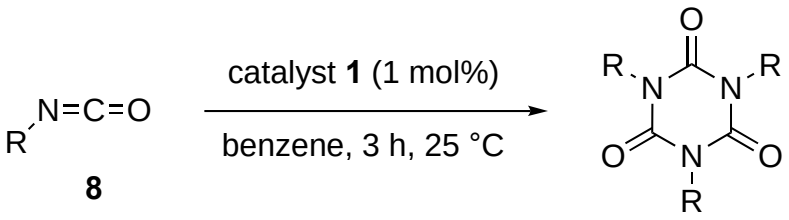
8 **9**

In a glovebox, a J. Young NMR tube was charged with 0.50 mL of benzene-d_6, isocyanate (0.24 mmol), pinacolborane (0.27 mmol, 1.1 equiv), and catalyst (0.012 or 0.0024 mmol). The reaction progress was monitored by ^{1}H NMR spectroscopy. At the specified time, 1,3,5-tris(trifluoromethyl)benzene (0.24 mmol) was added to the NMR tube as an internal standard to determine the reaction yield.

General Procedure for Competition Experiments

In a glovebox, a J. Young NMR tube was charged with 0.50 mL of benzene-d_6, substrate **A** (0.24 mmol), substrate **B** (0.24 mmol), pinacolborane (0.24 mmol), and catalyst (0.012 mmol). The reaction progress was monitored by ^{1}H NMR spectroscopy. After 1 h, 1,3,5-tris(trifluoromethyl)benzene (0.24 mmol) was added to the NMR tube as an internal standard to determine the reaction yield.

Isocyanate Cyclotrimerization Catalysis

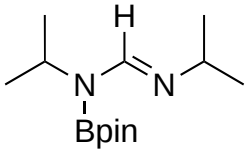


>95%

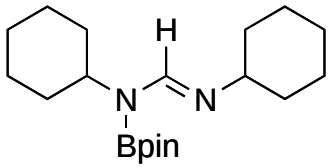
12a, R = Ph
12b, R = 4-OCH_3-Ph
12c, R = 4-Cl-Ph
12d, R = 1-Naph
12e, R = Hex (18 h)

In a glovebox, a scintillation vial was charged with isocyanate (0.80 mmol), benzene (2.0 mL), and catalyst **1** (0.0080 mmol). After stirring for 3 hours, the resulting precipitate was filtered, washed with pentane (5 mL), and dried under vacuum to afford the resulting isocyanurate products in >95% yield.

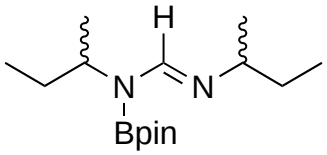
NMR Characterization Data for Carbodiimide Hydroboration Products



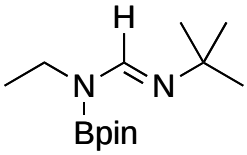
***N*,*N*'-diisopropyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formimidamide (7a).**[13] ^{1}H NMR (400 MHz, C_6D_6) δ 8.22 (s, 1H), 4.94 (hept, *J* = 6.9 Hz, 1H), 3.29 (hept, *J* = 6.3 Hz, 1H), 1.41 (d, *J* = 7.0 Hz, 6H), 1.17 (d, *J* = 6.2 Hz, 6H), 1.02 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 149.6, 82.4, 56.9, 43.2, 25.4, 24.2, 21.5. ^{11}B NMR (128 MHz, C_6D_6) δ 25.3.



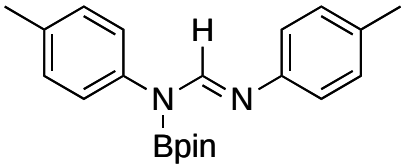
***N*,*N*'-dicyclohexyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formimidamide (7b).**[13] ^{1}H NMR (400 MHz, C_6D_6) δ 8.29 (s, 1H), 4.57 (m, 1H), 2.97 (m, 1H), 1.10 – 2.20 (m, 20H), 1.05 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 150.2, 82.4, 65.1, 51.4, 35.8, 31.7, 26.5, 26.0, 25.7, 25.0, 24.2. ^{11}B NMR (128 MHz, C_6D_6) δ 25.5.



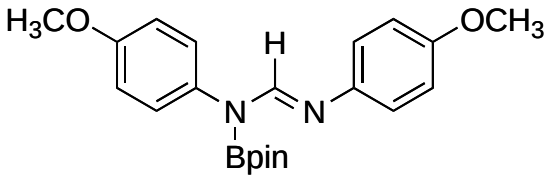
***N*,*N*'-di-*sec*-butyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formimidamide (7c).** ^{1}H NMR (400 MHz, C_6D_6) δ 8.22 (s, 1H), 4.62 (m, 1H), 2.95 (m, 2H), 2.13 (m, 2H), 1.64 (m, 1H), 1.51 (m, 1H), 1.44 (m, 4H), 1.16 (d, *J* = 6.4 Hz, 5H), 1.02 (s, 12H), 0.96 (q, *J* = 7.1 Hz, 4H), 0.85 (t, *J* = 7.2 Hz, 5H). ^{13}C NMR (101 MHz, C_6D_6) δ 150.1, 82.4, 63.2, 49.6, 49.3, 31.8, 31.7, 28.0, 27.8, 24.2, 24.2, 19.8, 19.7, 11.3, 11.0. ^{11}B NMR (128 MHz, C_6D_6) δ 25.4.



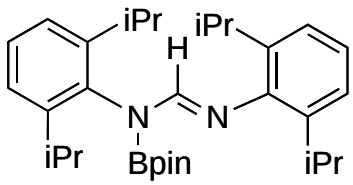
***N*'-*tert*-butyl-*N*-ethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formimidamide (7d).**[14] ^{1}H NMR (400 MHz, C_6D_6) δ 8.14 (s, 1H), 3.76 (q, *J* = 7.0 Hz, 2H), 1.30 (t, *J* = 7.0 Hz, 3H), 1.19 (s, 9H), 1.04 (s, 12H).



***N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-*N*,*N*'-di-*p*-tolylformimidamide (7e).**[15] ^{1}H NMR (400 MHz, C_6D_6) δ 8.63 (s, 1H), 7.53 – 6.48 (overlapping signals, 8H), 2.07 (s, 6H), 1.00 (s, 12H). 13C NMR (101 MHz, C_6D_6) δ 151.2, 132.3, 129.3, 121.4, 121.2, 83.6, 24.2, 20.6. ^{11}B NMR (128 MHz, C_6D_6) δ 25.4.

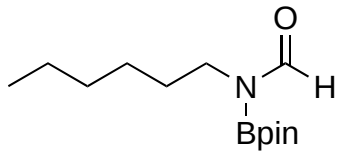


***N*,*N*'-bis(4-methoxyphenyl)-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formimidamide (7f).**[15] ^{1}H NMR (400 MHz, C_6D_6) δ 8.63 (s, 1H), 7.55 – 7.23 (br m, 2H), 7.20 – 6.91 (br m, 2H), 6.82 – 6.64 (br m, 4H), 3.27 (s, 6H), 1.03 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 151.1, 132.3, 129.3, 128.6, 121.9, 117.1, 113.6, 83.6, 54.6, 24.2. ^{11}B NMR (128 MHz, C_6D_6) δ 25.5.

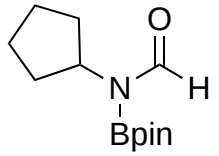


***N*,*N*'-bis(2,6-diisopropylphenyl)-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl) formimidamide (7g).**[13] ^{1}H NMR (400 MHz, C_6D_6) δ 8.31 (s, 1H), 7.22 – 7.07 (m, 6H), 3.54 – 3.05 (m, 4H), 1.44 – 1.33 (m, 12H), 1.19 (d, *J* = 7.0 Hz, 12H), 0.97 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 183.1, 152.1, 147.9, 145.9, 139.3, 133.9, 128.0, 123.4, 123.4, 122.9, 83.6, 28.7, 27.4, 25.0, 24.1, 23.9, 23.3. ^{11}B NMR (128 MHz, C_6D_6) δ 25.0.

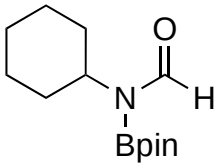
NMR Characterization Data for Isocyanate Hydroboration Products



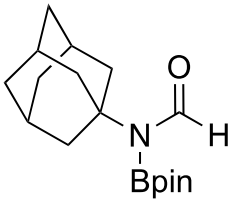
***N*-formyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexanamide (9a).**[16] ^{1}H NMR (400 MHz, C_6D_6) δ 8.97 (s, 1H), 3.45 (t, *J* = 6.0 Hz, 2H), 1.57 (m, 2H), 1.18 (m, 6H), 0.98 (s, 12H), 0.80 (m, 3H). ^{13}C NMR (101 MHz, C_6D_6) δ 164.7, 83.5, 40.0, 31.5, 29.9, 26.6, 24.1, 22.6, 13.9. ^{11}B NMR (128 MHz, C_6D_6) δ 25.8.



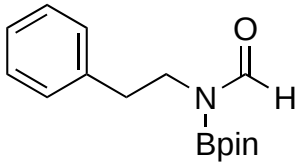
***N*-cyclopentyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (9b).**[17] ^{1}H NMR (400 MHz, C_6D_6) δ 9.03 (s, 1H), 4.72 (p, *J* = 8.7 Hz, 1H), 1.92 (m, 2H), 1.76 (m, 4H), 1.38 (m, 2H), 0.94 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 165.3, 83.2, 51.3, 30.9, 24.8, 24.0. ^{11}B NMR (128 MHz, C_6D_6) δ 25.7.



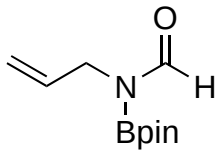
***N*-cyclohexyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (9c).**[14] ^{1}H NMR (400 MHz, C_6D_6) δ 9.04 (s, 1H), 4.28 (t, *J* = 11.7 Hz, 1H), 2.03 (q, *J* = 12.5 Hz, 2H), 1.65 (m, 4H), 1.45 (m, 1H), 1.26 – 1.03 (overlapping signals, 3H), 0.98 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 165.0, 83.0, 50.1, 31.5, 26.2, 25.4, 24.1. ^{11}B NMR (128 MHz, C_6D_6) δ 25.2.



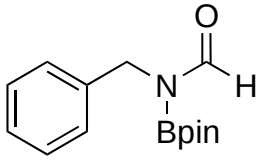
***N*-1-adamantyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (9d).**[17] ^{1}H NMR (400 MHz, Tol) δ 9.06 (s, 1H), 2.40 (d, *J* = 3.0 Hz, 6H), 2.12 (m, 3H), 2.01 (s, 6H), 1.00 (s, 12H).



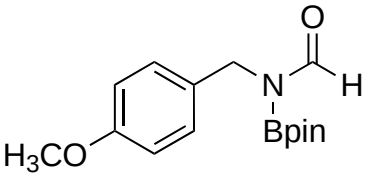
***N*-phenethyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (9e).** ^{1}H NMR (400 MHz, C_6D_6) δ 8.95 (s, 1H), 7.14 – 6.94 (m, 5H), 3.64 (t, *J* = 7.3 Hz, 2H), 2.84 (t, *J* = 7.3 Hz, 2H), 0.88 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 164.9, 139.3, 129.2, 128.2, 126.0, 83.5, 41.8, 35.6, 24.1. ^{11}B NMR (128 MHz, C_6D_6) δ 25.3.



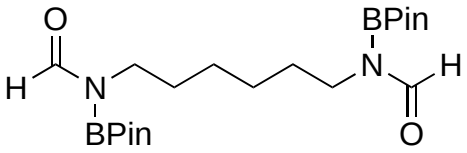
***N*-allyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (9f).**[17] ^{1}H NMR (400 MHz, C_6D_6) δ 8.95 (s, 1H), 5.91 – 5.74 (m, 1H), 5.11 (dd, *J* = 17.1, 1.6 Hz, 1H), 4.95 (dd, *J* = 10.2, 1.5 Hz, 1H), 3.98 (d, *J* = 5.5 Hz, 2H), 0.94 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 164.2, 134.7, 115.2, 83.7, 41.9, 24.0. ^{11}B NMR (128 MHz, C_6D_6) δ 25.7.



***N*-benzyl-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (9g).**[14] ^{1}H NMR (400 MHz, C_6D_6) δ 8.98 (s, 1H), 7.46 (d, *J* = 7.6 Hz, 2H), 7.13 (t, *J* = 7.5 Hz, 2H), 7.03 (t, *J* = 7.4 Hz, 1H), 4.56 (s, 2H), 0.93 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 164.6, 139.5, 128.4, 128.2, 126.9, 83.7, 43.4, 24.1. ^{11}B NMR (128 MHz, C_6D_6) δ 25.7.

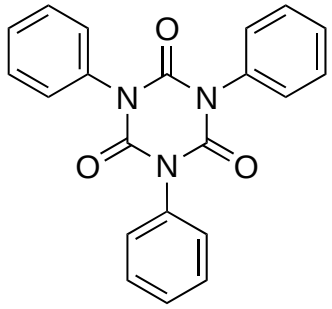


***N*-(4-methoxybenzyl)-*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (9h).**[17] ^{1}H NMR (400 MHz, C_6D_6) δ 8.97 (s, 1H), 7.44 (d, *J* = 8.2 Hz, 2H), 6.75 (d, *J* = 8.2 Hz, 2H), 4.54 (s, 2H), 3.29 (s, 3H), 0.94 (s, 12H). ^{13}C NMR (101 MHz, C_6D_6) δ 164.6, 159.0, 131.7, 129.9, 113.7, 83.8, 54.4, 42.8, 24.1. ^{11}B NMR (128 MHz, C_6D_6) δ 25.9.

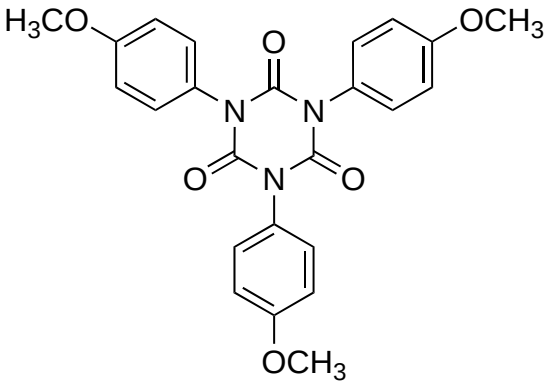


***N*,*N*'-(hexane-1,6-diyl)bis(*N*-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide) (9i).**[16] ^{1}H NMR (400 MHz, C_6D_6) δ 8.92 (s, 2H), 3.37 (t, *J* = 7.3 Hz, 4H), 1.48 (d, *J* = 7.2 Hz, 4H), 1.12 (p, *J* = 4.1 Hz, 4H), 1.00 (s, 24H). ^{13}C NMR (101 MHz, C_6D_6) δ 164.7, 83.6, 39.8, 29.7, 26.6, 24.1. ^{11}B NMR (128 MHz, C_6D_6) δ 26.2.

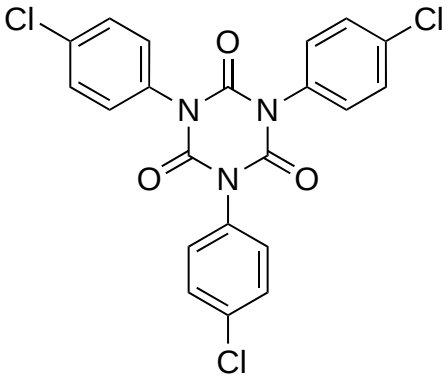
NMR Characterization Data for Isocyanate Cyclotrimerization Products



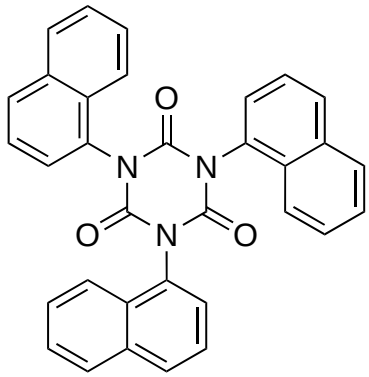
1,3,5-triphenyl-1,3,5-triazinane-2,4,6-trione (12a).[18] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.46 (overlapping signals, 9H), 7.43 (d, *J* = 7.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.7, 133.6, 129.4, 128.4.



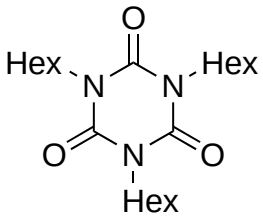
1,3,5-tris(4-methoxyphenyl)-1,3,5-triazinane-2,4,6-trione (12b).[18] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 7.8 Hz, 6H), 7.00 (d, *J* = 6.9 Hz, 6H), 3.84 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9, 149.2, 129.4, 126.3, 114.6, 55.5.



1,3,5-tris(4-chlorophenyl)-1,3,5-triazinane-2,4,6-trione (12c).[18] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.7 Hz, 6H), 7.35 (d, *J* = 8.7 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.2, 135.6, 131.8, 129.8, 128.4.



1,3,5-tri(naphthalen-1-yl)-1,3,5-triazinane-2,4,6-trione (12d).[18] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (dt, *J* = 11.3, 7.9 Hz, 9H), 7.73 (q, *J* = 8.2 Hz, 6H), 7.67 – 7.49 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.8, 134.59, 130.4, 129.0, 127.8, 127.3, 126.6, 125.5, 121.1, 120.8.



1,3,5-trihexanoyl-1,3,5-triazinane-2,4,6-trione (12e). ^{1}H NMR (400 MHz, C_6D_6) δ 3.82 (m, 6H), 1.62 (m, 6H), 1.18 (m, 18H), 0.83 (t, *J* = 6.5 Hz, 9H). ^{13}C NMR (101 MHz, C_6D_6) δ 148.7, 42.6, 30.9, 27.9, 26.4, 22.5, 13.8.

NMR Spectra

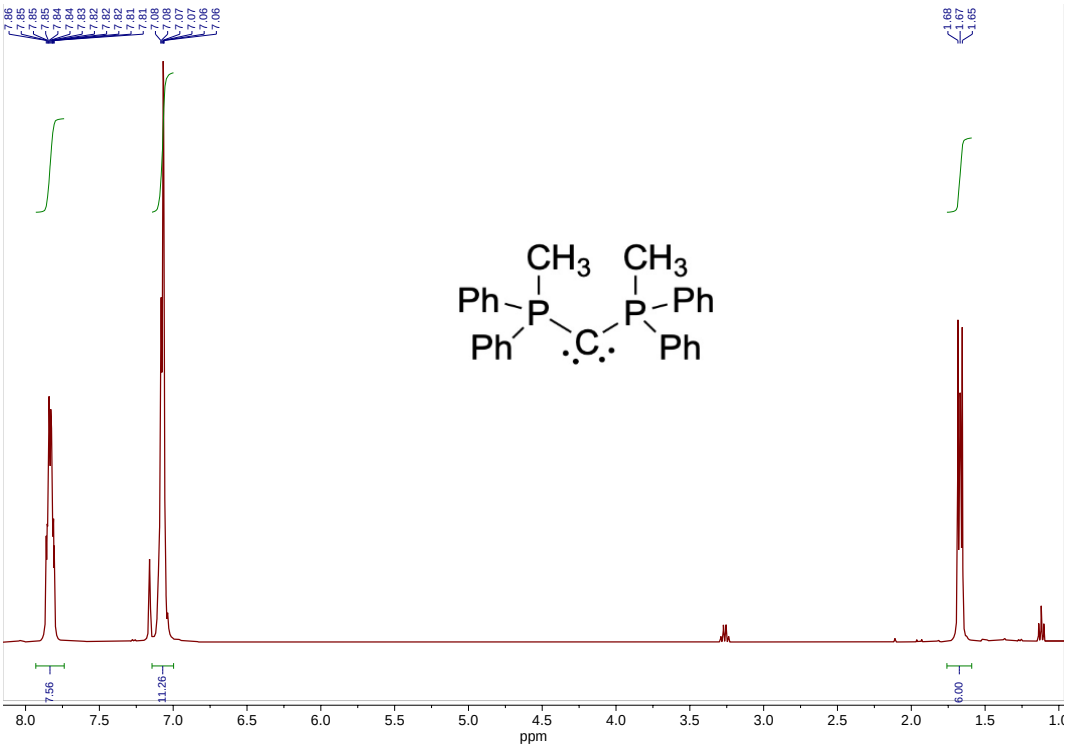


Figure S1. ^{1}H NMR spectrum of carbodiphosphorane **2** in benzene-d_6. Peaks at 1.11 and 3.25 ppm correspond to residual diethyl ether.

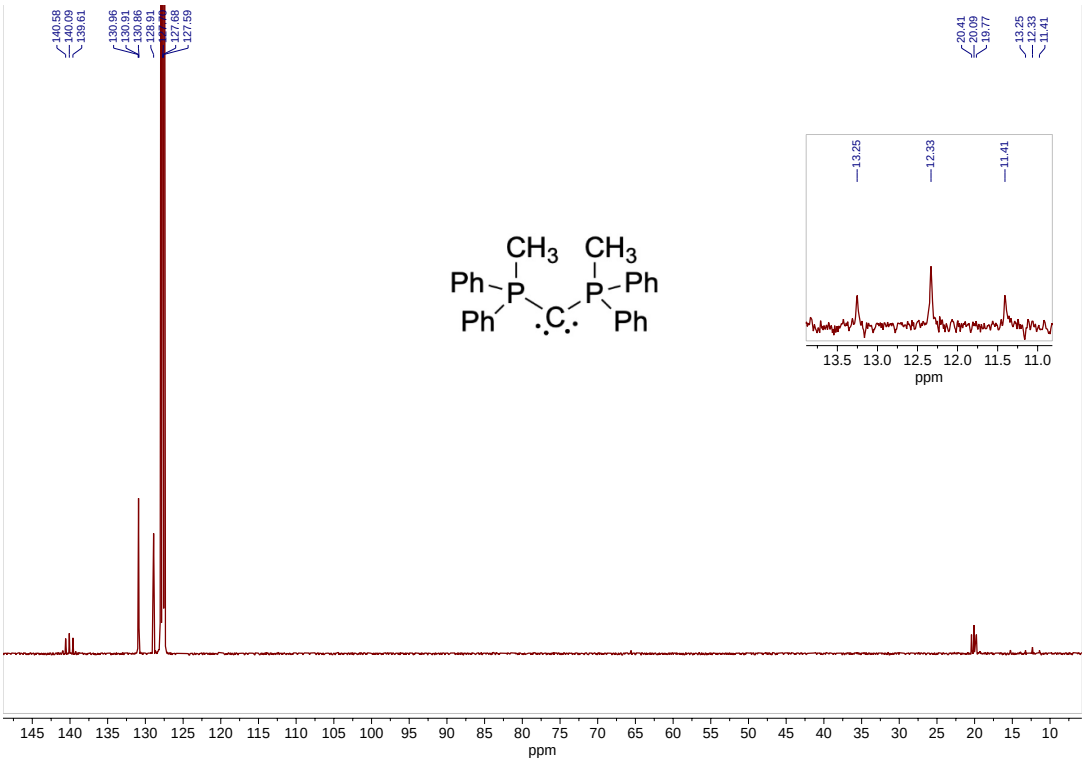


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of carbodiphosphorane **2** in benzene-d_6.

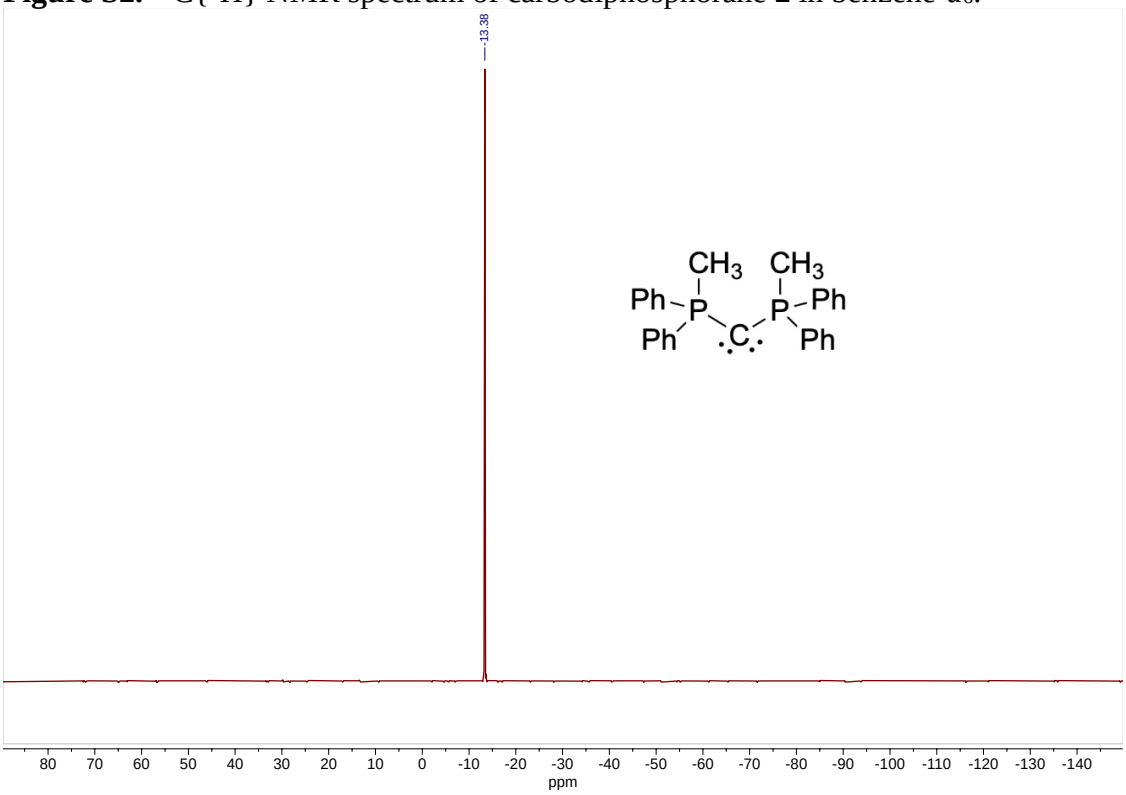


Figure S3. ^{31}P NMR spectrum of carbodiphosphorane **2** in benzene-d_6.

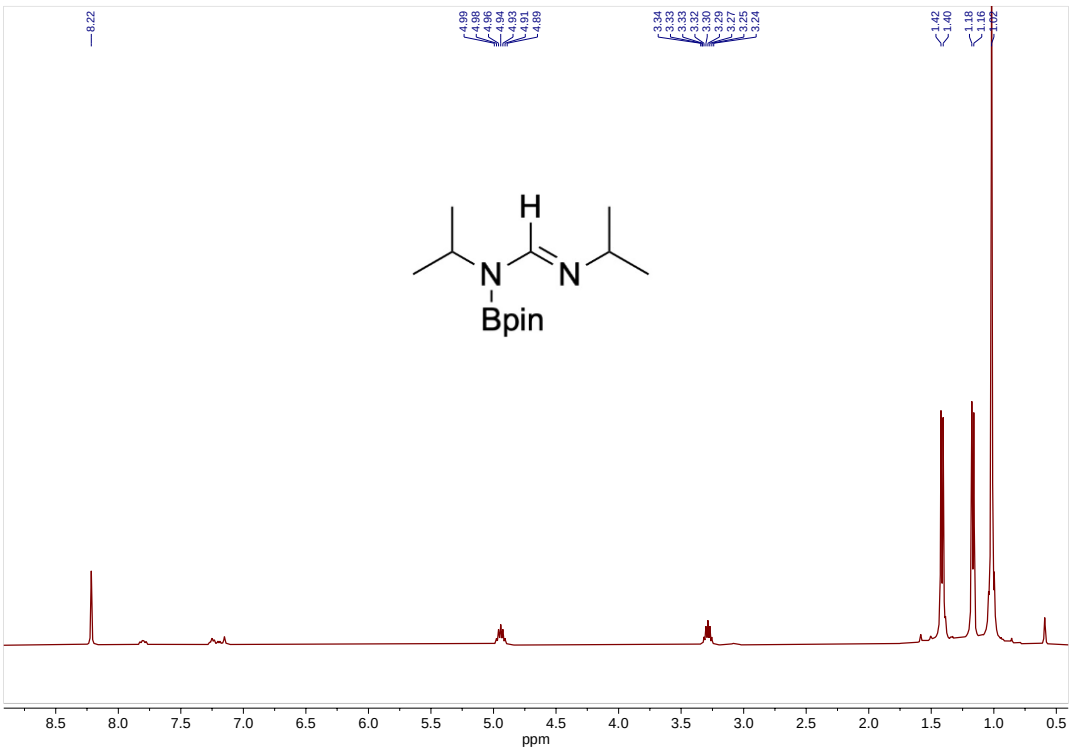


Figure S4. ^{1}H NMR spectrum of **7a** in benzene-d_6.

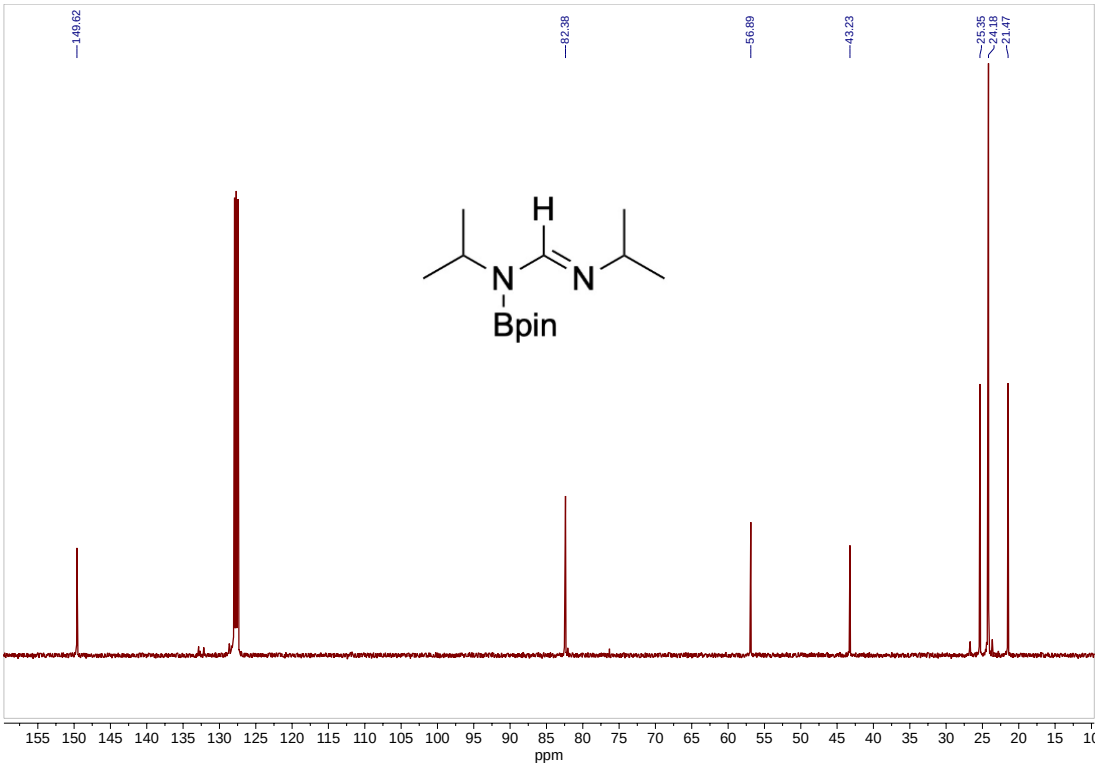


Figure S5. ^{13}C{^{1}H} NMR spectrum of **7a** in benzene-d_6.

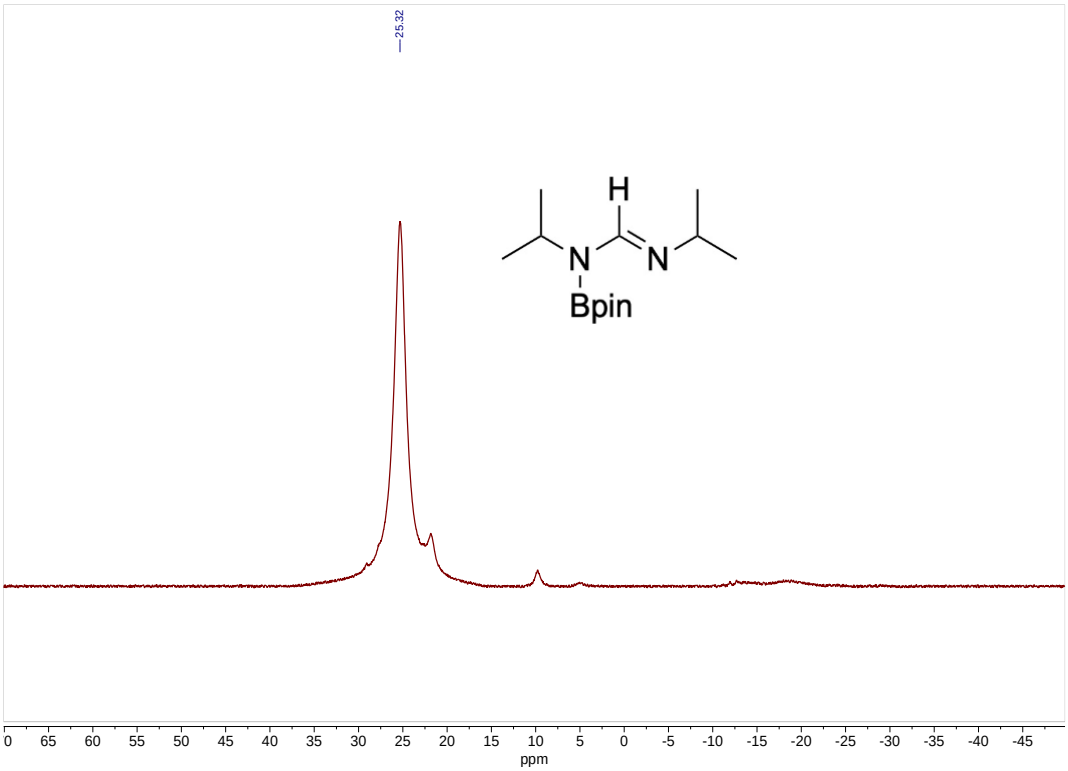


Figure S6. ^{11}B NMR spectrum of **7a** in benzene-d_6.

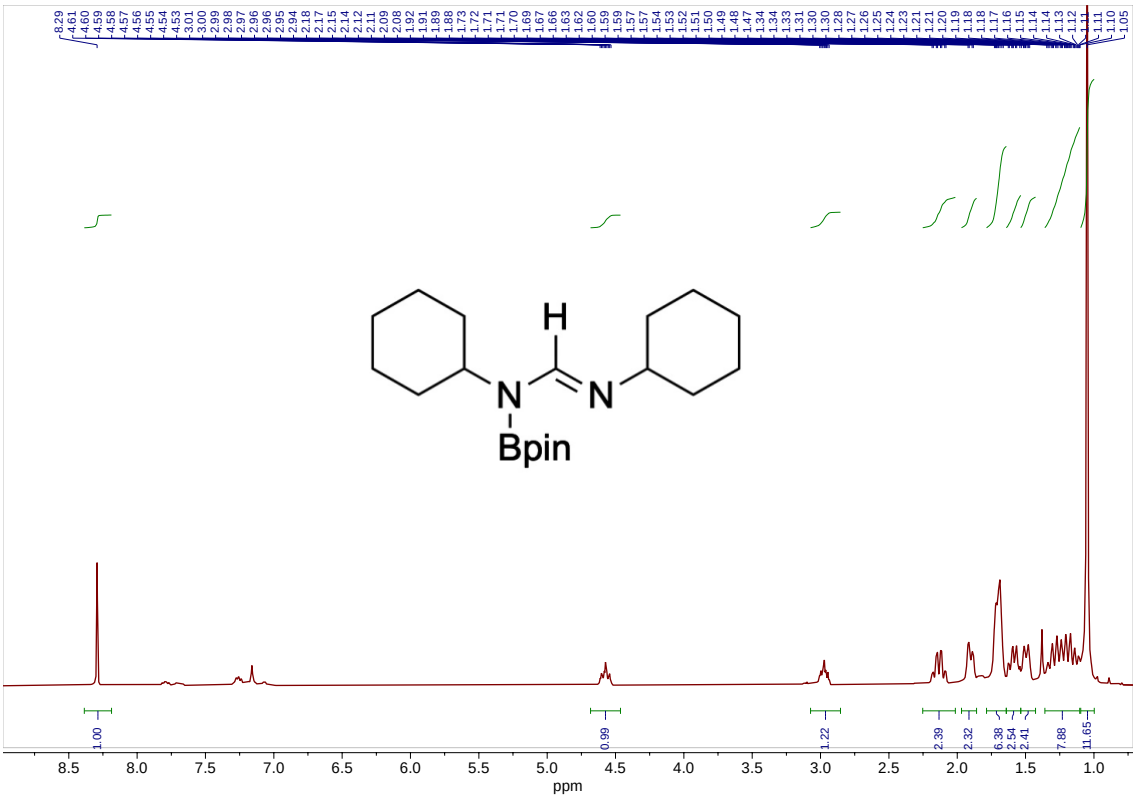


Figure S7. ^{1}H NMR spectrum of **7b** in benzene-d_6.

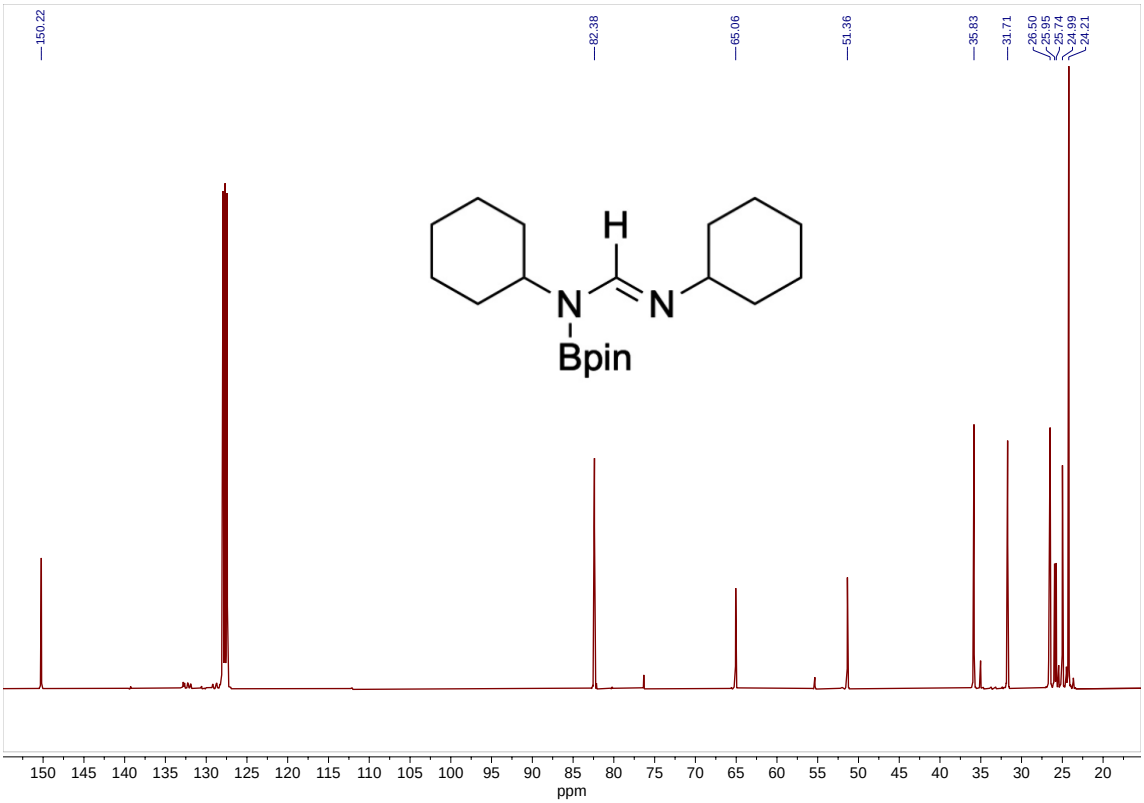


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of **7b** in benzene-d_6.

