Supporting Information for

On the Reactivity of Al-Group 11 (Cu, Ag, Au) Bonds

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1 Experimental and Supplementary Information

1.1 General information

Unless 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, ^{31}P at 202 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 was purchased from Sigma-Aldrich, dried over a potassium mirror before distilling and storage over molecular sieves. $[\{SiN^{Dipp}\}AlK]_2$ (**3**),[1] *N,N'*-diisopropyl-4,5-dimethyl-2-ylidene (NHC^{iPr}),[2] ^{cy}CAACAgCl,[3] *N,N'*-bis[2,6-bis(1-methylethyl)phenyl]-1,3-dihydro-2-ylidene (IPr)[4] were prepared according to reported procedures. All other chemicals were purchased from Merck and used without further purification.

Synthetic Procedures

*Synthesis of {SiN^{Dipp}}Al-Cu{IPr}(**13**)*

A solution of *N,N'*-bis{diisopropylphenyl}-2-ylidene (IPr, 0.388 g, 1.00 mmol) in toluene (25 mL) was added to a schlenk flask containing CuCl (0.099 g, 1.00 mmol). After stirring for 3 days at room temperature, the solution was put under vacuum to remove all volatile and afford an off-white solid. A solution of [{SiN^{Dipp}}AlK]$_2$ (**3**, 0.560 g, 1.00 mmol) in hexane (40 mL) was then added to the Schlenk flask, affording a pale-yellow reaction mixture. The resulting mixture was then left stirring at room temperature overnight before filtering. The colourless filtrate was then collected, and all volatiles were removed *in vacuo* yielding **13** as an off-white solid. Yield 0.75g, 77%. No meaningful result was obtained for elemental analysis after multiple attempts. ^{1}H NMR (500 MHz, 298 K, Benzene-*d$_6$*) δ 7.20 (t, *J* = 7.8 Hz, 2H, *p*-C$_6$*H$_3$* on IPr), 7.05 – 6.94 (m, 10H, C$_6$*H$_3$* on IPr and SiN^{Dipp}), 6.05 (s, 2H, NC*H* on IPr), 3.90 (sept, *J* = 6.9 Hz, 4H, C*H*Me$_2$ on SiN^{Dipp}), 2.39 (sept, *J* = 6.9 Hz, 4H, , C*H*Me$_2$ on IPr), 1.38 (d, *J* = 6.9 Hz, 12H, CH*Me$_2$* on SiN^{Dipp}), 1.07 (s, 4H, SiC*H$_2$*), 1.06 (d, *J* = 6.9 Hz, 12H, CH*Me$_2$* on SiN^{Dipp}), 1.01 (d, *J* = 6.9 Hz, 12H, CH*Me$_2$* on IPr), 0.91 (d, *J* = 6.9 Hz, 12H, CH*Me$_2$* on IPr), 0.22 (s, 12H, Si*Me$_2$*). ^{13}C{^{1}H} NMR (126 MHz, 298 K, Benzene-*d$_6$*) δ 185.1 (Cu*C*$_{carbene}$),146.9 (*C$_6$*H$_3$ on SiN^{Dipp}), 146.3 (*C$_6$*H$_3$ on SiN^{Dipp}), 145.1 (*C$_6$*H$_3$ on IPr), 136.0 (*C$_6$*H$_3$ on IPr), 130.1 (*C$_6$*H$_3$), 124.5 (*C$_6$*H$_3$ on IPr), 123.3 (*C$_6$*H$_3$ on SiN^{Dipp}), 123.0 (N*C*H on IPr), 122.5 (*C$_6$*H$_3$), 28.9 (*C*HMe2 on IPr), 28.2 (*C*HMe2 on SiN^{Dipp}), 25.8 (CH*Me$_2$* on SiN^{Dipp}), 24.5 (CH*Me$_2$* on IPr), 24.3 (CH*Me$_2$* on IPr), 24.1 (CH*Me$_2$* on SiN^{Dipp}), 14.6 (Si*C*H$_2$), 1.6 (Si*Me$_2$*).

Figure S1. ^{1}H NMR spectrum of **13**. (500 MHz, 298 K, Benzene-d_6) *grease

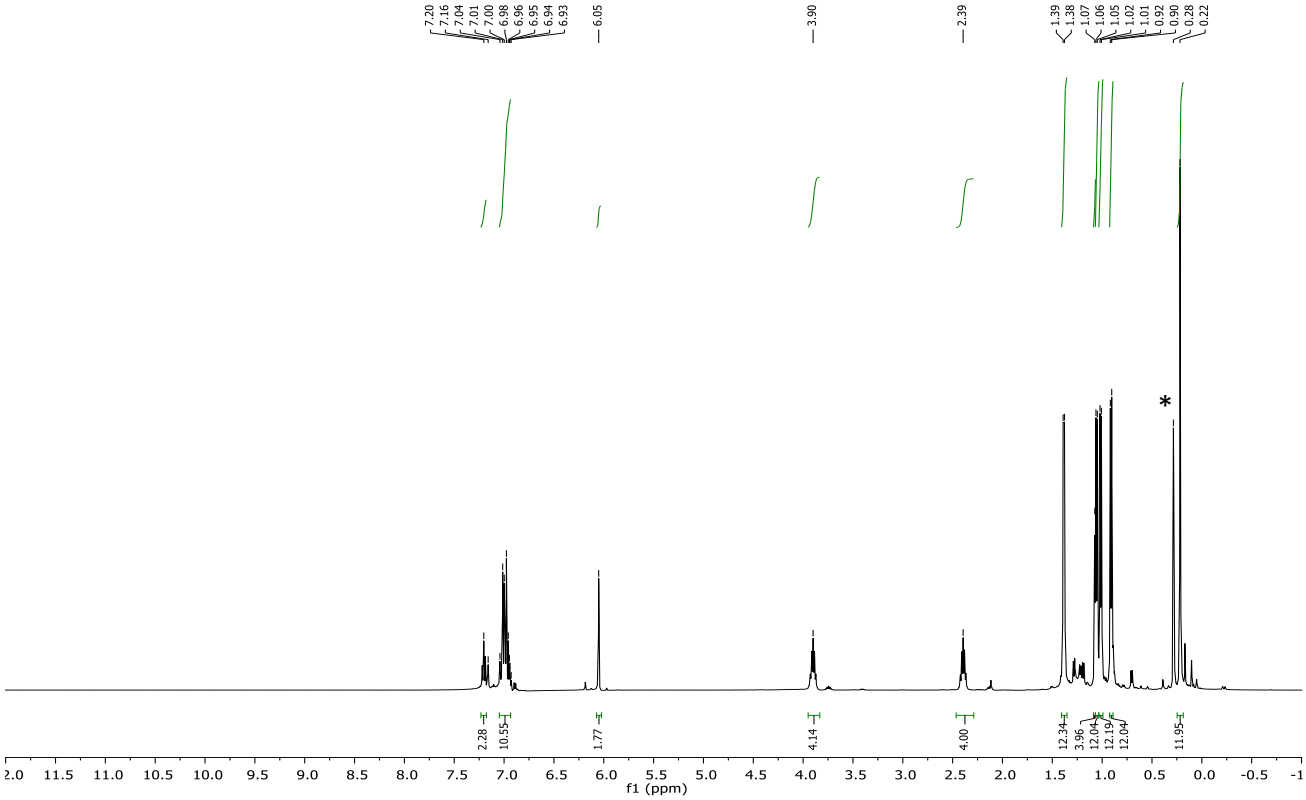


Figure S2. ^{13}C{^{1}H} NMR spectrum of **13**. (126 MHz, 298 K, Benzene-d_6)

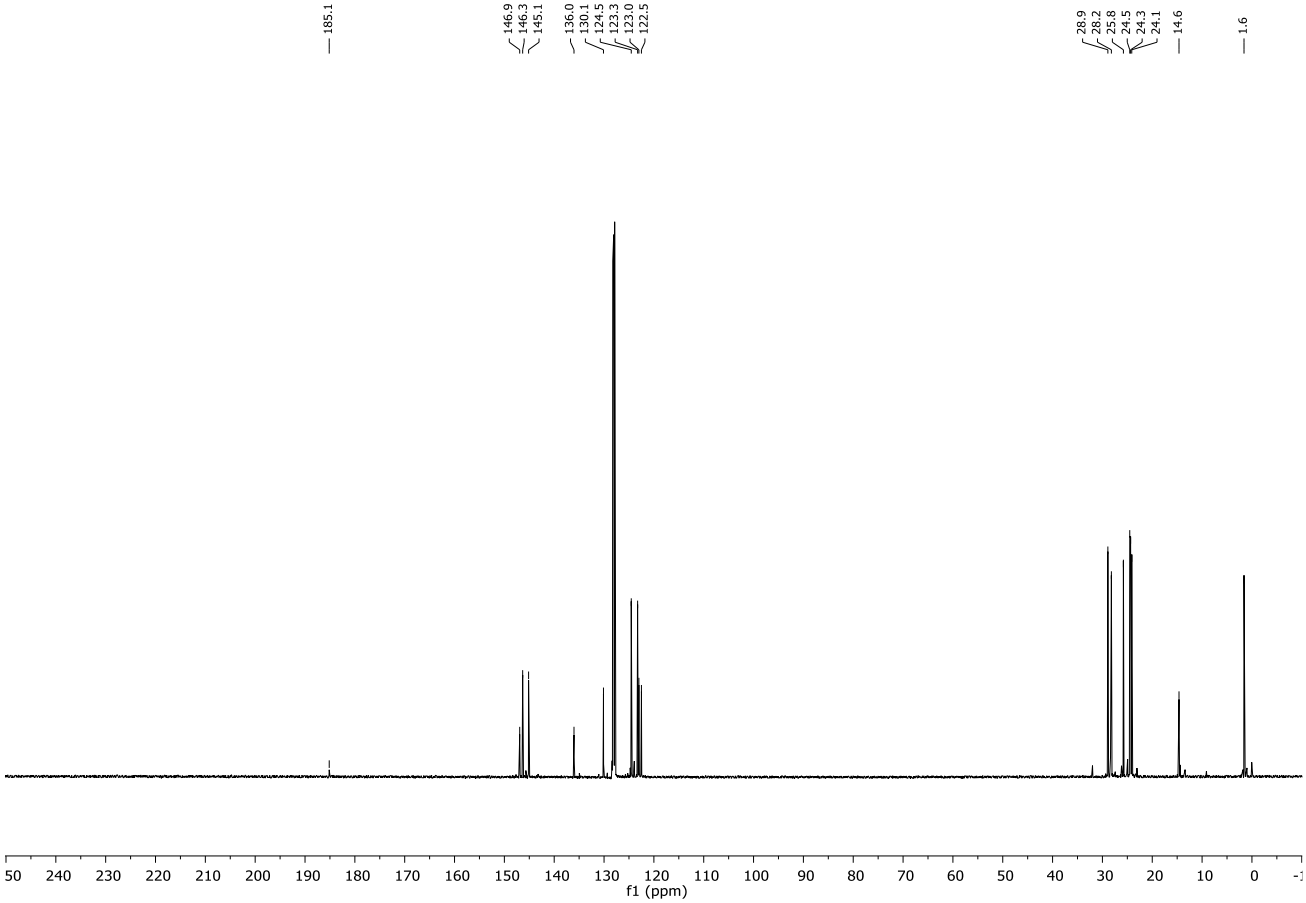


Figure S3. ^{1}H-^{1}H COSY NMR spectrum of **13**.

