# Structural Snapshots of an Al–Cu Bond-Mediated Transformation of Terminal Acetylenes

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## 1 Experimental and Supplementary Information

### 1.1. General information

Except stated otherwise, all the experiments were conducted using standard Schlenk line and/or glovebox techniques under an inert atmosphere of argon. NMR spectra were recorded with an Agilent ProPulse spectrometer ($^{1}$H at 500 MHz, $^{13}$C at 126 MHz). The spectra are referenced relative to residual protio solvent resonances. Elemental analyses were performed at Elemental Microanalysis Ltd., Okehampton, Devon, UK. Solvents were dried by passage through a commercially available solvent purification system and stored under argon in ampoules over 4 Å molecular sieves. $C_6D_6$ and $d_8$-THF was purchased from Sigma-Aldrich, dried over a potassium mirror before distilling and storage over molecular sieves. [(NHC$^{iPr}$)Cu-Al{SiN$^{Dipp}$}] (**1**) and [($^{Me_2}$CAAC)Cu-Al{SiN$^{Dipp}$}] (**4**) were prepared according to reported procedures. [1] All other chemicals were purchased from Merck and used without further purification.

## 1.2. Synthetic Procedures

Synthesis of [(NHC$^{iPr}$)Cu]…[(PhC$^{H}$C$^{H}$)(PhCC)-κ$^2$-C,C'-Al{SiN$^{Dipp}$}] (**2**)

In a J Young's tube, phenylacetylene (5.1 mg, 5.5 μL, 0.05 mmol) was added via micropipette to a colourless solution of [(NHC$^{iPr}$)Cu-Al{SiN$^{Dipp}$}] (**1**, 19 mg, 0.025 mmol) in $C_6D_6$. Quantitative generation of **2** was observed by NMR spectroscopy within 30 mins at room temperature. The colourless solution was then put under vacuum to remove all volatiles and give compound **2** as a colourless waxy solid. Yield 22.5mg, 93%. No meaningful elemental analysis was obtained after several attempts. The related structure of **2a** was characterised by X-ray diffraction analysis on a single crystals obtained by keeping a solution of **2** at –30 °C in hexanes. $^1$H NMR (500 MHz, 298 K, Benzene-$d_6$) δ 7.27-7.23 (m, 2H, *p*-C$_6$*H*$_5$ of AlCCPh), 7.21-7.16 (m, 4H, *m*-C$_6$*H*$_3$) 7.12 – 7.09 (m, 2H, *p*-C$_6$*H*$_3$), 7.00 – 6.91 (m, 4H, *o*- and *m*-C$_6$*H*$_5$ of AlC$_2$H$_2$Ph), 6.85 – 6.80 (m, 3H, C$_6$*H*$_5$ of AlCCPh), 6.79 – 6.73 (m, 1H, *p*-C$_6$*H*$_5$ of AlC$_2$H$_2$Ph), 6.08 (d, *J* = 21.3 Hz, 1H, AlC$_2$*H*$_2$), 5.26 (d, *J* = 21.3 Hz, 1H, AlC$_2$*H*$_2$), 4.60 (sept, *J* = 6.8 Hz, 2H, C*H*Me$_2$), 4.41 (sept, *J* = 6.8 Hz, 2H, C*H*Me$_2$), 4.08 (sept, *J* = 7.1 Hz, 2H, NC*H*Me$_2$), 1.58 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$ on SiN$^{Dipp}$), 1.52 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$ on SiN$^{Dipp}$), 1.47 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$ on SiN$^{Dipp}$), 1.41 (s$_{br}$, 4H, SiC*H*$_2$), 1.39 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$ on SiN$^{Dipp}$), 1.27 (s, 6H, NC*Me*), 0.78 (d, *J* = 7.1 Hz, 12H, NCH*Me*$_2$), 0.54 (s, 6H, Si*Me*$_2$), 0.47 (s, 6H, Si*Me*$_2$). $^{13}$C NMR (126 MHz, 298 K, Benzene-$d_6$) δ 180.6 (Cu*C*$_{carbene}$), 149.4, 147.9 (*i*- and *o*- *C*$_6$H$_3$ of SiN$^{Dipp}$), 147.8 (*i*-*C*$_6$H$_5$ of AlCCPh), 141.5 (*i*-*C*$_6$H$_5$ of AlC$_2$H$_2$Ph), 140.0 (Al*C*$_2$H$_2$), 132.0$^+$, 128.4*, 127.5$^+$ ($^+$*o*- and *m*-C$_6$*H*$_5$ of AlC$_2$H$_2$Ph; *Al*C*$_2$H$_2$), 127.3, 126.9 (*C*$_6$H$_5$ of AlCCPh), 126.7 (*p*-*C*$_6$H$_3$ of SiN$^{Dipp}$), 124.6 (N*C*Me), 123.7, 123.7 (*p*-*C*$_6$H$_5$ of AlC$_2$H$_2$Ph and C$_6$*H*$_5$ of AlCCPh), 122.2 (*m*-*C*$_6$H$_3$), 113.1 (AlC*C*Ph), 53.8 (N*C*HMe2), 27.9 (*C*HMe$_2$), 27.8(*C*HMe$_2$), 26.5 (CH*Me*$_2$), 26.5(CH*Me*$_2$), 26.2(CH*Me*$_2$), 26.1 (CH*Me*$_2$), 22.2 (NCH*Me*$_2$), 15.4 (Si*C*H$_2$), 9.7 (NC*Me*), 1.9 (Si*Me*$_2$), 1.8 (Si*Me*$_2$). $^{13}$C resonances correlated to Al*C*CPh were not observed.

**Figure S1.** $^{1}$H NMR (500 MHz, 298 K, $d_6$-benzene) spectrum of **2**. *grease

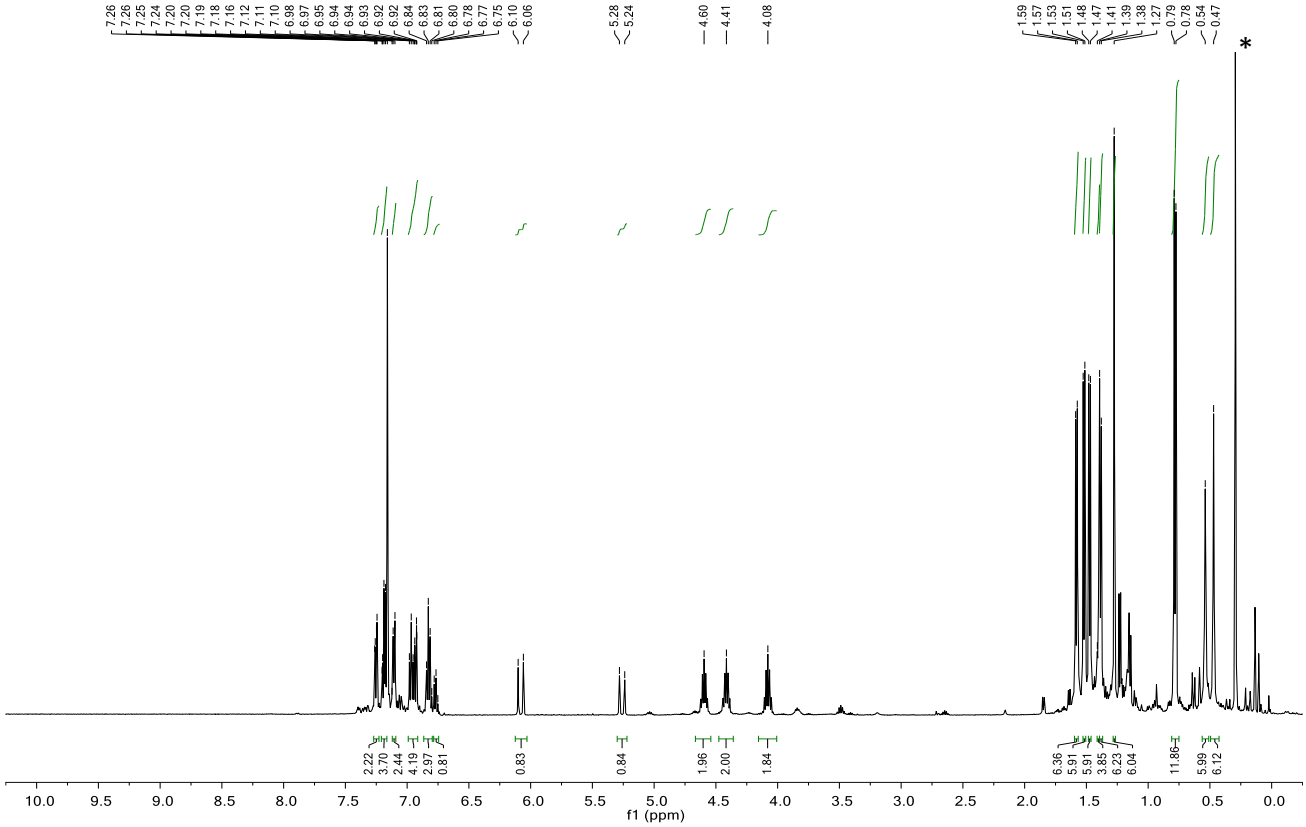



**Figure S2.** $^{13}$C NMR (126 MHz, 298 K, $d_6$-benzene) spectrum of **2**.

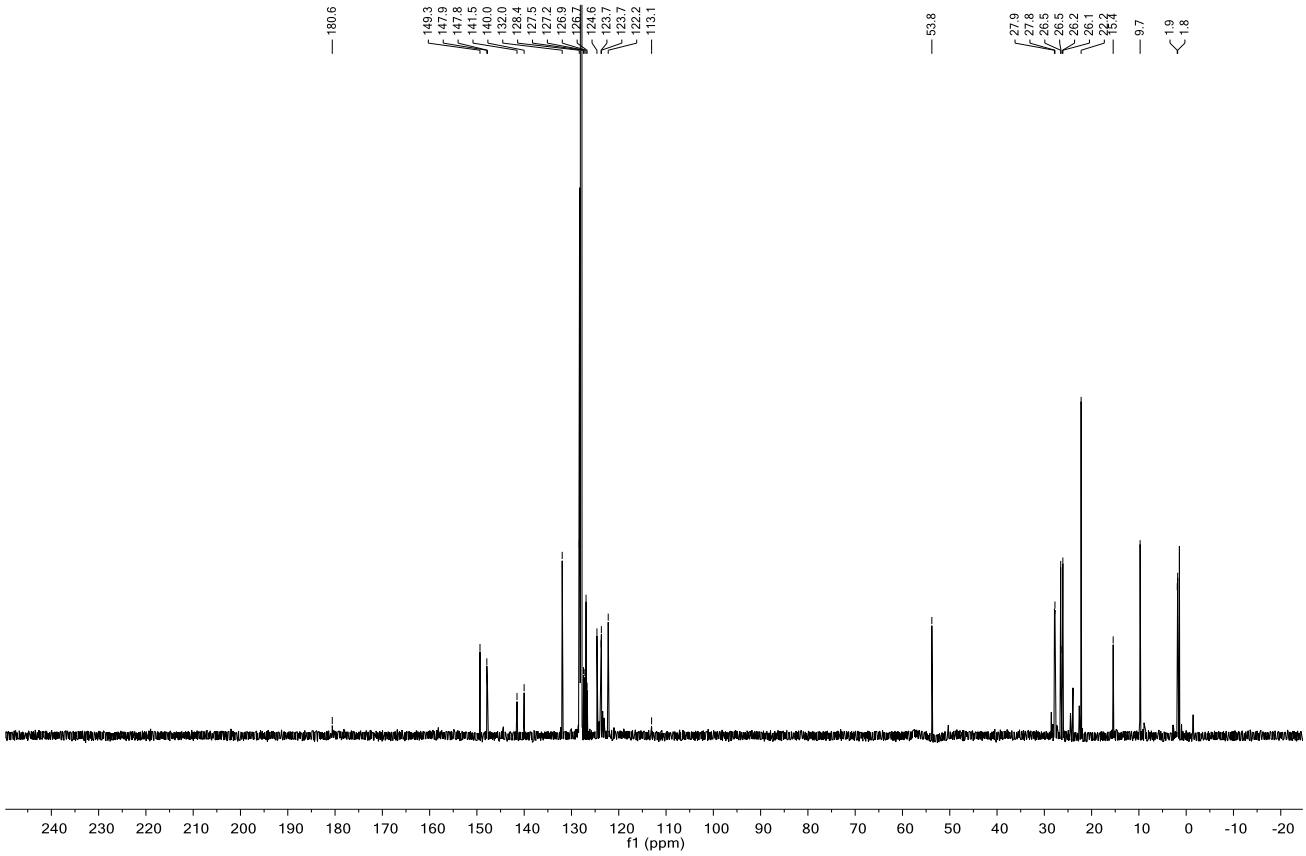


**Figure S3.** $^{1}$H-$^{1}$H COSY spectrum of **2**.

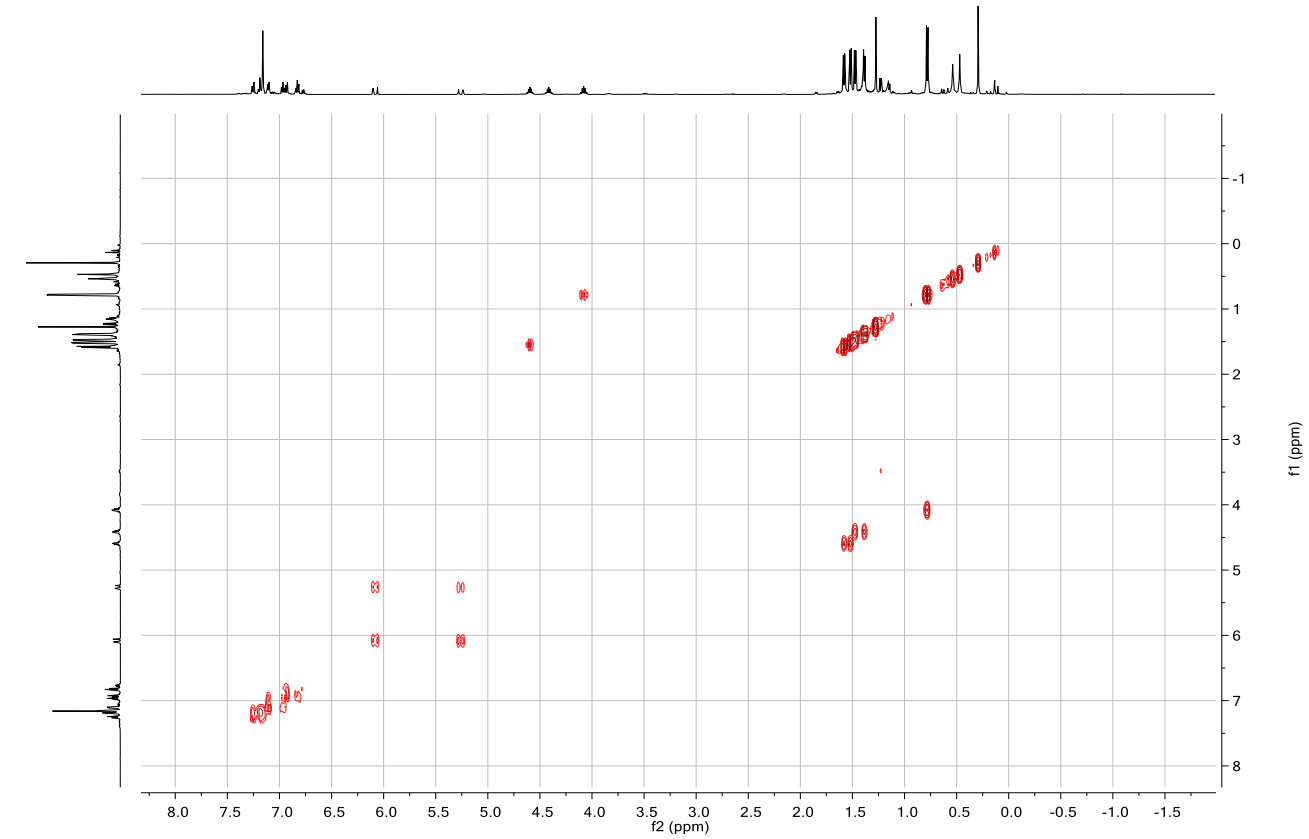



**Figure S4.** $^{1}$H-$^{13}$C HSQC spectrum of **2**.

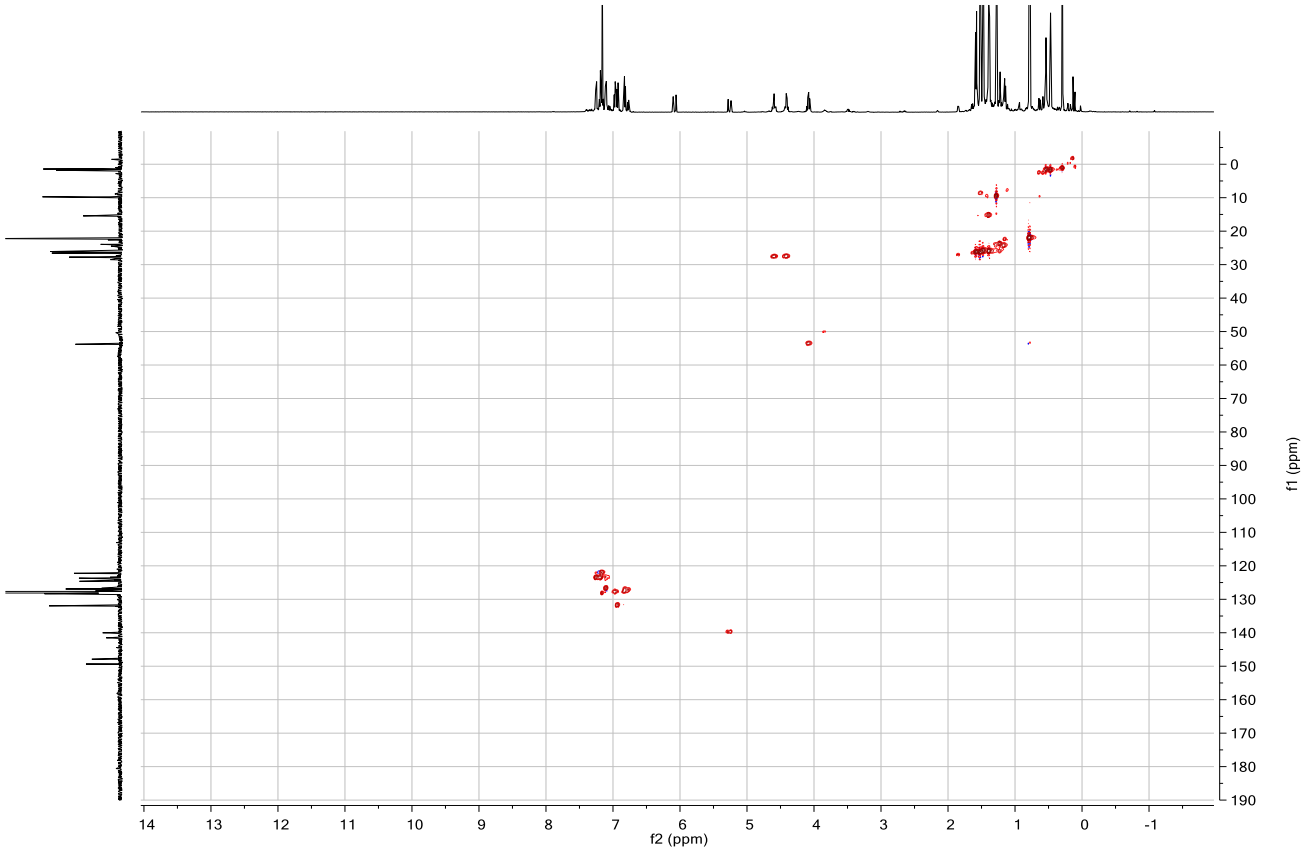
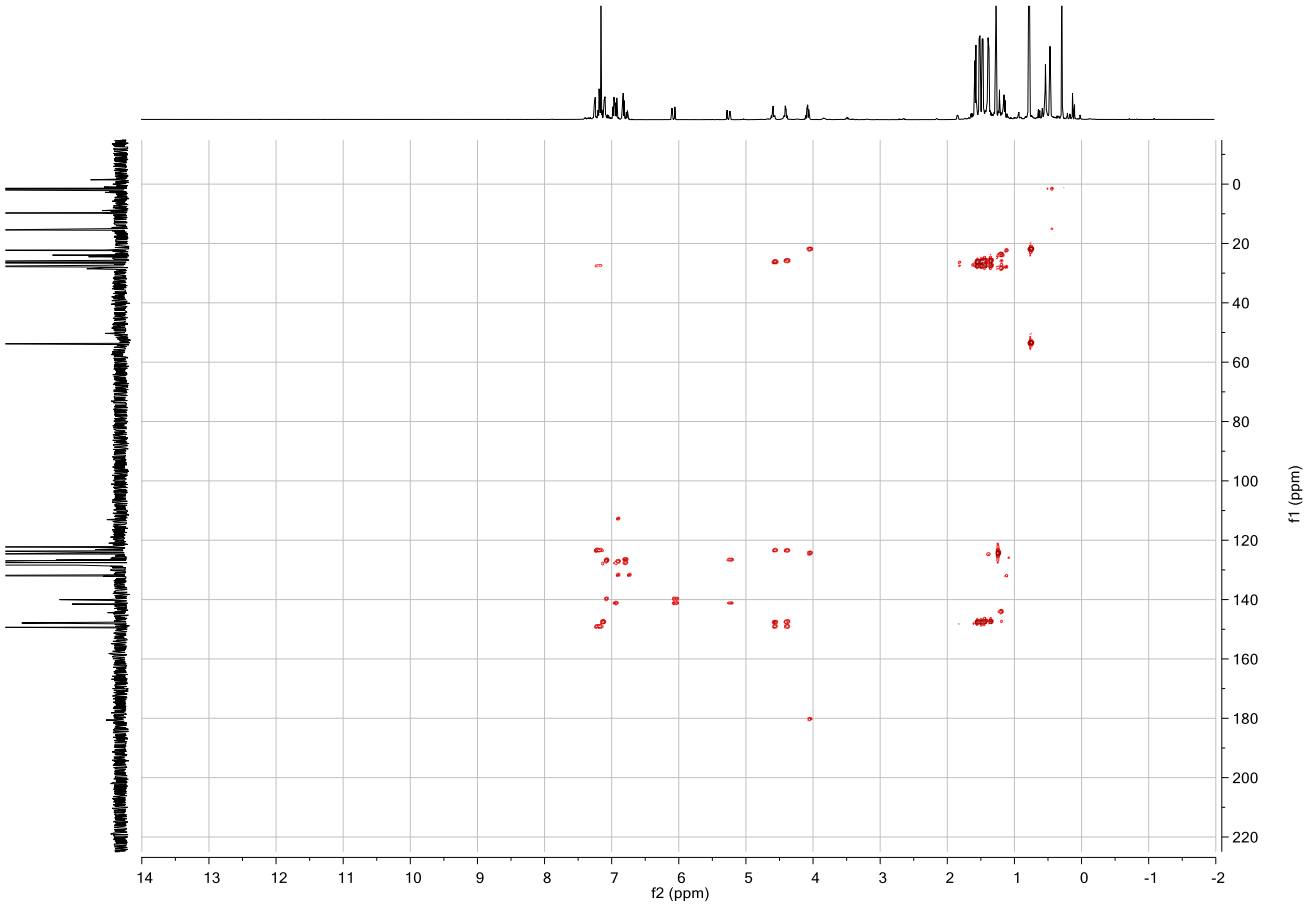


**Figure S5.** $^{1}H$-$^{13}C$ HMBC spectrum of **2**.



Synthesis of [(NHC$^{iPr}$)Cu…(PhCC)$_2$)-κ$^2$-C,C'-Al{SiN$^{Dipp}$}] (**3**)

In a J Young's tube, phenylacetylene (7.6 mg, 8.2 μL, 0.075 mmol) was added via micropipette to a colourless solution of [(NHC$^{iPr}$)Cu-Al{SiN$^{Dipp}$}] (**1**, 19 mg, 0.025 mmol) in $C_6D_6$. The colourless reaction mixture was then kept at 60 °C overnight before full conversion of **1** and generation of styrene was confirmed by NMR spectroscopy. All volatiles were then removed *in vacuo*, affording **3** as a white powder. Yield 20 mg, 83%. Colourless single crystals suitable for X-ray crystallography was obtained by slow evaporation of a hexane solution of **3** at room temperature. Anal Calc'd for $C_{57}H_{81}AlCuN_4Si_2$ (**3**, 969.00) C, 70.65; H, 8.43; N, 5.78 %. Found: C, 70.62; H, 8.36; N, 5.74 %. $^1$H NMR (500 MHz, 298 K, Benzene-$d_6$) δ 7.24 (d, $J$ = 7.5 Hz, 4H, *m*-C$_6$*H*$_3$ on SiN$^{Dipp}$), 7.13 (t, $J$ = 7.5 Hz, 2H, *p*-C$_6$*H*$_3$ on SiN$^{Dipp}$), 6.99 – 6.94 (m, 4H, *o*-C$_6$*H*$_5$ on AlCCPh), 6.86 – 6.81 (m, 4H, *m*-C$_6$*H*$_5$ on AlCCPh), 6.80 – 6.74 (m, 2H, *p*-C$_6$*H*$_5$ on AlCCPh), 4.47 (sept, $J$ = 6.8 Hz, 4H, C*H*Me$_2$ on SiN$^{Dipp}$), 4.14 (sept, $J$ = 7.0 Hz, 2H, NC*H*Me$_2$), 1.57 (d, $J$ = 6.8 Hz, 12H, C*H*Me$_2$ on SiN$^{Dipp}$), 1.50 (d, $J$ = 6.8 Hz, 12H, C*H*Me$_2$ on SiN$^{Dipp}$), 1.41 (s, 6H, NC*Me*), 1.40 (s, 4H, SiC*H*$_2$), 0.74 (d, $J$ = 7.0 Hz, 12H, NCH*Me*$_2$), 0.51 (s (br), 12H, Si*Me*$_2$). $^{13}$C NMR (126 MHz, 298 K, Benzene-$d_6$) δ 181.9 (Cu*C*$_{carbene}$), 148.5 (*i*-*C*$_6$H$_3$ on SiN$^{Dipp}$), 147.8 (*o*-*C*$_6$H$_3$ on SiN$^{Dipp}$), 132.1 (*o*-*C*$_6$H$_5$ of AlCCPh), 127.5 (*m*-*C*$_6$H$_5$ of AlCCPh), 126.6 (*p*-*C*$_6$H$_5$ of AlCCPh), 125.2 (N*C*Me), 123.4 (*m*-*C*$_6$H$_3$ on SiN$^{Dipp}$), 122.3 (*p*-*C*$_6$H$_3$ on SiN$^{Dipp}$), 110.9 (AlC*C*Ph), 53.9 (N*C*HMe$_2$), 27.9 (*C*HMe2 on SiN$^{Dipp}$), 26.6 (CH*Me*$_2$ on SiN$^{Dipp}$), 26.1 (CH*Me*$_2$ on SiN$^{Dipp}$), 22.1 (NCH*Me*$_2$), 15.5 (Si*C*H$_2$), 9.8 (NC*Me*), 1.5 (Si*Me*$_2$). $^{13}$C resonance correlated to Al*C*CPh and *i*-*C*$_6$H$_5$ on AlCCPh were not observed.

**Figure S6.** $^{1}$H NMR (500 MHz, 298 K, $d_6$-benzene) spectrum of **3**. *grease

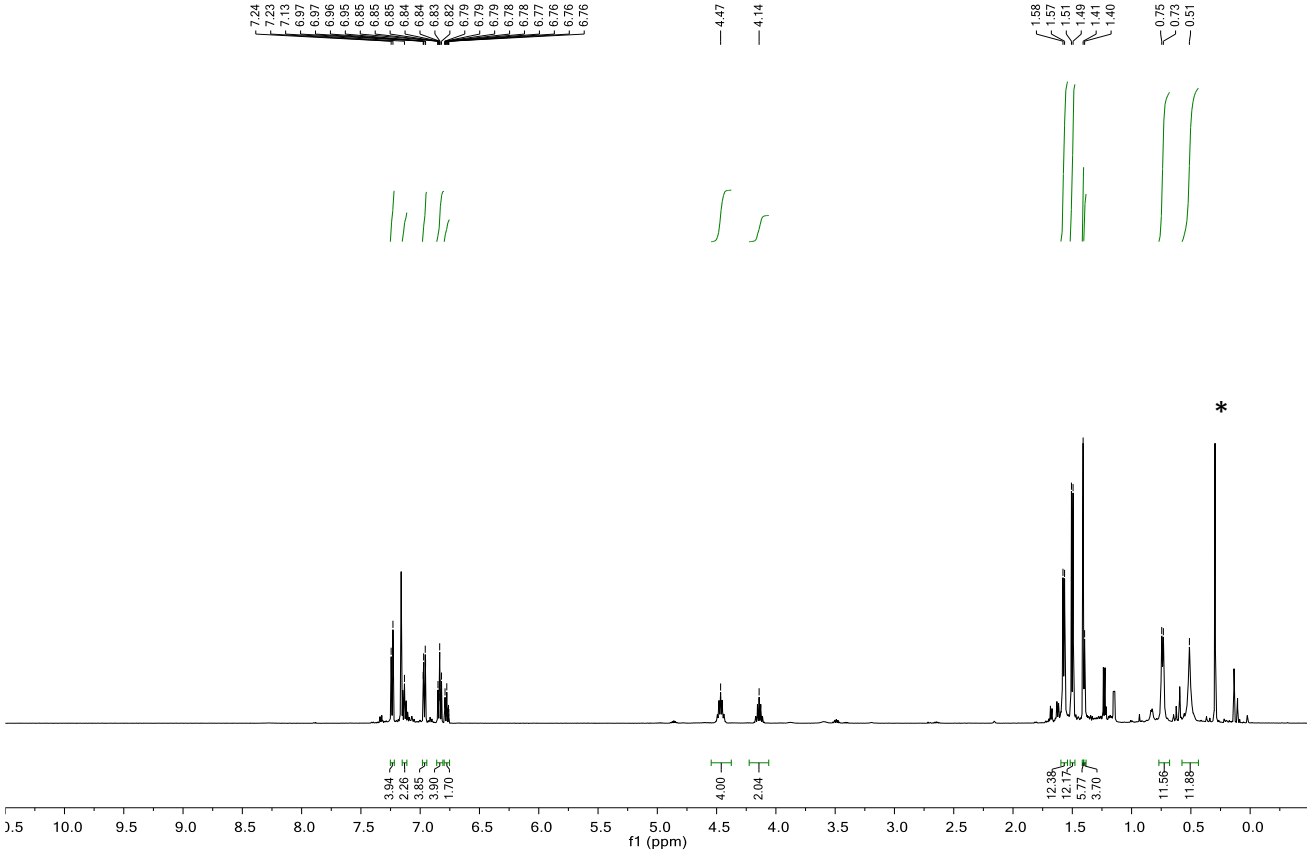



**Figure S7.** $^{13}$C NMR (126 MHz, 298 K, $d_6$-benzene) spectrum of **3**.

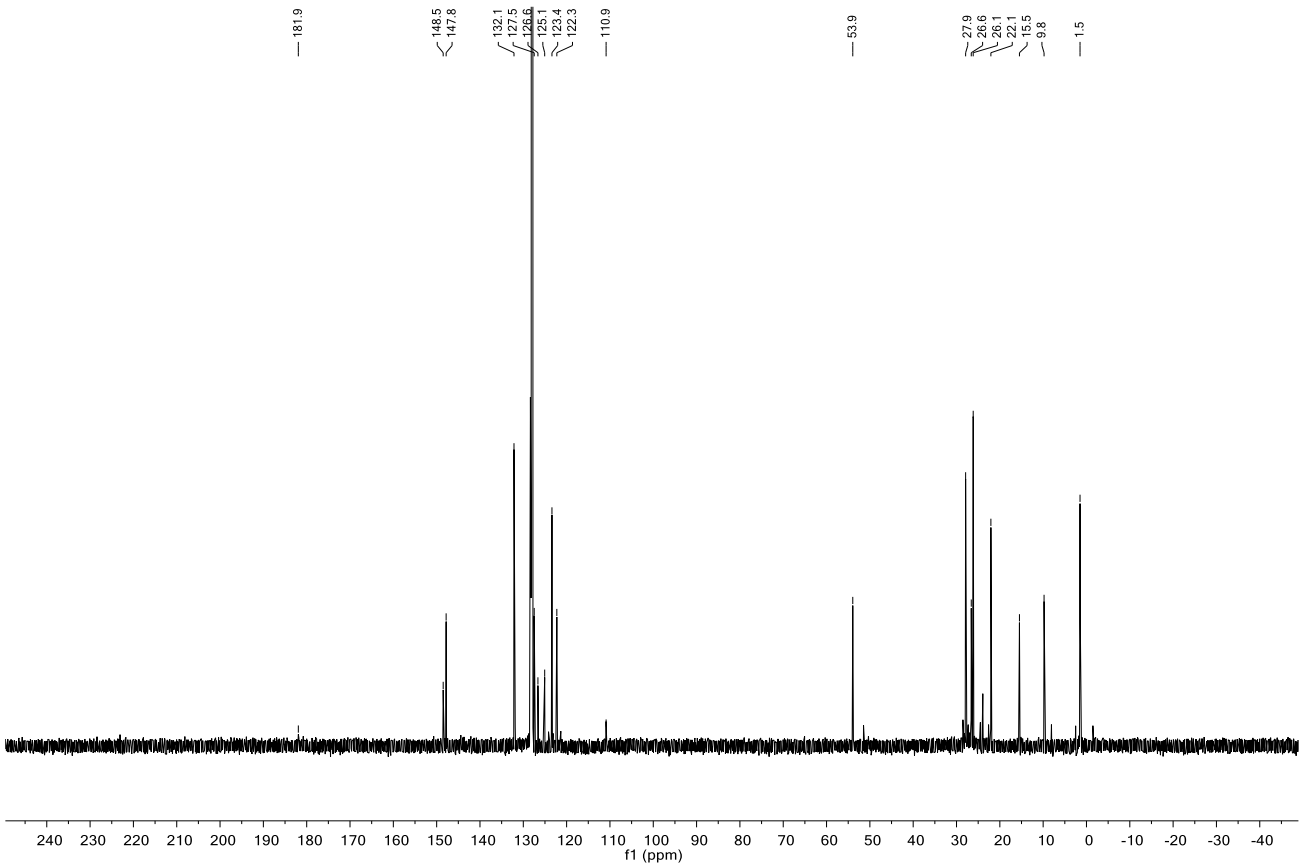


**Figure S8.** $^{1}$H-$^{1}$H COSY spectrum of **3**.

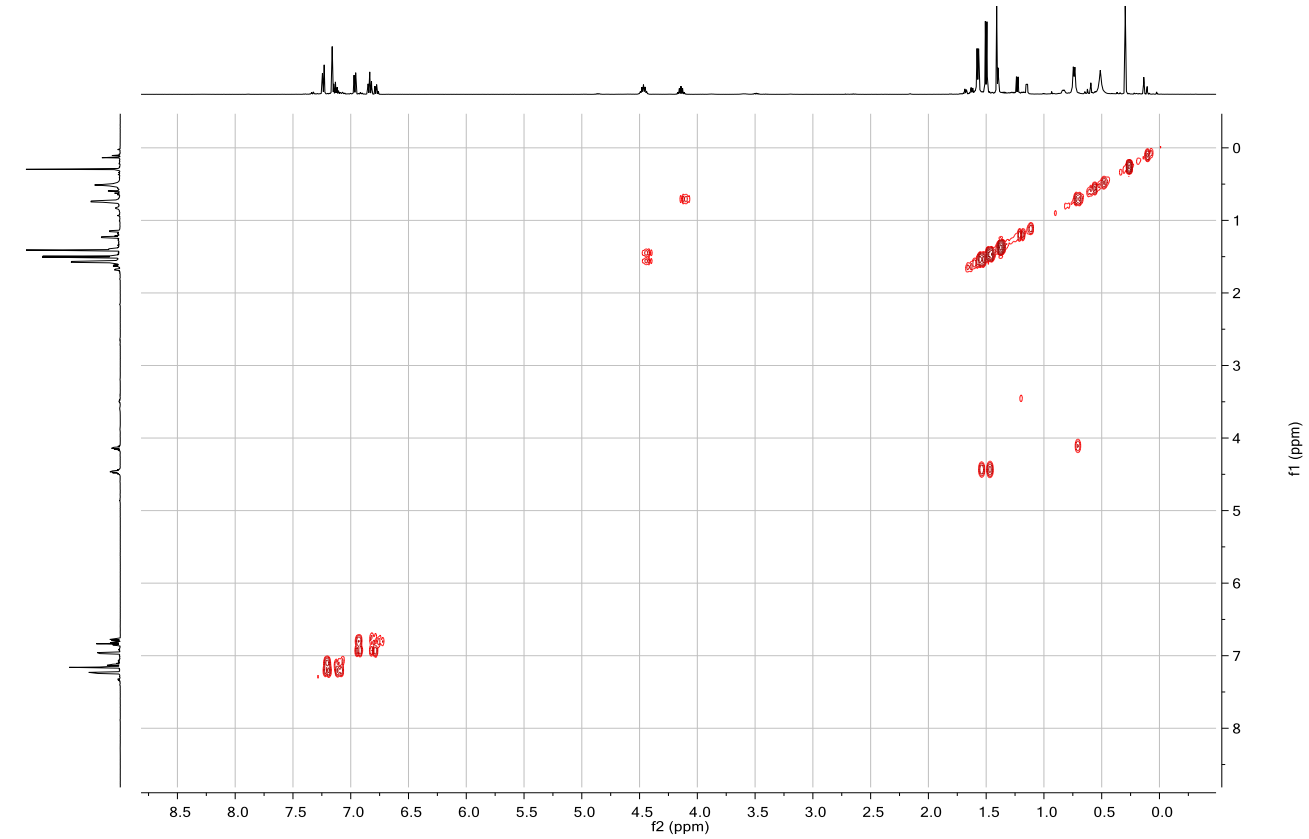



**Figure S9.** $^{1}$H-$^{13}$C HSQC spectrum of **3**.

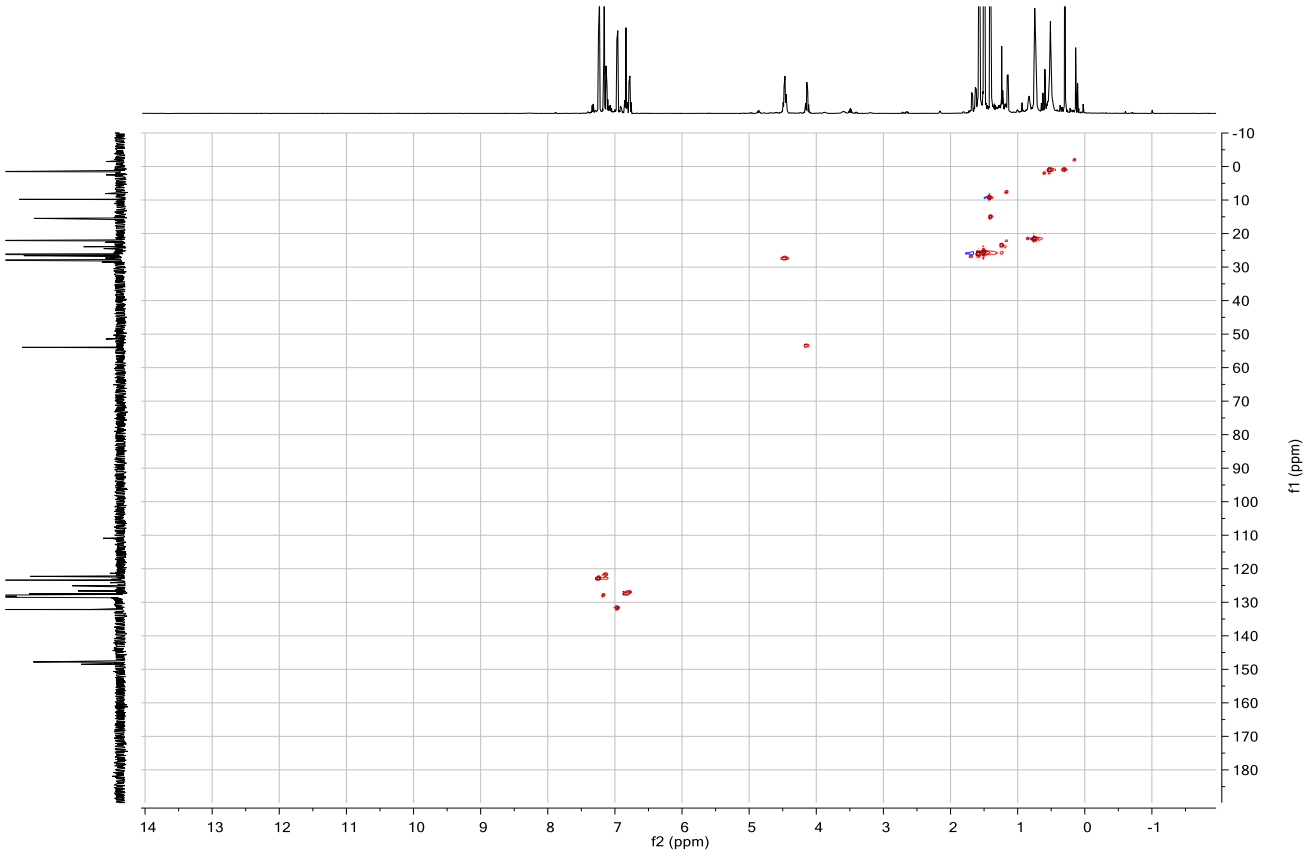
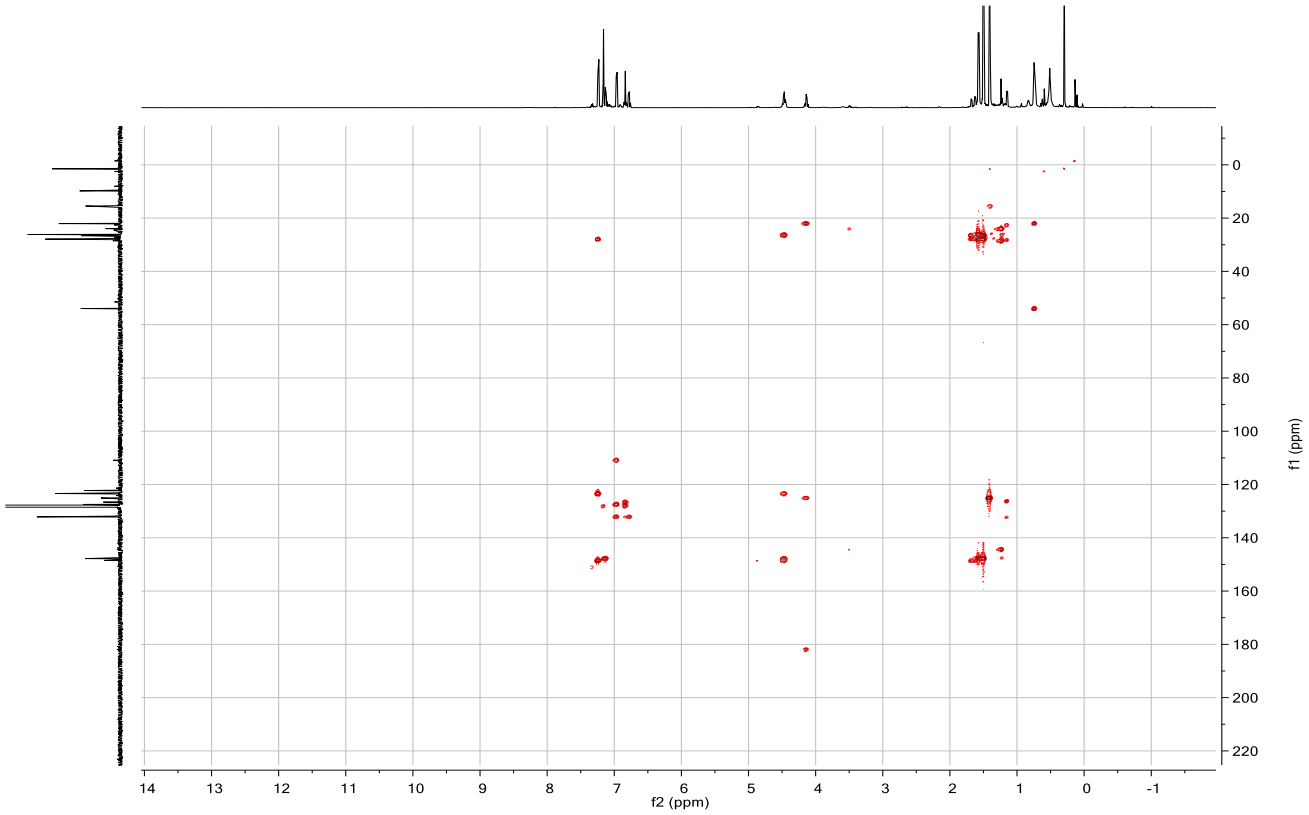


**Figure S10.** $^{1}H$-$^{13}C$ HMBC spectrum of **3**.



Heating reactions of [($^{Me_2}$CAAC)Cu-Al{SiN$^{Dipp}$}] with PhCCH; isolation of **5** and **6**

In a J Young's tube, phenylacetylene (7.6 mg, 8.2 μL, 0.075 mmol) was added via micropipette to a colourless solution of [($^{Me_2}$CAAC)Cu-Al{SiN$^{Dipp}$}] (**4**, 22 mg, 0.025 mmol) in $C_6D_6$. The colourless reaction mixture was then kept at 60$^{o}$C overnight. Multiple species were observed in the crude reaction mixture by NMR spectroscopy along with some grey precipitates. The reaction mixture was then put under vacuum to remove all volatiles, and a toluene/hexane (2:1) solution of the reaction mixture was then kept at -30$^{o}$C affording colourless single crystals of **5** along with some pale-green amorphous solids and black powders. The residual solution was then put under vacuum again to remove all volatiles, and slow evaporation of a hexane solution the residual solids at room temperature gives single crystals of **6** alongside dark red oil.

Synthesis of [(NHC$^{iPr}$)Cu]…[($^{n}$BuC$^{H}$C$^{H}$)($^{n}$BuCC)-κ$^{2}$-C,C'-Al{SiN$^{Dipp}$}] (**7a**)

In a J Young's tube, 1-hexyne (4.1 mg, 5.7 μL, 0.05 mmol) was added via micropipette to a colourless solution of [(NHC$^{iPr}$)Cu-Al{SiN$^{Dipp}$}] (**1**, 19 mg, 0.025 mmol) in $C_6D_6$. Quantitative generation of **7a** was observed by NMR spectroscopy within 30 mins at room temperature. The colourless solution was then put under vacuum to remove all volatiles and give compound **7a** as an off-white waxy solid. Yield 20.8 mg, 90%. No meaningful result of elemental analysis was obtained after several attempts. $^{1}$H NMR (500 MHz, 298 K, Benzene-$d_6$) δ 7.20 – 7.17 (m, 2H, *m*-$C_6H_3$), 7.15 – 7.13 (m, 2H, *m*-$C_6H_3$), 7.07– 7.04 (m, 2H, *p*-$C_6H_3$), 5.11 (d, *J* = 20.8 Hz, 1H, $AlC_2H_2$), 4.48 (sept, *J* = 6.8 Hz, 2H, C*H*Me$_2$), 4.36 (sept, *J* = 6.8 Hz, 2H, C*H*Me$_2$), 4.29 (d, *J* = 20.8 Hz, 1H, $AlC_2H_2$), 4.16 (sept, *J* = 7.0 Hz, 2H, NC*H*Me$_2$), 1.97 – 1.92 (m, 3H, $(CH_2)_3CH_3$), 1.80 – 1.74 (m, 2H, $(CH_2)_3CH_3$), 1.58 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$), 1.52 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$), 1.48 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$), 1.47 (s, 6H, NC*Me*), 1.44 (d, *J* = 6.8 Hz, 6H, CH*Me*$_2$), 1.39 (s, 4H, $SiCH_2$), 1.27 – 1.21 (m, 4H, $(CH_2)_3CH_3$), 1.17 – 1.09 (m, 4H, $(CH_2)_3CH_3$), 1.04 (d, *J* = 7.0 Hz, 12H, NCH*Me*$_2$), 0.79 – 0.77 (m, 2H, $(CH_2)_3CH_3$), 0.75 – 0.72 (m, 3H, $(CH_2)_3CH_3$), 0.50 (s, 6H, Si*Me*$_2$), 0.46 (s, 6H, Si*Me*$_2$). $^{13}$C NMR (126 MHz, 298 K, Benzene-$d_6$) δ 182.2 (Cu$C_{carbene}$), 149.4 (*i*-$C_6H_3$), 147.4 (*o*-$C_6H_3$), 147.0 (*o*-$C_6H_3$), 138.2 ($AlC_2H_2$), 124.7 (Al*C*C$^{n}$Bu), 123.9 (N*C*Me), 123.4 (*m*-$C_6H_3$), 123.3 (*m*-$C_6H_3$), 122.3 ($AlC_2H_2$), 122.0 (*p*-$C_6H_3$), 112.5 (AlC*C*$^{n}$Bu), 53.6 (N*C*HMe$_2$), 39.0 ((*C*H$_2$)$_3$CH$_3$), 32.0 ((*C*H$_2$)$_3$CH$_3$), 30.9 ((*C*H$_2$)$_3$CH$_3$), 28.0 (*C*HMe$_2$), 27.7 (*C*HMe2), 26.5 (CH*Me*$_2$), 26.2 (CH*Me*$_2$), 25.9 (CH*Me*$_2$), 24.5 (CH*Me*$_2$), 24.2 ((*C*H$_2$)$_3$CH$_3$), 24.0 ((*C*H$_2$)$_3$CH$_3$), 22.6 ((CH$_2$)$_3$*C*H$_3$), 22.4 (NCH*Me*$_2$), 15.5(Si*C*H$_2$), 14.2 ((CH$_2$)$_3$*C*H$_3$), 13.9 ((CH$_2$)$_3$*C*H$_3$), 9.8 (NC*Me*), 2.0 (Si*Me*$_2$), 1.0 (Si*Me*$_2$).

**Figure S11.** $^{1}$H NMR (500 MHz, 298 K, $d_6$-benzene) spectrum of **7a**. *grease

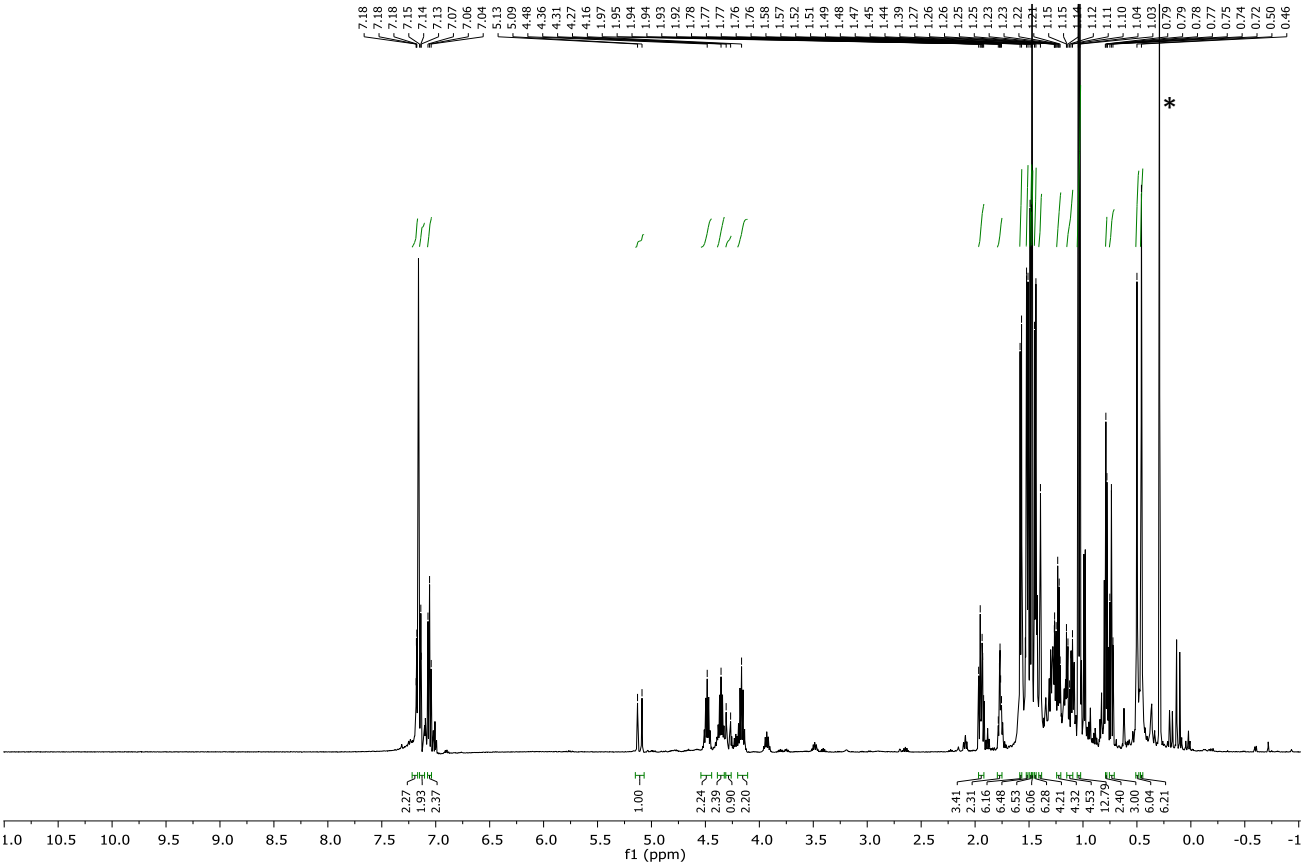



**Figure S12.** $^{13}$C NMR (126 MHz, 298 K, $d_6$-benzene) spectrum of **7a**.

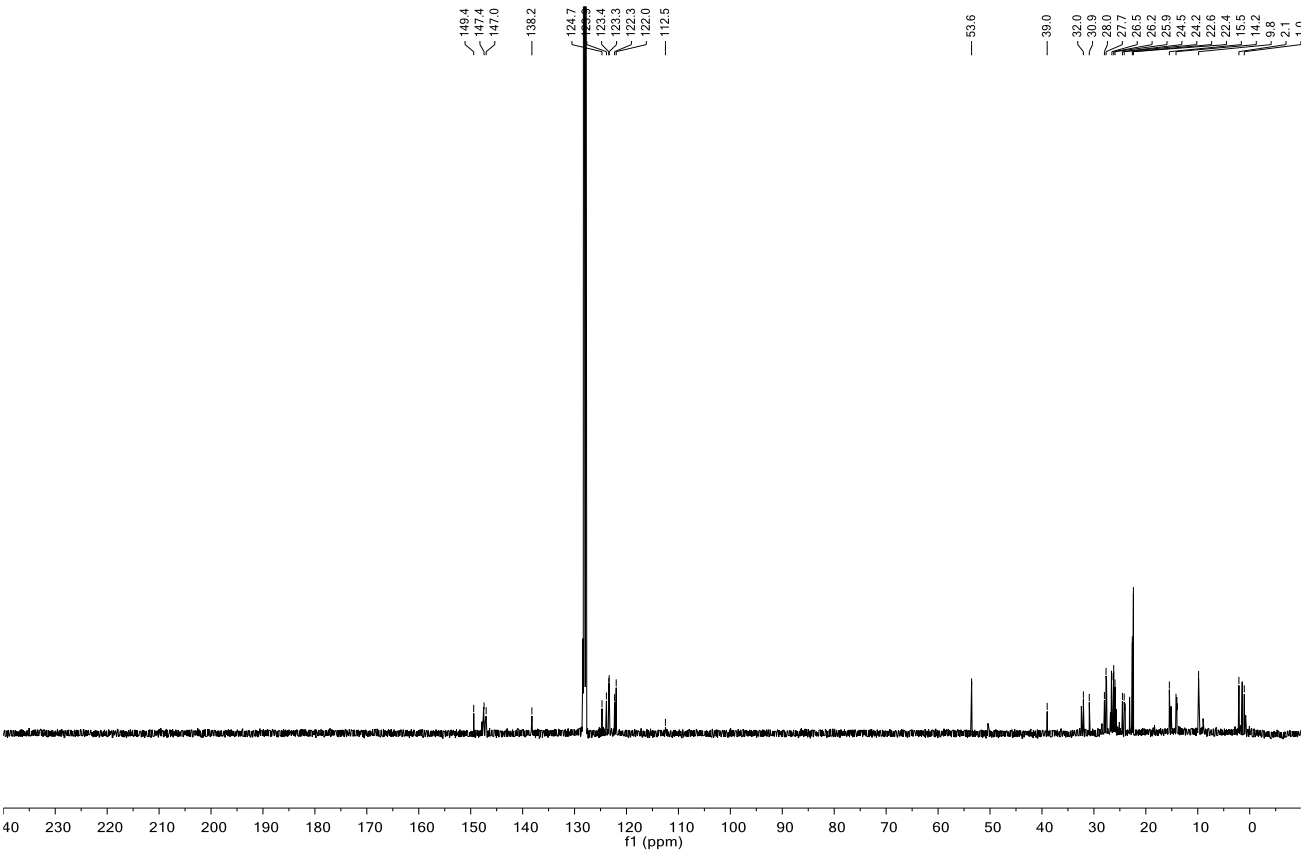


**Figure S13.** $^{1}$H-$^{1}$H COSY spectrum of **7a**.

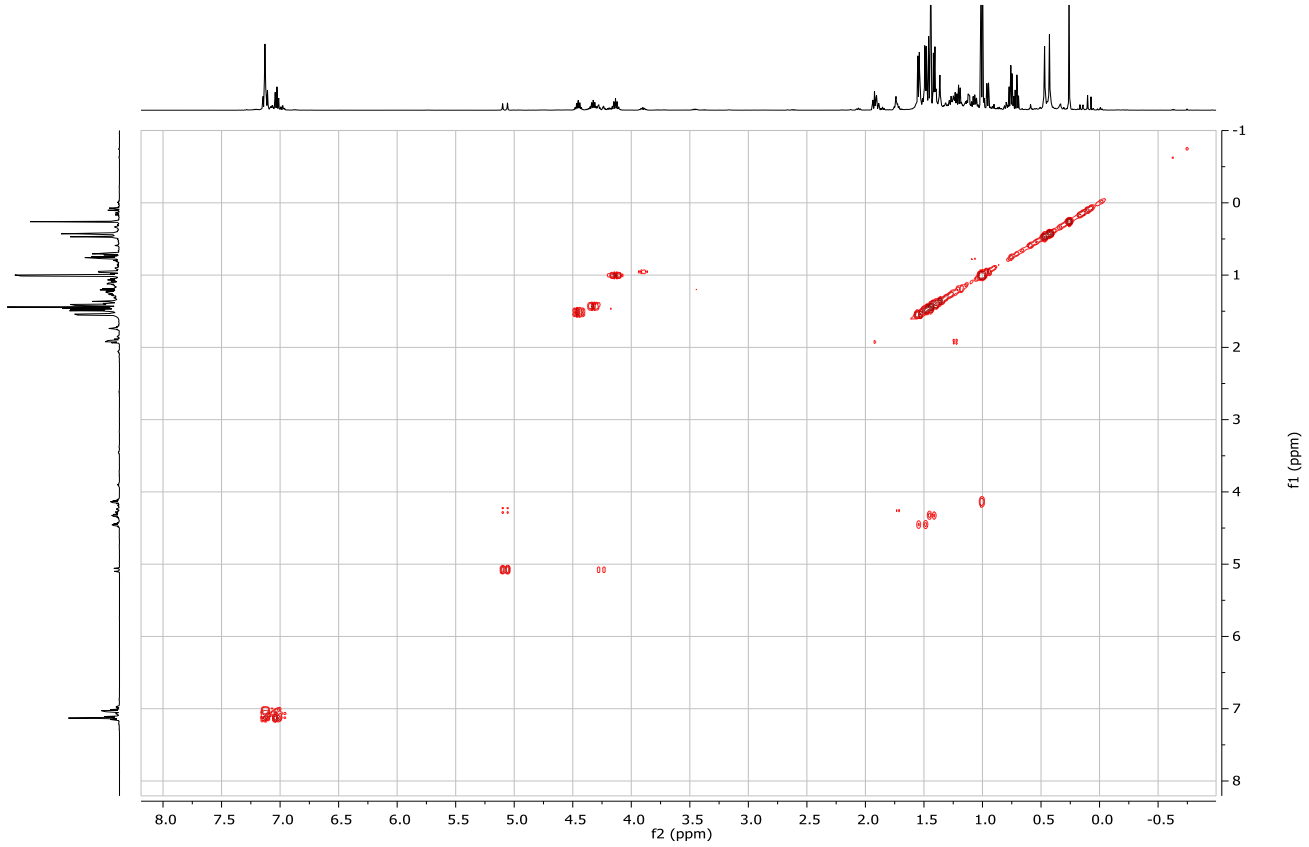



**Figure S14.** $^{1}$H-$^{13}$C HSQC spectrum of **7a**.

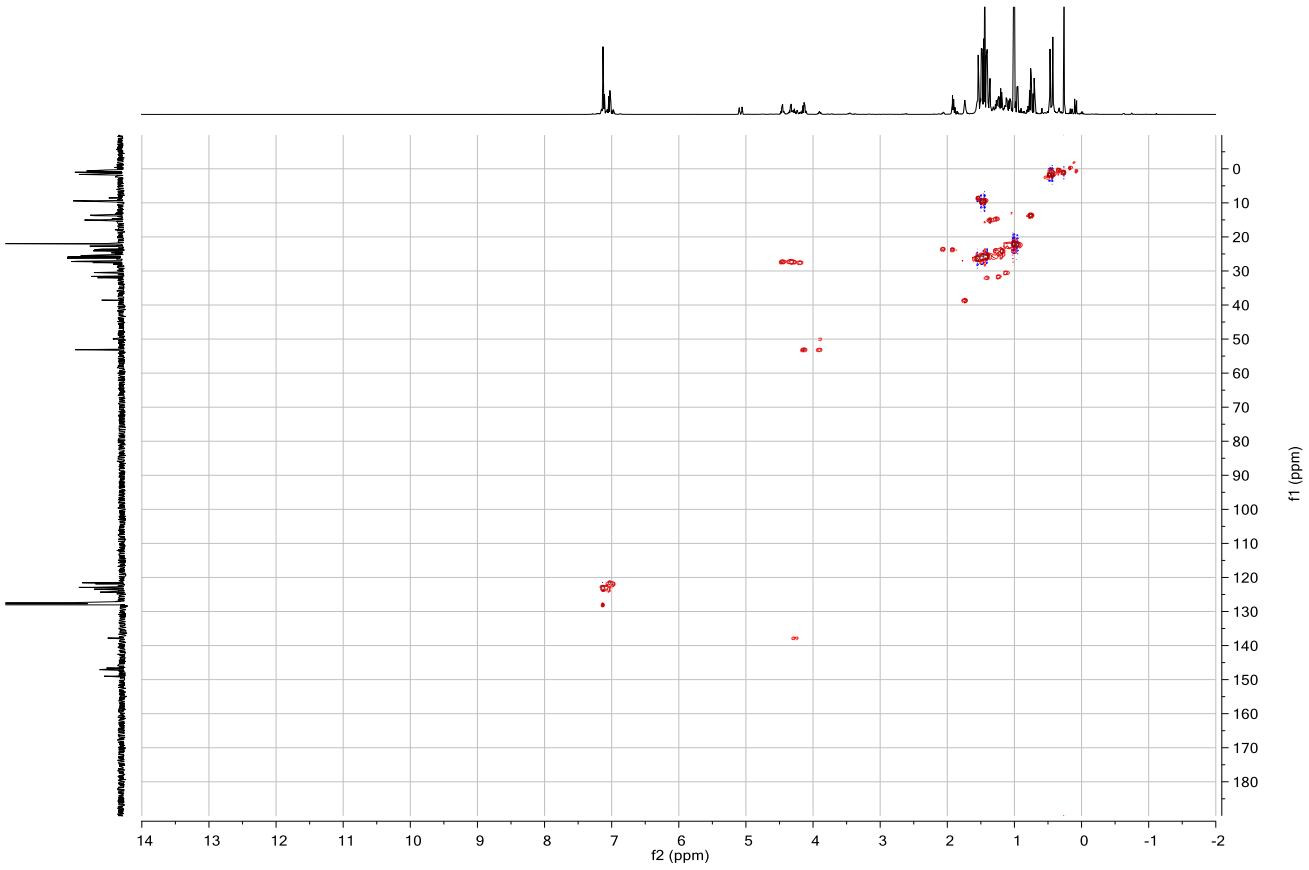
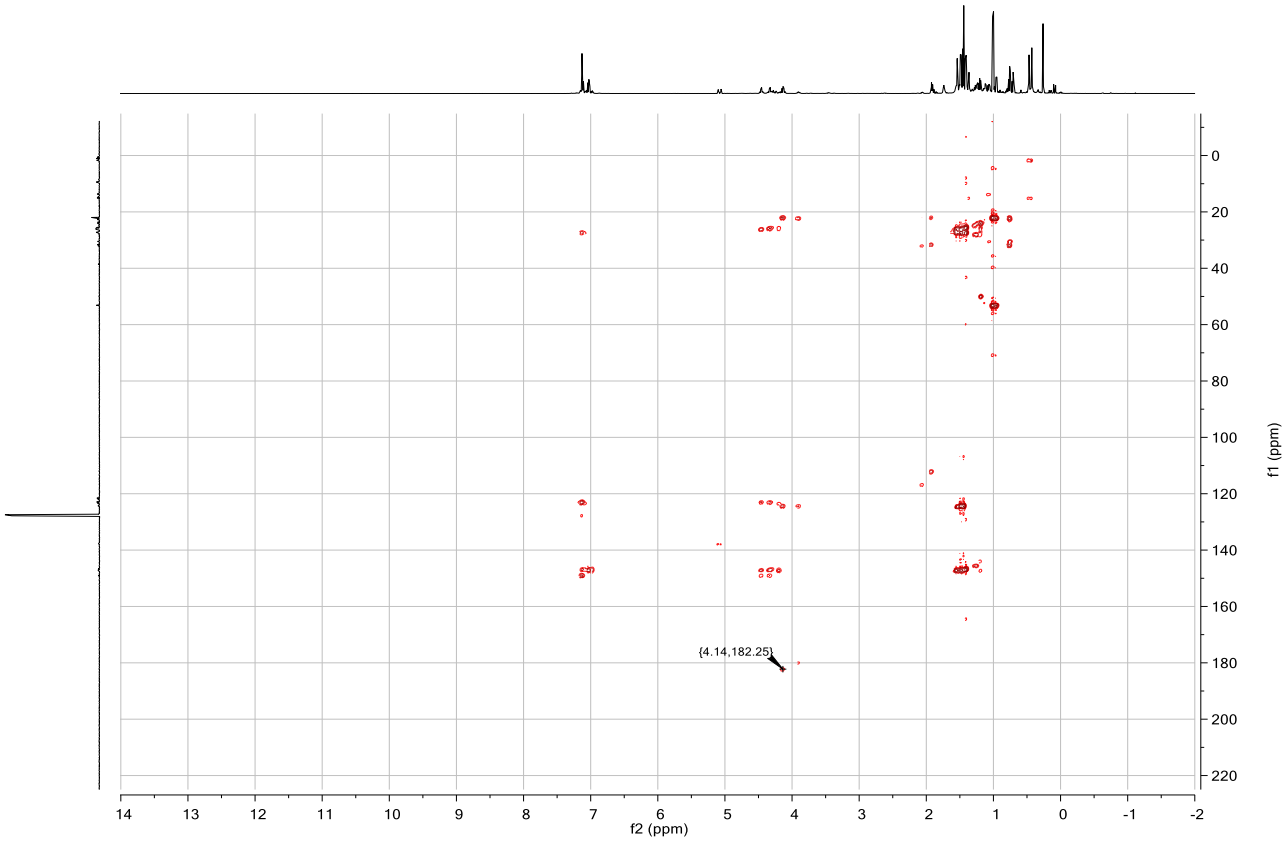


**Figure S15.** $^{1}H$-$^{13}C$ HMBC spectrum of **7a**.



Synthesis of [(NHC$^{iPr}$)Cu…($^{n}$BuCC)$_2$-κ$^2$-C,C'-Al{SiN$^{Dipp}$}] (**7**)

In a J Young's tube, 1-hexyne (6.1 mg, 8.5 μL, 0.075 mmol) was added via micropipette to a colourless solution of [(NHC$^{iPr}$)Cu-Al{SiN$^{Dipp}$}] (**1**, 19 mg, 0.025 mmol) in $C_6D_6$. The colourless reaction mixture was then kept at 60$^{o}$C overnight before full conversion of **7** and generation of 1-hexene was confirmed by NMR spectroscopy. All volatiles were then removed *in vacuo*, affording **7** as a white powder. Yield 20 mg, 83%. Colourless single crystals suitable for X-ray crystallography was obtained by slow evaporation of a hexane solution of **7** at room temperature. No meaningful elemental analysis was obtained after several attempts. $^{1}$H NMR (500 MHz, 298 K, Benzene-$d_6$) δ 7.18 – 7.15 (m, 4H, *m*-C$_6$*H*$_3$)*overlapping with $C_6D_6$, 7.07– 7.04 (m, 2H, *p*-C$_6$*H*$_3$), 4.39 (sept, *J* = 6.9 Hz, 4H, C*H*Me$_2$), 4.15 (sept, *J* = 7.2 Hz, 2H, NC*H*Me$_2$), 1.88 (t, *J* = 7.2 Hz, 4H, CCC*H*$_2$(CH$_2$)$_2$CH$_3$), 1.54 (d, *J* = 6.9 Hz, 12H, CH*Me*$_2$)*, 1.53 (s, 6H, NC*Me*)* *overlapping peaks, 1.51 (d, *J* = 6.9 Hz, 12H, CH*Me*$_2$), 1.34 (s, 4H, SiC*H*$_2$), 1.24 – 1.11 (m, 8H, CCCH$_2$(C*H*$_2$)$_2$CH$_3$), 1.02 (d, *J* = 7.2 Hz, 12H, NCH*Me*$_2$), 0.82 (t, *J* = 7.3 Hz, 6H, CCCH$_2$(CH$_2$)$_2$C*H*$_3$), 0.44 (s, 12H, SiMe$_2$). $^{13}$C NMR (126 MHz, 298 K, Benzene-$d_6$) δ 183.2 (Cu*C*$_{carbene}$), 148.6 (*i*-*C*$_6$H$_3$), 147.5 (*o*-*C*$_6$H$_3$), 124.8 (N*C*Me), 123.3 (*m*-*C*$_6$H$_3$), 122.1 (*p*-*C*$_6$H$_3$), 109.9 (C*C*CH$_2$(CH$_2$)$_2$*C*H$_3$), 53.6 (N*C*HMe$_2$), 32.1 (CC*C*H$_2$(CH$_2$)$_2$*C*H$_3$), 27.7 (*C*H*Me*$_2$), 26.7 (CH*Me*$_2$), 26.1 (CH*Me*$_2$), 24.1 (CCCH$_2$(*C*H$_2$)$_2$CH$_3$), 22.5 (NCH*Me*$_2$), 22.2 (CCCH$_2$(*C*H$_2$)$_2$*C*H$_3$), 15.5 (Si*C*H$_2$), 14.1 (CCCH$_2$(CH$_2$)$_2$*C*H$_3$), 9.9 (NC*Me*), 1.7 (Si*Me*$_2$). $^{13}$C resonance correlated to Al*C*C(CH$_2$)$_3$CH$_3$ not observed.

