Supporting Information for:

Snapshots of Magnesium-centred Diborane Heterolysis by an Outer Sphere S_N2 Process

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Experimental

General Experimental Procedures: All manipulations were carried out using standard Schlenk line and glovebox techniques under an inert atmosphere of argon. NMR experiments were conducted in J Young tap NMR tubes made up and sealed in a glovebox. NMR spectra were recorded on a Bruker AV300 spectrometer operating at 300.2 MHz (^{1}H), 75.5 MHz (^{13}C), 96.3 MHz (^{11}B) or an Agilent ProPulse spectrometer operating at 500 MHz (^{1}H), 126 MHz (^{13}C), 160.4 MHz (^{11}B). The spectra were referenced relative to residual solvent resonances or an external $BF_3.OEt_2$ standard (^{11}B). Solvents (toluene, hexane) were dried by passage through a commercially available (Innovative Technologies) solvent purification system, under nitrogen and stored in ampoules over molecular sieves. d_8-Toluene was purchased from Fluorochem Ltd. and Sigma-Aldrich Ltd. and dried over molten potassium before distilling under argon and storing over molecular sieves. Di-*n*-butylmagnesium (1.0 M solution in *n*-heptane) and B_2pin_2 were purchased from Sigma-Aldrich Ltd. [(BDI)Mg*n*-Bu] (BDI = HC{(Me)CNDipp}$_2$; Dipp = 2,6-*i*-$Pr_2C_6H_3$] was synthesized by a literature procedure.[1] Elemental analysis was carried out Mr Stephen Boyer of London Metropolitan Enterprises.

Compound 11

Toluene-d_8 (0.5 mL) was added to a J Young NMR tube containing a mixture of [(BDI)Mg*n*-Bu] (50 mg, 0.1 mmol) and bis(pinacolato)diboron (25.4 mg, 0.1 mmol). After 2 hours *N*,*N*'-di-*tert*-butylcarbodiimide (15.45 mg, 0.1 mmol) was added and the solution was heated at 80˚C for 2 hours. The solvent was removed under reduced pressure to afford a colorless solid and hexane was added to obtain crystals of compound **11** (40 mg, 52.5%). Colorless crystals suitable for X-ray diffraction analysis were obtained from a saturated hexane solution at –35˚C. ^{1}H NMR (300 MHz, d_8-tol): δ 7.15 (m, 6H, Ar-*H*), 4.89 (s, 1H, NC(CH$_3$)C*H*), 3.51 (hept, 4H, J_{HH} = 6.7 Hz, C*H*(CH$_3$)$_2$), 1.67 (s, 6H, NC(C*H*$_3$)CH), 1.39 (d, 12H, J_{HH} = 6.7 Hz, CH(C*H*$_3$)$_2$), 1.31 (d, 12H, JHH = 6.7 Hz, CH(C*H*$_3$)$_2$), 1.24 (s, 18H, NC(C*H*$_3$)$_3$), 1.10 (s, 12H, B(OC(C*H*$_3$)$_2$)$_2$) ppm. ^{11}B{^{1}H} NMR (96 MHz, d_8-tol): δ 31.4 (br s) ppm. ^{13}C{^{1}H} NMR (126 MHz, d_8-tol): δ 169.08 (N*C*(CH$_3$)CH), 145.22 (*C*$_{ipso}$), 142.52 (*C*$_{ortho}$), 124.73 (*C*$_{para}$), 123.53 (*C*$_{meta}$), 94.47 (NC(CH$_3$)*C*H), 83.80 ((B(O*C*(CH$_3$)$_2$)$_2$), 49.89 (N*C*(CH$_3$)$_3$), 33.19 (NC(*C*H$_3$)$_3$), 27.71(NC(*C*H$_3$)CH), 25.40 (B(OC(*C*H$_3$)$_2$)$_2$), 25.36 (CH(*C*H$_3$)$_2$), 24.41 (*C*H(CH$_3$)$_2$), 23.85 (CH(*C*H$_3$)$_2$) ppm. Elemental analysis: Found C, 72.97; H, 10.17; N, 7.69 %. $C_{44}H_{71}BMgN_4O_2$ requires: C, 73.08; H, 9.90; N, 7.75 %.

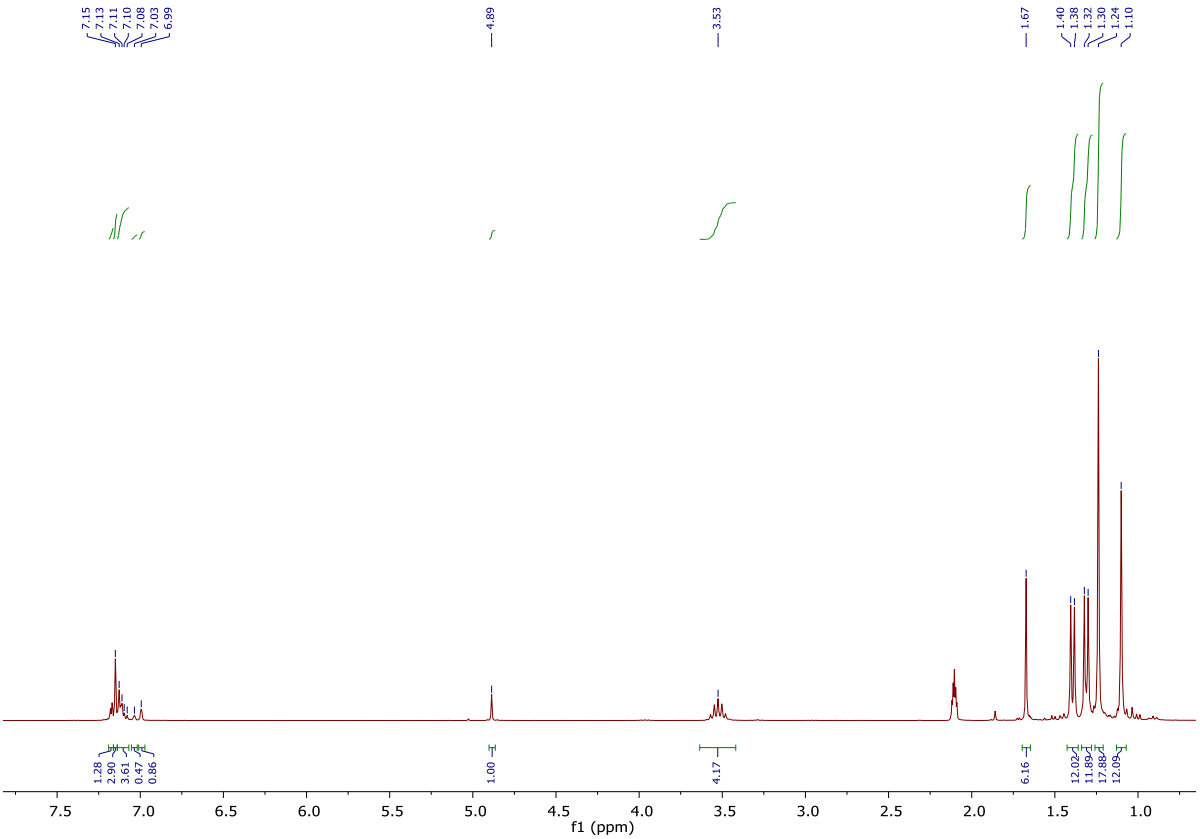


Figure S1: ^{1}H NMR spectrum (25°C, 300 MHz, d_8-tol) of compound **11**.

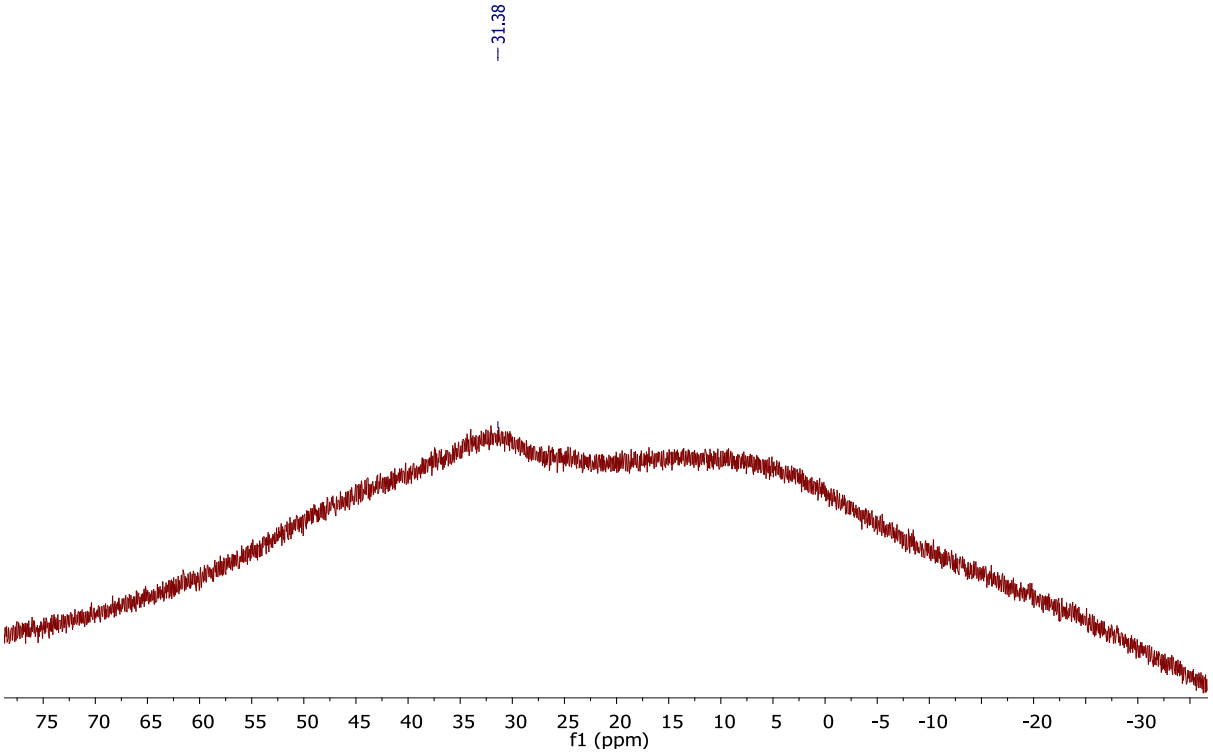


Figure S2: $^{11}B\{^{1}H\}$ NMR spectrum (25°C, 96 MHz, d_8-tol) of compound **11**.

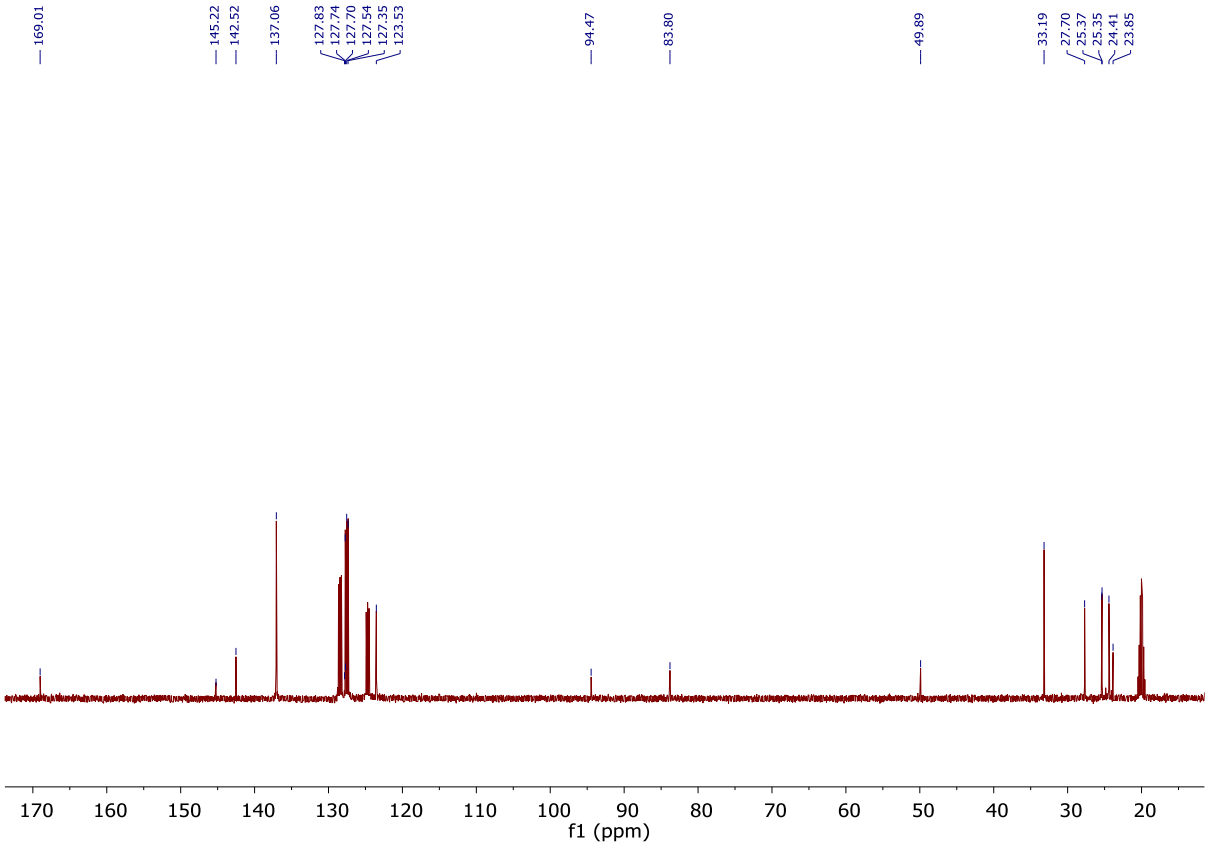


Figure S3: $^{13}C\{^{1}H\}$ NMR spectrum (25°C, 126 MHz, d_8-tol) of compound **11**.

Compound 12

Toluene-d_8 (0.5 mL) was added to a J Young NMR tube containing a mixture of [(BDI)Mg*n*-Bu] (50 mg, 0.1 mmol) and bis(pinacolato)diboron (25.4 mg, 0.1 mmol). After 2 hours *N*,*N*'-diisopropylcarbodiimide (12.64 mg, 0.1 mmol) was added and the solution was heated at 80˚C for 2 hours. Although attempts to crystallize compound **12** from the *n*-BuBpin also produced in the reaction were thwarted by its solubility in hydrocarbon solvents, its formation was clearly demonstrated by multinuclear NMR spectroscopy. ^{1}H NMR (300 MHz, d_8-tol): δ 7.11 (m, 6H, Ar-*H*), 4.85 (s, 1H, NC(CH$_3$)C*H*), 3.47 (m, 4H + 2H, J_{HH} = 6.8 Hz, (C$_6$H$_3$)C*H*(CH$_3$)$_2$ and NC*H*(CH$_3$)$_2$), 1.67 (s, 6H, NC(C*H*$_3$)CH), 1.34 (d, 12H, J_{HH} = 6.8 Hz, CH(C*H*$_3$)$_2$), 1.27 (d, 12H, J_{HH} = 6.8 Hz, CH(C*H*$_3$)$_2$), 1.01 (s, 12H, B(OC(C*H*$_3$)$_2$)$_2$), 0.97 (d, 12H, J_{HH} = 6.2 Hz, NCH(C*H*$_3$)$_2$) ppm. ^{11}B{^{1}H} NMR (96 MHz, d_8-tol): δ 37.2 (*n*-BuBpin), 12.5. (C-Bpin) ppm.

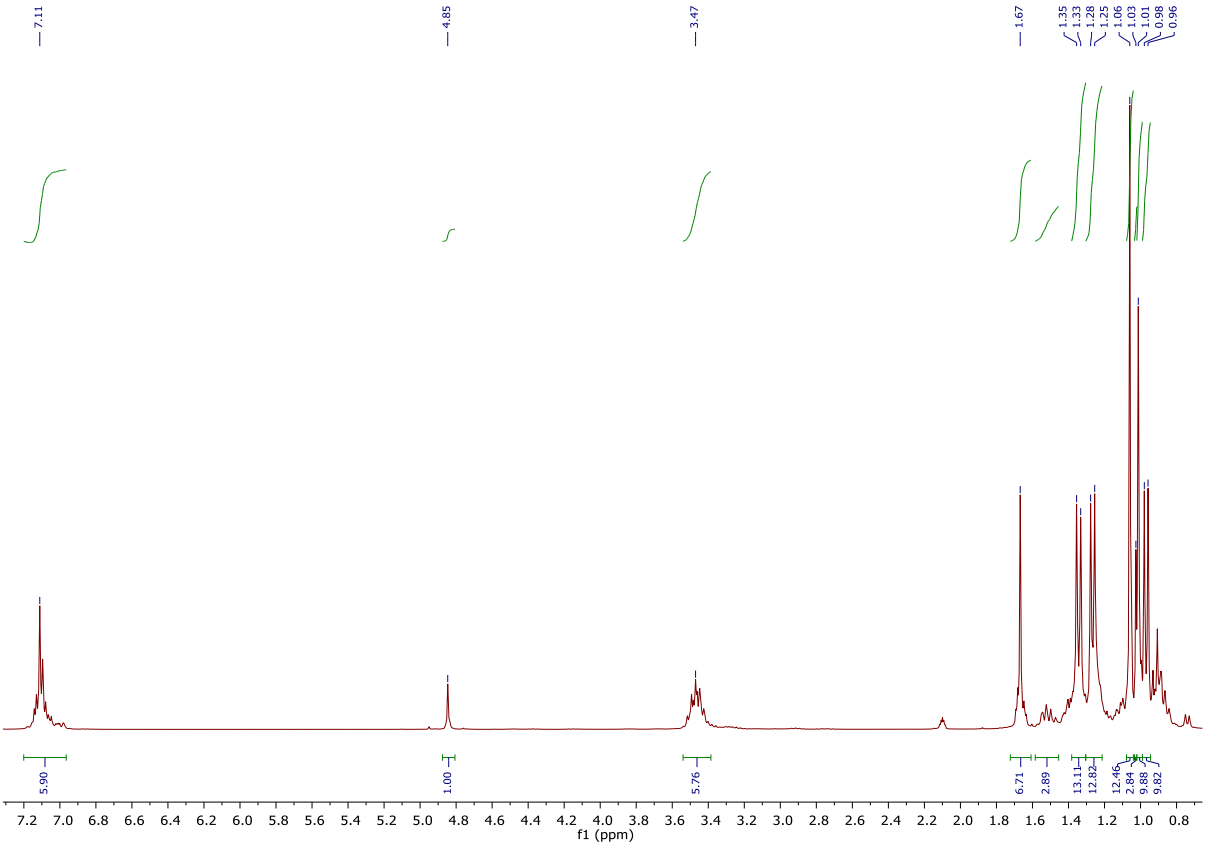


Figure S4: ^{1}H NMR spectrum (25°C, 300 MHz, d_8-tol) of compound **12**.

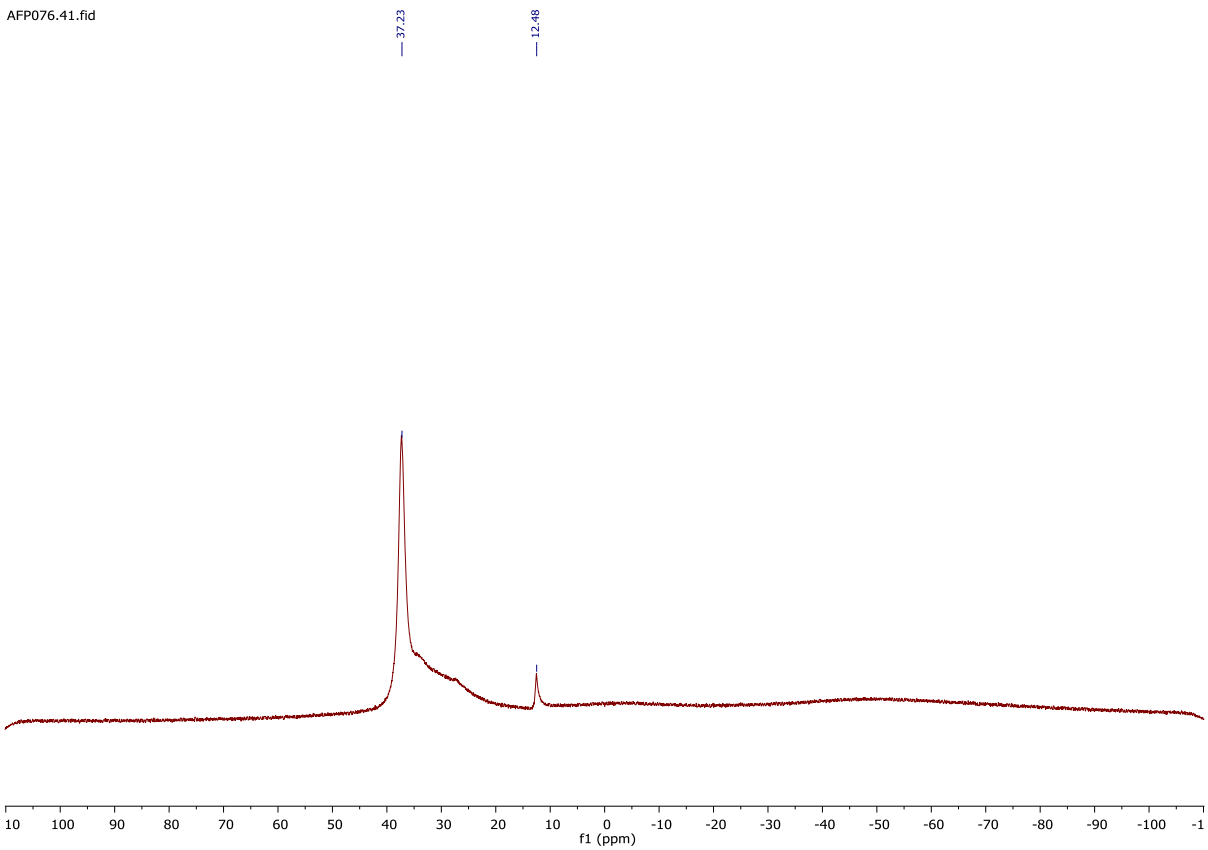


Figure S5: $^{11}B\{^{1}H\}$ NMR spectrum (25°C, 96 MHz, d_8-tol) of compound **12** in the presence of *n*-BuBpin.

Compound 13

Toluene-d_8 (0.5 mL) was added to a J Young NMR tube containing a mixture of [(BDI)Mg*n*-Bu] (50 mg, 0.1 mmol) and bis(pinacolato)diboron (25.4 mg, 0.1 mmol). After 2 hours *N*,*N*'-di-*p*-tolylcarbodiimide (22.26 mg, 0.1 mmol) was added and analysis by NMR spectroscopy demonstrated the formation of the compound **13** at room temperature. Although attempts to crystallize compound **13** from the *n*-BuBpin also produced in the reaction were thwarted by its solubility in hydrocarbon solvents, its formation was clearly demonstrated by multinuclear NMR spectroscopy. ^{1}H NMR (300 MHz, d_8-tol): δ 7.08 (m, 6H, Ar-*H*), 6.80 (d, 4H, J_{HH} = 8Hz, $CH_3(C_6H_4)$), 6.53 (d, 4H, J_{HH} = 8Hz, $CH_3(C_6H_4)$), 4.89 (s, 1H, $NC(CH_3)CH$), 3.31 (hept, 4H, J_{HH} = 6.8 Hz, $CH(CH_3)_2$), 2.1 (s, 6H, $CH_3(C_6H_4)$, 1.68 (s, 6H, $NC(CH_3)CH$), 1.18 (d, 12H, J_{HH} = 6.8 Hz, $CH(CH_3)_2$), 0.98 (d, 12H, J_{HH} = 6.7 Hz, $CH(CH_3)_2$), 0.67 (s, 12H, $B(OC(CH_3)_2)_2$) ppm. ^{11}B{^{1}H} NMR (96 MHz, d_8-tol): δ 37.2 (BuBpin), 8.6 (C-Bpin) ppm.

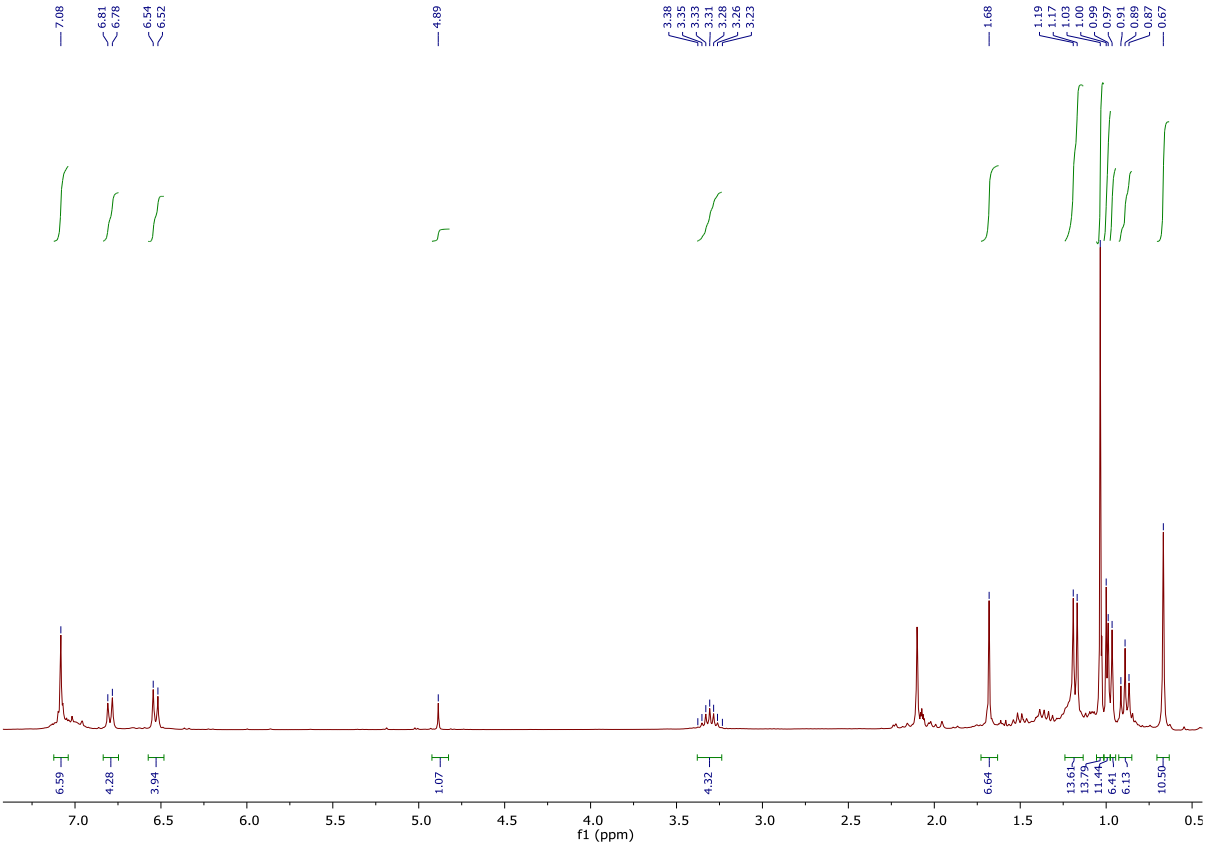


Figure S6: ^{1}H NMR spectrum (25°C, 300 MHz, d_8-tol) of compound **13**.

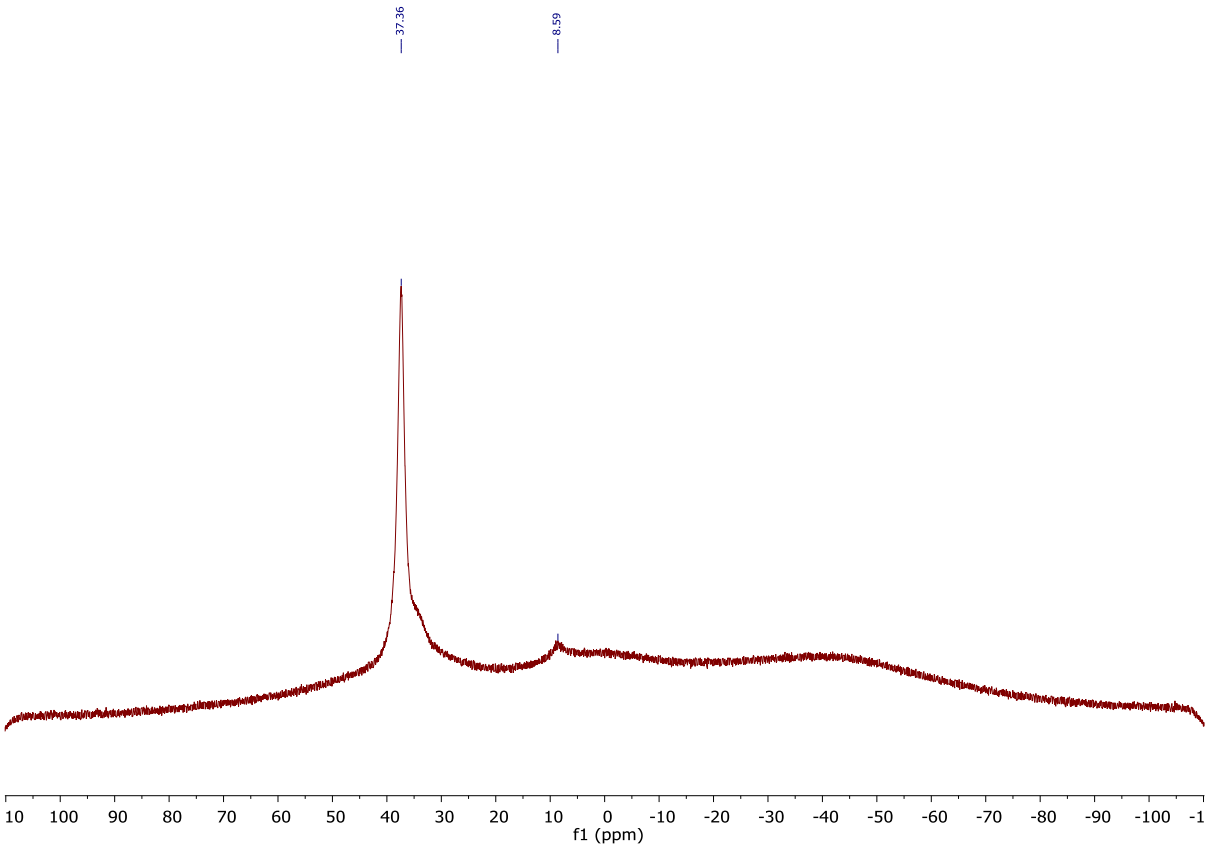


Figure S7: $^{11}B\{^{1}H\}$ NMR spectrum (25°C, 300 MHz, d_8-tol) of compound **12** in the presence of *n*-BuBpin.

Compound 14

Toluene-d_8 (0.5 mL) was added to a J Young NMR tube containing a mixture of [(BDI)Mg*n*-Bu] (50.1 mg, 0.1 mmol) and bis(pinacolato)diboron (25.4 mg, 0.1 mmol) and the resultant solution was left to react for 2 hours. *N,N'*-dimesitylcarbodiimide (27.9 mg, 0.1 mmol) was added with the immediate production of a viscous light yellow solution containing needle-like crystals. Volatiles were removed and the crystals were washed with hexane twice and then dried under vacuum to produce yellow crystals of compound **14** (37.1 mg, 43.6%), which were suitable for X-ray diffraction analysis but proved insufficiently soluble for analysis by NMR spectroscopy. Elemental analysis: Found C, 76.41; H, 9.03; N, 6.40%. $C_{54}H_{75}BMgN_4O_2$ requires: C, 76.55; H, 8.92; N, 6.61 %.

Compound $\mathbf{15_{BN}}$

Toluene-d_8 (0.5 mL) was added to a J Young NMR tube, containing a mixture of [(BDI)Mg*n*-Bu] (50 mg, 0.1 mmol) and bis(pinacolato)diboron (25.4 mg, 0.1 mmol). After 2 hours, *N*-benzylidenebutane-1-amine (16.15 mg, 0.1 mmol) was added. After 10 minutes, volatiles were removed under vacuum and the resultant solid was washed with hexane to yield compound **$\mathbf{15_{BN}}$** (68.6 mg, 94%). Colorless crystals suitable for X-ray diffraction analysis were obtained from a saturated hexane solution at room temperature. ^{1}H NMR (500 MHz,d_8-tol) δ 7.16 (m, 3H, CH ar), 7.06 (m, 5H, CH ar), 6.96 (m, 2H, CH ar), 6.65 (t, 1H, J_{HH} = 7.1 Hz, CH ar), 4.81 (s, 1H, NC(CH_3)C*H*), 3.71, 3.61 (hept, 1H, J_{HH} = 6.6 Hz C*H*(CH_3)$_2$), 3.44 (hept, 1H, J_{HH} = 6.6 Hz C*H*(CH_3)$_2$), 3.30 (hept, 1H, J_{HH} = 6.6 Hz C*H*(CH_3)$_2$), 3.20, 2.82 (hept, 1H, J_{HH} = 6.6 Hz C*H*(CH_3)$_2$), 1.69 (s, 3H, C*H*$_3$), 1.57 (s, 3H, C*H*$_3$), 1.43 (d, 3H, J_{HH} = 6.6 Hz CH(C*H*$_3$)$_2$), 1.38 (m, 6H, CH(C*H*$_3$)$_2$), 1.33 (d, 3H, J_{HH} = 6.7 Hz CH(C*H*$_3$)$_2$), 1.27 (d, 3H, J_{HH} = 6.7 Hz CH(C*H*$_3$)$_2$), 1.19 (m, 9H, C*H*$_3$), 0.99 (s, 3H, C*H*$_3$), 0.95 (m, 6H, C*H*$_3$), 0.90 (s, 3H, C*H*$_3$), 0.86-0.82 (m, 7H, 2 x CH_2 + CH_3) ppm. ^{11}B{^{1}H} NMR (160 MHz, d_8-tol) δ 24.5 ppm. ^{13}C{^{1}H} NMR (126 MHz, d_8-tol) δ 170.18 (N*C*(CH_3)CH), 169.38, 153.39, 145.13, 143.07, 142.63, 141.69, 141.57, 127.78 (CH ar), 125.13 (CH ar), 124.11 (CH ar), 123.75 (CH ar), 123.40 (CH ar), 121.32 (CH ar), 118.03(CH ar, at 6.65 ppm in ^{1}H), 94.01 (NC(CH_3)*C*H), 85.51, 81.64, 53.80(BuN-*C*H(Ph)), 44.90 (N*C*$H_2$$CH_2$), 28.14 (*C*H($CH_3$)$_2$), 28.08 (*C*H($CH_3$)$_2$), 28.04 (*C*H($CH_3$)$_2$), 27.49 (*C*H($CH_3$)$_2$), 26.29 ($CH_3$), 25.11 ($CH_3$), 24.86 ($CH_3$), 24.71 ($CH_3$), 24.57 ($CH_3$), 24.50 ($CH_3$), 24.45 ($CH_3$), 24.41 ($CH_3$), 24.24 ($CH_3$), 24.19 ($CH_3$), 24.12 ($CH_3$), 23.47 ($CH_2$), 13.87 ($CH_3$) ppm. Elemental analysis: Found C, 75.39; H, 9.60; N, 5.72 %. $C_{46}H_{68}BMgN_3O_2$ requires: C, 75.67; H, 9.39; N, 5.75 %.

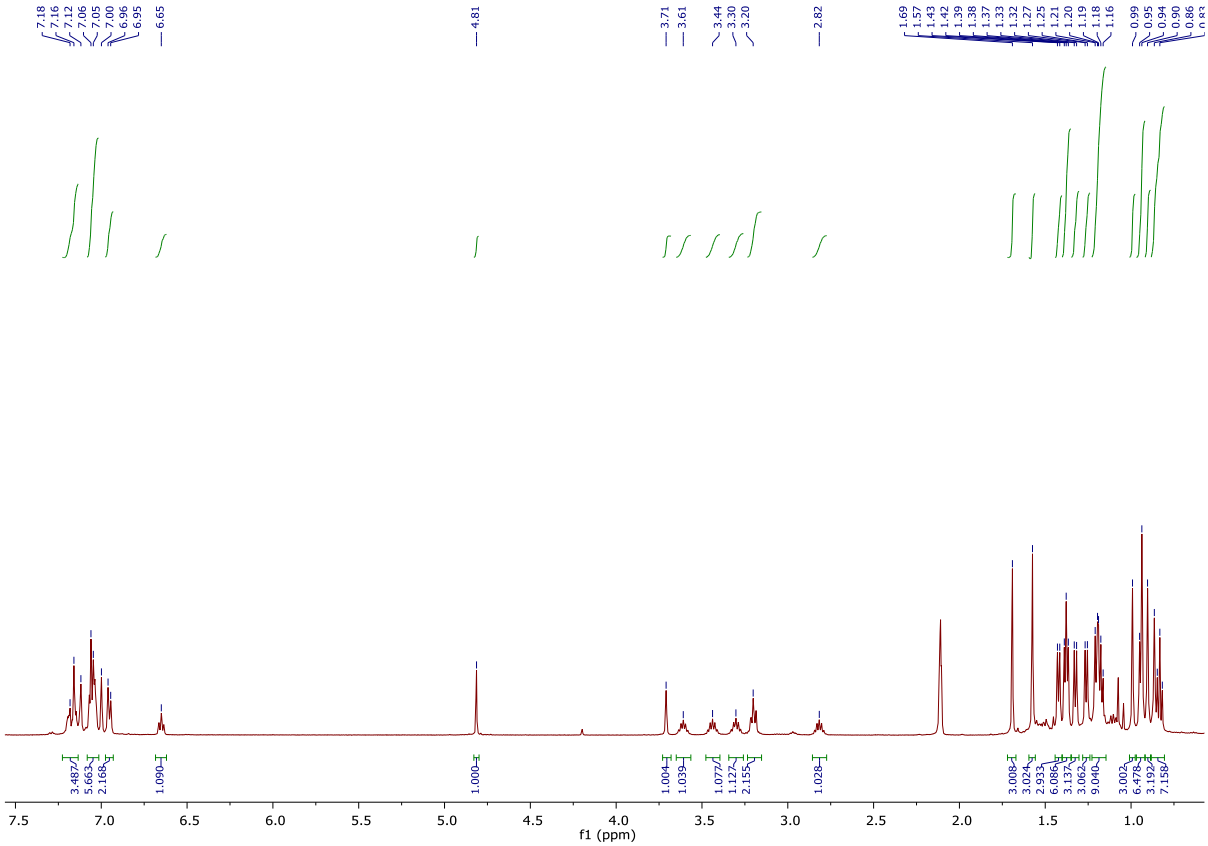


Figure S8: ^{1}H NMR spectrum (25°C, 500 MHz, d_8-tol) of compound **15$_{BN}$**.

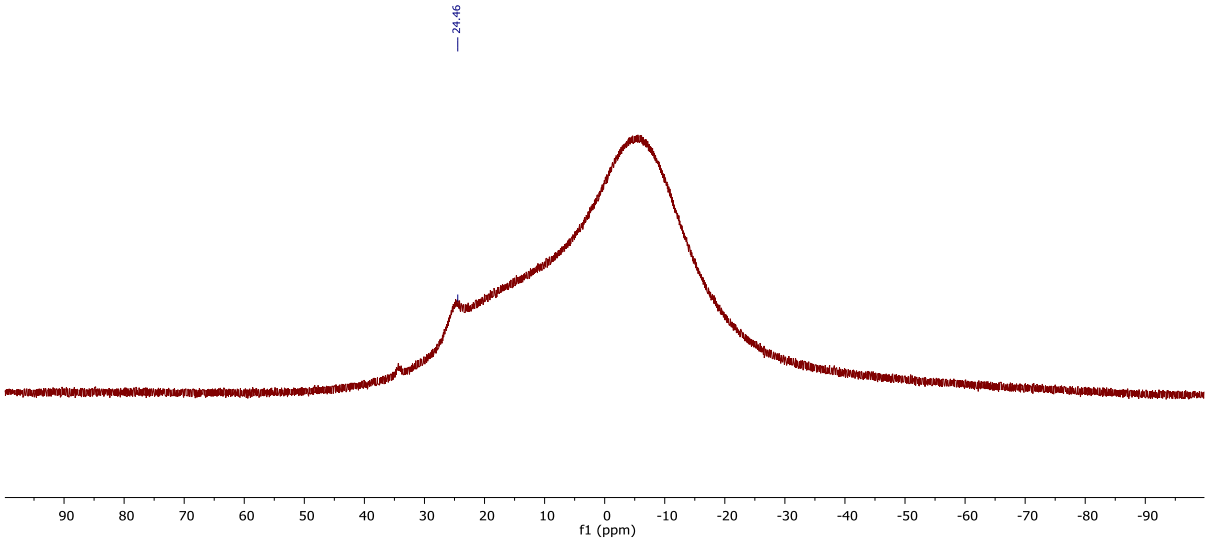


Figure S9: ^{11}B{^{1}H} NMR spectrum (25°C, 160 MHz, d_8-tol) of compound **15$_{BN}$.**

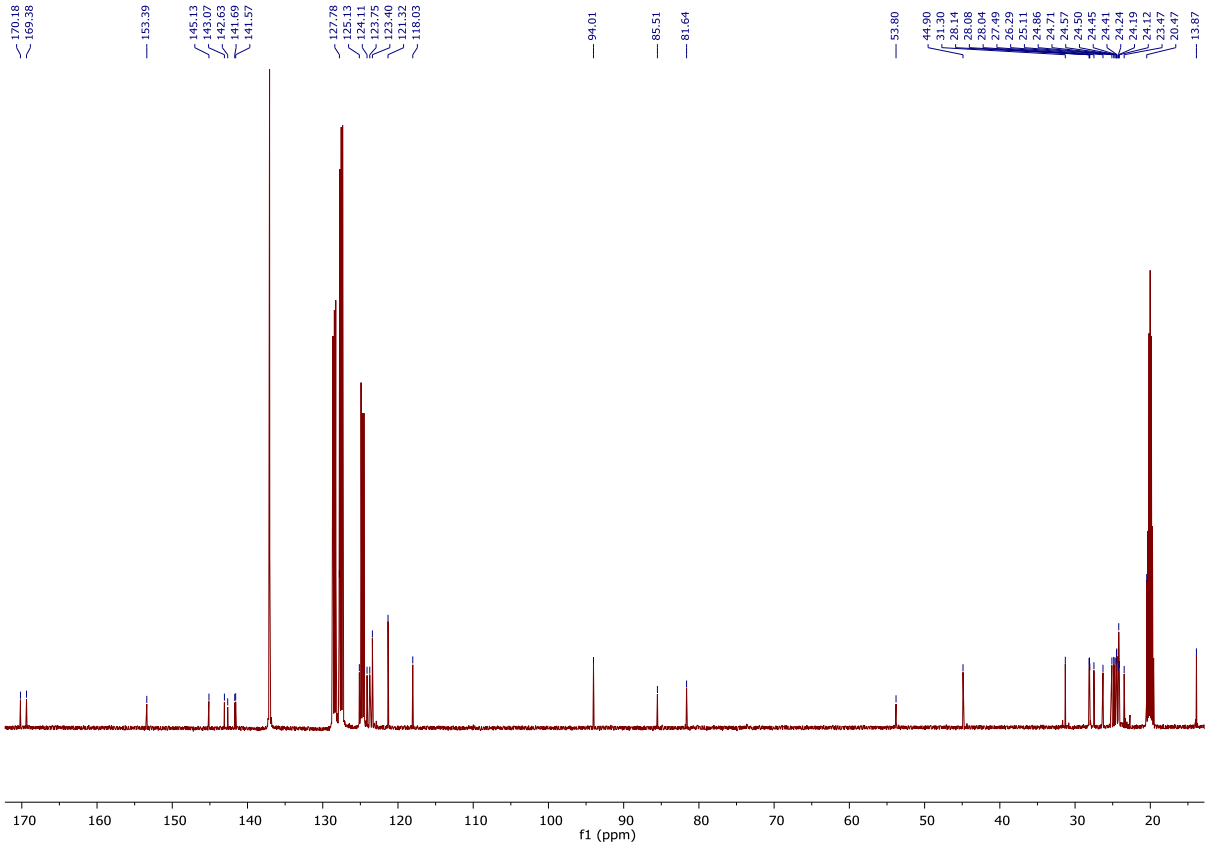


Figure S10: $^{13}C\{^{1}H\}$ NMR spectrum (25°C, 126 MHz, d_8-tol) of compound **15$_{BN}$**.

Compound 16_{BN}

Toluene-d_8 (0.5 mL) was added to a J Young NMR tube containing a mixture of [(BDI)Mg*n*-Bu] (50 mg, 0.1 mmol) and bis(pinacolato)diboron (25.4 mg, 0.1 mmol). After 2 hours *N*-benzylidene-*tert*-butylamine (16.15 mg, 0.1 mmol) was added. After 10 minutes, volatiles were removed under vacuum and the resultant solid was crystallized from hexane solution at –35˚C to yield compound **16_{BN}** (30 mg, 41%). ^{1}H NMR (500 MHz, d_8-tol) δ 7.19 (m, 1H, aromatic C*H*), 7.17 (m, 2H, aromatic C*H*), 7.12 (m, 1H, aromatic C*H*), 7.06-7.00 (m, 4H, aromatic C*H*), 6.85 (m, 2H, aromatic C*H*), 6.41 (m, 1H, aromatic C*H*), 4.77 (s, 1H, NC(CH_3)C*H*), 3.70 (s, 1H, N-C*H*Ph), 3.52 (hept, 1H, J_{HH} = 6.7 Hz C*H*(CH_3)$_2$), 3.38 (hept, 1H, J_{HH} = 6.7 Hz C*H*(CH_3)$_2$), 3.27 (hept, 1H, J_{HH} = 6.7 Hz C*H*(CH_3)$_2$), 2.79 (hept, 1H, J_{HH} = 6.7 Hz C*H*(CH_3)$_2$), 1.66 (s, 3H, C*H*$_3$), 1.56 (s, 3H, C*H*$_3$), 1.47 (d, 3H, J_{HH} = 6.7 Hz CH(C*H*$_3$)$_2$), 1.43 (d, 3H, J_{HH} = 6.7 Hz CH(C*H*$_3$)$_2$), 1.40-1.38 (m, 12H, C*H*$_3$), 1.30 (d, 3H, J_{HH} = 6.7 Hz CH(C*H*$_3$)$_2$), 1.27 (d, 3H, J_{HH} = 6.7 Hz CH(C*H*$_3$)$_2$), 1.20 (d, 3H, J_{HH} = 6.7 Hz CH(C*H*$_3$)$_2$), 1.17 (d, 3H, J_{HH} = 6.7 Hz CH(C*H*$_3$)$_2$), 1.11 (s, 3H, C*H*$_3$), 1.08 (s, 3H, C*H*$_3$), 1.02-1.00 (m, 6H, CH_3), 0.97 (s, 3H, C*H*$_3$) ppm. ^{11}B{^{1}H} NMR (160 MHz, d_8-tol) δ 24.99 ppm. ^{13}C{^{1}H} NMR (126 MHz, d_8-tol) δ 170.23 (N*C*(CH_3)CH), 169.29, 157.08, 145.48, 145.00, 142.84, 142.46, 141.90, 141.67, 127.99 (CH ar), 125.22 (CH ar), 124.04 (CH ar), 123.81 (CH ar), 123.51 (CH ar), 123.35 (CH ar), 117.08 (CH ar), 94.14 (NC(CH_3)*C*H), 84.60, 81.56, 56.72, 55.18 (tBuN-*C*H(Ph)), 30.74 (*C*H$_3$), 28.17 (*C*H(CH_3)$_2$), 28.02 (*C*H(CH_3)$_2$), 27.89 (*C*H(CH_3)$_2$), 27.40 (*C*H(CH_3)$_2$), 26.03 (*C*H$_3$), 25.39 (*C*H$_3$), 25.18 (*C*H$_3$), 25.08 (*C*H$_3$), 24.91 (*C*H$_3$), 24.79 (*C*H$_3$), 24.72 (*C*H$_3$), 24.63 (*C*H$_3$), 24.57 (*C*H$_3$), 24.39 (*C*H$_3$), 24.05 (*C*H$_3$), 23.91 (*C*H$_3$), 23.11 (*C*H$_3$) ppm. Elemental analysis: Found C, 75.48; H, 9.50; N, 5.68 %. $C_{46}H_{68}BMgN_3O_2$ requires: C, 75.67; H, 9.39; N, 5.75 %.

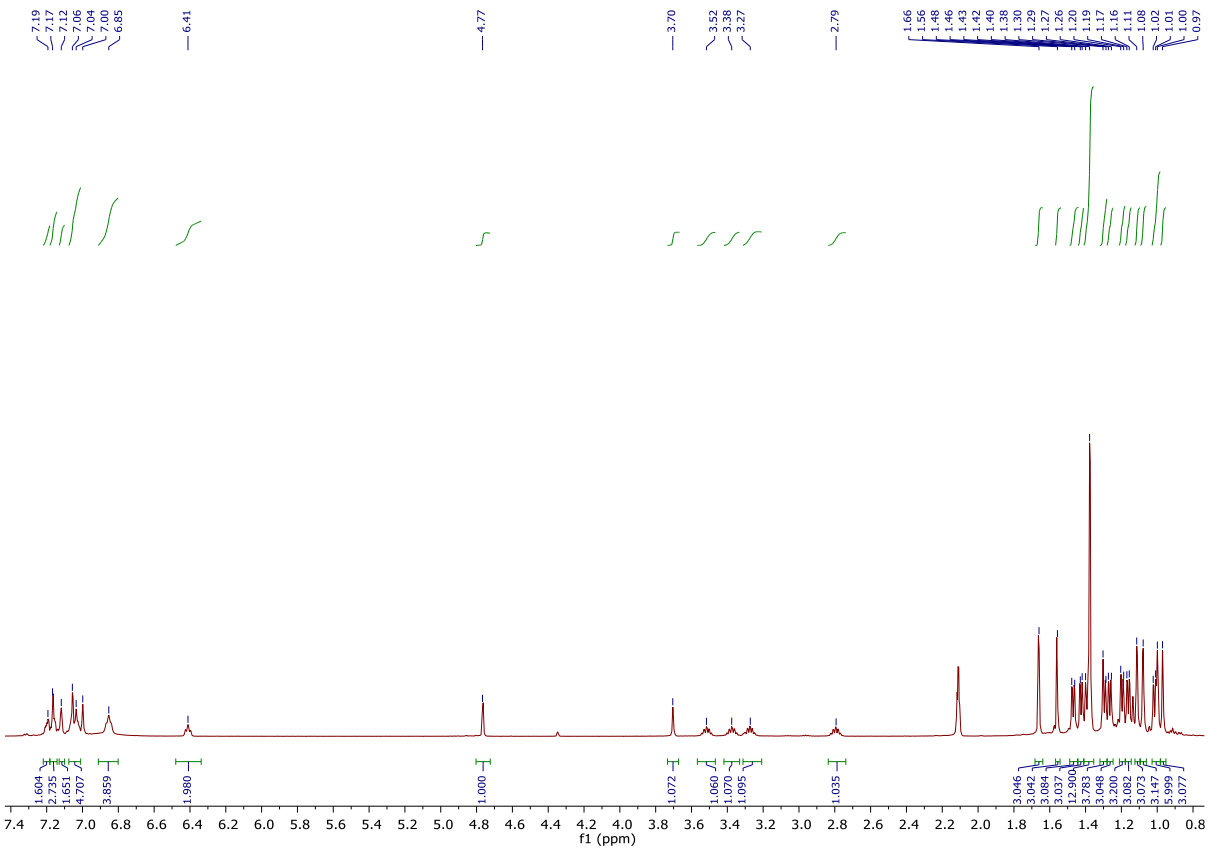


Figure S11: ^{1}H NMR spectrum (25°C, 500 MHz, d_8-tol) of compound **16$_{BN}$**.