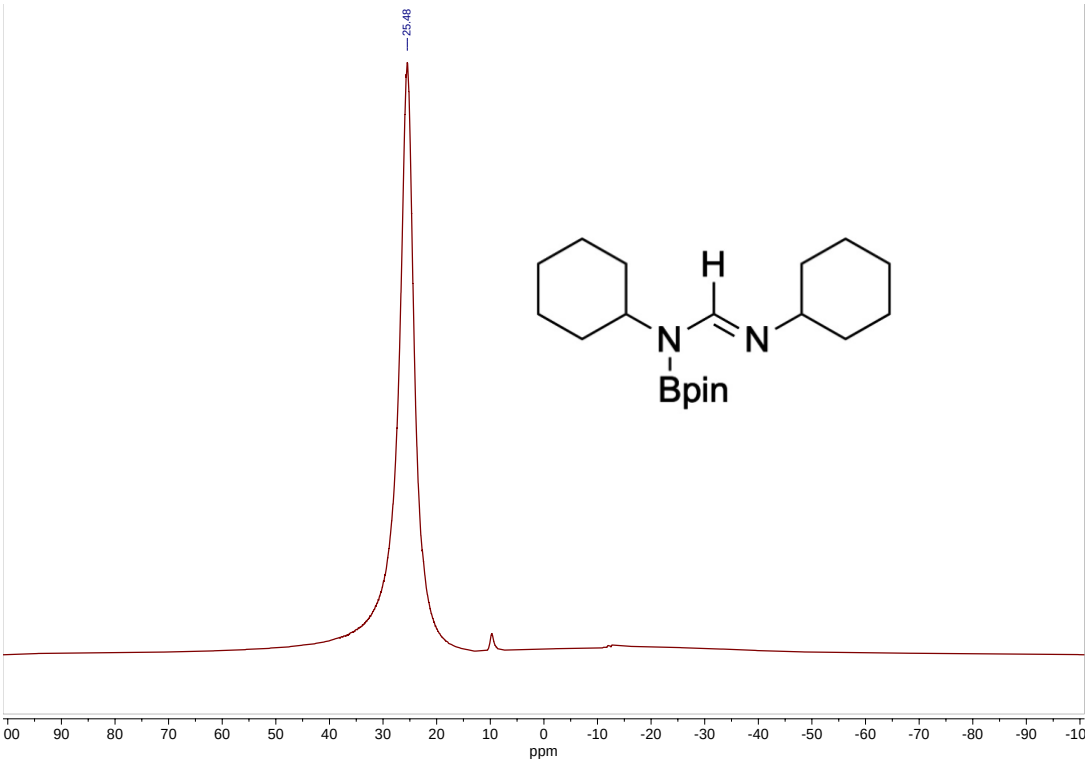


Figure S9. ^{11}B NMR spectrum of **7b** in benzene-d_6.

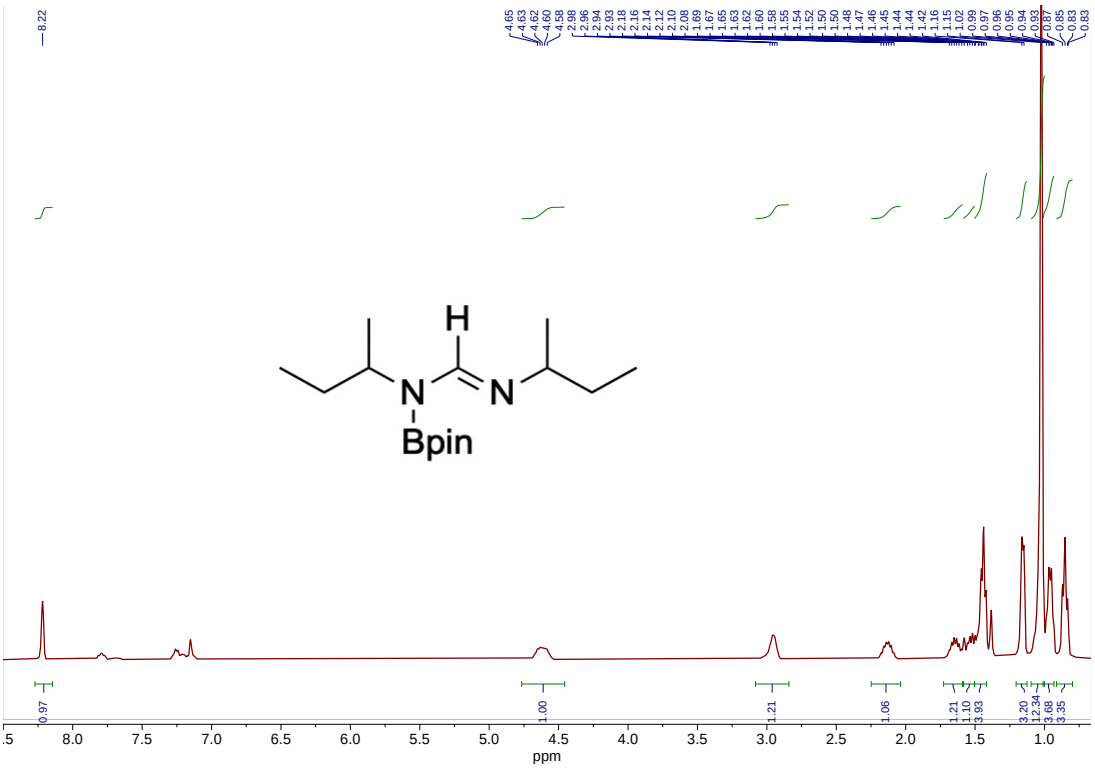


Figure S10. ^{1}H NMR spectrum of **7c** in benzene-d_6.

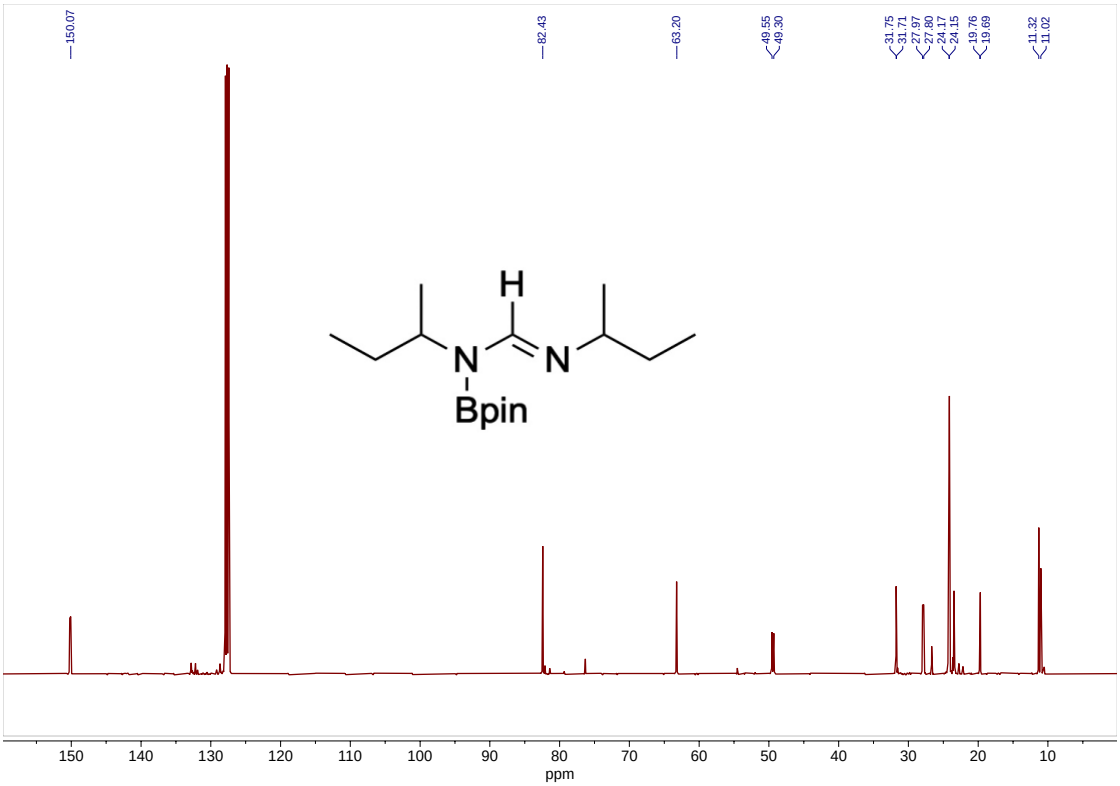


Figure S11. ^{13}C{^{1}H} NMR spectrum of **7c** in benzene-d_6.

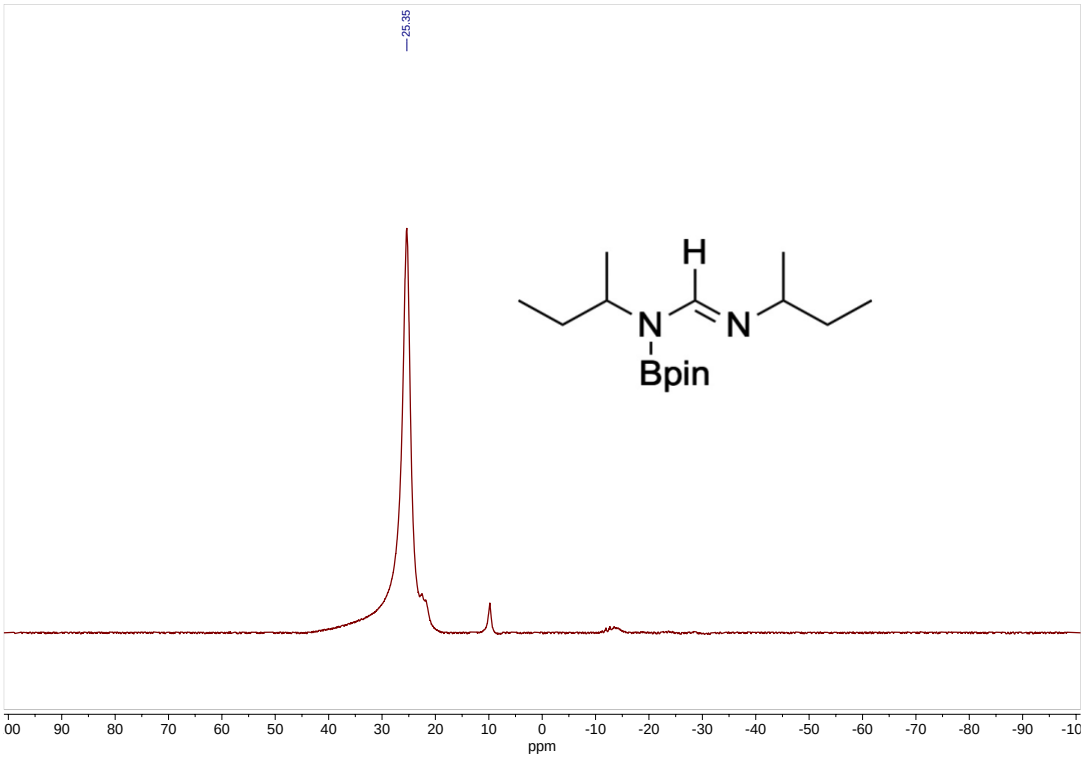


Figure S12. ^{11}B NMR spectrum of **7c** in benzene-d_6.

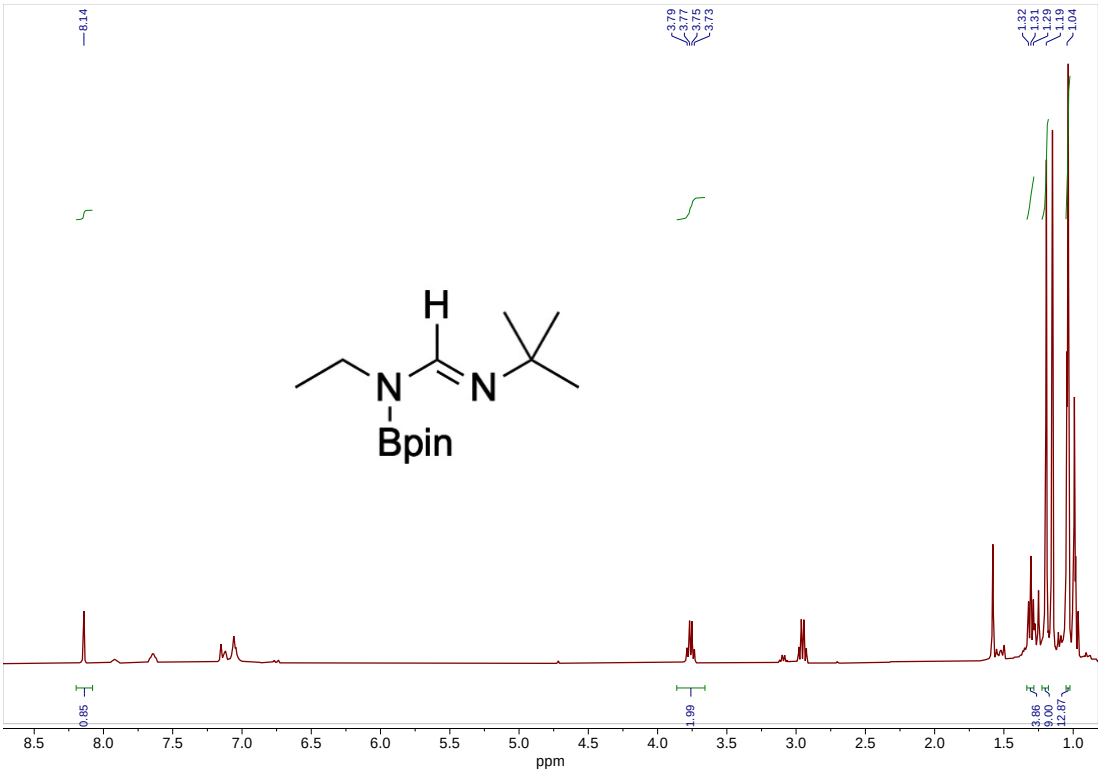


Figure S13. ^{1}H NMR spectrum of **7d** and remaining 1-tert-butyl-3-ethylcarbodiimide and pinacolborane in benzene-d_6.

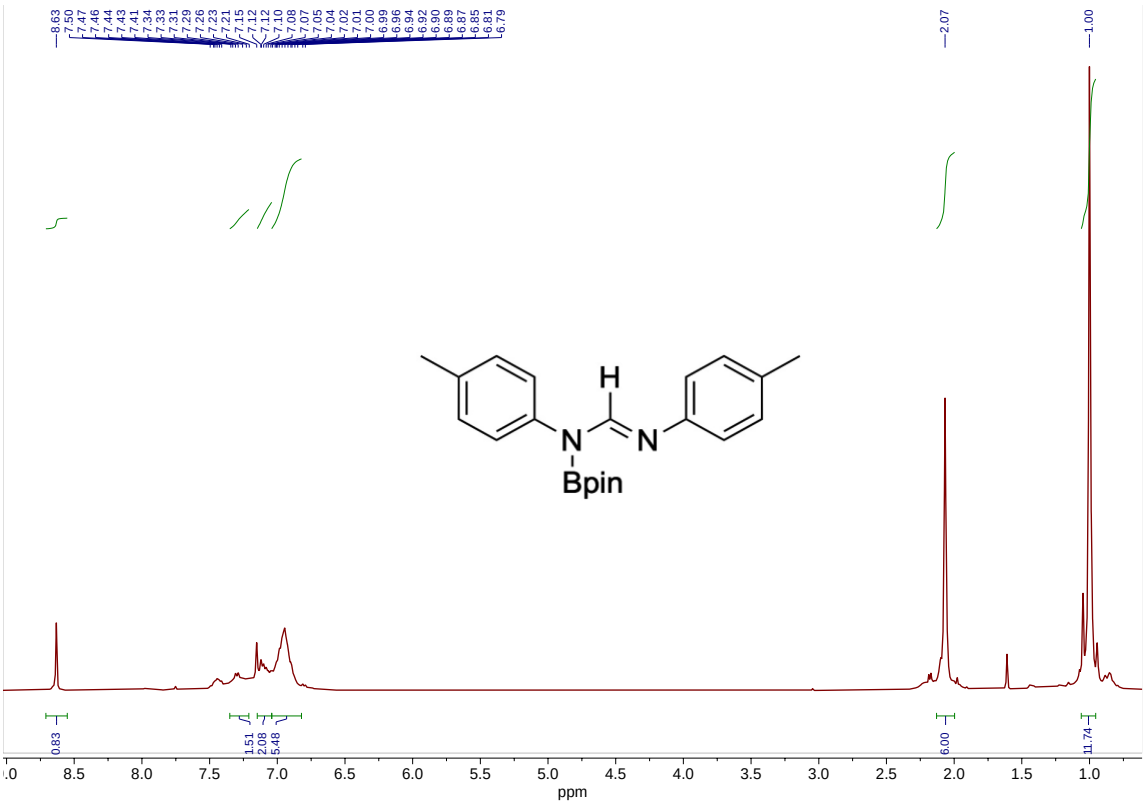


Figure S14. ^{1}H NMR spectrum of **7e** in benzene-d_6.

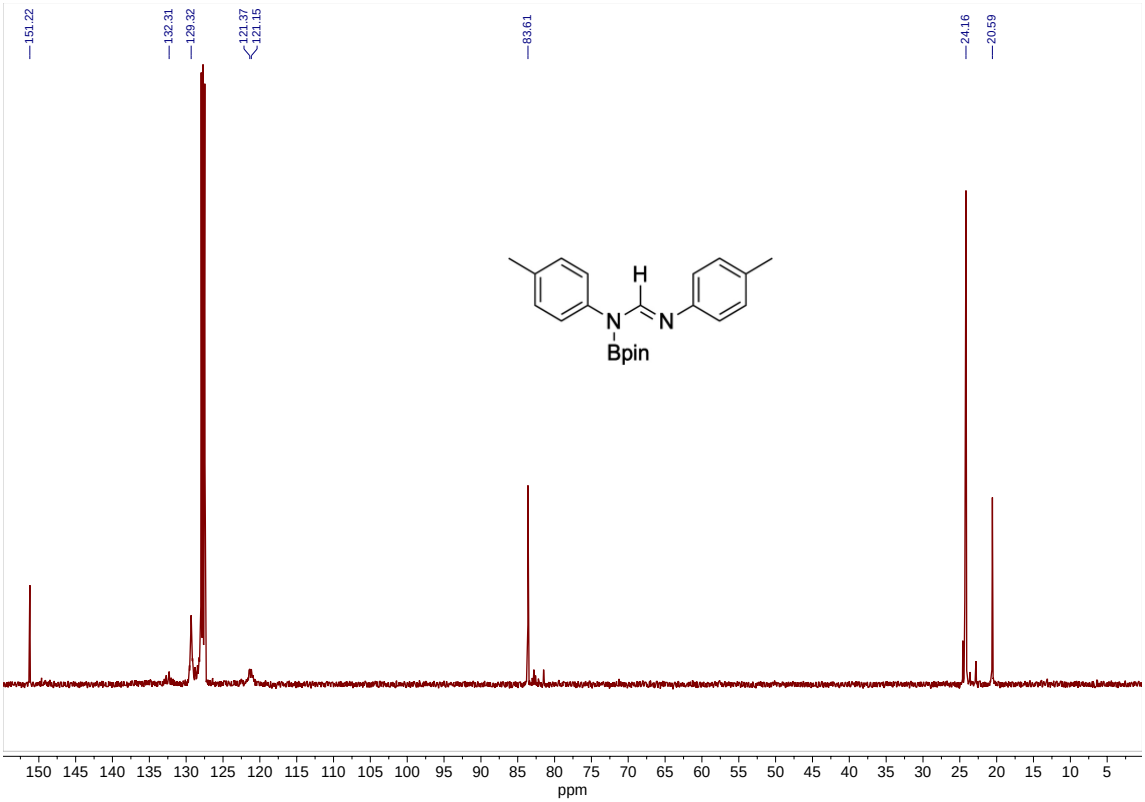


Figure S15. ^{13}C{^{1}H} NMR spectrum of **7e** in benzene-d_6.

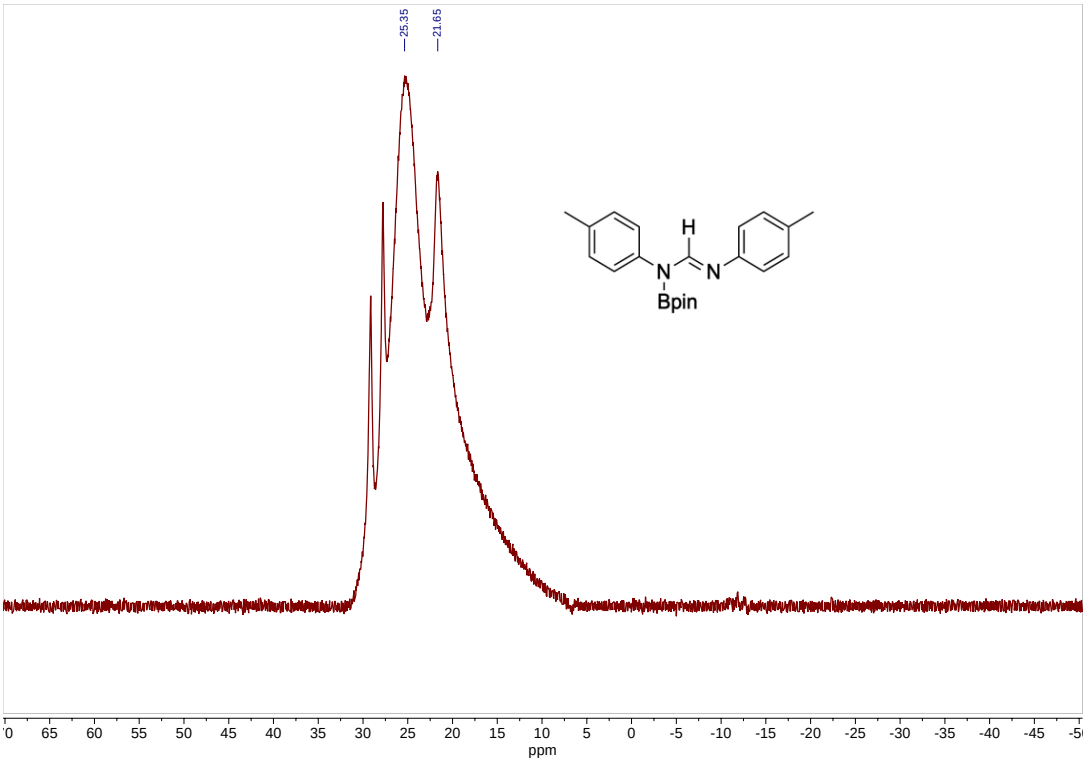


Figure S16. ^{11}B NMR spectrum of **7e** in benzene-d_6.

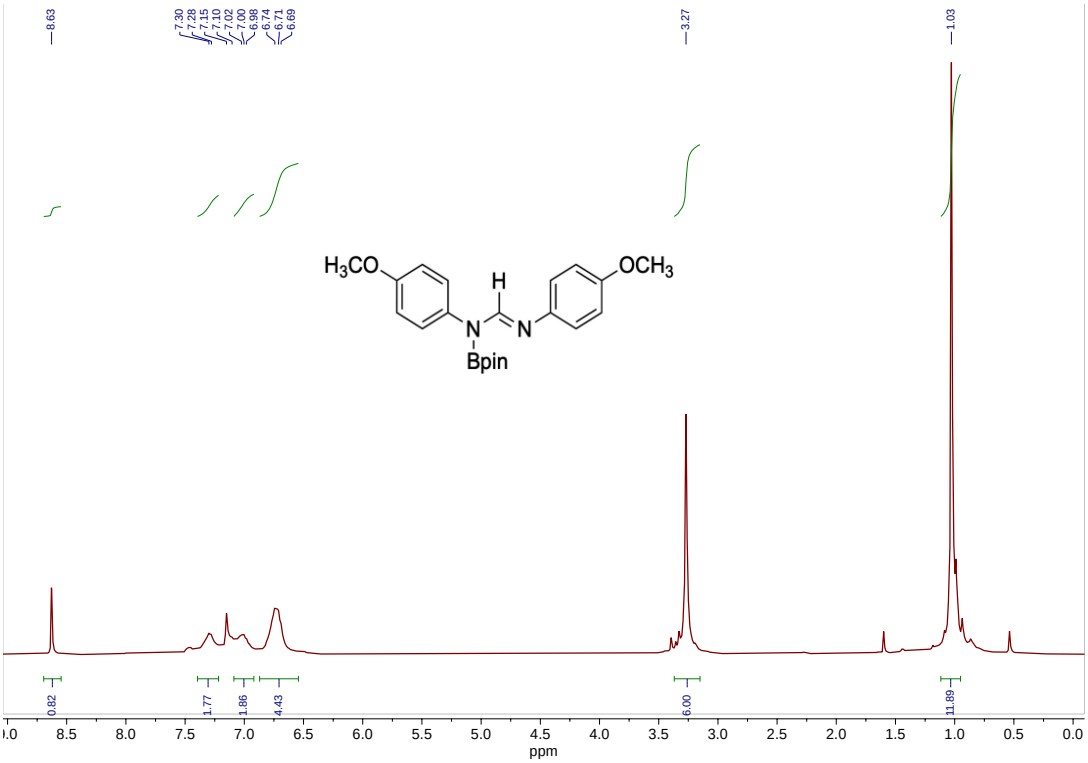


Figure S17. ^{1}H NMR spectrum of **7f** in benzene-d_6.

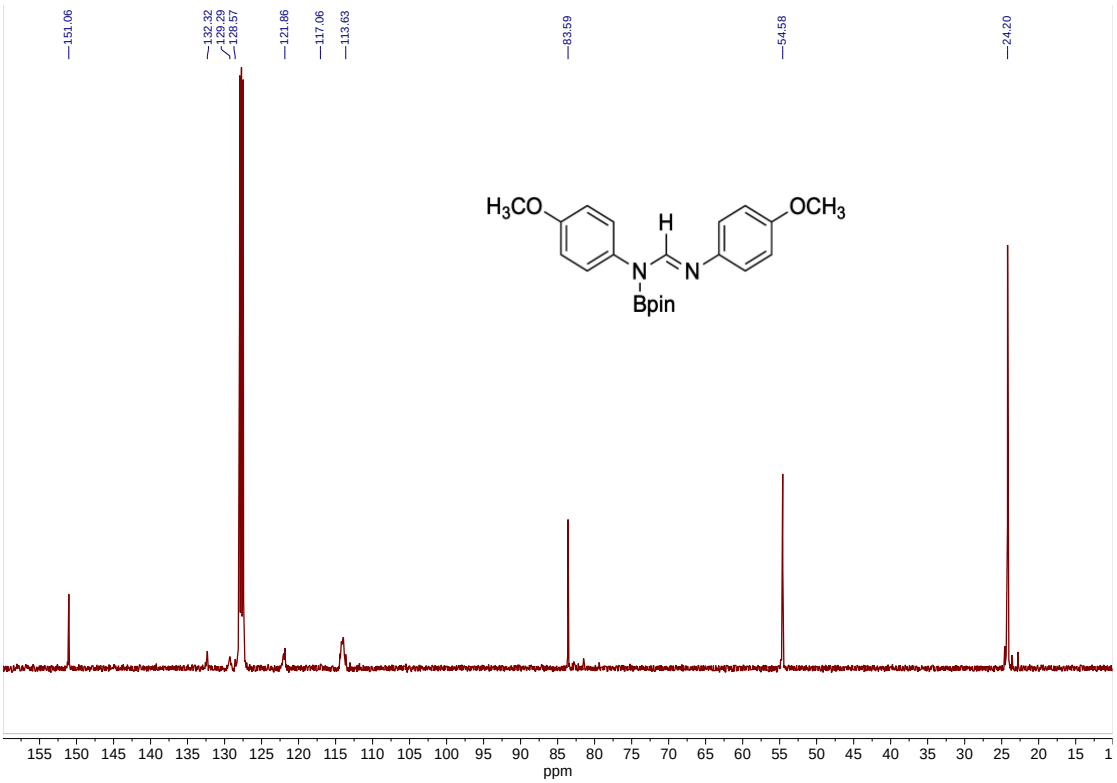


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of **7f** in benzene-d_6.

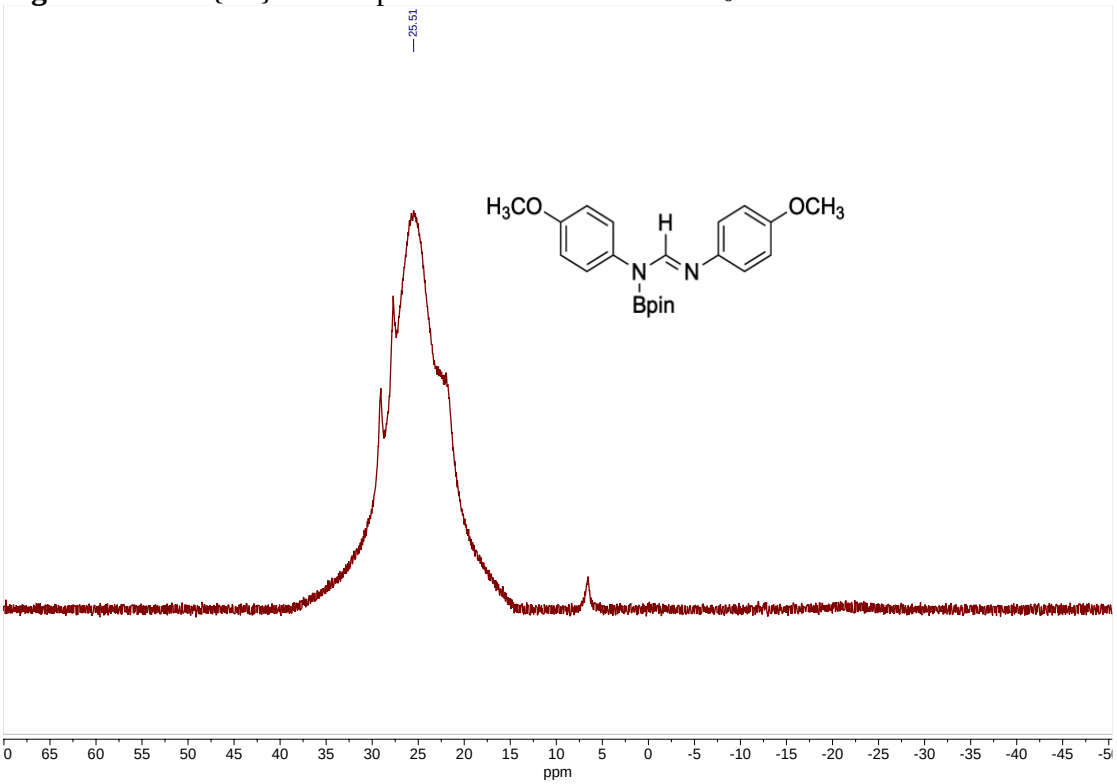


Figure S19. ^{11}B NMR spectrum of **7f** in benzene-d_6.

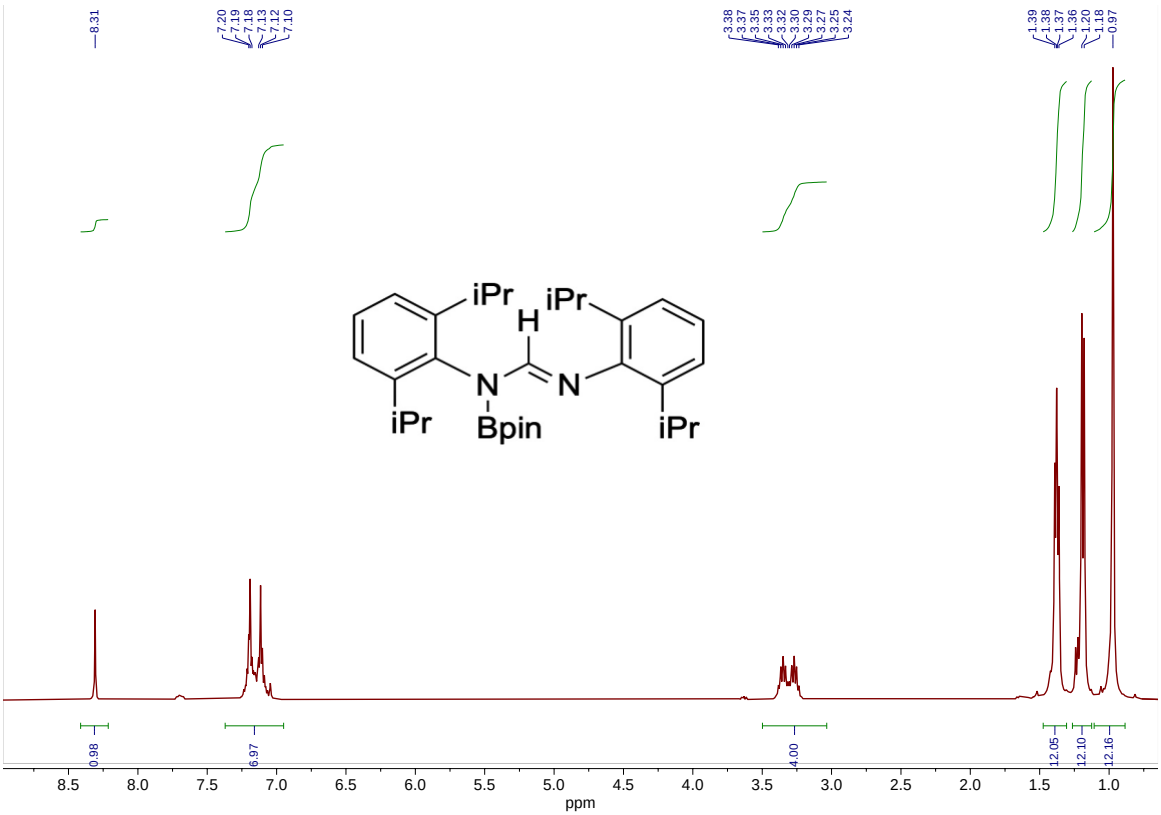


Figure S20. ^{1}H NMR spectrum of **7g** in benzene-d_6.

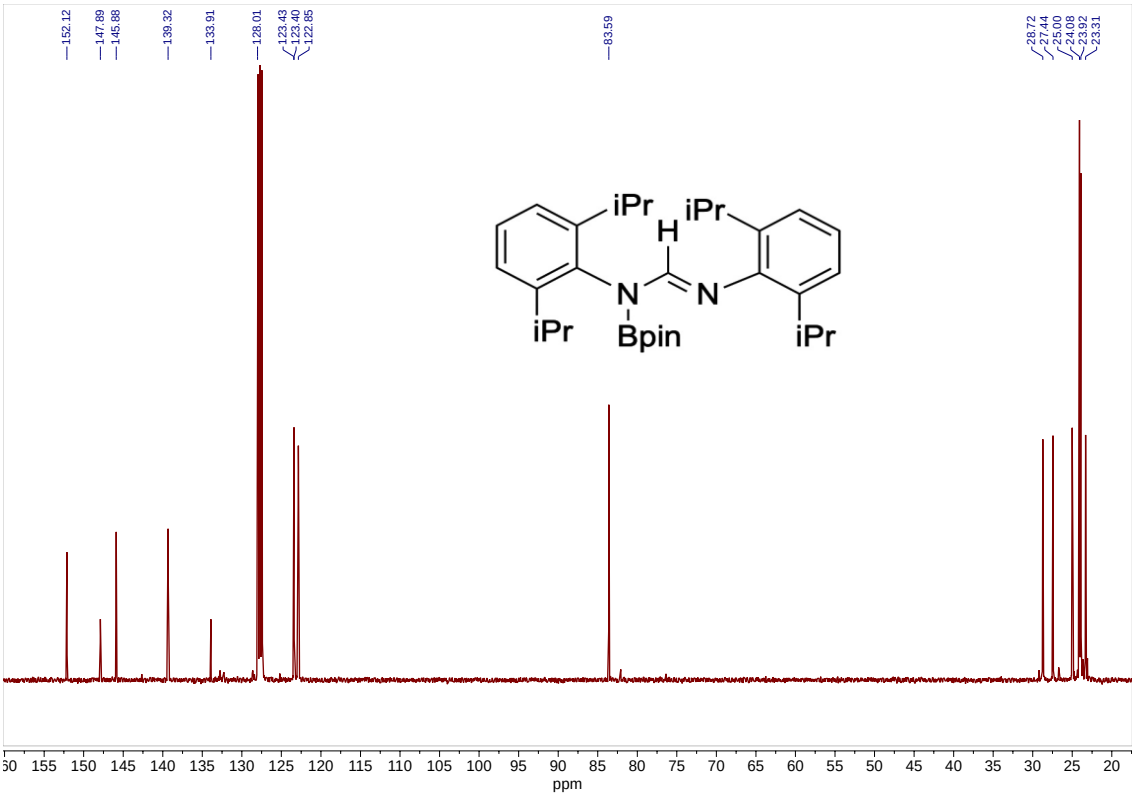


Figure S21. ^{13}C{^{1}H} NMR spectrum of **7g** in benzene-d_6.