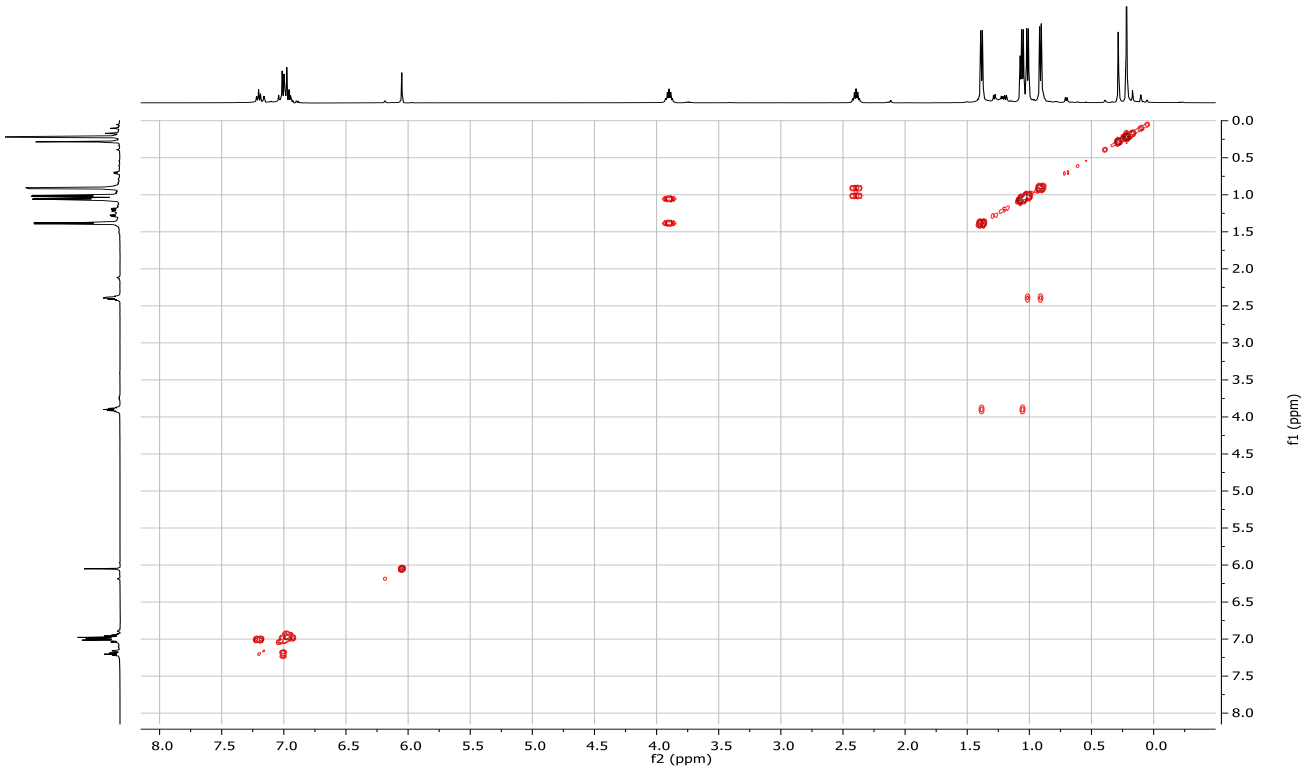


Figure S4. ^{1}H-^{13}C HSQC NMR spectrum of **13**.

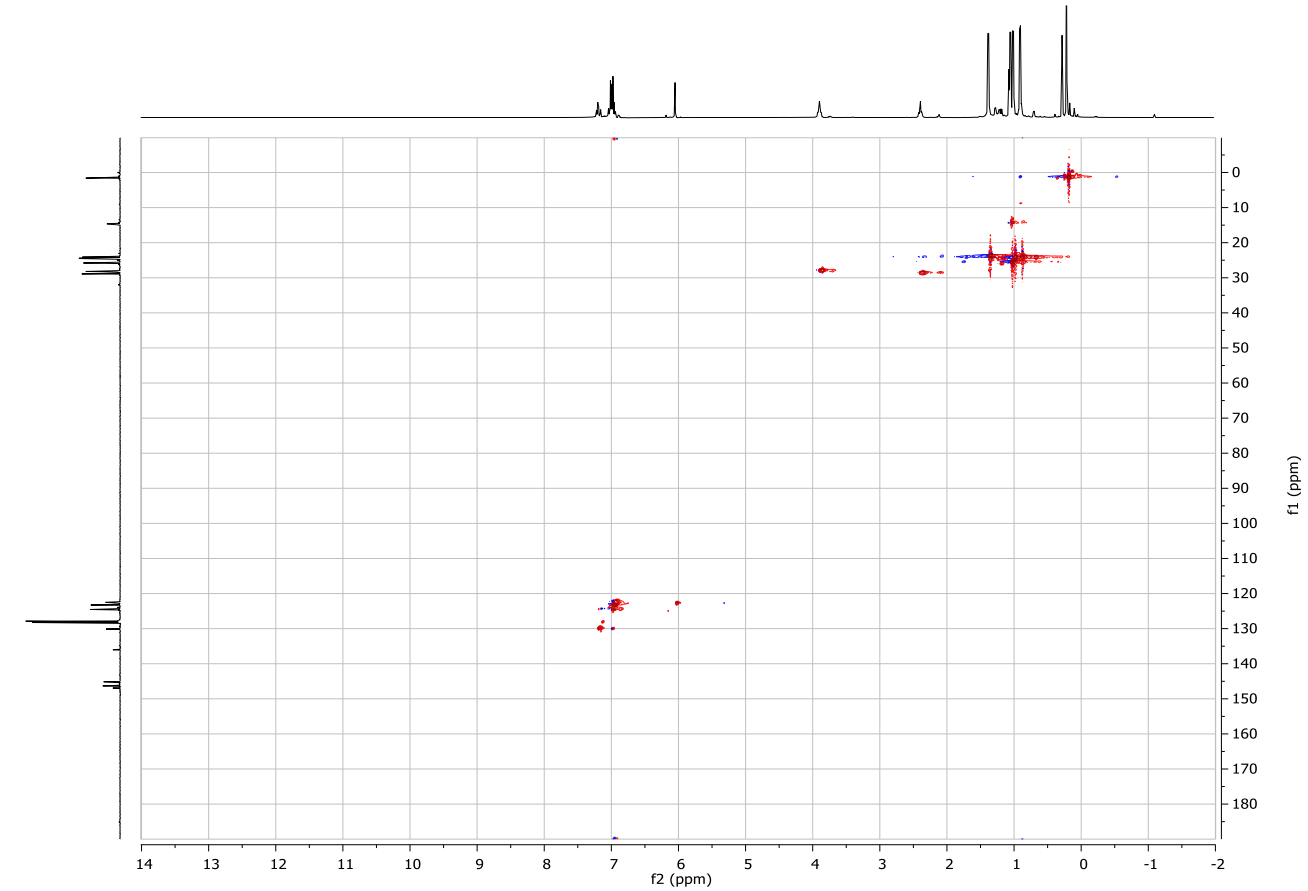
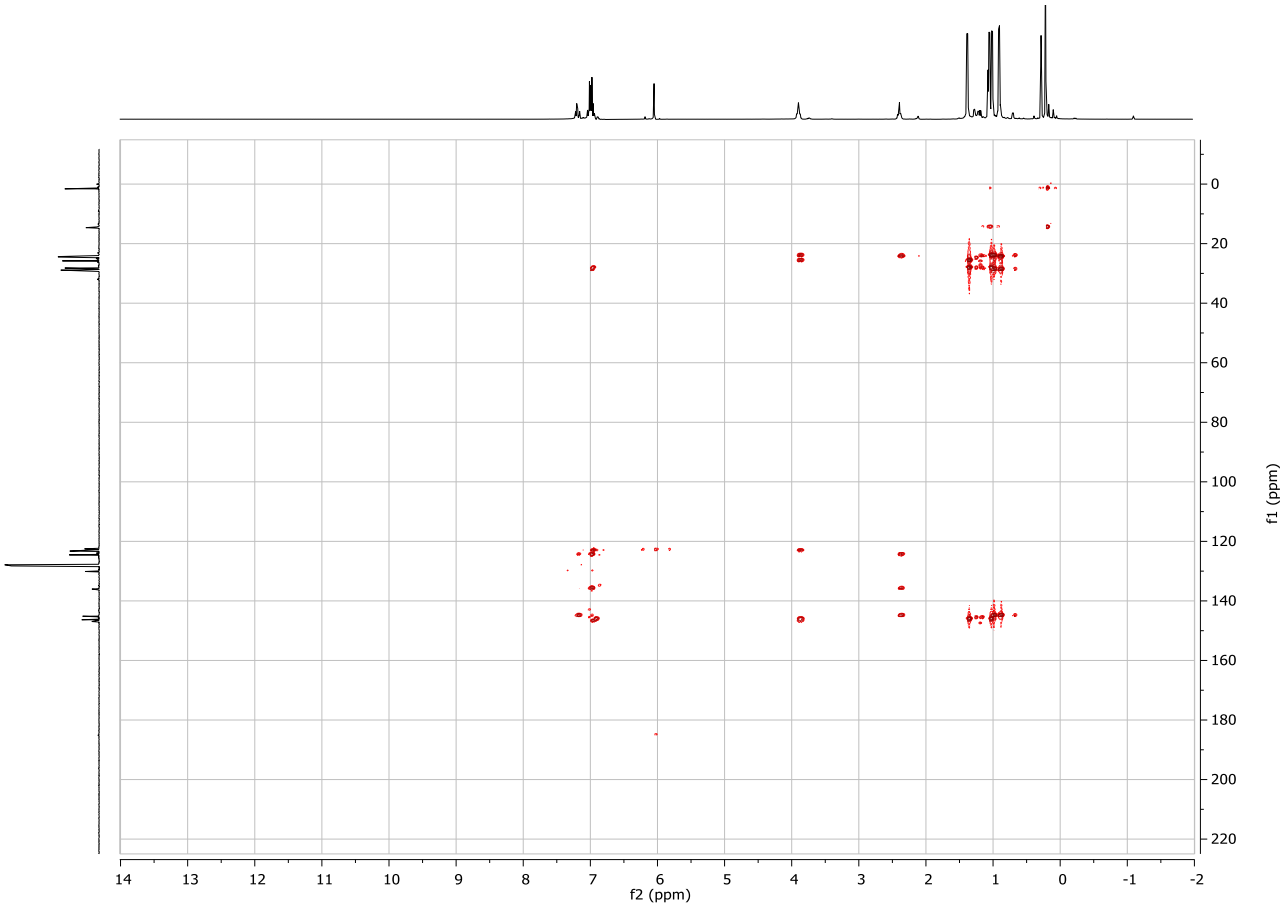


Figure S5. ^{1}H-^{13}C HMBC NMR spectrum of **13**.