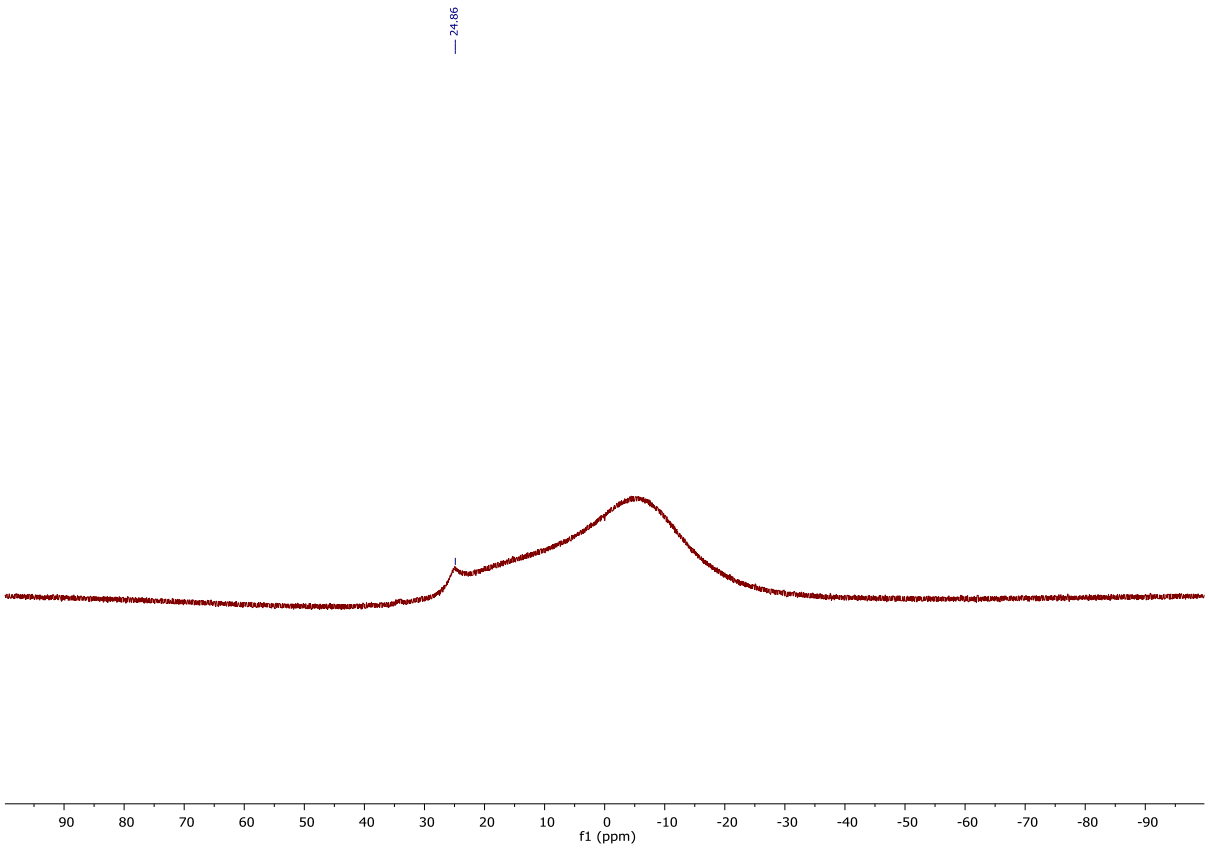


Figure S12: ^{11}B{^{1}H} NMR spectrum (25°C, 160 MHz, d_8-tol) of compound **16$_{BN}$**.

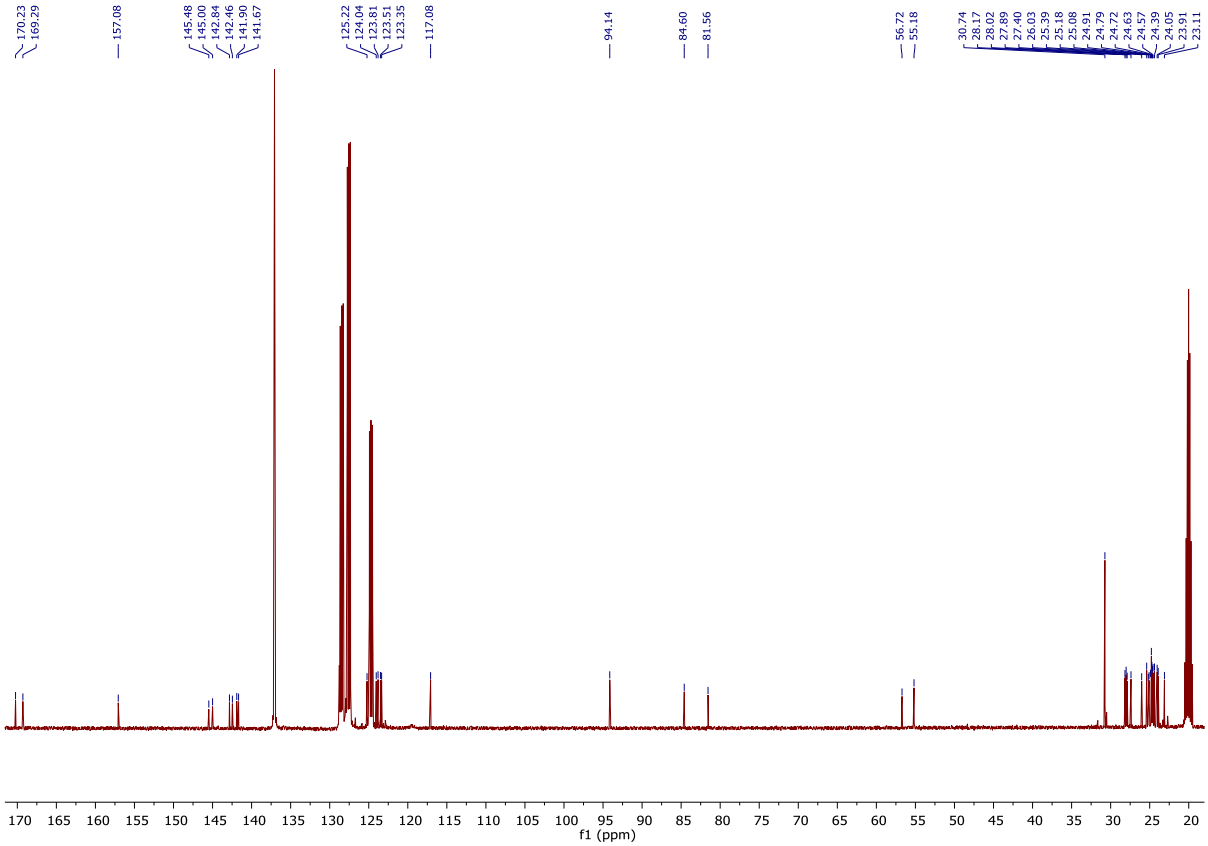


Figure S13: $^{13}C\{^{1}H\}$ NMR spectrum (25°C, 126 MHz, d_8-tol) of compound **16$_{BN}$**.

Compound 17$_{BN}$

Toluene-d_8 (0.5 mL) was added to a J Young NMR tube containing a mixture of [(BDI)Mg*n*-Bu] (50 mg, 0.1 mmol) and bis(pinacolato)diboron (25.4 mg, 0.1 mmol). After 2 hours *N*-1-diphenylmethanimine (18.15 mg, 0.1 mmol) was added. The solution became orange then pale yellow over a period of 3 hours. The solvent was removed under vacuum and the solid was washed with hexane and dried under vacuum to yield compound **17$_{BN}$** (70.5 mg, 94%). Despite repeated attempts, an accurate elemental analysis could not be obtained for this compound. ^{1}H NMR (500 MHz, d_8-tol) δ 7.66, 7.65, 7.11, 7.09, 7.06, 6.80, 6.67, 4.96 (s, 1H, NC(CH$_3$)C*H*), 4.51 (s, 1H, N-C*H*Ph), 3.74 (hept, 1H, J_{HH} = 6.7 Hz, C*H*(CH$_3$)$_2$), 3.38 (m, 2H, C*H*(CH$_3$)$_2$), 2.67 (hept, 1H, J_{HH} = 6.7 Hz, C*H*(CH$_3$)$_2$), 1.75 (s, 3H, CH$_3$), 1.65 (s, 3H, CH$_3$), 1.31 (m, 9H, CH$_3$), 1.20 (m, 12H, CH$_3$), 0.92 (s, 3H, CH$_3$), 0.77 (d, 3H, J_{HH} = 6.7 Hz, CH$_3$), 0.66 (m, 9H, CH$_3$) ppm. ^{11}B{^{1}H} NMR (160 MHz, d_8-tol) δ 24.8 ppm. ^{13}C{^{1}H} NMR (126 MHz, d_8-tol) δ 170.50(N*C*(CH$_3$)CH), 170.00, 152.79, 146.28, 145.11, 144.72, 143.43, 143.10, 141.58, 141.32, 128.04 (CH ar), 127.81 (CH ar), 125.14 (CH ar), 124.14 (CH ar), 123.85 (CH ar), 123.36 (CH ar), 123.31 (CH ar), 122.18 (CH ar), 120.71 (CH ar, reso at 6.80), 120.65 (CH ar, reso at 7.66), 118.52 (CH ar), 93.81 (NC(CH$_3$)*C*H), 85.30, 82.92, 53.91 (N*C*HPh), 28.38 (*C*H(CH$_3$)$_2$), 28.27 (*C*H(CH$_3$)$_2$), 28.13 (*C*H(CH$_3$)$_2$), 27.77 (*C*H(CH$_3$)$_2$), 25.48 (*C*H$_3$), 25.23 (*C*H$_3$), 24.74 (*C*H$_3$), 24.71 (*C*H$_3$), 24.63 (*C*H$_3$), 24.28 (*C*H$_3$), 24.13 (*C*H$_3$), 23.98 (*C*H$_3$), 23.89 (*C*H$_3$), 23.54 (*C*H$_3$), 23.06 (*C*H$_3$) ppm.

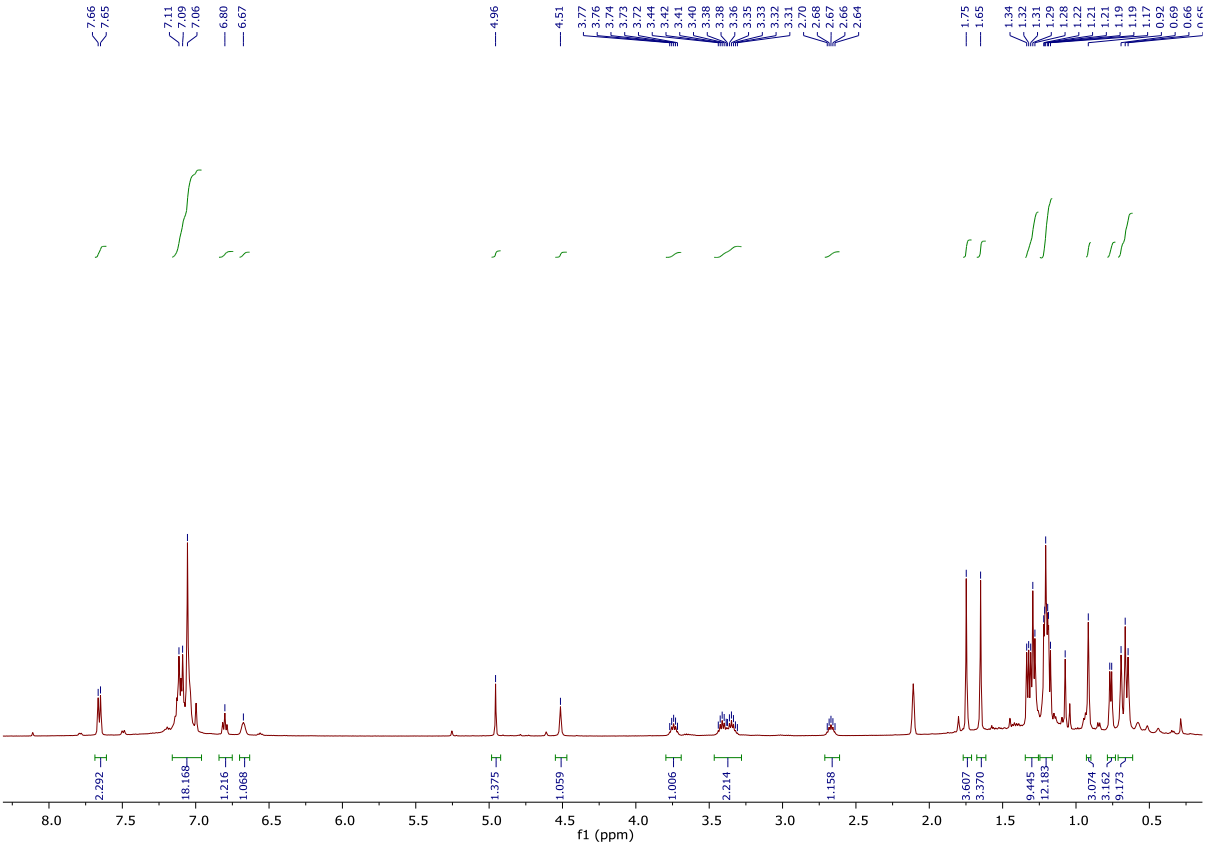


Figure S14: ^{1}H NMR spectrum (25°C, 500 MHz, d_8-tol) of compound **17$_{BN}$**.

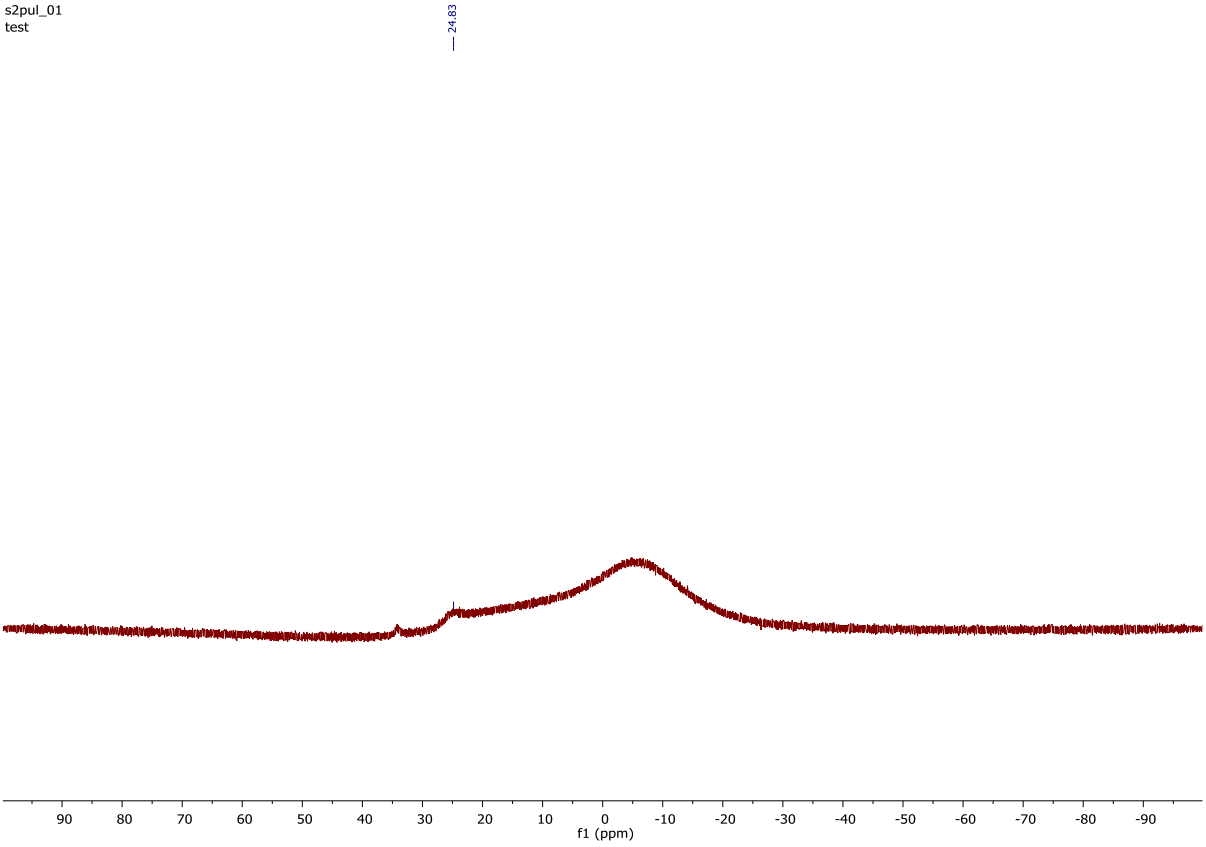


Figure S15: ^{11}B{^{1}H} NMR spectrum (25°C, 160 MHz, d_8-tol) of compound **17$_{BN}$**.

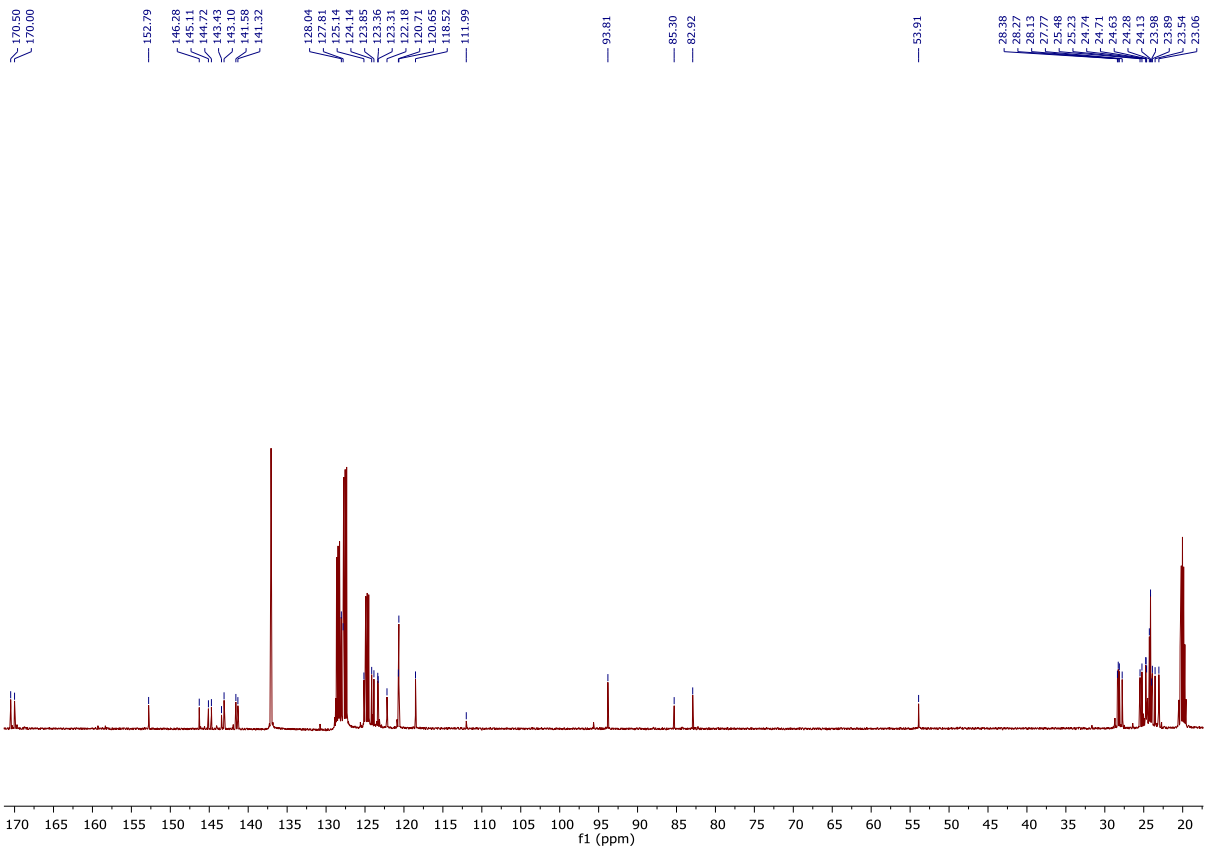


Figure S16: $^{13}C\{^{1}H\}$ NMR spectrum (25°C, 126 MHz, d_8-tol) of compound **17$_{BN}$**.

Compound 18$_{BN}$

Toluene-d_8 (0.5 mL) was added to a J Young NMR tube conaining a mixture of [(BDI)Mg*n*-Bu] (50 mg, 0.1 mmol) and bis(pinacolato)diboron (25.4 mg, 0.1 mmol). After 2 hours *N*-(diphenylmethylene)-benzenamine (25.7 mg, 0.1 mmol) was added. After a further 30 minutes, volatiles were removed under vacuum and the resultant solid was crystallized from a hexane solution at –35˚C to yield compounf **18$_{BN}$** (45 mg, 54%). ^{1}H NMR (500 MHz, d_8-toluene) δ 7.16-7.00 (m, 11H, aromatic C*H*), 6.86 (m, 3H, aromatic C*H*), 6.58 (m, 1H, aromatic C*H*), 6.50 (m, 6H, aromatic C*H*), 4.72 (s, 1H, NC(CH_3)C*H*), 3.22 (hept, 2H, J_{HH} = 6.7 Hz, C*H*(CH_3)$_2$), 3.06 (hept, 2H, J_{HH} = 6.7 Hz, C*H*(CH_3)$_2$), 1.58 (s, 6H, NC(C*H*$_3$)CH), 1.35 (s, 6H, C*H*$_3$), 1.18 (d, 6H, J_{HH} = 6.7 Hz, C*H*$_3$), 1.13 (m, 12H, C*H*$_3$), 1.08 (d, 6H, J_{HH} = 6.7 Hz, C*H*$_3$), 1.00 (d, 6H, J_{HH} = 6.7 Hz, C*H*$_3$) ppm. ^{11}B NMR (160 MHz, Tol) δ 26.0 ppm. ^{13}C NMR (126 MHz, toluene) δ 170.34 (N*C*(CH_3)CH), 146.70, 146.54, 143.26, 142.42, 142.15, 127.45 (CH ar), 127.06 (CH ar), 125.54 (CH ar), 123.97 (CH ar), 123.94 (CH ar), 123.21 (CH ar), 122.96 (CH ar), 120.67 (CH ar), 120.08 (CH ar), 93.72 (NC(CH_3)*C*H), 88.07, 83.14, 31.65, 28.37 (*C*H(CH_3)$_2$), 27.45 (*C*H(CH_3)$_2$), 25.13 (*C*H_3), 25.01 (*C*H_3), 24.79 (*C*H_3), 24.66 (*C*H_3), 24.59 (*C*H_3), 24.46 (*C*H_3), 23.96 (*C*H_3) ppm. Elemental analysis: Found C, 78.27; H, 8.14; N, 5.19 %. $C_{54}H_{68}BMgN_3O_2$ requires: C, 78.50; H, 8.30; N, 5.09 %.

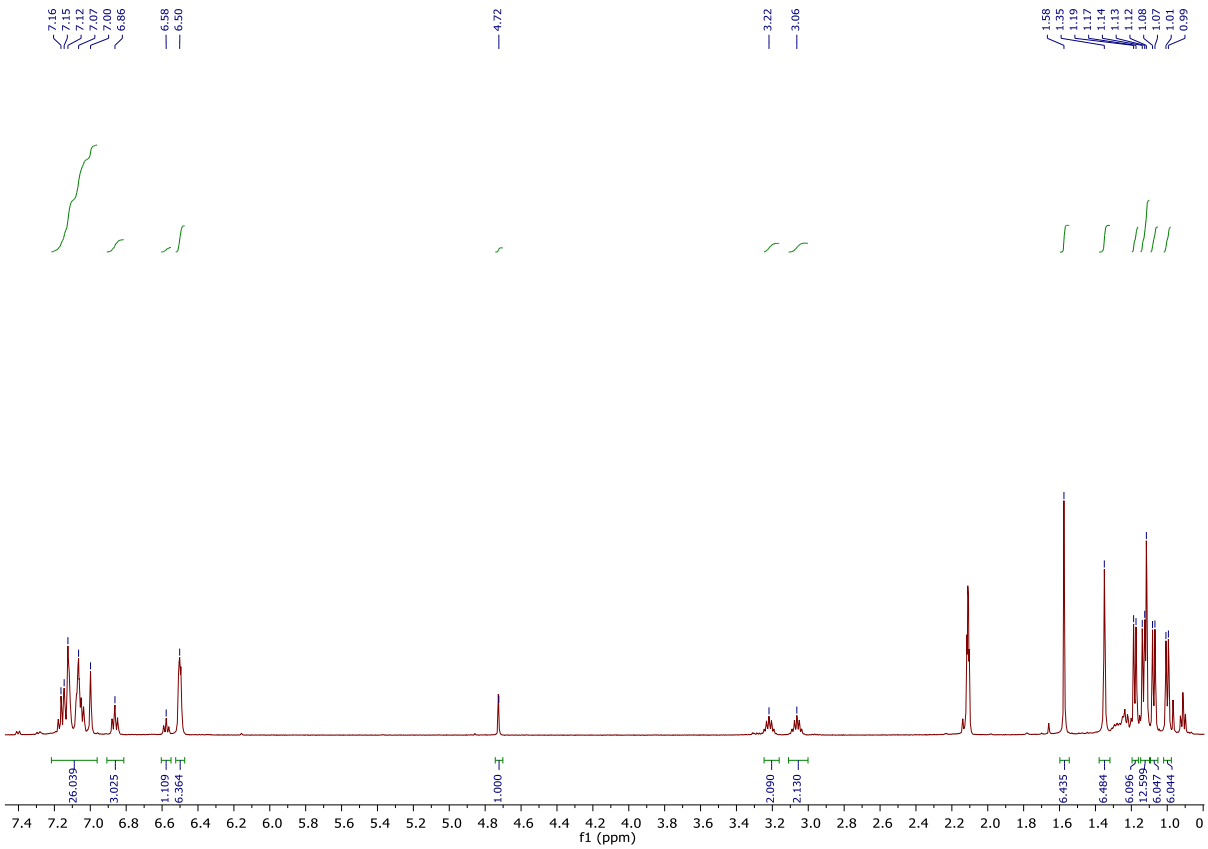


Figure S17: ^{1}H NMR spectrum (25°C, 500 MHz, d_8-tol) of compound **18$_{BN}$**.

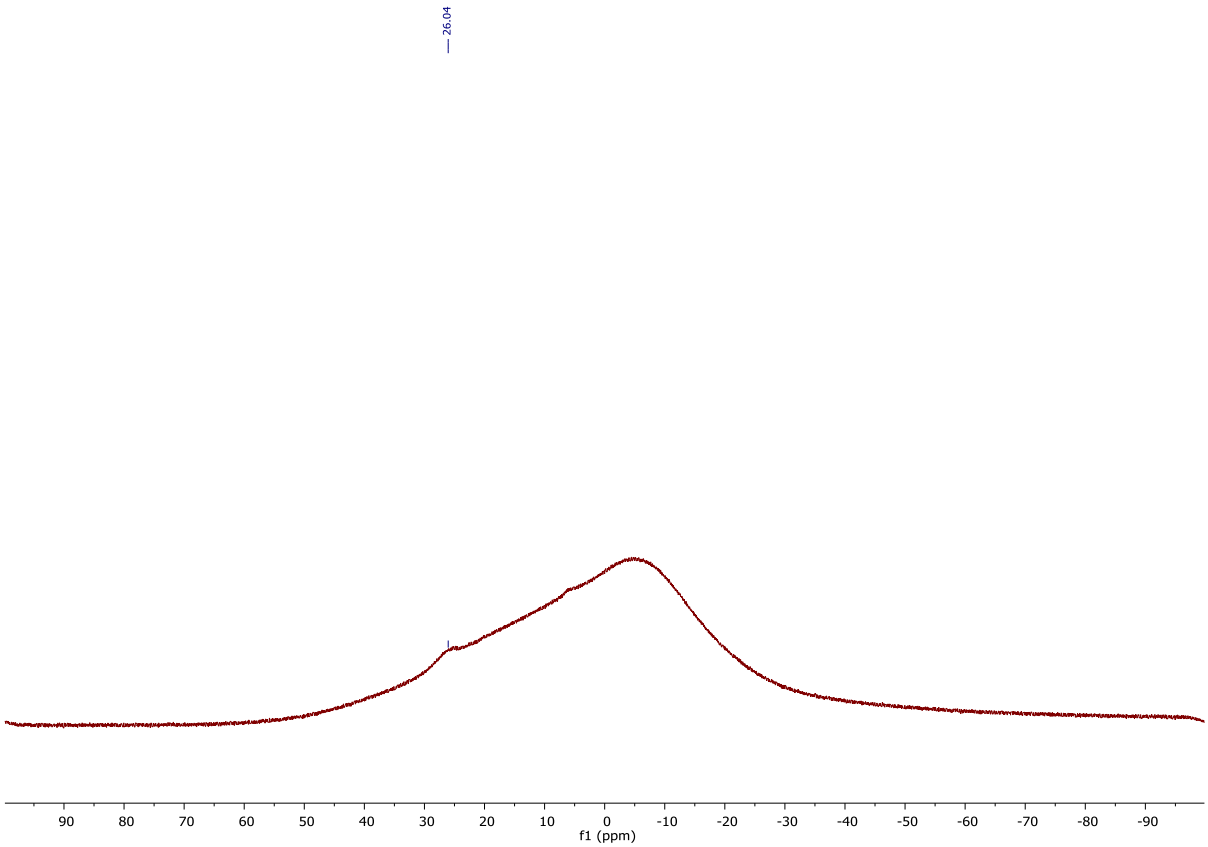


Figure S18: ^{11}B{^{1}H} NMR spectrum (25°C, 160 MHz, d_8-tol) of compound **18$_{BN}$**.

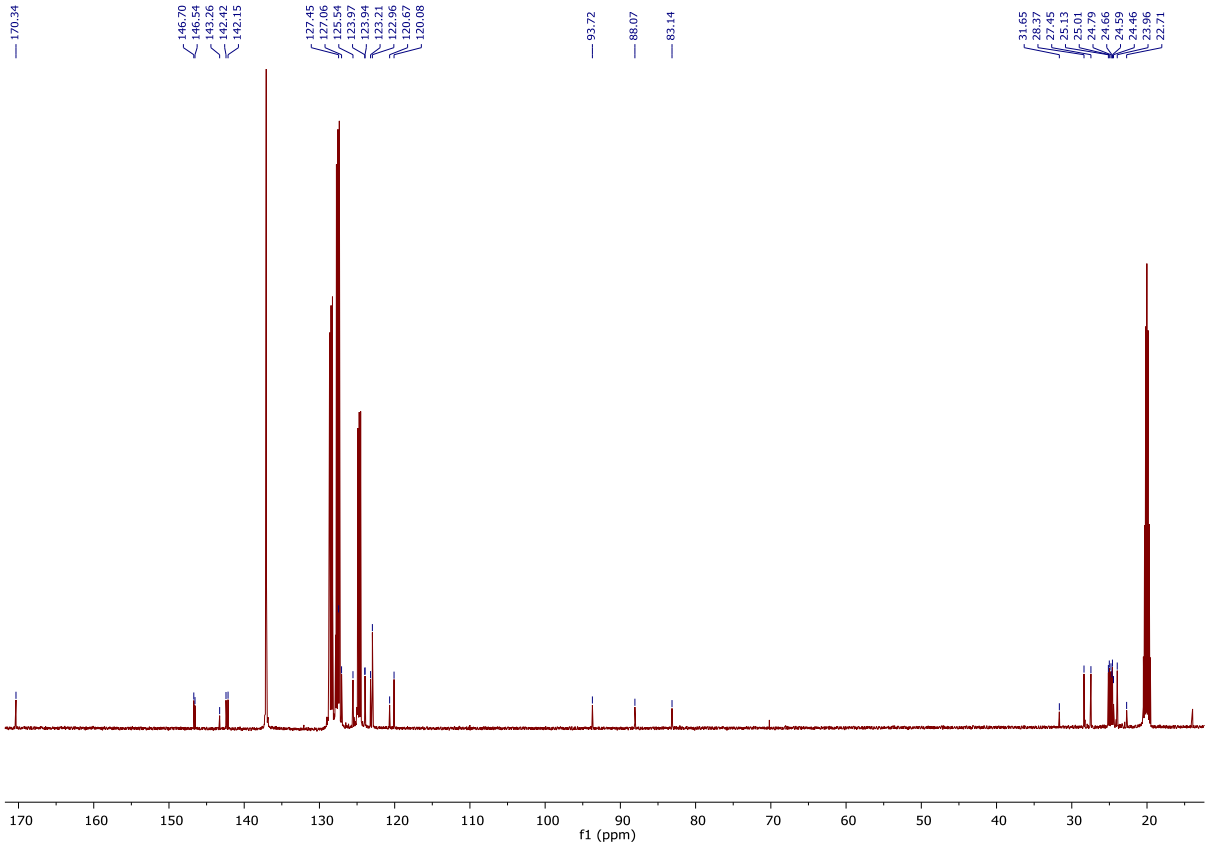


Figure S19: $^{13}C\{^{1}H\}$ NMR spectrum (25°C, 126 MHz, d_8-tol) of compound **18$_{BN}$**.

Compound 17$_{BC}$

A sample of compound **17$_{BN}$** in toluene-d_8 was prepared as described above and heated at 80°C for three hours. Volatiles were removed under vacuum to produce a colourless solid, which was washed with hexane and dried under vacuum. Recrystallization from hexane solution provided compound **17$_{BC}$** as colourless crystals (70.5 mg, 94.0%). ^{1}H NMR (500 MHz, d_8-toluene) δ 7.50 (d, 2H, J_{HH} = 7.6 Hz, aromatic C*H*), 7.14-7.02 (m, 13H, aromatic C*H*), 6.56 (t, 1H, J_{HH} = 7.1 Hz, aromatic C*H*), 5.25 (s, 1H, NC(CH$_3$)C*H*), 4.61 (s, 1H, NC*H*Ph), 3.65 (hept, 1H, J_{HH} = 6.6 Hz, C*H*(CH$_3$)$_2$), 3.38 (m, 3H, C*H*(CH$_3$)$_2$), 1.80 (s, 3H, C*H*$_3$), 1.74 (s, 3H, C*H*$_3$), 1.28 (m, 12H, C*H*$_3$), 1.23 (d, 3H, J_{HH} = 6.6 Hz, CH(C*H*$_3$)$_2$), 1.15 (d, 3H, J_{HH} = 6.6 Hz, CH(C*H*$_3$)$_2$), 0.94 (d, 3H, J_{HH} = 6.6 Hz, CH(C*H*$_3$)$_2$), 0.85 (d, 3H, J_{HH} = 6.6 Hz, CH(C*H*$_3$)$_2$), 0.58-0.51 (m, 9H, C*H*$_3$), 0.44 (s, 3H, C*H*$_3$) ppm. $^{13}C\{^{1}H\}$ NMR (126 MHz, d_8-toluene) δ 171.08 (N*C*(CH$_3$)CH), 170.48, 159.14, 146.90, 146.39, 144.85, 143.88, 142.71, 142.10, 128.49 (CH ar), 125.87, 124.93 (CH ar), 124.82 (CH ar), 124.27 (CH ar), 123.94 (CH ar), 112.78 (CH ar, CH at 6.6 ppm), 96.44 (NC(CH$_3$)*C*H), 88.80, 85.08, 49.43, 29.49 (*C*H(CH$_3$)$_2$), 29.07 (*C*H(CH$_3$)$_2$), 29.05 (*C*H(CH$_3$)$_2$), 28.49 (*C*H(CH$_3$)$_2$), 25.82 (*C*H$_3$), 25.32 (*C*H$_3$), 25.11 (*C*H$_3$), 24.91 (*C*H$_3$), 23.95 (*C*H$_3$), 23.82 (*C*H$_3$) ppm.

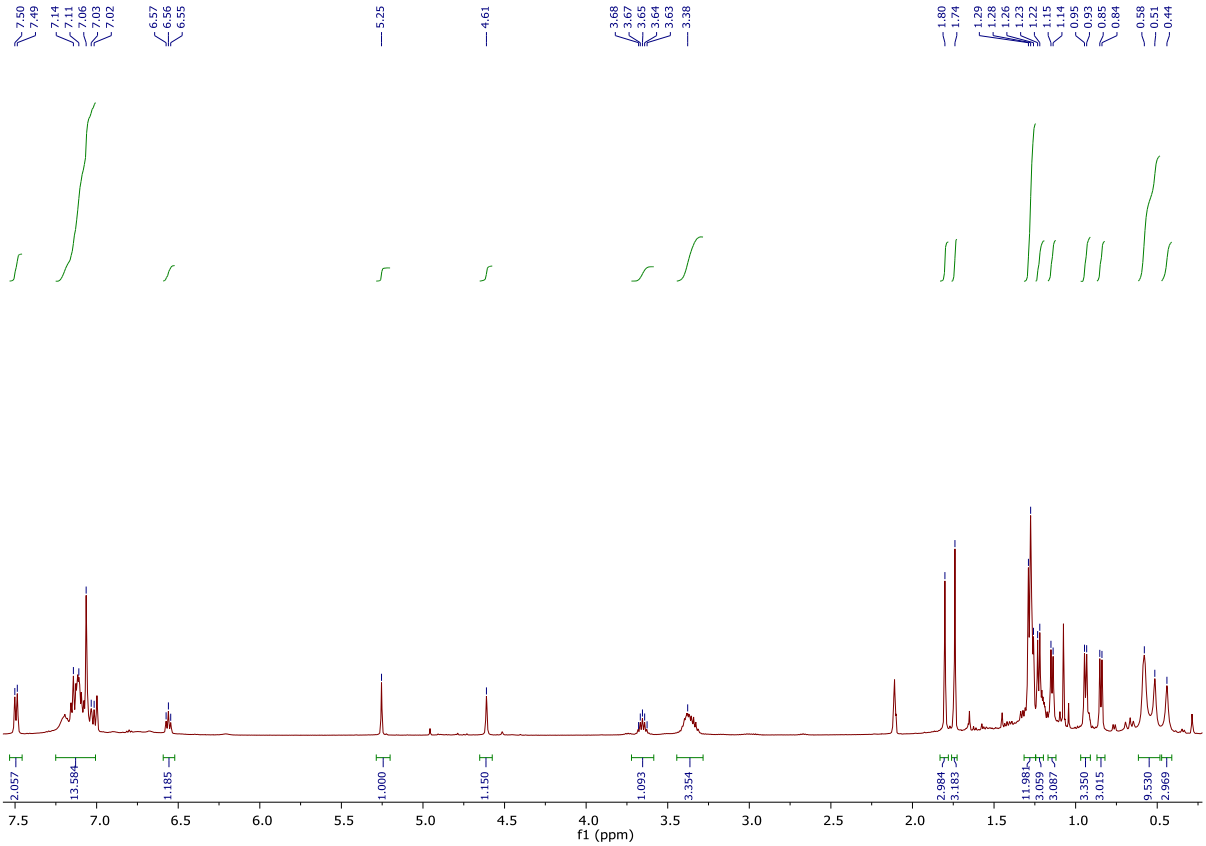


Figure S20: ^{1}H NMR spectrum (25°C, 500 MHz, d_8-tol) of compound **17$_{BC}$**.

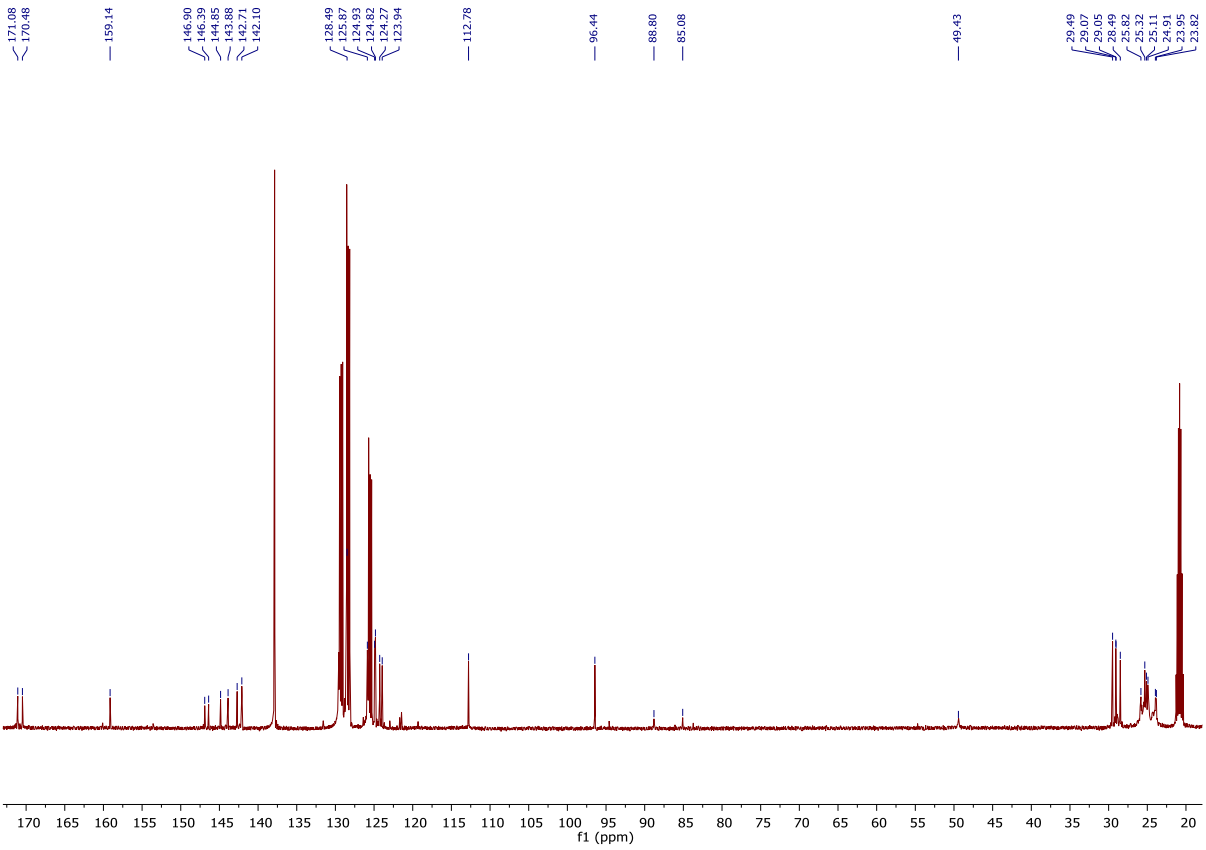


Figure S21: ^{13}C{^{1}H} NMR spectrum (25°C, 126 MHz, d_8-tol) of compound **17$_{BC}$**.

Compound $\mathbf{18_{Ph}}$

A sample of compound $\mathbf{18_{BN}}$ in toluene-d_8 was prepared as described above and heated at 80°C for three hours. Volatiles were removed under vacuum to produce a colourless solid, which was washed with hexane and dried under vacuum. Recrystallization from hexane solution provided compound $\mathbf{18_{Ph}}$ as colourless crystals. ^{1}H NMR (500 MHz, d_8-toluene) δ 7.49 (m, 2H, aromatic C*H*), 7.29 (m, 2H, aromatic C*H*), 7.16 (m, 4H, aromatic C*H*), 7.09 (s, 1H, aromatic C*H*), 6.96-6.85 (m, 6H, aromatic C*H*), 6.77 (m, 4H, aromatic C*H*), 6.54 (m, 2H, aromatic C*H*), 5.06 (s, 1H, NC(CH_3)C*H*), 3.63 (m, 1H, C*H*(CH_3)$_2$), 3.35 (m, 2H, C*H*(CH_3)$_2$), 2.50 (m, 1H, C*H*(CH_3)$_2$), 1.78 (s, 3H, C*H*$_3$), 1.55 (s, 6H, C*H*$_3$), 1.34 (d, 3H, C*H*$_3$), 1.29 (d, 3H, C*H*$_3$), 1.25 (d, 3H, C*H*$_3$), 1.21 (d, 3H, C*H*$_3$), 1.18 (d, 3H, C*H*$_3$), 1.00-0.97 (m, 9H, C*H*$_3$), 0.87 (s, 3H, C*H*$_3$), 0.77 (d, 3H, C*H*$_3$), 0.48 (d, 3H, C*H*$_3$) ppm. ^{11}B{^{1}H} NMR (160 MHz, d_8-toluene) δ 5.89 ppm. ^{13}C{^{1}H} NMR (126 MHz, d_8-toluene) δ 170.48 (N*C*(CH_3)CH), 169.94, 146.95, 146.53, 145.94, 142.78, 140.53, 132.07 (CH ar), 126.13 (CH ar), 125.86 (CH ar), 125.43 (CH ar), 124.34 (CH ar), 123.81 (CH ar), 123.24 (CH ar), 95.68 (NC(CH_3)*C*H), 82.82, 77.84, 31.65 (*C*H_3), 29.87 (*C*H(CH_3)$_2$), 28.38 (*C*H(CH_3)$_2$), 28.30 (*C*H(CH_3)$_2$), 28.10 (*C*H(CH_3)$_2$), 27.81 (*C*H_3), 26.04 (*C*H_3), 25.86 (*C*H_3), 25.66 (*C*H_3), 25.23 (*C*H_3), 24.91 (*C*H_3), 24.78 (*C*H_3), 24.37 (*C*H_3), 24.29 (*C*H_3), 24.15 (*C*H_3), 24.09 (*C*H_3), 23.90 (*C*H_3), 23.68 (*C*H_3), 23.51 (*C*H_3), 23.30 (*C*H_3), 22.71 (*C*H_3) ppm.