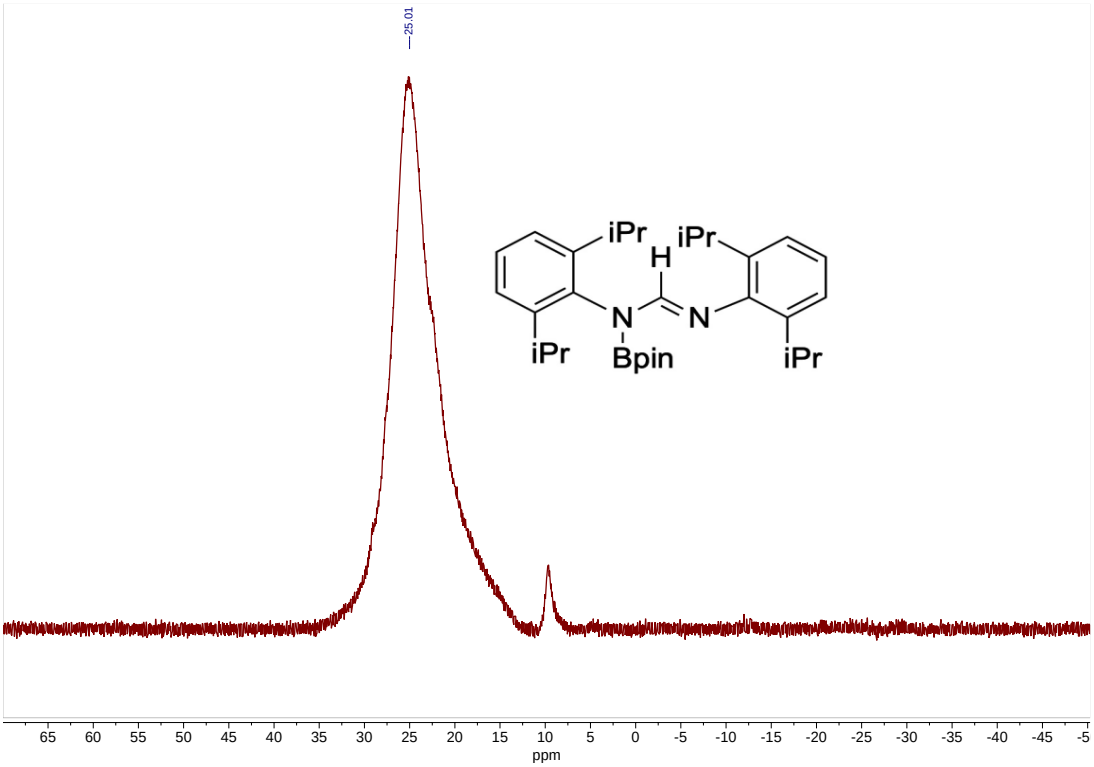


Figure S22. ^{11}B NMR spectrum of **7g** in benzene-d_6.

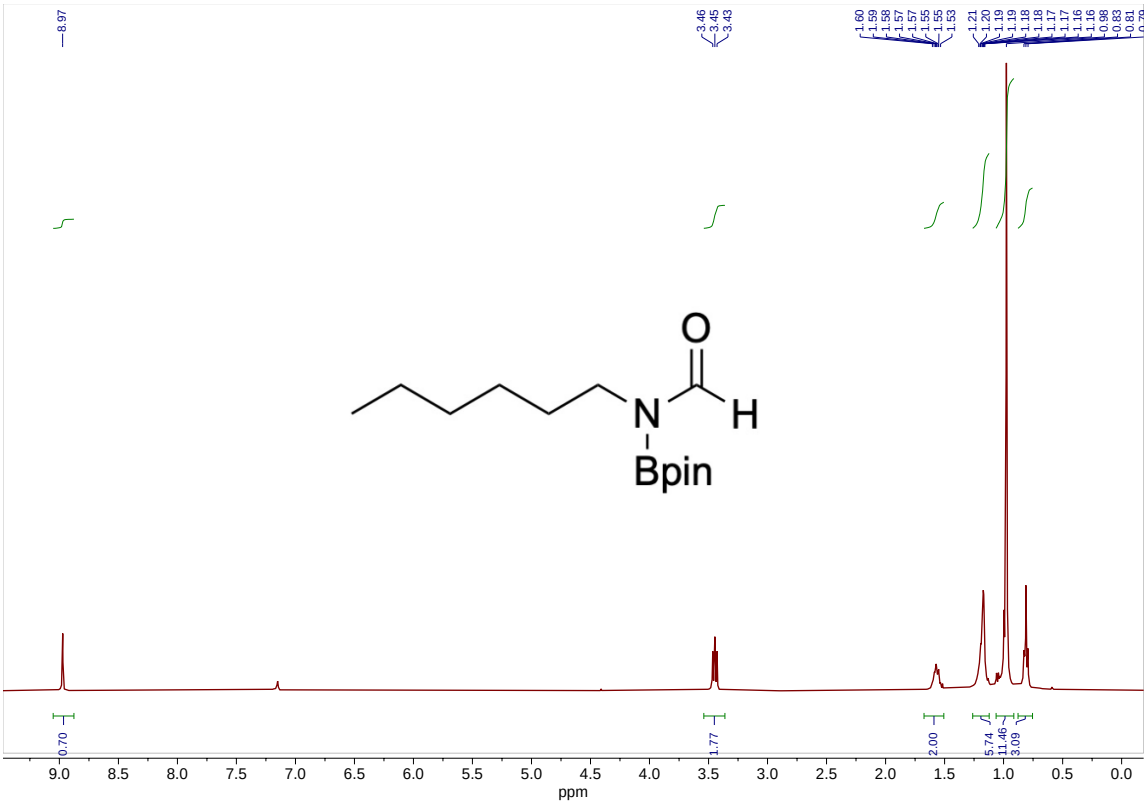


Figure S23. ^{1}H NMR spectrum of **9a** in benzene-d_6.

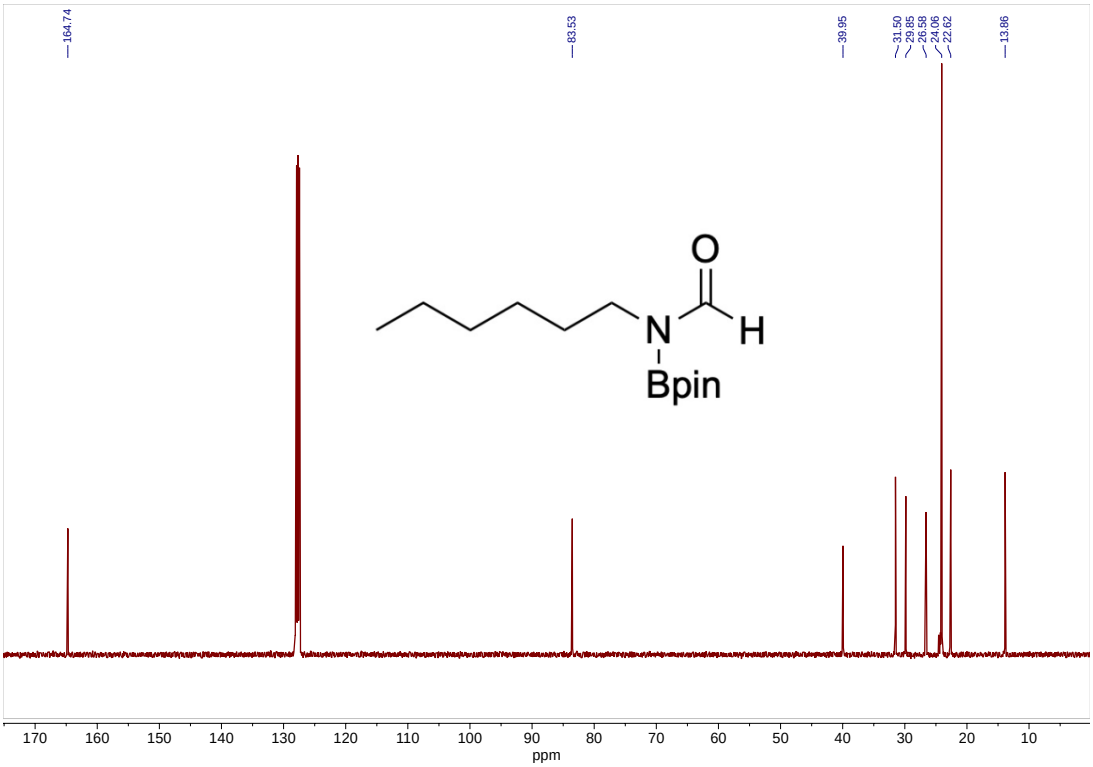


Figure S24. $^{13}C\{^{1}H\}$ NMR spectrum of **9a** in benzene-d_6.

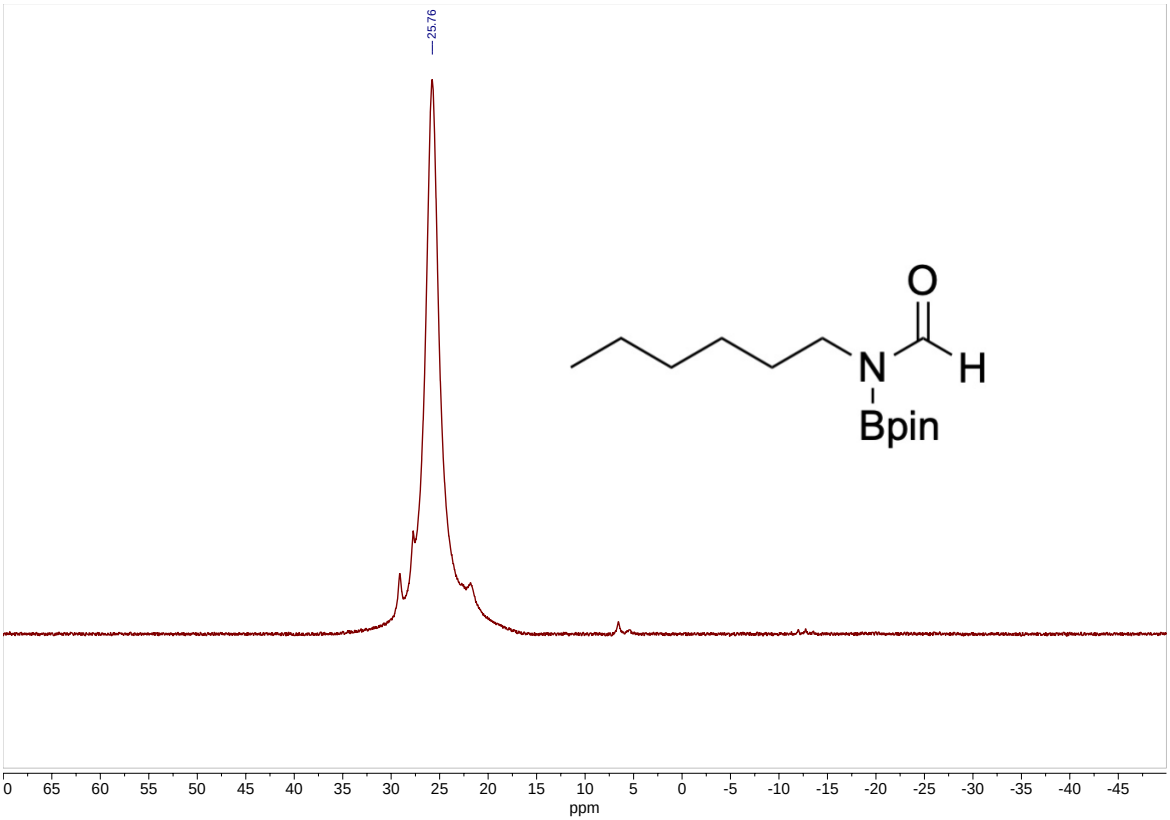


Figure S25. ^{11}B NMR spectrum of **9a** in benzene-d_6.

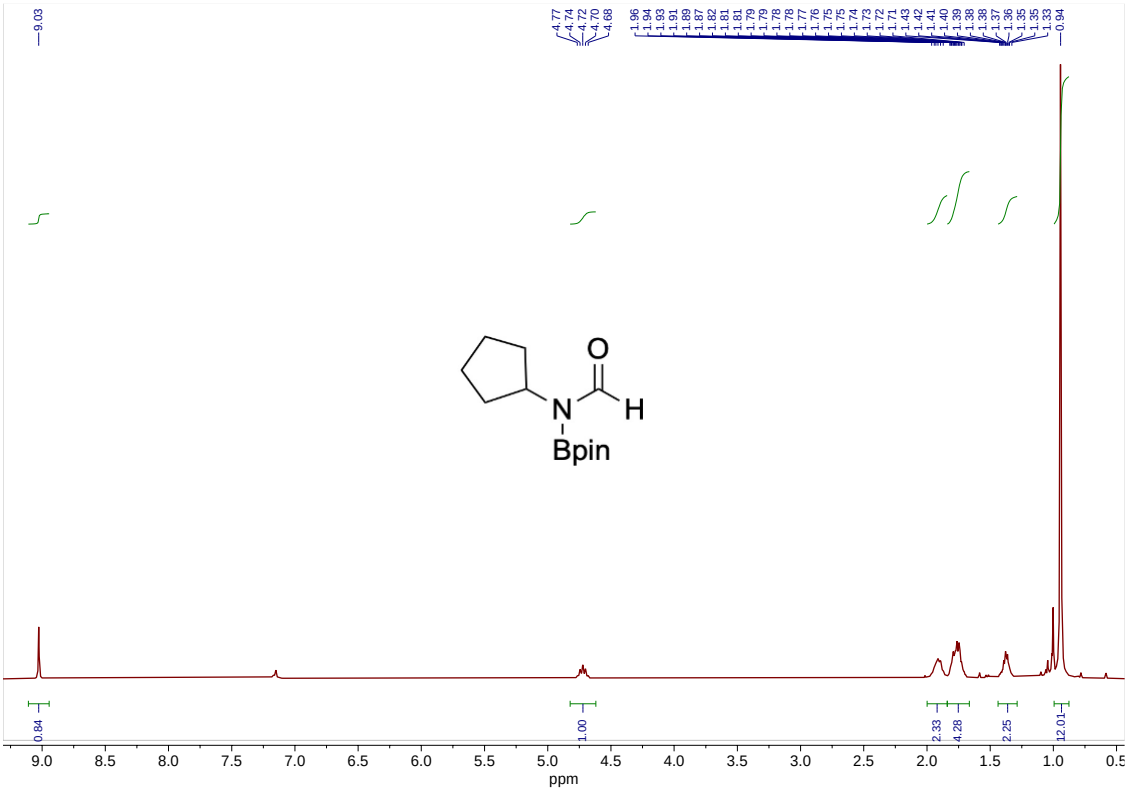


Figure S26. ^{1}H NMR spectrum of **9b** in benzene-d_6.

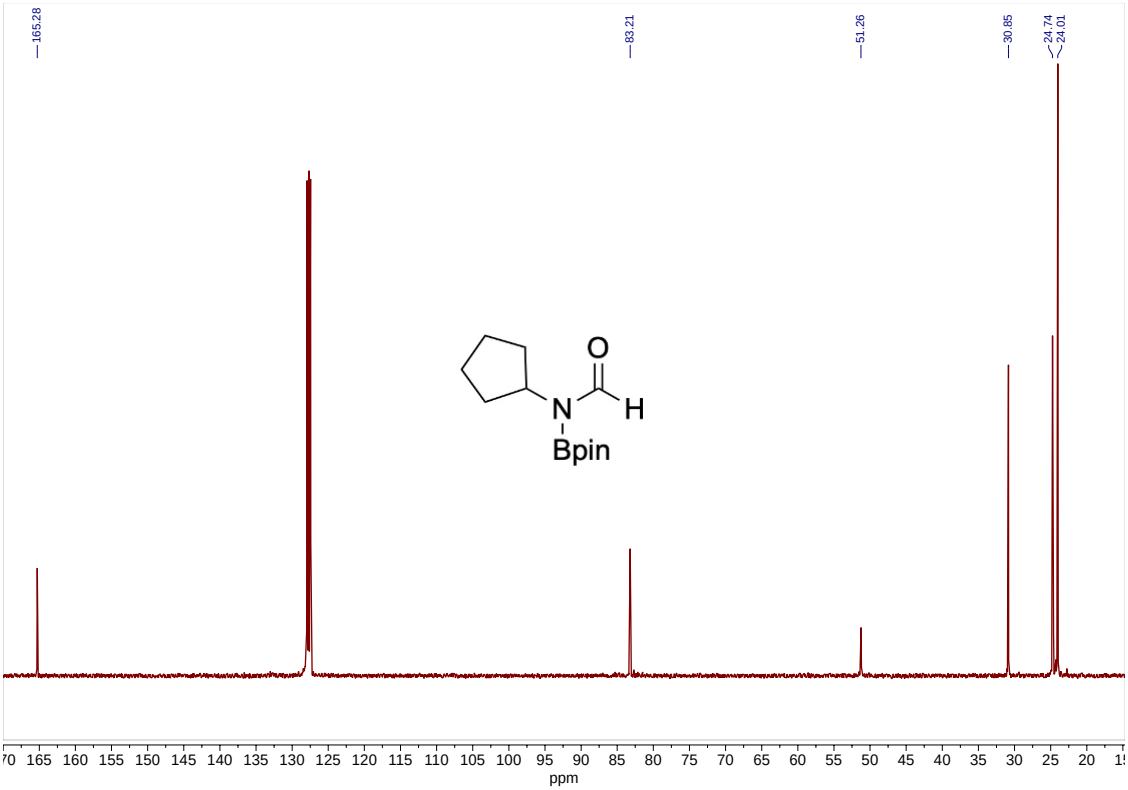


Figure S27. ^{13}C{^{1}H} NMR spectrum of **9b** in benzene-d_6.

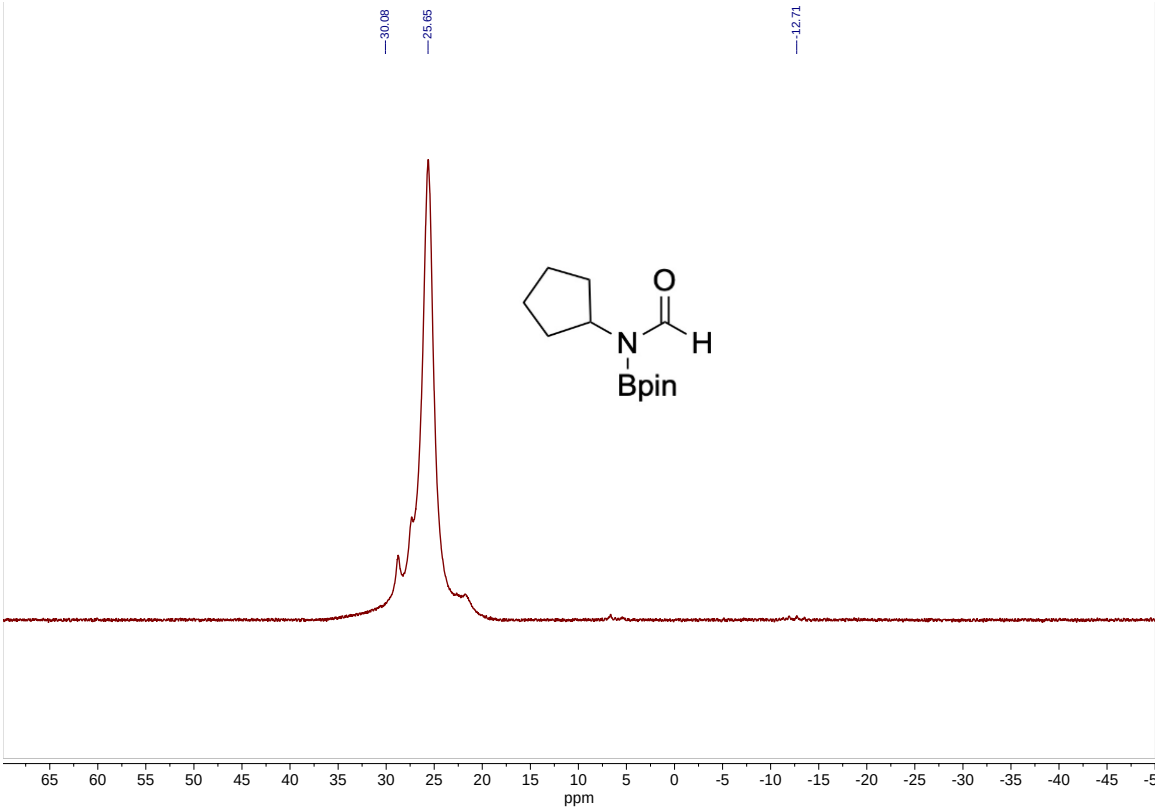


Figure S28. ^{11}B NMR spectrum of **9b** in benzene-d_6.

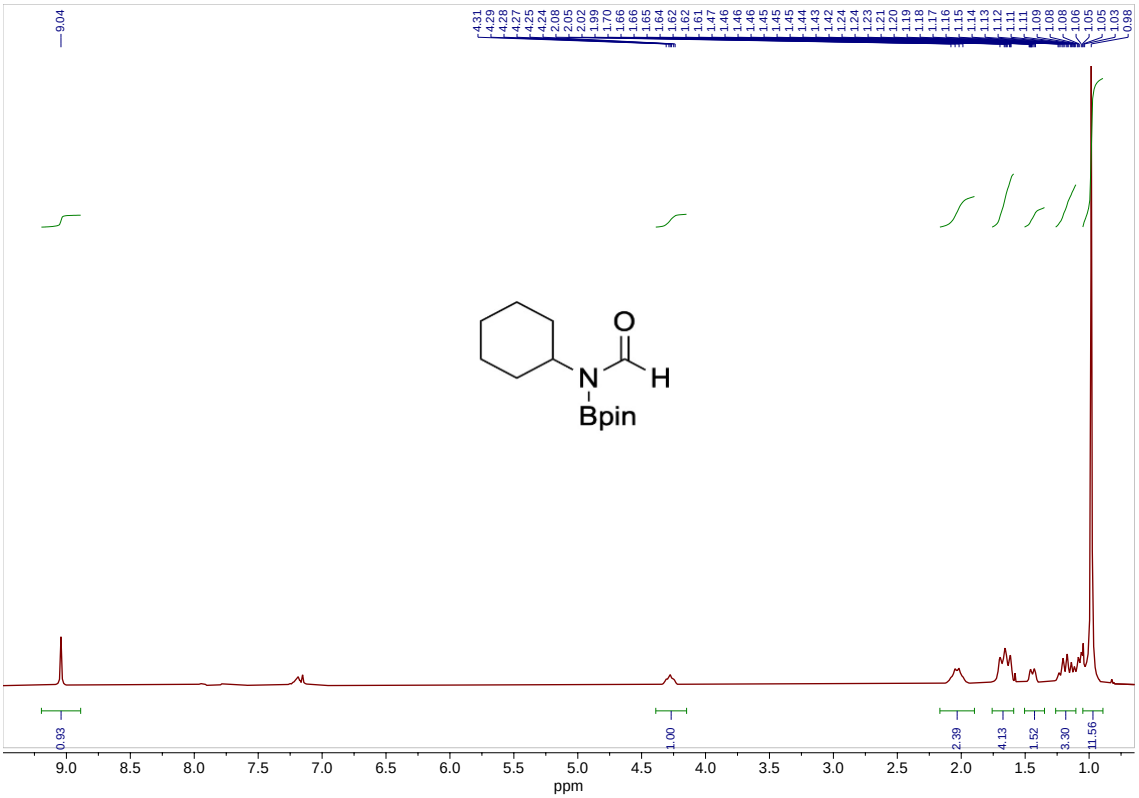


Figure S29. ^{1}H NMR spectrum of **9c** in benzene-d_6.

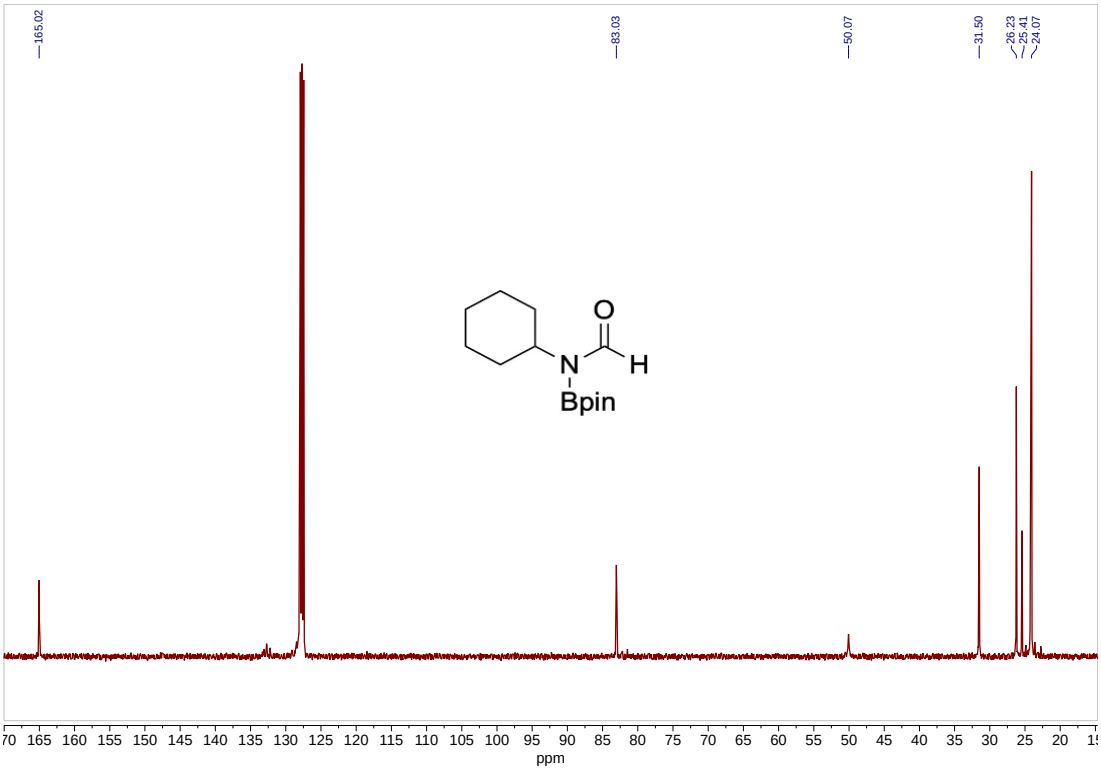


Figure S30. $^{13}C\{^{1}H\}$ NMR spectrum of **9c** in benzene-d_6.

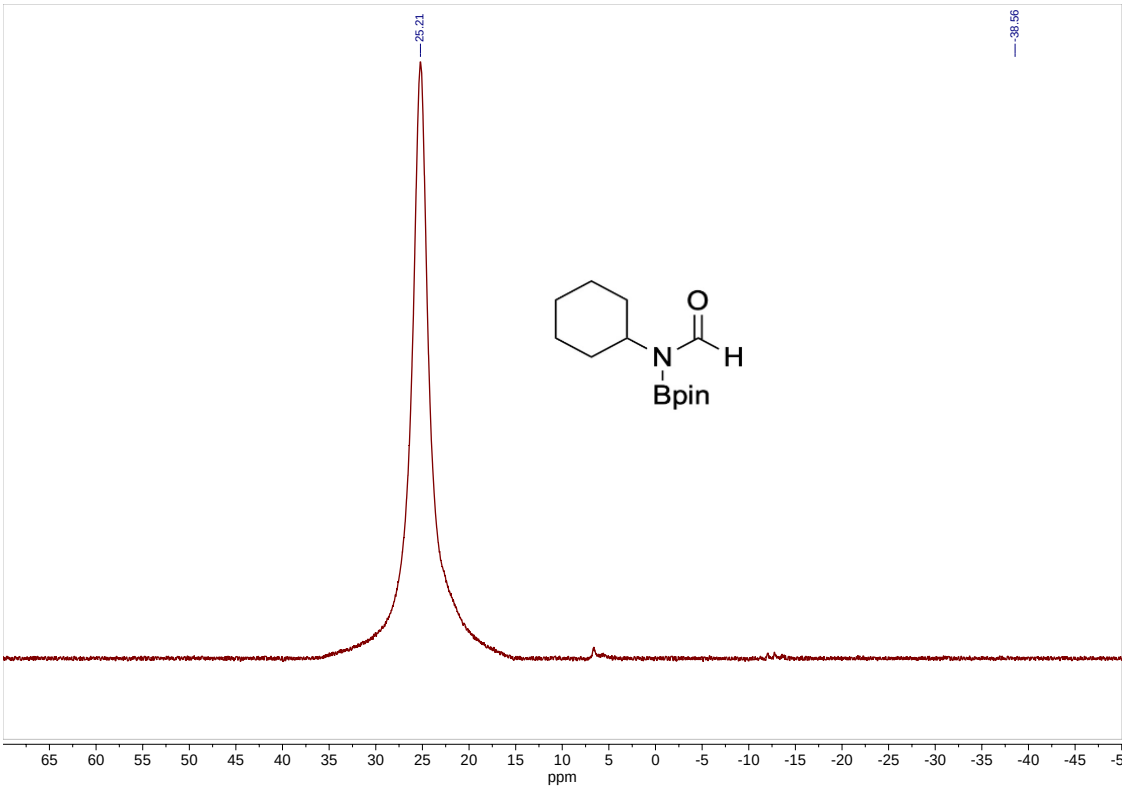


Figure S31. ^{11}B NMR spectrum of **9c** in benzene-d_6.

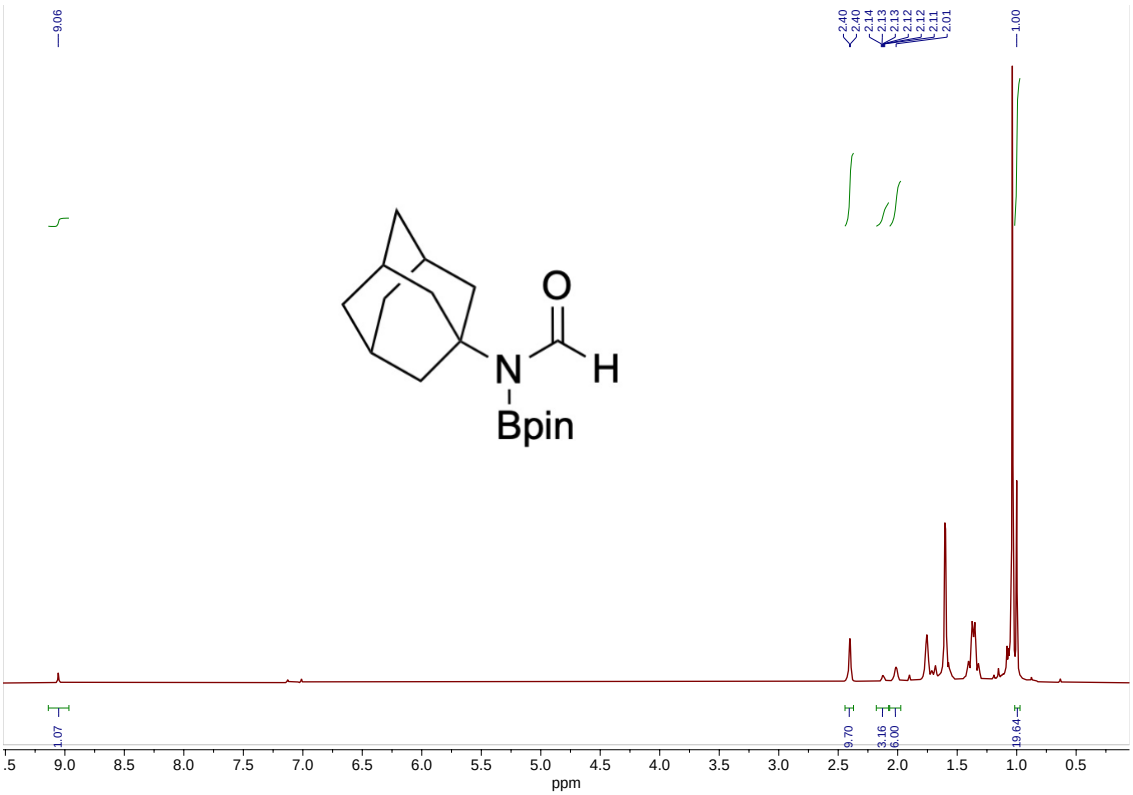


Figure S32. ^{1}H NMR spectrum of **9d** and remaining 1-adamantylisocyanate and pinacolborane in benzene-d_6.

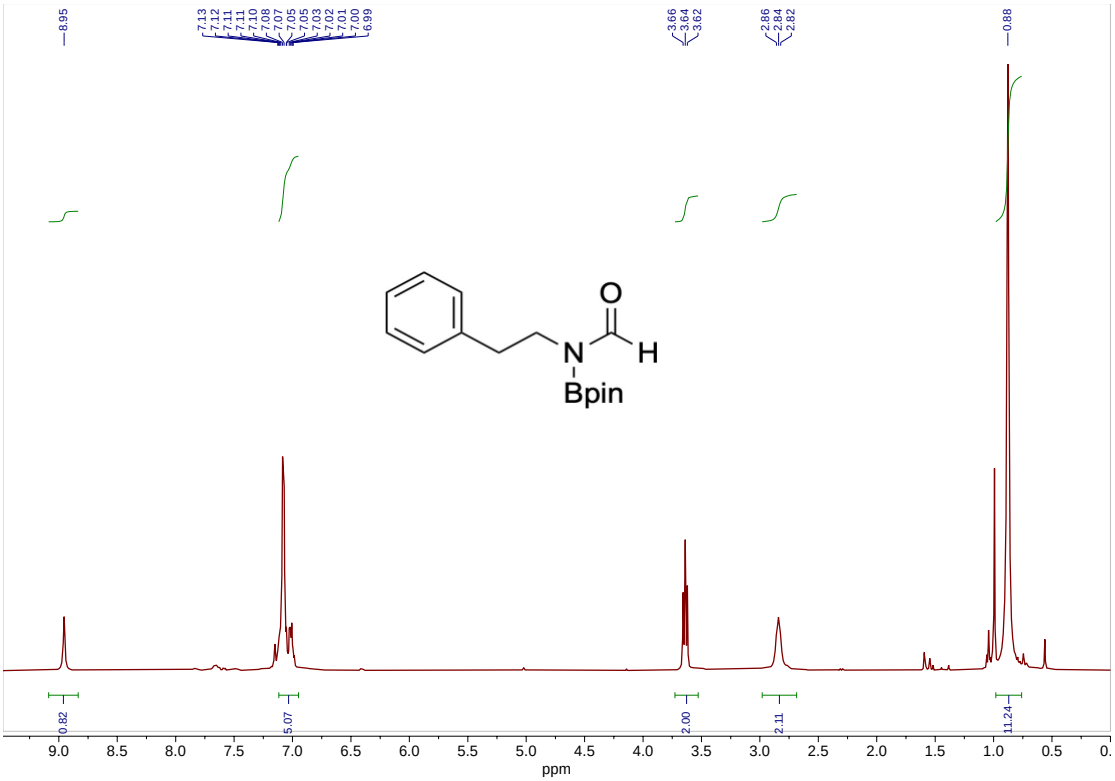


Figure S33. ^{1}H NMR spectrum of **9e** in benzene-d_6.

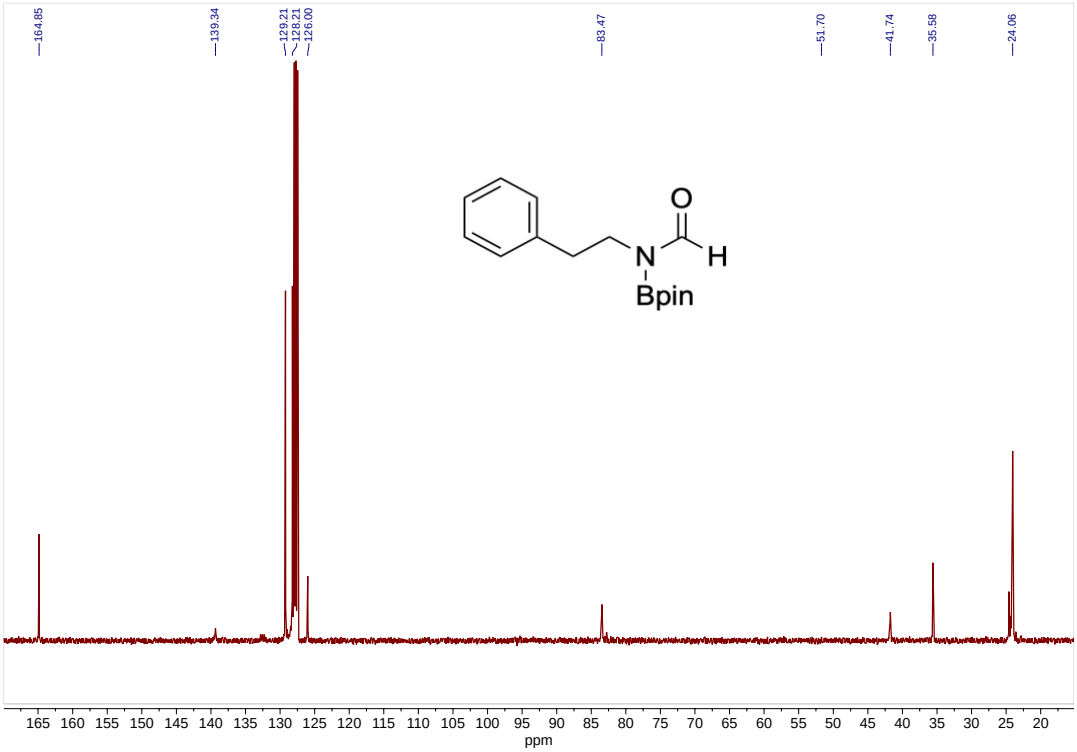


Figure S34. $^{13}C\{^{1}H\}$ NMR spectrum of **9e** in benzene-d_6.

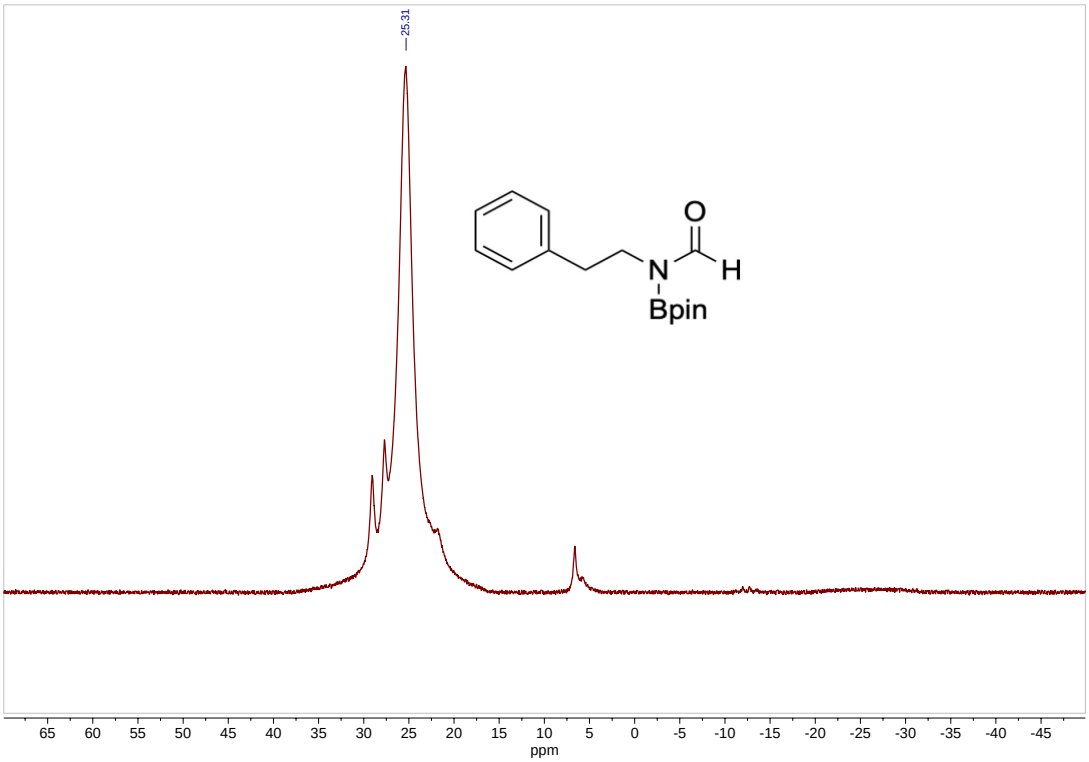


Figure S35. ^{11}B NMR spectrum of **9e** in benzene-d_6.