**Figure S16.** $^{1}$H NMR (500 MHz, 298 K, $d_6$-benzene) spectrum of **7**. *grease

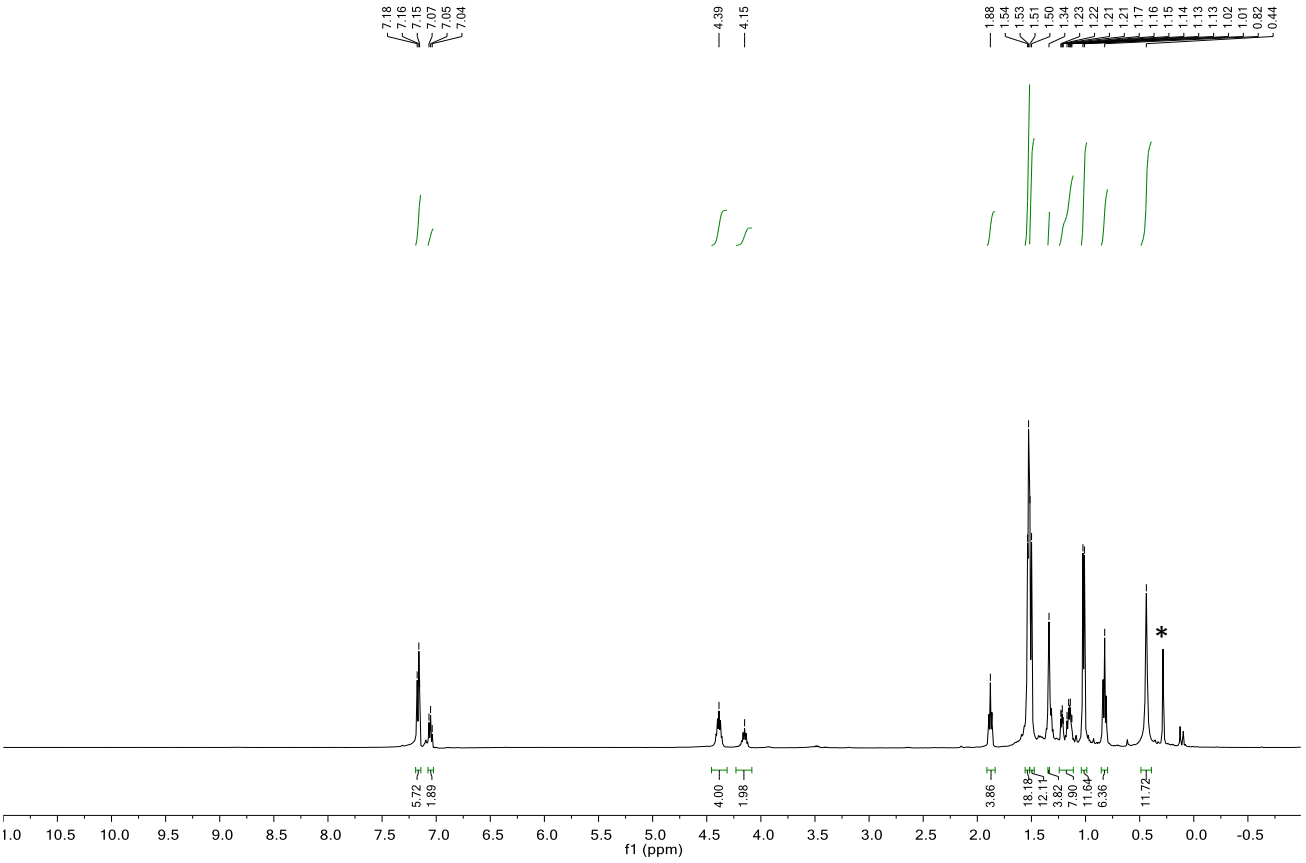



**Figure S17.** $^{13}$C NMR (126 MHz, 298 K, $d_6$-benzene) spectrum of **7**.

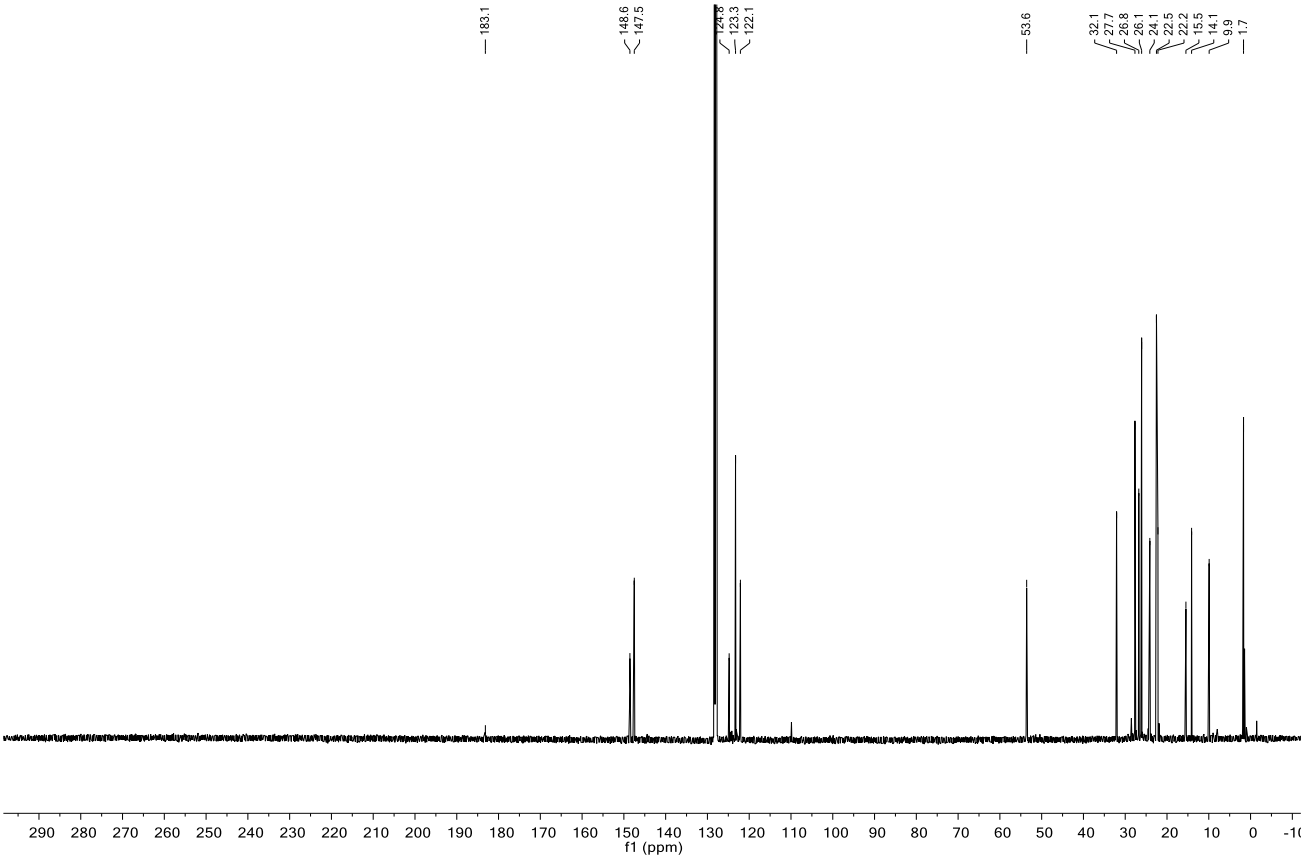


**Figure S18.** $^{1}$H-$^{1}$H COSY spectrum of **7**.

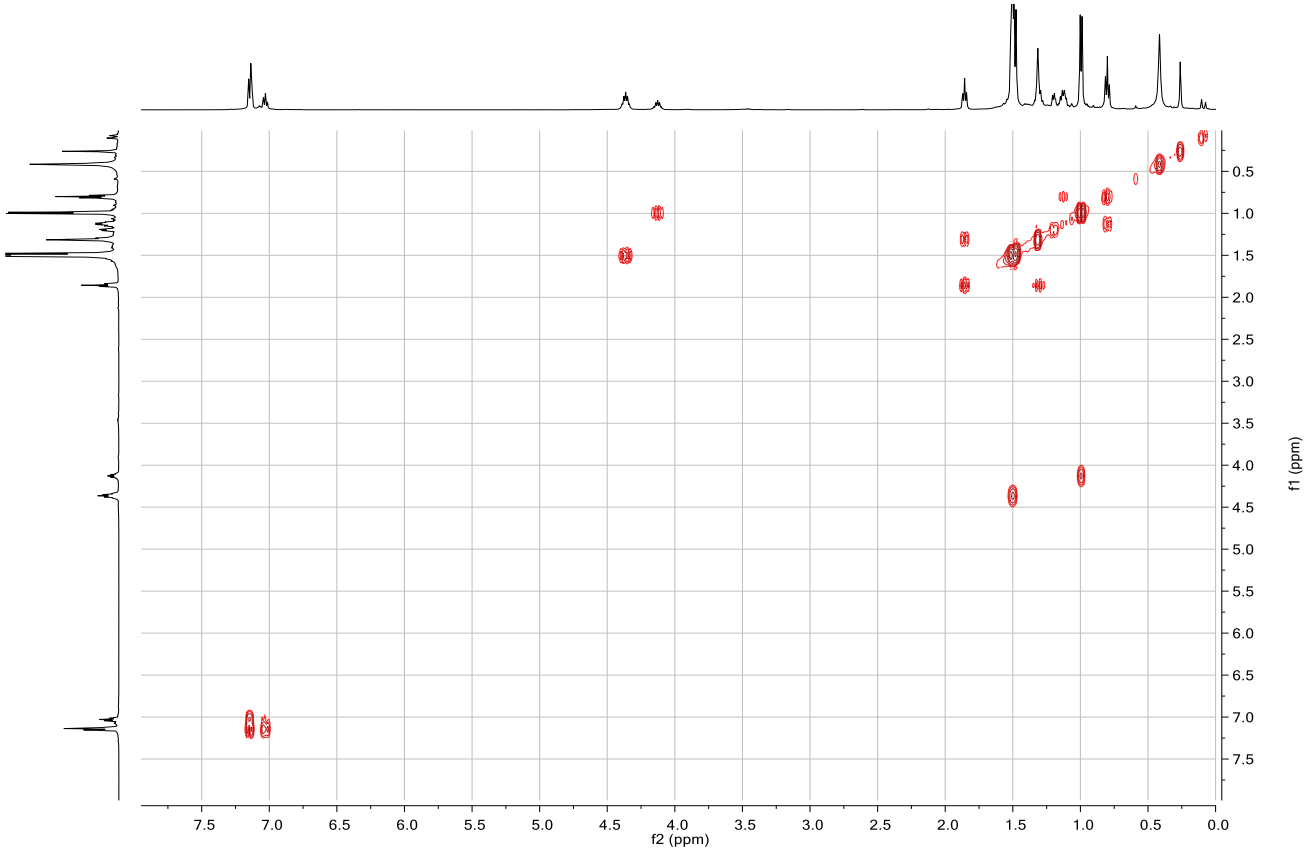



**Figure S19.** $^{1}$H-$^{13}$C HSQC spectrum of **7**.

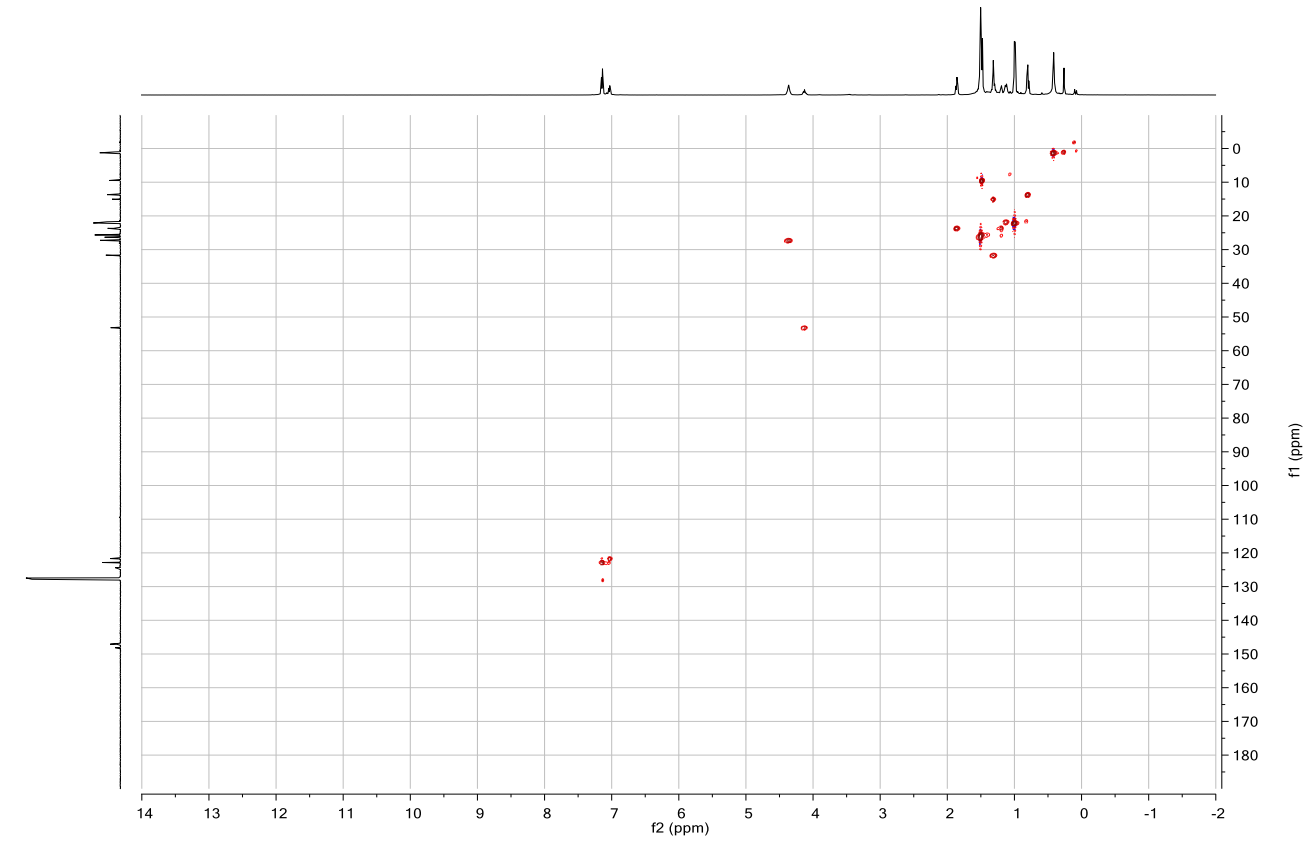
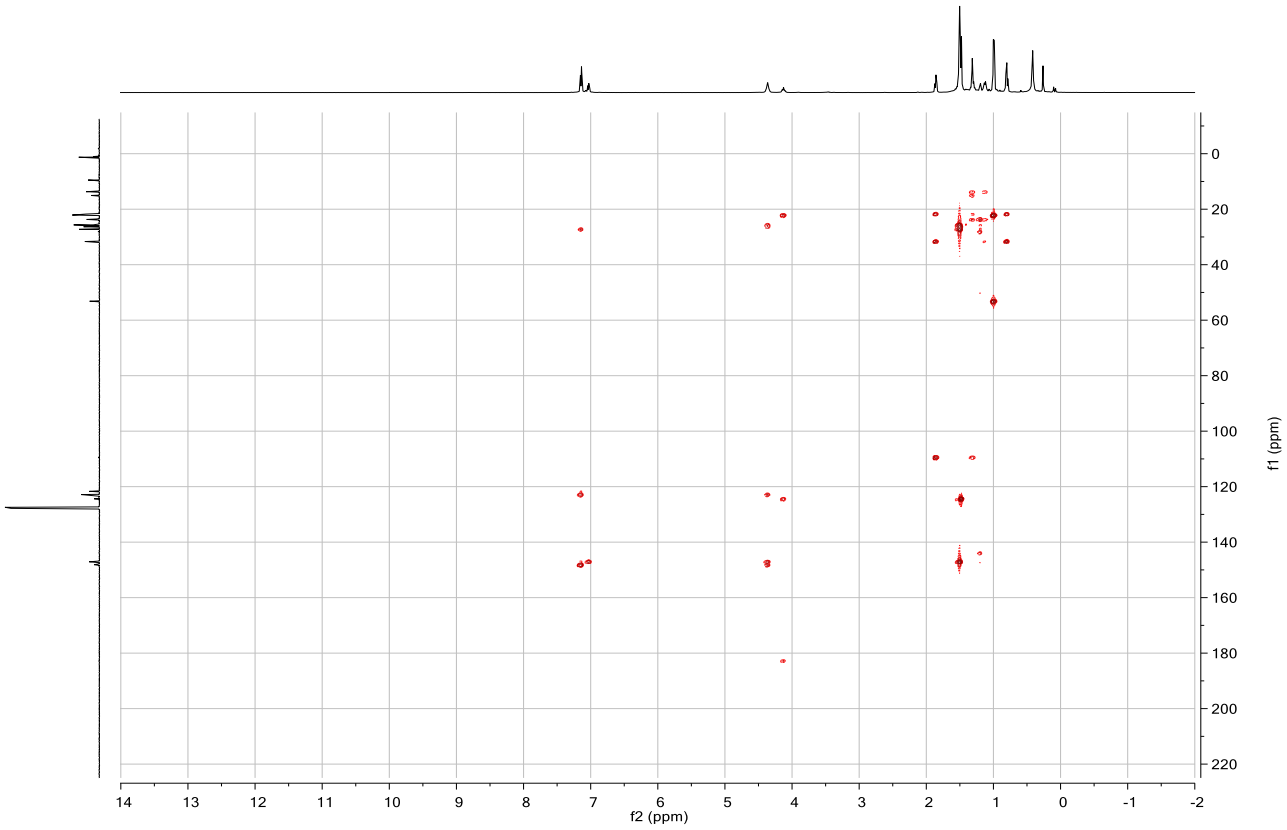


**Figure S20** $^{1}H$-$^{13}C$ HMBC spectrum of **7**.



Synthesis of [(NHC$^{iPr}$)Cu…(Me$_3$SiCC)$_2$-κ$^2$-C,C'-Al{SiN$^{Dipp}$}] (**8**)

In a J Young's tube, ethynyltrimethylsilane (6.1 mg, 9.2 μL, 0.075 mmol) was added via micropipette to a colourless solution of [(NHC$^{iPr}$)Cu-Al{SiN$^{Dipp}$}] (**1**, 19 mg, 0.025 mmol) in $C_6D_6$. The colourless reaction mixture was then kept at 60°C for three days before full conversion of **8** and generation of corresponding alkene was confirmed by NMR spectroscopy. The colourless solution was then put under vacuum to remove all volatiles and give compound **8** as a white powder. Single crystals suitable for X-ray crystallography was obtained by slow evaporation a hexane solution at room temperature. Yield 21 mg, 84 %. Anal Calc'd for $C_{51}H_{89}AlCuN_4Si_4$ (**8**, 961.17) C, 63.73; H, 9.33; N, 5.83 %. Found: C, 63.40; H, 8.90; N, 5.89 %.$^1$H NMR (500 MHz, 298 K, Benzene-$d_6$) δ 7.12 (d, $J$ = 7.5 Hz, 4H, *m*-C$_6$*H*$_3$), 7.04 (t, $J$ = 7.5 Hz, 2H, *p*-C$_6$*H*$_3$), 4.31 (sept, $J$ = 6.8 Hz, 4H, C*H*Me$_2$), 4.24 (sept, $J$ = 7.0 Hz, 2H, NC*H*Me$_2$), 1.55, (s, 6H, NC*Me*), 1.54 (d, $J$ = 6.8Hz, 12H, CH*Me*$_2$) *overlapping peaks, 1.46 (d, $J$ = 6.8 Hz, 12H, CH*Me*$_2$), 1.36 (s, 4H, SiC*H*$_2$), 1.07 (d, $J$ = 7.0 Hz, 12H, NCH*Me*$_2$), 0.43 (s, 12H, Si*Me*$_2$), -0.09 (s, 18H, Si*Me*$_3$). $^{13}$C{$^1$H} NMR (126 MHz, 298 K, Benzene-$d_6$) δ 182.6 (Cu*C*$_{carbene}$), 148.2 (*i*-*C*$_6$H$_3$), 147.1 (*o*-*C*$_6$H$_3$), 125.5 (N*C*Me), 123.3 (*m*-*C*$_6$H$_3$), 122.2 (*p*-*C*$_6$H$_3$), 111.3 (AlC*C*SiMe$_3$), 53.6 (N*C*HMe$_2$), 27.5 (*C*HMe$_2$), 27.3 (CH*Me*$_2$), 26.1 (CH*Me*$_2$), 22.7 (NCH*Me*$_2$), 15.4 (Si*C*H$_2$), 10.0 (NC*Me*), 1.7 (Si*Me*$_2$), 1.3 (Si*Me*$_3$). $^{13}$C resonance correlated to Al*C*CSiMe$_3$ was not observed.

**Figure S21.** $^{1}$H NMR (500 MHz, 298 K, $d_6$-benzene) spectrum of **8**. *grease

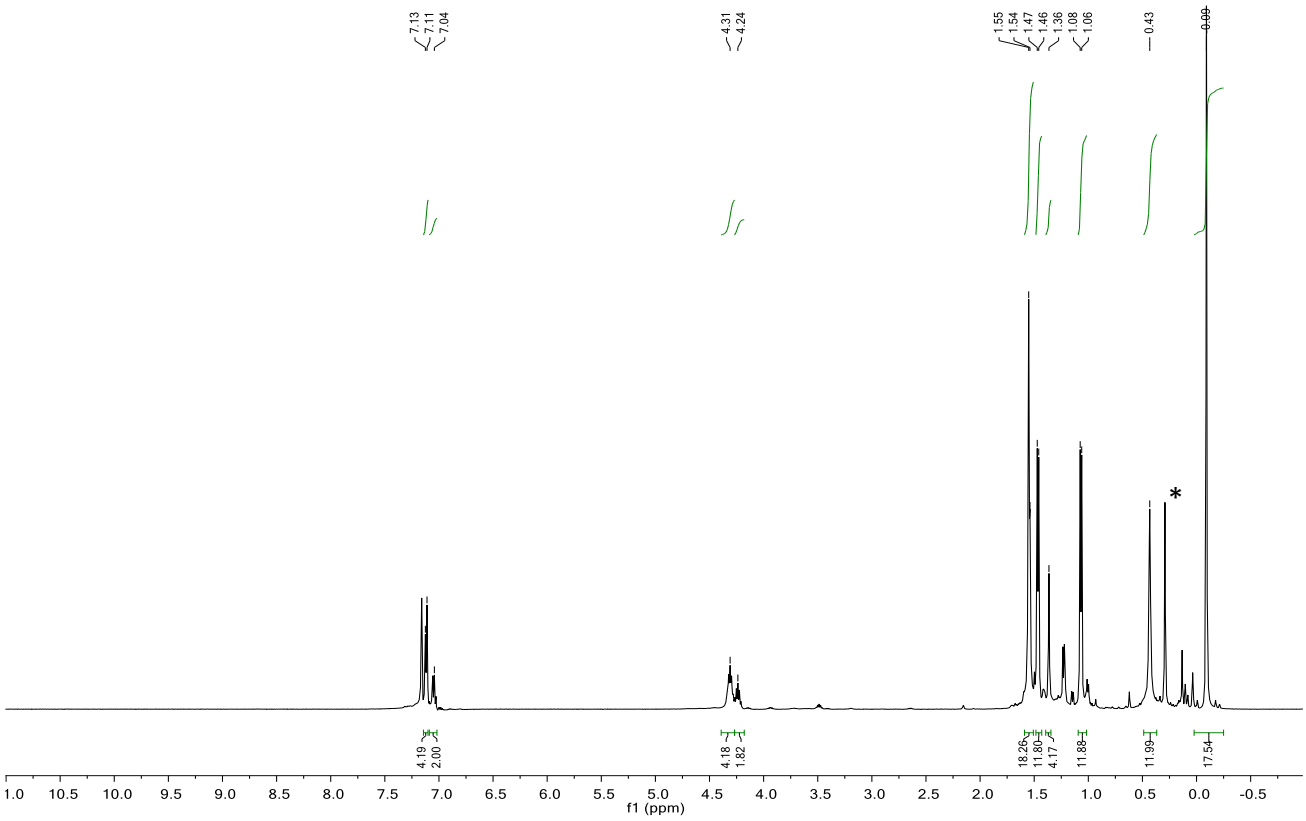



**Figure S22.** $^{13}$C NMR (126 MHz, 298 K, $d_6$-benzene) spectrum of **8**. *grease

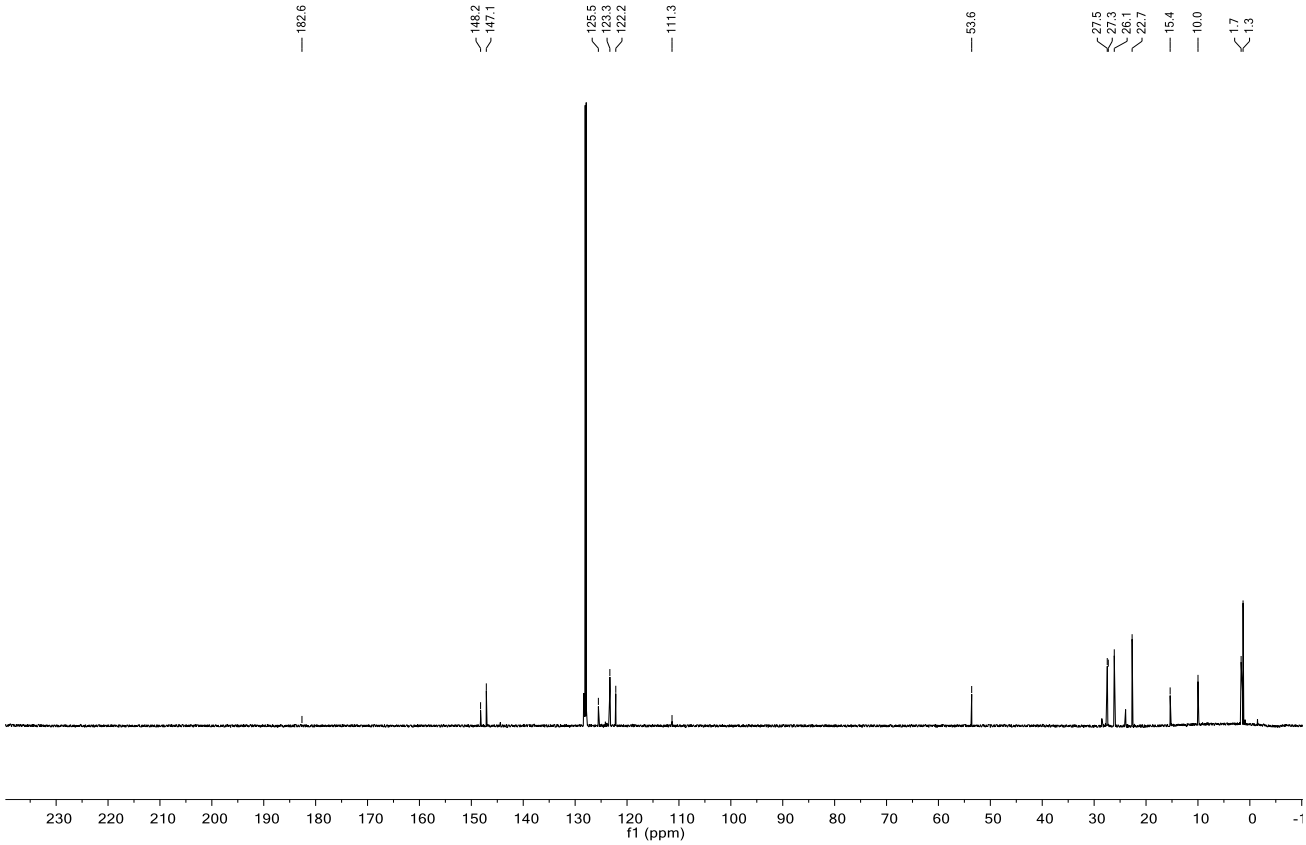


**Figure S23.** $^{1}$H-$^{1}$H COSY spectrum of **8**.

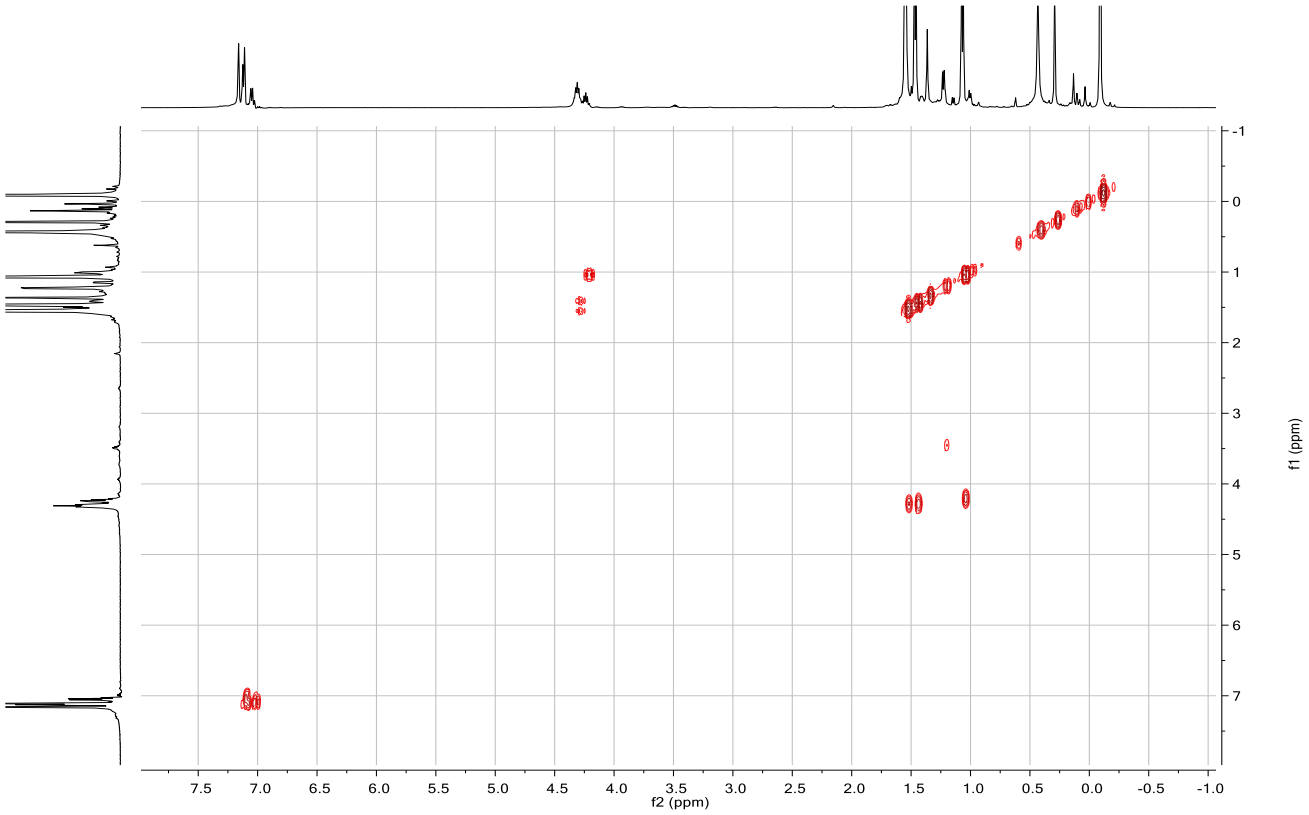



**Figure S24.** $^{1}$H-$^{13}$C HSQC spectrum of **8**.

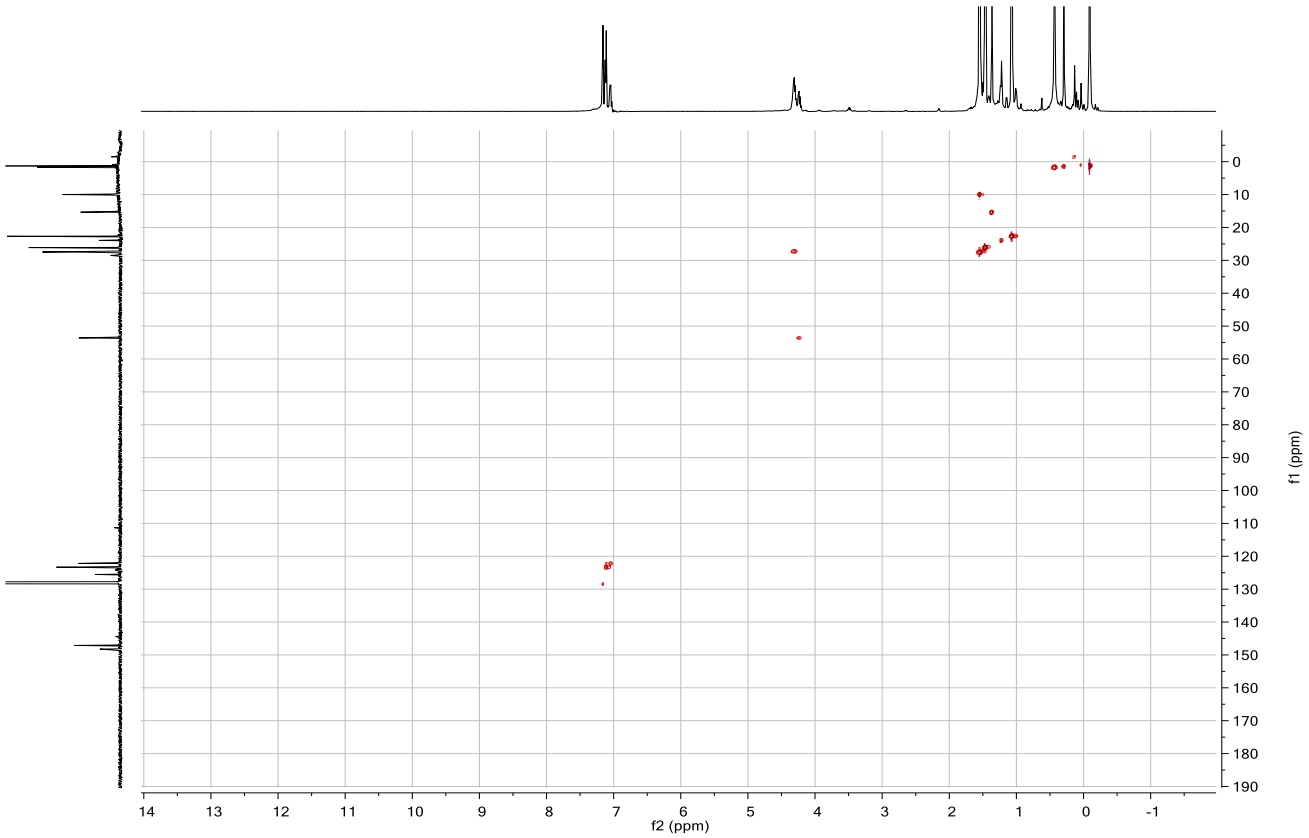
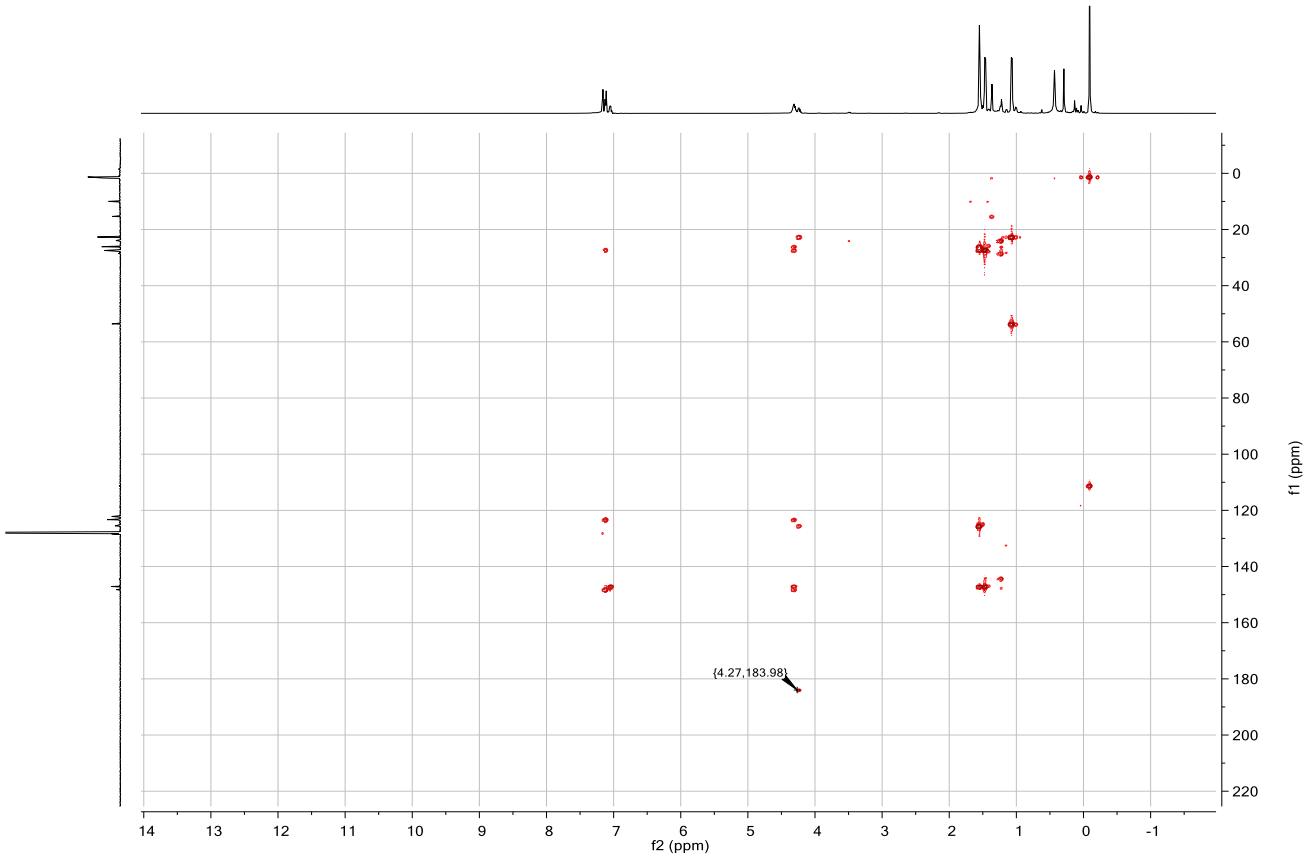


**Figure S25.** $^{1}H$-$^{13}C$ HMBC spectrum of **8**.



Synthesis of [(NHC$^{iPr}$)Cu…($^{t}$BuCC)$_2$-κ$^2$-C,C'-Al{SiN$^{Dipp}$}] (**9**)

In a J Young's tube, 3,3-dimethyl-1-butyne (6.1 mg, 9.2 μL, 0.075 mmol) was added via micropipette to a colourless solution of [(NHC$^{iPr}$)Cu-Al{SiN$^{Dipp}$}] (**1**, 19 mg, 0.025 mmol) in $C_6D_6$. The colourless reaction mixture was then kept at 60$^{o}$C overnight before full conversion of **9** and generation of 3,3-dimethyl-1-butene was confirmed by NMR spectroscopy. The colourless solution was then put under vacuum to remove all volatiles and give compound **9** as a pale-yellow waxy solid. Yield 19 mg, 76 %. No meaningful result of elemental analysis was obtained after several attempts. $^{1}$H NMR (500 MHz, 298 K, Benzene-$d_6$) δ 7.21 (m, 2H, *p*-C$_6$*H*$_3$), 7.13 – 7.03 (m, 4H, *m*-C$_6$*H*$_3$), 4.40 (sept, *J* = 7.0 Hz, 4H, C*H*Me$_2$ on SiN$^{Dipp}$), 3.92 (sept, *J* = 6.5 Hz, 1H, NC*H*Me$_2$), 3.79 (sept, *J* = 6.5 Hz, 1H, NC*H*Me$_2$), 1.59 (d, *J* = 7.0 Hz, 12H, CH*Me*$_2$ on SiN$^{Dipp}$), 1.54 – 1.49 (m, 12H, CH*Me*$_2$ on SiN$^{Dipp}$), 1.39 (s, 4H, SiC*H*$_2$), 1.23 (d, *J* = 6.5 Hz, 12H, NC*H*Me$_2$), 1.07 (s, 3H, NC*Me*), 1.06 (s, 3H, NC*Me*), 0.97 (s, 18H, C*Me*$_3$), 0.60 (s, 6H, Si*Me*$_2$), 0.43 (s, 6H, Si*Me*$_2$). $^{13}$C NMR (126 MHz, 298 K, Benzene-$d_6$) δ 167.3 ($C_{carbene}$), 148.8 (*i*-*C*$_6$H$_3$), 147.5 (*o*-*C*$_6$H$_3$), 145.9 (*o*-*C*$_6$H$_3$), 125.1 (N*C*Me), 124.0 (*m*-*C*$_6$H$_3$), 123.7 (*p*-*C*$_6$H$_3$), 122.1 (*m*-*C*$_6$H$_3$), 120.5 (AlC*C*Me$_3$), 53.8 (*C*Me$_3$), 50.4 (*C*Me$_3$), 31.8 (C*Me*$_3$), 28.2 (N*C*HMe$_2$), 27.3 (*C*HMe$_2$), 26.1 (CH*Me*$_2$), 25.1 (CH*Me*$_2$), 24.5 (CH*Me*$_2$), 22.6 (NCH*Me*$_2$), 15.1 (Si*C*H$_2$), 10.0 (NC*Me*), 9.0 (NC*Me*), 2.6 (Si*Me*$_2$), 0.1 (Si*Me*$_2$). $^{13}$C resonance correlates to Al*C*CMe$_3$ was not observed.

**Figure S26.** $^{1}$H NMR (500 MHz, 298 K, $d_6$-benzene) spectrum of **9**. *grease

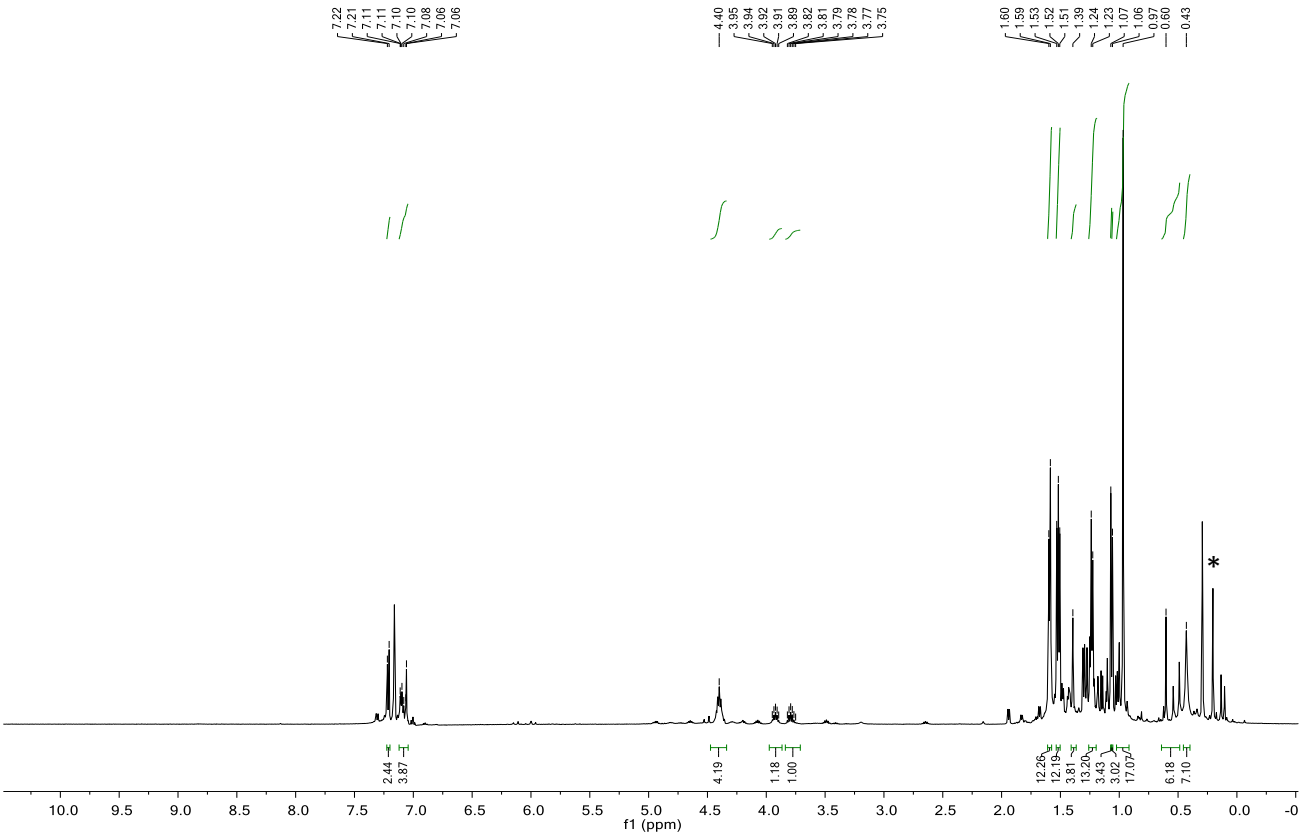



**Figure S27.** $^{13}$C NMR (126 MHz, 298 K, $d_6$-benzene) spectrum of **9**. *grease

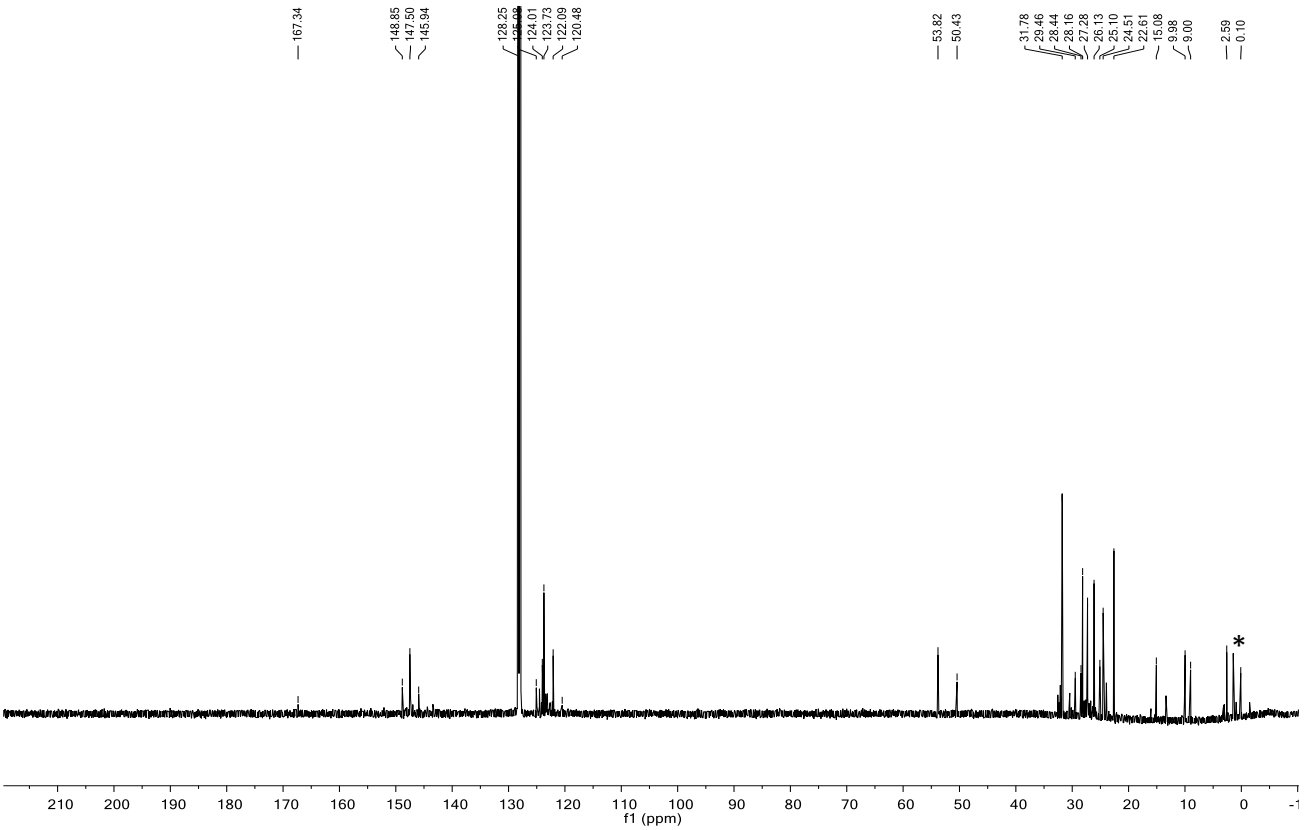


**Figure S28.** $^{1}$H-$^{1}$H COSY spectrum of **9**.

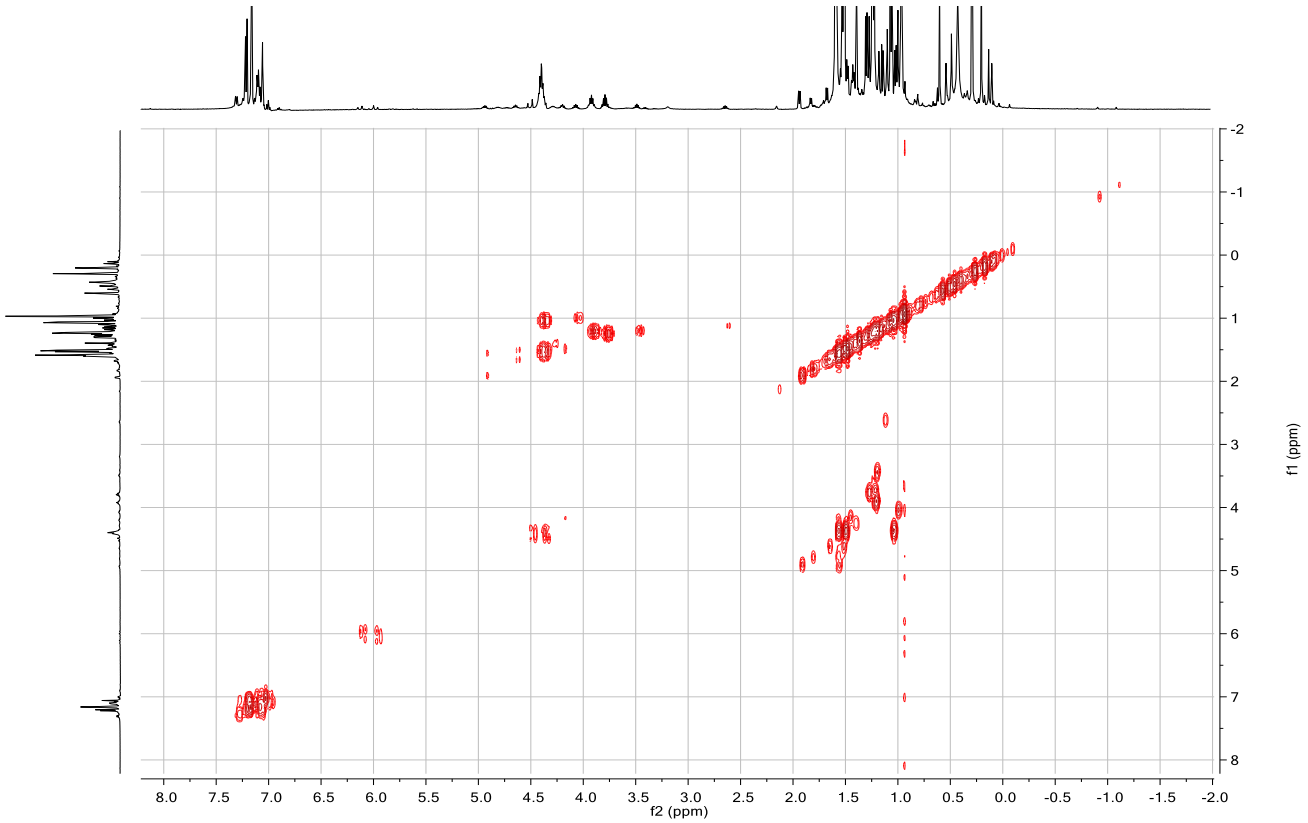



**Figure S29.** $^{1}$H-$^{13}$C HSQC spectrum of **9**.

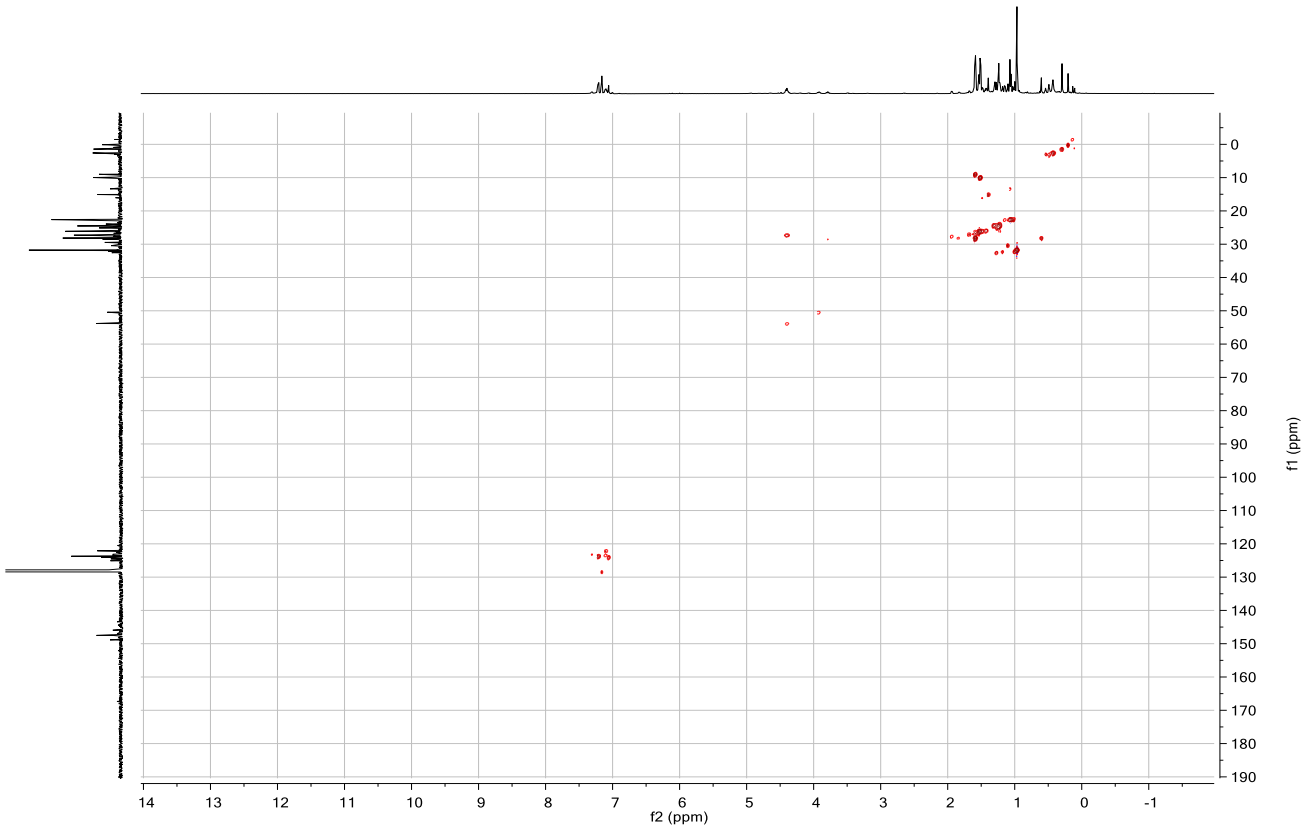
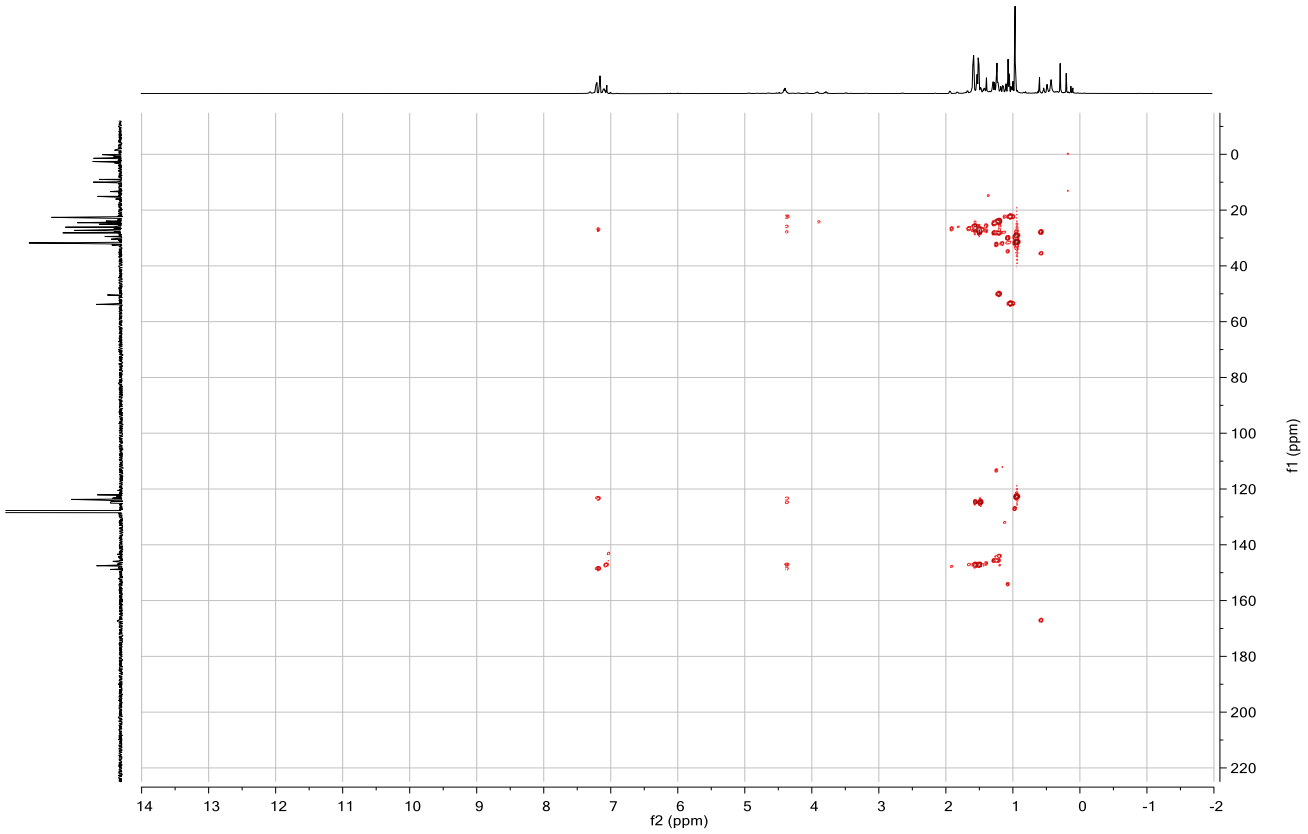


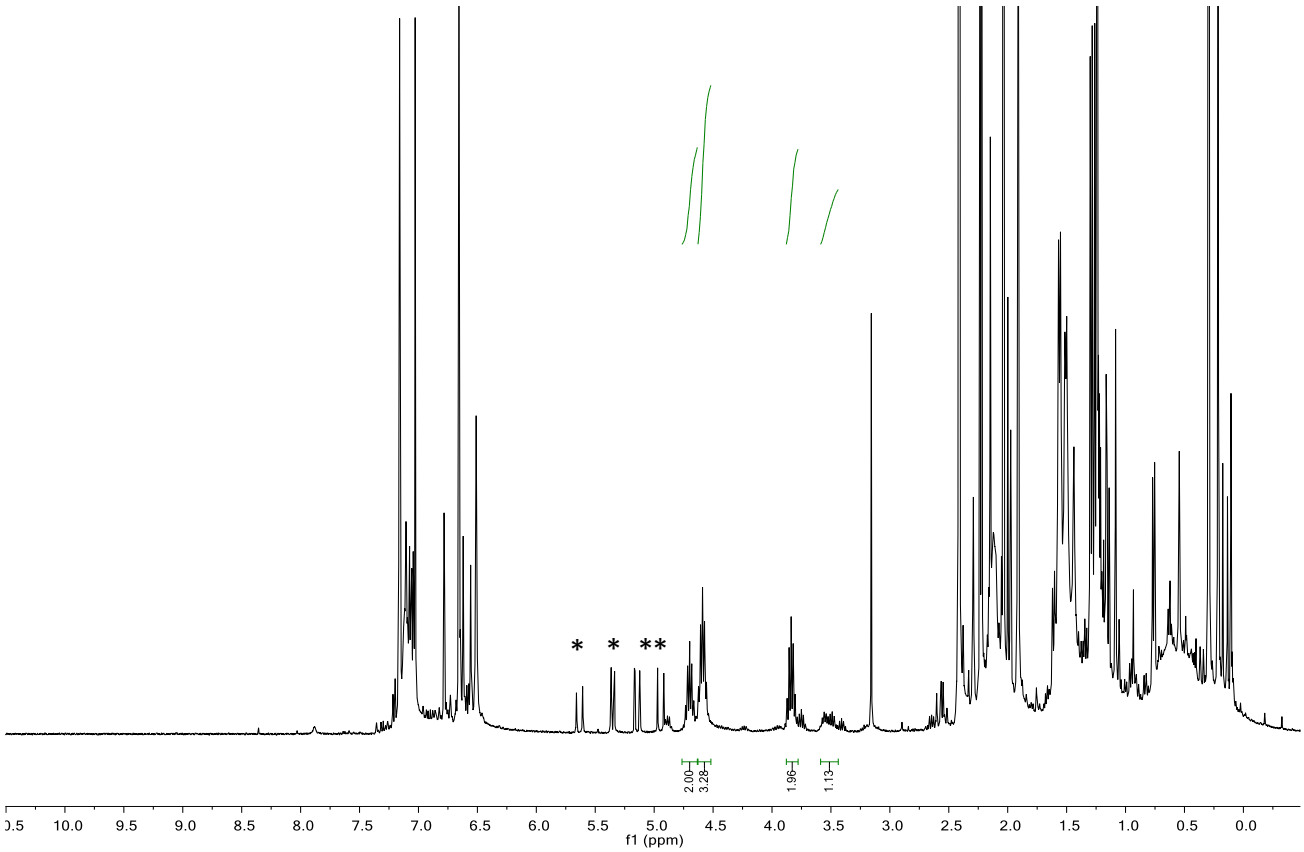
**Figure S30.** $^{1}H$-$^{13}C$ HMBC spectrum of **9**.



Heating reactions of [(NHC$^{iPr}$)Cu-Al{SiN$^{Dipp}$}] with MesCCH; Isolation of **10** and **10a**

In a J Young's tube, 2-ethynyl-1,3,5-trimethylbenzene (7.2 mg, 7.8 mL, 0.05 mmol) was added via micropipette to a colourless solution of [(NHC$^{iPr}$)Cu-Al{SiN$^{Dipp}$}] (**1**, 19 mg, 0.025 mmol) in $C_6D_6$. The tube was then immediately taken to a heating mantle and kept at 60$^{o}$C to prevent side reaction previously observed at room temperature. Full consumption of A was observed by NMR spectroscopy after the reaction mixture was kept at 60$^{o}$C for 3 days, along with the generation of related alkenes of 2-Ethynyl-1,3,5-trimethylbenzene. $^{1}$H NMR spectrum of the crude reaction mixture indicates there are more than one Cu-Al involving species, despite bulk sample of each product was not obtained, two species were identified by mechanical separation of colourless single crystals and subsequent X-ray diffraction analysis. The products of the reaction, along with the mesityl-stryene, were found to be [(NHC$^{iPr}$)Cu…(MesCC)$_2$-κ$^2$-C,C'-Al{SiN$^{Dipp}$}] (**10**) and [(NHC$^{iPr}$)Cu(NHC$^{iPr}$)][(MesCC)$_2$-κ$^2$-C,C'-Al{SiN$^{Dipp}$}] (**10a**), plausibly generated in the ratio of 4:1. (rough intepretation from the crude 1H NMR spectrum).

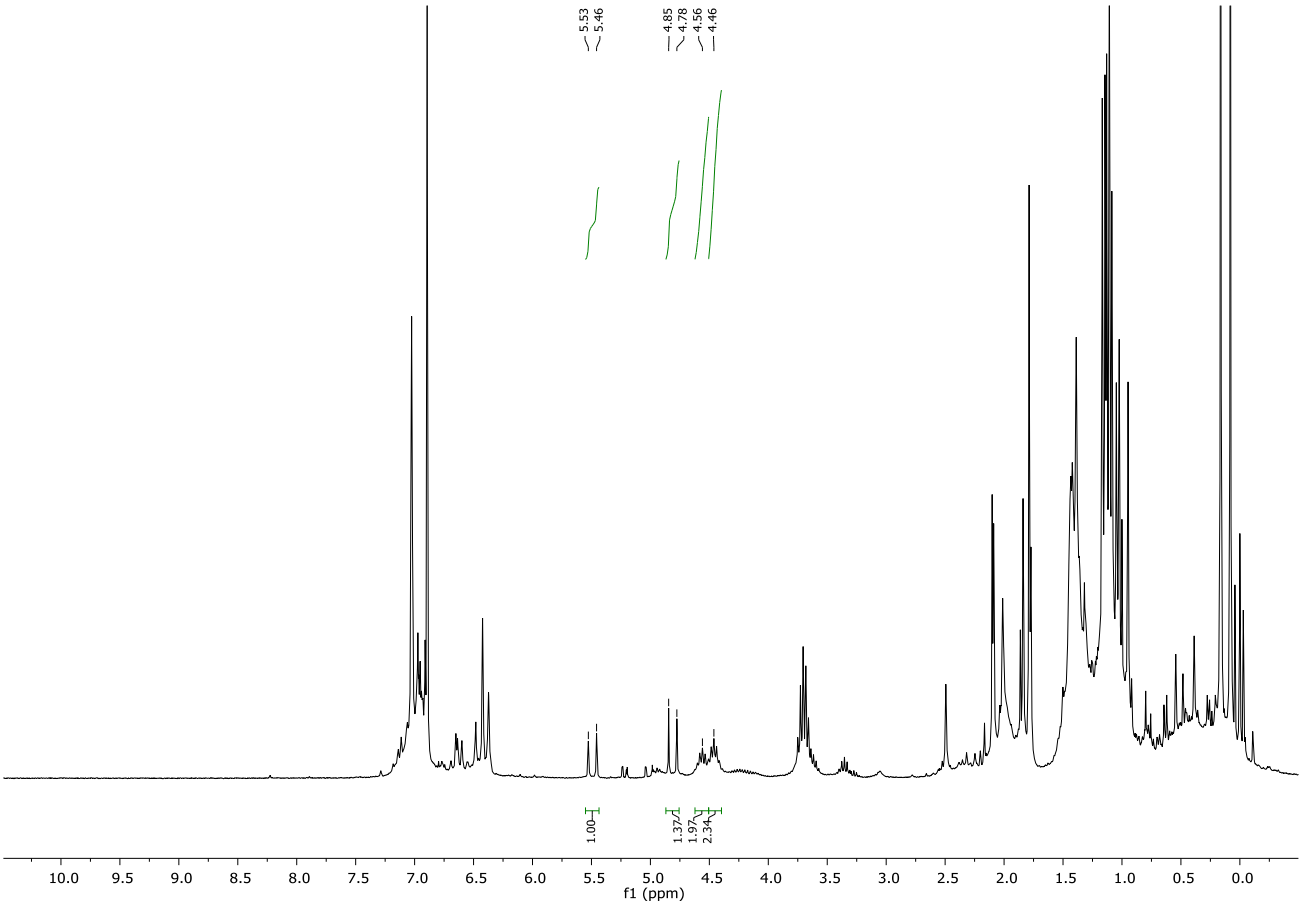
**Figure S31.** $^{1}$H NMR (500 MHz, 298 K, $d_6$-benzene) spectrum of the reaction mixture *alkenes



Room temperature reactions of [(NHC$^{iPr}$)Cu-Al{SiN$^{Dipp}$}] with MesCCH; Isolation of **11**.

In a J Young's tube, 2-ethynyl-1,3,5-trimethylbenzene (7.2 mg, 7.8 mL, 0.05 mmol) was added via micropipette to a colourless solution of [(NHC$^{iPr}$)Cu-Al{SiN$^{Dipp}$}] (**1**, 19 mg, 0.025 mmol) in $C_6D_6$. Upon addition of the acetylene, the reaction mixture transformed into a pale-yellow solution with significant amount of colourless crystalline solids precipitating within 15 mins, precluding in depth *in-situ* solution state characterisation of the reaction mixture. $^1$H NMR spectrum shows two diagnostic doublets at 5.49 and 4.81 ppm (each integrated to 1H, $J$ = 20.9Hz), alongside two septets at 4.56 and 4.46 ppm (each integrated to 2H), indicating some analogous reactivity to that between **1** with phenylacetylene or 1-hexyne taking place in the mixture. The identity of the colourless crystal was confirmed by X-ray diffraction analysis to be [(NHC$^{iPr}$)Cu(NHC$^{iPr}$)][(MesC$^{H}$C$^{H}$)(MesCC)-κ$^2$-C,C'-Al{SiN$^{Dipp}$}]. (**11**)

**Figure S32.** $^1$H NMR (500 MHz, 298 K, $d_6$-benzene) spectrum of the reaction mixture



Synthesis of [(NHC$^{iPr}$)Cu(H)($^{t}$BuCC)Al{SiN$^{Dipp}$}] (**12**)

In a J Young's tube, 3,3-dimethyl-1-butyne (2.0 mg, 3.1 µl, 0.025 mmol) was added via micropipette to a colourless solution of [(NHC$^{iPr}$)Cu-Al{SiN$^{Dipp}$}] (**1**, 19 mg, 0.025 mmol) in $C_6D_6$. Quantitative generation of **12** was observed by NMR spectroscopy in 2-3 hours at room temperature. The colourless solution was then put under vacuum to remove all volatiles and give compound **12** as a white crystalline solid. Yield 18.5 mg, 88 %. Single crystal suitable for X-ray crystallography was obtained by slow evaporation a concentrated benzene solution at room temperature. Anal Calc'd for $C_{54}H_{90}AlCuN_4Si_2$ (**12.**$C_6H_6$, 942.04): C, 68.85; H, 9.63; N, 5.95 %. Found: C, 68.90; H, 8.99; N, 5.45 %.$^{1}$H NMR (500 MHz, 298 K, Benzene-$d_6$) δ 7.14 (dd, $J$ = 7.5, 1.8 Hz, 2H, *m*-$C_6H_3$), 7.09 (dd, $J$ = 7.6, 1.8 Hz, 2H, *m*-$C_6H_3$), 7.00 (t, $J$ = 7.5 Hz, 2H, *p*-$C_6H_3$), 4.29 (sept, $J$ = 6.8 Hz, 2H, C*H*Me$_2$), 4.20 (sept, $J$ = 6.8 Hz, 2H, C*H*Me$_2$), 4.07 (sept, $J$ = 7.0 Hz, 2H, NC*H*Me$_2$), 1.59 (d, $J$ = 6.8 Hz, 6H, CH*Me*$_2$), 1.52 (s, 6H, NC*Me*), 1.48 (d, $J$ = 6.8 Hz, 6H, CH*Me*$_2$), 1.43 (d, $J$ = 6.8 Hz, 6H, CH*Me*$_2$), 1.42 (d, $J$ = 6.8 Hz, 6H, CH*Me*$_2$), 1.30-1.27 (br, 4H, SiC*H*$_2$), 1.02 (d, $J$ = 7.0 Hz, 12H, NCH*Me*$_2$), 1.00 (s, 9H, C*Me*$_3$), 0.53-0.42 (s br, 6H, Si*Me*$_2$), 0.39 – 0.30 (s br, 6H, Si*Me*$_2$). $^{1}$H resonance correlated to Al-*H* not observed. $^{13}$C NMR (126 MHz, 298 K, Benzene-$d_6$) δ 181.5 (Cu*C*$_{carbene}$), 147.6 (*i*-*C*$_6$H$_3$), 147.4 (*o*-*C*$_6$H$_3$), 147.0 (*o*-*C*$_6$H$_3$), 144.4 (AlC*C*CMe$_3$), 125.0 (N*C*Me), 123.9 (*m*-*C*$_6$H$_3$), 123.3 (*m*-*C*$_6$H$_3$), 122.2 (*p*-*C*$_6$H$_3$), 53.7 (N*C*HMe$_2$), 50.4 (*C*Me$_3$), 32.1 (C*Me*$_3$), 29.9 (CH*Me*$_2$), 27.9 (CH*Me*$_2$), 26.0 (CH*Me*$_2$), 23.9 (CH*Me*$_2$), 22.6 (NCH*Me*$_2$), 15.2 (Si*C*H$_2$), 10.1 (NC*Me*), 0.9 (Si*Me*$_2$), -1.5 (Si*Me*$_2$). $^{13}$C resonance correlated to Al-*C*C$^{t}$Bu not observed.

**Figure S33.** $^{1}$H NMR (500 MHz, 298 K, $d_6$-benzene) spectrum of **12**. *grease

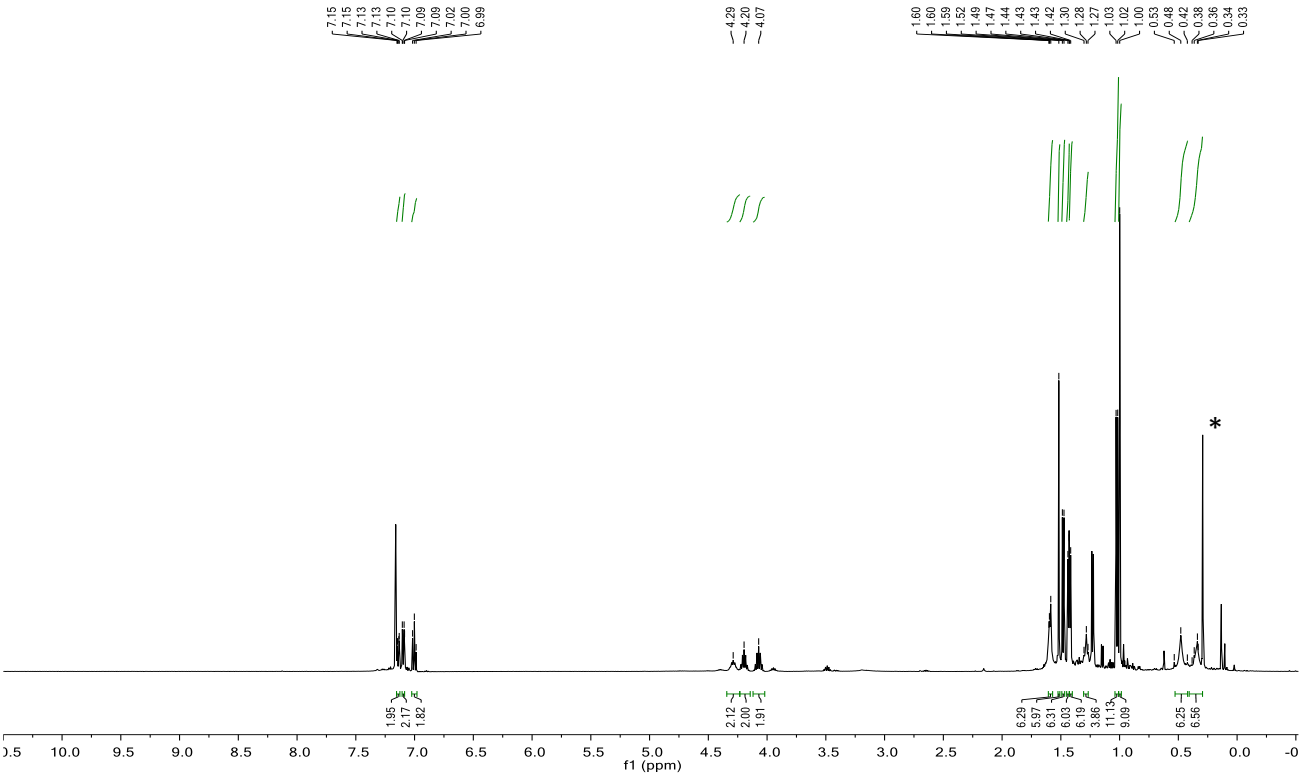



**Figure S34.** $^{13}$C NMR (126 MHz, 298 K, $d_6$-benzene) spectrum of **12**. *grease

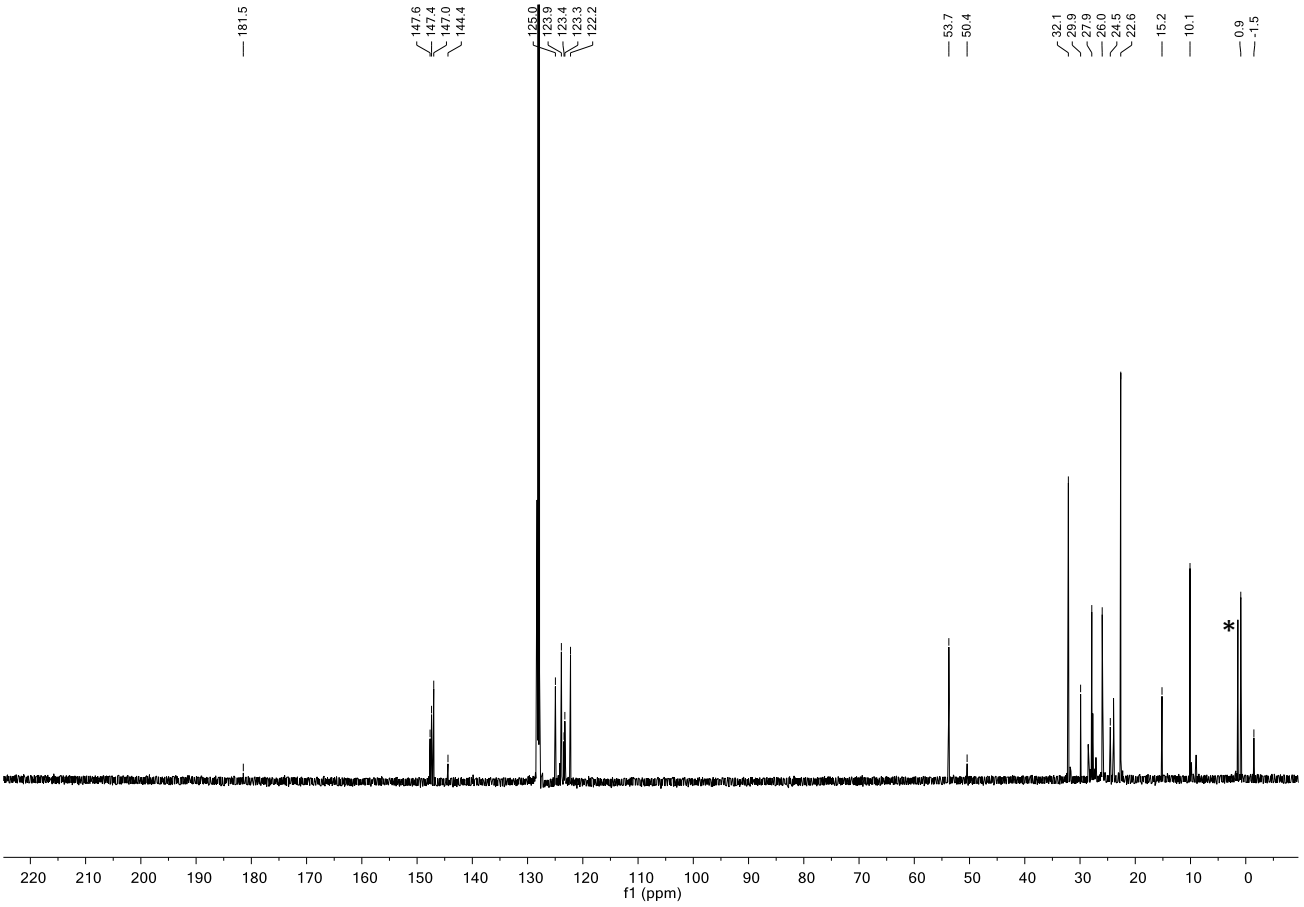


**Figure S35.** $^{1}$H-$^{1}$H COSY spectrum of **12**.

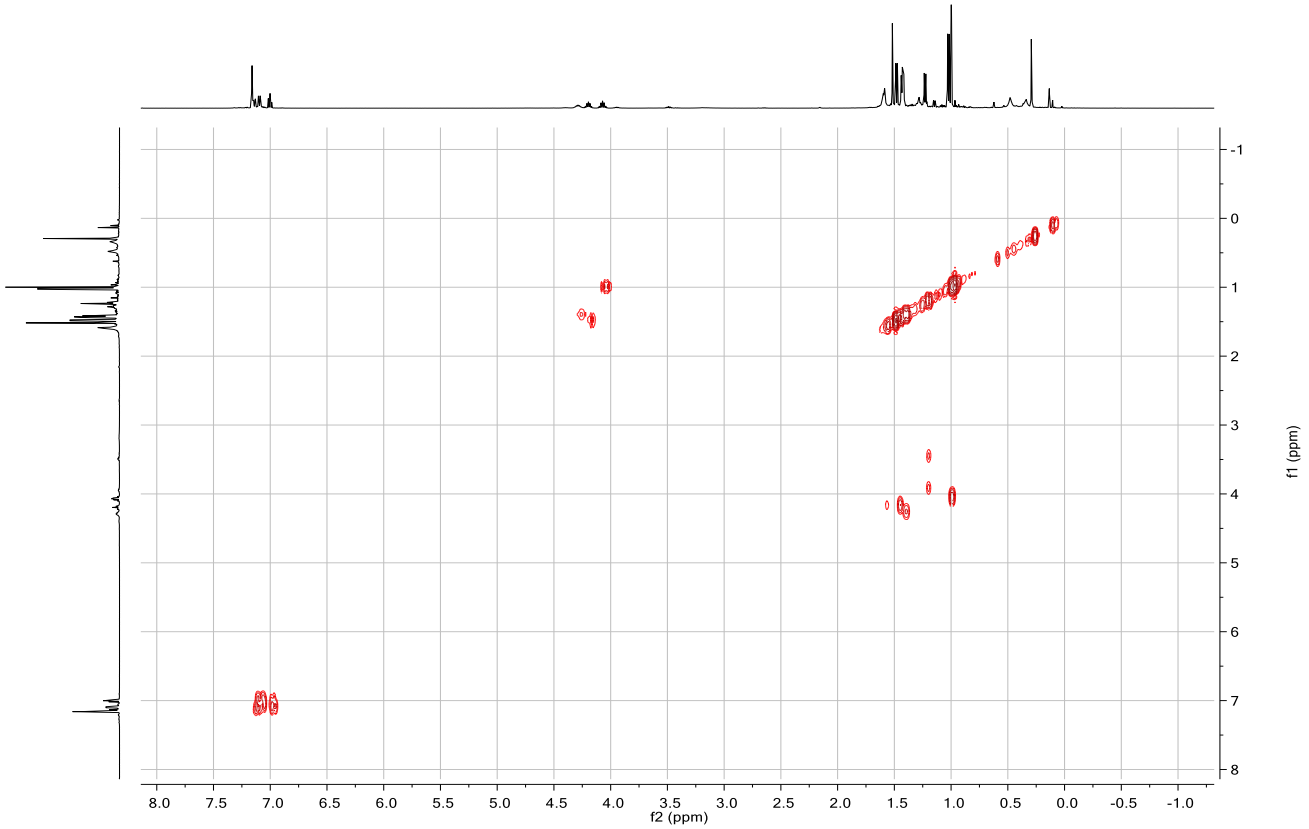



**Figure S36.** $^{1}$H-$^{13}$C HSQC spectrum of **12**.

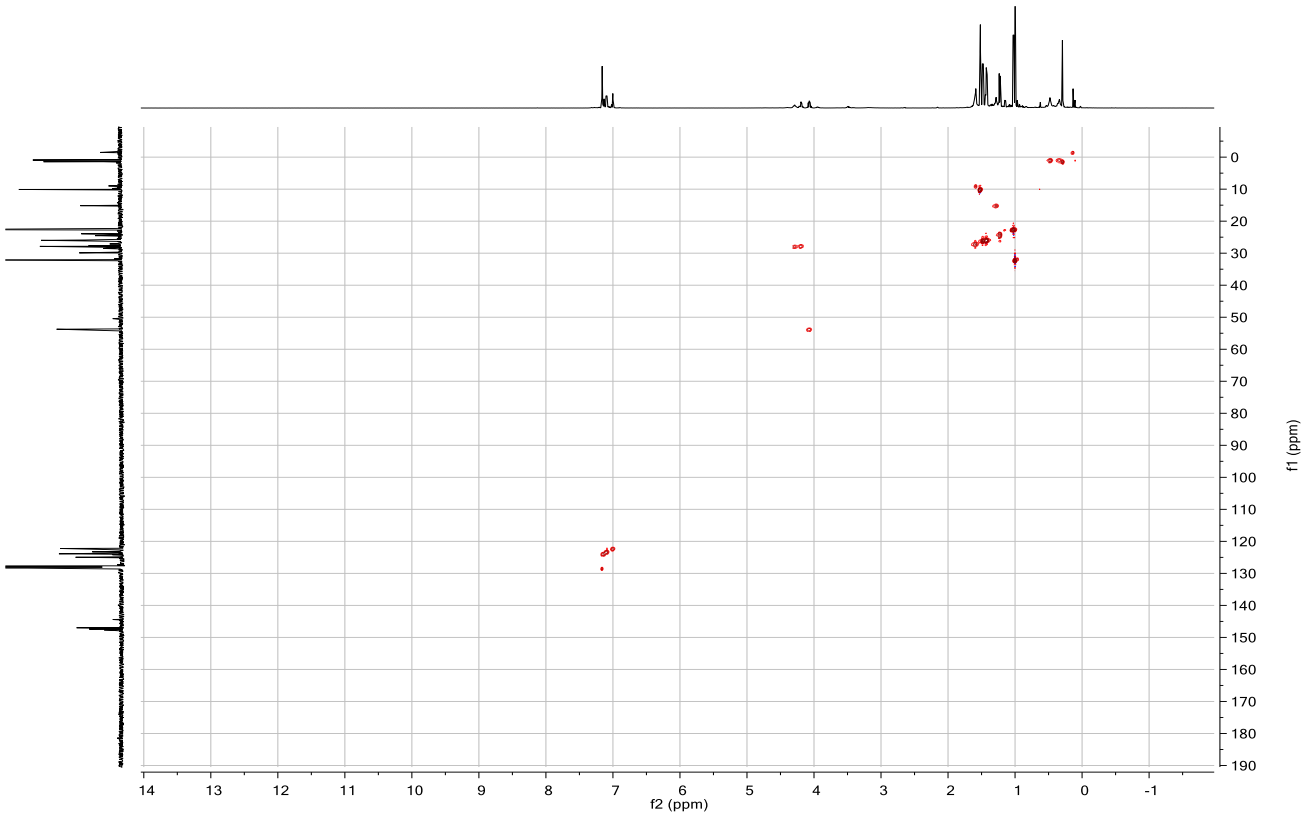
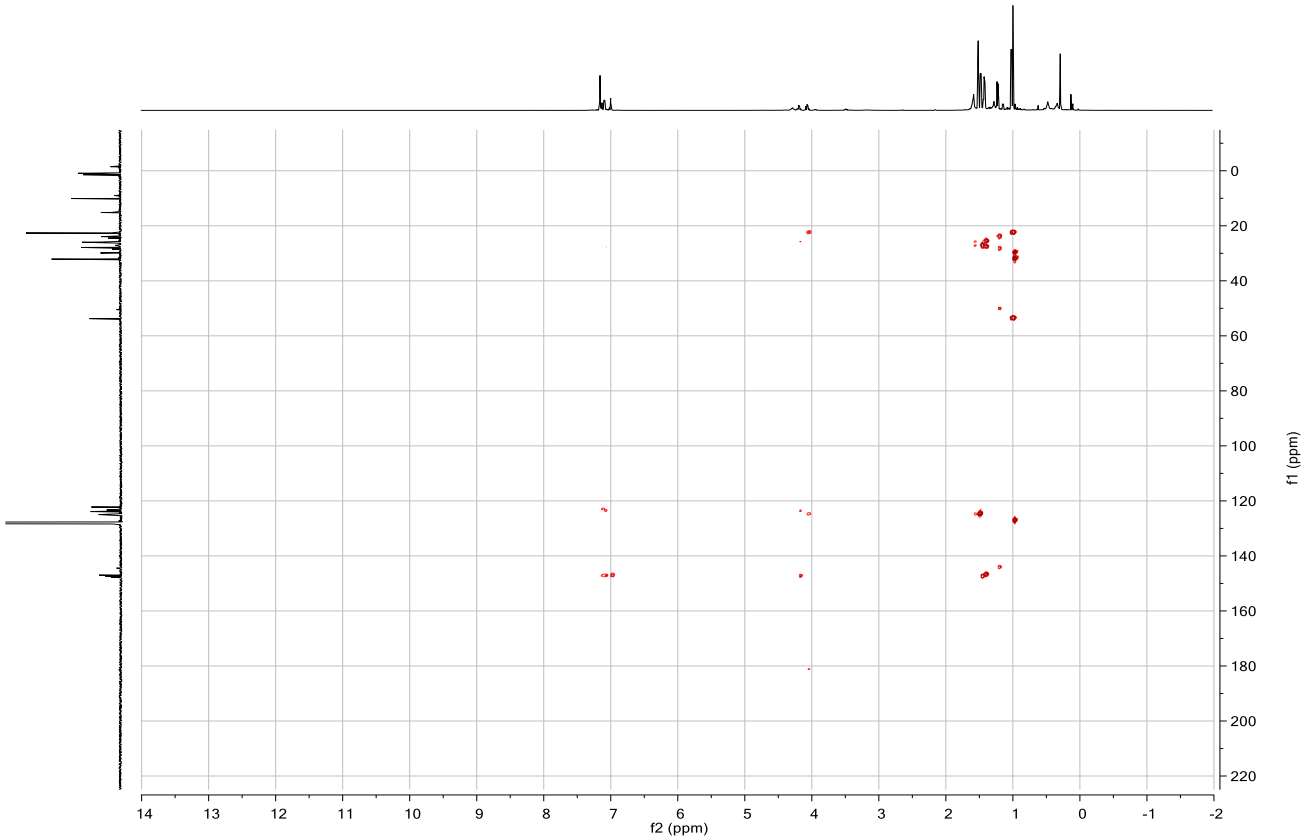


**Figure S37.** $^{1}H$-$^{13}C$ HMBC spectrum of **12**.



Synthesis of [(NHC$^{iPr}$)Cu(H)(Me$_3$SiCC)Al{SiN$^{Dipp}$}] (**13**)

In a J Young's tube, ethynyltrimethylsilane (2.4 mg, 3.1 µl, 0.025 mmol) was added via micropipette to a colourless solution of [(NHC$^{iPr}$)Cu-Al{SiN$^{Dipp}$}] (**1**, 19 mg, 0.025 mmol) in $C_6D_6$. Quantitative generation of **13** was observed by NMR spectroscopy overnight at room temperature. The colourless solution was then put under vacuum to remove all volatiles and give compound **13** as a white powder. Yield 19 mg, 89 %. Single crystal suitable for X-ray crystallography was obtained by slow evaporation a hexane solution at room temperature. Anal Calc'd for $C_{46}H_{80}AlCuN_4Si_3$ (**13**, 863.96) C, 63.95; H, 9.33; N, 6.49 %. Found: C, 64.38; H, 8.79; N, 6.28 %. $^1$H NMR (500 MHz, 298 K, Benzene-*d*$_6$) δ 7.13 – 7.11 (m, 2H, *m*-C$_6$*H*$_3$), 7.09 – 7.06 (m, 2H, *m*-C$_6$*H*$_3$), 7.00 – 6.97 (m, 2H, *p*-C$_6$*H*$_3$), 4.29 (sept, *J* = 6.7 Hz, 2H, C*H*Me$_2$), 4.14 (sept, *J* = 6.7 Hz, 2H, C*H*Me$_2$), 3.94 (sept, *J* = 7.1 Hz, 2H, NC*H*Me$_2$), 1.50 (s, 6H, NC*Me*), 1.47 (d, *J* = 6.7 Hz, 12H, CH*Me*$_2$), 1.41 (d, *J* = 6.7 Hz, 12H, CH*Me*$_2$), 1.27 (s br, 4H, SiC*H*$_2$), 1.01 (d, *J* = 7.1 Hz, 12H, NCH*Me*$_2$), 0.47 (s br, 6H, Si*Me*$_2$), 0.34 (s br, 6H, Si*Me*$_2$), 0.04 (s, 9H, Si*Me*$_3$). $^1$H resonance correlated to Al-*H* not observed. $^{13}$C{$^1$H} NMR (126 MHz, 298 K, Benzene-*d*$_6$) δ 180.9 (Cu*C*$_{carbene}$), 147.7 (*i*-*C*$_6$H$_3$), 147.3 (Al*C*CSiMe$_3$), 146.9 (*o*-*C*$_6$H$_3$), 146.8 (*o*-*C*$_6$H$_3$), 124.8 (N*C*Me), 123.8 (*m*-*C*$_6$H$_3$), 123.26 (*m*-*C*$_6$H$_3$), 122.3 (*p*-*C*$_6$H$_3$), 118.1 (AlC*C*SiMe$_3$), 53.6 (N*C*HMe$_2$), 27.8 (*C*HMe$_2$), 27.6 (*C*HMe$_2$), 26.0 (CH*Me*$_2$), 25.6 (CH*Me*$_2$), 24.5 (CH*Me*$_2$), 22.6 (CH*Me*$_2$), 15.1(Si*C*H$_2$), 10.0 (NC*Me*), 1.2 (Si*Me*$_2$), 0.9 (Si*Me*$_3$), 0.8 (Si*Me*$_2$).