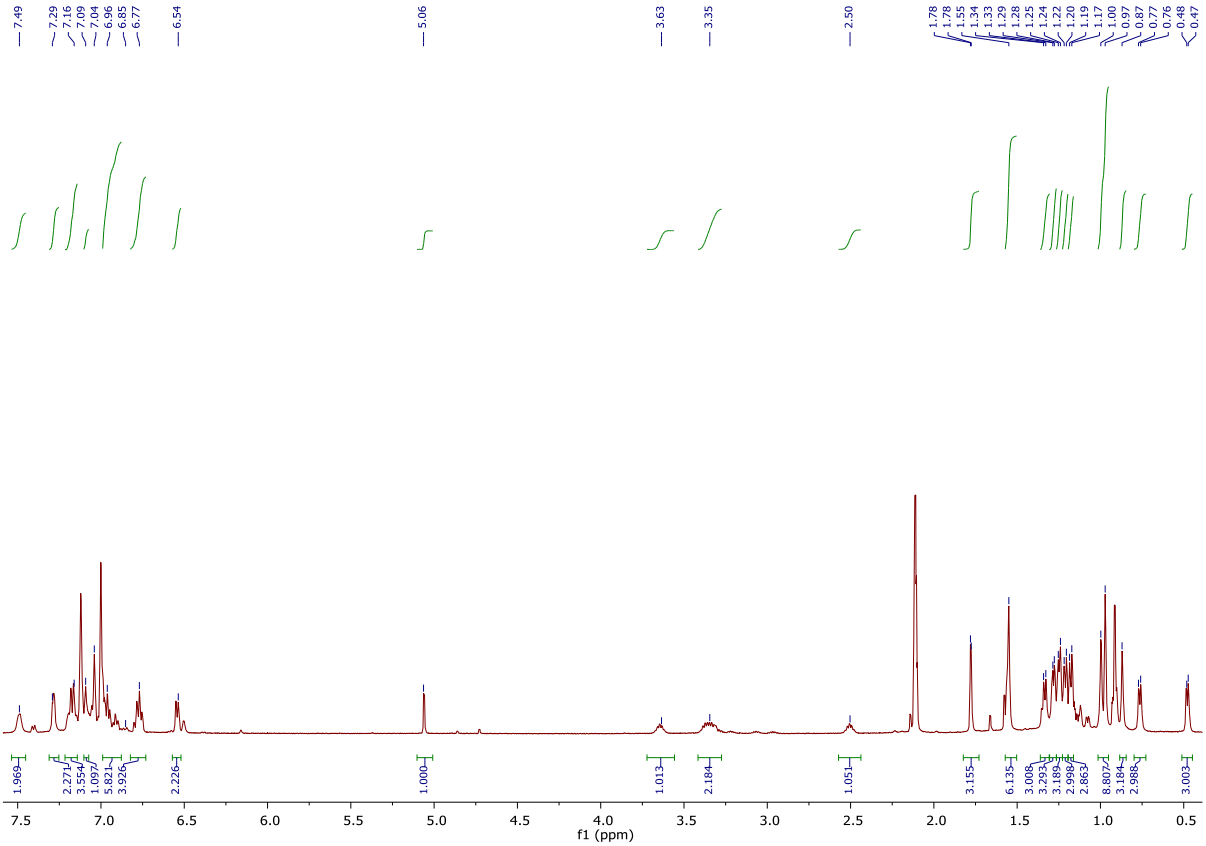


Figure S22: ^{1}H NMR spectrum (25°C, 500 MHz, d_8-tol) of compound **18$_{Ph}$.**

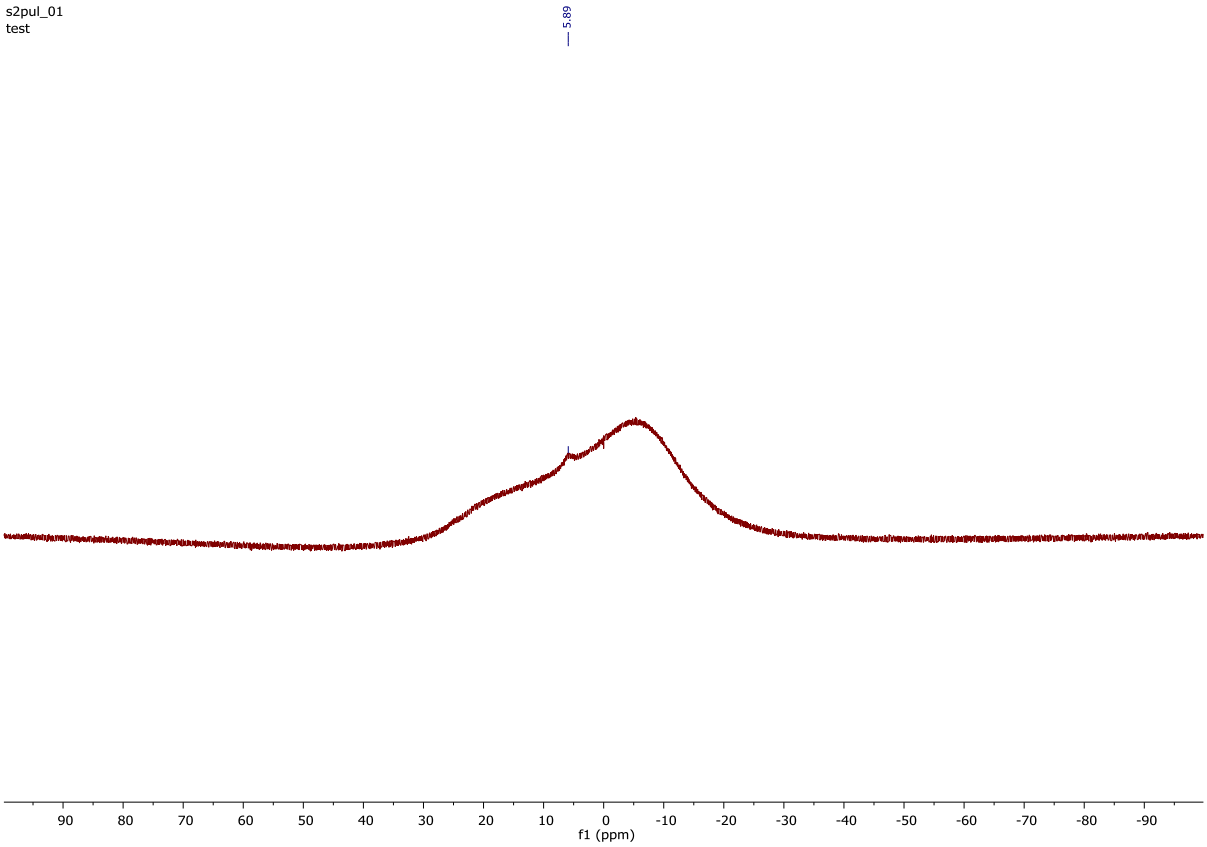


Figure S23: ^{11}B{^{1}H} NMR spectrum (25°C, 160 MHz, d_8-tol) of compound **18$_{Ph}$.**

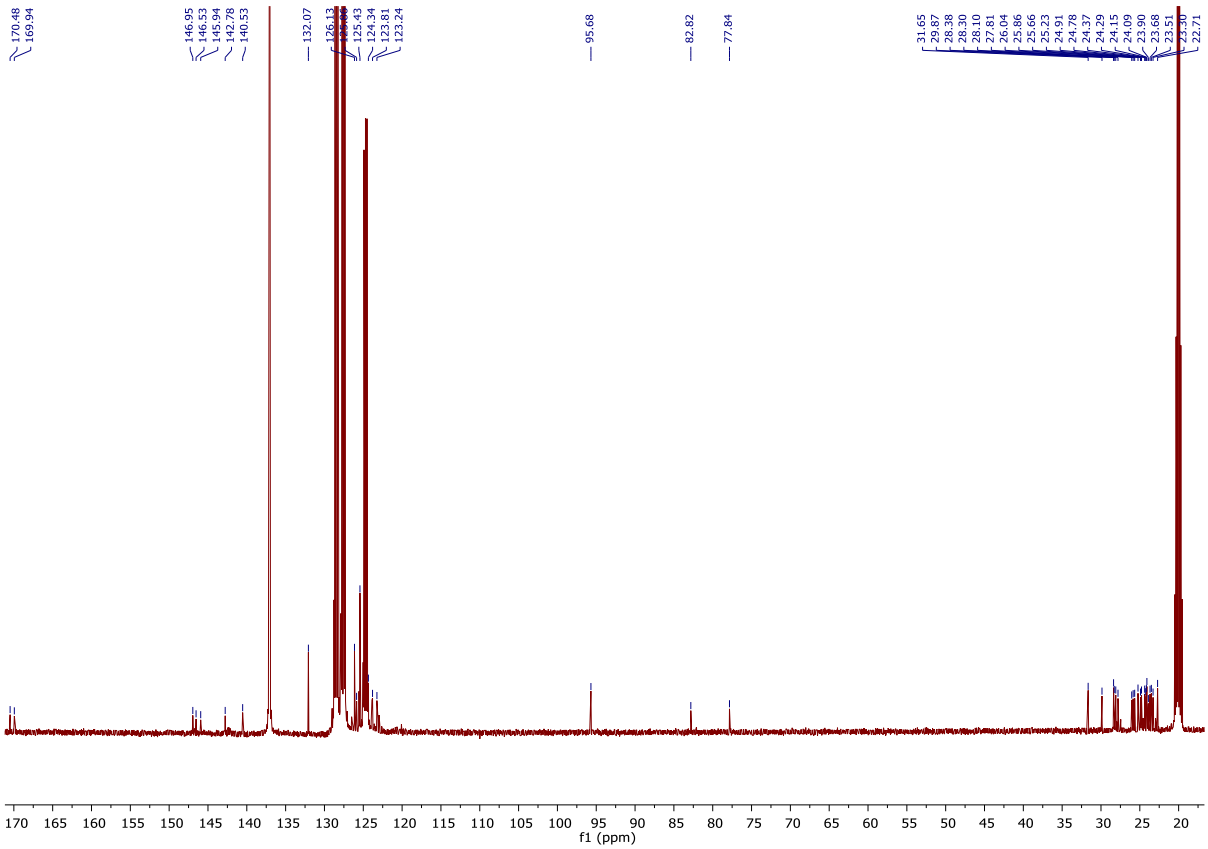


Figure S24: $^{13}C\{^{1}H\}$ NMR spectrum (25°C, 126 MHz, d_8-tol) of compound **18$_{Ph}$**.

Variable temperature kinetic analysis of the isomerization reactions of compounds 17_{BN} to 17_{BC} and 18_{BN} to 18_{Ph}

All NMR Data were recorded on a Bruker AV400 NMR operating at 400.13 MHz (^{1}H) and were recorded at 323 K unless stated otherwise. All data were processed using MestreNova data analysis software. In a glovebox, d_8-toluene solutions [0.05-0.07 M] of **17_{BN}** and **18_{BN}** were prepared in J. Young NMR tubes as described above. The NMR tubes were sealed, removed from the glovebox, and loaded into the NMR spectrometer which had been preheated to the chosen temperature. ^{1}H NMR spectra were recorded at regular intervals. Reaction kinetics were monitored using the intensity changes associated with the disappearance of the singlet resonances corresponding to the methine CH protons of the BDI ligand converting of the starting materials. Data were recorded at 60, 65, 70 and 75°C and were monitored by variable temperature ^{1}H NMR spectroscopy until 80% conversion (>3 half-lives) into the isomerized products had been achieved. Data were normalised against the initial substrate concentration $[Substrate]_{t=0}$ so that:

$$Ct = \frac{[Substrate]_{t=0}}{[Substrate]_{t=0} + [Substrate]_t}$$

Reaction rates were derived from the plot of Ln(Ct) vs. time by using linear trendlines generated by Microsoft Excel software.

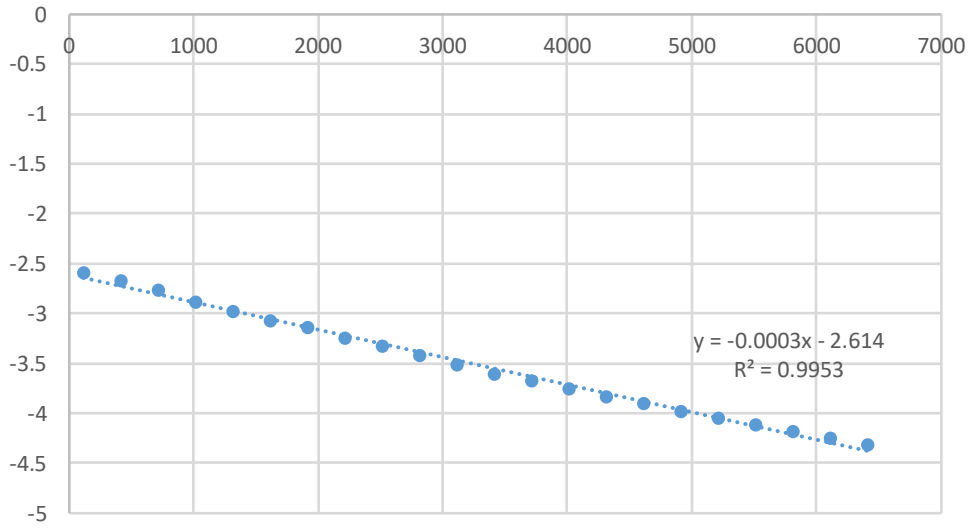


Figure S25: First order rate plot of ln([**Ct**]$_t$) vs time for consumption of **17_{BN}** at 60°C.

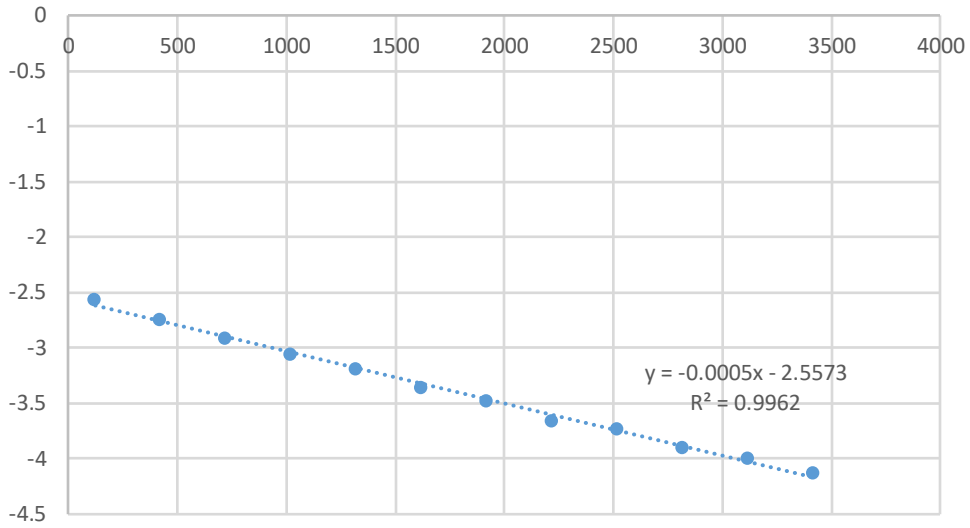


Figure S26: First order rate plot ln([**Ct**]$_t$) vs time for consumption of **17$_{BN}$** at 65°C.

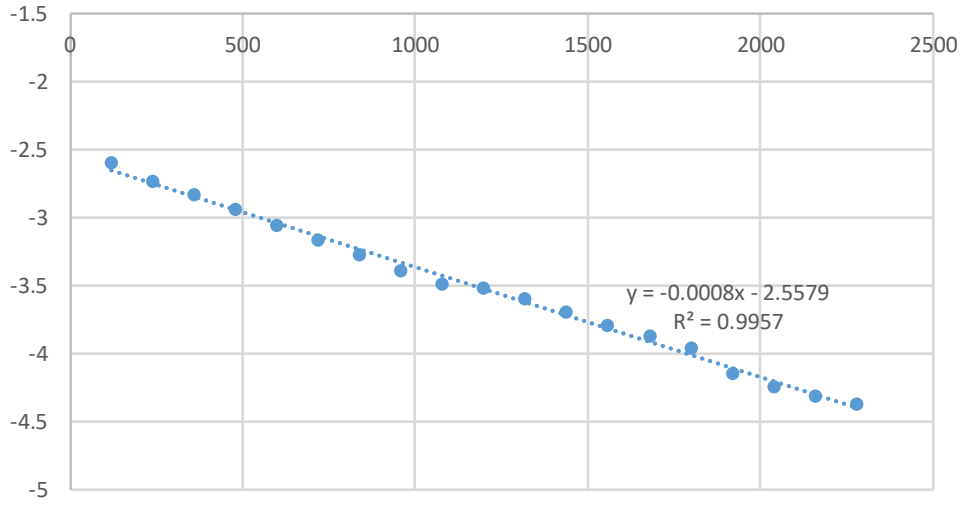


Figure S27: First order rate plot ln([**Ct**]$_t$) vs time for consumption of **17$_{BN}$** at 70°C.

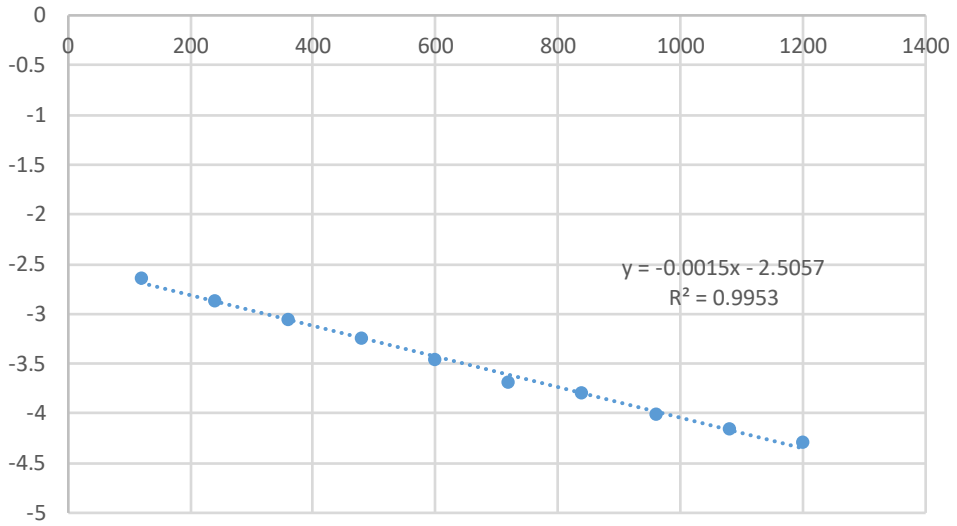


Figure S28: First order rate plot ln([**Ct**]$_t$) vs time for consumption of **17$_{BN}$** at 75°C.

Actual temp (K)	1/T	-k (s-1)	ln(k)
337.44717	0.002963427	0.0003	-8.111728083
343.09322	0.00291466	0.0005	-7.60090246
348.73927	0.002867472	0.0008	-7.13089883
354.38532	0.002821787	0.0015	-6.502290171

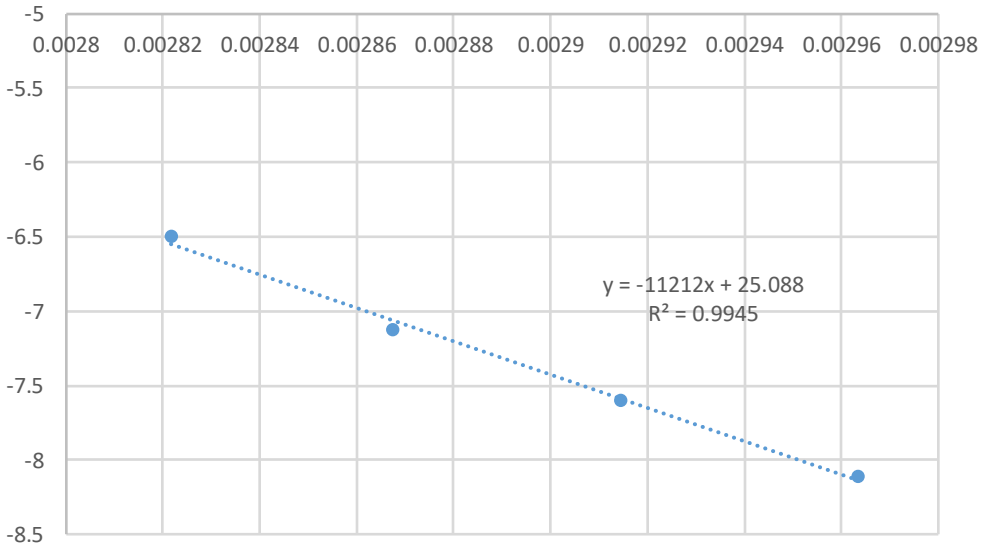


Figure S29: Arrhenius Plot - Ln(k) vs 1/T for conversion of **17$_{BN}$** to **17$_{BC}$**.

Actual temp (K)	1/T	-k (s-1)	kh/kBT	ln(kh/kbT)
337.44717	0.002963427	0.0003	4.26666E-17	-37.6931
343.09322	0.00291466	0.0005	6.99407E-17	-37.1989
348.73927	0.002867472	0.0008	1.10093E-16	-36.7452
354.38532	0.002821787	0.0015	2.03136E-16	-36.1327

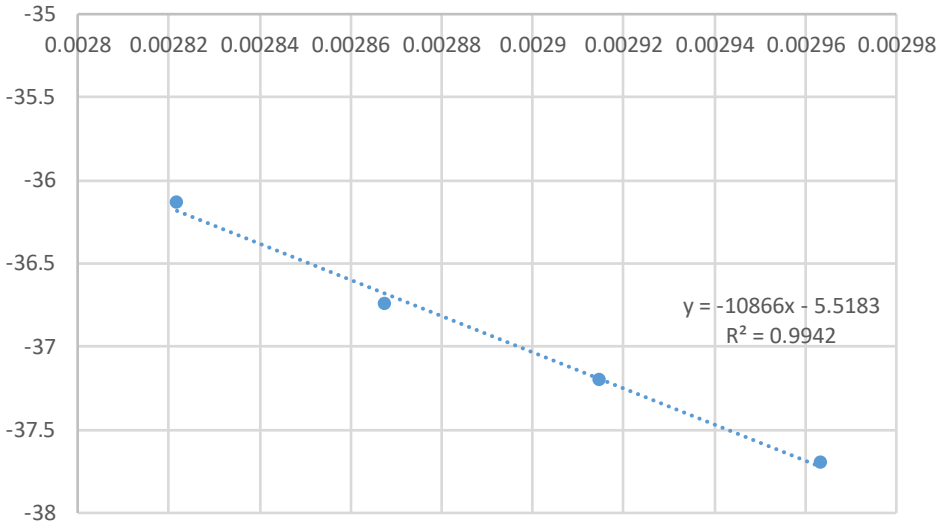


Figure S30: Eyring Plot - – Ln(k/T) vs 1/T for conversion of **17**$_{BN}$ to **17**$_{BC}$.

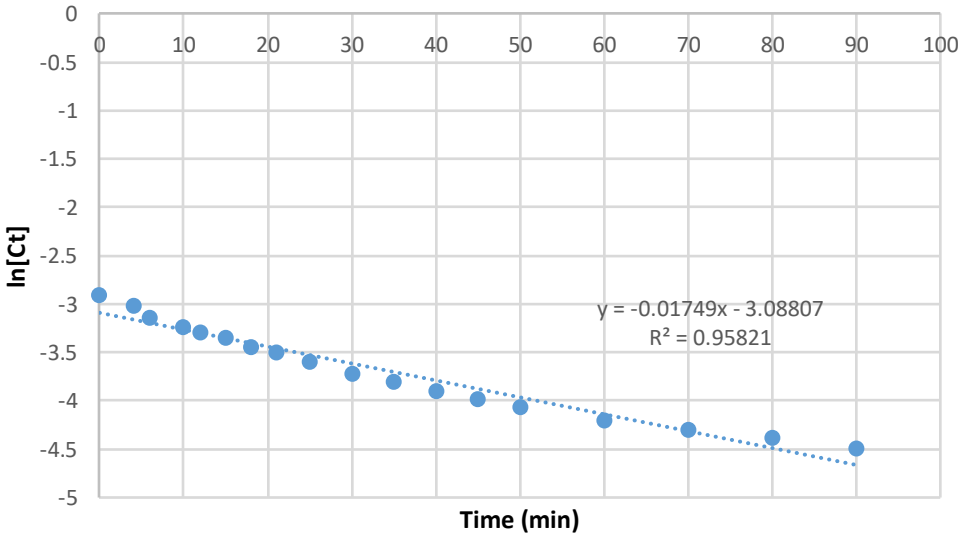


Figure S31: First order rate plot of ln([**Ct**]$_t$) vs time for consumption of **18**$_{BN}$ at 60°C.

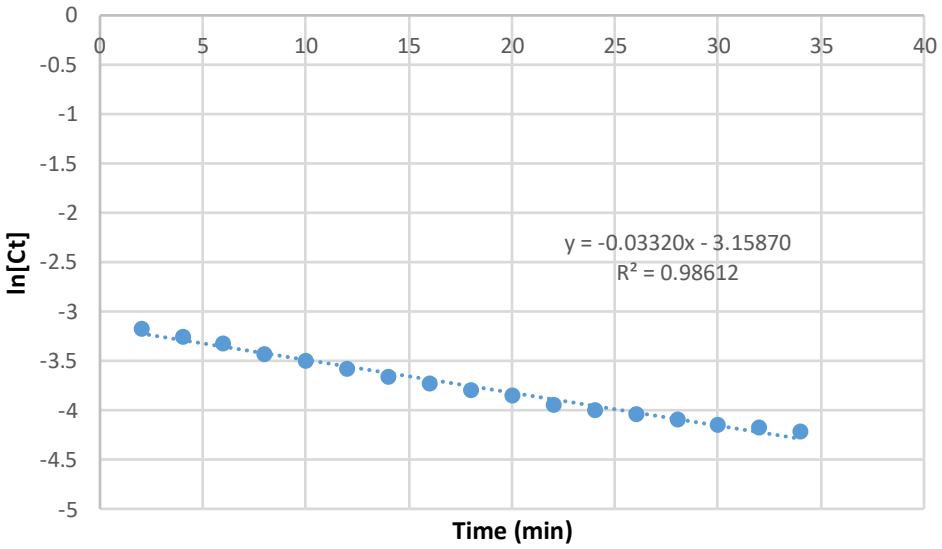


Figure S32: First order rate plot of ln([**Ct**]$_t$) vs time for consumption of **18**$_{BN}$ at 65°C.

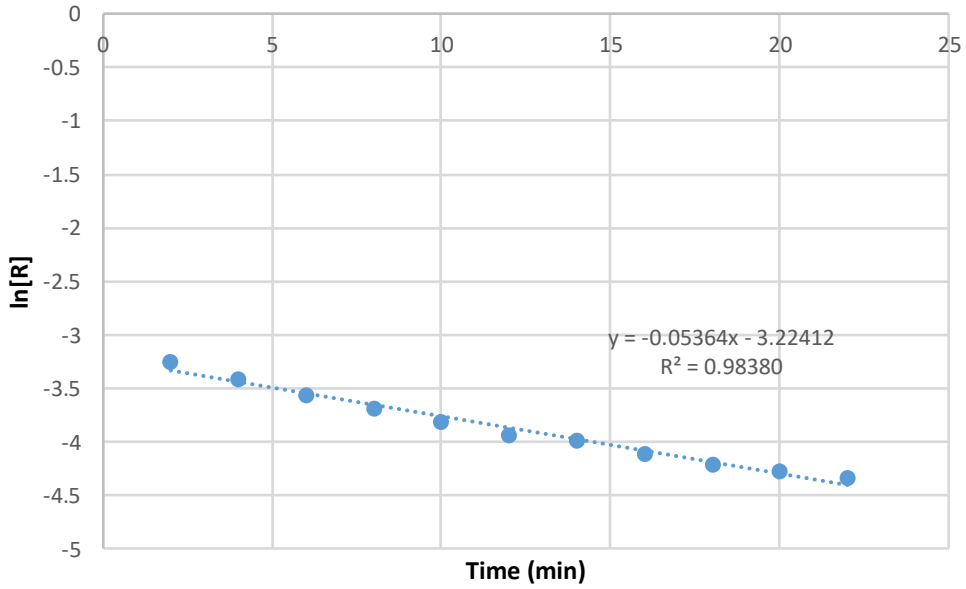


Figure S33: First order rate plot of ln([**Ct**]$_t$) vs time for consumption of **18**$_{BN}$ at 70°C.

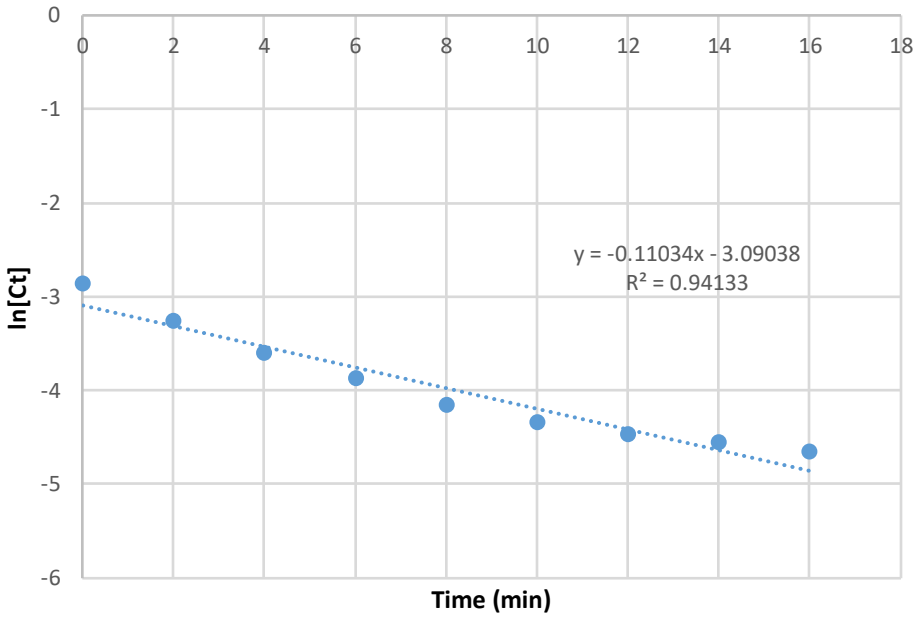


Figure S34: First order rate plot of ln([**Ct**]$_t$) vs time for consumption of **18**$_{BN}$ at 75°C.

Actual temp (K)	1/T	-k (s-1)	ln(k)
337.44717	0.00296343	0.00029	-8.14563
343.09322	0.00291466	0.00055	-7.50559
348.73927	0.00286747	0.00089	-7.02429
354.38532	0.00282179	0.00184	-6.29799

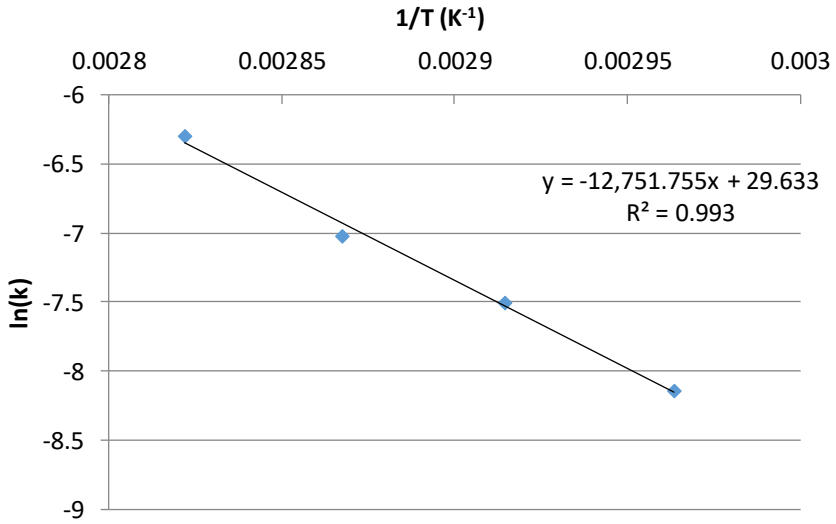


Figure S35: Arrhenius Plot - Ln(k) vs 1/T for conversion of **18**$_{BN}$ to **18**$_{Ph}$.

Actual temp (K)	1/T	-k (s-1)	kh/kBT	ln(kh/kBT)
337.4472	0.002963427	0.00029	4.12443E-17	-37.727
343.0932	0.00291466	0.00055	7.69348E-17	-37.1036
348.7393	0.002867472	0.00089	1.22479E-16	-36.6386
354.3853	0.002821787	0.00184	2.49181E-16	-35.9284

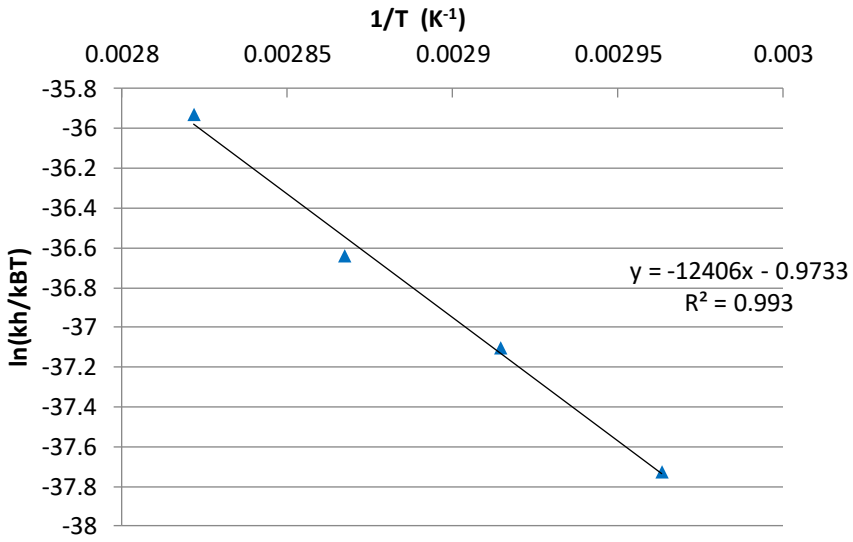


Figure S36: Eyring Plot - Ln(k/T) vs 1/T for conversion of **18**$_{BN}$ to **18**$_{Ph}$.

Single Crystal X-ray Diffraction analysis.

Single Crystal X-ray diffraction data for compounds **11**, **14**, **15$_{BN}$**, **16$_{BN}$**, **17$_{BN}$**, **18$_{BN}$**, **17$_{BC}$** and **18$_{Ph}$** were collected using Cu*K*α (λ = 1.54184 Å) on a SuperNova, Dual Cu at zero, EosS2 diffractometer. The crystals were kept at 150(2) K during data collections. The structures were solved using Olex2,[2] and refined with the ShelXL[3] refinement package using Least Squares minimisation.

For **15$_{BN}$** The ADPs pertaining to C37-C41 indicate some disorder in this region of the model. However, attempts to model this did not readily improve the convergence in a tangible way and, hence, were abandoned.

The asymmetric unit in **16$_{BN}$** contains 2 molecules of the magnesium complex. The Dipp moiety attached to N2 was modelled for 60:40 disorder over 2 proximate sites. There may also be some less well resolved disorder pertaining to the Dipp based on C6, but this has not been sculpted into the motif as presented. Phenyl rings in the disordered components were treated as rigid hexagons in the refinement, and ADP restraints were included for all fractional-occupancy carbon atoms.

In addition to one molecule of the magnesium complex, the asymmetric unit in **18$_{BN}$** also contains ½ of a hexane molecule. The latter is located proximate to an inversion centre that is present in the space group, which serves to generate the remainder of the solvent, by symmetry.

The isopropyl group based on C12 of **18$_{Ph}$** was modelled to take account of 55:45 disorder. C-C distance restraints plus some ADP restraints, were employed in the disordered region to assist convergence.

Table S1: Single Crystal X-ray Data Parameters for compounds **11**, **14**, **15$_{BN}$**, and **16$_{BN}$**.

Compound	**11**	**14**	**15$_{BN}$**	**16$_{BN}$**
Empirical formula	$C_{44}H_{71}BMgN_4O_2$	$C_{54}H_{75}BMgN_4O_2$	$C_{46}H_{68}BMgN_3O_2$	$C_{92}H_{136}B_2Mg_2N_6O_4$
Formula weight	723.16	847.30	730.15	1460.30
Temperature/K	150.01(10)	291.55(10)	150.01(10)	150.00(10)
Crystal system	orthorhombic	monoclinic	orthorhombic	monoclinic
Space group	*Pbca*	*Cc*	*Pbca*	$P2_1/c$
a/Å	21.3924(2)	18.6101(2)	20.5267(1)	23.0251(3)
b/Å	18.2770(1)	15.4868(2)	19.7717(1)	18.0591(2)
c/Å	22.9162(3)	17.9575(2)	21.7073(1)	22.6756(2)
α/°	90	90	90	90
β/°	90	103.0650(10)	90	112.2850(10)
γ/°	90	90	90	90
Volume/Å^3	8959.98(15)	5041.57(10)	8809.86(7)	8724.55(18)
Z	8	4	8	4
ρ_{calc} g/cm^3	1.072	1.116	1.101	1.112
μ/mm^{-1}	0.621	0.623	0.632	0.638
F(000)	3168.0	1840.0	3184.0	3184.0
Crystal size/mm^3	0.371 × 0.099 × 0.092	0.323 × 0.099 × 0.084	0.402 × 0.304 × 0.279	0.699 × 0.222 × 0.179
2Θ range /°	7.44 to 146.744	7.508 to 146.708	7.424 to 146.902	6.416 to 146.978
Reflections collected	119218	29358	126347	125364
Independent reflections	9008 [R_{int} = 0.0690]	7701 [R_{int} = 0.0414]	8859 [R_{int} = 0.0510]	17508 [R_{int} = 0.0515]
Data/restraints/parameters	9008/0/489	7701/2/579	8859/0/493	17508/162/1077
Goodness-of-fit on F^2	1.067	1.040	1.032	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0653, wR_2 = 0.1585	R_1 = 0.0383, wR_2 = 0.1013	R_1 = 0.0448, wR_2 = 0.1168	R_1 = 0.0592, wR_2 = 0.1484
Final R indexes [all data]	R_1 = 0.0765, wR_2 = 0.1655	R_1 = 0.0402, wR_2 = 0.1056	R_1 = 0.0480, wR_2 = 0.1198	R_1 = 0.0685, wR_2 = 0.1545
Largest diff. peak/hole/e Å^{-3}	0.42/-0.26	0.28/-0.21	0.55/-0.32	0.46/-0.42

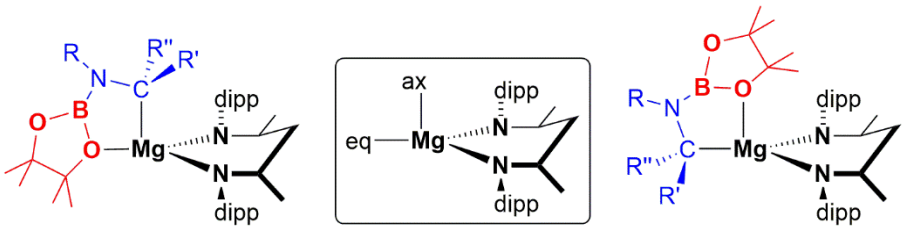
Table S2: Single Crystal X-ray Data Parameters for compounds **17$_{BN}$**, **18$_{BN}$**, **17$_{BC}$** and **18$_{Ph}$**.

Compound	**17$_{BN}$**	**18$_{BN}$**	**17$_{BC}$**	**18$_{Ph}$**
Empirical formula	$C_{48}H_{64}BMgN_3O_2$	$C_{57}H_{75}BMgN_3O_2$	$C_{48}H_{64}BMgN_3O_2$	$C_{54}H_{68}BMgN_3O_2$
Formula weight	750.14	869.32	750.14	826.23
Temperature/K	149.9(4)	150.00(10)	150.00(10)	149.9(3)
Crystal system	triclinic	monoclinic	monoclinic	monoclinic
Space group	*P*-1	$P2_1/c$	$P2_1/c$	$P2_1/n$
a/Å	11.0413(8)	11.9947(3)	11.8747(5)	12.10496(12)
b/Å	11.5237(7)	21.8853(5)	20.2674(6)	22.2539(2)
c/Å	17.5561(11)	19.2733(3)	18.1008(7)	18.11019(16)
α/°	82.531(5)	90	90	90
β/°	82.771(6)	98.837(2)	90.243(4)	98.9416(9)
γ/°	84.240(5)	90	90	90
Volume/Å^3	2189.2(2)	4999.33(19)	4356.3(3)	4819.28(8)
Z	2	4	4	4
ρ_{calc} g/cm^3	1.138	1.155	1.144	1.139
μ/mm^{-1}	0.652	0.636	0.655	0.637
F(000)	812.0	1884.0	1624.0	1784.0
Crystal size/mm^3	0.135 × 0.09 × 0.025	0.12 × 0.094 × 0.068	0.149 × 0.124 × 0.078	0.217 × 0.192 × 0.085
2Θ range /°	5.11 to 140.342	6.152 to 146.95	6.548 to 147.696	6.34 to 146.352
Reflections collected	14171	36973	54653	60632
Independent reflections	8031 [R_{int} = 0.0703]	9893 [R_{int} = 0.0565]	8726 [R_{int} = 0.1131]	9606 [R_{int} = 0.0657]
Data/restraints/parameters	8031/0/510	9893/0/592	8726/0/510	9606/16/587
Goodness-of-fit on F^2	1.033	1.033	1.056	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0684, wR_2 = 0.1173	R_1 = 0.0525, wR_2 = 0.1189	R_1 = 0.0675, wR_2 = 0.1491	R_1 = 0.0450, wR_2 = 0.1076
Final R indexes [all data]	R_1 = 0.1234, wR_2 = 0.1431	R_1 = 0.0783, wR_2 = 0.1316	R_1 = 0.0919, wR_2 = 0.1620	R_1 = 0.0561, wR_2 = 0.1142
Largest diff. peak/hole/e Å^{-3}	0.32/-0.27	0.69/-0.33	0.36/-0.37	0.24/-0.23

Computational Details / Methodology

DFT calculations were run with Gaussian 09 (Revision D.01). [4]The Mg center was described with the Stuttgart RECPs and associated basis sets,[5] and 6-31G** basis sets were used for all other atoms (BS1).[6] Initial BP86[7] optimizations were performed using the 'grid = ultrafine' option, with all stationary points being fully characterized via analytical frequency calculations as either minima (all positive eigenvalues) or transition states (one negative eigenvalue). IRC calculations and subsequent geometry optimizations were used to confirm the minima linked by each transition state. All energies were recomputed with a larger basis set (BS2) featuring 6-311++G** on all atoms. Corrections for the effect of toluene (ε = 2.3741) solvent were run using the polarizable continuum model and BS1.[8] Single-point dispersion corrections to the BP86 results employed Grimme's D3 parameter set with Becke-Johnson damping as implemented in Gaussian.[9]

Computed intermediate geometries were predominately taken from X-ray crystallography structure solutions. However, to confirm the lowest conformation had crystallised for each *N*-alkyl imine, the Ph and H positions were swapped at C for imines ^{n}BuNCHPh and ^{t}BuNCHPh (complexes **15** and **16**), with the lowest energy conformer included in the results herein. Likewise, due to the backbone chirality of the nacnac ligand, there are actually two different coordination conformations at the Mg center for the asymmetric "Bpin-imine" substrate, where either the Bpin is bound in the equatorial (eq) or axial (ax) position (see Scheme S1 below). Again both conformations were computed and the more stable intermediates are reported in the results herein.



Scheme S1: The two different coordination environments for the "Bpin-imine" substrate at the Mg center, either equatorial (eq) or axial (ax).

Breakdown of Energy Contributions

The following tables detail the evolution of the relative energies as the successive corrections to the initial SCF energy are included. Terms used are:

$\mathbf{\Delta E_{BS1}}$	SCF energy computed with the BP86 functional with BS1
$\mathbf{\Delta H_{BS1}}$	Enthalpy at 0 K with BS1
$\mathbf{\Delta G_{BS1}}$	Free energy at 298.15 K and 1 atm with BS1
$\mathbf{\Delta G_{BS1/tol}}$	Free energy corrected for toluene solvent with BS1
$\mathbf{\Delta G_{BS1/tol+D3}}$	Free energy corrected for toluene and dispersion effects with BS1
$\mathbf{\Delta G_{tol}}$	Free energy corrected for basis set (BS2), dispersion effects and toluene solvent

In each case the final data used in the main article is highlighted in bold.

Table S3: Relative energies (kcal/mol) for computed structures. Data in bold are those used in the main text. All energies are quoted relative to **5** at 0.0 kcal/mol.

	ΔE_{BS1}	ΔH_{BS1}	ΔG_{BS1}	$\Delta G_{BS1/tol}$	$\Delta G_{BS1/tol+D3}$	ΔE_{BS2}	ΔG_{tol}
5	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
8	-46.7	-44.5	-26.7	138.9	-55.0	-42.0	**-50.2**
11	-44.3	-43.2	-44.3	125.3	-34.1	-42.3	**-32.0**
12	-54.5	-53.7	-57.2	112.3	-41.9	-53.2	**-40.7**
12_{BN}	-47.0	-46.0	-47.1	122.7	-39.7	-45.6	**-38.3**
12_{BC}	-39.3	-38.3	-39.2	130.0	-34.4	-37.6	**-32.8**
TS(5-5b)	15.3	14.8	13.5	214.0	18.4	16.2	**19.4**
5b	6.8	6.1	1.8	201.7	11.4	6.6	**11.1**
5c	1.0	-0.4	-21.2	146.2	16.5	-2.6	**12.9**
15_{BN}	-36.6	-36.0	-39.5	123.4	-45.3	-37.1	**-45.8**
15_{BC}	-43.3	-42.4	-44.6	124.5	-38.5	-44.6	**-39.8**
TS(15_{BN}-15_{BCN})	-10.3	-10.1	-12.6	156.43	-6.7	-11.1	**-7.5**
15_{BCN}	-26.4	-25.6	-29.3	140.0	-20.3	-26.1	**-20.0**
TS(15_{BCN}-15_{BC})	-15.6	-15.1	-17.5	152.1	-10.4	-16.0	**-10.8**
16_{BN}	-30.1	-28.9	-30.4	138.9	-28.7	-29.9	**-28.5**
16_{BC}	-33.6	-32.5	-33.3	135.8	-34.1	-34.4	**-34.9**
TS(16_{BN}-16_{BCN})	-3.8	-3.6	-4.6	164.3	-3.9	-4.3	**-4.3**
16_{BCN}	-16.9	-15.9	-17.4	151.8	-14.5	-16.0	**-13.6**
TS(16_{BCN}-16_{BC})	-7.0	-6.8	-8.1	161.3	-4.4	-7.3	**-4.7**
5·PhNCHPh	0.2	0.9	10.5	210.8	1.1	2.1	**3.0**
TS(5-17_{BN})1	18.9	20.3	36.6	237.3	8.4	21.8	**11.3**
INT(5-17_{BN})	15.7	17.4	34.0	235.1	3.1	19.2	**6.7**
TS(5-17_{BN})2	27.3	28.3	45.0	245.3	10.8	30.0	**13.4**
17_{BN}	-36.5	-35.7	-38.7	130.4	-33.9	-37.4	**-34.8**
TS(17_{BN}-17_{BCN})	-9.3	-9.5	-12.1	156.3	-7.1	-10.8	**-8.6**
17_{BCN}	-23.5	-22.8	-25.1	143.9	-22.4	-24.0	**-22.8**
TS(17_{BCN}-17_{BC})	-18.6	-18.1	-19.8	149.2	-17.7	-19.6	**-18.7**
17_{BC}	-37.5	-36.4	-38.1	130.8	-36.8	-39.1	**-38.4**
TS(5-17_{BCN})	37.1	37.7	53.9	254.6	26.2	41.2	**30.3**
17_{BCN}-BpinBu	-3.7	-2.3	12.0	211.4	-14.2	-1.7	**-12.2**
18_{BN}	-28.9	-27.6	-26.8	142.2	-36.6	-29.5	**-37.1**
TS(18_{BN}-18_{BCN})	-10.2	-10.3	-10.4	159.0	-15.8	-9.9	**-15.5**
18_{BCN}	-16.3	-15.7	-15.3	154.2	-24.6	-15.5	**-23.8**
TS(18_{BCN}-18_{BC})	-10.9	-10.8	-9.9	159.3	-17.8	-10.4	**-17.2**
18_{BC}	-24.9	-24.1	-24.1	144.5	-30.1	-25.3	**-30.5**
TS(18_{BC}-18_{BPh})	-4.3	-4.9	-4.4	165.3	-10.9	-4.3	**-10.9**
18_{BPh}	-30.5	-30.2	-30.7	138.9	-36.8	-30.3	**-36.6**

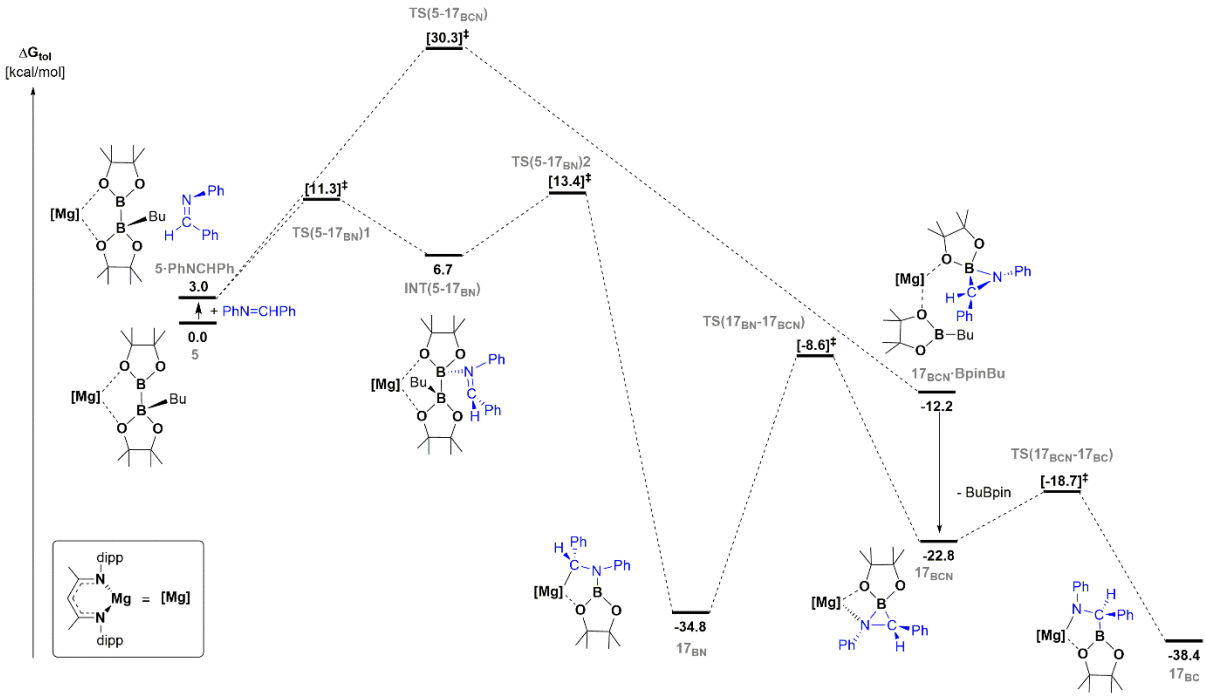


Figure S37: – DFT calculated free energy (kcal mol^{-1}) profile for the reaction of imine PhN=CHPh with compound **5** (in toluene), relative to **5** and the free substrates.

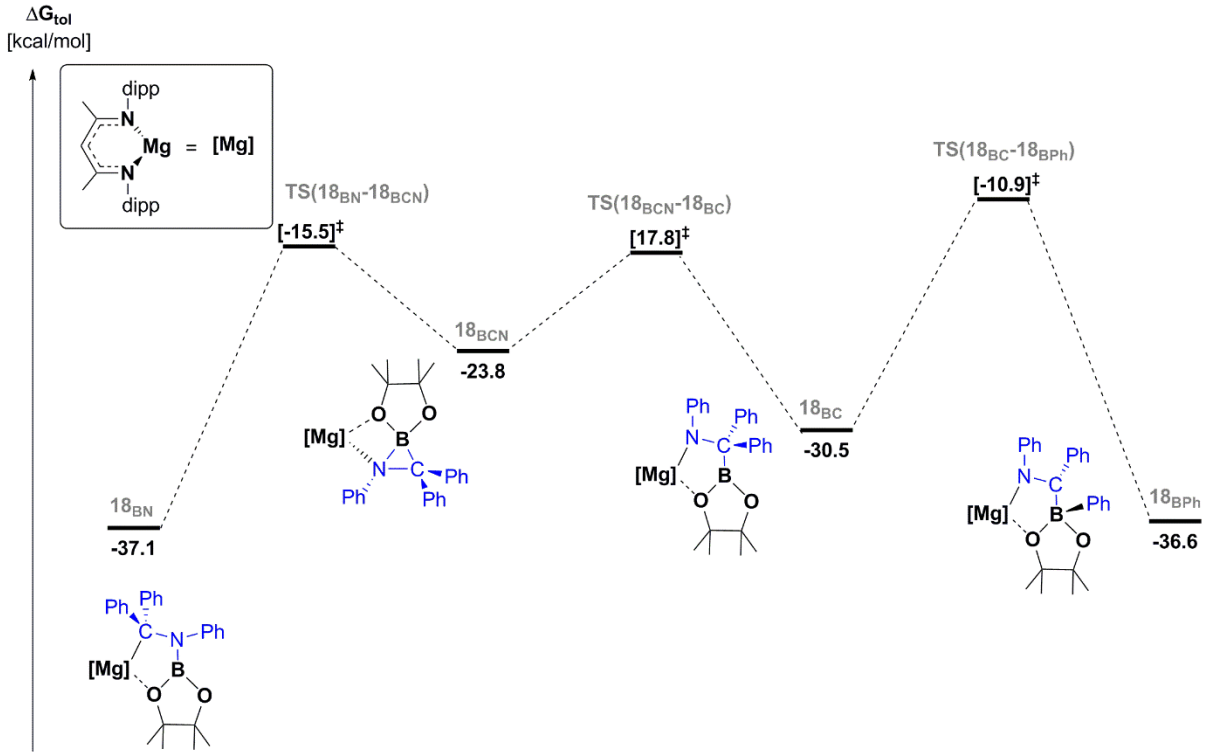


Figure S38: DFT calculated free energy (kcal mol^{-1}) profile for intermediates leading to **18$_{Ph}$** formed after PhN=CPh$_2$ reacts with compound **5** (in toluene), relative to **5** and the free substrates.

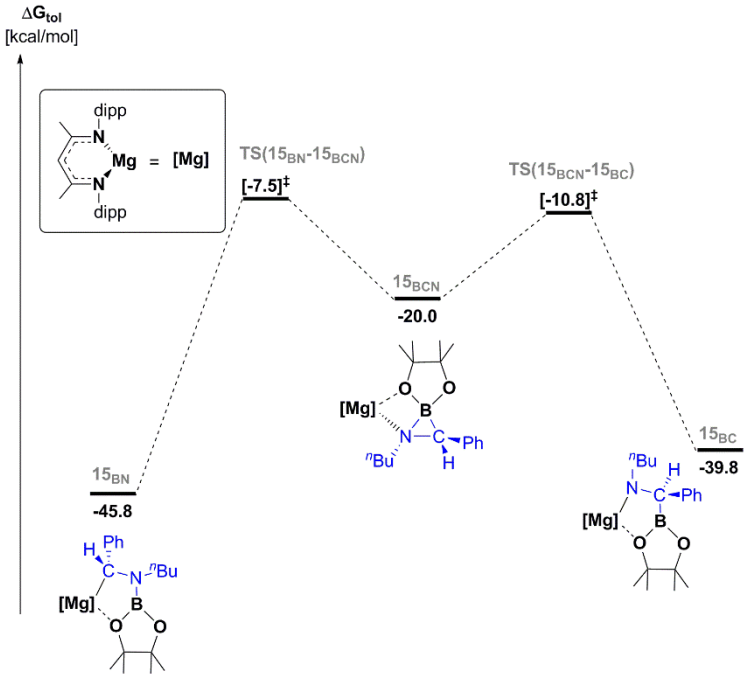


Figure S39: DFT calculated free energy (kcal mol^{-1}) profile for intermediates of **15** formed after imine *n*-BuN=CHPh reacts with compound **5** (in toluene), relative to **5** and the free substrates.