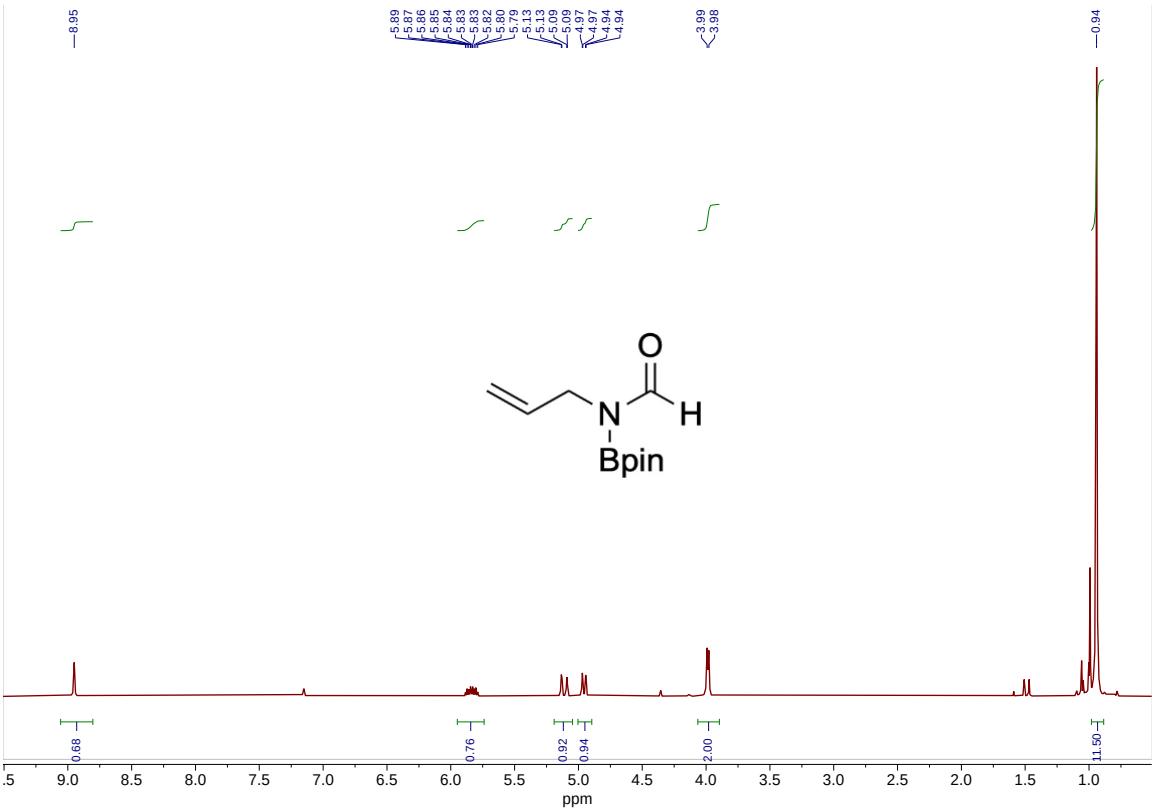


Figure S36. ^{1}H NMR spectrum of **9f** in benzene-d_6.

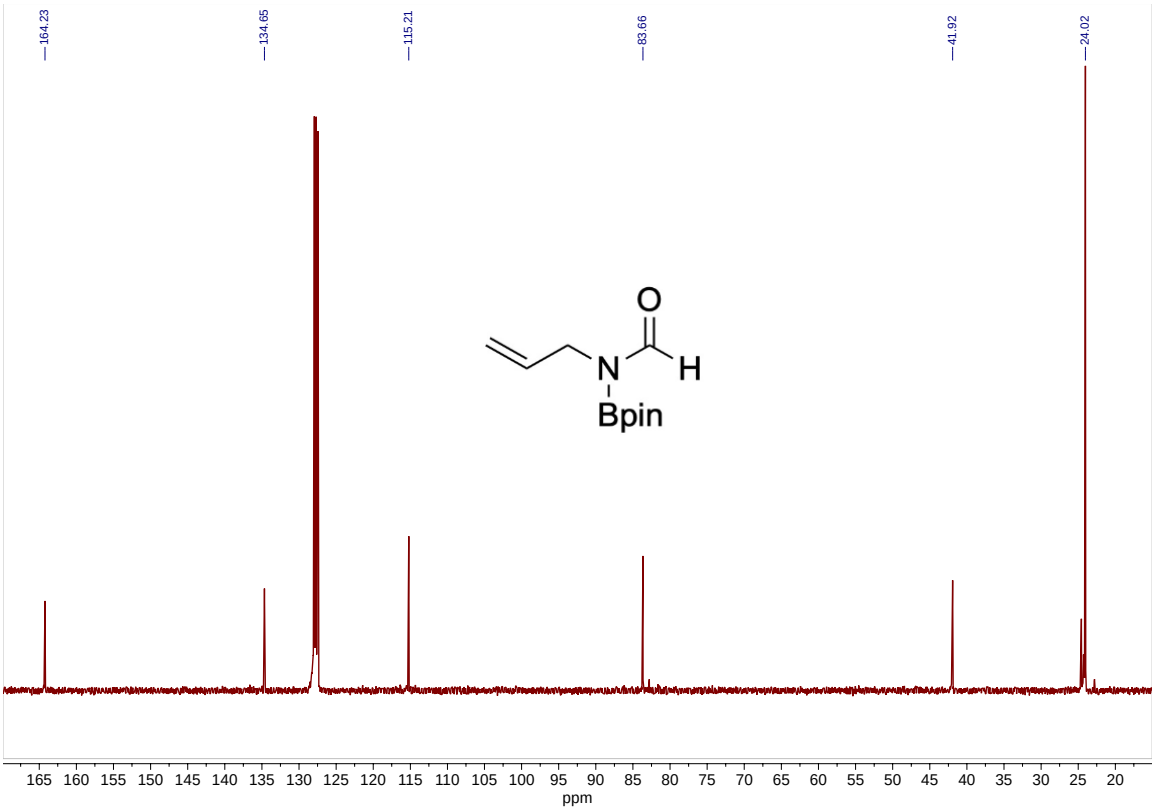


Figure S37. ^{13}C{^{1}H} NMR spectrum of **9f** in benzene-d_6.

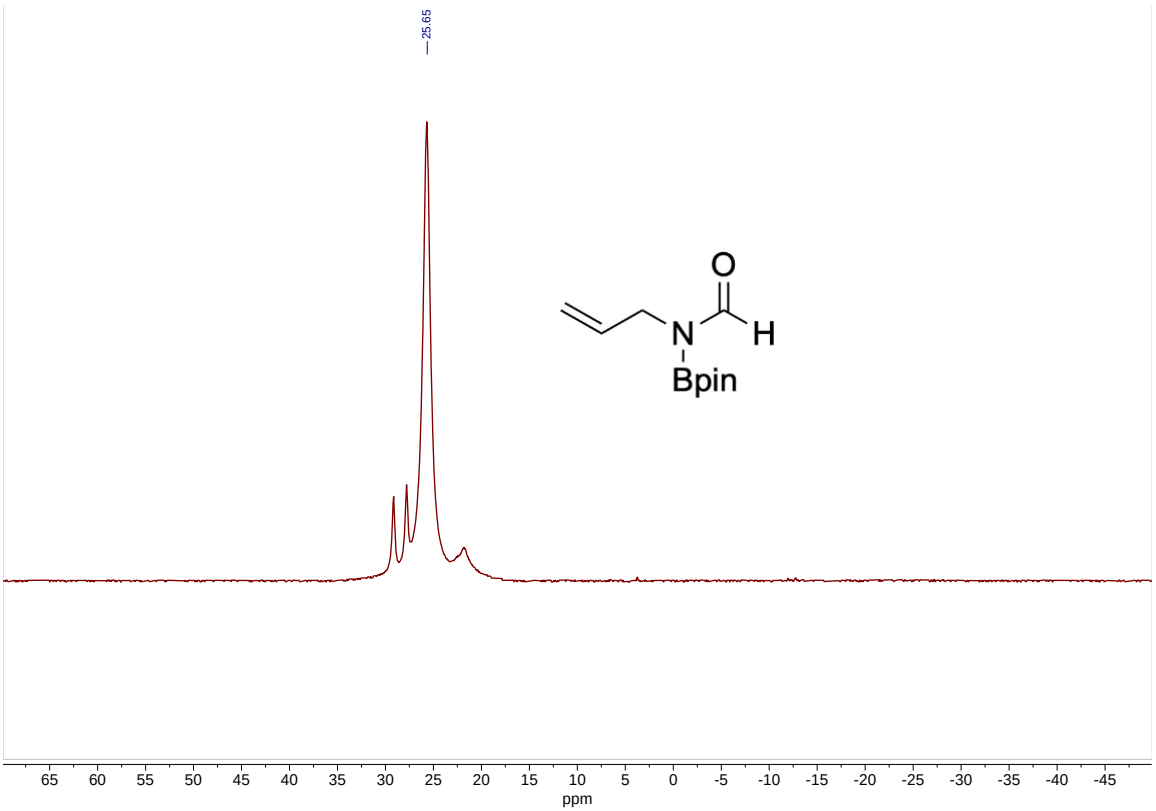


Figure S38. ^{11}B NMR spectrum of **9f** in benzene-d_6.

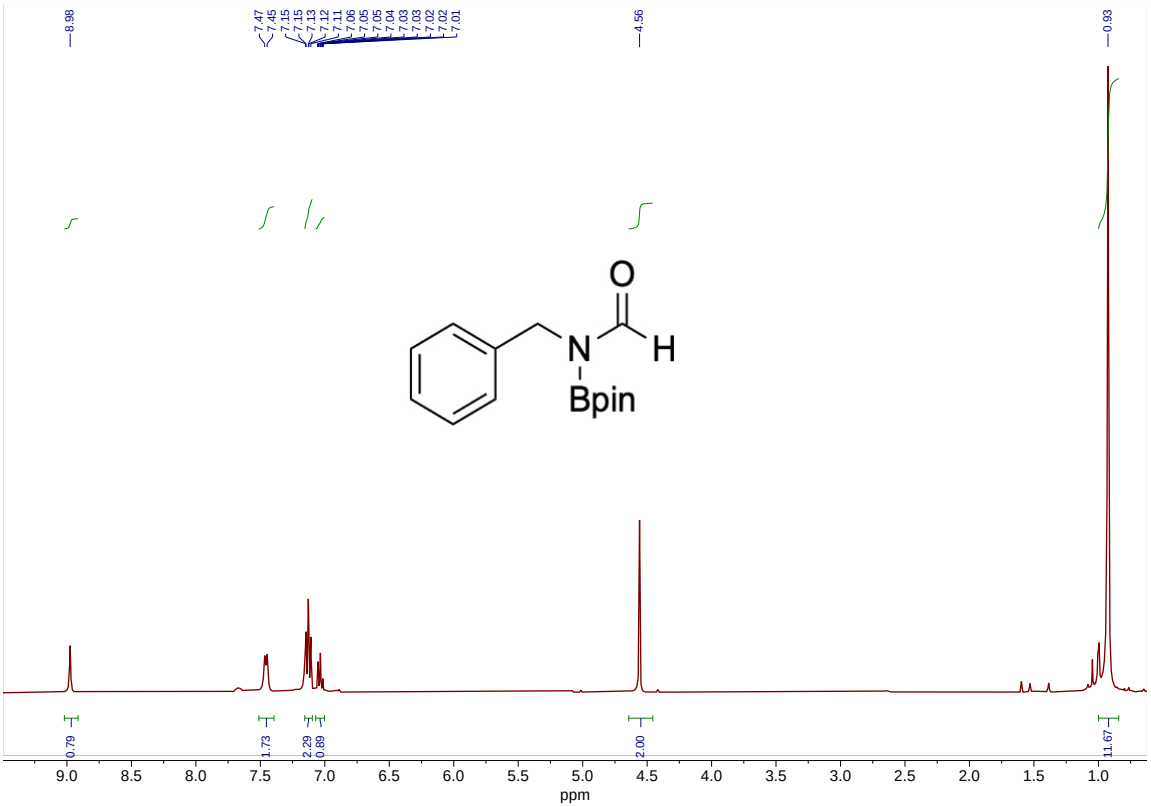


Figure S39. ^{1}H NMR spectrum of **9g** in benzene-d_6.

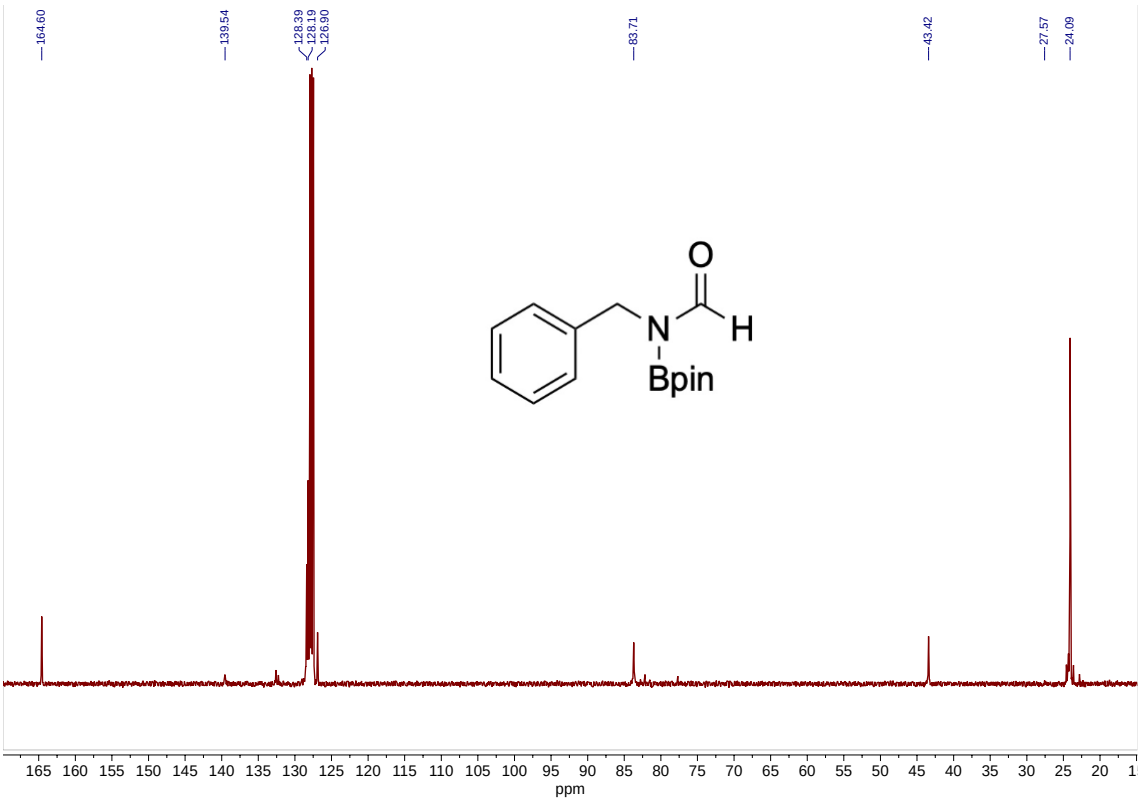


Figure S40. $^{13}C\{^{1}H\}$ NMR spectrum of **9g** in benzene-d_6.

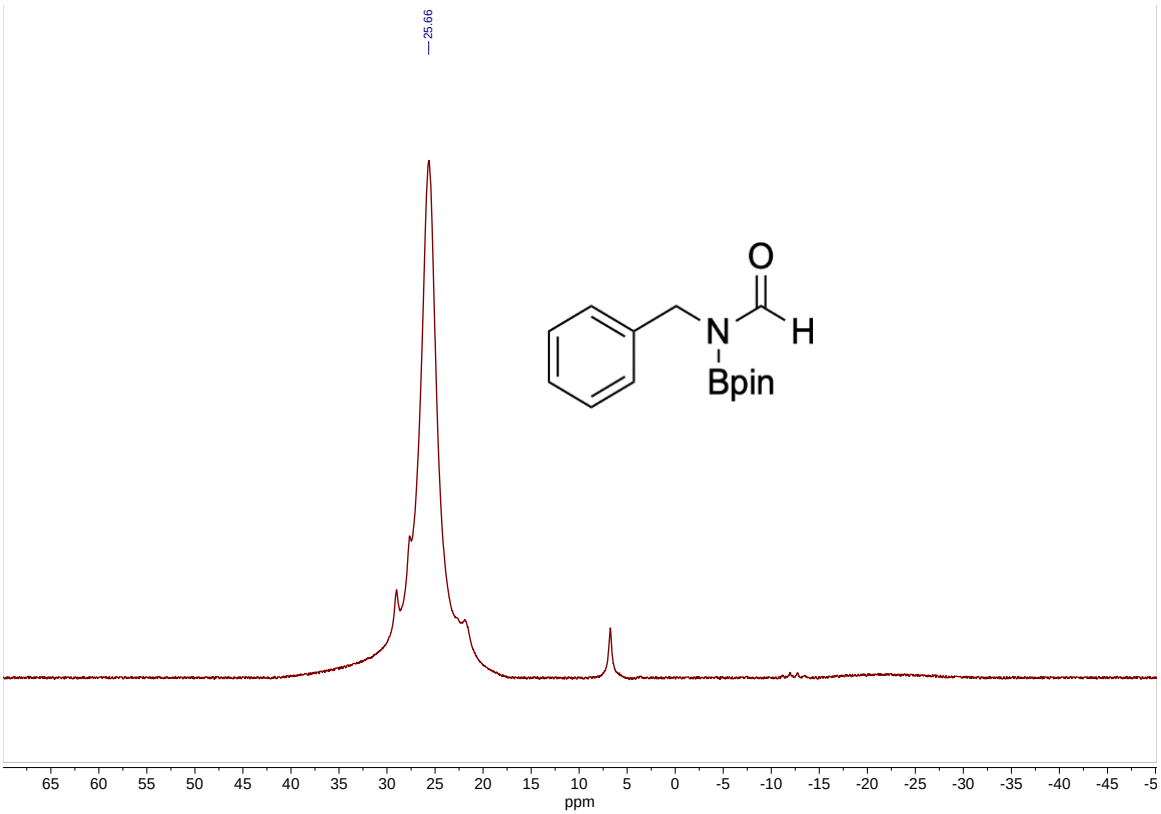


Figure S41. ^{11}B NMR spectrum of **9g** in benzene-d_6.

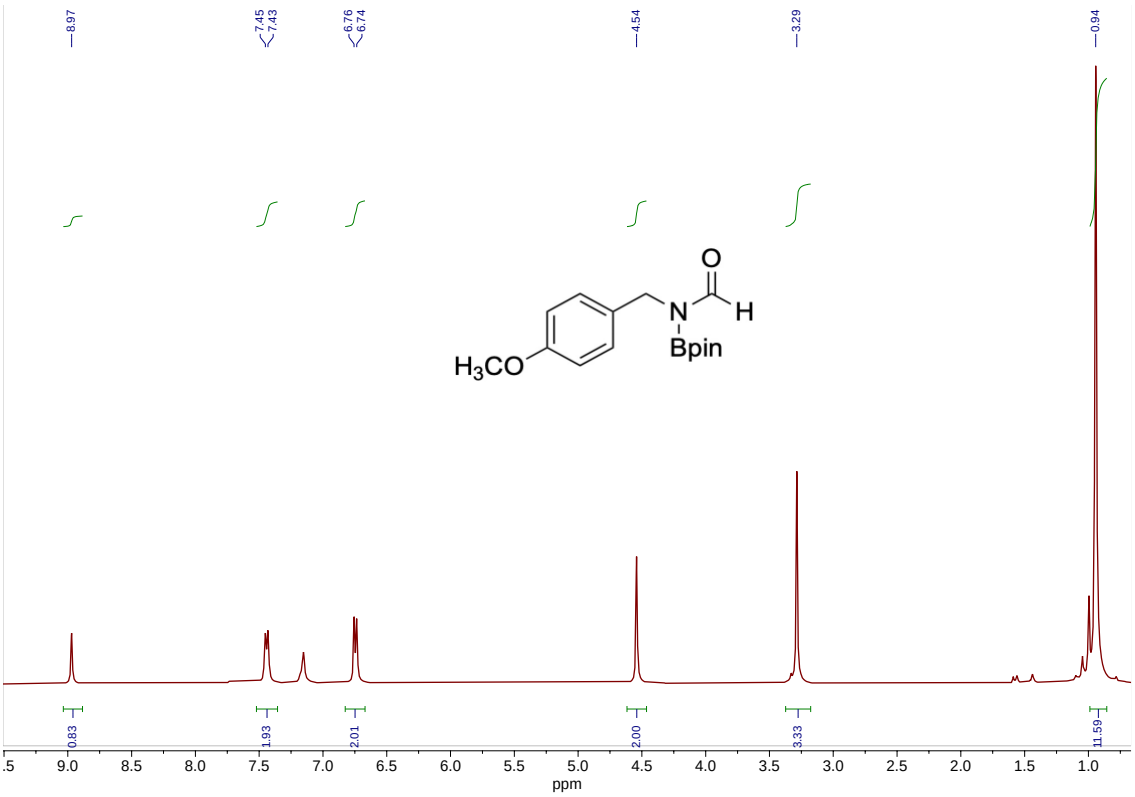


Figure S42. ^{1}H NMR spectrum of **9h** in benzene-d_6.

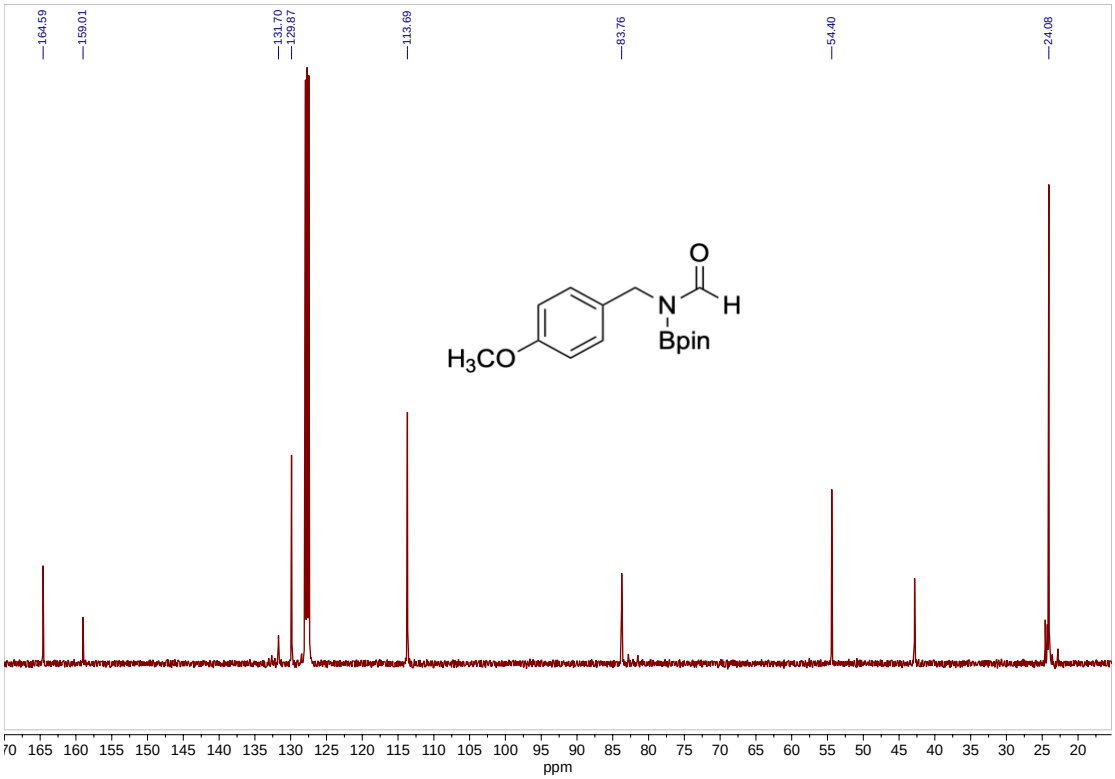


Figure S43. ^{13}C{^{1}H} NMR spectrum of **9h** in benzene-d_6.

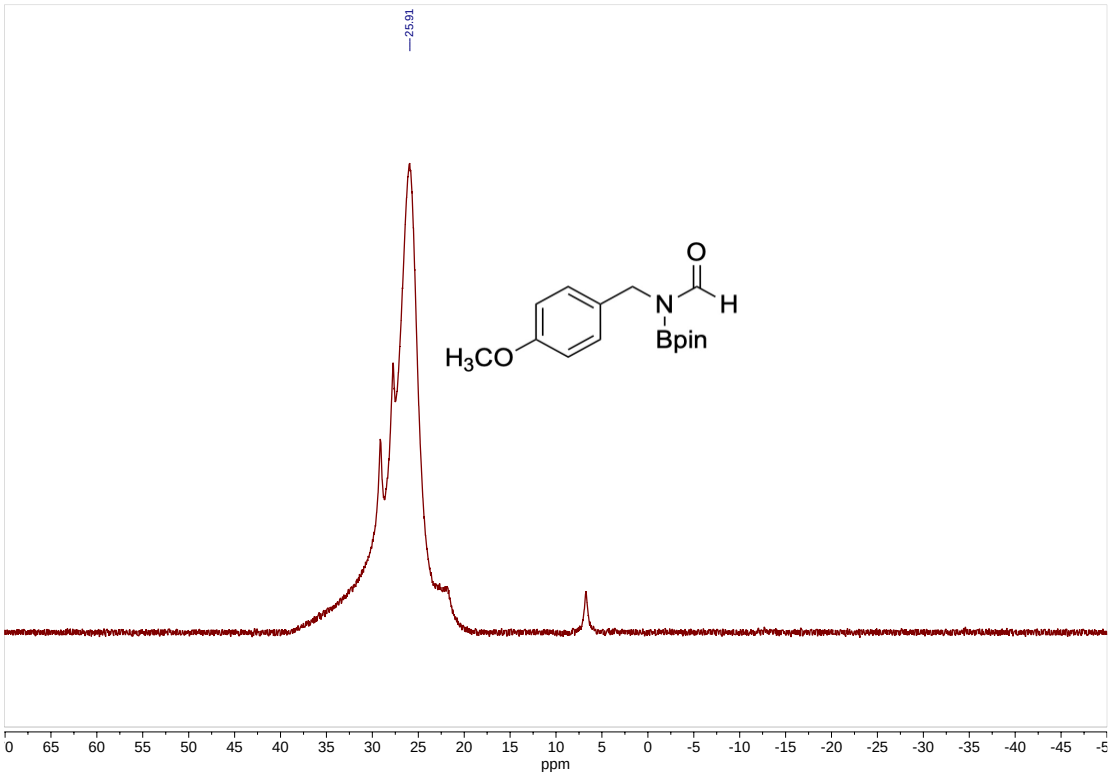


Figure S44. ^{11}B NMR spectrum of **9h** in benzene-d_6.

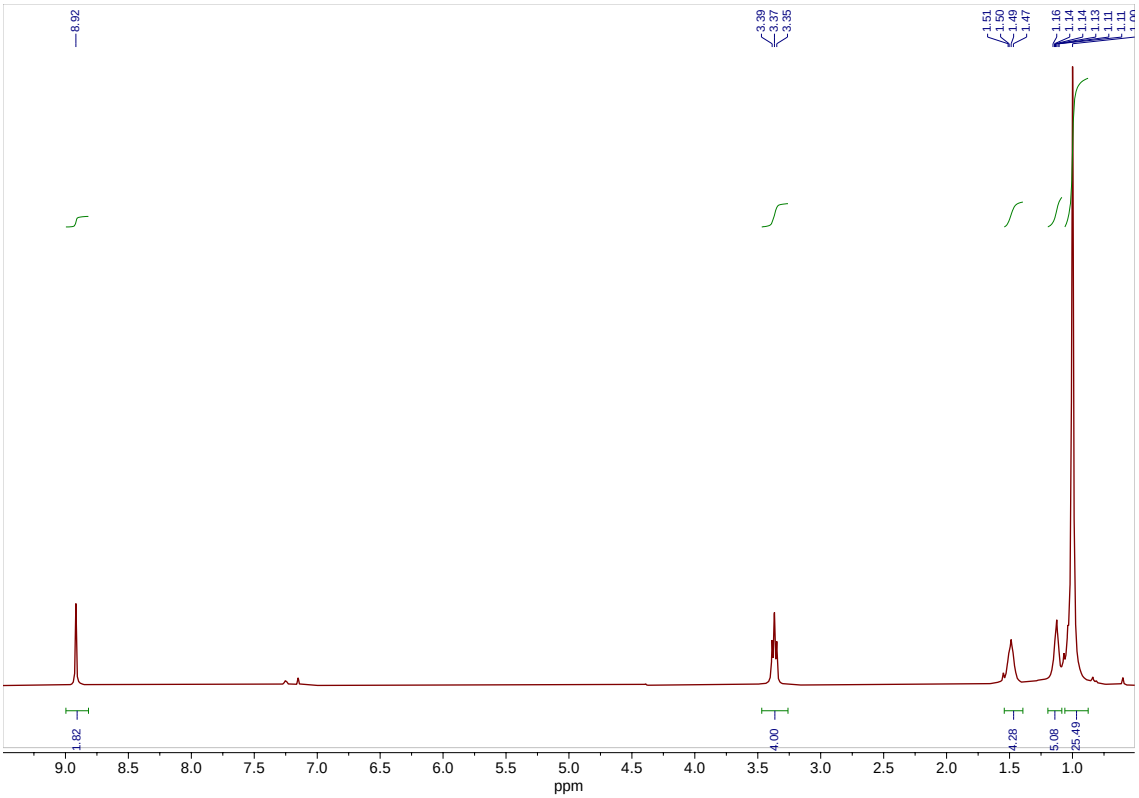


Figure S45. ^{1}H NMR spectrum of **9i** in benzene-d_6.

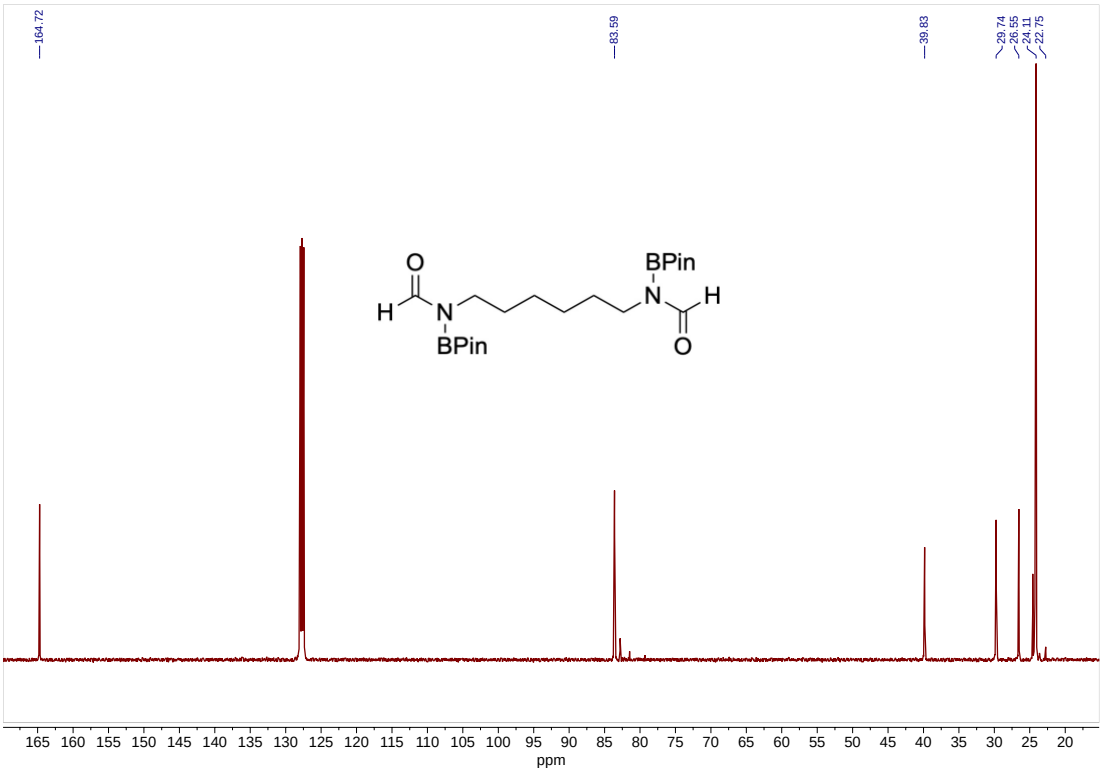


Figure S46. $^{13}C\{^{1}H\}$ NMR spectrum of **9i** in benzene-d_6.

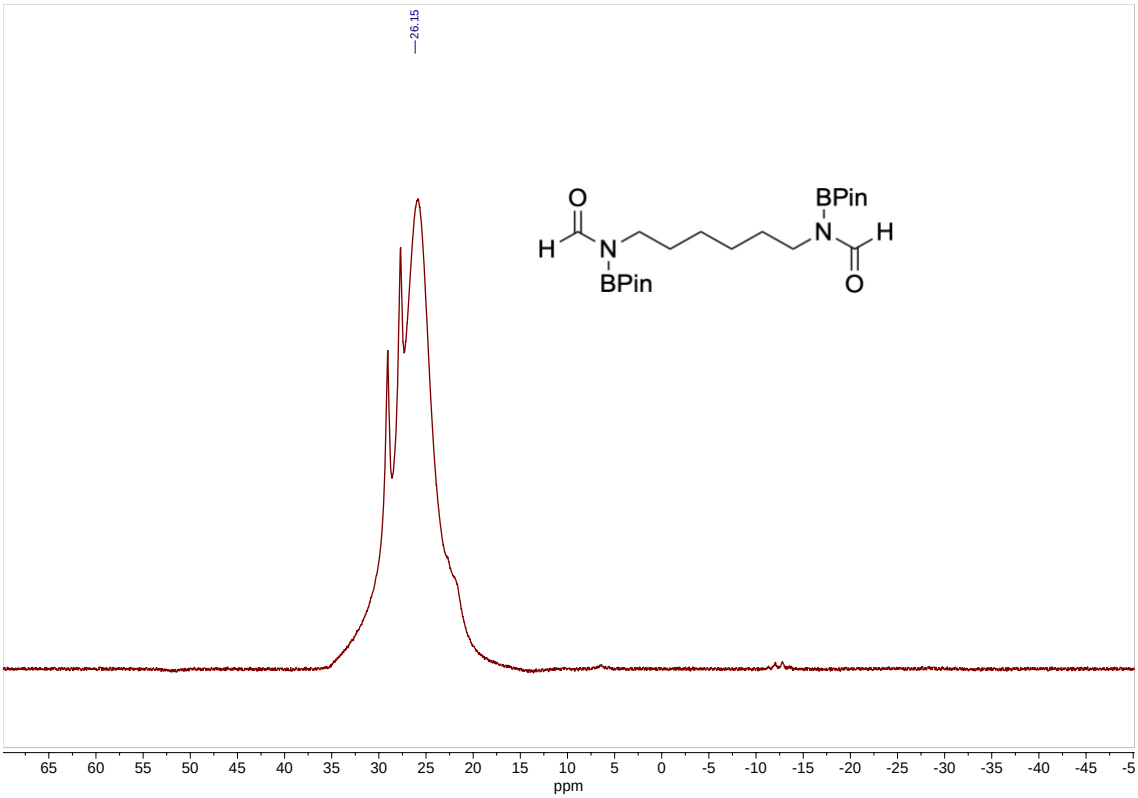


Figure S47. ^{11}B NMR spectrum of **9i** in benzene-d_6.

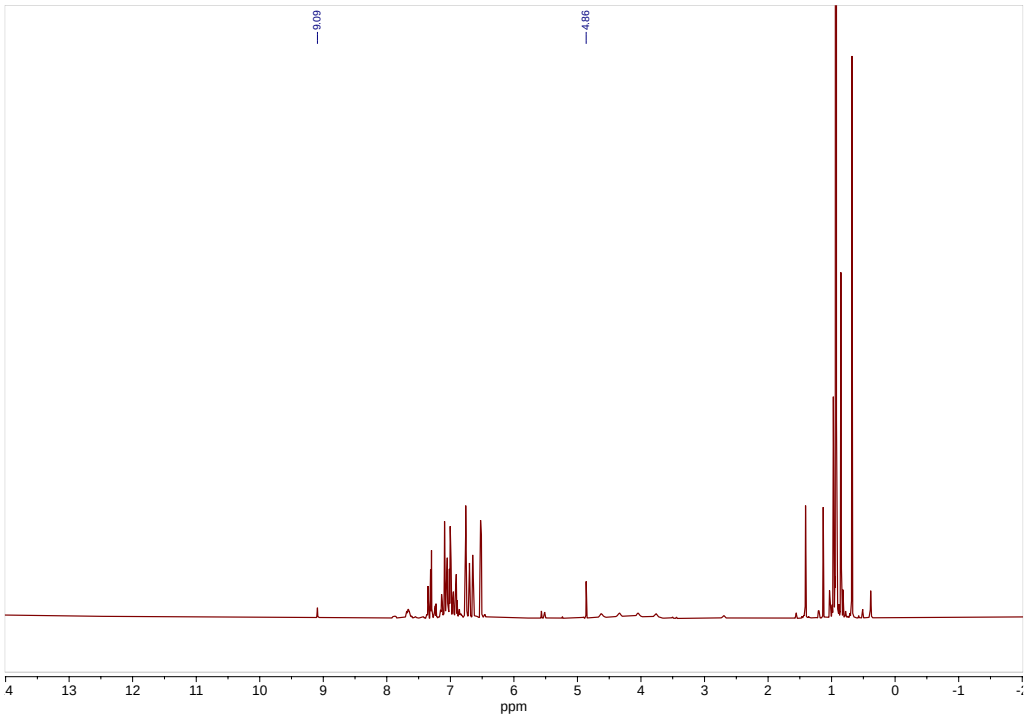


Figure S48. ^{1}H NMR spectrum for the reaction of phenyl isocyanate with HBpin in the presence of catalyst **1**. Singlet at 9.1 ppm corresponds to the monohydroboration product, and the singlet at 4.86 ppm corresponds to the dihydroboration product.