**Figure S38.** $^{1}$H NMR (500 MHz, 298 K, $d_6$-benzene) spectrum of **13**. *grease

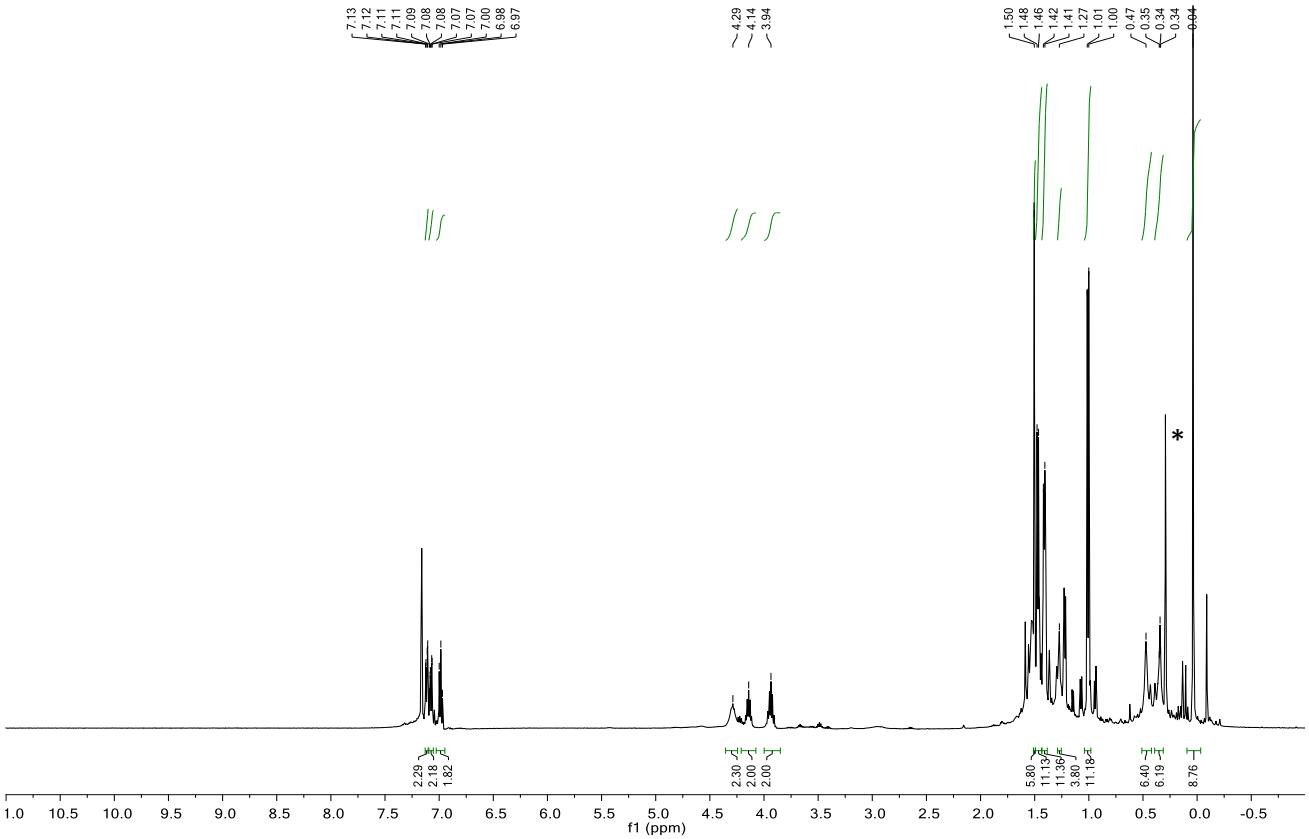



**Figure S39.** $^{13}$C NMR (126 MHz, 298 K, $d_6$-benzene) spectrum of **13**. *grease

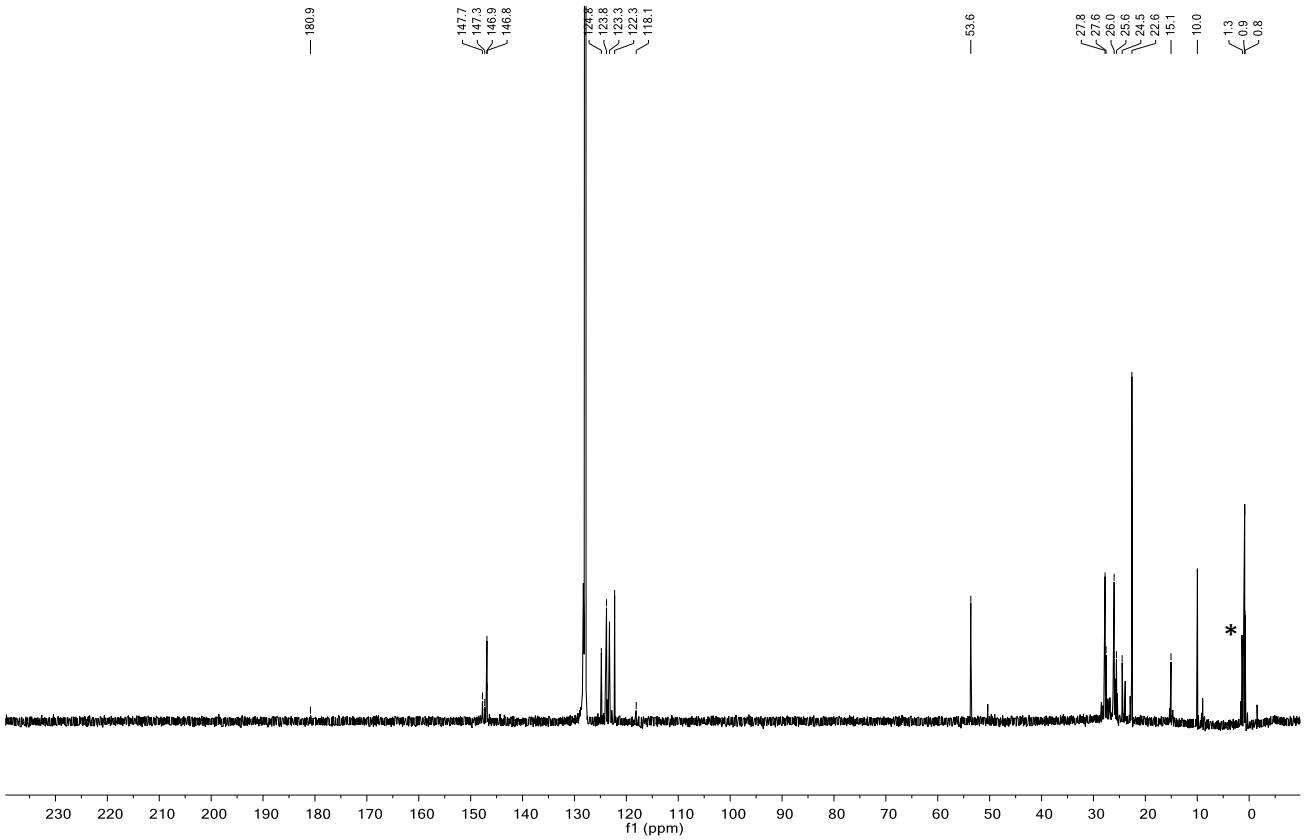


**Figure S40.** $^{1}$H-$^{1}$H COSY spectrum of **13**.

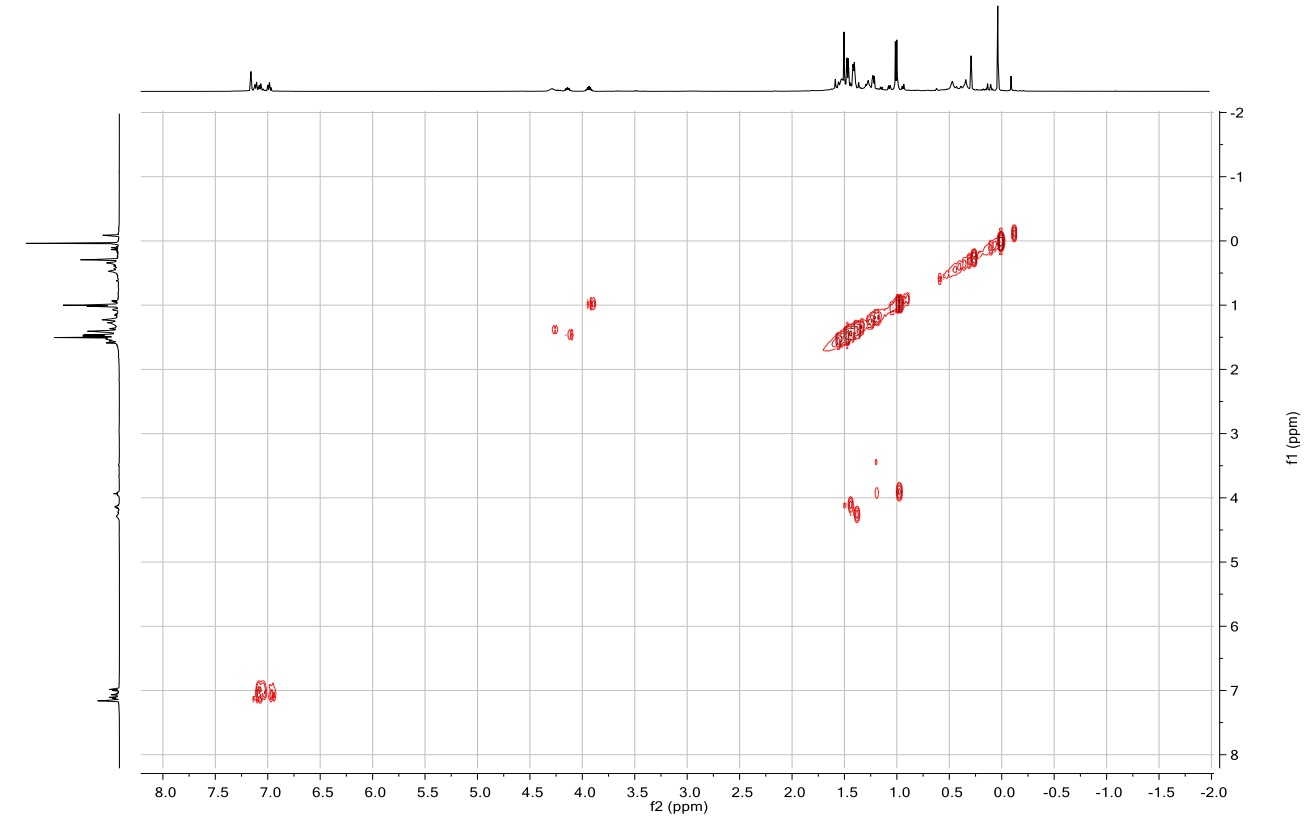



**Figure S41.** $^{1}$H-$^{13}$C HSQC spectrum of **13**.

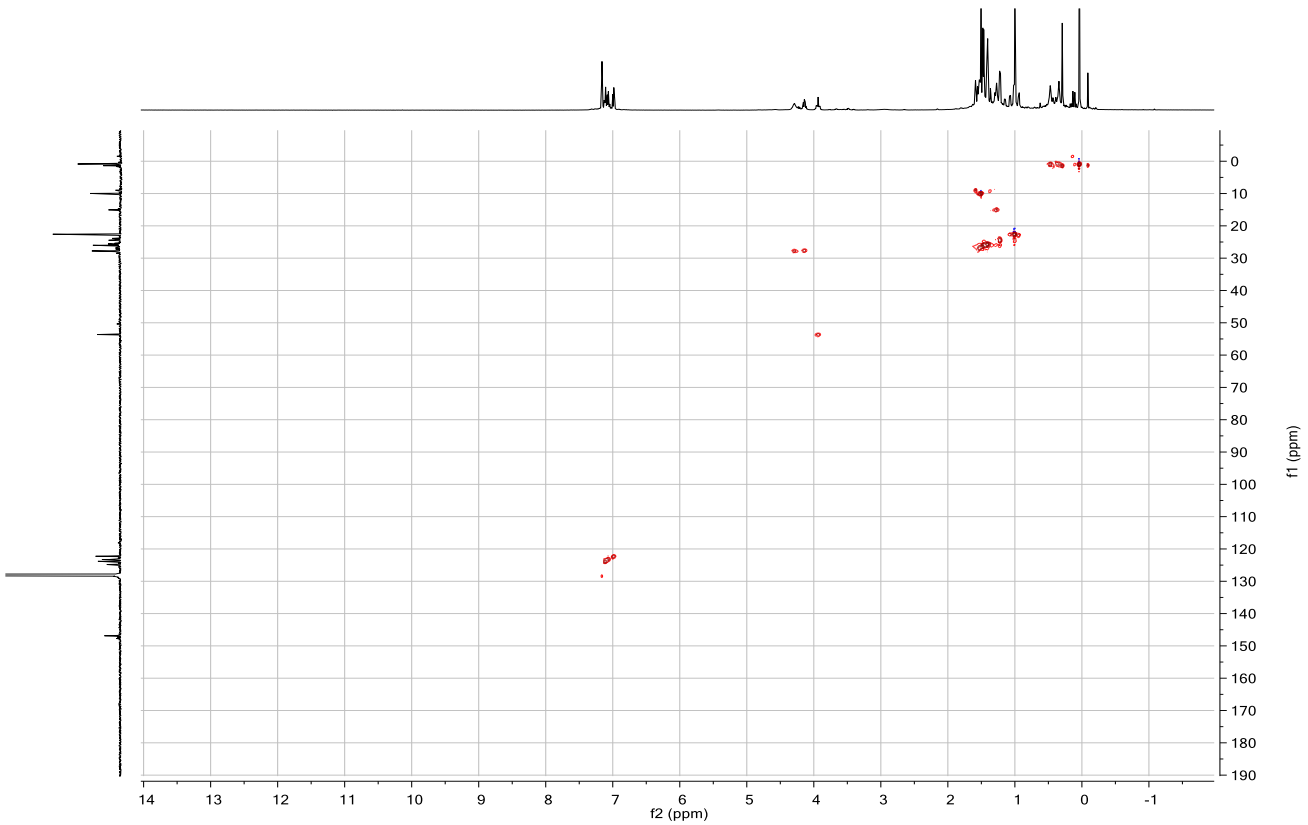
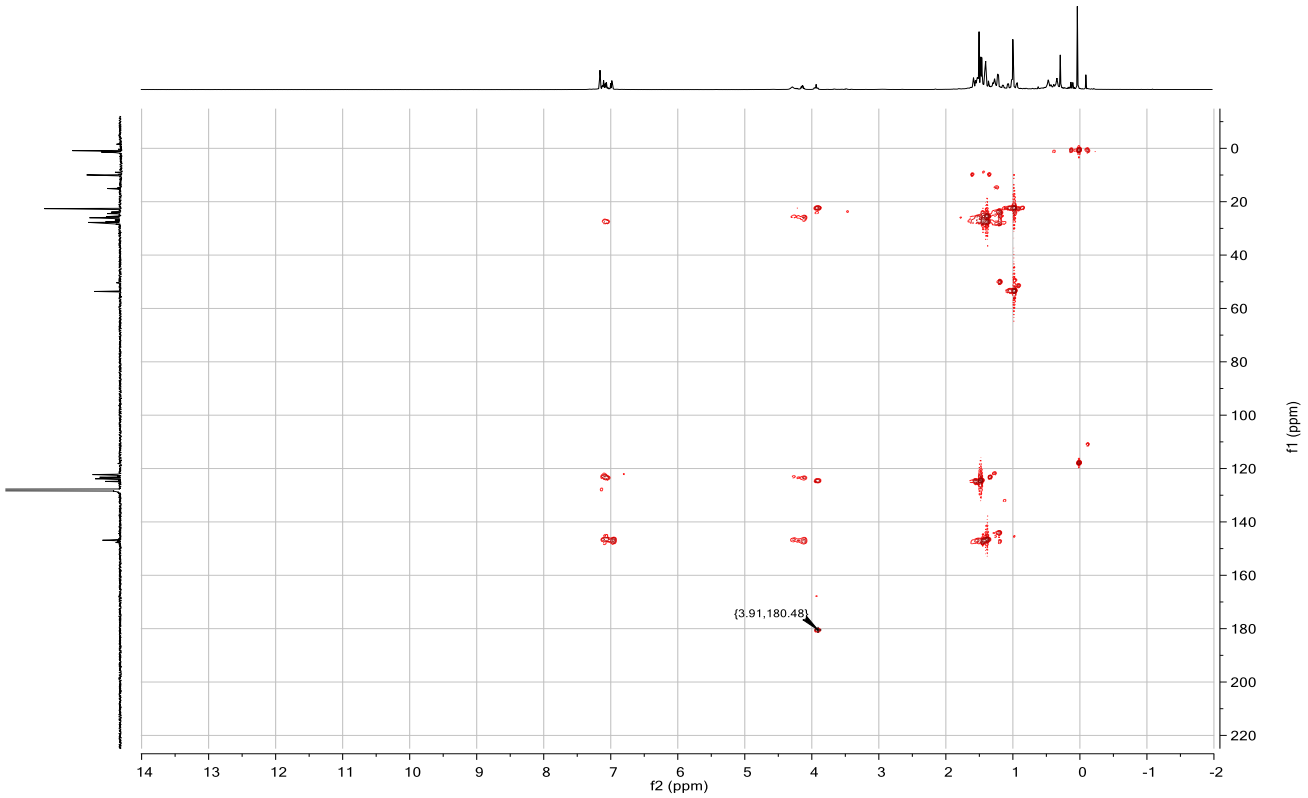


**Figure S42.** $^{1}H$-$^{13}C$ HMBC spectrum of **13**.



## 1.3. Generation of Alkenes from Corresponding Alkyne

**Figure S43:** $^{1}H$ NMR (500 MHz, $d_6$-benzene) spectrum of **1** with 3 equivalents of PhCCH (kept at 60°C overnight)

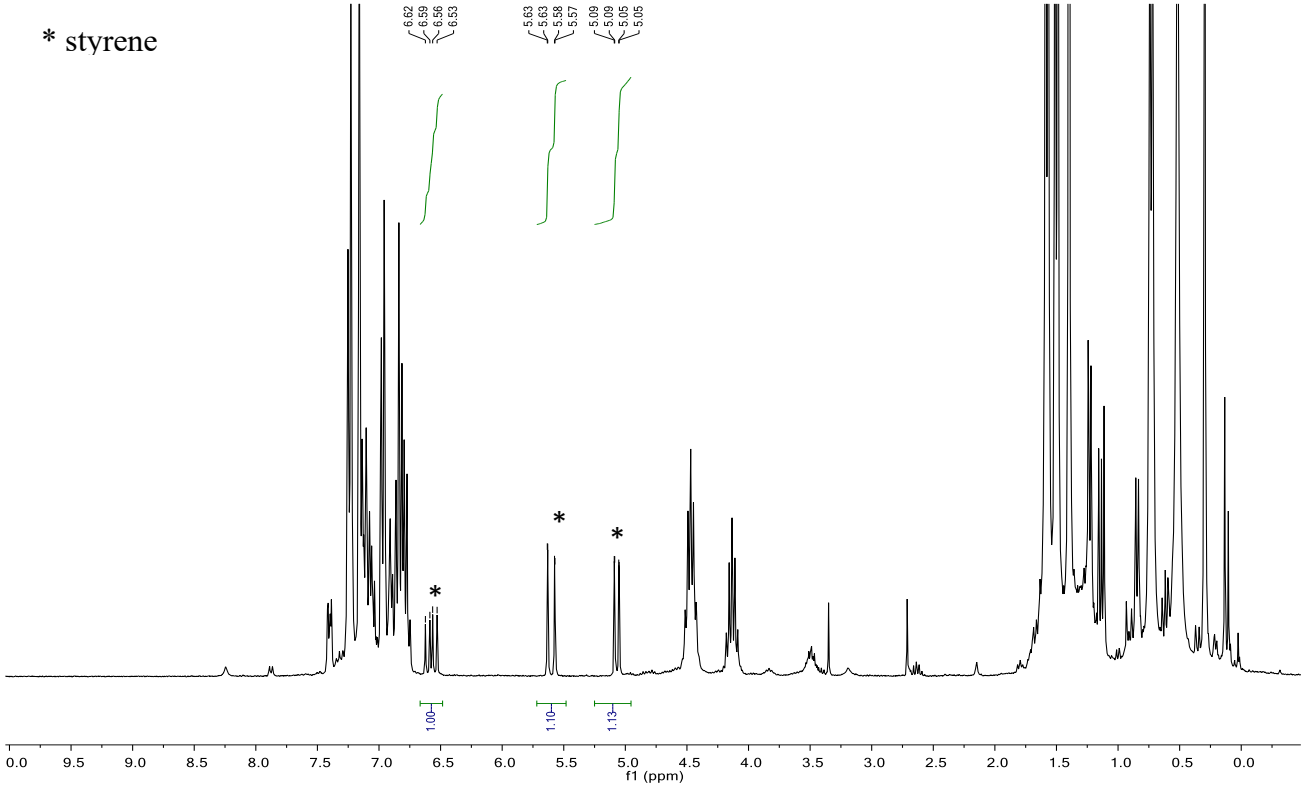


**Figure S44:** $^{1}$H NMR (500 MHz, $d_6$-benzene) spectrum of **1** with 3 equivalents of $^{n}$BuCCH (kept at 60°C overnight)

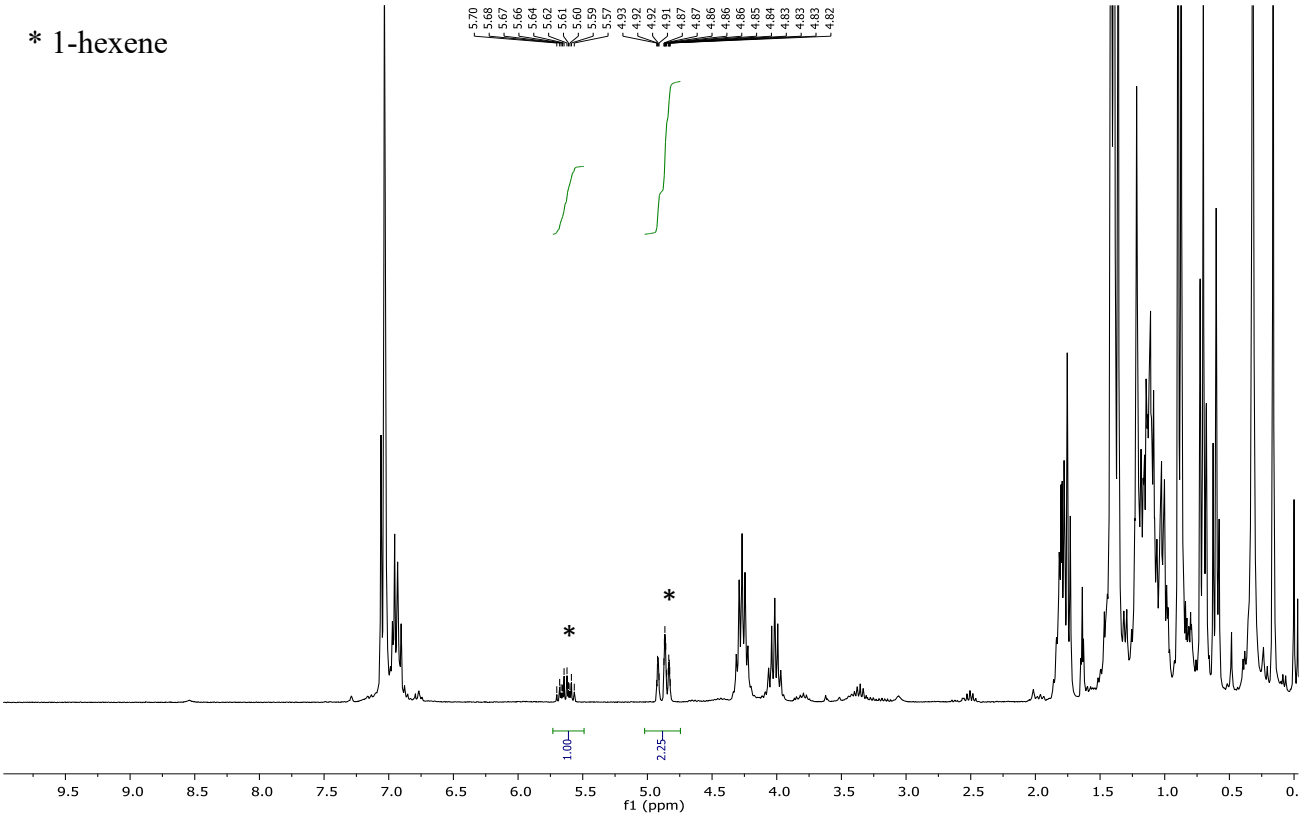



**Figure S45:** $^{1}$H NMR (500 MHz, $d_6$-benzene) spectrum of **1** with 3 equivalents of MesCCH (kept at 60°C 3 days).

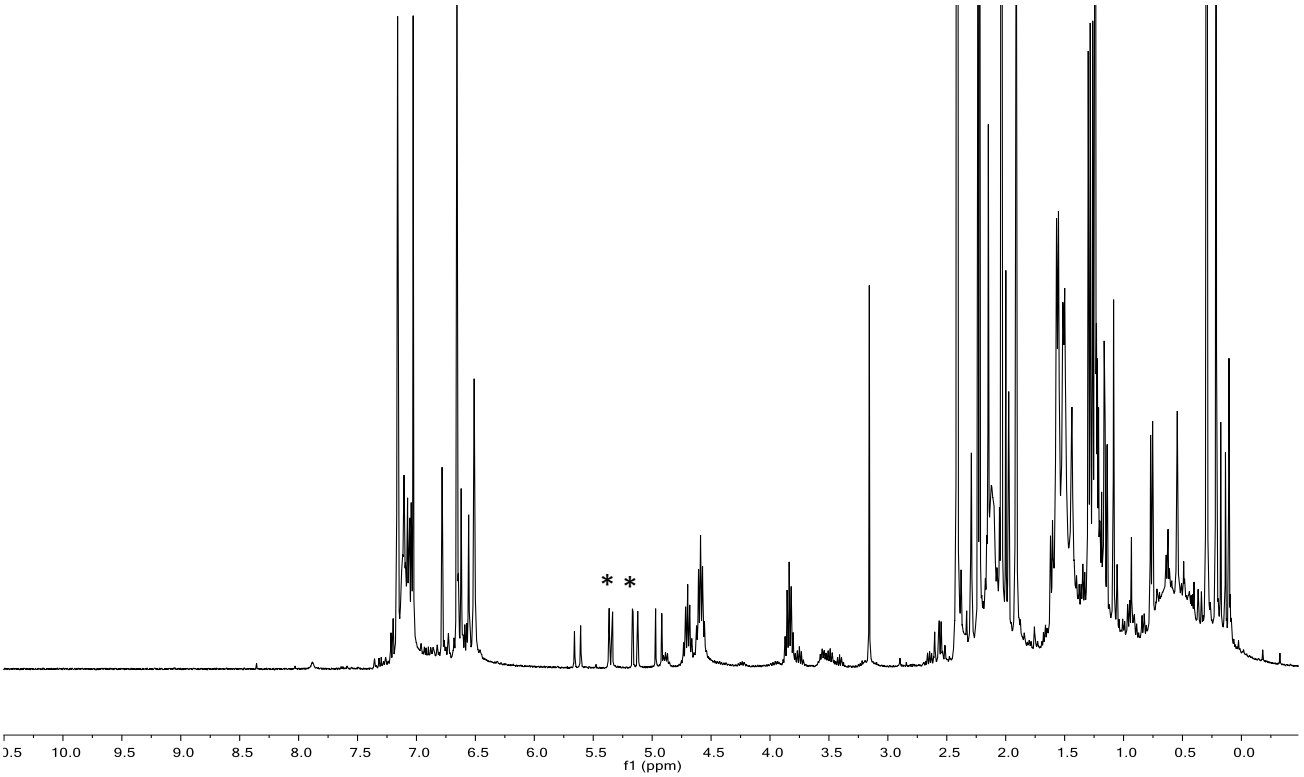


**Figure S46:** $^{1}$H NMR (500 MHz, $d_6$-benzene) spectrum of **1** with 3 equivalents of $^{t}$BuCCH (kept at 60°C overnight).

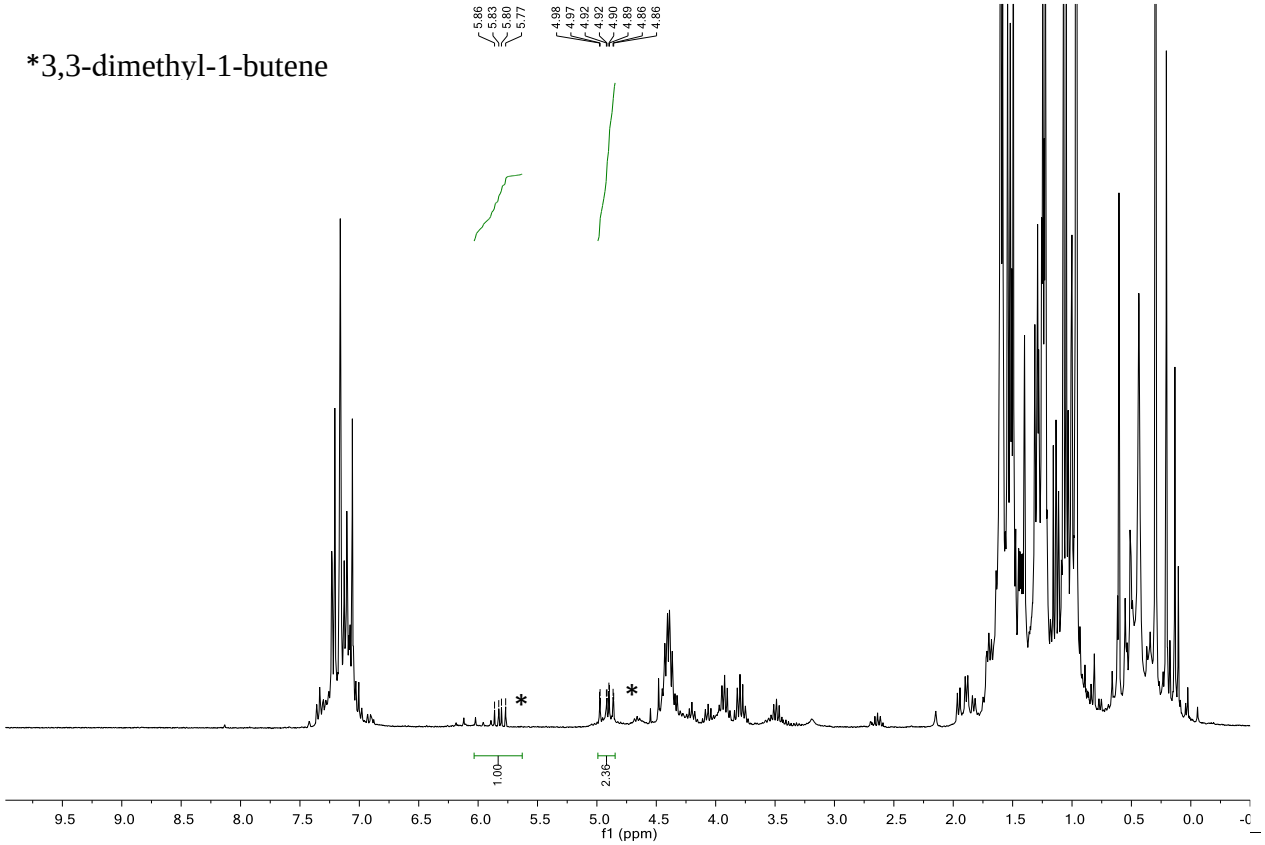
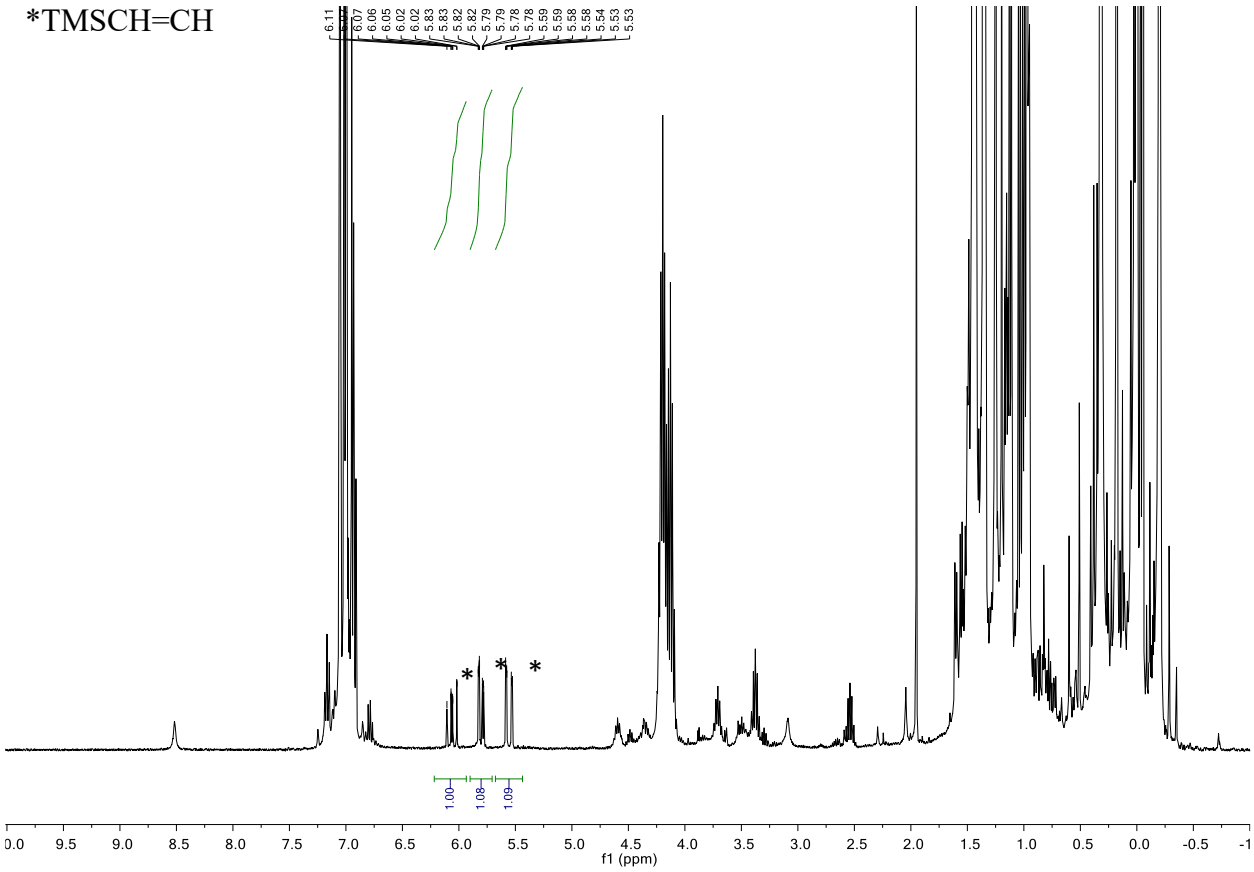


**Figure S47:** $^{1}$H NMR (500 MHz, $d_6$-benzene) spectrum of **1** with 3 equivalents of $Me_3SiCCH$ (kept at 60ºC 3 days).



### 1.4. Single Crystal X-ray Diffraction Analysis

Single Crystal X–ray diffraction data were collected either on a SuperNova EosS2 diffractometer using CuKα (λ = 1.54184 Å) radiation (compounds **2a**, **3**, **5**, **7**, **10**, **10a**, **11, 12**) or on a Rigaku Xcalibur diffractometer using Mo Kα (λ = 0.71073 Å) radiation (compounds **6**, **8** and **13**). The crystals were maintained at 150 K during data collection. Using Olex2,[2] the structures were solved with the olex2.solve[3] structure solution program or ShelXT and refined with the ShelXL[4] refinement package using Least Squares minimisation. Noteworthy points follow, and where disorder has been modelled, both distance and ADP restraints have been employed, on merit, in these regions to assist convergence. The hydrogen atoms attached to C31, C44 and C45 in the structure of **2a** were each located, and refined subject to being a distance of 0.98 Å from the relevant parent atom.

The asymmetric unit in **5** comprises one aluminium based complex and two crystallographically independent copper containing species. The metal centres in the latter are co-incident with inversion centres intrinsic to the space group and these symmetry elements serve to generate the remainder of transition metal complexes.

In the structure of **6**, the asymmetric unit contains two crystallographically (and chemically) distinct molecules, plus two regions of solvent. The mixed-metal complexes differ, most prominently, in the comparative Cu2 and Cu4 environments. Both solvent moieties were disordered in a manner that was accessible to modelling (disorder ratios of 55:45 and 75:25, for the moieties based on C1S and C1TS, respectively). There was evidence for some smearing of the electron density in the phenyl group based on C53 which was not modelled but this ring was treated as a rigid hexagon in the final least-squares cycles.

Structural refinement of **7** was unremarkable, with the exception of disorder modelling for C46-C49 for which each carbon was treated as being split over two sites in an 85:25 ratio. While there was some comparative smearing of electron density evident for C50-C53, this was not positionally divergent enough to lend itself to ready modelling.

In **8**, the $SiMe_3$ group based on Si3 was treated for 50:50 disorder over 2 proximate sites.

In the structure of **10**, the asymmetric unit comprises one molecule of benzene and half of the metal complex. Cu1, Al1 and C1, in the latter, are all located on a crystallographic 2-fold rotation axis, which serves to generate the remainder of the molecule.

The bridging hydride was located, and refined freely with a riding $U_{iso}$ value, in the structure of **12**.

The hydride was also located and refined in the structure of **13**, with a fixed $U_{iso}$ value in this instance.

**Figure S48:** X-ray structure of **5**: Symm ops: [1] 2 – *x*, –*y*, 2 – *z*; [2] –*x* 2 – *y*, 1 – *z*

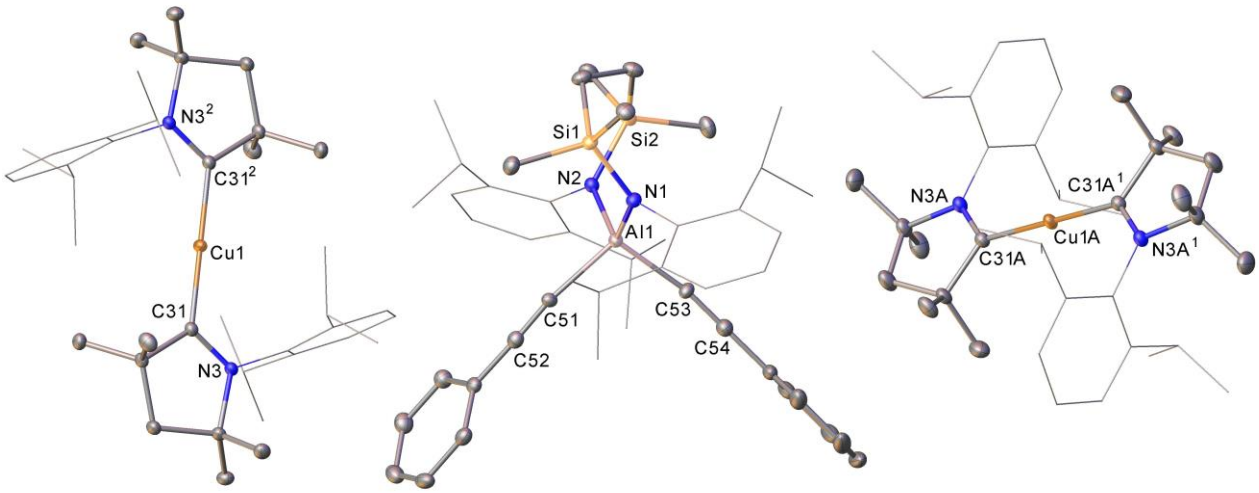



**Figure S49:** X-ray structure of **6**.

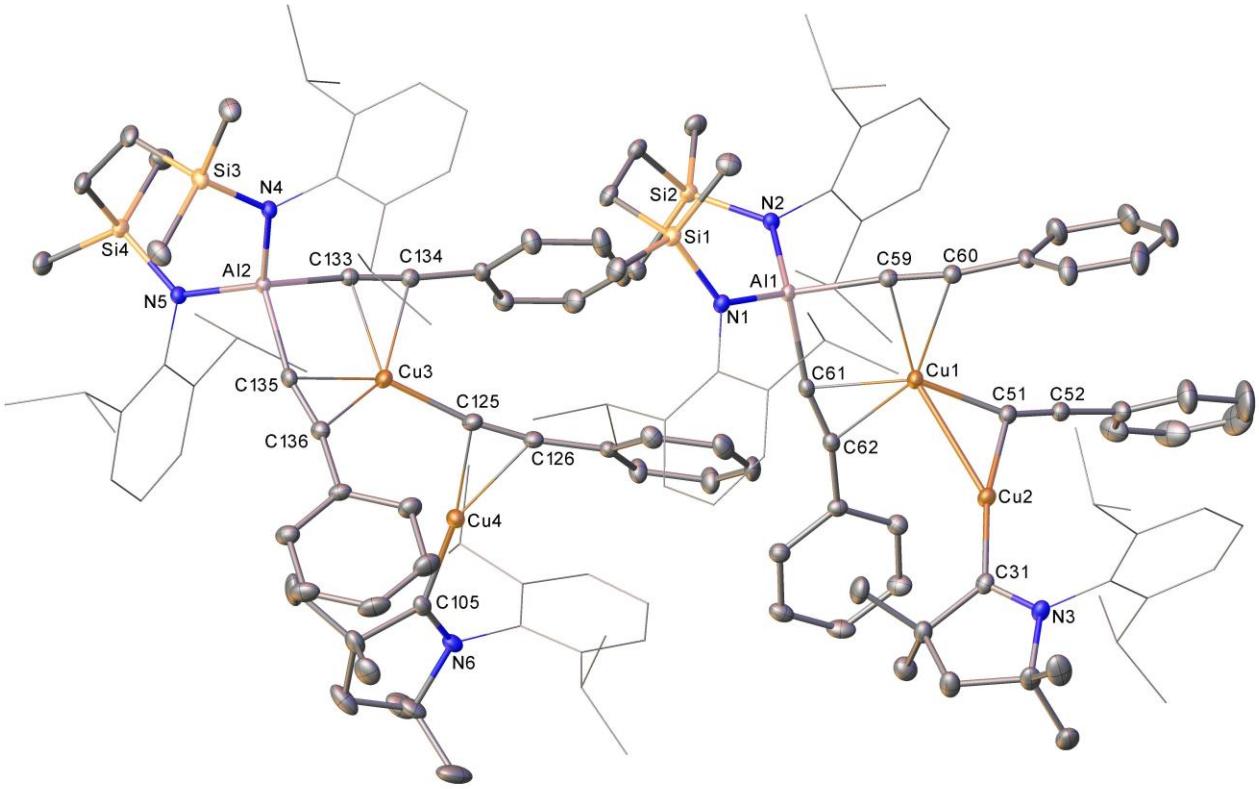


**Figure S50:** X-ray structure of **10a**.

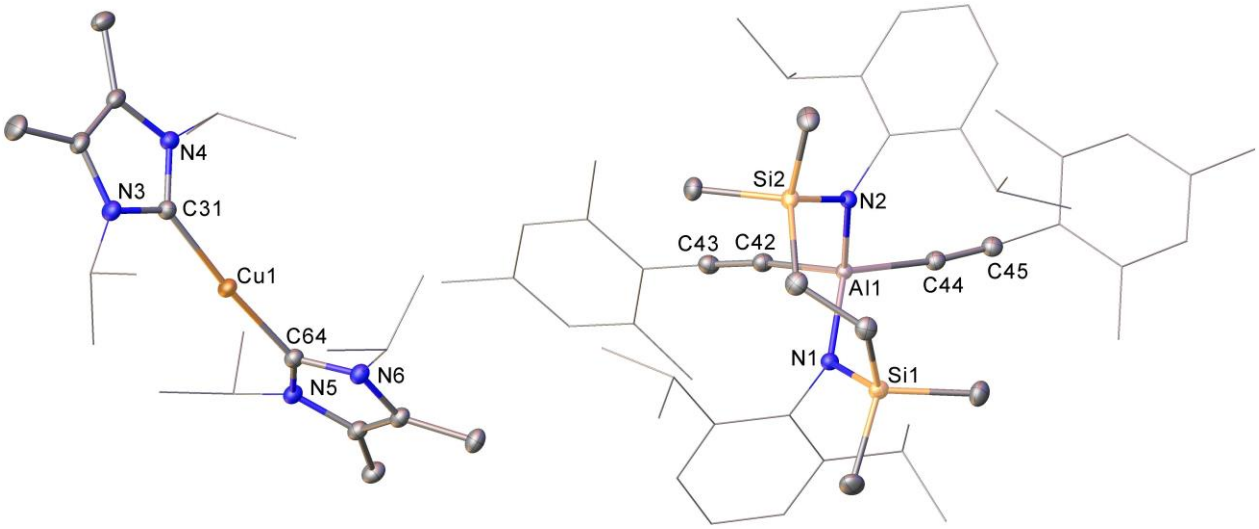



**Figure S51:** X-ray structure of **11**.

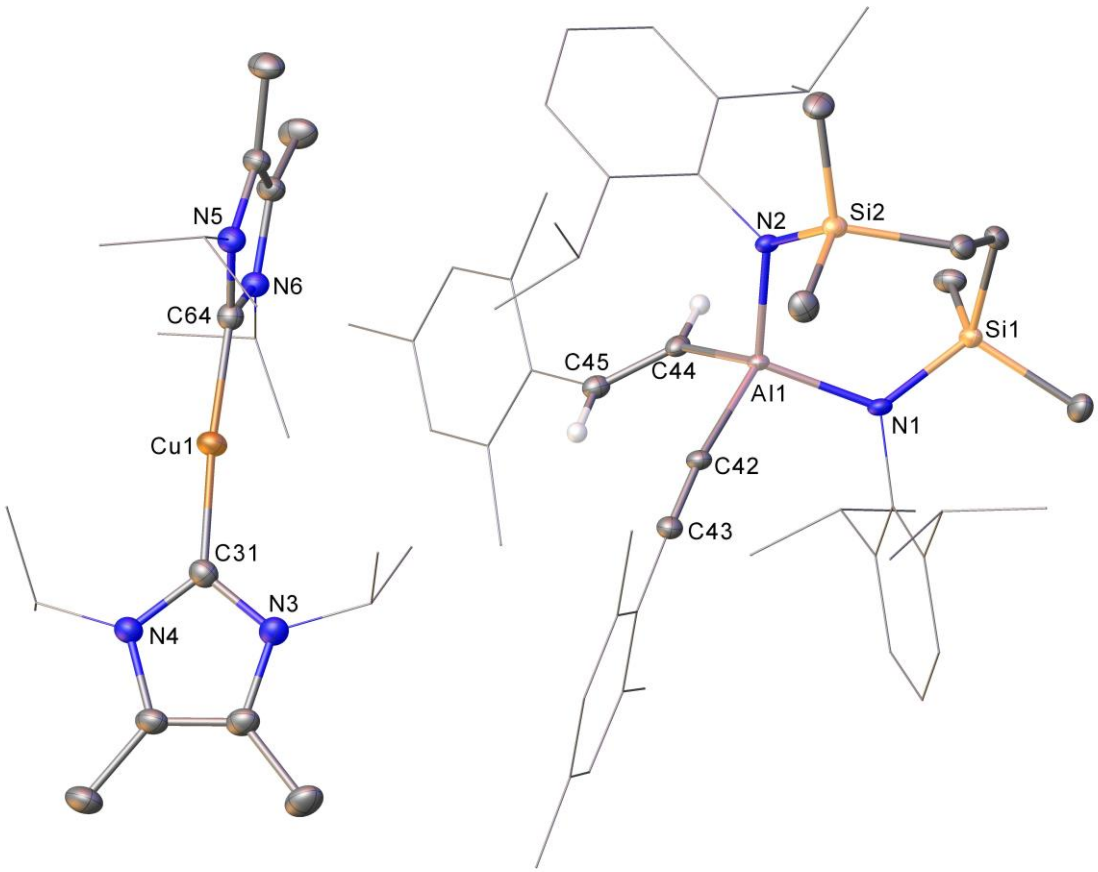


**Table S1:** Crystal data and structure refinement for compounds **2a**, **3, 5** and **6.**

| Compound | **2a** | **3** | **5** | **6** |
|---|---|---|---|---|
| Empirical formula | $C_{57}H_{83}AlN_4Si_2$ | $C_{57}H_{80}AlCuN_4Si_2$ | $C_{86}H_{122}AlCuN_4Si_2$ | $C_{160}H_{220}Al_2Cu_4N_6Si_4$ |
| Formula weight | 907.43 | 967.95 | 1358.57 | 2647.89 |
| Crystal system | monoclinic | monoclinic | triclinic | triclinic |
| Space group | $P2_1/c$ | $Cc$ | $P$-1 | $P$-1 |
| $a$/Å | 16.00380(10) | 20.8885(2) | 12.2250(2) | 13.2732(2) |
| $b$/Å | 13.50320(10) | 13.8728(1) | 12.4368(2) | 17.1411(3) |
| $c$/Å | 25.41530(10) | 19.6118(2) | 27.9562(4) | 34.2337(6) |
| $\alpha$/° | 90 | 90 | 81.885(1) | 97.978(1) |
| $\beta$/° | 97.5190(10) | 101.347(1) | 86.337(1) | 98.341(1) |
| $\gamma$/° | 90 | 90 | 74.292(2) | 96.908(2) |
| Volume/Å$^3$ | 5445.08(6) | 5572.06(9) | 4049.28(12) | 7553.0(2) |
| $Z$ | 4 | 4 | 2 | 2 |
| $\rho_{calc}$ g/cm$^3$ | 1.107 | 1.154 | 1.114 | 1.164 |
| $\mu$/mm$^{-1}$ | 1.031 | 1.400 | 1.093 | 0.649 |
| $F$(000) | 1976.0 | 2080.0 | 1472.0 | 2840.0 |
| Crystal size/mm$^3$ | 0.148 × 0.115 × 0.075 | 0.166 × 0.097 × 0.086 | 0.168 × 0.129 × 0.054 | 0.604 × 0.472 × 0.279 |
| 2θ range /° | 7.428 to 145.89 | 7.698 to 145.962 | 7.446 to 145.826 | 6 to 58.258 |
| Index ranges | -19 ≤ h ≤ 19, -16 ≤ k ≤ 16, -31 ≤ l ≤ 28 | -25 ≤ h ≤ 22, -17 ≤ k ≤ 17, -24 ≤ l ≤ 24 | -14 ≤ h ≤ 15, -15 ≤ k ≤ 15, -34 ≤ l ≤ 29 | -18 ≤ h ≤ 17, -23 ≤ k ≤ 23, -46 ≤ l ≤ 46 |
| Reflections collected | 75392 | 29874 | 56874 | 128297 |
| Independent reflections | 10831 [$R_{int}$ = 0.0409, $R_{sigma}$ = 0.0246] | 8301 [$R_{int}$ = 0.0423, $R_{sigma}$ = 0.0513] | 16041 [$R_{int}$ = 0.0327, $R_{sigma}$ = 0.0372] | 38945 [$R_{int}$ = 0.0311, $R_{sigma}$ = 0.0408] |
| Data/restraints/parameters | 10831/3/607 | 8301/2/605 | 16041/0/878 | 38945/291/1741 |
| Goodness-of-fit on $F^2$ | 1.012 | 1.031 | 1.025 | 1.050 |
| Final $R$ indexes [$I$>=2σ (I)] | $R_1$ = 0.0395, $wR_2$ = 0.1056 | $R_1$ = 0.0371, $wR_2$ = 0.0903 | $R_1$ = 0.0358, $wR_2$ = 0.0904 | $R_1$ = 0.0425, $wR_2$ = 0.0943 |
| Final $R$ indexes [all data] | $R_1$ = 0.0452, $wR_2$ = 0.1104 | $R_1$ = 0.0390, $wR_2$ = 0.0921 | $R_1$ = 0.0413, $wR_2$ = 0.0947 | $R_1$ = 0.0612, $wR_2$ = 0.1016 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.56/-0.24 | 0.34/-0.36 | 0.53/-0.36 | 0.61/-0.36 |
| Flack parameter | - | 0.17(3) | - | - |

**Table S1:** Crystal data and structure refinement for compounds **7**, **8**, **10** and **10a**.

| Compound | **7** | **8** | **10** | **10a** |
|---|---|---|---|---|
| Empirical formula | $C_{53}H_{88}AlCuN_4Si_2$ | $C_{51}H_{88}AlCuN_4Si_4$ | $C_{75}H_{104}AlCuN_4Si_2$ | $C_{74}H_{112}AlCuN_6Si_2$ |
| Formula weight | 927.97 | 960.13 | 1208.32 | 1232.39 |
| Crystal system | monoclinic | monoclinic | orthorhombic | monoclinic |
| Space group | *Cc* | $P2_1/n$ | *Pbcn* | $P2_1/c$ |
| *a*/Å | 21.4197(1) | 12.6138(3) | 15.0236(1) | 12.40965(5) |
| *b*/Å | 13.5245(1) | 20.7585(4) | 21.9618(1) | 23.21981(10) |
| *c*/Å | 19.6839(1) | 22.1325(4) | 21.1294(2) | 25.09012(11) |
| *α*/° | 90 | 90 | 90 | 90 |
| *β*/° | 103.151(1) | 93.689(2) | 90 | 92.1704(4) |
| *γ*/° | 90 | 90 | 90 | 90 |
| Volume/Å$^3$ | 5552.69(6) | 5783.2(2) | 6971.55(9) | 7224.52(5) |
| *Z* | 4 | 4 | 4 | 4 |
| $\rho_{calc}$ g/cm$^3$ | 1.110 | 1.103 | 1.151 | 1.133 |
| $\mu$/mm$^{-1}$ | 1.379 | 0.510 | 1.213 | 1.185 |
| *F*(000) | 2016.0 | 2080.0 | 2608.0 | 2672.0 |
| Crystal size/mm$^3$ | 0.198 × 0.131 × 0.066 | 0.882 × 0.689 × 0.557 | 0.164 × 0.085 × 0.066 | 0.216 × 0.153 × 0.055 |
| 2θ range /° | 7.79 to 145.704 | 5.872 to 60.604 | 7.128 to 145.926 | 7.052 to 146.126 |
| Index ranges | -26 ≤ h ≤ 26, -16 ≤ k ≤ 16, -24 ≤ l ≤ 21 | -17 ≤ h ≤ 17, -29 ≤ k ≤ 29, -29 ≤ l ≤ 31 | -18 ≤ h ≤ 17, -27 ≤ k ≤ 26, -25 ≤ l ≤ 26 | -14 ≤ h ≤ 15, -28 ≤ k ≤ 28, -30 ≤ l ≤ 29 |
| Reflections collected | 49961 | 98784 | 80334 | 97505 |
| Independent reflections | 9866 [$R_{int}$ = 0.0313, $R_{sigma}$ = 0.0265] | 15956 [$R_{int}$ = 0.0315, $R_{sigma}$ = 0.0263] | 6963 [$R_{int}$ = 0.0557, $R_{sigma}$ = 0.0251] | 14393 [$R_{int}$ = 0.0309, $\underline{R}_{sigma}$ = 0.0196] |
| Data/restraints/parameters | 9866/69/601 | 15956/100/613 | 6963/0/388 | 14393/0/787 |
| Goodness-of-fit on $F^2$ | 1.023 | 1.039 | 1.024 | 1.031 |
| Final *R* indexes [*I*>=2σ (I)] | $R_1$ = 0.0273, $wR_2$ = 0.0729 | $R_1$ = 0.0348, $wR_2$ = 0.0844 | $R_1$ = 0.0351, $wR_2$ = 0.0917 | $R_1$ = 0.0310, $wR_2$ = 0.0829 |
| Final *R* indexes [all data] | $R_1$ = 0.0278, $wR_2$ = 0.0734 | $R_1$ = 0.0509, $wR_2$ = 0.0920 | $R_1$ = 0.0424, $wR_2$ = 0.0965 | $R_1$ = 0.0346, $wR_2$ = 0.0857 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.41/-0.25 | 0.50/-0.37 | 0.27/-0.51 | 0.36/-0.40 |
| Flack parameter | 0.000(6) | - | - | - |

**Table S1:** Crystal data and structure refinement for compounds **11**, **12** and **13**.

| Compound | **11** | **12** | **13** |
|---|---|---|---|
| Empirical formula | $C_{74}H_{114}AlCuN_6Si_2$ | $C_{46}H_{80}AlCuN_4Si_3$ | $C_{188}H_{320}Al_4Cu_4N_{16}Si_8$ |
| Formula weight | 1234.41 | 863.93 | 3391.38 |
| Crystal system | monoclinic | Monoclinic | monoclinic |
| Space group | $P2_1/n$ | $P2_1/n$ | $P2_1/c$ |
| $a$/Å | 13.5126(1) | 15.0696(4) | 16.2074(3) |
| $b$/Å | 23.3252(1) | 16.5798(5) | 12.7848(2) |
| $c$/Å | 23.6673(2) | 20.4317(4) | 24.4265(5) |
| $\alpha$/° | 90 | 90 | 90 |
| $\beta$/° | 105.075(1) | 91.457(2) | 100.576(2) |
| $\gamma$/° | 90 | 90 | 90 |
| Volume/Å$^3$ | 7202.84(9) | 5103.2(2) | 4975.39(16) |
| $Z$ | 4 | 4 | 1 |
| $\rho_{calc}$ g/cm$^3$ | 1.138 | 1.124 | 1.132 |
| $\mu$/mm$^{-1}$ | 1.188 | 1.684 | 0.538 |
| $F$(000) | 2680.0 | 1872.0 | 1840.0 |
| Crystal size/mm$^3$ | 0.2 × 0.125 × 0.075 | 0.095 × 0.062 × 0.03 | 0.412 × 0.35 × 0.169 |
| 2θ range /° | 7.58 to 145.928 | 7.93 to 146.056 | 6 to 60.752 |
| Index ranges | -16 ≤ h ≤ 16, -28 ≤ k ≤ 28, -28 ≤ l ≤ 29 | -18 ≤ h ≤ 16, -17 ≤ k ≤ 20, -23 ≤ l ≤ 25 | -22 ≤ h ≤ 21, -14 ≤ k ≤ 18, -32 ≤ l ≤ 32 |
| Reflections collected | 104118 | 28989 | 52870 |
| Independent reflections | 14348 [$R_{int}$ = 0.0564, $R_{sigma}$ = 0.0341] | 10112 [$R_{int}$ = 0.0562, $R_{sigma}$ = 0.0631] | 13342 [$R_{int}$ = 0.0315, $R_{sigma}$ = 0.0342] |
| Data/restraints/parameters | 14348/0/787 | 10112/0/524 | 13342/0/520 |
| Goodness-of-fit on $F^2$ | 1.022 | 1.018 | 1.030 |
| Final $R$ indexes [$I$>=2σ (I)] | $R_1$ = 0.0432, $wR_2$ = 0.1129 | $R_1$ = 0.0480, $wR_2$ = 0.1087 | $R_1$ = 0.0368, $wR_2$ = 0.0853 |
| Final $R$ indexes [all data] | $R_1$ = 0.0495, $wR_2$ = 0.1185 | $R_1$ = 0.0710, $wR_2$ = 0.1207 | $R_1$ = 0.0537, $wR_2$ = 0.0928 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.96/-1.00 | 0.53/-0.42 | 0.47/-0.34 |

## 1.5. Computational Details

DFT calculations were performed with Gaussian 16 (C.01).[5] Cu, Al, and Si centres were described with the Stuttgart RECPs and associated basis sets,[6] while 6-31G** was employed for the remaining atoms (this basis set combination will herein, and throughout the manuscript is referred to as "BS1").[7,8] A polarization function was also added to Al (ζd = 0.190) and Si (ζd = 0.284).[9] Initial BP86 optimizations[10,11] were performed using the 'grid = ultrafine' option, with all stationary points being fully characterized via analytical frequency calculations as minima or transition states (all positive eigenvalues or one imaginary eigenvalue respectively). All energies were recomputed with a larger basis set featuring 6-311++G** basis sets on all atoms except Cu, for which cc-pVTZ-pp was employed (referred to as "BS2" throughout).[12,13] Corrections for the effect of benzene (ε = 2.3741) solvent were employed using the polarizable continuum model and BS1.[14] Single-point dispersion corrections to the BP86 results employed Grimme's D3 parameter set with Becke-Johnson damping as implemented in Gaussian.[14]

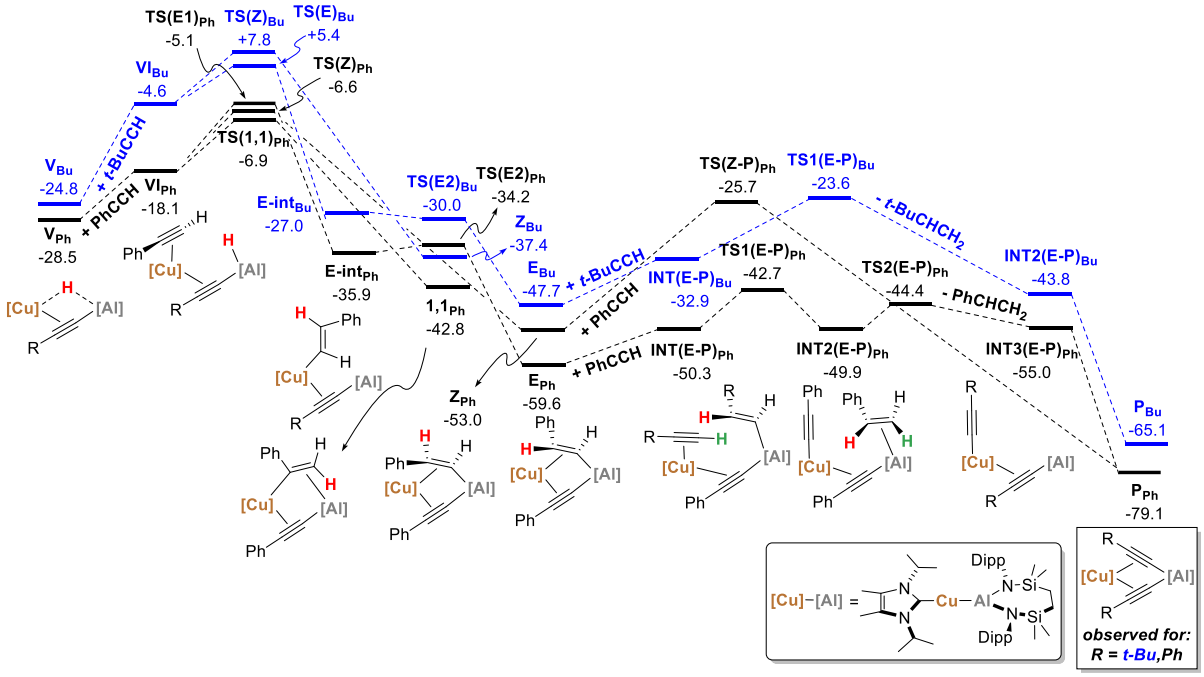



**Figure S52.** Full computed free energy profile (BP86-D3BJ,$C_6H_6$/BS2//BP86/BS1 level, energies quoted in kcal $mol^{-1}$) of onwards formation of **$P_{Ph}$** (black) and **$P_{Bu}$** (blue) from **$V_{Ph}$** and **$V_{Bu}$**, respectively, as well as alternative alkyne addition and H transfer processes to form **$1,1_{Ph}$**, **$Z_{Ph}$** and **$Z_{Bu}$**.