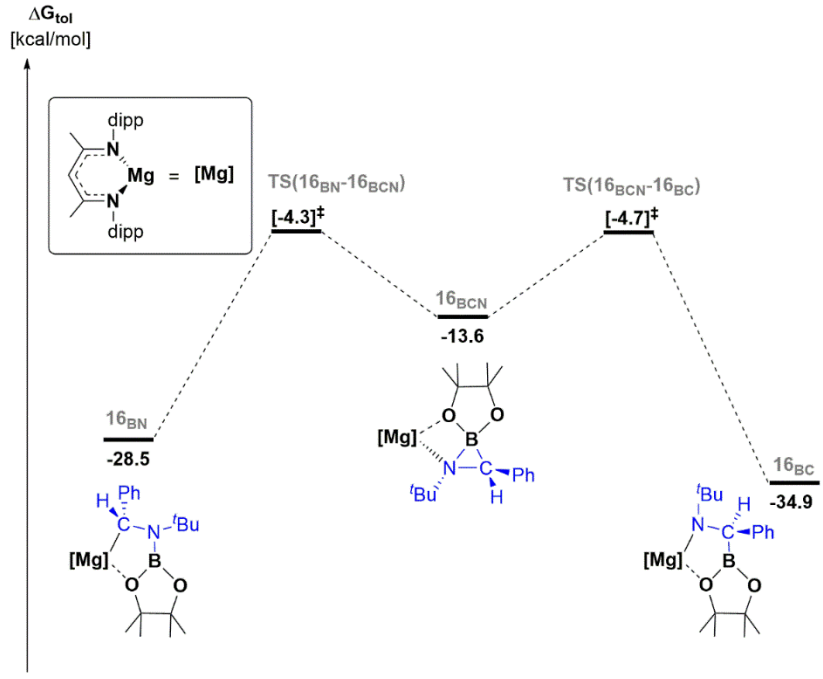
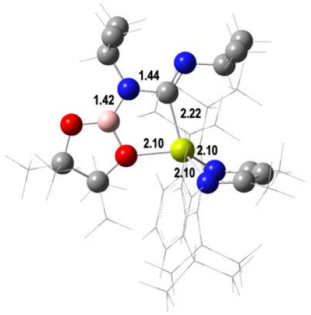
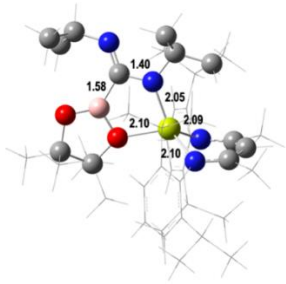


Figure S40: DFT calculated free energy (kcal mol^{-1}) profile for intermediates of **16** formed after imine *t*-BuN=CHPh reacts with compound **5** (in toluene), relative to **5** and the free substrates.

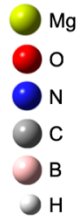
DFT- computed geometries for the addition of imines to copound **5**, relative to **5** and the free substrates. Bond lengths given in Ångstroms.

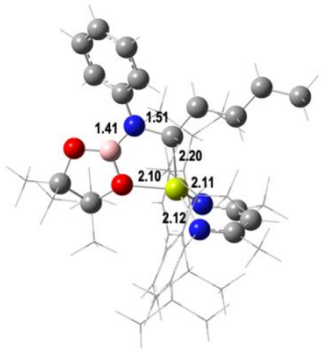


12$_{BN}$
-32.8

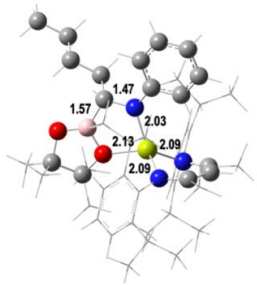


12$_{BC}$
-38.3

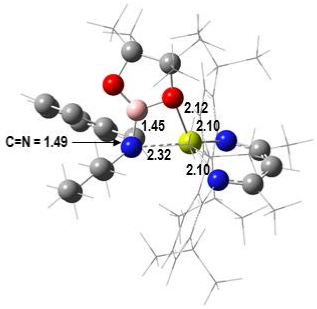




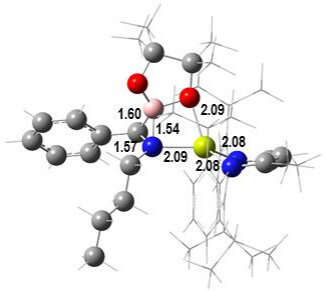
15$_{BN}$
-45.8



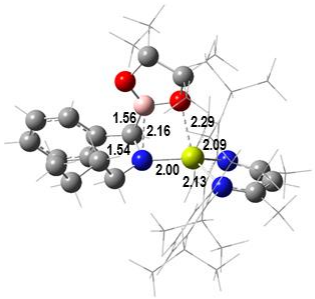
15$_{BC}$
-39.8



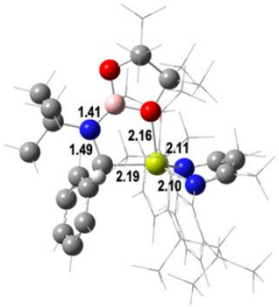
TS(15_{BN}-15_{BCN})
-7.5



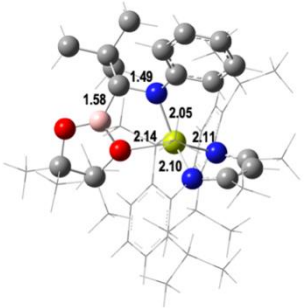
15_{BCN}
-20.0



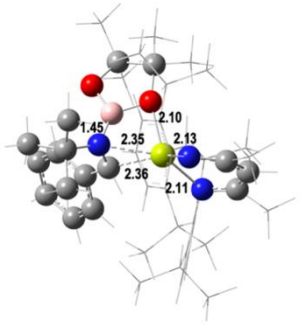
TS(15_{BCN}-15_{BC})
-10.8



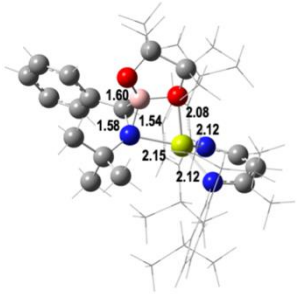
16_{BN}
-28.5



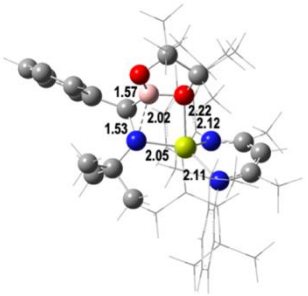
16_{BC}
-34.9



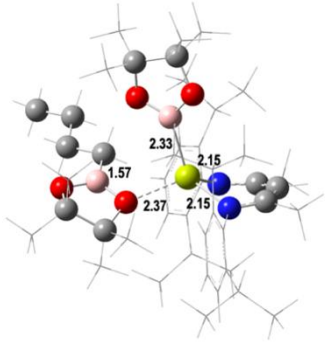
TS(16_{BN}-16_{BCN})
-4.3



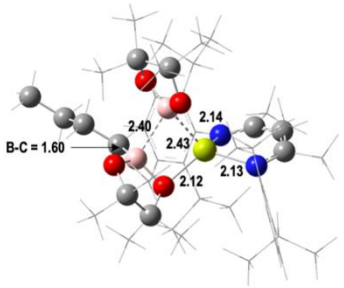
16_{BCN}
-13.6



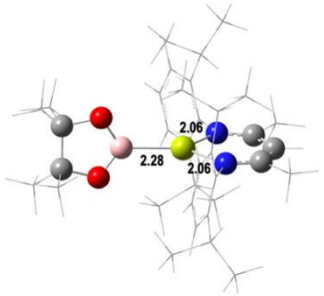
TS(16_{BCN}-16_{BC})
-4.7



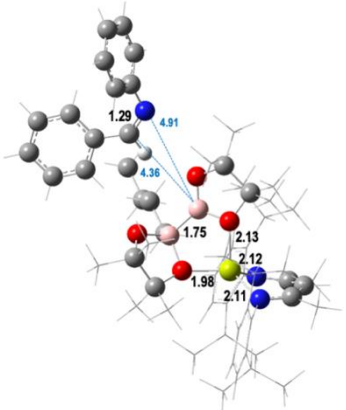
5b
11.1



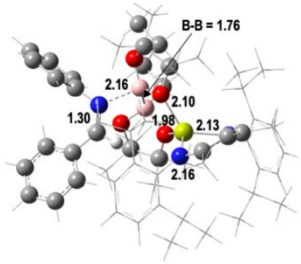
TS(5-5b)
[19.4]‡



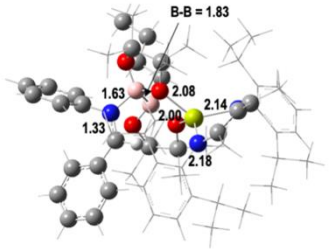
5c
12.9



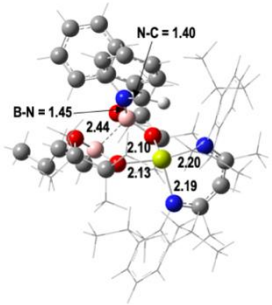
5·PhNCHPh
3.0



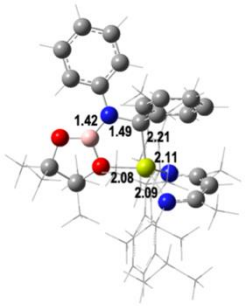
TS(5-17$_{BN}$)1
[11.3]‡



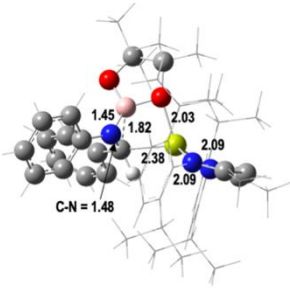
INT(5-17$_{BN}$)
6.7



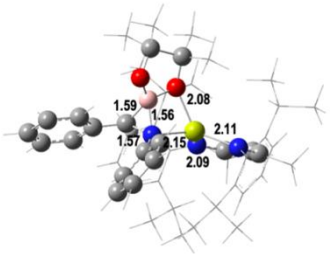
TS(5-17$_{BN}$)2
[13.4]‡



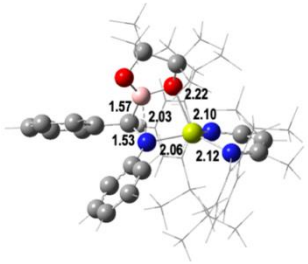
17$_{BN}$
-34.8



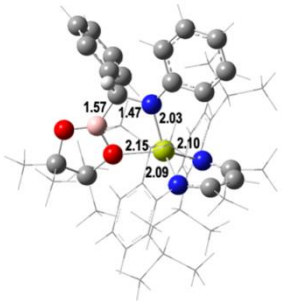
TS(17$_{BN}$-17$_{BCN}$)
[-8.6]‡



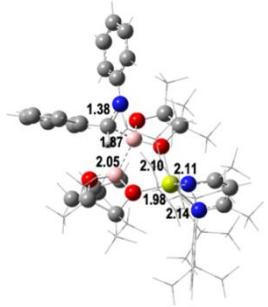
17_{BCN}
-22.8



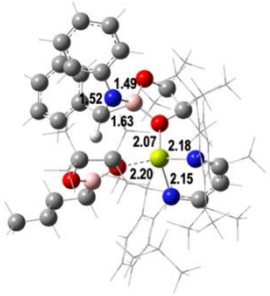
$TS(17_{BCN}\text{-}17_{BC})$
[-18.7]‡



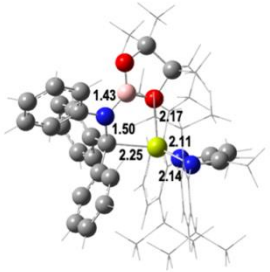
17_{BC}
-38.4



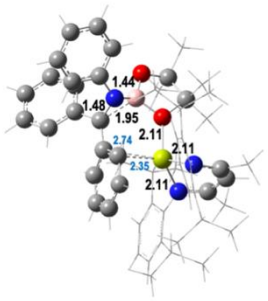
$TS(5\text{-}17_{BCN})$
[30.3]‡



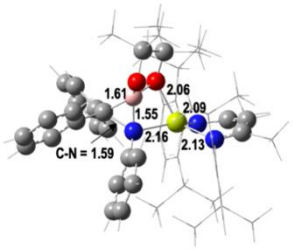
17_{BCN}-BpinBu
-12.2



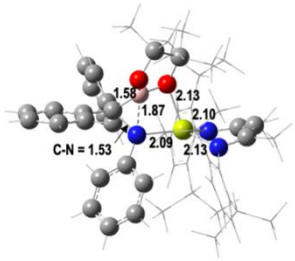
18_{BN}
-37.1



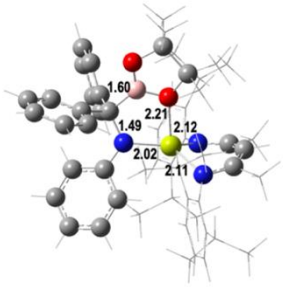
TS(18_{BN}-18_{BCN})
[-15.5]‡



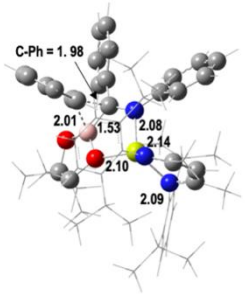
18_{BCN}
-23.8



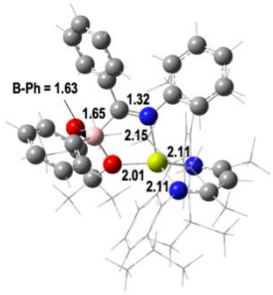
TS(18_{BCN}-18_{BC})
[-17.2]‡



18_{BC}
-30.5



TS(18_{BC}-18_{BPh})
[-10.9]‡



18_{BPh}
-36.6

Cartesian Coordinates and Computed Energies (in Hartrees)

pinBBu

SCF (BP86) Energy = -569.123611693
Enthalpy 0K = -568.827988
Enthalpy 298K = -568.811084
Free Energy 298K = -568.871244
Lowest Frequency = 17.1407 cm^{-1}
Second Frequency = 53.5275 cm^{-1}
SCF (BP86-D3BJ) Energy = -569.174139930
SCF (Toluene) Energy = -569.125385795
SCF (BS2) Energy = -569.267887458

O	-0.86955	1.32355	-0.42098
O	-0.18300	-0.73258	0.38809
C	-2.09600	0.61210	-0.04689
C	-2.54730	1.19499	1.30436
H	-2.67048	2.28517	1.20025
H	-3.50903	0.76697	1.63350
H	-1.79541	1.01090	2.08938
C	-3.15587	0.87903	-1.12021
H	-4.08214	0.31845	-0.90581
H	-3.40478	1.95284	-1.13647
H	-2.79923	0.59839	-2.12243
C	-1.60237	-0.88916	0.05313
C	-2.26924	-1.72283	1.15171
H	-3.35284	-1.82123	0.96660
H	-1.83363	-2.73543	1.16496
H	-2.12193	-1.27719	2.14676
C	-1.65455	-1.63812	-1.29038
H	-1.10344	-2.58741	-1.19226
H	-2.69080	-1.86796	-1.58998
H	-1.17991	-1.05036	-2.09324
B	0.19901	0.53546	-0.02082
C	1.69302	1.04254	-0.01374
H	1.83297	1.66855	0.89301
H	1.83638	1.74484	-0.85814
C	2.76818	-0.06372	-0.04099
H	2.59361	-0.76676	0.79568
H	2.65516	-0.66819	-0.96226
C	4.20767	0.47436	0.03493
H	4.32239	1.07303	0.96015
H	4.37762	1.17930	-0.80264
C	5.27346	-0.63192	0.00174
H	5.20596	-1.22365	-0.92865
H	6.29435	-0.21688	0.05981
H	5.14849	-1.33203	0.84698

DMAP (NC_5H_4-NMe_2)

SCF (BP86) Energy = -382.256098610
Enthalpy 0K = -382.098887
Enthalpy 298K = -382.089042
Free Energy 298K = -382.132978
Lowest Frequency = 63.0068 cm^{-1}
Second Frequency = 82.3186 cm^{-1}
SCF (BP86-D3BJ) Energy = -382.285474805
SCF (Toluene) Energy = -382.259778610
SCF (BS2) Energy = -382.353392958

N	2.69408	0.00000	0.02022
N	-1.56586	-0.00001	-0.08409
C	1.96745	1.13861	0.00953
H	2.54406	2.07381	0.02487
C	0.57117	1.20572	-0.01449
H	0.08321	2.18308	-0.01244
C	-0.18332	0.00002	-0.03751
C	0.57116	-1.20569	-0.01482
H	0.08318	-2.18303	-0.01314
C	1.96744	-1.13861	0.00919
H	2.54405	-2.07381	0.02429
C	-2.29344	1.25866	0.03158
H	-2.12529	1.76120	1.00588
H	-3.37040	1.06258	-0.07244
H	-2.00183	1.96192	-0.76982
C	-2.29335	-1.25870	0.03216
H	-2.00277	-1.96186	-0.76973
H	-3.37042	-1.06255	-0.07043
H	-2.12398	-1.76139	1.00615

PhNCHPh

SCF (BP86) Energy = -556.743441703
Enthalpy 0K = -556.546372
Enthalpy 298K = -556.534136
Free Energy 298K = -556.584766
Lowest Frequency = 41.1174 cm^{-1}
Second Frequency = 56.9383 cm^{-1}
SCF (BP86-D3BJ) Energy = -556.789039723
SCF (Toluene) Energy = -556.745924351
SCF (BS2) Energy = -556.879545901

C	0.40498	-0.40756	0.18195
H	0.09425	-1.41787	0.52529
N	-0.45918	0.51462	-0.09904
C	1.85378	-0.18399	0.08812
C	2.74134	-1.22778	0.43325
C	2.38219	1.05659	-0.34186
C	4.12806	-1.03979	0.35116
H	2.33411	-2.18970	0.76697
C	3.76552	1.24178	-0.42097
H	1.68091	1.85439	-0.60455
C	4.64276	0.19520	-0.07593
H	4.80749	-1.85511	0.62038
H	4.16849	2.20422	-0.75369
H	5.72573	0.34437	-0.14067
C	-1.83491	0.21956	-0.05944
C	-2.71162	1.23657	0.38652
C	-2.38143	-1.01334	-0.49319
C	-4.09145	1.00844	0.44527
H	-2.27953	2.19304	0.69659
C	-3.76622	-1.22601	-0.45132
H	-1.71705	-1.78343	-0.89945
C	-4.62619	-0.22308	0.02673
H	-4.75617	1.79972	0.80797
H	-4.17748	-2.17843	-0.80317
H	-5.70729	-0.39301	0.05576

PhNCHPh

SCF (BP86) Energy = -556.743441703
Enthalpy 0K = -556.546372
Enthalpy 298K = -556.534136
Free Energy 298K = -556.584766
Lowest Frequency = 41.1174 cm^{-1}
Second Frequency = 56.9383 cm^{-1}
SCF (BP86-D3BJ) Energy = -556.789039723
SCF (Toluene) Energy = -556.745924351
SCF (BS2) Energy = -556.879545901

C	0.40498	-0.40756	0.18195
H	0.09425	-1.41787	0.52529
N	-0.45918	0.51462	-0.09904
C	1.85378	-0.18399	0.08812
C	2.74134	-1.22778	0.43325
C	2.38219	1.05659	-0.34186
C	4.12806	-1.03979	0.35116
H	2.33411	-2.18970	0.76697
C	3.76552	1.24178	-0.42097
H	1.68091	1.85439	-0.60455
C	4.64276	0.19520	-0.07593
H	4.80749	-1.85511	0.62038
H	4.16849	2.20422	-0.75369
H	5.72573	0.34437	-0.14067
C	-1.83491	0.21956	-0.05944
C	-2.71162	1.23657	0.38652
C	-2.38143	-1.01334	-0.49319
C	-4.09145	1.00844	0.44527
H	-2.27953	2.19304	0.69659
C	-3.76622	-1.22601	-0.45132
H	-1.71705	-1.78343	-0.89945
C	-4.62619	-0.22308	0.02673
H	-4.75617	1.79972	0.80797
H	-4.17748	-2.17843	-0.80317
H	-5.70729	-0.39301	0.05576

$PhNCPh_2$

SCF (BP86) Energy = -787.787717127
Enthalpy 0K = -787.512142
Enthalpy 298K = -787.495034
Free Energy 298K = -787.557441
Lowest Frequency = 33.8488 cm^{-1}
Second Frequency = 40.2728 cm^{-1}
SCF (BP86-D3BJ) Energy = -787.864356061
SCF (Toluene) Energy = -787.790676788
SCF (BS2) Energy = -787.977621335

C	0.53917	0.31474	-0.05647
N	-0.26103	1.34074	-0.09049
C	2.00564	0.60348	-0.02760
C	2.96471	-0.36331	-0.40639
C	2.45316	1.88953	0.35768
C	4.33299	-0.05262	-0.39688
H	2.63537	-1.35700	-0.72381
C	3.81799	2.19446	0.37205
H	1.70148	2.63285	0.63885
C	4.76469	1.22373	-0.00422
H	5.06277	-0.81034	-0.70104
H	4.14907	3.19181	0.68062
H	5.83329	1.46327	0.00876
C	-1.66109	1.26729	0.01650
C	-2.32021	0.59249	1.07346
C	-2.43624	2.01630	-0.90150
C	-3.71521	0.65497	1.19017
H	-1.72655	0.03780	1.80610
C	-3.83225	2.04633	-0.79417
H	-1.91901	2.56303	-1.69636
C	-4.48081	1.36962	0.25359
H	-4.20822	0.13662	2.01994
H	-4.41697	2.61704	-1.52382
H	-5.57080	1.40992	0.34670
C	0.09574	-1.12229	-0.08049
C	0.57381	-2.04344	0.87823
C	-0.81094	-1.57240	-1.06511
C	0.14115	-3.37813	0.86230
H	1.27984	-1.70481	1.64374
C	-1.22680	-2.91056	-1.09078
H	-1.18568	-0.86575	-1.81169
C	-0.75669	-3.81603	-0.12464
H	0.51028	-4.07775	1.61967
H	-1.92271	-3.24713	-1.86627
H	-1.08776	-4.85965	-0.14240

^{n}BuNCHPh

SCF (BP86) Energy = -482.940112361
Enthalpy 0K = -482.711233
Enthalpy 298K = -482.697979
Free Energy 298K = -482.750748
Lowest Frequency = 35.1922 cm^{-1}
Second Frequency = 67.1735 cm^{-1}
SCF (BP86-D3BJ) Energy = -482.980766647
SCF (Toluene) Energy = -482.942072996
SCF (BS2) Energy = -483.057562321

C	0.08483	0.02080	-0.00007
H	-0.44254	-0.95630	0.00003
N	-0.52490	1.15407	-0.00023
C	1.55975	-0.07279	-0.00003
C	2.17548	-1.34256	-0.00013
C	2.37116	1.08487	0.00015
C	3.57347	-1.45827	-0.00008
H	1.54856	-2.24263	-0.00025
C	3.76487	0.96827	0.00020
H	1.87621	2.06088	0.00027
C	4.37107	-0.30281	0.00008
H	4.04041	-2.44883	-0.00017
H	4.38730	1.86960	0.00035
H	5.46282	-0.38994	0.00013
C	-1.98462	1.20897	-0.00019
H	-2.27342	1.82467	0.87661
H	-2.27351	1.82453	-0.87706
C	-2.80519	-0.09314	-0.00005
H	-2.54408	-0.70361	0.88678
H	-2.54422	-0.70369	-0.88687
C	-4.32060	0.17880	0.00006
H	-4.58118	0.79296	-0.88377
H	-4.58103	0.79306	0.88387
C	-5.16519	-1.10474	0.00021
H	-4.95312	-1.72273	0.89059
H	-6.24491	-0.87801	0.00029
H	-4.95327	-1.72284	-0.89013

^{t}BuNCHPh

SCF (BP86) Energy = -482.945225683
Enthalpy 0K = -482.717521
Enthalpy 298K = -482.704293
Free Energy 298K = -482.755857
Lowest Frequency = 36.0752 cm^{-1}
Second Frequency = 72.2391 cm^{-1}
SCF (BP86-D3BJ) Energy = -482.988902827
SCF (Toluene) Energy = -482.946967318
SCF (BS2) Energy = -483.062384733

C	-0.22723	-0.54882	-0.00003
H	-0.46464	-1.63332	-0.00014
N	-1.12426	0.37280	0.00007
C	1.21737	-0.23367	-0.00001
C	2.15830	-1.28531	0.00001

C	1.67931	1.10230	-0.00002
C	3.53426	-1.01222	0.00002
H	1.80283	-2.32301	0.00001
C	3.05132	1.37354	-0.00001
H	0.93466	1.90417	-0.00006
C	3.98349	0.31801	0.00002
H	4.25555	-1.83622	0.00004
H	3.40202	2.41125	-0.00002
H	5.05714	0.53428	0.00003
C	-2.56413	0.04606	0.00002
C	-2.91963	-1.45633	-0.00026
H	-2.52736	-1.97086	0.89458
H	-4.01542	-1.58110	-0.00037
H	-2.52720	-1.97053	-0.89522
C	-3.14804	0.72338	-1.26369
H	-2.88354	1.79310	-1.27977
H	-2.74363	0.25712	-2.17827
H	-4.24755	0.62875	-1.28221
C	-3.14807	0.72295	1.26393
H	-4.24759	0.62833	1.28237
H	-2.74371	0.25637	2.17836
H	-2.88357	1.79266	1.28039

^{i}PrNCN^{i}Pr

SCF (BP86) Energy = -384.663990780
Enthalpy 0K = -384.466088
Enthalpy 298K = -384.453420
Free Energy 298K = -384.504972
Lowest Frequency = 23.8349 cm^{-1}
Second Frequency = 27.2358 cm^{-1}
SCF (BP86-D3BJ) Energy = -384.692047877
SCF (Toluene) Energy = -384.665763511
SCF (BS2) Energy = -384.763019620

C	0.00004	-0.43121	-0.00060
N	1.18320	-0.53258	0.34928
N	-1.18311	-0.53175	-0.35072
C	2.94494	1.06614	0.93987
H	3.81509	1.63448	0.56922
H	2.21420	1.78001	1.35415
H	3.28031	0.40569	1.75737
C	3.33349	-0.75316	-0.79827
H	2.87718	-1.33277	-1.61703
H	4.20843	-0.21284	-1.19856
H	3.68147	-1.46215	-0.02808
C	-2.94691	1.06516	-0.93975
H	-3.81702	1.63301	-0.56825
H	-2.21727	1.77939	-1.35535
H	-3.28283	0.40403	-1.75647
C	2.32320	0.23544	-0.19421
H	1.97527	0.92226	-0.99222
C	-2.32304	0.23553	0.19394
H	-1.97466	0.92302	0.99117
C	-3.33174	-0.75361	0.79978
H	-2.87393	-1.33240	1.61829
H	-4.20664	-0.21382	1.20086
H	-3.68008	-1.46330	0.03040

^{t}BuNCN^{t}Bu

SCF (BP86) Energy = -463.293050800
Enthalpy 0K = -463.041521
Enthalpy 298K = -463.026103
Free Energy 298K = -463.083859
Lowest Frequency = 12.3444 cm^{-1}
Second Frequency = 16.6580 cm^{-1}
SCF (BP86-D3BJ) Energy = -463.335345849
SCF (Toluene) Energy = -463.294850749
SCF (BS2) Energy = -463.409039538

C	0.00001	-0.00459	0.00156
N	-1.21192	0.00158	0.00829
N	1.21195	-0.01150	-0.00462
C	-2.64140	0.00004	0.00013
C	-3.15968	0.31744	1.42585
H	-4.26369	0.32196	1.44580
H	-2.79921	-0.43878	2.14289
H	-2.79910	1.30638	1.75441
C	-3.14686	1.07784	-0.99233
H	-2.77720	0.86693	-2.00961
H	-4.25064	1.09646	-1.01679
H	-2.78601	2.07572	-0.69234
C	-3.14747	-1.39670	-0.44168
H	-4.25127	-1.42358	-0.45574
H	-2.77807	-1.63707	-1.45249
H	-2.78676	-2.17341	0.25301
C	2.64140	-0.00015	-0.00006
C	3.13907	1.40008	0.44030
H	2.77070	1.63799	1.45207
H	4.24269	1.43453	0.45145
H	2.77121	2.17424	-0.25347
C	3.15667	-1.07435	0.99125
H	2.80152	-2.07465	0.69252
H	4.26061	-1.08574	1.01262
H	2.78848	-0.86559	2.00949
C	3.15825	-0.31430	-1.42701
H	4.26222	-0.31158	-1.44967
H	2.80336	-1.30562	-1.75460
H	2.79108	0.43947	-2.14323

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SCF (BP86) Energy = -2220.57991976
Enthalpy 0K = -2219.487760
Enthalpy 298K = -2219.422702
Free Energy 298K = -2219.583100
Lowest Frequency = 18.9735 cm^{-1}
Second Frequency = 26.5885 cm^{-1}
SCF (BP86-D3BJ) Energy = -2220.90416120
SCF (Toluene) Energy = -2220.58694528
SCF (BS2) Energy = -2420.36376068

Mg	-0.34476	0.01378	-0.18714
O	1.54140	-2.22807	2.66404
O	0.23112	-0.49946	1.62808
O	2.35893	-3.05123	-0.58702
O	0.47307	-1.78737	-0.98025
N	0.51453	1.72437	-1.09139
N	-2.31856	0.35138	-0.85786
C	0.52128	3.21091	-3.10961
H	1.23137	3.83727	-2.55179
H	-0.27347	3.84981	-3.52516
H	1.06303	2.76611	-3.96307
C	-0.07685	2.11136	-2.23709
C	-1.29747	1.57224	-2.73842
H	-1.55178	1.93263	-3.74029
C	-2.37621	0.92362	-2.08493
C	-3.68846	0.97689	-2.86537
H	-4.44482	0.28346	-2.47490
H	-3.49885	0.74795	-3.92734

H	-4.11693	1.99339	-2.83081
C	-3.58012	0.07622	-0.19956
C	-4.27991	1.13606	0.45445
C	-5.50795	0.85688	1.08681
H	-6.04588	1.67243	1.58322
C	-6.05569	-0.42852	1.09327
H	-7.01385	-0.62228	1.58673
C	-5.36109	-1.46468	0.46179
H	-5.78584	-2.47393	0.46235
C	-4.12896	-1.24233	-0.18402
C	-3.45154	-2.41490	-0.89197
H	-2.39781	-2.12895	-1.05143
C	-4.08901	-2.67981	-2.27744
H	-5.16444	-2.90677	-2.16873
H	-3.61217	-3.54568	-2.76980
H	-3.99583	-1.81357	-2.95154
C	-3.47321	-3.71728	-0.06284
H	-4.49158	-4.13664	0.01548
H	-3.09036	-3.56385	0.95815
H	-2.84912	-4.48910	-0.54735
C	-3.75936	2.57485	0.51098
H	-2.77726	2.60376	0.00859
C	-4.69983	3.55854	-0.22462
H	-5.68564	3.61324	0.27025
H	-4.87252	3.26009	-1.27138
H	-4.27065	4.57572	-0.22645
C	-3.56264	3.03956	1.97213
H	-4.51365	3.02218	2.53234
H	-3.18275	4.07550	2.00169
H	-2.84709	2.39704	2.51180
C	1.66127	2.46199	-0.59421
C	1.46942	3.35241	0.50686
C	2.58182	4.02219	1.04927
H	2.43604	4.70200	1.89370
C	3.86843	3.84311	0.53151
H	4.72197	4.36877	0.97182
C	4.04690	2.99050	-0.55883
H	5.05064	2.85487	-0.97631
C	2.96910	2.29261	-1.14167
C	0.07563	3.66519	1.05162
H	-0.55049	2.76348	0.91397
C	-0.57072	4.80491	0.22652
H	0.04535	5.71953	0.28797
H	-1.57765	5.04808	0.60918
H	-0.66802	4.53353	-0.83720
C	0.06676	4.02383	2.55137
H	0.61356	3.27809	3.15151
H	-0.96954	4.07474	2.92381
H	0.52274	5.01173	2.74049
C	3.28221	1.39866	-2.34317
H	2.32990	0.97938	-2.70761
C	4.20878	0.22372	-1.95175
H	4.44417	-0.39762	-2.83533
H	3.76039	-0.42235	-1.18001
H	5.16769	0.59505	-1.55095
C	3.92666	2.19470	-3.50432
H	3.32408	3.07013	-3.79544
H	4.04744	1.54914	-4.39225
H	4.93023	2.56185	-3.22754
C	0.71923	-2.53986	-2.25600
C	1.30645	-1.54898	-3.26490
H	1.45104	-2.03087	-4.24660
H	2.27400	-1.15597	-2.92583
H	0.60746	-0.70550	-3.40091
C	-0.60019	-3.08965	-2.79294
H	-1.26580	-2.26321	-3.08956
H	-1.12198	-3.71574	-2.05601
H	-0.40765	-3.70185	-3.69148
C	1.73639	-3.64723	-1.76936
C	2.84369	-3.97658	-2.77714
H	3.44517	-3.08997	-3.02619
H	2.42159	-4.39293	-3.70824
H	3.51793	-4.73147	-2.34178
C	1.05731	-4.94472	-1.29309
H	0.62269	-5.51401	-2.13197
H	0.26546	-4.73848	-0.55488
H	1.81513	-5.57543	-0.80189
C	-0.37602	-0.86951	2.90607
C	-1.90023	-0.81125	2.79138
H	-2.24597	0.22419	2.62952
H	-2.37059	-1.17054	3.72328
H	-2.28208	-1.42729	1.96252
C	0.10443	0.12876	3.97487
H	1.19142	0.04849	4.12432
H	-0.40125	-0.04188	4.94089
H	-0.12774	1.15469	3.64460
C	0.20857	-2.32100	3.14062
C	0.25527	-2.73479	4.62236
H	0.66183	-3.75681	4.70278
H	-0.75003	-2.73021	5.08018
H	0.91376	-2.06703	5.19770
C	-0.55993	-3.40135	2.34292
H	-0.67724	-3.10688	1.28621
H	-1.56111	-3.60756	2.76108
H	0.02589	-4.33463	2.37468
B	1.63895	-1.29504	1.51821
B	1.53973	-2.08466	-0.04812
C	2.92915	-0.32134	1.71530
H	3.02134	0.42936	0.90451
H	2.79079	0.27020	2.64468
C	4.25417	-1.10467	1.82956
H	4.15187	-1.86253	2.63028
H	4.43212	-1.68159	0.89849
C	5.48588	-0.22655	2.11659
H	5.31879	0.33207	3.05884
H	5.57591	0.54480	1.32605
C	6.79762	-1.02175	2.21680
H	7.66256	-0.36830	2.42856
H	6.74423	-1.77660	3.02190
H	7.00958	-1.56239	1.27647

8

SCF (BP86) Energy = -2418.47374141
Enthalpy 0K = -2417.319202
Enthalpy 298K = -2417.247675
Free Energy 298K = -2417.427488
Lowest Frequency = 15.4632 cm^{-1}
Second Frequency = 16.4520 cm^{-1}
SCF (BP86-D3BJ) Energy = -2418.81793464
SCF (Toluene) Energy = -2418.48037868
SCF (BS2) Energy = -2618.30321429

C	-1.28709	-1.54818	-4.28094
H	-0.31190	-1.99159	-4.55567
H	-1.66091	-0.99533	-5.15651
H	-1.97072	-2.38188	-4.06178
C	-1.09994	-0.63175	-3.07525
C	-0.84716	0.73338	-3.38186

H	-0.76748	0.94445	-4.45295
C	-0.84369	1.89359	-2.56372
C	-0.77265	3.21297	-3.33086
H	-1.06152	4.07188	-2.70865
H	-1.40489	3.19144	-4.23296
H	0.26779	3.37838	-3.66718
C	-1.20387	3.08214	-0.49753
C	-2.57727	3.47896	-0.38438
C	-2.90294	4.59005	0.41901
H	-3.95233	4.89604	0.50124
C	-1.92187	5.31198	1.10803
H	-2.19871	6.16894	1.73173
C	-0.58118	4.93606	0.97271
H	0.19569	5.51497	1.48492
C	-0.19644	3.84155	0.17340
C	1.29331	3.56388	-0.02623
H	1.38969	2.59586	-0.54857
C	2.08031	3.46405	1.29666
H	2.11456	4.43163	1.82987
H	3.11971	3.15072	1.10039
H	1.63331	2.71556	1.96888
C	1.91651	4.65502	-0.93068
H	1.40669	4.71787	-1.90629
H	2.98428	4.44500	-1.11609
H	1.84486	5.64844	-0.45204
C	-3.70566	2.76302	-1.13474
H	-3.28554	1.83960	-1.56848
C	-4.24343	3.63461	-2.29563
H	-4.69588	4.56590	-1.90977
H	-5.02154	3.09164	-2.86101
H	-3.44663	3.91896	-3.00061
C	-4.87627	2.36007	-0.21063
H	-5.36534	3.24269	0.23889
H	-4.54455	1.70180	0.60858
H	-5.64787	1.82185	-0.78890
C	-1.65861	-2.45218	-1.60640
C	-3.06418	-2.61903	-1.39188
C	-3.56416	-3.90819	-1.12545
H	-4.64092	-4.04122	-0.97419
C	-2.71793	-5.02078	-1.04059
H	-3.12843	-6.01448	-0.83008
C	-1.34285	-4.84670	-1.22722
H	-0.67444	-5.71327	-1.16198
C	-0.79110	-3.58165	-1.51484
C	0.71598	-3.46882	-1.73965
H	0.94458	-2.40674	-1.93419
C	1.51764	-3.88330	-0.48710
H	1.23128	-3.27598	0.38610
H	2.59857	-3.73313	-0.65219
H	1.35731	-4.94723	-0.23422
C	1.16852	-4.29676	-2.96457
H	1.00154	-5.37690	-2.80227
H	2.24740	-4.15377	-3.15322
H	0.62029	-4.01072	-3.87784
C	-4.02874	-1.43230	-1.45337
H	-3.42203	-0.52279	-1.29551
C	-5.10623	-1.48173	-0.34881
H	-5.81703	-2.31370	-0.50164
H	-5.69619	-0.54960	-0.35312
H	-4.65605	-1.59837	0.65089
C	-4.70450	-1.31707	-2.84041
H	-3.96667	-1.18079	-3.64659
H	-5.39555	-0.45548	-2.86614
H	-5.28985	-2.22668	-3.06685
C	-1.87034	-1.59922	1.71728
H	-1.36375	-2.40034	1.16896
C	-2.65016	-1.91427	2.82809
H	-2.73681	-2.96008	3.12812
C	-3.31616	-0.87587	3.54080
C	-3.12767	0.44329	3.03819
H	-3.59422	1.30823	3.51318
C	-2.32547	0.64836	1.91734
H	-2.17831	1.66416	1.53475
C	-4.75159	-0.03218	5.34553
H	-4.02005	0.69492	5.74681
H	-5.32768	-0.43646	6.18941
H	-5.45137	0.51217	4.68352
C	-4.24737	-2.50164	5.12831
H	-4.70956	-3.15478	4.36401
H	-4.89925	-2.50009	6.01289
H	-3.27607	-2.94501	5.41947
C	2.42527	-0.17152	0.16763
C	3.01513	0.12911	-2.15528
H	3.97972	-0.31816	-1.81830
C	3.28468	1.61555	-2.46867
H	2.35417	2.10577	-2.80338
H	4.03984	1.72671	-3.26862
H	3.64955	2.14124	-1.57118
C	2.60429	-0.61473	-3.43710
H	2.51206	-1.69779	-3.25814
H	3.35285	-0.46158	-4.23485
H	1.63083	-0.23549	-3.79332
C	1.85038	-0.44780	2.50290
H	2.85795	-0.00092	2.67103
C	1.95239	-1.95096	2.84677
H	0.97001	-2.43799	2.71237
H	2.26582	-2.10268	3.89672
H	2.68096	-2.45477	2.19129
C	0.89297	0.24849	3.48604
H	0.78458	1.31989	3.25163
H	1.27063	0.15925	4.52015
H	-0.10874	-0.21064	3.45244
C	6.13626	0.44223	0.95620
C	6.02891	-1.13335	1.10745
C	7.07695	-1.93227	0.32578
H	6.89258	-3.01094	0.45783
H	8.09357	-1.71281	0.69523
H	7.03853	-1.71058	-0.75096
C	5.98299	-1.60957	2.56959
H	5.21804	-1.06466	3.14612
H	6.95808	-1.48157	3.06901
H	5.72205	-2.67995	2.58892
C	6.78022	0.89264	-0.36632
H	6.30441	0.40538	-1.23265
H	7.86065	0.67176	-0.38743
H	6.64735	1.98093	-0.47624
C	6.79741	1.16283	2.13572
H	6.78582	2.25047	1.95732
H	7.84917	0.84768	2.24812
H	6.26886	0.96811	3.08057
N	-1.13519	-1.13336	-1.82807
N	-0.86279	1.88518	-1.21524
N	-1.68615	-0.34039	1.24266
N	-4.09341	-1.13196	4.64531
N	1.45159	-0.22370	1.10676
N	2.00587	-0.02907	-1.09943
O	4.72711	0.85847	0.89827
O	4.70840	-1.42670	0.53091

Mg -0.12976 0.05638 -0.34887
B   3.97906 -0.25060 0.54009

11
SCF (BP86) Energy = -2114.81996899
Enthalpy 0K = -2113.770143
Enthalpy 298K = -2113.706621
Free Energy 298K = -2113.866339
Lowest Frequency = 12.2233 cm^{-1}
Second Frequency = 18.9542 cm^{-1}
SCF (BP86-D3BJ) Energy = -2115.12151716
SCF (Toluene) Energy = -2114.82520344
SCF (BS2) Energy = -2314.57224580

C   3.31293 2.52389 2.50583
H   4.07554 2.98453 1.85565
H   3.79891 2.20418 3.43906
H   2.58550 3.32050 2.73480
C   2.63623 1.35287 1.80502
C   2.83491 0.07505 2.39554
H   3.36361 0.09913 3.35205
C   2.65561 -1.23325 1.86561
C   3.35906 -2.34468 2.63567
H   3.39297 -2.09913 3.70900
H   4.40261 -2.46154 2.29520
H   2.85951 -3.31573 2.50023
C   2.11526 -2.80662 0.13474
C   3.31349 -3.10415 -0.58682
C   3.44633 -4.36414 -1.20161
H   4.36406 -4.58931 -1.75691
C   2.43768 -5.32907 -1.12287
H   2.56392 -6.30559 -1.60239
C   1.26322 -5.02708 -0.42712
H   0.47008 -5.77955 -0.36049
C   1.07374 -3.78016 0.20117
C -0.22254 -3.54586 0.97679
H -0.29501 -2.46758 1.21003
C -1.47260 -3.92427 0.15366
H -1.48975 -3.39682 -0.81310
H -2.39232 -3.65130 0.69715
H -1.52066 -5.00921 -0.04709
C -0.20378 -4.31339 2.32041
H -1.13325 -4.13443 2.88990
H   0.64525 -4.00582 2.95406
H -0.11773 -5.40155 2.15021
C   4.44908 -2.09411 -0.76987
H   4.21741 -1.19980 -0.16692
C   4.54222 -1.65336 -2.24850
H   4.75240 -2.51502 -2.90638
H   5.35639 -0.92025 -2.38628
H   3.60145 -1.19207 -2.59178
C   5.81554 -2.64327 -0.29847
H   5.78080 -3.00226 0.74372
H   6.58886 -1.85802 -0.36298
H   6.15068 -3.48794 -0.92597
C   1.99043 2.86947 0.06751
C   1.03262 3.88271 0.36650
C   1.18379 5.15760 -0.21456
H   0.45439 5.93933 0.02643
C   2.23972 5.44740 -1.08357
H   2.34758 6.44944 -1.51232
C   3.14294 4.43270 -1.41627
H   3.95525 4.64575 -2.12030
C   3.03266 3.13825 -0.87181
C   4.02277 2.06585 -1.33328
H   3.68263 1.10078 -0.91795
C   4.02874 1.94670 -2.87499
H   3.01978 1.73293 -3.26540
H   4.70073 1.13477 -3.19971
H   4.38167 2.87701 -3.35332
C   5.45483 2.32807 -0.81297
H   5.83894 3.29763 -1.17726
H   6.14643 1.54117 -1.16288
H   5.49495 2.34373 0.28878
C -0.17642 3.63833 1.26962
H -0.13094 2.59125 1.61967
C -1.48736 3.80808 0.46784
H -1.57650 4.83113 0.06157
H -2.36702 3.62126 1.10557
H -1.52793 3.10058 -0.37591
C -0.18066 4.55629 2.51338
H   0.73510 4.43868 3.11744
H -1.04461 4.32591 3.16163
H -0.25583 5.62044 2.22765
C -1.92310 -0.01930 -0.08693
C -1.23397 0.07348 -2.53098
C -1.76784 -1.28830 -3.04304
H -1.04883 -2.08935 -2.79920
H -1.90157 -1.27270 -4.13999
H -2.73175 -1.54511 -2.57732
C -2.17297 1.22718 -2.96174
H -3.17927 1.13658 -2.52232
H -2.28410 1.24876 -4.06052
H -1.76004 2.19780 -2.63815
C   0.14822 0.32562 -3.17770
H   0.56609 1.28729 -2.83157
H   0.07427 0.35529 -4.27856
H   0.85292 -0.48111 -2.90630
C -2.06315 -0.10953 2.44518
C -3.05181 -1.29638 2.55581
H -3.86100 -1.24148 1.80999
H -3.51623 -1.31972 3.55782
H -2.52581 -2.25197 2.39973
C -0.96146 -0.30934 3.51204
H -0.42492 -1.25921 3.34752
H -1.39358 -0.32688 4.52786
H -0.22245 0.50910 3.46446
C -2.80195 1.21593 2.75876
H -2.08355 2.05072 2.79866
H -3.30744 1.15654 3.73977
H -3.55563 1.45067 1.99157
C -5.58263 -0.83443 -1.00902
C -5.71514 0.63468 -0.40898
C -6.42524 1.64354 -1.31941
H -6.41018 2.63842 -0.84567
H -7.47919 1.35654 -1.47547
H -5.93590 1.72792 -2.30089
C -6.33480 0.68149 0.99768
H -5.81746 0.00569 1.69673
H -7.40343 0.41033 0.97469
H -6.24857 1.70626 1.39367
C -5.70898 -0.89733 -2.54040
H -5.02195 -0.19469 -3.03772
H -6.73762 -0.67216 -2.86793
H -5.45476 -1.91444 -2.87986
C -6.50583 -1.87966 -0.37171
H -6.29512 -2.86923 -0.80852
H -7.56474 -1.63939 -0.56796

H -6.35837 -1.95057 0.71603
N 1.94871 -1.51443 0.75035
N 1.90851 1.56821 0.68668
N -0.99161 0.04939 -1.07630
N -1.35898 -0.06054 1.14535
O -4.31464 1.06596 -0.26963
O -4.19553 -1.20414 -0.68301
Mg 0.58160 0.00712 0.28400
B -3.50575 -0.05216 -0.35220

12
SCF (BP86) Energy = -2036.20709192
Enthalpy 0K = -2035.211359
Enthalpy 298K = -2035.150229
Free Energy 298K = -2035.307959
Lowest Frequency = 14.4799 cm^{-1}
Second Frequency = 14.8527 cm^{-1}
SCF (BP86-D3BJ) Energy = -2036.48605846
SCF (Toluene) Energy = -2036.21254238
SCF (BS2) Energy = -2235.94374148

C -2.69874 3.15595 2.40235
H -1.93863 3.48374 3.13352
H -3.65917 3.06379 2.93075
H -2.77742 3.95356 1.64724
C -2.28781 1.83297 1.76931
C -2.90980 0.67144 2.30705
H -3.52957 0.86115 3.18754
C -3.01957 -0.64518 1.78926
C -4.03878 -1.54312 2.47995
H -4.98980 -1.57231 1.92125
H -4.25723 -1.17409 3.49360
H -3.67611 -2.58165 2.54201
C -2.78649 -2.31555 0.08887
C -3.95003 -2.26643 -0.74162
C -4.39175 -3.44677 -1.36856
H -5.28268 -3.40865 -2.00590
C -3.71788 -4.66154 -1.20235
H -4.08240 -5.57046 -1.69276
C -2.56597 -4.69594 -0.41129
H -2.02882 -5.64262 -0.28403
C -2.07730 -3.54312 0.23581
C -0.81131 -3.66868 1.08303
H -0.53609 -2.66029 1.44196
C 0.37135 -4.20167 0.24404
H 0.15957 -5.20598 -0.16316
H 1.28176 -4.27824 0.86106
H 0.59081 -3.52912 -0.60127
C -1.04875 -4.55537 2.32744
H -1.86379 -4.16120 2.95824
H -0.13607 -4.61088 2.94721
H -1.31929 -5.58652 2.03832
C -4.70310 -0.96538 -1.03398
H -4.27607 -0.17016 -0.39983
C -6.21389 -1.05958 -0.72122
H -6.71973 -1.79080 -1.37613
H -6.70093 -0.08179 -0.88119
H -6.40353 -1.36459 0.32173
C -4.49495 -0.55153 -2.50935
H -4.90429 -1.31310 -3.19644
H -3.42430 -0.43228 -2.74509
H -5.00581 0.40404 -2.72390
C -0.92517 3.04355 0.18445
C -1.53107 3.49365 -1.02859
C -1.06438 4.68240 -1.62236
H -1.53562 5.03886 -2.54440
C -0.01355 5.41671 -1.06108
H 0.33535 6.33810 -1.53948
C 0.58884 4.95683 0.11356
H 1.41876 5.52318 0.55139
C 0.15502 3.77958 0.75490
C 0.87531 3.33663 2.02879
H 0.35921 2.43547 2.40421
C 2.34269 2.95049 1.73494
H 2.40986 2.13714 0.99630
H 2.84748 2.61494 2.65837
H 2.90745 3.81483 1.34258
C 0.82595 4.41628 3.13518
H 1.39939 5.31428 2.84451
H 1.26949 4.03088 4.07003
H -0.20486 4.74208 3.35366
C -2.69757 2.74137 -1.67267
H -2.69079 1.71420 -1.26422
C -2.57205 2.64448 -3.20809
H -2.66968 3.63120 -3.69402
H -3.37111 2.00317 -3.61630
H -1.60157 2.21627 -3.51053
C -4.05183 3.38195 -1.28553
H -4.20432 3.38342 -0.19381
H -4.89169 2.83007 -1.74402
H -4.10298 4.42861 -1.63535
C 1.84805 -0.57855 -0.07927
C 2.18050 -0.77324 2.34339
H 3.11628 -0.18253 2.23236
C 2.57900 -2.25286 2.53886
H 1.68401 -2.86628 2.74158
H 3.27077 -2.36556 3.39368
H 3.07132 -2.65896 1.63976
C 1.44633 -0.26361 3.59375
H 1.20988 0.80890 3.50944
H 2.05705 -0.41309 4.50084
H 0.49688 -0.81313 3.72564
C 1.35796 -0.28220 -2.46748
H 2.30350 -0.84579 -2.62500
C 1.61018 1.19299 -2.84699
H 0.70174 1.79653 -2.67302
H 1.89472 1.29347 -3.91032
H 2.41603 1.62298 -2.22888
C 0.28747 -0.91434 -3.37275
H 0.12865 -1.97382 -3.11322
H 0.57571 -0.85215 -4.43644
H -0.67638 -0.38672 -3.25176
C 5.45427 -1.65787 -0.86761
C 5.58709 -0.08161 -0.75066
C 6.71175 0.40916 0.16602
H 6.69281 1.50992 0.21665
H 7.69687 0.10324 -0.22613
H 6.60451 0.01968 1.18914
C 5.66015 0.63296 -2.11046
H 4.84562 0.31083 -2.77917
H 6.62319 0.44645 -2.61437
H 5.55760 1.71830 -1.95058
C 5.96992 -2.41130 0.36958
H 5.54218 -2.00133 1.29855
H 7.06963 -2.36730 0.43987
H 5.67046 -3.46920 0.29569
C 6.04680 -2.26639 -2.14231
H 5.86495 -3.35336 -2.15153