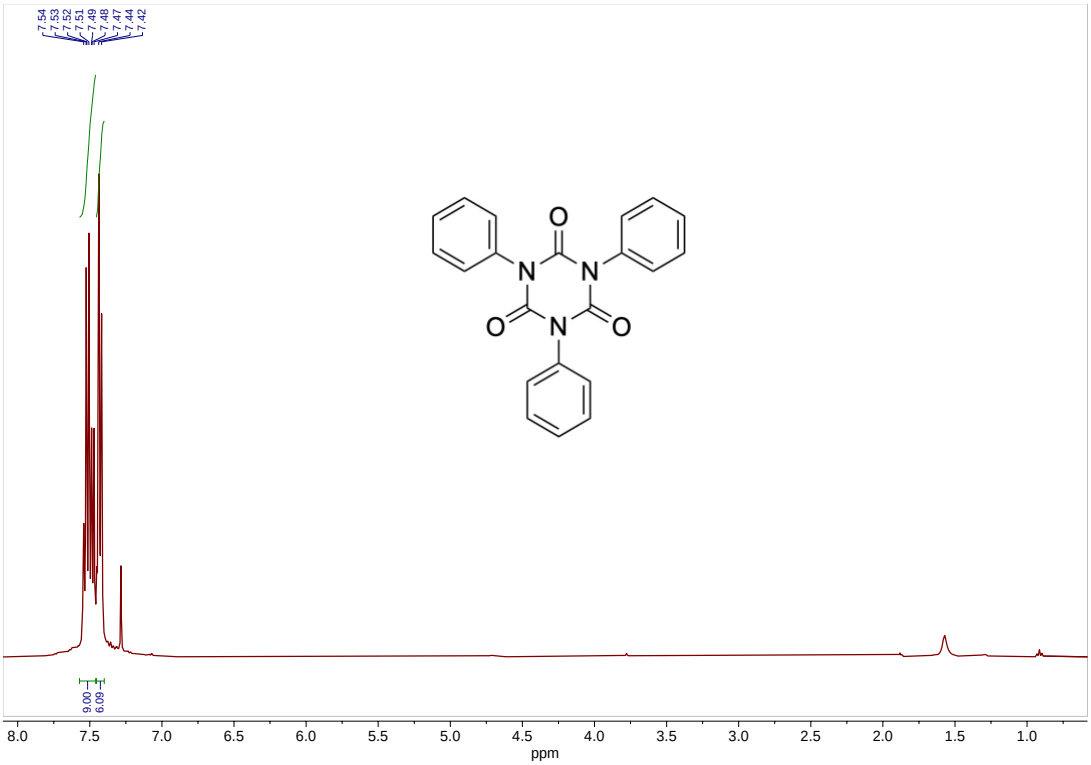


Figure S49. ^{1}H NMR spectrum of **10a** in chloroform-*d*.

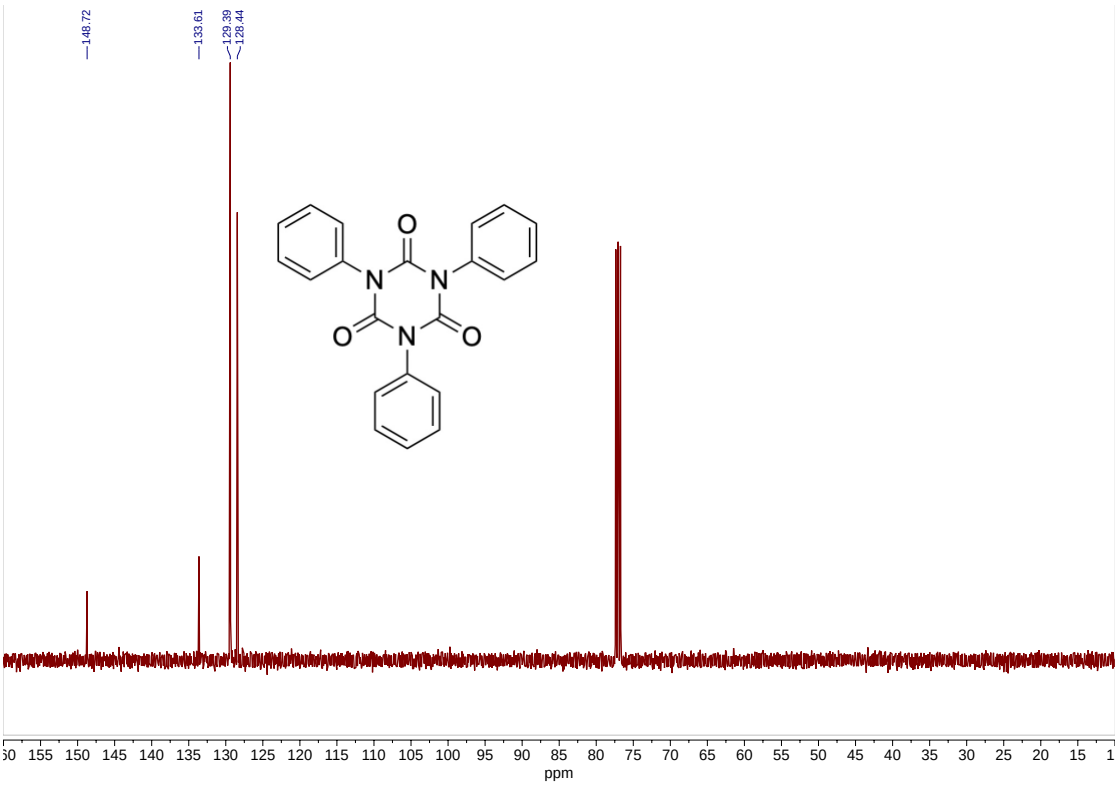


Figure S50. $^{13}C\{^{1}H\}$ NMR spectrum of **10a** in chloroform-*d*.

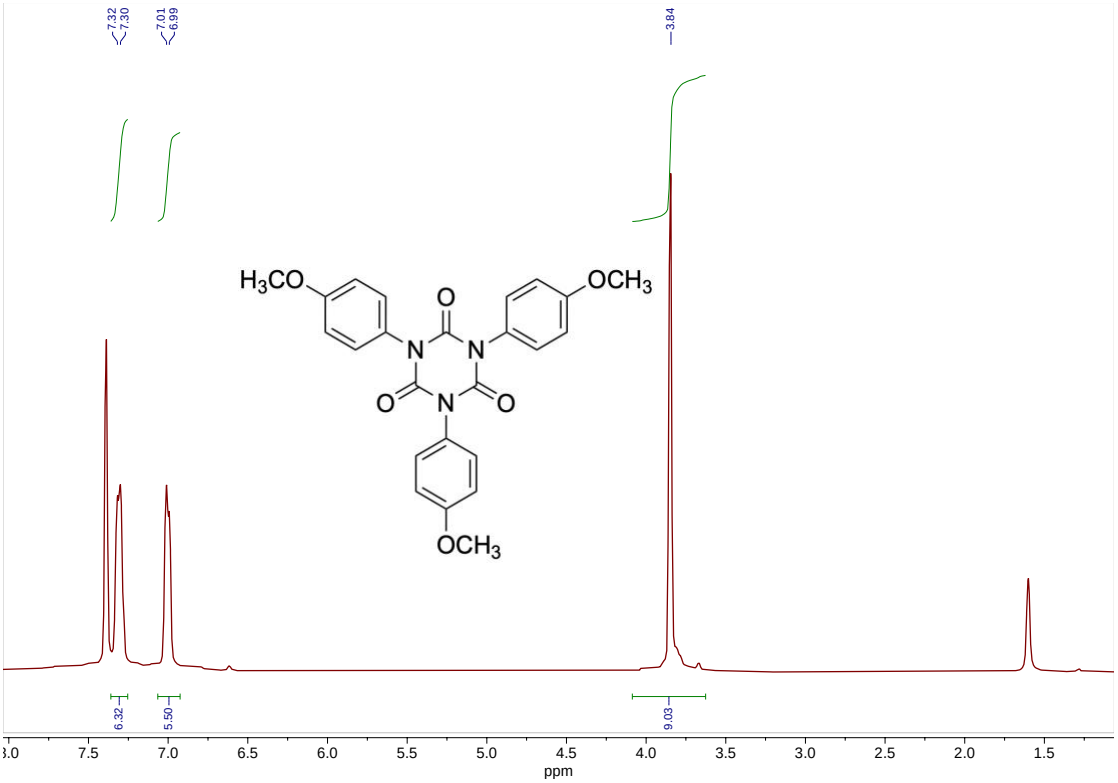


Figure S51. ^{1}H NMR spectrum of **10b** in chloroform-*d*.

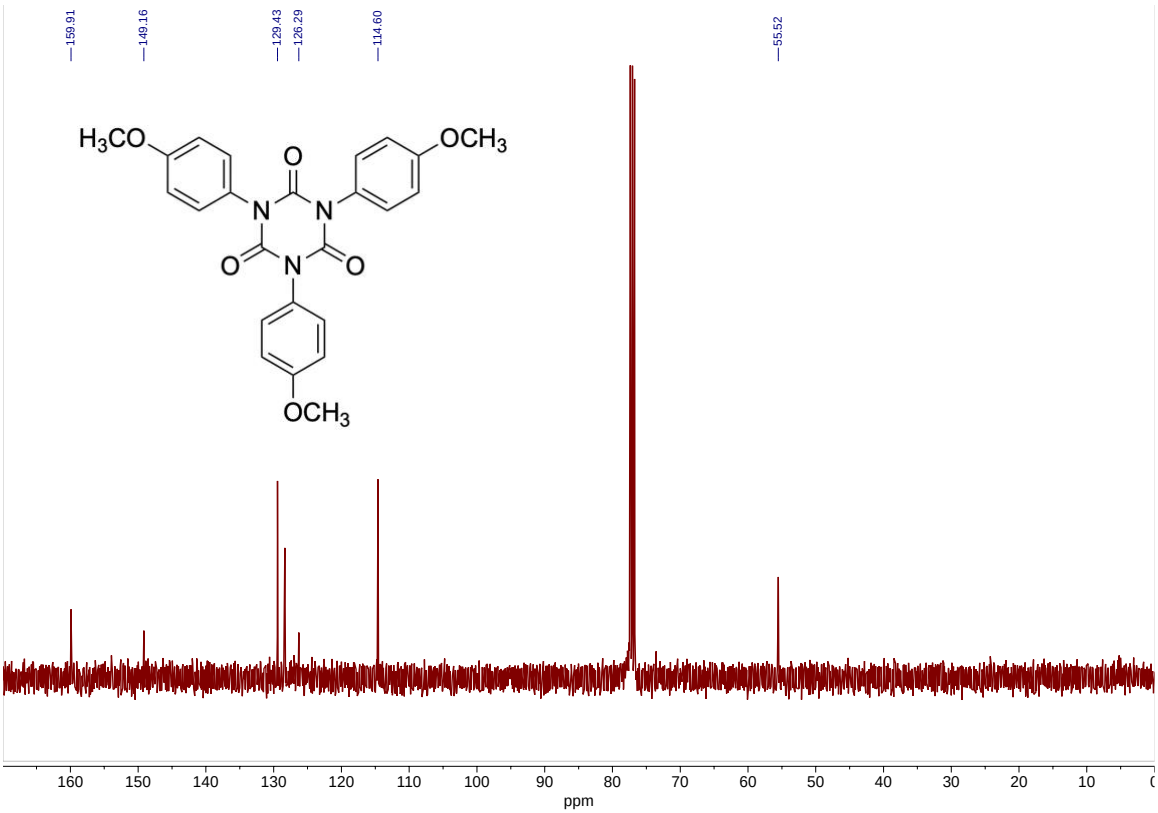


Figure S52. $^{13}C\{^{1}H\}$ NMR spectrum of **10b** in chloroform-*d*.

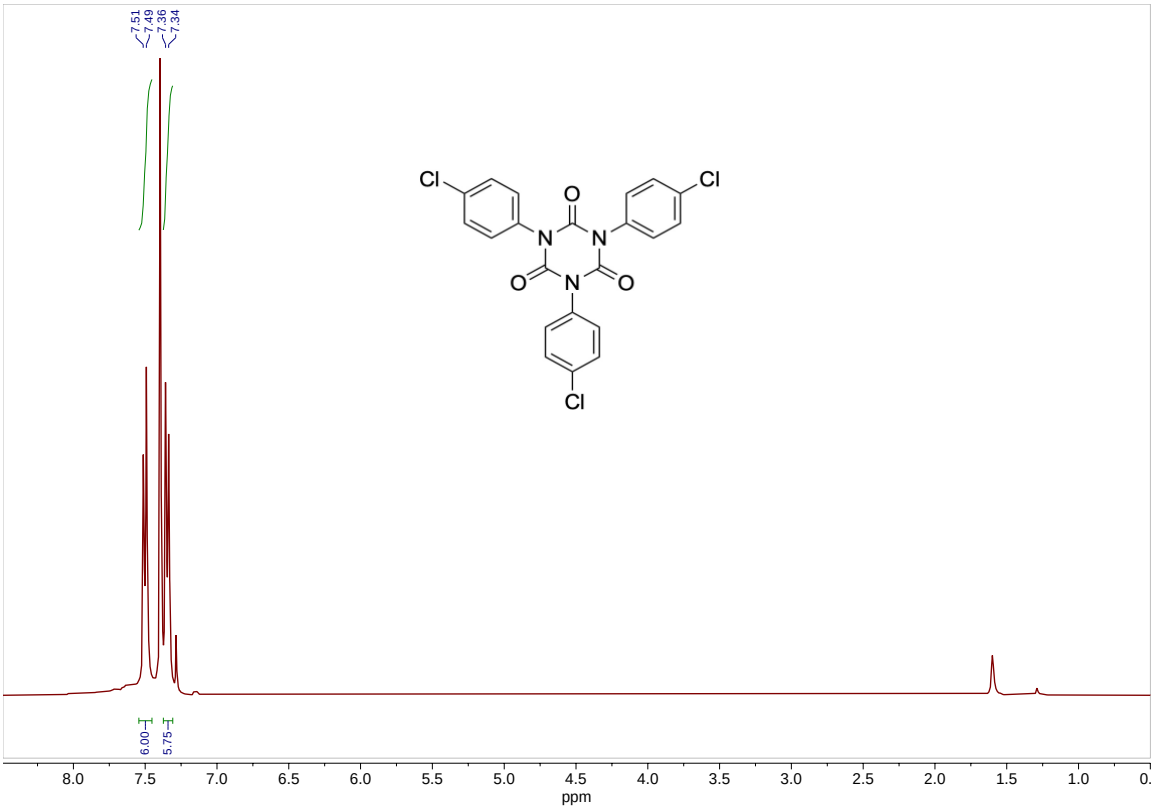


Figure S53. ^{1}H NMR spectrum of **10c** in chloroform-*d*.

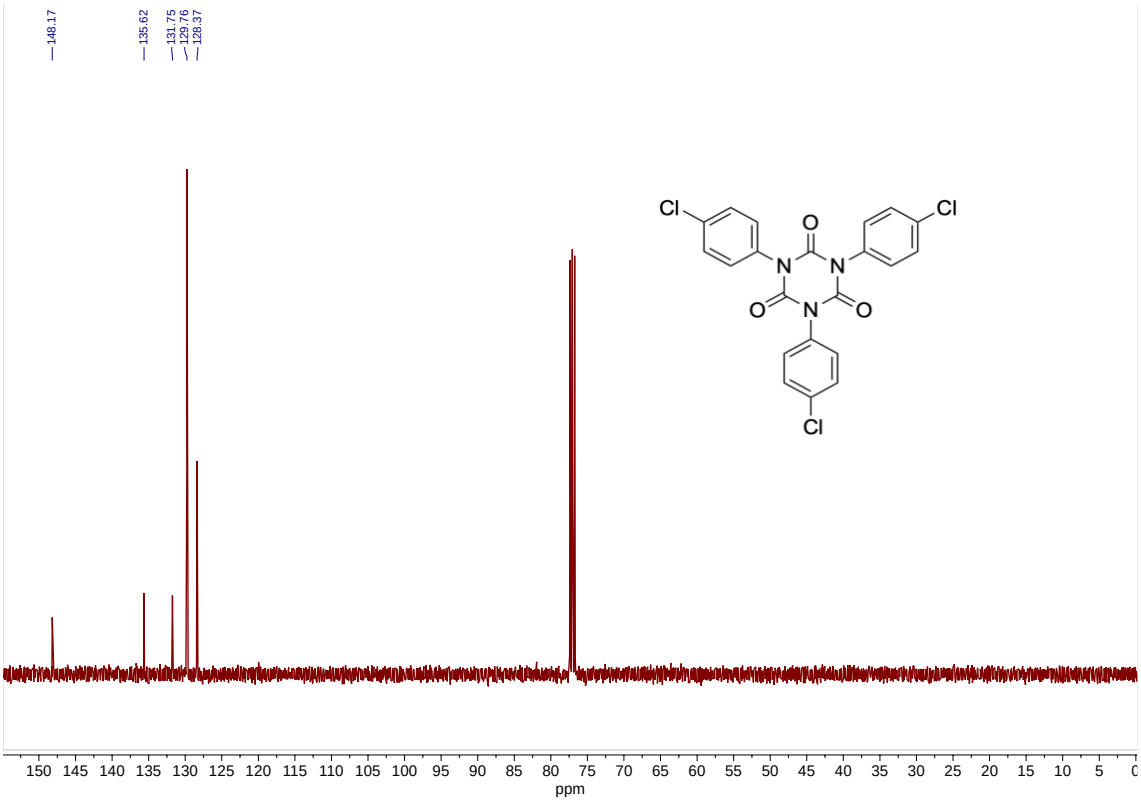


Figure S54. $^{13}C\{^{1}H\}$ NMR spectrum of **10c** in chloroform-*d*.

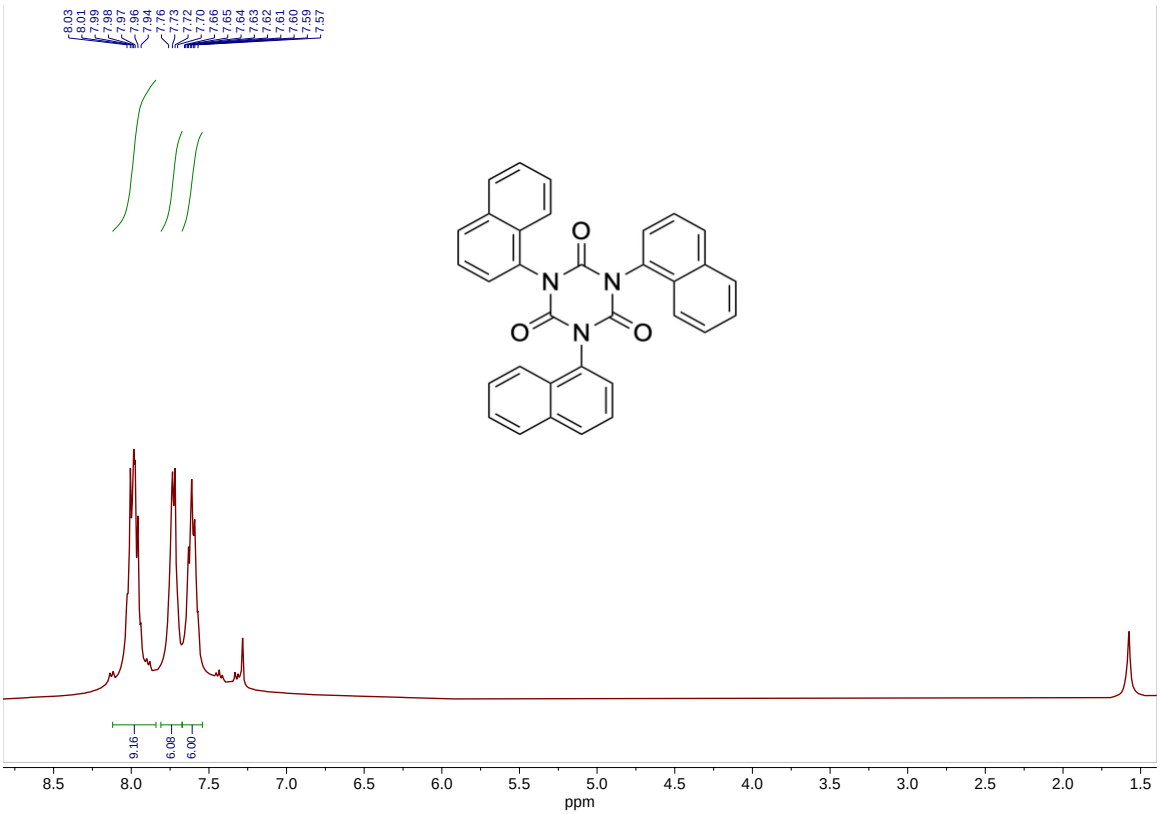


Figure S55. ^{1}H NMR spectrum of **10d** in chloroform-*d*.

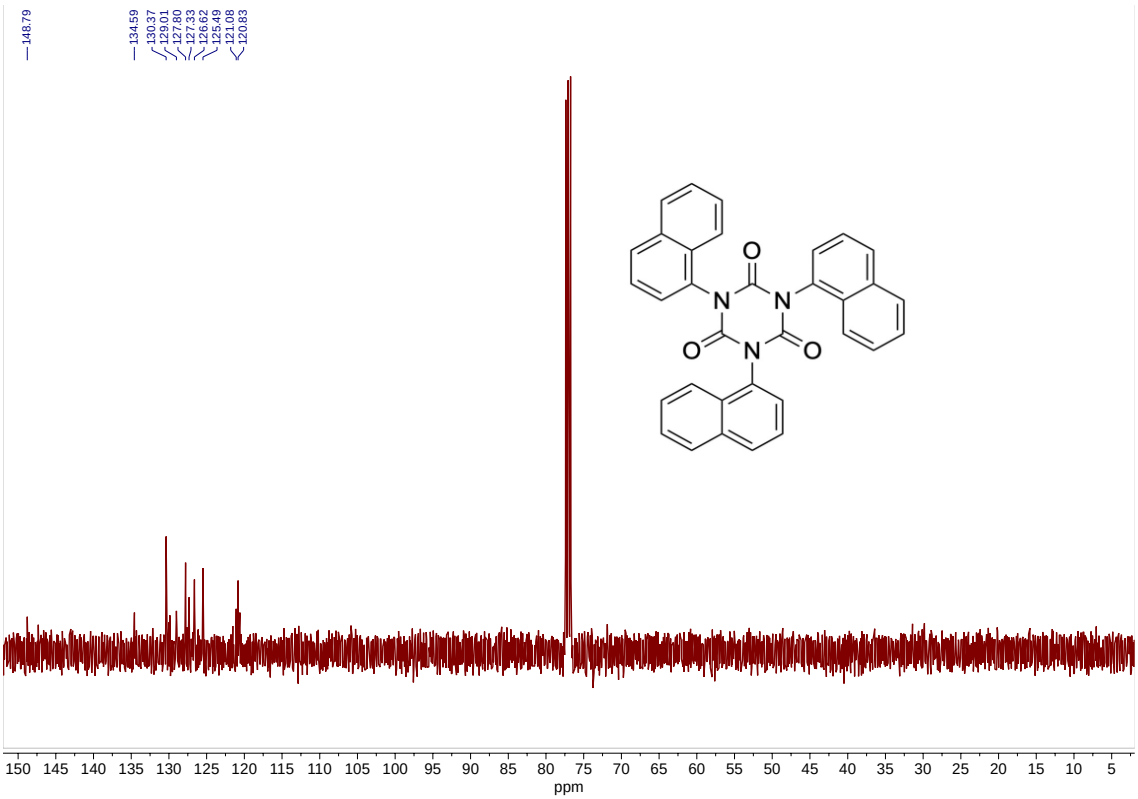


Figure S56. $^{13}C\{^{1}H\}$ NMR spectrum of **10d** in chloroform-*d*.

Full Authorship of Gaussian 16, Rev B.01

Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2016**.

Conformational Search Protocol

Conformational searches at all stationary points studied were performed using the parameters described below to locate conformational isomers reported in the manuscript. These structures were subject to further structural and energy refinements using quantum mechanics, from which the lowest energy minimum and transition state structures were obtained.

Conformational Search Parameters

Potential:

Force field: Optimized Polarizable Liquid Simulation (OPLS)
Solvent: None
Electrostatic cutoff: None

Minimization:

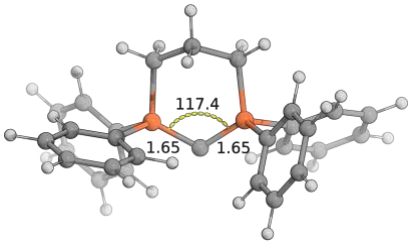
Minimization method: Polak-Ribier Conjugate Gradient (PRCG)
Maximum iteration: 2500
Convergence on gradient with threshold of 0.05

Conformational Sampling:

Method: Torsional sampling (MCMM)
Maximum number of steps: 1000
Energy window: 10.00 kcal/mol
Redundancy window: 0.5 Å maximum atom deviation

Calculation Parameters, Geometries, Energies, and Vibrational Frequencies

Carbodiphosphorane 1



Gaussian 16: ES64L-G16RevB.01 20-Dec-2017

# wb97xd/6-31G(d,p) gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc
) opt=(maxcycle=250) freq=noraman

Full point group C1 NOp 1
Stoichiometry C28H26P2 Framework group C1[X(C28H26P2)]

Num atoms: 56
Charge = 0 Multiplicity = 1

SCF = -1764.91653344 | Predicted change in Energy=-
8.650337D-09

Optimization completed.
Maximum Force 0.000010 0.000450 YES
RMS Force 0.000002 0.000300 YES
Maximum Displacement 0.001797 0.001800 YES
RMS Displacement 0.000386 0.001200 YES

Atom Coordinates (in Angstroms)
Type X Y Z

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C 5.174186 -4.390218 -1.809321
C 5.015361 -3.383792 -2.961479
C 4.029141 -2.252850 -2.626605
P 2.316269 -2.905445 -2.382338
C 2.203578 -4.354517 -1.597276
H 5.957020 -5.117449 -2.046789
H 5.462758 -3.867942 -0.890001
H 4.685243 -3.909394 -3.867020
H 5.993682 -2.949536 -3.192579
H 4.310483 -1.775004 -1.681689
H 4.054046 -1.474659 -3.394354
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C -0.168689 -3.839331 -5.483941
C 0.489632 -3.785247 -4.260748
C 1.532375 -2.876553 -4.052118
C 1.905193 -2.027245 -5.096777
C 1.250547 -2.084988 -6.324731
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H -0.977241 -4.548592 -5.630863
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C 0.418552 -0.766882 0.530392
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C 1.275015 -0.281454 -2.073593
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H 0.078947 -0.958733 1.543490
H 1.181523 -2.774679 0.216190
H 1.586734 -0.090793 -3.096829
H 0.521200 1.710900 -1.790337
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C 5.124725 -7.006785 1.927009
C 5.031711 -6.428996 0.663897
C 3.790031 -6.037139 0.156037
C 2.645062 -6.216746 0.934904
C 2.737976 -6.800088 2.193693
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H 5.937219 -6.277188 0.082744
H 1.693110 -5.871491 0.540667
H 1.842988 -6.938360 2.792189
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C 2.988131 -7.630671 -4.783803
C 2.906398 -6.627267 -3.822289
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C 4.529700 -7.785204 -2.472795
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H 3.902403 -9.498863 -5.335977
H 2.381373 -7.567241 -5.681747
H 2.232539 -5.786710 -3.957557
H 5.121591 -7.867058 -1.566086
H 5.267172 -9.638699 -3.269706

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -1764.91653344 | Predicted change in Energy=-
8.650337D-09
Zero-point correction (ZPE) = -1764.45298844 0.463545
Internal Energy (U) = -1764.4269724399999 0.489561
Enthalpy (H) = -1764.42602844 0.490505
Gibbs Free Energy (G) = -1764.51244844 0.404085

Frequencies
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96.1104 102.4615 132.6648
162.8968 189.3770 198.3007
222.1230 238.1541 247.1715
250.3160 257.4963 267.4281
293.5439 316.2112 346.4130
383.4653 405.6521 412.3412
413.5884 415.4208 416.3168
417.5764 457.0113 464.6135
485.2771 503.5263 520.8383

529.6752 566.8688 635.9137
637.1573 637.2590 638.3314
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716.3285 721.1644 722.5937
723.7458 725.0671 727.2257
733.4409 767.1960 769.4074
779.1584 780.6232 813.7468
824.2997 871.3382 880.6503
881.9803 885.7382 887.2229
939.7406 954.7855 957.3539
958.4799 960.7055 995.5635
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1010.3775 1022.4843 1023.3626
1023.9946 1025.3964 1025.7596
1029.8548 1030.9315 1032.8833
1059.7068 1065.7862 1066.4280
1066.9920 1067.1423 1102.6191
1113.7540 1117.8583 1121.0695
1124.6059 1136.5797 1139.6629
1146.1560 1151.7183 1174.5443
1195.0104 1195.3388 1195.8130
1195.9302 1215.9117 1219.2877
1221.0546 1224.2134 1246.3750
1262.9064 1303.9174 1331.8218
1334.1725 1337.0084 1339.5545
1341.0523 1363.8061 1364.5301
1368.1280 1370.7210 1386.6794
1466.2101 1481.0783 1489.5902
1490.4716 1492.7548 1493.6029
1515.8069 1538.4536 1538.7138
1541.2794 1541.7426 1662.6190
1663.7559 1665.3534 1666.9445
1682.4794 1682.8084 1684.4080
1684.7348 3057.6982 3072.8779
3083.0416 3108.5144 3136.6799
3143.2699 3199.2418 3200.4233
3201.2544 3202.6138 3205.1300
3205.6092 3205.7286 3211.0214
3211.9202 3212.9382 3213.8740
3219.7622 3221.7396 3221.9503
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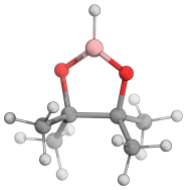
Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -1765.338915 Hartrees

Pinacolborane (HBpin)



Gaussian 16: ES64L-G16RevB.01 20-Dec-2017

# wB97xd/6-31G(d,p) gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc
) opt=(maxcycle=250) freq=noraman

Full point group C1 NOp 1
Stoichiometry C6H13BO2 Framework group C1[X(C6H13BO2)]

Num atoms: 22
Charge = 0 Multiplicity = 1

SCF = -411.766637846 | Predicted change in Energy=-6.355293D-09

Optimization completed.
Maximum Force 0.000008 0.000450 YES
RMS Force 0.000003 0.000300 YES
Maximum Displacement 0.000656 0.001800 YES
RMS Displacement 0.000124 0.001200 YES

Atom Coordinates (in Angstroms)
Type X Y Z

C -0.294668 1.887688 3.459973
O 0.827205 0.975816 3.463642
B 1.960508 1.736353 3.433427
O 1.732198 3.070367 3.612278
C 0.347144 3.214353 4.000934
H 3.045775 1.279247 3.266767
C -0.769654 1.995306 2.010055
H -1.011044 0.994991 1.642915
H -1.662419 2.621149 1.926549
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C -1.401033 1.310512 4.331212
H -1.779809 0.389329 3.881538
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H -2.232385 2.017834 4.412951
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H 0.302123 5.357144 3.814506
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C 0.326619 3.315461 5.526975
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Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -411.766637846 | Predicted change in Energy=-6.355293D-09
Zero-point correction (ZPE) = -411.57378584599996 0.192852
Internal Energy (U) = -411.564505846 0.202132
Enthalpy (H) = -411.56356184599997 0.203076
Gibbs Free Energy (G) = -411.606599846 0.160038

Frequencies
101.8252 238.4397 249.5038
284.6417 297.3340 299.1576
311.5659 323.0596 368.6740
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677.7657 755.0992 831.5993
893.8621 908.5312 948.1924
954.4059 974.6052 995.9380

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1160.4084 1206.3661 1208.2842
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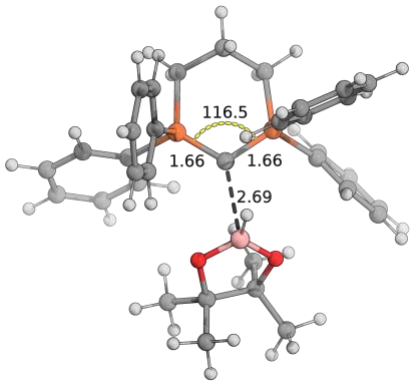
Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -411.909858 Hartrees

TS(1-12)



Gaussian 16: EM64L-G16RevC.01 3-Jul-2019

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) opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman

Full point group C1 NOp 1
Stoichiometry C34H39BO2P2 Framework group
C1[X(C34H39BO2P2)]

Num atoms: 78
Charge = 0 Multiplicity = 1

SCF = -2176.70627974 | Predicted change in Energy=-6.979680D-10

Optimization completed.
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RMS Force 0.000000 0.000300 YES
Maximum Displacement 0.000367 0.001800 YES
RMS Displacement 0.000079 0.001200 YES

Atom Coordinates (in Angstroms)
Type X Y Z

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C -0.042826 -2.631525 -2.566226
C -1.290806 -1.729537 -2.576998
P -1.403630 -0.800357 -0.981298
H 2.142157 -2.492429 -2.618740
H 1.312341 -1.129685 -3.354383
H -0.102478 -3.315749 -1.710070
H -0.046563 -3.256963 -3.465242
H -1.218851 -1.013157 -3.402046
H -2.196348 -2.325688 -2.724006
C -3.005971 -4.203069 1.723667
C -3.836026 -3.666101 0.740565
C -3.381759 -2.622577 -0.056913
C -2.095210 -2.103185 0.122423
C -1.273117 -2.642758 1.111093
C -1.726231 -3.691349 1.908053
H -3.361488 -5.018057 2.346650
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H -1.076858 -4.102349 2.674429
C -4.706461 2.402872 -1.316593
C -4.514656 1.713935 -0.122484
C -3.555442 0.710191 -0.041379
C -2.779115 0.385170 -1.156478
C -2.969448 1.088779 -2.347652
C -3.931567 2.089631 -2.430270
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H -5.105547 1.963611 0.752843
H -3.391495 0.198372 0.900039
H -2.354667 0.872500 -3.216060
H -4.072431 2.628671 -3.361731
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C 4.077343 0.093344 -1.380198
C 5.026703 1.023895 -1.791405
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H 2.950629 3.558626 -2.685969
H 1.257701 1.887066 -1.940394
H 4.396831 -0.872062 -0.998161
H 6.082694 0.778666 -1.736955
C 3.246335 -3.378274 2.383044
C 2.901558 -3.991801 1.183901
C 2.399790 -3.230659 0.130476
C 2.238097 -1.850574 0.268491
C 2.584180 -1.239497 1.481182
C 3.087590 -2.001245 2.528391
H 3.635155 -3.971406 3.204950
H 3.019957 -5.064340 1.065425
H 2.127280 -3.729938 -0.794098
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H 3.349862 -1.518247 3.464231
C 0.006471 -0.073918 -0.498898
B -0.186050 0.901176 2.001445
O -1.280346 1.726524 1.888379
C -0.801995 3.037486 1.536473

C 0.688640 3.002178 2.046238
O 1.003587 1.599595 2.039774
H -0.280141 -0.227160 2.363043
C -0.921925 3.193910 0.020053
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H -0.549362 4.168693 -0.309531
H -1.974485 3.113598 -0.264005
C -1.687867 4.067172 2.228292
H -2.702779 3.989858 1.828772
H -1.734165 3.905461 3.306604
H -1.322527 5.081884 2.038748
C 1.684683 3.730155 1.154361
H 2.689752 3.637187 1.575055
H 1.700302 3.302877 0.151636
H 1.438934 4.795118 1.086033
C 0.840897 3.475358 3.494296
H 1.856691 3.253817 3.831906
H 0.670035 4.551742 3.589786
H 0.143966 2.949333 4.152356

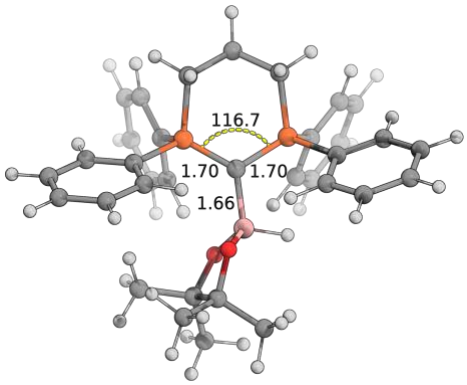
Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -2176.70627974 | Predicted change in Energy=-6.979680D-10
Zero-point correction (ZPE) = -2176.04824874 0.658031
Internal Energy (U) = -2176.01231974 0.69396
Enthalpy (H) = -2176.01137574 0.694904
Gibbs Free Energy (G) = -2176.11638874 0.589891

Frequencies
-32.4223 21.7286 22.8150
31.0019 40.4590 42.1488
45.0261 54.9886 57.3056
61.6772 69.0850 70.1875
80.7681 86.4815 94.7467
96.8479 110.7141 138.6022
142.7166 185.7893 192.3255
213.3311 219.0989 233.4155
245.3130 250.3146 257.5404
263.0199 269.3551 273.1311
276.4821 301.2667 307.0787
318.3332 324.5001 337.0755
344.1085 356.3809 357.0468
375.1516 383.8579 407.0472
409.1665 411.0931 419.0096
420.2956 420.7542 425.0477
463.7465 469.6357 480.4733
497.6773 501.3146 510.6071
525.3032 529.8333 533.2036
567.7516 592.4416 635.2013
635.5152 636.5034 637.1747
651.0884 678.1642 686.8426
712.6420 716.5286 718.8655
724.9262 727.5300 728.3424
730.9832 737.0003 753.0341
767.8169 773.2096 773.9750
778.2482 806.0295 816.6088
840.4333 860.3310 870.7862
884.5847 887.2335 889.1405
897.2583 906.6968 943.2660
943.3843 946.7951 951.0891
959.5591 962.0046 964.0277
976.4921 992.2363 994.6370
997.8459 1010.3501 1011.2893
1013.1390 1018.1913 1022.2938
1023.1342 1023.8697 1025.0951
1026.2959 1028.7678 1029.7700
1034.9860 1041.3959 1058.7553
1064.7793 1066.0583 1067.3452
1067.8431 1068.7139 1102.1052
1117.0034 1120.7361 1126.1329
1129.5036 1138.9289 1147.2508
1150.0448 1156.4156 1162.0727
1175.2126 1187.1546 1195.5764
1195.6439 1197.4304 1198.0875
1202.0580 1212.0193 1214.0575
1220.2007 1223.3468 1230.1599
1237.8250 1263.1978 1263.3400
1284.8333 1304.5367 1316.6494
1332.8226 1334.4186 1339.2216
1341.0526 1343.5925 1363.4773
1367.0135 1368.5095 1372.9377
1380.8051 1388.0571 1418.4028
1419.8564 1430.3088 1439.9155
1463.8087 1486.8970 1487.0461
1489.7408 1490.8385 1493.6725
1494.0385 1498.5263 1500.4507
1504.8971 1516.7133 1522.3083
1524.1841 1530.2606 1540.8399
1541.1954 1545.7555 1548.2728
1548.9401 1663.2172 1664.3921
1666.7924 1667.3951 1683.5539
1684.1970 1684.6394 1686.5260
2708.7768 3057.6106 3063.7244
3066.2944 3068.6531 3072.1149
3077.6560 3081.2001 3107.3727
3136.4553 3144.2947 3144.4543
3146.9324 3154.4752 3156.6268
3157.7444 3167.5415 3172.9136
3192.5798 3196.9224 3203.1452
3203.6568 3204.6372 3208.4033
3209.1766 3209.9772 3213.0470
3216.8153 3217.1609 3220.1305
3223.2173 3224.3686 3226.4451
3230.5000 3232.4503 3233.0183
3234.1682 3239.4743 3245.2681

Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -2177.263957 Hartrees

Adduct **12**



Gaussian 16: ES64L-G16RevB.01 20-Dec-2017

# wB97xd/6-31G(d,p) gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc
) opt=(maxcycle=250) freq=noraman

Full point group C1 NOp 1
Stoichiometry C34H39BO2P2 Framework group
C1[X(C34H39BO2P2)]

Num atoms: 78
Charge = 0 Multiplicity = 1

SCF = -2176.73043812 | Predicted change in Energy=-
1.901628D-08

Optimization completed.
Maximum Force 0.000014 0.000450 YES
RMS Force 0.000003 0.000300 YES
Maximum Displacement 0.001480 0.001800 YES
RMS Displacement 0.000245 0.001200 YES

Atom Coordinates (in Angstroms)
Type X Y Z

P -6.907076 4.453911 -2.887892
C -6.368216 5.970236 -2.006072
C -6.439261 5.818717 -0.481697
C -7.882849 5.653285 0.005020
P -8.707035 4.145352 -0.641980
H -7.044652 6.762075 -2.344462
H -5.365559 6.250718 -2.337833
H -6.007145 6.708381 -0.012330
H -5.832391 4.964479 -0.157608
H -7.931957 5.653498 1.096913
H -8.497297 6.492090 -0.338744
C -13.107047 5.071089 0.343456
C -12.230250 4.720213 1.365710
C -10.909908 4.401293 1.067244
C -10.461046 4.438998 -0.254803
C -11.343864 4.782450 -1.282033
C -12.663700 5.095849 -0.975885
H -14.139483 5.314093 0.574778
H -12.574847 4.685163 2.394195
H -10.239423 4.103972 1.867878
H -11.010709 4.757096 -2.315691
H -13.351224 5.347964 -1.776683
C -7.160059 0.607020 1.906274
C -7.483893 0.444355 0.562614
C -7.959382 1.518400 -0.181336
C -8.123788 2.770429 0.421859
C -7.793302 2.927171 1.772092
C -7.313738 1.850573 2.511233
H -6.783043 -0.232837 2.481418
H -7.361560 -0.522316 0.085272
H -8.201482 1.387447 -1.231745
H -7.898437 3.890288 2.262863
H -7.056432 1.985786 3.556903
C -3.447801 1.405843 -2.470401
C -4.726378 1.002208 -2.844811
C -5.752659 1.932091 -2.969957
C -5.499166 3.287525 -2.727100
C -4.211434 3.688694 -2.355383
C -3.191119 2.750773 -2.225369
H -2.652142 0.674397 -2.368005
H -4.931097 -0.046096 -3.038237
H -6.757596 1.621355 -3.259803
H -3.984687 4.731803 -2.160966
H -2.197356 3.073423 -1.931416
C -7.074986 5.752443 -7.291185
C -5.881768 5.259969 -6.768797
C -5.822750 4.847819 -5.442453
C -6.961230 4.928465 -4.636506
C -8.159584 5.418510 -5.161026
C -8.209324 5.831120 -6.488470
H -7.122653 6.064593 -8.329829
H -5.000129 5.185680 -7.397013
H -4.898003 4.442495 -5.043344
H -9.057428 5.396547 -4.553482
H -9.145546 6.192958 -6.900992
C -8.413206 3.926163 -2.301182
B -9.403111 2.814826 -3.025562
O -8.687854 1.694140 -3.689783
C -9.260137 1.446776 -4.960814
C -10.537173 2.379466 -4.988296
O -10.184423 3.428498 -4.113358
H -10.127946 2.364204 -2.121140
C -8.225030 1.820178 -6.030459
H -7.998222 2.886927 -6.003322
H -8.560788 1.558904 -7.039693
H -7.298322 1.273650 -5.827471
C -9.576368 -0.045023 -5.085234
H -8.644392 -0.619064 -5.066232
H -10.198070 -0.386035 -4.255398
H -10.091543 -0.267706 -6.026595
C -10.849923 2.968030 -6.362603
H -11.738075 3.603737 -6.292404
H -10.022711 3.579839 -6.727900
H -11.053427 2.179049 -7.094979
C -11.796398 1.680104 -4.449471

H -12.586072 2.429926 -4.343434
H -12.153052 0.893778 -5.122410
H -11.614670 1.246686 -3.463544

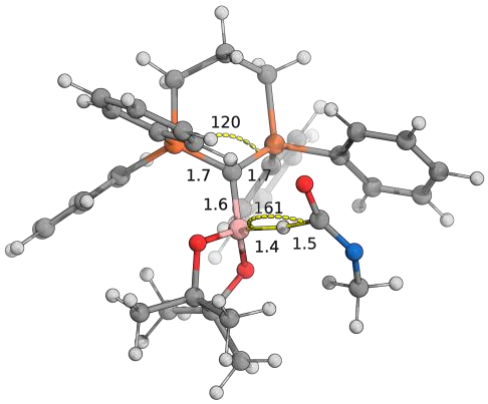
Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -2176.73043812 | Predicted change in Energy=-1.901628D-08
Zero-point correction (ZPE) = -2176.07086712 0.659571
Internal Energy (U) = -2176.0350641200002 0.695374
Enthalpy (H) = -2176.0341201200004 0.696318
Gibbs Free Energy (G) = -2176.13843312 0.592005

Frequencies
15.7187 26.1060 32.6312
37.6438 40.5011 47.5705
49.4583 62.7102 66.3587
68.9857 80.0593 90.9624
98.3959 110.0869 121.8893
132.5508 148.6245 158.5617
176.0354 184.6473 206.4838
220.2676 234.0340 238.8065
249.0649 254.2662 259.3151
264.0901 268.7681 270.7894
290.3224 297.6174 311.7399
321.8771 323.6460 359.4008
370.9405 378.4785 382.8850
402.8332 409.5798 411.3017
413.3798 416.9427 419.2963
423.4383 439.5604 450.0523
470.2650 477.1726 493.9535
496.9123 509.8296 520.1744
529.9209 533.2229 576.7635
584.5254 633.4953 633.8539
635.4461 636.6361 649.1647
672.0599 677.6596 703.9290
710.7341 714.3995 719.2477
725.8910 729.1805 732.2523
733.9273 740.9116 747.4962
769.2014 774.9197 780.3619
781.2400 814.6560 869.9078
875.4978 879.3886 882.3682
883.6859 892.0821 894.0661
925.2965 935.9733 940.5680
943.6650 954.9523 959.0838
960.9315 966.0618 967.3248
1002.1006 1006.7063 1009.2860
1010.7961 1012.1265 1016.4030
1016.9741 1020.3619 1021.2229
1021.9393 1023.6664 1024.1416
1029.0150 1029.3280 1034.6804
1037.5456 1054.1269 1067.4343
1067.8968 1069.0948 1069.4503
1071.7715 1102.3434 1108.9083
1126.0541 1127.2494 1128.2055
1131.4283 1132.5458 1145.2830
1146.0432 1150.9369 1153.5461
1155.2497 1188.5127 1193.2172
1198.6738 1198.8033 1199.6892
1199.9517 1219.5495 1224.9096
1230.8914 1232.2901 1236.6998
1242.9077 1263.6027 1266.7909
1273.6591 1283.3659 1307.0022
1319.8272 1335.6458 1339.4659
1342.0810 1343.2070 1348.5980
1374.9627 1376.6994 1379.6040
1390.2168 1390.6356 1410.0113
1411.4163 1422.2489 1431.9062
1465.4761 1485.5642 1487.5037
1490.3024 1491.3593 1493.5277
1494.4132 1498.5490 1501.2290
1501.7084 1519.7281 1521.2936
1523.6374 1526.6810 1544.3157
1544.7123 1546.8284 1548.1886
1551.4910 1661.8465 1662.9433
1665.6422 1666.9836 1682.7818
1683.7049 1684.2098 1684.6091
2272.0607 3056.5505 3059.9856
3062.4420 3066.1022 3067.4748
3089.3217 3093.4828 3118.9468
3128.3900 3134.3555 3135.9786
3143.0785 3148.7758 3149.0378
3151.8147 3164.6015 3170.1086
3170.4492 3196.1230 3203.1194
3205.6585 3206.0687 3207.4755
3212.5796 3215.1119 3216.1979
3216.6832 3221.0649 3223.2033
3225.8489 3226.0444 3228.3111
3230.9139 3234.3572 3234.8180
3235.2397 3237.3294 3250.0301

Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -2177.284283 Hartrees

TS(12-13)



Gaussian 16: ES64L-G16RevB.01 20-Dec-2017

# wB97xd/6-31G(d,p) gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc
) opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman

Full point group C1 NOp 1
Stoichiometry C36H42BNO3P2 Framework group
C1[X(C36H42BNO3P2)]

Num atoms: 85
Charge = 0 Multiplicity = 1

SCF = -2384.65595167 | Predicted change in Energy=-
3.283146D-09

Optimization completed.

Maximum Force	0.000009	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.001204	0.001800	YES
RMS Displacement	0.000246	0.001200	YES

Atom Coordinates (in Angstroms)
Type X Y Z

P	1.418629	0.175431	-1.332306
C	1.143905	0.756294	-3.052415
C	-0.039139	0.016024	-3.683646
C	-1.376898	0.524175	-3.140648
P	-1.508041	0.483168	-1.293250
H	2.068205	0.573288	-3.606254
H	0.967729	1.837022	-3.057458
H	0.062093	-1.061168	-3.512942
H	-0.027423	0.167229	-4.767403
H	-1.532259	1.559946	-3.458304
H	-2.205504	-0.067936	-3.537870
C	-5.047630	-2.283054	-0.345158
C	-5.034308	-0.997935	0.185842
C	-3.974592	-0.139869	-0.091023
C	-2.932119	-0.571273	-0.911413
C	-2.948505	-1.863445	-1.445009
C	-4.003907	-2.716807	-1.158225
H	-5.865281	-2.956871	-0.111130
H	-5.840735	-0.665546	0.831191
H	-3.955388	0.855425	0.339742
H	-2.105683	-2.226702	-2.024589
H	-3.994983	-3.730234	-1.542827
C	-2.725252	4.782667	-0.136468
C	-1.747126	4.105244	0.583659
C	-1.395132	2.803331	0.235676
C	-2.024365	2.178834	-0.842104
C	-3.020762	2.856690	-1.554115
C	-3.367354	4.155755	-1.203678
H	-2.996046	5.798067	0.135494
H	-1.256659	4.585283	1.424574
H	-0.659547	2.249353	0.811561
H	-3.537367	2.368544	-2.376760
H	-4.138553	4.679154	-1.759545
C	4.003008	3.418978	0.688818
C	2.829197	3.757018	0.019550
C	2.081073	2.769385	-0.608574
C	2.502998	1.436001	-0.580794
C	3.671757	1.101666	0.103063
C	4.420434	2.092765	0.731241
H	4.585118	4.188085	1.186147
H	2.489749	4.787351	-0.003228
H	1.145457	3.039025	-1.091021
H	3.980863	0.064623	0.169114
H	5.323761	1.822422	1.268283
C	3.886690	-3.640981	-2.030297
C	2.635583	-3.716236	-1.429120
C	1.896186	-2.560172	-1.190065
C	2.421167	-1.322881	-1.556984
C	3.678305	-1.246157	-2.170042
C	4.409851	-2.403276	-2.403453
H	4.459035	-4.545529	-2.211971
H	2.219758	-4.674286	-1.135735
H	0.919304	-2.636929	-0.720572
H	4.095914	-0.283097	-2.453993
H	5.385878	-2.340675	-2.873918
C	-0.078506	-0.061019	-0.553111
B	-0.036076	-0.540787	0.993405
O	-0.517923	0.361607	2.019899
C	0.438985	0.421848	3.072250
C	1.383901	-0.803792	2.784602
O	1.289293	-0.944979	1.372165
C	1.164309	1.768543	2.962062
H	1.698363	1.847548	2.012648
H	1.876538	1.923630	3.778704
H	0.420213	2.570615	3.004754
C	-0.286325	0.349023	4.413648
H	-0.929769	1.226085	4.530401
H	0.426796	0.335366	5.245219
H	-0.914693	-0.540661	4.475875
C	2.844133	-0.575397	3.161781
H	3.431252	-1.456501	2.886839

H 3.262939 0.289828 2.646960
H 2.945069 -0.421826 4.241441
C 0.903884 -2.105923 3.437147
H 1.493788 -2.932021 3.031421
H -0.143981 -2.312297 3.215532
H 1.033935 -2.084863 4.523503
H -0.883160 -1.615390 1.023489
C -1.388093 -2.987873 0.919822
O -0.803821 -3.530291 0.010462
N -2.273590 -3.149364 1.794702
C -2.751651 -2.117616 2.673498
H -3.838660 -2.020051 2.571189
H -2.548628 -2.383249 3.719795
H -2.297402 -1.139070 2.470001

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -2384.65595167 | Predicted change in Energy=-3.283146D-09
Zero-point correction (ZPE) = -2383.94526267 0.710689
Internal Energy (U) = -2383.9046656699998 0.751286
Enthalpy (H) = -2383.90372167 0.75223
Gibbs Free Energy (G) = -2384.01750167 0.63845

Frequencies
-412.0328 10.8337 29.0628
31.9401 36.8326 50.4789
53.1587 59.8108 63.1963
65.8301 71.7586 77.4235
85.6780 88.7862 94.2989
104.0565 114.2367 120.3552
130.1379 138.6437 145.8816
152.0336 167.5586 174.0315
183.7911 205.8292 212.4159
223.6035 227.1927 234.0035
234.6688 240.7465 249.0499
254.7643 260.6413 265.2597
274.8371 280.5032 294.8292
304.0770 308.4939 323.1770
342.4645 344.8829 352.8900
371.3571 381.1108 391.9478
405.5759 409.5366 412.1661
415.9844 417.2772 421.7972
431.9951 441.7220 464.1577
476.1805 482.8475 495.1718
503.9115 510.1715 520.2906
527.3222 534.4366 585.8874
588.2102 608.6108 634.1952
635.2336 636.5158 637.2562
667.2566 680.5851 702.0002
709.9808 715.1030 718.5440
719.3183 724.0408 728.4716
735.1111 737.2345 742.8346
761.0705 769.1724 776.3009
777.3865 783.4134 817.9180
846.0009 871.0513 873.8785
877.3822 884.0008 888.3012
890.7623 902.5187 939.9309
941.9439 949.5810 951.9199
954.2471 962.2596 970.3127
975.7153 986.1059 994.1708
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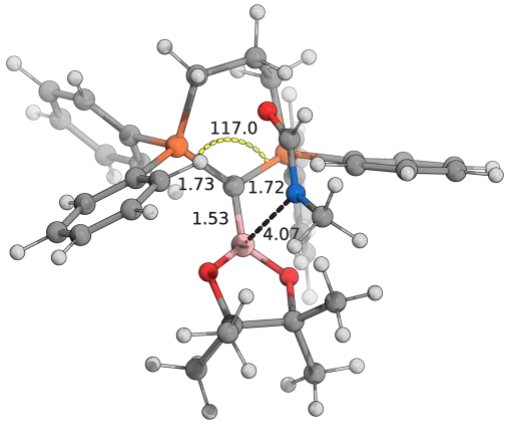
1014.8021 1017.2701 1018.5368
1022.3081 1022.6129 1023.0589
1024.6074 1027.0847 1028.3027
1032.4032 1043.2480 1047.2595
1056.0130 1064.8398 1067.3522
1067.6711 1068.9026 1076.2345
1082.0671 1122.3486 1126.5157
1127.2632 1128.6873 1133.5198
1134.2308 1146.0809 1150.7312
1152.7880 1153.5428 1155.0701
1160.5391 1172.0320 1195.7181
1197.7126 1199.4924 1199.6396
1200.8902 1202.2095 1214.6498
1226.7375 1229.5881 1232.2750
1234.9319 1237.2112 1264.1283
1274.1346 1275.8499 1296.9387
1313.3318 1321.6598 1332.3462
1338.6421 1340.4605 1344.9106
1345.2184 1347.6110 1373.7487
1378.9907 1379.4761 1380.7502
1395.0170 1410.2724 1416.6357
1426.7229 1436.0066 1471.7511
1474.9681 1486.7940 1488.4193
1490.0746 1492.5727 1495.2737
1495.7989 1496.7231 1498.9346
1504.5321 1512.0804 1514.6202
1518.2767 1524.6769 1525.7667
1528.0116 1543.0577 1543.4564
1544.9897 1545.7189 1548.0501
1664.0750 1665.3913 1667.8928
1668.5018 1682.4314 1683.9687
1685.2590 1685.4825 1719.3568
2049.0771 3017.4953 3061.9662
3065.9749 3067.1350 3074.4179
3078.7523 3084.6635 3089.7271
3091.8286 3109.3335 3127.6420
3135.1236 3141.1416 3142.5742
3152.6297 3153.3261 3155.1888
3179.2999 3182.4669 3185.7860
3190.7163 3195.6737 3197.8202
3203.7537 3210.3459 3210.6407
3213.3537 3214.0706 3215.2197
3221.5349 3222.0038 3225.0818
3227.2376 3227.4635 3229.0026
3234.8440 3236.3103 3236.7124
3237.8954 3245.2271 3248.8106

Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -2385.290837 Hartrees

13



Gaussian 16: ES64L-G16RevB.01 20-Dec-2017

# wB97xd/6-31G(d,p) gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc
) opt=(maxcycle=250) freq=noraman

Full point group C1 NOp 1
Stoichiometry C36H42BNO3P2 Framework group
C1[X(C36H42BNO3P2)]

Num atoms: 85
Charge = 0 Multiplicity = 1

SCF = -2384.70412622 | Predicted change in Energy=-
2.633172D-08

Optimization completed.
Maximum Force 0.000077 0.000450 YES
RMS Force 0.000008 0.000300 YES
Maximum Displacement 0.001009 0.001800 YES
RMS Displacement 0.000235 0.001200 YES

Atom Coordinates (in Angstroms)
Type X Y Z

P 1.390090 0.647363 -1.132563
C 0.846430 0.837121 -2.868812
C -0.268071 -0.172574 -3.185087
C -1.633543 0.165900 -2.567228
P -1.531986 0.906827 -0.890296
H 1.720757 0.662188 -3.502424
H 0.509968 1.867869 -3.031721
H -0.001688 -1.176000 -2.839329
H -0.388143 -0.231023 -4.270346
H -2.202710 0.857677 -3.195476
H -2.180108 -0.775199 -2.459147
C -4.892203 -0.678246 1.769876
C -4.081332 -1.552911 1.052060
C -3.091388 -1.060550 0.211642
C -2.925464 0.321953 0.092663
C -3.731757 1.204867 0.813615
C -4.720149 0.698949 1.649902
H -5.660448 -1.069094 2.430522
H -4.196621 -2.626397 1.156380
H -2.427972 -1.736259 -0.329179
H -3.586819 2.277447 0.735416
H -5.350828 1.379734 2.212526
C -2.119191 5.442418 -1.553756
C -3.050176 4.542443 -2.070773
C -2.882921 3.178249 -1.870084
C -1.783585 2.701391 -1.146081
C -0.864348 3.608584 -0.618654
C -1.029409 4.975676 -0.827554
H -2.248810 6.507744 -1.715826
H -3.906116 4.905288 -2.630367
H -3.619758 2.484278 -2.265693
H -0.021500 3.237673 -0.043409
H -0.305142 5.672746 -0.419007
C 4.184689 4.163118 -0.090977
C 3.756249 4.004989 -1.404238
C 2.922764 2.941700 -1.741641
C 2.514019 2.033020 -0.763338
C 2.950330 2.193159 0.558358
C 3.782768 3.255716 0.887304
H 4.833585 4.992618 0.171483
H 4.068525 4.708113 -2.169412
H 2.598115 2.831304 -2.770936
H 2.635761 1.482551 1.318409
H 4.119585 3.375780 1.911798
C 3.819501 -3.230930 -0.967843
C 4.486321 -2.023495 -1.177242
C 3.771846 -0.832496 -1.213774
C 2.384259 -0.858139 -1.042004
C 1.714507 -2.063635 -0.832538
C 2.439456 -3.249931 -0.797465
H 4.384065 -4.157757 -0.932459
H 5.564302 -2.009830 -1.302119
H 4.293268 0.109128 -1.359093
H 0.634357 -2.093337 -0.700529
H 1.903080 -4.175865 -0.618303
C -0.013383 0.587637 -0.132031
B 0.096022 0.043382 1.290367
O -0.963135 -0.254316 2.098958
C -0.470236 -0.794515 3.333733
C 1.047617 -1.094700 3.017105
O 1.312012 -0.228244 1.890026
C -0.677682 0.285015 4.395640
H -0.111182 1.189160 4.154646
H -0.380542 -0.061702 5.389600
H -1.738162 0.548403 4.420559
C -1.305196 -2.030588 3.646617
H -2.335495 -1.724681 3.849429

H -0.919625 -2.555867 4.526435
H -1.315153 -2.705056 2.786942
C 2.016927 -0.729957 4.133564
H 3.038447 -0.950324 3.812097
H 1.959987 0.329151 4.393050
H 1.808708 -1.321539 5.030416
C 1.296239 -2.526898 2.548136
H 2.323694 -2.600633 2.180561
H 1.171865 -3.235583 3.372872
H 0.615902 -2.808480 1.735570
H -1.420815 -4.666391 -1.542761
C -1.196893 -3.704578 -1.013878
O -1.258845 -2.643400 -1.704850
N -0.893975 -3.771597 0.255359
C -0.880977 -5.090899 0.840070
H -1.107396 -5.902548 0.123642
H 0.100991 -5.316217 1.284325
H -1.611134 -5.171952 1.659573

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -2384.70412622 | Predicted change in Energy=-2.633172D-08
Zero-point correction (ZPE) = -2383.98969822 0.714428
Internal Energy (U) = -2383.94816222 0.755964
Enthalpy (H) = -2383.94721822 0.756908
Gibbs Free Energy (G) = -2384.06482122 0.639305

Frequencies
19.9425 24.9064 30.4138
35.3448 36.0161 41.2130
46.9669 52.2795 57.5187
58.9122 62.6086 71.6425
76.8481 81.7111 84.7755
91.8453 100.5928 102.0207
116.5264 119.5348 128.6504
135.7735 155.3960 160.9659
191.4207 196.1255 213.1540
213.7776 226.9956 230.0984
236.9006 252.5045 257.7032
262.4799 280.4187 284.1712
285.9176 292.8458 302.9030
312.3881 318.2809 328.5939
331.7905 351.8295 357.4662
377.5551 389.4032 399.4955
401.8643 408.2778 409.2034
412.8028 417.1300 420.0022
422.2585 454.2049 464.9512
468.9199 490.3464 494.6799
499.4771 520.4925 528.0110
532.8272 543.4572 581.6843
593.0382 633.8529 634.3450
635.4408 635.6469 660.6281
677.6829 686.9877 693.8000
705.0554 711.8924 718.0904
719.6985 721.2163 729.4914
741.3198 744.1121 750.6880
769.9994 773.8142 776.3191
781.6675 798.8606 821.0967
865.6650 882.4058 882.8440
885.9490 888.1681 893.3578
900.7271 951.4398 954.9125
956.5916 964.9089 965.3864
966.7161 970.8760 987.9379
999.8729 1003.0021 1011.3668
1014.3682 1015.0210 1016.6355
1020.8301 1023.0601 1023.7567
1023.9680 1028.8338 1032.5964
1033.7742 1035.0050 1036.7884
1042.6386 1055.5194 1064.6968
1066.0283 1067.8036 1068.4903
1076.3244 1083.1404 1088.4224
1093.7797 1120.9939 1127.8232
1130.6578 1132.5340 1144.6385
1147.6156 1151.5326 1153.1886
1154.5129 1154.6398 1162.9114
1168.7315 1197.7183 1197.8687
1198.8201 1200.2080 1204.8629
1205.0734 1211.1869 1221.8966
1236.3079 1242.8081 1245.8026
1258.7974 1277.5426 1290.6573
1310.9456 1317.5933 1333.8913
1337.9335 1347.7331 1348.7065
1350.8018 1358.7798 1368.4827
1383.5975 1386.0109 1394.7946
1395.7995 1406.5123 1410.9376
1419.5281 1426.6888 1435.6590
1445.9497 1450.7791 1453.0323
1467.1341 1475.8509 1489.6265
1491.3058 1491.9599 1494.3263
1496.0822 1497.5410 1500.1251
1500.9327 1510.5516 1524.9254
1526.7828 1528.3453 1532.5647
1532.8196 1540.3527 1548.3999
1549.7016 1550.5192 1554.9519
1662.9619 1663.8097 1665.2777
1665.3848 1683.0094 1683.5483
1685.6262 1685.9545 1711.3884
2815.6880 2949.5824 3021.9690
3033.3809 3040.5191 3061.6981
3066.8105 3071.6430 3075.0412
3086.7583 3091.1223 3133.8115
3140.9320 3144.9801 3145.6198
3147.6165 3151.4220 3154.1813
3154.7337 3160.1945 3162.5949
3168.2381 3169.4454 3199.1576
3204.0715 3205.2406 3205.6111
3205.7485 3212.4896 3213.6584
3214.4271 3219.1603 3221.7963
3223.2857 3228.3994 3230.6501
3231.1038 3231.2521 3236.9962
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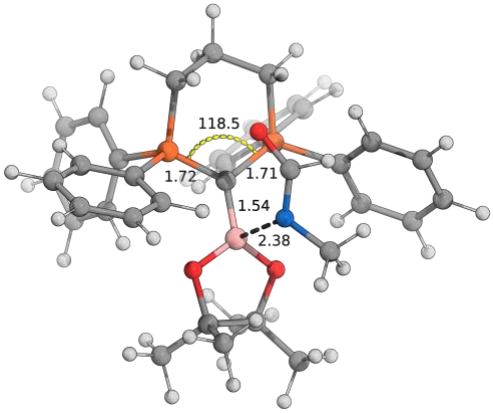
Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -2385.337124 Hartrees

TS(13-14)



Gaussian 16: ES64L-G16RevB.01 20-Dec-2017

# wB97XD/6-31G(d,p) gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc
) opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman

Full point group C1 NOp 1
Stoichiometry C36H42BNO3P2 Framework group
C1[X(C36H42BNO3P2)]

Num atoms: 85
Charge = 0 Multiplicity = 1

SCF = -2384.69995451 | Predicted change in Energy=-
2.132588D-08

Optimization completed.
Maximum Force 0.000013 0.000450 YES
RMS Force 0.000002 0.000300 YES
Maximum Displacement 0.001171 0.001800 YES
RMS Displacement 0.000270 0.001200 YES

Atom Coordinates (in Angstroms)
Type X Y Z

P -1.503383 0.605706 -1.014952
C -1.290982 1.338947 -2.671223
C -0.037881 2.210571 -2.826086
C 1.244717 1.389643 -2.645348
P 1.430702 0.802219 -0.927906
H -2.202658 1.886687 -2.927290
H -1.214241 0.460122 -3.319385
H -0.049546 3.058007 -2.129298
H -0.037534 2.635387 -3.834630
H 1.178930 0.488301 -3.263363
H 2.130642 1.971666 -2.914060
C 2.539446 4.620562 1.424565
C 1.394232 3.903098 1.750554
C 1.077154 2.741502 1.050496
C 1.902781 2.298033 0.018704
C 3.059556 3.018349 -0.299398
C 3.375569 4.175398 0.400613
H 2.787602 5.525952 1.969580
H 0.741812 4.242850 2.548332
H 0.189285 2.169223 1.299100
H 3.723849 2.665187 -1.084026
H 4.274696 4.730049 0.152217
C 5.175767 -1.859652 -0.721408
C 4.746364 -1.161634 0.403814
C 3.620971 -0.351368 0.332116
C 2.914504 -0.238598 -0.868291
C 3.349864 -0.937575 -1.995452
C 4.478831 -1.745481 -1.919713
H 6.053581 -2.495495 -0.663196
H 5.285400 -1.251853 1.341114
H 3.279967 0.180514 1.212775
H 2.798487 -0.879882 -2.926418
H 4.805303 -2.293195 -2.797334
C -4.964279 -2.358035 -1.613289
C -5.207497 -0.992598 -1.498696
C -4.147299 -0.119490 -1.284178
C -2.840072 -0.609753 -1.194346
C -2.593899 -1.978999 -1.312964
C -3.663847 -2.844048 -1.516277
H -5.790803 -3.043597 -1.774588
H -6.219430 -0.606682 -1.567635
H -4.345994 0.942962 -1.174907
H -1.582749 -2.363659 -1.224980
H -3.472709 -3.908999 -1.600369
C -3.107273 3.806967 1.905258
C -2.934335 2.480715 2.302693
C -2.500111 1.529844 1.389850
C -2.237644 1.895665 0.062142
C -2.423200 3.219843 -0.331878
C -2.854632 4.173742 0.589318
H -3.441548 4.550462 2.621943
H -3.137618 2.188938 3.328321
H -2.343573 0.497819 1.694563
H -2.227880 3.525736 -1.354720
H -2.989862 5.203411 0.274189
C -0.007280 0.088700 -0.349642
B 0.027101 -1.108399 0.622569
O -1.171958 -1.489590 1.236560
C -0.863727 -2.311723 2.362298
C 0.612010 -1.880212 2.692132
O 1.116306 -1.444538 1.428051
C -1.871627 -2.012339 3.467639
H -1.897174 -0.949017 3.715711
H -1.631080 -2.574985 4.375588
H -2.870906 -2.308216 3.137177
C -1.003480 -3.770830 1.929311
H -2.019647 -3.922464 1.555301
H -0.830351 -4.460031 2.761480
H -0.314159 -4.000778 1.117972
C 0.682041 -0.669728 3.629989
H 1.714968 -0.312249 3.662349
H 0.056506 0.146381 3.254922
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C 1.497112 -3.002773 3.216153
H 2.508006 -2.622581 3.388748
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H 1.560981 -3.819829 2.495924

H 1.367678 -2.947055 -2.955347
C 0.628286 -2.364375 -2.345722
O -0.021103 -1.472134 -2.947535
N 0.563758 -2.694326 -1.070055
C 1.516555 -3.700046 -0.657043
H 2.205402 -3.998800 -1.465386
H 2.129122 -3.319496 0.170401
H 1.026150 -4.621112 -0.306372

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -2384.69995451 | Predicted change in Energy=-2.132588D-08
Zero-point correction (ZPE) = -2383.98560451 0.71435
Internal Energy (U) = -2383.9452345100003 0.75472
Enthalpy (H) = -2383.9442905100004 0.755664
Gibbs Free Energy (G) = -2384.05808151 0.641873

Frequencies
-131.1049 16.6372 27.8731
31.0144 33.2672 44.8677
48.2711 50.0320 53.7840
58.4153 60.2997 65.3149
70.7549 80.7075 101.4783
102.9251 105.3617 126.2044
136.4070 139.7604 154.3897
163.9588 179.8198 190.6570
203.1746 212.7347 216.2460
220.0843 229.7261 238.3857
243.5527 250.6288 251.7778
261.6272 268.2721 273.4989
282.8324 293.3486 301.3513
311.9703 323.4851 337.1534
341.4124 350.9529 361.1372
370.3799 386.4438 389.7558
408.3348 409.5906 413.4309
416.0663 416.9512 420.0889
431.6356 448.6528 462.5822
477.7103 486.8419 493.8794
500.3598 514.0160 523.9116
529.7686 534.3201 567.5716
592.8729 604.0889 634.2996
635.0430 635.3930 636.0488
677.2138 682.7264 690.4213
702.3506 706.4143 714.7594
719.6903 722.3654 732.3523
736.6123 744.1262 749.7695
764.0513 771.9662 775.8448
778.4243 792.7265 832.2250
861.2068 879.9200 882.2407
883.4016 885.2435 892.5534
900.2390 942.9132 945.0261
949.4975 954.5085 956.3066
963.4542 965.0270 983.8813
989.8235 990.4322 1008.6047
1010.7851 1010.9907 1018.2415
1020.2207 1021.0941 1023.2395
1023.8798 1025.6581 1027.9281
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1146.9842 1147.6785 1153.0336
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1233.8493 1234.3409 1239.8276
1263.3284 1281.7794 1288.0990
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1336.4207 1340.7453 1344.9579
1346.4608 1351.6504 1357.8245
1372.6319 1378.1504 1379.5255
1386.0177 1397.1948 1416.9654
1419.4339 1423.5675 1429.8491
1438.7269 1442.7696 1455.9415
1470.1797 1482.5106 1486.6891
1491.1672 1492.2952 1494.3023
1495.6608 1497.3929 1499.3258
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1520.6620 1523.3982 1526.3034
1538.5499 1542.6352 1544.8321
1546.7632 1547.4667 1548.8087
1663.4810 1665.7509 1666.2398
1668.7385 1683.7409 1684.4971
1684.8999 1687.5174 1708.5522
2792.0265 2976.6014 3031.0015
3060.3756 3063.0648 3067.0337
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3152.6812 3154.5465 3157.7673
3160.0420 3165.9413 3178.3741
3198.0718 3199.6802 3202.4342
3208.6913 3209.5769 3210.7156
3210.8216 3213.5635 3214.4958
3217.7414 3222.6878 3223.0070
3224.4695 3226.8853 3231.6171
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Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -2385.330597 Hartrees

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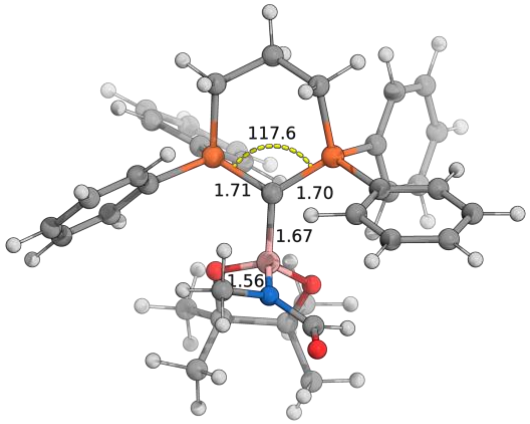

Gaussian 16: ES64L-G16RevB.01 20-Dec-2017

# wB97xd/6-31G(d,p) gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc
) opt=(maxcycle=250) freq=noraman

Full point group C1 NOp 1
Stoichiometry C36H42BNO3P2 Framework group
C1[X(C36H42BNO3P2)]

Num atoms: 85
Charge = 0 Multiplicity = 1

SCF = -2384.72949546 | Predicted change in Energy=-
8.851369D-09

Optimization completed.
Maximum Force 0.000017 0.000450 YES
RMS Force 0.000002 0.000300 YES
Maximum Displacement 0.001097 0.001800 YES
RMS Displacement 0.000163 0.001200 YES

Atom Coordinates (in Angstroms)
Type X Y Z

P 4.900430 -1.043001 9.374708
C 5.587511 0.525561 8.695618
C 4.546368 1.396126 7.988562
C 3.955038 0.686628 6.764312
P 2.950222 -0.774424 7.222185
H 6.388351 0.272277 7.995349
H 6.044664 1.066048 9.529396
H 5.022561 2.329021 7.670094
H 3.751907 1.672514 8.691866
H 3.347680 1.359554 6.153808
H 4.753105 0.309156 6.116495
C 2.047056 -2.920040 3.264819
C 1.104884 -2.037064 3.786314
C 1.350474 -1.386544 4.990253
C 2.553070 -1.610454 5.665973
C 3.503143 -2.481396 5.129129
C 3.244280 -3.145554 3.936749
H 1.839449 -3.447512 2.339358
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H 3.960199 -3.867636 3.562804
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C -0.776307 -0.494271 8.878019
C 0.426062 -0.968780 8.367570
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C 1.049893 1.284967 7.770930
C -0.155378 1.754813 8.286347
H -2.007674 1.234405 9.245697
H -1.484211 -1.193702 9.311737
H 0.674440 -2.027149 8.426951
H 1.742716 2.001508 7.343308
H -0.376108 2.816889 8.252944
C 2.993553 0.449689 13.301550
C 2.211583 -0.085479 12.283002
C 2.813505 -0.561515 11.122500
C 4.196947 -0.499218 10.972073
C 4.979327 0.045622 11.994476
C 4.378424 0.513913 13.157425
H 2.526921 0.816859 14.210159
H 1.132771 -0.140877 12.388522
H 2.218921 -1.001233 10.329245
H 6.060693 0.089326 11.892788
H 4.989972 0.927755 13.952753
C 8.656288 -3.566926 10.265540
C 7.657003 -3.455703 11.228619
C 6.527917 -2.685433 10.979067
C 6.393999 -2.010901 9.764242
C 7.395839 -2.132874 8.799589
C 8.523928 -2.906209 9.048610
H 9.532881 -4.176702 10.459575
H 7.748974 -3.982840 12.172585
H 5.733331 -2.631046 11.713060
H 7.286120 -1.658928 7.828899
H 9.291160 -3.001931 8.287587
C 3.805983 -1.783328 8.295789
B 3.355357 -3.341645 8.707997
O 1.915790 -3.548012 8.868649
C 1.661717 -4.331142 10.025724
C 3.087557 -4.496482 10.723733
O 3.907109 -3.566243 10.047022
C 0.639752 -3.570277 10.880418
H -0.267852 -3.414291 10.288308
H 0.362046 -4.129170 11.779226
H 1.016592 -2.592531 11.184449
C 1.024197 -5.658796 9.602795
H 0.804666 -6.291435 10.469606
H 0.083192 -5.453915 9.083584
H 1.667014 -6.215058 8.919685

C 3.101003 -4.137118 12.211232
H 4.116687 -4.264351 12.599280
H 2.806036 -3.098964 12.376674
H 2.439976 -4.791116 12.789189
C 3.699993 -5.896387 10.561961
H 4.716062 -5.871624 10.967364
H 3.131846 -6.660701 11.101816
H 3.768891 -6.180518 9.511094
N 3.915342 -4.371149 7.678059
C 5.347085 -4.564653 7.594361
H 5.558348 -5.503938 7.080388
H 5.835970 -3.752644 7.034097
H 5.773648 -4.577146 8.600435
C 3.160859 -5.017773 6.763280
O 3.578902 -5.755200 5.871193
H 2.085567 -4.814398 6.891385

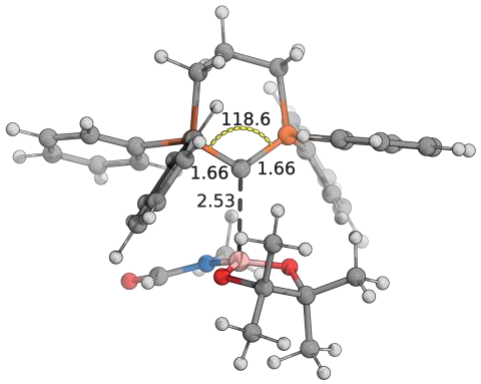
Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -2384.72949546 | Predicted change in Energy=-8.851369D-09
Zero-point correction (ZPE) = -2384.01247946 0.717016
Internal Energy (U) = -2383.97232846 0.757167
Enthalpy (H) = -2383.97138446 0.758111
Gibbs Free Energy (G) = -2384.08407846 0.645417

Frequencies
19.2255 27.8795 28.0785
39.9262 44.2218 48.7240
53.2453 56.5826 65.6021
68.8690 78.3209 80.0534
90.5241 93.6367 99.6422
103.5332 119.8196 124.4393
139.9875 150.3081 164.0440
167.1895 194.7796 197.6595
208.0330 222.7156 231.7150
239.4587 248.4326 258.0959
262.0523 267.1699 276.2045
278.5559 289.1200 295.2601
298.6173 308.8589 315.2358
336.0830 342.7779 351.9455
361.2279 370.6963 380.6177
395.2500 401.4019 411.7320
413.7893 421.3417 424.2666
426.5801 428.3740 435.4488
442.3546 457.1068 483.1341
485.4807 490.7802 495.4691
503.0149 519.4504 525.4721
529.6274 545.7300 579.7493
602.7491 635.0623 635.9696
636.3729 637.0268 662.7283
678.2207 700.0786 709.6131
719.4574 721.3486 722.7420
727.2176 730.3571 737.0874
739.2283 744.9919 766.7331
771.9084 773.7767 778.0880
798.3950 822.4410 863.3345
867.6863 879.9944 882.8141
887.9430 889.5078 897.0463
917.0116 931.5334 937.6953
944.8279 951.6745 964.7230
965.5535 970.9957 973.4442
981.8198 993.5139 1004.0633
1013.4178 1015.4698 1016.2664
1017.8506 1019.0115 1020.6237
1022.5118 1024.2775 1025.1302
1025.5063 1027.3167 1030.9896
1041.9393 1048.4295 1052.2403
1062.2522 1066.5275 1067.5407
1068.6360 1070.6805 1073.5990
1077.3979 1078.0483 1116.4730
1125.2255 1127.6117 1131.1121
1134.2790 1135.0182 1148.7620
1150.7907 1153.8563 1156.5394
1161.4263 1184.7647 1195.9013
1196.7511 1199.6258 1200.6939
1201.3240 1212.8813 1219.5156
1227.3239 1229.1044 1232.4640
1247.9417 1251.1529 1260.9003
1271.0259 1276.2131 1292.4241
1324.5691 1337.8850 1339.7993
1344.7388 1345.3798 1351.9836
1372.6234 1374.3730 1375.1664
1394.0335 1395.9390 1400.7199
1410.3716 1416.0023 1423.3398
1429.0981 1437.4354 1449.9942
1467.7461 1485.5960 1489.5610
1491.2630 1493.2667 1494.7895
1496.1742 1496.4869 1502.1570
1507.9567 1511.3336 1515.6014
1517.6749 1519.5660 1525.7476
1529.0024 1543.0800 1543.7761
1546.6584 1550.2571 1555.2640
1662.6217 1665.9067 1667.0439
1669.2104 1684.3361 1684.7408
1686.1543 1686.5898 1779.1143
3011.5146 3044.1898 3060.5428
3063.3437 3066.0424 3069.1796
3070.7641 3090.9718 3096.1714
3118.0357 3119.2666 3132.8559
3137.2452 3141.4645 3145.7946
3151.1487 3155.6443 3166.8771
3175.1004 3176.6475 3177.3150
3183.1228 3185.7592 3201.5479
3207.8600 3209.0769 3211.9037
3212.7161 3216.3786 3217.7618
3224.1575 3224.4387 3226.5686
3228.7444 3235.0877 3235.3874
3236.6738 3237.6352 3240.4046
3249.6481 3253.9115 3254.5258

Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -2385.360977 Hartrees

TS(14-11)



Gaussian 16: ES64L-G16RevB.01 20-Dec-2017

# wB97xd/6-31G(d,p) gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc
) opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman

Full point group C1 NOp 1
Stoichiometry C36H42BNO3P2 Framework group
C1[X(C36H42BNO3P2)]

Num atoms: 85
Charge = 0 Multiplicity = 1

SCF = -2384.70164779 | Predicted change in Energy=-
2.069151D-08

Optimization completed on the basis of negligible forces.