*Synthesis of {SiN^{Dipp}}Al-C(N^{i}Pr)$_2$-Cu{IPr} (**14**)*

Inside a J Young's tube, {SiN^{Dipp}}Al-Cu{IPr} (**13**, 48.5mg, 0.05mmol) was dissolved in 0.4mL of C_6D_6, *N,N'*-diisopropylcarbodiimide (7.8µL, 0.05mmol) was then added *via* a micropipette. No significant change was observed in the ^{1}H NMR spectrum when the reaction mixture was left at room temperature overnight. The reaction mixture was then kept at 40 °C, and full conversion into compound **14** in quantitative yields was determined by ^{1}H NMR after 3 days. ^{1}H NMR (500 MHz, 298 K, Benzene-*d*$_6$) δ 7.14 – 7.12 (m, 2H, *p*-C$_6$*H*$_3$), 7.10-7.08 (m, 4H, *m*-C$_6$*H*$_3$), 7.06 – 7.02 (m, 2H, *p*-C$_6$*H*$_3$), 6.98 (d$_{app}$, 4H, *m*-C$_6$*H*$_3$), 4.13 (s, 2H, NC*H* on IPr), 4.26-3.90(m, 4H, C*H*Me$_2$ on SiN^{Dipp}), 3.38(sept, *J* = 6.9 Hz, 1H, NC*H*Me$_2$ on carbodiimide) 2.99 (sept, *J* = 6.9 Hz, 1H, NC*H*Me$_2$ on carbodiimide), 2.52 (sept, *J* = 6.8 Hz, 4H, C*H*Me$_2$ on IPr), 1.44-1.43 (m, 12H, CH*Me*$_2$ on SiN^{Dipp}), 1.42 – 1.36 (m, 12H, CH*Me*$_2$ on SiN^{Dipp}), 1.33 (d, *J* = 6.9 Hz, 6H, NCH*Me*$_2$ on carbodiimide), 1.28 (s, 4H, SiC*H*$_2$), 1.23 (d, *J* = 6.9 Hz, 12H, CH*Me*$_2$ on IPr), 1.05 (d, *J* = 6.9 Hz, 6H, NCH*Me*$_2$ on carbodiimide), 0.94 (d, *J* = 6.8 Hz, 12H CH*Me*$_2$ on IPr), 0.33 – 0.02 (s, br, 12H, Si*Me*$_2$) *Si*Me*$_2$ peak overlapping with the grease. ^{13}C{^{1}H} NMR (126 MHz, 298 K, Benzene-*d*$_6$) δ 182.1 (Cu*C*$_{carbene}$), 149.6 (*i*-*C*$_6$H$_3$), 148.4 (*i*-*C*$_6$H$_3$), 146.7 (*o*-*C*$_6$H$_3$), 146.4(*o*-*C*$_6$H$_3$), 145.3(*o*-*C*$_6$H$_3$), 135.7 (*o*-*C*$_6$H$_3$), 130.7 (*m*-*C*$_6$H$_3$), 128.4 (*m*-*C*$_6$H$_3$), 124.6 (*m*-*C*$_6$H$_3$) 123.7 (*p*-*C*$_6$H$_3$), 123.6 (*p*-*C*$_6$H$_3$) , 123.4 (N*C*H on IPr), 122.5 (*m*-*C*$_6$H$_3$), 58.0 (N*C*HMe$_2$ on carbodiimide), 45.9 (N*C*HMe$_2$ on carbodiimide), 44.4 ((NCH*Me*$_2$ on carbodiimide), 28.9 (*C*HMe$_2$ on IPr), 27.8 (*C*HMe$_2$ on SiN^{Dipp}), 27.4 (NCH*Me*$_2$ on carbodiimide), 26.2 (CH*Me*$_2$ on SiN^{Dipp}), 26.1 (CH*Me*$_2$ on SiN^{Dipp}), 24.8 (CH*Me*$_2$ on IPr), 23.8 (CH*Me*$_2$ on IPr), 15.1 (Si*C*H$_2$), 1.4 (Si*Me*$_2$). ^{13}C resonance correlated to Al*C*N not observed.

Figure S6. ^{1}H NMR spectrum of **14**. (500 MHz, 298 K, Benzene-d_6) *grease

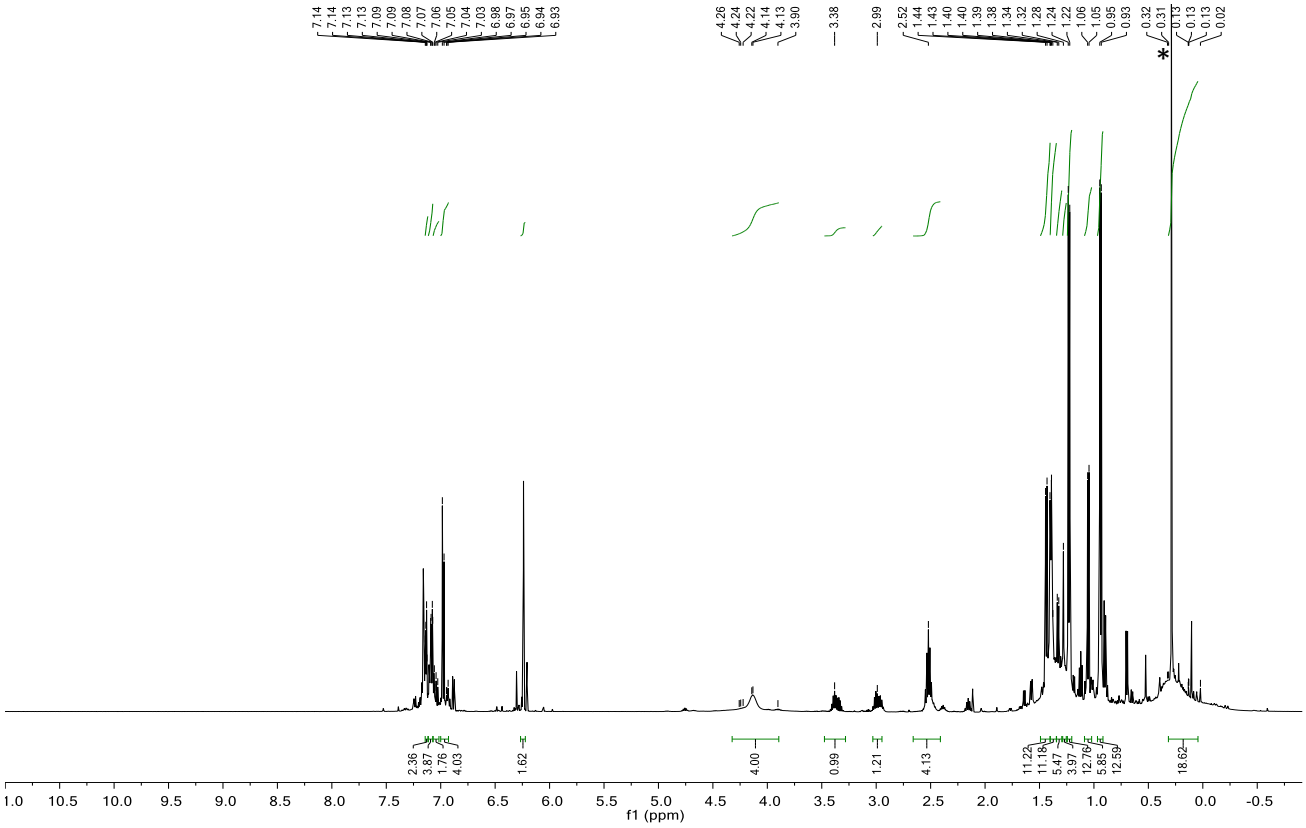


Figure S7. ^{13}C{^{1}H} NMR spectrum of **14**. (126 MHz, 298 K, Benzene-d_6)

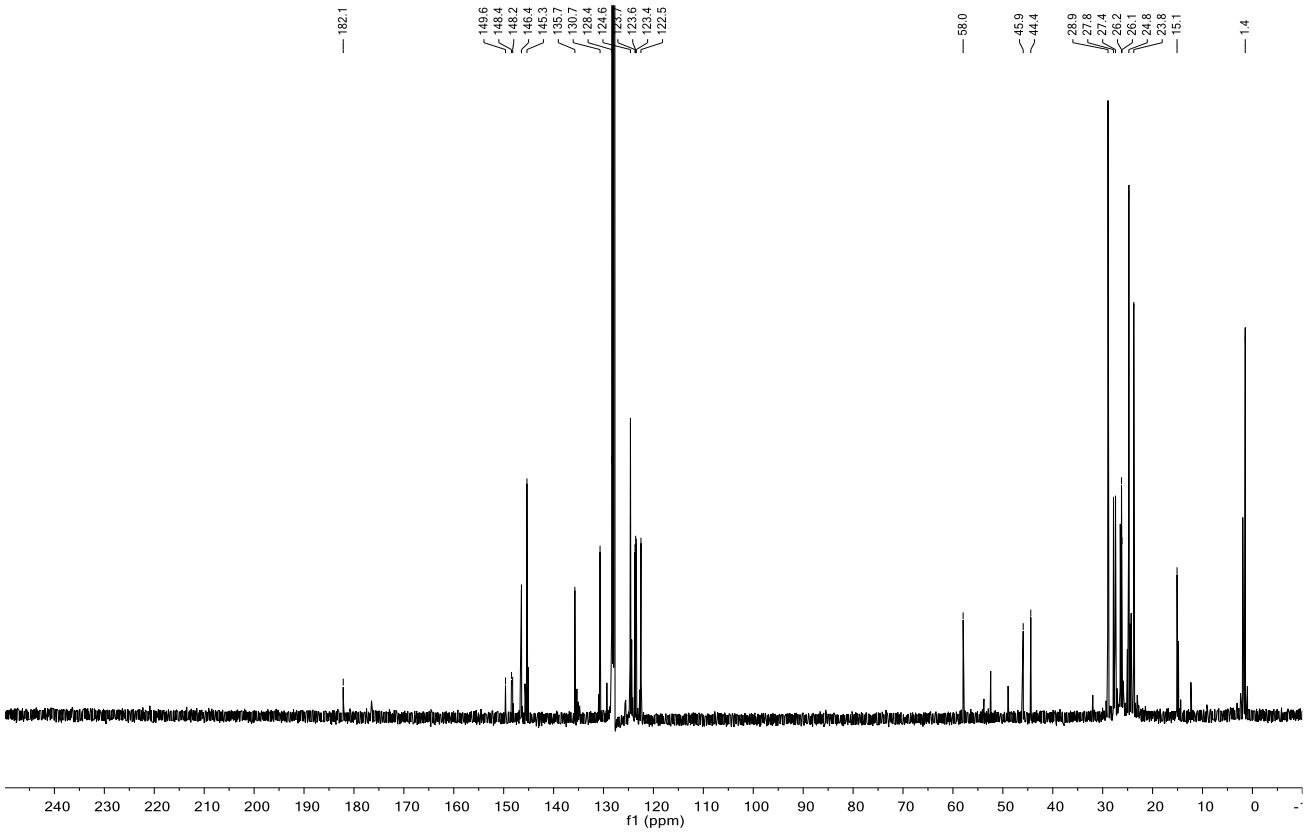


Figure S8. ^{1}H-^{1}H COSY NMR spectrum of **14**.

