Supporting Information for:

Snapshots of Magnesium-centred Diborane Heterolysis by an Outer Sphere SN2 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 (1H), 75.5 MHz (13C), 96.3 MHz (11B) or an Agilent ProPulse spectrometer operating at 500 MHz (1H), 126 MHz (13C), 160.4 MHz (11B). The spectra were referenced relative to residual solvent resonances or an external BF3.OEt2 standard (11B). 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. d8-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 B2pin2 were purchased from Sigma-Aldrich Ltd. [(BDI)Mgn-Bu] (BDI = HC{(Me)CNDipp}2; Dipp = 2,6-i-Pr2C6H3) was synthesized by a literature procedure.¹ Elemental analysis was carried out Mr Stephen Boyer of London Metropolitan Enterprises.
**Compound 11**

Toluene-\textsubscript{d8} (0.5 mL) was added to a J Young NMR tube containing a mixture of [(BDI)Mg-Bu] (50 mg, 0.1 mmol) and bis(pinacolato)diboron (25.4 mg, 0.1 mmol). After 2 hours \(N,N'\)-di-\textit{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, \textit{d}_8-tol): \(\delta\) 7.15 (m, 6H, Ar-H), 4.89 (s, 1H, NC(CH\(_3\))CH), 3.51 (hept, 4H, \(J_{HH} = 6.7\) Hz, CH(CH\(_3\))\(_2\)), 1.67 (s, 6H, NC(CH\(_3\))CH), 1.39 (d, 12H, \(J_{HH} = 6.7\) Hz, CH(CH\(_3\))\(_2\)), 1.31 (d, 12H, J\(_{HH}\) = 6.7 Hz, CH(CH\(_3\))\(_2\)), 1.24 (s, 18H, NC(CH\(_3\))\(_3\)), 1.10 (s, 12H, B(OC(CH\(_3\))\(_2\))\(_2\)) ppm. \(^{11}\)B\{\(^1\)H\} NMR (96 MHz, \textit{d}_8-tol): \(\delta\) 31.4 (br s) ppm. \(^{13}\)C\{\(^1\)H\} NMR (126 MHz, \textit{d}_8-tol): \(\delta\) 169.08 (NC(CH\(_3\))CH), 145.22 (C\(_{ipso}\)), 142.52 (C\(_{ortho}\)), 124.73 (C\(_{para}\)), 123.53 (C\(_{meta}\)), 94.47 (NC(CH\(_3\))CH), 83.80 (B(OC(CH\(_3\))\(_2\))\(_2\)), 49.89 (NC(CH\(_3\))\(_3\)), 33.19 (NC(CH\(_3\))\(_3\)), 27.71 (NC(CH\(_3\))CH), 25.40 (B(OC(CH\(_3\))\(_2\))\(_2\)), 25.36 (CH(CH\(_3\))\(_2\)), 24.41 (CH(CH\(_3\))\(_2\)), 23.85 (CH(CH\(_3\))\(_2\)) ppm. Elemental analysis: Found C, 72.97; H, 10.17; N, 7.69 %. \(C_{44}H_{71}BMgN_{4}O_{2}\) requires: C, 73.08; H, 9.90; N, 7.75 %.

**Figure S1:** \(^1\)H NMR spectrum (25˚C, 300 MHz, \textit{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$_3$)CH), 3.47 (m, 4H + 2H, $J_{HH} = 6.8$ Hz, (C$_6$H$_5$)CH(CH$_3$)$_2$ and NCH(CH$_3$)$_2$), 1.67 (s, 6H, NC(CH$_3$)CH), 1.34 (d, 12H, $J_{HH} = 6.8$ Hz, CH(CH$_3$)$_2$), 1.27 (d, 12H, $J_{HH} = 6.8$ Hz, CH(CH$_3$)$_2$), 1.01 (s, 12H, B(OC(CH$_3$)$_2$)$_2$), 0.97 (d, 12H, $J_{HH} = 6.2$ Hz, NCH(CH$_3$)$_2$) 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:** $^{11}\text{B}\{^1\text{H}\}$ 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, $J_{HH} = 8$Hz, $CH_3(C_6H_4)$), 6.53 (d, 4H, $J_{HH} = 8$Hz, $CH_3(C_6H_4)$), 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)MgBu] (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$_4$O$_2$ requires: C, 76.55; H, 8.92; N, 6.61 %.
Compound 15BN

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 15BN (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) $\delta$ 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$_3$)CH), 3.71, 3.61 (hept, 1H, $J_{HH} = 6.6$ Hz C(CH$_3$)$_2$), 3.44 (hept, 1H, $J_{HH} = 6.6$ Hz C(CH$_3$)$_2$), 3.30 (hept, 1H, $J_{HH} = 6.6$ Hz CH(CH$_3$)$_2$), 1.69 (s, 3H, CH$_3$), 1.57 (s, 3H, CH$_3$), 1.43 (d, 3H, $J_{HH} = 6.6$ Hz CH(CH$_3$)$_2$), 1.38 (m, 6H, CH(CH$_3$)$_2$), 1.33 (d, 3H, $J_{HH} = 6.7$ Hz CH(CH$_3$)$_2$), 1.27 (d, 3H, $J_{HH} = 6.7$ Hz CH(CH$_3$)$_2$), 1.19 (m, 9H, CH$_3$), 0.99 (s, 3H, CH$_3$), 0.95 (m, 6H, CH$_3$), 0.90 (s, 3H, CH$_3$), 0.86-0.82 (m, 7H, 2 x CH$_2$ + CH$_3$) ppm. $^{11}$B{$^1$H} NMR (160 MHz, $d_8$-tol) $\delta$ 24.5 ppm. $^{13}$C{$^1$H} NMR (126 MHz, $d_8$-tol) $\delta$ 170.18 (NC(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$_3$)CH), 85.51, 81.64, 53.80(BuN-CH(Ph)), 44.90 (NCH$_2$CH$_2$), 28.14 (CH(CH$_3$)$_2$), 28.08 (CH(CH$_3$)$_2$), 28.04 (CH(CH$_3$)$_2$), 27.49 (CH(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$_{88}$BMgN$_3$O$_2$ 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 15BN.

Figure S9: $^{11}$B{$^1$H} NMR spectrum (25°C, 160 MHz, d$_8$-tol) of compound 15BN.
Figure S10: $^{13}$C{$^1$H} NMR spectrum (25°C, 126 MHz, d$_8$-tol) of compound 15$_{BN}$. 
Compound 16BN

Toluene-$d_8$ (0.5 mL) was added to a J Young NMR tube containing a mixture of [(BDI)Mg-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 $-35^\circ$C to yield compound 16BN (30 mg, 41%). $^1$H NMR (500 MHz, d$_8$-tol) $\delta$ 7.19 (m, 1H, aromatic CH), 7.17 (m, 2H, aromatic CH), 7.12 (m, 1H, aromatic CH), 7.06-7.00 (m, 4H, aromatic CH), 6.85 (m, 2H, aromatic CH), 6.41 (m, 1H, aromatic CH), 4.77 (s, 1H, NC(CH$_3$)CH), 3.70 (s, 1H, N-C$\text{H}_\text{Ph}$), 3.52 (hept, 1H, $J_{\text{HH}}$ = 6.7 Hz C$\text{H}$ (CH$_3$)$_2$), 3.37 (hept, 1H, $J_{\text{HH}}$ = 6.7 Hz C$\text{H}$ (CH$_3$)$_2$), 1.87 (s, 3H, C$\text{H}$), 1.56 (s, 3H, CH$_3$), 1.47 (d, 3H, $J_{\text{HH}}$ = 6.7 Hz CH(CH$_3$)$_2$), 1.43 (d, 3H, $J_{\text{HH}}$ = 6.7 Hz CH(CH$_3$)$_2$), 1.40-1.38 (m, 12H, C$\text{H}$), 1.27 (d, 3H, $J_{\text{HH}}$ = 6.7 Hz CH(CH$_3$)$_2$), 1.20 (d, 3H, $J_{\text{HH}}$ = 6.7 Hz CH(CH$_3$)$_2$), 1.17 (d, 3H, $J_{\text{HH}}$ = 6.7 Hz CH(CH$_3$)$_2$), 1.11 (s, 3H, CH$_3$), 1.08 (s, 3H, CH$_3$), 1.02-1.00 (m, 6H, CH$_3$), 0.97 (s, 3H, CH$_3$) ppm. $^{11}$B $^1$H NMR (160 MHz, d$_8$-tol) $\delta$ 24.99 ppm. $^{13}$C $^1$H NMR (126 MHz, d$_8$-tol) $\delta$ 170.23 (NC(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$_3$)CH), 84.60, 81.56, 56.72, 55.18 (tBuN-CH(Ph)), 30.74 (CH$_3$), 28.17 (CH(CH$_3$)$_2$), 28.02 (CH(CH$_3$)$_2$), 27.89 (CH(CH$_3$)$_2$), 27.40 (CH(CH$_3$)$_2$), 26.03 (CH$_3$), 25.39 (CH$_3$), 25.18 (CH$_3$), 25.08 (CH$_3$), 24.91 (CH$_3$), 24.79 (CH$_3$), 24.72 (CH$_3$), 24.63 (CH$_3$), 24.57 (CH$_3$), 24.39 (CH$_3$), 24.05 (CH$_3$), 23.91 (CH$_3$), 23.11 (CH$_3$) ppm. Elemental analysis: Found C, 75.48; H, 9.50; N, 5.68 %. C$_{46}$H$_{68}$BMgN$_3$O$_2$ requires: C, 75.67; H, 9.39; N, 5.75 %. 