H	7.13749	-2.10317	-2.18299
H	5.59349	-1.83820	-3.04846
N	-1.38084	1.80843	0.77344
N	-2.31817	-1.11407	0.73152
N	0.94272	-0.40412	-1.06914
N	1.32646	-0.57074	1.16712
O	3.99465	-1.85954	-0.90294
O	4.30138	0.30710	-0.14589
Mg	-0.56000	-0.06632	0.34377
B	3.41111	-0.72287	-0.37959

12_{BN}

SCF (BP86) Energy = -2036.19519119
Enthalpy 0K = -2035.199092
Enthalpy 298K = -2035.138420
Free Energy 298K = -2035.291832
Lowest Frequency = 14.5321 cm^{-1}
Second Frequency = 25.0163 cm^{-1}
SCF (BP86-D3BJ) Energy = -2036.48724138
SCF (Toluene) Energy = -2036.20021570
SCF (BS2) Energy = -2235.93155449

Mg	0.01388	-0.26467	-0.35032
O	-0.11405	-0.59749	1.72092
O	-0.31470	-2.23505	3.36419
N	1.63838	0.86492	-1.05814
N	-1.41148	1.04921	-1.16732
C	2.67925	1.51354	-3.22820
H	3.48026	2.01993	-2.66880
H	2.40738	2.12400	-4.10222
H	3.10037	0.56078	-3.59785
C	1.46902	1.22765	-2.34816
C	0.20263	1.32955	-2.98567
H	0.25385	1.54549	-4.05622
C	-1.11210	1.36578	-2.44502
C	-2.21681	1.74609	-3.42375
H	-3.05234	2.25617	-2.92219
H	-2.62602	0.82813	-3.88428
H	-1.83619	2.38484	-4.23526
C	-2.71322	1.36376	-0.63389
C	-4.63614	-1.12368	-2.49187
H	-5.67543	-1.13096	-2.11830
H	-4.46706	-2.07874	-3.01918
H	-4.55455	-0.30624	-3.22760
C	-4.17639	2.91482	0.56200
H	-4.34434	3.88903	1.03236
C	-5.21319	1.97379	0.54958
H	-6.18004	2.21011	1.00664
C	-5.00029	0.73222	-0.05534
H	-5.81077	-0.00532	-0.07390
C	-3.76791	0.40561	-0.65713
C	-3.62516	-0.95730	-1.33290
H	-2.60701	-1.01764	-1.75720
C	-3.77480	-2.11475	-0.32237
H	-3.02221	-2.04626	0.48000
H	-3.63263	-3.08676	-0.82386
H	-4.77673	-2.11391	0.14275
C	-2.92160	2.63713	-0.01390
C	-1.82607	3.70604	0.00817
H	-0.85950	3.17230	-0.05013
C	-1.83129	4.55968	1.29412
H	-2.70818	5.22955	1.33909
H	-0.93726	5.20601	1.32237
H	-1.83572	3.93926	2.20532
C	-1.91165	4.63970	-1.22373
H	-2.88852	5.15479	-1.25273
H	-1.78964	4.08886	-2.16857
H	-1.12253	5.41133	-1.18026
C	2.92860	1.02533	-0.43638
C	3.23360	2.25753	0.22412
C	4.47785	2.39457	0.86990
H	4.72011	3.33990	1.36692
C	5.40896	1.34957	0.89321
H	6.36960	1.47548	1.40389
C	5.09750	0.14430	0.25734
H	5.82334	-0.67666	0.27279
C	3.87353	-0.04182	-0.41637
C	3.61697	-1.38011	-1.10756
H	2.63266	-1.31851	-1.60517
C	4.68211	-1.67798	-2.18867
H	4.75892	-0.86096	-2.92569
H	4.43374	-2.60685	-2.73091
H	5.68207	-1.81427	-1.74015
C	3.54935	-2.53884	-0.08864
H	4.50855	-2.65649	0.44661
H	3.32385	-3.49047	-0.59862
H	2.75654	-2.37072	0.65831
C	2.25333	3.43246	0.22288
H	1.25421	3.01453	0.00198
C	2.18321	4.15769	1.58424
H	2.00109	3.45697	2.41631
H	1.36859	4.90206	1.57820
H	3.11570	4.70525	1.80785
C	2.58512	4.45134	-0.89350
H	3.59917	4.86654	-0.75280
H	1.86934	5.29236	-0.87833
H	2.54309	3.99225	-1.89361
C	0.10803	0.07805	3.02916
C	-0.56655	-0.95118	4.01721
C	0.06042	-0.99332	5.41378
H	-0.45722	-1.74950	6.02591
H	-0.04212	-0.01810	5.91970
H	1.12656	-1.26062	5.37210
C	-2.09308	-0.78181	4.11677
H	-2.55977	-0.72792	3.11949
H	-2.36652	0.12635	4.67921
H	-2.51257	-1.65384	4.64344
C	-0.55092	1.45357	2.97639
H	-0.02540	2.09731	2.25221
H	-0.48974	1.94338	3.96329
H	-1.60785	1.39085	2.67751
C	1.62669	0.19140	3.22019
H	2.09842	-0.80354	3.26624
H	1.86787	0.73401	4.14932
H	2.07173	0.74410	2.37665
B	-0.21323	-2.00059	2.00256
N	-0.20665	-2.97480	0.97435
C	-0.31561	-4.42303	1.35374
H	-0.37379	-4.41692	2.45710
C	-1.60449	-5.07301	0.82045
H	-1.68362	-6.10668	1.20187
H	-2.49512	-4.51672	1.15715
H	-1.59240	-5.09514	-0.27881
C	0.93909	-5.21933	0.95366
H	0.86314	-6.25155	1.33953
H	1.03540	-5.25070	-0.14131
H	1.84822	-4.76216	1.37893
N	-0.12131	-3.38405	-1.31469

C	-0.10933	-2.48161	-0.38037
C	-0.03480	-2.94116	-2.70132
H	0.04862	-1.82377	-2.76491
C	1.21214	-3.55890	-3.36366
H	1.29217	-3.25579	-4.42267
H	2.13168	-3.24741	-2.84222
H	1.15576	-4.66069	-3.31953
C	-1.30286	-3.37549	-3.46221
H	-2.20491	-2.92863	-3.01361
H	-1.25431	-3.07256	-4.52322
H	-1.41189	-4.47334	-3.41780

12_{BC}

SCF (BP86) Energy = -2036.18284545
Enthalpy 0K = -2035.186963
Enthalpy 298K = -2035.126466
Free Energy 298K = -2035.279289
Lowest Frequency = 13.0580 cm^{-1}
Second Frequency = 21.4557 cm^{-1}
SCF (BP86-D3BJ) Energy = -2036.47823631
SCF (Toluene) Energy = -2036.18866606
SCF (BS2) Energy = -2235.91887674

Mg	-0.07101	-0.00638	-0.63505
O	-0.76340	0.75918	1.19642
O	-2.06271	2.45415	2.05462
N	-0.03884	-2.08776	-0.79269
N	1.97176	0.20242	-1.06177
N	-1.53663	1.19100	-1.41041
C	0.43094	-3.92761	-2.40938
H	0.11636	-4.64531	-1.63692
H	1.31329	-4.32419	-2.93392
H	-0.39439	-3.86057	-3.14154
C	0.70383	-2.54821	-1.82315
C	1.73096	-1.79926	-2.45506
H	2.17002	-2.28312	-3.33274
C	2.39546	-0.60925	-2.05486
C	3.64451	-0.27365	-2.86371
H	4.14900	0.62993	-2.49428
H	3.35624	-0.10714	-3.91690
H	4.36224	-1.11040	-2.85819
C	2.86470	1.16520	-0.47424
C	2.17335	3.30804	-2.99761
H	2.96925	4.07275	-2.94841
H	1.41080	3.65515	-3.71678
H	2.62044	2.38278	-3.39643
C	4.74609	1.70419	0.99378
H	5.58655	1.37438	1.61522
C	4.47878	3.07064	0.87196
H	5.09846	3.80645	1.39542
C	3.41880	3.48720	0.05831
H	3.22410	4.55756	-0.06221
C	2.60612	2.56419	-0.62843
C	1.54530	3.08366	-1.60022
H	0.76070	2.31207	-1.70963
C	0.83549	4.36781	-1.12709
H	0.41974	4.25774	-0.11149
H	-0.00204	4.60116	-1.80472
H	1.50907	5.24324	-1.12579
C	3.96317	0.73300	0.33706
C	4.35046	-0.73898	0.52176
H	3.61607	-1.36146	-0.01706
C	4.32508	-1.16585	2.00692
H	5.06707	-0.60428	2.60141
H	4.57019	-2.23846	2.10283
H	3.33703	-0.99811	2.46340
C	5.75144	-1.03279	-0.06837
H	6.53569	-0.48789	0.48642
H	5.82669	-0.73331	-1.12545
H	5.98262	-2.11032	0.00125
C	-0.88038	-2.99420	-0.05043
C	-0.34119	-3.63624	1.11002
C	-1.17901	-4.47215	1.87389
H	-0.77328	-4.97225	2.75906
C	-2.52079	-4.67548	1.52859
H	-3.15593	-5.32583	2.13940
C	-3.03876	-4.04156	0.39622
H	-4.08726	-4.20152	0.12066
C	-2.24336	-3.20405	-0.41236
C	-2.87731	-2.57970	-1.65605
H	-2.09548	-1.99685	-2.17208
C	-3.38878	-3.66135	-2.63694
H	-2.59990	-4.38471	-2.90362
H	-3.75598	-3.19297	-3.56660
H	-4.22732	-4.23315	-2.20157
C	-4.01879	-1.60407	-1.29448
H	-4.82020	-2.11712	-0.73329
H	-4.46837	-1.18056	-2.20886
H	-3.65562	-0.75894	-0.68929
C	1.12581	-3.45914	1.51491
H	1.44837	-2.47010	1.13655
C	1.34591	-3.49221	3.04275
H	0.66269	-2.81110	3.57762
H	2.38191	-3.19866	3.28231
H	1.19688	-4.50523	3.45627
C	2.03468	-4.51932	0.84626
H	1.71635	-5.53782	1.13181
H	3.08319	-4.38893	1.16837
H	2.01011	-4.44958	-0.25190
C	-0.55401	0.72280	2.67324
C	-1.04955	2.16160	3.08059
C	-1.72690	2.23798	4.45165
H	-2.06450	3.27014	4.63749
H	-1.01822	1.96264	5.25132
H	-2.60324	1.57626	4.51285
C	0.03647	3.24210	2.95666
H	0.56059	3.18765	1.98877
H	0.78526	3.15211	3.76098
H	-0.43734	4.23346	3.03607
C	0.91845	0.44299	2.95481
H	1.17112	-0.57899	2.63008
H	1.11588	0.50509	4.03867
H	1.58460	1.14799	2.43560
C	-1.44948	-0.40621	3.20221
H	-2.51470	-0.19887	3.00991
H	-1.31116	-0.54314	4.28749
H	-1.19102	-1.35149	2.69792
C	-2.44429	1.75020	-0.51099
B	-1.80691	1.69715	0.93912
N	-3.60029	2.22426	-0.92182
C	-4.62691	2.80780	-0.05286
H	-5.50363	2.94518	-0.71959
C	-5.11756	1.89097	1.09207
H	-4.35873	1.77573	1.88274
H	-6.02461	2.31174	1.56291
H	-5.37157	0.89210	0.69783
C	-4.25481	4.22033	0.45273
H	-5.12256	4.70322	0.93834

H -3.43084 4.17952 1.18274
H -3.94014 4.85423 -0.39358
C -1.92999 1.24942 -2.83406
H -2.97450 0.88046 -2.91533
C -1.92339 2.68526 -3.40235
H -0.89972 3.09974 -3.40051
H -2.28878 2.68843 -4.44546
H -2.58187 3.32747 -2.79999
C -1.00226 0.35673 -3.67116
H 0.04280 0.71701 -3.62191
H -1.01313 -0.69464 -3.33200
H -1.30140 0.36330 -4.73387

15_{BN}
SCF (BP86) Energy = -2134.45466683
Enthalpy 0K = -2133.428368
Enthalpy 298K = -2133.366521
Free Energy 298K = -2133.525475
Lowest Frequency = 13.0509 cm^{-1}
Second Frequency = 16.6011 cm^{-1}
SCF (BP86-D3BJ) Energy = -2134.75588762
SCF (Toluene) Energy = -2134.46030550
SCF (BS2) Energy = -2334.21254798

Mg -0.05617 -0.03522 -0.34213
O 0.60862 0.11913 1.64078
O 2.48372 0.30632 3.00518
N -1.52791 1.36963 -0.89554
N -1.21698 -1.69444 -0.96406
C -2.56172 2.23018 -2.99501
H -3.12440 2.96300 -2.39781
H -3.20810 1.84718 -3.79870
H -1.72405 2.77782 -3.46473
C -2.00656 1.10240 -2.13288
C -1.99761 -0.18457 -2.72981
H -2.36190 -0.20331 -3.76063
C -1.77434 -1.47677 -2.17144
C -2.18804 -2.64313 -3.06280
H -2.43519 -3.54099 -2.47813
H -1.35161 -2.90701 -3.73513
H -3.04781 -2.37540 -3.69600
C -1.22831 -3.02333 -0.40153
C 1.06646 -4.55796 -2.79711
H 1.24582 -5.60612 -2.49878
H 1.88666 -4.26002 -3.47350
H 0.12461 -4.53457 -3.36933
C -2.30045 -4.68101 1.04201
H -3.12332 -4.97267 1.70209
C -1.27188 -5.59553 0.78687
H -1.29160 -6.59189 1.24107
C -0.21892 -5.21945 -0.05037
H 0.58987 -5.93117 -0.25105
C -0.17037 -3.94613 -0.65432
C 1.01737 -3.62609 -1.56309
H 0.89886 -2.58886 -1.92288
C 2.35295 -3.71043 -0.78923
H 2.36960 -3.02315 0.07260
H 3.19995 -3.44998 -1.44763
H 2.53144 -4.73190 -0.40940
C -2.30148 -3.39468 0.46938
C -3.45976 -2.43851 0.76334
H -3.05811 -1.41196 0.67219
C -4.04124 -2.60579 2.18319
H -4.60331 -3.55066 2.28799
H -4.74833 -1.78820 2.40210
H -3.25533 -2.59514 2.95654
C -4.59500 -2.57969 -0.27925
H -4.99515 -3.60931 -0.27971
H -4.24854 -2.34797 -1.29809
H -5.42709 -1.89277 -0.04232
C -1.89405 2.60730 -0.25501
C -3.15203 2.69768 0.42326
C -3.48556 3.89425 1.08738
H -4.45294 3.96842 1.59644
C -2.61349 4.98835 1.11053
H -2.89179 5.90871 1.63479
C -1.38508 4.89169 0.45049
H -0.70169 5.74850 0.45620
C -1.00643 3.72371 -0.24124
C 0.33090 3.71921 -0.97949
H 0.44688 2.72765 -1.45185
C 0.36024 4.77884 -2.10601
H -0.48357 4.65467 -2.80517
H 1.29889 4.70273 -2.68227
H 0.30268 5.80261 -1.69554
C 1.51879 3.93150 -0.01438
H 1.42819 4.88923 0.52785
H 2.47403 3.94969 -0.56633
H 1.58199 3.12132 0.73051
C -4.16184 1.54683 0.42854
H -3.63780 0.64720 0.06144
C -4.69977 1.24335 1.84424
H -3.88483 1.04631 2.56082
H -5.35881 0.35820 1.82066
H -5.29840 2.08018 2.24483
C -5.34645 1.82478 -0.52774
H -5.89569 2.73209 -0.21856
H -6.05819 0.98033 -0.52037
H -5.01093 1.97297 -1.56631
C 0.11015 0.33423 3.02568
C 1.37568 -0.08403 3.87079
C 1.52261 0.65824 5.20264
H 2.44080 0.32128 5.71037
H 0.66822 0.44594 5.86790
H 1.59465 1.74591 5.05514
C 1.48262 -1.60416 4.09074
H 1.36166 -2.15840 3.14542
H 0.72838 -1.96819 4.80818
H 2.48252 -1.83296 4.49236
C -1.12233 -0.54276 3.23194
H -1.94823 -0.19265 2.59099
H -1.46432 -0.48090 4.27913
H -0.92015 -1.59673 2.98946
C -0.24004 1.82222 3.15526
H 0.65066 2.45510 3.01279
H -0.66666 2.04051 4.14832
H -0.98625 2.10102 2.39379
C 4.24897 0.20919 0.56919
C 5.00730 -0.59301 -0.31258
H 4.48844 -1.21637 -1.04645
C 6.40781 -0.60431 -0.24338
H 6.97307 -1.23759 -0.93636
C 7.08466 0.18154 0.70284
H 8.17830 0.17233 0.75300
C 6.33712 0.98679 1.57774
H 6.84724 1.61523 2.31640
C 4.93754 1.01189 1.50722
H 4.36580 1.65168 2.18441

B	2.04195	0.23229	1.69048
N	2.81735	0.21881	0.50838
C	2.62125	0.90751	-1.91714
H	2.40741	1.96689	-1.68169
H	3.72691	0.85044	-2.01772
C	2.00639	0.56006	-3.28438
H	2.20254	-0.50884	-3.50987
H	0.90099	0.65670	-3.23967
C	2.54183	1.41925	-4.44389
H	3.64370	1.32047	-4.49044
H	2.34368	2.48729	-4.22669
C	1.93455	1.05178	-5.80670
H	2.33574	1.68455	-6.61722
H	2.14858	-0.00020	-6.06772
H	0.83639	1.17209	-5.80085
C	2.09598	-0.01319	-0.79687
H	2.34682	-1.04994	-1.11262

15_{BC}

SCF (BP86) Energy = -2134.46541571
Enthalpy 0K = -2133.438515
Enthalpy 298K = -2133.377004
Free Energy 298K = -2133.533611
Lowest Frequency = 13.2027 cm^{-1}
Second Frequency = 22.3442 cm^{-1}
SCF (BP86-D3BJ) Energy = -2134.77093851
SCF (Toluene) Energy = -2134.47176486
SCF (BS2) Energy = -2334.22455299

Mg	0.11032	0.09423	0.34586
O	-0.36490	-0.45243	-1.65956
O	-1.79086	-1.76669	-2.91543
N	0.61213	2.05563	0.88243
N	1.91862	-0.69164	1.04409
N	-1.68329	-0.77447	0.74228
C	1.33743	3.52615	2.76782
H	1.21957	4.37510	2.07845
H	2.27836	3.64169	3.32745
H	0.50907	3.57932	3.49689
C	1.29614	2.18889	2.03828
C	1.98588	1.12644	2.68004
H	2.39673	1.38310	3.66043
C	2.33896	-0.16651	2.21638
C	3.20976	-0.98656	3.16080
H	3.85094	-1.69983	2.62295
H	2.55396	-1.57426	3.82866
H	3.83721	-0.34178	3.79519
C	2.56564	-1.86991	0.52455
C	1.15636	-4.20708	2.90840
H	1.49479	-5.22779	2.65437
H	0.27291	-4.29568	3.56323
H	1.96302	-3.72521	3.48507
C	4.33631	-2.85874	-0.83919
H	5.23544	-2.74870	-1.45430
C	3.80770	-4.13780	-0.62195
H	4.29010	-5.01649	-1.06349
C	2.66199	-4.28122	0.16639
H	2.25107	-5.28134	0.34536
C	2.02431	-3.16857	0.75354
C	0.79796	-3.40393	1.63569
H	0.41076	-2.42212	1.95830
C	-0.33570	-4.11843	0.86858
H	-0.57998	-3.59381	-0.06970
H	-1.25009	-4.14843	1.48473
H	-0.06024	-5.15706	0.61099
C	3.73737	-1.71100	-0.28428
C	4.36163	-0.33243	-0.53042
H	3.54557	0.40889	-0.44012
C	4.99948	-0.18479	-1.92914
H	5.92885	-0.77476	-2.01934
H	5.27412	0.86937	-2.10782
H	4.32174	-0.50473	-2.73709
C	5.42297	0.02110	0.54040
H	6.23056	-0.73256	0.54874
H	4.99202	0.07030	1.55102
H	5.87812	1.00346	0.32176
C	0.05216	3.21588	0.23616
C	0.77034	3.80788	-0.85078
C	0.18031	4.87793	-1.55058
H	0.72182	5.33871	-2.38285
C	-1.08458	5.36795	-1.20028
H	-1.52910	6.19744	-1.76055
C	-1.76793	4.79673	-0.12295
H	-2.75094	5.18917	0.16088
C	-1.22259	3.72793	0.61810
C	-2.01463	3.18180	1.80870
H	-1.40749	2.39934	2.29538
C	-2.30327	4.28460	2.85479
H	-1.38468	4.80194	3.17897
H	-2.78537	3.84655	3.74577
H	-2.98879	5.05107	2.45179
C	-3.33227	2.51458	1.36100
H	-3.98936	3.23215	0.83746
H	-3.88032	2.12432	2.23552
H	-3.12906	1.66629	0.69031
C	2.18063	3.33413	-1.21479
H	2.22991	2.25489	-0.97141
C	2.53657	3.51563	-2.70503
H	1.76609	3.09918	-3.37537
H	3.49362	3.01344	-2.92883
H	2.66617	4.58062	-2.96691
C	3.25200	4.03755	-0.34602
H	3.21265	5.13123	-0.49525
H	4.26395	3.69243	-0.62318
H	3.10966	3.83393	0.72596
C	0.05367	-0.27092	-3.08157
C	-0.60454	-1.53652	-3.75480
C	-1.07235	-1.31834	-5.19595
H	-1.54006	-2.24168	-5.57363
H	-0.21782	-1.07796	-5.85125
H	-1.81183	-0.50730	-5.26790
C	0.25948	-2.80450	-3.65257
H	0.62080	-2.97221	-2.62480
H	1.13198	-2.75397	-4.32458
H	-0.35136	-3.67324	-3.94549
C	1.57613	-0.23438	-3.14270
H	1.95722	0.67511	-2.65165
H	1.91209	-0.20998	-4.19348
H	2.02388	-1.10955	-2.64880
C	-0.56659	1.05634	-3.53880
H	-1.66773	1.01480	-3.51291
H	-0.25165	1.30654	-4.56527
H	-0.24079	1.86957	-2.86980
C	-2.44148	-1.34613	-0.38469
H	-2.64476	-2.43178	-0.21965
C	-2.12067	-1.08504	2.02112
C	-3.21838	-1.94948	2.32959
H	-3.79953	-2.40401	1.52204

C	-3.57379	-2.23879	3.65599
H	-4.42365	-2.90770	3.83938
C	-2.87203	-1.69003	4.74024
H	-3.16004	-1.91741	5.77126
C	-1.78849	-0.83439	4.46298
H	-1.21768	-0.38776	5.28612
C	-1.42382	-0.53868	3.14691
H	-0.57185	0.13533	2.97547
B	-1.55504	-1.22618	-1.67760
C	-3.84058	-0.67854	-0.63857
H	-4.30492	-0.49137	0.34699
H	-3.70091	0.31876	-1.10158
C	-4.79233	-1.52099	-1.50507
H	-4.31781	-1.74241	-2.48042
H	-4.95180	-2.50390	-1.01655
C	-6.15618	-0.84777	-1.74172
H	-5.99834	0.13255	-2.23276
H	-6.62671	-0.62393	-0.76474
C	-7.11284	-1.69923	-2.59116
H	-6.68222	-1.91194	-3.58601
H	-7.31916	-2.67041	-2.10712
H	-8.08037	-1.19182	-2.74700

TS(15_{BN}-15_{BCN})

SCF (BP86) Energy = -2134.41275196
Enthalpy 0K = -2133.387025
Enthalpy 298K = -2133.325926
Free Energy 298K = -2133.482632
Lowest Frequency = -237.2014 cm^{-1}
Second Frequency = 11.4130 cm^{-1}
SCF (BP86-D3BJ) Energy = -2134.71858440
SCF (Toluene) Energy = -2134.41911188
SCF (BS2) Energy = -2334.17113756

Mg	0.03910	0.25768	-0.50679
O	-0.40965	-3.55934	-0.01744
O	-0.26514	-1.65332	-1.36328
N	1.62998	1.52850	-1.02753
N	-1.44874	1.70623	-0.84567
C	2.52982	3.42651	-2.39050
H	3.48278	2.88106	-2.43095
H	2.68377	4.30974	-1.74643
H	2.28097	3.79982	-3.39689
C	1.38585	2.57175	-1.85202
C	0.09458	3.01613	-2.23101
H	0.10039	3.85229	-2.93607
C	-1.17470	2.75191	-1.65636
C	-2.23234	3.81127	-1.95509
H	-2.07912	4.23153	-2.96178
H	-2.13447	4.64600	-1.23833
H	-3.25924	3.42972	-1.87421
C	-2.74289	1.69353	-0.19965
C	-2.93418	2.39925	1.02406
C	-4.21200	2.39607	1.61916
H	-4.36290	2.94098	2.55795
C	-5.28769	1.72468	1.03364
H	-6.27689	1.74527	1.50295
C	-5.08588	1.01435	-0.15618
H	-5.92763	0.47713	-0.60242
C	-3.82628	0.96878	-0.78631
C	-3.64857	0.15128	-2.07132
H	-2.62305	-0.26341	-2.03966
C	-3.75779	1.00513	-3.35810
H	-4.73046	1.52692	-3.40090
H	-3.68558	0.35879	-4.25125
H	-2.95916	1.75797	-3.42785
C	-4.63628	-1.03026	-2.16970
H	-5.67116	-0.68424	-2.33977
H	-4.63103	-1.65201	-1.25885
H	-4.37448	-1.67280	-3.02680
C	-1.81168	3.16621	1.72793
H	-0.89697	3.06396	1.11776
C	-2.13137	4.67450	1.85179
H	-3.00750	4.84632	2.50169
H	-2.35215	5.13132	0.87288
H	-1.27760	5.21510	2.29630
C	-1.52110	2.57239	3.12527
H	-2.41981	2.59828	3.76593
H	-0.73063	3.14659	3.63739
H	-1.18740	1.52364	3.05825
C	2.96884	1.41391	-0.49239
C	3.37663	2.25747	0.58423
C	4.68920	2.13738	1.08418
H	5.00434	2.78381	1.91108
C	5.59237	1.21616	0.54931
H	6.60992	1.14099	0.94682
C	5.17840	0.37848	-0.49271
H	5.88391	-0.35258	-0.89691
C	3.87680	0.44931	-1.02524
C	2.44604	3.27548	1.24976
H	1.48573	3.26927	0.70553
C	3.01088	4.71435	1.19512
H	3.93725	4.80527	1.78914
H	2.28085	5.43074	1.61062
H	3.24837	5.02907	0.16543
C	2.16461	2.88244	2.71847
H	1.70273	1.88390	2.79464
H	1.48719	3.61337	3.19347
H	3.09741	2.86119	3.30874
C	3.46820	-0.49002	-2.16297
H	2.41191	-0.76641	-1.97861
C	4.29864	-1.78949	-2.19991
H	3.86481	-2.49923	-2.92542
H	4.33904	-2.28431	-1.21585
H	5.33515	-1.59906	-2.53062
C	3.52680	0.19102	-3.55143
H	2.83018	1.03922	-3.62604
H	3.26301	-0.53078	-4.34508
H	4.54630	0.56108	-3.76057
C	-0.31768	-2.81651	-2.27452
C	0.61621	-2.58375	-3.46178
H	0.59963	-3.46019	-4.13239
H	1.65306	-2.41142	-3.14378
H	0.27896	-1.71016	-4.04454
C	-1.76438	-2.95168	-2.76679
H	-2.05217	-2.03755	-3.30925
H	-2.46073	-3.09258	-1.92565
H	-1.87022	-3.80399	-3.45854
C	0.10867	-3.99874	-1.30827
C	1.63177	-4.14377	-1.16186
H	2.09563	-3.17815	-0.90612
H	2.09781	-4.53661	-2.08106
H	1.84331	-4.84162	-0.33669
C	-0.52884	-5.35165	-1.64130
H	-0.22873	-5.69284	-2.64703
H	-1.62723	-5.30766	-1.59455
H	-0.18716	-6.10445	-0.91263
B	-0.37215	-2.16918	0.00694

C	0.71703	-1.05374	1.28825
H	0.95839	0.01629	1.50884
C	1.53025	-1.89095	2.20108
C	2.76550	-1.36821	2.67504
C	1.18734	-3.20304	2.62668
C	3.60535	-2.10607	3.51581
H	3.06788	-0.36105	2.36220
C	2.02853	-3.93481	3.48001
H	0.26782	-3.66909	2.26440
C	3.24305	-3.39920	3.93488
H	4.54973	-1.66339	3.85366
H	1.72414	-4.94133	3.79131
H	3.89449	-3.97463	4.60088
N	-0.74655	-1.25245	1.07157
C	-1.69072	-1.47349	2.19399
H	-1.82113	-0.50949	2.72113
H	-1.25161	-2.17938	2.92526
C	-3.05003	-1.99260	1.71224
H	-3.47741	-1.27091	0.99031
H	-2.89858	-2.94579	1.16895
C	-4.04472	-2.21154	2.86603
H	-4.18341	-1.25810	3.41096
H	-3.61076	-2.92234	3.59572
C	-5.41018	-2.73080	2.38996
H	-5.30952	-3.69774	1.86533
H	-6.10537	-2.87990	3.23393
H	-5.88095	-2.01883	1.68923

15_{BCN}

SCF (BP86) Energy = -2134.43841047
Enthalpy 0K = -2133.411866
Enthalpy 298K = -2133.350189
Free Energy 298K = -2133.509294
Lowest Frequency = 9.2700 cm^{-1}
Second Frequency = 14.6642 cm^{-1}
SCF (BP86-D3BJ) Energy = -2134.73968426
SCF (Toluene) Energy = -2134.44437774
SCF (BS2) Energy = -2334.19501395

Mg	0.18424	-0.12734	-0.63670
O	-1.93270	2.97108	-0.71281
O	-1.37017	0.86319	-1.62058
N	-0.00477	-2.17824	-0.94770
N	2.22858	0.00151	-1.00721
C	0.68626	-4.10330	-2.37552
H	-0.35788	-4.44714	-2.38517
H	1.23718	-4.77599	-1.69366
H	1.12121	-4.22334	-3.37932
C	0.82008	-2.66351	-1.89686
C	1.90202	-1.93573	-2.47933
H	2.36358	-2.44205	-3.33094
C	2.62636	-0.80612	-2.02177
C	3.92709	-0.50653	-2.75685
H	4.27551	-1.37186	-3.33963
H	4.72257	-0.19709	-2.06209
H	3.77015	0.33572	-3.45526
C	3.21848	0.81390	-0.32969
C	4.01766	0.21274	0.69483
C	4.94245	1.00920	1.39729
H	5.55907	0.54620	2.17510
C	5.09200	2.37336	1.12720
H	5.81230	2.97571	1.69066
C	4.31700	2.95203	0.11950
H	4.44259	4.01560	-0.11277
C	3.38938	2.19763	-0.62745
C	2.65614	2.89461	-1.77075
H	1.99160	2.14644	-2.23493
C	3.64536	3.37908	-2.85825
H	4.30371	4.17739	-2.47269
H	3.09707	3.78940	-3.72452
H	4.29312	2.56175	-3.21664
C	1.79366	4.07829	-1.27525
H	2.40186	4.80482	-0.70886
H	0.96663	3.74751	-0.62561
H	1.35214	4.62259	-2.12921
C	3.93469	-1.27700	1.03479
H	3.01236	-1.67080	0.57405
C	5.12813	-2.06098	0.43740
H	6.08468	-1.68870	0.84571
H	5.17345	-1.97053	-0.65960
H	5.04982	-3.13436	0.68483
C	3.85411	-1.53032	2.55548
H	4.78255	-1.23115	3.07246
H	3.70783	-2.60591	2.75494
H	3.01957	-0.97655	3.01673
C	-0.95304	-3.08891	-0.33670
C	-0.57812	-3.82323	0.82716
C	-1.48255	-4.75792	1.36799
H	-1.18745	-5.32937	2.25521
C	-2.73958	-4.97391	0.79715
H	-3.42293	-5.71731	1.22092
C	-3.12079	-4.21051	-0.30992
H	-4.11482	-4.35844	-0.74565
C	-2.26166	-3.25190	-0.88447
C	0.75818	-3.62037	1.54029
H	1.31123	-2.83413	0.99798
C	1.62445	-4.90017	1.52887
H	1.13025	-5.72435	2.07293
H	2.59765	-4.71672	2.01729
H	1.82131	-5.25104	0.50179
C	0.52933	-3.12908	2.98888
H	-0.04113	-2.18552	3.00688
H	1.49067	-2.95790	3.50111
H	-0.03520	-3.87155	3.57950
C	-2.78420	-2.43404	-2.06856
H	-2.05327	-1.63421	-2.27641
C	-4.12824	-1.75639	-1.71498
H	-4.50991	-1.18219	-2.57644
H	-4.01665	-1.06665	-0.86270
H	-4.90487	-2.49601	-1.45475
C	-2.94131	-3.29035	-3.34702
H	-1.98706	-3.74312	-3.66290
H	-3.31259	-2.67133	-4.18278
H	-3.66531	-4.10979	-3.19058
C	-1.75578	1.72742	-2.74334
C	-2.58969	0.92195	-3.74593
H	-2.94224	1.57547	-4.56320
H	-3.46398	0.45917	-3.26983
H	-1.97557	0.12405	-4.19733
C	-0.48151	2.22405	-3.43682
H	0.13811	1.35944	-3.73295
H	0.10287	2.86891	-2.76795
H	-0.71746	2.79431	-4.35145
C	-2.55972	2.89585	-2.01182
C	-4.05448	2.55779	-1.82159
H	-4.18511	1.57844	-1.33415
H	-4.60475	2.55467	-2.77777
H	-4.50459	3.32028	-1.16576

C	-2.42565	4.26632	-2.68815
H	-2.81827	4.24345	-3.71956
H	-1.37868	4.60402	-2.71378
H	-3.00716	5.01123	-2.12048
B	-1.66530	1.61603	-0.33210
C	-2.22460	0.78873	0.91808
H	-2.35969	-0.30426	0.87667
C	-3.01854	1.38634	2.03171
C	-3.63490	0.53398	2.98021
C	-3.23218	2.78179	2.16595
C	-4.42433	1.04513	4.02041
H	-3.49011	-0.54959	2.89024
C	-4.00620	3.29378	3.21839
H	-2.81629	3.45540	1.41040
C	-4.60594	2.43180	4.15129
H	-4.89206	0.35899	4.73543
H	-4.15484	4.37651	3.30060
H	-5.21504	2.83577	4.96706
N	-0.70036	1.14176	0.76989
C	-0.03790	1.97832	1.78603
H	0.88011	2.39157	1.32527
H	-0.67110	2.84414	2.06231
C	0.32750	1.19794	3.05701
H	0.96872	0.33686	2.78036
H	-0.59768	0.77664	3.49388
C	1.04742	2.06623	4.10343
H	1.97591	2.47680	3.66161
H	0.41093	2.93834	4.34851
C	1.38521	1.30306	5.39354
H	2.04719	0.44284	5.18821
H	1.89825	1.95036	6.12545
H	0.47218	0.91058	5.87505

TS(15_{BCN}-15_{BC})

SCF (BP86) Energy = -2134.42123496
Enthalpy 0K = -2133.395028
Enthalpy 298K = -2133.333967
Free Energy 298K = -2133.490482
Lowest Frequency = -116.9987 cm^{-1}
Second Frequency = 15.0937 cm^{-1}
SCF (BP86-D3BJ) Energy = -2134.72603057
SCF (Toluene) Energy = -2134.42669435
SCF (BS2) Energy = -2334.17889509

Mg	0.22391	0.45934	0.29815
O	-1.14271	-3.13950	1.45921
O	-0.81210	-0.86331	1.85498
N	-0.88537	2.21785	0.54929
N	2.13392	1.38797	0.28169
C	-1.04808	4.64020	1.12023
H	-2.08600	4.46729	1.43706
H	-1.09318	5.17765	0.15564
H	-0.55044	5.30435	1.84375
C	-0.26446	3.34350	0.95122
C	1.13518	3.46627	1.15138
H	1.44018	4.44874	1.52388
C	2.22424	2.66395	0.72296
C	3.56311	3.40015	0.75637
H	3.45244	4.41417	0.34023
H	4.34828	2.87441	0.19750
H	3.89858	3.51709	1.80174
C	3.29218	0.78648	-0.35325
C	3.33599	0.74735	-1.78550
C	4.43599	0.13753	-2.41802
H	4.47249	0.10415	-3.51026
C	5.48863	-0.42129	-1.68536
H	6.33512	-0.88831	-2.19968
C	5.44650	-0.37078	-0.29176
H	6.27316	-0.79868	0.28615
C	4.36808	0.22092	0.39925
C	4.44538	0.22892	1.92984
H	3.49912	0.64931	2.31554
C	5.60993	1.10489	2.45547
H	6.58200	0.69644	2.12742
H	5.61191	1.11893	3.55983
H	5.55162	2.14450	2.10105
C	4.62179	-1.20124	2.49520
H	5.62897	-1.59183	2.26764
H	3.89291	-1.90771	2.07102
H	4.51365	-1.20108	3.59420
C	2.25291	1.40645	-2.64768
H	1.27552	1.22639	-2.15828
C	2.45767	2.93891	-2.73165
H	3.44440	3.17162	-3.17001
H	2.39827	3.42034	-1.74382
H	1.68519	3.39547	-3.37568
C	2.16014	0.82985	-4.07565
H	3.03299	1.11436	-4.69007
H	1.26717	1.23161	-4.58200
H	2.08159	-0.26978	-4.07720
C	-2.27527	2.31291	0.16150
C	-2.59957	2.64951	-1.18651
C	-3.95441	2.72051	-1.56510
H	-4.20450	2.97345	-2.60170
C	-4.98229	2.48734	-0.64602
H	-6.03026	2.55884	-0.95568
C	-4.65588	2.15651	0.67309
H	-5.46042	1.97236	1.39332
C	-3.31720	2.04958	1.10093
C	-1.52908	2.92103	-2.24465
H	-0.54666	2.91167	-1.74127
C	-1.70065	4.30779	-2.90517
H	-2.63912	4.37022	-3.48373
H	-0.86930	4.50690	-3.60398
H	-1.71806	5.11810	-2.15651
C	-1.52012	1.80211	-3.31064
H	-1.28400	0.82391	-2.85617
H	-0.76651	2.01290	-4.08984
H	-2.50093	1.72320	-3.81262
C	-3.03933	1.67020	2.55799
H	-1.96631	1.42550	2.63522
C	-3.84021	0.41814	2.97722
H	-3.56356	0.10998	4.00117
H	-3.64934	-0.42467	2.29410
H	-4.92759	0.60894	2.98426
C	-3.34475	2.83246	3.53262
H	-2.73022	3.72295	3.32440
H	-3.14683	2.52529	4.57505
H	-4.40560	3.13340	3.46738
C	-0.14980	-1.58471	2.96312
C	-0.41526	-0.83095	4.26775
H	0.02166	-1.37675	5.12183
H	-1.49093	-0.69776	4.45034
H	0.05448	0.16640	4.23084
C	1.34803	-1.60610	2.65423
H	1.72466	-0.57113	2.57845
H	1.54833	-2.12117	1.70001
H	1.92011	-2.10482	3.45225

C	-0.80421	-3.02142	2.87298
C	-2.12115	-3.14463	3.66076
H	-2.81243	-2.32153	3.42086
H	-1.94548	-3.15132	4.74977
H	-2.61159	-4.09164	3.38405
C	0.13401	-4.17709	3.24244
H	0.46787	-4.09669	4.29136
H	1.01838	-4.20989	2.58941
H	-0.40429	-5.13244	3.13158
B	-1.25992	-1.86623	0.91557
C	-1.78362	-1.42410	-0.48220
H	-2.36688	-0.48041	-0.45015
C	-2.54430	-2.36338	-1.39668
C	-3.29538	-1.81512	-2.46067
C	-2.54176	-3.76765	-1.24382
C	-4.01291	-2.63396	-3.34549
H	-3.31937	-0.72622	-2.58389
C	-3.25849	-4.59013	-2.12812
H	-1.99444	-4.21314	-0.40830
C	-3.99428	-4.02886	-3.18386
H	-4.59186	-2.18213	-4.15875
H	-3.24697	-5.67664	-1.98574
H	-4.55479	-4.67244	-3.87065
N	-0.33446	-1.07252	-0.86598
C	0.33499	-1.91123	-1.85829
H	-0.37068	-2.23793	-2.65099
H	1.09155	-1.28140	-2.36897
C	1.07339	-3.16146	-1.32204
H	0.35864	-3.81074	-0.78348
H	1.82331	-2.83290	-0.57356
C	1.77485	-3.96641	-2.42931
H	1.02137	-4.28956	-3.17385
H	2.47594	-3.30267	-2.97306
C	2.53674	-5.19393	-1.90553
H	3.02555	-5.75229	-2.72303
H	3.32246	-4.89893	-1.18699
H	1.85754	-5.89198	-1.38416

16_{BN}

SCF (BP86) Energy = -2134.44943684
Enthalpy 0K = -2133.423276
Enthalpy 298K = -2133.362047
Free Energy 298K = -2133.516100
Lowest Frequency = 13.3083 cm^{-1}
Second Frequency = 19.4865 cm^{-1}
SCF (BP86-D3BJ) Energy = -2134.76552308
SCF (Toluene) Energy = -2134.45510288
SCF (BS2) Energy = -2334.20589535

Mg	-0.00011	-0.19366	0.08449
O	-2.02928	-0.36620	0.80990
O	-4.23699	0.05054	0.21075
N	1.08170	1.18842	1.25712
N	1.08652	-1.87864	0.70629
N	-2.46447	0.36145	-1.54901
C	1.70029	-3.13924	2.76785
H	1.18132	-4.00727	2.33238
H	1.44044	-3.05662	3.83476
H	2.78212	-3.34729	2.70782
C	1.34803	-1.85172	2.03166
C	1.34815	-0.67480	2.83193
H	1.52982	-0.86404	3.89363
C	1.40358	0.70573	2.47366
C	1.84785	1.65258	3.58278
H	2.36190	1.11173	4.39093
H	0.97379	2.16914	4.01828
H	2.51550	2.43623	3.19288
C	1.41060	2.56387	0.93184
C	2.63764	2.83415	0.25123
C	2.94841	4.16463	-0.08868
H	3.88968	4.37476	-0.60492
C	2.08166	5.22180	0.20576
H	2.34306	6.24777	-0.07437
C	0.87846	4.94891	0.85903
H	0.19224	5.77081	1.09327
C	0.52470	3.63866	1.23733
C	-0.79626	3.44291	1.97711
H	-0.84858	2.38358	2.27008
C	-0.87665	4.29756	3.26423
H	0.00022	4.14705	3.91603
H	-1.78316	4.04282	3.84163
H	-0.92989	5.37514	3.02963
C	-2.01207	3.74363	1.07102
H	-1.95284	4.76430	0.65428
H	-2.95628	3.67698	1.64144
H	-2.07456	3.03832	0.22628
C	3.64057	1.72974	-0.08825
H	3.07139	0.78617	-0.18033
C	4.66836	1.54197	1.05405
H	5.40134	0.75746	0.79426
H	4.18581	1.25031	2.00093
H	5.22630	2.47901	1.23097
C	4.37203	1.97836	-1.42414
H	5.07683	2.82608	-1.35466
H	3.65987	2.18594	-2.23911
H	4.96741	1.09304	-1.70061
C	1.47065	-3.05186	-0.04238
C	0.48774	-3.96304	-0.53300
C	0.90090	-5.09305	-1.26653
H	0.14232	-5.79611	-1.62828
C	2.24943	-5.34414	-1.53171
H	2.54969	-6.23159	-2.09862
C	3.20778	-4.43810	-1.06869
H	4.26640	-4.61772	-1.28780
C	2.85091	-3.29129	-0.33353
C	3.97142	-2.32582	0.06070
H	3.53216	-1.50701	0.65526
C	5.07004	-2.99968	0.91521
H	4.66087	-3.47921	1.82020
H	5.81757	-2.25360	1.23639
H	5.60528	-3.77852	0.34395
C	4.60349	-1.70494	-1.20646
H	5.04727	-2.48415	-1.85071
H	5.40828	-1.00015	-0.93415
H	3.85536	-1.16072	-1.80593
C	-1.00716	-3.79809	-0.26332
H	-1.15615	-2.82047	0.22787
C	-1.51883	-4.89717	0.69821
H	-1.37501	-5.90082	0.26105
H	-2.59845	-4.77687	0.90076
H	-0.98451	-4.87668	1.66338
C	-1.83085	-3.80110	-1.57008
H	-1.48072	-3.02078	-2.26542
H	-2.89896	-3.61708	-1.36033
H	-1.76379	-4.77191	-2.09136
C	-3.48769	0.50251	-2.67731
C	-2.81569	0.74660	-4.04323
H	-2.27185	1.70121	-4.07928

H	-3.60632	0.77087	-4.81301
H	-2.11269	-0.05842	-4.30976
C	-4.31582	-0.80186	-2.78842
H	-3.65464	-1.65931	-3.00244
H	-5.04761	-0.72579	-3.61224
H	-4.86782	-1.00344	-1.85792
C	-4.41401	1.70040	-2.36778
H	-4.94620	1.56312	-1.41420
H	-5.16718	1.81574	-3.16760
H	-3.82758	2.63307	-2.31406
C	-2.84481	-0.58466	2.03887
C	-4.30445	-0.72154	1.44021
C	-4.67075	-2.16761	1.05773
H	-5.61813	-2.15835	0.49506
H	-4.80471	-2.80504	1.94762
H	-3.89821	-2.61993	0.41518
C	-5.41166	-0.12330	2.31697
H	-5.25308	0.95010	2.49713
H	-5.47215	-0.64246	3.28872
H	-6.38188	-0.24205	1.80789
C	-2.32479	-1.82649	2.76463
H	-2.34871	-2.72418	2.13276
H	-2.93784	-2.01749	3.66249
H	-1.28560	-1.65586	3.09288
C	-2.68117	0.63711	2.94674
H	-1.62106	0.73991	3.22784
H	-3.26330	0.51207	3.87472
H	-3.01129	1.56040	2.44809
B	-2.91752	0.05116	-0.24623
C	-0.24662	1.14964	-2.54470
C	-0.46928	2.54153	-2.38267
C	0.81825	0.76996	-3.40616
C	0.31859	3.49375	-3.04454
H	-1.29343	2.87240	-1.74246
C	1.60757	1.72134	-4.06632
H	1.00276	-0.29875	-3.57952
C	1.36458	3.09609	-3.89456
H	0.11101	4.55912	-2.89410
H	2.40565	1.38521	-4.73888
H	1.97300	3.84060	-4.41805
C	-1.02941	0.09431	-1.82966
H	-0.93201	-0.85562	-2.39721

16_{BC}

SCF (BP86) Energy = -2134.45503574
Enthalpy 0K = -2133.429046
Enthalpy 298K = -2133.367904
Free Energy 298K = -2133.520714
Lowest Frequency = 11.9488 cm^{-1}
Second Frequency = 27.5425 cm^{-1}
SCF (BP86-D3BJ) Energy = -2134.77478314
SCF (Toluene) Energy = -2134.46107222
SCF (BS2) Energy = -2334.21300088

Mg	0.18310	-0.08806	-0.22870
O	-0.35118	-0.22866	1.83784
O	-1.06152	-1.75881	3.41355
N	1.58046	1.28061	-1.01779
N	-1.38690	0.69267	-1.38597
N	0.52606	-2.09452	0.00421
C	2.55722	2.30204	-3.08523
H	3.28871	2.77580	-2.41484
H	2.15118	3.06148	-3.77199
H	3.09996	1.56242	-3.70060
C	1.43243	1.61825	-2.31504
C	0.26033	1.35633	-3.07239
H	0.35703	1.57230	-4.14024
C	-1.04505	0.99485	-2.66132
C	-2.08469	0.91500	-3.77300
H	-3.09319	1.18007	-3.42403
H	-2.12664	-0.12806	-4.13630
H	-1.81768	1.55542	-4.62755
C	-2.77988	0.74846	-1.01768
C	-3.73581	-2.33780	-2.61089
H	-4.81028	-2.52745	-2.43532
H	-3.26686	-3.28422	-2.92898
H	-3.65761	-1.62076	-3.44429
C	-4.69900	2.07702	-0.28557
H	-5.14274	3.04651	-0.03565
C	-5.48523	0.92111	-0.19924
H	-6.53299	0.98759	0.11302
C	-4.91969	-0.31632	-0.52115
H	-5.53531	-1.22137	-0.46755
C	-3.57612	-0.43139	-0.93586
C	-3.04586	-1.80956	-1.33030
H	-1.96912	-1.71479	-1.55266
C	-3.20376	-2.84303	-0.19453
H	-2.73347	-2.49913	0.74196
H	-2.72418	-3.79277	-0.48336
H	-4.26708	-3.04957	0.02337
C	-3.34938	2.02191	-0.68522
C	-2.53672	3.31966	-0.77636
H	-1.47154	3.03926	-0.67975
C	-2.87362	4.33538	0.33814
H	-3.87179	4.78569	0.19398
H	-2.14570	5.16529	0.32212
H	-2.85464	3.88142	1.34187
C	-2.70976	4.01581	-2.14886
H	-3.77282	4.25578	-2.32983
H	-2.35575	3.38910	-2.98022
H	-2.13977	4.96150	-2.17485
C	2.78049	1.63516	-0.30301
C	2.73676	2.73287	0.61333
C	3.86030	2.98345	1.42381
H	3.83710	3.81746	2.13213
C	5.01194	2.19001	1.33744
H	5.87115	2.39328	1.98537
C	5.06330	1.15304	0.40154
H	5.97509	0.55178	0.31314
C	3.97153	0.86275	-0.44267
C	4.12788	-0.24146	-1.49282
H	3.22876	-0.23376	-2.13132
C	5.35327	0.01274	-2.40218
H	5.33080	1.01803	-2.85563
H	5.38352	-0.73257	-3.21590
H	6.29965	-0.07682	-1.84051
C	4.20625	-1.64435	-0.85721
H	5.04129	-1.71584	-0.13776
H	4.36022	-2.41168	-1.63564
H	3.26668	-1.88113	-0.33346
C	1.52621	3.67025	0.65605
H	0.62786	3.05082	0.46558
C	1.33995	4.40399	1.99953
H	1.35450	3.71799	2.86257
H	0.37559	4.94062	2.00528
H	2.12771	5.16094	2.16111
C	1.59465	4.71570	-0.48448
H	2.50477	5.33363	-0.38649