Maximum Force	0.000004	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.004387	0.001800	NO
RMS Displacement	0.000624	0.001200	YES

Atom Coordinates (in Angstroms)
Type X Y Z

P	1.501520	-0.104450	-1.316439
C	1.440510	-0.551914	-3.109009
C	0.541690	-1.783074	-3.302109
C	-0.932669	-1.454004	-3.033520
P	-1.251145	-0.876324	-1.293997
H	2.459259	-0.746584	-3.455663
H	1.041067	0.283263	-3.693683
H	0.884446	-2.593887	-2.647427
H	0.642695	-2.145171	-4.330511
H	-1.247497	-0.636689	-3.691060
H	-1.583309	-2.303071	-3.261853
C	-3.076829	-4.415124	1.054624
C	-3.333370	-3.104799	1.448242
C	-2.817057	-2.039766	0.718936
C	-2.052663	-2.275143	-0.428985
C	-1.791755	-3.593612	-0.811579
C	-2.298636	-4.658379	-0.072892
H	-3.474003	-5.245010	1.630442
H	-3.923118	-2.909152	2.338198
H	-2.963154	-1.023112	1.068220
H	-1.175400	-3.803059	-1.680895
H	-2.084334	-5.677466	-0.378540
C	-4.557285	2.268981	-2.138905
C	-4.941122	1.003636	-1.708536
C	-3.980166	0.030150	-1.444108
C	-2.622726	0.319794	-1.591405
C	-2.249740	1.588659	-2.045497
C	-3.206434	2.558095	-2.318427
H	-5.307821	3.027532	-2.337464
H	-5.992710	0.770147	-1.575156
H	-4.295882	-0.953221	-1.113399
H	-1.193922	1.820661	-2.161385
H	-2.898248	3.541714	-2.658374
C	3.119928	4.204790	-0.905835
C	2.383445	3.852197	-2.033276
C	1.937963	2.543790	-2.191429
C	2.230447	1.572014	-1.231738
C	2.964836	1.937525	-0.100406
C	3.407861	3.245303	0.060954
H	3.465426	5.225990	-0.779684
H	2.153094	4.596462	-2.788925
H	1.349752	2.291771	-3.068881
H	3.183657	1.198585	0.662571
H	3.972872	3.515285	0.947141
C	4.827672	-2.954332	0.146794
C	3.501473	-3.168111	0.501691
C	2.515775	-2.289628	0.061118
C	2.853129	-1.185618	-0.716434
C	4.189961	-0.975627	-1.073489
C	5.172161	-1.859660	-0.645867
H	5.599280	-3.632937	0.496441
H	3.232060	-3.999378	1.143404
H	1.475567	-2.431614	0.336606
H	4.465516	-0.111266	-1.672253
H	6.209041	-1.690038	-0.918752
C	0.068703	-0.267800	-0.487425
B	-0.010134	0.314303	1.975170
O	-1.392286	0.441911	2.047237
C	-1.671158	1.805301	2.399728
C	-0.358819	2.565896	1.970339
O	0.637766	1.534587	2.039236
C	-2.932533	2.249791	1.671028
H	-3.784063	1.657776	2.019433
H	-3.147116	3.303815	1.875770
H	-2.840579	2.111794	0.593154
C	-1.906116	1.825666	3.912994
H	-2.722243	1.138179	4.150375
H	-1.015788	1.489676	4.451669
H	-2.177907	2.823183	4.270348
C	-0.405347	3.087262	0.537448
H	0.566165	3.515964	0.280982
H	-0.602218	2.260148	-0.143504
H	-1.170586	3.859372	0.413780
C	0.059725	3.689233	2.912011
H	0.989727	4.133216	2.546643
H	-0.704258	4.473023	2.942462
H	0.232585	3.325681	3.926257

N 0.663810 -0.884634 2.468805
C -0.062244 -2.133492 2.622146
H -1.042603 -1.939519 3.061390
H -0.219311 -2.621113 1.654213
H 0.516434 -2.794479 3.267542
C 1.968993 -0.848540 2.869746
O 2.590410 -1.785199 3.342451
H 2.419777 0.148127 2.735218

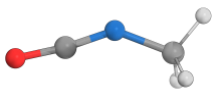
Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -2384.70164779 | Predicted change in Energy=-2.069151D-08
Zero-point correction (ZPE) = -2383.9862497900003 0.715398
Internal Energy (U) = -2383.9458787900003 0.755769
Enthalpy (H) = -2383.94493479 0.756713
Gibbs Free Energy (G) = -2384.0585797900003 0.643068

Frequencies
-107.0713 16.7598 19.1008
29.4920 36.5128 41.7868
51.2748 57.4891 60.6850
69.8809 71.2313 76.2211
85.4628 87.3559 90.0791
93.1981 107.9298 113.6516
122.9770 134.2834 147.7928
149.8392 180.0711 185.0893
197.2117 201.0104 225.7679
230.9740 241.6202 243.8951
249.4436 258.0235 261.2293
269.6040 275.9297 279.7006
283.9136 291.6821 308.6476
316.8922 325.1342 327.6033
340.9659 352.9584 357.8533
363.2441 376.5373 396.7940
401.4117 408.7334 411.4436
416.5262 422.7176 425.2724
429.9387 438.4874 457.9546
474.2325 483.9062 498.7914
502.5077 511.1093 524.7080
531.6736 536.4147 558.1984
567.4506 595.3916 635.5352
636.2036 636.6602 636.9276
650.3703 683.6849 685.4632
712.9614 715.3494 719.4170
720.1526 727.3821 728.0830
730.6383 732.8510 766.3808
770.0337 771.5383 772.8382
775.6394 809.1239 825.8545
864.4836 871.4356 871.6035
879.0027 884.1325 887.0311
892.2700 916.8441 939.6942
943.6772 945.0161 951.9879
953.5461 964.5307 966.0879
991.5476 995.9188 995.9801
1001.7428 1003.7408 1012.2305
1015.7542 1018.7674 1020.3934
1023.4875 1024.1847 1024.7733
1025.1761 1027.6037 1029.9144
1030.2563 1033.9163 1056.2259
1064.2629 1065.7781 1067.2230
1068.3238 1069.7285 1069.9940
1104.1467 1118.6696 1121.9132
1126.4844 1128.1444 1138.5633
1144.3044 1151.6651 1153.9589
1159.6155 1162.8467 1177.5246
1186.6740 1196.9741 1197.0454
1197.9565 1198.7393 1202.4115
1215.7351 1216.6702 1222.3843
1226.4895 1230.8854 1233.9021
1264.7770 1266.8588 1285.9918
1309.3308 1313.5664 1316.5076
1332.0236 1333.6728 1338.5273
1341.9521 1343.2938 1369.1097
1369.6619 1373.3028 1376.2587
1387.7714 1392.3650 1414.1263
1418.3370 1419.4619 1430.1464
1439.1591 1452.3143 1464.4073
1468.5815 1485.2764 1486.6375
1488.7315 1490.1639 1494.1540
1494.8811 1498.4236 1499.0395
1505.9597 1510.6051 1513.2948
1520.1679 1523.1105 1532.8542
1534.8673 1540.3787 1541.8427
1545.0063 1546.7610 1547.5638
1663.0615 1663.8634 1665.7470
1667.7168 1684.3116 1685.0825
1685.3687 1685.6507 1817.6098
3041.2731 3063.1732 3065.4066
3068.3045 3070.4319 3071.6694
3080.2536 3082.3536 3085.0196
3112.7611 3140.5270 3143.0512
3146.9111 3147.2163 3148.3486
3156.1947 3156.8244 3165.3471
3173.7414 3190.2386 3191.8861
3197.4735 3199.3273 3204.7426
3204.8518 3208.5918 3210.8797
3211.9126 3213.0136 3213.1030
3219.8609 3222.2827 3223.3421
3226.6205 3231.7424 3232.8171
3233.4209 3233.5763 3239.3273
3241.4321 3242.3836 3245.4396

Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -2385.336088 Hartrees

Methyl Isocyanate



Gaussian 16: ES64L-G16RevB.01 20-Dec-2017
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wb97xd/6-31G(d,p) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
---
Full point group CS NOp 2
Stoichiometry C2H3NO Framework group CS[SG(C2HNO),X(H2)]

Num atoms: 7
Charge = 0 Multiplicity = 1

SCF = -207.919317494 | Predicted change in Energy=-5.647155D-07

Optimization completed.
Maximum Force 0.000418 0.000450 YES
RMS Force 0.000135 0.000300 YES
Maximum Displacement 0.001755 0.001800 YES
RMS Displacement 0.000733 0.001200 YES

Atom Coordinates (in Angstroms)
Type X Y Z

C 0.032479 0.003553 0.003553
H -0.613869 -0.617801 -0.617801
H 0.667827 0.605732 -0.652674
H 0.667827 -0.652674 0.605732
N -0.783359 0.838331 0.838331
C -0.684003 1.684583 1.684583
O -0.724022 2.516172 2.516172

Statistical Thermodynamic Analysis

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -207.919317494 | Predicted change in Energy=-5.647155D-07
Zero-point correction (ZPE) = -207.868019494 0.051298
Internal Energy (U) = -207.86332249400002 0.055995
Enthalpy (H) = -207.862378494 0.056939
Gibbs Free Energy (G) = -207.895229494 0.024088

Frequencies
57.3764 163.0200 584.7668
629.7591 905.7861 1141.2300
1168.7419 1481.1097 1507.8761
1524.2673 1550.0884 2438.7094
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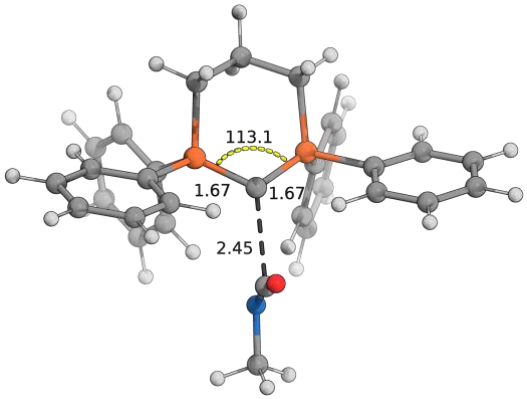
Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -208.005287 Hartrees

TS(1-15)



Gaussian 16: ES64L-G16RevB.01 20-Dec-2017
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wB97XD/6-31G(d,p) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
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Full point group C1 NOp 1
Stoichiometry C30H29NOP2 Framework group C1[X(C30H29NOP2)]

Num atoms: 63
Charge = 0 Multiplicity = 1

SCF = -1972.83925316 | Predicted change in Energy=-3.258543D-09

Optimization completed.
Maximum Force 0.000011 0.000450 YES
RMS Force 0.000001 0.000300 YES
Maximum Displacement 0.001774 0.001800 YES
RMS Displacement 0.000307 0.001200 YES

Atom Coordinates (in Angstroms)
Type X Y Z

P -1.333425 -0.206334 -0.958815
C -1.007383 0.067007 -2.755395
C 0.285759 0.868574 -2.978653
C 1.530102 0.138799 -2.446113
P 1.430129 -0.127976 -0.621957
H -1.860295 0.547832 -3.242697
H -0.914979 -0.933408 -3.191737
H 0.198966 1.849834 -2.494194
H 0.410986 1.057937 -4.050058
H 1.600969 -0.862262 -2.884995
H 2.446892 0.669650 -2.717787
C 2.420390 3.937624 1.372292
C 1.721107 2.940489 2.047319
C 1.447465 1.729585 1.421968
C 1.881866 1.498604 0.112142
C 2.583102 2.504300 -0.559149
C 2.850006 3.718868 0.067574
H 2.625861 4.885649 1.859774
H 1.378393 3.109642 3.063430
H 0.879980 0.956612 1.936452
H 2.925066 2.356431 -1.578883
H 3.390235 4.494371 -0.466492
C 4.999386 -2.919677 0.219746
C 3.694844 -3.400531 0.277032
C 2.622833 -2.545028 0.039004
C 2.856707 -1.200421 -0.251966
C 4.167676 -0.718124 -0.298887
C 5.235985 -1.577118 -0.067790
H 5.834031 -3.588601 0.406057
H 3.508088 -4.443391 0.512678

H 1.598759 -2.900363 0.096266
H 4.355522 0.333253 -0.498230
H 6.252497 -1.198070 -0.103064
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C -5.073867 -1.869731 -1.324710
C -4.031069 -0.950795 -1.298415
C -2.744852 -1.359356 -0.934860
C -2.512869 -2.690737 -0.587104
C -3.561113 -3.606441 -0.607577
H -5.654752 -3.914691 -0.994611
H -6.071738 -1.547877 -1.605568
H -4.224040 0.089775 -1.544169
H -1.514267 -2.988635 -0.283247
H -3.378388 -4.638812 -0.326890
C -2.999227 3.783604 0.712237
C -3.089535 3.550565 -0.656062
C -2.612494 2.357210 -1.192291
C -2.038406 1.387332 -0.365526
C -1.945369 1.632818 1.008811
C -2.428401 2.822142 1.542111
H -3.368405 4.715238 1.129816
H -3.527782 4.298591 -1.309420
H -2.690367 2.197813 -2.263358
H -1.476100 0.888987 1.649675
H -2.350117 3.002866 2.609705
C -0.015795 -0.792996 -0.118532
C -0.257219 -1.812590 2.099962
O -0.186347 -2.948875 1.782915
N -0.369799 -0.789572 2.786109
C -0.541494 -0.935104 4.230547
H -1.482411 -0.464007 4.530093
H -0.553185 -1.978199 4.566578
H 0.272789 -0.414876 4.743670

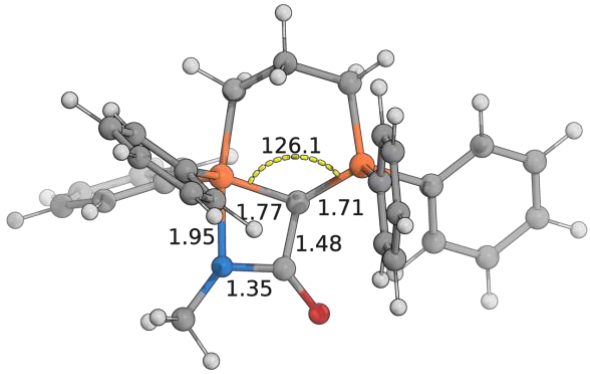
Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -1972.83925316 | Predicted change in Energy=-3.258543D-09
Zero-point correction (ZPE) = -1972.32355416 0.515699
Internal Energy (U) = -1972.29227916 0.546974
Enthalpy (H) = -1972.29133416 0.547919
Gibbs Free Energy (G) = -1972.38994316 0.44931

Frequencies
-179.4164 15.2095 18.5886
22.6456 32.5343 38.0055
41.6993 45.8819 53.8727
60.8524 65.4101 74.9011
83.7726 84.4165 97.9532
109.7220 134.1172 144.1048
145.8484 176.4156 183.6080
209.6784 227.6619 235.3387
235.6048 251.0833 256.4988
261.8190 269.1717 284.0563
343.1382 383.0810 389.2025
409.5033 412.1400 415.6441
416.4369 420.2590 422.6668
463.0674 470.3992 489.8092
498.2003 508.6672 531.1443
564.1124 586.9406 615.7974
634.6328 635.4743 635.6733
637.6391 665.6924 690.6642
716.8775 717.5308 719.2248
726.0135 727.3955 729.8704
730.6502 737.7032 768.7050
769.8057 778.7354 780.5002
811.9715 841.7544 867.4699
880.9144 884.3578 885.2121
889.1309 935.8124 955.0686
959.6557 961.5782 962.5459
963.3344 998.3062 1007.9784
1010.0637 1010.7372 1012.1013
1020.2993 1022.3157 1023.3496
1024.8614 1030.4233 1031.7509
1034.6067 1058.1358 1063.4194
1064.3657 1065.0677 1067.1218
1069.0613 1098.8378 1116.2010
1117.4380 1126.6729 1127.4636
1134.9471 1139.9379 1143.9214
1145.4257 1145.9443 1150.8849
1170.7120 1182.1027 1195.3614
1195.5101 1197.5098 1197.9421
1218.0546 1218.3675 1231.3362
1233.3869 1257.1093 1304.6518
1334.0868 1336.7498 1336.8829
1338.5856 1342.2315 1365.0798
1365.4513 1373.9779 1374.8534
1381.5926 1386.7227 1466.9813
1469.2673 1481.8583 1490.2489
1490.8133 1492.6514 1493.3635
1511.8184 1517.6454 1524.6317
1539.4210 1539.6264 1545.0683
1546.3814 1663.0403 1663.5321
1665.2661 1666.0531 1683.1373
1683.6485 1683.7277 1684.3646
2214.8312 3041.4979 3056.1290
3082.8183 3085.6584 3107.8193
3124.6733 3133.1941 3141.5523
3142.3206 3189.3661 3197.1875
3202.7763 3202.8069 3203.3359
3204.2089 3210.8993 3210.9499
3211.5266 3212.2984 3220.8491
3221.2783 3221.4178 3221.4769
3230.4324 3230.8014 3231.8335
3232.2083 3236.8648 3237.9726

Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -1973.339088 Hartrees

15



Gaussian 16: ES64L-G16RevB.01 20-Dec-2017

# wB97xd/6-31G(d,p) gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc
) opt=(maxcycle=250) freq=noraman

Full point group C1 NOp 1
Stoichiometry C30H29NOP2 Framework group
C1[X(C30H29NOP2)]

Num atoms: 63
Charge = 0 Multiplicity = 1

SCF = -1972.89864244 | Predicted change in Energy=-
6.063297D-09

Optimization completed.
Maximum Force 0.000015 0.000450 YES
RMS Force 0.000002 0.000300 YES
Maximum Displacement 0.001696 0.001800 YES
RMS Displacement 0.000223 0.001200 YES

Atom Coordinates (in Angstroms)
Type X Y Z

P 9.679063 1.254039 2.752001
C 9.350872 3.119181 2.513960
C 8.256168 3.450995 1.495645
C 8.694853 3.176944 0.048163
P 8.990157 1.408660 -0.261835
H 10.287281 3.597845 2.203141
H 9.093001 3.561186 3.481304
H 7.987754 4.511149 1.564808
H 7.343717 2.885889 1.725810
H 7.959689 3.548356 -0.671809
H 9.640426 3.685332 -0.166533
C 11.187350 0.981842 -4.274640
C 11.493091 0.133626 -3.214634
C 10.835680 0.264241 -1.994775
C 9.858513 1.252225 -1.846351
C 9.538624 2.093210 -2.916474
C 10.208304 1.961542 -4.127060
H 11.708937 0.877779 -5.220930
H 12.247972 -0.636552 -3.334097
H 11.047585 -0.412555 -1.169036
H 8.768123 2.852325 -2.813193
H 9.965443 2.620494 -4.954327
C 4.953841 -0.777495 -0.726125
C 4.953303 0.606596 -0.595382
C 6.157688 1.297962 -0.493497
C 7.369212 0.605200 -0.521361
C 7.366812 -0.790743 -0.652844
C 6.161047 -1.473268 -0.754884
H 4.014292 -1.315608 -0.802450
H 4.015795 1.152437 -0.567264
H 6.135578 2.376907 -0.379271
H 8.306854 -1.338992 -0.633981
H 6.165134 -2.554065 -0.850951
C 5.622144 0.489736 4.870258
C 5.956579 -0.189439 3.701246
C 7.195445 0.013978 3.105070
C 8.107630 0.920934 3.652683
C 7.758753 1.607166 4.818233
C 6.529154 1.381825 5.432291
H 4.658917 0.322638 5.342097
H 5.254897 -0.884916 3.251755
H 7.458650 -0.534494 2.206704
H 8.451775 2.315567 5.263207
H 6.279489 1.910764 6.346817
C 13.347616 1.808153 5.519095
C 13.381021 2.261388 4.203408
C 12.266814 2.111820 3.384413
C 11.111301 1.495794 3.868822
C 11.091398 1.022640 5.182793
C 12.201178 1.187874 6.006187
H 14.214854 1.931101 6.160094
H 14.277491 2.732362 3.812356
H 12.303870 2.452729 2.353669
H 10.209653 0.516188 5.563937
H 12.171288 0.823023 7.028164
C 9.861984 0.776450 1.061166
C 10.113664 -0.659269 1.328150
O 10.278706 -1.598856 0.536652
N 10.093920 -0.654543 2.675837
C 10.324583 -1.805417 3.499471
H 9.445168 -2.031060 4.118512
H 10.530050 -2.669363 2.858694
H 11.180449 -1.653054 4.170289

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -1972.89864244 | Predicted change in Energy=-
6.063297D-09
Zero-point correction (ZPE) = -1972.37897144 0.519671
Internal Energy (U) = -1972.34882244 0.54982
Enthalpy (H) = -1972.34787844 0.550764
Gibbs Free Energy (G) = -1972.44145044 0.457192

Frequencies
17.8745 26.6094 29.9507
41.3944 45.8159 51.5408
57.1988 57.8916 72.4824
79.9206 92.3805 105.4206
123.4411 142.1100 148.2064
173.6920 178.0184 183.8685
203.7920 213.6010 225.5542
244.6523 251.8397 256.0963
269.4924 279.8142 287.1141
300.2211 329.5029 342.2619
352.5829 393.8252 398.5745
407.9717 410.3461 412.0091
420.4383 444.9798 470.7760
504.9348 505.8658 513.1142
521.5861 542.9681 546.6208
583.5840 626.1008 634.4164
635.3793 637.7509 641.7859
704.6303 705.1391 715.6523
720.8497 722.1726 727.2732
735.6459 740.6528 753.1646
769.9989 772.2250 773.8409
780.4768 781.8231 813.8396
816.8368 871.9027 879.9930
882.8168 885.1492 886.7772
939.1674 949.8235 958.8703
960.8200 962.3766 990.4606
997.3454 1003.6667 1008.1614
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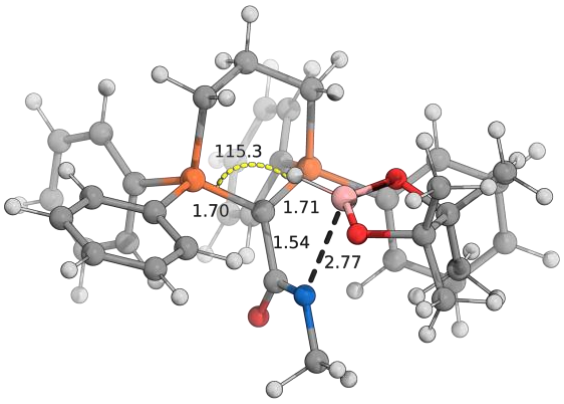
1019.5991 1021.3944 1022.1900
1024.2745 1024.6779 1027.5908
1037.8509 1044.3822 1067.1800
1067.3206 1068.5202 1068.7791
1077.2061 1117.8248 1120.2041
1126.8703 1130.0907 1131.9474
1145.5960 1150.5131 1155.2342
1156.4423 1157.7267 1191.4668
1195.7458 1196.4529 1199.8939
1200.6242 1207.0665 1224.5385
1227.5161 1235.2393 1239.0584
1271.6227 1285.3255 1315.1354
1332.4797 1336.9113 1338.5326
1341.4224 1347.5911 1369.7318
1372.1037 1383.5923 1385.0749
1391.4494 1437.7429 1452.3009
1471.3002 1487.5699 1489.3220
1492.1680 1493.5771 1495.1313
1508.4644 1518.1277 1529.2471
1543.0204 1543.6956 1547.6334
1548.7653 1663.0973 1663.1603
1665.0398 1665.6821 1684.0855
1684.4262 1685.0352 1685.6355
1762.2298 3014.1694 3057.5548
3072.7445 3073.2398 3087.9080
3105.2209 3123.9897 3133.2769
3145.0561 3187.4685 3189.6968
3201.4980 3202.4763 3203.3756
3207.8907 3209.3097 3212.0669
3212.3809 3216.2338 3219.6924
3221.1728 3224.1259 3226.1116
3229.7148 3230.5315 3233.8988
3235.3588 3237.2465 3238.8825

Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -1973.393898 Hartrees

$TS_{15\text{-}16}$



Gaussian 16: ES64L-G16RevB.01 20-Dec-2017
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wB97XD/6-31G(d,p) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
---
Full point group C1 NOp 1
Stoichiometry C36H42BNO3P2 Framework group C1[X(C36H42BNO3P2)]

Num atoms: 85
Charge = 0 Multiplicity = 1

SCF = -2384.66606729 | Predicted change in Energy=-8.145623D-10

Optimization completed.
Maximum Force 0.000005 0.000450 YES
RMS Force 0.000001 0.000300 YES
Maximum Displacement 0.000385 0.001800 YES
RMS Displacement 0.000082 0.001200 YES

Atom Coordinates (in Angstroms)
Type X Y Z

P 1.495899 1.264470 -0.535598
C 1.337673 1.151112 -2.358472
C 1.343517 -0.279193 -2.917607
C 0.214432 -1.170951 -2.370680
P 0.367107 -1.387243 -0.565651

H	2.120134	1.754250	-2.828403
H	0.381573	1.639374	-2.573526
H	2.311636	-0.754487	-2.719949
H	1.239980	-0.221277	-4.005697
H	-0.769104	-0.714479	-2.527212
H	0.226554	-2.139143	-2.878778
C	4.204128	-3.815597	0.255746
C	3.568261	-3.978237	-0.972079
C	2.403229	-3.270359	-1.249333
C	1.878192	-2.388878	-0.301191
C	2.514201	-2.232232	0.934547
C	3.673558	-2.949502	1.207643
H	5.115343	-4.365614	0.469397
H	3.978827	-4.655711	-1.714016
H	1.913456	-3.411448	-2.208523
H	2.092380	-1.539650	1.665714
H	4.169483	-2.820732	2.164157
C	-2.768572	-4.337490	1.011687
C	-1.965650	-3.623704	1.897916
C	-1.055905	-2.685634	1.424754
C	-0.958262	-2.455117	0.047670
C	-1.779098	-3.152806	-0.839125
C	-2.680339	-4.096544	-0.355888
H	-3.471512	-5.073873	1.387915
H	-2.045850	-3.795715	2.965964
H	-0.434245	-2.125928	2.120348
H	-1.733157	-2.961663	-1.905602
H	-3.316011	-4.637917	-1.049080
C	0.757261	5.716955	0.314716
C	-0.231369	4.791250	0.628537
C	-0.025119	3.431662	0.408674
C	1.192654	3.004407	-0.126762
C	2.194616	3.935180	-0.430187
C	1.973300	5.288673	-0.214592
H	0.586422	6.774978	0.488279
H	-1.175392	5.119828	1.050165
H	-0.783756	2.700835	0.681278
H	3.152694	3.603685	-0.820672
H	2.751413	6.007367	-0.450325
C	5.867761	0.497507	0.718447
C	4.840731	0.585929	1.656437
C	3.536233	0.826225	1.245660
C	3.256814	1.000187	-0.115842
C	4.286642	0.909522	-1.052838
C	5.590639	0.653810	-0.635066
H	6.884343	0.298971	1.043169
H	5.054100	0.451902	2.711992
H	2.719174	0.827236	1.967569
H	4.085742	1.031512	-2.113077
H	6.387084	0.576528	-1.368210
C	0.406691	0.156881	0.164444
C	-0.119957	0.312296	1.599238
O	0.607933	-0.089917	2.553812
N	-1.317943	0.838889	1.642063
C	-1.833665	1.006527	2.987746
H	-1.989971	0.043813	3.499902
H	-1.154162	1.584557	3.630236
H	-2.795781	1.529662	2.938909
B	-2.606804	1.257310	-0.779548
C	-4.827223	1.310681	-0.343144
C	-4.335791	-0.176905	-0.487846
H	-1.576264	1.686519	-1.182219
O	-3.598622	2.052987	-0.269895
O	-3.029592	-0.014619	-1.084330
C	-5.641068	1.591873	0.912773
H	-5.920513	2.648567	0.937107
H	-6.558609	0.994418	0.924033
H	-5.064264	1.370718	1.811901
C	-5.576016	1.821848	-1.576793
H	-5.716745	2.901434	-1.481249
H	-5.001228	1.635853	-2.488423
H	-6.557931	1.350494	-1.679349
C	-4.156200	-0.877487	0.855471
H	-5.114971	-1.002548	1.367283
H	-3.730862	-1.865716	0.685002
H	-3.464419	-0.320411	1.488133
C	-5.178727	-1.043110	-1.415150
H	-4.744417	-2.045747	-1.461172
H	-6.201373	-1.132830	-1.034603
H	-5.216023	-0.638918	-2.428470

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -2384.66606729 | Predicted change in Energy=-8.145623D-10
Zero-point correction (ZPE) = -2383.9520772899996 0.71399
Internal Energy (U) = -2383.9118272899996 0.75424
Enthalpy (H) = -2383.9108832899997 0.755184
Gibbs Free Energy (G) = -2384.0245592899996 0.641508

Frequencies
-55.5898 21.8775 25.0956
33.2439 34.9959 38.5565
44.9354 50.3309 50.7754
57.9670 70.7357 79.1962
88.5709 91.1029 94.9923
100.1825 101.2705 110.4594
120.4968 125.6420 137.6031
149.4557 153.0467 174.9265
188.7435 207.1032 220.0712
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253.3788 260.3056 265.4813
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286.9783 291.0521 308.7590
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532.4128 579.8719 591.4584
596.6081 632.5872 633.8046
634.3447 635.7365 679.3151
688.3131 696.4397 715.7957
718.5173 721.0715 728.1622
733.3195 736.8561 742.3304
751.1362 754.6729 769.2950
771.9289 776.2169 779.4969
783.9639 831.1620 839.5591
839.9982 870.5808 883.0709
885.2130 887.8383 890.8979
894.0352 896.9980 941.1400
945.7551 954.4762 958.8150
961.7877 966.1364 973.9261
976.1579 996.7140 1009.9539
1012.2597 1013.1299 1015.1000
1018.1911 1018.7903 1019.7854
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1057.6622 1060.6282 1066.7440
1067.3778 1069.2049 1069.4685
1073.4498 1074.7025 1088.1186
1096.5184 1122.7545 1125.2114
1126.9917 1129.9353 1131.1472
1135.1491 1136.2012 1148.6585
1149.4332 1151.1850 1159.2129
1161.6565 1177.0603 1198.7385

1199.9338 1200.2708 1200.4545
1201.2705 1203.3675 1206.3375
1211.4166 1238.5828 1239.8164
1242.3115 1243.9441 1262.7998
1271.1584 1287.6294 1319.6108
1321.4277 1337.5748 1339.8918
1344.5757 1345.3815 1356.3156
1375.4305 1380.1814 1387.8605
1388.6810 1390.3481 1393.3603
1401.6185 1419.3661 1420.6886
1430.6652 1440.1159 1445.4878
1474.5309 1485.9652 1490.3793
1492.5641 1493.1733 1494.5015
1495.8124 1497.2080 1499.9524
1501.7021 1504.6203 1506.5710
1519.7009 1521.7508 1523.5044
1532.8976 1545.6527 1546.8870
1550.0514 1551.0702 1552.0956
1662.0434 1663.3129 1664.8333
1665.1750 1684.1379 1684.5212
1685.1916 1685.3147 1692.4248
2729.4268 2992.8300 3049.8661
3065.7347 3068.6414 3070.9482
3071.1519 3086.7112 3089.3134
3090.0138 3096.6636 3120.6840
3141.8862 3147.3637 3147.5286
3147.6750 3150.3081 3154.7363
3159.1129 3168.8630 3171.2386
3172.6042 3179.7341 3187.1244
3197.1622 3204.3064 3205.2942
3206.1206 3211.5077 3213.4050
3213.6374 3214.8638 3219.5376
3223.3869 3224.5456 3225.4409
3228.1436 3234.1187 3234.6933
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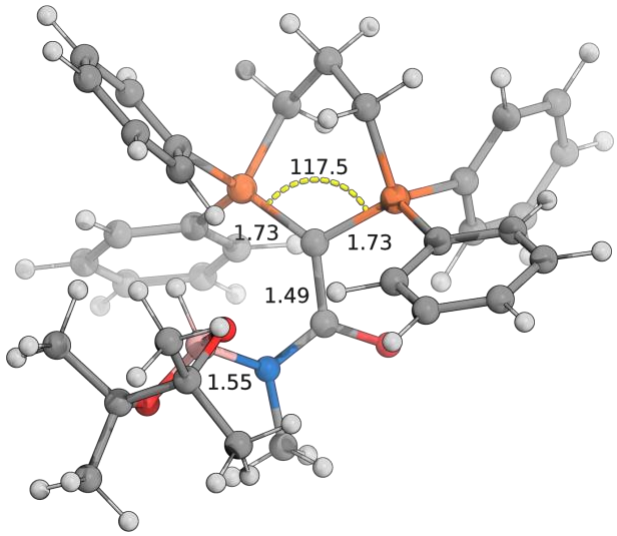
Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -2385.299922 Hartrees

16



Gaussian 16: ES64L-G16RevB.01 20-Dec-2017

# wB97xd/6-31G(d,p) gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc
) opt=(maxcycle=250) freq=noraman

Full point group C1 NOp 1
Stoichiometry C36H42BNO3P2 Framework group
C1[X(C36H42BNO3P2)]

Num atoms: 85
Charge = 0 Multiplicity = 1

SCF = -2384.70746730 | Predicted change in Energy=-
1.599803D-08

Optimization completed.
Maximum Force 0.000016 0.000450 YES
RMS Force 0.000002 0.000300 YES
Maximum Displacement 0.001604 0.001800 YES
RMS Displacement 0.000303 0.001200 YES

Atom Coordinates (in Angstroms)

Type	X	Y	Z
P	0.281916	3.928689	-0.569596
C	-1.146335	2.911555	-1.104485
C	-2.352555	2.951677	-0.143822
C	-2.003674	3.190252	1.337130
P	-0.418940	2.400197	1.858311
H	-0.739143	1.897514	-1.169179
H	-1.440269	3.188885	-2.119772
H	-2.886590	2.002114	-0.238829
H	-3.041895	3.741311	-0.456178
H	-1.887137	4.259937	1.537032
H	-2.813066	2.830569	1.977492
C	-1.532741	-1.977733	0.948026
C	-0.383086	-1.422004	0.393285
C	-0.009915	-0.117626	0.700728
C	-0.801206	0.639242	1.567136
C	-1.957960	0.082284	2.122431
C	-2.317028	-1.227147	1.819191
H	-1.814504	-2.998146	0.708301
H	0.240234	-2.009906	-0.273122
H	0.928348	0.290931	0.329664
H	-2.574372	0.657736	2.807973
H	-3.208501	-1.658579	2.262732
C	-0.155423	3.432135	6.321222