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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\{H\} NMR spectrum (25°C, 126 MHz, d$_8$-tol) of compound 16$_{\text{BN}}$. 
Compound 17BN
Toluene-$d_8$ (0.5 mL) was added to a J Young NMR tube containing a mixture of [(BDI)Mg$_2$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 17BN (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) $\delta$ 7.66, 7.65, 7.11, 7.09, 7.06, 6.80, 6.67, 4.96 (s, 1H, NC(CH$_3$)CH), 4.51 (s, 1H, N-CHPh), 3.74 (hept, 1H, $J_{HH} = 6.7$ Hz, CH(CH$_3$)$_2$), 3.38 (m, 2H, CH(CH$_3$)$_2$), 2.67 (hept, 1H, $J_{HH} = 6.7$ Hz, CH(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) $\delta$ 24.8 ppm. $^{13}$C{$^1$H} NMR (126 MHz, d$_8$-tol) $\delta$ 170.50(NC(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$_3$)CH), 85.30, 82.92, 53.91 (NCHPh), 28.38 (CH(CH$_3$)$_2$), 28.27 (CH(CH$_3$)$_2$), 28.13 (CH(CH$_3$)$_2$), 27.77 (CH(CH$_3$)$_2$), 25.48 (CH$_3$), 25.23 (CH$_3$), 24.74 (CH$_3$), 24.71 (CH$_3$), 24.63 (CH$_3$), 24.28 (CH$_3$), 24.13 (CH$_3$), 23.98 (CH$_3$), 23.89 (CH$_3$), 23.54 (CH$_3$), 23.06 (CH$_3$) ppm.
Figure S14: $^1$H NMR spectrum (25°C, 500 MHz, d$_8$-tol) of compound 17$_{\text{BN}}$.

Figure S15: $^{11}$B{$^1$H} NMR spectrum (25°C, 160 MHz, d$_8$-tol) of compound 17$_{\text{BN}}$.  

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**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 containing a mixture of [(BDI)Mg-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 compound $^{18}$BN (45 mg, 54%). $^1$H NMR (500 MHz, d$_8$-toluene) δ 7.16-7.00 (m, 11H, aromatic CH), 6.86 (m, 3H, aromatic CH), 6.58 (m, 1H, aromatic CH), 6.50 (m, 6H, aromatic CH), 4.72 (s, 1H, NC(CH$_3$)CCH), 3.22 (hept, 2H, $J_{HH}$ = 6.7 Hz, C(CH$_3$)$_2$), 3.06 (hept, 2H, $J_{HH}$ = 6.7 Hz, C(CH$_3$)$_2$), 1.58 (s, 1H, NC(CH$_3$)CH), 1.35 (s, 6H, CH$_3$), 1.18 (d, 6H, $J_{HH}$ = 6.7 Hz, CH$_3$), 1.13 (m, 12H, CH$_3$), 1.08 (d, 6H, $J_{HH}$ = 6.7 Hz, CH$_3$), 1.00 (d, 6H, $J_{HH}$ = 6.7 Hz, CH$_3$) ppm. $^{11}$B NMR (160 MHz, Tol) δ 26.0 ppm. $^{13}$C NMR (126 MHz, toluene) δ 170.34 (NC(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$_3$)CH), 88.07, 83.14, 31.65, 28.37 (CH(CH$_3$)$_2$), 27.45 (CH(CH$_3$)$_2$), 25.13 (CH$_3$), 25.01 (CH$_3$), 24.79 (CH$_3$), 24.66 (CH$_3$), 24.59 (CH$_3$), 24.46 (CH$_3$), 23.96 (CH$_3$) ppm. Elemental analysis: Found C, 78.27; H, 8.14; N, 5.19 %. C$_{54}$H$_{68}$BМgN$_3$O$_2$ requires: C, 78.50; H, 8.30; N, 5.09 %.

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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$^{18}$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 CH), 7.14-7.02 (m, 13H, aromatic CH), 6.56 (t, 1H, $J_{HH} = 7.1$ Hz, aromatic CH), 5.25 (s, 1H, NC(CH$_3$)C(CH$_3$)), 4.61 (s, 1H, NCHPh), 3.65 (hept, 1H, $J_{HH} = 6.6$ Hz, CH(CH$_3$)$_2$), 3.38 (m, 3H, CH(CH$_3$)$_2$), 1.80 (s, 3H, CH$_3$), 1.74 (s, 3H, CH$_3$), 1.28 (m, 12H, CH$_3$), 1.23 (d, 3H, $J_{HH} = 6.6$ Hz, CH(CH$_3$)$_2$), 1.15 (d, 3H, $J_{HH} = 6.6$ Hz, CH(CH$_3$)$_2$), 0.94 (d, 3H, $J_{HH} = 6.6$ Hz, CH(CH$_3$)$_2$), 0.85 (d, 3H, $J_{HH} = 6.6$ Hz, CH(CH$_3$)$_2$), 0.58-0.51 (m, 9H, CH$_3$), 0.44 (s, 3H, CH$_3$) ppm. $^{13}$C{$^1$H} NMR (126 MHz, d$_8$-toluene) δ 171.08 (NC(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$_3$)CH), 88.80, 85.08, 49.43, 29.49 (CH(CH$_3$)$_2$), 29.07 (CH(CH$_3$)$_2$), 29.05 (CH(CH$_3$)$_2$), 28.49 (CH(CH$_3$)$_2$), 25.82 (CH$_3$), 25.32 (CH$_3$), 25.11 (CH$_3$), 24.91 (CH$_3$), 23.95 (CH$_3$), 23.82 (CH$_3$) 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$_{BC}$. 

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Compound 18\text{Ph}

A sample of compound 18\text{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 18\text{Ph} as colourless crystals. $^1$H NMR (500 MHz, d$_8$-toluene) $\delta$ 7.49 (m, 2H, aromatic CH), 7.29 (m, 2H, aromatic CH), 7.16 (m, 4H, aromatic CH), 7.09 (s, 1H, aromatic CH), 6.96-6.85 (m, 6H, aromatic CH), 6.77 (m, 4H, aromatic CH), 6.54 (m, 2H, CH(CH$_3$)$_2$), 6.06 (s, 1H, NC(CH$_3$)CH), 3.63 (m, 1H, CH(CH$_3$)$_2$), 3.35 (m, 2H, CH(CH$_3$)$_2$), 2.50 (m, 1H, CH(CH$_3$)$_2$), 1.78 (s, 3H, CH$_3$), 1.55 (s, 6H, CH$_3$), 1.34 (d, 3H, CH$_3$), 1.29 (d, 3H, CH$_3$), 1.25 (d, 3H, CH$_3$), 1.21 (d, 3H, CH$_3$), 1.18 (d, 3H, CH$_3$), 1.00-0.97 (m, 9H, CH$_3$), 0.87 (s, 3H, CH$_3$), 0.77 (d, 3H, CH$_3$), 0.48 (d, 3H, CH$_3$) ppm. $^{13}$B\{$^1$H\} NMR (160 MHz, d$_8$-toluene) $\delta$ 5.89 ppm. $^{13}$C\{$^1$H\} NMR (126 MHz, d$_8$-toluene) $\delta$ 170.48 (N\text{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$_3$)CH), 82.82, 77.84, 31.65 (CH$_3$), 29.87 (CH(CH$_3$)$_2$), 28.38 (CH(CH$_3$)$_2$), 28.30 (CH(CH$_3$)$_2$), 28.10 (CH(CH$_3$)$_2$), 27.81 (CH$_3$), 26.04 (CH$_3$), 25.86 (CH$_3$), 25.66 (CH$_3$), 25.23 (CH$_3$), 24.91 (CH$_3$), 24.78 (CH$_3$), 24.37 (CH$_3$), 24.29 (CH$_3$), 24.15 (CH$_3$), 24.09 (CH$_3$), 23.90 (CH$_3$), 23.68 (CH$_3$), 23.51 (CH$_3$), 23.30 (CH$_3$), 22.71 (CH$_3$) 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$_{ph}$.

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Figure S24: $^{13}$C($^1$H) NMR spectrum (25°C, 126 MHz, d$_8$-tol) of compound 18ph.
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 $[\text{Substrate}]_{t=0}$ so that:

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

Reaction rates were derived from the plot of $\ln(C_t)$ vs. time by using linear trendlines generated by Microsoft Excel software.

![Graph](image)

**Figure S25:** First order rate plot of $\ln([C_t])$ vs time for consumption of $17_{BN}$ at 60°C.
**Figure S26:** First order rate plot ln([Ct]₀) vs time for consumption of 17BN at 65°C.

**Figure S27:** First order rate plot ln([Ct]₀) vs time for consumption of 17BN at 70°C.
**Figure S28:** First order rate plot \( \ln([C_t]_k) \) vs time for consumption of \( 17BN \) 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          | -7.6090246 |
| 348.73927      | 0.002867472 | 0.0008          | -7.13089883 |
| 354.38532      | 0.00281787  | 0.0015          | -6.50290171 |

**Figure S29:** Arrhenius Plot - \( \ln(k) \) vs \( 1/T \) for conversion of \( 17BN \) to \( 17BC \).
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 17BN to 17BC.

**Figure S31:** First order rate plot of ln([Ct]₀) vs time for consumption of 18BN at 60°C.

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**Figure S32:** First order rate plot of \( \ln([Ct]_0) \) vs time for consumption of 18BN at 65°C.

**Figure S33:** First order rate plot of \( \ln([Ct]_0) \) vs time for consumption of 18BN at 70°C.
**Figure S34**: First order rate plot of ln([Ct]), vs time for consumption of 18BN 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 18BN to 18Ph.

\[ y = -12,751.755x + 29.633 \]
\[ R^2 = 0.993 \]
Figure S36: Eyring Plot - Ln(k/T) vs 1/T for conversion of 18BN to 18ph.
Single Crystal X-ray Diffraction analysis.

Single Crystal X-ray diffraction data for compounds 11, 14, 15BN, 16BN, 17BN, 18BN, 17BC and 18Ph were collected using CuKα (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 ShelXL³ refinement package using Least Squares minimisation.