H	0.71997	5.38917	-0.44593
H	1.60987	4.24040	-1.47649
C	-0.78839	0.57304	3.02151
C	-1.67419	-0.47769	3.79519
C	-1.61509	-0.35631	5.32084
H	-2.24082	-1.14129	5.77498
H	-2.00597	0.62173	5.64967
H	-0.59047	-0.47378	5.70313
C	-3.13462	-0.52126	3.31782
H	-3.20973	-0.58382	2.22014
H	-3.69352	0.36817	3.65241
H	-3.61965	-1.41346	3.74508
C	-1.54281	1.80507	2.53735
H	-0.85702	2.49406	2.01912
H	-1.96601	2.34699	3.40062
H	-2.36122	1.54395	1.85034
C	0.49253	0.96458	3.77080
H	1.01558	0.08308	4.17343
H	0.26481	1.64621	4.60690
H	1.18024	1.47885	3.08067
C	0.42677	-2.88098	-1.14105
C	-0.00324	-4.24354	-1.19860
H	-0.23551	-4.78181	-0.27610
C	-0.13634	-4.92313	-2.41868
H	-0.47061	-5.96783	-2.40439
C	0.15465	-4.30087	-3.64330
H	0.05546	-4.84233	-4.58904
C	0.59462	-2.96433	-3.61502
H	0.84514	-2.44767	-4.54929
C	0.73106	-2.27865	-2.40451
H	1.09906	-1.24315	-2.42634
B	-0.39358	-1.59661	2.22563
C	1.50357	-3.38918	2.07033
C	0.97768	-4.20487	3.27412
H	0.29678	-5.00880	2.94013
H	1.81806	-4.68254	3.80957
H	0.42848	-3.57681	3.99483
C	2.27680	-4.34870	1.14038
H	2.59657	-3.85401	0.21105
H	3.17915	-4.72263	1.65867
H	1.66702	-5.22338	0.86098
C	2.47145	-2.29883	2.58216
H	2.00683	-1.69334	3.38237
H	3.38444	-2.75008	3.00981
H	2.77851	-1.61779	1.77145
C	0.26191	-2.71456	1.31970
H	-0.49848	-3.52406	1.23399

TS(16_{BN}-16_{BCN})

SCF (BP86) Energy = -2134.40764375
Enthalpy 0K = -2133.382995
Enthalpy 298K = -2133.322176
Free Energy 298K = -2133.474995
Lowest Frequency = -216.4922 cm^{-1}
Second Frequency = 17.4887 cm^{-1}
SCF (BP86-D3BJ) Energy = -2134.72453548
SCF (Toluene) Energy = -2134.41400679
SCF (BS2) Energy = -2334.16512633

Mg	-0.28118	-0.02984	-0.37164
O	1.31651	-3.47897	0.41036
O	0.24804	-1.96261	-1.00549
N	0.50559	1.72648	-1.22504
N	-2.30084	0.48845	-0.78436
C	0.36706	3.52533	-2.96324
H	1.46374	3.51830	-3.02784
H	0.08104	4.45442	-2.43887
H	-0.05788	3.57999	-3.97782
C	-0.19287	2.31750	-2.21719
C	-1.50752	1.94620	-2.60106
H	-1.87893	2.46924	-3.48704
C	-2.51304	1.25687	-1.87939
C	-3.92624	1.51384	-2.40078
H	-3.92543	1.49371	-3.50312
H	-4.26433	2.52073	-2.10092
H	-4.66173	0.78884	-2.02814
C	-3.46639	0.14402	0.00249
C	-4.03428	1.11058	0.88777
C	-5.15620	0.75105	1.66207
H	-5.58784	1.49032	2.34625
C	-5.73356	-0.51647	1.56736
H	-6.60867	-0.77536	2.17263
C	-5.18193	-1.45410	0.68685
H	-5.63918	-2.44456	0.61294
C	-4.05203	-1.15674	-0.10089
C	-3.50162	-2.21541	-1.06290
H	-2.39950	-2.12296	-1.04568
C	-3.95979	-1.97979	-2.52325
H	-5.06229	-1.96275	-2.58879
H	-3.60184	-2.79770	-3.17442
H	-3.57520	-1.03437	-2.93248
C	-3.86271	-3.65883	-0.65554
H	-4.93995	-3.86307	-0.78902
H	-3.60143	-3.87460	0.39329
H	-3.32479	-4.37568	-1.29790
C	-3.49919	2.53918	1.02962
H	-2.65514	2.66108	0.32939
C	-4.57304	3.59311	0.66644
H	-5.40519	3.58280	1.39231
H	-5.00628	3.41870	-0.33187
H	-4.13634	4.60696	0.67828
C	-2.97567	2.81071	2.45767
H	-3.77360	2.67312	3.20835
H	-2.61484	3.85059	2.54463
H	-2.14610	2.13686	2.72478
C	1.73892	2.37420	-0.83093
C	1.71191	3.43367	0.12198
C	2.91104	4.11443	0.41640
H	2.89151	4.93887	1.13814
C	4.11821	3.76013	-0.19068
H	5.03784	4.30764	0.04103
C	4.14594	2.67674	-1.07642
H	5.10016	2.37538	-1.51799
C	2.97924	1.95893	-1.40250
C	0.44423	3.84549	0.87435
H	-0.37259	3.17636	0.54988
C	0.01743	5.29753	0.56041
H	0.79078	6.01896	0.87819
H	-0.91453	5.55251	1.09510
H	-0.15776	5.45164	-0.51730
C	0.63441	3.66432	2.39911
H	0.89929	2.62392	2.65320
H	-0.28862	3.92695	2.94256
H	1.44175	4.31285	2.78150
C	3.07008	0.75471	-2.34421
H	2.27235	0.05484	-2.02953
C	4.42051	0.01630	-2.22739
H	4.38262	-0.93474	-2.78590

H	4.67601	-0.20504	-1.17835
H	5.24620	0.60471	-2.66550
C	2.81070	1.11797	-3.82585
H	1.78991	1.49439	-3.99091
H	2.94734	0.22972	-4.46849
H	3.52267	1.89006	-4.16842
C	0.67080	-3.09335	-1.85481
C	1.19846	-2.55600	-3.18653
H	1.55077	-3.38797	-3.82039
H	2.02973	-1.85099	-3.04660
H	0.39094	-2.03848	-3.73111
C	-0.56007	-3.97622	-2.09844
H	-1.33762	-3.39072	-2.61367
H	-0.97393	-4.35038	-1.14916
H	-0.30723	-4.83971	-2.73604
C	1.75845	-3.80537	-0.93995
C	3.17017	-3.22507	-1.11463
H	3.16686	-2.13273	-0.97976
H	3.59178	-3.46658	-2.10492
H	3.83054	-3.64937	-0.34251
C	1.79503	-5.33247	-1.06957
H	2.06248	-5.63575	-2.09642
H	0.83028	-5.79007	-0.80460
H	2.56117	-5.73570	-0.38777
B	0.67175	-2.24364	0.37318
C	1.30581	-0.56433	1.29680
H	1.02445	0.51334	1.36892
C	2.64707	-0.71458	1.92039
C	3.42366	0.46543	2.09820
C	3.27298	-1.93792	2.28842
C	4.72715	0.43064	2.60746
H	2.98889	1.43209	1.81706
C	4.57425	-1.96743	2.81201
H	2.73947	-2.87946	2.14830
C	5.31863	-0.78879	2.97950
H	5.27995	1.37009	2.72390
H	5.01111	-2.93394	3.09130
H	6.33328	-0.81895	3.39010
N	0.11704	-1.45131	1.45712
C	-0.53159	-1.86236	2.75813
C	-0.98789	-0.57893	3.47096
H	-1.43526	-0.81323	4.45166
H	-0.13125	0.09623	3.64117
H	-1.74631	-0.04889	2.86879
C	-1.74506	-2.73432	2.39172
H	-2.46314	-2.17402	1.77119
H	-1.42174	-3.63502	1.84006
H	-2.26843	-3.06882	3.30397
C	0.40903	-2.66655	3.68085
H	1.28767	-2.07587	3.98009
H	-0.13442	-2.96415	4.59596
H	0.76047	-3.58401	3.18061

16_{BCN}

SCF (BP86) Energy = -2134.42852105
Enthalpy 0K = -2133.402653
Enthalpy 298K = -2133.341489
Free Energy 298K = -2133.495513
Lowest Frequency = 13.3749 cm^{-1}
Second Frequency = 19.7027 cm^{-1}
SCF (BP86-D3BJ) Energy = -2134.74250519
SCF (Toluene) Energy = -2134.43424321
SCF (BS2) Energy = -2334.18376464

Mg	-0.44649	-0.08345	-0.34815
O	1.55591	-3.29964	0.27834
O	0.65453	-1.65152	-1.15996
N	0.16344	1.71004	-1.29727
N	-2.52867	0.22851	-0.55927
C	-0.29690	3.35866	-3.12557
H	0.78694	3.52616	-3.17985
H	-0.75766	4.27828	-2.72328
H	-0.69531	3.22018	-4.14362
C	-0.67287	2.16854	-2.24698
C	-1.98767	1.67397	-2.48361
H	-2.46233	2.11559	-3.36348
C	-2.87734	0.93432	-1.66797
C	-4.34165	1.00899	-2.08600
H	-4.46337	1.61399	-2.99586
H	-4.95814	1.45277	-1.28659
H	-4.75368	0.00526	-2.27285
C	-3.62361	-0.13095	0.32634
C	-3.96667	0.77332	1.38144
C	-5.07212	0.48104	2.20336
H	-5.34293	1.17942	3.00137
C	-5.83069	-0.68009	2.02506
H	-6.69115	-0.88583	2.67041
C	-5.46369	-1.58095	1.02353
H	-6.04130	-2.50297	0.89297
C	-4.36977	-1.33703	0.16790
C	-4.03319	-2.41163	-0.86730
H	-3.16306	-2.05592	-1.44555
C	-5.18966	-2.68944	-1.85721
H	-6.07369	-3.09424	-1.33405
H	-4.87858	-3.43676	-2.60794
H	-5.51424	-1.78541	-2.39809
C	-3.64940	-3.73521	-0.16390
H	-4.50627	-4.14123	0.40166
H	-2.82210	-3.59330	0.55042
H	-3.34615	-4.49848	-0.90097
C	-3.17707	2.05886	1.64142
H	-2.16783	1.91514	1.21193
C	-3.80953	3.27563	0.92517
H	-4.85058	3.42727	1.26212
H	-3.81772	3.14797	-0.16910
H	-3.24381	4.19681	1.15167
C	-3.01129	2.35713	3.14730
H	-3.96584	2.65153	3.61764
H	-2.31116	3.19619	3.29303
H	-2.61836	1.48496	3.69534
C	1.38590	2.45580	-1.06924
C	1.37604	3.58928	-0.20432
C	2.57279	4.30706	-0.00554
H	2.56483	5.17977	0.65721
C	3.76007	3.93680	-0.64112
H	4.67847	4.51159	-0.48172
C	3.76427	2.81604	-1.47864
H	4.69746	2.52045	-1.96678
C	2.60170	2.05308	-1.70520
C	0.12201	4.07119	0.52688
H	-0.70912	3.39655	0.25806
C	-0.27713	5.50472	0.10492
H	0.49492	6.23794	0.39784
H	-1.22109	5.80414	0.59337
H	-0.41603	5.58922	-0.98546
C	0.31683	4.00640	2.05860
H	0.54242	2.98152	2.39620
H	-0.59147	4.35200	2.58216

H	1.14950	4.65457	2.38344
C	2.67624	0.83670	-2.63330
H	1.89255	0.12828	-2.31087
C	4.03155	0.10421	-2.53657
H	3.99106	-0.84132	-3.10419
H	4.29605	-0.13106	-1.49259
H	4.85551	0.69525	-2.97467
C	2.39835	1.20892	-4.10968
H	1.38454	1.61238	-4.25434
H	2.49785	0.31753	-4.75425
H	3.12089	1.96469	-4.46687
C	0.70432	-2.90477	-1.91564
C	1.14209	-2.60593	-3.35457
H	1.24338	-3.54198	-3.93145
H	2.10274	-2.07234	-3.38639
H	0.38425	-1.98154	-3.85806
C	-0.70034	-3.51601	-1.92085
H	-1.40787	-2.80105	-2.37309
H	-1.03019	-3.74007	-0.89612
H	-0.73905	-4.44543	-2.51402
C	1.74040	-3.77470	-1.07119
C	3.20469	-3.53165	-1.49167
H	3.45702	-2.46093	-1.45521
H	3.41482	-3.91295	-2.50560
H	3.86740	-4.05706	-0.78493
C	1.44961	-5.28209	-1.08696
H	1.50246	-5.68988	-2.11147
H	0.45915	-5.50884	-0.66479
H	2.20446	-5.80358	-0.47569
B	1.32513	-1.88416	0.19121
C	2.17099	-0.67639	0.80551
H	2.19736	0.31027	0.31591
C	3.36951	-0.80503	1.69950
C	4.01265	0.36724	2.16546
C	3.97184	-2.05004	2.00627
C	5.19204	0.30339	2.92405
H	3.58172	1.34323	1.91153
C	5.14544	-2.11590	2.77088
H	3.50220	-2.96373	1.62975
C	5.76077	-0.94111	3.23722
H	5.66738	1.22833	3.26950
H	5.59110	-3.09190	2.99457
H	6.68035	-0.99606	3.82989
N	0.68696	-0.97260	1.25126
C	0.24779	-1.25763	2.65497
C	0.98340	-2.44160	3.32771
H	2.03100	-2.19964	3.55429
H	0.48131	-2.68932	4.27996
H	0.96457	-3.33204	2.67957
C	0.42300	0.01723	3.50336
H	-0.15004	0.85610	3.06944
H	0.06291	-0.14513	4.53461
H	1.48462	0.30979	3.55337
C	-1.24649	-1.62638	2.56363
H	-1.65850	-1.84082	3.56496
H	-1.84819	-0.80938	2.12928
H	-1.38317	-2.52913	1.94329

TS(16_{BCN}-16_{BC})

SCF (BP86) Energy = -2134.41270561
Enthalpy 0K = -2133.388114
Enthalpy 298K = -2133.327188
Free Energy 298K = -2133.480543
Lowest Frequency = -116.9586 cm^{-1}
Second Frequency = 14.2054 cm^{-1}
SCF (BP86-D3BJ) Energy = -2134.72563437
SCF (Toluene) Energy = -2134.41835252
SCF (BS2) Energy = -2334.16992856

Mg	-0.35491	-0.07587	-0.16187
O	2.50009	-2.78417	-0.42481
O	1.22241	-1.07392	-1.36085
N	-0.17198	1.84234	-1.03764
N	-2.41231	-0.30322	-0.59258
C	-0.79290	3.26531	-3.00518
H	-0.03737	3.96604	-2.62555
H	-1.75888	3.79197	-3.08381
H	-0.51113	2.96303	-4.02871
C	-0.94177	2.03270	-2.11879
C	-1.98700	1.14704	-2.53390
H	-2.40296	1.39914	-3.51383
C	-2.74233	0.18954	-1.81676
C	-4.02338	-0.29001	-2.49089
H	-4.17049	0.19312	-3.46796
H	-4.90621	-0.08824	-1.86288
H	-3.99258	-1.38363	-2.63957
C	-3.49320	-0.84987	0.20758
C	-4.30576	0.04869	0.96961
C	-5.33716	-0.47226	1.77496
H	-5.96387	0.21972	2.34795
C	-5.57706	-1.84663	1.86660
H	-6.37777	-2.23027	2.50762
C	-4.78231	-2.72047	1.12147
H	-4.96800	-3.79906	1.17742
C	-3.75526	-2.24997	0.27895
C	-2.98194	-3.27324	-0.54639
H	-2.33770	-2.70210	-1.23111
C	-3.91326	-4.15498	-1.41011
H	-4.54521	-4.81294	-0.78833
H	-3.31867	-4.80483	-2.07619
H	-4.58713	-3.54635	-2.03684
C	-2.07835	-4.15751	0.34331
H	-2.67388	-4.68932	1.10598
H	-1.31628	-3.55912	0.87146
H	-1.55585	-4.92200	-0.25985
C	-4.11498	1.56701	0.93577
H	-3.15049	1.77026	0.43897
C	-5.22262	2.26291	0.10899
H	-6.22003	2.06493	0.54060
H	-5.23334	1.91678	-0.93718
H	-5.07002	3.35660	0.09906
C	-4.06109	2.17340	2.35552
H	-5.02052	2.05613	2.88875
H	-3.85416	3.25594	2.30175
H	-3.27719	1.70080	2.97027
C	0.81576	2.82849	-0.65572
C	0.53331	3.70310	0.43812
C	1.51042	4.63173	0.84348
H	1.29155	5.30538	1.67759
C	2.74921	4.71831	0.20008
H	3.49475	5.45054	0.52751
C	3.02130	3.85802	-0.86586
H	3.98986	3.92269	-1.37382
C	2.08432	2.90224	-1.30997
C	-0.83023	3.71083	1.12809
H	-1.27138	2.70493	1.00113
C	-1.77265	4.72246	0.43217
H	-1.35535	5.74324	0.49498

H	-2.76697	4.73273	0.91238
H	-1.91191	4.48087	-0.63395
C	-0.75110	4.00624	2.64021
H	-0.02975	3.34503	3.14837
H	-1.73818	3.85766	3.10784
H	-0.45414	5.05048	2.84197
C	2.48877	2.00526	-2.48311
H	1.68551	1.26606	-2.63865
C	3.78889	1.22869	-2.17335
H	4.05656	0.57313	-3.02136
H	3.68634	0.60814	-1.26976
H	4.64069	1.91319	-2.01689
C	2.67771	2.81412	-3.78946
H	1.78029	3.39311	-4.05774
H	2.91241	2.13835	-4.63103
H	3.51584	3.52707	-3.69426
C	1.26996	-2.14378	-2.38231
C	1.54252	-1.49386	-3.74289
H	1.62240	-2.26600	-4.52760
H	2.46889	-0.90264	-3.74009
H	0.70544	-0.82681	-4.00897
C	-0.09557	-2.82834	-2.40777
H	-0.87083	-2.08027	-2.64548
H	-0.32308	-3.28457	-1.43394
H	-0.13996	-3.61484	-3.17935
C	2.43240	-3.08822	-1.84392
C	3.81646	-2.75768	-2.43561
H	4.06184	-1.69110	-2.31409
H	3.87812	-3.01546	-3.50642
H	4.57857	-3.34028	-1.89391
C	2.15653	-4.59005	-1.99979
H	2.06690	-4.87030	-3.06345
H	1.23983	-4.89535	-1.47406
H	2.99770	-5.15743	-1.56966
B	1.97903	-1.51149	-0.20710
C	2.28372	-0.51334	0.96002
H	2.40239	0.55937	0.69536
C	3.47511	-0.85766	1.84364
C	4.29724	0.19746	2.30309
C	3.87589	-2.17817	2.15754
C	5.45705	-0.04487	3.05600
H	4.01453	1.22913	2.06067
C	5.02950	-2.42385	2.91739
H	3.29215	-3.02064	1.77900
C	5.82613	-1.36058	3.37427
H	6.06976	0.79758	3.39602
H	5.31448	-3.45748	3.14436
H	6.72739	-1.55709	3.96491
N	0.83371	-0.83928	1.31874
C	0.39877	-0.95945	2.74155
C	0.74795	-2.33058	3.37622
H	1.83382	-2.45458	3.49652
H	0.28500	-2.43013	4.37544
H	0.37419	-3.15113	2.73973
C	-1.13915	-0.82944	2.73685
H	-1.45445	0.16704	2.36964
H	-1.60884	-1.59771	2.09918
H	-1.55527	-0.94625	3.75274
C	0.96568	0.18207	3.62050
H	0.73846	1.16243	3.16488
H	0.51253	0.15871	4.62836
H	2.05655	0.10576	3.74025

17_{BN}

SCF (BP86) Energy = -2208.25788647
Enthalpy 0K = -2207.262970
Enthalpy 298K = -2207.202172
Free Energy 298K = -2207.358246
Lowest Frequency = 11.4842 cm^{-1}
Second Frequency = 17.6245 cm^{-1}
SCF (BP86-D3BJ) Energy = -2208.57055484
SCF (Toluene) Energy = -2208.26459428
SCF (BS2) Energy = -2408.03508430

Mg	-0.17137	-0.00682	-0.31183
O	0.52980	0.05565	1.65025
O	2.39286	0.21102	3.02372
N	-1.17015	1.64790	-1.16353
N	-1.68319	-1.36536	-0.79025
C	-1.96254	2.41482	-3.40228
H	-2.36847	3.31710	-2.92021
H	-2.67569	2.05921	-4.16066
H	-1.03740	2.71873	-3.92414
C	-1.65170	1.32614	-2.38235
C	-1.88177	-0.00911	-2.82211
H	-2.14679	-0.09099	-3.87957
C	-2.01511	-1.22197	-2.09482
C	-2.52819	-2.41757	-2.88719
H	-3.14817	-3.08381	-2.26990
H	-1.66269	-3.01141	-3.23456
H	-3.10201	-2.10513	-3.77250
C	-2.21451	-2.48377	-0.05051
C	0.12943	-4.95445	-1.26548
H	-0.06166	-5.92144	-0.76619
H	1.13982	-4.98424	-1.70611
H	-0.59984	-4.85516	-2.08684
C	-4.06733	-3.50949	1.17454
H	-5.10417	-3.47439	1.52737
C	-3.27759	-4.62377	1.47756
H	-3.68899	-5.45337	2.06241
C	-1.95850	-4.66536	1.01744
H	-1.33815	-5.54110	1.23905
C	-1.40724	-3.61897	0.25023
C	0.02051	-3.77768	-0.26729
H	0.29833	-2.86057	-0.81625
C	1.02751	-3.96037	0.88822
H	1.02285	-3.08508	1.56017
H	2.04817	-4.07574	0.49075
H	0.79298	-4.85288	1.49479
C	-3.56361	-2.42902	0.42479
C	-4.49333	-1.24765	0.13423
H	-3.87995	-0.43759	-0.29650
C	-5.16021	-0.70830	1.41912
H	-5.83488	-1.45391	1.87492
H	-5.77066	0.18262	1.18989
H	-4.41293	-0.42828	2.18056
C	-5.58145	-1.61717	-0.90202
H	-6.22163	-2.43507	-0.52586
H	-5.14347	-1.94744	-1.85729
H	-6.23141	-0.74883	-1.11006
C	-1.16391	3.02898	-0.74477
C	-2.25261	3.51276	0.04763
C	-2.23750	4.85163	0.48424
H	-3.07371	5.22801	1.08190
C	-1.17803	5.71095	0.17211
H	-1.18527	6.74886	0.52141
C	-0.10976	5.22647	-0.58684
H	0.72503	5.89391	-0.82864

C	-0.07648	3.89793	-1.05751
C	1.13952	3.45562	-1.87247
H	0.96937	2.41194	-2.19109
C	1.33753	4.31386	-3.14387
H	0.43301	4.33569	-3.77430
H	2.16956	3.91559	-3.75012
H	1.58623	5.35893	-2.88833
C	2.42219	3.48956	-1.00960
H	2.64055	4.51675	-0.66798
H	3.29490	3.13577	-1.58439
H	2.33010	2.85136	-0.11536
C	-3.44573	2.62084	0.39829
H	-3.08617	1.57488	0.37329
C	-4.01854	2.90028	1.80440
H	-3.23344	2.88665	2.57925
H	-4.77137	2.13863	2.06583
H	-4.52304	3.88109	1.85661
C	-4.56710	2.74496	-0.66097
H	-4.92790	3.78717	-0.72328
H	-5.42678	2.10369	-0.39718
H	-4.21858	2.44513	-1.66190
C	0.03798	0.49763	2.98446
C	1.23950	0.06584	3.90997
C	1.45844	0.96997	5.12768
H	2.32456	0.60585	5.70346
H	0.57772	0.95265	5.79212
H	1.65993	2.00989	4.83212
C	1.17578	-1.40729	4.34762
H	1.00651	-2.08004	3.49152
H	0.37504	-1.57567	5.08673
H	2.13654	-1.68253	4.81123
C	-1.28891	-0.20550	3.26383
H	-2.06245	0.15020	2.56270
H	-1.63506	0.02669	4.28532
H	-1.20673	-1.29716	3.15857
C	-0.13893	2.02033	2.90879
H	0.82099	2.52674	2.71760
H	-0.55940	2.41603	3.84804
H	-0.82920	2.28240	2.09052
C	4.17742	0.17292	0.50873
C	4.83226	0.52529	-0.69376
H	4.25520	0.62341	-1.61495
C	6.21938	0.73028	-0.72148
H	6.69655	1.00139	-1.66971
C	6.99228	0.58303	0.43951
H	8.07526	0.74090	0.41341
C	6.35062	0.21620	1.63311
H	6.93370	0.08259	2.55131
C	4.96551	0.00605	1.67337
H	4.49023	-0.28255	2.61198
C	2.40706	-1.24698	-1.64925
C	1.95384	-1.25282	-2.99666
H	1.31523	-0.42973	-3.34525
C	2.30032	-2.27582	-3.88714
H	1.93338	-2.23921	-4.91959
C	3.12118	-3.33969	-3.46846
H	3.40023	-4.13676	-4.16528
C	3.58272	-3.35162	-2.14316
H	4.23782	-4.16071	-1.79915
C	3.23367	-2.32509	-1.24881
H	3.62930	-2.34269	-0.22892
B	1.96816	0.06932	1.71090
N	2.75204	-0.01436	0.52912
C	1.99304	-0.12208	-0.75091
H	2.12975	0.82271	-1.31543

17_{BC}

SCF (BP86) Energy = -2208.25946427
Enthalpy 0K = -2207.264226
Enthalpy 298K = -2207.203776
Free Energy 298K = -2207.357367
Lowest Frequency = 16.7499 cm^{-1}
Second Frequency = 21.4148 cm^{-1}
SCF (BP86-D3BJ) Energy = -2208.57744814
SCF (Toluene) Energy = -2208.26641057
SCF (BS2) Energy = -2408.03774976

Mg	0.14157	-0.13214	-0.31713
O	0.26021	0.74926	1.64058
O	0.02065	2.81600	2.65748
N	-0.46983	-2.08833	-0.75582
N	2.02085	-0.36555	-1.19458
N	-1.07999	1.44473	-0.67760
C	-0.61613	-3.90112	-2.47431
H	-1.24160	-4.43271	-1.74307
H	0.16699	-4.58261	-2.84356
H	-1.25359	-3.64000	-3.33715
C	0.00578	-2.63897	-1.88864
C	1.08861	-2.10646	-2.64037
H	1.26494	-2.61638	-3.59185
C	2.04344	-1.11058	-2.32430
C	3.11394	-0.86895	-3.38274
H	4.06591	-0.53295	-2.94697
H	2.76679	-0.07125	-4.06427
H	3.29230	-1.76935	-3.99036
C	3.18907	0.39527	-0.83370
C	2.79048	2.94582	-3.36381
H	3.59870	3.69062	-3.25042
H	1.99045	3.40355	-3.97027
H	3.20325	2.09395	-3.92864
C	5.34704	0.50949	0.30760
H	6.14900	0.02615	0.87501
C	5.45700	1.86997	-0.00883
H	6.33720	2.44016	0.30707
C	4.43461	2.49115	-0.73273
H	4.52189	3.55351	-0.98749
C	3.29388	1.77963	-1.15977
C	2.23529	2.51193	-1.98638
H	1.39675	1.81710	-2.16590
C	1.66480	3.74131	-1.24607
H	1.30766	3.47977	-0.23664
H	0.81216	4.15958	-1.80713
H	2.42305	4.53746	-1.13605
C	4.22752	-0.24996	-0.08530
C	4.15302	-1.73988	0.27476
H	3.07924	-1.99900	0.33980
C	4.81900	-2.08215	1.62601
H	5.91993	-2.01555	1.56661
H	4.57850	-3.12129	1.90968
H	4.48848	-1.41911	2.44170
C	4.77664	-2.63941	-0.82111
H	5.83205	-2.36334	-0.99463
H	4.24061	-2.56267	-1.77785
H	4.75089	-3.69815	-0.50761
C	-1.54765	-2.70758	-0.02616
C	-1.23280	-3.42176	1.17345
C	-2.28640	-3.91126	1.96801
H	-2.05767	-4.45756	2.88837

C	-3.62463	-3.71898	1.59971
H	-4.43112	-4.10133	2.23451
C	-3.92042	-3.05334	0.40676
H	-4.96633	-2.92540	0.10606
C	-2.90684	-2.54462	-0.43282
C	-3.31774	-1.89366	-1.75833
H	-2.40331	-1.56246	-2.27934
C	-4.05222	-2.91086	-2.66720
H	-3.47511	-3.83820	-2.81565
H	-4.24811	-2.46321	-3.65703
H	-5.02801	-3.19518	-2.23478
C	-4.20365	-0.64404	-1.56712
H	-5.14287	-0.89230	-1.04080
H	-4.46822	-0.21707	-2.54907
H	-3.68318	0.13793	-0.99621
C	0.22247	-3.71841	1.54968
H	0.82837	-2.85126	1.22005
C	0.45465	-3.92904	3.05965
H	0.03417	-3.11280	3.67044
H	1.53627	-3.99214	3.27021
H	0.00579	-4.87446	3.41215
C	0.75455	-4.95156	0.77876
H	0.15610	-5.84656	1.02478
H	1.80454	-5.15766	1.05252
H	0.71298	-4.80298	-0.31051
C	0.77403	0.59018	3.03679
C	1.03834	2.09351	3.43662
C	0.80923	2.40287	4.91864
H	0.99443	3.47338	5.10209
H	1.50522	1.82460	5.55018
H	-0.22183	2.17784	5.22855
C	2.40778	2.61978	2.97836
H	2.60382	2.39311	1.91761
H	3.22582	2.19322	3.58192
H	2.42447	3.71444	3.10202
C	2.01635	-0.28978	3.00852
H	1.75238	-1.31932	2.71738
H	2.46881	-0.33486	4.01400
H	2.76642	0.09426	2.30141
C	-0.36942	-0.05746	3.82934
H	-1.26069	0.59045	3.85378
H	-0.06020	-0.27230	4.86538
H	-0.65564	-1.00708	3.34952
C	-1.32069	2.39587	0.41645
H	-1.12554	3.44457	0.09649
C	-2.71850	2.39405	1.07648
C	-3.34623	1.18295	1.43420
H	-2.87165	0.23377	1.16163
C	-4.57959	1.18230	2.10520
H	-5.05319	0.22924	2.36474
C	-5.20304	2.39547	2.43978
H	-6.16678	2.39621	2.96010
C	-4.58305	3.60861	2.09715
H	-5.06365	4.56097	2.34727
C	-3.35047	3.60501	1.42611
H	-2.86940	4.55482	1.16122
C	-1.57459	1.79353	-1.92793
C	-2.41583	2.91843	-2.18533
H	-2.75255	3.54592	-1.35622
C	-2.85849	3.21683	-3.48273
H	-3.50820	4.08804	-3.63059
C	-2.49732	2.42185	-4.58157
H	-2.84920	2.66163	-5.58980
C	-1.67153	1.30503	-4.35123
H	-1.36850	0.66456	-5.18832
C	-1.21962	0.99908	-3.06414
H	-0.56751	0.12381	-2.92870
B	-0.33192	2.03824	1.58945

18_{BN}

SCF (BP86) Energy = -2439.29014287
Enthalpy 0K = -2438.215832
Enthalpy 298K = -2438.150779
Free Energy 298K = -2438.312050
Lowest Frequency = 18.2919 cm^{-1}
Second Frequency = 29.4770 cm^{-1}
SCF (BP86-D3BJ) Energy = -2439.65696479
SCF (Toluene) Energy = -2439.29750054
SCF (BS2) Energy = -2639.12042748

Mg	0.28666	-0.17686	0.38884
O	-0.51837	1.51291	1.49085
O	-2.19792	3.12049	1.37058
N	-0.48768	-1.96065	1.28248
N	2.31398	-0.56304	0.84460
N	-1.73021	1.71637	-0.67177
C	-0.35868	-3.39034	3.33799
H	-0.15028	-3.11038	4.38383
H	0.14821	-4.35422	3.15778
H	-1.43685	-3.55613	3.21276
C	0.18723	-2.31964	2.39582
C	1.46579	-1.82299	2.77800
H	1.80067	-2.19920	3.74855
C	2.49759	-1.20223	2.02158
C	3.89812	-1.33007	2.60947
H	4.58723	-1.77603	1.87317
H	3.89489	-1.95766	3.51213
H	4.31787	-0.34465	2.86898
C	-1.58829	-2.81975	0.87967
C	-1.31345	-4.03467	0.18269
C	-2.38647	-4.86721	-0.19173
H	-2.17056	-5.80014	-0.72419
C	-3.71240	-4.53369	0.09613
H	-4.53093	-5.19794	-0.20060
C	-3.97725	-3.33793	0.77061
H	-5.01309	-3.07077	1.00584
C	-2.94184	-2.47075	1.17090
C	0.09765	-4.48058	-0.20361
H	0.80777	-3.71210	0.14667
C	0.48633	-5.82183	0.46149
H	0.39767	-5.78150	1.55980
H	1.52911	-6.08720	0.21416
H	-0.15871	-6.64566	0.10802
C	0.23176	-4.59421	-1.73907
H	-0.45522	-5.35883	-2.14227
H	1.25665	-4.89841	-2.01438
H	-0.00321	-3.64200	-2.24175
C	-3.31280	-1.21887	1.96299
H	-2.41792	-0.57521	1.97818
C	-3.67501	-1.57575	3.42541
H	-4.53322	-2.27027	3.45055
H	-3.96142	-0.67295	3.99384
H	-2.83872	-2.05811	3.95651
C	-4.46988	-0.41432	1.33180
H	-4.27294	-0.14562	0.28173
H	-4.62991	0.52240	1.89504
H	-5.42192	-0.97239	1.36416
C	3.50148	-0.18466	0.09988

C	3.94804	-1.02345	-0.96607
C	5.11258	-0.66720	-1.67519
H	5.46438	-1.31995	-2.48078
C	5.83017	0.49388	-1.37196
H	6.73468	0.75055	-1.93359
C	5.37239	1.32378	-0.34523
H	5.91959	2.24384	-0.11235
C	4.22118	1.00980	0.40249
C	3.23193	-2.32059	-1.34644
H	2.22185	-2.28672	-0.89976
C	3.96212	-3.54673	-0.74883
H	4.99641	-3.61049	-1.13146
H	3.44334	-4.48320	-1.01975
H	4.01232	-3.49439	0.35158
C	3.06881	-2.47963	-2.87399
H	2.54502	-1.61773	-3.31941
H	2.47957	-3.38195	-3.10305
H	4.04170	-2.58757	-3.38429
C	3.78228	1.99413	1.48534
H	2.97126	1.51392	2.05656
C	4.91550	2.34989	2.47587
H	5.38651	1.45493	2.91710
H	4.52163	2.96904	3.30102
H	5.71426	2.93281	1.98501
C	3.22108	3.28492	0.84611
H	3.98795	3.77774	0.22427
H	2.91405	4.00856	1.62373
H	2.35819	3.07777	0.19305
C	-0.58068	1.00491	-1.32359
C	0.46549	1.97412	-1.82123
C	1.71842	1.51766	-2.31336
H	1.93968	0.44557	-2.30801
C	2.69756	2.39802	-2.79295
H	3.64604	1.98978	-3.15704
C	2.47797	3.78559	-2.77979
H	3.24131	4.47592	-3.15332
C	1.26670	4.26748	-2.26040
H	1.07209	5.34586	-2.23099
C	0.28321	3.38330	-1.78816
H	-0.66079	3.79388	-1.41893
C	-1.04162	-0.07988	-2.27513
C	-2.14638	-0.89790	-1.92056
H	-2.65206	-0.71592	-0.96815
C	-2.61720	-1.91892	-2.75436
H	-3.46953	-2.52288	-2.42582
C	-1.99942	-2.17177	-3.99094
H	-2.36245	-2.97098	-4.64528
C	-0.91220	-1.37007	-4.37174
H	-0.42584	-1.52937	-5.34124
C	-0.44462	-0.34279	-3.53678
H	0.37683	0.28724	-3.88853
C	-2.81092	2.24371	-1.45810
C	-4.04170	2.57745	-0.84547
H	-4.16292	2.44247	0.23132
C	-5.10224	3.09284	-1.60282
H	-6.04189	3.34733	-1.09994
C	-4.97396	3.26877	-2.98954
H	-5.80701	3.66249	-3.58070
C	-3.76128	2.92346	-3.60529
H	-3.63837	3.04795	-4.68661
C	-2.68987	2.41770	-2.85535
H	-1.75554	2.15921	-3.35546
C	-0.63935	2.11391	2.85772
C	-1.38478	3.46711	2.53430
C	0.75424	2.27365	3.45664
H	1.21161	1.28227	3.61467
H	0.68128	2.77027	4.43955
H	1.41168	2.87149	2.81239
C	-1.47107	1.16427	3.72393
H	-2.50311	1.07721	3.35424
H	-1.50515	1.52529	4.76527
H	-1.00847	0.16410	3.72453
C	-2.32010	3.95987	3.64330
H	-2.81274	4.88991	3.31707
H	-1.75479	4.18001	4.56491
H	-3.10389	3.22415	3.87626
C	-0.43563	4.59804	2.09889
H	0.24906	4.26801	1.30069
H	0.16264	4.97558	2.94494
H	-1.03931	5.43096	1.70445
B	-1.52953	2.12151	0.68008

18_{BC}

SCF (BP86) Energy = -2439.28371212
Enthalpy 0K = -2438.210197
Enthalpy 298K = -2438.144930
Free Energy 298K = -2438.307756
Lowest Frequency = 19.8777 cm^{-1}
Second Frequency = 22.1832 cm^{-1}
SCF (BP86-D3BJ) Energy = -2439.64386415
SCF (Toluene) Energy = -2439.29164156
SCF (BS2) Energy = -2639.11383695

Mg	0.43888	0.15661	0.35464
O	-1.14453	-0.66838	1.65357
O	-2.87009	-2.20351	1.58466
N	2.39515	-0.15548	1.07567
N	0.42159	2.24710	0.71770
N	-0.58010	-0.87518	-1.05641
C	3.81086	0.18896	3.10661
H	4.77834	0.54902	2.71860
H	3.89832	-0.90519	3.19343
H	3.66936	0.62320	4.10845
C	2.65994	0.58425	2.18504
C	1.97252	1.76623	2.55336
H	2.33524	2.21883	3.48163
C	1.13566	2.63605	1.78524
C	1.16265	4.08652	2.25547
H	0.83698	4.15301	3.30782
H	0.52560	4.74050	1.64614
H	2.19747	4.46723	2.21690
C	3.49888	-0.95873	0.58736
C	4.60216	-0.30391	-0.04899
C	5.71736	-1.06628	-0.44606
H	6.56366	-0.55838	-0.92223
C	5.76693	-2.45001	-0.25631
H	6.64742	-3.02372	-0.56402
C	4.66366	-3.09232	0.31061
H	4.68504	-4.17957	0.44129
C	3.52307	-2.37805	0.72912
C	4.61094	1.19070	-0.38586
H	3.66189	1.62824	-0.03262
C	5.76713	1.95730	0.29663
H	5.72369	1.88362	1.39599
H	5.72589	3.02812	0.03115
H	6.75135	1.57363	-0.02528
C	4.68246	1.38189	-1.91913
H	5.61068	0.95079	-2.33311

H	4.67280	2.45443	-2.17835
H	3.83131	0.89607	-2.42371
C	2.37181	-3.17078	1.34287
H	1.50771	-2.48781	1.41615
C	2.71945	-3.66613	2.76613
H	3.61071	-4.31757	2.74211
H	1.88860	-4.25381	3.19564
H	2.93609	-2.83244	3.45507
C	1.95943	-4.36732	0.45660
H	1.75087	-4.05026	-0.57789
H	1.05481	-4.85324	0.86331
H	2.74900	-5.13796	0.42056
C	-0.35863	3.21904	-0.02132
C	0.09263	3.65020	-1.30351
C	-0.69687	4.55768	-2.03763
H	-0.34210	4.89356	-3.01780
C	-1.90308	5.05460	-1.53620
H	-2.49653	5.76715	-2.11889
C	-2.33509	4.63499	-0.27503
H	-3.27857	5.02109	0.12642
C	-1.59220	3.72139	0.49754
C	1.44986	3.25034	-1.88062
H	1.85999	2.43571	-1.25719
C	2.42186	4.45166	-1.78256
H	2.04304	5.30922	-2.36637
H	3.41698	4.18933	-2.18075
H	2.54585	4.78836	-0.73917
C	1.35455	2.73421	-3.33218
H	0.68708	1.86114	-3.41270
H	2.34978	2.42535	-3.69260
H	0.98570	3.51519	-4.02018
C	-2.16412	3.31658	1.85733
H	-1.45085	2.62152	2.33087
C	-2.34964	4.52729	2.80307
H	-1.41496	5.09266	2.94578
H	-2.69975	4.19034	3.79498
H	-3.10586	5.22876	2.40938
C	-3.51099	2.57906	1.68815
H	-4.26508	3.23184	1.21629
H	-3.91358	2.27512	2.67170
H	-3.41048	1.68729	1.04874
C	-1.95974	-1.33290	-0.75014
C	-2.24991	-2.75906	-1.30400
C	-1.32739	-3.77855	-0.99041
H	-0.44070	-3.51620	-0.40616
C	-1.50816	-5.09303	-1.43846
H	-0.77064	-5.86102	-1.17958
C	-2.62606	-5.42207	-2.22342
H	-2.77175	-6.44742	-2.57969
C	-3.54783	-4.41796	-2.55178
H	-4.41845	-4.65381	-3.17394
C	-3.36273	-3.10099	-2.09617
H	-4.09272	-2.33430	-2.37144
C	-3.08313	-0.31317	-1.09942
C	-2.79473	0.86885	-1.81011
H	-1.76610	1.05437	-2.12983
C	-3.80791	1.79135	-2.11952
H	-3.55340	2.69664	-2.67949
C	-5.12943	1.56218	-1.70633
H	-5.91878	2.28179	-1.94903
C	-5.42830	0.40303	-0.97166
H	-6.45327	0.21433	-0.63297
C	-4.41658	-0.52173	-0.66831
H	-4.66177	-1.42369	-0.09813
C	-0.07516	-1.00788	-2.35406
C	1.34235	-0.98155	-2.52598
H	1.98404	-0.94154	-1.63499
C	1.94096	-1.06766	-3.78835
H	3.03488	-1.05939	-3.86071
C	1.15600	-1.19886	-4.94773
H	1.62139	-1.27615	-5.93534
C	-0.23981	-1.24747	-4.80252
H	-0.87670	-1.35707	-5.68847
C	-0.84949	-1.15598	-3.54272
H	-1.93865	-1.19148	-3.47799
C	-1.38036	-1.05990	3.07955
C	-2.78087	-1.80838	2.99399
C	-1.37010	0.20498	3.93660
H	-0.38363	0.69495	3.86408
H	-1.54425	-0.05639	4.99453
H	-2.14201	0.92147	3.62375
C	-0.22368	-1.97696	3.48286
H	-0.19189	-2.88551	2.86235
H	-0.31333	-2.27921	4.53907
H	0.72979	-1.43904	3.36122
C	-2.87381	-3.08194	3.84327
H	-3.85731	-3.55150	3.68238
H	-2.78058	-2.84645	4.91712
H	-2.10107	-3.81607	3.57301
C	-3.99289	-0.90665	3.27504
H	-3.99111	-0.01231	2.63422
H	-4.02319	-0.58879	4.33049
H	-4.91301	-1.47362	3.06085
B	-2.01236	-1.43417	0.84461

18_{BPh}

SCF (BP86) Energy = -2439.29263263
Enthalpy 0K = -2438.219999
Enthalpy 298K = -2438.154496
Free Energy 298K = -2438.318145
Lowest Frequency = 19.2612 cm^{-1}
Second Frequency = 24.9713 cm^{-1}
SCF (BP86-D3BJ) Energy = -2439.65448597
SCF (Toluene) Energy = -2439.29911452
SCF (BS2) Energy = -2639.12174260

Mg	-0.55450	0.19199	0.16613
O	0.40435	0.18542	-1.60201
O	1.65041	-1.46711	-2.77495
N	-0.66833	1.96082	1.30934
N	-2.50666	-0.44414	0.65374
N	0.95341	-1.22450	0.75298
C	-1.46731	3.13773	3.36448
H	-1.19015	4.08605	2.88076
H	-0.71492	2.94387	4.14949
H	-2.44217	3.25760	3.86051
C	-1.50432	1.98350	2.36882
C	-2.45210	0.96915	2.66250
H	-2.96103	1.10045	3.62121
C	-2.96919	-0.08924	1.87510
C	-4.12032	-0.85853	2.51459
H	-3.71074	-1.72699	3.06142
H	-4.82927	-1.24644	1.76911
H	-4.66582	-0.23631	3.24008
C	-3.34882	-1.28147	-0.17405
C	-4.31545	-0.64385	-1.01820
C	-5.10698	-1.44180	-1.86611
H	-5.84754	-0.96152	-2.51361

C	-4.96694	-2.83444	-1.90059
H	-5.59032	-3.43627	-2.57037
C	-4.03060	-3.44790	-1.06480
H	-3.93252	-4.53924	-1.07691
C	-3.21601	-2.70085	-0.18822
C	-4.53422	0.87321	-0.99134
H	-3.58538	1.33212	-0.65747
C	-4.89717	1.46783	-2.36927
H	-4.20204	1.14370	-3.16002
H	-4.87282	2.57040	-2.31992
H	-5.91870	1.18675	-2.68133
C	-5.62297	1.27426	0.03426
H	-6.58324	0.78526	-0.20865
H	-5.78435	2.36668	0.01618
H	-5.34774	0.99442	1.06214
C	0.16073	3.11692	1.05207
C	-0.24779	4.03635	0.03625
C	0.58679	5.12850	-0.26607
H	0.28319	5.83629	-1.04346
C	1.79731	5.32982	0.40843
H	2.43379	6.18445	0.15616
C	2.18180	4.43394	1.41013
H	3.12564	4.59434	1.94280
C	1.38422	3.32389	1.75609
C	1.87160	2.39972	2.87516
H	1.06916	1.67202	3.08211
C	3.12408	1.59743	2.45739
H	2.94493	1.00574	1.54631
H	3.42755	0.91348	3.26998
H	3.97465	2.26820	2.24499
C	2.15685	3.17299	4.18445
H	3.02048	3.85120	4.07064
H	2.39928	2.46902	4.99962
H	1.29683	3.78590	4.50238
C	-1.59550	3.88413	-0.67326
H	-1.81989	2.80100	-0.71663
C	-1.60826	4.43021	-2.11515
H	-1.55448	5.53305	-2.13667
H	-2.54963	4.14677	-2.61667
H	-0.76992	4.03971	-2.71513
C	-2.73378	4.54498	0.14178
H	-2.84136	4.09276	1.13983
H	-3.69959	4.43629	-0.38310
H	-2.53858	5.62412	0.27331
C	0.89826	-1.93551	2.00086
C	0.39603	-1.24072	3.12212
H	0.10675	-0.19057	3.01426
C	0.25678	-1.87985	4.36317
H	-0.12470	-1.31449	5.21983
C	0.59145	-3.23546	4.50082
H	0.47841	-3.73917	5.46621
C	1.05855	-3.94446	3.38074
H	1.30661	-5.00759	3.46896
C	1.21302	-3.30749	2.14190
H	1.57169	-3.87303	1.28018
C	1.86306	-1.41953	-0.18730
C	3.06407	-2.29222	-0.00974
C	3.38777	-3.24671	-1.00163
H	2.73693	-3.33276	-1.87647
C	4.53271	-4.04667	-0.86650
H	4.76343	-4.79396	-1.63339
C	5.39064	-3.87804	0.23209
H	6.29146	-4.49356	0.32756
C	5.09669	-2.90338	1.20123
H	5.77227	-2.75096	2.04967
C	3.93866	-2.12365	1.08911
H	3.71245	-1.36865	1.84790
C	3.05369	0.41903	-1.71116
C	3.10198	1.71822	-1.15694
H	2.22541	2.11821	-0.63353
C	4.23738	2.53747	-1.28392
H	4.22936	3.54449	-0.85158
C	5.36982	2.06816	-1.96814
H	6.25829	2.70209	-2.06882
C	5.35041	0.77968	-2.52896
H	6.22638	0.40525	-3.07207
C	4.20818	-0.02625	-2.39965
H	4.19442	-1.02081	-2.85942
C	0.45512	-1.20159	-3.52074
C	-0.01085	0.22234	-3.01311
C	0.72166	1.37826	-3.71843
H	1.80537	1.20546	-3.77513
H	0.56133	2.30843	-3.14960
H	0.32742	1.52090	-4.73884
C	-1.51876	0.46204	-3.07987
H	-1.86740	0.39458	-4.12492
H	-1.75999	1.47727	-2.72015
H	-2.09088	-0.27128	-2.48960
C	-0.58215	-2.30104	-3.21420
H	-0.91511	-2.26028	-2.16501
H	-0.11245	-3.28408	-3.38278
H	-1.47579	-2.23307	-3.85863
C	0.80086	-1.23871	-5.02045
H	-0.07115	-0.97391	-5.64480
H	1.11529	-2.25940	-5.29532
H	1.63007	-0.55573	-5.25653
B	1.75804	-0.56891	-1.60068
C	-2.28016	-3.46246	0.75370
H	-1.71315	-2.72151	1.34396
C	-3.08145	-4.34571	1.74190
H	-3.59605	-5.16707	1.21214
H	-2.40215	-4.79820	2.48485
H	-3.85005	-3.77102	2.28350
C	-1.26621	-4.34406	-0.00835
H	-0.58789	-3.74369	-0.63477
H	-0.65267	-4.91890	0.70515
H	-1.77780	-5.06809	-0.66660

TS(5-5b)

SCF (BP86) Energy = -2220.55559966
Enthalpy 0K = -2219.464203
Enthalpy 298K = -2219.398983
Free Energy 298K = -2219.561573
Lowest Frequency = -135.2496 cm^{-1}
Second Frequency = 16.4369 cm^{-1}
SCF (BP86-D3BJ) Energy = -2220.87424985
SCF (Toluene) Energy = -2220.56037645
SCF (BS2) Energy = -2420.33788036