C	-0.217092	2.094784	5.939098
C	-0.286489	1.755694	4.593155
C	-0.306005	2.761694	3.628155
C	-0.228319	4.102759	4.009109
C	-0.154838	4.435518	5.356620
H	-0.091552	3.692268	7.372922
H	-0.192734	1.311752	6.689476
H	-0.290497	0.713953	4.290284
H	-0.194352	4.882209	3.252734
H	-0.084044	5.477119	5.651636
C	-1.360213	8.244171	-0.485515
C	-1.883113	7.326700	-1.391688
C	-1.378637	6.030999	-1.436503
C	-0.340751	5.646510	-0.579093
C	0.186939	6.575158	0.324767
C	-0.327398	7.866599	0.368219
H	-1.756311	9.254040	-0.447731
H	-2.685773	7.616321	-2.062075
H	-1.800613	5.328122	-2.148111
H	1.017831	6.266724	0.953605
H	0.088117	8.583664	1.068747
C	3.364199	3.281348	-3.900325
C	3.362383	2.462715	-2.774303
C	2.451045	2.676260	-1.745669
C	1.532766	3.725084	-1.859688
C	1.536923	4.554531	-2.982513
C	2.453256	4.328859	-4.003718
H	4.082539	3.108989	-4.695729
H	4.081160	1.654106	-2.686033
H	2.482127	2.043773	-0.857432
H	0.840745	5.384776	-3.055330
H	2.461409	4.976882	-4.874049
C	0.777089	3.230610	0.930698
C	2.123820	3.692370	1.355445
O	2.497974	4.791455	0.888188
N	2.877863	2.934599	2.157640
C	4.159500	3.509704	2.533241
H	4.019263	4.494657	2.987559
H	4.634512	2.833423	3.243027
H	4.812533	3.644151	1.662017
B	2.659167	1.398332	2.201125
C	3.985873	-0.464436	2.498570
C	3.968694	-0.128786	0.967158
H	1.481664	1.196281	2.530605
O	3.612527	0.763618	3.086491
O	2.879538	0.766750	0.865747
C	5.350669	-0.878634	3.039852
H	5.270129	-1.107676	4.106468
H	5.725130	-1.770799	2.525702
H	6.078336	-0.073207	2.922984
C	2.942145	-1.530711	2.867286
H	2.844481	-1.553828	3.956247
H	1.964011	-1.282296	2.445064
H	3.231005	-2.529269	2.522793
C	5.245713	0.593577	0.518516
H	5.078216	1.020955	-0.475047
H	5.483187	1.413676	1.199851
H	6.107244	-0.080343	0.464589
C	3.712847	-1.325974	0.054661
H	3.709463	-0.999444	-0.990796
H	4.490859	-2.088651	0.169412
H	2.743881	-1.782174	0.270711

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -2384.70746730 | Predicted change in Energy=-1.599803D-08
Zero-point correction (ZPE) = -2383.9922923000004 0.715175
Internal Energy (U) = -2383.9520083 0.755459
Enthalpy (H) = -2383.9510643000003 0.756403
Gibbs Free Energy (G) = -2384.0649553000003 0.642512

Frequencies

20.4439 21.4584 32.8909
35.5118 39.0261 43.2862
47.8239 52.7519 61.6232
65.4787 70.1366 76.3855
81.3099 89.2525 96.8857
106.5324 120.9118 130.4216
145.3267 149.7084 163.9932
171.0719 185.7753 202.9112
208.0323 219.9133 225.9207
228.5933 234.3750 246.1685
252.0526 258.4960 265.2472
271.2972 275.1512 284.8775
294.3268 305.7428 313.9100
324.6055 332.9651 338.8799
353.2829 359.4034 368.5341
381.4463 384.1845 408.7971
412.5932 417.4670 418.1084
425.8522 428.8638 465.7911
470.2567 474.2603 489.9895
496.3056 501.9871 505.6301
516.6217 530.2814 536.3133
559.8246 587.8943 588.3182
632.5261 634.3723 636.4539
637.3231 676.0545 684.4254
702.1922 710.9352 714.4509
716.6816 719.4956 722.2330
723.9896 736.4790 742.7771
747.4204 754.0127 764.4041
773.8502 775.1622 779.3898
783.1852 790.8993 857.2431
875.0333 879.7423 886.7258
889.4071 891.9489 893.4805
907.1597 932.8507 939.7926
942.8525 943.9019 955.9064
964.3635 968.4467 974.0486
988.1861 989.2415 1002.8036
1009.0840 1012.2370 1017.8219
1018.4774 1019.3184 1019.8773
1021.5753 1022.8231 1024.4045
1026.3657 1027.8406 1041.9807
1050.7830 1054.8414 1067.1932
1067.5271 1068.6187 1070.2904
1072.5098 1082.0248 1097.3979
1114.6554 1122.8645 1126.7915
1128.5983 1128.9734 1134.3807
1146.7064 1147.8813 1152.2790
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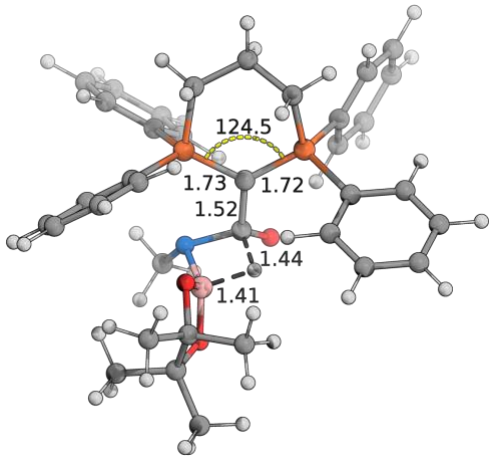
1177.0277 1181.8809 1194.2280
1199.3534 1199.9195 1199.9627
1200.3510 1220.3577 1227.7191
1230.6289 1236.1004 1236.9169
1240.5104 1241.4657 1269.6378
1274.1610 1277.5398 1283.5981
1302.6946 1318.5146 1339.4965
1339.7216 1340.6322 1345.9813
1354.2625 1373.4876 1378.8165
1382.6933 1384.3802 1385.9700
1409.8064 1410.6452 1421.8124
1430.1800 1444.6565 1471.8999
1481.1542 1487.9731 1489.2615
1491.7212 1492.7494 1494.5777
1496.1355 1497.3942 1498.7884
1501.8952 1506.9213 1511.3926
1518.6178 1520.0307 1523.8525
1525.7273 1541.0911 1543.7706
1544.9264 1547.6278 1548.7515

1660.8110 1663.7990 1666.4648
1669.4037 1682.0589 1682.3281
1682.7808 1685.6144 1689.8777
2322.0153 3046.4684 3054.7597
3057.6935 3060.9436 3064.1317
3088.2149 3096.0305 3098.8344
3116.2037 3129.0468 3137.1501
3137.4141 3138.9010 3143.7163
3152.5755 3154.5767 3156.8227
3158.7959 3158.9272 3166.1117

3168.4971 3190.3820 3190.6892
3202.1771 3204.2921 3207.2408
3207.7498 3212.7711 3212.9427
3214.1829 3214.4671 3219.4306
3223.9266 3224.5017 3225.4543
3228.8168 3233.7094 3234.9264
3235.0760 3237.2341 3241.0651

Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -2385.337170 Hartrees

TS(16-17)



Gaussian 16: ES64L-G16RevB.01 20-Dec-2017

# wB97xd/6-31G(d,p) gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc
) opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman

Full point group C1 NOp 1
Stoichiometry C36H42BNO3P2 Framework group
C1[X(C36H42BNO3P2)]

Num atoms: 85
Charge = 0 Multiplicity = 1

SCF = -2384.64185470 | Predicted change in Energy=-
5.459165D-09

Optimization completed.
Maximum Force 0.000013 0.000450 YES
RMS Force 0.000002 0.000300 YES
Maximum Displacement 0.000656 0.001800 YES
RMS Displacement 0.000144 0.001200 YES

Atom Coordinates (in Angstroms)
Type X Y Z

P 2.041862 0.882558 0.709963
C 2.297611 0.441490 2.461199
C 2.374931 -1.081172 2.622245
C 0.996572 -1.725036 2.477577
P 0.122967 -1.480439 0.854675
H 1.449317 0.853012 3.017628
H 3.192400 0.943495 2.834128
H 2.766802 -1.318319 3.616629
H 3.081656 -1.503956 1.898799
H 1.062388 -2.805862 2.630528
H 0.344980 -1.341463 3.266615
C -4.263937 -1.993767 2.193902
C -3.793128 -2.684261 1.079920
C -2.474667 -2.532387 0.671064
C -1.609783 -1.701855 1.384441
C -2.092124 -0.998543 2.486861
C -3.413156 -1.144529 2.892046
H -5.296931 -2.106708 2.507593
H -4.458217 -3.332202 0.518254
H -2.121421 -3.040529 -0.219137
H -1.455941 -0.292530 3.011971
H -3.781592 -0.581243 3.743138
C 1.570415 -5.214035 -1.433714
C 0.777640 -5.370598 -0.298921
C 0.310395 -4.251750 0.380368
C 0.630178 -2.968054 -0.073382
C 1.421429 -2.815156 -1.212988
C 1.888515 -3.938817 -1.888669
H 1.934492 -6.087846 -1.964877
H 0.521660 -6.363796 0.055852
H -0.315218 -4.381206 1.259721
H 1.640226 -1.819282 -1.588006
H 2.496592 -3.812221 -2.778285
C 6.113622 0.180518 -1.370512
C 4.930942 0.184368 -2.103194
C 3.708261 0.395463 -1.473620
C 3.666145 0.605893 -0.090161
C 4.859998 0.606860 0.642739
C 6.077085 0.393667 0.004165
H 7.063924 0.012924 -1.867821
H 4.954643 0.022888 -3.176073
H 2.769828 0.405800 -2.031023
H 4.862250 0.773319 1.714453
H 6.995080 0.393481 0.582987
C 1.141831 5.381255 0.668698
C 2.448309 4.950049 0.456265
C 2.736510 3.589942 0.437872
C 1.713053 2.661573 0.640021
C 0.398695 3.093278 0.845232
C 0.119969 4.455179 0.859602
H 0.917351 6.443218 0.674416

H 3.241998 5.671894 0.294226
H 3.751565 3.252650 0.252725
H -0.399509 2.363506 0.960587
H -0.901693 4.790145 1.004024
C 0.680888 -0.003197 0.155693
C 0.112378 0.220575 -1.234560
O 0.853048 0.467172 -2.218257
N -1.057591 -0.675923 -1.310630
C -1.229286 -1.391933 -2.567665
H -2.266219 -1.312247 -2.902631
H -0.581726 -0.964303 -3.341217
H -0.974776 -2.453345 -2.451315
B -1.889048 0.572723 -1.109764
C -3.651909 1.688110 -0.167807
C -3.958272 1.387136 -1.673395
O -2.609234 0.765282 0.113588
O -2.676987 1.058783 -2.192535
C -4.813642 1.425713 0.783454
H -4.511852 1.661961 1.808537
H -5.677525 2.048821 0.527328
H -5.109431 0.375896 0.758265
C -3.124693 3.112838 0.043026
H -2.753821 3.195565 1.070160
H -2.299556 3.325249 -0.642925
H -3.906000 3.865620 -0.100563
C -4.859984 0.156487 -1.837845
H -4.848925 -0.143994 -2.889185
H -4.480169 -0.676028 -1.237321
H -5.895416 0.359363 -1.545200
C -4.529989 2.562119 -2.457977
H -4.723640 2.256277 -3.489914
H -5.473858 2.905327 -2.020043
H -3.826561 3.396442 -2.482517
H -0.729973 1.363650 -1.011531

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -2384.64185470 | Predicted change in Energy=-5.459165D-09
Zero-point correction (ZPE) = -2383.9290766999998 0.712778
Internal Energy (U) = -2383.8892907 0.752564
Enthalpy (H) = -2383.8883467 0.753508
Gibbs Free Energy (G) = -2384.0011446999997 0.64071

Frequencies
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31.0384 33.5789 40.0490
50.9138 53.0461 58.6575
64.2260 66.8419 71.0502
75.3992 84.2410 94.4529
98.9797 105.1329 108.2095
112.4111 142.3086 153.1184
162.9432 192.4444 202.1110
207.9767 218.1223 224.3729
232.2666 237.1769 237.9458
247.8180 265.6432 269.8567
274.2006 278.1548 281.7924
294.8094 307.0917 312.1647
324.5442 337.5303 340.3882
357.5716 362.4819 381.6869
383.1466 393.4219 406.8778
409.4720 410.4787 422.1275
422.3402 426.2630 442.0148
450.0418 466.2593 475.2457
491.3224 499.3134 501.0593
514.7412 524.3062 532.8493
546.9915 567.6957 586.3398
596.9853 633.7963 633.9021
636.1114 637.3388 663.9352
685.9940 699.1814 708.0596
714.1146 718.4842 720.7139
724.4709 733.6311 736.6329
741.7651 750.7118 763.4934
774.5503 774.7607 780.7883
784.8237 813.5938 866.0456
874.4900 876.2800 887.4152
888.9983 891.1291 891.4481
906.5405 922.8951 942.7329
946.1768 948.3520 952.2928
966.8499 972.1123 972.6756
992.3399 996.5975 1005.7205
1010.1387 1014.2607 1016.5561
1018.2424 1019.7064 1020.8133
1021.0521 1021.5285 1022.7690
1024.5774 1034.5811 1040.8581
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1069.8522 1070.5664 1077.7975
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1198.9816 1199.3696 1200.9701
1202.4008 1205.3229 1224.3599
1229.8701 1231.6942 1236.7989
1241.9135 1253.2021 1273.5329
1274.8901 1279.3204 1291.1372
1298.0006 1321.7704 1329.5227
1337.8484 1339.2907 1342.3934
1345.5784 1349.7166 1373.1785
1373.8171 1382.8445 1388.5409
1390.1280 1412.5102 1414.3584
1425.4163 1433.7582 1443.7224
1472.2971 1489.2004 1489.2902
1491.7082 1493.5471 1494.3706
1496.4015 1496.7840 1502.4361
1506.4327 1509.5058 1519.6217
1521.5902 1524.7606 1528.3995
1531.2210 1542.1118 1545.1212
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1593.4842 1660.7899 1665.5484
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3204.0285 3204.6129 3209.3606
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3218.9506 3220.9547 3221.9410
3223.1357 3227.5102 3230.8660
3232.3142 3233.3778 3236.6035
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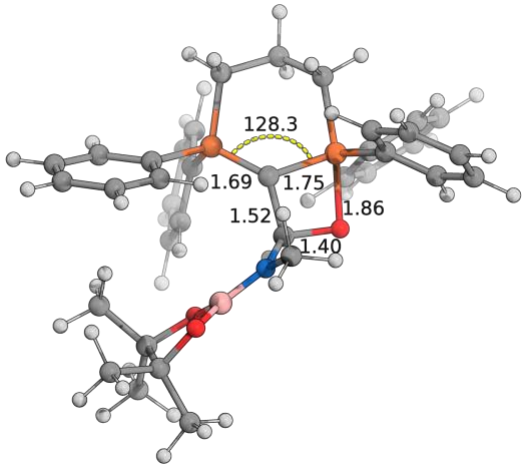
Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -2385.271911 Hartrees

17



Gaussian 16: ES64L-G16RevB.01 20-Dec-2017

# wB97xd/6-31G(d,p) gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc
) opt=(maxcycle=250) freq=noraman

Full point group C1 NOp 1
Stoichiometry C36H42BNO3P2 Framework group
C1[X(C36H42BNO3P2)]

Num atoms: 85
Charge = 0 Multiplicity = 1

SCF = -2384.71519336 | Predicted change in Energy=-
1.746411D-08

Optimization completed.
Maximum Force 0.000029 0.000450 YES
RMS Force 0.000003 0.000300 YES
Maximum Displacement 0.000795 0.001800 YES
RMS Displacement 0.000159 0.001200 YES

Atom Coordinates (in Angstroms)
Type X Y Z

P 9.177647 3.278714 -6.597116
C 8.840298 4.833241 -7.663567
C 8.180840 4.550416 -9.017334
C 9.148699 3.892680 -10.014124
P 9.679667 2.237329 -9.471999
H 9.782969 5.364370 -7.839310
H 8.208910 5.518559 -7.089327
H 7.827351 5.485683 -9.466588
H 7.293514 3.919956 -8.877064
H 8.721717 3.809936 -11.018616
H 10.062386 4.489216 -10.104283
C 13.488896 1.232690 -11.856553
C 12.243913 1.048349 -12.455881
C 11.082002 1.320092 -11.742604
C 11.163763 1.790144 -10.428957
C 12.411964 1.969028 -9.829794
C 13.573055 1.686608 -10.543307
H 14.394263 1.010659 -12.412627
H 12.179603 0.683657 -13.475838
H 10.111632 1.153785 -12.202023
H 12.457594 2.311960 -8.801012
H 14.539924 1.810109 -10.067170
C 6.443910 -0.878012 -10.536196
C 7.671540 -1.269089 -10.007048
C 8.654106 -0.322458 -9.742569
C 8.413993 1.032388 -10.007744
C 7.178504 1.418975 -10.532949
C 6.199232 0.465838 -10.798464
H 5.677390 -1.619118 -10.739178
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H 9.598289 -0.641278 -9.307686
H 6.962332 2.463709 -10.730792
H 5.243080 0.777175 -11.206418
C 4.656980 2.592977 -5.809877
C 5.268715 3.737533 -5.308878
C 6.629661 3.949151 -5.514734
C 7.400113 3.007914 -6.200118
C 6.779230 1.853817 -6.685224
C 5.415652 1.653317 -6.503338
H 3.593903 2.432628 -5.658983
H 4.686156 4.472100 -4.761272
H 7.093995 4.851312 -5.125666
H 7.367647 1.109149 -7.212393
H 4.947900 0.756864 -6.898587
C 11.403736 5.530542 -3.204951
C 11.829208 5.662512 -4.522323
C 11.144065 5.012121 -5.545051
C 10.036992 4.211104 -5.263296
C 9.635991 4.058282 -3.933013
C 10.304857 4.725897 -2.913467
H 11.931693 6.043363 -2.406975
H 12.696001 6.272723 -4.757112
H 11.496840 5.111293 -6.567481
H 8.806907 3.399654 -3.695517
H 9.976182 4.605388 -1.885778
C 9.960179 2.280160 -7.803621
C 10.176303 1.107812 -6.864518
H 9.620676 0.197254 -7.137818
O 9.648597 1.709931 -5.721849
N 11.567471 0.686618 -6.706686
B 12.051812 -0.456337 -7.351350
C 12.099057 -2.298774 -8.695688
C 13.453006 -2.150200 -7.910829
O 11.238393 -1.382415 -8.002361
O 13.391224 -0.802237 -7.428237
C 13.536426 -3.068706 -6.689282
H 14.400144 -2.774623 -6.087942
H 12.643083 -2.973145 -6.065809
H 13.653120 -4.117707 -6.976488
C 14.701895 -2.302228 -8.768975
H 15.591753 -2.183251 -8.145265

H 14.738253 -3.294238 -9.230690
H 14.733932 -1.545426 -9.554947
C 11.477004 -3.687799 -8.637739
H 10.543369 -3.695065 -9.207631
H 12.148734 -4.431250 -9.078780
H 11.249708 -3.982133 -7.612165
C 12.199012 -1.832878 -10.148604
H 11.197753 -1.795210 -10.586510
H 12.631287 -0.832448 -10.209729
H 12.807434 -2.515526 -10.748900
C 12.447467 1.622974 -6.035567
H 12.531145 2.567872 -6.591322
H 12.054218 1.863483 -5.044876
H 13.441112 1.182605 -5.942132

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -2384.71519336 | Predicted change in Energy=-1.746411D-08
Zero-point correction (ZPE) = -2383.99715936 0.718034
Internal Energy (U) = -2383.95739436 0.757799
Enthalpy (H) = -2383.9564493599996 0.758744
Gibbs Free Energy (G) = -2384.06871336 0.64648

Frequencies
20.5991 26.4849 29.2897
37.4103 42.9990 47.5159
54.2845 55.0988 62.1093
68.1611 73.2029 76.6742
82.1544 90.4241 98.7454
105.7364 120.8182 134.9545
143.4196 154.0723 183.4379
196.6405 206.5559 212.2755
219.3627 222.2255 237.8825
241.4300 242.9350 257.3715
260.1109 262.9326 275.1338
276.1312 286.5155 292.4533
298.7176 311.0852 325.7390
330.2402 340.8587 352.4720
361.6588 379.2516 383.4084
396.5773 405.5347 410.5846
413.2728 415.7082 418.8431
420.1537 446.0411 456.1090
463.1099 483.7554 495.8221
502.8290 515.7949 527.5243
529.1792 536.9687 541.7910
573.8348 591.2865 597.2569
619.8952 635.4789 635.6355
638.8412 640.3722 661.3016
676.7507 690.3903 706.9240
715.5047 715.7782 719.2835
724.6553 727.7902 733.0907
741.3641 750.3644 769.7543
770.8947 774.0611 780.8132
804.5537 831.0669 858.0846
868.2087 876.2035 881.6053
882.6814 890.2218 892.6128
912.6709 938.9737 945.8092
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962.4165 965.2103 989.0236
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1023.5747 1024.2176 1024.5067
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1066.0252 1067.5592 1068.2488
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1127.4510 1136.1842 1146.8983
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1160.9188 1164.9521 1186.4010
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1286.1691 1307.9469 1318.3092
1326.5678 1333.5034 1335.3836
1339.2944 1341.6162 1343.9784
1352.4915 1370.8122 1371.3074
1372.8127 1381.2169 1385.6184
1421.7318 1422.6071 1432.0682
1432.9484 1441.8633 1465.2021
1473.2245 1482.4175 1489.1963
1489.8302 1490.4749 1493.1463
1493.9733 1498.2730 1498.8903
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1532.3959 1541.0352 1543.9494
1544.9372 1546.5937 1548.5477
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1665.3490 1666.2751 1682.4605
1684.2323 1685.1527 1685.6179
3013.5176 3028.3722 3054.1338
3066.4673 3068.7155 3070.8775
3073.5726 3076.5969 3083.9439
3101.6234 3122.9818 3131.3453
3140.3920 3144.2054 3149.1755
3154.3084 3156.7408 3160.6688
3171.8323 3177.9493 3178.2778
3185.8682 3198.2717 3199.7038
3205.2329 3205.6405 3207.0246
3207.7021 3211.5120 3214.8764
3215.2499 3216.7915 3219.3416
3224.7549 3226.4072 3226.8506
3228.1198 3232.2706 3233.6206
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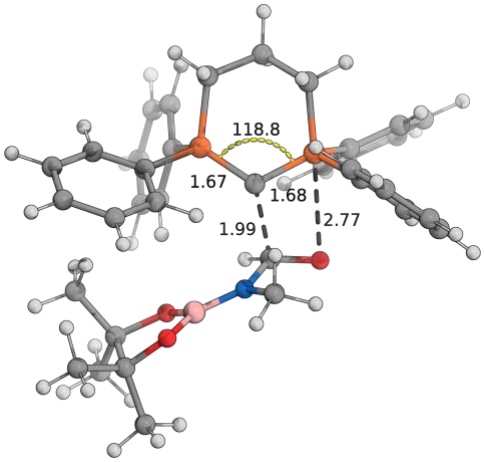
Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -2385.347700 Hartrees

TS(17-11)



Gaussian 16: EM64L-G16RevC.01 3-Jul-2019

# wB97xd/6-31G(d,p) gfprint gfinput
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) opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman

Full point group C1 NOp 1
Stoichiometry C36H42BNO3P2 Framework group
C1[X(C36H42BNO3P2)]

Num atoms: 85
Charge = 0 Multiplicity = 1

SCF = -2384.68213344 | Predicted change in Energy=-
4.878327D-09

Optimization completed.
Maximum Force 0.000084 0.000450 YES
RMS Force 0.000005 0.000300 YES
Maximum Displacement 0.001135 0.001800 YES
RMS Displacement 0.000191 0.001200 YES

Atom Coordinates (in Angstroms)
Type X Y Z

P -2.491136 -0.250538 0.476479
C -3.189844 0.458279 2.033120
C -2.609793 1.840008 2.361092
C -1.114246 1.773211 2.700350
P -0.110381 1.178954 1.274695
H -2.985543 -0.233682 2.855739
H -4.276239 0.515671 1.918757
H -3.150452 2.259650 3.215912
H -2.781174 2.518425 1.516095
H -0.732518 2.736768 3.051069
H -0.944062 1.052353 3.507177
C 3.810997 -0.180845 3.275532
C 3.525190 1.181857 3.192018
C 2.363578 1.609906 2.559952
C 1.472939 0.673997 2.025967
C 1.760272 -0.687385 2.114230
C 2.934205 -1.113697 2.729938
H 4.725692 -0.512510 3.757183
H 4.215454 1.909033 3.607359
H 2.156176 2.672845 2.468039
H 1.063915 -1.396484 1.678047
H 3.166090 -2.172669 2.767278
C 0.922197 4.824744 -1.383120
C 1.493968 3.574952 -1.611819
C 1.199025 2.505936 -0.774674
C 0.328000 2.676109 0.308950
C -0.245817 3.930317 0.528363
C 0.051487 4.999885 -0.313384
H 1.151651 5.658202 -2.039535
H 2.168731 3.426471 -2.449155
H 1.644103 1.534951 -0.976077
H -0.935200 4.089446 1.351459
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C -4.870035 0.516768 -0.850387
C -3.478696 0.628175 -0.788314
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H -5.497890 2.762228 -3.315578
H -6.674877 1.183901 -1.807176
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C -3.065158 -1.981713 0.508676
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H -4.145103 -5.702240 0.662653
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H -2.287167 -2.306075 2.495646
H -3.812182 -2.011523 -1.504151
H -4.550020 -4.370327 -1.390195
C -0.820816 -0.051907 0.393391
C -0.285538 -0.857521 -1.343205
H 0.171530 0.050921 -1.768426
O -1.355261 -1.312348 -1.817275
N 0.755815 -1.777273 -0.966722
B 2.118849 -1.465946 -1.087423
C 4.034299 -0.302128 -1.525040
C 4.355973 -1.814478 -1.230063
O 2.607485 -0.313413 -1.691729
O 3.138231 -2.291794 -0.644130
C 4.596806 -2.633254 -2.500798
H 4.624309 -3.692887 -2.234956
H 3.786232 -2.487684 -3.220330
H 5.543603 -2.370138 -2.981251
C 5.490688 -2.038513 -0.239023
H 5.637839 -3.111410 -0.088851
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C 4.663024 0.244884 -2.800538
H 4.379525 1.293633 -2.926231
H 5.755227 0.192751 -2.746499
H 4.326652 -0.303967 -3.681249
C 4.362394 0.618818 -0.350692
H 3.969833 1.618889 -0.553158
H 3.904048 0.256575 0.570017
H 5.442188 0.701114 -0.196347
C 0.296691 -3.048389 -0.443752
H -0.493218 -3.440672 -1.088145
H 1.130227 -3.750343 -0.394025
H -0.131017 -2.925811 0.561282

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -2384.68213344 | Predicted change in Energy=-4.878327D-09
Zero-point correction (ZPE) = -2383.96646444 0.715669
Internal Energy (U) = -2383.92640244 0.755731
Enthalpy (H) = -2383.92545844 0.756675
Gibbs Free Energy (G) = -2384.0386114400003 0.643522

Frequencies
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255.0154 259.4649 265.9621
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419.5721 423.5816 434.8414
453.8585 457.7078 472.9439
482.5452 493.6383 503.9410
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534.6292 540.9201 576.2057
593.4559 635.2411 635.5236
635.8112 636.7248 652.8413
664.5126 682.5391 696.0049
709.6841 716.3335 718.1794
725.5464 727.3977 732.1221
733.3700 740.6629 744.3135
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882.8996 884.1878 890.5639
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943.8293 948.8609 951.1301
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1014.4243 1016.8879 1022.0259
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1165.7560 1165.9343 1182.5851
1196.0575 1196.3307 1197.1294
1198.5732 1204.3397 1205.4601
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1246.0950 1265.1742 1268.1355
1286.7136 1313.4071 1316.9541
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1341.7919 1344.0636 1357.6422
1367.1867 1368.2876 1370.5312
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1421.1434 1422.3472 1431.8927
1441.1489 1441.8659 1466.4829
1484.0255 1489.4280 1490.2117
1490.7033 1493.3177 1495.2503
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1597.0913 1663.5819 1665.1190
1665.5949 1668.5915 1682.7572
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3145.5661 3148.5866 3149.5286
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3217.7308 3220.7776 3221.5328
3226.0751 3227.1229 3230.2531
3232.3028 3233.2067 3235.0483
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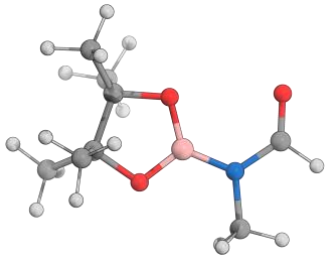
Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -2385.317336 Hartrees

11



Gaussian 16: ES64L-G16RevB.01 20-Dec-2017

# wB97xd/6-31G(d,p) gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc
) opt=(maxcycle=250) freq=noraman

Full point group C1 NOp 1
Stoichiometry C8H16BNO3 Framework group
C1[X(C8H16BNO3)]

Num atoms: 29
Charge = 0 Multiplicity = 1

SCF = -619.749820314 | Predicted change in Energy=-
3.917519D-10

Optimization completed.
Maximum Force 0.000006 0.000450 YES
RMS Force 0.000001 0.000300 YES
Maximum Displacement 0.000246 0.001800 YES
RMS Displacement 0.000040 0.001200 YES

Atom Coordinates (in Angstroms)
Type X Y Z

N 2.286634 1.119113 0.316833
C 2.679698 1.347082 1.622201
O 2.742521 0.521723 2.500814
H 2.943930 2.410710 1.793626
B 1.884359 -0.176772 -0.178258
C 1.194702 -2.311502 -0.307815
C 1.348788 -1.706000 -1.747524
C 2.267104 2.243311 -0.615981
H 2.578101 3.155110 -0.099883
H 2.947825 2.069564 -1.452951
H 1.263545 2.398743 -1.019041
O 1.441630 -0.291176 -1.474068
O 1.896750 -1.352212 0.510524
C 1.836411 -3.677596 -0.116803
H 1.683798 -4.012737 0.911835
H 1.381298 -4.412254 -0.788653
H 2.910386 -3.644993 -0.305165
C -0.254535 -2.335640 0.180269
H -0.260142 -2.560883 1.249033
H -0.737044 -1.364736 0.036513
H -0.840879 -3.097246 -0.341230
C 2.653789 -2.113839 -2.432607
H 2.791127 -1.499577 -3.325896
H 3.512035 -1.955284 -1.773712
H 2.636191 -3.164763 -2.733690
C 0.167937 -1.951923 -2.674625
H 0.360962 -1.493916 -3.648077
H 0.018488 -3.025482 -2.826130
H -0.751607 -1.523325 -2.273538

Statistical Thermodynamic Analysis
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

SCF = -619.749820314 | Predicted change in Energy=-
3.917519D-10
Zero-point correction (ZPE) = -619.5003813139999 0.249439
Internal Energy (U) = -619.4861463139999 0.263674
Enthalpy (H) = -619.4852023139999 0.264618
Gibbs Free Energy (G) = -619.540700314 0.20912

Frequencies
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111.3751 124.6858 217.6134
227.8838 233.4108 251.1478
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313.5230 325.7057 338.3823
370.4298 384.7300 404.4550
458.9906 514.2223 529.0865
560.6498 592.2670 677.8417
686.4457 690.8326 861.0258
881.9837 913.0889 950.4506
953.2864 990.0588 1004.5333
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1266.7534 1287.8273 1316.1504
1328.0120 1412.9127 1424.1326
1424.6496 1434.5079 1443.8184
1454.9344 1472.2851 1489.3239
1498.0309 1500.4807 1503.8568
1505.0274 1506.2501 1521.3550
1525.4844 1526.6059 1540.7179
1544.8864 1869.6794 2953.1976
3069.1913 3069.3027 3070.7526
3074.3196 3076.8507 3150.6668
3153.2168 3155.2261 3157.3983
3157.9100 3158.2984 3163.6573
3167.9327 3179.7773 3180.1071

Single point energy at ωB97XD/def2-TZVPP/PCM(Benzene): -
-619.982264 Hartrees

Intrinsic Reaction Coordinate (IRC) Analysis

Protocol and Summary

Intrinsic reaction coordinate (IRC) analysis was performed on the highest energy transition states for the carbodiphosphorane–borane adduct cycle **TS(12-13)** and the carbodiphosphorane–isocyanate adduct cycle **TS(16-17)** (Figure S57 and Figure S58, respectively). The following parameters were used for each calculation:

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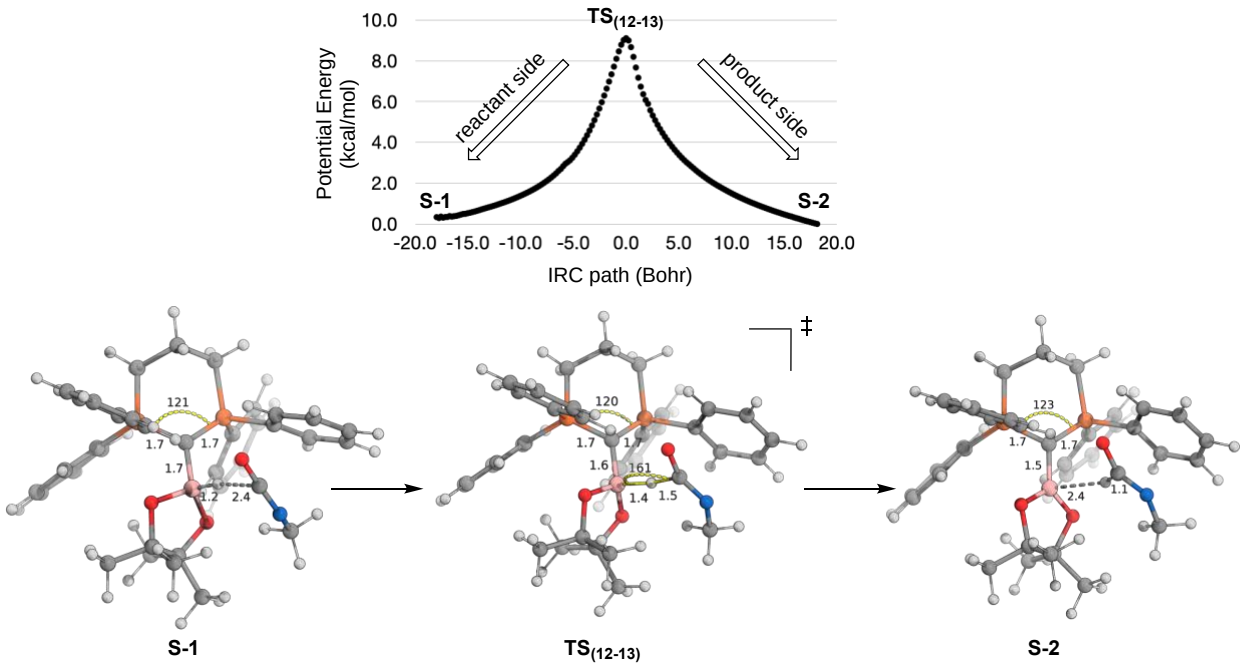

Figure S57. Computed intrinsic reaction coordinate plot from the highest energy transition states for the carbodiphosphorane–borane adduct cycle **TS(12-13)**. Computations performed at the ωB97XD/6-31G(d,p) level. Distances are reported in Ångströms (Å).

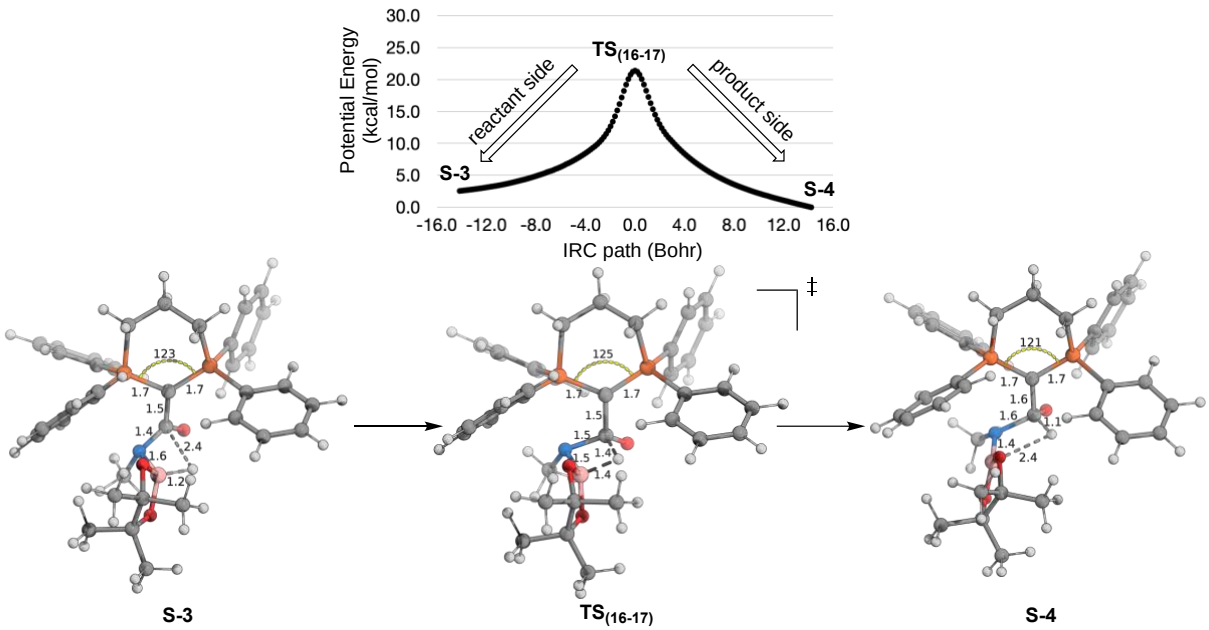

Figure S58. Computed intrinsic reaction coordinate plot from the highest energy transition states for the carbodiphosphorane–isocyanate adduct cycle **TS$_{(16\text{-}17)}$**. Computations performed at the ωB97XD/6-31G(d,p) level. Distances are reported in Ångströms (Å).

Natural Bond Order (NBO) Analysis

NBO analysis was performed on the geometry optimized carbodiphosphorane catalyst **1**. All NBO calculations were performed using the same level of theory as that used in the rest of the manuscript – ωB97XD/def2-TZVPP/PCM(Benzene)//ωB97XD /6-31G(d,p).

The following parameters were used in the calculations.

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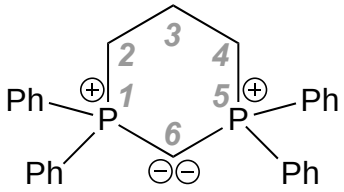
Natural Atomic Charges



Carbodiphosphorane **1**

Atom	Natural Charge
P 1	1.62049
C 6	–1.52374
P 5	1.61523
C 2	–0.75028
C 4	–0.74232
C 3	–0.39850

Natural Bond Orbitals

HOMO-1

Occupancy: 1.69344 (lone pair) on C 6
Orbital composition: s(32.41%) p 2.06(66.63%) d 0.03(0.95%) f 0.00(0.01%)

HOMO

Occupancy: 1.53766 (lone pair) on C 6
Orbital composition: s(2.29%) p 42.19(96.78%) d 0.39(0.90%) f 0.01(0.03%)

References

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