For 15BN 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 16BN 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 18BN 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 18Ph 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_{4}O_{2} | C_{54}H_{75}BMgN_{4}O_{2} | C_{92}H_{136}B_{2}Mg_{2}N_{6}O_{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 | P_{2\text{I}}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/Å³ | 8959.98(15) | 5041.57(10) | 8809.867 | 8724.55(18) |
| Z | 8 | 4 | 8 | 4 |
| ρ_{calc} g/cm³ | 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/mm³ | 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 F² | 1.067 | 1.040 | 1.032 | 1.032 |
| Final R indexes [I>2σ (I)] | R₁ = 0.0653, wR₂ = 0.1585 | R₁ = 0.0383, wR₂ = 0.1013 | R₁ = 0.0448, wR₂ = 0.1168 | R₁ = 0.0592, wR₂ = 0.1484 |
| Final R indexes [all data] | R₁ = 0.0765, wR₂ = 0.1655 | R₁ = 0.0402, wR₂ = 0.1056 | R₁ = 0.0480, wR₂ = 0.1198 | R₁ = 0.0685, wR₂ = 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 17BN, 18BN, 17BC and 18Ph.

| Compound | 17BN | 18BN | 17BC | 18Ph |
|----------|------|------|------|------|
| **Empirical formula** | C₄₈H₆₂BMgN₃O₂ | C₅₇H₇₂BMgN₃O₂ | C₄₈H₆₂BMgN₃O₂ | C₅₄H₆₂BMgN₃O₂ |
| **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 | P2₁/c | P2₁/c | P2₁/c |
| **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) | 90.000(2) | 90.000(2) | 90.000(2) |
| **β/°** | 82.771(6) | 98.837(2) | 90.243(4) | 98.9416(9) |
| **γ/°** | 84.240(5) | 90.000(2) | 90.000(2) | 90.000(2) |
| **Volume/Å³** | 2189.2(2) | 4999.33(19) | 4356.3(3) | 4819.28(8) |
| **Z** | 2 | 4 | 4 | 4 |
| **ρcalc g/cm³** | 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/mm³** | 0.135 × 0.09 × 0.025 | 0.12 × 0.094 × 0.068 | 0.149 × 0.124 × 0.078 | 0.217 × 0.192 × 0.085 |
| **Reflections collected** | 14171 | 36973 | 54653 | 60632 |
| **Independent reflections** | 8031 [Rint = 0.0703] | 9893 [Rint = 0.0565] | 8726 [Rint = 0.1131] | 9606 [Rint = 0.0657] |
| **Data/restraints/parameters** | 8031/0/510 | 9893/0/592 | 8726/0/510 | 9606/16/587 |
| **Goodness-of-fit on F²** | 1.033 | 1.033 | 1.056 | 1.025 |
| **Final R indexes [I>2σ (I)]** | R₁ = 0.0684, wR₂ = 0.1173 | R₁ = 0.0525, wR₂ = 0.1189 | R₁ = 0.0675, wR₂ = 0.1491 | R₁ = 0.0450, wR₂ = 0.1076 |
| **Final R indexes [all data]** | R₁ = 0.1234, wR₂ = 0.1431 | R₁ = 0.0783, wR₂ = 0.1316 | R₁ = 0.0919, wR₂ = 0.1620 | R₁ = 0.0561, wR₂ = 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). The Mg center was described with the Stuttgart RECPs and associated basis sets, and 6-31G** basis sets were used for all other atoms (BS1). Initial BP86 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 ($\varepsilon = 2.3741$) solvent were run using the polarizable continuum model and BS1. Single-point dispersion corrections to the BP86 results employed Grimme’s D3 parameter set with Becke-Johnson damping as implemented in Gaussian.

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 $'\text{BuNCHPh}$ and $'\text{BuNCHPh}$ (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:

| Term          | Description                                                                 |
|---------------|-----------------------------------------------------------------------------|
| $\Delta E_{BS1}$ | SCF energy computed with the BP86 functional with BS1                      |
| $\Delta H_{BS1}$ | Enthalpy at 0 K with BS1                                                    |
| $\Delta G_{BS1}$ | Free energy at 298.15 K and 1 atm with BS1                                  |
| $\Delta G_{BS1/tol}$ | Free energy corrected for toluene solvent with BS1                        |
| $\Delta G_{BS1/tol+D3}$ | Free energy corrected for toluene and dispersion effects with BS1        |
| $\Delta G_{tol}$ | 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.

|        | \(\Delta E_{BS1}\) | \(\Delta H_{BS1}\) | \(\Delta G_{BS1}\) | \(\Delta G_{BS1\text{tol}}\) | \(\Delta E_{BS2}\) | \(\Delta G_{\text{mol}}\) |
|--------|-------------------|-------------------|-------------------|-----------------|------------------|-----------------|
| 5      | 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           |
| 5_{b}  | 6.8               | 6.1               | 1.8              | 201.7           | 11.4             | 6.6           | 11.1           |
| 5_{c}  | 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 compound 5, relative to 5 and the free substrates. Bond lengths given in Ångstroms.

12_{SN} -32.8
12_{BC} -38.3

15_{SN} -45.8
15_{BC} -39.8
$^{17}_{\text{BCN}}$ -22.8

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

$^{17}_{\text{BC}}$ -38.4

$\text{TS}(5-^{17}_{\text{BCN}})$ [30.3]$^\dagger$

$^{17}_{\text{BCN}}$-BpinBu -12.2

$^{18}_{\text{BN}}$ -37.1
| X       | Y       | Z       |
|---------|---------|---------|
| 2.54406 | 2.07381 | 0.02487 |

**Cartesian Coordinates and Computed Energies (in Hartrees)**

**pinBBu**

| Energy (BP86) | -569.123611693 |
|--------------|-----------------|
| Enthalpy OK  | -568.827988     |
| SCF 298K     | -568.811084     |
| Free Energy  | -568.871244     |

**SCF (Toluene)**

| Energy (BP86) | -569.125385795 |
|--------------|-----------------|
| SCF (BS2)    | -569.267887458 |

**PhNCHPh**

| Energy (BP86) | -556.743441703 |
|--------------|-----------------|
| Enthalpy OK  | -556.546372     |
| SCF 298K     | -556.534136     |
| Free Energy  | -556.584766     |

**SCF (Toluene)**

| Energy (BP86-D3BJ) | -556.789039723 |
|--------------------|-----------------|
| SCF (BS2) Energy   | -556.745924351 |

**PhNCPh**

| Energy (BP86) | -556.879545901 |
|--------------|-----------------|
| Enthalpy OK  | -556.546372     |
| SCF 298K     | -556.534136     |
| Free Energy  | -556.584766     |

**SCF (Toluene)**

| Energy (BP86-D3BJ) | -556.789039723 |
|--------------------|-----------------|
| SCF (BS2) Energy   | -556.745924351 |

**DMPAP (N(CH_3)_{2}NMe_2)**

| Energy (BP86) | -382.256098610 |
|--------------|-----------------|
| Enthalpy OK  | -382.098887     |
| SCF 298K     | -382.132978     |
| Free Energy  | -382.132978     |

**SCF (Toluene)**

| Energy (BP86-D3BJ) | -382.285474805 |
|--------------------|-----------------|
| SCF (BS2) Energy   | -382.259778610 |

**PhNCPh**

| Energy (BP86) | -556.743441703 |
|--------------|-----------------|
| Enthalpy OK  | -556.546372     |
| SCF 298K     | -556.534136     |
| Free Energy  | -556.584766     |

**SCF (Toluene)**

| Energy (BP86-D3BJ) | -556.789039723 |
|--------------------|-----------------|
| SCF (BS2) Energy   | -556.745924351 |
|    |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |   S45   |
\[
\begin{align*}
C & \quad 1.67931 \quad 1.10230 \quad -0.00002 \\
C & \quad 3.53426 \quad -1.01222 \quad 0.00002 \\
H & \quad 1.80283 \quad -2.32301 \quad 0.00001 \\
C & \quad 3.05132 \quad 1.37354 \quad -0.00001 \\
H & \quad 0.93466 \quad 1.90417 \quad -0.00006 \\
C & \quad 3.98349 \quad 0.31801 \quad 0.00002 \\
H & \quad 4.25555 \quad -1.83622 \quad 0.00004 \\
H & \quad 3.40202 \quad 2.41122 \quad -0.00002 \\
H & \quad 5.05714 \quad 0.53428 \quad 0.00003 \\
C & \quad -2.56413 \quad 0.04606 \quad 0.00002 \\
C & \quad -2.91963 \quad -1.45633 \quad -0.00026 \\
H & \quad -2.52736 \quad -1.97086 \quad 0.89458 \\
H & \quad -4.01542 \quad -1.58110 \quad -0.00037 \\
H & \quad -2.52720 \quad -1.97053 \quad -0.89522 \\
C & \quad -3.14604 \quad 0.72338 \quad -1.26369 \\
H & \quad -2.88354 \quad 1.79310 \quad -1.27977 \\
H & \quad -2.74363 \quad 0.25712 \quad -2.17827 \\
H & \quad -4.24755 \quad 0.62875 \quad -1.28221 \\
C & \quad -3.14807 \quad 0.72295 \quad 1.26393 \\
C & \quad -4.24759 \quad 0.62833 \quad 1.28237 \\
H & \quad -2.74371 \quad 0.25637 \quad 2.17836 \\
H & \quad -2.88357 \quad 1.79266 \quad 1.28039 \\
\end{align*}
\]

\[
\begin{align*}
\text{SCF (BP86) Energy} & = -384.663990780 \\
\text{Enthalpy 298K} & = -384.460688 \\
\text{Enthalpy 298K} & = -384.453420 \\
\text{Free Energy 298K} & = -384.504972 \\
\text{Lowest Frequency} & = 23.8349 \text{ cm}^{-1} \\
\text{Second Frequency} & = 27.2538 \text{ cm}^{-1} \\
\text{SCF (BP86-D3BJ) Energy} & = -384.692047877 \\
\text{SCF (Toluene) Energy} & = -384.665763511 \\
\text{SCF (BS2) Energy} & = -384.763019620 \\
\end{align*}
\]