Mg	-0.32142	0.19964	-0.27727
O	1.10101	-2.09990	2.39477
O	-0.20968	-0.24940	1.79385
O	2.44987	-1.96098	-0.81597
O	0.34966	-2.86043	-1.02158
N	0.40108	2.04054	-1.09514
N	-2.26708	0.45999	-1.09207
C	0.32569	3.81422	-2.86964

H	1.14792	4.28793	-2.31723
H	-0.48264	4.55107	-3.00746
H	0.69269	3.54904	-3.87644
C	-0.21582	2.57123	-2.16726
C	-1.42115	2.07954	-2.73280
H	-1.72253	2.59590	-3.64947
C	-2.41213	1.22666	-2.19949
C	-3.75034	1.28793	-2.93397
H	-4.37103	0.39762	-2.76376
H	-3.57905	1.40715	-4.01601
H	-4.33162	2.16544	-2.60066
C	-3.47500	-0.06272	-0.50421
C	-4.32669	0.80629	0.24519
C	-5.46640	0.26454	0.87191
H	-6.11634	0.92369	1.45875
C	-5.78759	-1.09107	0.75595
H	-6.67999	-1.49293	1.24764
C	-4.96278	-1.93010	-0.00364
H	-5.22608	-2.98720	-0.10229
C	-3.80272	-1.44740	-0.64264
C	-2.94506	-2.39413	-1.48870
H	-1.88308	-2.13119	-1.32924
C	-3.22192	-2.23590	-3.00368
H	-4.28815	-2.41616	-3.23100
H	-2.62766	-2.97025	-3.57611
H	-2.95376	-1.23431	-3.37070
C	-3.10303	-3.87806	-1.10248
H	-4.08632	-4.28184	-1.40493
H	-2.98422	-4.04187	-0.01899
H	-2.33368	-4.47535	-1.61873
C	-4.05439	2.30795	0.40050
H	-3.21965	2.57716	-0.26812
C	-5.27742	3.16417	-0.00505
H	-6.11824	3.03080	0.69826
H	-5.64672	2.90555	-1.01142
H	-5.01337	4.23605	-0.00115
C	-3.62280	2.66805	1.84035
H	-4.39440	2.37453	2.57439
H	-3.46496	3.75696	1.93746
H	-2.68108	2.16620	2.11727
C	1.57933	2.69550	-0.57684
C	1.45759	3.47895	0.61051
C	2.61085	4.06784	1.16171
H	2.52093	4.67359	2.06948
C	3.86740	3.90189	0.56853
H	4.75471	4.36534	1.01246
C	3.97589	3.14663	-0.60329
H	4.95695	3.02744	-1.07662
C	2.85429	2.53595	-1.20105
C	0.09395	3.75460	1.24569
H	-0.59870	2.96647	0.89804
C	-0.46972	5.10674	0.74645
H	0.19523	5.93783	1.04196
H	-1.46802	5.30009	1.17807
H	-0.56275	5.12584	-0.35182
C	0.11883	3.71768	2.78684
H	0.56163	2.77918	3.15844
H	-0.90728	3.79976	3.18573
H	0.69651	4.55720	3.21214
C	3.06698	1.75701	-2.50329
H	2.08998	1.35280	-2.82136
C	4.03051	0.56450	-2.31088
H	4.16378	0.02919	-3.26852
H	3.65126	-0.15505	-1.56995
H	5.02868	0.91067	-1.98817
C	3.60356	2.67210	-3.63188
H	2.96905	3.55753	-3.79589
H	3.66456	2.11233	-4.58186
H	4.62069	3.03263	-3.39677
C	1.23944	-3.76249	-1.77344
C	1.03885	-3.43631	-3.26414
H	1.61899	-4.11466	-3.91295
H	1.33350	-2.39800	-3.48653
H	-0.02837	-3.54818	-3.51634
C	0.82715	-5.20968	-1.48806
H	-0.18063	-5.40135	-1.89234
H	0.80782	-5.42004	-0.40859
H	1.52311	-5.91761	-1.97177
C	2.65928	-3.35889	-1.22779
C	3.78699	-3.39818	-2.26416
H	3.57714	-2.74660	-3.12525
H	3.94351	-4.42769	-2.63168
H	4.72783	-3.05792	-1.80155
C	3.07303	-4.13633	0.03461
H	3.25872	-5.20095	-0.18814
H	2.30505	-4.05720	0.82023
H	4.00353	-3.70367	0.43593
C	-0.86999	-0.89772	2.95694
C	-2.38583	-0.89613	2.79095
H	-2.78399	0.12866	2.83219
H	-2.84509	-1.46243	3.62018
H	-2.70854	-1.35212	1.84429
C	-0.47077	-0.07349	4.19375
H	0.61982	-0.08205	4.35102
H	-0.95841	-0.45773	5.10532
H	-0.79012	0.97093	4.04958
C	-0.22450	-2.34043	2.94223
C	-0.04214	-2.95270	4.33884
H	0.42695	-3.94562	4.24442
H	-1.01587	-3.08370	4.84206
H	0.60553	-2.33173	4.97529
C	-0.95800	-3.33682	2.03150
H	-1.05989	-2.95395	1.00573
H	-1.95494	-3.58890	2.43022
H	-0.36728	-4.26609	1.97770
B	1.11696	-0.89995	1.67268
B	1.08933	-1.75114	-0.57522
C	2.44500	-0.01238	1.69895
H	2.55932	0.62351	0.80403
H	2.27248	0.70454	2.53394
C	3.76113	-0.77000	1.96501
H	3.62270	-1.46528	2.81516
H	3.98931	-1.39839	1.08572
C	4.95397	0.15885	2.25356
H	4.72648	0.78100	3.14204
H	5.07291	0.86983	1.41350
C	6.27056	-0.60000	2.48289
H	7.10897	0.08682	2.69321
H	6.18747	-1.29647	3.33678
H	6.54495	-1.19940	1.59621

5b

SCF (BP86) Energy = -2220.56913551
Enthalpy 0K = -2219.478107
Enthalpy 298K = -2219.411349
Free Energy 298K = -2219.580203
Lowest Frequency = 14.3165 cm^{-1}
Second Frequency = 17.9582 cm^{-1}

SCF (BP86-D3BJ) Energy = -2220.87954776
SCF (Toluene) Energy = -2220.57479419
SCF (BS2) Energy = -2420.35330441

Mg	0.32233	0.05980	-0.40496
O	-1.54899	0.56611	3.62572
O	-0.21797	-0.19885	1.88484
O	-1.76725	2.66086	-0.04460
O	-0.17843	3.10699	-1.64336
N	-0.36795	-1.63443	-1.53458
N	2.35332	-0.25679	-1.04354
C	-0.34979	-2.82155	-3.73955
H	-1.03052	-3.55462	-3.28318
H	0.44476	-3.35743	-4.28160
H	-0.92913	-2.25113	-4.48686
C	0.25270	-1.87364	-2.70552
C	1.48795	-1.29235	-3.09386
H	1.78374	-1.52003	-4.12176
C	2.48870	-0.64521	-2.33186
C	3.81868	-0.44950	-3.05125
H	4.29780	0.49978	-2.76776
H	3.67413	-0.46791	-4.14211
H	4.52946	-1.25402	-2.79456
C	3.55762	0.08915	-0.33532
C	4.37852	-0.94937	0.20865
C	5.50345	-0.59631	0.97953
H	6.12838	-1.39066	1.40437
C	5.84316	0.74198	1.20867
H	6.72314	0.99555	1.80956
C	5.05479	1.75125	0.64520
H	5.33344	2.80023	0.79898
C	3.91568	1.45582	-0.13062
C	3.13869	2.61096	-0.76673
H	2.25197	2.19550	-1.27428
C	3.99052	3.34293	-1.83128
H	4.87982	3.81780	-1.37902
H	3.39389	4.13387	-2.31765
H	4.34455	2.65655	-2.61857
C	2.63120	3.62507	0.27997
H	3.46009	4.08119	0.85022
H	1.94110	3.15145	0.99861
H	2.07690	4.43488	-0.22248
C	4.08310	-2.43737	-0.01432
H	3.20605	-2.51256	-0.67899
C	5.26464	-3.16671	-0.69644
H	6.15421	-3.19216	-0.04237
H	5.56399	-2.67916	-1.63907
H	4.99178	-4.21158	-0.92616
C	3.72923	-3.15478	1.30770
H	4.56350	-3.10349	2.02974
H	3.50892	-4.22175	1.12610
H	2.84516	-2.70352	1.78730
C	-1.57772	-2.34939	-1.22792
C	-1.51389	-3.42907	-0.29228
C	-2.70289	-4.09129	0.06577
H	-2.66269	-4.91956	0.77995
C	-3.93813	-3.71601	-0.47827
H	-4.85269	-4.24420	-0.18847
C	-3.99035	-2.66556	-1.39950
H	-4.95565	-2.37588	-1.82984
C	-2.83081	-1.96640	-1.79379
C	-0.16980	-3.90044	0.26706
H	0.47778	-3.00702	0.35243
C	0.52857	-4.87259	-0.71463
H	-0.09759	-5.76638	-0.88565
H	1.49717	-5.20994	-0.30431
H	0.72195	-4.39895	-1.68957
C	-0.27364	-4.55480	1.65886
H	-0.83585	-3.92631	2.36914
H	0.73531	-4.72587	2.07244
H	-0.77018	-5.54046	1.61308
C	-2.97837	-0.83620	-2.81742
H	-1.96867	-0.46608	-3.06582
C	-3.77781	0.35525	-2.24269
H	-3.94372	1.11479	-3.02794
H	-3.24391	0.83697	-1.40837
H	-4.76917	0.03270	-1.87849
C	-3.64836	-1.32987	-4.12266
H	-3.14349	-2.21584	-4.54149
H	-3.63440	-0.53211	-4.88579
H	-4.70503	-1.60218	-3.95262
C	-1.16109	4.19277	-1.76496
C	-1.98416	3.89902	-3.03245
H	-2.71669	4.69764	-3.24209
H	-2.52087	2.94178	-2.94286
H	-1.29880	3.82354	-3.89247
C	-0.40857	5.51741	-1.94068
H	0.18433	5.48446	-2.86972
H	0.27942	5.71556	-1.10512
H	-1.11332	6.36423	-2.01879
C	-1.98709	4.06566	-0.42654
C	-3.49620	4.29605	-0.56735
H	-3.94911	3.60062	-1.28953
H	-3.70993	5.32928	-0.89370
H	-3.98762	4.14125	0.40760
C	-1.43451	4.92599	0.72409
H	-1.61223	6.00207	0.55463
H	-0.35232	4.76561	0.85667
H	-1.93932	4.63728	1.66052
C	0.64939	-0.11222	3.10983
C	2.03852	0.38260	2.73542
H	2.57753	-0.35472	2.12122
H	2.63426	0.54349	3.65047
H	2.00631	1.33159	2.18160
C	0.70773	-1.53081	3.69303
H	-0.28753	-1.87316	4.02021
H	1.39527	-1.57770	4.55364
H	1.07390	-2.22814	2.92417
C	-0.17281	0.88009	4.00654
C	-0.02201	0.65371	5.51401
H	-0.65144	1.37620	6.05835
H	1.02371	0.80811	5.83065
H	-0.33501	-0.35890	5.80884
C	0.06085	2.35883	3.65422
H	-0.04922	2.53080	2.57070
H	1.05923	2.70124	3.97305
H	-0.69546	2.96950	4.17320
B	-1.53971	0.06512	2.34276
B	-0.63196	2.16298	-0.71059
C	-2.86120	-0.16500	1.53490
H	-2.95811	0.71527	0.86573
H	-2.77929	-1.04130	0.86709
C	-4.12365	-0.27883	2.42161
H	-4.04483	-1.17512	3.06793
H	-4.16773	0.58405	3.11268
C	-5.43178	-0.35692	1.61609
H	-5.37440	-1.21412	0.91835
H	-5.51923	0.54644	0.98135

C -6.68031 -0.48860 2.50198
H -7.60438 -0.53879 1.90043
H -6.63608 -1.40218 3.12180
H -6.77606 0.37084 3.18965

5c
SCF (BP86) Energy = -1651.45464818
Enthalpy 0K = -1650.660452
Enthalpy 298K = -1650.611010
Free Energy 298K = -1650.745698
Lowest Frequency = 12.0445 cm^{-1}
Second Frequency = 14.6298 cm^{-1}
SCF (BP86-D3BJ) Energy = -1651.66661818
SCF (Toluene) Energy = -1651.46147313
SCF (BS2) Energy = -1851.09995036

Mg -0.00008 -0.20722 -0.00009
O 0.07341 2.85658 1.15026
O -0.07258 2.85676 -1.15016
N -1.50160 -1.61722 0.01309
N 1.50114 -1.61754 -0.01330
C -2.47866 -3.89409 0.01844
H -3.10716 -3.72462 0.90958
H -2.15785 -4.94585 0.00844
H -3.12796 -3.71358 -0.85539
C -1.28733 -2.94897 0.01012
C -0.00043 -3.54353 -0.00021
H -0.00055 -4.63609 -0.00028
C 1.28659 -2.94924 -0.01046
C 2.47772 -3.89461 -0.01883
H 3.10642 -3.72506 -0.90981
H 2.15669 -4.94631 -0.00913
H 3.12691 -3.71445 0.85517
C -2.84990 -1.10752 0.02523
C -3.48272 -0.81564 1.26831
C -2.78737 -1.07420 2.60667
H -1.86178 -1.63844 2.39566
C -2.38212 0.25845 3.28058
H -1.73850 0.87204 2.62627
H -1.83623 0.07011 4.22208
H -3.27414 0.86259 3.52411
C -3.64428 -1.93137 3.56434
H -3.08311 -2.15279 4.48894
H -3.93438 -2.89135 3.10400
H -4.57186 -1.40972 3.85890
C -4.76565 -0.23515 1.25211
H -5.25940 -0.00533 2.20314
C -5.41767 0.05912 0.04861
H -6.41593 0.50954 0.05770
C -4.78007 -0.21839 -1.16646
H -5.28502 0.02441 -2.10836
C -3.49730 -0.79812 -1.20596
C -2.81868 -1.03902 -2.55609
H -1.88542 -1.59699 -2.36262
C -3.68207 -1.89692 -3.50739
H -4.62004 -1.38255 -3.78120
H -3.95403 -2.86418 -3.05122
H -3.13420 -2.10378 -4.44329
C -2.43523 0.30228 -3.22566
H -1.89932 0.12495 -4.17505
H -1.79059 0.91949 -2.57582
H -3.33684 0.89765 -3.45545
C 2.84955 -1.10811 -0.02530
C 3.49694 -0.79900 1.20596
C 2.81821 -1.03994 2.55603
H 1.88485 -1.59769 2.36243
C 2.43500 0.30135 3.22575
H 1.89897 0.12401 4.17507
H 1.79053 0.91879 2.57594
H 3.33670 0.89651 3.45569
C 3.68138 -1.89814 3.50725
H 4.61944 -1.38399 3.78117
H 3.95317 -2.86539 3.05097
H 3.13343 -2.10501 4.44311
C 4.77983 -0.21952 1.16660
H 5.28478 0.02306 2.10855
C 5.41755 0.05801 -0.04840
H 6.41591 0.50823 -0.05739
C 4.76553 -0.23598 -1.25198
H 5.25938 -0.00615 -2.20296
C 3.48249 -0.81620 -1.26831
C 2.78718 -1.07447 -2.60675
H 1.86143 -1.63850 -2.39586
C 3.64397 -1.93177 -3.56441
H 3.08284 -2.15296 -4.48910
H 3.93377 -2.89188 -3.10413
H 4.57172 -1.41033 -3.85881
C 2.38231 0.25832 -3.28060
H 1.73877 0.87201 -2.62630
H 1.83649 0.07018 -4.22217
H 3.27450 0.86228 -3.52399
B 0.00028 2.06803 0.00000
C 0.26460 4.25977 0.74321
C -0.26330 4.25995 -0.74294
C -0.51728 5.15158 1.71336
H -0.10063 5.04836 2.72894
H -0.44096 6.21382 1.42140
H -1.58127 4.87462 1.75351
C 1.77280 4.54533 0.85967
H 2.09910 4.32896 1.88987
H 2.35307 3.90222 0.17848
H 2.00832 5.60016 0.63668
C 0.51889 5.15162 -1.71297
H 0.44293 6.21385 -1.42087
H 1.58278 4.87430 -1.75315
H 0.10219 5.04868 -2.72856
C -1.77141 4.54603 -0.85936
H -2.09777 4.32990 -1.88960
H -2.35189 3.90304 -0.17826
H -2.00657 5.60091 -0.63625

5·PhNCHPh
SCF (BP86) Energy = -2777.32309001
Enthalpy 0K = -2776.032747
Enthalpy 298K = -2775.953958
Free Energy 298K = -2776.151154
Lowest Frequency = 5.9775 cm^{-1}
Second Frequency = 10.8467 cm^{-1}
SCF (BP86-D3BJ) Energy = -2777.71000612
SCF (Toluene) Energy = -2777.33053942
SCF (BS2) Energy = -2977.23992250

Mg -1.87955 0.17132 0.25307
O 1.48285 -0.29575 -2.09017
O -0.80949 -0.08727 -1.39341
O 2.11577 -0.13651 1.28409
O -0.09575 0.49807 1.36403
N -2.98951 -1.45746 1.04075

N	-3.32946	1.65854	0.60238
C	-4.59313	-2.17710	2.82944
H	-4.58707	-3.15552	2.33023
H	-5.63589	-1.85952	2.98738
H	-4.13675	-2.30116	3.82740
C	-3.83155	-1.12076	2.03442
C	-4.12620	0.21835	2.43349
H	-4.72405	0.27073	3.34784
C	-4.02809	1.45399	1.74919
C	-4.79206	2.60952	2.38712
H	-5.32069	3.21248	1.63322
H	-4.08695	3.28865	2.89828
H	-5.51848	2.25136	3.13099
C	-3.66524	2.82988	-0.18682
C	-4.72487	2.72959	-1.14304
C	-5.03814	3.84776	-1.94006
H	-5.85547	3.77166	-2.66501
C	-4.33511	5.05128	-1.82640
H	-4.59191	5.90691	-2.45971
C	-3.30835	5.14773	-0.88450
H	-2.76342	6.09239	-0.77655
C	-2.96294	4.06434	-0.05120
C	-1.87270	4.28781	0.99403
H	-1.74405	3.33481	1.53185
C	-2.27413	5.37441	2.02063
H	-2.34047	6.36648	1.54019
H	-1.51978	5.44619	2.82410
H	-3.25239	5.16985	2.48507
C	-0.52109	4.66947	0.35126
H	-0.59681	5.62385	-0.19885
H	-0.17186	3.90407	-0.35867
H	0.25801	4.80226	1.12335
C	-5.57040	1.46345	-1.29992
H	-5.03242	0.63999	-0.79888
C	-6.94053	1.61976	-0.59688
H	-7.51452	2.45402	-1.03828
H	-6.82702	1.82199	0.48035
H	-7.54135	0.69971	-0.70583
C	-5.78054	1.07014	-2.77831
H	-6.37510	1.82224	-3.32545
H	-6.33241	0.11696	-2.84498
H	-4.82241	0.94957	-3.31142
C	-2.89177	-2.84730	0.62974
C	-3.52585	-3.24196	-0.58867
C	-3.39191	-4.56984	-1.03456
H	-3.87612	-4.87053	-1.96813
C	-2.66074	-5.51534	-0.30902
H	-2.56553	-6.54317	-0.67400
C	-2.05958	-5.13035	0.88998
H	-1.49348	-5.86893	1.46798
C	-2.15590	-3.81242	1.38284
C	-4.42150	-2.28420	-1.37324
H	-4.02649	-1.26095	-1.22913
C	-5.85820	-2.31292	-0.79711
H	-6.27698	-3.33255	-0.86587
H	-6.52366	-1.63478	-1.35960
H	-5.88020	-2.00845	0.26165
C	-4.45259	-2.56758	-2.88888
H	-3.43722	-2.66626	-3.30655
H	-4.96509	-1.74687	-3.41741
H	-5.00694	-3.49370	-3.12268
C	-1.45845	-3.51402	2.71208
H	-1.65108	-2.45896	2.96756
C	0.07149	-3.71279	2.60271
H	0.56170	-3.50965	3.57189
H	0.52067	-3.05957	1.83733
H	0.31550	-4.75335	2.32766
C	-2.00454	-4.39323	3.86387
H	-3.09958	-4.32317	3.96169
H	-1.55322	-4.09035	4.82518
H	-1.75452	-5.45669	3.70499
C	0.45660	0.79576	2.73137
C	-0.05111	-0.29908	3.67241
H	0.28576	-0.11075	4.70557
H	0.30759	-1.29064	3.36592
H	-1.15437	-0.30180	3.67012
C	-0.05331	2.15326	3.20714
H	-1.14743	2.12260	3.34159
H	0.19904	2.96053	2.50698
H	0.39590	2.39377	4.18649
C	2.01157	0.73950	2.45952
C	2.84293	0.11124	3.58319
H	2.52162	-0.91718	3.80643
H	2.77715	0.71271	4.50650
H	3.89716	0.08471	3.26293
C	2.62339	2.09296	2.05997
H	2.62873	2.79765	2.90882
H	2.07603	2.55493	1.22184
H	3.66698	1.92285	1.74700
C	-0.64175	0.53262	-2.70691
C	-1.53166	1.77253	-2.81058
H	-2.59896	1.49322	-2.79286
H	-1.34787	2.30090	-3.76224
H	-1.35703	2.48530	-1.98969
C	-1.05006	-0.49320	-3.77970
H	-0.37552	-1.36238	-3.76727
H	-1.03792	-0.04718	-4.78910
H	-2.07471	-0.84364	-3.57441
C	0.91057	0.83703	-2.73543
C	1.49133	0.93171	-4.15678
H	2.56864	1.16101	-4.09945
H	1.00518	1.73259	-4.74165
H	1.37666	-0.02139	-4.69470
C	1.27481	2.11953	-1.95429
H	0.83462	2.09840	-0.94330
H	0.93990	3.04030	-2.46297
H	2.37047	2.16458	-1.84414
B	0.59089	-0.79656	-1.00944
B	0.93204	-0.15095	0.58364
C	0.49938	-2.42081	-1.08818
H	-0.23231	-2.83138	-0.36281
H	0.10637	-2.70476	-2.08704
C	1.85669	-3.12502	-0.88089
H	2.59369	-2.70926	-1.59544
H	2.25679	-2.88549	0.12634
C	1.80774	-4.65483	-1.04937
H	1.43796	-4.89240	-2.06648
H	1.05340	-5.07330	-0.35416
C	3.16341	-5.34229	-0.82101
H	3.09896	-6.43650	-0.95625
H	3.92602	-4.96280	-1.52444
H	3.53981	-5.15361	0.20071
C	5.23283	0.11918	-0.04658
H	4.15220	-0.08599	0.03694
C	5.81578	-0.27554	-1.34923
C	4.88988	-0.59171	-2.37537
C	7.20262	-0.38783	-1.61688
C	5.34194	-0.98576	-3.64257

H	3.81102	-0.51764	-2.17761
C	7.64432	-0.79537	-2.88176
H	7.93003	-0.16814	-0.83255
C	6.71875	-1.08907	-3.89926
H	4.61502	-1.22171	-4.42669
H	8.71838	-0.88625	-3.07568
H	7.07253	-1.40451	-4.88690
C	7.08969	1.09249	1.12899
C	7.51574	2.29879	0.52218
C	7.98237	0.40511	1.98501
C	8.81028	2.78519	0.75026
H	6.81856	2.84276	-0.12294
C	9.27980	0.89390	2.19236
H	7.64418	-0.51525	2.47158
C	9.70319	2.08578	1.57974
H	9.12391	3.71942	0.27129
H	9.96306	0.34074	2.84627
H	10.71381	2.46881	1.75307
N	5.75591	0.65392	1.01026

TS(5-17$_{BN}$)1

SCF (BP86) Energy = -2777.29323700
Enthalpy 0K = -2776.001746
Enthalpy 298K = -2775.925332
Free Energy 298K = -2776.109556
Lowest Frequency = -104.3516 cm^{-1}
Second Frequency = 18.1144 cm^{-1}
SCF (BP86-D3BJ) Energy = -2777.71057216
SCF (Toluene) Energy = -2777.30016521
SCF (BS2) Energy = -2977.20860540

Mg	1.09472	0.00397	0.44606
O	-1.83592	1.31376	-2.03976
O	0.29183	0.84453	-1.16246
O	-2.23949	2.29540	1.55147
O	-0.49872	0.75255	1.59033
N	3.13522	0.55852	0.67606
N	1.34773	-2.03488	1.12870
C	5.00855	0.54262	2.35236
H	5.35102	1.46039	1.85719
H	5.80044	-0.21859	2.25157
H	4.89346	0.73687	3.43280
C	3.68601	0.02434	1.78902
C	3.14649	-1.07106	2.51448
H	3.71376	-1.30663	3.42070
C	2.26618	-2.11879	2.11662
C	2.51301	-3.42076	2.88184
H	1.70914	-4.15829	2.76748
H	2.65602	-3.20632	3.95363
H	3.44990	-3.88535	2.52834
C	0.66413	-3.26981	0.77622
C	1.20229	-4.11951	-0.23940
C	0.57987	-5.35774	-0.50104
H	1.00589	-6.01287	-1.26784
C	-0.55014	-5.77530	0.20477
H	-1.00855	-6.74818	-0.00155
C	-1.09508	-4.92556	1.17148
H	-1.99229	-5.24038	1.71223
C	-0.52440	-3.67123	1.46990
C	-1.19820	-2.81788	2.55046
H	-0.95016	-1.76371	2.33423
C	-0.69168	-3.15837	3.97470
H	-0.78236	-4.24244	4.16666
H	-1.30103	-2.63641	4.73358
H	0.35619	-2.86820	4.13444
C	-2.73836	-2.95879	2.54732
H	-3.06030	-3.92582	2.97301
H	-3.16729	-2.87362	1.53693
H	-3.18424	-2.17146	3.17881
C	2.46045	-3.77895	-1.04067
H	2.65745	-2.69983	-0.91164
C	3.69293	-4.54968	-0.51024
H	3.52269	-5.63967	-0.56344
H	3.91884	-4.29545	0.53688
H	4.58754	-4.31930	-1.11505
C	2.28373	-4.06703	-2.54973
H	2.25399	-5.15137	-2.75526
H	3.13237	-3.65522	-3.12027
H	1.35636	-3.62447	-2.94618
C	4.00957	1.34165	-0.17925
C	4.97112	0.66988	-0.99769
C	5.82697	1.43095	-1.81960
H	6.56526	0.91136	-2.44063
C	5.75700	2.82411	-1.85949
H	6.43151	3.39811	-2.50351
C	4.80857	3.47625	-1.06598
H	4.74888	4.56791	-1.09572
C	3.92951	2.76856	-0.22295
C	5.12876	-0.85258	-1.04652
H	4.36665	-1.30060	-0.38632
C	6.51968	-1.30757	-0.54404
H	7.32222	-0.93964	-1.20748
H	6.58282	-2.40971	-0.52472
H	6.73518	-0.93554	0.47035
C	4.89809	-1.38690	-2.47853
H	3.89466	-1.12772	-2.85461
H	5.00523	-2.48502	-2.50434
H	5.63504	-0.96896	-3.18599
C	2.96373	3.56196	0.65583
H	2.06782	2.93427	0.79895
C	2.50284	4.89166	0.02449
H	1.67815	5.32123	0.61770
H	2.13579	4.75520	-1.00467
H	3.31338	5.64215	0.01091
C	3.57390	3.85187	2.04858
H	3.80722	2.93115	2.60511
H	2.87572	4.44943	2.66067
H	4.50943	4.42993	1.94390
C	-0.54576	1.39396	2.94172
C	0.55576	2.45800	2.97688
H	0.60028	2.94799	3.96375
H	0.38879	3.23031	2.21007
H	1.53527	1.98471	2.79738
C	-0.27574	0.35209	4.02616
H	0.72325	-0.09715	3.88661
H	-1.02392	-0.45011	4.03037
H	-0.28919	0.83803	5.01774
C	-1.99303	2.01553	2.95331
C	-2.10505	3.34098	3.72069
H	-1.45633	4.11708	3.28846
H	-1.84693	3.21035	4.78627
H	-3.14480	3.70191	3.66467
C	-3.06636	1.03809	3.46414
H	-2.97422	0.86524	4.55026
H	-3.00238	0.07206	2.94022
H	-4.06063	1.46474	3.26129
C	0.38751	0.55817	-2.59198
C	0.63384	-0.95120	-2.72881

H	1.58424	-1.21508	-2.23031
H	0.72741	-1.25848	-3.78400
H	-0.17490	-1.54189	-2.26943
C	1.59629	1.31136	-3.17481
H	1.51446	2.39600	-3.01632
H	1.69498	1.12492	-4.25868
H	2.52569	0.97348	-2.68618
C	-1.03634	1.03411	-3.18857
C	-0.94376	2.28205	-4.10385
H	-1.96873	2.57555	-4.38504
H	-0.38585	2.07139	-5.03342
H	-0.47595	3.14210	-3.60550
C	-1.76136	-0.05957	-3.99997
H	-1.93561	-0.97031	-3.40966
H	-1.20453	-0.32784	-4.91510
H	-2.74721	0.32710	-4.30663
B	-0.99787	1.75290	-0.91136
B	-1.52602	1.41371	0.73167
C	-0.59014	3.35567	-0.92586
H	-0.06245	3.62455	0.01320
H	0.14282	3.58153	-1.72965
C	-1.80338	4.29421	-1.07482
H	-2.32751	4.06022	-2.02262
H	-2.52772	4.07860	-0.26557
C	-1.46015	5.79542	-1.05088
H	-0.72666	6.01713	-1.85179
H	-0.94615	6.03577	-0.09864
C	-2.68721	6.70740	-1.21291
H	-2.41327	7.77696	-1.18869
H	-3.20065	6.51616	-2.17250
H	-3.42243	6.53141	-0.40722
C	-2.71511	-1.10956	-0.37723
H	-1.67638	-1.44071	-0.21308
C	-3.46471	-1.98984	-1.29506
C	-2.83943	-3.22129	-1.62221
C	-4.72799	-1.70134	-1.87325
C	-3.45536	-4.13959	-2.48126
H	-1.86410	-3.45966	-1.18319
C	-5.33275	-2.61985	-2.73957
H	-5.22242	-0.75318	-1.65953
C	-4.70686	-3.84177	-3.04386
H	-2.95501	-5.08559	-2.71209
H	-6.30333	-2.37723	-3.18478
H	-5.19104	-4.55415	-3.72023
C	-4.37193	0.48468	0.25288
C	-5.37464	-0.05537	1.08678
C	-4.65996	1.60372	-0.55754
C	-6.65695	0.51316	1.10102
H	-5.14138	-0.92172	1.71351
C	-5.94735	2.16118	-0.53207
H	-3.87778	1.98532	-1.21969
C	-6.94989	1.62499	0.29387
H	-7.42968	0.08208	1.74698
H	-6.16684	3.02517	-1.16875
H	-7.95079	2.06862	0.30822
N	-3.05140	-0.05241	0.29757

INT(5-17$_{BN}$)

SCF (BP86) Energy = -2777.29838430
Enthalpy 0K = -2776.006465
Enthalpy 298K = -2775.929772
Free Energy 298K = -2776.113704
Lowest Frequency = 20.9488 cm^{-1}
Second Frequency = 21.9833 cm^{-1}
SCF (BP86-D3BJ) Energy = -2777.72065409
SCF (Toluene) Energy = -2777.30461093
SCF (BS2) Energy = -2977.21265449

Mg	-1.02512	-0.02819	0.46670
O	1.91183	-1.38807	-2.07861
O	-0.16608	-0.90073	-1.11747
O	2.45069	-2.09618	1.57460
O	0.67175	-0.54311	1.55302
N	-3.04052	-0.69846	0.69379
N	-1.42898	2.02044	1.08193
C	-4.90482	-0.76647	2.38098
H	-5.17523	-1.72942	1.92911
H	-5.75098	-0.07291	2.24021
H	-4.78353	-0.89978	3.46979
C	-3.62025	-0.17686	1.79942
C	-3.15157	0.96605	2.49833
H	-3.72820	1.18177	3.40340
C	-2.34814	2.06313	2.07134
C	-2.68942	3.36264	2.80359
H	-1.93495	4.14959	2.68336
H	-2.83499	3.16275	3.87774
H	-3.64917	3.75624	2.42539
C	-0.83025	3.29467	0.71261
C	-1.41218	4.08473	-0.32596
C	-0.88008	5.36196	-0.59870
H	-1.33991	5.96983	-1.38476
C	0.19943	5.87751	0.12178
H	0.58479	6.87992	-0.09234
C	0.78836	5.08766	1.11307
H	1.64807	5.47780	1.66611
C	0.31138	3.79672	1.41907
C	1.03425	3.00861	2.51571
H	0.81656	1.94084	2.34286
C	0.54754	3.38750	3.93645
H	0.62650	4.47816	4.09361
H	1.17481	2.89656	4.70131
H	-0.49445	3.09035	4.12203
C	2.56869	3.19498	2.46477
H	2.87292	4.19679	2.81639
H	2.97213	3.05573	1.44933
H	3.05402	2.46468	3.13522
C	-2.62908	3.63888	-1.13818
H	-2.76102	2.55430	-0.97557
C	-3.91600	4.34837	-0.65352
H	-3.81362	5.44437	-0.74368
H	-4.14114	4.11781	0.39955
H	-4.78521	4.04123	-1.26113
C	-2.43835	3.88756	-2.65241
H	-2.46315	4.96474	-2.89308
H	-3.25118	3.41097	-3.22493
H	-1.47953	3.48520	-3.01578
C	-3.88152	-1.54524	-0.13494
C	-4.88699	-0.94083	-0.95332
C	-5.72160	-1.76210	-1.73832
H	-6.49378	-1.29372	-2.35887
C	-5.58854	-3.15113	-1.74216
H	-6.24837	-3.77297	-2.35631
C	-4.59445	-3.73701	-0.95268
H	-4.48388	-4.82506	-0.95624
C	-3.73308	-2.96747	-0.14619
C	-5.11095	0.57152	-1.04540
H	-4.36338	1.07134	-0.40614
C	-6.51585	0.98303	-0.54481

H	-7.30774	0.56021	-1.18800
H	-6.62563	2.08151	-0.56032
H	-6.70690	0.63607	0.48331
C	-4.91362	1.07035	-2.49546
H	-3.90041	0.84898	-2.86952
H	-5.07421	2.16048	-2.55586
H	-5.63258	0.59413	-3.18436
C	-2.70688	-3.69151	0.72426
H	-1.83251	-3.02509	0.81216
C	-2.21451	-5.02269	0.12045
H	-1.34563	-5.39260	0.68974
H	-1.90045	-4.90972	-0.92923
H	-2.99033	-5.80771	0.16914
C	-3.25107	-3.95800	2.14841
H	-3.49650	-3.02874	2.68469
H	-2.50591	-4.50771	2.74973
H	-4.16667	-4.57431	2.10038
C	0.71783	-1.18747	2.89615
C	-0.34697	-2.28885	2.92805
H	-0.40055	-2.76063	3.92339
H	-0.13165	-3.06879	2.18249
H	-1.34111	-1.85790	2.71854
C	0.39734	-0.16031	3.98493
H	-0.61625	0.25382	3.84107
H	1.11585	0.66870	4.00457
H	0.41849	-0.65292	4.97323
C	2.18251	-1.77002	2.94781
C	2.31620	-3.06062	3.77212
H	1.70759	-3.87296	3.34819
H	2.02232	-2.90207	4.82465
H	3.36871	-3.38801	3.75897
C	3.21289	-0.74229	3.46209
H	3.10116	-0.55818	4.54474
H	3.12071	0.21940	2.93381
H	4.22527	-1.13418	3.27827
C	-0.33244	-0.65965	-2.55470
C	-0.59485	0.84240	-2.72945
H	-1.51770	1.12135	-2.18855
H	-0.75156	1.10884	-3.78818
H	0.23588	1.45237	-2.34111
C	-1.55902	-1.44475	-3.04766
H	-1.46255	-2.52064	-2.84303
H	-1.70444	-1.30913	-4.13364
H	-2.47022	-1.09146	-2.53751
C	1.05968	-1.15008	-3.19961
C	0.93569	-2.44259	-4.04474
H	1.94859	-2.74272	-4.35991
H	0.32989	-2.28709	-4.95470
H	0.50268	-3.27807	-3.47645
C	1.74151	-0.08771	-4.08480
H	1.94976	0.83953	-3.53222
H	1.13559	0.15281	-4.97601
H	2.70784	-0.48843	-4.43278
B	1.14423	-1.75039	-0.88587
B	1.81941	-1.14366	0.70452
C	0.81724	-3.35510	-0.72601
H	0.34184	-3.55942	0.25317
H	0.06134	-3.65940	-1.48222
C	2.05344	-4.26354	-0.85872
H	2.53827	-4.07710	-1.83784
H	2.79128	-3.97707	-0.08550
C	1.75439	-5.76907	-0.73067
H	1.00221	-6.06096	-1.49054
H	1.28006	-5.96273	0.25221
C	3.00236	-6.65470	-0.87794
H	2.76100	-7.72760	-0.77778
H	3.47806	-6.51051	-1.86484
H	3.75768	-6.40794	-0.11043
C	2.49538	1.13981	-0.35503
H	1.47205	1.44851	-0.10332
C	3.18329	2.03857	-1.27840
C	2.53022	3.27784	-1.53972
C	4.40627	1.78120	-1.96226
C	3.07558	4.21928	-2.41862
H	1.58452	3.49883	-1.03380
C	4.93781	2.72569	-2.84615
H	4.92457	0.83300	-1.82054
C	4.28723	3.95157	-3.07686
H	2.54800	5.16339	-2.58910
H	5.87432	2.49835	-3.36661
H	4.71738	4.68441	-3.76735
C	4.25411	-0.40542	0.15070
C	5.21339	0.32559	0.87904
C	4.64328	-1.52679	-0.60451
C	6.55906	-0.06659	0.85414
H	4.89707	1.19781	1.45841
C	5.99387	-1.91095	-0.61866
H	3.89574	-2.04585	-1.20760
C	6.95478	-1.18907	0.10728
H	7.29859	0.50764	1.42221
H	6.29447	-2.78153	-1.21118
H	8.00587	-1.49537	0.08877
N	2.87169	0.01130	0.23224

TS(5-17$_{BN}$)2

SCF (BP86) Energy = -2777.27977665
Enthalpy 0K = -2775.989006
Enthalpy 298K = -2775.912279
Free Energy 298K = -2776.096178
Lowest Frequency = -244.8013 cm^{-1}
Second Frequency = 22.1079 cm^{-1}
SCF (BP86-D3BJ) Energy = -2777.70610566
SCF (Toluene) Energy = -2777.28734662
SCF (BS2) Energy = -2977.19551702

Mg	-0.78779	-0.03291	0.34978
O	2.08941	-1.62494	-2.31212
O	0.10240	-1.24871	-1.14985
O	3.00123	-1.36157	1.72088
O	0.84597	-0.44034	1.59632
N	-2.64017	-1.13821	0.70235
N	-1.60538	1.84681	1.13694
C	-4.38987	-1.61450	2.45018
H	-4.40500	-2.64749	2.08164
H	-5.37055	-1.16612	2.21499
H	-4.29886	-1.62059	3.54922
C	-3.26152	-0.77343	1.85054
C	-3.01817	0.42207	2.56928
H	-3.60179	0.49400	3.49215
C	-2.48636	1.67314	2.14407
C	-3.10341	2.85500	2.89463
H	-2.52360	3.78244	2.82179
H	-3.24472	2.59601	3.95639
H	-4.10782	3.05905	2.48167
C	-1.32442	3.23943	0.80541
C	-2.07002	3.89196	-0.21828
C	-1.87842	5.27136	-0.43799
H	-2.46376	5.76903	-1.21854

C	-0.97406	6.01635	0.32118
H	-0.85053	7.09007	0.14623
C	-0.21120	5.36297	1.29322
H	0.52091	5.93455	1.87255
C	-0.34995	3.98345	1.54455
C	0.56042	3.35934	2.60559
H	0.50872	2.26604	2.46862
C	0.11367	3.69013	4.05000
H	0.06253	4.78319	4.20060
H	0.84020	3.29015	4.77975
H	-0.87340	3.26883	4.29425
C	2.03311	3.79081	2.41562
H	2.18208	4.85832	2.65394
H	2.36715	3.61876	1.37997
H	2.68794	3.21819	3.09547
C	-3.09509	3.17610	-1.09523
H	-3.01858	2.09389	-0.88675
C	-4.53286	3.62629	-0.74592
H	-4.64541	4.71623	-0.88274
H	-4.79026	3.39322	0.30069
H	-5.27377	3.13128	-1.39742
C	-2.80353	3.40234	-2.59730
H	-3.00551	4.44637	-2.89420
H	-3.44677	2.75716	-3.21933
H	-1.74960	3.18886	-2.83950
C	-3.36593	-2.12935	-0.07971
C	-4.49735	-1.70931	-0.84850
C	-5.24118	-2.66796	-1.56579
H	-6.10819	-2.33802	-2.14900
C	-4.90400	-4.02164	-1.54513
H	-5.49831	-4.75413	-2.10135
C	-3.79035	-4.42722	-0.80423
H	-3.52211	-5.48757	-0.78740
C	-3.00591	-3.51390	-0.07098
C	-4.94922	-0.25045	-0.96674
H	-4.26774	0.37087	-0.36153
C	-6.38507	-0.03674	-0.43259
H	-7.12436	-0.59582	-1.03279
H	-6.65796	1.03167	-0.47963
H	-6.49080	-0.36795	0.61322
C	-4.86616	0.22819	-2.43536
H	-3.83601	0.17833	-2.82507
H	-5.21564	1.27036	-2.52674
H	-5.49964	-0.39097	-3.09387
C	-1.83117	-4.06758	0.73798
H	-1.08486	-3.25942	0.82363
C	-1.14908	-5.27590	0.05936
H	-0.19342	-5.50178	0.56024
H	-0.93834	-5.08934	-1.00659
H	-1.77082	-6.18634	0.12579
C	-2.25803	-4.48975	2.16535
H	-2.64063	-3.64708	2.76085
H	-1.40283	-4.92587	2.71098
H	-3.05129	-5.25696	2.11609
C	1.00319	-1.00389	2.97719
C	0.22239	-2.31792	3.05459
H	0.20306	-2.69422	4.09089
H	0.65749	-3.10114	2.41532
H	-0.81919	-2.13994	2.74497
C	0.40740	-0.02409	3.99035
H	-0.67541	0.09936	3.81467
H	0.88545	0.96232	3.95138
H	0.54112	-0.42844	5.00902
C	2.57434	-1.18393	3.09376
C	3.00448	-2.41827	3.89639
H	2.62285	-3.34815	3.44946
H	2.65670	-2.35573	4.94188
H	4.10486	-2.47466	3.90667
C	3.29251	0.06529	3.64340
H	3.07422	0.23613	4.71113
H	3.01481	0.96826	3.07634
H	4.37804	-0.07888	3.52684
C	-0.23101	-1.05399	-2.60590
C	-0.56949	0.42353	-2.81098
H	-1.45724	0.69109	-2.20256
H	-0.85070	0.61821	-3.85940
H	0.26114	1.08781	-2.53235
C	-1.45753	-1.91291	-2.92603
H	-1.31048	-2.97004	-2.66305
H	-1.68645	-1.85146	-4.00392
H	-2.33931	-1.55526	-2.37498
C	1.09152	-1.54068	-3.35646
C	0.97650	-2.95759	-3.96530
H	1.96541	-3.24057	-4.36012
H	0.25156	-2.99806	-4.79536
H	0.68994	-3.71092	-3.21403
C	1.58274	-0.57926	-4.44617
H	1.76638	0.43274	-4.05834
H	0.85603	-0.52230	-5.27537
H	2.53129	-0.96285	-4.85673
B	1.45019	-1.83984	-1.07823
B	2.14013	-0.60029	0.91137
C	1.67207	-3.24889	-0.34260
H	1.27279	-3.25984	0.68484
H	1.00511	-3.92701	-0.92173
C	3.09021	-3.84470	-0.36665
H	3.48477	-3.79663	-1.40017
H	3.75678	-3.22557	0.25907
C	3.14761	-5.30274	0.12606
H	2.46286	-5.92573	-0.48308
H	2.75841	-5.35150	1.16312
C	4.56205	-5.90229	0.08339
H	4.57564	-6.94551	0.44373
H	4.96411	-5.89879	-0.94546
H	5.26016	-5.32086	0.71128
C	1.80316	1.52454	-0.41489
H	1.08397	1.89454	0.32550
C	2.10039	2.37500	-1.54615
C	1.40399	3.61896	-1.68459
C	3.04714	2.07557	-2.57862
C	1.63761	4.48668	-2.75474
H	0.67584	3.90346	-0.92111
C	3.28042	2.95968	-3.63997
H	3.60330	1.13658	-2.54415
C	2.58458	4.17609	-3.74901
H	1.07651	5.42746	-2.80309
H	4.02196	2.68438	-4.39969
H	2.77267	4.85993	-4.58280
C	4.03193	0.49604	-0.18892
C	4.73532	1.65248	0.20650
C	4.73748	-0.59153	-0.73292
C	6.12869	1.70626	0.07996
H	4.17698	2.50075	0.61094
C	6.13601	-0.53088	-0.85064
H	4.18849	-1.45950	-1.09858
C	6.83933	0.61296	-0.44607
H	6.66228	2.60893	0.39674
H	6.67362	-1.38427	-1.27808

H 7.92848 0.65965 -0.54942
N 2.59803 0.45720 0.02324

TS(5-17$_{BCN}$)
SCF (BP86) Energy = -2777.26428012
Enthalpy 0K = -2775.974104
Enthalpy 298K = -2775.897493
Free Energy 298K = -2776.081972
Lowest Frequency = -154.0755 cm^{-1}
Second Frequency = 18.8854 cm^{-1}
SCF (BP86-D3BJ) Energy = -2777.68097799
SCF (Toluene) Energy = -2777.27110341
SCF (BS2) Energy = -2977.17766923

Mg -1.08736 -0.20926 -0.38861
O 1.64162 1.13901 2.46439
O -0.23487 0.65055 1.18317
O 2.86494 1.02686 -1.38747
O 0.83163 -0.08255 -1.22566
N -2.76874 0.87504 -1.14695
N -1.98524 -2.12201 -0.50918
C -4.45341 0.83441 -3.01782
H -4.57177 1.91110 -2.84021
H -5.42508 0.34416 -2.83698
H -4.21571 0.66944 -4.08278
C -3.37160 0.19876 -2.14747
C -3.08632 -1.15596 -2.48890
H -3.52143 -1.46577 -3.44474
C -2.60089 -2.24079 -1.71244
C -2.80205 -3.61006 -2.36109
H -2.59823 -4.43728 -1.66912
H -2.10856 -3.69847 -3.21751
H -3.82121 -3.72212 -2.76386
C -2.02551 -3.27782 0.36819
C -3.27358 -3.67231 0.95264
C -3.31518 -4.80578 1.78832
H -4.27519 -5.10978 2.21985
C -2.16848 -5.54595 2.08123
H -2.22191 -6.42346 2.73422
C -0.95107 -5.14626 1.52616
H -0.04713 -5.72154 1.74616
C -0.85021 -4.03153 0.66823
C 0.51036 -3.75313 0.03430
H 0.55623 -2.69011 -0.26826
C 0.68827 -4.60408 -1.24676
H 0.63147 -5.67960 -1.00072
H 1.67238 -4.40799 -1.70485
H -0.08974 -4.39218 -1.99857
C 1.69110 -4.02591 0.99109
H 1.88290 -5.10778 1.10651
H 1.50780 -3.61237 1.99758
H 2.59639 -3.55129 0.57604
C -4.59376 -2.92793 0.73290
H -4.38404 -2.01388 0.15235
C -5.61265 -3.77454 -0.06677
H -5.88946 -4.68765 0.48944
H -5.21268 -4.09069 -1.04273
H -6.53809 -3.19945 -0.24618
C -5.22092 -2.50741 2.08158
H -5.49721 -3.38605 2.68957
H -6.14347 -1.92490 1.91529
H -4.52533 -1.89612 2.67933
C -3.33722 2.15915 -0.76334
C -4.45076 2.20769 0.13238
C -5.02764 3.45585 0.44535
H -5.89166 3.48541 1.11738
C -4.53121 4.64793 -0.08142
H -4.99728 5.60629 0.17007
C -3.42006 4.59998 -0.92696
H -3.01893 5.53384 -1.32982
C -2.80348 3.38311 -1.28005
C -5.08594 0.96909 0.76909
H -4.41777 0.10975 0.58110
C -6.46227 0.65600 0.13499
H -7.16396 1.49364 0.29545
H -6.90806 -0.24574 0.58956
H -6.38858 0.48813 -0.95070
C -5.24877 1.13256 2.29908
H -4.29475 1.38593 2.78848
H -5.62941 0.20119 2.74788
H -5.97016 1.93010 2.54682
C -1.61100 3.43382 -2.23866
H -0.96169 2.57421 -1.98601
C -0.77002 4.72051 -2.09284
H 0.16130 4.63094 -2.67580
H -0.49678 4.92159 -1.04516
H -1.30415 5.60260 -2.48716
C -2.04354 3.29045 -3.71809
H -2.52408 2.32311 -3.92515
H -1.16906 3.38385 -4.38609
H -2.75741 4.08929 -3.98613
C 1.21490 -0.14587 -2.67768
C 0.00565 0.19923 -3.54529
H 0.29899 0.16505 -4.60901
H -0.39988 1.19836 -3.34051
H -0.80218 -0.54167 -3.40838
C 1.63945 -1.59077 -2.95659
H 0.75886 -2.24614 -2.85540
H 2.40020 -1.92316 -2.23368
H 2.02676 -1.69956 -3.98273
C 2.38689 0.91695 -2.75675
C 1.93234 2.32523 -3.17804
H 1.11188 2.68813 -2.54290
H 1.61079 2.35700 -4.23278
H 2.78232 3.01631 -3.05707
C 3.54773 0.48033 -3.66241
H 3.20833 0.39474 -4.71016
H 3.98374 -0.47623 -3.34543
H 4.34305 1.24202 -3.62577
C -0.68373 0.67070 2.58822
C -1.66867 -0.48019 2.81085
H -2.59342 -0.31571 2.23006
H -1.96039 -0.53263 3.87369
H -1.24904 -1.45751 2.52631
C -1.38372 2.01894 2.83101
H -0.68898 2.86362 2.71009
H -1.81179 2.06628 3.84650
H -2.20150 2.14729 2.10310
C 0.68764 0.52963 3.35863
C 0.73752 1.29914 4.69040
H 1.72861 1.15767 5.15076
H -0.02430 0.92627 5.39750
H 0.58678 2.37866 4.54254
C 1.08883 -0.93416 3.62358
H 0.98002 -1.56041 2.72438
H 0.48176 -1.38191 4.42929
H 2.14689 -0.95743 3.92835
B 1.14324 1.32680 1.14363