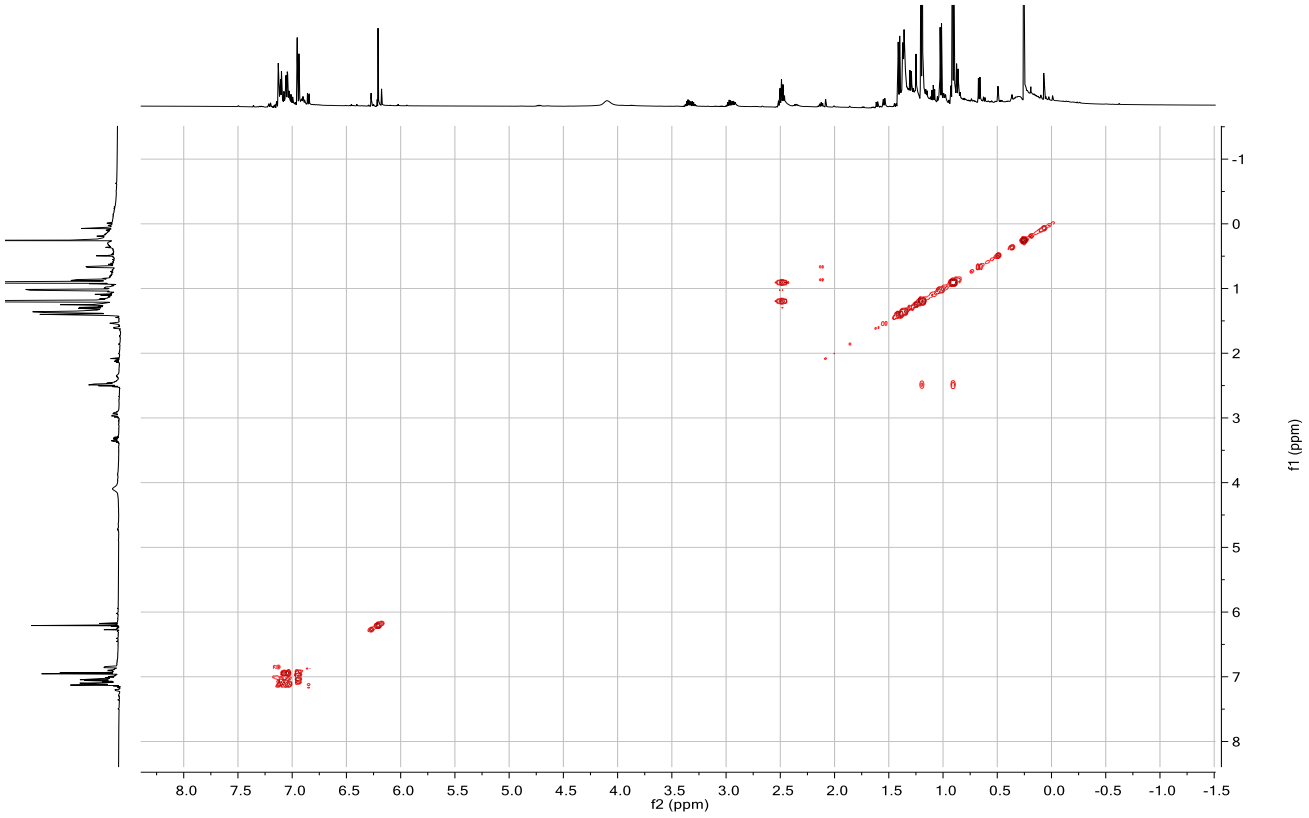


Figure S9. ^{1}H-^{13}C HSQC NMR spectrum of **14**.

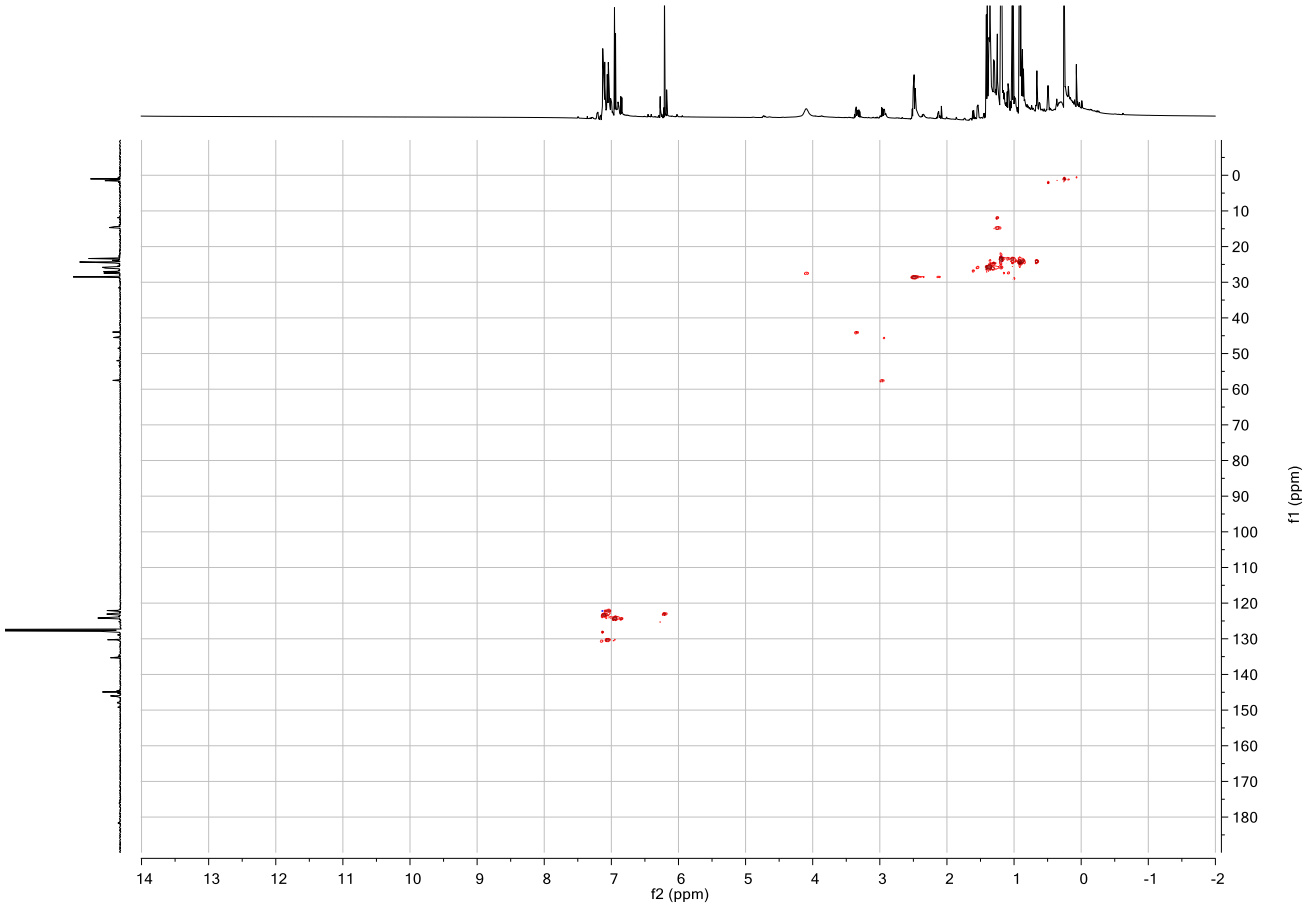
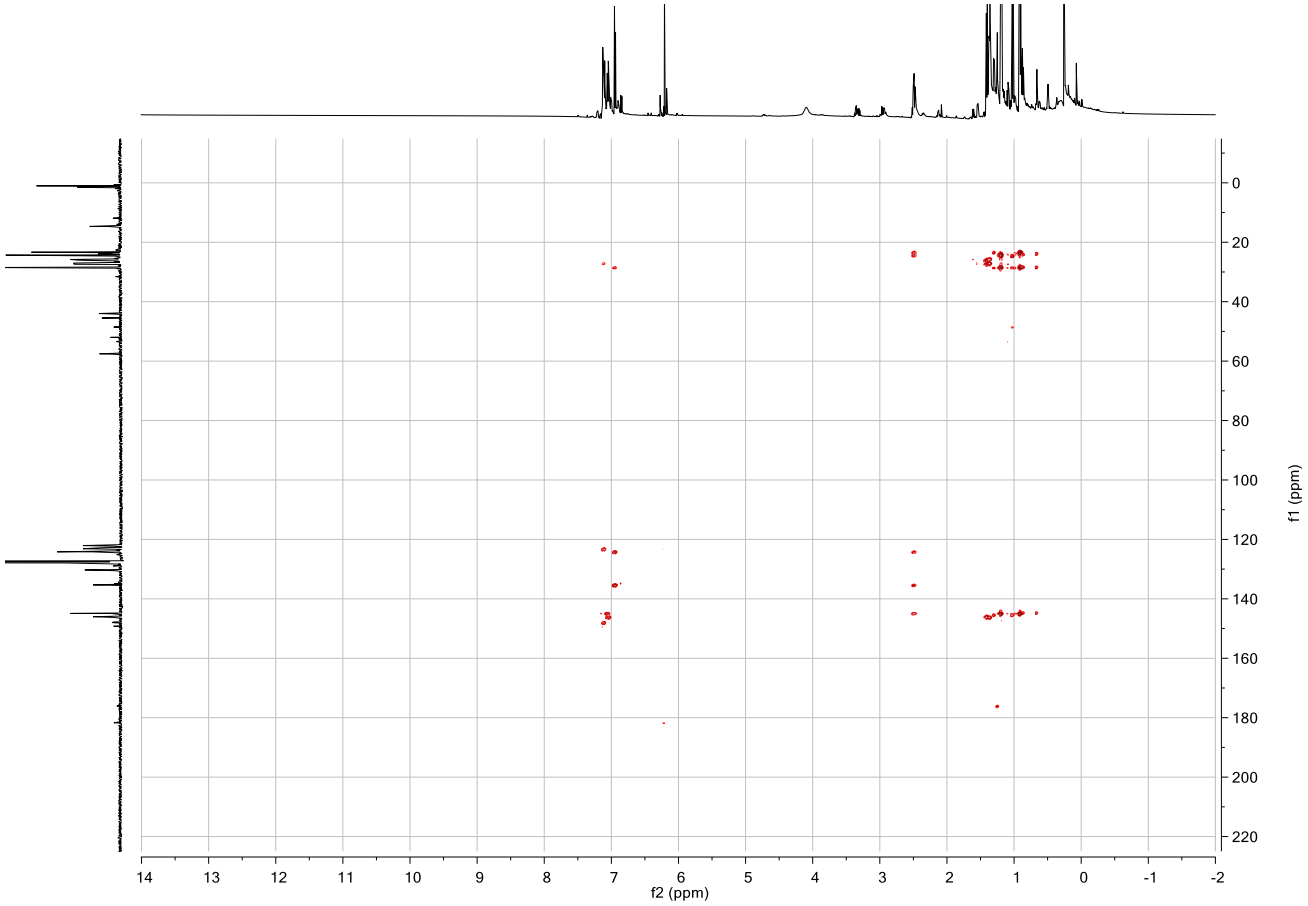


Figure S10. ^{1}H-^{13}C HMBC NMR spectrum of **14**.