\[
\begin{align*}
C & \quad 0.00004 \quad -0.43121 \quad -0.00060 \\
N & \quad 1.18320 \quad -0.53258 \quad 0.39428 \\
N & \quad -1.18311 \quad -0.53175 \quad -0.35072 \\
C & \quad 2.94494 \quad 1.06614 \quad 0.93987 \\
H & \quad 3.81509 \quad 1.63448 \quad 0.56922 \\
H & \quad 2.21420 \quad 1.78001 \quad 1.35415 \\
H & \quad 3.28031 \quad 0.40569 \quad 1.75737 \\
C & \quad 3.33349 \quad -0.75316 \quad -0.79827 \\
H & \quad 2.87718 \quad -1.33277 \quad -1.61703 \\
H & \quad 4.20843 \quad -0.21284 \quad -1.19856 \\
H & \quad 3.68147 \quad -1.46215 \quad -0.02808 \\
C & \quad -2.94691 \quad 1.06516 \quad -0.93975 \\
H & \quad -3.81702 \quad 1.63301 \quad -0.56825 \\
H & \quad -2.21727 \quad 1.77939 \quad -1.35535 \\
H & \quad -3.28283 \quad 0.40403 \quad -1.75647 \\
C & \quad 2.32320 \quad 0.23544 \quad -0.19421 \\
H & \quad 1.97527 \quad 0.92226 \quad -0.99222 \\
C & \quad -2.32304 \quad 0.23553 \quad 0.19394 \\
H & \quad -1.97466 \quad 0.92302 \quad 0.91117 \\
C & \quad -3.33174 \quad -0.75361 \quad 0.79978 \\
H & \quad -2.87393 \quad -1.33240 \quad 1.61829 \\
H & \quad -4.20664 \quad -0.21382 \quad 1.20086 \\
H & \quad -3.68008 \quad -1.46330 \quad 0.03040 \\
\end{align*}
\]

\[
\begin{align*}
\text{SCF (BP86) Energy} & = -463.293050800 \\
\text{Enthalpy 0K} & = -463.041521 \\
\text{Enthalpy 298K} & = -463.026103 \\
\text{Free Energy 298K} & = -463.083859 \\
\text{Lowest Frequency} & = 12.3444 \text{ cm}^{-1} \\
\end{align*}
\]
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 (B2) Energy = -2235.94374148

H -6.35837 -1.95057 0.71603 C -1.06438 4.68240 -1.62236
N 1.94871 -1.51443 0.75035 H -1.53562 5.03886 -2.54440
N 1.90851 1.56821 0.68668 C -0.01355 5.41671 -1.06108
N -0.99161 0.04939 -1.07630 H 0.33535 6.33810 -1.53948
N -1.35898 -0.06054 1.14535 C 0.58884 4.95683 0.11356
O -4.31464 1.06596 -0.26963 H 1.41876 5.52318 0.55139
O -4.19553 -1.20414 -0.68301 C 0.15502 3.77958 0.75490
Mg 0.58160 0.00712 0.28400 H 0.87531 3.33663 2.02879
B -3.50575 -0.05216 -0.35220 H 3.5921 2.43547 2.40421

12
|原子 | 碳 | 氧 | 镁 |
|-----|-----|-----|-----|
| N   | 1.3964 | 0.8684 | 0.0081 |
| N   | -2.0917 | -0.0532 | -0.7390 |
| C   | 0.62516 | -0.95730 | -1.33290 |
| C   | -2.0701 | -1.01764 | -1.75720 |
| C   | -3.77480 | -2.11475 | -3.22277 |
| C   | -3.0222 | -2.04627 | 0.4800 |
| H   | -3.63263 | -3.08676 | -0.82386 |
| H   | -4.77673 | -2.11391 | 0.14275 |
| C   | -2.92160 | 2.63712 | -0.01390 |
| C   | -1.82607 | 3.70604 | 0.00817 |
| O   | -0.85950 | 3.17232 | -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 |

**SCF (BP86) Enthalpy** = 2036.1951119
**SCF (BP86) Enthalpy** = 2035.199092
**Free Energy** BP86 = 2035.291832

- **SCF (BP86-D3BJ) Energy** = 2036.48724138
- **SCF (Toluene) Energy** = 2036.20021570
- **SCF (BP86) Energy** = 2036.20021570

| 原子 | 碳 | 氧 | 镁 |
|-----|-----|-----|-----|
| N   | 1.12100 | -1.3678 | -2.44502 |
| C   | 2.67925 | 1.51354 | -3.22820 |
| H   | 3.48026 | 2.01993 | -2.66880 |
| H   | 2.40738 | 2.12400 | -4.10222 |
| C   | 3.10037 | 0.56078 | -3.59785 |
| C   | 1.46902 | 1.22765 | -2.34816 |
| C   | 0.20263 | 1.32955 | -2.98567 |
| C   | 0.25398 | 1.54549 | -4.05622 |
| C   | -3.05234 | 2.25617 | -2.92219 |
| C   | -2.62602 | 0.82813 | -3.88428 |
| H   | -1.83619 | 2.38848 | -4.23526 |
| C   | -2.71322 | 1.36376 | -0.63389 |
| C   | -4.63614 | -1.12368 | -2.49187 |
| C   | -5.67543 | -1.13096 | -2.11830 |
| C   | -4.46706 | -2.07874 | -3.01918 |
| C   | -4.55455 | -0.30624 | -3.27670 |
| C   | -4.17639 | 2.91482 | 0.56200 |
| C   | -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 | -0.0532 | -0.7390 |
| C   | -3.76723 | 0.40616 | -0.65713 |
| C   | -3.62516 | -0.95730 | -1.33290 |
| C   | -2.60701 | -1.01764 | -1.75720 |
| C   | -3.77480 | -2.11475 | -3.22277 |
| C   | -3.0222 | -2.04627 | 0.4800 |
| H   | -3.63263 | -3.08676 | -0.82386 |
| H   | -4.77673 | -2.11391 | 0.14275 |
| C   | -2.92160 | 2.63712 | -0.01390 |
| C   | -1.82607 | 3.70604 | 0.00817 |
| O   | -0.85950 | 3.17232 | -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  | -0.10933  | -2.48161  | -0.38037  | H  | 4.57019  | -2.23846  | 2.10283  |
| C  | -0.03480  | -2.94116  | -2.70132  | C  | 3.33703  | -0.99811  | 2.46340  |
| H  | 0.04862   | -1.82377  | -2.76491  | C  | 5.75144  | -1.03279  | -0.06837  |
| C  | 1.21214   | -3.55890  | -3.36636  | H  | 6.53569  | -0.48789  | 0.48642  |
| H  | 1.29217   | -3.25579  | -4.42267  | C  | 5.82669  | -0.73331  | -1.12545  |
| C  | 2.13168   | -3.24741  | -2.84222  | C  | 5.98262  | -2.11032  | 0.00125  |
| H  | 1.15576   | -4.66099  | -3.31953  | C  | -0.88038  | -2.99440  | -0.05043  |
| C  | -1.30286  | -3.37549  | -3.46221  | H  | -0.34119  | -3.63624  | 1.11002  |
| H  | -2.20491  | -2.92863  | -3.01361  | C  | -1.17901  | -4.47215  | 1.87389  |
| C  | -1.25431  | -3.07256  | -4.52322  | H  | -0.77328  | -4.97225  | 2.75906  |
| H  | -1.41189  | -4.47334  | -4.1780  | C  | -2.52079  | -4.67548  | 1.52859  |
| C  | -3.15593  | -5.32583  | 2.13940  | C  | -3.03876  | -4.04156  | 0.39622  |

**SCF (BP86) Energy = -2036.1828454**

Enthalpy 0K = -2035.186963

Enthalpy 298K = -2035.126466

Free Energy 298K = -2025.279289

Lowest Frequency = 13.0580 cm⁻¹

Second Frequency = 21.4557 cm⁻¹

**SCF (BP86-D3BJ) Energy = -2036.4782363**

**SCF (Toluene) Energy = -2036.1886660**

**SCF (BS2) Energy = -2235.91887674**

Mg -0.07101  -0.00638  -0.63505  
O -0.76340  0.75918  1.19642  
C -2.06271  2.45415  2.05462  
N -0.03884  -2.08776  -0.79269  
C  1.97176  0.20242  -1.06717  
H  0.11366  -4.64531  -1.63692  
C  1.31329  -3.42149  -2.93392  
C  -0.39439  -3.86057  -3.14914  
C  0.70383  -2.54821  -1.82215  
C  1.73096  -1.79926  -2.45506  
C  2.17002  -2.28331  -3.32324  
C  2.39546  -0.60925  -2.05486  
C  3.64451  -0.27365  -2.86371  
H  4.14900  -0.62993  -2.49428  
C  3.35624  -0.10714  -3.91690  
C  4.36224  -1.11040  -2.85819  
C  2.86470  1.16520  -0.47424  
C  2.17335  3.30804  -2.99761  
C  2.96925  4.07275  -2.94841  
C  1.41080  3.65515  -3.71678  
C  2.62044  2.38278  -3.39643  
C  4.74609  1.70419  0.99378  
H  5.58655  1.37438  1.61522  
C  4.47879  3.07064  0.87196  
H  5.09846  3.80645  1.39542  
C  3.41880  3.48720  0.5831  
C  3.22410  4.55756  -0.06221  
C  2.60612  2.56419  -0.62843  
C  1.54530  3.08366  -1.60022  
C  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  
C  1.50907  5.24324  -1.12579  
C  3.96317  0.73300  0.33706  
C  4.35046  -0.73898  0.52176  
C  3.61607  -1.36146  -0.01706  
C  4.32508  -1.16585  2.00692  
H  5.06707  -0.60428  2.60141  