**Breakdown of Energy Contributions**

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

$\mathbf{\Delta E_{BS1}}$ SCF energy computed with the BP86 functional with BS1

$\mathbf{\Delta H_{BS1}}$ Enthalpy at 298.15 K with BS1

$\mathbf{\Delta G_{BS1}}$ Free energy at 298.15 K and 1 atm with BS1

$\mathbf{\Delta G_{BS1/\mathit{bnz}}}$ Free energy corrected for benzene solvent with BS1

$\mathbf{\Delta G_{BS1/\mathit{bnz}+D3BJ}}$ Free energy corrected for benzene and dispersion effects with BS1

$\mathbf{\Delta E_{BS2}}$ SCF energy computed with the BP86 functional with BS2

$\mathbf{\Delta G_{bnz}}$ Free energy corrected for basis set (BS2), dispersion effects and benzene solvent

**Table S2.** Energies breakdown table (kcal/mol) of all stationary points in the free energy profiles in Figures 5, 6 and S52. In each case the final data used in the main article are highlighted in bold.

| | $\Delta E_{BS1}$ | $\Delta H_{BS1}$ | $\Delta G_{BS1}$ | $\Delta G_{BS1/bnz}$ | $\Delta G_{BS1/bnz+D3}$ | $\Delta E_{BS2}$ | $\Delta G_{bnz}$ |
|---|---|---|---|---|---|---|---|
| **I** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| **TS(I-III)$_{Ph}$** | 21.7 | 22.4 | 38.8 | 39.8 | 15.8 | 25.9 | 20.0 |
| **TS(I-II)$_{Ph}$** | 6.1 | 6.9 | 20.7 | 21.6 | 7.2 | 8.8 | 10.0 |
| **II$_{Ph}$** | -3.5 | -1.8 | 13.1 | 13.4 | -5.8 | -2.7 | -5.0 |
| **TS(II-INT)$_{Ph}$** | -3.5 | -2.3 | 14.8 | 16.0 | -2.8 | -2.8 | -2.2 |
| **INT$_{Ph}$** | -3.8 | -2.0 | 13.3 | 14.4 | -4.0 | -2.9 | -3.1 |
| **TS(II-II)$_{Ph}$** | -1.5 | -0.6 | 15.5 | 16.3 | -1.3 | 0.7 | 0.9 |
| **III$_{Ph}$** | -23.4 | -21.4 | -8.3 | -8.5 | -17.8 | -20.8 | -15.2 |
| **TS(III-IV)$_{Ph}$** | 1.7 | 0.3 | 12.8 | 12.3 | 5.6 | 3.7 | 7.6 |
| **IV$_{Ph}$** | -13.0 | -13.2 | 1.0 | 0.2 | -17.2 | -10.9 | -15.2 |
| **TS(IV-V)$_{Ph}$** | -10.1 | -10.9 | 4.8 | 3.7 | -10.2 | -8.7 | -8.8 |
| **V$_{Ph}$** | -27.7 | -27.6 | -12.7 | -12.0 | -29.8 | -26.4 | -28.5 |
| **VI$_{Ph}$** | -15.6 | -14.7 | 11.4 | 12.2 | -23.0 | -10.6 | -18.1 |
| **TS(E)$_{Ph}$** | -2.2 | -2.5 | 24.6 | 25.3 | -9.7 | 2.3 | -5.1 |
| **E-INT1$_{Ph}$** | -42.9 | -39.0 | -13.5 | -12.8 | -39.3 | -39.4 | -35.9 |
| **TS(E2)$_{Ph}$** | -41.9 | -38.3 | -10.8 | -9.6 | -38.3 | -37.8 | -34.2 |
| **E$_{Ph}$** | -63.2 | -58.8 | -29.4 | -27.9 | -67.2 | -55.7 | -59.6 |
| **INT(E-P)$_{Ph}$** | -55.8 | -50.6 | -11.1 | -10.3 | -59.9 | -46.1 | -50.3 |
| **TS(E-P)$_{Ph}$** | -48.8 | -46.3 | -3.9 | -1.9 | -52.8 | -38.7 | -42.7 |
| **INT2(E-P)$_{Ph}$** | -56.6 | -50.4 | -10.2 | -8.4 | -58.6 | -48.0 | -49.9 |
| **TS2(E-P)$_{Ph}$** | -54.1 | -48.2 | -8.1 | -6.3 | -52.5 | -45.9 | -44.4 |
| **INT2(E-P)$_{Ph}$** | -65.6 | -60.5 | -36.2 | -35.3 | -60.0 | -60.6 | -55.0 |
| **P$_{Ph}$** | -85.7 | -80.7 | -52.2 | -50.7 | -87.6 | -77.2 | -79.1 |
| **TS(1,1)$_{Ph}$** | -5.8 | -5.6 | 22.5 | 24.0 | -13.0 | 0.3 | -6.9 |
| **1,1$_{Ph}$** | -44.9 | -41.2 | -11.8 | -10.2 | -49.0 | -38.7 | -42.8 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **TS(Z)$_{Ph}$** | -2.7 | -2.9 | 24.9 | 26.4 | -12.6 | 3.3 | -6.6 |
| **Z$_{Ph}$** | -56.0 | -51.6 | -22.3 | -20.9 | -60.6 | -48.4 | -53.0 |
| **TS(Z-P)Ph** | -24.6 | -23.5 | 20.4 | 22.4 | -36.6 | -13.8 | -25.7 |
| **TS(I-II)$_{Bu}$** | 11.1 | 11.9 | 25.7 | 26.5 | 11.3 | 14.1 | 14.3 |
| **II$_{Bu}$** | 0.7 | 2.3 | 17.9 | 19.1 | -0.9 | 2.4 | 0.8 |
| **TS(II-III)$_{Bu}$** | 3.5 | 4.3 | 22.1 | 23.1 | 4.4 | 6.7 | 7.6 |
| **III)$_{Bu}$** | -18.2 | -16.6 | -2.7 | -2.4 | -13.6 | -14.8 | -10.2 |
| **TS(I-III)$_{Bu}$** | 25.4 | 25.9 | 44.2 | 44.9 | 19.8 | 30.1 | 24.5 |
| **III$_{Bu}$** | -18.2 | -16.6 | -2.7 | -2.4 | -13.6 | -14.8 | -10.1 |
| **TS(III-IV)$_{Bu}$** | 4.6 | 3.0 | 17.1 | 17.0 | 7.9 | 7.2 | 10.6 |
| **IV$_{Bu}$** | -11.2 | -11.5 | 2.2 | 1.0 | -13.1 | -8.8 | -10.7 |
| **V$_{Bu}$** | -24.5 | -24.4 | -8.1 | -7.4 | -27.1 | -22.2 | -24.8 |
| **VI$_{Bu}$** | -5.2 | -4.2 | 23.7 | 23.5 | -11.0 | 1.2 | -4.6 |
| **TS(E)$_{Bu}$** | 3.9 | 3.7 | 34.3 | 34.8 | -0.9 | 10.2 | 5.4 |
| **E-int$_{Bu}$** | -36.7 | -32.8 | -3.9 | -2.2 | -33.3 | -30.4 | -27.0 |
| **TS(E2)$_{Bu}$** | -35.7 | -32.2 | -0.4 | 1.3 | -37.6 | -28.0 | -30.0 |
| **E$_{Bu}$** | -51.3 | -47.1 | -16.5 | -15.3 | -57.1 | -41.9 | -47.7 |
| **INT(E-P)$_{Bu}$** | -39.5 | -34.6 | 7.9 | 8.6 | -45.5 | -26.8 | -32.9 |
| **TS1(E-P)$_{Bu}$** | -30.2 | -27.9 | 18.1 | 19.8 | -36.6 | -17.2 | -23.6 |
| **INT2(E-P)$_{Bu}$** | -57.3 | -52.2 | -23.9 | -22.1 | -51.6 | -49.4 | -43.8 |
| **P$_{Bu}$** | -73.1 | -68.1 | -37.7 | -36.6 | -75.2 | -63.0 | -65.1 |
| **TS(Z)$_{Bu}$** | 9.4 | 9.3 | 39.6 | 40.6 | 0.1 | 17.1 | 7.8 |
| **Z$_{Bu}$** | -40.9 | -36.6 | -6.2 | -5.1 | -46.6 | -31.8 | -37.4 |

## Cartesian Coordinates and Energies

**PhCCH**

SCF (BP86) Energy = -308.384259635
Enthalpy 0K = -308.278156
Enthalpy 298K = -308.270491
Free Energy 298K = -308.308773
Lowest Frequency = 139.6409 $cm^{-1}$
Second Frequency = 150.8438 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -308.406625348
SCF (C6H6) Energy = -308.386067353
SCF (BS2) Energy = -308.463936022

| | | | |
|---|---|---|---|
| C | 0.59981 | 0.00003 | -0.00005 |
| C | -0.12011 | 1.22148 | -0.00004 |
| H | 0.43363 | 2.16500 | -0.00009 |
| C | 2.02973 | 0.00002 | -0.00001 |
| C | -0.12004 | -1.22147 | -0.00002 |
| H | 0.43374 | -2.16496 | -0.00002 |
| C | 3.25261 | -0.00002 | 0.00005 |
| C | -1.52033 | -1.21573 | 0.00000 |
| H | -2.06498 | -2.16566 | -0.00008 |
| C | -2.22515 | -0.00006 | 0.00004 |
| H | -3.32000 | -0.00003 | 0.00015 |
| C | -1.52036 | 1.21573 | 0.00001 |
| H | -2.06508 | 2.16562 | 0.00003 |
| H | 4.32575 | 0.00009 | 0.00010 |

**$HPhCCH_2$**

SCF (BP86) Energy = -309.639886019
Enthalpy 0K = -309.510361
Enthalpy 298K = -309.502438
Free Energy 298K = -309.541911
Lowest Frequency = 46.8166 $cm^{-1}$
Second Frequency = 200.8464 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -309.664911102
SCF (C6H6) Energy = -309.641276383
SCF (BS2) Energy = -309.716310235

| | | | |
|---|---|---|---|
| C | 1.79075 | -1.05182 | 0.00018 |
| C | 2.27665 | 0.26478 | 0.00015 |
| C | 0.40909 | -1.28967 | -0.00003 |
| H | 3.35471 | 0.45613 | 0.00025 |
| H | 0.03361 | -2.31985 | -0.00003 |
| C | 1.36717 | 1.33822 | -0.00007 |
| C | -0.52001 | -0.22268 | -0.00012 |
| H | 1.73781 | 2.36894 | -0.00020 |
| C | -0.01147 | 1.09908 | -0.00024 |
| H | -0.70392 | 1.94729 | -0.00055 |
| H | 2.48838 | -1.89608 | 0.00028 |
| C | -1.96058 | -0.53379 | -0.00023 |
| H | -2.19345 | -1.60801 | -0.00093 |
| C | -2.99166 | 0.33698 | 0.00036 |
| H | -2.85088 | 1.42295 | 0.00110 |
| H | -4.02599 | -0.01801 | 0.00008 |

***t*-BuCCH**

SCF (BP86) Energy = -234.586239247
Enthalpy 0K = -234.449586
Enthalpy 298K = -234.440796
Free Energy 298K = -234.480163
Lowest Frequency = 169.1734 $cm^{-1}$
Second Frequency = 169.3137 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -234.606343592
SCF (C6H6) Energy = -234.587510303
SCF (BS2) Energy = -234.647660256

| | | | |
|---|---|---|---|
| C | -1.17636 | 0.00006 | 0.00001 |
| C | -2.39700 | 0.00004 | 0.00005 |
| H | -3.47013 | -0.00003 | 0.00005 |
| C | 0.29934 | 0.00001 | -0.00003 |
| C | 0.81206 | 0.25834 | 1.44227 |
| H | 1.91626 | 0.26087 | 1.45420 |
| H | 0.45810 | 1.23236 | 1.81822 |
| H | 0.45868 | -0.52496 | 2.13285 |
| C | 0.81200 | 1.11988 | -0.94489 |
| H | 0.45916 | 2.10963 | -0.61136 |
| H | 1.91621 | 1.12857 | -0.95366 |
| H | 0.45743 | 0.95887 | -1.97625 |
| C | 0.81192 | -1.37828 | -0.49741 |
| H | 1.91612 | -1.39005 | -0.50114 |
| H | 0.45782 | -2.19082 | 0.15814 |
| H | 0.45854 | -1.58466 | -1.52107 |

***t*-$BuHCCH_2$**

SCF (BP86) Energy = -235.840752982
Enthalpy 0K = -235.680612
Enthalpy 298K = -235.671784
Free Energy 298K = -235.711379
Lowest Frequency = 102.8285 $cm^{-1}$
Second Frequency = 228.1389 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -235.863887196
SCF (C6H6) Energy = -235.841261783
SCF (BS2) Energy = -235.898749957

| | | | |
|---|---|---|---|
| C | -1.00872 | 0.67322 | 0.00002 |
| H | -0.96247 | 1.77377 | 0.00004 |
| C | -2.21645 | 0.08531 | 0.00002 |
| H | -2.33995 | -1.00265 | 0.00001 |
| H | -3.13608 | 0.67941 | 0.00002 |
| C | 0.35479 | -0.00249 | 0.00001 |
| C | 1.12695 | 0.46412 | 1.26230 |
| H | 2.14818 | 0.04272 | 1.27177 |
| H | 1.21630 | 1.56454 | 1.29236 |
| H | 0.61241 | 0.14140 | 2.18346 |
| C | 1.12670 | 0.46369 | -1.26261 |
| H | 2.14792 | 0.04229 | -1.27213 |
| H | 0.61197 | 0.14065 | -2.18354 |
| H | 1.21603 | 1.56411 | -1.29306 |
| C | 0.24977 | -1.54020 | 0.00027 |
| H | -0.28436 | -1.90738 | 0.89369 |
| H | -0.28455 | -1.90766 | -0.89293 |
| H | 1.25639 | -1.99311 | 0.00025 |

**$TS(I\text{-}III)_{Ph}$**

SCF (BP86) Energy = -2339.39427809
Enthalpy 0K = -2338.281759
Enthalpy 298K = -2338.209426
Free Energy 298K = -2338.387728
Lowest Frequency = -260.1585 $cm^{-1}$
Second Frequency = 11.8749 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2339.77270026
SCF (C6H6) Energy = -2339.39854675
SCF (BS2) Energy = -3151.59032159

| | | | |
|---|---|---|---|
| Cu | -1.35951 | -0.08342 | -0.05529 |
| Si | 3.69122 | -0.91434 | -1.71796 |
| Si | 3.58617 | 2.18993 | 0.68223 |
| Al | 1.07692 | 0.06546 | 0.15184 |
| N | 2.28506 | -1.22644 | -0.65109 |
| N | 1.86149 | 1.81893 | 0.32516 |
| N | -3.95163 | 1.32034 | -0.60755 |
| N | -4.28991 | -0.82120 | -0.70020 |
| C | 1.82002 | -2.58713 | -0.59420 |
| C | 2.26132 | -3.47777 | 0.44522 |
| C | 1.77868 | -4.80279 | 0.47923 |
| H | 2.13030 | -5.47425 | 1.27122 |
| C | 0.87246 | -5.28379 | -0.47250 |
| H | 0.51140 | -6.31723 | -0.42591 |
| C | 0.45949 | -4.42956 | -1.50150 |
| H | -0.22060 | -4.80849 | -2.27442 |
| C | 0.92291 | -3.10233 | -1.59203 |
| C | 3.29096 | -3.06559 | 1.50107 |
| H | 3.41189 | -1.97211 | 1.40793 |
| C | 2.84806 | -3.40182 | 2.94342 |
| H | 1.84934 | -3.00128 | 3.17536 |
| H | 3.56584 | -2.98212 | 3.67131 |
| H | 2.82250 | -4.49321 | 3.11321 |
| C | 4.66666 | -3.72238 | 1.23646 |
| H | 4.59339 | -4.82330 | 1.29711 |
| H | 5.40531 | -3.39364 | 1.98966 |
| H | 5.05694 | -3.46943 | 0.23973 |
| C | 0.51794 | -2.28176 | -2.81826 |
| H | 0.94545 | -1.27405 | -2.68731 |

| | | | |
|---|---|---|---|
| C | -1.00733 | -2.11897 | -2.95442 |
| H | -1.51310 | -3.09559 | -3.06020 |
| H | -1.25551 | -1.51463 | -3.84583 |
| H | -1.41918 | -1.60073 | -2.06797 |
| C | 1.10087 | -2.89694 | -4.11283 |
| H | 2.19536 | -3.01404 | -4.05498 |
| H | 0.86842 | -2.26056 | -4.98583 |
| H | 0.67158 | -3.89670 | -4.30616 |
| C | 4.51316 | -2.55312 | -2.27941 |
| H | 5.39357 | -2.79959 | -1.66291 |
| H | 4.86688 | -2.43805 | -3.31922 |
| H | 3.82854 | -3.41525 | -2.24724 |
| C | 3.27914 | 0.01005 | -3.34487 |
| H | 2.77298 | -0.65172 | -4.06633 |
| H | 4.22317 | 0.34783 | -3.81112 |
| H | 2.64473 | 0.89688 | -3.19868 |
| C | 5.05685 | 0.10372 | -0.85091 |
| H | 5.29119 | -0.37468 | 0.11927 |
| H | 5.95847 | -0.05593 | -1.47915 |
| C | 4.80626 | 1.61611 | -0.67530 |
| H | 4.49377 | 2.07139 | -1.63475 |
| H | 5.75582 | 2.12753 | -0.40941 |
| C | 4.22844 | 1.43552 | 2.32216 |
| H | 3.60556 | 1.71563 | 3.18800 |
| H | 5.24885 | 1.81461 | 2.51099 |
| H | 4.29860 | 0.33544 | 2.27819 |
| C | 3.83644 | 4.07990 | 0.77811 |
| H | 3.61699 | 4.55931 | -0.19053 |
| H | 4.89072 | 4.29172 | 1.02979 |
| H | 3.19873 | 4.56611 | 1.53232 |
| C | 1.02221 | 2.98993 | 0.27789 |
| C | 0.48015 | 3.57062 | 1.47224 |
| C | -0.23904 | 4.78083 | 1.39810 |
| H | -0.62742 | 5.22375 | 2.32354 |
| C | -0.45016 | 5.43934 | 0.18129 |
| H | -0.98988 | 6.39239 | 0.14845 |
| C | 0.05033 | 4.86131 | -0.99223 |
| H | -0.10570 | 5.36828 | -1.95213 |
| C | 0.77582 | 3.65494 | -0.96954 |
| C | 0.64748 | 2.91846 | 2.84500 |
| H | 1.26090 | 2.01482 | 2.69505 |
| C | -0.71765 | 2.46329 | 3.40578 |
| H | -1.38812 | 3.32376 | 3.58250 |
| H | -0.58722 | 1.93787 | 4.36974 |
| H | -1.21998 | 1.78010 | 2.69946 |
| C | 1.36548 | 3.82872 | 3.86640 |
| H | 2.36833 | 4.12516 | 3.51751 |
| H | 1.48399 | 3.30597 | 4.83259 |
| H | 0.79361 | 4.75368 | 4.06121 |
| C | 1.29454 | 3.08190 | -2.28432 |
| H | 1.98592 | 2.27050 | -2.00333 |
| C | 0.14669 | 2.45605 | -3.10917 |
| H | -0.38250 | 1.68262 | -2.52355 |
| H | 0.53443 | 1.98435 | -4.03012 |
| H | -0.58894 | 3.22499 | -3.40799 |
| C | 2.08128 | 4.10489 | -3.13061 |
| H | 1.43630 | 4.92538 | -3.49333 |
| H | 2.51506 | 3.61342 | -4.01944 |
| H | 2.90666 | 4.55848 | -2.55591 |
| C | -3.31367 | 0.11411 | -0.43656 |
| C | -3.24184 | 2.60637 | -0.37539 |
| H | -2.18794 | 2.29344 | -0.24472 |
| C | -3.31243 | 3.54162 | -1.59142 |
| H | -3.05755 | 3.00288 | -2.51836 |
| H | -2.57377 | 4.34637 | -1.45220 |
| H | -4.30383 | 4.00754 | -1.71156 |
| C | -3.70052 | 3.27544 | 0.92987 |
| H | -3.63498 | 2.56955 | 1.77329 |
| H | -4.73551 | 3.65331 | 0.86851 |
| H | -3.03622 | 4.12827 | 1.14313 |
| C | -5.29586 | 1.14958 | -0.96305 |
| C | -6.27221 | 2.25105 | -1.24750 |
| H | -6.25022 | 3.03988 | -0.47851 |
| H | -7.29600 | 1.84562 | -1.26957 |
| H | -6.08972 | 2.73334 | -2.22394 |
| C | -5.51160 | -0.21274 | -1.02561 |
| C | -6.77053 | -0.92469 | -1.42025 |
| H | -7.04767 | -1.72546 | -0.71570 |
| H | -6.69864 | -1.37634 | -2.42557 |
| H | -7.60785 | -0.20986 | -1.44578 |
| C | -4.03357 | -2.27661 | -0.55851 |
| H | -2.94994 | -2.32171 | -0.34947 |
| C | -4.77666 | -2.86252 | 0.65273 |
| H | -4.55051 | -2.29121 | 1.56553 |
| H | -4.44707 | -3.90156 | 0.81461 |
| H | -5.86913 | -2.87979 | 0.50328 |
| C | -4.31297 | -3.05421 | -1.85550 |
| H | -5.39154 | -3.17474 | -2.04659 |
| H | -3.87978 | -4.06444 | -1.76883 |
| H | -3.85166 | -2.55998 | -2.72429 |
| C | 0.24328 | -0.92401 | 2.20824 |
| C | 1.40174 | -0.45098 | 2.32818 |
| H | 2.30845 | -0.31991 | 2.90122 |
| C | -0.92031 | -1.70812 | 2.55431 |
| C | -1.83044 | -1.22181 | 3.52750 |
| C | -1.04395 | -3.04463 | 2.09400 |
| C | -2.81581 | -2.06788 | 4.05411 |
| C | -2.02747 | -3.88039 | 2.63722 |
| C | -2.90983 | -3.40212 | 3.62290 |
| H | -1.73145 | -0.19306 | 3.88328 |
| H | -0.34044 | -3.42089 | 1.34553 |
| H | -3.50120 | -1.68715 | 4.81883 |
| H | -2.09216 | -4.91993 | 2.29872 |
| H | -3.66874 | -4.06547 | 4.05085 |

**TS(I-II)$_{Ph}$**

SCF (BP86) Energy = -2339.41916970
Enthalpy 0K = -2338.307146
Enthalpy 298K = -2338.234110
Free Energy 298K = -2338.416624
Lowest Frequency = -28.4714 $cm^{-1}$
Second Frequency = 13.8854 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2339.78221749
SCF (C6H6) Energy = -2339.42349916
SCF (BS2) Energy = -3151.61758361

| | | | |
|---|---|---|---|
| Cu | 0.96066 | -0.74376 | 0.16531 |
| Si | -2.83374 | 2.96325 | -1.40331 |
| Si | -4.12269 | 0.71039 | 1.54089 |
| Al | -1.16594 | 0.40882 | 0.05919 |
| N | -1.38169 | 2.10510 | -0.77740 |
| N | -2.80053 | -0.24971 | 0.79225 |
| N | 1.92653 | -3.38400 | -0.85498 |
| N | 3.56282 | -1.95924 | -0.94964 |
| C | -0.11925 | 2.73134 | -1.09365 |
| C | 0.45020 | 3.69070 | -0.19437 |
| C | 1.69853 | 4.26813 | -0.49732 |
| H | 2.12463 | 5.00773 | 0.19081 |
| C | 2.39569 | 3.93582 | -1.66685 |
| H | 3.36145 | 4.40305 | -1.88976 |
| C | 1.82733 | 3.02076 | -2.55973 |
| H | 2.35558 | 2.77710 | -3.48957 |
| C | 0.57906 | 2.41756 | -2.30455 |
| C | -0.27236 | 4.10260 | 1.08988 |
| H | -1.31836 | 3.76603 | 0.98214 |
| C | 0.31596 | 3.37739 | 2.31992 |
| H | 0.29895 | 2.28262 | 2.18608 |
| H | -0.24976 | 3.62801 | 3.23555 |
| H | 1.36934 | 3.66838 | 2.48329 |
| C | -0.28271 | 5.62872 | 1.32152 |
| H | 0.72719 | 6.02021 | 1.53912 |
| H | -0.91916 | 5.87816 | 2.18868 |
| H | -0.66927 | 6.17511 | 0.44456 |
| C | -0.01130 | 1.48427 | -3.36372 |
| H | -0.97511 | 1.12140 | -2.96842 |
| C | 0.87235 | 0.24766 | -3.63030 |
| H | 1.84878 | 0.53610 | -4.06125 |
| H | 0.38285 | -0.42978 | -4.35339 |
| H | 1.05502 | -0.31480 | -2.69727 |
| C | -0.28717 | 2.23728 | -4.68611 |
| H | -0.94037 | 3.11219 | -4.52994 |
| H | -0.77575 | 1.57126 | -5.41994 |
| H | 0.65058 | 2.60287 | -5.14198 |
| C | -2.35362 | 4.70910 | -2.00303 |

H -3.22771 5.17924 -2.48757
H -1.52910 4.68872 -2.73377
H -2.04200 5.35813 -1.16831
C -3.65089 2.07395 -2.88567
H -3.01204 2.11000 -3.78299
H -4.60596 2.57111 -3.13470
H -3.87137 1.01603 -2.67141
C -4.19130 3.19782 -0.07986
H -3.75157 3.70774 0.79838
H -4.88412 3.93991 -0.52929
C -4.97767 1.94306 0.35365
H -5.34290 1.38488 -0.52977
H -5.89506 2.24466 0.90221
C -3.44940 1.72403 3.01229
H -3.09623 1.07324 3.82901
H -4.22929 2.39058 3.42186
H -2.60100 2.35658 2.69869
C -5.52912 -0.44298 2.11761
H -6.08215 -0.83925 1.24878
H -6.24335 0.12737 2.73737
H -5.17850 -1.30660 2.70262
C -2.95945 -1.68089 0.83758
C -2.55562 -2.45077 1.97899
C -2.79122 -3.84118 1.99695
H -2.50425 -4.41619 2.88561
C -3.38760 -4.50398 0.91827
H -3.57056 -5.58338 0.95990
C -3.75460 -3.76134 -0.21060
H -4.22420 -4.26994 -1.06099
C -3.55955 -2.36820 -0.26957
C -1.87422 -1.82380 3.19796
H -1.65128 -0.77420 2.93243
C -0.54525 -2.53731 3.53670
H -0.71824 -3.57242 3.88067
H -0.01479 -2.01236 4.35191
H 0.12193 -2.58900 2.65948
C -2.78293 -1.82043 4.44953
H -3.71529 -1.25851 4.28305
H -2.25985 -1.36322 5.30873
H -3.06011 -2.85066 4.73697
C -3.99546 -1.61692 -1.52611
H -3.94149 -0.54372 -1.27648
C -3.01682 -1.87402 -2.69433
H -1.98558 -1.58742 -2.42037
H -3.30701 -1.29460 -3.58905
H -3.00459 -2.94343 -2.97227
C -5.44623 -1.93161 -1.94896
H -5.56545 -2.98118 -2.27243
H -5.74534 -1.29257 -2.79856
H -6.15543 -1.75506 -1.12262
C 2.25809 -2.08822 -0.53462
C 0.59097 -3.93448 -0.50294
H 0.05108 -3.04406 -0.12547
C -0.17739 -4.46095 -1.72382
H -0.16653 -3.72477 -2.54354
H -1.22647 -4.62769 -1.42976
H 0.22452 -5.41680 -2.09840
C 0.67909 -4.95766 0.64055
H 1.25780 -4.55187 1.48608
H 1.14413 -5.90612 0.32173
H -0.33984 -5.18166 0.99622
C 2.99718 -4.05387 -1.46270
C 2.97040 -5.47046 -1.95176
H 2.63811 -6.17749 -1.17354
H 3.98165 -5.77896 -2.25888
H 2.30640 -5.60109 -2.82400
C 4.03733 -3.14715 -1.52717
C 5.41286 -3.35852 -2.08445
H 6.18711 -3.39459 -1.29808
H 5.70219 -2.57051 -2.79914
H 5.45151 -4.31611 -2.62650
C 4.30020 -0.68105 -0.77448
H 3.59467 -0.06937 -0.18629
C 5.58326 -0.85750 0.05278
H 5.38659 -1.43304 0.97114
H 5.95697 0.13511 0.35106
H 6.38336 -1.35797 -0.51660
C 4.54894 0.03659 -2.11084
H 5.28631 -0.49063 -2.73954
H 4.94346 1.04598 -1.90893
H 3.61179 0.14427 -2.67698
C 2.77761 0.49519 2.39029
C 4.00863 1.20671 2.42490
C 1.69807 -0.10629 2.24910
H 0.79231 -0.50670 2.67711
C 5.41197 3.07666 1.70601
H 5.54613 3.97856 1.09936
C 4.19735 2.38203 1.64630
H 3.38686 2.73059 0.99798
C 5.06826 0.76179 3.26256
H 4.92312 -0.13852 3.86743
C 6.45256 2.62846 2.53925
H 7.39725 3.18012 2.58457
C 6.27353 1.47068 3.31742
H 7.07899 1.11907 3.97079

**$II_{Ph}$**
SCF (BP86) Energy = -2339.43439826
Enthalpy 0K = -2338.320602
Enthalpy 298K = -2338.247942
Free Energy 298K = -2338.428634
Lowest Frequency = 11.7563 $cm^{-1}$
Second Frequency = 15.7290 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2339.80501031
SCF (C6H6) Energy = -2339.43990402
SCF (BS2) Energy = -3151.63590605

Cu -1.22879 0.36112 0.16027
Si 3.21058 -2.45088 -1.30202
Si 3.96326 0.15400 1.53904
Al 1.09962 -0.22893 -0.03446
N 1.60261 -1.93474 -0.67083
N 2.49717 0.79216 0.71012
N -2.45970 2.53380 -1.44518
N -3.71030 0.74912 -1.38686
C 0.48994 -2.83206 -0.89093
C 0.10998 -3.77521 0.12072
C -0.98916 -4.62619 -0.10748
H -1.26910 -5.35124 0.66548
C -1.72030 -4.57960 -1.30030
H -2.56749 -5.25598 -1.45893
C -1.33845 -3.67342 -2.29557
H -1.89026 -3.65042 -3.24298
C -0.24528 -2.80100 -2.12102
C 0.89903 -3.93647 1.42340
H 1.56849 -3.06009 1.49761
C 0.00911 -3.98568 2.68480
H -0.67461 -3.12515 2.74542
H 0.63718 -3.99263 3.59332
H -0.60375 -4.90448 2.71297
C 1.78774 -5.20291 1.38535
H 1.16565 -6.11135 1.29333
H 2.37833 -5.29210 2.31478
H 2.48538 -5.19036 0.53470
C 0.15525 -1.89698 -3.28989
H 0.97632 -1.25212 -2.93318
C -0.98564 -0.96926 -3.75658
H -1.83659 -1.54551 -4.16378
H -0.63127 -0.30063 -4.56184
H -1.35140 -0.34486 -2.92487
C 0.68197 -2.72983 -4.48265
H 1.52438 -3.37802 -4.19082
H 1.02297 -2.06900 -5.30003
H -0.11123 -3.38198 -4.89047
C 3.15468 -4.25707 -1.93587
H 3.62725 -4.95233 -1.22210
H 3.71887 -4.32791 -2.88222
H 2.12977 -4.61355 -2.12385
C 3.81052 -1.39233 -2.77522
H 3.20544 -1.57905 -3.67746
H 4.85533 -1.66421 -3.01296
H 3.78679 -0.31138 -2.56930
C 4.56047 -2.36079 0.04653
H 4.20478 -2.91653 0.93506

| | | | |
|---|---|---|---|
| H | 5.40059 | -2.96355 | -0.35783 |
| C | 5.06949 | -0.95785 | 0.44209 |
| H | 5.35664 | -0.38043 | -0.45767 |
| H | 6.00580 | -1.05251 | 1.03197 |
| C | 3.47953 | -0.86698 | 3.07873 |
| H | 2.98734 | -0.24409 | 3.84356 |
| H | 4.37686 | -1.31947 | 3.53746 |
| H | 2.79284 | -1.69277 | 2.82259 |
| C | 5.09251 | 1.59960 | 2.05771 |
| H | 5.56108 | 2.06636 | 1.17476 |
| H | 5.90193 | 1.21860 | 2.70495 |
| H | 4.56012 | 2.39294 | 2.60414 |
| C | 2.35267 | 2.23114 | 0.68829 |
| C | 1.75104 | 2.94109 | 1.77903 |
| C | 1.67045 | 4.34830 | 1.72793 |
| H | 1.22483 | 4.88289 | 2.57520 |
| C | 2.14830 | 5.07771 | 0.63389 |
| H | 2.08177 | 6.17121 | 0.62126 |
| C | 2.72740 | 4.38657 | -0.43699 |
| H | 3.11679 | 4.94855 | -1.29421 |
| C | 2.84935 | 2.98363 | -0.42689 |
| C | 1.19726 | 2.24031 | 3.02182 |
| H | 1.25889 | 1.15449 | 2.83743 |
| C | -0.28628 | 2.59225 | 3.26768 |
| H | -0.41643 | 3.66470 | 3.49896 |
| H | -0.67974 | 2.01638 | 4.12366 |
| H | -0.90364 | 2.35046 | 2.38687 |
| C | 2.02339 | 2.56167 | 4.28962 |
| H | 3.07859 | 2.26202 | 4.18369 |
| H | 1.60682 | 2.03383 | 5.16609 |
| H | 2.00532 | 3.64349 | 4.51298 |
| C | 3.52135 | 2.29917 | -1.61545 |
| H | 3.68782 | 1.25222 | -1.31112 |
| C | 2.59619 | 2.28661 | -2.85304 |
| H | 1.63403 | 1.79258 | -2.62753 |
| H | 3.06745 | 1.74941 | -3.69538 |
| H | 2.37419 | 3.31501 | -3.19005 |
| C | 4.89344 | 2.91166 | -1.97012 |
| H | 4.79993 | 3.94640 | -2.34525 |
| H | 5.38371 | 2.31994 | -2.76323 |
| H | 5.56558 | 2.93437 | -1.09580 |
| C | -2.50328 | 1.25074 | -0.95637 |
| C | -1.33695 | 3.44589 | -1.10637 |
| H | -0.58654 | 2.76107 | -0.66677 |
| C | -0.70426 | 4.10582 | -2.34036 |
| H | -0.49716 | 3.36257 | -3.12699 |
| H | 0.25481 | 4.55518 | -2.03613 |
| H | -1.33109 | 4.90683 | -2.76409 |
| C | -1.75096 | 4.46142 | -0.02900 |
| H | -2.19579 | 3.94931 | 0.83921 |
| H | -2.47835 | 5.19914 | -0.40989 |
| H | -0.85655 | 5.00542 | 0.31530 |
| C | -3.62350 | 2.83790 | -2.16700 |
| C | -3.90149 | 4.14219 | -2.85035 |
| H | -3.72799 | 5.00631 | -2.18807 |
| H | -4.95583 | 4.17955 | -3.16584 |
| H | -3.28300 | 4.28586 | -3.75387 |
| C | -4.41268 | 1.70560 | -2.13487 |
| C | -5.73607 | 1.48199 | -2.80138 |
| H | -6.48979 | 1.06158 | -2.11566 |
| H | -5.65744 | 0.80153 | -3.66758 |
| H | -6.13126 | 2.43985 | -3.17394 |
| C | -4.19991 | -0.58422 | -0.94144 |
| H | -3.31962 | -1.01455 | -0.43261 |
| C | -5.32044 | -0.44251 | 0.10199 |
| H | -5.00313 | 0.20958 | 0.93020 |
| H | -5.54901 | -1.43283 | 0.52809 |
| H | -6.25040 | -0.04068 | -0.33517 |
| C | -4.57642 | -1.50705 | -2.11035 |
| H | -5.52486 | -1.21643 | -2.59048 |
| H | -4.70008 | -2.53234 | -1.72521 |
| H | -3.78123 | -1.52728 | -2.87122 |
| C | -1.80360 | -0.49318 | 1.92345 |
| C | -2.91090 | -0.76939 | 2.80000 |
| C | -0.53076 | -0.63990 | 1.66750 |
| H | 0.32133 | -1.04710 | 2.22870 |
| C | -4.57378 | -2.34019 | 3.69243 |
| H | -4.98429 | -3.35574 | 3.72899 |
| C | -3.47410 | -2.07597 | 2.86616 |
| H | -3.03395 | -2.87351 | 2.25920 |
| C | -3.51025 | 0.25427 | 3.58602 |
| H | -3.10087 | 1.26806 | 3.53659 |
| C | -5.14424 | -1.32311 | 4.47769 |
| H | -6.00096 | -1.53596 | 5.12499 |
| C | -4.60008 | -0.02740 | 4.41824 |
| H | -5.03313 | 0.77623 | 5.02458 |

**TS(II-INT)$_{Ph}$**

SCF (BP86) Energy = -2339.43433110
Enthalpy 0K = -2338.320554
Enthalpy 298K = -2338.248759
Free Energy 298K = -2338.425881
Lowest Frequency = -5.0704 $cm^{-1}$
Second Frequency = 13.8268 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2339.80436868
SCF (C6H6) Energy = -2339.43841358
SCF (BS2) Energy = -3151.63610354

| | | | |
|---|---|---|---|
| Cu | 1.24456 | -0.29002 | 0.17394 |
| Si | -3.36270 | 2.45583 | -0.92502 |
| Si | -3.88210 | -0.44198 | 1.66584 |
| Al | -1.10241 | 0.20438 | 0.02505 |
| N | -1.70549 | 1.93256 | -0.44021 |
| N | -2.44210 | -0.94047 | 0.70668 |
| N | 2.50315 | -2.17497 | -1.74587 |
| N | 3.67477 | -0.35251 | -1.50861 |
| C | -0.66433 | 2.91318 | -0.66083 |
| C | -0.26995 | 3.79984 | 0.39544 |
| C | 0.72543 | 4.76586 | 0.14826 |
| H | 1.01399 | 5.44941 | 0.95519 |
| C | 1.34623 | 4.88097 | -1.10041 |
| H | 2.11226 | 5.64530 | -1.27158 |
| C | 0.96518 | 4.01358 | -2.12998 |
| H | 1.43943 | 4.10619 | -3.11459 |
| C | -0.02944 | 3.03349 | -1.94125 |
| C | -0.90851 | 3.75813 | 1.78852 |
| H | -1.50747 | 2.83041 | 1.83520 |
| C | 0.13841 | 3.72383 | 2.92426 |
| H | 0.86442 | 2.90934 | 2.78170 |
| H | -0.35902 | 3.57673 | 3.89946 |
| H | 0.69824 | 4.67405 | 2.98834 |
| C | -1.86750 | 4.94772 | 2.03140 |
| H | -1.33529 | 5.90959 | 1.92224 |
| H | -2.28135 | 4.90700 | 3.05491 |
| H | -2.71314 | 4.95022 | 1.32708 |
| C | -0.41608 | 2.15820 | -3.13786 |
| H | -1.20017 | 1.46348 | -2.79174 |
| C | 0.76338 | 1.30236 | -3.64801 |
| H | 1.58084 | 1.93618 | -4.03816 |
| H | 0.43449 | 0.64761 | -4.47544 |
| H | 1.16806 | 0.66667 | -2.84335 |
| C | -0.99680 | 2.99508 | -4.30176 |
| H | -1.87075 | 3.58954 | -3.98864 |
| H | -1.31149 | 2.33784 | -5.13227 |
| H | -0.24497 | 3.69824 | -4.70275 |
| C | -3.38036 | 4.30169 | -1.40817 |
| H | -3.26776 | 4.98255 | -0.55089 |
| H | -4.34906 | 4.52477 | -1.88994 |
| H | -2.58075 | 4.54579 | -2.12548 |
| C | -4.03582 | 1.53889 | -2.46045 |
| H | -3.48773 | 1.82816 | -3.37199 |
| H | -5.09619 | 1.81363 | -2.60827 |
| H | -3.98587 | 0.44366 | -2.36889 |
| C | -4.62124 | 2.20306 | 0.48905 |
| H | -4.21860 | 2.66803 | 1.40874 |
| H | -5.49796 | 2.82238 | 0.20688 |
| C | -5.07399 | 0.75113 | 0.75965 |
| H | -5.40400 | 0.26560 | -0.17882 |
| H | -5.97401 | 0.75554 | 1.41058 |
| C | -3.34333 | 0.42301 | 3.28100 |
| H | -2.79117 | -0.26005 | 3.94712 |
| H | -4.22422 | 0.79603 | 3.83334 |
| H | -2.69522 | 1.29327 | 3.07544 |
| C | -4.95104 | -1.96841 | 2.06867 |

H -5.46116 -2.33475 1.16159
H -5.72912 -1.69068 2.80125
H -4.37371 -2.80922 2.48197
C -2.26032 -2.36244 0.51301
C -1.59498 -3.17676 1.48838
C -1.47183 -4.56392 1.26418
H -0.97691 -5.17958 2.02451
C -1.96838 -5.17442 0.10758
H -1.86600 -6.25514 -0.04021
C -2.61380 -4.38197 -0.84880
H -3.02049 -4.85107 -1.75258
C -2.78066 -2.99589 -0.66395
C -1.01471 -2.61316 2.78759
H -1.09884 -1.51497 2.73114
C 0.48074 -2.96213 2.95018
H 0.63438 -4.05013 3.06532
H 0.89445 -2.47017 3.84769
H 1.06506 -2.62029 2.08025
C -1.79492 -3.09451 4.03378
H -2.85622 -2.80040 3.99879
H -1.35475 -2.66831 4.95303
H -1.75692 -4.19485 4.12551
C -3.53033 -2.20260 -1.73206
H -3.71714 -1.20625 -1.29747
C -2.66784 -2.00857 -2.99929
H -1.71768 -1.49711 -2.76224
H -3.20157 -1.40381 -3.75392
H -2.41895 -2.98136 -3.46000
C -4.89683 -2.82243 -2.09605
H -4.78703 -3.79979 -2.59887
H -5.44632 -2.15943 -2.78749
H -5.52271 -2.97732 -1.20105
C 2.51656 -0.96705 -1.09254
C 1.43424 -3.17337 -1.48564
H 0.68323 -2.58845 -0.92042
C 0.76112 -3.68217 -2.76890
H 0.48760 -2.84612 -3.43241
H -0.16477 -4.20882 -2.48650
H 1.39268 -4.38968 -3.33004
C 1.93817 -4.31029 -0.58190
H 2.41350 -3.90615 0.32621
H 2.66627 -4.96047 -1.09718
H 1.08117 -4.93082 -0.27338
C 3.63756 -2.32130 -2.55824
C 3.93382 -3.50884 -3.42271
H 3.83374 -4.46010 -2.87444
H 4.96999 -3.45221 -3.79112
H 3.27350 -3.56289 -4.30620
C 4.37640 -1.16406 -2.41301
C 5.64821 -0.78577 -3.10932
H 6.42221 -0.42523 -2.41227
H 5.49035 0.00128 -3.86774
H 6.06124 -1.66292 -3.63133
C 4.11844 0.94138 -0.92197
H 3.25585 1.23860 -0.30004
C 5.32379 0.74732 0.01324
H 5.11968 -0.03566 0.75969
H 5.51487 1.68588 0.55852
H 6.24371 0.48723 -0.53744
C 4.34349 2.03205 -1.97979
H 5.25401 1.85990 -2.57654
H 4.45920 3.00237 -1.46982
H 3.47912 2.11038 -2.65662
C 1.89893 0.25492 2.03285
C 3.07280 0.34561 2.86041
C 0.62315 0.44252 1.85459
H -0.23006 0.73333 2.47662
C 4.77996 1.69462 3.99811
H 5.17799 2.68113 4.26144
C 3.61985 1.61043 3.21783
H 3.12153 2.52184 2.87330
C 3.74810 -0.82247 3.31285
H 3.34993 -1.80352 3.03627
C 5.42557 0.53197 4.45343
H 6.32883 0.60327 5.06769
C 4.89630 -0.72450 4.10743
H 5.38772 -1.64012 4.45521

**INT$_{Ph}$**
SCF (BP86) Energy = -2339.43485699
Enthalpy 0K = -2338.320702
Enthalpy 298K = -2338.248177
Free Energy 298K = -2338.428412
Lowest Frequency = 12.5680 $cm^{-1}$
Second Frequency = 15.9793 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2339.80421328
SCF (C6H6) Energy = -2339.43896522
SCF (BS2) Energy = -3151.63623133

Cu 1.29220 -0.17414 0.13951
Si -3.58785 2.28874 -0.31361
Si -3.72764 -1.18616 1.55055
Al -1.08050 0.13168 0.10403
N -1.85791 1.84038 -0.05912
N -2.27438 -1.28014 0.49602
N 2.77102 -1.42472 -2.09814
N 3.57308 0.53216 -1.56845
C -0.93087 2.94555 -0.18034
C -0.50588 3.66635 0.98390
C 0.34354 4.78066 0.83312
H 0.65090 5.33828 1.72537
C 0.79612 5.19732 -0.42337
H 1.44501 6.07513 -0.51746
C 0.40117 4.47979 -1.55792
H 0.75238 4.79988 -2.54629
C -0.45277 3.36320 -1.46617
C -0.94309 3.27980 2.40065
H -1.44103 2.29645 2.32371
C 0.26149 3.14262 3.35846
H 1.02403 2.46451 2.94540
H -0.07079 2.74482 4.33456
H 0.73917 4.11928 3.55367
C -1.96118 4.27597 3.00356
H -1.54369 5.29840 3.03172
H -2.21424 3.98863 4.03989
H -2.89901 4.31160 2.42774
C -0.85309 2.65300 -2.76236
H -1.55272 1.84595 -2.48714
C 0.35760 1.99391 -3.45940
H 1.09376 2.75234 -3.78373
H 0.03241 1.44466 -4.36156
H 0.86409 1.28407 -2.78441
C -1.57737 3.60068 -3.74599
H -2.46185 4.07362 -3.28764
H -1.91143 3.04767 -4.64214
H -0.91014 4.41163 -4.08889
C -3.78566 4.18495 -0.37043
H -3.52889 4.68666 0.57460
H -4.83949 4.41926 -0.60448
H -3.15735 4.63205 -1.15775
C -4.33006 1.67864 -1.96668
H -3.88387 2.20207 -2.82753
H -5.41345 1.89848 -1.96978
H -4.21139 0.59680 -2.12872
C -4.69739 1.60278 1.08138
H -4.24720 1.85734 2.05935
H -5.63043 2.20077 1.02314
C -5.03744 0.09738 1.00246
H -5.38372 -0.17048 -0.01408
H -5.89953 -0.12651 1.66626
C -3.23612 -0.72253 3.33866
H -2.60725 -1.49487 3.81052
H -4.13726 -0.59089 3.96391
H -2.67956 0.23146 3.36809
C -4.65853 -2.84972 1.52431
H -5.17314 -2.98459 0.55748
H -5.42771 -2.85754 2.31636
H -4.00346 -3.72142 1.67135
C -1.94297 -2.58133 -0.04444
C -1.21447 -3.55680 0.71517
C -0.95249 -4.82098 0.14629
H -0.41142 -5.56485 0.74294
C -1.36814 -5.15381 -1.14731
H -1.15850 -6.14583 -1.56239

C -2.07037 -4.20139 -1.89467
H -2.41270 -4.45300 -2.90555
C -2.37418 -2.93178 -1.36697
C -0.70439 -3.30251 2.13593
H -0.89081 -2.23957 2.36190
C 0.81580 -3.54761 2.25597
H 1.07003 -4.61019 2.09204
H 1.17128 -3.27296 3.26408
H 1.37728 -2.94031 1.52844
C -1.44706 -4.16007 3.18805
H -2.53071 -3.96171 3.19919
H -1.05399 -3.95370 4.19968
H -1.30742 -5.23820 2.99109
C -3.17503 -1.95768 -2.22697
H -3.44949 -1.12183 -1.56206
C -2.31851 -1.38128 -3.37651
H -1.41448 -0.87798 -2.98867
H -2.89273 -0.64447 -3.96604
H -1.98786 -2.18109 -4.06343
C -4.48024 -2.57340 -2.77574
H -4.28210 -3.38404 -3.49944
H -5.07662 -1.80565 -3.29992
H -5.09995 -2.99428 -1.96603
C 2.56448 -0.35169 -1.26756
C 1.88977 -2.61901 -2.03477
H 1.06070 -2.28046 -1.38459
C 1.29105 -2.98937 -3.40016
H 0.87239 -2.10227 -3.90195
H 0.46963 -3.70544 -3.23632
H 2.02555 -3.46407 -4.07089
C 2.58518 -3.80227 -1.34257
H 3.00516 -3.49543 -0.37134
H 3.39707 -4.22764 -1.95735
H 1.84325 -4.59645 -1.15910
C 3.90707 -1.22751 -2.90012
C 4.41308 -2.18966 -3.93126
H 4.48886 -3.21851 -3.54243
H 5.42081 -1.88908 -4.25829
H 3.77264 -2.22036 -4.83058
C 4.41435 0.01176 -2.56457
C 5.60240 0.71550 -3.14653
H 6.27658 1.11340 -2.36992
H 5.31458 1.55729 -3.80073
H 6.18818 0.01168 -3.75829
C 3.72998 1.80101 -0.80762
H 2.77569 1.88105 -0.25681
C 4.86743 1.69722 0.22151
H 4.71247 0.83801 0.89241
H 4.88840 2.61199 0.83727
H 5.85403 1.59855 -0.26322
C 3.85288 3.03424 -1.71579
H 4.84927 3.12099 -2.17828
H 3.68522 3.93753 -1.10760
H 3.08791 3.02109 -2.50736
C 1.84903 -0.18579 2.06346
C 2.87921 -0.33824 3.07396
C 0.55571 -0.00033 1.92014
H -0.32079 0.01746 2.58119
C 3.79593 0.14874 5.29756
H 3.70400 0.65282 6.26615
C 2.78275 0.29662 4.34188
H 1.90355 0.90989 4.56226
C 4.02930 -1.12773 2.81221
H 4.11383 -1.61019 1.83247
C 4.91977 -0.65157 5.02628
H 5.70679 -0.77007 5.77842
C 5.02705 -1.29504 3.78117
H 5.89905 -1.92074 3.56088

**TS(II_II)Ph**
SCF (BP86) Energy = -2339.43117042
Enthalpy 0K = -2338.317863
Enthalpy 298K = -2338.246017
Free Energy 298K = -2338.424872
Lowest Frequency = -112.1346 $cm^{-1}$
Second Frequency = 13.0915 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2339.79935006
SCF (C6H6) Energy = -2339.43575771
SCF (BS2) Energy = -3151.63050939

Cu -1.54326 0.47873 0.39445
Si 3.00292 -2.82620 -0.47497
Si 4.08994 0.78291 0.82800
Al 1.08162 -0.26994 0.32303
N 1.41057 -2.06443 -0.06327
N 2.47345 0.96395 0.05951
N -2.88416 1.57752 -1.99217
N -3.86676 -0.19951 -1.19263
C 0.30916 -3.00335 0.03480
C -0.09278 -3.54000 1.30266
C -1.10332 -4.52244 1.33916
H -1.39454 -4.94464 2.30723
C -1.73479 -4.97981 0.17833
H -2.50560 -5.75643 0.23410
C -1.36248 -4.43364 -1.05440
H -1.85480 -4.78321 -1.96968
C -0.35511 -3.45443 -1.15307
C 0.52830 -3.10880 2.63626
H 1.10841 -2.18824 2.44654
C -0.54844 -2.77638 3.69215
H -1.26930 -2.03706 3.31028
H -0.07572 -2.35949 4.59854
H -1.10513 -3.67713 4.00666
C 1.50082 -4.16630 3.21021
H 0.99467 -5.13970 3.33980
H 1.87289 -3.84757 4.20031
H 2.37536 -4.32454 2.56001
C 0.00113 -2.92971 -2.54694
H 0.84637 -2.23217 -2.42676
C -1.16411 -2.13582 -3.17739
H -2.04483 -2.78335 -3.34206
H -0.86742 -1.72666 -4.15998
H -1.47243 -1.29777 -2.53069
C 0.44046 -4.06284 -3.50256
H 1.27213 -4.65583 -3.08698
H 0.76740 -3.64707 -4.47248
H -0.39044 -4.76112 -3.70826
C 2.88329 -4.71975 -0.28858
H 2.66478 -5.05356 0.73643
H 3.84975 -5.15985 -0.59253
H 2.10110 -5.13880 -0.94210
C 3.61533 -2.56817 -2.26726
H 2.97983 -3.09337 -2.99726
H 4.63078 -2.99916 -2.34264
H 3.68220 -1.51280 -2.56914
C 4.38819 -2.18103 0.67565
H 4.02879 -2.19211 1.72212
H 5.16915 -2.96802 0.62915
C 5.01041 -0.81193 0.31111
H 5.22277 -0.75874 -0.77338
H 6.00006 -0.70895 0.80426
C 3.93724 0.71394 2.73232
H 3.57783 1.66694 3.15350
H 4.92040 0.49318 3.18518
H 3.24182 -0.07900 3.06037
C 5.22325 2.22360 0.31514
H 5.49194 2.14979 -0.75203
H 6.15781 2.18444 0.90150
H 4.76061 3.21018 0.47079
C 2.21205 2.20669 -0.63827
C 1.80883 3.39678 0.05451
C 1.61718 4.59007 -0.67290
H 1.32195 5.49524 -0.12927
C 1.80577 4.65404 -2.05737
H 1.66483 5.59728 -2.59660
C 2.19245 3.49362 -2.73721
H 2.35521 3.53039 -3.82114
C 2.40141 2.27789 -2.05796
C 1.57940 3.45165 1.56619
H 1.72817 2.43071 1.95427
C 0.13562 3.88025 1.91071
H -0.06479 4.91711 1.58576
H -0.03233 3.83216 3.00034
H -0.60207 3.21744 1.43024

| | | | |
|---|---|---|---|
| C | 2.58641 | 4.38321 | 2.28050 |
| H | 3.63067 | 4.07040 | 2.11630 |
| H | 2.40010 | 4.38645 | 3.36921 |
| H | 2.49107 | 5.42483 | 1.92529 |
| C | 2.84529 | 1.06299 | -2.86646 |
| H | 3.04448 | 0.26695 | -2.13092 |
| C | 1.72740 | 0.56522 | -3.80870 |
| H | 0.80699 | 0.32678 | -3.24796 |
| H | 2.04428 | -0.34622 | -4.34628 |
| H | 1.47247 | 1.32982 | -4.56460 |
| C | 4.14626 | 1.31950 | -3.65844 |
| H | 4.00417 | 2.08566 | -4.44137 |
| H | 4.48240 | 0.39470 | -4.16052 |
| H | 4.96044 | 1.66538 | -2.99963 |
| C | -2.72851 | 0.56781 | -1.07094 |
| C | -1.87160 | 2.65657 | -2.12327 |
| H | -1.00642 | 2.25508 | -1.56376 |
| C | -1.42822 | 2.88890 | -3.57575 |
| H | -1.20973 | 1.93492 | -4.08212 |
| H | -0.50155 | 3.48453 | -3.56317 |
| H | -2.17752 | 3.44105 | -4.16531 |
| C | -2.32984 | 3.94501 | -1.42062 |
| H | -2.62366 | 3.73618 | -0.37931 |
| H | -3.18146 | 4.42000 | -1.93770 |
| H | -1.49423 | 4.66368 | -1.40494 |
| C | -4.11492 | 1.46634 | -2.65712 |
| C | -4.60924 | 2.39696 | -3.72245 |
| H | -4.52415 | 3.45526 | -3.42453 |
| H | -5.67372 | 2.19965 | -3.92396 |
| H | -4.06670 | 2.27507 | -4.67653 |
| C | -4.73520 | 0.34070 | -2.15102 |
| C | -6.05853 | -0.24220 | -2.54430 |
| H | -6.69836 | -0.45608 | -1.67190 |
| H | -5.95155 | -1.18022 | -3.11674 |
| H | -6.60360 | 0.47058 | -3.18254 |
| C | -4.12396 | -1.33432 | -0.26337 |
| H | -3.13293 | -1.51723 | 0.18949 |
| C | -5.08222 | -0.91124 | 0.86185 |
| H | -4.67162 | -0.04543 | 1.40509 |
| H | -5.19764 | -1.74115 | 1.57886 |
| H | -6.08442 | -0.65475 | 0.47725 |
| C | -4.56407 | -2.61871 | -0.98122 |
| H | -5.61721 | -2.58604 | -1.30337 |
| H | -4.45251 | -3.46455 | -0.28414 |
| H | -3.92646 | -2.82455 | -1.85500 |
| C | -1.33038 | 0.47126 | 2.31351 |
| C | -1.76919 | 0.96778 | 3.61651 |
| C | -0.04461 | 0.30664 | 1.89632 |
| H | 0.81329 | 0.70876 | 2.49376 |
| C | -1.48905 | 1.19833 | 6.04619 |
| H | -0.91273 | 0.98786 | 6.95448 |
| C | -1.03636 | 0.72342 | 4.80878 |
| H | -0.10839 | 0.14408 | 4.74994 |
| C | -2.97424 | 1.70831 | 3.72439 |
| H | -3.55083 | 1.88728 | 2.80951 |
| C | -2.67605 | 1.94839 | 6.12705 |
| H | -3.02885 | 2.31944 | 7.09532 |
| C | -3.41200 | 2.20861 | 4.95736 |
| H | -4.33875 | 2.79097 | 5.01193 |

**III$_{Ph}$**

SCF (BP86) Energy = -2339.46606117
Enthalpy 0K = -2338.351869
Enthalpy 298K = -2338.279212
Free Energy 298K = -2338.462693
Lowest Frequency = 10.6029 $cm^{-1}$
Second Frequency = 13.9752 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2339.82100094
SCF (C6H6) Energy = -2339.47229551
SCF (BS2) Energy = -3151.66478097

| | | | |
|---|---|---|---|
| Cu | -2.23491 | -0.55044 | 0.42408 |
| Si | 4.02557 | 0.01270 | -2.19559 |
| Al | 1.68356 | 0.28980 | 0.11105 |
| Si | 2.96704 | 3.27081 | -0.24036 |
| N | -5.02494 | 0.35068 | -0.13999 |
| N | 3.08624 | -0.55153 | -0.76955 |
| N | -4.32713 | -1.12430 | -1.57570 |
| N | 1.58360 | 2.13526 | -0.00194 |
| C | -3.91475 | -0.37305 | -0.50112 |
| H | 1.30142 | -1.41327 | 1.97914 |
| C | 1.70447 | -2.92516 | -1.98867 |
| H | 1.58478 | -1.85200 | -2.21638 |
| C | 2.71172 | -3.03195 | -0.84220 |
| C | 0.30870 | 2.75602 | 0.28999 |
| C | 4.30263 | -2.07602 | 0.78191 |
| C | 3.94084 | 2.95382 | -1.85510 |
| H | 3.23602 | 2.96389 | -2.70832 |
| H | 4.55192 | 3.87297 | -1.97628 |
| C | -1.09782 | -2.11163 | 2.48171 |
| C | 4.85635 | 1.71026 | -1.91401 |
| H | 5.49302 | 1.64884 | -1.01101 |
| H | 5.56597 | 1.80847 | -2.76217 |
| C | 3.36541 | -1.88965 | -0.28293 |
| C | 4.21382 | 3.16209 | 1.19961 |
| H | 3.77982 | 3.53393 | 2.14166 |
| H | 5.10908 | 3.76971 | 0.97615 |
| H | 4.54967 | 2.12558 | 1.37122 |
| C | 3.90457 | -4.49177 | 0.72642 |
| H | 4.10926 | -5.49447 | 1.11679 |
| C | -3.40787 | -2.11272 | -2.19815 |
| H | -2.44352 | -1.89031 | -1.70302 |
| C | -0.06578 | 3.09685 | 1.62681 |
| C | 5.42138 | -1.22602 | -2.56651 |
| H | 6.17511 | -1.23153 | -1.76150 |
| H | 5.92931 | -0.94168 | -3.50463 |
| H | 5.04881 | -2.25675 | -2.67604 |
| C | -4.99165 | 1.23186 | 1.05725 |
| H | -3.91094 | 1.30337 | 1.27998 |
| C | 4.54650 | -3.37394 | 1.27007 |
| H | 5.25688 | -3.50895 | 2.09380 |
| C | -2.20182 | -1.88019 | 3.34117 |
| H | -2.75604 | -0.93931 | 3.23353 |
| C | 0.81720 | 2.79428 | 2.83869 |
| H | 1.70537 | 2.25377 | 2.46769 |
| C | -6.12185 | 0.04538 | -0.95986 |
| C | -0.71060 | -1.10240 | 1.44398 |
| C | 0.31660 | -3.47331 | -1.58894 |
| H | 0.36089 | -4.54920 | -1.34261 |
| H | -0.39303 | -3.35755 | -2.42946 |
| H | -0.08314 | -2.93526 | -0.71355 |
| C | -5.67675 | -0.88978 | -1.87491 |
| C | 2.21337 | -3.63189 | -3.26634 |
| H | 3.18418 | -3.22911 | -3.60061 |
| H | 1.49106 | -3.51008 | -4.09386 |
| H | 2.34524 | -4.71556 | -3.09756 |
| C | 2.99862 | -4.31064 | -0.32390 |
| H | 2.49482 | -5.18360 | -0.75558 |
| C | 5.02969 | -0.89721 | 1.43057 |
| H | 4.84225 | -0.01761 | 0.79003 |
| C | -0.39691 | -3.33546 | 2.63815 |
| H | 0.44704 | -3.55011 | 1.97338 |
| C | 0.63180 | -0.84480 | 1.29225 |
| C | -0.57574 | 3.07483 | -0.78954 |
| C | -0.77924 | -4.27348 | 3.60905 |
| H | -0.22623 | -5.21583 | 3.69902 |
| C | -5.68743 | 0.56398 | 2.25525 |
| H | -5.54619 | 1.18293 | 3.15718 |
| H | -5.25613 | -0.43149 | 2.44805 |
| H | -6.77320 | 0.44963 | 2.09488 |
| C | -0.22758 | 2.69304 | -2.22858 |
| H | 0.86498 | 2.53755 | -2.25867 |
| C | -1.86366 | -4.01316 | 4.46349 |
| H | -2.15957 | -4.74565 | 5.22239 |
| C | -1.29092 | 3.75900 | 1.84465 |
| H | -1.56945 | 4.03227 | 2.86926 |
| C | 2.91070 | 0.18770 | -3.73661 |
| H | 2.56325 | -0.79236 | -4.10212 |
| H | 3.46357 | 0.67787 | -4.55790 |
| H | 2.01979 | 0.80195 | -3.52086 |
| C | 4.45216 | -0.59134 | 2.83233 |
| H | 4.59309 | -1.45035 | 3.51217 |
| H | 3.36837 | -0.38401 | 2.79109 |
| H | 4.95137 | 0.28452 | 3.28414 |

C -6.43520 -1.51705 -3.00494
H -6.12283 -1.12444 -3.98898
H -7.51041 -1.30543 -2.89662
H -6.31929 -2.61302 -3.03251
C -0.89172 1.34916 -2.60798
H -0.62858 0.54890 -1.89081
H -0.58543 1.02302 -3.61869
H -1.99240 1.44080 -2.58891
C 2.30049 5.05023 -0.35178
H 1.68272 5.19491 -1.25372
H 3.14906 5.75467 -0.40492
H 1.68310 5.32146 0.51913
C 0.10344 1.87897 3.85859
H -0.78906 2.37208 4.28469
H 0.77984 1.63889 4.69831
H -0.21264 0.93593 3.38598
C -2.56992 -2.80523 4.32858
H -3.41418 -2.58656 4.99289
C -3.79573 -3.55379 -1.82853
H -4.74869 -3.86534 -2.28867
H -3.87982 -3.66224 -0.73534
H -3.01245 -4.24490 -2.18149
C 1.30182 4.09047 3.52980
H 1.83865 4.75647 2.83314
H 1.98100 3.85218 4.36774
H 0.45262 4.66240 3.94491
C -5.50852 2.64963 0.77172
H -6.60301 2.68777 0.65292
H -5.03477 3.06832 -0.13018
H -5.24676 3.29924 1.62275
C 6.55803 -1.10293 1.50852
H 7.04891 -0.19389 1.89871
H 6.98867 -1.32590 0.51760
H 6.82735 -1.93490 2.18298
C -0.57718 3.77968 -3.26578
H -1.66785 3.92307 -3.36718
H -0.19517 3.49382 -4.26149
H -0.13542 4.75429 -2.99741
C -3.23160 -1.89176 -3.70816
H -2.39097 -2.51000 -4.06478
H -2.99602 -0.83808 -3.92851
H -4.12248 -2.18450 -4.28707
C -1.78801 3.73551 -0.51829
H -2.45393 3.99514 -1.34896
C -7.48566 0.65707 -0.85065
H -7.87291 0.63526 0.18161
H -8.19667 0.09570 -1.47676
H -7.50666 1.70696 -1.19246
C -2.14620 4.08984 0.78872
H -3.07858 4.63198 0.97968

**TS(III-IV)$_{Ph}$**
SCF (BP86) Energy = -2339.42609115
Enthalpy 0K = -2338.317417
Enthalpy 298K = -2338.244571
Free Energy 298K = -2338.429075
Lowest Frequency = -581.8128 $cm^{-1}$
Second Frequency = 8.7433 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2339.77682576
SCF (C6H6) Energy = -2339.43283547
SCF (BS2) Energy = -3151.62576198

Cu -2.46529 -0.53660 0.42642
Si 3.74179 -0.49269 -2.45192
Al 1.75097 0.21448 0.04827
Si 3.58813 2.86482 -0.33428
N -4.98252 0.81140 -0.35074
N 2.80364 -0.92007 -0.98620
N -4.95453 -1.27803 -0.95815
N 2.01080 2.05099 -0.05791
C -4.18092 -0.30174 -0.38021
H 1.55980 -0.49044 1.60985
C 0.91902 -2.92612 -2.15796
H 0.97184 -1.83536 -2.31691
C 1.95282 -3.27152 -1.08390
C 0.88846 2.89662 0.27098
C 3.77095 -2.69613 0.47933
C 4.38103 2.38457 -2.00807
H 3.65461 2.60247 -2.81444
H 5.19335 3.12965 -2.14329
C -0.92670 -1.64178 2.76709
C 4.95711 0.95794 -2.16274
H 5.60318 0.70138 -1.30132
H 5.62871 0.92316 -3.04649
C 2.84035 -2.29286 -0.53242
C 4.84896 2.45341 1.03854
H 4.54050 2.87885 2.00752
H 5.84128 2.86853 0.78627
H 4.96874 1.36535 1.17517
C 2.93413 -4.99685 0.35551
H 2.97241 -6.03791 0.69429
C -4.43056 -2.66085 -1.12216
H -3.36717 -2.55230 -0.83845
C 0.61864 3.27869 1.62369
C 4.81128 -1.97638 -2.98457
H 5.64391 -2.14220 -2.28096
H 5.24573 -1.77928 -3.98031
H 4.23610 -2.91385 -3.03940
C -4.49566 2.08068 0.25643
H -3.41338 1.89698 0.38621
C 3.79339 -4.03873 0.90435
H 4.50947 -4.33796 1.67914
C -2.03985 -1.54087 3.63562
H -2.88537 -0.91093 3.33488
C 1.46255 2.78374 2.79996
H 2.22008 2.09470 2.38856
C -6.24788 0.53687 -0.88679
C -0.89664 -0.92168 1.48371
C -0.51823 -3.26315 -1.70183
H -0.64822 -4.34872 -1.54024
H -1.24439 -2.95190 -2.47551
H -0.76231 -2.74240 -0.76099
C -6.22937 -0.79043 -1.27557
C 1.22364 -3.62689 -3.50215
H 2.22363 -3.36532 -3.88562
H 0.48040 -3.34151 -4.26883
H 1.18695 -4.72602 -3.39547
C 2.02463 -4.60411 -0.63167
H 1.34655 -5.34937 -1.06463
C 4.75482 -1.71617 1.11996
H 4.58802 -0.73849 0.63445
C 0.15953 -2.46467 3.15382
H 1.01550 -2.56790 2.47925
C 0.05663 -0.39388 0.75580
C 0.03871 3.38777 -0.77128
C 0.13177 -3.14868 4.37711
H 0.97680 -3.78731 4.65676
C -5.10739 2.30667 1.64838
H -4.62440 3.17793 2.12041
H -4.93962 1.42962 2.29414
H -6.19169 2.50565 1.60207
C 0.23812 2.96372 -2.22582
H 1.22133 2.46450 -2.27357
C -0.97113 -3.02446 5.23933
H -0.98806 -3.56139 6.19386
C -0.45724 4.14836 1.89250
H -0.65017 4.44680 2.92984
C 2.60430 -0.00157 -3.90624
H 2.02866 -0.86533 -4.27765
H 3.20367 0.39218 -4.74672
H 1.88382 0.78115 -3.61486
C 4.49387 -1.54691 2.63374
H 4.65415 -2.49607 3.17628
H 3.45844 -1.21695 2.82124
H 5.18024 -0.79670 3.06603
C -7.31624 -1.57619 -1.94399
H -7.10668 -1.75618 -3.01327
H -8.26604 -1.02208 -1.88739
H -7.48066 -2.55628 -1.46722
C -0.83190 1.92680 -2.64218
H -0.83789 1.06058 -1.95748
H -0.65029 1.55761 -3.66784
H -1.84130 2.37732 -2.61907
C 3.32440 4.75022 -0.37802

| | | | |
|---|---|---|---|
| H | 2.71026 | 5.05329 | -1.24226 |
| H | 4.30167 | 5.25713 | -0.46122 |
| H | 2.82199 | 5.12089 | 0.52969 |
| C | 0.61660 | 1.98941 | 3.81999 |
| H | -0.15808 | 2.62600 | 4.28505 |
| H | 1.25701 | 1.60056 | 4.63136 |
| H | 0.11505 | 1.13439 | 3.34039 |
| C | -2.05668 | -2.21444 | 4.86462 |
| H | -2.92123 | -2.11170 | 5.52986 |
| C | -5.08228 | -3.63609 | -0.12843 |
| H | -6.14967 | -3.80901 | -0.34598 |
| H | -4.99040 | -3.25906 | 0.90279 |
| H | -4.56909 | -4.61042 | -0.18351 |
| C | 2.20178 | 3.94444 | 3.50516 |
| H | 2.84590 | 4.50690 | 2.80821 |
| H | 2.83753 | 3.55954 | 4.32248 |
| H | 1.48902 | 4.66229 | 3.94972 |
| C | -4.65573 | 3.28684 | -0.68026 |
| H | -5.69834 | 3.63559 | -0.75179 |
| H | -4.28706 | 3.05432 | -1.69246 |
| H | -4.04934 | 4.11663 | -0.28440 |
| C | 6.22520 | -2.12163 | 0.87018 |
| H | 6.91289 | -1.36807 | 1.29382 |
| H | 6.44532 | -2.21796 | -0.20626 |
| H | 6.46195 | -3.09069 | 1.34474 |
| C | 0.25936 | 4.14872 | -3.21413 |
| H | -0.71632 | 4.66502 | -3.26146 |
| H | 0.49047 | 3.79465 | -4.23436 |
| H | 1.01853 | 4.89818 | -2.93333 |
| C | -4.48317 | -3.14199 | -2.58013 |
| H | -3.88694 | -4.06428 | -2.67399 |
| H | -4.05314 | -2.38896 | -3.26030 |
| H | -5.50743 | -3.37541 | -2.91272 |
| C | -1.02161 | 4.25659 | -0.45112 |
| H | -1.65264 | 4.64598 | -1.25891 |
| C | -7.36582 | 1.52576 | -1.02025 |
| H | -7.54068 | 2.08689 | -0.08762 |
| H | -8.30167 | 0.99981 | -1.26524 |
| H | -7.18325 | 2.26132 | -1.82317 |
| C | -1.27183 | 4.64840 | 0.87043 |
| H | -2.08350 | 5.34869 | 1.10024 |

**$IV_{Ph}$**

SCF (BP86) Energy = -2339.44954105
Enthalpy 0K = -2338.339016
Enthalpy 298K = -2338.266138
Free Energy 298K = -2338.447969
Lowest Frequency = 7.5166 $cm^{-1}$
Second Frequency = 13.3122 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2339.81743728
SCF (C6H6) Energy = -2339.45671607
SCF (BS2) Energy = -3151.64900747

| | | | |
|---|---|---|---|
| Cu | -1.80162 | -0.23659 | 0.13004 |
| Si | 4.32896 | 0.56045 | -1.38688 |
| Al | 1.78973 | 0.50547 | 0.70511 |
| Si | 2.53284 | 3.61591 | 0.45892 |
| N | -4.71789 | 0.05137 | 0.62417 |
| N | 3.16719 | -0.29845 | -0.33905 |
| N | -4.29064 | -0.53707 | -1.42690 |
| N | 1.33856 | 2.29869 | 0.25016 |
| C | -3.68436 | -0.16668 | -0.25222 |
| H | 2.07066 | 0.36010 | 2.29110 |
| C | 2.18727 | -2.23506 | -2.39322 |
| H | 2.09157 | -1.13677 | -2.35576 |
| C | 2.85130 | -2.66481 | -1.08354 |
| C | -0.04046 | 2.65563 | 0.15895 |
| C | 3.99120 | -2.21024 | 1.05502 |
| C | 3.98874 | 3.45786 | -0.76931 |
| H | 3.59391 | 3.53082 | -1.80060 |
| H | 4.57872 | 4.38651 | -0.61672 |
| C | -0.86348 | -3.08769 | 1.14294 |
| C | 4.91148 | 2.22305 | -0.62629 |
| H | 5.18951 | 2.05578 | 0.43205 |
| H | 5.87242 | 2.41953 | -1.14698 |
| C | 3.33738 | -1.71145 | -0.12406 |
| C | 3.30625 | 3.61913 | 2.20789 |
| H | 2.59816 | 3.98456 | 2.96968 |
| H | 4.19729 | 4.27174 | 2.23339 |
| H | 3.61883 | 2.60460 | 2.50839 |
| C | 3.64023 | -4.52394 | 0.30676 |
| H | 3.76217 | -5.60064 | 0.46950 |
| C | -3.48265 | -0.92607 | -2.61490 |
| H | -2.45712 | -0.64069 | -2.31812 |
| C | -0.84121 | 2.87836 | 1.33248 |
| C | 5.89969 | -0.49886 | -1.62447 |
| H | 6.55404 | -0.44887 | -0.73841 |
| H | 6.47579 | -0.12085 | -2.48730 |
| H | 5.66628 | -1.56029 | -1.80693 |
| C | -4.45434 | 0.42254 | 2.04159 |
| H | -3.38000 | 0.67807 | 2.03270 |
| C | 4.11729 | -3.60217 | 1.24473 |
| H | 4.62315 | -3.96712 | 2.14681 |
| C | -2.20054 | -3.55470 | 1.11637 |
| H | -2.99397 | -2.87119 | 0.79615 |
| C | -0.26554 | 2.72934 | 2.74290 |
| H | 0.78603 | 2.41635 | 2.63060 |
| C | -5.95607 | -0.18959 | 0.01390 |
| C | -0.50716 | -1.74131 | 0.77629 |
| C | 0.77012 | -2.82479 | -2.56713 |
| H | 0.78912 | -3.92848 | -2.61343 |
| H | 0.32027 | -2.46331 | -3.51039 |
| H | 0.11452 | -2.53097 | -1.73230 |
| C | -5.68493 | -0.56151 | -1.29001 |
| C | 3.06124 | -2.61191 | -3.61264 |
| H | 4.07868 | -2.19492 | -3.53295 |
| H | 2.61024 | -2.23967 | -4.55073 |
| H | 3.16101 | -3.70868 | -3.70384 |
| C | 3.01646 | -4.04364 | -0.85014 |
| H | 2.64724 | -4.75662 | -1.59730 |
| C | 4.61517 | -1.29399 | 2.11161 |
| H | 4.39273 | -0.25585 | 1.81160 |
| C | 0.17081 | -3.97241 | 1.54539 |
| H | 1.20754 | -3.62339 | 1.55158 |
| C | 0.10660 | -0.65704 | 0.53645 |
| C | -0.65595 | 2.83529 | -1.12777 |
| C | -0.14204 | -5.28509 | 1.91918 |
| H | 0.66533 | -5.95791 | 2.22579 |
| C | -4.65803 | -0.77447 | 2.98478 |
| H | -4.34707 | -0.49238 | 4.00433 |
| H | -4.04668 | -1.63496 | 2.66920 |
| H | -5.71351 | -1.09222 | 3.03344 |
| C | 0.14797 | 2.62851 | -2.40898 |
| H | 1.19969 | 2.53337 | -2.08905 |
| C | -1.47140 | -5.74082 | 1.89633 |
| H | -1.70587 | -6.76922 | 2.18998 |
| C | -2.18135 | 3.29432 | 1.19127 |
| H | -2.76692 | 3.50126 | 2.09567 |
| C | 3.68534 | 0.98945 | -3.13925 |
| H | 3.58209 | 0.09553 | -3.77463 |
| H | 4.40302 | 1.66964 | -3.63374 |
| H | 2.70919 | 1.49944 | -3.10982 |
| C | 4.00924 | -1.52008 | 3.51433 |
| H | 4.20092 | -2.54619 | 3.87796 |
| H | 2.92150 | -1.34777 | 3.50492 |
| H | 4.45785 | -0.82179 | 4.24369 |
| C | -6.65881 | -0.89050 | -2.38050 |
| H | -6.74341 | -0.07964 | -3.12528 |
| H | -7.66096 | -1.04390 | -1.95101 |
| H | -6.39003 | -1.81293 | -2.92043 |
| C | -0.24284 | 1.31058 | -3.11300 |
| H | -0.11118 | 0.44747 | -2.43700 |
| H | 0.38107 | 1.13834 | -4.00835 |
| H | -1.29881 | 1.34099 | -3.43937 |
| C | 1.70753 | 5.30439 | 0.13777 |
| H | 1.39277 | 5.40549 | -0.91448 |
| H | 2.42375 | 6.11592 | 0.35520 |
| H | 0.81598 | 5.45928 | 0.76710 |
| C | -0.97835 | 1.62487 | 3.55375 |
| H | -2.04387 | 1.87193 | 3.72328 |
| H | -0.50589 | 1.50701 | 4.54496 |
| H | -0.91873 | 0.65225 | 3.03634 |
| C | -2.49820 | -4.87148 | 1.49113 |
| H | -3.53616 | -5.22047 | 1.46711 |

| | | | |
|---|---|---|---|
| C | -3.50280 | -2.44715 | -2.83739 |
| H | -4.49760 | -2.81334 | -3.14229 |
| H | -3.19628 | -2.98047 | -1.92338 |
| H | -2.79105 | -2.70809 | -3.63771 |
| C | -0.29447 | 4.06476 | 3.52097 |
| H | 0.23940 | 4.86391 | 2.98018 |
| H | 0.18154 | 3.94641 | 4.51064 |
| H | -1.32955 | 4.41361 | 3.69068 |
| C | -5.22724 | 1.67515 | 2.48171 |
| H | -6.29552 | 1.47539 | 2.66101 |
| H | -5.13234 | 2.47964 | 1.73574 |
| H | -4.79903 | 2.03911 | 3.43029 |
| C | 6.15180 | -1.46373 | 2.17104 |
| H | 6.59290 | -0.74528 | 2.88502 |
| H | 6.62096 | -1.30194 | 1.18701 |
| H | 6.43052 | -2.47899 | 2.50676 |
| C | 0.04288 | 3.81609 | -3.38928 |
| H | -0.97828 | 3.92745 | -3.79730 |
| H | 0.72264 | 3.66712 | -4.24671 |
| H | 0.31171 | 4.76879 | -2.90283 |
| C | -3.85048 | -0.11928 | -3.86944 |
| H | -3.07758 | -0.28322 | -4.63800 |
| H | -3.88749 | 0.95974 | -3.64904 |
| H | -4.81557 | -0.42640 | -4.30284 |
| C | -2.00402 | 3.23532 | -1.21335 |
| H | -2.45197 | 3.38872 | -2.20280 |
| C | -7.29323 | -0.03346 | 0.67226 |
| H | -7.33311 | -0.52151 | 1.65978 |
| H | -8.07211 | -0.49733 | 0.04735 |
| H | -7.57244 | 1.02565 | 0.81108 |
| C | -2.76958 | 3.47899 | -0.06617 |
| H | -3.80641 | 3.82371 | -0.15324 |