B	2.01216	0.40547	-0.46378
C	1.16743	2.88009	0.58879
H	1.70219	2.98799	-0.37012
H	0.11311	3.15621	0.37855
C	1.77372	3.88905	1.59072
H	1.21948	3.85500	2.54906
H	2.80237	3.57642	1.84885
C	1.79444	5.33989	1.07562
H	0.75985	5.66376	0.84525
H	2.34443	5.37906	0.11488
C	2.42635	6.32675	2.07083
H	2.42888	7.35844	1.67828
H	1.87639	6.33500	3.02889
H	3.47202	6.05075	2.29504
C	3.05789	-0.70439	0.61479
H	2.26853	-1.12188	1.26048
C	4.09226	0.02720	1.47255
C	4.72500	-0.73684	2.47670
C	4.49016	1.36803	1.30837
C	5.71253	-0.17613	3.30162
H	4.44157	-1.78781	2.60482
C	5.47783	1.93230	2.13158
H	4.02948	1.96769	0.51810
C	6.09178	1.16514	3.13431
H	6.18767	-0.79065	4.07446
H	5.77086	2.97789	1.98458
H	6.86235	1.60661	3.77539
C	4.67683	-1.67449	-0.96213
C	5.62863	-0.61965	-1.11264
C	4.98305	-2.91532	-1.60448
C	6.81485	-0.82200	-1.82980
H	5.42172	0.36022	-0.68620
C	6.17479	-3.10952	-2.30653
H	4.25596	-3.72815	-1.50295
C	7.10653	-2.06138	-2.42454
H	7.52442	0.00807	-1.92640
H	6.37887	-4.08192	-2.76895
H	8.04010	-2.20634	-2.97815
N	3.46422	-1.66212	-0.28618

17_{BCN}-BpinBu

SCF (BP86) Energy = -2777.32932966
Enthalpy 0K = -2776.037771
Enthalpy 298K = -2775.959928
Free Energy 298K = -2776.148744
Lowest Frequency = 13.8896 cm^{-1}
Second Frequency = 19.1549 cm^{-1}
SCF (BP86-D3BJ) Energy = -2777.74146040
SCF (Toluene) Energy = -2777.33835846
SCF (BS2) Energy = -2977.24595430

Mg	0.77265	0.10147	-0.46418
O	-0.54156	-1.21955	3.63344
O	0.22273	-0.34635	1.62164
O	-2.90645	1.76441	-2.11295
O	-0.80683	0.74499	-1.63850
N	1.63167	-1.70680	-1.24078
N	2.57745	1.29398	-0.71250
C	3.03604	-2.62914	-3.11253
H	2.50656	-3.57756	-2.95866
H	4.10612	-2.79490	-2.89851
H	2.96861	-2.34702	-4.17686
C	2.49697	-1.49031	-2.25017
C	3.01113	-0.21410	-2.61977
H	3.54537	-0.22581	-3.57472
C	3.15578	0.99938	-1.91041
C	4.01685	2.03494	-2.63632
H	4.83242	1.56015	-3.20315
H	4.44308	2.78649	-1.95935
H	3.38096	2.56427	-3.37033
C	3.27435	2.30037	0.07697
C	4.50419	1.93317	0.72097
C	5.19566	2.89536	1.48275
H	6.13878	2.61367	1.96278
C	4.71253	4.19729	1.63676
H	5.26656	4.93003	2.23286
C	3.51400	4.55036	1.01309
H	3.13557	5.57187	1.12016
C	2.78186	3.63514	0.22880
C	1.53141	4.15778	-0.48270
H	0.93238	3.28509	-0.79420
C	1.92132	4.95459	-1.75196
H	2.52265	5.83915	-1.47642
H	1.01972	5.31010	-2.28011
H	2.51644	4.35512	-2.45762
C	0.64066	5.05335	0.40707
H	1.12853	6.01751	0.63401
H	0.37633	4.57396	1.36152
H	-0.30087	5.28485	-0.11669
C	5.13557	0.54020	0.59765
H	4.36434	-0.14297	0.20169
C	6.32406	0.53714	-0.39472
H	7.11799	1.22372	-0.05053
H	6.02399	0.85091	-1.40525
H	6.76138	-0.47405	-0.46901
C	5.62253	-0.01811	1.95517
H	6.48400	0.55077	2.34610
H	5.95954	-1.06196	1.83372
H	4.83382	0.00066	2.72376
C	1.38904	-3.09734	-0.89262
C	2.28112	-3.76337	0.00078
C	2.08234	-5.13217	0.27203
H	2.77487	-5.64575	0.94795
C	1.03039	-5.84699	-0.30736
H	0.90083	-6.91382	-0.09751
C	0.13961	-5.17793	-1.15255
H	-0.69343	-5.73144	-1.59731
C	0.28422	-3.80871	-1.45210
C	3.45361	-3.06117	0.68717
H	3.37696	-1.98360	0.46155
C	4.81302	-3.56809	0.15205
H	4.93664	-4.64748	0.35035
H	5.64935	-3.04095	0.64369
H	4.90820	-3.41688	-0.93512
C	3.39561	-3.23095	2.22300
H	2.42021	-2.91656	2.63023
H	4.18346	-2.62974	2.70799
H	3.55345	-4.28191	2.52187
C	-0.73121	-3.16385	-2.39888
H	-0.63007	-2.06887	-2.29740
C	-2.19261	-3.53157	-2.05753
H	-2.88302	-2.99924	-2.73217
H	-2.46347	-3.25613	-1.02573
H	-2.38737	-4.61068	-2.18371
C	-0.44097	-3.54119	-3.87219
H	0.56060	-3.21777	-4.19695
H	-1.18350	-3.07715	-4.54493
H	-0.50253	-4.63534	-4.01032

C	-0.84252	1.19178	-3.06905
C	-0.12338	0.20331	-3.98460
H	-0.25862	0.52531	-5.03256
H	-0.52304	-0.81472	-3.89253
H	0.95973	0.17991	-3.78026
C	-0.16135	2.56199	-3.14893
H	0.87433	2.48099	-2.78456
H	-0.69833	3.30272	-2.53595
H	-0.12451	2.92709	-4.18924
C	-2.39190	1.28800	-3.35476
C	-3.03268	-0.07860	-3.67869
H	-2.76947	-0.82346	-2.91181
H	-2.73682	-0.45955	-4.67123
H	-4.12753	0.04041	-3.66103
C	-2.75886	2.29958	-4.45181
H	-2.28915	2.04150	-5.41705
H	-2.46320	3.32168	-4.17119
H	-3.85183	2.29399	-4.59463
C	0.62769	0.62615	2.72700
C	0.39591	2.04411	2.23281
H	1.16073	2.32077	1.49095
H	0.51027	2.74940	3.07396
H	-0.60825	2.15618	1.79374
C	2.10533	0.34846	3.00220
H	2.26613	-0.67553	3.37496
H	2.50089	1.06172	3.74369
H	2.68267	0.48415	2.07552
C	-0.31703	0.19955	3.90534
C	0.31011	0.33032	5.29733
H	-0.41706	-0.00527	6.05401
H	0.56271	1.38208	5.51389
H	1.21871	-0.28126	5.40158
C	-1.69239	0.87792	3.86354
H	-2.13153	0.82485	2.85575
H	-1.63440	1.93915	4.15351
H	-2.36350	0.36262	4.56930
B	-0.37867	-1.45612	2.29491
B	-2.20505	1.10152	-1.05204
C	-0.81869	-2.82875	1.67230
H	-1.23302	-2.68304	0.65821
H	0.07917	-3.45787	1.51291
C	-1.82551	-3.59604	2.56280
H	-1.39088	-3.72487	3.57187
H	-2.73489	-2.98220	2.71125
C	-2.22454	-4.97048	1.99996
H	-1.31077	-5.57169	1.82933
H	-2.68609	-4.83784	1.00237
C	-3.19051	-5.73662	2.91696
H	-3.46344	-6.71747	2.49130
H	-2.74072	-5.91639	3.90985
H	-4.12522	-5.17034	3.07637
C	-2.91911	0.15085	0.06077
H	-2.34435	-0.61050	0.61576
C	-4.36767	-0.19385	0.00528
C	-4.79208	-1.45367	0.49497
C	-5.35630	0.65204	-0.56063
C	-6.12953	-1.86644	0.40856
H	-4.05006	-2.12098	0.95172
C	-6.69591	0.24399	-0.63274
H	-5.06134	1.62480	-0.96015
C	-7.09485	-1.01545	-0.15352
H	-6.41964	-2.85084	0.79375
H	-7.43803	0.92075	-1.07190
H	-8.14321	-1.32706	-0.21375
C	-3.17377	2.60915	0.84692
C	-2.96413	3.92021	0.34624
C	-4.12826	2.43914	1.88293
C	-3.64797	5.01581	0.88769
H	-2.27087	4.05391	-0.48951
C	-4.81055	3.54256	2.41460
H	-4.34202	1.43186	2.25140
C	-4.57322	4.84057	1.93204
H	-3.46503	6.01723	0.48045
H	-5.54361	3.38132	3.21355
H	-5.10974	5.69795	2.35115
N	-2.40046	1.54668	0.35139

TS(17_{BN}-17_{BCN})

SCF (BP86) Energy = -2208.21455414
Enthalpy 0K = -2207.221271
Enthalpy 298K = -2207.161081
Free Energy 298K = -2207.315888
Lowest Frequency = -127.7457 cm^{-1}
Second Frequency = 13.1916 cm^{-1}
SCF (BP86-D3BJ) Energy = -2208.52581262
SCF (Toluene) Energy = -2208.22232772
SCF (BS2) Energy = -2407.99270097

Mg	0.14554	0.36268	-0.68115
O	-0.28776	-3.47420	-0.68364
O	-0.22007	-1.35583	-1.69611
N	1.82371	1.60409	-0.75510
N	-1.27535	1.87489	-0.89002
C	2.88436	3.69873	-1.63207
H	3.84521	3.16892	-1.58216
H	2.89965	4.48848	-0.86077
H	2.79861	4.20470	-2.60728
C	1.68605	2.77911	-1.41389
C	0.45821	3.30013	-1.89123
H	0.56458	4.22493	-2.46508
C	-0.88174	2.99926	-1.52881
C	-1.88208	4.10719	-1.84600
H	-1.55140	4.67893	-2.72715
H	-1.94316	4.81427	-1.00020
H	-2.89808	3.72671	-2.01868
C	-2.63881	1.86293	-0.39430
C	-2.93700	2.46827	0.86038
C	-4.28135	2.54444	1.27524
H	-4.51571	3.01707	2.23564
C	-5.31563	2.02802	0.49215
H	-6.35581	2.10481	0.82563
C	-5.00633	1.38190	-0.70998
H	-5.81637	0.94632	-1.30192
C	-3.67989	1.27163	-1.17104
C	-3.39335	0.52544	-2.47854
H	-2.38976	0.07270	-2.37166
C	-3.35071	1.45670	-3.71399
H	-4.30400	2.00362	-3.82592
H	-3.19452	0.86628	-4.63492
H	-2.53715	2.19533	-3.65025
C	-4.39924	-0.61730	-2.73364
H	-5.40285	-0.23137	-2.98491
H	-4.49841	-1.27595	-1.85484
H	-4.07357	-1.22879	-3.59160
C	-1.85824	3.00338	1.80506
H	-0.87556	2.81651	1.33638
C	-1.98188	4.52457	2.04992
H	-2.94581	4.77466	2.52709

H	-1.91499	5.10274	1.11334
H	-1.17828	4.87510	2.72126
C	-1.89808	2.24363	3.15146
H	-2.84831	2.42539	3.68321
H	-1.07945	2.57582	3.81249
H	-1.80908	1.15515	3.00328
C	3.08618	1.36140	-0.09038
C	3.34906	1.96056	1.17772
C	4.58704	1.70900	1.80403
H	4.79203	2.16690	2.77823
C	5.55443	0.89561	1.20964
H	6.51208	0.71665	1.70953
C	5.28458	0.30348	-0.02978
H	6.04083	-0.34094	-0.48651
C	4.06260	0.51338	-0.69710
C	2.34631	2.86293	1.90244
H	1.45418	2.96662	1.26069
C	2.91615	4.27924	2.15304
H	3.77055	4.24905	2.85193
H	2.14546	4.93080	2.60027
H	3.26819	4.75574	1.22334
C	1.89823	2.23863	3.24386
H	1.42508	1.25265	3.10324
H	1.17445	2.89755	3.75375
H	2.75623	2.09867	3.92444
C	3.81054	-0.15402	-2.05182
H	2.73948	-0.43566	-2.06525
C	4.64367	-1.43455	-2.26463
H	4.29403	-1.96745	-3.16554
H	4.57535	-2.12539	-1.40885
H	5.70988	-1.19882	-2.43031
C	4.03965	0.79926	-3.24966
H	3.34623	1.65266	-3.24153
H	3.89334	0.25779	-4.20125
H	5.07205	1.19142	-3.24228
C	-0.09807	-2.36457	-2.76921
C	0.87582	-1.86650	-3.83703
H	0.98624	-2.62726	-4.62889
H	1.87218	-1.65542	-3.42471
H	0.48914	-0.94770	-4.30986
C	-1.49038	-2.55691	-3.38542
H	-1.83797	-1.60204	-3.80907
H	-2.21835	-2.88991	-2.62934
H	-1.46426	-3.30033	-4.19941
C	0.38383	-3.63539	-1.95488
C	1.89853	-3.64929	-1.69077
H	2.23202	-2.69693	-1.24958
H	2.47919	-3.84177	-2.60853
H	2.11997	-4.44615	-0.96355
C	-0.05818	-4.97343	-2.56088
H	0.35473	-5.10758	-3.57575
H	-1.15442	-5.05342	-2.60868
H	0.31356	-5.79803	-1.93137
B	-0.42565	-2.10372	-0.40839
C	0.23042	-1.25724	1.06487
H	0.37890	-0.20373	1.42641
C	1.02970	-2.15419	1.96131
C	2.26744	-1.69052	2.46959
C	0.63106	-3.46988	2.29586
C	3.07278	-2.50352	3.27822
H	2.60887	-0.67994	2.21437
C	1.43843	-4.27959	3.11001
H	-0.31460	-3.86208	1.91458
C	2.66216	-3.80616	3.60874
H	4.02626	-2.11376	3.65213
H	1.10015	-5.29187	3.35906
H	3.28687	-4.44153	4.24547
C	-2.21746	-1.96139	1.55423
C	-3.34114	-2.62613	1.01155
C	-2.18160	-1.69845	2.94132
C	-4.40791	-3.00071	1.83811
H	-3.36100	-2.84908	-0.06023
C	-3.25614	-2.07789	3.75925
H	-1.29628	-1.22020	3.37135
C	-4.37683	-2.72721	3.21694
H	-5.27111	-3.51477	1.40061
H	-3.20972	-1.86965	4.83394
H	-5.21195	-3.02315	3.85974
N	-1.17702	-1.53777	0.70093

17_{BCN}

SCF (BP86) Energy = -2208.23727553
Enthalpy 0K = -2207.242482
Enthalpy 298K = -2207.182069
Free Energy 298K = -2207.336604
Lowest Frequency = 11.9617 cm^{-1}
Second Frequency = 15.7536 cm^{-1}
SCF (BP86-D3BJ) Energy = -2208.55313127
SCF (Toluene) Energy = -2208.24412220
SCF (BS2) Energy = -2408.01367666

Mg	0.40988	0.40678	0.50792
O	-1.01289	-3.03280	1.28679
O	-0.49444	-0.81427	1.93196
N	-0.42445	2.31602	0.60524
N	2.42221	1.00053	0.32770
C	-0.18525	4.75470	1.08751
H	-1.23656	4.75683	1.40762
H	-0.13946	5.28138	0.11759
H	0.41496	5.33714	1.80400
C	0.38051	3.34592	0.94016
C	1.78694	3.25557	1.09381
H	2.25486	4.19466	1.40444
C	2.72197	2.27381	0.67570
C	4.15237	2.80690	0.59947
H	4.18065	3.73194	0.00053
H	4.85511	2.08724	0.16153
H	4.50216	3.07389	1.61178
C	3.45666	0.19770	-0.30100
C	3.46537	0.10640	-1.72843
C	4.46078	-0.66707	-2.35469
H	4.46952	-0.74208	-3.44563
C	5.43904	-1.33956	-1.61508
H	6.20799	-1.93105	-2.12319
C	5.42190	-1.24978	-0.22183
H	6.18826	-1.77435	0.35923
C	4.44487	-0.49685	0.46269
C	4.52775	-0.46007	1.99276
H	3.62027	0.04847	2.36609
C	5.76201	0.32600	2.50083
H	6.69500	-0.15457	2.15696
H	5.78069	0.33725	3.60499
H	5.77637	1.36807	2.15050
C	4.58339	-1.88461	2.59548
H	5.55678	-2.36296	2.38938
H	3.80011	-2.54046	2.18728
H	4.46746	-1.84486	3.69255
C	2.45938	0.86972	-2.59560

H	1.50586	0.92478	-2.03511
C	2.92598	2.32443	-2.84510
H	3.90467	2.33208	-3.35693
H	3.02555	2.89474	-1.90873
H	2.20302	2.85544	-3.48949
C	2.16168	0.18010	-3.94160
H	3.01966	0.25128	-4.63414
H	1.31076	0.67836	-4.43506
H	1.90387	-0.88251	-3.81218
C	-1.79137	2.62337	0.24850
C	-2.08854	3.07879	-1.06986
C	-3.42803	3.35704	-1.40657
H	-3.66205	3.70189	-2.42004
C	-4.45947	3.20527	-0.47524
H	-5.49385	3.43584	-0.75141
C	-4.15928	2.74669	0.81333
H	-4.97164	2.61714	1.53444
C	-2.84016	2.43864	1.20097
C	-1.01418	3.24567	-2.14698
H	-0.02951	3.08535	-1.67502
C	-1.01312	4.66334	-2.76335
H	-1.94270	4.86314	-3.32478
H	-0.17206	4.77441	-3.46972
H	-0.91746	5.44722	-1.99314
C	-1.18227	2.18034	-3.25455
H	-1.10320	1.15814	-2.84868
H	-0.40770	2.30125	-4.03234
H	-2.16699	2.27049	-3.74615
C	-2.56331	1.92195	2.61645
H	-1.69024	1.24839	2.54865
C	-3.73582	1.09848	3.18884
H	-3.43329	0.61802	4.13526
H	-4.06191	0.31045	2.49006
H	-4.61139	1.72964	3.42414
C	-2.20293	3.06129	3.59967
H	-1.28117	3.58646	3.30566
H	-2.04668	2.65592	4.61522
H	-3.01815	3.80488	3.65598
C	-0.19410	-1.70054	3.06644
C	-0.56464	-0.98766	4.36939
H	-0.41479	-1.66006	5.23208
H	-1.61275	-0.65599	4.36412
H	0.07785	-0.10283	4.51811
C	1.30459	-2.00654	3.03206
H	1.87336	-1.06289	3.07034
H	1.56609	-2.53960	2.10384
H	1.62123	-2.62300	3.88974
C	-1.07109	-2.97917	2.72833
C	-2.54264	-2.82176	3.16464
H	-2.96798	-1.87288	2.80098
H	-2.65595	-2.86259	4.26145
H	-3.12831	-3.64383	2.72326
C	-0.50374	-4.29327	3.28027
H	-0.43468	-4.26743	4.38168
H	0.49229	-4.50962	2.86569
H	-1.17257	-5.12394	3.00168
B	-1.08056	-1.68209	0.83579
C	-2.11960	-1.02616	-0.17935
H	-2.38869	0.03769	-0.10689
C	-3.17318	-1.80588	-0.88996
C	-4.31226	-1.12062	-1.37663
C	-3.12655	-3.21285	-1.04999
C	-5.36923	-1.80918	-1.99036
H	-4.36501	-0.03101	-1.26278
C	-4.17717	-3.89660	-1.67779
H	-2.27003	-3.76888	-0.66010
C	-5.30408	-3.20260	-2.15016
H	-6.24162	-1.25339	-2.35223
H	-4.11741	-4.98468	-1.79306
H	-6.12333	-3.74318	-2.63640
C	-0.16128	-1.96420	-1.65309
C	0.94668	-2.82646	-1.48581
C	-0.78891	-1.90387	-2.91805
C	1.42134	-3.59475	-2.55811
H	1.42507	-2.89470	-0.50380
C	-0.31571	-2.68538	-3.98263
H	-1.66005	-1.25755	-3.05310
C	0.79139	-3.53336	-3.81312
H	2.28386	-4.25268	-2.40673
H	-0.82021	-2.62886	-4.95339
H	1.15679	-4.14156	-4.64688
N	-0.59747	-1.16519	-0.55549

TS(17_{BCN}-17_{BC})

SCF (BP86) Energy = -2208.22936077
Enthalpy 0K = -2207.235016
Enthalpy 298K = -2207.175013
Free Energy 298K = -2207.328105
Lowest Frequency = -87.0444 cm^{-1}
Second Frequency = 13.5824 cm^{-1}
SCF (BP86-D3BJ) Energy = -2208.54623642
SCF (Toluene) Energy = -2208.23625006
SCF (BS2) Energy = -2408.00663807

Mg	0.35809	0.40345	0.38198
O	-1.68228	-2.64552	1.88964
O	-0.83808	-0.47076	2.02869
N	-0.48667	2.32142	0.28322
N	2.38248	1.02527	0.32807
C	-0.29179	4.79941	0.52562
H	-1.37050	4.82605	0.73096
H	-0.14293	5.22655	-0.48260
H	0.23249	5.45546	1.23810
C	0.28341	3.38802	0.57404
C	1.67457	3.33015	0.84508
H	2.11044	4.30050	1.10121
C	2.64491	2.32731	0.59240
C	4.07646	2.86278	0.60362
H	4.13499	3.81024	0.04468
H	4.79731	2.15580	0.17345
H	4.38135	3.08351	1.64173
C	3.46523	0.19995	-0.18158
C	3.54862	0.00035	-1.59636
C	4.58392	-0.80142	-2.11189
H	4.64674	-0.95926	-3.19194
C	5.53069	-1.40349	-1.27687
H	6.32950	-2.02163	-1.70015
C	5.44485	-1.20518	0.10221
H	6.18871	-1.66981	0.75896
C	4.42848	-0.41353	0.67744
C	4.45015	-0.25104	2.20111
H	3.55253	0.32394	2.49321
C	5.69539	0.52677	2.69469
H	6.62010	-0.02585	2.45230
H	5.66086	0.65144	3.79154
H	5.77770	1.52509	2.24040
C	4.41972	-1.62363	2.91631
H	5.37679	-2.15702	2.78179

H	3.62414	-2.27706	2.52753
H	4.26930	-1.49398	4.00262
C	2.57990	0.67926	-2.56958
H	1.59444	0.74748	-2.06945
C	3.03478	2.12445	-2.88768
H	4.03854	2.11881	-3.34858
H	3.07600	2.75555	-1.98613
H	2.33801	2.59921	-3.60120
C	2.37113	-0.10432	-3.88058
H	3.27168	-0.07696	-4.52026
H	1.55512	0.35592	-4.46163
H	2.10445	-1.15620	-3.69284
C	-1.83999	2.56508	-0.16537
C	-2.09352	2.75345	-1.55624
C	-3.41980	2.95740	-1.98549
H	-3.61695	3.09700	-3.05439
C	-4.48321	2.99773	-1.07808
H	-5.50608	3.16979	-1.42945
C	-4.22496	2.81693	0.28528
H	-5.05710	2.85041	0.99663
C	-2.92087	2.58900	0.76787
C	-0.98051	2.74284	-2.60537
H	-0.01862	2.62273	-2.07709
C	-0.91842	4.07423	-3.38944
H	-1.83075	4.23214	-3.99125
H	-0.06014	4.07283	-4.08391
H	-0.81150	4.94141	-2.71598
C	-1.14033	1.54987	-3.57421
H	-1.07671	0.58541	-3.04363
H	-0.34978	1.56766	-4.34446
H	-2.11268	1.58609	-4.09633
C	-2.71536	2.39036	2.27208
H	-1.70075	1.98132	2.41400
C	-3.71860	1.37080	2.85353
H	-3.47766	1.15667	3.90992
H	-3.70165	0.42379	2.29067
H	-4.75369	1.75467	2.83486
C	-2.81701	3.72057	3.05619
H	-2.05482	4.45024	2.74009
H	-2.68232	3.54243	4.13797
H	-3.80859	4.18612	2.91370
C	-0.34049	-1.19701	3.22208
C	-0.41859	-0.25644	4.42546
H	-0.11364	-0.78389	5.34565
H	-1.43538	0.13700	4.56788
H	0.26560	0.59736	4.28505
C	1.10981	-1.58821	2.93596
H	1.70554	-0.67922	2.74598
H	1.17828	-2.24490	2.05273
H	1.56649	-2.10584	3.79405
C	-1.30255	-2.45194	3.28205
C	-2.59897	-2.19718	4.07193
H	-3.09880	-1.27423	3.74016
H	-2.40884	-2.12595	5.15625
H	-3.28874	-3.03795	3.89584
C	-0.63705	-3.74048	3.78326
H	-0.27825	-3.62421	4.82054
H	0.20787	-4.03998	3.14598
H	-1.37603	-4.55782	3.77016
B	-1.50494	-1.45508	1.20298
C	-2.00123	-1.10756	-0.24225
H	-2.35912	-0.07461	-0.41286
C	-3.01159	-2.05686	-0.84563
C	-4.17461	-1.52294	-1.44296
C	-2.87518	-3.46315	-0.79269
C	-5.17477	-2.35990	-1.96266
H	-4.29311	-0.43392	-1.49726
C	-3.86956	-4.29910	-1.31989
H	-1.98671	-3.90155	-0.33152
C	-5.02447	-3.75417	-1.90596
H	-6.06908	-1.91978	-2.41775
H	-3.74070	-5.38605	-1.27202
H	-5.79894	-4.41139	-2.31594
C	-0.00205	-2.10040	-1.51662
C	1.25568	-2.72459	-1.28857
C	-0.64868	-2.38380	-2.75279
C	1.83658	-3.57653	-2.23588
H	1.77487	-2.52503	-0.34376
C	-0.06697	-3.24874	-3.69099
H	-1.61251	-1.91929	-2.97380
C	1.17649	-3.85569	-3.44613
H	2.80994	-4.03137	-2.02079
H	-0.59493	-3.44393	-4.63164
H	1.62275	-4.53149	-4.18282
N	-0.50040	-1.21993	-0.54117

TS(18_{BN}-18_{BCN})

SCF (BP86) Energy = -2439.26021924
Enthalpy 0K = -2438.188280
Enthalpy 298K = -2438.123378
Free Energy 298K = -2438.285815
Lowest Frequency = -155.4803 cm^{-1}
Second Frequency = 13.1197 cm^{-1}
SCF (BP86-D3BJ) Energy = -2439.62063283
SCF (Toluene) Energy = -2439.26702349
SCF (BS2) Energy = -2639.08927379

Mg	-0.65235	0.08171	0.21772
O	1.07860	-0.00056	1.42020
O	3.37955	-0.19532	1.85367
N	-1.90571	1.71794	0.65060
N	-2.05490	-1.42776	0.65158
N	2.80599	0.75315	-0.38519
C	-3.31599	2.63979	2.50477
H	-4.41519	2.58434	2.43452
H	-2.99381	3.62170	2.13148
H	-3.06227	2.56175	3.57618
C	-2.65753	1.49126	1.74745
C	-2.90884	0.20133	2.29434
H	-3.45689	0.22889	3.24161
C	-2.78736	-1.10643	1.74504
C	-3.51270	-2.18847	2.54255
H	-2.84825	-2.54315	3.35217
H	-3.77636	-3.05836	1.92649
H	-4.42410	-1.79386	3.01701
C	-2.05352	2.97218	-0.05383
C	-3.26059	3.25310	-0.77096
C	-3.35750	4.45387	-1.50253
H	-4.28274	4.66526	-2.05010
C	-2.30875	5.37479	-1.55054
H	-2.40544	6.29955	-2.12884
C	-1.13562	5.09926	-0.84296
H	-0.31467	5.82247	-0.86327
C	-0.98424	3.91902	-0.08908
C	-4.46951	2.31394	-0.81256
H	-4.24667	1.42310	-0.20131
C	-5.74036	2.98323	-0.23568
H	-5.57566	3.38250	0.77811

H	-6.57101	2.25746	-0.18859
H	-6.07167	3.82431	-0.86982
C	-4.74697	1.83735	-2.25591
H	-4.94867	2.68944	-2.92789
H	-5.63312	1.17984	-2.28121
H	-3.89075	1.27850	-2.66757
C	0.28552	3.75501	0.74362
H	0.40041	2.68303	0.98461
C	0.13914	4.52798	2.07758
H	-0.01357	5.60360	1.87946
H	1.04754	4.42466	2.69626
H	-0.72155	4.17333	2.66945
C	1.56426	4.21124	0.01294
H	1.66650	3.74438	-0.97996
H	2.45954	3.93765	0.59404
H	1.59013	5.30664	-0.12370
C	-2.30581	-2.72307	0.04009
C	-3.43455	-2.87155	-0.82801
C	-3.73333	-4.14702	-1.34613
H	-4.60685	-4.26611	-1.99413
C	-2.94137	-5.26253	-1.05918
H	-3.19780	-6.24639	-1.46589
C	-1.80835	-5.09716	-0.26151
H	-1.17284	-5.96283	-0.04729
C	-1.46367	-3.84635	0.29079
C	-4.33373	-1.69764	-1.22755
H	-3.72854	-0.77796	-1.13035
C	-5.56672	-1.55602	-0.30283
H	-6.16065	-2.48751	-0.30115
H	-6.22238	-0.74023	-0.65622
H	-5.28341	-1.32977	0.73640
C	-4.80904	-1.80641	-2.69456
H	-3.97421	-2.02542	-3.38011
H	-5.27970	-0.86302	-3.01462
H	-5.56621	-2.59969	-2.82340
C	-0.21409	-3.78901	1.16967
H	0.00827	-2.72421	1.36374
C	-0.45305	-4.49155	2.52801
H	-1.30821	-4.06057	3.07378
H	0.44103	-4.41708	3.17187
H	-0.66583	-5.56445	2.37647
C	1.01588	-4.41368	0.47222
H	0.86276	-5.48592	0.26201
H	1.90982	-4.33838	1.11324
H	1.24324	-3.91075	-0.47951
C	2.47333	-0.53666	-1.02581
C	3.59120	-1.44460	-1.43882
C	4.70241	-1.69124	-0.58983
H	4.73025	-1.23198	0.40116
C	5.76562	-2.50811	-0.99587
H	6.60370	-2.67448	-0.30920
C	5.76652	-3.11479	-2.26279
H	6.59634	-3.75812	-2.57390
C	4.69114	-2.86465	-3.12903
H	4.68160	-3.29968	-4.13512
C	3.63287	-2.03584	-2.72944
H	2.83262	-1.82331	-3.44526
C	1.19177	-0.54591	-1.71390
C	0.38951	0.65285	-1.81410
H	0.83379	1.59118	-1.45857
C	-0.81915	0.67963	-2.55336
H	-1.35039	1.63330	-2.64770
C	-1.32738	-0.48028	-3.14868
H	-2.25561	-0.45570	-3.72519
C	-0.60850	-1.68817	-2.97886
H	-1.00370	-2.61780	-3.40243
C	0.59500	-1.72898	-2.27771
H	1.12862	-2.67878	-2.19402
C	3.90241	1.55698	-0.74867
C	4.61840	2.28904	0.22915
H	4.36165	2.15831	1.28459
C	5.66487	3.14170	-0.14932
H	6.20767	3.69817	0.62342
C	6.03130	3.27472	-1.49899
H	6.85305	3.93701	-1.78945
C	5.33462	2.53327	-2.46921
H	5.61235	2.61712	-3.52594
C	4.28347	1.68231	-2.10536
H	3.75043	1.10170	-2.86411
C	1.27340	-0.00115	2.90564
C	2.70801	-0.64297	3.04883
C	0.17186	-0.79617	3.60135
H	-0.80872	-0.30678	3.47438
H	0.38830	-0.83750	4.68326
H	0.10154	-1.82750	3.22990
C	1.22900	1.46132	3.36643
H	2.01715	2.06032	2.88285
H	1.35401	1.53558	4.45938
H	0.25156	1.89685	3.10789
C	3.50142	-0.13276	4.26051
H	4.49062	-0.61829	4.27647
H	2.98748	-0.37885	5.20574
H	3.66030	0.95485	4.21519
C	2.70019	-2.17984	3.04364
H	2.13580	-2.56409	2.18179
H	2.27054	-2.59613	3.97021
H	3.73860	-2.53687	2.95351
B	2.45522	0.06217	0.82566

18_{BCN}

SCF (BP86) Energy = -2439.27004036
Enthalpy 0K = -2438.196938
Enthalpy 298K = -2438.131944
Free Energy 298K = -2438.293696
Lowest Frequency = 19.0957 cm^{-1}
Second Frequency = 23.4392 cm^{-1}
SCF (BP86-D3BJ) Energy = -2439.63687215
SCF (Toluene) Energy = -2439.27663597
SCF (BS2) Energy = -2639.09819571

Mg	0.23541	-0.51658	0.49408
O	0.35957	1.16192	1.68552
O	-1.71683	2.24802	1.66440
N	-1.12584	-2.11679	0.84603
N	1.98709	-1.65902	0.51795
N	-0.66536	1.13426	-0.56231
C	-1.48137	-4.28120	2.06738
H	-1.38324	-5.14373	1.38552
H	-2.54688	-4.02277	2.11820
H	-1.13957	-4.61621	3.06028
C	-0.60679	-3.12637	1.58155
C	0.76751	-3.28372	1.90752
H	0.95822	-4.12589	2.57753
C	1.94215	-2.75316	1.31538
C	3.21266	-3.55014	1.58543
H	3.98924	-2.93200	2.06108
H	3.64769	-3.91307	0.63870
H	3.00659	-4.41664	2.22960

C	-2.46040	-2.35530	0.31760
C	-2.60376	-3.18176	-0.83675
C	-3.89598	-3.46901	-1.31887
H	-4.00260	-4.10111	-2.20752
C	-5.03706	-2.97548	-0.68492
H	-6.03485	-3.22108	-1.06374
C	-4.88941	-2.15174	0.43587
H	-5.78407	-1.75469	0.92378
C	-3.62216	-1.81357	0.95023
C	-1.41427	-3.76976	-1.60033
H	-0.48952	-3.47773	-1.07363
C	-1.45539	-5.31491	-1.65344
H	-1.50884	-5.76410	-0.64792
H	-0.55155	-5.70667	-2.15192
H	-2.33017	-5.67470	-2.22329
C	-1.34988	-3.19560	-3.03380
H	-2.25565	-3.45938	-3.60756
H	-0.48229	-3.60936	-3.57743
H	-1.27317	-2.09597	-3.02868
C	-3.54709	-0.89785	2.17643
H	-2.64642	-0.26689	2.05617
C	-3.41289	-1.69390	3.49744
H	-4.26004	-2.39347	3.61211
H	-3.42583	-1.01074	4.36572
H	-2.48035	-2.27643	3.54384
C	-4.75021	0.06293	2.29921
H	-4.96009	0.59349	1.35632
H	-4.54559	0.82106	3.07250
H	-5.67018	-0.46782	2.60265
C	3.25399	-1.39450	-0.13591
C	3.45026	-1.84463	-1.47590
C	4.71435	-1.67674	-2.07605
H	4.87324	-2.04609	-3.09507
C	5.76964	-1.06061	-1.39522
H	6.74900	-0.94986	-1.87276
C	5.55102	-0.57133	-0.10405
H	6.36506	-0.05912	0.42067
C	4.30935	-0.71725	0.54562
C	2.34553	-2.53071	-2.28137
H	1.39474	-2.37906	-1.73932
C	2.58180	-4.05589	-2.37749
H	3.54242	-4.27417	-2.87707
H	1.78005	-4.54087	-2.96203
H	2.60509	-4.52660	-1.38059
C	2.19101	-1.91678	-3.69092
H	2.04447	-0.82439	-3.64404
H	1.32181	-2.35541	-4.20868
H	3.07754	-2.10679	-4.32077
C	4.15482	-0.09956	1.93862
H	3.15199	-0.36682	2.31733
C	5.20581	-0.61242	2.95172
H	5.20653	-1.71107	3.04999
H	5.00883	-0.18660	3.95112
H	6.22630	-0.30684	2.66151
C	4.24032	1.44165	1.84473
H	5.20163	1.75316	1.40136
H	4.17392	1.89603	2.84835
H	3.43342	1.85465	1.22038
C	-0.05547	2.60490	-0.52021
C	-0.88841	3.64298	-1.25069
C	-2.10267	4.14316	-0.72458
H	-2.45359	3.77203	0.24161
C	-2.84802	5.10759	-1.42001
H	-3.78149	5.48279	-0.98547
C	-2.40431	5.59697	-2.65827
H	-2.98604	6.35337	-3.19633
C	-1.20555	5.10588	-3.19914
H	-0.84708	5.47299	-4.16730
C	-0.46187	4.14068	-2.50544
H	0.47462	3.77279	-2.93602
C	1.41194	2.70811	-0.82846
C	2.14140	1.71589	-1.51188
H	1.63261	0.79229	-1.81100
C	3.49494	1.90185	-1.84312
H	4.03342	1.10819	-2.37032
C	4.15006	3.09140	-1.49464
H	5.20319	3.23961	-1.75524
C	3.44161	4.08865	-0.80034
H	3.94117	5.02193	-0.51730
C	2.09377	3.89794	-0.47042
H	1.54007	4.69176	0.04324
C	-1.73384	0.90590	-1.49085
C	-3.07976	0.85693	-1.07997
H	-3.31364	1.02736	-0.02648
C	-4.09810	0.61803	-2.01583
H	-5.13857	0.57211	-1.67776
C	-3.79244	0.44717	-3.37435
H	-4.59026	0.26724	-4.10219
C	-2.45311	0.51834	-3.79394
H	-2.20152	0.39996	-4.85353
C	-1.43063	0.74232	-2.86136
H	-0.38742	0.81215	-3.18659
C	0.08327	1.52520	3.07912
C	-1.10555	2.58607	2.93309
C	1.35083	2.11294	3.71188
H	2.11801	1.32891	3.81363
H	1.13176	2.50070	4.72228
H	1.77175	2.92677	3.10499
C	-0.29850	0.24208	3.83062
H	-1.20742	-0.21881	3.42027
H	-0.45956	0.43417	4.90482
H	0.52472	-0.48911	3.74327
C	-2.16839	2.48120	4.03261
H	-2.97412	3.20697	3.83422
H	-1.73678	2.71526	5.02113
H	-2.61458	1.47669	4.07564
C	-0.60187	4.04444	2.85258
H	0.14754	4.16777	2.05454
H	-0.16162	4.38572	3.80422
H	-1.45612	4.69835	2.61388
B	-0.63027	1.88642	0.79570

TS(18_{BCN}-18_{BC})

SCF (BP86) Energy = -2439.26143864
Enthalpy 0K = -2438.189083
Enthalpy 298K = -2438.124421
Free Energy 298K = -2438.285076
Lowest Frequency = -133.4255 cm^{-1}
Second Frequency = 19.9829 cm^{-1}
SCF (BP86-D3BJ) Energy = -2439.62560732
SCF (Toluene) Energy = -2439.26840736
SCF (BS2) Energy = -2639.09002504

Mg	-0.29675	-0.37980	0.42420
O	1.07138	0.63523	1.70258
O	0.80788	2.94812	1.59056
N	-2.36300	-0.44446	0.92252
N	0.01242	-2.45280	0.59735

N	0.50585	1.13402	-0.78125
C	-3.93857	-1.25767	2.68396
H	-4.79752	-1.63291	2.10307
H	-4.16976	-0.21133	2.93773
H	-3.87297	-1.84790	3.61061
C	-2.63855	-1.35954	1.89069
C	-1.82569	-2.46978	2.21719
H	-2.22233	-3.08820	3.02768
C	-0.75552	-3.08450	1.50199
C	-0.59322	-4.57160	1.79675
H	-0.60331	-4.74918	2.88488
H	0.32357	-4.99777	1.37069
H	-1.45430	-5.12037	1.37578
C	-3.53300	0.23818	0.39974
C	-4.41044	-0.48309	-0.47178
C	-5.59370	0.13391	-0.92006
H	-6.26811	-0.42728	-1.57679
C	-5.92138	1.44396	-0.55631
H	-6.85050	1.90412	-0.90873
C	-5.03169	2.16462	0.24418
H	-5.26638	3.20089	0.51066
C	-3.83595	1.59355	0.72678
C	-4.09278	-1.88542	-1.00059
H	-3.11792	-2.19184	-0.58548
C	-5.13767	-2.94152	-0.57372
H	-5.20492	-3.03797	0.52263
H	-4.87026	-3.93225	-0.98111
H	-6.14424	-2.68827	-0.95109
C	-3.96415	-1.85429	-2.54173
H	-4.92346	-1.58610	-3.01846
H	-3.67204	-2.84696	-2.92621
H	-3.21198	-1.11666	-2.86667
C	-2.92569	2.47446	1.58157
H	-1.96919	1.93916	1.71015
C	-3.54170	2.72753	2.97782
H	-4.53475	3.20080	2.88298
H	-2.90878	3.40743	3.57499
H	-3.67191	1.79400	3.55130
C	-2.59823	3.81899	0.89221
H	-2.23465	3.66414	-0.13671
H	-1.81233	4.34983	1.45437
H	-3.48227	4.47883	0.84224
C	1.04118	-3.20323	-0.09132
C	0.82503	-3.61274	-1.43857
C	1.83678	-4.33583	-2.10155
H	1.66638	-4.66141	-3.13382
C	3.03583	-4.66754	-1.46314
H	3.80402	-5.24389	-1.98973
C	3.24109	-4.25533	-0.14233
H	4.18192	-4.50714	0.35939
C	2.27113	-3.51770	0.56366
C	-0.49352	-3.36726	-2.17241
H	-1.13030	-2.74100	-1.52254
C	-1.23603	-4.70611	-2.39782
H	-0.64689	-5.38244	-3.04206
H	-2.20889	-4.53823	-2.89167
H	-1.41981	-5.23074	-1.44495
C	-0.29607	-2.61603	-3.50731
H	0.16958	-1.62731	-3.35766
H	-1.26767	-2.45348	-4.00351
H	0.34103	-3.18753	-4.20503
C	2.59365	-3.09498	2.00017
H	1.72530	-2.53706	2.39249
C	2.83988	-4.30877	2.92804
H	1.98730	-5.00667	2.94186
H	3.01780	-3.96859	3.96348
H	3.73166	-4.87786	2.61156
C	3.81709	-2.15259	2.03506
H	4.71303	-2.64981	1.62551
H	4.04705	-1.85865	3.07431
H	3.64221	-1.24072	1.44386
C	1.89544	1.72881	-0.55399
C	2.10534	3.10167	-1.21394
C	1.11294	4.10589	-1.11320
H	0.18621	3.89691	-0.57414
C	1.29162	5.36842	-1.69299
H	0.50165	6.12107	-1.59375
C	2.46787	5.67021	-2.39848
H	2.60714	6.65780	-2.85113
C	3.45610	4.68389	-2.52077
H	4.37702	4.89182	-3.07704
C	3.27418	3.41717	-1.94112
H	4.05748	2.66403	-2.06166
C	3.07504	0.78822	-0.72328
C	3.01166	-0.36754	-1.52467
H	2.06411	-0.62999	-2.00586
C	4.14556	-1.17296	-1.72555
H	4.06563	-2.06369	-2.35587
C	5.36646	-0.84289	-1.11821
H	6.25142	-1.46775	-1.27875
C	5.44050	0.29316	-0.29382
H	6.38474	0.55848	0.19472
C	4.30633	1.09403	-0.09603
H	4.37994	1.99761	0.52022
C	-0.14951	1.40371	-2.01660
C	-1.55825	1.51991	-2.06257
H	-2.12833	1.48903	-1.13113
C	-2.23906	1.68999	-3.27839
H	-3.33085	1.77796	-3.26603
C	-1.53120	1.76589	-4.48795
H	-2.05904	1.90734	-5.43646
C	-0.12952	1.66807	-4.45649
H	0.44513	1.73057	-5.38754
C	0.55553	1.49046	-3.24695
H	1.64572	1.42009	-3.25014
C	1.02164	1.08913	3.11022
C	1.18575	2.67193	2.96767
C	2.16958	0.41223	3.86928
H	1.98925	-0.67311	3.92803
H	2.22854	0.80018	4.90095
H	3.13896	0.56997	3.37658
C	-0.30898	0.63797	3.72376
H	-1.17755	1.09109	3.22608
H	-0.35213	0.89596	4.79520
H	-0.40276	-0.45889	3.63944
C	0.28108	3.48801	3.89635
H	0.42787	4.56160	3.69521
H	0.53295	3.30273	4.95464
H	-0.78123	3.25229	3.74246
C	2.64347	3.15173	3.13379
H	3.32996	2.59824	2.47303
H	2.99901	3.04688	4.17240
H	2.69360	4.21554	2.85270
B	1.15716	1.81746	0.83573

TS(18_{BC}-18_{BPh})

SCF (BP86) Energy = -2439.25093285

Enthalpy 0K = -2438.179694

Enthalpy 298K = -2438.114548
Free Energy 298K = -2438.276342
Lowest Frequency = -410.8202 cm^{-1}
Second Frequency = 19.8920 cm^{-1}
SCF (BP86-D3BJ) Energy = -2439.61365025
SCF (Toluene) Energy = -2439.25716733
SCF (BS2) Energy = -2639.08027854

Mg	-0.46866	-0.01810	0.31990
O	0.27401	-0.39270	-1.60752
O	2.16582	-1.17771	-2.74590
N	-1.72472	1.61198	0.92393
N	-1.78033	-1.47859	1.03283
N	1.55024	-0.08657	0.83453
C	-3.24185	2.53231	2.69793
H	-3.37281	3.39598	2.03080
H	-2.70334	2.87935	3.59751
H	-4.23226	2.18199	3.02890
C	-2.47313	1.39665	2.02759
C	-2.62259	0.13803	2.66700
H	-3.13618	0.18933	3.63134
C	-2.38185	-1.17855	2.20776
C	-2.83172	-2.29306	3.14536
H	-1.97355	-2.59788	3.77150
H	-3.16993	-3.18596	2.59969
H	-3.63353	-1.95697	3.82018
C	-1.95471	-2.80369	0.48956
C	-3.12960	-3.07568	-0.28418
C	-3.29028	-4.35732	-0.84532
H	-4.18830	-4.57447	-1.43312
C	-2.32796	-5.35919	-0.66860
H	-2.47309	-6.34959	-1.11319
C	-1.18286	-5.08231	0.08357
H	-0.43295	-5.86754	0.23174
C	-0.97219	-3.81885	0.67456
C	-4.22364	-2.02121	-0.48725
H	-3.74742	-1.03251	-0.35381
C	-4.86242	-2.06417	-1.89283
H	-4.10747	-2.06028	-2.69538
H	-5.52029	-1.18868	-2.03406
H	-5.49346	-2.96020	-2.02991
C	-5.34204	-2.14176	0.57693
H	-5.81155	-3.14085	0.53447
H	-6.12971	-1.38902	0.39540
H	-4.96096	-1.98793	1.59745
C	-1.73491	2.91209	0.29151
C	-2.48403	3.07100	-0.91885
C	-2.39129	4.28393	-1.62652
H	-2.95488	4.40733	-2.55604
C	-1.60123	5.34197	-1.16061
H	-1.53536	6.27525	-1.72969
C	-0.92341	5.20344	0.05319
H	-0.33936	6.04519	0.44235
C	-0.98141	4.01204	0.80793
C	-0.28652	4.00449	2.17528
H	-0.50925	3.04068	2.66192
C	1.25018	4.13407	2.08264
H	1.70409	3.29911	1.52835
H	1.69140	4.14381	3.09419
H	1.54096	5.07338	1.57983
C	-0.84296	5.12629	3.08760
H	-0.56666	6.12498	2.70670
H	-0.42168	5.03489	4.10400
H	-1.94180	5.09404	3.16563
C	-3.45047	1.98269	-1.39537
H	-2.98851	1.00399	-1.16053
C	-3.75851	2.02475	-2.90564
H	-4.37444	2.90254	-3.16994
H	-4.33650	1.13063	-3.19564
H	-2.84542	2.05615	-3.52249
C	-4.78156	2.04773	-0.60605
H	-4.62790	1.89894	0.47310
H	-5.47826	1.26647	-0.95846
H	-5.26788	3.02845	-0.75229
C	1.90742	-0.14438	2.19970
C	1.16356	0.65064	3.11244
H	0.42751	1.34919	2.70275
C	1.34872	0.56714	4.49859
H	0.75071	1.20592	5.15874
C	2.29813	-0.31526	5.03851
H	2.45293	-0.37972	6.12023
C	3.03611	-1.12327	4.15724
H	3.76924	-1.83561	4.55341
C	2.84466	-1.05399	2.77027
H	3.41730	-1.71932	2.12285
C	2.42191	-0.33134	-0.23283
C	3.88616	-0.66127	-0.04851
C	4.42476	-1.82891	-0.62680
H	3.77601	-2.47561	-1.22405
C	5.78309	-2.15222	-0.45997
H	6.18306	-3.06441	-0.91614
C	6.62319	-1.30798	0.28032
H	7.68185	-1.55774	0.40921
C	6.10001	-0.13109	0.84663
H	6.75161	0.54056	1.41585
C	4.74752	0.18975	0.68147
H	4.34537	1.11031	1.11477
C	2.59792	1.25839	-1.39336
C	1.84260	2.37998	-1.03674
H	1.03818	2.28185	-0.29653
C	2.11285	3.63838	-1.60306
H	1.49669	4.50078	-1.32740
C	3.17086	3.77800	-2.51595
H	3.39360	4.75748	-2.95311
C	3.94971	2.65834	-2.86182
H	4.78079	2.76512	-3.56868
C	3.66412	1.40239	-2.30290
H	4.25702	0.52763	-2.59093
C	1.00974	-1.51180	-3.56463
C	-0.11446	-0.53548	-3.03471
C	-0.04798	0.86102	-3.67043
H	0.97778	1.25975	-3.67058
H	-0.67711	1.55773	-3.09330
H	-0.41998	0.83610	-4.70836
C	-1.52754	-1.10670	-3.10362
H	-1.79044	-1.33813	-4.15023
H	-2.25753	-0.36727	-2.73717
H	-1.62874	-2.02432	-2.50495
C	0.68600	-2.99672	-3.31489
H	0.38158	-3.17820	-2.27151
H	1.59155	-3.59185	-3.51568
H	-0.11677	-3.35882	-3.97901
C	1.38280	-1.29559	-5.03675
H	0.51755	-1.48101	-5.69661
H	2.18057	-2.00223	-5.31805
H	1.75396	-0.27575	-5.21495
B	1.72228	-0.54631	-1.57624
C	0.28268	-3.60964	1.52297

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H    0.30344 -2.55641  1.85365
C    0.26850 -4.50085  2.78767
H    0.32475 -5.57174  2.52175
H    1.13475 -4.26407  3.42883
H   -0.64767 -4.35572  3.38321
C    1.56917 -3.87207  0.71195
H    1.63377 -3.20985 -0.16637
H    2.45983 -3.69165  1.33607
H    1.61712 -4.91620  0.35470
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