**SCF (Toluene) Energy = -2036.1886660**
SCF (BP86) Energy = -2134.46541571
Enthalpy 0K = -2.75094 5.18917 0.16088
Enthalpy 298K = -2.01463 3.18180 1.80870
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 -0.25076 0.45627 1.00595
O -1.17086 -1.76699 -2.10543
N 0.1213 2.05563 0.88243
N 1.91562 -0.69164 1.04409
N -1.68329 -0.77447 0.74282
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
C 2.39673 1.38310 3.66043
C 2.33896 -0.16651 2.21638
C 3.30976 -0.98656 3.16080
C 3.85094 -1.69983 2.62295
C 2.55396 -1.57426 3.82866
C 3.83721 -0.34178 3.79519
C 2.56564 -1.86991 0.52455
C 1.15636 -4.20780 2.0840
C 1.49479 -5.22779 2.65437
C 0.27291 -4.29568 3.56323
C 1.96302 -3.72521 3.48507
C 4.33631 -2.85874 -0.83919
C 5.23546 -2.74120 -1.45429
C 3.80770 -4.13780 -0.62195
C 4.29010 -5.01649 -1.06349
C 2.66199 -4.28122 0.16639
C 2.25107 -5.28134 0.34536
C 2.02431 -3.16857 0.75354
C 0.79796 -3.40393 1.63569
C 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
| 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 | -0.53685 | 3.14691 |
| H     | -0.57185 | 0.13553  | 2.97547 |
| B     | -1.55054 | -1.22618 | -1.67760 |
| C     | -3.84058 | -0.67854 | -0.63857 |
| H     | -4.30492 | -0.49137 | 0.34699 |
| C     | -3.70091 | 0.31876  | -1.10158 |
| C     | -4.79233 | -1.50299 | -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\text{NM}-15\text{SCN})**

| SCF (BP86) Energy = -2134.41275196 |
| Enthalpy 0K = -2133.3870725 |
| 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 |
| C  | 3.48278 | 2.88106 | -2.43095 |
| H  | 2.68377 | 4.30974 | -1.74643 |
| C  | 2.28097 | 3.79982 | -3.36989 |
| C  | 1.38585 | 2.57175 | -1.85202 |
| C  | 0.09458 | 3.01613 | -2.23101 |
| C  | 0.10039 | 3.85229 | -2.93607 |
| C  | -1.17470 | 2.75191 | -1.65636 |
| C  | -2.23234 | 3.81127 | -1.95509 |
| C  | -2.07912 | 4.23153 | -2.96178 |
| C  | -2.13447 | 4.64600 | -1.23833 |
| C  | -3.25924 | 3.42972 | -1.87421 |
| C  | -2.74289 | 1.69353 | -0.19965 |
| C  | -2.93418 | 2.39925 | 1.02406 |
| C  | -4.21200 | 2.39603 | 1.61916 |
| C  | -4.36290 | 2.94098 | 2.55795 |
| C  | -5.28769 | 1.72468 | 1.03364 |
| C  | -6.26789 | 1.74527 | 1.50295 |
| C  | -5.08588 | 1.01435 | -0.15618 |
| C  | -5.92763 | 0.47713 | -0.60242 |
| C  | -3.82628 | 0.96878 | -0.78631 |
| C  | -3.64857 | 0.15128 | -2.07132 |
| C  | -2.62305 | -0.26341 | -2.03966 |
| C  | -3.75779 | 1.00513 | -3.35810 |
| C  | -4.73046 | 1.52692 | -3.40090 |
| Element | X  | Y  | Z  |
|---------|----|----|----|
| 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       | 3.18734 | -2.30304 | 2.62668 |
| C       | 3.60535 | -2.10607 | 3.51581 |
| H       | 3.06788 | -0.36105 | 2.36220 |
| C       | 2.02853 | -3.93841 | 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 |
| C       | 3.89449 | -3.97463 | 4.60088 |
| N       | -0.74655 | -1.25224 | 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 |
| C       | -4.18341 | -1.25810 | 3.41096 |
| C       | -3.61076 | -2.92234 | 3.59572 |
| C       | -5.41018 | -2.73080 | 2.38996 |
| C       | -5.30952 | -3.69774 | 1.86533 |
| H       | -6.10537 | -2.87990 | 3.23393 |
| H       | -5.88095 | -2.01883 | 1.68923 |

**SCF (BP86) Energy** = \(-2134.34841047\)

**Enthalpy 0K** = \(-2133.411866\)

**Enthalpy 298K** = \(-2133.350189\)

**Free Energy 298K** = \(-2133.509294\)

**Lowest Frequency** = \(9.2700 \text{ cm}^{-1}\)

**Second Frequency** = \(14.6642 \text{ cm}^{-1}\)

**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 |
| C      | 2.22885 | 0.00151 | 0.01072 |
| C      | 0.68626 | -4.10330 | -2.37552 |
| H      | -0.35788 | -4.44714 | -2.38517 |
| C      | 1.23718 | -4.77559 | -1.69366 |
| H      | 1.12121 | -4.22334 | -3.37932 |
| C      | 0.82008 | -2.66351 | -1.89686 |
| C      | 1.90202 | -1.93573 | -2.47933 |
| C      | 2.36358 | -2.44205 | -3.33094 |
| C      | 2.62636 | -0.80612 | -2.02177 |
| C      | 3.92709 | -0.50653 | -2.75685 |
| C      | 4.27551 | -1.37196 | 27.33963 |
| C      | 4.72257 | -0.19709 | -2.06209 |
| C      | 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 |
| C      | 5.55907 | 0.54620 | 2.17510 |
| C      | 5.09200 | 2.37336 | 1.12720 |
| C      | 5.81230 | 2.97571 | 1.69066 |
| C      | 4.31700 | 2.95203 | 0.11950 |
| C      | 4.44259 | 4.01560 | -0.11277 |
| Element | SCF (BS2) Energy | SCF (BP86) Energy | SCF (BP86-D3BJ) Energy | SCF (Toluene) Energy |
|---------|------------------|-------------------|------------------------|---------------------|
| Mg      | 0.00011          | -0.19366          | -0.08449               | 0.00061             |
| O       | -0.20928         | -0.36620          | -0.08909               | -0.10015            |
| N       | -0.23699         | 0.05054           | 0.21075                | 0.00176             |
| N       | 1.08170          | 1.19842           | 1.25712                | 1.01561             |
| N       | 1.08652          | -1.93864          | -0.10299               | -1.51874            |
| N       | -2.46447         | 0.36145           | -1.54901               | -1.37501            |
| C       | 1.70029          | -3.13924          | 2.76785                | 1.50700             |
| C       | 1.18132          | -4.00727          | 2.33238                | -1.38085            |
| C       | 2.78212          | -3.34729          | 2.70782                | -1.48072            |
| C       | 1.34803          | -1.85172          | 2.03166                | -2.89896            |
| C       | 1.34815          | -0.67480          | 2.83193                | -2.18569            |
| H       | 1.52982          | -0.86404          | 3.89363                | -3.48769            |
| C       | 1.40358          | 0.70573           | 2.47366                | -2.21785            |

**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
SCF (Toluene) Energy = -2134.42852105
Enthalpy OK = -2133.402653

SCF (Toluene) Energy = -2134.74250519
SCF (Toluene) Energy = -2334.18376464

Mg -0.44649 -0.08345 -0.34815
O 1.55591 -3.29964 0.27834
N 0.65453 -1.65152 -1.15996
H 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
H -1.98767 1.67397 -2.48361
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
H -3.96667 0.77332 1.38144
C -5.07212 0.48104 2.20336
H -5.34293 1.17942 3.00137
H -5.83069 -0.68009 2.02506
H -6.69115 -0.88583 2.67041
H -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
H -3.17707 2.05886 1.64142
C -2.16783 1.91514 1.21193
C -3.80953 3.27563 0.92517
H -4.85058 3.42727 1.26212
C -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
H -1.42174 -3.63502 1.84006
C 1.38590 2.45580 -1.06924
C -2.26843 -3.06888 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

Enthalpy = -2133.402653

Free Energy 298K = -2133.495513
Lowest Frequency = 13.3749 cm⁻¹
Second Frequency = 19.7027 cm⁻¹

SCF (BP86-D3BJ) Energy = -2133.43424321
SCF (BS2) Energy = -2334.18376464

16_3CM
Enthalpy 0K =

\[ \begin{align*}
\text{TS} & : H = 0.96457 \\
& : C = 0.423 \\
H & : 2.03100 \\
C & : 0.98340 \\
& : 6.68035 \\
H & : 5.59110 \\
C & : 3.50220 \\
& : 3.58172 \\
H & : 1.32458 \\
C & : 4.01265 \\
& : 0.45915 \\
H & : 1.50246 \\
C & : 4.59155 \\
& : 0.79975 \\
H & : 3.94923 \\
C & : 5.80358 \\
& : 4.54678 \\
H & : 2.92405 \\
C & : 5.96387 \\
& : 4.58713 \\
H & : 2.03100 \\
C & : 3.56542 \\
& : 0.79975 \\
H & : 2.35542 \\
C & : 4.18571 \\
& : 3.33204 \\
H & : 2.97957 \\
C & : 3.80420 \\
& : 2.1298 \\
H & : 1.43297 \\
C & : 4.71831 \\
& : 0.79975 \\
H & : 5.49475 \\
C & : 3.02130 \\
& : 3.98863 \\
H & : -0.07587 \\
O & : 2.50009 \\
& : 1.07392 \\
N & : -0.17198 \\
& : 1.84234 \\
N & : -0.41231 \\
C & : -0.79290 \\
& : 3.26531 \\
H & : -0.03737 \\
H & : 3.96604 \\
H & : -1.75888 \\
H & : 2.96303 \\
C & : -0.94177 \\
& : 2.03270 \\
C & : -1.98700 \\
& : 1.14704 \\
& : 1.84663 \\
& : 2.50762 \\
& : 3.79906 \\
& : 2.24997 \\
& : -0.29001 \\
& : 0.19312 \\
& : -0.88241 \\
& : 3.83633 \\
& : -2.63957 \\
& : 0.28795 \\
& : -0.54639 \\
& : -1.23111 \\
& : -1.41011 \\
& : -0.78633 \\
& : -0.20761 \\
& : 3.54635 \\
& : 0.34331 \\
& : 1.62975 \\
& : 0.87146 \\
& : 0.93577 \\
& : 0.43897 \\
& : 0.10899 \\
& : 0.54060 \\
& : 0.93718 \\
& : 0.09906 \\
& : 3.25552 \\
& : 2.88875 \\
& : 3.25594 \\
& : 2.30175 \\
& : 2.97027 \\
& : 2.82849 \\
& : 0.43812 \\
& : 0.84348 \\
& : 1.67759 \\
& : 0.20008 \\
& : 0.52751 \\
& : 0.86586 \\
& : -0.37382 \\
& : 0.03907 \\
& : 1.12009 \\
& : 0.43217 \\
& : 0.49498
\end{align*} \]