**TS(IV-V)$_{Ph}$**

SCF (BP86) Energy = -2339.44491055
Enthalpy 0K = -2338.334570
Enthalpy 298K = -2338.262485
Free Energy 298K = -2338.441922
Lowest Frequency = -7.0331 $cm^{-1}$
Second Frequency = 13.2723 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2339.80717069
SCF (C6H6) Energy = -2339.45256520
SCF (BS2) Energy = -3151.64547846

| | | | |
|---|---|---|---|
| Cu | 1.92998 | 0.14526 | -0.06012 |
| Si | -4.75178 | -0.25733 | -0.08422 |
| Al | -1.55890 | -0.45898 | 0.68557 |
| Si | -2.63970 | -3.50093 | 0.95009 |
| N | 4.40252 | 0.76476 | 1.35628 |
| N | -3.16280 | 0.48987 | 0.25018 |
| N | 4.85923 | -0.38897 | -0.43236 |
| N | -1.52073 | -2.30927 | 0.22295 |
| C | 3.81487 | 0.11321 | 0.29990 |
| H | -1.11248 | -0.27667 | 2.23258 |
| C | -3.19312 | 2.15678 | -2.25135 |
| H | -3.19115 | 1.05957 | -2.14489 |
| C | -3.06501 | 2.74254 | -0.84272 |
| C | -0.32654 | -2.79812 | -0.39371 |
| C | -3.03012 | 2.58172 | 1.61712 |
| C | -4.45636 | -3.15360 | 0.48144 |
| H | -4.57328 | -3.25119 | -0.61393 |
| H | -5.01605 | -4.00949 | 0.91457 |
| C | 1.04390 | 2.84943 | -1.14849 |
| C | -5.06224 | -1.82029 | 0.98136 |
| H | -4.77510 | -1.61681 | 2.03085 |
| H | -6.16970 | -1.89860 | 0.99734 |
| C | -3.08538 | 1.92365 | 0.33946 |
| C | -2.61227 | -3.49283 | 2.86757 |
| H | -1.75268 | -4.04645 | 3.27940 |
| H | -3.53204 | -3.96331 | 3.25914 |
| H | -2.56529 | -2.46296 | 3.26137 |
| C | -2.89066 | 4.77516 | 0.52090 |
| H | -2.82255 | 5.86670 | 0.59075 |
| C | 4.62016 | -1.11977 | -1.70687 |
| H | 3.53337 | -1.31871 | -1.68470 |
| C | 0.80951 | -3.20915 | 0.38582 |
| C | -6.14726 | 0.97121 | 0.35357 |
| H | -6.31139 | 1.01066 | 1.44358 |
| H | -7.09256 | 0.64575 | -0.11525 |
| H | -5.92991 | 1.99575 | 0.01145 |
| C | 3.57913 | 1.49592 | 2.36000 |
| H | 2.54658 | 1.21184 | 2.08379 |
| C | -2.91935 | 3.98616 | 1.67570 |
| H | -2.88285 | 4.47143 | 2.65877 |
| C | 1.98208 | 2.96982 | -2.20465 |
| H | 2.32836 | 2.06353 | -2.71120 |
| C | 0.80635 | -3.13771 | 1.91454 |
| H | -0.18569 | -2.76512 | 2.21516 |
| C | 5.79893 | 0.68353 | 1.28386 |
| C | 0.56117 | 1.56190 | -0.71561 |
| C | -2.01598 | 2.53467 | -3.17622 |
| H | -1.93585 | 3.62806 | -3.31227 |
| H | -2.15677 | 2.08640 | -4.17611 |
| H | -1.05733 | 2.17363 | -2.77440 |
| C | 6.09007 | -0.04562 | 0.14561 |
| C | -4.52426 | 2.58970 | -2.91140 |
| H | -5.39725 | 2.33437 | -2.28854 |
| H | -4.65019 | 2.10410 | -3.89624 |
| H | -4.54551 | 3.68228 | -3.07570 |
| C | -2.97361 | 4.14298 | -0.72483 |
| H | -2.96816 | 4.75130 | -1.63730 |
| C | -3.15457 | 1.82976 | 2.94558 |
| H | -3.20136 | 0.75382 | 2.70786 |
| C | 0.56785 | 4.02242 | -0.50794 |
| H | -0.17937 | 3.93477 | 0.28588 |
| C | -0.04246 | 0.53288 | -0.28941 |
| C | -0.24304 | -2.89846 | -1.82274 |
| C | 1.03433 | 5.27862 | -0.91699 |
| H | 0.65350 | 6.17826 | -0.42269 |
| C | 3.70161 | 3.01906 | 2.19196 |
| H | 2.97976 | 3.51584 | 2.86103 |
| H | 3.47020 | 3.31892 | 1.15769 |
| H | 4.70646 | 3.39171 | 2.45217 |
| C | -1.40302 | -2.46647 | -2.71599 |
| H | -2.19721 | -2.11636 | -2.03463 |
| C | 1.97415 | 5.38922 | -1.95612 |
| H | 2.33372 | 6.37496 | -2.26917 |
| C | 1.94939 | -3.72826 | -0.26274 |
| H | 2.79713 | -4.06736 | 0.34635 |
| C | -5.04694 | -0.82745 | -1.89059 |
| H | -5.23844 | 0.01362 | -2.57460 |
| H | -5.93484 | -1.48588 | -1.91642 |
| H | -4.19606 | -1.40338 | -2.29050 |
| C | -1.93391 | 2.05409 | 3.86449 |
| H | -1.82571 | 3.11843 | 4.14334 |
| H | -1.00724 | 1.72250 | 3.36936 |
| H | -2.04443 | 1.47565 | 4.79945 |
| C | 7.43793 | -0.43416 | -0.38198 |
| H | 7.66531 | -1.50137 | -0.21351 |
| H | 8.21888 | 0.15039 | 0.12865 |
| H | 7.53767 | -0.23764 | -1.46200 |
| C | -1.00766 | -1.28847 | -3.63327 |
| H | -0.64287 | -0.43272 | -3.04166 |
| H | -1.87442 | -0.95030 | -4.22867 |
| H | -0.21035 | -1.57946 | -4.34219 |
| C | -2.22500 | -5.25414 | 0.32560 |
| H | -2.43566 | -5.35343 | -0.75261 |
| H | -2.84364 | -5.99597 | 0.86033 |
| H | -1.16620 | -5.51697 | 0.48055 |
| C | 1.83766 | -2.12387 | 2.45109 |
| H | 2.86910 | -2.39438 | 2.16025 |
| H | 1.79242 | -2.06777 | 3.55403 |
| H | 1.62300 | -1.11221 | 2.05602 |
| C | 2.44336 | 4.23130 | -2.60057 |
| H | 3.16503 | 4.31262 | -3.42018 |
| C | 4.92946 | -0.23048 | -2.92262 |
| H | 6.00729 | -0.01575 | -3.01942 |
| H | 4.39092 | 0.72813 | -2.85163 |
| H | 4.60617 | -0.74190 | -3.84438 |
| C | 1.03105 | -4.51901 | 2.57019 |
| H | 0.28631 | -5.25725 | 2.23004 |
| H | 0.95633 | -4.44287 | 3.66980 |
| H | 2.03190 | -4.92411 | 2.33458 |
| C | 3.83064 | 1.01181 | 3.79601 |

| | | | |
|---|---|---|---|
| H | 4.80309 | 1.34656 | 4.19131 |
| H | 3.77919 | -0.08690 | 3.85752 |
| H | 3.04769 | 1.42506 | 4.45270 |
| C | -4.45397 | 2.21742 | 3.69050 |
| H | -4.56785 | 1.61551 | 4.61001 |
| H | -5.34587 | 2.05801 | 3.06298 |
| H | -4.44511 | 3.28169 | 3.98801 |
| C | -1.96563 | -3.63981 | -3.54858 |
| H | -1.21503 | -4.02963 | -4.26008 |
| H | -2.84188 | -3.31348 | -4.13668 |
| H | -2.28037 | -4.47865 | -2.90520 |
| C | 5.33614 | -2.47741 | -1.75620 |
| H | 4.94605 | -3.04923 | -2.61333 |
| H | 5.13878 | -3.06197 | -0.84373 |
| H | 6.42462 | -2.38054 | -1.89231 |
| C | 0.91799 | -3.42080 | -2.42206 |
| H | 0.95543 | -3.51341 | -3.51458 |
| C | 6.75375 | 1.25087 | 2.28986 |
| H | 6.52610 | 2.29930 | 2.54127 |
| H | 7.77821 | 1.22634 | 1.88728 |
| H | 6.75915 | 0.67480 | 3.23187 |
| C | 2.01046 | -3.84891 | -1.65680 |
| H | 2.88802 | -4.29321 | -2.13930 |

**$V_{Ph}$**

SCF (BP86) Energy = -2339.47302367
Enthalpy 0K = -2338.361628
Enthalpy 298K = -2338.289057
Free Energy 298K = -2338.469842
Lowest Frequency = 9.7888 $cm^{-1}$
Second Frequency = 14.1242 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2339.84146110
SCF (C6H6) Energy = -2339.47781242
SCF (BS2) Energy = -3151.67375291

| | | | |
|---|---|---|---|
| Cu | 1.32102 | -0.00859 | 0.10103 |
| Si | -3.87271 | 1.55819 | -1.20501 |
| Al | -1.30896 | -0.06841 | -0.08488 |
| Si | -3.94192 | -1.53886 | 1.26422 |
| N | 3.56408 | 1.55167 | 1.24075 |
| N | -2.22747 | 1.51466 | -0.49126 |
| N | 4.05567 | -0.56847 | 1.21201 |
| N | -2.29769 | -1.52891 | 0.55650 |
| C | 3.06180 | 0.32385 | 0.88915 |
| H | -0.02875 | 0.38549 | 1.04675 |
| C | -0.65694 | 2.70530 | -2.76578 |
| H | -1.07281 | 1.68695 | -2.67689 |
| C | -0.82089 | 3.37875 | -1.40034 |
| C | -1.51793 | -2.74325 | 0.58628 |
| C | -1.61882 | 3.46801 | 0.93100 |
| C | -5.23534 | -0.74894 | 0.09859 |
| H | -5.17661 | -1.25679 | -0.88327 |
| H | -6.21099 | -1.06158 | 0.52727 |
| C | 2.27835 | -1.00033 | -2.85299 |
| C | -5.21376 | 0.78593 | -0.07735 |
| H | -5.17162 | 1.29175 | 0.90654 |
| H | -6.16928 | 1.12256 | -0.53279 |
| C | -1.54816 | 2.77339 | -0.32162 |
| C | -4.06751 | -0.62114 | 2.93771 |
| H | -3.55531 | -1.17046 | 3.74424 |
| H | -5.13030 | -0.52059 | 3.22395 |
| H | -3.63747 | 0.39269 | 2.89603 |
| C | -0.32042 | 5.32964 | 0.00611 |
| H | 0.12820 | 6.32269 | 0.12231 |
| C | 3.89586 | -2.02701 | 0.95993 |
| H | 2.84084 | -2.10950 | 0.64267 |
| C | -0.69976 | -3.06298 | 1.71992 |
| C | -4.42793 | 3.36460 | -1.45774 |
| H | -4.66257 | 3.83982 | -0.49016 |
| H | -5.34557 | 3.38435 | -2.07155 |
| H | -3.66901 | 3.98870 | -1.95350 |
| C | 2.76649 | 2.78978 | 1.02622 |
| H | 1.79040 | 2.40098 | 0.68117 |
| C | -1.00173 | 4.72612 | 1.07036 |
| H | -1.07912 | 5.25205 | 2.02989 |
| C | 2.08330 | -2.01612 | -3.82418 |
| H | 1.15225 | -2.58971 | -3.81086 |
| C | -0.74212 | -2.23776 | 3.00840 |
| H | -1.33951 | -1.33580 | 2.79362 |
| C | 4.85752 | 1.43762 | 1.77158 |
| C | 1.23833 | -0.71868 | -1.89081 |
| C | 0.82981 | 2.57245 | -3.16313 |
| H | 1.29636 | 3.55992 | -3.33192 |
| H | 0.92891 | 1.99477 | -4.09863 |
| H | 1.40419 | 2.04879 | -2.38230 |
| C | 5.16958 | 0.09201 | 1.75402 |
| C | -1.42224 | 3.44900 | -3.88552 |
| H | -2.50436 | 3.50151 | -3.68574 |
| H | -1.28121 | 2.93758 | -4.85463 |
| H | -1.05334 | 4.48451 | -3.99887 |
| C | -0.23462 | 4.64792 | -1.21356 |
| H | 0.29431 | 5.11464 | -2.05332 |
| C | -2.36418 | 2.88512 | 2.12988 |
| H | -2.81759 | 1.94170 | 1.78124 |
| C | 3.48886 | -0.26410 | -2.87523 |
| H | 3.64349 | 0.51388 | -2.12131 |
| C | 0.05940 | -0.62596 | -1.42301 |
| C | -1.53234 | -3.64275 | -0.53033 |
| C | 4.46651 | -0.52768 | -3.84422 |
| H | 5.39254 | 0.05724 | -3.85213 |
| C | 3.34780 | 3.66271 | -0.09690 |
| H | 2.62107 | 4.45460 | -0.34006 |
| H | 3.51907 | 3.06838 | -1.00889 |
| H | 4.29673 | 4.14572 | 0.19162 |
| C | -2.47271 | -3.44708 | -1.72231 |
| H | -3.08480 | -2.55574 | -1.49853 |
| C | 4.26279 | -1.53664 | -4.80085 |
| H | 5.02878 | -1.74289 | -5.55553 |
| C | 0.11805 | -4.21064 | 1.68231 |
| H | 0.73451 | -4.45269 | 2.55679 |
| C | -3.91241 | 0.61447 | -2.86376 |
| H | -3.31633 | 1.12688 | -3.63649 |
| H | -4.94781 | 0.52141 | -3.23736 |
| H | -3.50549 | -0.40548 | -2.75208 |
| C | -1.40211 | 2.54942 | 3.29178 |
| H | -0.91204 | 3.46033 | 3.68117 |
| H | -0.61466 | 1.85093 | 2.96242 |
| H | -1.94957 | 2.08132 | 4.12955 |
| C | 6.41983 | -0.57362 | 2.24376 |
| H | 6.26354 | -1.11487 | 3.19352 |
| H | 7.19784 | 0.18425 | 2.42536 |
| H | 6.82788 | -1.29211 | 1.51424 |
| C | -1.71767 | -3.18002 | -3.04330 |
| H | -1.08919 | -2.27898 | -2.96338 |
| H | -2.42959 | -3.03613 | -3.87590 |
| H | -1.06732 | -4.03468 | -3.30668 |
| C | -4.50839 | -3.33591 | 1.55900 |
| H | -4.85006 | -3.80611 | 0.62234 |
| H | -5.35656 | -3.34392 | 2.26572 |
| H | -3.70854 | -3.96727 | 1.97806 |
| C | 0.64853 | -1.77151 | 3.48528 |
| H | 1.28908 | -2.62835 | 3.76228 |
| H | 0.55207 | -1.13206 | 4.38112 |
| H | 1.16297 | -1.18694 | 2.70352 |
| C | 3.06936 | -2.27892 | -4.78339 |
| H | 2.90292 | -3.06728 | -5.52523 |
| C | 4.78150 | -2.51321 | -0.19900 |
| H | 5.85328 | -2.49960 | 0.06246 |
| H | 4.62824 | -1.90047 | -1.10048 |
| H | 4.51439 | -3.55457 | -0.44449 |
| C | -1.44236 | -3.02662 | 4.14118 |
| H | -2.45755 | -3.34559 | 3.85330 |
| H | -1.52279 | -2.41125 | 5.05560 |
| H | -0.87080 | -3.93649 | 4.39914 |
| C | 2.52100 | 3.56456 | 2.32938 |
| H | 3.42353 | 4.08595 | 2.68830 |
| H | 2.15678 | 2.89385 | 3.12409 |
| H | 1.74278 | 4.32166 | 2.14127 |
| C | -3.50485 | 3.80529 | 2.61845 |
| H | -4.06516 | 3.32447 | 3.43999 |
| H | -4.21715 | 4.03354 | 1.80777 |
| H | -3.11707 | 4.76663 | 3.00069 |
| C | -3.42095 | -4.65577 | -1.90264 |
| H | -2.86332 | -5.56197 | -2.20033 |

H -4.16288 -4.45040 -2.69475
H -3.96476 -4.89432 -0.97426
C 4.07650 -2.86778 2.23427
H 3.69018 -3.88295 2.04663
H 3.51167 -2.44072 3.07722
H 5.13472 -2.96514 2.52614
C -0.68972 -4.77083 -0.52016
H -0.69866 -5.44846 -1.38242
C 5.68671 2.57610 2.28324
H 5.73506 3.41440 1.56936
H 6.71925 2.23642 2.45949
H 5.30609 2.97544 3.23990
C 0.14395 -5.05646 0.56738
H 0.78716 -5.94350 0.55615

**$VI_{Ph}$**
SCF (BP86) Energy = -2647.83787465
Enthalpy 0K = -2646.620103
Enthalpy 298K = -2646.538890
Free Energy 298K = -2646.740068
Lowest Frequency = 11.5071 $cm^{-1}$
Second Frequency = 13.6260 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2648.25642866
SCF (C6H6) Energy = -2647.84444456
SCF (BS2) Energy = -3460.11250129

Cu 1.90691 0.18164 -0.09730
Si -3.95446 -0.84191 2.17014
Al -1.76749 0.16961 -0.10113
Si -4.00014 2.60825 0.19931
N 4.67126 -1.01753 -0.03956
N -2.91539 -1.10326 0.74538
N 4.74299 1.12254 -0.41724
N -2.32995 2.00979 -0.03402
C 3.87212 0.08942 -0.17650
H -1.52358 -0.34811 -1.60927
C -1.03861 -3.19919 1.79461
H -1.10496 -2.12690 2.04470
C -2.02391 -3.44556 0.65182
C -1.33763 2.90573 -0.55332
C -3.75722 -2.74393 -0.94458
C -4.71617 2.03012 1.87776
H -3.97501 2.23670 2.67322
H -5.55637 2.73001 2.07129
C 1.62889 -0.17489 3.01083
C -5.22835 0.57288 1.96212
H -5.87120 0.33650 1.09267
H -5.88943 0.46080 2.84794
C -2.89699 -2.41981 0.15734
C -5.27304 2.06720 -1.12668
H -5.12353 2.60343 -2.07757
H -6.28606 2.31869 -0.76079
H -5.25598 0.98796 -1.34085
C -2.89393 -5.03806 -1.00012
H -2.90410 -6.04501 -1.43255
C 4.23929 2.50359 -0.64447
H 3.15847 2.41188 -0.43323
C -1.23780 3.18262 -1.96138
C -4.98522 -2.40465 2.53859
H -5.75828 -2.56348 1.76809
H -5.49716 -2.29319 3.51060
H -4.37028 -3.31770 2.57632
C 4.07952 -2.35428 0.24321
H 3.00646 -2.12244 0.37171
C -3.73461 -4.03724 -1.50011
H -4.40308 -4.26395 -2.33968
C 2.99003 0.14858 3.23258
H 3.58111 0.53060 2.39527
C -2.23170 2.61938 -2.97952
H -2.89024 1.92407 -2.43402
C 6.02621 -0.68847 -0.20133
C 0.98745 -0.00155 1.72338
C 0.41504 -3.49306 1.35961
H 0.56382 -4.56754 1.14746
H 1.12126 -3.20620 2.15941
H 0.67319 -2.92768 0.44881
C 6.07196 0.67132 -0.44278
C -1.38208 -4.01915 3.05904
H -2.39158 -3.78689 3.43622
H -0.65889 -3.80900 3.86814
H -1.34638 -5.10444 2.85406
C -2.04783 -4.72952 0.07024
H -1.38414 -5.50535 0.47154
C -4.71492 -1.71915 -1.54496
H -4.58844 -0.80022 -0.94872
C 0.86543 -0.66273 4.10301
H -0.18972 -0.90038 3.94845
C 0.06780 0.11031 0.84885
C -0.39844 3.54276 0.33371
C 1.45050 -0.82416 5.36543
H 0.84216 -1.20045 6.19469
C 4.58916 -2.95306 1.56368
H 3.97119 -3.83001 1.81732
H 4.49962 -2.22733 2.38770
H 5.63476 -3.29519 1.49545
C -0.47207 3.35612 1.85129
H -0.96455 2.38359 2.02374
C 2.80279 -0.50334 5.57161
H 3.25542 -0.62890 6.56063
C -0.22627 4.04422 -2.43694
H -0.17057 4.25244 -3.51225
C -2.92985 -0.41078 3.72731
H -2.37709 -1.29393 4.09076
H -3.58530 -0.06563 4.54684
H -2.20141 0.39204 3.52125
C -4.35621 -1.39081 -3.01135
H -4.46156 -2.28042 -3.65882
H -3.31747 -1.03040 -3.08785
H -5.02648 -0.60805 -3.41025
C 7.27695 1.53576 -0.65873
H 7.16892 2.19605 -1.53462
H 8.16226 0.90472 -0.83345
H 7.49910 2.17410 0.21467
C 0.90976 3.33511 2.53656
H 1.60333 2.64054 2.03590
H 0.80673 3.01176 3.58651
H 1.37545 4.33775 2.55383
C -4.05043 4.52771 0.16023
H -4.16993 4.96142 1.16723
H -4.91718 4.85557 -0.43993
H -3.14477 4.96654 -0.28881
C -1.55433 1.81582 -4.11013
H -0.85995 2.44068 -4.70143
H -2.31730 1.42436 -4.80608
H -0.99364 0.96067 -3.70256
C 3.56742 -0.01384 4.49941
H 4.61998 0.24924 4.65159
C 4.82148 3.51649 0.35369
H 5.88087 3.74606 0.15574
H 4.72452 3.15365 1.38973
H 4.25775 4.46013 0.27191
C -3.09852 3.75213 -3.57930
H -3.60689 4.33910 -2.79652
H -3.86859 3.33744 -4.25439
H -2.48202 4.45357 -4.17048
C 4.21521 -3.31300 -0.95002
H 5.25754 -3.63367 -1.11488
H 3.83575 -2.85245 -1.87575
H 3.61860 -4.21877 -0.75265
C -6.19167 -2.15946 -1.43320
H -6.86208 -1.36843 -1.81458
H -6.47547 -2.37241 -0.38869
H -6.38768 -3.07289 -2.02330
C -1.34072 4.44908 2.51747
H -0.92024 5.45310 2.32590
H -1.37573 4.29962 3.61175
H -2.37223 4.43872 2.13892
C 4.39266 2.93442 -2.11192
H 3.84221 3.87633 -2.27078
H 3.96658 2.17334 -2.78455
H 5.44495 3.10871 -2.39272
C 0.59198 4.39491 -0.19538
H 1.28883 4.88852 0.49130
C 7.17157 -1.64871 -0.09299

| | | | |
|---|---|---|---|
| H | 7.35044 | -1.97387 | 0.94701 |
| H | 8.09649 | -1.16730 | -0.44686 |
| H | 7.01996 | -2.55400 | -0.70291 |
| C | 0.69185 | 4.64921 | -1.57038 |
| H | 1.45620 | 5.33307 | -1.95737 |
| C | 1.41048 | -1.52903 | -3.22376 |
| C | 0.37892 | -2.44337 | -2.87744 |
| H | -0.40629 | -2.11655 | -2.18696 |
| C | 1.40069 | -0.22103 | -2.66100 |
| C | 2.41510 | -1.92213 | -4.14783 |
| H | 3.19982 | -1.21014 | -4.42199 |
| C | 1.35939 | 0.87636 | -2.08164 |
| C | 2.38451 | -3.20515 | -4.70749 |
| H | 3.15610 | -3.50259 | -5.42525 |
| C | 1.36663 | -4.10905 | -4.35147 |
| H | 1.35030 | -5.11168 | -4.79171 |
| C | 0.36819 | -3.72568 | -3.43846 |
| H | -0.42997 | -4.42072 | -3.15922 |
| H | 1.08864 | 1.92461 | -1.98933 |

**TS(E)$_{Ph}$**

SCF (BP86) Energy = -2647.81661593
Enthalpy 0K = -2646.600107
Enthalpy 298K = -2646.519573
Free Energy 298K = -2646.719110
Lowest Frequency = -411.4563 $cm^{-1}$
Second Frequency = 8.7198 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2648.23487911
SCF (C6H6) Energy = -2647.82316581
SCF (BS2) Energy = -3460.09183382

| | | | |
|---|---|---|---|
| Cu | 1.98684 | -0.13358 | -0.16803 |
| Si | -3.68951 | 0.13363 | 2.46758 |
| Al | -1.48477 | 0.29816 | 0.05296 |
| Si | -3.44817 | 2.95142 | -0.27022 |
| N | 4.60337 | -1.59105 | -0.39835 |
| N | -2.81840 | -0.59169 | 1.08214 |
| N | 4.85720 | 0.54384 | -0.72416 |
| N | -1.85587 | 2.11861 | -0.38251 |
| C | 3.91711 | -0.40327 | -0.41049 |
| H | -1.09580 | -0.70167 | -1.22939 |
| C | -1.05435 | -2.67383 | 2.34580 |
| H | -0.95983 | -1.57590 | 2.36915 |
| C | -2.24668 | -3.00688 | 1.44886 |
| C | -0.77629 | 2.87855 | -0.96864 |
| C | -4.15584 | -2.41711 | 0.01400 |
| C | -4.20008 | 2.88511 | 1.49202 |
| H | -3.43089 | 3.22729 | 2.21061 |
| H | -4.96223 | 3.69295 | 1.47832 |
| C | 2.02565 | 0.06189 | 3.02991 |
| C | -4.85215 | 1.57054 | 1.97552 |
| H | -5.57458 | 1.19646 | 1.22516 |
| H | -5.45583 | 1.76582 | 2.88709 |
| C | -3.06362 | -1.99439 | 0.84375 |
| C | -4.77307 | 2.26964 | -1.46577 |
| H | -4.55080 | 2.54333 | -2.50947 |
| H | -5.75264 | 2.71149 | -1.20564 |
| H | -4.87563 | 1.17635 | -1.41919 |
| C | -3.60087 | -4.77213 | 0.41275 |
| H | -3.81021 | -5.83587 | 0.25501 |
| C | 4.48440 | 1.98368 | -0.78217 |
| H | 3.38273 | 1.96070 | -0.68719 |
| C | -0.61796 | 2.96157 | -2.39395 |
| C | -4.77109 | -1.17184 | 3.33779 |
| H | -5.59291 | -1.52110 | 2.69172 |
| H | -5.21745 | -0.73172 | 4.24687 |
| H | -4.19039 | -2.05936 | 3.63597 |
| C | 3.88627 | -2.87036 | -0.14588 |
| H | 2.87570 | -2.52875 | 0.14367 |
| C | -4.39873 | -3.79067 | -0.18502 |
| H | -5.24265 | -4.09232 | -0.81745 |
| C | 3.41430 | -0.21071 | 3.09308 |
| H | 3.95750 | -0.37288 | 2.15767 |
| C | -1.60202 | 2.31396 | -3.37251 |
| H | -2.27591 | 1.67344 | -2.77839 |
| C | 5.96108 | -1.39510 | -0.70140 |
| C | 1.30465 | 0.12643 | 1.77808 |
| C | 0.26005 | -3.24445 | 1.76638 |
| H | 0.24716 | -4.34958 | 1.75052 |
| H | 1.12142 | -2.92383 | 2.37898 |
| H | 0.41893 | -2.89129 | 0.73355 |
| C | 6.12323 | -0.03764 | -0.90318 |
| C | -1.25357 | -3.16821 | 3.79679 |
| H | -2.15778 | -2.73344 | 4.25493 |
| H | -0.38732 | -2.88775 | 4.42242 |
| H | -1.35641 | -4.26757 | 3.83952 |
| C | -2.53375 | -4.36770 | 1.22044 |
| H | -1.90240 | -5.12809 | 1.69578 |
| C | -5.07638 | -1.41727 | -0.68151 |
| H | -4.76690 | -0.42045 | -0.32728 |
| C | 1.32553 | 0.28276 | 4.24534 |
| H | 0.25572 | 0.50404 | 4.20948 |
| C | 0.34296 | 0.24368 | 0.95279 |
| C | 0.14147 | 3.60726 | -0.13597 |
| C | 1.99637 | 0.22409 | 5.47320 |
| H | 1.43754 | 0.39717 | 6.39911 |
| C | 4.47216 | -3.65566 | 1.03781 |
| H | 3.77871 | -4.47088 | 1.30161 |
| H | 4.58601 | -3.01029 | 1.92373 |
| H | 5.44592 | -4.11446 | 0.80195 |
| C | 0.01136 | 3.64562 | 1.38942 |
| H | -0.59571 | 2.77038 | 1.67879 |
| C | 3.37370 | -0.05122 | 5.52255 |
| H | 3.89359 | -0.09487 | 6.48516 |
| C | 0.43011 | 3.73190 | -2.93612 |
| H | 0.52972 | 3.79715 | -4.02618 |
| C | -2.45451 | 0.82521 | 3.75119 |
| H | -1.91090 | -0.00201 | 4.23841 |
| H | -2.97613 | 1.40053 | 4.53657 |
| H | -1.71455 | 1.49425 | 3.27936 |
| C | -4.89651 | -1.45744 | -2.21626 |
| H | -5.16846 | -2.44865 | -2.62193 |
| H | -3.85245 | -1.25324 | -2.50558 |
| H | -5.54221 | -0.70761 | -2.70743 |
| C | 7.37263 | 0.70818 | -1.26150 |
| H | 7.33854 | 1.11587 | -2.28680 |
| H | 8.24022 | 0.03296 | -1.20469 |
| H | 7.57043 | 1.54926 | -0.57612 |
| C | 1.36855 | 3.55807 | 2.11854 |
| H | 1.97297 | 2.71560 | 1.74850 |
| H | 1.21170 | 3.41359 | 3.20159 |
| H | 1.95677 | 4.48653 | 2.00115 |
| C | -3.28132 | 4.81638 | -0.70025 |
| H | -3.41201 | 5.44956 | 0.19360 |
| H | -4.07553 | 5.09745 | -1.41389 |
| H | -2.31184 | 5.07324 | -1.15463 |
| C | -0.91569 | 1.42537 | -4.43220 |
| H | -0.25711 | 2.01686 | -5.09436 |
| H | -1.67462 | 0.94344 | -5.07369 |
| H | -0.31101 | 0.63626 | -3.96223 |
| C | 4.07784 | -0.26604 | 4.32638 |
| H | 5.15273 | -0.47624 | 4.35318 |
| C | 5.04165 | 2.76250 | 0.42006 |
| H | 6.13969 | 2.86208 | 0.38196 |
| H | 4.76393 | 2.27200 | 1.36670 |
| H | 4.61338 | 3.77809 | 0.42381 |
| C | -2.45138 | 3.39266 | -4.08845 |
| H | -2.96998 | 4.05491 | -3.37724 |
| H | -3.21019 | 2.92278 | -4.74011 |
| H | -1.81349 | 4.03054 | -4.72698 |
| C | 3.74714 | -3.70636 | -1.42809 |
| H | 4.71768 | -4.08647 | -1.78903 |
| H | 3.27709 | -3.11302 | -2.22820 |
| H | 3.10154 | -4.57726 | -1.22751 |
| C | -6.56345 | -1.61351 | -0.31252 |
| H | -7.18276 | -0.82762 | -0.78047 |
| H | -6.72440 | -1.56843 | 0.77768 |
| H | -6.94655 | -2.58798 | -0.66495 |
| C | -0.73005 | 4.91710 | 1.86617 |
| H | -0.17966 | 5.82561 | 1.56101 |
| H | -0.81355 | 4.92696 | 2.96807 |
| H | -1.74402 | 4.98500 | 1.44636 |
| C | 4.82198 | 2.62934 | -2.13482 |
| H | 4.27722 | 3.58365 | -2.21501 |

| | | | |
|---|---|---|---|
| H | 4.49973 | 1.98986 | -2.97279 |
| H | 5.89760 | 2.84284 | -2.24592 |
| C | 1.16728 | 4.36806 | -0.73269 |
| H | 1.84367 | 4.94202 | -0.08878 |
| C | 6.99794 | -2.47546 | -0.76341 |
| H | 7.22632 | -2.89698 | 0.23114 |
| H | 7.93636 | -2.06931 | -1.17120 |
| H | 6.69522 | -3.31088 | -1.41645 |
| C | 1.32301 | 4.43637 | -2.12244 |
| H | 2.11109 | 5.05612 | -2.56609 |
| C | -0.24132 | -2.30676 | -2.94545 |
| C | -1.40478 | -2.95229 | -2.47176 |
| H | -1.87241 | -2.59762 | -1.54964 |
| C | 0.40741 | -1.18454 | -2.31111 |
| C | 0.37898 | -2.79887 | -4.13068 |
| H | 1.28476 | -2.30747 | -4.49982 |
| C | 1.40061 | -0.41440 | -2.11054 |
| C | -0.17435 | -3.87869 | -4.82477 |
| H | 0.30588 | -4.23085 | -5.74413 |
| C | -1.33493 | -4.51221 | -4.34385 |
| H | -1.75892 | -5.36575 | -4.88317 |
| C | -1.93862 | -4.04744 | -3.16563 |
| H | -2.83292 | -4.53588 | -2.76686 |
| H | 2.17958 | 0.02928 | -2.72632 |

**E-INT1$_{Ph}$**

SCF (BP86) Energy = -2647.88140373
Enthalpy 0K = -2646.658345
Enthalpy 298K = -2646.577658
Free Energy 298K = -2646.779877
Lowest Frequency = 8.6472 $cm^{-1}$
Second Frequency = 11.5935 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2648.28613415
SCF (C6H6) Energy = -2647.88795625
SCF (BS2) Energy = -3460.15837300

| | | | |
|---|---|---|---|
| Cu | 1.73377 | 0.26920 | -0.13079 |
| Si | -4.26979 | -1.55719 | 1.71151 |
| Al | -1.92403 | 0.02051 | 0.11124 |
| Si | -4.51163 | 0.06003 | -1.90720 |
| N | 4.35803 | 1.00523 | 1.16071 |
| N | -2.55470 | -1.32398 | 1.19421 |
| N | 4.48061 | 1.14334 | -1.00451 |
| N | -3.01082 | 0.75929 | -1.17951 |
| C | 3.60329 | 0.89345 | 0.02021 |
| H | 3.13518 | -2.47046 | 0.41275 |
| C | -1.24079 | -0.74276 | 3.83813 |
| H | -1.92765 | -0.10861 | 3.25055 |
| C | -0.93964 | -1.98567 | 2.99804 |
| C | -2.60649 | 2.06020 | -1.68356 |
| C | -1.29285 | -3.46399 | 1.05253 |
| C | -5.79694 | -0.47276 | -0.59604 |
| H | -6.02668 | 0.39407 | 0.05262 |
| H | -6.72079 | -0.63928 | -1.18903 |
| C | 0.99667 | 3.04064 | 1.21712 |
| C | -5.49383 | -1.72776 | 0.25238 |
| H | -5.16887 | -2.56752 | -0.39068 |
| H | -6.42744 | -2.08279 | 0.73747 |
| C | -1.58316 | -2.25109 | 1.75103 |
| C | -4.12414 | -1.46427 | -2.98263 |
| H | -3.54604 | -1.19213 | -3.88061 |
| H | -5.06327 | -1.94020 | -3.31714 |
| H | -3.54513 | -2.21999 | -2.42685 |
| C | 0.30634 | -4.08725 | 2.79663 |
| H | 1.04119 | -4.79366 | 3.19738 |
| C | 4.04485 | 1.04020 | -2.42117 |
| H | 2.95675 | 0.87878 | -2.32843 |
| C | -1.77167 | 2.17239 | -2.83643 |
| C | -4.40574 | -3.16652 | 2.71495 |
| H | -4.23023 | -4.04932 | 2.07812 |
| H | -5.42300 | -3.24865 | 3.13623 |
| H | -3.68432 | -3.21010 | 3.54563 |
| C | 3.76141 | 0.75039 | 2.49662 |
| H | 2.68501 | 0.65827 | 2.26802 |
| C | -0.33949 | -4.35177 | 1.58378 |
| H | -0.09936 | -5.26917 | 1.03664 |
| C | 1.95106 | 3.88088 | 0.59200 |
| H | 2.43764 | 3.52799 | -0.32178 |
| C | -1.27116 | 0.95230 | -3.61054 |
| H | -1.64409 | 0.05569 | -3.08637 |
| C | 5.69616 | 1.31025 | 0.85808 |
| C | 0.65565 | 1.74697 | 0.65637 |
| C | 0.03061 | 0.08450 | 4.12669 |
| H | 0.75785 | -0.49078 | 4.72725 |
| H | -0.21998 | 0.99532 | 4.69988 |
| H | 0.52019 | 0.38589 | 3.18671 |
| C | 5.77320 | 1.40038 | -0.51670 |
| C | -1.94599 | -1.10784 | 5.16554 |
| H | -2.88620 | -1.65787 | 4.99448 |
| H | -2.18403 | -0.19766 | 5.74514 |
| H | -1.30004 | -1.74514 | 5.79538 |
| C | -0.00507 | -2.91675 | 3.49482 |
| H | 0.48531 | -2.71654 | 4.45493 |
| C | -1.99201 | -3.81240 | -0.26230 |
| H | -2.90308 | -3.19030 | -0.31294 |
| C | 0.38463 | 3.49315 | 2.41457 |
| H | -0.34709 | 2.85067 | 2.91168 |
| C | -0.17608 | 0.80777 | 0.36538 |
| C | -3.06709 | 3.24683 | -1.03207 |
| C | 0.71715 | 4.74045 | 2.96045 |
| H | 0.23720 | 5.06840 | 3.88897 |
| C | 3.93764 | 1.93294 | 3.46247 |
| H | 3.28931 | 1.77532 | 4.34015 |
| H | 3.63836 | 2.87985 | 2.98569 |
| H | 4.97218 | 2.02684 | 3.83085 |
| C | -3.98291 | 3.18064 | 0.19131 |
| H | -4.44446 | 2.17727 | 0.19187 |
| C | 1.65447 | 5.56956 | 2.32154 |
| H | 1.90845 | 6.54578 | 2.74754 |
| C | -1.39507 | 3.45354 | -3.28701 |
| H | -0.75302 | 3.53758 | -4.17182 |
| C | -4.85882 | -0.08507 | 2.77225 |
| H | -4.31263 | -0.02910 | 3.72791 |
| H | -5.93488 | -0.18241 | 3.00215 |
| H | -4.71659 | 0.87494 | 2.24745 |
| C | -1.11113 | -3.44243 | -1.47547 |
| H | -0.16406 | -4.00781 | -1.46391 |
| H | -0.84022 | -2.37127 | -1.46953 |
| H | -1.63280 | -3.66144 | -2.42479 |
| C | 6.96309 | 1.75116 | -1.35740 |
| H | 7.11496 | 1.04469 | -2.18981 |
| H | 7.87480 | 1.72832 | -0.74012 |
| H | 6.88836 | 2.76473 | -1.79039 |
| C | -3.16503 | 3.31103 | 1.49567 |
| H | -2.39821 | 2.51840 | 1.56868 |
| H | -3.81621 | 3.24205 | 2.38566 |
| H | -2.63056 | 4.27624 | 1.53093 |
| C | -5.35350 | 1.38634 | -2.97997 |
| H | -5.72244 | 2.22601 | -2.36792 |
| H | -6.21907 | 0.93866 | -3.49910 |
| H | -4.67548 | 1.80398 | -3.74086 |
| C | 0.27079 | 0.87575 | -3.62189 |
| H | 0.71218 | 1.74369 | -4.14429 |
| H | 0.61075 | -0.03826 | -4.14057 |
| H | 0.66640 | 0.85362 | -2.59185 |
| C | 2.26541 | 5.13446 | 1.13218 |
| H | 2.99623 | 5.77423 | 0.62560 |
| C | 4.27121 | 2.34340 | -3.20439 |
| H | 5.33615 | 2.52866 | -3.41945 |
| H | 3.86707 | 3.21238 | -2.65930 |
| H | 3.74736 | 2.27645 | -4.17235 |
| C | -1.82093 | 0.92336 | -5.05537 |
| H | -2.92374 | 0.93692 | -5.07526 |
| H | -1.48092 | 0.01414 | -5.58267 |
| H | -1.46914 | 1.79551 | -5.63486 |
| C | 4.23282 | -0.59151 | 3.08151 |
| H | 5.30184 | -0.57818 | 3.35336 |
| H | 4.06319 | -1.40940 | 2.36332 |
| H | 3.65880 | -0.81335 | 3.99646 |
| C | -2.43073 | -5.28985 | -0.34733 |
| H | -3.03992 | -5.45377 | -1.25354 |
| H | -3.03195 | -5.58868 | 0.52844 |
| H | -1.56697 | -5.97437 | -0.41068 |
| C | -5.12385 | 4.21924 | 0.16292 |

H -4.74776 5.25211 0.26801
H -5.82105 4.04210 1.00050
H -5.69801 4.16698 -0.77765
C 4.63425 -0.20199 -3.10833
H 4.18910 -0.30691 -4.11216
H 4.39157 -1.10534 -2.52709
H 5.72768 -0.13573 -3.23699
C -2.65340 4.50220 -1.51564
H -2.99624 5.41047 -1.00820
C 6.78466 1.52665 1.86490
H 6.66842 2.47808 2.41384
H 7.76107 1.56015 1.35660
H 6.83418 0.71675 2.61127
C -1.82090 4.61483 -2.63501
H -1.51323 5.60084 -2.99950
C 2.86724 -3.83489 -1.23980
C 3.55730 -4.86198 -0.54789
H 3.89636 -4.66717 0.47718
C 2.63544 -2.53668 -0.56880
C 2.44657 -4.11772 -2.56493
H 1.92313 -3.34145 -3.13417
C 1.89492 -1.47660 -0.99873
C 2.69502 -5.36184 -3.15765
H 2.35819 -5.54850 -4.18402
C 3.37654 -6.36865 -2.44985
H 3.57102 -7.34022 -2.91639
C 3.80765 -6.10826 -1.13865
H 4.34211 -6.88035 -0.57319
H 1.40664 -1.62039 -1.98398

**TS(E2)$_{Ph}$**
SCF (BP86) Energy = -2647.88540071
Enthalpy 0K = -2646.661614
Enthalpy 298K = -2646.582066
Free Energy 298K = -2646.779031
Lowest Frequency = -4.9996 $cm^{-1}$
Second Frequency = 12.8080 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2648.29573228
SCF (C6H6) Energy = -2647.89078853
SCF (BS2) Energy = -3460.16065729

Cu -1.55492 -0.26268 -0.07474
Si 4.05142 0.75846 2.21371
Al 1.73814 -0.22809 0.19658
Si 4.06622 0.96379 -1.74209
N -4.20887 0.13012 1.21737
N 2.30837 0.61127 1.73860
N -4.46422 -0.86706 -0.69726
N 2.77233 -0.22672 -1.32604
C -3.50726 -0.38585 0.15818
H -3.21289 2.04616 -1.14077
C 1.32141 -1.34619 3.81174
H 1.90617 -1.55408 2.89850
C 0.92088 0.13152 3.77327
C 2.53187 -1.30055 -2.27763
C 0.93133 2.40391 2.80072
C 5.40885 1.12949 -0.38849
H 5.85668 0.13132 -0.22046
H 6.20495 1.71793 -0.89170
C -1.39793 -3.43687 0.42181
C 5.04673 1.79924 0.95710
H 4.51437 2.75409 0.78906
H 5.97649 2.07421 1.49720
C 1.36708 1.03901 2.75860
C 3.31768 2.69240 -2.03366
H 2.67133 2.70471 -2.92627
H 4.11548 3.44197 -2.18068
H 2.70949 3.01912 -1.17259
C -0.30613 1.95092 4.87034
H -0.92759 2.30883 5.69880
C -4.07821 -1.47019 -1.99973
H -2.97872 -1.53740 -1.91756
C 1.67750 -1.10952 -3.40874
C 4.20193 1.58160 3.92377
H 3.82339 2.61421 3.94761
H 5.26959 1.60162 4.20611
H 3.65765 1.01719 4.69725
C -3.49375 0.78622 2.34569
H -2.43079 0.60524 2.10123
C 0.10941 2.82915 3.86334
H -0.20190 3.87906 3.90326
C -2.61135 -3.66943 1.11400
H -3.14344 -2.81425 1.54112
C 0.92258 0.19383 -3.67477
H 1.07289 0.84823 -2.79894
C -5.59350 -0.01563 1.02847
C -0.83725 -2.10792 0.28710
C 0.08896 -2.27761 3.80672
H -0.50893 -2.15891 4.72813
H 0.40464 -3.33424 3.75225
H -0.56099 -2.07125 2.94312
C -5.75641 -0.64733 -0.18866
C 2.21126 -1.67360 5.03427
H 3.12929 -1.06405 5.05812
H 2.50878 -2.73735 5.02224
H 1.66846 -1.49120 5.97895
C 0.09236 0.61147 4.80804
H -0.23020 -0.08324 5.59241
C 1.32406 3.43808 1.74069
H 1.79677 2.88308 0.91020
C -0.71909 -4.54422 -0.15122
H 0.21174 -4.36749 -0.69862
C 0.17100 -1.32298 0.17828
C 3.17560 -2.56663 -2.10102
C -1.24084 -5.83798 -0.02643
H -0.70703 -6.68087 -0.47860
C -3.78995 0.12049 3.69808
H -3.06424 0.49358 4.43895
H -3.67740 -0.97442 3.63571
H -4.80164 0.35109 4.07073
C 4.10268 -2.84549 -0.91969
H 4.26978 -1.87617 -0.41970
C -2.43753 -6.05898 0.67739
H -2.83929 -7.07275 0.77675
C 1.50390 -2.16853 -4.32305
H 0.85643 -2.01313 -5.19362
C 4.89977 -0.94339 2.37082
H 4.43975 -1.54584 3.17075
H 5.96403 -0.79712 2.63021
H 4.86584 -1.53424 1.44235
C 0.09632 4.19094 1.18298
H -0.35315 4.85201 1.94560
H -0.67894 3.49444 0.82842
H 0.39238 4.83165 0.33463
C -7.03175 -1.06608 -0.85489
H -7.07750 -0.75124 -1.91058
H -7.88980 -0.60571 -0.34034
H -7.18256 -2.15999 -0.82771
C 3.43989 -3.79884 0.10109
H 2.47442 -3.40036 0.45976
H 4.09318 -3.95838 0.97741
H 3.24113 -4.78535 -0.35477
C 4.98817 0.37312 -3.29775
H 5.58966 -0.52570 -3.08118
H 5.67664 1.16556 -3.63977
H 4.31017 0.12379 -4.12816
C -0.59592 -0.04765 -3.81851
H -0.82581 -0.65118 -4.71526
H -1.12844 0.91371 -3.90763
H -0.99384 -0.56882 -2.93252
C -3.11704 -4.96961 1.24953
H -4.04954 -5.13337 1.80069
C -4.62465 -2.89529 -2.17948
H -5.71060 -2.91116 -2.36706
H -4.40287 -3.51643 -1.29687
H -4.13411 -3.35785 -3.05206
C 1.45165 0.93091 -4.92752
H 2.52356 1.17575 -4.84669
H 0.89690 1.87332 -5.08155
H 1.32066 0.31345 -5.83434
C -3.70553 2.30761 2.35372
H -4.73813 2.58979 2.62111
H -3.45843 2.73313 1.36858
H -3.02797 2.75617 3.09866

| | | | |
|---|---|---|---|
| C | 2.35332 | 4.46708 | 2.26600 |
| H | 2.57474 | 5.21824 | 1.48708 |
| H | 3.30560 | 3.99954 | 2.56168 |
| H | 1.95562 | 5.00545 | 3.14501 |
| C | 5.48215 | -3.38765 | -1.35328 |
| H | 5.40253 | -4.38498 | -1.82071 |
| H | 6.14885 | -3.48781 | -0.47851 |
| H | 5.97044 | -2.71774 | -2.08104 |
| C | -4.40520 | -0.53447 | -3.17492 |
| H | -3.98955 | -0.95593 | -4.10527 |
| H | -3.95342 | 0.45729 | -3.01570 |
| H | -5.49164 | -0.41119 | -3.32162 |
| C | 2.94940 | -3.59854 | -3.03216 |
| H | 3.44274 | -4.56624 | -2.88408 |
| C | -6.64766 | 0.41064 | 2.00437 |
| H | -6.66472 | -0.22320 | 2.90879 |
| H | -7.64186 | 0.33703 | 1.53639 |
| H | -6.51720 | 1.45465 | 2.33359 |
| C | 2.12594 | -3.40795 | -4.14623 |
| H | 1.97140 | -4.21612 | -4.86931 |
| C | -2.02300 | 3.61859 | -2.02710 |
| C | -3.18651 | 4.36325 | -2.34238 |
| H | -4.16215 | 3.97453 | -2.02402 |
| C | -2.15989 | 2.34467 | -1.28653 |
| C | -0.77824 | 4.14275 | -2.45801 |
| H | 0.13952 | 3.58462 | -2.24342 |
| C | -1.18446 | 1.53090 | -0.78599 |
| C | -0.70424 | 5.35420 | -3.15633 |
| H | 0.27214 | 5.73418 | -3.47792 |
| C | -1.87156 | 6.08125 | -3.45265 |
| H | -1.81055 | 7.02717 | -4.00117 |
| C | -3.11571 | 5.57616 | -3.04149 |
| H | -4.03464 | 6.12915 | -3.26699 |
| H | -0.15608 | 1.91203 | -0.95867 |

**$E_{ph}$**

SCF (BP86) Energy = -2647.91378909
Enthalpy 0K = -2646.689251
Enthalpy 298K = -2646.609315
Free Energy 298K = -2646.805168
Lowest Frequency = 14.4255 $cm^{-1}$
Second Frequency = 16.8134 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2648.33882086
SCF (C6H6) Energy = -2647.91910097
SCF (BS2) Energy = -3460.18425945

| | | | |
|---|---|---|---|
| Si | 4.14030 | 0.67395 | 1.71480 |
| Al | 1.47815 | -0.12644 | -0.01182 |
| Si | 4.00190 | -1.77296 | -1.37448 |
| N | 2.29485 | -1.64343 | -0.83389 |
| N | 2.65503 | 1.12346 | 0.81725 |
| C | 1.44585 | -2.77261 | -1.11662 |
| C | 2.70536 | 3.42268 | -0.15677 |
| C | 2.28325 | 2.51476 | 0.87128 |
| C | 1.24704 | -3.80452 | -0.13549 |
| C | 0.81527 | -2.92883 | -2.39928 |
| C | 5.25804 | -1.53233 | 0.04965 |
| H | 4.98522 | -2.23035 | 0.86442 |
| H | 6.20950 | -1.92924 | -0.36420 |
| C | -0.43287 | 2.04035 | -1.00025 |
| H | -0.22571 | 2.54839 | -0.04493 |
| C | 0.99174 | 2.16703 | 3.10891 |
| H | 1.23518 | 1.12076 | 2.85774 |
| C | 1.49835 | 3.03822 | 1.95563 |
| C | 3.56727 | 2.96525 | -1.33133 |
| H | 3.74412 | 1.88797 | -1.17578 |
| C | 0.09590 | -0.75221 | 1.32208 |
| C | 1.00752 | -1.92525 | -3.53938 |
| H | 1.52929 | -1.05069 | -3.11374 |
| C | -1.20488 | 2.87114 | -1.95004 |
| C | 0.03355 | -4.07346 | -2.66065 |
| H | -0.40937 | -4.19580 | -3.65688 |
| C | 4.97419 | 2.22345 | 2.45499 |
| H | 5.47914 | 2.81348 | 1.67193 |
| H | 5.74266 | 1.90932 | 3.18337 |
| H | 4.26980 | 2.89620 | 2.96735 |
| C | -1.76852 | -1.35982 | 3.12923 |
| C | 0.13518 | 0.80553 | -1.22723 |
| H | -0.05136 | 0.41240 | -2.24044 |
| C | -0.95076 | -0.96945 | 2.00553 |
| C | 1.16872 | 4.40921 | 1.97941 |
| H | 0.58110 | 4.79751 | 2.82014 |
| C | 1.94228 | -3.77281 | 1.22610 |
| H | 2.33246 | -2.74851 | 1.35512 |
| C | -3.18286 | -1.40709 | 3.06672 |
| H | -3.67586 | -1.13121 | 2.13029 |
| C | -1.96184 | 5.10480 | -2.62238 |
| H | -1.99301 | 6.18477 | -2.44160 |
| C | -1.27951 | 4.26788 | -1.72741 |
| H | -0.76374 | 4.69166 | -0.85750 |
| C | 2.33740 | 4.78022 | -0.09239 |
| H | 2.66918 | 5.45714 | -0.88890 |
| C | 1.57522 | 5.28543 | 0.96683 |
| H | 1.31302 | 6.34848 | 1.00990 |
| C | 3.75784 | -0.54987 | 3.13218 |
| H | 3.17313 | -0.06259 | 3.93028 |
| H | 4.69376 | -0.92924 | 3.58013 |
| H | 3.17926 | -1.41972 | 2.77862 |
| C | 2.85018 | 3.14614 | -2.68771 |
| H | 1.88492 | 2.61551 | -2.70466 |
| H | 3.47430 | 2.75619 | -3.51182 |
| H | 2.65171 | 4.21253 | -2.89793 |
| C | 4.44540 | -0.52596 | -2.75326 |
| H | 3.92917 | -0.77093 | -3.69594 |
| H | 5.53285 | -0.56244 | -2.94805 |
| H | 4.18840 | 0.51160 | -2.49098 |
| C | -1.85557 | 2.33795 | -3.08906 |
| H | -1.81926 | 1.25861 | -3.26947 |
| C | 0.44689 | -4.92131 | -0.44492 |
| H | 0.31842 | -5.70612 | 0.30945 |
| C | 5.48683 | -0.11052 | 0.60364 |
| H | 5.69615 | 0.59827 | -0.22081 |
| H | 6.40137 | -0.09714 | 1.23399 |
| C | -0.54123 | 2.26617 | 3.27574 |
| H | -0.85280 | 3.28132 | 3.58172 |
| H | -0.89194 | 1.56196 | 4.05006 |
| H | -1.06328 | 2.01629 | 2.33655 |
| C | 4.36976 | -3.51826 | -2.08146 |
| H | 4.89846 | -4.14635 | -1.34491 |
| H | 5.03201 | -3.42309 | -2.96009 |
| H | 3.46553 | -4.06279 | -2.39452 |
| C | -1.13324 | -1.70566 | 4.35208 |
| H | -0.04186 | -1.66789 | 4.40912 |
| C | 4.93999 | 3.67483 | -1.35680 |
| H | 4.82894 | 4.76218 | -1.51861 |
| H | 5.56520 | 3.27925 | -2.17717 |
| H | 5.48995 | 3.53490 | -0.41133 |
| C | -2.60228 | 4.56101 | -3.74810 |
| H | -3.14050 | 5.21191 | -4.44527 |
| C | 1.67465 | 2.51880 | 4.45155 |
| H | 2.76737 | 2.38596 | 4.40688 |
| H | 1.28780 | 1.87639 | 5.26316 |
| H | 1.47795 | 3.56860 | 4.73518 |
| C | -0.33353 | -1.44886 | -4.14209 |
| H | -0.84634 | -2.26312 | -4.68488 |
| H | -0.16519 | -0.63029 | -4.86442 |
| H | -1.02382 | -1.08515 | -3.36211 |
| C | -3.93479 | -1.79628 | 4.18396 |
| H | -5.02744 | -1.83011 | 4.11491 |
| C | 0.99245 | -4.08530 | 2.40075 |
| H | 0.65721 | -5.13824 | 2.38835 |
| H | 0.09968 | -3.44298 | 2.37980 |
| H | 1.51284 | -3.92664 | 3.36225 |
| C | -2.54802 | 3.17301 | -3.97513 |
| H | -3.04899 | 2.74184 | -4.84893 |
| C | -0.16109 | -5.06927 | -1.69708 |
| H | -0.75633 | -5.96033 | -1.92678 |
| C | 1.88590 | -2.50733 | -4.67297 |
| H | 2.87293 | -2.82929 | -4.30695 |
| H | 2.04267 | -1.75726 | -5.46919 |
| H | 1.39970 | -3.38671 | -5.13297 |
| C | -1.89263 | -2.08886 | 5.46410 |
| H | -1.38468 | -2.35166 | 6.39807 |
| C | -3.29534 | -2.13851 | 5.38678 |

H -3.88499 -2.43980 6.25866
C 3.14269 -4.74793 1.26531
H 3.65643 -4.69355 2.24205
H 3.87896 -4.52442 0.47832
H 2.80453 -5.78995 1.11977
N -4.33324 0.86868 -0.06803
N -4.03366 -1.13858 -0.85048
C -5.60326 0.38612 -0.41980
C -5.41223 -0.88863 -0.91716
C -3.35835 -0.06577 -0.31909
Cu -1.46486 -0.04185 0.16256
C -3.99606 2.17573 0.55701
H -2.89190 2.18372 0.52218
C -6.43942 -1.83346 -1.46330
H -6.40119 -1.90556 -2.56457
H -7.44830 -1.48333 -1.19426
H -6.32762 -2.85263 -1.05881
C -6.88671 1.15104 -0.30294
H -7.00348 1.62866 0.68361
H -7.74028 0.46847 -0.43841
H -6.97534 1.94190 -1.06858
C -3.31367 -2.38698 -1.22689
H -2.24933 -2.09939 -1.14250
C -4.42802 2.22688 2.03226
H -5.52570 2.23255 2.14366
H -4.04274 3.15133 2.49341
H -4.02290 1.36993 2.59347
C -4.50070 3.37227 -0.26349
H -4.22783 3.26970 -1.32544
H -4.02321 4.28982 0.11660
H -5.59089 3.50933 -0.18020
C -3.56675 -3.52511 -0.22563
H -3.36748 -3.19490 0.80588
H -2.87968 -4.35603 -0.45468
H -4.59988 -3.90920 -0.28096
C -3.57500 -2.80274 -2.68234
H -4.57281 -3.24912 -2.82108
H -2.82531 -3.55883 -2.96499
H -3.46992 -1.94697 -3.36860

**INT(E-P)$_{Ph}$**
SCF (BP86) Energy = -2956.28626824
Enthalpy 0K = -2954.955219
Enthalpy 298K = -2954.866735
Free Energy 298K = -2955.084743
Lowest Frequency = 4.8412 $cm^{-1}$
Second Frequency = 9.7038 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2956.75028442
SCF (C6H6) Energy = -2956.29447745
SCF (BS2) Energy = -3768.63298786

Si -4.29311 -1.84772 1.23971
Al -1.81581 0.18668 0.35916
Si -3.42060 1.60614 2.87634
N -1.90313 1.13158 2.03728
N -3.29542 -0.99542 0.02213
C -0.69155 1.68766 2.58244
C -4.70678 -0.44531 -1.97988
C -3.69562 -1.24400 -1.34602
C 0.12517 0.91992 3.48555
C -0.28881 3.03866 2.29637
C -4.49730 0.12290 3.43138
H -3.86026 -0.55373 4.03285
H -5.20013 0.57989 4.16080
C -1.58148 1.01438 -2.55718
H -1.62944 -0.05854 -2.79914
C -2.01798 -3.22457 -1.54042
H -1.77228 -2.84989 -0.53325
C -3.11491 -2.31718 -2.10144
C -5.39455 0.72053 -1.27040
H -4.91519 0.80700 -0.28154
C -0.07093 -0.94594 0.44976
C -1.10109 3.97675 1.39818
H -1.92365 3.38073 0.96854
C -1.51053 1.87334 -3.75906
C 0.86847 3.56960 2.90206
H 1.14393 4.61044 2.69240
C -5.57325 -2.98773 0.40186
H -6.29628 -2.42663 -0.21113
H -6.13597 -3.53015 1.18242
H -5.10076 -3.73251 -0.25767
C 1.03505 -3.36582 0.79273
C -1.62200 1.39336 -1.24514
H -1.61898 2.48661 -1.08368
C 0.65255 -1.99194 0.53417
C -3.54836 -2.56188 -3.42068
H -3.10133 -3.39377 -3.97872
C -0.26239 -0.49342 3.92391
H -0.96950 -0.87374 3.16678
C 2.17833 -3.96455 0.20820
H 2.81469 -3.35704 -0.44070
C -1.69260 2.06086 -6.20047
H -1.88549 1.58936 -7.17056
C -1.74168 1.29152 -5.02967
H -1.98641 0.22410 -5.08161
C -5.10075 -0.72963 -3.30134
H -5.87509 -0.10830 -3.76700
C -4.53553 -1.78122 -4.02959
H -4.86313 -1.99186 -5.05368
C -3.23526 -2.95514 2.38185
H -2.82322 -3.80597 1.81400
H -3.84980 -3.36144 3.20507
H -2.39881 -2.39619 2.83396
C -5.20064 2.05847 -2.01939
H -4.13398 2.27656 -2.18178
H -5.64417 2.89050 -1.44298
H -5.69564 2.04249 -3.00695
C -4.52981 2.75983 1.82667
H -4.16478 3.79942 1.86017
H -5.56023 2.75528 2.22632
H -4.57916 2.45858 0.76924
C -1.21457 3.25780 -3.70786
H -1.01615 3.72899 -2.73922
C 1.27640 1.49711 4.05591
H 1.87081 0.90749 4.76341
C -5.29046 -0.67595 2.37651
H -5.89062 0.00401 1.74330
H -6.03038 -1.33234 2.88154
C -0.73650 -3.15502 -2.40250
H -0.91927 -3.52912 -3.42616
H 0.06251 -3.77350 -1.95717
H -0.36429 -2.11976 -2.48013
C -3.04841 2.54879 4.50661
H -3.07147 1.87565 5.37995
H -3.83225 3.31104 4.66397
H -2.07286 3.05880 4.50664
C 0.22580 -4.15721 1.64851
H -0.65694 -3.70807 2.10855
C -6.90308 0.46330 -1.04885
H -7.43480 0.35528 -2.01142
H -7.36435 1.30873 -0.50718
H -7.08572 -0.45298 -0.46366
C -1.40081 3.43294 -6.13031
H -1.35897 4.03684 -7.04316
C -2.47446 -4.69560 -1.40770
H -3.35586 -4.79313 -0.75273
H -1.66478 -5.31299 -0.97910
H -2.74183 -5.12556 -2.38992
C -0.26391 4.55415 0.23470
H 0.54197 5.21350 0.60480
H -0.90192 5.16355 -0.43081
H 0.20722 3.75929 -0.36396
C 2.49495 -5.30649 0.46197
H 3.38120 -5.74986 -0.00489
C 0.93637 -1.46056 4.00284
H 1.62380 -1.19596 4.82707
H 1.50811 -1.46982 3.06134
H 0.58662 -2.48930 4.19720
C -1.16138 4.02589 -4.87720
H -0.92843 5.09476 -4.81372
C 1.65609 2.81568 3.77813
H 2.53702 3.25626 4.25954
C -1.71979 5.14690 2.20024
H -2.35353 4.79423 3.02863

H -2.33824 5.78323 1.54174
H -0.93123 5.78750 2.63506
C 0.54841 -5.49766 1.89673
H -0.09285 -6.08959 2.55835
C 1.68210 -6.08090 1.30618
H 1.92995 -7.12905 1.50265
C -0.98751 -0.47953 5.29034
H -1.28270 -1.50259 5.58622
H -1.89367 0.14336 5.26585
H -0.32528 -0.07666 6.07813
N 4.32981 -1.18714 -1.72751
N 4.81207 -1.05748 0.38949
C 5.70208 -1.46277 -1.61592
C 6.00805 -1.38012 -0.27110
C 3.77328 -0.93863 -0.49689
Cu 1.89145 -0.50945 -0.13776
C 3.49196 -1.17487 -2.95807
H 2.51402 -0.82285 -2.58212
C 7.34419 -1.54419 0.38707
H 7.76401 -0.58087 0.72652
H 8.06113 -1.97852 -0.32696
H 7.30399 -2.21634 1.25953
C 6.62628 -1.74119 -2.76221
H 6.22994 -2.50895 -3.44655
H 7.59131 -2.11073 -2.38196
H 6.83613 -0.83719 -3.36094
C 4.58636 -0.89884 1.85265
H 3.53128 -0.57303 1.90369
C 3.29575 -2.58402 -3.54109
H 4.22918 -3.00236 -3.95326
H 2.56203 -2.53686 -4.36254
H 2.90498 -3.27765 -2.78012
C 3.98759 -0.15703 -3.99648
H 4.16717 0.82318 -3.52764
H 3.21427 -0.02800 -4.77136
H 4.91127 -0.48415 -4.50073
C 4.70184 -2.23925 2.59683
H 4.06768 -3.00655 2.12540
H 4.36086 -2.10598 3.63666
H 5.74011 -2.61005 2.63305
C 5.45110 0.21309 2.46570
H 6.51220 -0.07404 2.54476
H 5.08901 0.42194 3.48580
H 5.37573 1.14358 1.88048
C 1.52499 1.42760 -0.97914
C 2.50529 2.17149 -0.79469
H 0.47505 1.27520 -1.28018
C 3.66337 2.95837 -0.54678
C 3.95824 3.40656 0.76992
C 4.51928 3.33947 -1.61514
C 5.08856 4.20014 1.00113
C 5.64273 4.13657 -1.36908
C 5.93342 4.56564 -0.06204
H 3.28064 3.13536 1.58627
H 4.27625 3.01829 -2.63239
H 5.30719 4.54476 2.01719
H 6.29250 4.42949 -2.20017
H 6.81228 5.19097 0.12610

**TS(E-P)$_{Ph}$**
SCF (BP86) Energy = -2956.27516013
Enthalpy 0K = -2954.947130
Enthalpy 298K = -2954.859858
Free Energy 298K = -2955.073226
Lowest Frequency = -723.4943 $cm^{-1}$
Second Frequency = 6.9962 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2956.74107316
SCF (C6H6) Energy = -2956.28157242
SCF (BS2) Energy = -3768.62122810

Si -4.15821 -2.26331 0.30017
Al -1.58450 -0.24301 0.45632
Si -3.25305 0.06550 3.30785
N -1.72969 0.01131 2.34686
N -3.14648 -0.95272 -0.39713
C -0.51673 0.30069 3.07940
C -4.53903 0.41088 -1.96679
C -3.51889 -0.57465 -1.73851
C 0.31853 -0.76656 3.56003
C -0.13984 1.65144 3.39512
C -4.32253 -1.51528 3.14695
H -3.67998 -2.39070 3.36100
H -5.01143 -1.44376 4.01554
C -1.32604 1.79265 -1.80378
H -1.15319 0.95449 -2.49464
C -1.85632 -2.29953 -2.76339
H -1.63201 -2.42224 -1.69156
C -2.92328 -1.20834 -2.88270
C -5.26447 1.11414 -0.81936
H -4.86358 0.68191 0.11184
C 0.01746 -1.42044 0.04635
C -0.99623 2.86613 3.02234
H -1.81573 2.49978 2.38066
C -1.70718 3.03563 -2.47614
C 1.03379 1.89468 4.13699
H 1.29662 2.93024 4.38483
C -5.44865 -2.87614 -0.96214
H -6.19706 -2.10460 -1.20281
H -5.98149 -3.74374 -0.53394
H -4.99045 -3.19149 -1.91247
C 1.26384 -3.71468 -0.53965
C -1.09931 1.58238 -0.45496
H -1.29007 2.45495 0.19015
C 0.82271 -2.36194 -0.26133
C -3.33923 -0.84302 -4.17926
H -2.88421 -1.34560 -5.04156
C -0.05335 -2.24023 3.37723
H -0.74884 -2.29012 2.52211
C 2.56117 -4.00246 -1.02959
H 3.25358 -3.17113 -1.18861
C -2.40816 4.16481 -4.53772
H -2.68513 4.11245 -5.59605
C -2.05827 2.99626 -3.85032
H -2.07778 2.02778 -4.36155
C -4.91337 0.74177 -3.28303
H -5.69233 1.49782 -3.43725
C -4.32613 0.12522 -4.39274
H -4.64050 0.38788 -5.40890
C -3.09112 -3.76870 0.78923
H -2.72362 -4.27818 -0.11739
H -3.68390 -4.49628 1.37168
H -2.22098 -3.47688 1.40089
C -4.98695 2.63351 -0.80039
H -3.91076 2.84786 -0.71056
H -5.50629 3.11197 0.04934
H -5.34468 3.11833 -1.72607
C -4.37593 1.54836 2.86195
H -4.01783 2.47915 3.33062
H -5.40073 1.36195 3.23176
H -4.43736 1.72164 1.77719
C -1.70455 4.29435 -1.81998
H -1.41013 4.35233 -0.76733
C 1.48213 -0.46458 4.29544
H 2.09747 -1.28850 4.67420
C -5.13647 -1.74077 1.85629
H -5.74122 -0.84644 1.61462
H -5.87316 -2.55686 2.01305
C -0.54264 -1.90099 -3.47385
H -0.69225 -1.77602 -4.56177
H 0.22465 -2.68094 -3.32493
H -0.14005 -0.95521 -3.07334
C -2.88292 0.20007 5.18617
H -2.99115 -0.77654 5.68709
H -3.61579 0.88426 5.64944
H -1.87403 0.57935 5.40953
C 0.37435 -4.79853 -0.31739
H -0.62455 -4.59259 0.07400
C -6.78989 0.86433 -0.84332
H -7.25551 1.28899 -1.75069
H -7.27055 1.34205 0.02905
H -7.03384 -0.21047 -0.81691
C -2.40355 5.40189 -3.87133
H -2.67114 6.31785 -4.40882
C -2.34492 -3.66126 -3.30991

H -3.25098 -4.01107 -2.78833
H -1.56170 -4.42924 -3.18010
H -2.58383 -3.60300 -4.38715
C -0.20905 3.93810 2.23673
H 0.57181 4.40670 2.86180
H -0.88708 4.74789 1.91016
H 0.28963 3.51528 1.35107
C 2.95134 -5.32200 -1.29616
H 3.96025 -5.52159 -1.67382
C 1.15677 -3.14552 3.06873
H 1.81373 -3.26647 3.94928
H 1.75933 -2.74626 2.23799
H 0.81456 -4.15537 2.78374
C -2.04725 5.46081 -2.51091
H -2.03199 6.42442 -1.99064
C 1.85106 0.85369 4.58674
H 2.74738 1.06457 5.18130
C -1.62115 3.52607 4.27569
H -2.22109 2.81747 4.86705
H -2.27252 4.37035 3.98537
H -0.83396 3.92777 4.93893
C 0.77135 -6.11458 -0.58582
H 0.06847 -6.93517 -0.40605
C 2.05946 -6.38492 -1.07841
H 2.36606 -7.41532 -1.28638
C -0.78879 -2.79226 4.62143
H -1.06063 -3.85308 4.47332
H -1.70949 -2.23063 4.83714
H -0.14146 -2.73017 5.51493
N 4.34458 -0.67092 -2.01221
N 4.82231 -0.73599 0.10711
C 5.74624 -0.62024 -1.92037
C 6.04927 -0.66812 -0.57372
C 3.76928 -0.73530 -0.76835
Cu 1.86244 -0.60725 -0.32579
C 3.49316 -0.56460 -3.22550
H 2.48011 -0.76191 -2.82869
C 7.39790 -0.63925 0.07868
H 7.57407 0.29796 0.63457
H 8.18511 -0.72102 -0.68661
H 7.54181 -1.47574 0.78307
C 6.68660 -0.55007 -3.08507
H 6.70335 -1.48566 -3.67160
H 7.71161 -0.36933 -2.72627
H 6.43668 0.27140 -3.77744
C 4.58078 -0.82210 1.57206
H 3.48125 -0.73431 1.64715
C 3.80586 -1.64436 -4.27325
H 4.76152 -1.46718 -4.79235
H 3.01089 -1.64158 -5.03708
H 3.83001 -2.64636 -3.81502
C 3.50152 0.86433 -3.79233
H 3.22472 1.58485 -3.00643
H 2.76462 0.94082 -4.60943
H 4.48618 1.14460 -4.20312
C 4.98718 -2.19402 2.13395
H 4.51282 -3.00760 1.56200
H 4.65202 -2.27226 3.18124
H 6.08010 -2.34431 2.12156
C 5.18922 0.35937 2.34231
H 6.28341 0.27737 2.44927
H 4.75340 0.38085 3.35445
H 4.94674 1.31530 1.85122
C 1.60057 1.35782 -0.17135
C 2.24756 2.42524 -0.03633
H 0.21070 1.26174 -0.29326
C 3.02187 3.60349 0.14830
C 3.46490 3.97712 1.44918
C 3.38010 4.43066 -0.95239
C 4.24224 5.12645 1.63185
C 4.15446 5.57951 -0.75624
C 4.59143 5.93195 0.53323
H 3.17676 3.35084 2.29905
H 3.03382 4.15749 -1.95389
H 4.57518 5.40015 2.63887
H 4.41909 6.20679 -1.61427
H 5.19742 6.83179 0.68142

**INT2(E-P)$_{Ph}$**
SCF (BP86) Energy = -2956.28760809
Enthalpy 0K = -2954.954559
Enthalpy 298K = -2954.866385
Free Energy 298K = -2955.083338
Lowest Frequency = 7.6525 $cm^{-1}$
Second Frequency = 12.1926 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2956.75240609
SCF (C6H6) Energy = -2956.29424798
SCF (BS2) Energy = -3768.63592102

Si -4.23079 -2.01995 -0.89676
Al -1.60375 -0.55179 0.29860
Si -3.32671 -1.62339 2.88451
N -1.77020 -1.28392 2.02876
N -3.14288 -0.58191 -0.79644
C -0.58250 -1.58324 2.80869
C -4.49864 1.42261 -1.43811
C -3.46734 0.46819 -1.73741
C 0.10573 -2.83193 2.63915
C -0.11059 -0.67529 3.81678
C -4.49115 -2.80878 1.92921
H -3.91392 -3.71883 1.67860
H -5.21401 -3.13334 2.70755
C -0.89377 2.37206 -0.40587
H -0.09665 1.97554 -1.04961
C -1.75651 -0.45924 -3.47282
H -1.54061 -1.12206 -2.61918
C -2.82505 0.53822 -3.01901
C -5.28137 1.40796 -0.12270
H -4.89387 0.56070 0.46560
C 0.12515 -1.03002 -0.55506
C -0.75825 0.68454 4.09952
H -1.56941 0.81625 3.36379
C -1.49478 3.62865 -0.84818
C 0.98953 -1.03767 4.61962
H 1.33143 -0.33881 5.39172
C -5.45461 -1.84036 -2.34555
H -6.12977 -0.97800 -2.23872
H -6.07257 -2.75438 -2.39847
H -4.93401 -1.72721 -3.30958
C 1.31991 -2.75448 -2.18722
C -1.12327 1.68027 0.75858
H -1.84457 2.02830 1.50520
C 0.97573 -1.69487 -1.25207
C -3.21179 1.53658 -3.93587
H -2.72455 1.56913 -4.91779
C -0.32369 -3.87985 1.61061
H -0.95250 -3.35801 0.86846
C 2.65166 -3.01783 -2.58611
H 3.44995 -2.40082 -2.16540
C -1.85449 5.26384 -2.63609
H -1.75549 5.55028 -3.68807
C -1.36690 4.02530 -2.20256
H -0.89569 3.33951 -2.91335
C -4.83639 2.40469 -2.38787
H -5.62268 3.12884 -2.14425
C -4.20556 2.47162 -3.63389
H -4.49116 3.23789 -4.36241
C -3.24812 -3.62166 -1.23051
H -2.88551 -3.63481 -2.27226
H -3.90534 -4.49960 -1.09629
H -2.38219 -3.75300 -0.56156
C -5.06391 2.69620 0.69966
H -3.99857 2.85513 0.92636
H -5.61622 2.64572 1.65489
H -5.41756 3.58824 0.15325
C -4.29727 -0.02721 3.28261
H -3.86222 0.49755 4.14869
H -5.34516 -0.27340 3.53184
H -4.31155 0.67652 2.43651
C -2.09648 4.53170 0.06530
H -2.13847 4.27338 1.12767
C 1.19630 -3.14396 3.47487
H 1.69411 -4.11257 3.35424
C -5.25852 -2.30343 0.68930

H -5.82051 -1.38141 0.92694
H -6.02983 -3.04728 0.39831
C -0.43526 0.23831 -3.86577
H -0.57173 0.90722 -4.73493
H 0.32639 -0.51325 -4.13659
H -0.03230 0.83402 -3.03038
C -3.00677 -2.52049 4.53985
H -2.78635 -3.59035 4.39554
H -3.92104 -2.44873 5.15590
H -2.17260 -2.08936 5.11298
C 0.28781 -3.56624 -2.72677
H -0.74303 -3.38430 -2.41401
C -6.79788 1.19099 -0.33410
H -7.24447 2.01498 -0.91846
H -7.31917 1.15529 0.63918
H -7.01447 0.25071 -0.86585
C -2.46263 6.13937 -1.72138
H -2.83302 7.11376 -2.05702
C -2.24438 -1.33710 -4.64931
H -3.15289 -1.90510 -4.38943
H -1.46165 -2.06143 -4.93619
H -2.47968 -0.72457 -5.53809
C 0.24845 1.84791 3.93986
H 1.01283 1.81828 4.73702
H -0.26866 2.82040 4.02508
H 0.77946 1.81902 2.97496
C 2.94084 -4.04848 -3.49136
H 3.98032 -4.23697 -3.78182
C 0.87000 -4.51435 0.86556
H 1.44888 -5.18863 1.52201
H 1.55338 -3.74730 0.47015
H 0.51157 -5.12024 0.01581
C -2.57688 5.77137 -0.36836
H -3.02508 6.46292 0.35237
C 1.64166 -2.26407 4.46705
H 2.47813 -2.53659 5.12043
C -1.38552 0.75533 5.51283
H -2.15178 -0.01926 5.67483
H -1.85748 1.74124 5.67429
H -0.61448 0.62810 6.29347
C 0.58084 -4.59200 -3.63396
H -0.23286 -5.20586 -4.03513
C 1.90883 -4.83857 -4.02339
H 2.13626 -5.64217 -4.73164
C -1.17339 -5.00300 2.24994
H -1.46698 -5.74931 1.48987
H -2.09164 -4.61405 2.71576
H -0.59663 -5.52772 3.03279
N 4.66589 0.10647 -1.81652
N 4.87791 -0.96801 0.06044
C 6.04748 -0.02132 -1.58697
C 6.18125 -0.70395 -0.39427
C 3.94263 -0.46076 -0.80062
Cu 2.01545 -0.23225 -0.39882
C 3.97451 0.84678 -2.90284
H 2.91247 0.59397 -2.72943
C 7.43867 -1.13922 0.29439
H 7.44847 -0.86104 1.36125
H 8.30921 -0.65674 -0.17703
H 7.59600 -2.23094 0.23349
C 7.12490 0.46452 -2.50796
H 7.19316 -0.13599 -3.43286
H 8.10235 0.40013 -2.00470
H 6.98006 1.51658 -2.80476
C 4.45454 -1.57128 1.35254
H 3.35766 -1.65349 1.24117
C 4.35611 0.34284 -4.30376
H 5.38196 0.62488 -4.59054
H 3.67317 0.79100 -5.04454
H 4.25634 -0.75282 -4.37046
C 4.12642 2.36645 -2.72498
H 3.78945 2.66394 -1.71883
H 3.50481 2.88802 -3.47265
H 5.16796 2.70079 -2.86764
C 5.01272 -2.98724 1.56004
H 4.84076 -3.61721 0.67188
H 4.48905 -3.45061 2.41215
H 6.09018 -2.98867 1.79208
C 4.72384 -0.61812 2.52713
H 5.80197 -0.49270 2.72666
H 4.25168 -1.02559 3.43621
H 4.27494 0.36628 2.31831
C 2.16199 1.43766 0.53242
C 2.48848 2.54717 1.00181
H -0.25918 1.09433 1.12304
C 2.82834 3.82284 1.54876
C 3.45209 3.93437 2.82198
C 2.55477 5.02333 0.83696
C 3.78434 5.18662 3.35312
C 2.89300 6.27125 1.37447
C 3.50947 6.36300 2.63447
H 3.66684 3.02015 3.38400
H 2.06914 4.95590 -0.14161
H 4.26319 5.24550 4.33709
H 2.67149 7.18140 0.80568
H 3.77174 7.34064 3.05235

**TS2(E-P)$_{Ph}$**
SCF (BP86) Energy = -2956.28351390
Enthalpy 0K = -2954.950760
Enthalpy 298K = -2954.862891
Free Energy 298K = -2955.079964
Lowest Frequency = -28.5763 $cm^{-1}$
Second Frequency = 9.2527 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2956.74211890
SCF (C6H6) Energy = -2956.29012861
SCF (BS2) Energy = -3768.63259723