*Synthesis of { SiN^{Dipp}}Al-O_2C-Cu{IPr} (**15**)*

{SiN^{Dipp}}Al-Cu{IPr}(**13**, 25 mg, 0.026mmol),was dissolved in 0.4mL of C_6D_6 inside a J Young's tube. The solution was then degassed by three cycles of freeze-pump-thaw before the tube was charged with 2 atm of $^{13}CO_2$. Full Conversion of the starting material was determined by ^{1}H and ^{13}C NMR spectra within 30 minutes of the addition of the CO_2 to the solution. No meaningful result was obtained for elemental analysis after multiple attempts. ^{1}H NMR (500 MHz, 298 K, Benzene-d_6) δ 7.25-7.22 (m, 2H, *p*-C_6H_3), 7.12 – 7.08 (m, 2H, *p*-C_6H_3), 7.04-7.01 (m, 8H, *m*-C_6H_3), 6.09 (s, 2H, NC*H*), 3.95 (sept, *J* = 6.8 Hz, 4H,C*H*Me_2 on SiN^{Dipp}), 2.24 (sept, *J* = 6.9 Hz, 4H, C*H*Me_2 on IPr), 1.41 (d, *J* = 6.8 Hz, 12H, CH*Me*$_2$ on SiN^{Dipp}), 1.20 (s, 4H, SiCH_2), 1.13 (d, *J* = 6.8 Hz, 12H, CH*Me*$_2$ on SiN^{Dipp}), 1.06 (d, *J* = 6.9 Hz, 12H CH*Me*$_2$ on IPr), 1.01 (d, *J* = 6.9 Hz, 12H CH*Me*$_2$ on IPr), 0.29 (s, 12H, Si*Me*$_2$)*overlapping with grease. ^{13}C NMR (126 MHz, 298 K, Benzene-d_6) δ 234.0 (Cu*C*O_2), 165.8 (*i*-C_6H_3), 163.2 (*i*-C_6H_3), 146.5 (*o*-C_6H_3), 145.4 (*o*-C_6H_3), 124.3 (*m*-C_6H_3), 123.3 (*m*-C_6H_3), 122.8 (*p*-C_6H_3), 122.7 (*p*-C_6H_3), 28.8 (*C*HMe_2), 27.7 (*C*HMe_2), 25.5 (CH*Me*$_2$), 25.1 (CH*Me*$_2$), 23.9 (CH*Me*$_2$), 23.7 (CH*Me*$_2$), 14.4 (Si*C*H_2), 0.5 (Si*Me*$_2$) ^{13}C resonance correlated to Cu$C_{carbene}$ was not observed.

Figure S11. ^{1}H NMR spectrum of **15**. (500 MHz, 298 K, Benzene-d_6) *grease

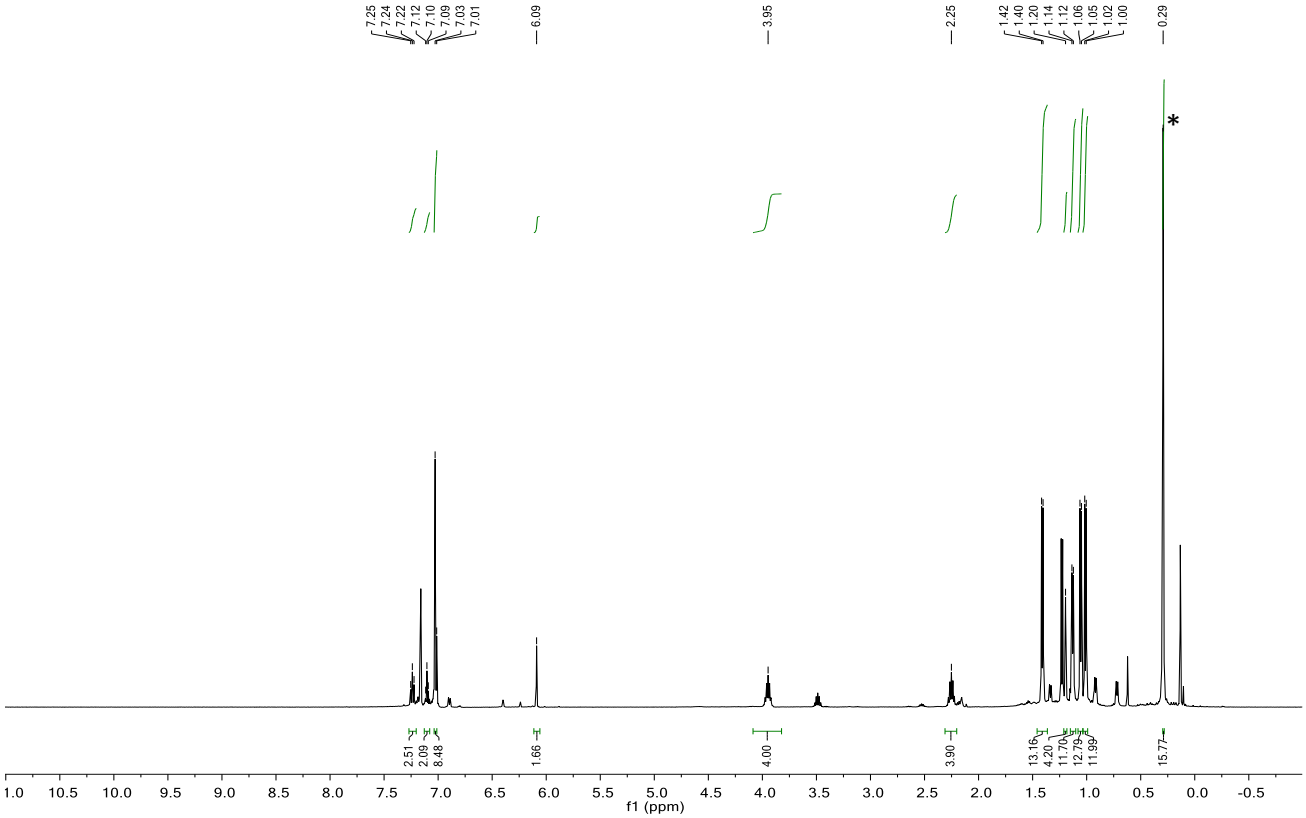
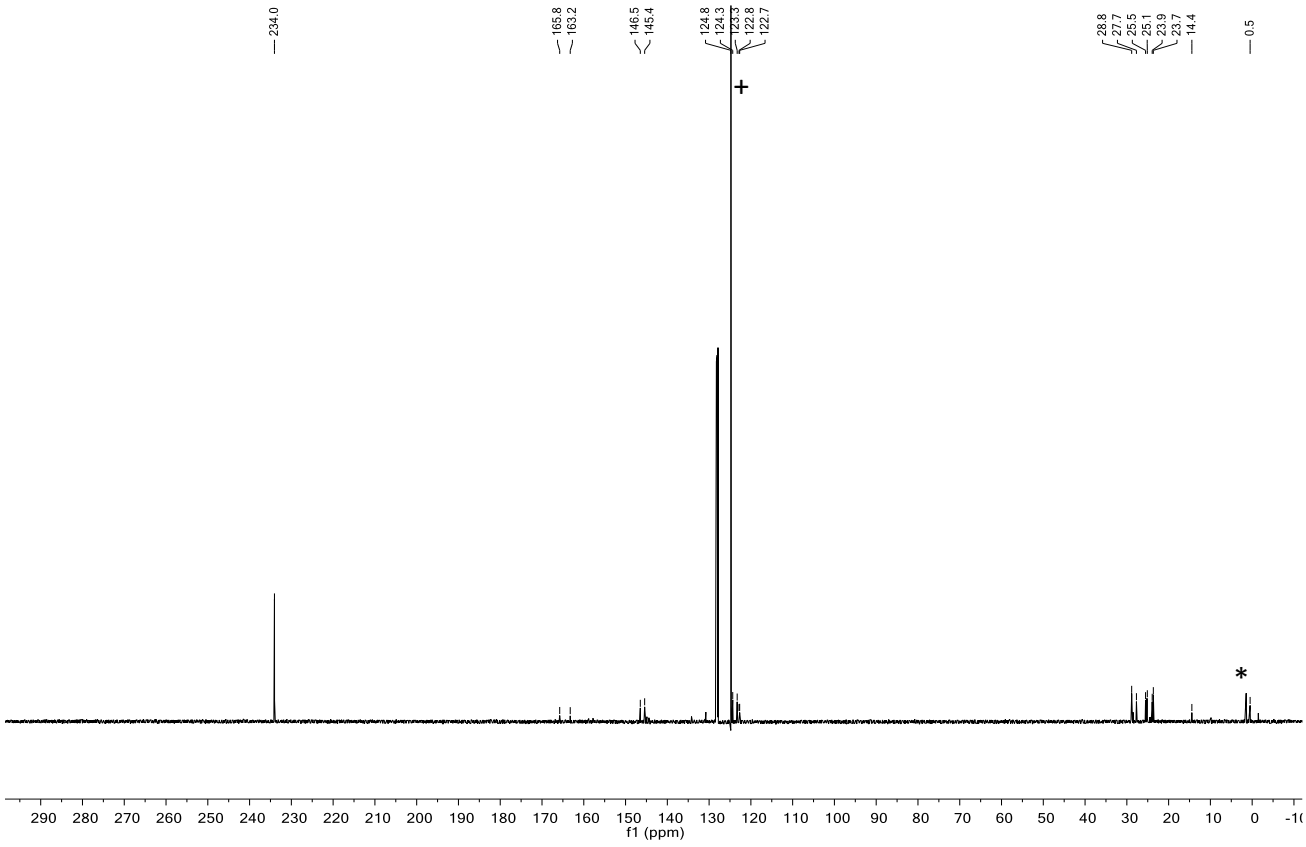


Figure S12. ^{13}C{^{1}H} NMR spectrum of **15**. (126 MHz, 298 K, Benzene-d_6) $^{+}$ residual $^{13}CO_2$ *grease



Synthesis of {SiN^{Dipp}}Al-Ag{NHC^{iPr}} (**16**)

Hexane (25 mL) was cannula transferred into a foil wrapped Schlenk flask containing *N,N'*-diisopropyl-4,5-dimethyl-2-ylidene (NHC^{iPr}, 0.180 g, 1.00 mmol) and AgCl (0.143 g, 1.00 mmol). After the suspension was stirred for 3 days at 40^{o}C, a solution of [{SiN^{Dipp}}AlK]$_2$ (**3**, 0.560 g, 1.00 mmol) in hexane (20 mL) was then added to the stirring white suspension, and the resulting pale yellow reaction mixture was stirred at room temperature overnight before filtering. The colourless filtrate was then collected, all volatiles were then removed *in vacuo* yielding **16** as an off-white solid. Yield 0.528 g, 65.2%. Anal Calc'd for $C_{41}H_{70}AlAgN_4Si_2$ (**16**, 810.06) C, 60.79; H, 8.71; N, 6.92 %. Found: C, 60.04; H, 8.32; N, 6.63 %. ^{1}H NMR (500 MHz, 298 K, Benzene-d_6) δ 7.16-7.14 (m, 4H, *m*-C$_6$*H*$_3$), 7.06 – 6.99 (m, 2H, *p*-C$_6$*H*$_3$), 4.17 (sept, *J* = 6.9 Hz, 4H, C*H*Me$_2$ on SiN^{Dipp}), 3.63 (sept, *J* = 6.7 Hz, 2H, NC*H*Me$_2$ on NHC^{iPr}), 1.51 (d, *J* = 6.9 Hz, 12H, CH*Me*$_2$ on SiN^{Dipp}), 1.47 (d, *J* = 6.9 Hz, 12H, CH*Me*$_2$ on SiN^{Dipp}), 1.34 (s, 6H, NC*Me*), 1.27 (s, 4H, SiC*H*$_2$), 1.00 (d, *J* = 6.7 Hz, 12H, NCH*Me*$_2$ on NHC^{iPr}), 0.37 (s, 12H, Si*Me*$_2$). ^{13}C{^{1}H} NMR (126 MHz, 298 K, Benzene-d_6) δ 230.5 (Ag*C*$_{carbene}$). 147.4(*o*-C$_6$H$_3$), 146.6 (*i*-*C*$_6$H$_3$), 123.1 (*m*-*C*$_6$H$_3$), 122.8 (*p*-*C*$_6$H$_3$), 122.5 (N*C*Me), 49.7 (N*C*HMe$_2$ on NHC^{iPr}), 28.3 (*C*HMe$_2$ on SiN^{Dipp}), 26.0 (CH*Me*$_2$ on SiN^{Dipp}), 24.7 (CH*Me*$_2$ on SiN^{Dipp}), 24.2 (NCH*Me*$_2$ on NHC^{iPr}), 14.3 (Si*C*H$_2$), 8.7 (NC*Me*), 1.3 (Si*Me*$_2$).