Second Frequency = 14.2054 cm⁻¹

SCF (BP86-D3BJ) Energy = -2134.41270561
Enthalpy OK = -2133.388114
Enthalpy 298K = -2133.327188
Free Energy 298K = -2133.480543
Lowest Frequency = -116.9586 cm⁻¹
|    |    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|----|
|    |    |    |    |    |    |    |    |
|    |    |    |    |    |    |    |    |
|    |    |    |    |    |    |    |    |
|    |    |    |    |    |    |    |    |
|    |    |    |    |    |    |    |    |
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|    |    |    |    |    |    |    |    |
|    |    |    |    |    |    |    |    |
|    |    |    |    |    |    |    |    |

### 18$_{\text{Be}}$

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 = -2439.6596479

SCF (Toluene) Energy = -2439.29750054

SCF (B22) Energy = -2639.12042748

### Mg

| Nucleus | X (Å) | Y (Å) | Z (Å) |
|---------|-------|-------|-------|
| O       | -0.51837 | 1.51291 | 1.49085 |
| N       | -0.219792 | 3.12049 | 1.37058 |
| C       | -0.48768 | -1.96065 | 1.28248 |
| H       | 2.31398 | -0.56304 | 0.84460 |
| N       | -1.73021 | 1.71637 | -0.67177 |
| C       | -0.35868 | -3.39034 | 3.33799 |
| H       | -0.150283 | -3.11038 | 4.38383 |
| C       | 0.14821 | -4.35422 | 3.15778 |
| H       | -1.43685 | -3.55613 | 3.21276 |
| C       | 0.18723 | -2.31964 | 2.39582 |
| H       | 1.46579 | -1.82299 | 2.77800 |
| C       | 1.80067 | -2.19920 | 3.74855 |
| C       | 2.49759 | -1.20223 | 2.02158 |
| O       | 3.89812 | -1.33007 | 2.60947 |
| C       | 4.58723 | -1.77603 | 1.87317 |
| C       | 3.89489 | -1.95766 | 3.51213 |
| H       | 4.31787 | -0.34465 | 2.86898 |
| C       | -1.58829 | -2.81975 | 0.87967 |
| H       | -1.31345 | -0.04347 | 0.18269 |
| C       | -2.38647 | -4.86721 | -0.19173 |
| H       | -2.17056 | -5.80014 | -0.72419 |
| C       | -3.71240 | -4.53369 | 0.09613 |
| C       | -4.53093 | -5.19794 | -0.20060 |
| C       | -3.97725 | -3.33793 | 0.77061 |
| C       | -5.01309 | -3.07077 | 1.00584 |
| C       | -2.94184 | -2.47075 | 1.17090 |
| C       | 0.09765 | -4.48058 | -0.20361 |
| C       | 0.80777 | -3.71210 | 0.14667 |
| C       | 0.48633 | -5.82183 | 0.46149 |
| H       | 0.39767 | -5.78150 | 1.55980 |
| C       | 1.52911 | -6.08720 | 0.21416 |
| C       | -0.15871 | -6.64566 | 0.10802 |
| C       | 0.23176 | -4.59421 | -1.73907 |
| C       | -0.45522 | -5.35883 | -2.14227 |
| C       | 1.25665 | -4.89841 | -2.01438 |
| C       | -0.00321 | -3.64200 | -2.24175 |
| C       | 0.31228 | -1.21877 | 1.96299 |
| H       | -2.41792 | -0.57521 | 1.97818 |
| C       | -3.67501 | -1.57575 | 3.42541 |
| C       | -4.53322 | -2.27027 | 3.45055 |
| C       | -3.96142 | -0.67295 | 3.99384 |
| C       | -2.83872 | -2.05811 | 3.95651 |
| C       | -4.46988 | -0.41432 | 1.33180 |
| C       | -4.72794 | -0.14562 | 0.28173 |
| C       | -6.42291 | 0.52240 | 1.89504 |
| C       | -5.42192 | -0.97239 | 1.36416 |
| C       | 3.50148 | -0.18466 | 0.09988 |

**Enthalpy 298K**

-2438.215832 cm$^{-1}$

**Free Energy 298K**

-2438.312050 cm$^{-1}$

**Lowest Frequency**

18.2919 cm$^{-1}$

**Second Frequency**

29.4770 cm$^{-1}$

-2439.6596479 cm$^{-1}$

-2439.29750054 cm$^{-1}$

-2639.12042748 cm$^{-1}$
SCF (BP86) Energy = -2439.29263263
Enthalpy 0K = -2438.219999
Enthalpy 298K = -2438.154496
Free Energy 298K = -2438.318145

SCF (BP86-D3BJ) Energy = -2439.65448579
SCF (Toluene) Energy = -2439.29911452
SCF (BS2) Energy = -2639.12174260

|   |   |
|---|---|
|   |   |
|   |   |
|   |   |

-67-
SCF (BP86) Energy = -2220.5559966
Enthalpy HK = -2219.464203
Enthalpy HK' = -2219.398983
Free Energy 298K = -2219.561573
Lowest Frequency = -135.2496 cm⁻¹
Second Frequency = 16.4369 cm⁻¹
SCF (BP86-D3BJ) Energy = -2220.8742985
SCF (Toluene) Energy = -2220.56037645
SCF (B82) 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

TS (5-5b)

SCF (BP86) Energy = -2220.5559966
Enthalpy HK = -2219.464203
Enthalpy HK' = -2219.398983
Free Energy 298K = -2219.561573
Lowest Frequency = -135.2496 cm⁻¹
Second Frequency = 16.4369 cm⁻¹
SCF (BP86-D3BJ) Energy = -2220.8742985
SCF (Toluene) Energy = -2220.56037645
SCF (B82) 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

TS (5-5b)

SCF (BP86) Energy = -2220.5559966
Enthalpy HK = -2219.464203
Enthalpy HK' = -2219.398983
Free Energy 298K = -2219.561573
Lowest Frequency = -135.2496 cm⁻¹
Second Frequency = 16.4369 cm⁻¹
SCF (BP86-D3BJ) Energy = -2220.8742985
SCF (Toluene) Energy = -2220.56037645
SCF (B82) 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
Second Frequency = 17.9582
Free Energy 298K = -2219.580203
SCF (BP86) Energy = -2220.56913551
Enthalpy OK = -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 = -2350.330441

Mg  0.32233  0.05980 -0.40496
O  -1.54899  0.56611  3.62572
O  -0.21797  -1.9885  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  0.65420
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 -1.72478
C  3.99052  3.34293 -1.83128
C  4.87982  3.81870 -1.37902
C  3.39389  4.13387 -2.31765
C  4.43455  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
C  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
C  4.99178  -4.21158 -0.92616
C  3.79293  -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
H  -1.57772  -2.34939 -2.21792
C  -1.51398  -3.42907 -2.74228
C  -2.70289  -4.01929  0.05677
H  -2.66269  -4.91956  0.77995
C  -3.93813  -3.71601 -0.47827
H  -4.85269  -4.24420 -1.88471
C  -3.90035  -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  0.17463
5c
SCF (BP86) Energy = -1651.45464818
Enthalpy 0K = -1650.660452
Enthalpy 298K = -1650.661100
Free Energy 298K = -1650.745698
Lowest Frequency = 12.0445 cm⁻¹
Second Frequency = 14.6298 cm⁻¹
SCF (BP86-D3BJ) Energy = -1651.6661818
SCF (Toluene) Energy = -1651.46147313
SCF (BS2) Energy = -1851.09995036

Mg

O 0.07341 2.85658 1.15026
-0.07258 2.85676 -1.15016
-1.50160 -1.61722 0.01309
1.50114 -1.61754 -0.01330
-2.47866 -3.89409 0.01844
-3.10716 -3.72462 0.90958
-2.15785 -4.94585 0.00844
-3.12796 -3.71358 -0.85539
-3.34906 -3.98497 0.01012
-3.00043 -3.54353 -0.00021
-0.00055 -4.63609 -0.00028
1.28659 -2.94924 -0.01046
2.47772 -3.89461 -0.01883
3.10642 -3.72506 -0.90981
2.15669 -4.94631 -0.00913
3.12691 -3.71445 0.85517
-2.84990 -1.10752 0.02523
-3.48272 -0.81564 1.26831
-2.78737 -0.07420 2.60667
-1.86178 -1.63844 2.39566
-2.328212 0.25845 3.28058
-1.73850 0.87204 2.62627
-1.83623 0.07011 4.22208
-3.27414 0.86259 3.52411
-3.64428 -1.93137 3.56434
-3.08311 -2.15279 4.48894
-3.93438 -2.89135 3.10400
-4.57186 -1.40972 3.85890
-4.76565 -0.23515 1.25211
-5.25940 -0.05533 2.20314
-5.41767 0.05912 0.04861
-6.41593 0.50954 0.05770
-4.78007 -0.21839 -1.16464
-5.28502 0.02441 -2.10836
-3.49730 -0.79812 -1.20596
-2.81668 -1.03902 -2.55609
-1.88545 -1.59899 -2.32622
-3.68207 -1.89692 -3.50739
-4.62004 -1.38255 -3.78120
-3.95403 -2.86418 -3.05122
-3.13420 -2.10378 -4.44329
-2.43523 0.30228 -3.22566
-1.89932 0.12495 -4.17505
-1.79059 0.91949 -2.57582
-3.33684 0.89765 -3.45545
2.84955 -1.10811 -0.02530
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 0.23596 -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
C 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