Si -3.70980 -2.89551 -0.77897
Al -1.42647 -0.94223 0.22934
Si -3.19674 -1.58306 2.87910
N -1.62267 -1.19582 2.05842
N -2.88369 -1.28965 -0.89344
C -0.47728 -1.18320 2.95448
C -4.52991 0.30519 -1.90940
C -3.31637 -0.45609 -1.99863
C 0.31606 -2.36132 3.14950
C -0.17288 -0.01162 3.72232
C -4.05555 -3.13367 2.14377
H -3.30269 -3.94501 2.13067
H -4.77458 -3.42583 2.93798
C -2.01299 2.58696 -1.16077
H -2.13934 2.22338 -2.18889
C -1.29837 -1.22647 -3.45675
H -1.06211 -1.74785 -2.51472
C -2.57184 -0.41280 -3.22317
C -5.41525 0.32862 -0.66107
H -4.92910 -0.31610 0.08789
C 0.41283 -1.19421 -0.40854
C -0.94814 1.30242 3.59090
H -1.68113 1.17036 2.77566
C -2.71319 3.84578 -0.86335
C 0.87629 -0.05376 4.66197
H 1.09232 0.84396 5.25236
C -4.79683 -3.19615 -2.31114
H -5.55781 -2.41728 -2.46668
H -5.31250 -4.16618 -2.19788
H -4.18515 -3.24385 -3.22674
C 1.98186 -3.01304 -1.55181
C -1.20927 1.87497 -0.32755
H -0.97898 2.18740 0.69403
C 1.40797 -1.85318 -0.88878
C -3.03104 0.38725 -4.28955
H -2.45168 0.40955 -5.21990
C 0.08290 -3.66384 2.38140
H -0.61048 -3.42837 1.55518
C 3.37616 -3.25336 -1.58800
H 4.04055 -2.53278 -1.10378
C -4.23665 5.60905 -1.63090
H -4.88444 6.02242 -2.41141
C -3.55586 4.40503 -1.85516
H -3.67870 3.86948 -2.80306
C -4.94906 1.07546 -3.01218
H -5.88049 1.64769 -2.93095

| | | | |
|---|---|---|---|
| C | -4.21190 | 1.13024 | -4.19923 |
| H | -4.55834 | 1.73343 | -5.04550 |
| C | -2.43096 | -4.31314 | -0.75107 |
| H | -2.01756 | -4.46896 | -1.76178 |
| H | -2.91985 | -5.25473 | -0.44293 |
| H | -1.58624 | -4.14342 | -0.06345 |
| C | -5.53119 | 1.74704 | -0.05991 |
| H | -4.54567 | 2.16213 | 0.20107 |
| H | -6.15166 | 1.72778 | 0.85335 |
| H | -6.00424 | 2.44890 | -0.76875 |
| C | -4.38387 | -0.09335 | 2.85213 |
| H | -4.17263 | 0.58234 | 3.69718 |
| H | -5.43316 | -0.42601 | 2.94220 |
| H | -4.29172 | 0.49405 | 1.92742 |
| C | -2.56499 | 4.54566 | 0.36003 |
| H | -1.89689 | 4.15233 | 1.13236 |
| C | 1.35135 | -2.34732 | 4.10590 |
| H | 1.93686 | -3.26034 | 4.26342 |
| C | -4.79275 | -3.06737 | 0.78696 |
| H | -5.54727 | -2.25987 | 0.79487 |
| H | -5.37004 | -4.00338 | 0.63381 |
| C | -0.08988 | -0.33027 | -3.80867 |
| H | -0.24044 | 0.19231 | -4.77041 |
| H | 0.82326 | -0.94441 | -3.89903 |
| H | 0.09170 | 0.43177 | -3.03307 |
| C | -2.89708 | -2.02783 | 4.70891 |
| H | -2.40991 | -3.00692 | 4.83721 |
| H | -3.87787 | -2.07023 | 5.21593 |
| H | -2.27627 | -1.28309 | 5.22959 |
| C | 1.12354 | -3.94940 | -2.18459 |
| H | 0.04470 | -3.77839 | -2.15574 |
| C | -6.83316 | -0.22936 | -0.92798 |
| H | -7.37117 | 0.38260 | -1.67364 |
| H | -7.43039 | -0.21622 | 0.00122 |
| H | -6.81405 | -1.26626 | -1.30061 |
| C | -4.08780 | 6.28367 | -0.40823 |
| H | -4.61683 | 7.22579 | -0.22990 |
| C | -1.49697 | -2.29758 | -4.55481 |
| H | -2.31996 | -2.98937 | -4.30806 |
| H | -0.57608 | -2.89389 | -4.68178 |
| H | -1.73511 | -1.83525 | -5.52928 |
| C | -0.01380 | 2.47749 | 3.22379 |
| H | 0.68934 | 2.69891 | 4.04667 |
| H | -0.60139 | 3.39817 | 3.05328 |
| H | 0.58634 | 2.27088 | 2.32249 |
| C | 3.89201 | -4.38859 | -2.22797 |
| H | 4.97412 | -4.55919 | -2.23702 |
| C | 1.38562 | -4.22513 | 1.77097 |
| H | 2.06118 | -4.61784 | 2.55191 |
| H | 1.92794 | -3.45407 | 1.20403 |
| H | 1.16122 | -5.06004 | 1.08469 |
| C | -3.24778 | 5.74637 | 0.58429 |
| H | -3.11745 | 6.27339 | 1.53537 |
| C | 1.63433 | -1.21023 | 4.86922 |
| H | 2.42920 | -1.22815 | 5.62324 |
| C | -1.72537 | 1.65421 | 4.88196 |
| H | -2.43317 | 0.86328 | 5.17782 |
| H | -2.29773 | 2.58871 | 4.74350 |
| H | -1.03294 | 1.81251 | 5.72806 |
| C | 1.64449 | -5.07693 | -2.83147 |
| H | 0.96280 | -5.78516 | -3.31459 |
| C | 3.03129 | -5.30378 | -2.85644 |
| H | 3.43673 | -6.18726 | -3.36051 |
| C | -0.57708 | -4.75483 | 3.25690 |
| H | -0.71316 | -5.68574 | 2.67776 |
| H | -1.56346 | -4.44621 | 3.63683 |
| H | 0.05815 | -4.99204 | 4.12906 |
| N | 4.83256 | 0.27053 | -1.67983 |
| N | 5.00591 | -0.23069 | 0.42839 |
| C | 6.19015 | 0.42252 | -1.34607 |
| C | 6.29956 | 0.10485 | -0.00662 |
| C | 4.09945 | -0.11579 | -0.59114 |
| Cu | 2.13569 | -0.08828 | -0.36890 |
| C | 4.15523 | 0.58303 | -2.96534 |
| H | 3.12362 | 0.22884 | -2.78739 |
| C | 7.53092 | 0.06717 | 0.84606 |
| H | 7.39828 | 0.61253 | 1.79522 |
| H | 8.36993 | 0.54011 | 0.31201 |
| H | 7.84013 | -0.96370 | 1.09514 |
| C | 7.27592 | 0.81170 | -2.30245 |
| H | 7.51078 | 0.00889 | -3.02416 |
| H | 8.20099 | 1.03163 | -1.74683 |
| H | 7.02047 | 1.71472 | -2.88118 |
| C | 4.54247 | -0.53752 | 1.80840 |
| H | 3.48588 | -0.82537 | 1.65669 |
| C | 4.73107 | -0.21335 | -4.14677 |
| H | 5.73271 | 0.13642 | -4.44474 |
| H | 4.06787 | -0.09048 | -5.01914 |
| H | 4.78512 | -1.28837 | -3.90926 |
| C | 4.08864 | 2.09971 | -3.20724 |
| H | 3.62329 | 2.60010 | -2.34289 |
| H | 3.47280 | 2.30153 | -4.09994 |
| H | 5.08518 | 2.53866 | -3.38425 |
| C | 5.27095 | -1.73873 | 2.42997 |
| H | 5.28959 | -2.59638 | 1.73742 |
| H | 4.72735 | -2.04722 | 3.33789 |
| H | 6.30559 | -1.50087 | 2.72605 |
| C | 4.55075 | 0.71890 | 2.69259 |
| H | 5.57390 | 1.07408 | 2.90479 |
| H | 4.06287 | 0.48601 | 3.65346 |
| H | 3.97855 | 1.52300 | 2.20226 |
| C | 1.96147 | 1.76560 | 0.07601 |
| C | 2.07438 | 2.99886 | 0.22601 |
| H | -0.55392 | 1.09798 | -0.74474 |
| C | 2.14925 | 4.41666 | 0.39684 |
| C | 3.13599 | 5.00709 | 1.23268 |
| C | 1.23611 | 5.28102 | -0.26723 |
| C | 3.20379 | 6.39641 | 1.39461 |
| C | 1.31307 | 6.66955 | -0.10241 |
| C | 2.29537 | 7.23681 | 0.72796 |
| H | 3.84589 | 4.35436 | 1.75077 |
| H | 0.46610 | 4.84019 | -0.90745 |
| H | 3.97268 | 6.82786 | 2.04557 |
| H | 0.59677 | 7.31418 | -0.62374 |
| H | 2.35189 | 8.32311 | 0.85528 |

**INT2(E-P)$_{Ph}$**

SCF (BP86) Energy = -2646.66192283
Enthalpy 0K = -2645.460543
Enthalpy 298K = -2645.379925
Free Energy 298K = -2645.582936
Lowest Frequency = 6.4462 $cm^{-1}$
Second Frequency = 12.1534 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2647.06108760
SCF (C6H6) Energy = -2646.66853118
SCF (BS2) Energy = -3458.93966499

| | | | |
|---|---|---|---|
| Si | 4.10531 | 1.58850 | 1.90891 |
| Al | 1.88264 | 0.01677 | 0.18448 |
| Si | 4.40751 | 0.35696 | -1.84883 |
| N | 3.01229 | -0.55273 | -1.14638 |
| N | 2.39851 | 1.31754 | 1.37403 |
| C | 2.72157 | -1.85946 | -1.70767 |
| C | 1.02922 | 3.39637 | 1.48854 |
| C | 1.37060 | 2.11382 | 2.02280 |
| C | 3.29581 | -3.02974 | -1.11825 |
| C | 1.87611 | -1.99460 | -2.85230 |
| C | 5.67691 | 0.89072 | -0.52153 |
| H | 6.01273 | -0.01130 | 0.02500 |
| H | 6.55925 | 1.21057 | -1.11488 |
| C | 1.08527 | 0.32951 | 3.89429 |
| H | 1.77201 | -0.21246 | 3.22055 |
| C | 0.71776 | 1.64749 | 3.20701 |
| C | 1.73015 | 3.97956 | 0.25985 |
| H | 2.58334 | 3.31630 | 0.03500 |
| C | 0.24408 | -0.97057 | 0.39334 |
| C | 1.22424 | -0.79644 | -3.54449 |
| H | 1.46763 | 0.10112 | -2.95052 |
| C | 1.62618 | -3.28168 | -3.36969 |
| H | 0.98096 | -3.38173 | -4.25014 |
| C | 4.16955 | 3.05383 | 3.11861 |
| H | 4.02456 | 4.01414 | 2.59813 |
| H | 5.16202 | 3.07803 | 3.60190 |
| H | 3.40476 | 2.98474 | 3.90773 |

C -0.98406 -3.20530 1.13752
C -0.60920 -1.86993 0.71458
C -0.27490 2.45382 3.80088
H -0.76433 2.10243 4.71697
C 4.20354 -2.95207 0.11001
H 4.47621 -1.88980 0.23575
C -2.08201 -3.43506 2.00114
H -2.67300 -2.57961 2.34027
C 0.02204 4.15420 2.11495
H -0.24513 5.13081 1.69598
C -0.63336 3.69455 3.26253
H -1.40328 4.30738 3.74444
C 4.79258 0.04046 2.78488
H 4.25282 -0.16320 3.72397
H 5.85945 0.18618 3.03196
H 4.71887 -0.86024 2.15339
C 0.80427 3.98840 -0.97574
H 0.38121 2.99298 -1.18747
H 1.35048 4.34082 -1.86930
H -0.05309 4.66690 -0.82247
C 3.80697 1.91910 -2.75660
H 3.23840 1.66413 -3.66568
H 4.66638 2.54389 -3.05847
H 3.15297 2.53542 -2.11714
C 3.00375 -4.29367 -1.66752
H 3.44351 -5.18788 -1.21105
C 5.28564 2.01425 0.46512
H 4.87673 2.88728 -0.07789
H 6.19645 2.39396 0.97422
C -0.14000 -0.57580 4.14439
H -0.84189 -0.11889 4.86483
H 0.17838 -1.54506 4.56693
H -0.68360 -0.77343 3.20751
C 5.34194 -0.77725 -3.05577
H 5.83153 -1.61054 -2.52474
H 6.12681 -0.19616 -3.57076
H 4.68165 -1.21462 -3.82090
C -0.23400 -4.31728 0.67435
H 0.60481 -4.14780 -0.00797
C 2.28876 5.39817 0.51266
H 1.47814 6.13111 0.67143
H 2.86965 5.74055 -0.36180
H 2.94686 5.43567 1.39719
C 1.82786 0.58123 5.22869
H 2.74142 1.18196 5.08784
H 2.11703 -0.37510 5.70039
H 1.18175 1.12422 5.94155
C -0.31399 -0.92236 -3.58606
H -0.63166 -1.78240 -4.20337
H -0.76269 -0.01096 -4.01579
H -0.72833 -1.04335 -2.57197
C -2.40454 -4.73561 2.41119
H -3.24871 -4.89540 3.09074
C 3.45025 -3.39720 1.38496
H 3.13558 -4.45301 1.30795
H 2.53749 -2.79713 1.54880
H 4.09077 -3.29921 2.27955
C 2.17747 -4.42864 -2.78945
H 1.96924 -5.41854 -3.20975
C 1.77949 -0.58856 -4.97302
H 2.87297 -0.44449 -4.97536
H 1.31755 0.29833 -5.44177
H 1.55880 -1.45924 -5.61631
C -0.57482 -5.61547 1.07692
H 0.00991 -6.46442 0.70667
C -1.65508 -5.83168 1.94944
H -1.91440 -6.84791 2.26439
C 5.51324 -3.75316 -0.05260
H 6.17575 -3.58391 0.81437
H 6.05995 -3.45764 -0.96399
H 5.32747 -4.84004 -0.11327
N -4.39262 -0.18469 1.23890
N -4.37221 -1.62026 -0.39304
C -5.72405 -0.59611 1.05613
C -5.71172 -1.50678 0.01844
C -3.56037 -0.80201 0.34395
Cu -1.67078 -0.33019 0.02272
C -3.86984 0.86763 2.15152
H -2.77570 0.79909 2.01010
C -6.86108 -2.27485 -0.55942
H -6.89363 -2.21573 -1.66004
H -7.81088 -1.86345 -0.18326
H -6.83500 -3.34432 -0.28413
C -6.88851 -0.14234 1.88266
H -6.86549 -0.55679 2.90644
H -7.82918 -0.47579 1.41708
H -6.93800 0.95559 1.96954
C -3.82393 -2.38428 -1.54347
H -2.73301 -2.26808 -1.41483
C -4.17722 0.57699 3.62866
H -5.23899 0.73274 3.87979
H -3.58500 1.26395 4.25523
H -3.89910 -0.45470 3.90061
C -4.29798 2.27061 1.69515
H -4.00229 2.42805 0.64571
H -3.77999 3.02230 2.31378
H -5.38410 2.43440 1.79995
C -4.14708 -3.88465 -1.47374
H -3.89336 -4.29605 -0.48350
H -3.54133 -4.41497 -2.22718
H -5.20531 -4.10106 -1.69202
C -4.20998 -1.72467 -2.87772
H -5.29313 -1.79085 -3.07707
H -3.68627 -2.23259 -3.70480
H -3.91288 -0.66381 -2.87732
C -1.84743 1.29358 -0.96577
C -2.21785 2.24637 -1.67931
C -2.62164 3.35830 -2.47961
C -2.70937 3.25565 -3.89518
C -2.95499 4.60711 -1.88500
C -3.11061 4.34837 -4.67331
C -3.35493 5.69530 -2.67054
C -3.43612 5.57506 -4.06867
H -2.45645 2.30187 -4.36927
H -2.89165 4.70234 -0.79638
H -3.16950 4.24263 -5.76255
H -3.60577 6.64658 -2.18754
H -3.74895 6.42779 -4.68036

**$P_{Ph}$**
SCF (BP86) Energy = -2646.69404035
Enthalpy 0K = -2645.492058
Enthalpy 298K = -2645.412147
Free Energy 298K = -2645.608280
Lowest Frequency = 16.3582 $cm^{-1}$
Second Frequency = 17.5552 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2647.11270110
SCF (C6H6) Energy = -2646.69989499
SCF (BS2) Energy = -3458.96621035

Cu -1.42963 0.01380 0.05826
Si 4.17156 -1.57946 -1.38529
Al 1.61170 -0.07642 0.03465
Si 4.23190 0.90885 1.69007
N -4.03653 -1.18045 -0.71856
N 2.47090 -1.52975 -0.81236
N -4.34677 0.78397 0.16599
N 2.69936 1.24441 0.82790
C -3.36597 -0.10875 -0.18231
C 0.15885 -0.76305 1.24721
C 1.10220 -1.75597 -3.47206
H 1.63614 -0.89193 -3.04108
C 0.96345 -2.79828 -2.35904
C -0.90571 -0.98596 1.89732
C 2.20695 2.60184 0.84823
C -1.70160 -1.40609 3.02826
C 1.51121 -3.74057 -0.14559
C 5.59222 0.17927 0.55688
H 5.74878 0.88644 -0.28059
H 6.51792 0.24714 1.16717
C -1.65955 2.29636 -2.30178
C 5.42675 -1.26142 0.02464
H 5.19414 -1.96027 0.85124
H 6.39321 -1.61772 -0.39101

| | | | |
|---|---|---|---|
| C | 1.64530 | -2.67683 | -1.10097 |
| C | 3.94924 | -0.32011 | 3.12593 |
| H | 3.33547 | 0.13233 | 3.92267 |
| H | 4.91067 | -0.63152 | 3.57201 |
| H | 3.43050 | -1.23141 | 2.78194 |
| C | -1.03277 | -1.70163 | 4.24722 |
| H | 0.05474 | -1.59620 | 4.29058 |
| C | 0.04691 | -4.97239 | -1.68085 |
| H | -0.54881 | -5.86316 | -1.91104 |
| C | -4.00368 | 2.07705 | 0.81968 |
| H | -2.90196 | 2.10346 | 0.74082 |
| C | 1.39285 | 3.08412 | 1.92656 |
| C | 4.60161 | -3.30620 | -2.09078 |
| H | 5.04034 | -3.96460 | -1.32298 |
| H | 5.35446 | -3.18989 | -2.89031 |
| H | 3.73009 | -3.82713 | -2.51727 |
| C | -3.29561 | -2.38190 | -1.19792 |
| H | -2.23781 | -2.06788 | -1.12739 |
| C | 0.71303 | -4.85896 | -0.45508 |
| H | 0.62792 | -5.66878 | 0.27909 |
| C | -2.73895 | 1.81863 | -3.08438 |
| H | -2.95079 | 0.74585 | -3.09798 |
| C | -3.82332 | -1.96200 | 4.11754 |
| H | -4.91275 | -2.06139 | 4.06235 |
| C | 0.97935 | 2.20397 | 3.10893 |
| H | 1.29511 | 1.17322 | 2.87373 |
| C | -3.15046 | -2.25564 | 5.31442 |
| H | -3.70995 | -2.58473 | 6.19605 |
| C | -5.42451 | -0.97029 | -0.69489 |
| C | -0.80745 | 1.41137 | -1.54639 |
| C | -0.26073 | -1.25466 | -3.99520 |
| H | -0.82821 | -2.06091 | -4.49449 |
| H | -0.11452 | -0.44887 | -4.73611 |
| H | -0.87457 | -0.85075 | -3.17468 |
| C | -5.62160 | 0.27658 | -0.13292 |
| C | 1.93451 | -2.30514 | -4.65568 |
| H | 2.93268 | -2.64547 | -4.33720 |
| H | 2.06773 | -1.52952 | -5.43139 |
| H | 1.42654 | -3.16575 | -5.12776 |
| C | 0.18261 | -3.94323 | -2.61999 |
| H | -0.30762 | -4.03786 | -3.59690 |
| C | 2.25050 | -3.73346 | 1.19397 |
| H | 2.69725 | -2.72961 | 1.30217 |
| C | -3.11063 | -1.53791 | 2.98665 |
| H | -3.63567 | -1.30080 | 2.05828 |
| C | -1.75252 | -2.12035 | 5.37239 |
| H | -1.21695 | -2.34314 | 6.30129 |
| C | -1.38814 | 3.68949 | -2.28360 |
| H | -0.55492 | 4.05894 | -1.67738 |
| C | 0.21847 | 0.87585 | -1.04698 |
| C | 2.53766 | 3.51013 | -0.21047 |
| C | -2.17603 | 4.57024 | -3.03653 |
| H | -1.95396 | 5.64246 | -3.01627 |
| C | -3.59047 | -2.70742 | -2.66969 |
| H | -2.84750 | -3.44283 | -3.01781 |
| H | -3.50099 | -1.81172 | -3.30546 |
| H | -4.59121 | -3.14627 | -2.81294 |
| C | 3.42160 | 3.09489 | -1.38415 |
| H | 3.71834 | 2.05100 | -1.18832 |
| C | -3.24084 | 4.08646 | -3.81634 |
| H | -3.85071 | 4.77887 | -4.40592 |
| C | 0.94850 | 4.42207 | 1.91892 |
| H | 0.33956 | 4.78245 | 2.75678 |
| C | 4.53475 | -0.32686 | -2.78132 |
| H | 4.02328 | -0.61050 | -3.71558 |
| H | 5.62084 | -0.30883 | -2.98594 |
| H | 4.22558 | 0.69852 | -2.52841 |
| C | 1.31351 | -3.98117 | 2.39509 |
| H | 0.90454 | -5.00774 | 2.38745 |
| H | 0.46666 | -3.27940 | 2.39407 |
| H | 1.86753 | -3.86104 | 3.34348 |
| C | -6.91538 | 0.99869 | 0.09130 |
| H | -6.99067 | 1.42052 | 1.10687 |
| H | -7.75825 | 0.30160 | -0.03655 |
| H | -7.06298 | 1.82607 | -0.62496 |
| C | 2.65628 | 3.13259 | -2.72584 |
| H | 1.76259 | 2.48831 | -2.69246 |
| H | 3.30084 | 2.78635 | -3.55377 |
| H | 2.32673 | 4.15894 | -2.96922 |
| C | 4.97730 | 2.52348 | 2.37964 |
| H | 5.42971 | 3.12486 | 1.57321 |
| H | 5.77505 | 2.28167 | 3.10384 |
| H | 4.23456 | 3.15951 | 2.88507 |
| C | -0.55207 | 2.19291 | 3.30949 |
| H | -0.93016 | 3.18695 | 3.60967 |
| H | -0.83418 | 1.47681 | 4.10094 |
| H | -1.06933 | 1.89366 | 2.38275 |
| C | -3.51728 | 2.70820 | -3.83743 |
| H | -4.34202 | 2.32335 | -4.44691 |
| C | -4.55899 | 3.29203 | 0.06061 |
| H | -5.64754 | 3.40606 | 0.19016 |
| H | -4.32862 | 3.23002 | -1.01453 |
| H | -4.08398 | 4.20415 | 0.45762 |
| C | 1.66719 | 2.63505 | 4.42570 |
| H | 2.76544 | 2.58145 | 4.35494 |
| H | 1.34902 | 1.98589 | 5.26156 |
| H | 1.40098 | 3.67436 | 4.69054 |
| C | -3.48150 | -3.59301 | -0.27024 |
| H | -4.49705 | -4.01979 | -0.33461 |
| H | -3.27615 | -3.32496 | 0.77775 |
| H | -2.76317 | -4.37524 | -0.56557 |
| C | 3.39693 | -4.77144 | 1.21646 |
| H | 3.93953 | -4.73025 | 2.17801 |
| H | 4.12238 | -4.60004 | 0.40649 |
| H | 3.00143 | -5.79647 | 1.09803 |
| C | 4.70858 | 3.94513 | -1.47671 |
| H | 4.47957 | 5.00421 | -1.69266 |
| H | 5.35983 | 3.57487 | -2.28857 |
| H | 5.28465 | 3.91607 | -0.53667 |
| C | -4.37302 | 2.07443 | 2.31231 |
| H | -3.96954 | 2.98358 | 2.78778 |
| H | -3.94204 | 1.19987 | 2.82472 |
| H | -5.46486 | 2.07329 | 2.47090 |
| C | 2.05420 | 4.83282 | -0.17920 |
| H | 2.32089 | 5.51396 | -0.99662 |
| C | -6.45228 | -1.92494 | -1.22220 |
| H | -6.46840 | -1.95802 | -2.32597 |
| H | -7.45540 | -1.61394 | -0.89098 |
| H | -6.29206 | -2.95379 | -0.86086 |
| C | 1.26536 | 5.30042 | 0.87762 |
| H | 0.91107 | 6.33714 | 0.89479 |

**TS(1,1)$_{Ph}$**

SCF (BP86) Energy = -2647.82234971
Enthalpy 0K = -2646.604752
Enthalpy 298K = -2646.524536
Free Energy 298K = -2646.722522
Lowest Frequency = -523.2578 $cm^{-1}$
Second Frequency = 11.1792 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2648.24372376
SCF (C6H6) Energy = -2647.82765950
SCF (BS2) Energy = -3460.09509483

| | | | |
|---|---|---|---|
| Cu | -1.73362 | -0.23841 | -0.09446 |
| Si | 3.78201 | 1.37928 | 2.10249 |
| Al | 1.71930 | -0.09779 | 0.06667 |
| Si | 4.41782 | -2.01070 | 0.12845 |
| N | -4.68117 | 0.54871 | 0.00431 |
| N | 2.66562 | 1.40891 | 0.70121 |
| N | -4.34372 | -1.46032 | -0.75660 |
| N | 2.65605 | -1.74224 | -0.09053 |
| C | -3.69024 | -0.36251 | -0.25496 |
| H | 0.95344 | 0.21091 | -1.44704 |
| C | 0.60460 | 3.19939 | 1.99363 |
| H | 0.85225 | 2.15026 | 2.22649 |
| C | 1.42085 | 3.59020 | 0.75977 |
| C | 1.85010 | -2.83006 | -0.58877 |
| C | 2.97526 | 3.11780 | -1.08954 |
| C | 5.01442 | -1.32985 | 1.81471 |
| H | 4.31578 | -1.66124 | 2.60633 |
| H | 5.96086 | -1.87528 | 2.01279 |
| C | -1.76375 | -0.40720 | 3.08177 |
| C | 5.26956 | 0.19303 | 1.89677 |
| H | 5.86842 | 0.53322 | 1.03085 |

| | | | |
|---|---|---|---|
| H | 5.89565 | 0.41946 | 2.78622 |
| C | 2.34673 | 2.69399 | 0.12764 |
| C | 5.54839 | -1.19686 | -1.18280 |
| H | 5.42077 | -1.64363 | -2.18120 |
| H | 6.59904 | -1.36062 | -0.87824 |
| H | 5.39751 | -0.11063 | -1.27299 |
| C | 1.86138 | 5.29644 | -0.94917 |
| H | 1.69714 | 6.30455 | -1.34596 |
| C | -3.58230 | -2.66337 | -1.19051 |
| H | -2.55672 | -2.44530 | -0.83918 |
| C | 1.77855 | -3.11985 | -1.99554 |
| C | 4.55936 | 3.10080 | 2.35883 |
| H | 5.28077 | 3.32284 | 1.55409 |
| H | 5.10775 | 3.12256 | 3.31689 |
| H | 3.81794 | 3.91407 | 2.36639 |
| C | -4.36031 | 1.88685 | 0.57013 |
| H | -3.27486 | 1.81527 | 0.75806 |
| C | 2.72142 | 4.40494 | -1.60005 |
| H | 3.22363 | 4.71686 | -2.52355 |
| C | -3.08435 | -0.90821 | 3.17282 |
| H | -3.58126 | -1.24492 | 2.25844 |
| C | 2.62037 | -2.37295 | -3.03488 |
| H | 3.09217 | -1.52071 | -2.51740 |
| C | -5.94240 | 0.03807 | -0.34498 |
| C | -1.03470 | -0.35605 | 1.83115 |
| C | -0.91036 | 3.26134 | 1.69346 |
| H | -1.24395 | 4.29880 | 1.51036 |
| H | -1.48921 | 2.86355 | 2.54612 |
| H | -1.15597 | 2.66502 | 0.79904 |
| C | -5.72708 | -1.23750 | -0.82969 |
| C | 0.92293 | 4.06864 | 3.23132 |
| H | 1.98333 | 4.00166 | 3.52342 |
| H | 0.31174 | 3.75123 | 4.09560 |
| H | 0.69776 | 5.13341 | 3.04068 |
| C | 1.21300 | 4.87458 | 0.21657 |
| H | 0.52038 | 5.55750 | 0.72338 |
| C | 3.93951 | 2.21421 | -1.85207 |
| H | 3.94279 | 1.24762 | -1.32132 |
| C | -1.11913 | 0.02684 | 4.26971 |
| H | -0.09413 | 0.40440 | 4.20902 |
| C | 0.00025 | -0.30310 | 1.09244 |
| C | 1.09369 | -3.64946 | 0.31936 |
| C | -1.78224 | -0.03669 | 5.50167 |
| H | -1.26914 | 0.30302 | 6.40766 |
| C | -5.05440 | 2.13509 | 1.91902 |
| H | -4.62811 | 3.04354 | 2.37585 |
| H | -4.88500 | 1.29635 | 2.61290 |
| H | -6.13881 | 2.30031 | 1.81061 |
| C | 1.16028 | -3.46056 | 1.83763 |
| H | 1.50126 | -2.42588 | 2.01582 |
| C | -3.09338 | -0.53691 | 5.57982 |
| H | -3.60699 | -0.58829 | 6.54542 |
| C | 0.95597 | -4.17177 | -2.44914 |
| H | 0.91438 | -4.38552 | -3.52363 |
| C | 2.88671 | 0.81285 | 3.69723 |
| H | 2.17855 | 1.57494 | 4.06226 |
| H | 3.61478 | 0.61295 | 4.50350 |
| H | 2.32189 | -0.11927 | 3.52008 |
| C | 3.47284 | 1.95591 | -3.30111 |
| H | 3.46425 | 2.88469 | -3.89948 |
| H | 2.45550 | 1.53163 | -3.32093 |
| H | 4.15273 | 1.24500 | -3.80354 |
| C | -6.73847 | -2.23164 | -1.31407 |
| H | -6.45183 | -2.68533 | -2.27693 |
| H | -7.70939 | -1.73398 | -1.46343 |
| H | -6.89982 | -3.05326 | -0.59383 |
| C | -0.20340 | -3.64823 | 2.53498 |
| H | -0.99403 | -3.05835 | 2.04606 |
| H | -0.13887 | -3.32325 | 3.58762 |
| H | -0.51718 | -4.70800 | 2.54462 |
| C | 4.82638 | -3.88375 | 0.06019 |
| H | 5.07393 | -4.28179 | 1.05870 |
| H | 5.71012 | -4.04370 | -0.58171 |
| H | 3.99968 | -4.48735 | -0.34683 |
| C | 1.79704 | -1.80868 | -4.21400 |
| H | 1.31079 | -2.61203 | -4.79634 |
| H | 2.45881 | -1.25924 | -4.90636 |
| H | 1.01337 | -1.11381 | -3.87358 |
| C | -3.73841 | -0.97490 | 4.41102 |
| H | -4.75689 | -1.37484 | 4.46410 |
| C | -4.04961 | -3.94660 | -0.48617 |
| H | -5.01801 | -4.31061 | -0.86576 |
| H | -4.12976 | -3.79736 | 0.60309 |
| H | -3.30340 | -4.73770 | -0.66537 |
| C | 3.73712 | -3.29466 | -3.58312 |
| H | 4.36058 | -3.71291 | -2.77640 |
| H | 4.39502 | -2.74230 | -4.27817 |
| H | 3.30316 | -4.14497 | -4.13967 |
| C | -4.58979 | 3.01731 | -0.44529 |
| H | -5.66118 | 3.19405 | -0.63961 |
| H | -4.08775 | 2.80080 | -1.40090 |
| H | -4.16974 | 3.95332 | -0.04155 |
| C | 5.38110 | 2.77069 | -1.83214 |
| H | 6.07466 | 2.08230 | -2.34767 |
| H | 5.74532 | 2.91291 | -0.80044 |
| H | 5.43938 | 3.74856 | -2.34312 |
| C | 2.19101 | -4.41641 | 2.48369 |
| H | 1.91912 | -5.47015 | 2.29121 |
| H | 2.22052 | -4.26958 | 3.57844 |
| H | 3.20483 | -4.25506 | 2.09014 |
| C | -3.52806 | -2.78222 | -2.72109 |
| H | -2.85275 | -3.61008 | -2.99421 |
| H | -3.12308 | -1.85265 | -3.15323 |
| H | -4.51699 | -2.99343 | -3.16222 |
| C | 0.29337 | -4.69158 | -0.19073 |
| H | -0.26916 | -5.31876 | 0.50966 |
| C | -7.24634 | 0.75720 | -0.17761 |
| H | -7.55036 | 0.83842 | 0.88104 |
| H | -8.04378 | 0.20924 | -0.70346 |
| H | -7.22003 | 1.77676 | -0.59519 |
| C | 0.21087 | -4.95662 | -1.56313 |
| H | -0.40881 | -5.78050 | -1.93502 |
| C | -1.73142 | 1.62221 | -2.81414 |
| C | -0.96030 | 2.73585 | -2.38991 |
| H | -0.11116 | 2.58040 | -1.71584 |
| C | -1.40643 | 0.27247 | -2.39253 |
| C | -2.81407 | 1.84465 | -3.70189 |
| H | -3.40416 | 0.98451 | -4.03464 |
| C | -0.46573 | -0.43627 | -1.85907 |
| C | -3.11129 | 3.13644 | -4.15906 |
| H | -3.94372 | 3.29044 | -4.85428 |
| C | -2.34318 | 4.23097 | -3.72515 |
| H | -2.57749 | 5.24049 | -4.07986 |
| C | -1.27043 | 4.02611 | -2.83912 |
| H | -0.65916 | 4.86810 | -2.49860 |
| H | -0.14894 | -1.47638 | -1.80710 |

**1,1$_{Ph}$**

SCF (BP86) Energy = -2647.88456029
Enthalpy 0K = -2646.661133
Enthalpy 298K = -2646.581118
Free Energy 298K = -2646.777076
Lowest Frequency = 10.6893 $cm^{-1}$
Second Frequency = 15.5103 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2648.30895512
SCF (C6H6) Energy = -2647.88972898
SCF (BS2) Energy = -3460.15716635

| | | | |
|---|---|---|---|
| Cu | -1.74975 | 0.25633 | -0.22410 |
| Si | 3.98142 | 0.56169 | 1.97357 |
| Al | 1.54701 | -0.21958 | 0.01935 |
| Si | 4.04587 | -2.28423 | -0.71673 |
| N | -4.67836 | 0.89163 | 0.22314 |
| N | 2.73901 | 1.03674 | 0.75550 |
| N | -4.38296 | -0.53646 | -1.38854 |
| N | 2.30771 | -1.90059 | -0.45737 |
| C | -3.70092 | 0.20037 | -0.44971 |
| H | 1.32616 | 0.98335 | -2.62591 |
| C | 0.79893 | 2.63927 | 2.39751 |
| H | 0.91301 | 1.54343 | 2.34034 |
| C | 1.73811 | 3.25293 | 1.35589 |
| C | 1.36044 | -2.97462 | -0.66795 |
| C | 3.46987 | 3.13398 | -0.39378 |
| C | 5.14086 | -1.91174 | 0.80890 |

H  4.71878 -2.48109  1.65999
H  6.09886 -2.42216  0.57211
C -2.18095 -1.20018  2.58911
C  5.41906 -0.45248  1.22252
H  5.82822  0.12032  0.36883
H  6.21597 -0.42846  1.99546
C  2.63045  2.46375  0.55766
C  4.77131 -1.37205 -2.23111
H  4.38954 -1.80544 -3.17074
H  5.87180 -1.47179 -2.24049
H  4.53205 -0.29735 -2.23683
C  2.55185  5.30430  0.28282
H  2.52858  6.39523  0.18706
C -3.64574 -1.39466 -2.35202
H -2.60318 -1.32874 -1.98872
C  0.81069 -3.24356 -1.96944
C  4.79311  2.10476  2.74456
H  5.39033  2.67166  2.01264
H  5.46986  1.77895  3.55453
H  4.05796  2.80269  3.17377
C -4.32259  1.83394  1.31622
H -3.24454  1.64185  1.45890
C  3.41446  4.53769 -0.50752
H  4.07072  5.03702 -1.23059
C -3.30470 -2.02042  2.31617
H -3.50381 -2.30980  1.28043
C  1.33225 -2.58080 -3.25199
H  1.97874 -1.73830 -2.95010
C -5.95359  0.60444 -0.29174
C -1.29273 -0.75869  1.54071
C -0.67870  2.97202  2.09512
H -0.87532  4.05630  2.17633
H -1.33896  2.45624  2.81589
H -0.95872  2.65300  1.07707
C -5.76640 -0.30464 -1.31398
C  1.14759  3.08277  3.83750
H  2.17097  2.79020  4.12369
H  0.45067  2.62501  4.56283
H  1.07058  4.17912  3.95024
C  1.72023  4.65296  1.19909
H  1.03877  5.24644  1.82003
C  4.44200  2.37805 -1.29981
H  4.31943  1.30863 -1.06055
C -1.93281 -0.81919  3.93429
H -1.06348 -0.19238  4.15463
C -0.20953 -0.49544  0.92635
C  0.95920 -3.81529  0.42484
C -2.78211 -1.24553  4.96406
H -2.57370 -0.94097  5.99540
C -5.03629  1.50759  2.63768
H -4.56577  2.08835  3.44824
H -4.93983  0.43878  2.88644
H -6.10453  1.77856  2.61893
C  1.65644 -3.77705  1.78704
H  2.41777 -2.98038  1.73082
C -3.88771 -2.06559  4.68188
H -4.54603 -2.40162  5.48963
C -0.18527 -4.23285 -2.11002
H -0.59437 -4.43419 -3.10737
C  3.17884 -0.44087  3.38353
H  2.52141  0.20538  3.98935
H  3.95122 -0.86095  4.05230
H  2.56868 -1.27853  3.00945
C  4.11516  2.57879 -2.79738
H  4.24846  3.63276 -3.10045
H  3.07517  2.29654 -3.03071
H  4.78448  1.96588 -3.42713
C -6.80384 -0.97283 -2.16432
H -6.57083 -0.91374 -3.24034
H -7.77949 -0.48448 -2.01485
H -6.93150 -2.04021 -1.91041
C  0.70686 -3.44857  2.95721
H  0.23690 -2.46338  2.82907
H  1.26051 -3.44874  3.91325
H -0.10064 -4.19739  3.04320
C  4.29198 -4.15962 -1.01625
H  4.62032 -4.66031 -0.08994
H  5.08280 -4.31471 -1.77095
H  3.38090 -4.66890 -1.36648
C  0.21412 -2.03375 -4.16886
H -0.40265 -2.85156 -4.58296
H  0.65359 -1.49431 -5.02627
H -0.45395 -1.33564 -3.63922
C -4.14020 -2.45354  3.35362
H -4.99643 -3.09740  3.12449
C -4.07579 -2.86804 -2.28357
H -5.06527 -3.04109 -2.73751
H -4.09555 -3.22657 -1.24183
H -3.34223 -3.48036 -2.83260
C  2.20403 -3.56953 -4.06574
H  3.05551 -3.94904 -3.48006
H  2.60206 -3.08032 -4.97314
H  1.60679 -4.44119 -4.38822
C -4.48622  3.29993  0.88159
H -5.54250  3.57055  0.71327
H -3.91758  3.50217 -0.04008
H -4.09691  3.96028  1.67437
C  5.91602  2.76187 -1.03632
H  6.59126  2.17094 -1.68067
H  6.20696  2.58373  0.01183
H  6.09773  3.82932 -1.25540
C  2.38170 -5.11489  2.07189
H  1.65767 -5.93922  2.20200
H  2.97166 -5.04269  3.00311
H  3.06179 -5.39806  1.25313
C -3.68310 -0.81514 -3.77568
H -3.00833 -1.39744 -4.42462
H -3.34046  0.23195 -3.77928
H -4.69148 -0.85783 -4.22054
C -0.04564 -4.78166  0.22951
H -0.35303 -5.40413  1.07817
C -7.24287  1.16787  0.22416
H -7.52665  0.74192  1.20286
H -8.05838  0.93996 -0.48006
H -7.20651  2.26388  0.33755
C -0.63863 -4.98405 -1.02097
H -1.41597 -5.74473 -1.15316
C -0.78874  2.58289 -1.90711
C  0.22842  3.56253 -2.04175
H  1.25030  3.32297 -1.73491
C -0.53683  1.19230 -1.47369
C -2.11476  2.95632 -2.25268
H -2.91006  2.21408 -2.12800
C  0.63070  0.55428 -1.88565
C -2.40201  4.23019 -2.76292
H -3.42907  4.48274 -3.04986
C -1.37991  5.18646 -2.88784
H -1.60556  6.19003 -3.26430
C -0.06894  4.84858 -2.51053
H  0.73291  5.59138 -2.57818
H  0.60415 -0.54998 -1.90223

**TS(Z)$_{Ph}$**
SCF (BP86) Energy = -2647.81743667
Enthalpy 0K = -2646.600516
Enthalpy 298K = -2646.520189
Free Energy 298K = -2646.718656
Lowest Frequency = -557.6960 $cm^{-1}$
Second Frequency = 12.2297 $cm^{-1}$
SCF (BP86-D3BJ) Energy =  -2648.24208227
SCF (C6H6) Energy = -2647.82275374
SCF (BS2) Energy =  -3460.09023606

Cu  1.87521  0.15671 -0.04608
Si -3.81025 -1.03575  2.13600
Al -1.59533  0.17117  0.07297
Si -4.05936  2.39489  0.17795
N  4.61015 -1.04699 -0.46321
N -2.72988 -1.20555  0.71373
N  4.65813  1.12588 -0.53294
N -2.33799  1.91701 -0.04869
C  3.81609  0.06301 -0.32586
H -0.86038 -0.25556 -1.44524
C -0.81077 -3.22764  1.86143

H -0.91741 -2.15757 2.10527
C -1.76768 -3.52445 0.70557
C -1.42859 2.95612 -0.47484
C -3.44552 -2.89246 -0.98138
C -4.76305 1.76580 1.84232
H -4.05459 2.02332 2.65261
H -5.65049 2.41011 2.01626
C 1.85604 -0.12657 3.11497
C -5.17930 0.28040 1.91992
H -5.79547 0.00216 1.04379
H -5.83867 0.12051 2.79944
C -2.63749 -2.52987 0.14628
C -5.27063 1.78274 -1.17044
H -5.10518 2.29006 -2.13371
H -6.29932 2.02157 -0.84199
H -5.22311 0.69782 -1.34591
C -2.55820 -5.17604 -0.92975
H -2.53952 -6.19560 -1.33064
C 4.13925 2.52011 -0.50935
H 3.09476 2.38661 -0.17432
C -1.34722 3.35079 -1.85399
C -4.73484 -2.66983 2.46184
H -5.45918 -2.87676 1.65602
H -5.29750 -2.59041 3.40863
H -4.06492 -3.54046 2.53029
C 4.05480 -2.41017 -0.24699
H 2.97990 -2.21074 -0.08859
C -3.38566 -4.20098 -1.49789
H -4.01383 -4.45997 -2.35860
C 3.26588 -0.04048 3.20979
H 3.83926 0.14444 2.29646
C -2.23984 2.74729 -2.94215
H -2.79395 1.91256 -2.48075
C 5.93475 -0.68870 -0.76314
C 1.14957 0.02987 1.86015
C 0.65618 -3.46336 1.43615
H 0.85079 -4.53284 1.23630
H 1.34724 -3.13448 2.23199
H 0.89081 -2.89913 0.51836
C 5.96404 0.69169 -0.81001
C -1.12533 -4.05159 3.13058
H -2.14370 -3.85879 3.50590
H -0.41313 -3.80294 3.93784
H -1.04269 -5.13622 2.93664
C -1.75639 -4.82499 0.16154
H -1.09690 -5.57915 0.60774
C -4.37862 -1.88892 -1.65057
H -4.31029 -0.96739 -1.04962
C 1.11029 -0.35917 4.30044
H 0.01995 -0.41863 4.23871
C 0.13875 0.16977 1.09774
C -0.59870 3.63542 0.48337
C 1.76109 -0.50523 5.53183
H 1.16890 -0.68467 6.43552
C 4.60308 -3.05663 1.03609
H 4.04624 -3.98669 1.23705
H 4.47171 -2.38822 1.90191
H 5.67012 -3.32201 0.95008
C -0.67646 3.34819 1.98610
H -1.10973 2.33947 2.09955
C 3.16178 -0.42010 5.61266
H 3.66610 -0.53350 6.57788
C -0.44844 4.36775 -2.23543
H -0.39805 4.66086 -3.29055
C -2.81739 -0.53483 3.69165
H -2.16063 -1.35578 4.02465
H -3.49343 -0.27860 4.52662
H -2.18598 0.34801 3.48943
C -3.92034 -1.55497 -3.08778
H -3.96328 -2.44615 -3.73968
H -2.88312 -1.18061 -3.09986
H -4.57092 -0.78174 -3.53406
C 7.13433 1.58831 -1.07914
H 6.92563 2.32287 -1.87442
H 7.99587 0.98826 -1.41012
H 7.45016 2.14931 -0.18213
C 0.69975 3.36204 2.68418
H 1.42927 2.72770 2.15662
H 0.60530 2.98207 3.71599
H 1.11441 4.38401 2.75505
C -4.23520 4.30580 0.18540
H -4.39785 4.69333 1.20516
H -5.11725 4.59063 -0.41445
H -3.35889 4.82374 -0.23459
C -1.44702 2.17927 -4.14039
H -0.89548 2.97278 -4.67642
H -2.13887 1.71554 -4.86563
H -0.71935 1.41774 -3.82279
C 3.90923 -0.18498 4.44676
H 5.00088 -0.11138 4.50099
C 4.85468 3.39827 0.52931
H 5.87917 3.66588 0.22392
H 4.89628 2.89971 1.51144
H 4.29110 4.33798 0.64944
C -3.25958 3.79350 -3.45437
H -3.85923 4.22483 -2.63677
H -3.95028 3.33927 -4.18765
H -2.74192 4.62886 -3.95967
C 4.18713 -3.30871 -1.48524
H 5.22677 -3.62864 -1.66389
H 3.80416 -2.80198 -2.38503
H 3.58404 -4.21837 -1.33068
C -5.85123 -2.35461 -1.64131
H -6.50695 -1.57428 -2.06733
H -6.20154 -2.57280 -0.61811
H -5.99272 -3.26991 -2.24363
C -1.61438 4.34765 2.70372
H -1.24917 5.38321 2.57965
H -1.65561 4.13062 3.78639
H -2.63921 4.30455 2.30755
C 4.09657 3.13617 -1.91609
H 3.54836 4.09192 -1.87435
H 3.55673 2.46489 -2.60294
H 5.10327 3.34181 -2.31745
C 0.28550 4.64153 0.04340
H 0.90574 5.16141 0.78193
C 7.05869 -1.65021 -1.00367
H 7.19502 -2.35880 -0.16963
H 8.00400 -1.09745 -1.11628
H 6.91296 -2.24309 -1.92325
C 0.37219 5.01205 -1.30409
H 1.05583 5.80802 -1.62040
C 0.75308 -1.33840 -2.81629
C -0.01413 -2.49167 -2.54246
H -0.76777 -2.46231 -1.74993
C 0.60340 -0.07859 -2.08393
C 1.70526 -1.38687 -3.87009
H 2.28574 -0.48453 -4.08378
C 1.24528 1.03710 -1.94285
C 1.87903 -2.55737 -4.61797
H 2.60732 -2.57296 -5.43635
C 1.11507 -3.70348 -4.32942
H 1.24873 -4.61676 -4.91920
C 0.17269 -3.66427 -3.28965
H -0.43596 -4.54274 -3.05433
H 0.94176 2.02503 -1.59404

**$Z_{Ph}$**

SCF (BP86) Energy = -2647.90230884
Enthalpy 0K = -2646.677639
Enthalpy 298K = -2646.597829
Free Energy 298K = -2646.793912
Lowest Frequency = 9.6988 $cm^{-1}$
Second Frequency = 14.8811 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2648.32796050
SCF (C6H6) Energy = -2647.90779511
SCF (BS2) Energy = -3460.17273959

Cu 1.58966 0.05008 -0.11811
Si -3.98266 -1.00445 1.78119
Al -1.50294 0.13092 -0.00984
Si -4.12892 2.10041 -0.61724
N 4.50416 -0.80982 -0.32432
N -2.62747 -1.25417 0.62484

| | | | |
|---|---|---|---|
| N | 4.15903 | 1.25070 | -0.93196 |
| N | -2.37313 | 1.81086 | -0.36875 |
| C | 3.51568 | 0.12826 | -0.47108 |
| H | 1.47736 | 0.00413 | -2.89179 |
| C | -0.84544 | -2.86751 | 2.44765 |
| H | -1.04284 | -1.78202 | 2.45568 |
| C | -1.56910 | -3.44752 | 1.22921 |
| C | -1.51654 | 2.96004 | -0.53202 |
| C | -2.93567 | -3.26944 | -0.81292 |
| C | -5.20539 | 1.53988 | 0.86103 |
| H | -4.80462 | 2.00802 | 1.78043 |
| H | -6.18106 | 2.03984 | 0.68221 |
| C | 1.99755 | 0.59094 | 3.05884 |
| C | -5.42429 | 0.02842 | 1.06803 |
| H | -5.75606 | -0.45106 | 0.12700 |
| H | -6.25530 | -0.13780 | 1.78599 |
| C | -2.35938 | -2.64268 | 0.34074 |
| C | -4.83527 | 1.23333 | -2.16859 |
| H | -4.42860 | 1.66257 | -3.09828 |
| H | -5.93244 | 1.36713 | -2.19034 |
| H | -4.63276 | 0.15125 | -2.18199 |
| C | -2.01878 | -5.43804 | -0.13616 |
| H | -1.90750 | -6.51486 | -0.30589 |
| C | 3.40225 | 2.50771 | -1.18714 |
| H | 2.35186 | 2.20178 | -1.02304 |
| C | -1.08838 | 3.40294 | -1.83448 |
| C | -4.78666 | -2.67495 | 2.23150 |
| H | -4.07020 | -3.42694 | 2.59431 |
| H | -5.30195 | -3.11046 | 1.35882 |
| H | -5.54218 | -2.50830 | 3.01976 |
| C | 4.19972 | -2.16792 | 0.20567 |
| H | 3.09661 | -2.16936 | 0.25159 |
| C | -2.75195 | -4.64800 | -1.02863 |
| H | -3.20648 | -5.11196 | -1.91208 |
| C | 3.37247 | 0.91729 | 2.97501 |
| H | 3.82039 | 1.05681 | 1.98740 |
| C | -1.54807 | 2.73425 | -3.13630 |
| H | -2.03546 | 1.78321 | -2.85938 |
| C | 5.75702 | -0.28420 | -0.68233 |
| C | 1.14541 | 0.46575 | 1.89660 |
| C | 0.68331 | -3.06467 | 2.33166 |
| H | 0.95412 | -4.13594 | 2.35260 |
| H | 1.20375 | -2.56691 | 3.16858 |
| H | 1.06637 | -2.63670 | 1.39034 |
| C | 5.53737 | 1.02386 | -1.06862 |
| C | -1.34117 | -3.46507 | 3.78459 |
| H | -2.41643 | -3.28574 | 3.94527 |
| H | -0.79268 | -3.01886 | 4.63376 |
| H | -1.17632 | -4.55697 | 3.82277 |
| C | -1.42687 | -4.82746 | 0.97515 |
| H | -0.83907 | -5.43626 | 1.67301 |
| C | -3.75307 | -2.47492 | -1.82698 |
| H | -3.82578 | -1.45208 | -1.42139 |
| C | 1.42432 | 0.40303 | 4.34495 |
| H | 0.36096 | 0.15714 | 4.41685 |
| C | 0.03930 | 0.41088 | 1.27361 |
| C | -1.09172 | 3.72078 | 0.61269 |
| C | 2.20511 | 0.53773 | 5.49909 |
| H | 1.74461 | 0.38867 | 6.48149 |
| C | 4.73571 | -2.35768 | 1.63439 |
| H | 4.34900 | -3.30663 | 2.04134 |
| H | 4.40399 | -1.54087 | 2.29446 |
| H | 5.83731 | -2.41059 | 1.66348 |
| C | -1.58000 | 3.39817 | 2.02631 |
| H | -1.96237 | 2.36324 | 1.99918 |
| C | 3.56849 | 0.86639 | 5.40232 |
| H | 4.17518 | 0.97410 | 6.30728 |
| C | -0.26188 | 4.54048 | -1.94926 |
| H | 0.03498 | 4.87960 | -2.94920 |
| C | -3.38693 | -0.14475 | 3.38081 |
| H | -2.72298 | -0.80400 | 3.96436 |
| H | -4.24720 | 0.12260 | 4.02020 |
| H | -2.83146 | 0.78304 | 3.16322 |
| C | -3.03834 | -2.39588 | -3.19469 |
| H | -2.92891 | -3.39763 | -3.64792 |
| H | -2.03020 | -1.96116 | -3.09337 |
| H | -3.61522 | -1.76997 | -3.89915 |
| C | 6.52999 | 2.02308 | -1.58008 |
| H | 6.42460 | 2.20136 | -2.66490 |
| H | 7.55340 | 1.65464 | -1.40870 |
| H | 6.44365 | 2.99795 | -1.07300 |
| C | -0.47069 | 3.48104 | 3.09476 |
| H | 0.41250 | 2.89047 | 2.81015 |
| H | -0.84493 | 3.09730 | 4.06028 |
| H | -0.14646 | 4.52291 | 3.27004 |
| C | -4.50542 | 3.97389 | -0.81337 |
| H | -4.98040 | 4.37442 | 0.09841 |
| H | -5.22184 | 4.12245 | -1.64045 |
| H | -3.61408 | 4.58552 | -1.02115 |
| C | -0.38536 | 2.41657 | -4.10499 |
| H | 0.07141 | 3.33835 | -4.50798 |
| H | -0.75613 | 1.83354 | -4.96623 |
| H | 0.41260 | 1.83049 | -3.62144 |
| C | 4.14600 | 1.05704 | 4.13636 |
| H | 5.20684 | 1.31627 | 4.05106 |
| C | 3.72568 | 3.60382 | -0.15977 |
| H | 4.73651 | 4.02416 | -0.29573 |
| H | 3.63776 | 3.21837 | 0.86831 |
| H | 2.99634 | 4.42216 | -0.27556 |
| C | -2.57974 | 3.61275 | -3.88563 |
| H | -3.45739 | 3.84551 | -3.26458 |
| H | -2.93107 | 3.10453 | -4.80188 |
| H | -2.12416 | 4.57264 | -4.18932 |
| C | 4.62833 | -3.28769 | -0.75371 |
| H | 5.72203 | -3.42065 | -0.78319 |
| H | 4.25600 | -3.10131 | -1.77307 |
| H | 4.18911 | -4.23733 | -0.40749 |
| C | -5.18798 | -3.02202 | -1.99116 |
| H | -5.76907 | -2.38303 | -2.67985 |
| H | -5.72236 | -3.05652 | -1.02651 |
| H | -5.18893 | -4.04464 | -2.40944 |
| C | -2.74923 | 4.32540 | 2.43547 |
| H | -2.42045 | 5.38038 | 2.45392 |
| H | -3.11450 | 4.06782 | 3.44605 |
| H | -3.59575 | 4.25291 | 1.73644 |
| C | 3.52621 | 2.98685 | -2.64127 |
| H | 2.76669 | 3.76526 | -2.81948 |
| H | 3.34191 | 2.16237 | -3.34922 |
| H | 4.51433 | 3.42447 | -2.85842 |
| C | -0.26348 | 4.84664 | 0.43917 |
| H | 0.03913 | 5.42240 | 1.32110 |
| C | 7.04918 | -1.04314 | -0.67629 |
| H | 7.21610 | -1.58265 | 0.27017 |
| H | 7.89122 | -0.34573 | -0.80768 |
| H | 7.10521 | -1.78187 | -1.49517 |
| C | 0.15938 | 5.26372 | -0.82834 |
| H | 0.78377 | 6.15730 | -0.94246 |
| C | 1.18136 | -2.06656 | -2.45673 |
| C | 2.06217 | -2.38241 | -3.52171 |
| H | 2.49272 | -1.56434 | -4.11241 |
| C | 0.87719 | -0.63664 | -2.22142 |
| C | 0.62813 | -3.13277 | -1.71176 |
| H | -0.06921 | -2.92321 | -0.89577 |
| C | -0.12464 | -0.01825 | -1.48438 |
| C | 0.94897 | -4.46201 | -2.02367 |
| H | 0.49768 | -5.26518 | -1.43366 |
| C | 1.81458 | -4.75948 | -3.09045 |
| H | 2.05006 | -5.80057 | -3.33619 |
| C | 2.36986 | -3.71139 | -3.84387 |
| H | 3.03998 | -3.92867 | -4.68296 |
| H | -0.06896 | 1.07148 | -1.69738 |

**TS(Z-P)$_{Ph}$**

SCF (BP86) Energy = -2956.23659084
Enthalpy 0K = -2954.910771
Enthalpy 298K = -2954.823523
Free Energy 298K = -2955.034558
Lowest Frequency = -870.5779 $cm^{-1}$
Second Frequency = 11.9700 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2956.71547481
SCF (C6H6) Energy = -2956.24290349
SCF (BS2) Energy = -3768.58141851

| | | | |
|---|---|---|---|
| Cu | -1.23194 | 0.68126 | -0.18891 |

| | | | |
|---|---|---|---|
| Si | 4.64102 | -1.28385 | -1.13348 |
| Al | 1.72588 | -0.22875 | 0.14230 |
| Si | 3.79245 | -0.71915 | 2.65210 |
| N | -3.53631 | 1.89354 | -1.71479 |
| N | 2.83893 | -1.16610 | -1.07285 |
| N | -4.20522 | 1.21821 | 0.23918 |
| N | 2.61146 | 0.28598 | 1.74960 |
| C | -3.09127 | 1.28050 | -0.56530 |
| H | -1.88830 | -2.08340 | 0.85590 |
| C | 2.35595 | 0.21428 | -3.67572 |
| H | 2.68858 | 0.62907 | -2.70874 |
| C | 2.06299 | -1.27103 | -3.44566 |
| C | 2.39268 | 1.60354 | 2.31476 |
| C | 1.88717 | -3.28026 | -2.02250 |
| C | 5.42534 | -1.08325 | 1.72047 |
| H | 5.90178 | -0.11435 | 1.47700 |
| H | 6.07895 | -1.53530 | 2.49652 |
| C | -0.42852 | 3.83717 | -0.53729 |
| C | 5.38705 | -1.99572 | 0.47765 |
| H | 4.86323 | -2.94304 | 0.70743 |
| H | 6.41962 | -2.29344 | 0.19837 |
| C | 2.23817 | -1.89513 | -2.16563 |
| C | 3.02618 | -2.40105 | 3.14234 |
| H | 2.30388 | -2.27180 | 3.96710 |
| H | 3.80871 | -3.09664 | 3.49407 |
| H | 2.50153 | -2.88809 | 2.30302 |
| C | 1.32411 | -3.40099 | -4.40842 |
| H | 0.99816 | -3.98797 | -5.27412 |
| C | -4.15321 | 0.64049 | 1.60706 |
| H | -3.15054 | 0.18038 | 1.64830 |
| C | 1.42506 | 1.80955 | 3.35170 |
| C | 5.17376 | -2.46387 | -2.54044 |
| H | 4.91380 | -2.05900 | -3.53197 |
| H | 4.73066 | -3.46853 | -2.47626 |
| H | 6.27302 | -2.56898 | -2.49837 |
| C | -2.64983 | 2.10201 | -2.89199 |
| H | -1.65272 | 1.83800 | -2.49894 |
| C | 1.44532 | -4.00040 | -3.14943 |
| H | 1.19882 | -5.06258 | -3.03626 |
| C | -1.53098 | 4.33066 | 0.20223 |
| H | -2.07480 | 3.64365 | 0.85608 |
| C | 0.51810 | 0.68760 | 3.84911 |
| H | 0.82800 | -0.22562 | 3.31629 |
| C | -4.90016 | 2.20772 | -1.63171 |
| C | 0.01013 | 2.46844 | -0.42560 |
| C | 1.08269 | 0.97971 | -4.10057 |
| H | 0.69220 | 0.60905 | -5.06578 |
| H | 1.29848 | 2.05700 | -4.21793 |
| H | 0.28824 | 0.87046 | -3.34413 |
| C | -5.32453 | 1.78552 | -0.38900 |
| C | 3.47851 | 0.44295 | -4.71314 |
| H | 4.41895 | -0.04764 | -4.41421 |
| H | 3.68303 | 1.52218 | -4.83212 |
| H | 3.19592 | 0.04766 | -5.70541 |
| C | 1.61786 | -2.03951 | -4.54104 |
| H | 1.51360 | -1.55794 | -5.52116 |
| C | 1.99497 | -4.02397 | -0.68754 |
| H | 2.22639 | -3.26382 | 0.07936 |
| C | 0.27645 | 4.73054 | -1.38523 |
| H | 1.13144 | 4.35741 | -1.95590 |
| C | 0.76723 | 1.45771 | -0.38692 |
| C | 3.16361 | 2.73308 | 1.88825 |
| C | -0.11469 | 6.07147 | -1.48567 |
| H | 0.44160 | 6.74775 | -2.14329 |
| C | -2.60600 | 3.56740 | -3.35727 |
| H | -1.73472 | 3.70009 | -4.01917 |
| H | -2.49373 | 4.25933 | -2.50871 |
| H | -3.50064 | 3.84798 | -3.93629 |
| C | 4.23936 | 2.62433 | 0.81244 |
| H | 4.24905 | 1.57258 | 0.48478 |
| C | -1.21016 | 6.55013 | -0.74644 |
| H | -1.51119 | 7.59987 | -0.82543 |
| C | 1.25667 | 3.08808 | 3.91802 |
| H | 0.51319 | 3.22182 | 4.71351 |
| C | 5.55321 | 0.35372 | -1.54020 |
| H | 4.93302 | 1.04060 | -2.13736 |
| H | 6.45198 | 0.11333 | -2.13583 |
| H | 5.88960 | 0.89432 | -0.64255 |
| C | 0.67141 | -4.71990 | -0.29815 |
| H | 0.43263 | -5.54856 | -0.98890 |
| H | -0.17347 | -4.01555 | -0.30673 |
| H | 0.75035 | -5.14976 | 0.71586 |
| C | -6.70290 | 1.87725 | 0.19387 |
| H | -7.20535 | 0.89566 | 0.24512 |
| H | -7.32640 | 2.53355 | -0.43250 |
| H | -6.70510 | 2.30471 | 1.20995 |
| C | 3.91953 | 3.49815 | -0.41987 |
| H | 2.94995 | 3.21101 | -0.85856 |
| H | 4.69979 | 3.38127 | -1.19281 |
| H | 3.86782 | 4.56922 | -0.15407 |
| C | 4.36281 | 0.17023 | 4.23949 |
| H | 4.94372 | 1.07675 | 4.00135 |
| H | 5.01438 | -0.50725 | 4.81937 |
| H | 3.52825 | 0.48112 | 4.88559 |
| C | -0.95006 | 0.98150 | 3.47876 |
| H | -1.31274 | 1.88919 | 3.99372 |
| H | -1.60262 | 0.13651 | 3.76076 |
| H | -1.05232 | 1.14787 | 2.38987 |
| C | -1.91352 | 5.67449 | 0.09863 |
| H | -2.76376 | 6.04139 | 0.68344 |
| C | -4.22846 | 1.73440 | 2.68538 |
| H | -5.21034 | 2.23642 | 2.69947 |
| H | -3.44795 | 2.49613 | 2.53250 |
| H | -4.07009 | 1.28266 | 3.67811 |
| C | 0.62755 | 0.42654 | 5.36793 |
| H | 1.65367 | 0.16006 | 5.66945 |
| H | -0.03805 | -0.40419 | 5.66513 |
| H | 0.32883 | 1.31346 | 5.95485 |
| C | -2.98836 | 1.13180 | -4.03466 |
| H | -3.95829 | 1.36698 | -4.50464 |
| H | -3.00831 | 0.09024 | -3.68138 |
| H | -2.21454 | 1.21302 | -4.81628 |
| C | 3.13521 | -5.06966 | -0.68029 |
| H | 3.16762 | -5.59669 | 0.29011 |
| H | 4.12309 | -4.61290 | -0.84798 |
| H | 2.97820 | -5.82943 | -1.46726 |
| C | 5.64088 | 2.96950 | 1.36558 |
| H | 5.69224 | 4.02047 | 1.70215 |
| H | 6.41438 | 2.83411 | 0.58788 |
| H | 5.90732 | 2.33323 | 2.22654 |
| C | -5.19562 | -0.46978 | 1.81812 |
| H | -4.92029 | -1.06399 | 2.70398 |
| H | -5.22631 | -1.15366 | 0.95530 |
| H | -6.20829 | -0.07024 | 1.98721 |
| C | 2.95335 | 3.99446 | 2.47898 |
| H | 3.55476 | 4.84512 | 2.13631 |
| C | -5.70518 | 2.88737 | -2.69814 |
| H | -5.42212 | 3.94627 | -2.82726 |
| H | -6.77267 | 2.86110 | -2.43076 |
| H | -5.60566 | 2.39398 | -3.67878 |
| C | 2.01130 | 4.18550 | 3.49328 |
| H | 1.86853 | 5.17257 | 3.94643 |
| C | -2.01867 | -1.99367 | -1.33112 |
| C | -3.34691 | -2.47731 | -1.23300 |
| H | -3.82113 | -2.52518 | -0.24698 |
| C | -1.30688 | -1.60265 | -0.09359 |
| C | -1.40351 | -1.97600 | -2.60410 |
| H | -0.36817 | -1.63925 | -2.69866 |
| C | -0.09782 | -1.16665 | 0.29114 |
| C | -2.09974 | -2.42747 | -3.73467 |
| H | -1.59053 | -2.42563 | -4.70346 |
| C | -3.42122 | -2.89356 | -3.62657 |
| H | -3.95663 | -3.24847 | -4.51366 |
| C | -4.04388 | -2.91517 | -2.36697 |
| H | -5.06905 | -3.28764 | -2.26484 |
| H | -0.18392 | -1.55492 | 1.64032 |
| C | -1.82123 | -2.75877 | 2.36448 |
| C | -0.66814 | -2.28311 | 2.63883 |
| H | 0.09845 | -2.36450 | 3.40687 |
| C | -3.00677 | -3.50799 | 2.69505 |
| C | -3.70033 | -3.24980 | 3.90932 |
| C | -3.50358 | -4.52696 | 1.84069 |
| C | -4.84274 | -3.98572 | 4.25002 |
| C | -4.63918 | -5.26573 | 2.19667 |

C -5.31818 -4.99748 3.39781
H -3.31697 -2.47545 4.58146
H -2.97981 -4.73488 0.90272
H -5.35952 -3.77427 5.19255
H -4.99866 -6.05606 1.52894
H -6.20874 -5.57357 3.66903

**TS(I-II)$_{Bu}$**
SCF (BP86) Energy = -2265.61309437
Enthalpy 0K = -2264.470528
Enthalpy 298K = -2264.396458
Free Energy 298K = -2264.580033
Lowest Frequency = -85.8570 $cm^{-1}$
Second Frequency = 11.8584 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2265.97508653
SCF (C6H6) Energy = -2265.61716629
SCF (BS2) Energy = -3077.79282014

Cu 1.29949 -0.08776 0.38018
Si -3.66925 2.22595 -0.38403
Si -3.87011 -1.27056 1.36669
Al -1.09754 0.12098 0.22052
N -1.95381 1.81071 -0.00851
N -2.36467 -1.30036 0.39193
N 3.06907 -1.28016 -1.72313
N 3.95334 0.57212 -1.01222
C -1.05269 2.93738 -0.05542
C -0.65575 3.60737 1.15036
C 0.13651 4.76999 1.06599
H 0.41661 5.29278 1.98689
C 0.56958 5.27864 -0.16359
H 1.16925 6.19461 -0.20539
C 0.23646 4.59176 -1.33586
H 0.59447 4.96942 -2.30124
C -0.55496 3.42683 -1.30859
C -1.07299 3.10021 2.53464
H -1.26684 2.01390 2.42571
C 0.02067 3.30078 3.60836
H 1.01060 2.95761 3.26553
H -0.24130 2.74699 4.52736
H 0.11670 4.36302 3.89572
C -2.38668 3.74294 3.03659
H -2.28014 4.84109 3.09623
H -2.64101 3.37222 4.04597
H -3.23330 3.51977 2.37115
C -0.84283 2.71307 -2.63196
H -1.56811 1.91183 -2.41507
C 0.42977 2.03655 -3.19141
H 1.20681 2.78499 -3.43206
H 0.19971 1.48402 -4.12077
H 0.85216 1.32563 -2.45955
C -1.46369 3.64689 -3.69405
H -2.37729 4.14078 -3.32232
H -1.72863 3.07699 -4.60249
H -0.75973 4.44137 -4.00035
C -3.91710 4.12022 -0.37926
H -4.96036 4.33990 -0.66882
H -3.25355 4.61243 -1.10886
H -3.73082 4.58833 0.59947
C -4.26828 1.66298 -2.11221
H -3.82668 2.27492 -2.91513
H -5.36545 1.78743 -2.16559
H -4.04249 0.60759 -2.32689
C -4.89570 1.47130 0.87508
H -4.56246 1.70975 1.90227
H -5.83085 2.05116 0.72825
C -5.18978 -0.03867 0.73520
H -5.43569 -0.29338 -0.31339
H -6.09911 -0.29975 1.31697
C -3.48780 -0.78208 3.17549
H -2.87556 -1.54447 3.68460
H -4.42063 -0.65400 3.75330
H -2.93856 0.17499 3.21924
C -4.72178 -2.97649 1.32090
H -5.15885 -3.16631 0.32572
H -5.54338 -3.00100 2.05827
H -4.03634 -3.80916 1.54158
C -1.95820 -2.58023 -0.13361
C -1.19659 -3.51223 0.64621
C -0.84131 -4.75850 0.08963
H -0.27481 -5.46951 0.70317
C -1.20047 -5.11569 -1.21469
H -0.92105 -6.09352 -1.62240
C -1.93704 -4.20609 -1.98292
H -2.23390 -4.47742 -3.00316
C -2.32820 -2.95532 -1.46792
C -0.74857 -3.21691 2.07824
H -1.03361 -2.17385 2.29865
C 0.78379 -3.32065 2.22374
H 1.14444 -4.34624 2.02571
H 1.08800 -3.04790 3.24908
H 1.29096 -2.62988 1.52825
C -1.43707 -4.13922 3.11101
H -2.53451 -4.04270 3.08400
H -1.10038 -3.89433 4.13455
H -1.19142 -5.20026 2.92467
C -3.15161 -2.02467 -2.35470
H -3.47969 -1.19733 -1.70355
C -2.29177 -1.41951 -3.48670
H -1.42826 -0.86524 -3.07878
H -2.88467 -0.72100 -4.10395
H -1.89895 -2.20902 -4.15266
C -4.41171 -2.70463 -2.93232
H -4.15680 -3.51466 -3.63898
H -5.02649 -1.97081 -3.48316
H -5.03561 -3.14323 -2.13528
C 2.91383 -0.29954 -0.77066
C 2.13546 -2.43610 -1.77237
H 1.34374 -2.13937 -1.05694
C 1.47315 -2.60979 -3.14687
H 1.08615 -1.64856 -3.52135
H 0.62030 -3.29946 -3.03805
H 2.15838 -3.03511 -3.89847
C 2.79042 -3.72612 -1.25457
H 3.25397 -3.56176 -0.26857
H 3.56194 -4.11104 -1.94369
H 2.01420 -4.50129 -1.14553
C 4.17513 -1.02924 -2.54777
C 4.62590 -1.89782 -3.68339
H 4.72142 -2.95576 -3.38720
H 5.61594 -1.56942 -4.03608
H 3.93688 -1.85596 -4.54507
C 4.73140 0.15445 -2.10455
C 5.92537 0.87716 -2.65205
H 6.79989 0.82730 -1.97955
H 5.71564 1.94270 -2.84559
H 6.22336 0.42794 -3.61211
C 4.10262 1.81630 -0.21366
H 3.42358 1.64300 0.64033
C 5.52802 2.00774 0.33346
H 5.92885 1.07439 0.76161
H 5.50530 2.76902 1.13113
H 6.22966 2.36717 -0.43602
C 3.60090 3.04848 -0.98098
H 4.22294 3.26226 -1.86749
H 3.63498 3.93290 -0.32352
H 2.55762 2.91250 -1.30177
C 2.63315 -0.24673 2.95372
C 1.53884 0.24603 2.64148
H 0.62051 0.76352 2.85427
C 3.91539 -0.83296 3.39208
C 3.64584 -1.72452 4.63825
H 3.18762 -1.13957 5.45248
H 2.97230 -2.56004 4.38964
H 4.59960 -2.14376 5.00473
C 4.88249 0.31330 3.79824
H 5.83932 -0.11188 4.14931
H 5.09077 0.98011 2.94717
H 4.45297 0.91974 4.61256
C 4.55603 -1.69675 2.27461
H 3.89363 -2.53474 2.00360
H 4.73674 -1.10146 1.36598
H 5.51682 -2.11081 2.62873