Figure S13. ^{1}H NMR spectrum of **16**. (500 MHz, 298 K, Benzene-d_6)

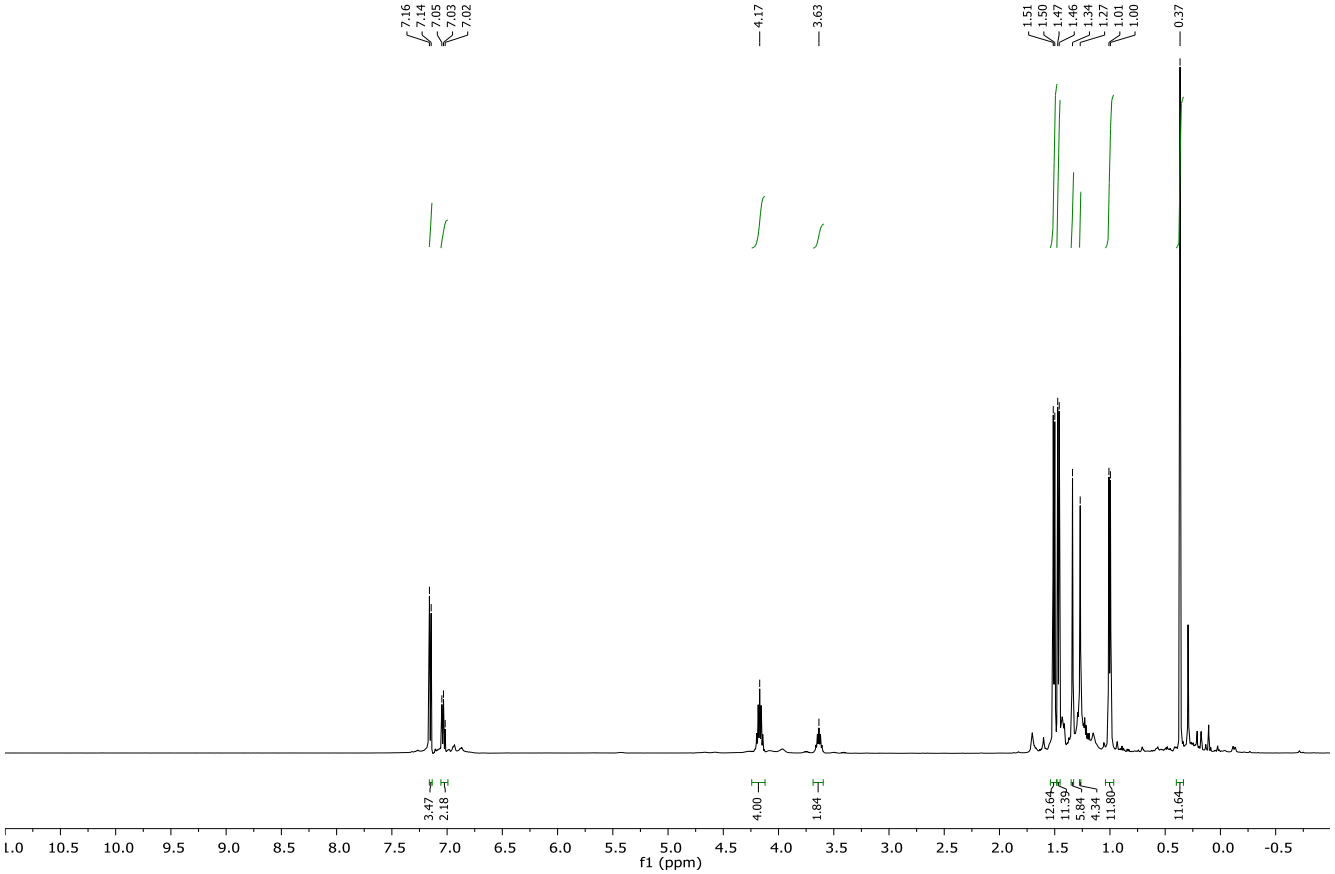


Figure S14. ^{13}C{^{1}H} NMR spectrum of **16**. (126 MHz, 298 K, Benzene-d_6)

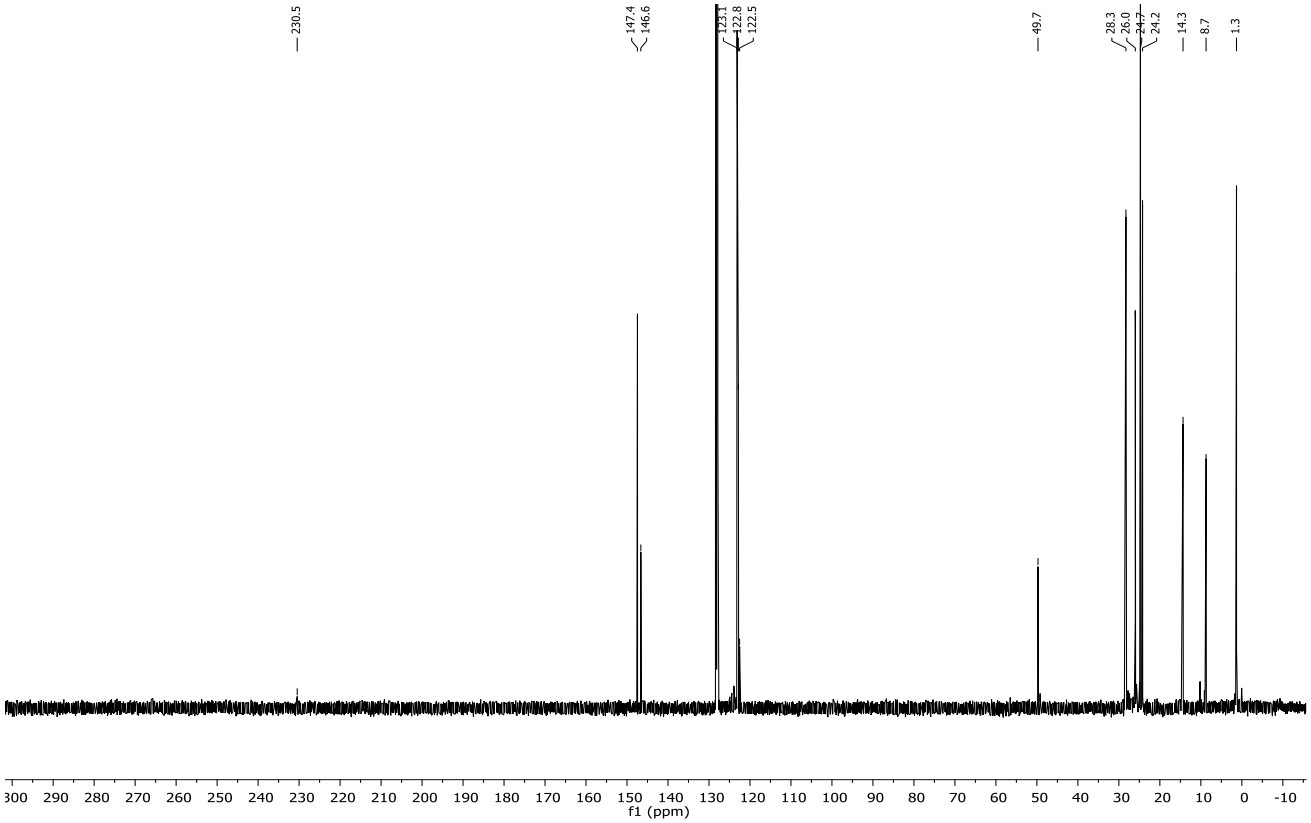


Figure S15. ^{1}H-^{1}H COSY NMR spectrum of **16**.