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 = -2777.7100612
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
The page contains a table of data with columns labeled with chemical symbols (H, C, etc.) and numerical values. The data appears to be related to molecular geometries or structural parameters. The table includes columns for atom counts, bond distances, or similar properties. The values are presented in a structured format, likely indicating coordinates or energies associated with a molecular system. The data is organized in a tabular format with rows and columns designed to represent specific data points or measurements.
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 -0.32764 -4.91510
H -2.74721  0.32710 -4.30663
B -0.99787  1.75290 -0.9136
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 -2.65577
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
C -3.42243  6.53141 -0.40722
C -2.71511 -1.10956 -0.37723
H -1.67638 -1.44071 -2.21308
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
C -2.95501 -5.08559 -2.71209
H -6.30333 -2.37723 -3.18478
C -5.19104 -4.55415 -3.72023
C -4.37193  0.48648  0.25288
C -5.37464 -0.05537  1.08679
C -4.65996  1.60372 -0.55754
H -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 -6.16695  3.92517 -1.68759
H -7.95079  2.06862  0.30822
N -0.05140 -0.05241  0.29757

INT (5-17es)
SCF (BP86) Energy = -2777.29838430
Enthalpy OK = -2777.006456
Enthalpy 298K = -2775.929772
Free Energy 298K = -2776.113704
Lowest Frequency = 20.9488 cm⁻¹
Second Frequency = 21.9833 cm⁻¹
\[ \begin{align*} 
&H \quad 7.92488 \quad 0.65965 \quad -0.54942 
&N \quad 2.59803 \quad 0.45720 \quad 0.02324 
&\textbf{TS (5-17\textsubscript{aii})} 
&\text{SCF (BP86) Energy} = -2777.26428012 
&\text{Enthalpy OK} = -2777.974104 
&\text{Enthalpy 298K} = -2775.894793 
&\text{Free Energy 298K} = -2776.081972 
&\text{Lowest Frequency} = -154.0755 \text{ cm}^{-1} 
&\text{Second Frequency} = 18.8854 \text{ cm}^{-1} 
&\text{SCF (BP86-D3BJ) Energy} = -2777.68097799 
&\text{SCF (Toluene) Energy} = -2777.27110341 
&\text{SCF (BS2) Energy} = -2977.17766923 

&Mg \quad -1.08736 \quad -0.20926 \quad -0.38861 
&O \quad 1.64162 \quad 1.13901 \quad 2.46493 
&N \quad -0.23487 \quad 0.65055 \quad 1.18317 
&O \quad 2.86494 \quad 1.02686 \quad -1.38747 
&O \quad 0.83163 \quad -0.08255 \quad -1.22566 
&N \quad -2.76874 \quad 0.87504 \quad -1.14695 
&C \quad -1.98524 \quad -2.12201 \quad -0.59198 
&C \quad -4.45341 \quad 0.83441 \quad -3.01782 
&C \quad -4.51777 \quad 1.91110 \quad -2.84021 
&C \quad -5.42508 \quad 0.34416 \quad -2.83698 
&C \quad -4.21571 \quad 0.66944 \quad -4.08278 
&C \quad -3.37160 \quad 0.19876 \quad -2.14747 
&C \quad -3.08632 \quad -1.15596 \quad -2.48890 
&C \quad -3.52143 \quad -1.46577 \quad -3.44474 
&C \quad -2.60089 \quad -2.24079 \quad -1.71244 
&C \quad -2.82085 \quad -3.61006 \quad -2.36109 
&C \quad -2.59823 \quad -4.43728 \quad -1.66912 
&C \quad -2.10856 \quad -3.69847 \quad -3.21751 
&C \quad -3.82121 \quad -3.72212 \quad -2.76386 
&C \quad -2.02551 \quad -3.27762 \quad 0.3619 
&C \quad -3.27358 \quad -3.67231 \quad 0.95264 
&C \quad -3.31518 \quad -4.80578 \quad 1.78832 
&C \quad -4.47519 \quad -5.10978 \quad 2.21985 
&C \quad -2.16848 \quad -5.54595 \quad 2.08123 
&C \quad -2.22191 \quad -6.42346 \quad 2.73422 
&C \quad -0.95107 \quad -5.14626 \quad 1.52616 
&C \quad -0.04713 \quad -5.72154 \quad 1.74616 
&C \quad -0.85021 \quad -4.03153 \quad 0.66823 
&C \quad 0.51036 \quad -3.75313 \quad 0.03430 
&C \quad 0.55623 \quad -2.69011 \quad -0.26826 
&C \quad 0.68827 \quad -4.60408 \quad -1.24676 
&C \quad 0.63147 \quad -5.67960 \quad -1.00072 
&C \quad 1.67238 \quad -4.40799 \quad -1.70485 
&C \quad -0.08974 \quad -4.39218 \quad -1.99857 
&C \quad 1.69110 \quad -4.02519 \quad 0.99109 
&C \quad 1.88290 \quad -5.10778 \quad 1.10651 
&C \quad 1.50780 \quad -3.61237 \quad 1.99758 
&C \quad 2.59639 \quad -3.55129 \quad 0.57064 
&C \quad -4.59376 \quad -2.92793 \quad 0.73290 
&C \quad -4.38404 \quad -2.01888 \quad 0.5525 
&C \quad -5.61265 \quad -3.77454 \quad -0.06677 
&C \quad -5.88946 \quad -4.68765 \quad 0.4984 
&C \quad -5.21268 \quad -4.09069 \quad -1.04273 
&C \quad -6.53809 \quad -3.19945 \quad -0.24618 
&C \quad -5.22092 \quad -2.50741 \quad 2.08158 
&C \quad -5.49721 \quad -3.38605 \quad 2.68957 
&C \quad -6.14347 \quad -1.92490 \quad 1.91529 
&C \quad -4.52533 \quad -1.89612 \quad 2.67933 
&C \quad -3.33722 \quad 2.15915 \quad -0.76334 
&C \quad -4.45076 \quad 2.20769 \quad 0.13238 
&W \quad 0.22100 \quad 0.31571 \quad 2.23006 
&W \quad -1.96039 \quad -0.53263 \quad 3.87369 
&W \quad 1.24904 \quad -1.45751 \quad 5.25263 
&W \quad 1.38372 \quad 2.01894 \quad 2.83101 
&W \quad -0.68898 \quad 2.86362 \quad 2.71009 
&W \quad -1.81179 \quad 2.06628 \quad 3.48650 
&W \quad -2.20116 \quad 2.14724 \quad 2.10310 
&W \quad 0.68764 \quad 0.52963 \quad 3.35863 
&W \quad 0.73752 \quad 1.29914 \quad 4.69040 
&W \quad 1.72861 \quad 1.15767 \quad 5.15076 
&W \quad -0.02430 \quad 0.92627 \quad 5.39750 
&W \quad 0.58678 \quad 2.37866 \quad 4.54254 
&W \quad 1.08883 \quad -0.93416 \quad 3.62358 
&W \quad 0.98002 \quad -1.56041 \quad 2.72438 
&W \quad 0.48176 \quad -1.38191 \quad 4.42929 
&W \quad 2.14689 \quad -0.95743 \quad 3.92835 
&W \quad 1.14324 \quad 1.32680 \quad 1.14363 
\end{align*} \]
B  2.01216  0.40547  -0.46378  H  3.54537  -0.22581  -3.57472
C  1.16743  2.88009  0.58879  C  3.15578  0.99938  -1.91041
H  1.70219  2.98799  -0.37012  C  4.01685  2.03494  -2.63632
H  0.11311  3.15621  0.37855  H  4.83242  1.56015  -3.20315
C  1.73732  3.88905  1.59072  H  4.44308  2.78649  -1.95935
H  1.21948  3.85500  2.54906  H  3.38096  2.56427  -3.37033
C  2.80237  3.57642  1.84885  C  3.27435  2.30037  0.07697
C  1.79444  5.33989  1.07562  C  4.50419  1.93317  0.72097
H  0.75985  5.66376  0.84525  H  5.19566  2.89536  1.48275
H  2.34443  5.37906  0.11488  H  6.13878  2.61367  1.96278
C  2.42635  6.32675  2.07083  H  4.71253  4.19729  1.63676
H  2.42888  7.35844  1.67828  H  5.26656  4.93003  2.23286
H  1.87639  6.33500  3.02889  C  3.51400  4.55036  1.01309
C  3.47202  6.00575  2.29504  H  3.13557  5.57187  1.12016
C  3.05789  -0.70439  0.61479  C  2.78186  3.63514  0.22880
H  2.26853  -1.12188  1.26048  C  1.53141  4.15778  -0.48270
C  4.09226  0.02720  1.47255  H  0.93238  3.28509  -0.79420
C  4.72500  -0.73684  2.47670  H  1.92132  4.95459  -1.75196
C  4.49016  1.36803  1.30837  H  2.52265  5.83915  -1.47642
C  5.71253  -0.17613  3.30162  H  1.01972  5.31010  -2.28011
H  4.44157  -1.78781  2.60482  H  2.51644  4.35512  -2.45762
C  5.47783  1.93230  2.13158  C  0.64066  5.05335  0.40707
H  4.02948  1.96769  0.51810  H  1.12853  6.01751  0.63401
C  6.09178  1.16514  3.13431  C  0.37633  4.57396  1.36152
H  6.18767  -0.79065  4.07446  H  -0.30087  5.28485  -0.11669
C  5.77086  2.97789  1.98458  C  5.13557  0.54020  0.59765
H  6.86235  1.60661  3.77539  H  4.36434  -0.14297  0.20169
C  4.67865  -1.67449  -0.96213  C  6.32406  0.53714  -0.39472
C  5.62663  -0.61965  -1.11264  H  7.11799  1.22372  -0.05053
C  4.98305  -2.91532  -1.60448  H  6.02399  0.85091  -1.40525
C  6.81485  -0.82200  -1.82980  H  6.76138  -0.47405  -0.46901
C  5.42172  0.36022  -0.68620  C  5.62253  0.01811  1.95517
C  6.17479  -3.10952  -2.30653  H  6.48400  0.55077  2.34610
H  4.25596  -3.72815  -1.50295  H  5.95954  -1.06196  1.83372
C  7.10653  -2.06138  -2.42454  H  4.83382  0.00066  2.72376
H  7.52442  0.00807  -1.92640  C  1.38904  -3.09734  -0.89262
H  6.37887  -4.08192  -2.76895  C  2.28112  -3.76337  0.00078
H  8.04010  -2.20634  -2.97815  C  2.08234  -5.13217  0.27203
N  3.46422  -1.66212  -0.28618  C  1.03039  -5.84699  -0.30736