**$II_{Bu}$**
SCF (BP86) Energy = -2265.62975510
Enthalpy 0K = -2264.485145
Enthalpy 298K = -2264.411641
Free Energy 298K = -2264.592417
Lowest Frequency = 12.7154 $cm^{-1}$
Second Frequency = 15.3565 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2265.99947866
SCF (C6H6) Energy = -2265.63320952
SCF (BS2) Energy = -3077.81150290

| | | | |
|---|---|---|---|
| Cu | 1.36791 | -0.35230 | 0.63757 |
| Si | -2.92502 | 2.65256 | -1.09430 |
| Si | -3.94421 | -0.48630 | 1.03038 |
| Al | -0.89158 | 0.23260 | 0.02666 |
| N | -1.36966 | 2.00040 | -0.44702 |
| N | -2.37344 | -0.92704 | 0.27190 |
| N | 2.87156 | -2.01567 | -1.30216 |
| N | 3.99589 | -0.24050 | -0.72342 |
| C | -0.29460 | 2.96963 | -0.45588 |
| C | -0.03862 | 3.78005 | 0.69908 |
| C | 0.97038 | 4.76225 | 0.64139 |
| H | 1.15145 | 5.38974 | 1.52194 |
| C | 1.73676 | 4.96431 | -0.51141 |
| H | 2.50796 | 5.74206 | -0.53677 |
| C | 1.49708 | 4.16395 | -1.63406 |
| H | 2.08910 | 4.32203 | -2.54387 |
| C | 0.49746 | 3.17130 | -1.63411 |
| C | -0.83036 | 3.63350 | 2.00384 |
| H | -1.44681 | 2.72199 | 1.90235 |
| C | 0.09753 | 3.45745 | 3.22600 |
| H | 0.80017 | 2.62529 | 3.06917 |
| H | -0.49772 | 3.24644 | 4.13266 |
| H | 0.68249 | 4.37277 | 3.42702 |
| C | -1.78601 | 4.82227 | 2.26242 |
| H | -1.23038 | 5.77670 | 2.29099 |
| H | -2.29404 | 4.70183 | 3.23606 |
| H | -2.56422 | 4.90897 | 1.48848 |
| C | 0.27858 | 2.36422 | -2.91744 |
| H | -0.57002 | 1.68466 | -2.72996 |
| C | 1.50060 | 1.48784 | -3.26926 |
| H | 2.38954 | 2.10778 | -3.48772 |
| H | 1.29428 | 0.88098 | -4.16968 |
| H | 1.74842 | 0.80515 | -2.43977 |
| C | -0.08558 | 3.26631 | -4.11906 |
| H | -0.97316 | 3.88791 | -3.91497 |
| H | -0.29705 | 2.65316 | -5.01345 |
| H | 0.74391 | 3.94914 | -4.37613 |
| C | -2.79271 | 4.53387 | -1.38655 |
| H | -2.57193 | 5.11510 | -0.47942 |
| H | -3.75494 | 4.89060 | -1.79559 |
| H | -2.00640 | 4.77038 | -2.12166 |
| C | -3.44046 | 1.96082 | -2.80030 |
| H | -2.71862 | 2.24234 | -3.58390 |
| H | -4.41613 | 2.40271 | -3.07417 |
| H | -3.55561 | 0.86745 | -2.82062 |
| C | -4.37325 | 2.32642 | 0.10778 |
| H | -4.07562 | 2.65051 | 1.12289 |
| H | -5.17163 | 3.03150 | -0.20349 |
| C | -4.92867 | 0.88537 | 0.12785 |
| H | -5.14199 | 0.53783 | -0.90116 |
| H | -5.91219 | 0.86979 | 0.64412 |
| C | -3.67586 | 0.12475 | 2.82134 |
| H | -3.24580 | -0.65961 | 3.46549 |
| H | -4.63469 | 0.44300 | 3.26811 |
| H | -2.99913 | 0.99747 | 2.85214 |
| C | -5.12263 | -1.98601 | 1.01352 |
| H | -5.50814 | -2.15814 | -0.00601 |
| H | -5.98867 | -1.78329 | 1.66777 |
| H | -4.64988 | -2.92179 | 1.34681 |
| C | -2.20758 | -2.31692 | -0.09370 |
| C | -1.78146 | -3.30466 | 0.85554 |
| C | -1.67167 | -4.65210 | 0.45204 |
| H | -1.36344 | -5.40069 | 1.19147 |
| C | -1.95472 | -5.06090 | -0.85541 |
| H | -1.86795 | -6.11486 | -1.14144 |
| C | -2.36671 | -4.10006 | -1.78569 |
| H | -2.60601 | -4.40803 | -2.81052 |
| C | -2.50896 | -2.74518 | -1.42940 |
| C | -1.45096 | -2.97410 | 2.31288 |
| H | -1.47500 | -1.87589 | 2.41133 |
| C | -0.03350 | -3.44586 | 2.70049 |
| H | 0.06778 | -4.54326 | 2.62540 |
| H | 0.18825 | -3.16655 | 3.74564 |
| H | 0.73175 | -2.97988 | 2.05903 |
| C | -2.48114 | -3.57591 | 3.29805 |
| H | -3.50228 | -3.20852 | 3.10896 |
| H | -2.21595 | -3.31715 | 4.33893 |
| H | -2.50442 | -4.67812 | 3.22534 |
| C | -3.00583 | -1.76312 | -2.48625 |
| H | -3.20893 | -0.82186 | -1.94966 |
| C | -1.92329 | -1.47229 | -3.54905 |
| H | -1.00672 | -1.06648 | -3.08526 |
| H | -2.28450 | -0.73607 | -4.28887 |
| H | -1.64492 | -2.39207 | -4.09428 |
| C | -4.31837 | -2.21977 | -3.15937 |
| H | -4.17514 | -3.13068 | -3.76764 |
| H | -4.69813 | -1.43228 | -3.83439 |
| H | -5.10125 | -2.43770 | -2.41349 |
| C | 2.79923 | -0.89040 | -0.51563 |
| C | 1.78192 | -3.02444 | -1.29800 |
| H | 0.95854 | -2.49531 | -0.78069 |
| C | 1.29177 | -3.38540 | -2.70825 |
| H | 1.12802 | -2.48066 | -3.31532 |
| H | 0.32722 | -3.90992 | -2.61554 |
| H | 1.98782 | -4.05143 | -3.24318 |
| C | 2.16250 | -4.25818 | -0.46347 |
| H | 2.50410 | -3.96138 | 0.54101 |
| H | 2.95950 | -4.85338 | -0.94220 |
| H | 1.27562 | -4.90279 | -0.34970 |
| C | 4.09246 | -2.07422 | -1.99124 |
| C | 4.49710 | -3.16108 | -2.94037 |
| H | 4.34070 | -4.16562 | -2.51366 |
| H | 5.56909 | -3.07093 | -3.17544 |
| H | 3.94527 | -3.11602 | -3.89570 |
| C | 4.80074 | -0.94536 | -1.63373 |
| C | 6.13212 | -0.49122 | -2.15066 |
| H | 6.85210 | -0.26555 | -1.34693 |
| H | 6.04733 | 0.40971 | -2.78347 |
| H | 6.57698 | -1.28315 | -2.77290 |
| C | 4.36146 | 0.97405 | 0.05031 |
| H | 3.45633 | 1.16068 | 0.65656 |
| C | 5.52531 | 0.69452 | 1.01727 |
| H | 5.32198 | -0.19732 | 1.63124 |
| H | 5.65289 | 1.55695 | 1.69275 |
| H | 6.48368 | 0.54787 | 0.49249 |
| C | 4.60926 | 2.20058 | -0.83938 |
| H | 5.53933 | 2.11313 | -1.42498 |
| H | 4.70081 | 3.09425 | -0.20033 |
| H | 3.76448 | 2.36762 | -1.52384 |
| C | 1.51950 | -0.14509 | 2.63321 |
| C | 0.32103 | 0.14309 | 2.19196 |
| H | -0.65692 | 0.40668 | 2.61375 |
| C | 2.26417 | -0.25546 | 3.94479 |
| C | 3.18477 | 0.98161 | 4.10897 |
| H | 3.89644 | 1.05798 | 3.27162 |
| H | 2.59999 | 1.91522 | 4.14887 |
| H | 3.76321 | 0.89882 | 5.04694 |
| C | 1.27019 | -0.30403 | 5.13396 |
| H | 1.80964 | -0.38517 | 6.09538 |
| H | 0.65166 | 0.60904 | 5.16533 |
| H | 0.59375 | -1.17111 | 5.04721 |
| C | 3.14171 | -1.53101 | 3.94832 |
| H | 3.72132 | -1.59876 | 4.88692 |
| H | 2.52330 | -2.43938 | 3.85998 |
| H | 3.84585 | -1.51974 | 3.09934 |

**$TS(II-III)_{Bu}$**
SCF (BP86) Energy = -2265.62518328
Enthalpy 0K = -2264.481085
Enthalpy 298K = -2264.408541
Free Energy 298K = -2264.585769
Lowest Frequency = -140.5798 $cm^{-1}$
Second Frequency = 18.3386 $cm^{-1}$

SCF (BP86-D3BJ) Energy = -2265.99276069
SCF (C6H6) Energy = -2265.62889450
SCF (BS2) Energy = -3077.80464524

Cu 1.59167 -0.21821 0.82799
Si -2.99949 2.31452 -1.53773
Si -4.08863 -0.84871 0.58142
Al -1.06959 0.26775 0.23683
N -1.49875 1.88047 -0.62229
N -2.35615 -1.10405 0.16216
N 3.22946 -1.94489 -0.93112
N 4.13011 0.00621 -0.55381
C -0.46912 2.90403 -0.58159
C -0.42458 3.85808 0.48724
C 0.63643 4.78357 0.53796
H 0.67615 5.49808 1.36833
C 1.62325 4.82887 -0.45249
H 2.43350 5.56423 -0.39623
C 1.53395 3.94972 -1.53717
H 2.27186 4.01395 -2.34549
C 0.50364 2.99282 -1.62976
C -1.51621 3.96238 1.55687
H -2.29586 3.22450 1.29684
C -0.99430 3.62431 2.96957
H -0.54244 2.62217 2.99276
H -1.81550 3.66377 3.70796
H -0.22648 4.35227 3.28905
C -2.16214 5.36885 1.58230
H -1.44676 6.12759 1.94650
H -3.02825 5.38064 2.26756
H -2.50436 5.69168 0.58664
C 0.41606 2.14703 -2.90318
H -0.42466 1.44573 -2.77055
C 1.68016 1.30525 -3.17059
H 2.56069 1.94685 -3.35733
H 1.53992 0.67707 -4.06865
H 1.90967 0.64670 -2.31719
C 0.11243 3.03994 -4.13034
H -0.79377 3.65041 -3.98193
H -0.03136 2.42376 -5.03621
H 0.94761 3.73506 -4.32990
C -3.08308 4.19907 -1.81463
H -3.46156 4.72442 -0.92376
H -3.78461 4.40103 -2.64317
H -2.10806 4.63802 -2.07920
C -3.14359 1.54546 -3.28150
H -2.42830 1.99866 -3.98579
H -4.16039 1.75045 -3.66402
H -2.99542 0.45608 -3.29959
C -4.58486 1.83678 -0.58459
H -4.51386 2.22400 0.44988
H -5.37422 2.45021 -1.06755
C -5.00240 0.35053 -0.59341
H -4.95634 -0.06175 -1.61951
H -6.06717 0.25710 -0.29213
C -4.23571 -0.12388 2.34219
H -3.89688 -0.84160 3.10724
H -5.28430 0.14154 2.56619
H -3.63376 0.79499 2.45746
C -5.05057 -2.48775 0.45551
H -5.16963 -2.78862 -0.59900
H -6.06005 -2.35135 0.88155
H -4.56420 -3.32262 0.98155
C -1.96863 -2.47369 -0.10135
C -1.63703 -3.38093 0.95877
C -1.33965 -4.72524 0.65173
H -1.10634 -5.41398 1.47229
C -1.34987 -5.20611 -0.66173
H -1.12929 -6.25839 -0.87209
C -1.66083 -4.32042 -1.69962
H -1.68281 -4.68530 -2.73354
C -1.97343 -2.97094 -1.44631
C -1.59971 -2.96922 2.43226
H -1.78708 -1.88300 2.47309
C -0.21155 -3.23132 3.05503
H 0.04234 -4.30634 3.04345
H -0.19534 -2.90108 4.10870
H 0.57600 -2.68094 2.51543
C -2.68774 -3.67873 3.27246
H -3.70432 -3.46195 2.90664
H -2.63150 -3.35336 4.32659
H -2.55459 -4.77528 3.25664
C -2.33341 -2.07441 -2.62709
H -2.66304 -1.11792 -2.18972
C -1.10608 -1.78843 -3.52069
H -0.28754 -1.32488 -2.94287
H -1.37086 -1.10261 -4.34518
H -0.71593 -2.71908 -3.97049
C -3.49750 -2.63778 -3.47131
H -3.22065 -3.58165 -3.97394
H -3.78631 -1.91886 -4.25861
H -4.38708 -2.84010 -2.85137
C 2.96923 -0.71678 -0.36499
C 2.23200 -3.04298 -0.87689
H 1.30407 -2.52268 -0.57477
C 1.98513 -3.69605 -2.24550
H 1.85052 -2.93507 -3.03100
H 1.05759 -4.28705 -2.18408
H 2.79913 -4.37540 -2.54487
C 2.58128 -4.06283 0.21962
H 2.73643 -3.55624 1.18574
H 3.49078 -4.63873 -0.02453
H 1.74545 -4.77259 0.33198
C 4.53773 -2.00208 -1.43690
C 5.15213 -3.18659 -2.11894
H 5.01198 -4.11780 -1.54527
H 6.23698 -3.03136 -2.22743
H 4.74185 -3.35398 -3.13044
C 5.10512 -0.76620 -1.20042
C 6.47213 -0.28739 -1.58512
H 7.00969 0.17693 -0.74155
H 6.44255 0.44974 -2.40677
H 7.08002 -1.13782 -1.93108
C 4.30079 1.35241 0.05479
H 3.27083 1.62840 0.34512
C 5.14248 1.26534 1.33842
H 4.68971 0.54667 2.03994
H 5.17360 2.25334 1.82770
H 6.18263 0.95873 1.13380
C 4.82207 2.40669 -0.93330
H 5.90120 2.30614 -1.13222
H 4.65474 3.40662 -0.50112
H 4.27748 2.35940 -1.88894
C 1.11377 0.33724 2.60981
C -0.10769 0.30063 2.02830
H -1.06194 0.20433 2.61238
C 1.46389 0.41683 4.08740
C 2.20655 1.75968 4.32322
H 3.09581 1.82873 3.67503
H 1.55759 2.62283 4.10179
H 2.53341 1.83534 5.37682
C 0.23014 0.34698 5.01940
H 0.53167 0.40848 6.08049
H -0.47100 1.17684 4.82369
H -0.32112 -0.59965 4.88066
C 2.43710 -0.73647 4.43677
H 2.78351 -0.64723 5.48310
H 1.95200 -1.71976 4.31973
H 3.31644 -0.71337 3.77070

**III$_{Bu}$**
SCF (BP86) Energy = -2265.65978926
Enthalpy 0K = -2264.515317
Enthalpy 298K = -2264.441832
Free Energy 298K = -2264.625192
Lowest Frequency = 8.9551 $cm^{-1}$
Second Frequency = 16.5029 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2266.01550161
SCF (C6H6) Energy = -2265.66466563
SCF (BS2) Energy = -3077.83887587

Cu 2.21377 0.67212 0.83659
Si -3.85173 0.49955 -2.16655
Si -2.79603 -3.10500 -0.99252

Al -1.57686 -0.27098  0.11110
N  -2.97591  0.72463 -0.61154
N  -1.44674 -2.04115 -0.43355
N   5.01516 -0.08916  0.15114
N   4.32011  1.58551 -1.04691
C  -3.32393  1.90226  0.16161
C  -4.29467  1.80476  1.20821
C  -4.60405  2.94523  1.97400
H  -5.34032  2.86074  2.78183
C  -3.99750  4.18072  1.72345
H  -4.25287  5.05797  2.32757
C  -3.06261  4.27994  0.68772
H  -2.58644  5.24657  0.48458
C  -2.71008  3.16689 -0.10055
C  -4.99953  0.48768  1.53674
H  -4.72975 -0.22361  0.73653
C  -4.50167 -0.09865  2.87825
H  -3.40909 -0.25647  2.87350
H  -4.98726 -1.06812  3.09020
H  -4.72976  0.58406  3.71608
C  -6.53819  0.62199  1.54550
H  -6.88686  1.28533  2.35675
H  -7.01043 -0.36405  1.70205
H  -6.91526  1.03471  0.59448
C  -1.67329  3.36324 -1.20826
H  -1.51677  2.37966 -1.68317
C  -0.31299  3.82641 -0.64264
H  -0.39616  4.80816 -0.14260
H   0.42257  3.93612 -1.46157
H   0.07677  3.09888  0.08848
C  -2.16664  4.34728 -2.29387
H  -3.11435  4.01622 -2.75054
H  -1.41706  4.44591 -3.10003
H  -2.33569  5.35477 -1.87367
C  -5.26417  1.76882 -2.29422
H  -6.05196  1.56390 -1.55025
H  -5.72240  1.71117 -3.29711
H  -4.91942  2.80199 -2.13181
C  -2.68397  0.70740 -3.66448
H  -2.35066  1.75165 -3.78023
H  -3.19964  0.41253 -4.59597
H  -1.78481  0.07547 -3.56667
C  -4.65882 -1.22440 -2.32814
H  -5.32881 -1.38607 -1.46239
H  -5.33467 -1.12730 -3.20355
C  -3.71871 -2.43360 -2.52632
H  -2.98432 -2.23369 -3.32985
H  -4.30322 -3.30810 -2.88212
C  -4.09852 -3.36620  0.37755
H  -3.69357 -3.95678  1.21504
H  -4.97208 -3.90833 -0.02700
H  -4.46169 -2.40865  0.78681
C  -2.08747 -4.79828 -1.49902
H  -1.42375 -4.71310 -2.37558
H  -2.91887 -5.47383 -1.76686
H  -1.50780 -5.27091 -0.69057
C  -0.17653 -2.71322 -0.25989
C   0.14896 -3.39013  0.95610
C   1.36984 -4.08919  1.04376
H   1.61126 -4.61805  1.97339
C   2.26641 -4.14001 -0.02825
H   3.19510 -4.71510  0.05306
C   1.95557 -3.45957 -1.21273
H   2.65358 -3.50057 -2.05643
C   0.75048 -2.74648 -1.35002
C  -0.78253 -3.40516  2.16907
H  -1.67336 -2.81095  1.90210
C  -0.12727 -2.73608  3.39760
H   0.77364 -3.28769  3.72250
H  -0.83118 -2.71909  4.24906
H   0.16381 -1.69987  3.16250
C  -1.25033 -4.83650  2.52037
H  -1.74602 -5.33097  1.66779
H  -1.96271 -4.81455  3.36432
H  -0.39983 -5.47334  2.82289
C   0.44918 -2.00461 -2.65202
H  -0.64714 -1.88133 -2.69855
C   1.06727 -0.58812 -2.61909
H   0.73390 -0.01628 -1.73197
H   0.79616 -0.01169 -3.52238
H   2.16848 -0.64748 -2.55700
C   0.89343 -2.75718 -3.92239
H   1.99307 -2.82608 -4.00308
H   0.53654 -2.22797 -4.82326
H   0.49077 -3.78394 -3.94758
C   3.90359  0.67946 -0.09959
C   4.98082 -1.14349  1.19912
H   3.90168 -1.22530  1.42711
C   5.46279 -2.50935  0.68880
H   4.96364 -2.77367 -0.25635
H   5.20035 -3.27851  1.43344
H   6.55448 -2.54821  0.54469
C   5.70773 -0.68423  2.47431
H   5.30827  0.28131  2.82391
H   6.79493 -0.57735  2.31906
H   5.55610 -1.42861  3.27374
C   6.11319  0.33449 -0.61239
C   7.47393 -0.29345 -0.60080
H   7.86268 -0.43383  0.42141
H   8.18770  0.35338 -1.13455
H   7.48787 -1.27831 -1.10031
C   5.67055  1.39797 -1.37571
C   6.43196  2.18747 -2.39686
H   6.31992  3.27541 -2.25784
H   6.11930  1.95019 -3.42931
H   7.50638  1.95817 -2.32145
C   3.40542  2.65971 -1.51341
H   2.43881  2.36604 -1.06243
C   3.79605  4.02651 -0.92696
H   3.87764  3.96807  0.17019
H   3.01641  4.76650 -1.17282
H   4.75163  4.40097 -1.33143
C   3.23629  2.67939 -3.04036
H   4.12872  3.06252 -3.56122
H   2.39522  3.34426 -3.29854
H   3.00459  1.67371 -3.42587
C   0.64332  0.90446  1.92675
C  -0.64765  0.56961  1.60334
H  -1.43058  0.87839  2.33210
C   0.93220  1.63677  3.27529
C   1.55603  3.02089  2.96042
H   2.45478  2.90706  2.32529
H   0.84035  3.66417  2.42005
H   1.85396  3.54131  3.89056
C  -0.30086  1.85883  4.18048
H  -0.00054  2.36825  5.11426
H  -1.06385  2.48672  3.68880
H  -0.77752  0.90313  4.46075
C   1.97307  0.80814  4.07049
H   2.26893  1.33088  4.99992
H   1.57022 -0.18184  4.34628
H   2.88168  0.64154  3.46229

**TS(I-III)$_{Bu}$**
SCF (BP86) Energy = -2265.59027108
Enthalpy 0K = -2264.446778
Enthalpy 298K = -2264.374017
Free Energy 298K = -2264.550541
Lowest Frequency = -228.6282 $cm^{-1}$
Second Frequency = 12.2951 $cm^{-1}$
SCF (BP86-D3BJ) Energy =  -2265.96821032
SCF (C6H6) Energy =  -2265.59438757
SCF (BS2) Energy =  -3077.76728717

Cu  1.33975  0.28842  0.17900
Si -3.65065  0.90911 -1.61112
Si -3.32484 -2.57787  0.25288
Al -1.09157 -0.10810  0.30956
N  -2.24844  1.20632 -0.54122
N  -1.65108 -1.94461  0.08408
N   4.13994 -0.67768 -0.35343
N   4.15374  1.48774 -0.19445
C  -1.77060  2.55984 -0.42041
C  -2.26743  3.44151  0.60137

C -1.68203 4.71429 0.76667
H -2.06285 5.37296 1.55672
C -0.64953 5.16772 -0.06030
H -0.20991 6.16016 0.08984
C -0.22948 4.35242 -1.11811
H 0.52234 4.72939 -1.82276
C -0.78077 3.07326 -1.32876
C -3.48217 3.10685 1.47530
H -3.81708 2.09572 1.18319
C -3.17162 3.09461 2.98780
H -2.40563 2.34621 3.23510
H -4.08281 2.85815 3.56683
H -2.81424 4.08301 3.32980
C -4.63741 4.10990 1.22961
H -4.37959 5.10942 1.62385
H -5.55389 3.77827 1.75015
H -4.86970 4.22770 0.16101
C -0.40399 2.32596 -2.60973
H -0.84283 1.31695 -2.53444
C 1.11215 2.16099 -2.82172
H 1.61775 3.13783 -2.92861
H 1.31192 1.58506 -3.74297
H 1.57255 1.61729 -1.97631
C -1.02231 3.04240 -3.83561
H -2.11186 3.17236 -3.72947
H -0.83156 2.47159 -4.76261
H -0.58203 4.04789 -3.96421
C -4.60189 2.52915 -1.96619
H -5.35350 2.73440 -1.18743
H -5.13854 2.42401 -2.92544
H -3.94048 3.40743 -2.04204
C -3.25842 0.20390 -3.34942
H -2.74445 0.94033 -3.98721
H -4.21671 -0.04733 -3.84116
H -2.64953 -0.71179 -3.32881
C -4.91009 -0.30131 -0.83332
H -5.08832 -0.01217 0.22035
H -5.86205 -0.07801 -1.35892
C -4.58955 -1.80584 -0.95518
H -4.27938 -2.05344 -1.98806
H -5.50854 -2.40450 -0.77829
C -4.10549 -2.34122 1.99093
H -3.43724 -2.63645 2.81519
H -5.01314 -2.96792 2.05590
H -4.42804 -1.29911 2.15857
C -3.36461 -4.44057 -0.16766
H -3.07713 -4.61063 -1.21888
H -4.39457 -4.81680 -0.03515
H -2.69279 -5.05129 0.45398
C -0.66546 -2.97393 -0.12810
C -0.17545 -3.77899 0.95526
C 0.67927 -4.86783 0.68738
H 1.01973 -5.49145 1.52326
C 1.08844 -5.18322 -0.61342
H 1.73086 -6.05063 -0.80239
C 0.65289 -4.37207 -1.66859
H 0.96545 -4.60555 -2.69399
C -0.20537 -3.27682 -1.45316
C -0.53420 -3.49813 2.41607
H -1.16362 -2.59265 2.42285
C 0.73440 -3.19189 3.24173
H 1.38915 -4.07846 3.32290
H 0.46750 -2.88236 4.26860
H 1.31780 -2.38318 2.77427
C -1.31957 -4.65093 3.08199
H -2.26970 -4.85927 2.56493
H -1.55424 -4.40244 4.13290
H -0.73051 -5.58576 3.08805
C -0.64659 -2.45093 -2.65695
H -1.34389 -1.69259 -2.26426
C 0.54120 -1.70808 -3.30646
H 1.05134 -1.06240 -2.56959
H 0.19317 -1.06835 -4.13720
H 1.28367 -2.41645 -3.71754
C -1.39961 -3.29587 -3.70820
H -0.74893 -4.07502 -4.14450
H -1.75512 -2.65889 -4.53779
H -2.27604 -3.80184 -3.26923
C 3.30994 0.39954 -0.15437
C 3.60656 -2.06716 -0.36205
H 2.51023 -1.91742 -0.33580
C 3.95236 -2.81638 -1.65717
H 3.71990 -2.20314 -2.54275
H 3.33540 -3.72725 -1.70390
H 5.01093 -3.11960 -1.70134
C 4.00479 -2.83905 0.90575
H 3.75272 -2.26313 1.81055
H 5.08113 -3.08071 0.93253
H 3.44067 -3.78523 0.93460
C 5.47548 -0.27994 -0.50207
C 6.63622 -1.19389 -0.75580
H 6.64125 -2.06324 -0.07888
H 7.58071 -0.65023 -0.59654
H 6.65023 -1.57778 -1.79105
C 5.48518 1.09758 -0.40107
C 6.65844 2.02216 -0.52644
H 6.69407 2.77283 0.27982
H 6.66518 2.56526 -1.48802
H 7.59412 1.44380 -0.47373
C 3.64852 2.86794 0.02067
H 2.55188 2.73549 0.01689
C 4.06636 3.41513 1.39608
H 3.80227 2.70722 2.19668
H 3.54006 4.36474 1.58833
H 5.14927 3.61725 1.45102
C 4.01194 3.82225 -1.12893
H 5.06852 4.13324 -1.10078
H 3.39703 4.73311 -1.04198
H 3.80229 3.36323 -2.10754
C -0.53323 0.47585 2.53555
C -1.70854 0.03045 2.41171
H -2.66892 -0.22262 2.84202
C 0.53344 1.19439 3.32175
C 0.77193 2.59586 2.71982
H 1.53265 3.13273 3.31296
H 1.12368 2.50407 1.67735
H -0.15205 3.19346 2.70050
C -0.03217 1.33107 4.76570
H 0.71479 1.84051 5.39980
H -0.96002 1.92410 4.78225
H -0.24169 0.34146 5.20422
C 1.86076 0.40942 3.38611
H 2.25079 0.21768 2.36889
H 2.60993 0.99778 3.94575
H 1.72973 -0.55775 3.89621

**III$_{Bu}$**
SCF (BP86) Energy = -2265.65978921
Enthalpy 0K = -2264.515316
Enthalpy 298K = -2264.441832
Free Energy 298K = -2264.625184
Lowest Frequency = 8.9740 $cm^{-1}$
Second Frequency = 16.4997 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2266.01549617
SCF (C6H6) Energy = -2265.66466621
SCF (BS2) Energy = -3077.83887609

Cu 2.21407 0.67185 0.83667
Si -3.85182 0.49974 -2.16641
Si -2.79651 -3.10498 -0.99231
Al -1.57693 -0.27095 0.11096
N -2.97594 0.72489 -0.61142
N -1.44708 -2.04114 -0.43368
N 5.01543 -0.08938 0.15107
N 4.32046 1.58556 -1.04664
C -3.32395 1.90251 0.16172
C -4.29470 1.80504 1.20831
C -4.60413 2.94555 1.97402
H -5.34043 2.86108 2.78184
C -3.99760 4.18104 1.72343
H -4.25302 5.05832 2.32749
C -3.06265 4.28022 0.68775
H -2.58647 5.24683 0.48459
C -2.71007 3.16712 -0.10045

| | | | |
|---|---|---|---|
| C | -4.99955 | 0.48798 | 1.53692 |
| H | -4.72961 | -0.22342 | 0.73685 |
| C | -4.50191 | -0.09814 | 2.87859 |
| H | -3.40932 | -0.25588 | 2.87405 |
| H | -4.98746 | -1.06763 | 3.09057 |
| H | -4.73021 | 0.58464 | 3.71630 |
| C | -6.53823 | 0.62223 | 1.54537 |
| H | -6.88704 | 1.28577 | 2.35641 |
| H | -7.01047 | -0.36378 | 1.70208 |
| H | -6.91515 | 1.03472 | 0.59420 |
| C | -1.67315 | 3.36341 | -1.20804 |
| H | -1.51669 | 2.37982 | -1.68297 |
| C | -0.31286 | 3.82637 | -0.64220 |
| H | -0.39600 | 4.80806 | -0.14206 |
| H | 0.42281 | 3.93609 | -1.46103 |
| H | 0.07673 | 3.09870 | 0.08887 |
| C | -2.16619 | 4.34756 | -2.29368 |
| H | -3.11385 | 4.01663 | -2.75056 |
| H | -1.41645 | 4.44615 | -3.09969 |
| H | -2.33521 | 5.35505 | -1.87346 |
| C | -5.26404 | 1.76923 | -2.29419 |
| H | -6.05144 | 1.56506 | -1.54961 |
| H | -5.72286 | 1.71099 | -3.29677 |
| H | -4.91894 | 2.80243 | -2.13272 |
| C | -2.68406 | 0.70728 | -3.66438 |
| H | -2.34957 | 1.75122 | -3.77947 |
| H | -3.20022 | 0.41363 | -4.59598 |
| H | -1.78561 | 0.07425 | -3.56715 |
| C | -4.65921 | -1.22410 | -2.32777 |
| H | -5.32911 | -1.38556 | -1.46191 |
| H | -5.33518 | -1.12695 | -3.20309 |
| C | -3.71938 | -2.43351 | -2.52598 |
| H | -2.98507 | -2.23384 | -3.32963 |
| H | -4.30415 | -3.30790 | -2.88163 |
| C | -4.09882 | -3.36622 | 0.37791 |
| H | -3.69361 | -3.95624 | 1.21567 |
| H | -4.97210 | -3.90896 | -0.02644 |
| H | -4.46250 | -2.40868 | 0.78673 |
| C | -2.08801 | -4.79824 | -1.49897 |
| H | -1.42321 | -4.71279 | -2.37469 |
| H | -2.91933 | -5.47334 | -1.76815 |
| H | -1.50944 | -5.27154 | -0.69012 |
| C | -0.17683 | -2.71321 | -0.26028 |
| C | 0.14878 | -3.39043 | 0.95551 |
| C | 1.36969 | -4.08946 | 1.04289 |
| H | 1.61121 | -4.61855 | 1.97237 |
| C | 2.26620 | -4.13994 | -0.02919 |
| H | 3.19493 | -4.71499 | 0.05192 |
| C | 1.95526 | -3.45917 | -1.21345 |
| H | 2.65323 | -3.49988 | -2.05720 |
| C | 0.75011 | -2.74613 | -1.35048 |
| C | -0.78258 | -3.40571 | 2.16857 |
| H | -1.67345 | -2.81149 | 1.90179 |
| C | -0.12722 | -2.73675 | 3.39712 |
| H | 0.77374 | -3.28837 | 3.72187 |
| H | -0.83105 | -2.71987 | 4.24865 |
| H | 0.16382 | -1.70052 | 3.16209 |
| C | -1.25025 | -4.83712 | 2.51972 |
| H | -1.74599 | -5.33153 | 1.66714 |
| H | -1.96255 | -4.81534 | 3.36375 |
| H | -0.39968 | -5.47395 | 2.82208 |
| C | 0.44865 | -2.00393 | -2.65225 |
| H | -0.64770 | -1.88090 | -2.69873 |
| C | 1.06640 | -0.58731 | -2.61891 |
| H | 0.73289 | -0.01579 | -1.73163 |
| H | 0.79517 | -0.01068 | -3.52204 |
| H | 2.16762 | -0.64642 | -2.55681 |
| C | 0.89306 | -2.75603 | -3.92284 |
| H | 1.99272 | -2.82468 | -4.00356 |
| H | 0.53606 | -2.22664 | -4.82356 |
| H | 0.49061 | -3.78287 | -3.94834 |
| C | 3.90391 | 0.67938 | -0.09946 |
| C | 4.98102 | -1.14391 | 1.19885 |
| H | 3.90189 | -1.22564 | 1.42689 |
| C | 5.46282 | -2.50972 | 0.68823 |
| H | 4.96363 | -2.77377 | -0.25697 |
| H | 5.20028 | -3.27901 | 1.43271 |
| H | 6.55450 | -2.54869 | 0.54411 |
| C | 5.70804 | -0.68496 | 2.47409 |
| H | 5.30867 | 0.28053 | 2.82390 |
| H | 6.79524 | -0.57813 | 2.31881 |
| H | 5.55639 | -1.42950 | 3.27338 |
| C | 6.11345 | 0.33429 | -0.61246 |
| C | 7.47414 | -0.29376 | -0.60098 |
| H | 7.86291 | -0.43423 | 0.42121 |
| H | 8.18794 | 0.35305 | -1.13472 |
| H | 7.48799 | -1.27858 | -1.10055 |
| C | 5.67087 | 1.39797 | -1.37554 |
| C | 6.43232 | 2.18761 | -2.39655 |
| H | 6.32034 | 3.27553 | -2.25734 |
| H | 6.11965 | 1.95053 | -3.42905 |
| H | 7.50672 | 1.95824 | -2.32118 |
| C | 3.40587 | 2.65997 | -1.51287 |
| H | 2.43923 | 2.36629 | -1.06196 |
| C | 3.79666 | 4.02658 | -0.92607 |
| H | 3.87820 | 3.96786 | 0.17108 |
| H | 3.01714 | 4.76673 | -1.17178 |
| H | 4.75232 | 4.40100 | -1.33041 |
| C | 3.23675 | 2.68006 | -3.03981 |
| H | 4.12922 | 3.06324 | -3.56058 |
| H | 2.39575 | 3.34509 | -3.29782 |
| H | 3.00494 | 1.67451 | -3.42559 |
| C | 0.64353 | 0.90409 | 1.92674 |
| C | -0.64743 | 0.56936 | 1.60317 |
| H | -1.43039 | 0.87808 | 2.33193 |
| C | 0.93238 | 1.63617 | 3.27541 |
| C | 1.55643 | 3.02024 | 2.96083 |
| H | 1.85432 | 3.54048 | 3.89109 |
| H | 2.45525 | 2.90639 | 2.32579 |
| H | 0.84092 | 3.66372 | 2.42047 |
| C | -0.30074 | 1.85827 | 4.18051 |
| H | -0.00046 | 2.36756 | 5.11438 |
| H | -1.06361 | 2.48628 | 3.68882 |
| H | -0.77753 | 0.90260 | 4.46066 |
| C | 1.97306 | 0.80727 | 4.07058 |
| H | 2.88171 | 0.64064 | 3.46243 |
| H | 2.26892 | 1.32985 | 5.00010 |
| H | 1.57006 | -0.18268 | 4.34620 |

**TS(III-IV)$_{Bu}$**

SCF (BP86) Energy = -2265.62351600
Enthalpy 0K = -2264.484144
Enthalpy 298K = -2264.410535
Free Energy 298K = -2264.593691
Lowest Frequency = -657.2197 $cm^{-1}$
Second Frequency = 12.2099 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2265.97578276
SCF (C6H6) Energy = -2265.62907146
SCF (BS2) Energy = -3077.80382199

| | | | |
|---|---|---|---|
| Cu | -2.32649 | -0.85328 | 0.86767 |
| Si | 3.74646 | -0.67382 | -2.16681 |
| Al | 1.63973 | 0.31036 | 0.15463 |
| Si | 3.06981 | 3.02686 | -0.90137 |
| N | -5.04239 | 0.13018 | 0.30934 |
| N | 2.85551 | -0.87294 | -0.62500 |
| N | -4.51673 | -1.49200 | -1.04138 |
| N | 1.62190 | 2.08407 | -0.40586 |
| C | -4.02153 | -0.73016 | -0.01258 |
| H | 1.59142 | -0.04277 | 1.84881 |
| C | 1.33407 | -3.36789 | -1.26159 |
| H | 1.22961 | -2.35324 | -1.68285 |
| C | 2.36624 | -3.27788 | -0.13540 |
| C | 0.38564 | 2.82226 | -0.30389 |
| C | 4.05980 | -2.08332 | 1.19975 |
| C | 3.94612 | 2.28903 | -2.43391 |
| H | 3.20502 | 2.20242 | -3.25175 |
| H | 4.64069 | 3.09241 | -2.75863 |
| C | 4.72765 | 0.96678 | -2.26234 |
| H | 5.39740 | 1.01969 | -1.38254 |
| H | 5.40483 | 0.82011 | -3.13030 |
| C | 3.09233 | -2.07597 | 0.14314 |
| C | 4.35437 | 3.13457 | 0.50622 |
| H | 3.98392 | 3.75354 | 1.33990 |

| | | | |
|---|---|---|---|
| H | 5.29246 | 3.58771 | 0.13859 |
| H | 4.60194 | 2.14033 | 0.91461 |
| C | 3.54503 | -4.43168 | 1.67896 |
| H | 3.71850 | -5.33757 | 2.26998 |
| C | -3.70567 | -2.59398 | -1.62199 |
| H | -2.72486 | -2.45700 | -1.13080 |
| C | 0.04206 | 3.52851 | 0.89237 |
| C | 5.04283 | -2.05903 | -2.34794 |
| H | 5.90053 | -1.89151 | -1.67542 |
| H | 5.42590 | -2.07178 | -3.38346 |
| H | 4.63550 | -3.05608 | -2.11912 |
| C | -4.89856 | 1.08218 | 1.44419 |
| H | -3.83311 | 0.96777 | 1.72020 |
| C | 4.25809 | -3.25886 | 1.94968 |
| H | 4.99724 | -3.25295 | 2.75969 |
| C | 0.91050 | 3.47558 | 2.15049 |
| H | 1.76524 | 2.81432 | 1.92678 |
| C | -6.16464 | -0.09004 | -0.50112 |
| C | -0.72236 | -0.94774 | 1.94409 |
| C | -0.05315 | -3.80649 | -0.74509 |
| H | -0.02368 | -4.81952 | -0.30494 |
| H | -0.77616 | -3.83584 | -1.58192 |
| H | -0.42850 | -3.10910 | 0.02228 |
| C | -5.83043 | -1.12087 | -1.36012 |
| C | 1.79850 | -4.31704 | -2.39103 |
| H | 2.76359 | -4.00432 | -2.82218 |
| H | 1.05488 | -4.34553 | -3.20850 |
| H | 1.92151 | -5.34939 | -2.01706 |
| C | 2.61196 | -4.43092 | 0.63688 |
| H | 2.05689 | -5.34964 | 0.41207 |
| C | 4.90632 | -0.85609 | 1.54144 |
| H | 4.62214 | -0.06648 | 0.82380 |
| C | 0.11667 | -0.35855 | 1.12660 |
| C | -0.50141 | 2.88880 | -1.42508 |
| C | -5.74775 | 0.64968 | 2.65110 |
| H | -5.49934 | 1.28364 | 3.51838 |
| H | -5.53913 | -0.39847 | 2.92022 |
| H | -6.82975 | 0.75340 | 2.46376 |
| C | -0.21574 | 2.11568 | -2.71110 |
| H | 0.81619 | 1.73438 | -2.62224 |
| C | -1.13859 | 4.29681 | 0.92525 |
| H | -1.38643 | 4.84890 | 1.83994 |
| C | 2.57959 | -0.72873 | -3.67944 |
| H | 2.15594 | -1.73622 | -3.82455 |
| H | 3.13051 | -0.45850 | -4.59825 |
| H | 1.73869 | -0.02267 | -3.57487 |
| C | 4.61684 | -0.33095 | 2.96550 |
| H | 4.88233 | -1.08214 | 3.73099 |
| H | 3.54822 | -0.08568 | 3.08322 |
| H | 5.20789 | 0.57940 | 3.17286 |
| C | -6.65745 | -1.71938 | -2.45703 |
| H | -6.30709 | -1.41506 | -3.45919 |
| H | -7.70228 | -1.38518 | -2.36198 |
| H | -6.66298 | -2.82123 | -2.42677 |
| C | -1.15733 | 0.89472 | -2.83479 |
| H | -1.08679 | 0.24686 | -1.94351 |
| H | -0.90635 | 0.29168 | -3.72660 |
| H | -2.20945 | 1.22138 | -2.92702 |
| C | 2.54303 | 4.79084 | -1.38970 |
| H | 1.90300 | 4.78716 | -2.28769 |
| H | 3.44147 | 5.39160 | -1.61563 |
| H | 1.98276 | 5.29898 | -0.58896 |
| C | 0.14125 | 2.85297 | 3.33702 |
| H | -0.72184 | 3.47796 | 3.63080 |
| H | 0.79915 | 2.75856 | 4.21950 |
| H | -0.23323 | 1.85112 | 3.07170 |
| C | -4.24521 | -3.97291 | -1.20756 |
| H | -5.21747 | -4.20360 | -1.67457 |
| H | -4.35894 | -4.03306 | -0.11316 |
| H | -3.53180 | -4.75278 | -1.52153 |
| C | 1.46529 | 4.86465 | 2.53957 |
| H | 2.05576 | 5.31471 | 1.72386 |
| H | 2.11638 | 4.78719 | 3.42865 |
| H | 0.65039 | 5.56886 | 2.78633 |
| C | -5.12166 | 2.54258 | 1.02771 |
| H | -6.17504 | 2.75857 | 0.78643 |
| H | -4.48834 | 2.80669 | 0.16639 |
| H | -4.83347 | 3.19820 | 1.86580 |
| C | 6.41794 | -1.12989 | 1.36935 |
| H | 7.00216 | -0.21131 | 1.55680 |
| H | 6.65640 | -1.48558 | 0.35305 |
| H | 6.77132 | -1.89817 | 2.08010 |
| C | -0.28968 | 2.99094 | -3.98010 |
| H | -1.31036 | 3.37474 | -4.15762 |
| H | -0.00088 | 2.40450 | -4.87039 |
| H | 0.38522 | 3.86084 | -3.91210 |
| C | -3.50125 | -2.44580 | -3.13719 |
| H | -2.73118 | -3.16332 | -3.46585 |
| H | -3.15109 | -1.43238 | -3.39054 |
| H | -4.41697 | -2.66069 | -3.71137 |
| C | -1.67368 | 3.66377 | -1.34039 |
| H | -2.33992 | 3.71952 | -2.20975 |
| C | -7.44126 | 0.69276 | -0.44630 |
| H | -7.83172 | 0.79021 | 0.57981 |
| H | -8.21567 | 0.18658 | -1.04338 |
| H | -7.32545 | 1.71139 | -0.85688 |
| C | -1.99305 | 4.37974 | -0.18009 |
| H | -2.89381 | 5.00255 | -0.14077 |
| C | -0.67571 | -1.50338 | 3.36903 |
| C | -0.94726 | -3.02786 | 3.28827 |
| H | -0.16280 | -3.53614 | 2.70332 |
| H | -0.96385 | -3.46783 | 4.30240 |
| H | -1.92088 | -3.22676 | 2.80568 |
| C | -1.79455 | -0.84035 | 4.21001 |
| H | -1.81525 | -1.26720 | 5.22937 |
| H | -1.63619 | 0.24814 | 4.29690 |
| H | -2.78303 | -1.00749 | 3.74460 |
| C | 0.68811 | -1.26820 | 4.04848 |
| H | 0.67837 | -1.69461 | 5.06775 |
| H | 1.50667 | -1.74480 | 3.48423 |
| H | 0.91908 | -0.19280 | 4.13130 |

**$IV_{Bu}$**

SCF (BP86) Energy = -2265.64860749
Enthalpy 0K = -2264.507754
Enthalpy 298K = -2264.433706
Free Energy 298K = -2264.617409
Lowest Frequency = 7.1646 $cm^{-1}$
Second Frequency = 18.0949 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2266.00902988
SCF (C6H6) Energy = -2265.65583773
SCF (BS2) Energy = -3077.82934187

| | | | |
|---|---|---|---|
| Cu | -1.89305 | -0.62126 | 0.42103 |
| Si | 3.89761 | -0.00571 | -1.90657 |
| Al | 1.73456 | 0.49778 | 0.56036 |
| Si | 2.59262 | 3.41597 | -0.41001 |
| N | -4.81033 | -0.08300 | 0.44966 |
| N | 2.97210 | -0.52716 | -0.47024 |
| N | -4.24094 | -1.38653 | -1.19854 |
| N | 1.29797 | 2.20026 | -0.16636 |
| C | -3.72310 | -0.67082 | -0.14717 |
| H | 2.23353 | 0.60501 | 2.09572 |
| C | 1.75671 | -2.96336 | -1.68678 |
| H | 1.59158 | -1.89789 | -1.92101 |
| C | 2.67218 | -3.00806 | -0.46136 |
| C | -0.04371 | 2.69880 | -0.14722 |
| C | 4.16190 | -1.96565 | 1.20299 |
| C | 3.73259 | 2.97784 | -1.88191 |
| H | 3.11056 | 2.88401 | -2.79271 |
| H | 4.34828 | 3.88836 | -2.04190 |
| C | 4.65376 | 1.74628 | -1.72346 |
| H | 5.20140 | 1.78756 | -0.76225 |
| H | 5.44271 | 1.76997 | -2.50499 |
| C | 3.26701 | -1.82136 | 0.08823 |
| C | 3.70914 | 3.57221 | 1.13285 |
| H | 3.17262 | 4.04923 | 1.96983 |
| H | 4.60033 | 4.18449 | 0.90593 |
| H | 4.05536 | 2.58600 | 1.48551 |
| C | 3.81933 | -4.39775 | 1.20093 |
| H | 4.03480 | -5.38424 | 1.62623 |
| C | -3.36893 | -2.24925 | -2.04223 |
| H | -2.35184 | -1.96839 | -1.71279 |
| C | -0.64173 | 3.20367 | 1.05709 |

| | | | |
|---|---|---|---|
| C | 5.38719 | -1.16919 | -2.19098 |
| H | 6.23264 | -0.90358 | -1.53468 |
| H | 5.73485 | -1.07374 | -3.23482 |
| H | 5.14372 | -2.22734 | -2.00546 |
| C | -4.66148 | 0.71228 | 1.70025 |
| H | -3.56831 | 0.85933 | 1.77123 |
| C | 4.40746 | -3.24714 | 1.73592 |
| H | 5.09463 | -3.34237 | 2.58529 |
| C | 0.09046 | 3.17858 | 2.40072 |
| H | 1.07432 | 2.70979 | 2.22790 |
| C | -5.99618 | -0.43078 | -0.21000 |
| C | -0.46832 | -1.49693 | 1.69483 |
| C | 0.37744 | -3.60486 | -1.42248 |
| H | 0.46501 | -4.67845 | -1.17460 |
| H | -0.25738 | -3.52953 | -2.32564 |
| H | -0.13688 | -3.09879 | -0.58931 |
| C | -5.63425 | -1.25694 | -1.25859 |
| C | 2.41693 | -3.64147 | -2.91035 |
| H | 3.39342 | -3.19140 | -3.15150 |
| H | 1.77147 | -3.55635 | -3.80399 |
| H | 2.58617 | -4.71730 | -2.72271 |
| C | 2.96250 | -4.26621 | 0.10208 |
| H | 2.51189 | -5.16408 | -0.33913 |
| C | 4.91759 | -0.78474 | 1.81917 |
| H | 4.56220 | 0.12645 | 1.30795 |
| C | 0.03011 | -0.61191 | 0.93956 |
| C | -0.81080 | 2.75232 | -1.35908 |
| C | -5.12480 | -0.09583 | 2.92398 |
| H | -4.87488 | 0.45621 | 3.84509 |
| H | -4.62258 | -1.07604 | 2.96154 |
| H | -6.21495 | -0.26486 | 2.92251 |
| C | -0.24921 | 2.20090 | -2.66616 |
| H | 0.80575 | 1.95362 | -2.46026 |
| C | -1.93075 | 3.77161 | 1.00824 |
| H | -2.36155 | 4.18529 | 1.92884 |
| C | 2.88679 | 0.00504 | -3.53310 |
| H | 2.66884 | -1.01596 | -3.88620 |
| H | 3.46504 | 0.51627 | -4.32434 |
| H | 1.92849 | 0.53646 | -3.42270 |
| C | 4.63101 | -0.62282 | 3.32802 |
| H | 4.96429 | -1.50629 | 3.90251 |
| H | 3.55470 | -0.47065 | 3.50610 |
| H | 5.17018 | 0.25416 | 3.72947 |
| C | -6.51832 | -1.87034 | -2.30151 |
| H | -6.41250 | -1.37453 | -3.28239 |
| H | -7.57271 | -1.77425 | -1.99974 |
| H | -6.31659 | -2.94404 | -2.44670 |
| C | -0.96964 | 0.89440 | -3.06544 |
| H | -0.89012 | 0.14231 | -2.25968 |
| H | -0.53391 | 0.46150 | -3.98408 |
| H | -2.04336 | 1.08274 | -3.25151 |
| C | 1.83488 | 5.12321 | -0.79424 |
| H | 1.29648 | 5.12243 | -1.75661 |
| H | 2.63973 | 5.87648 | -0.85710 |
| H | 1.12199 | 5.44793 | -0.01931 |
| C | -0.65290 | 2.30871 | 3.43892 |
| H | -1.65424 | 2.71941 | 3.66780 |
| H | -0.08588 | 2.26648 | 4.38607 |
| H | -0.77552 | 1.27761 | 3.06832 |
| C | -3.57273 | -3.73773 | -1.71503 |
| H | -4.56587 | -4.10344 | -2.02543 |
| H | -3.45340 | -3.91991 | -0.63511 |
| H | -2.81478 | -4.33483 | -2.24800 |
| C | 0.32610 | 4.59841 | 2.96443 |
| H | 0.89310 | 5.22864 | 2.25910 |
| H | 0.89567 | 4.54951 | 3.90967 |
| H | -0.62764 | 5.11446 | 3.17821 |
| C | -5.31358 | 2.09897 | 1.61235 |
| H | -6.41323 | 2.05584 | 1.65881 |
| H | -5.00378 | 2.61877 | 0.69322 |
| H | -4.97049 | 2.70273 | 2.46831 |
| C | 6.44212 | -0.90739 | 1.58612 |
| H | 6.96697 | -0.01801 | 1.97874 |
| H | 6.68673 | -1.00537 | 0.51606 |
| H | 6.85559 | -1.79275 | 2.10215 |
| C | -0.29152 | 3.21672 | -3.82745 |
| H | -1.32751 | 3.47900 | -4.10915 |
| H | 0.19705 | 2.79730 | -4.72487 |
| H | 0.22826 | 4.15323 | -3.56465 |
| C | -3.48506 | -1.93460 | -3.54107 |
| H | -2.66461 | -2.44205 | -4.07447 |
| H | -3.39103 | -0.85347 | -3.72813 |
| H | -4.43138 | -2.29277 | -3.97664 |
| C | -2.09738 | 3.32385 | -1.35565 |
| H | -2.65903 | 3.37921 | -2.29638 |
| C | -7.36741 | 0.04992 | 0.15635 |
| H | -7.58017 | -0.06678 | 1.23155 |
| H | -8.12449 | -0.53275 | -0.39087 |
| H | -7.52125 | 1.11218 | -0.10174 |
| C | -2.65823 | 3.85078 | -0.18617 |
| H | -3.63943 | 4.33875 | -0.21033 |
| C | -0.71229 | -2.52524 | 2.74584 |
| C | -1.63043 | -3.65642 | 2.22024 |
| H | -1.17969 | -4.15830 | 1.34865 |
| H | -1.78430 | -4.40971 | 3.01262 |
| H | -2.61715 | -3.25962 | 1.92345 |
| C | -1.36307 | -1.85599 | 3.98426 |
| H | -1.51223 | -2.60744 | 4.77967 |
| H | -0.72231 | -1.05160 | 4.37956 |
| H | -2.34493 | -1.42127 | 3.73074 |
| C | 0.67390 | -3.10917 | 3.13568 |
| H | 0.54033 | -3.86022 | 3.93472 |
| H | 1.16457 | -3.58983 | 2.27466 |
| H | 1.34335 | -2.31712 | 3.50632 |

**$V_{Bu}$**

SCF (BP86) Energy = -2265.66982162
Enthalpy 0K = -2264.527603
Enthalpy 298K = -2264.454202
Free Energy 298K = -2264.633859
Lowest Frequency = 15.1349 $cm^{-1}$
Second Frequency = 18.4728 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2266.03900020
SCF (C6H6) Energy = -2265.67408047
SCF (BS2) Energy = -3077.85070970

| | | | |
|---|---|---|---|
| Cu | -1.46714 | -0.08352 | 0.30081 |
| Al | 1.18246 | -0.08186 | 0.13308 |
| Si | 3.84528 | 1.54647 | 0.95630 |
| Si | 3.69247 | -1.69665 | -1.31369 |
| N | 2.16895 | 1.50802 | 0.31998 |
| N | 2.08013 | -1.59580 | -0.54197 |
| N | -3.72910 | 1.48118 | -0.77177 |
| C | 1.24589 | -2.77339 | -0.52744 |
| N | -4.32874 | -0.59689 | -0.53814 |
| C | -3.26263 | 0.25561 | -0.36346 |
| C | 0.00947 | -0.52855 | 1.67976 |
| C | 1.53825 | 2.77498 | 0.05455 |
| C | 0.40652 | 5.34491 | -0.47418 |
| H | -0.00704 | 6.34056 | -0.66987 |
| C | 1.28794 | -3.68652 | 0.57848 |
| C | -1.08096 | -0.65523 | 2.31544 |
| C | -5.24158 | -2.51749 | 0.80338 |
| H | -6.26324 | -2.56272 | 0.39306 |
| H | -5.24662 | -1.86039 | 1.68762 |
| H | -4.97766 | -3.53516 | 1.13623 |
| C | -3.21653 | -0.08550 | 3.51661 |
| H | -3.85659 | -0.36492 | 4.37233 |
| H | -3.79737 | -0.19702 | 2.58654 |
| H | -2.94728 | 0.97840 | 3.62019 |
| C | 1.01901 | 4.61249 | -1.49830 |
| H | 1.07803 | 5.03963 | -2.50688 |
| C | 0.88370 | 3.51532 | 1.09484 |
| C | 0.34403 | 4.78680 | 0.80783 |
| H | -0.12704 | 5.35679 | 1.61797 |
| C | 1.58821 | 3.34692 | -1.25963 |
| C | -5.06236 | 1.40358 | -1.19877 |
| C | -4.21445 | -2.04838 | -0.24076 |
| H | -3.20389 | -2.12860 | 0.19996 |
| C | -4.23965 | -2.90608 | -1.51633 |
| H | -5.24175 | -2.94615 | -1.97519 |
| H | -3.94682 | -3.93812 | -1.26272 |
| H | -3.52438 | -2.52262 | -2.25861 |
| C | 2.31993 | -3.56434 | 1.70324 |

| | | | |
|---|---|---|---|
| H | 2.97105 | -2.71093 | 1.44453 |
| C | 5.11301 | 0.63600 | -0.15293 |
| H | 5.06637 | 1.07965 | -1.16617 |
| H | 6.09651 | 0.95349 | 0.25444 |
| C | -1.95153 | -0.97673 | 3.48978 |
| C | -2.83600 | 2.67190 | -0.78678 |
| H | -1.90685 | 2.29245 | -0.32328 |
| C | -5.88975 | 2.56080 | -1.66998 |
| H | -5.37939 | 3.15485 | -2.44518 |
| H | -6.15672 | 3.24669 | -0.84677 |
| H | -6.83147 | 2.19336 | -2.10652 |
| C | 0.34598 | -3.04594 | -1.61122 |
| C | -5.44369 | 0.08445 | -1.05314 |
| C | -2.48787 | 3.10756 | -2.21839 |
| H | -2.12726 | 2.25062 | -2.80883 |
| H | -1.67903 | 3.85477 | -2.17321 |
| H | -3.34539 | 3.56305 | -2.74214 |
| C | 0.74982 | 2.98754 | 2.52600 |
| H | 1.12868 | 1.95115 | 2.52809 |
| C | 2.25888 | 2.61842 | -2.42090 |
| H | 2.71222 | 1.71048 | -1.98925 |
| C | -3.36551 | 3.81927 | 0.08589 |
| H | -4.23121 | 4.32979 | -0.36708 |
| H | -2.56037 | 4.56192 | 0.20741 |
| H | -3.65097 | 3.45771 | 1.08715 |
| C | 3.91640 | 0.73381 | 2.68229 |
| H | 3.37511 | 1.33163 | 3.43388 |
| H | 4.96116 | 0.62128 | 3.02274 |
| H | 3.46011 | -0.27128 | 2.66656 |
| C | 0.38731 | -4.76869 | 0.61552 |
| H | 0.41892 | -5.45626 | 1.46935 |
| C | -1.13091 | -0.74143 | 4.78717 |
| H | -1.74952 | -0.97956 | 5.67100 |
| H | -0.80601 | 0.30885 | 4.86275 |
| H | -0.23384 | -1.38084 | 4.80804 |
| C | 5.05602 | -0.90587 | -0.23116 |
| H | 5.00050 | -1.34887 | 0.78180 |
| H | 6.00273 | -1.29239 | -0.66418 |
| C | -2.36319 | -2.47088 | 3.41489 |
| H | -1.47556 | -3.12297 | 3.39939 |
| H | -2.94964 | -2.67536 | 2.50512 |
| H | -2.98038 | -2.73491 | 4.29238 |
| C | 1.57715 | 3.81282 | 3.53930 |
| H | 1.24609 | 4.86686 | 3.56099 |
| H | 2.65198 | 3.80663 | 3.29809 |
| H | 1.45759 | 3.40535 | 4.55933 |
| C | 1.22891 | 2.17368 | -3.48344 |
| H | 0.45447 | 1.52794 | -3.03603 |
| H | 1.72200 | 1.60811 | -4.29434 |
| H | 0.72526 | 3.04468 | -3.94078 |
| C | 1.68007 | -3.26757 | 3.07724 |
| H | 1.00753 | -4.08931 | 3.38583 |
| H | 1.09471 | -2.33588 | 3.04584 |
| H | 2.45940 | -3.16892 | 3.85447 |
| C | 3.38720 | 3.44951 | -3.07020 |
| H | 2.99681 | 4.36464 | -3.55066 |
| H | 3.90057 | 2.86059 | -3.85104 |
| H | 4.14057 | 3.76031 | -2.32676 |
| C | 4.18679 | -3.52240 | -1.56479 |
| H | 4.58043 | -3.96540 | -0.63578 |
| H | 4.98353 | -3.58236 | -2.32675 |
| H | 3.34353 | -4.14545 | -1.90437 |
| C | 3.80625 | -0.87423 | -3.03756 |
| H | 3.23530 | -1.43510 | -3.79500 |
| H | 4.86344 | -0.85976 | -3.36033 |
| H | 3.44326 | 0.16519 | -3.04330 |
| C | 0.36844 | -2.22776 | -2.90443 |
| H | 1.02485 | -1.35989 | -2.72338 |
| C | -0.72626 | 2.94861 | 2.97831 |
| H | -0.80533 | 2.52346 | 3.99502 |
| H | -1.33279 | 2.32432 | 2.30167 |
| H | -1.17127 | 3.95937 | 3.01049 |
| C | 3.19499 | -4.83580 | 1.81183 |
| H | 4.01116 | -4.68158 | 2.54004 |
| H | 3.64292 | -5.11440 | 0.84471 |
| H | 2.60201 | -5.69998 | 2.16176 |
| C | -6.78204 | -0.52681 | -1.33855 |
| H | -7.33662 | -0.77830 | -0.41706 |
| H | -6.70655 | -1.44510 | -1.94325 |
| H | -7.40178 | 0.18510 | -1.90558 |
| C | -0.52981 | -4.99978 | -0.41657 |
| H | -1.21552 | -5.85338 | -0.36946 |
| C | -0.52777 | -4.14884 | -1.52790 |
| H | -1.20707 | -4.35296 | -2.36449 |
| C | -1.01394 | -1.68717 | -3.32357 |
| H | -0.91824 | -1.04175 | -4.21518 |
| H | -1.47016 | -1.09057 | -2.51567 |
| H | -1.70547 | -2.50716 | -3.59137 |
| C | 4.47907 | 3.34338 | 1.03417 |
| H | 4.68844 | 3.72519 | 0.02041 |
| H | 5.42349 | 3.37608 | 1.60531 |
| H | 3.76793 | 4.03896 | 1.50480 |
| C | 0.97210 | -3.06165 | -4.06055 |
| H | 0.33473 | -3.93482 | -4.28972 |
| H | 1.97569 | -3.44350 | -3.81079 |
| H | 1.05395 | -2.45568 | -4.98108 |
| H | -0.23073 | 0.29568 | -0.83971 |

**$VI_{Bu}$**

SCF (BP86) Energy = -2500.22536733
Enthalpy 0K = -2498.945831
Enthalpy 298K = -2498.862882
Free Energy 298K = -2499.063243
Lowest Frequency = 16.5878 $cm^{-1}$
Second Frequency = 17.6092 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2500.63831815
SCF (C6H6) Energy = -2500.23240616
SCF (BS2) Energy = -3312.46112005

| | | | |
|---|---|---|---|
| Cu | -2.01667 | -0.10990 | -0.29142 |
| Si | 3.81490 | -1.70344 | -1.81937 |
| Al | 1.62776 | 0.03273 | -0.00733 |
| Si | 3.95954 | 2.19856 | -0.97235 |
| N | -4.75632 | -1.37783 | 0.09663 |
| N | 2.80015 | -1.44261 | -0.37620 |
| N | -4.85535 | 0.78961 | -0.04496 |
| N | 2.30222 | 1.80520 | -0.42405 |
| C | -3.97300 | -0.26343 | -0.10368 |
| H | 1.20006 | -0.09372 | 1.54043 |
| C | 0.89603 | -3.75572 | -0.59386 |
| H | 0.94642 | -2.83331 | -1.19717 |
| C | 1.96224 | -3.64065 | 0.49519 |
| C | 1.48055 | 2.88449 | 0.05921 |
| C | 3.76459 | -2.48042 | 1.68926 |
| C | 4.51415 | 1.10373 | -2.44248 |
| H | 3.69392 | 1.05001 | -3.18383 |
| H | 5.30073 | 1.71751 | -2.92995 |
| C | 5.07853 | -0.30196 | -2.12856 |
| H | 5.77834 | -0.25744 | -1.27267 |
| H | 5.68742 | -0.66241 | -2.98454 |
| C | 2.83172 | -2.50644 | 0.60074 |
| C | 5.35837 | 2.07329 | 0.33227 |
| H | 5.37266 | 1.12421 | 0.88777 |
| H | 5.30569 | 2.89415 | 1.06477 |
| H | 6.32573 | 2.16512 | -0.19608 |
| C | 2.99068 | -4.67095 | 2.46959 |
| H | 3.05874 | -5.50448 | 3.17739 |
| C | -4.40398 | 2.18348 | -0.30607 |
| H | -3.30936 | 2.07187 | -0.39901 |
| C | 1.54193 | 3.32103 | 1.43107 |
| C | 4.81463 | -3.32127 | -1.67711 |
| H | 5.53150 | -3.28756 | -0.84052 |
| H | 5.38587 | -3.48179 | -2.60851 |
| H | 4.16910 | -4.19911 | -1.51490 |
| C | -4.18226 | -2.74704 | 0.01501 |
| H | -3.10415 | -2.55137 | -0.12570 |
| C | 3.82584 | -3.55658 | 2.59469 |
| H | 4.55313 | -3.51695 | 3.41484 |
| C | 2.53490 | 2.74746 | 2.44309 |
| H | 3.10090 | 1.95052 | 1.93332 |
| C | -6.10280 | -1.02797 | 0.29126 |
| C | -0.95277 | -0.52295 | -2.03024 |
| C | -0.51573 | -3.83020 | 0.02861 |
| H | -0.62366 | -4.71500 | 0.68188 |

| | | | |
|---|---|---|---|
| H | -1.28331 | -3.90093 | -0.76345 |
| H | -0.72024 | -2.93144 | 0.63537 |
| C | -6.16442 | 0.34865 | 0.20028 |
| C | 1.13202 | -4.96637 | -1.52510 |
| H | 2.11358 | -4.90945 | -2.02387 |
| H | 0.35522 | -5.01735 | -2.31034 |
| H | 1.09917 | -5.91870 | -0.96582 |
| C | 2.06365 | -4.69609 | 1.42382 |
| H | 1.39783 | -5.56179 | 1.31803 |
| C | 4.70306 | -1.29993 | 1.91298 |
| H | 4.47711 | -0.57785 | 1.11109 |
| C | -0.11550 | -0.22511 | -1.12232 |
| C | 0.55722 | 3.56961 | -0.81276 |
| C | -4.69338 | -3.50891 | -1.22034 |
| H | -4.09072 | -4.42214 | -1.35812 |
| H | -4.60264 | -2.89722 | -2.13167 |
| H | -5.74470 | -3.82350 | -1.11417 |
| C | 0.43838 | 3.27613 | -2.31151 |
| H | 1.07293 | 2.39675 | -2.51944 |
| C | 0.69368 | 4.35011 | 1.88657 |
| H | 0.75866 | 4.66044 | 2.93614 |
| C | 2.76423 | -1.79050 | -3.41233 |
| H | 2.04064 | -2.62192 | -3.38177 |
| H | 3.40499 | -1.92298 | -4.30221 |
| H | 2.20200 | -0.85091 | -3.54053 |
| C | 4.42787 | -0.61375 | 3.26861 |
| H | 4.66533 | -1.28412 | 4.11467 |
| H | 3.36829 | -0.32450 | 3.35178 |
| H | 5.04761 | 0.29452 | 3.38025 |
| C | -7.36096 | 1.23479 | 0.37186 |
| H | -7.33053 | 1.79887 | 1.32057 |
| H | -8.27810 | 0.62591 | 0.38378 |
| H | -7.46626 | 1.96558 | -0.44614 |
| C | -1.01365 | 2.95067 | -2.72569 |
| H | -1.40448 | 2.08187 | -2.17342 |
| H | -1.06602 | 2.72549 | -3.80642 |
| H | -1.68231 | 3.81282 | -2.54815 |
| C | 4.08499 | 4.01021 | -1.57470 |
| H | 5.13319 | 4.34387 | -1.47852 |
| H | 3.45823 | 4.69899 | -0.98482 |
| H | 3.80435 | 4.10874 | -2.63572 |
| C | 1.82896 | 2.11576 | 3.66218 |
| H | 1.21402 | 2.85770 | 4.20364 |
| H | 2.57258 | 1.71768 | 4.37480 |
| H | 1.17957 | 1.28739 | 3.33639 |
| C | -4.93733 | 2.71251 | -1.64796 |
| H | -6.02215 | 2.90858 | -1.62477 |
| H | -4.72712 | 2.00072 | -2.46171 |
| H | -4.43455 | 3.66405 | -1.88685 |
| C | 3.52841 | 3.83551 | 2.91614 |
| H | 4.01573 | 4.34459 | 2.06791 |
| H | 4.31563 | 3.39360 | 3.55259 |
| H | 3.01583 | 4.61161 | 3.51299 |
| C | -4.35631 | -3.55269 | 1.31227 |
| H | -5.39802 | -3.87660 | 1.46883 |
| H | -4.03127 | -2.97471 | 2.19133 |
| H | -3.73271 | -4.45999 | 1.25507 |
| C | 6.19309 | -1.69175 | 1.80094 |
| H | 6.83952 | -0.80529 | 1.93302 |
| H | 6.42640 | -2.13701 | 0.81928 |
| H | 6.47542 | -2.42712 | 2.57588 |
| C | 0.92321 | 4.46995 | -3.17015 |
| H | 0.25394 | 5.34026 | -3.04170 |
| H | 0.91672 | 4.20313 | -4.24246 |
| H | 1.93842 | 4.79290 | -2.90170 |
| C | -4.67706 | 3.12847 | 0.87297 |
| H | -4.15142 | 4.08091 | 0.69483 |
| H | -4.28911 | 2.70106 | 1.81051 |
| H | -5.74819 | 3.35755 | 0.99368 |
| C | -0.26344 | 4.59803 | -0.30155 |
| H | -0.94640 | 5.11678 | -0.98513 |
| C | -7.21579 | -1.98633 | 0.58983 |
| H | -7.27902 | -2.80650 | -0.14378 |
| H | -8.17970 | -1.45509 | 0.56610 |
| H | -7.11988 | -2.44102 | 1.59136 |
| C | -0.21371 | 4.99158 | 1.03941 |
| H | -0.85728 | 5.79614 | 1.41218 |
| C | -1.84032 | 0.76875 | 2.37041 |
| C | -1.43701 | 1.38699 | 1.38233 |
| H | -0.94057 | 2.12817 | 0.76752 |
| C | -2.23900 | 0.00219 | 3.56511 |
| C | -1.73828 | 0.77934 | 4.81661 |
| H | -0.64367 | 0.89461 | 4.79944 |
| H | -2.19220 | 1.78269 | 4.86945 |
| H | -2.01948 | 0.22098 | 5.72668 |
| C | -1.56226 | -1.39358 | 3.51964 |
| H | -1.79952 | -1.95535 | 4.44019 |
| H | -1.91747 | -1.97531 | 2.65307 |
| H | -0.46864 | -1.29791 | 3.43023 |
| C | -3.78107 | -0.14072 | 3.63962 |
| H | -4.26639 | 0.84632 | 3.72280 |
| H | -4.18001 | -0.64557 | 2.74549 |
| H | -4.05545 | -0.73338 | 4.52992 |
| C | -1.53092 | -0.93285 | -3.35735 |
| C | -2.94706 | -0.34731 | -3.57793 |
| H | -3.64268 | -0.67324 | -2.78789 |
| H | -2.92047 | 0.75497 | -3.57701 |
| H | -3.33724 | -0.68110 | -4.55572 |
| C | -0.60409 | -0.42034 | -4.49223 |
| H | -1.03909 | -0.69264 | -5.47060 |
| H | -0.49500 | 0.67454 | -4.45358 |
| H | 0.39596 | -0.87277 | -4.42264 |
| C | -1.59903 | -2.47989 | -3.42998 |
| H | -0.59932 | -2.92420 | -3.30029 |
| H | -1.99478 | -2.79286 | -4.41282 |
| H | -2.25893 | -2.88549 | -2.64652 |

**TS(E)$_{Bu}$**

SCF (BP86) Energy = -2500.21084028
Enthalpy 0K = -2498.932201
Enthalpy 298K = -2498.850279
Free Energy 298K = -2499.046440
Lowest Frequency = -165.3391 $cm^{-1}$
Second Frequency = 10.7565 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2500.62569856
SCF (C6H6) Energy = -2500.21667501
SCF (BS2) Energy = -3312.44672491

| | | | |
|---|---|---|---|
| Cu | 2.13231 | -0.47796 | 0.02489 |
| Si | -3.89134 | -0.19820 | 2.01504 |
| Al | -1.39335 | 0.12408 | -0.07226 |
| Si | -3.40620 | 2.65705 | -0.55525 |
| N | 4.98423 | -1.56338 | 0.01032 |
| N | -2.86286 | -0.84519 | 0.69803 |
| N | 4.91171 | 0.60026 | -0.19252 |
| N | -1.75190 | 2.00613 | -0.27754 |
| C | 4.11120 | -0.50096 | -0.01173 |
| H | -1.01190 | -0.69627 | -1.45256 |
| C | -1.21267 | -3.09454 | 1.83393 |
| H | -1.08713 | -2.00874 | 1.97672 |
| C | -2.39294 | -3.30123 | 0.88500 |
| C | -0.69477 | 2.97913 | -0.40270 |
| C | -4.22017 | -2.54402 | -0.56936 |
| C | -4.57284 | 2.50173 | 0.96313 |
| H | -4.05145 | 2.99535 | 1.80627 |
| H | -5.41529 | 3.18309 | 0.71641 |
| C | -5.13137 | 1.13571 | 1.41609 |
| H | -5.73886 | 0.68839 | 0.60813 |
| H | -5.83868 | 1.28559 | 2.25910 |
| C | -3.14470 | -2.21265 | 0.32631 |
| C | -4.20455 | 1.87229 | -2.10623 |
| H | -3.83590 | 0.85228 | -2.28899 |
| H | -3.96359 | 2.47506 | -2.99831 |
| H | -5.30456 | 1.82697 | -2.01873 |
| C | -3.77789 | -4.94316 | -0.30228 |
| H | -4.02436 | -5.98487 | -0.53512 |
| C | 4.30848 | 1.94881 | -0.38671 |
| H | 3.24223 | 1.78110 | -0.14550 |
| C | -0.01871 | 3.19014 | -1.65398 |
| C | -4.93060 | -1.58514 | 2.81361 |
| H | -5.61472 | -2.07218 | 2.10085 |
| H | -5.53559 | -1.16137 | 3.63479 |
| H | -4.28845 | -2.37398 | 3.23852 |
| C | 4.48099 | -2.95985 | 0.10576 |

H 3.41511 -2.81925 0.36132
C -4.51039 -3.89200 -0.85934
H -5.34017 -4.11751 -1.54006
C -0.40834 2.45523 -2.94026
H -1.05806 1.61062 -2.65263
C 6.31239 -1.13545 -0.16095
C 1.23728 -0.18618 1.88970
C 0.08896 -3.64532 1.20853
H 0.00952 -4.72887 1.00583
H 0.94475 -3.49706 1.89030
H 0.31951 -3.13353 0.25958
C 6.26480 0.23883 -0.28914
C -1.45534 -3.73459 3.21977
H -2.35769 -3.32512 3.70392
H -0.59687 -3.54948 3.89148
H -1.58608 -4.82920 3.14670
C -2.72426 -4.63200 0.56053
H -2.13962 -5.44555 1.00704
C -5.09325 -1.48771 -1.24508
H -4.70691 -0.50643 -0.92856
C 0.36303 -0.05039 0.97913
C -0.33237 3.82469 0.70207
C 5.14492 -3.76530 1.23523
H 4.55975 -4.68322 1.40966
H 5.16843 -3.19502 2.17742
H 6.17228 -4.07376 0.98477
C -1.04389 3.75745 2.05339
H -1.87365 3.04078 1.93943
C 0.99238 4.16890 -1.74816
H 1.47506 4.33720 -2.71834
C -2.80830 0.54654 3.39671
H -2.32371 -0.25824 3.97464
H -3.41514 1.15027 4.09488
H -2.01406 1.19206 2.99084
C -4.99639 -1.56896 -2.78538
H -5.39912 -2.52590 -3.16330
H -3.95233 -1.49037 -3.12941
H -5.57459 -0.75474 -3.25662
C 7.40455 1.19805 -0.45149
H 7.24629 1.90110 -1.28574
H 8.33280 0.64436 -0.66178
H 7.57936 1.79688 0.45961
C -0.10373 3.21709 3.14880
H 0.29435 2.23524 2.85207
H -0.63443 3.10899 4.11201
H 0.75059 3.90008 3.31113
C -3.36267 4.54033 -0.88811
H -4.30820 4.82601 -1.38335
H -2.53061 4.84629 -1.54112
H -3.28765 5.12683 0.04130
C 0.81343 1.88983 -3.69462
H 1.48126 2.69376 -4.05353
H 0.48557 1.32597 -4.58611
H 1.39456 1.20651 -3.05679
C 4.85115 3.00507 0.58757
H 5.86968 3.33697 0.32845
H 4.85258 2.63279 1.62444
H 4.18926 3.88548 0.54489
C -1.20552 3.38061 -3.89128
H -2.11182 3.78385 -3.41346
H -1.51430 2.83259 -4.79975
H -0.58749 4.23969 -4.21025
C 4.55040 -3.67965 -1.25217
H 5.58927 -3.82610 -1.59264
H 4.00288 -3.11605 -2.02373
H 4.08432 -4.67525 -1.16365
C -6.57567 -1.58504 -0.81607
H -7.17109 -0.78513 -1.29234
H -6.69702 -1.49271 0.27562
H -7.01744 -2.55150 -1.11858
C -1.63010 5.11605 2.49905
H -0.83355 5.85528 2.69828
H -2.20666 4.99587 3.43357
H -2.29939 5.54983 1.73913
C 4.39084 2.39416 -1.85531
H 3.77351 3.29712 -1.98715
H 3.99410 1.61506 -2.52546
H 5.42266 2.63394 -2.16381
C 0.69870 4.77337 0.55981
H 0.96097 5.40294 1.41879
C 7.51808 -2.02577 -0.15816
H 7.75001 -2.41840 0.84767
H 8.39925 -1.45960 -0.49800
H 7.40591 -2.88942 -0.83457
C 1.37024 4.95430 -0.65352
H 2.14843 5.71956 -0.75508
C 0.69688 -1.56931 -2.48229
C 1.74449 -1.10899 -1.94934
H 2.76303 -1.04408 -2.32922
C -0.20428 -2.31849 -3.38709
C -1.16669 -1.38438 -4.15581
H -1.80028 -0.82897 -3.44773
H -0.61162 -0.65781 -4.77139
H -1.81041 -1.98582 -4.82041
C -1.00038 -3.41140 -2.63481
H -1.59153 -3.99429 -3.36192
H -0.32454 -4.10132 -2.10355
H -1.68715 -2.96482 -1.90053
C 0.76161 -3.00548 -4.40789
H 1.35385 -2.26003 -4.96391
H 1.45105 -3.69782 -3.89775
H 0.16037 -3.58246 -5.13196
C 1.92158 -0.28032 3.22304
C 2.89270 0.91331 3.41599
H 3.68430 0.88505 2.64899
H 2.37031 1.87906 3.34362
H 3.36930 0.84768 4.41033
C 0.84286 -0.27851 4.33893
H 1.33372 -0.35228 5.32582
H 0.23781 0.63975 4.31990
H 0.16297 -1.13836 4.22465
C 2.74280 -1.58824 3.33714
H 2.09985 -2.47742 3.23831
H 3.23803 -1.62928 4.32372
H 3.51745 -1.62400 2.55512

**E-int$_{Bu}$**
SCF (BP86) Energy = -2500.27547793
Enthalpy 0K = -2498.990391
Enthalpy 298K = -2498.908352
Free Energy 298K = -2499.107300
Lowest Frequency = 11.0064 $cm^{-1}$
Second Frequency = 18.1707 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2500.68298076
SCF (C6H6) Energy = -2500.27938816
SCF (BS2) Energy = -3312.51147397

Cu 1.76641 -0.36063 -0.23311
Si -4.09456 2.24609 0.04349
Al -1.72313 0.03895 -0.16285
Si -3.87525 -1.21750 1.91847
N 4.26902 1.05279 -0.85955
N -2.34314 1.77880 -0.05089
N 4.73646 -1.05743 -0.63610
N -2.74260 -1.34223 0.51679
C 3.68438 -0.17526 -0.66919
H 3.77987 0.12765 2.10695
C -1.58185 2.84971 -2.76212
H -2.14356 1.93043 -2.51917
C -1.09384 3.45119 -1.44221
C -2.57187 -2.65594 -0.08335
C -0.94754 3.55364 1.01881
C -5.28274 0.04897 1.64066
H -5.83367 -0.24283 0.72604
H -5.98620 -0.15531 2.47524
C -4.94230 1.55652 1.61189
H -4.33230 1.83748 2.49114
H -5.87582 2.14969 1.70481
C -1.44008 2.91108 -0.16256
C -2.92394 -0.70921 3.48958
H -2.35987 0.22719 3.33871
H -2.20215 -1.48532 3.79153
H -3.62063 -0.54517 4.33090
C 0.18398 5.24114 -0.35440