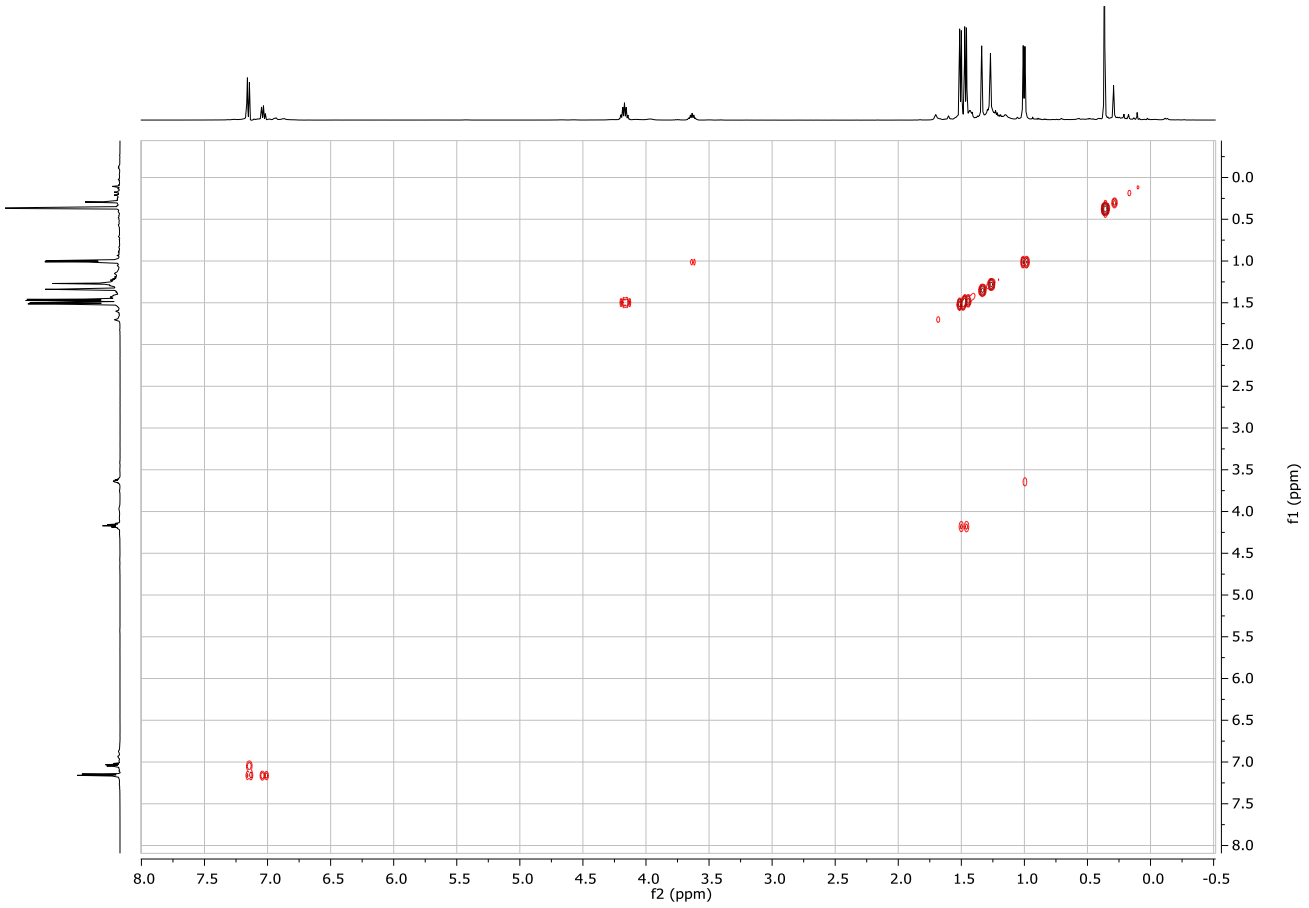


Figure S16. ^{1}H-^{13}C HSQC NMR spectrum of **16**.

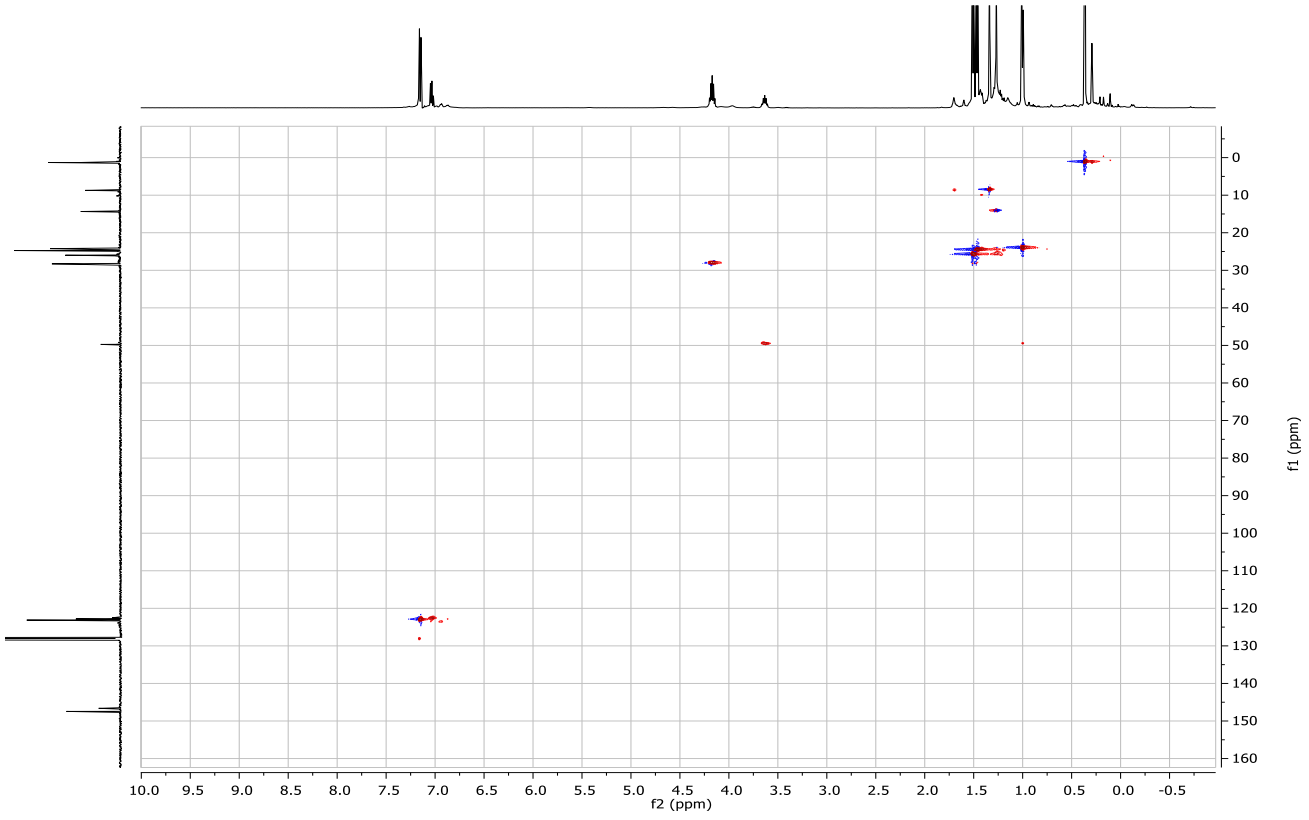
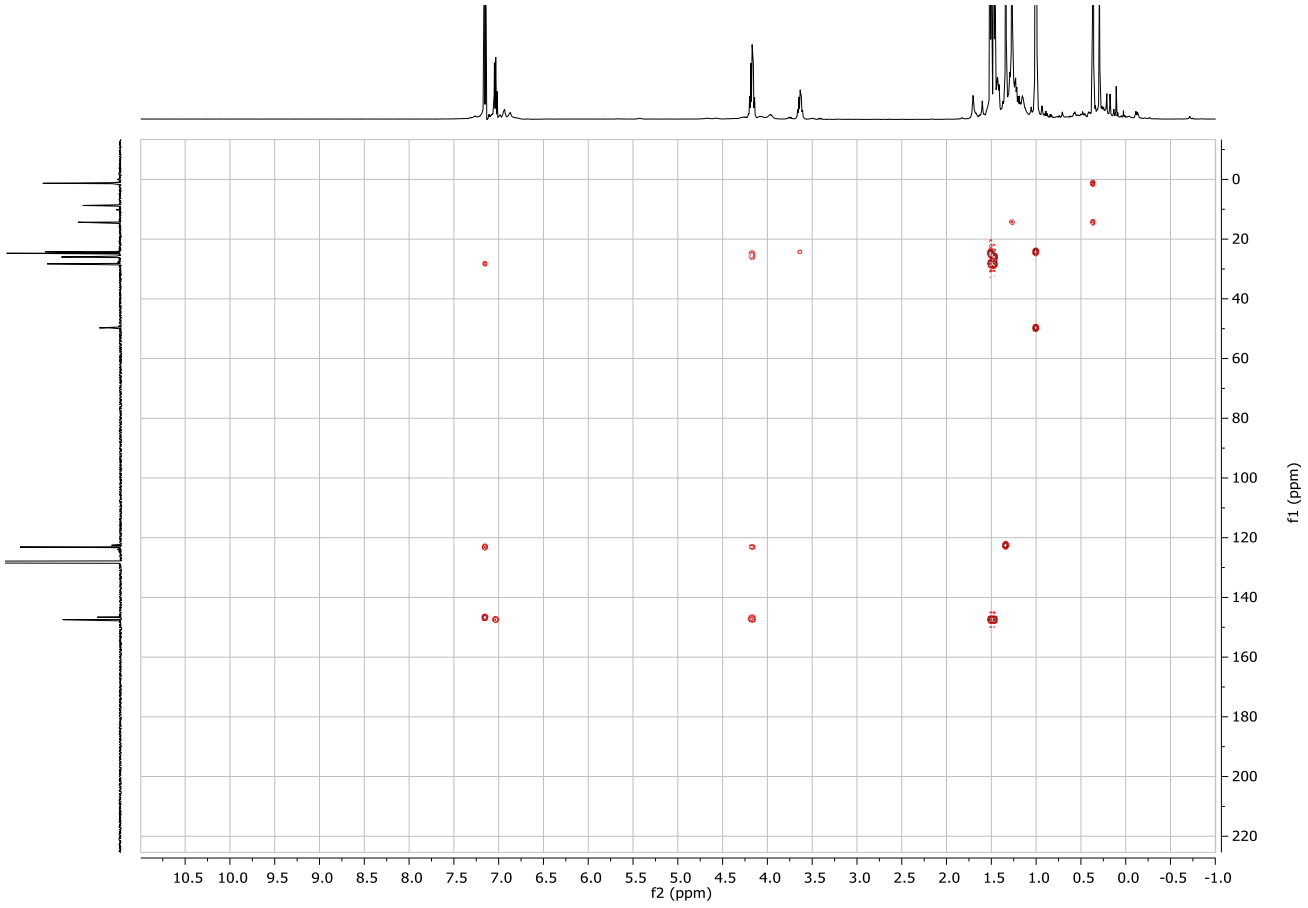


Figure S17. ^{1}H-^{13}C HMBC NMR spectrum of **16**.



Synthesis of {SiN^{Dipp}}Al-Au{NHC^{iPr}} (**17**)

Hexane (30 mL) was cannula transferred into a Schlenk flask charged with *N,N'*-diisopropyl-4,5-reaction mixture was then stirred at room temperature overnight before filtering. The pale-yellow filtrate was then collected, and all volatiles were removed *in vacuo*, giving **17** as a light brown fine powder. Yield 0.617 g, 69%. Colourless crystals suitable for X-ray crystallography were obtained by slow evaporation of a methylcyclohexane solution at room temperature. No meaningful result was obtained for elemental analysis after multiple attempts. ^{1}H NMR (500 MHz, 298 K, Benzene-d$_6$) δ 7.15 – 7.13 (m, 4H, *m*-C$_6$*H$_3$*), 7.04 – 6.98 (m, 2H, *p*-C$_6$*H$_3$*), 4.15 (sept, *J* = 6.9 Hz, 4H, C*H*Me$_2$ on SiN^{Dipp}), 3.84 (sept, *J* = 6.9 Hz, 2H, C*H*Me$_2$ on NHC^{iPr}), 1.57 (d, *J* = 6.9 Hz, 12H, CH*Me$_2$* on SiN^{Dipp}), 1.47 (d, *J* = 6.9 Hz, 12H, CH*Me$_2$* on SiN^{Dipp}), 1.33 (s, 6H, NC*Me*), 1.24 (s, 4H, SiC*H$_2$*), 1.07 (d, *J* = 6.9 Hz, 12H, CH*Me$_2$* on NHC^{iPr}), 0.35 (s, 12H, Si*Me$_2$*). ^{13}C{^{1}H} NMR (126 MHz, 298 K, Benzene-d$_6$) δ 216.1 (Au*C*$_{carbene}$) 147.3 (*o*-*C*$_6$H$_3$), 146.3 (*i*-*C*$_6$H$_3$), 123.1 (*m*-*C*$_6$H$_3$), 123.0 (*p*-*C*$_6$H$_3$), 122.7 (N*C*Me), 50.1 (N*C*HMe$_2$ on NHC), 28.4 (*C*HMe$_2$ on SiN^{Dipp}), 26.0 (CH*Me$_2$* on SiN^{Dipp}), 24.7 (CH*Me$_2$* on SiN^{Dipp}), 23.5 (NCH*Me$_2$* on NHC^{iPr}), 14.2 (Si*C*H$_2$), 9.1 (NC*Me*), 1.1 (Si*Me$_2$*).