17*bn-BpinBu

SCF (BP86) Energy = -2777.32932966
Enthalpy OK = -2777.037771
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 = -2797.24595430

Mg  0.77265  0.10147  -0.46418
O  -0.54156  -1.21955  3.63443
O  0.22273  -0.36615  1.62164
O  -2.90645  1.76441  -2.11295
O  -0.80683  0.74499  -1.63850
N  1.63167  -1.70680  -1.24078
C  2.57745  1.29398  -0.71250
C  3.03604  -2.62914  -3.11253
H  2.50565  -3.57756  -2.95866
C  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
SCF (Toluene) Energy = -2208.21455414
Enthalpy 0K = -2207.221771
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

TS(17\text{BM}-17\text{BCN})

\begin{align*}
\text{SCF (BP86) Energy} & = -2208.21455414 \\
\text{Enthalpy 0K} & = -2207.221771 \\
\text{Enthalpy 298K} & = -2207.161081 \\
\text{Free Energy 298K} & = -2207.315888 \\
\text{Lowest Frequency} & = -127.7457 \text{ cm}^{-1} \\
\text{Second Frequency} & = 13.1916 \text{ cm}^{-1} \\
\text{SCF (BP86-D3BJ) Energy} & = -2208.52581262 \\
\text{SCF (Toluene) Energy} & = -2208.22232772 \\
\text{SCF (BS2) Energy} & = -2407.99270097
\end{align*}
$\text{SCF (BP86) Energy} = -2208.22936077$

$\text{Enthalpy OK} = -2207.235016$

$\text{Enthalpy 298K} = -2207.175013$

$\text{Free Energy 298K} = -2207.328105$

$\text{Lowest Frequency} = -87.0444 \text{ cm}^{-1}$

$\text{Second Frequency} = 13.5824 \text{ cm}^{-1}$

$\text{SCF (BP86-D3BJ) Energy} = -2208.54623642$

$\text{SCF (Tolene) Energy} = -2208.23625006$

$\text{SCF (BS2) Energy} = -2408.00663807$

| Bond   | Length (Å) | Angle (°) | Torsion (°) | Energy (kcal/mol) | TS (17ac-17bc) |
|--------|------------|-----------|-------------|--------------------|-----------------|
| Mg-0   | 0.35809    | 0.40345   | 0.38198     |                    |                 |
| O-1    | -1.68228   | -2.64552  | 1.89964     |                    |                 |
| O-2    | -0.38308   | -0.47076  | 2.02869     |                    |                 |
| N-3    | -0.48667   | 2.32142   | 0.28322     |                    |                 |
| N-4    | 0.38248    | 1.02527   | 0.32807     |                    |                 |
| N-5    | -0.29179   | 4.79941   | 0.52562     |                    |                 |
| H-6    | -1.37050   | 4.82605   | 0.73096     |                    |                 |
| H-7    | -0.14293   | 5.22655   | -0.48260    |                    |                 |
| C-8    | 0.23249    | 5.45546   | 1.23810     |                    |                 |
| C-9    | 0.28341    | 3.38802   | 0.57404     |                    |                 |
| C-10   | 1.67457    | 3.33015   | 0.84508     |                    |                 |
| C-11   | 2.11044    | 4.30050   | 1.10121     |                    |                 |
| C-12   | 2.64491    | 2.32731   | 0.59240     |                    |                 |
| C-13   | 4.07646    | 2.86278   | 0.60362     |                    |                 |
| C-14   | 4.13499    | 3.81024   | 0.04468     |                    |                 |
| C-15   | 4.79731    | 2.15580   | 0.17345     |                    |                 |
| C-16   | 4.38135    | 3.08351   | 1.64173     |                    |                 |
| C-17   | 3.46523    | 0.19959   | -0.18158    |                    |                 |
| C-18   | 3.54862    | 0.00035   | -1.59636    |                    |                 |
| C-19   | 4.58392    | -0.80142  | -2.11189    |                    |                 |
| C-20   | 4.64674    | -0.95926  | -3.19194    |                    |                 |
| C-21   | 5.53069    | -1.40349  | -1.27687    |                    |                 |
| C-22   | 6.32950    | -2.02163  | -1.70015    |                    |                 |
| C-23   | 6.18871    | -1.66981  | 0.75896     |                    |                 |
| C-24   | 4.42848    | -0.41353  | 0.67744     |                    |                 |
| C-25   | 4.45015    | -0.25104  | 2.20111     |                    |                 |
| C-26   | 3.55253    | 0.32394   | 2.49321     |                    |                 |
| C-27   | 5.69539    | 0.52677   | 2.69469     |                    |                 |
| C-28   | 6.62010    | -0.02585  | 2.45230     |                    |                 |
| C-29   | 5.66086    | 0.65144   | 3.79154     |                    |                 |
| C-30   | 5.77770    | 1.52509   | 2.24040     |                    |                 |
| C-31   | 4.41972    | -1.62363  | 2.91631     |                    |                 |
| C-32   | 5.37679    | -2.15702  | 2.78179     |                    |                 |

-S81-
18BCN

SCF (BP86) Energy = -2439.27004051
Enthalpy (K) = -2428.19699
Enthalpy 298K = -2438.19194
Free Energy 298K = -2438.293696
Lowest Frequency = 19.0957 cm⁻¹
Second Frequency = 23.4392 cm⁻¹
SCF (BP86-D3BJ) Energy = -2439.6367215
SCF (Toluene) Energy = -2439.7663597
SCF (BS2) Energy = -2639.0915971

Mg 0.23541 -0.51658 0.49408
O 0.35957 1.16192 1.68552
N -1.71683 2.24802 1.66440
H -1.12584 -2.11679 0.84603
N 1.98709 -1.65902 0.41795
N -0.66536 1.13426 -0.56231
C -1.48137 4.28120 2.06738
C -1.38324 -5.14373 1.38552
H -2.54688 -4.02277 2.11820
H -1.13957 4.61621 3.06028
O -0.60779 -3.12637 1.58155
H 0.76751 -3.28372 1.90752
H 0.95822 -4.12589 2.57753
C 1.94215 -2.75316 1.31358
C 3.21266 -3.55014 1.58543
C 3.98924 -2.93200 2.06108
H 3.64769 -3.91307 0.63870
C 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 | 0.43578 |
| H  | -5.78407 | -1.75469 | 0.92378 |
| C  | -3.62216 | -1.81357 | 0.95023 |
| C  | -1.41427 | -3.76976 | -1.60033 |
| C  | -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 | -3.45393 | -3.60756 |
| H  | -0.48229 | -3.60936 | -3.57743 |
| H  | -1.27317 | -2.09597 | -3.02868 |
| C  | -3.54709 | -0.89785 | 2.17643 |
| H  | -2.66462 | -0.26689 | 2.05617 |
| H  | -3.41289 | -1.69390 | 3.49744 |
| C  | -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 |
| C  | -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 |
| H  | 5.76964 | -1.06061 | -1.39522 |
| C  | 6.74900 | -0.94986 | -1.87276 |
| C  | 5.55102 | -0.57133 | -0.10405 |
| H  | 6.36506 | -0.05912 | 0.42067 |
| C  | 4.35395 | -0.71725 | 0.54562 |
| C  | 2.34553 | -2.53071 | -2.28137 |
| H  | 1.39747 | -2.37906 | -1.73932 |
| C  | 2.58180 | -4.05589 | -2.37749 |
| C  | 3.54242 | -4.27417 | -2.87707 |
| H  | 1.78005 | -4.54087 | -2.96203 |
| C  | 2.60509 | -4.52660 | -1.38059 |
| H  | 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 |
| C  | 5.00883 | -0.18660 | 3.95112 |
| C  | 6.22630 | -0.30684 | 2.96151 |
| C  | 4.24032 | 1.44165 | 1.84473 |
| H  | 5.20163 | 1.75316 | 1.40136 |
| C  | 4.17392 | 1.89603 | 2.84835 |
| C  | 3.43342 | 1.85465 | 2.12038 |
| C  | -0.05547 | 2.60490 | -0.52021 |
| C  | -0.88841 | 3.64298 | -1.25069 |
| C  | -2.10267 | 4.14136 | -0.72458 |
| H  | -2.45359 | 3.77203 | 0.24161 |
| C  | -2.84802 | 5.10759 | -1.42001 |
| H  | -3.78149 | 5.48279 | -0.98547 |

### TS(18_{B86}-18_{B86})

| SCF (BP86) Energy | -2439.2614386 |
| Enthalpy DK | -2438.189083 |
| Enthalpy 298K | -2438.124421 |
| Free Energy 298K | -2438.28576 |
| Lowest Frequency | -133.4255 cm⁻¹ |
| Second Frequency | 19.2892 cm⁻¹ |
| SCF (BP86-D3BJ) Energy | -2439.6250732 |
| SCF (Toluene) Energy | -2439.26840736 |
| SCF (BS2) Energy | -2439.0902504 |

| 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 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 0.3034  | -2.5564 | 1.8536  |
| C    | 0.2685  | -4.5008 | 2.7876  |
| H    | 0.3248  | -5.5717 | 2.5217  |
| H    | 1.1347  | -4.2640 | 3.4288  |
| H    | -0.6476 | -4.3557 | 3.3832  |
| C    | 1.5692  | -3.8720 | 0.7119  |
| H    | 1.6338  | -3.2098 | -0.1664 |
| H    | 2.4598  | -3.6916 | 1.3360  |
| H    | 1.6171  | -4.9162 | 0.3547  |
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