H  0.79269  6.14903 -0.42804
C  4.51066 -2.50407 -0.39373
H  3.41058 -2.58833 -0.44016
C -1.60122 -3.58073  0.41672
C -4.26566  4.14194  0.07538
H -3.80507  4.60722  0.95952
H -5.34126  4.39310  0.07738
H -3.81033  4.60866 -0.81237
C  3.43788  2.28641 -0.88070
H  2.40632  1.88714 -0.87750
C -0.14731  4.70636  0.89504
H  0.21489  5.19902  1.80472
C -0.66702 -3.26225  1.58485
H -0.76997 -2.18672  1.81020
C  5.66768  0.94849 -0.93235
C  0.77670 -0.78195 -1.93934
C -0.40032  2.45692 -3.67476
H  0.19441  3.34000 -3.96900
H -0.76839  1.98662 -4.60416
H  0.26707  1.74599 -3.16236
C  5.96655 -0.39100 -0.79050
C -2.53362  3.80563 -3.51902
H -3.41401  4.07902 -2.91457
H -2.89371  3.33596 -4.45177
H -2.01823  4.74263 -3.79570
C -0.28615  4.60474 -1.50795
H -0.03908  5.02294 -2.49090
C -1.25200  3.04322  2.42900
H -1.83456  2.11203  2.31626
C -0.10271 -0.41660 -1.08108
C -3.40254 -3.05168 -1.17999
C  3.62269  3.10569 -2.16696
H  2.82393  3.86389 -2.21721
H  3.54421  2.46514 -3.06059
H  4.58851  3.63642 -2.19643
C -4.47807 -2.13318 -1.75764
H -4.54956 -1.26893 -1.07596
C -1.48945 -4.85093 -0.18531
H -0.75053 -5.55793  0.20852
C -5.07486  1.65887 -1.48229
H -4.69154  2.12706 -2.40366
H -6.13428  1.95289 -1.37167
H -5.04683  0.56780 -1.62137
C  0.04505  2.70973  3.19636
H  0.64814  3.61884  3.37290
H  0.67204  1.98772  2.64835
H -0.19645  2.28267  4.18617
C  7.31216 -1.04977 -0.82716
H  7.46353 -1.74593  0.01446
H  8.10209 -0.28501 -0.76196
H  7.48258 -1.61492 -1.76106
C -4.07728 -1.60585 -3.15395
H -3.12331 -1.05183 -3.11843
H -4.84990 -0.92902 -3.56030
H -3.94925 -2.43890 -3.86793
C -4.73912 -2.89069  2.19002
H -5.29355 -2.86521  3.14446
H -4.03369 -3.73493  2.22426
H -5.46385 -3.09798  1.38515
C  0.81192 -3.52498  1.22767
H  1.01206 -4.60333  1.08998
H  1.46993 -3.15338  2.03045
H  1.08808 -2.99596  0.30029
C  5.11316 -3.39053 -1.49710
H  6.21095 -3.45662 -1.42961
H  4.84563 -3.02051 -2.50028
H  4.71654 -4.41445 -1.39424
C -1.04244 -4.05885  2.85688
H -2.07237 -3.85171  3.19050
H -0.35911 -3.80560  3.68714
H -0.96354 -5.14638  2.67800
C  3.61048  3.11148  0.40351
H  4.61332  3.56572  0.48040
H  3.43160  2.47709  1.28596
H  2.86627  3.92506  0.40907
C -2.10018  4.03626  3.25744
H -2.27619  3.63466  4.27114
H -3.08279  4.23408  2.79998
H -1.58194  5.00520  3.37006
C -5.86936 -2.80183 -1.81390
H -5.88994 -3.64662 -2.52479
H -6.63224 -2.07538 -2.14564
H -6.17357 -3.19119 -0.82781
C  4.94564 -2.92365  1.01905
H  4.64874 -3.97094  1.19805
H  4.45283 -2.28918  1.77135
H  6.03829 -2.85964  1.15704
C -3.23505 -4.32489 -1.75777
H -3.87087 -4.61300 -2.60299
C  6.60796  2.09205 -1.16426
H  6.55114  2.48072 -2.19672
H  7.64559  1.76307 -0.99652
H  6.41761  2.93626 -0.48126
C -2.28930 -5.23024 -1.26748
H -2.17980 -6.22169 -1.72013
C  2.79109 -0.07991  2.56053
C  1.71623 -0.21924  1.74110
H  0.76763 -0.41745  2.28004
C  2.88162 -0.16104  4.09278
C  3.32808  1.22114  4.63877
H  4.28202  1.53710  4.17890
H  2.57482  1.99622  4.41960
H  3.47841  1.18651  5.73411
C  3.96614 -1.20262  4.47185
H  4.12120 -1.23355  5.56643
H  3.67667 -2.21588  4.14184
H  4.93633 -0.95591  4.00339
C  1.55040 -0.57043  4.75144
H  0.74810  0.15222  4.52975
H  1.21737 -1.56021  4.39291
H  1.66324 -0.62628  5.84921
C  1.10572 -1.37895 -3.28155
C  1.54254 -2.85200 -3.06875
H  2.45069 -2.90738 -2.44822
H  0.74698 -3.43067 -2.57104
H  1.76047 -3.32322 -4.04426
C -0.16242 -1.36874 -4.17331
H  0.06040 -1.81730 -5.15843
H -0.96976 -1.95250 -3.70221
H -0.52541 -0.34169 -4.33688
C  2.24592 -0.60042 -3.97867
H  1.94785  0.44115 -4.18608
H  2.49762 -1.08114 -4.94082
H  3.14719 -0.58028 -3.34480

**TS(E2)$_{Bu}$**
SCF (BP86) Energy = -2500.27386835
Enthalpy 0K = -2498.988578
Enthalpy 298K = -2498.907484
Free Energy 298K = -2499.101802
Lowest Frequency = -32.9543 $cm^{-1}$
Second Frequency = 16.5960 $cm^{-1}$
SCF (BP86-D3BJ) Energy =  -2500.69392376
SCF (C6H6) Energy =  -2500.27768424
SCF (BS2) Energy =  -3312.50762595

Cu  1.47473 -0.35453 -0.30516
Si -3.80346  2.24768 -0.21133
Al -1.42834  0.02984 -0.18502
Si -3.76074 -1.14569  1.78024
N  4.07876  1.06671 -0.48012
N -2.04720  1.78946 -0.12229
N  4.49412 -1.06167 -0.36954
N -2.50423 -1.32198  0.49759
C  3.45829 -0.15752 -0.42983
H  3.07777 -0.13512  2.13665
C -1.06683  2.79845 -2.80254
H -1.57770  1.84454 -2.58475
C -0.73607  3.46254 -1.46279
C -2.38465 -2.65086 -0.08360
C -0.84353  3.67361  0.99243
C -5.14327  0.10409  1.33949
H -5.61393 -0.22035  0.39179
H -5.91534 -0.07501  2.11737

| | | | |
|---|---|---|---|
| C | -4.80279 | 1.61039 | 1.28928 |
| H | -4.28224 | 1.92390 | 2.21378 |
| H | -5.74071 | 2.20375 | 1.26831 |
| C | -1.17903 | 2.94963 | -0.19940 |
| C | -2.97810 | -0.58835 | 3.42438 |
| H | -2.38961 | 0.33720 | 3.30580 |
| H | -2.30378 | -1.36118 | 3.82748 |
| H | -3.76109 | -0.39150 | 4.17828 |
| C | 0.30617 | 5.38204 | -0.34048 |
| H | 0.85609 | 6.32786 | -0.39719 |
| C | 4.24074 | -2.51991 | -0.26122 |
| H | 3.15159 | -2.59030 | -0.42830 |
| C | -1.54489 | -3.64465 | 0.51118 |
| C | -3.98768 | 4.14576 | -0.26191 |
| H | -3.54065 | 4.66385 | 0.59844 |
| H | -5.06663 | 4.38230 | -0.28361 |
| H | -3.53204 | 4.57346 | -1.16919 |
| C | 3.28427 | 2.32479 | -0.50032 |
| H | 2.24381 | 1.96030 | -0.58947 |
| C | -0.11295 | 4.87414 | 0.89363 |
| H | 0.11850 | 5.42995 | 1.80978 |
| C | -0.66002 | -3.36855 | 1.72635 |
| H | -0.73653 | -2.29250 | 1.95555 |
| C | 5.47628 | 0.93890 | -0.44368 |
| C | 0.82111 | -0.89239 | -2.21547 |
| C | 0.20721 | 2.47857 | -3.61328 |
| H | 0.77235 | 3.39459 | -3.86129 |
| H | -0.05944 | 1.99210 | -4.56841 |
| H | 0.87011 | 1.79962 | -3.05433 |
| C | 5.74200 | -0.41271 | -0.37053 |
| C | -2.01359 | 3.67203 | -3.66021 |
| H | -2.95579 | 3.90212 | -3.13754 |
| H | -2.26617 | 3.15661 | -4.60413 |
| H | -1.53710 | 4.63338 | -3.92324 |
| C | -0.00205 | 4.66645 | -1.50176 |
| H | 0.30911 | 5.06416 | -2.47508 |
| C | -1.25250 | 3.20627 | 2.39180 |
| H | -1.73772 | 2.22166 | 2.27305 |
| C | -0.19648 | -0.55695 | -1.52743 |
| C | -3.14592 | -3.00635 | -1.24318 |
| C | 3.59195 | 3.19615 | -1.72717 |
| H | 2.82172 | 3.98117 | -1.79818 |
| H | 3.56236 | 2.60166 | -2.65492 |
| H | 4.57319 | 3.69361 | -1.65714 |
| C | -4.07167 | -2.01528 | -1.94162 |
| H | -4.07911 | -1.10848 | -1.31531 |
| C | -1.50082 | -4.93890 | -0.04620 |
| H | -0.86336 | -5.69547 | 0.42614 |
| C | -4.67236 | 1.64859 | -1.80277 |
| H | -4.10537 | 1.93245 | -2.70371 |
| H | -5.66207 | 2.13690 | -1.86268 |
| H | -4.83985 | 0.56264 | -1.83659 |
| C | -0.01507 | 3.02813 | 3.29554 |
| H | 0.50635 | 3.98818 | 3.46053 |
| H | 0.69724 | 2.31773 | 2.84785 |
| H | -0.31528 | 2.64673 | 4.28769 |
| C | 7.07783 | -1.09173 | -0.33357 |
| H | 7.14182 | -1.85449 | 0.45992 |
| H | 7.86576 | -0.34879 | -0.13315 |
| H | 7.33044 | -1.58384 | -1.28974 |
| C | -3.53293 | -1.62353 | -3.33556 |
| H | -2.52101 | -1.19151 | -3.25937 |
| H | -4.19123 | -0.87954 | -3.81862 |
| H | -3.47642 | -2.50431 | -4.00034 |
| C | -4.66217 | -2.80317 | 2.03618 |
| H | -5.33861 | -2.71625 | 2.90469 |
| H | -3.97504 | -3.64337 | 2.21805 |
| H | -5.27378 | -3.06514 | 1.15692 |
| C | 0.81977 | -3.67063 | 1.40850 |
| H | 0.98351 | -4.74684 | 1.21795 |
| H | 1.46381 | -3.37101 | 2.25190 |
| H | 1.14569 | -3.10518 | 0.51966 |
| C | 4.95321 | -3.33231 | -1.35657 |
| H | 6.03461 | -3.42922 | -1.17038 |
| H | 4.80684 | -2.88315 | -2.35197 |
| H | 4.53298 | -4.35173 | -1.37835 |
| C | -1.10184 | -4.16494 | 2.97569 |
| H | -2.13184 | -3.91846 | 3.28146 |
| H | -0.43527 | -3.94675 | 3.82947 |
| H | -1.06075 | -5.25360 | 2.79135 |
| C | 3.38707 | 3.08605 | 0.82972 |
| H | 4.38944 | 3.51743 | 0.99310 |
| H | 3.14165 | 2.41781 | 1.66974 |
| H | 2.65721 | 3.91201 | 0.82395 |
| C | -2.25787 | 4.15697 | 3.08301 |
| H | -2.48433 | 3.79564 | 4.10192 |
| H | -3.21094 | 4.23303 | 2.53659 |
| H | -1.84209 | 5.17613 | 3.17743 |
| C | -5.52559 | -2.52662 | -2.04558 |
| H | -5.59832 | -3.42050 | -2.69013 |
| H | -6.17769 | -1.75065 | -2.48516 |
| H | -5.93475 | -2.79600 | -1.05721 |
| C | 4.53296 | -3.04868 | 1.15165 |
| H | 4.21216 | -4.10134 | 1.22386 |
| H | 3.97757 | -2.46728 | 1.90251 |
| H | 5.60789 | -3.00985 | 1.39663 |
| C | -3.05035 | -4.30714 | -1.77344 |
| H | -3.63616 | -4.56038 | -2.66499 |
| C | 6.45463 | 2.07181 | -0.51870 |
| H | 6.49960 | 2.52121 | -1.52658 |
| H | 7.46614 | 1.70784 | -0.27922 |
| H | 6.21967 | 2.87862 | 0.19423 |
| C | -2.24119 | -5.28106 | -1.18132 |
| H | -2.18968 | -6.29324 | -1.59711 |
| C | 2.04541 | -0.17650 | 2.53000 |
| C | 1.01652 | -0.12798 | 1.63714 |
| H | 0.02422 | -0.16976 | 2.13438 |
| C | 2.04535 | -0.31421 | 4.06186 |
| C | 2.74510 | 0.92620 | 4.67984 |
| H | 3.75853 | 1.05618 | 4.25854 |
| H | 2.17705 | 1.85019 | 4.48686 |
| H | 2.85012 | 0.81166 | 5.77465 |
| C | 2.88857 | -1.55968 | 4.44342 |
| H | 2.96361 | -1.65931 | 5.54207 |
| H | 2.43745 | -2.48696 | 4.04955 |
| H | 3.91670 | -1.48267 | 4.04582 |
| C | 0.63583 | -0.47403 | 4.65821 |
| H | -0.00862 | 0.38795 | 4.42342 |
| H | 0.14093 | -1.37908 | 4.26591 |
| H | 0.68963 | -0.56671 | 5.75778 |
| C | 1.40373 | -1.46863 | -3.47445 |
| C | 1.64690 | -2.98490 | -3.24961 |
| H | 2.36289 | -3.15771 | -2.43119 |
| H | 0.70590 | -3.49810 | -2.99355 |
| H | 2.05689 | -3.43932 | -4.16962 |
| C | 0.37926 | -1.30302 | -4.62800 |
| H | 0.78521 | -1.74015 | -5.55819 |
| H | -0.56601 | -1.81494 | -4.38718 |
| H | 0.15908 | -0.23979 | -4.81287 |
| C | 2.72859 | -0.77261 | -3.86350 |
| H | 2.56517 | 0.29875 | -4.06920 |
| H | 3.14316 | -1.23607 | -4.77641 |
| H | 3.47117 | -0.85252 | -3.05417 |

**$E_{Bu}$**

SCF (BP86) Energy = -2500.29882861
Enthalpy 0K = -2499.012939
Enthalpy 298K = -2498.931179
Free Energy 298K = -2499.127426
Lowest Frequency = 16.8691 $cm^{-1}$
Second Frequency = 22.0538 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2500.72332069
SCF (C6H6) Energy = -2500.30357021
SCF (BS2) Energy = -3312.52982717

| | | | |
|---|---|---|---|
| Si | -3.48040 | -1.58987 | 1.88115 |
| Al | -1.20383 | 0.05093 | 0.20237 |
| Si | -3.76665 | 2.14214 | 0.60356 |
| N | -2.04860 | 1.77702 | 0.22248 |
| N | -2.40445 | -1.42142 | 0.45518 |
| C | -1.26476 | 2.94412 | -0.09528 |
| C | -3.12803 | -2.64070 | -1.60380 |
| C | -2.33394 | -2.57318 | -0.41139 |
| C | -0.54667 | 3.65458 | 0.93039 |

| | | | |
|---|---|---|---|
| C | -1.23232 | 3.47426 | -1.43220 |
| C | -4.32276 | 1.26272 | 2.21361 |
| H | -3.51685 | 1.34658 | 2.96734 |
| H | -5.15721 | 1.87952 | 2.60679 |
| C | 0.25760 | -1.23971 | -2.12728 |
| C | -0.55334 | -3.71346 | 1.10675 |
| H | -0.66688 | -2.74702 | 1.62585 |
| C | -1.48251 | -3.68923 | -0.10893 |
| C | -4.06916 | -1.50927 | -1.99962 |
| H | -3.97954 | -0.75240 | -1.20502 |
| C | 0.15123 | -0.12936 | 1.72994 |
| C | -2.00750 | 2.83945 | -2.59013 |
| H | -2.47252 | 1.91807 | -2.20042 |
| C | -0.51486 | 4.65646 | -1.70288 |
| H | -0.51513 | 5.05367 | -2.72529 |
| C | -4.48224 | -3.20885 | 1.76626 |
| H | -5.18656 | -3.18207 | 0.91804 |
| H | -5.07201 | -3.34056 | 2.69047 |
| H | -3.84724 | -4.09854 | 1.63413 |
| C | 0.08938 | -0.12729 | -1.35159 |
| H | 0.60403 | 0.77975 | -1.72339 |
| C | 1.05844 | -0.35104 | 2.58203 |
| C | -1.45620 | -4.80498 | -0.97033 |
| H | -0.80701 | -5.65283 | -0.71914 |
| C | -0.50633 | 3.19281 | 2.39274 |
| H | -0.91579 | 2.16878 | 2.42078 |
| C | -3.05373 | -3.77070 | -2.44082 |
| H | -3.66969 | -3.79847 | -3.34793 |
| C | -2.22903 | -4.85829 | -2.13508 |
| H | -2.19253 | -5.73539 | -2.79044 |
| C | -2.52014 | -1.57753 | 3.53580 |
| H | -1.82079 | -2.42573 | 3.61594 |
| H | -3.22766 | -1.63430 | 4.38243 |
| H | -1.93716 | -0.64796 | 3.64119 |
| C | -3.65432 | -0.84569 | -3.33032 |
| H | -2.61920 | -0.47018 | -3.27952 |
| H | -4.32050 | 0.00439 | -3.56277 |
| H | -3.71485 | -1.55737 | -4.17388 |
| C | -5.07731 | 1.70292 | -0.72441 |
| H | -6.02070 | 2.20448 | -0.43902 |
| H | -5.29014 | 0.62766 | -0.80500 |
| H | -4.79938 | 2.07045 | -1.72445 |
| C | 0.14048 | 4.84260 | 0.60517 |
| H | 0.65098 | 5.39466 | 1.40356 |
| C | -4.79078 | -0.20436 | 2.06248 |
| H | -5.51210 | -0.29449 | 1.22888 |
| H | -5.35870 | -0.51037 | 2.96695 |
| C | 0.92519 | -3.83483 | 0.67291 |
| H | 1.11182 | -4.77410 | 0.12170 |
| H | 1.58831 | -3.82687 | 1.55614 |
| H | 1.20951 | -2.99484 | 0.01457 |
| C | -4.01936 | 4.02975 | 0.79653 |
| H | -3.30232 | 4.53235 | 1.45978 |
| H | -5.03643 | 4.20668 | 1.19006 |
| H | -3.95439 | 4.53106 | -0.18363 |
| C | -5.54155 | -1.97294 | -2.06576 |
| H | -5.69277 | -2.72776 | -2.85841 |
| H | -6.20803 | -1.12050 | -2.28917 |
| H | -5.87065 | -2.42223 | -1.11349 |
| C | -0.90490 | -4.84755 | 2.09638 |
| H | -1.93735 | -4.75827 | 2.47158 |
| H | -0.22557 | -4.83022 | 2.96849 |
| H | -0.80773 | -5.84081 | 1.62224 |
| C | -1.09338 | 2.44823 | -3.77121 |
| H | -0.59366 | 3.33052 | -4.21055 |
| H | -1.68457 | 1.97049 | -4.57283 |
| H | -0.31622 | 1.73660 | -3.45300 |
| C | 0.93981 | 3.14412 | 2.92916 |
| H | 1.39606 | 4.14919 | 2.97637 |
| H | 1.57765 | 2.50145 | 2.30232 |
| H | 0.95043 | 2.73901 | 3.95661 |
| C | 0.16579 | 5.35226 | -0.69794 |
| H | 0.69248 | 6.28662 | -0.92244 |
| C | -3.12556 | 3.77688 | -3.10593 |
| H | -3.81575 | 4.08154 | -2.30298 |
| H | -3.71786 | 3.27793 | -3.89401 |
| H | -2.70014 | 4.69793 | -3.54373 |
| C | -1.35272 | 4.07732 | 3.33969 |
| H | -1.21080 | 3.75793 | 4.38799 |
| H | -2.42845 | 4.01522 | 3.11882 |
| H | -1.05197 | 5.13847 | 3.27042 |
| N | 4.65528 | -0.88621 | -0.25699 |
| N | 4.09966 | 1.18109 | -0.64881 |
| C | 5.78154 | -0.27174 | -0.82646 |
| C | 5.42695 | 1.03957 | -1.07625 |
| C | 3.60894 | 0.00089 | -0.14240 |
| Cu | 1.83053 | -0.22495 | 0.59044 |
| C | 4.56154 | -2.26793 | 0.28248 |
| H | 3.48969 | -2.36242 | 0.53247 |
| C | 6.24723 | 2.11421 | -1.72265 |
| H | 5.90092 | 2.34307 | -2.74554 |
| H | 7.29667 | 1.78955 | -1.79679 |
| H | 6.23525 | 3.05509 | -1.14909 |
| C | 7.08059 | -0.95268 | -1.13465 |
| H | 7.48137 | -1.51170 | -0.27304 |
| H | 7.83564 | -0.20154 | -1.41353 |
| H | 6.99433 | -1.65830 | -1.97955 |
| C | 3.28717 | 2.43028 | -0.61894 |
| H | 2.29430 | 2.07453 | -0.28624 |
| C | 5.37563 | -2.42110 | 1.57942 |
| H | 6.46150 | -2.35950 | 1.39684 |
| H | 5.17161 | -3.40819 | 2.02724 |
| H | 5.10312 | -1.64688 | 2.31356 |
| C | 4.90986 | -3.34944 | -0.75330 |
| H | 4.40766 | -3.16319 | -1.71515 |
| H | 4.56719 | -4.32722 | -0.37672 |
| H | 5.99432 | -3.42706 | -0.93087 |
| C | 3.80998 | 3.41587 | 0.43809 |
| H | 3.92354 | 2.92223 | 1.41647 |
| H | 3.08003 | 4.23417 | 0.54728 |
| H | 4.77881 | 3.85991 | 0.15342 |
| C | 3.11536 | 3.07363 | -2.00275 |
| H | 4.02726 | 3.59178 | -2.34188 |
| H | 2.30528 | 3.81862 | -1.94038 |
| H | 2.83078 | 2.32374 | -2.75699 |
| H | -0.27298 | -2.15885 | -1.83483 |
| C | 1.79108 | -0.62504 | 3.85618 |
| C | 2.14574 | -2.13275 | 3.93621 |
| H | 1.23731 | -2.75447 | 3.88295 |
| H | 2.81238 | -2.42608 | 3.10895 |
| H | 2.66026 | -2.34778 | 4.88975 |
| C | 3.09071 | 0.21370 | 3.94701 |
| H | 3.63720 | -0.04245 | 4.87183 |
| H | 3.74693 | 0.01777 | 3.08255 |
| H | 2.86702 | 1.29186 | 3.96471 |
| C | 0.85972 | -0.26606 | 5.04599 |
| H | -0.06485 | -0.86433 | 5.01825 |
| H | 1.38053 | -0.46965 | 5.99852 |
| H | 0.58060 | 0.79952 | 5.02431 |
| C | 1.03326 | -1.43868 | -3.43083 |
| C | 2.02709 | -0.30486 | -3.73897 |
| H | 2.57044 | -0.51437 | -4.67780 |
| H | 1.51192 | 0.66265 | -3.86570 |
| H | 2.76769 | -0.19614 | -2.92806 |
| C | 0.00118 | -1.55663 | -4.58591 |
| H | 0.51115 | -1.81299 | -5.53303 |
| H | -0.74286 | -2.34285 | -4.37222 |
| H | -0.54001 | -0.60700 | -4.73137 |
| C | 1.79690 | -2.78273 | -3.32978 |
| H | 1.10360 | -3.61675 | -3.12489 |
| H | 2.33250 | -3.00329 | -4.27107 |
| H | 2.53526 | -2.75113 | -2.51056 |

**INT(E-P)$_{Bu}$**

SCF (BP86) Energy = -2734.86622080
Enthalpy 0K = -2733.443331
Enthalpy 298K = -2733.352098
Free Energy 298K = -2733.568712
Lowest Frequency = 13.6405 $cm^{-1}$
Second Frequency = 18.7265 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2735.33059650
SCF (C6H6) Energy = -2734.87292209
SCF (BS2) Energy = -3547.15342883

| | | | |
|---|---|---|---|
| Si | 4.22226 | -0.10681 | -2.11919 |
| Al | 1.67176 | 0.22220 | -0.04730 |
| Si | 3.28907 | 3.14432 | -0.16680 |
| N | 1.78587 | 2.15631 | -0.13093 |
| N | 3.23208 | -0.68572 | -0.73847 |
| C | 0.58115 | 2.92158 | 0.06769 |
| C | 4.84119 | -1.81415 | 0.83444 |
| C | 3.77115 | -1.88167 | -0.12172 |
| C | -0.20534 | 3.35032 | -1.05756 |
| C | 0.16869 | 3.34959 | 1.37766 |
| C | 4.37563 | 2.82064 | -1.70843 |
| H | 3.73222 | 2.93718 | -2.60191 |
| H | 5.06193 | 3.69433 | -1.73026 |
| C | 0.99415 | -1.75158 | 2.13087 |
| H | 0.67349 | -2.42571 | 1.31593 |
| C | 2.12754 | -3.41662 | -1.44551 |
| H | 1.60769 | -2.44961 | -1.56259 |
| C | 3.31136 | -3.18778 | -0.50183 |
| C | 5.37605 | -0.49366 | 1.38146 |
| H | 4.82640 | 0.30783 | 0.86408 |
| C | -0.02787 | -0.32927 | -1.16315 |
| C | 0.99797 | 3.07360 | 2.63503 |
| H | 1.82078 | 2.40289 | 2.33742 |
| C | -0.99088 | 4.13662 | 1.52649 |
| H | -1.28026 | 4.46646 | 2.53158 |
| C | 5.55731 | -1.38535 | -2.59888 |
| H | 6.31241 | -1.50409 | -1.80489 |
| H | 6.07462 | -1.03818 | -3.51115 |
| H | 5.14136 | -2.38471 | -2.80031 |
| C | 1.37759 | -0.49039 | 1.80950 |
| H | 1.68436 | 0.13307 | 2.66798 |
| C | -0.74636 | -0.78483 | -2.10903 |
| C | 3.95918 | -4.33702 | -0.00409 |
| H | 3.61634 | -5.32388 | -0.33585 |
| C | 0.20850 | 3.03920 | -2.49698 |
| H | 0.93839 | 2.21337 | -2.44177 |
| C | 5.44069 | -2.99382 | 1.31790 |
| H | 6.26369 | -2.91048 | 2.03800 |
| C | 5.02642 | -4.25816 | 0.89345 |
| H | 5.51845 | -5.16501 | 1.26157 |
| C | 3.15061 | 0.22466 | -3.66362 |
| H | 2.85916 | -0.71850 | -4.15318 |
| H | 3.71827 | 0.82474 | -4.39723 |
| H | 2.22891 | 0.77701 | -3.41752 |
| C | 5.09723 | -0.36954 | 2.89687 |
| H | 4.01772 | -0.45263 | 3.10531 |
| H | 5.45382 | 0.60086 | 3.28636 |
| H | 5.61254 | -1.16576 | 3.46359 |
| C | 4.38244 | 2.92681 | 1.39501 |
| H | 4.17118 | 3.72421 | 2.12646 |
| H | 5.45358 | 2.99185 | 1.13193 |
| H | 4.21861 | 1.96484 | 1.90076 |
| C | -1.35091 | 4.14475 | -0.85275 |
| H | -1.91919 | 4.49134 | -1.72460 |
| C | 5.19015 | 1.51490 | -1.79401 |
| H | 5.81354 | 1.38864 | -0.88999 |
| H | 5.91179 | 1.57783 | -2.63631 |
| C | 1.13147 | -4.44169 | -0.85242 |
| H | 1.57628 | -5.44965 | -0.78048 |
| H | 0.23243 | -4.53658 | -1.48511 |
| H | 0.80637 | -4.14989 | 0.15977 |
| C | 2.90210 | 5.02683 | -0.24666 |
| H | 3.01789 | 5.42604 | -1.26807 |
| H | 3.62854 | 5.56183 | 0.39060 |
| H | 1.89040 | 5.28783 | 0.10051 |
| C | 6.88372 | -0.29567 | 1.10628 |
| H | 7.49400 | -1.04997 | 1.63475 |
| H | 7.21323 | 0.69899 | 1.45698 |
| H | 7.11975 | -0.37265 | 0.03183 |
| C | 2.58325 | -3.89204 | -2.84520 |
| H | 3.21419 | -3.14028 | -3.34622 |
| H | 1.71529 | -4.09592 | -3.49942 |
| H | 3.16982 | -4.82568 | -2.77218 |
| C | 0.19384 | 2.37834 | 3.75455 |
| H | -0.59793 | 3.04263 | 4.14822 |
| H | 0.85619 | 2.12708 | 4.60226 |
| H | -0.28393 | 1.45261 | 3.39973 |
| C | -0.97552 | 2.58781 | -3.37226 |
| H | -1.68684 | 3.41268 | -3.56202 |
| H | -1.51993 | 1.76028 | -2.89231 |
| H | -0.61633 | 2.24318 | -4.35879 |
| C | -1.75646 | 4.53821 | 0.42802 |
| H | -2.63844 | 5.17446 | 0.56490 |
| C | 1.61174 | 4.37928 | 3.19676 |
| H | 2.20385 | 4.91833 | 2.44108 |
| H | 2.26853 | 4.16083 | 4.05795 |
| H | 0.81962 | 5.06591 | 3.54703 |
| C | 0.89733 | 4.24602 | -3.17535 |
| H | 1.18298 | 3.99683 | -4.21343 |
| H | 1.80465 | 4.55463 | -2.63753 |
| H | 0.21616 | 5.11572 | -3.21099 |
| N | -4.63771 | -1.85359 | -0.31300 |
| N | -4.91473 | 0.18180 | -1.03086 |
| C | -6.02220 | -1.66694 | -0.45214 |
| C | -6.19818 | -0.37504 | -0.90921 |
| C | -3.94675 | -0.71655 | -0.65412 |
| Cu | -2.02230 | -0.42074 | -0.53288 |
| C | -3.92149 | -3.07581 | 0.14353 |
| H | -2.86300 | -2.82333 | -0.05369 |
| C | -7.48150 | 0.31630 | -1.25814 |
| H | -7.54190 | 1.33128 | -0.83322 |
| H | -8.33345 | -0.25605 | -0.85909 |
| H | -7.62919 | 0.40256 | -2.34917 |
| C | -7.07019 | -2.70359 | -0.18032 |
| H | -7.11285 | -3.47691 | -0.96758 |
| H | -8.06243 | -2.22787 | -0.13819 |
| H | -6.91347 | -3.21691 | 0.78234 |
| C | -4.55317 | 1.55268 | -1.48668 |
| H | -3.44996 | 1.51320 | -1.54250 |
| C | -4.28172 | -4.31658 | -0.69064 |
| H | -5.27735 | -4.71661 | -0.44115 |
| H | -3.54722 | -5.11204 | -0.48327 |
| H | -4.25115 | -4.09896 | -1.77058 |
| C | -4.07229 | -3.30646 | 1.65500 |
| H | -3.71734 | -2.42684 | 2.21367 |
| H | -3.45793 | -4.17144 | 1.95551 |
| H | -5.11505 | -3.52296 | 1.94294 |
| C | -5.09249 | 1.86828 | -2.89116 |
| H | -4.87687 | 1.05079 | -3.59710 |
| H | -4.59546 | 2.77837 | -3.26487 |
| H | -6.17730 | 2.06135 | -2.89246 |
| C | -4.92343 | 2.62338 | -0.45058 |
| H | -6.01424 | 2.72936 | -0.32461 |
| H | -4.52274 | 3.59614 | -0.77733 |
| H | -4.46850 | 2.39021 | 0.52376 |
| C | -1.92378 | 0.00828 | 1.74460 |
| C | -2.83546 | 0.33771 | 2.51277 |
| H | -0.87203 | -0.25328 | 1.54591 |
| C | 0.95195 | -2.44417 | 3.49495 |
| C | -0.46961 | -3.02499 | 3.70790 |
| H | -1.22599 | -2.22159 | 3.73919 |
| H | -0.73999 | -3.71539 | 2.88807 |
| H | -0.52495 | -3.59146 | 4.65559 |
| C | 1.96990 | -3.61485 | 3.46630 |
| H | 1.74486 | -4.32043 | 2.64779 |
| H | 2.99560 | -3.24489 | 3.30478 |
| H | 1.94244 | -4.17710 | 4.41827 |
| C | 1.29287 | -1.49520 | 4.65930 |
| H | 1.23431 | -2.03407 | 5.62177 |
| H | 2.31510 | -1.09122 | 4.56503 |
| H | 0.59483 | -0.64154 | 4.70306 |
| C | -3.91950 | 0.73437 | 3.43152 |
| C | -5.30259 | 0.31790 | 2.86233 |
| H | -6.09511 | 0.62584 | 3.56669 |
| H | -5.49787 | 0.79669 | 1.89005 |
| H | -5.36600 | -0.77345 | 2.72651 |
| C | -3.68882 | 0.01591 | 4.79205 |
| H | -4.47891 | 0.31249 | 5.50414 |
| H | -3.71957 | -1.07989 | 4.67508 |
| H | -2.71235 | 0.28958 | 5.22272 |
| C | -3.88383 | 2.27054 | 3.65312 |
| H | -2.91895 | 2.58059 | 4.08386 |
| H | -4.01953 | 2.81664 | 2.70601 |
| H | -4.69032 | 2.56432 | 4.34779 |

C -1.19071 -1.39607 -3.41286
C -2.47770 -0.74263 -3.97379
H -2.33086 0.32671 -4.18776
H -2.75615 -1.24533 -4.91686
H -3.31224 -0.84984 -3.26225
C -0.04775 -1.22839 -4.44538
H 0.86980 -1.72761 -4.09939
H -0.35038 -1.68057 -5.40675
H 0.18386 -0.16572 -4.61697
C -1.46962 -2.90618 -3.21220
H -2.26554 -3.06317 -2.46596
H -1.79527 -3.35567 -4.16727
H -0.56614 -3.43232 -2.87195

**TS1(E-P)$_{Bu}$**
SCF (BP86) Energy = -2734.85145687
Enthalpy 0K = -2733.431147
Enthalpy 298K = -2733.341434
Free Energy 298K = -2733.552467
Lowest Frequency = -796.8211 $cm^{-1}$
Second Frequency = 14.6666 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2735.31934963
SCF (C6H6) Energy = -2734.85662956
SCF (BS2) Energy = -3547.13808802

Si 4.00382 -0.38518 -2.18058
Al 1.48280 0.22512 -0.22405
Si 3.37154 2.97717 -0.36645
N 1.78550 2.12400 -0.24723
N 3.03097 -0.81059 -0.72074
C 0.67187 3.02985 -0.05563
C 4.65952 -2.01541 0.76503
C 3.50002 -2.02284 -0.08694
C -0.11170 3.47273 -1.17441
C 0.37546 3.58319 1.23772
C 4.37342 2.52455 -1.93300
H 3.70071 2.64246 -2.80419
H 5.10786 3.35343 -2.02020
C 0.92636 -1.62179 2.15671
H 0.60248 -2.39963 1.44605
C 1.66073 -3.46016 -1.25921
H 1.20079 -2.46554 -1.38606
C 2.89834 -3.29777 -0.37227
C 5.36385 -0.72786 1.18940
H 4.85463 0.09815 0.67034
C -0.12894 -0.30606 -1.36076
C 1.21123 3.27926 2.48508
H 1.94707 2.50835 2.20075
C -0.68351 4.50116 1.38067
H -0.89103 4.91916 2.37303
C 5.19956 -1.79501 -2.65630
H 5.99256 -1.93870 -1.90528
H 5.68304 -1.53447 -3.61490
H 4.69358 -2.76445 -2.78216
C 0.88086 -0.31572 1.73377
H 1.16952 0.42833 2.49157
C -0.95235 -0.74790 -2.22728
C 3.48181 -4.47977 0.12927
H 3.02684 -5.44332 -0.12764
C 0.18594 3.03173 -2.60918
H 0.83963 2.14559 -2.54240
C 5.19698 -3.22648 1.24423
H 6.09096 -3.19265 1.87842
C 4.63087 -4.46254 0.92376
H 5.07291 -5.39518 1.29057
C 2.88161 -0.04885 -3.68502
H 2.50889 -0.99213 -4.11432
H 3.45362 0.47812 -4.46961
H 2.00617 0.57063 -3.43103
C 5.22602 -0.49165 2.71018
H 4.16597 -0.43058 3.00750
H 5.71979 0.44984 3.00896
H 5.68982 -1.31176 3.28730
C 4.49097 2.71143 1.16855
H 4.40722 3.56546 1.86053
H 5.55115 2.62883 0.86923
H 4.22781 1.80395 1.73067
C -1.15488 4.39915 -0.97527
H -1.72887 4.74546 -1.84283
C 5.10349 1.16946 -1.99234
H 5.76908 1.04940 -1.11861
H 5.77630 1.14123 -2.87580
C 0.60804 -4.40203 -0.62795
H 0.95443 -5.45057 -0.60394
H -0.32707 -4.38526 -1.21376
H 0.36198 -4.11399 0.40791
C 3.14202 4.87614 -0.51413
H 3.06779 5.20369 -1.56370
H 4.03727 5.36195 -0.08561
H 2.25791 5.26179 0.01540
C 6.85785 -0.69761 0.79456
H 7.43344 -1.47899 1.32228
H 7.30613 0.27631 1.06126
H 7.00310 -0.85206 -0.28716
C 2.03659 -3.99185 -2.66293
H 2.68946 -3.28843 -3.20330
H 1.13458 -4.15745 -3.27979
H 2.57038 -4.95650 -2.58806
C 0.36065 2.73141 3.65221
H -0.29646 3.51789 4.06626
H 1.01058 2.38805 4.47740
H -0.27731 1.89354 3.32870
C -1.08674 2.63382 -3.38068
H -1.74022 3.50340 -3.57599
H -1.66218 1.88135 -2.82024
H -0.81967 2.20604 -4.36381
C -1.45504 4.91284 0.29036
H -2.26286 5.64155 0.42119
C 1.98121 4.52724 2.98115
H 2.62630 4.95937 2.20116
H 2.61568 4.27129 3.84882
H 1.27866 5.31655 3.30429
C 0.93519 4.12287 -3.40918
H 1.11959 3.78592 -4.44536
H 1.90601 4.37070 -2.95598
H 0.33987 5.05265 -3.45676
N -4.58277 -1.90483 -0.15960
N -4.95160 0.11433 -0.87343
C -5.97506 -1.71797 -0.11779
C -6.20915 -0.43507 -0.57141
C -3.94040 -0.77501 -0.60412
Cu -2.01072 -0.38458 -0.50691
C -3.80609 -3.09725 0.26799
H -2.78503 -2.86028 -0.08365
C -7.52445 0.25892 -0.75738
H -7.52444 1.27673 -0.33355
H -8.32020 -0.30689 -0.24781
H -7.81201 0.34113 -1.82067
C -6.97637 -2.74808 0.30928
H -7.10565 -3.54943 -0.43989
H -7.96035 -2.27414 0.45116
H -6.70452 -3.22674 1.26473
C -4.64138 1.48973 -1.34677
H -3.56407 1.42830 -1.58498
C -4.26395 -4.38967 -0.42845
H -5.21699 -4.77032 -0.02785
H -3.50423 -5.17197 -0.26567
H -4.37378 -4.24411 -1.51555
C -3.75147 -3.22213 1.79848
H -3.32814 -2.30360 2.23454
H -3.10359 -4.07061 2.07624
H -4.74740 -3.40581 2.23652
C -5.39386 1.86469 -2.63363
H -5.31698 1.06842 -3.39149
H -4.94216 2.77799 -3.05456
H -6.45940 2.07909 -2.45318
C -4.80480 2.52498 -0.22489
H -5.85810 2.64843 0.08073
H -4.43222 3.50323 -0.57008
H -4.20434 2.22647 0.64796
C -1.81373 0.20053 1.40853
C -2.48329 0.55568 2.40618
H -0.38403 -0.06020 1.35007
C 1.18212 -2.17609 3.54966

| | | | |
|---|---|---|---|
| C | -0.15567 | -2.84589 | 3.98231 |
| H | -0.98200 | -2.11551 | 3.99500 |
| H | -0.43137 | -3.66569 | 3.29589 |
| H | -0.05048 | -3.27351 | 4.99555 |
| C | 2.27997 | -3.26596 | 3.49648 |
| H | 2.03831 | -4.04526 | 2.75453 |
| H | 3.25529 | -2.84070 | 3.21477 |
| H | 2.37903 | -3.74995 | 4.48494 |
| C | 1.55728 | -1.09129 | 4.57651 |
| H | 1.70857 | -1.54840 | 5.56984 |
| H | 2.49252 | -0.57605 | 4.30069 |
| H | 0.76481 | -0.32982 | 4.67075 |
| C | -3.32657 | 0.94995 | 3.55913 |
| C | -4.73901 | 0.31783 | 3.40426 |
| H | -5.38268 | 0.63035 | 4.24634 |
| H | -5.21627 | 0.63847 | 2.46389 |
| H | -4.68349 | -0.78275 | 3.40201 |
| C | -2.69152 | 0.43716 | 4.88123 |
| H | -3.32670 | 0.72393 | 5.73855 |
| H | -2.59620 | -0.66142 | 4.87594 |
| H | -1.69012 | 0.87059 | 5.03552 |
| C | -3.47388 | 2.49377 | 3.63384 |
| H | -2.49207 | 2.98151 | 3.72553 |
| H | -3.96421 | 2.89119 | 2.73086 |
| H | -4.08767 | 2.76913 | 4.51037 |
| C | -1.47896 | -1.34340 | -3.50770 |
| C | -2.73299 | -0.59609 | -4.02485 |
| H | -2.51035 | 0.45513 | -4.26262 |
| H | -3.09618 | -1.08643 | -4.94560 |
| H | -3.53620 | -0.62672 | -3.27161 |
| C | -0.37483 | -1.28766 | -4.59244 |
| H | 0.50619 | -1.87249 | -4.28662 |
| H | -0.76029 | -1.70915 | -5.53814 |
| H | -0.05006 | -0.25207 | -4.78032 |
| C | -1.87428 | -2.82210 | -3.26674 |
| H | -2.66943 | -2.89046 | -2.50692 |
| H | -2.25058 | -3.26598 | -4.20583 |
| H | -1.01134 | -3.41498 | -2.92652 |

**INT2(E-P)$_{Bu}$**

SCF (BP86) Energy = -2499.05378531
Enthalpy 0K = -2497.790282
Enthalpy 298K = -2497.708320
Free Energy 298K = -2497.907964
Lowest Frequency = 10.9348 $cm^{-1}$
Second Frequency = 14.1376 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2499.45578811
SCF (C6H6) Energy = -2499.05830424
SCF (BS2) Energy = -3311.29069158

| | | | |
|---|---|---|---|
| Si | -4.05835 | 2.20832 | -0.11833 |
| Al | -1.65237 | 0.04787 | -0.19686 |
| Si | -3.85680 | -1.22241 | 1.80119 |
| N | -2.67393 | -1.34708 | 0.44095 |
| N | -2.29419 | 1.78095 | -0.10505 |
| C | -2.47244 | -2.66426 | -0.14069 |
| C | -1.00134 | 3.59381 | 1.02780 |
| C | -1.39757 | 2.92231 | -0.17357 |
| C | -3.28068 | -3.08979 | -1.24287 |
| C | -1.49456 | -3.56505 | 0.38786 |
| C | -5.29310 | -0.01334 | 1.42776 |
| H | -5.78216 | -0.33850 | 0.48949 |
| H | -6.03561 | -0.22565 | 2.22564 |
| C | -1.38481 | 2.84138 | -2.77717 |
| H | -1.94726 | 1.91519 | -2.56443 |
| C | -0.95592 | 3.43757 | -1.43435 |
| C | -1.45372 | 3.13939 | 2.41649 |
| H | -2.14784 | 2.29415 | 2.26906 |
| C | -0.07185 | -0.41646 | -1.18267 |
| C | -0.57091 | -3.20933 | 1.55382 |
| H | -0.65788 | -2.12557 | 1.74365 |
| C | -1.36278 | -4.84685 | -0.18540 |
| H | -0.62014 | -5.53644 | 0.23139 |
| C | -4.27489 | 4.09878 | -0.07934 |
| H | -4.00780 | 4.53877 | 0.89341 |
| H | -5.33732 | 4.32919 | -0.27446 |
| H | -3.66964 | 4.60479 | -0.84766 |
| C | 0.83732 | -0.78385 | -2.00005 |
| C | -0.12452 | 4.57617 | -1.46010 |
| H | 0.19644 | 4.97577 | -2.42932 |
| C | -4.34846 | -2.19171 | -1.86518 |
| H | -4.42910 | -1.30389 | -1.21583 |
| C | -0.16504 | 4.72380 | 0.94415 |
| H | 0.13439 | 5.22975 | 1.86917 |
| C | 0.27681 | 5.22205 | -0.28600 |
| H | 0.91185 | 6.11372 | -0.33022 |
| C | -4.91930 | 1.60829 | -1.70965 |
| H | -4.53268 | 2.14281 | -2.59276 |
| H | -6.00322 | 1.81193 | -1.64156 |
| H | -4.79472 | 0.52997 | -1.88818 |
| C | -0.25994 | 2.63706 | 3.25573 |
| H | 0.28353 | 1.81563 | 2.75959 |
| H | -0.60978 | 2.28151 | 4.24209 |
| H | 0.45970 | 3.45632 | 3.43780 |
| C | -2.97207 | -0.63461 | 3.38129 |
| H | -2.24766 | -1.38551 | 3.73585 |
| H | -3.69965 | -0.45000 | 4.19160 |
| H | -2.41619 | 0.30294 | 3.21074 |
| C | -3.09393 | -4.37388 | -1.78985 |
| H | -3.71464 | -4.68583 | -2.63792 |
| C | -4.99836 | 1.50310 | 1.38973 |
| H | -4.46777 | 1.82063 | 2.30740 |
| H | -5.95425 | 2.06773 | 1.39963 |
| C | -0.17334 | 2.46861 | -3.65744 |
| H | 0.41908 | 3.35939 | -3.93221 |
| H | -0.51048 | 1.99947 | -4.59910 |
| H | 0.48734 | 1.76142 | -3.13182 |
| C | -4.67286 | -2.91544 | 2.09666 |
| H | -5.36609 | -3.17191 | 1.27845 |
| H | -5.25565 | -2.87999 | 3.03378 |
| H | -3.94084 | -3.73346 | 2.17736 |
| C | -2.20326 | 4.24467 | 3.19575 |
| H | -1.54566 | 5.10746 | 3.40294 |
| H | -2.54881 | 3.85469 | 4.16943 |
| H | -3.08371 | 4.62297 | 2.65138 |
| C | -2.31812 | 3.80102 | -3.55327 |
| H | -3.21640 | 4.06580 | -2.97198 |
| H | -2.64850 | 3.34016 | -4.50138 |
| H | -1.79690 | 4.74236 | -3.80328 |
| C | 0.90913 | -3.49631 | 1.22192 |
| H | 1.11177 | -4.58087 | 1.15142 |
| H | 1.55771 | -3.06657 | 2.00190 |
| H | 1.18886 | -3.02624 | 0.26383 |
| C | -3.92676 | -1.71569 | -3.27402 |
| H | -3.79114 | -2.57401 | -3.95595 |
| H | -2.97222 | -1.16261 | -3.24337 |
| H | -4.69197 | -1.05272 | -3.71596 |
| C | -2.14714 | -5.25937 | -1.26670 |
| H | -2.02329 | -6.26005 | -1.69482 |
| C | -0.96425 | -3.95957 | 2.84817 |
| H | -1.99177 | -3.72585 | 3.17137 |
| H | -0.28006 | -3.69064 | 3.67274 |
| H | -0.90166 | -5.05352 | 2.70413 |
| C | -5.73946 | -2.86121 | -1.91738 |
| H | -6.49579 | -2.14915 | -2.29254 |
| H | -6.06142 | -3.20830 | -0.92122 |
| H | -5.74821 | -3.73549 | -2.59196 |
| N | 4.32022 | 1.07658 | -0.79933 |
| N | 4.76977 | -1.03282 | -0.53928 |
| C | 5.72028 | 0.97316 | -0.76106 |
| C | 6.00778 | -0.36627 | -0.59672 |
| C | 3.72600 | -0.15020 | -0.64847 |
| Cu | 1.78687 | -0.33495 | -0.27824 |
| C | 3.49345 | 2.31327 | -0.81710 |
| H | 2.46550 | 1.92250 | -0.93526 |
| C | 7.35100 | -1.02780 | -0.53721 |
| H | 7.44442 | -1.71508 | 0.32017 |
| H | 8.13690 | -0.26394 | -0.42844 |
| H | 7.58009 | -1.60371 | -1.45182 |
| C | 6.67406 | 2.11770 | -0.92104 |
| H | 6.69016 | 2.51083 | -1.95320 |
| H | 7.69709 | 1.78821 | -0.68067 |
| H | 6.43448 | 2.95854 | -0.24920 |
| C | 4.52259 | -2.46598 | -0.24504 |

| | | | |
|---|---|---|---|
| H | 3.43200 | -2.55968 | -0.38947 |
| C | 3.79039 | 3.21872 | -2.02183 |
| H | 4.74896 | 3.75399 | -1.92580 |
| H | 2.99248 | 3.97607 | -2.09268 |
| H | 3.80041 | 2.64242 | -2.96170 |
| C | 3.55374 | 3.03885 | 0.53586 |
| H | 3.27503 | 2.34324 | 1.34407 |
| H | 2.82946 | 3.87018 | 0.53194 |
| H | 4.55508 | 3.45593 | 0.74050 |
| C | 5.22433 | -3.41130 | -1.23405 |
| H | 5.04796 | -3.10310 | -2.27774 |
| H | 4.81997 | -4.42934 | -1.10641 |
| H | 6.31150 | -3.46761 | -1.06485 |
| C | 4.81756 | -2.79117 | 1.22743 |
| H | 5.89070 | -2.70074 | 1.46774 |
| H | 4.51239 | -3.82869 | 1.44457 |
| H | 4.24387 | -2.11525 | 1.88057 |
| C | 1.76538 | -0.12945 | 1.64249 |
| C | 2.01640 | -0.18107 | 2.86151 |
| C | 2.29543 | -0.24757 | 4.31709 |
| C | 3.37522 | -1.32649 | 4.60316 |
| H | 3.57859 | -1.39006 | 5.68813 |
| H | 3.04227 | -2.31973 | 4.25726 |
| H | 4.32066 | -1.08137 | 4.09034 |
| C | 2.82295 | 1.12292 | 4.82307 |
| H | 3.04279 | 1.07453 | 5.90560 |
| H | 3.74926 | 1.40296 | 4.29352 |
| H | 2.07982 | 1.91888 | 4.65621 |
| C | 1.00517 | -0.61955 | 5.09663 |
| H | 0.21063 | 0.12329 | 4.92143 |
| H | 0.62589 | -1.60374 | 4.77353 |
| H | 1.20748 | -0.66527 | 6.18272 |
| C | 1.25477 | -1.38208 | -3.31574 |
| C | 1.70329 | -2.84678 | -3.07313 |
| H | 0.89689 | -3.43458 | -2.60465 |
| H | 1.96886 | -3.32007 | -4.03553 |
| H | 2.58649 | -2.88382 | -2.41596 |
| C | 0.03178 | -1.39067 | -4.26918 |
| H | -0.33463 | -0.36817 | -4.45349 |
| H | 0.31171 | -1.83841 | -5.23972 |
| H | -0.79126 | -1.98328 | -3.83823 |
| C | 2.41568 | -0.58763 | -3.95835 |
| H | 3.28598 | -0.55435 | -3.28368 |
| H | 2.71796 | -1.06825 | -4.90566 |
| H | 2.11327 | 0.44879 | -4.18307 |

**$P_{Bu}$**

SCF (BP86) Energy = -2499.07895187
Enthalpy 0K = -2497.815323
Enthalpy 298K = -2497.733748
Free Energy 298K = -2497.929942
Lowest Frequency = 3.8397 $cm^{-1}$
Second Frequency = 23.4100 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2499.49533578
SCF (C6H6) Energy = -2499.08466624
SCF (BS2) Energy = -3311.31229168

| | | | |
|---|---|---|---|
| Cu | 1.68314 | -0.00228 | 0.00060 |
| Al | -1.40321 | 0.00054 | -0.00049 |
| Si | -4.05636 | -1.50156 | -1.24811 |
| Si | -4.05538 | 1.50955 | 1.24235 |
| C | 1.77535 | 1.59117 | -3.08855 |
| C | 1.77127 | -1.59880 | 3.08718 |
| N | -2.43091 | 1.52500 | 0.48050 |
| N | -2.43388 | -1.52161 | -0.48215 |
| N | 4.50541 | -1.04810 | -0.29382 |
| N | 4.50389 | 1.04567 | 0.29547 |
| C | 0.03175 | 0.58640 | -1.28455 |
| C | 0.02979 | -0.58849 | 1.28417 |
| C | -1.83018 | -2.82377 | -0.33002 |
| C | -1.82235 | 2.82516 | 0.33074 |
| C | 1.03658 | 0.93611 | -1.96009 |
| C | 3.65855 | -0.00190 | 0.00111 |
| C | 1.03374 | -0.94079 | 1.95968 |
| C | -0.98719 | 3.37500 | 1.35981 |
| C | -0.99476 | -3.37742 | -1.35679 |
| C | -2.08312 | -3.61675 | 0.83818 |
| C | -0.76921 | -2.67457 | -2.69871 |
| H | -1.17922 | -1.65429 | -2.60673 |
| C | -2.06977 | 3.61988 | -0.83748 |
| C | 0.72486 | -2.55091 | -3.05606 |
| H | 1.26865 | -1.98215 | -2.28499 |
| H | 0.84817 | -2.02146 | -4.01799 |
| H | 1.20208 | -3.54127 | -3.16815 |
| C | 5.85176 | 0.66305 | 0.18939 |
| C | -0.76904 | 2.67125 | 2.70250 |
| H | -1.18201 | 1.65234 | 2.60873 |
| C | -5.42493 | 0.76515 | 0.12860 |
| H | -6.37197 | 1.05938 | 0.62935 |
| H | -5.42260 | 1.32425 | -0.82693 |
| C | 5.85273 | -0.66313 | -0.18909 |
| C | -1.45408 | -4.86802 | 0.98642 |
| H | -1.65082 | -5.45740 | 1.89028 |
| C | -4.03896 | -0.54653 | -2.90003 |
| H | -3.60152 | 0.45761 | -2.78669 |
| H | -5.06603 | -0.42538 | -3.28881 |
| H | -3.44969 | -1.08345 | -3.66200 |
| C | -5.42672 | -0.75360 | -0.13774 |
| H | -6.37334 | -1.04519 | -0.64084 |
| H | -5.42829 | -1.31270 | 0.81778 |
| C | -3.03560 | 3.17123 | -1.93462 |
| H | -3.51603 | 2.24754 | -1.57069 |
| C | 3.98691 | -2.38264 | -0.69991 |
| H | 2.89890 | -2.28959 | -0.52826 |
| C | -0.60710 | -5.38561 | 0.00061 |
| H | -0.13499 | -6.36608 | 0.12879 |
| C | -0.38727 | 4.63689 | 1.17052 |
| H | 0.23944 | 5.05185 | 1.96944 |
| C | -4.65126 | 3.29015 | 1.59498 |
| H | -3.86107 | 3.94583 | 1.99150 |
| H | -5.47187 | 3.25459 | 2.33343 |
| H | -5.04785 | 3.76594 | 0.68287 |
| C | -0.40064 | -4.64176 | -1.16569 |
| H | 0.22628 | -5.05958 | -1.96296 |
| C | -4.65604 | -3.28042 | -1.60275 |
| H | -3.86740 | -3.93688 | -2.00106 |
| H | -5.47730 | -3.24222 | -2.34035 |
| H | -5.05250 | -3.75698 | -0.69099 |
| C | -1.43524 | 4.86859 | -0.98374 |
| H | -1.62777 | 5.45933 | -1.88760 |
| C | -0.58800 | 5.38204 | 0.00403 |
| H | -0.11149 | 6.36057 | -0.12271 |
| C | 3.98347 | 2.37874 | 0.70398 |
| H | 2.89540 | 2.28409 | 0.53349 |
| C | -3.04861 | -3.16314 | 1.93351 |
| H | -3.52497 | -2.23802 | 1.56790 |
| C | -4.14233 | 4.21325 | -2.21265 |
| H | -3.72879 | 5.13960 | -2.65021 |
| H | -4.68150 | 4.49489 | -1.29324 |
| H | -4.87756 | 3.81049 | -2.93187 |
| C | -1.51224 | -3.39698 | -3.84833 |
| H | -1.14180 | -4.43101 | -3.97048 |
| H | -1.35451 | -2.86879 | -4.80623 |
| H | -2.59733 | -3.45264 | -3.66765 |
| C | 0.72300 | 2.54270 | 3.06646 |
| H | 1.20302 | 3.53144 | 3.18084 |
| H | 1.26847 | 1.97208 | 2.29798 |
| H | 0.84013 | 2.01293 | 4.02899 |
| C | 3.24044 | 1.12080 | -3.22146 |
| H | 3.72770 | 1.66112 | -4.05233 |
| H | 3.28688 | 0.04279 | -3.44622 |
| H | 3.81365 | 1.30067 | -2.29995 |
| C | -2.29506 | 2.82659 | -3.24362 |
| H | -3.00101 | 2.48509 | -4.02199 |
| H | -1.55778 | 2.02696 | -3.06786 |
| H | -1.75971 | 3.70853 | -3.64082 |
| C | -4.04565 | 0.55523 | 2.89476 |
| H | -3.61165 | -0.45059 | 2.78331 |
| H | -5.07428 | 0.43813 | 3.28065 |
| H | -3.45665 | 1.09044 | 3.65814 |
| C | 3.23594 | -1.12793 | 3.22312 |
| H | 3.28127 | -0.05058 | 3.45141 |
| H | 3.81018 | -1.30431 | 2.30158 |
| H | 3.72276 | -1.67054 | 4.05275 |

| | | | |
|---|---|---|---|
| C | 7.03545 | -1.55305 | -0.42785 |
| H | 6.98307 | -2.07394 | -1.39800 |
| H | 7.15110 | -2.32073 | 0.35685 |
| H | 7.95695 | -0.95107 | -0.43573 |
| C | -2.30795 | -2.81982 | 3.24279 |
| H | -3.01331 | -2.47537 | 4.02042 |
| H | -1.56801 | -2.02269 | 3.06683 |
| H | -1.77565 | -3.70313 | 3.64103 |
| C | 7.03312 | 1.55519 | 0.42665 |
| H | 6.98135 | 2.07549 | 1.39715 |
| H | 7.14585 | 2.32348 | -0.35786 |
| H | 7.95582 | 0.95504 | 0.43266 |
| C | 4.51188 | 3.52461 | -0.17725 |
| H | 5.54695 | 3.80382 | 0.07695 |
| H | 3.88314 | 4.41561 | -0.01546 |
| H | 4.46877 | 3.26994 | -1.24751 |
| C | -1.51459 | 3.39614 | 3.84896 |
| H | -1.36289 | 2.86733 | 4.80750 |
| H | -2.59866 | 3.45571 | 3.66355 |
| H | -1.14098 | 4.42884 | 3.97277 |
| C | 4.21687 | 2.65537 | 2.19784 |
| H | 3.80631 | 1.84695 | 2.82051 |
| H | 3.70829 | 3.59209 | 2.47781 |
| H | 5.28729 | 2.77263 | 2.43531 |
| C | 4.21892 | -2.66134 | -2.19360 |
| H | 5.28927 | -2.77655 | -2.43238 |
| H | 3.80556 | -1.85507 | -2.81717 |
| H | 3.71213 | -3.59975 | -2.47119 |
| C | 1.73349 | -3.13337 | 2.85211 |
| H | 2.23168 | -3.65485 | 3.68960 |
| H | 2.24833 | -3.40397 | 1.91688 |
| H | 0.69654 | -3.49489 | 2.77374 |
| C | 4.51840 | -3.52617 | 0.18255 |
| H | 3.89162 | -4.41882 | 0.02231 |
| H | 4.47536 | -3.27015 | 1.25248 |
| H | 5.55393 | -3.80341 | -0.07192 |
| C | -4.15982 | -4.20038 | 2.21143 |
| H | -3.75058 | -5.12805 | 2.65021 |
| H | -4.69931 | -4.48056 | 1.29174 |
| H | -4.89409 | -3.79394 | 2.92957 |
| C | 1.73685 | 3.12641 | -2.85801 |
| H | 2.25027 | 3.39989 | -1.92286 |
| H | 0.69975 | 3.48792 | -2.78212 |
| H | 2.23605 | 3.64552 | -3.69636 |
| C | 1.03642 | -1.26823 | 4.41610 |
| H | 1.03398 | -0.18261 | 4.60527 |
| H | 1.55260 | -1.76626 | 5.25652 |
| H | -0.00667 | -1.61700 | 4.39574 |
| C | 1.04210 | 1.25646 | -4.41734 |
| H | 1.55855 | 1.75286 | -5.25855 |
| H | -0.00140 | 1.60416 | -4.39887 |
| H | 1.04095 | 0.17036 | -4.60375 |

**TS(Z)$_{Bu}$**

SCF (BP86) Energy = -2500.20203910
Enthalpy 0K = -2498.922996
Enthalpy 298K = -2498.841294
Free Energy 298K = -2499.037967
Lowest Frequency = -537.2026 $cm^{-1}$
Second Frequency = 11.0225 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2500.62457061
SCF (C6H6) Energy = -2500.21667501
SCF (BS2) Energy = -3312.43579972

| | | | |
|---|---|---|---|
| Cu | 2.05224 | -0.13710 | 0.07833 |
| Si | -3.70164 | -1.45598 | 1.96271 |
| Al | -1.43337 | 0.03532 | 0.11985 |
| Si | -3.77072 | 2.29985 | 0.71989 |
| N | 4.87186 | -1.23292 | -0.37153 |
| N | -2.68514 | -1.35478 | 0.48800 |
| N | 4.80367 | 0.93799 | -0.28513 |
| N | -2.09244 | 1.82082 | 0.25789 |
| C | 4.00753 | -0.17761 | -0.18335 |
| H | -0.73567 | -0.20444 | -1.45554 |
| C | -1.09424 | -3.87785 | 1.05264 |
| H | -1.02388 | -2.90417 | 1.56762 |
| C | -1.97755 | -3.67480 | -0.18414 |
| C | -1.25803 | 2.96578 | -0.04092 |
| C | -3.54388 | -2.41428 | -1.60539 |
| C | -4.31832 | 1.44926 | 2.34878 |
| H | -3.47552 | 1.47808 | 3.06537 |
| H | -5.08875 | 2.12340 | 2.77720 |
| C | -4.89097 | 0.02015 | 2.22479 |
| H | -5.66552 | -0.01933 | 1.43595 |
| H | -5.42486 | -0.25389 | 3.16013 |
| C | -2.72396 | -2.47192 | -0.42855 |
| C | -5.14877 | 1.96207 | -0.57113 |
| H | -4.79484 | 2.06785 | -1.60764 |
| H | -5.95401 | 2.70316 | -0.41711 |
| H | -5.59925 | 0.96353 | -0.46996 |
| C | -2.84989 | -4.67301 | -2.25296 |
| H | -2.89854 | -5.51770 | -2.94876 |
| C | 4.23558 | 2.30637 | -0.14180 |
| H | 3.19033 | 2.10649 | 0.15199 |
| C | -1.27955 | 3.57866 | -1.34126 |
| C | -4.85116 | -2.98327 | 1.90065 |
| H | -5.83656 | -2.70228 | 1.49113 |
| H | -5.01752 | -3.37427 | 2.91966 |
| H | -4.45457 | -3.79998 | 1.27872 |
| C | 4.40180 | -2.64009 | -0.30373 |
| H | 3.33596 | -2.52697 | -0.03224 |
| C | -3.57782 | -3.50447 | -2.49576 |
| H | -4.21194 | -3.43975 | -3.38808 |
| C | -2.09516 | 3.02421 | -2.51242 |
| H | -2.51745 | 2.05786 | -2.18590 |
| C | 6.18411 | -0.78441 | -0.60014 |
| C | 1.23834 | -0.53424 | 1.94812 |
| C | 0.33969 | -4.31993 | 0.68284 |
| H | 0.34107 | -5.24709 | 0.08322 |
| H | 0.92699 | -4.52179 | 1.59493 |
| H | 0.86042 | -3.53993 | 0.10636 |
| C | 6.13830 | 0.59393 | -0.54549 |
| C | -1.70599 | -4.91101 | 2.02959 |
| H | -2.71132 | -4.61775 | 2.36888 |
| H | -1.06620 | -5.02864 | 2.92341 |
| H | -1.79267 | -5.90291 | 1.55038 |
| C | -2.06934 | -4.74733 | -1.09608 |
| H | -1.50942 | -5.66704 | -0.88914 |
| C | -4.46422 | -1.22938 | -1.88624 |
| H | -4.23183 | -0.46802 | -1.12583 |
| C | 0.27688 | -0.24094 | 1.17117 |
| C | -0.44736 | 3.57262 | 0.98053 |
| C | 5.09800 | -3.43441 | 0.81505 |
| H | 4.56086 | -4.38442 | 0.97295 |
| H | 5.09280 | -2.87635 | 1.76491 |
| H | 6.14041 | -3.68571 | 0.56106 |
| C | -0.31774 | 2.99971 | 2.39724 |
| H | -0.70373 | 1.96632 | 2.36814 |
| C | -0.54257 | 4.75701 | -1.57288 |
| H | -0.57979 | 5.21665 | -2.56739 |
| C | -2.62633 | -1.50887 | 3.54167 |
| H | -2.00374 | -2.41690 | 3.59217 |
| H | -3.26350 | -1.47951 | 4.44353 |
| H | -1.95499 | -0.63424 | 3.57774 |
| C | -4.24867 | -0.59309 | -3.27479 |
| H | -4.43392 | -1.31254 | -4.09267 |
| H | -3.22164 | -0.20963 | -3.38801 |
| H | -4.94352 | 0.25326 | -3.41887 |
| C | 7.27219 | 1.56323 | -0.69252 |
| H | 7.02776 | 2.39419 | -1.37332 |
| H | 8.15200 | 1.04829 | -1.10881 |
| H | 7.57784 | 2.00215 | 0.27366 |
| C | 1.15708 | 2.94623 | 2.85030 |
| H | 1.77043 | 2.36640 | 2.14139 |
| H | 1.23725 | 2.47036 | 3.84320 |
| H | 1.59680 | 3.95457 | 2.94736 |
| C | -3.86281 | 4.19179 | 0.98255 |
| H | -4.87512 | 4.43557 | 1.35235 |
| H | -3.71354 | 4.73532 | 0.03555 |
| H | -3.13124 | 4.58947 | 1.69998 |
| C | -1.21876 | 2.77262 | -3.76055 |
| H | -0.85008 | 3.72072 | -4.19211 |
| H | -1.80781 | 2.26518 | -4.54542 |
| H | -0.34389 | 2.15030 | -3.51822 |

| | | | |
|---|---|---|---|
| C | 4.90013 | 3.09988 | 0.99462 |
| H | 5.91606 | 3.44021 | 0.73730 |
| H | 4.95096 | 2.50354 | 1.92028 |
| H | 4.29455 | 3.99753 | 1.20070 |
| C | -3.25821 | 3.96839 | -2.90125 |
| H | -3.93867 | 4.16680 | -2.05854 |
| H | -3.85397 | 3.53277 | -3.72363 |
| H | -2.86994 | 4.94163 | -3.25197 |
| C | 4.47679 | -3.35525 | -1.66345 |
| H | 5.51467 | -3.57916 | -1.96004 |
| H | 4.00731 | -2.75371 | -2.45647 |
| H | 3.93874 | -4.31562 | -1.59858 |
| C | -5.94635 | -1.63868 | -1.71555 |
| H | -6.61169 | -0.76608 | -1.84529 |
| H | -6.13430 | -2.07082 | -0.71870 |
| H | -6.23819 | -2.39643 | -2.46495 |
| C | -1.13483 | 3.78683 | 3.44942 |
| H | -0.85277 | 4.85532 | 3.45298 |
| H | -0.94469 | 3.38658 | 4.46177 |
| H | -2.21794 | 3.72344 | 3.26629 |
| C | 4.19720 | 3.05723 | -1.48101 |
| H | 3.65378 | 4.00697 | -1.34407 |
| H | 3.64886 | 2.45900 | -2.22591 |
| H | 5.20423 | 3.29773 | -1.86158 |
| C | 0.26132 | 4.75743 | 0.69264 |
| H | 0.84902 | 5.23001 | 1.48789 |
| C | 7.37972 | -1.65930 | -0.82667 |
| H | 7.69329 | -2.19424 | 0.08721 |
| H | 8.23339 | -1.04257 | -1.14793 |
| H | 7.21021 | -2.41281 | -1.61297 |
| C | 0.21861 | 5.36012 | -0.56840 |
| H | 0.76684 | 6.28858 | -0.76277 |
| C | 0.71752 | 0.11051 | -2.03270 |
| C | 1.35761 | 1.15109 | -1.61049 |
| H | 1.01476 | 1.97877 | -0.98513 |
| C | 0.84035 | -0.98037 | -3.07681 |
| C | -0.32653 | -0.88944 | -4.08883 |
| H | -1.29041 | -1.06394 | -3.58564 |
| H | -0.35796 | 0.09312 | -4.58593 |
| H | -0.19996 | -1.66699 | -4.86258 |
| C | 0.81134 | -2.37512 | -2.42056 |
| H | 0.90211 | -3.16117 | -3.19073 |
| H | 1.64743 | -2.49019 | -1.70945 |
| H | -0.13291 | -2.53848 | -1.87685 |
| C | 2.18131 | -0.76637 | -3.82402 |
| H | 2.18592 | 0.20371 | -4.34637 |
| H | 3.02698 | -0.76758 | -3.11723 |
| H | 2.32780 | -1.57088 | -4.56786 |
| C | 1.93757 | -0.92217 | 3.22262 |
| C | 3.29711 | -0.19755 | 3.37486 |
| H | 3.96895 | -0.44190 | 2.53632 |
| H | 3.16365 | 0.89595 | 3.39902 |
| H | 3.77903 | -0.50722 | 4.31920 |
| C | 1.02669 | -0.56259 | 4.42645 |
| H | 1.52876 | -0.84610 | 5.36881 |
| H | 0.81461 | 0.51725 | 4.45988 |
| H | 0.06721 | -1.09955 | 4.36993 |
| C | 2.17583 | -2.45300 | 3.23466 |
| H | 1.21934 | -2.99769 | 3.20101 |
| H | 2.70780 | -2.74155 | 4.15893 |
| H | 2.78165 | -2.76982 | 2.37109 |

**$Z_{Bu}$**

SCF (BP86) Energy = -2500.28228281
Enthalpy 0K = -2498.995965
Enthalpy 298K = -2498.914463
Free Energy 298K = -2499.110972
Lowest Frequency = 11.1875 $cm^{-1}$
Second Frequency = 18.1785 $cm^{-1}$
SCF (BP86-D3BJ) Energy = -2500.70635428
SCF (C6H6) Energy = -2500.27938922
SCF (BS2) Energy = -3312.51359339

| | | | |
|---|---|---|---|
| Cu | 1.79900 | -0.14937 | 0.28795 |
| Si | -3.52727 | -1.72154 | 1.78180 |
| Al | -1.28733 | 0.03255 | 0.18327 |
| Si | -3.90246 | 2.06688 | 0.69324 |
| N | 4.71179 | -0.92084 | -0.26983 |
| N | -2.42531 | -1.49081 | 0.37841 |
| N | 4.28669 | 1.19417 | -0.54749 |
| N | -2.17523 | 1.75658 | 0.29623 |
| C | 3.70082 | 0.00847 | -0.17043 |
| H | 1.64771 | 0.96179 | -2.58416 |
| C | -0.67285 | -3.85761 | 1.12916 |
| H | -0.77033 | -2.89036 | 1.65044 |
| C | -1.49074 | -3.76530 | -0.16388 |
| C | -1.41248 | 2.94385 | -0.01242 |
| C | -3.04169 | -2.67249 | -1.73066 |
| C | -4.46129 | 1.07832 | 2.23295 |
| H | -3.68120 | 1.14285 | 3.01518 |
| H | -5.32465 | 1.65062 | 2.63186 |
| C | -4.88064 | -0.38457 | 1.97571 |
| H | -5.55756 | -0.44474 | 1.10286 |
| H | -5.48047 | -0.76327 | 2.83105 |
| C | -2.30342 | -2.62928 | -0.50124 |
| C | -5.18577 | 1.65860 | -0.66958 |
| H | -5.07836 | 2.31075 | -1.54998 |
| H | -6.19061 | 1.84179 | -0.24455 |
| H | -5.15962 | 0.61522 | -1.01411 |
| C | -2.12384 | -4.88004 | -2.26015 |
| H | -2.05186 | -5.74201 | -2.93237 |
| C | 3.52599 | 2.47255 | -0.49261 |
| H | 2.49428 | 2.13714 | -0.27783 |
| C | -1.42511 | 3.51579 | -1.33323 |
| C | -4.52337 | -3.33871 | 1.58670 |
| H | -5.33990 | -3.19350 | 0.85868 |
| H | -4.98438 | -3.60635 | 2.55385 |
| H | -3.92423 | -4.19339 | 1.24008 |
| C | 4.50647 | -2.33482 | 0.14141 |
| H | 3.44015 | -2.35081 | 0.43041 |
| C | -2.91991 | -3.77961 | -2.59187 |
| H | -3.48577 | -3.78515 | -3.53139 |
| C | -2.28558 | 2.95655 | -2.46772 |
| H | -2.75388 | 2.03043 | -2.09381 |
| C | 5.90658 | -0.32803 | -0.71625 |
| C | 1.17266 | -0.38852 | 2.32420 |
| C | 0.82934 | -4.08119 | 0.84567 |
| H | 0.99992 | -4.97955 | 0.22643 |
| H | 1.38458 | -4.21688 | 1.78964 |
| H | 1.26052 | -3.21607 | 0.31639 |
| C | 5.63530 | 1.01469 | -0.88728 |
| C | -1.18263 | -4.98004 | 2.06474 |
| H | -2.23839 | -4.84072 | 2.34457 |
| H | -0.58713 | -5.00957 | 2.99562 |
| H | -1.09336 | -5.97082 | 1.58392 |
| C | -1.43218 | -4.86447 | -1.04505 |
| H | -0.81864 | -5.73088 | -0.76949 |
| C | -4.01721 | -1.56319 | -2.10920 |
| H | -4.01270 | -0.86158 | -1.25988 |
| C | 0.16549 | -0.17772 | 1.58675 |
| C | -0.64063 | 3.61564 | 0.99929 |
| C | 5.34459 | -2.69903 | 1.38007 |
| H | 5.00420 | -3.67019 | 1.77642 |
| H | 5.23221 | -1.94577 | 2.17551 |
| H | 6.41632 | -2.80113 | 1.14362 |
| C | -0.60942 | 3.16115 | 2.46149 |
| H | -1.05178 | 2.15075 | 2.49865 |
| C | -0.66701 | 4.67061 | -1.61078 |
| H | -0.69434 | 5.08955 | -2.62380 |
| C | -2.58504 | -1.71585 | 3.44777 |
| H | -1.94191 | -2.60216 | 3.57020 |
| H | -3.30007 | -1.69343 | 4.28950 |
| H | -1.94312 | -0.82186 | 3.52323 |
| C | -3.57683 | -0.78337 | -3.36496 |
| H | -3.50193 | -1.44568 | -4.24670 |
| H | -2.59429 | -0.30702 | -3.21180 |
| H | -4.30452 | 0.01247 | -3.60500 |
| C | 6.55222 | 2.09514 | -1.37478 |
| H | 6.29169 | 2.43736 | -2.39155 |
| H | 7.58710 | 1.72119 | -1.40957 |
| H | 6.54696 | 2.97842 | -0.71522 |
| C | 0.82827 | 3.08168 | 3.01382 |
| H | 1.44836 | 2.40071 | 2.41043 |
| H | 0.81798 | 2.70996 | 4.05364 |

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H   1.31557  4.07282  3.03714
C  -4.21502  3.92647  1.05844
H  -5.16673  4.22753  0.58658
H  -3.42405  4.58896  0.67436
H  -4.31881  4.11443  2.14029
C  -1.46440  2.59991 -3.72576
H  -0.98770  3.49393 -4.16727
H  -2.11897  2.16095 -4.49946
H  -0.67412  1.87033 -3.49158
C   3.98068  3.35424  0.68140
H   4.98989  3.77157  0.52544
H   3.97736  2.78407  1.62378
H   3.27799  4.19671  0.78710
C  -3.40410  3.95684 -2.84844
H  -4.00449  4.25769 -1.97439
H  -4.08350  3.51729 -3.60094
H  -2.97614  4.87731 -3.28518
C   4.70447 -3.33559 -1.00859
H   5.76211 -3.42770 -1.30454
H   4.11269 -3.05423 -1.89268
H   4.36709 -4.33172 -0.67727
C  -5.45675 -2.09786 -2.28377
H  -6.16182 -1.26406 -2.45219
H  -5.79215 -2.65560 -1.39326
H  -5.53580 -2.77809 -3.15077
C  -1.44191  4.09473  3.37193
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H  -2.49325  4.14664  3.05592
C   3.50581  3.22625 -1.83180
H   2.70427  3.98239 -1.79522
H   3.29249  2.54461 -2.67111
H   4.45418  3.74974 -2.03531
C   0.08919  4.77647  0.66829
H   0.64971  5.29137  1.45749
C   7.18821 -1.05335 -0.99429
H   7.55207 -1.62801 -0.12659
H   7.97413 -0.32804 -1.25534
H   7.09777 -1.75254 -1.84384
C   0.09449  5.30741 -0.62603
H   0.65919  6.21816 -0.85540
C   1.02303  0.11642 -2.23842
C   0.13779  0.38237 -1.21980
H   0.26014  1.45915 -0.95913
C   1.21833 -1.09077 -3.15607
C   0.30513 -0.88920 -4.39713
H   0.49124  0.08423 -4.88429
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H  -0.75801 -0.93639 -4.11616
C   0.87633 -2.42415 -2.48153
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C   2.68718 -1.10211 -3.64606
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H   2.86669 -1.95933 -4.31917
C   1.94838 -0.67264  3.57501
C   3.24607  0.16952  3.64042
H   3.88265 -0.02120  2.76054
H   3.01727  1.24708  3.66862
H   3.81399 -0.08530  4.55276
C   1.04702 -0.33661  4.79437
H   1.58926 -0.55893  5.73091
H   0.76536  0.72754  4.80042
H   0.12301 -0.93673  4.77536
C   2.30758 -2.17863  3.63907
H   1.39579 -2.79697  3.64785
H   2.87942 -2.38896  4.56062
H   2.91844 -2.48108  2.77458
```

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