Figure S18. ^{1}H NMR spectrum of **17**. (500 MHz, 298 K, Benzene-d_6)

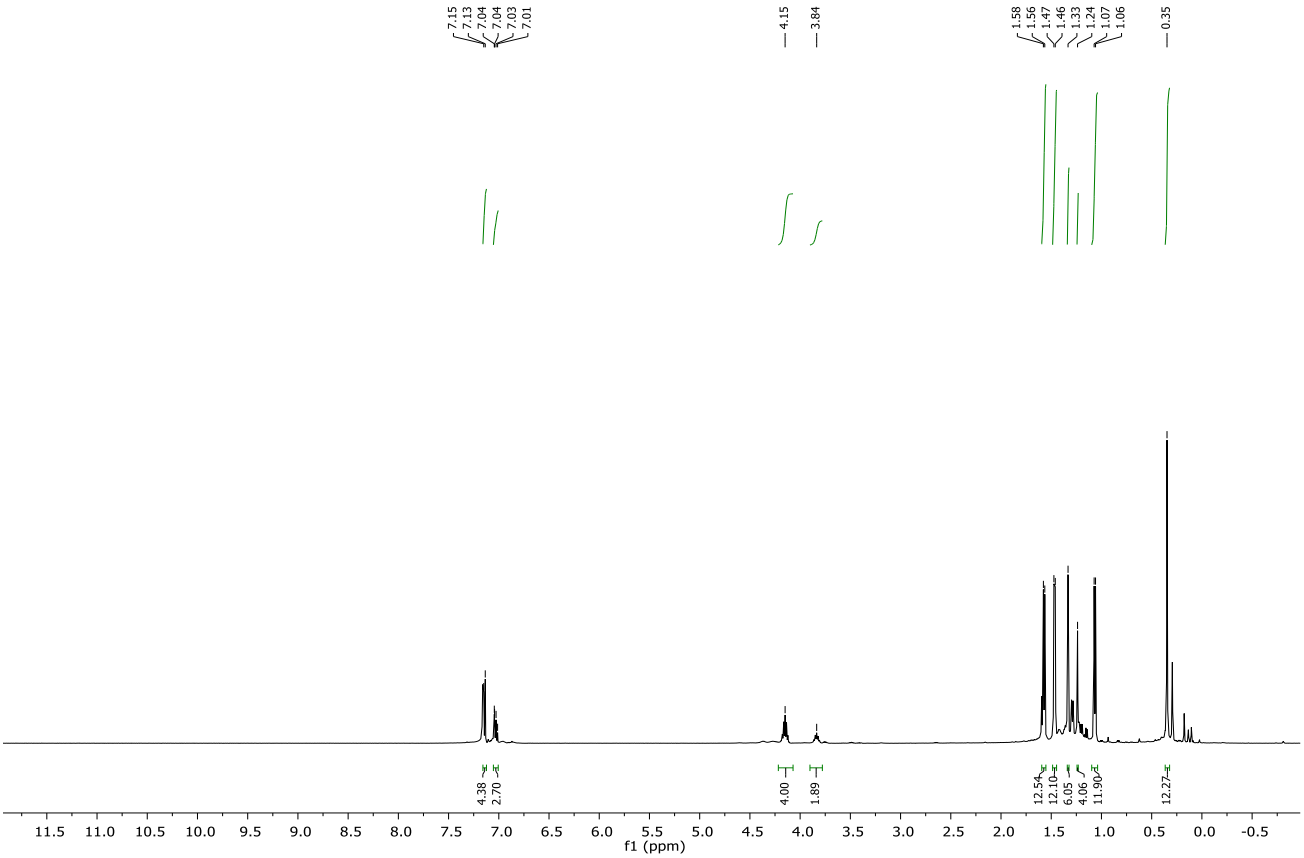


Figure S19. ^{13}C{^{1}H} NMR spectrum of **17**. (126 MHz, 298 K, Benzene-d_6)

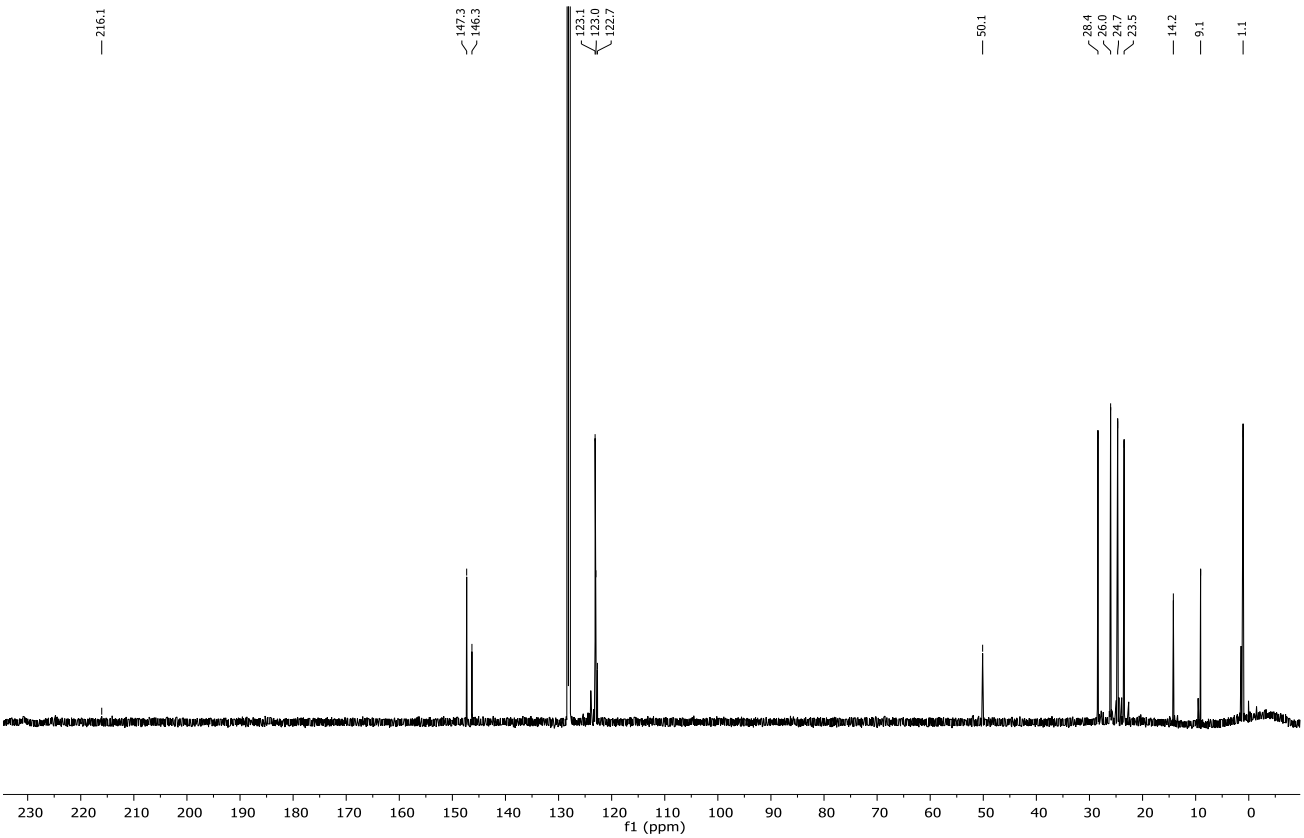


Figure S20. ^{1}H-^{1}H COSY NMR spectrum of **17**.

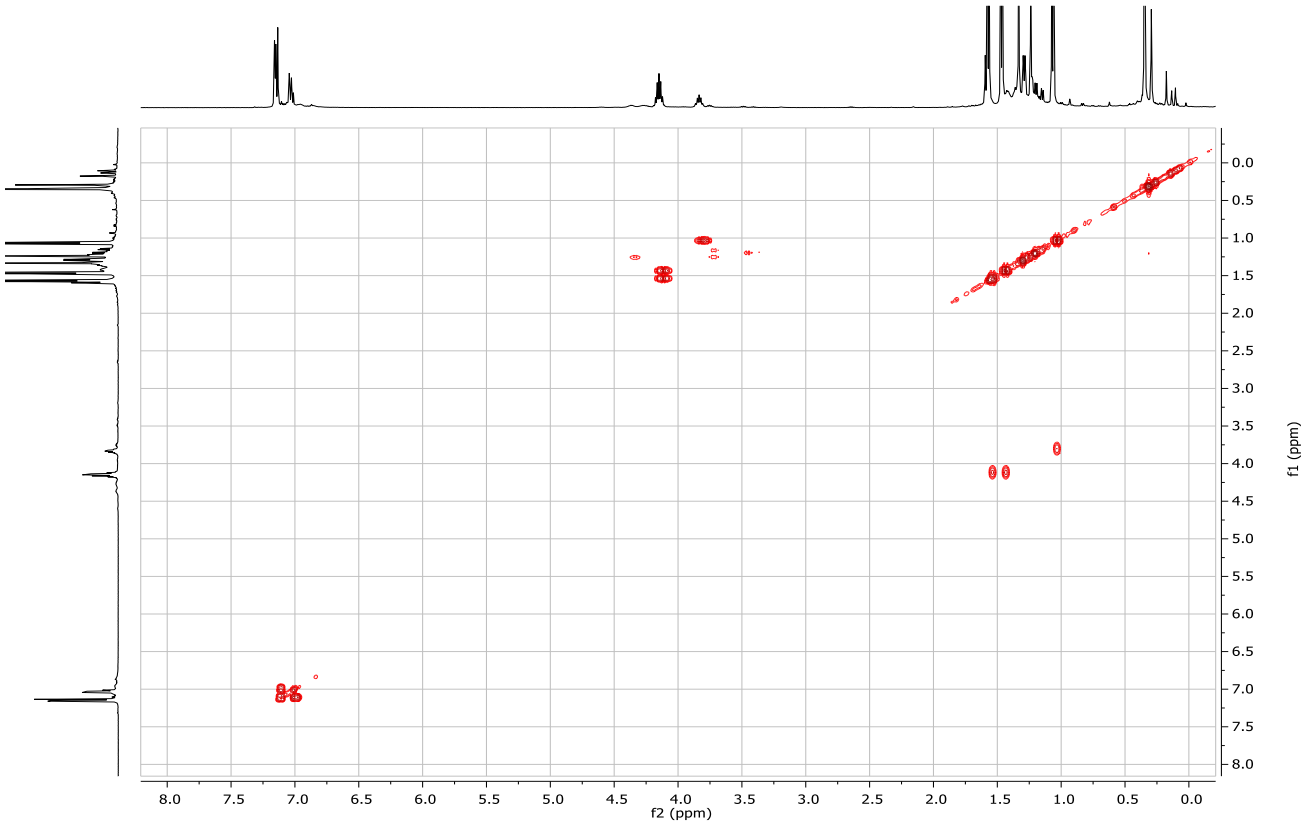


Figure S21. ^{1}H-^{13}C HSQC NMR spectrum of **17**.

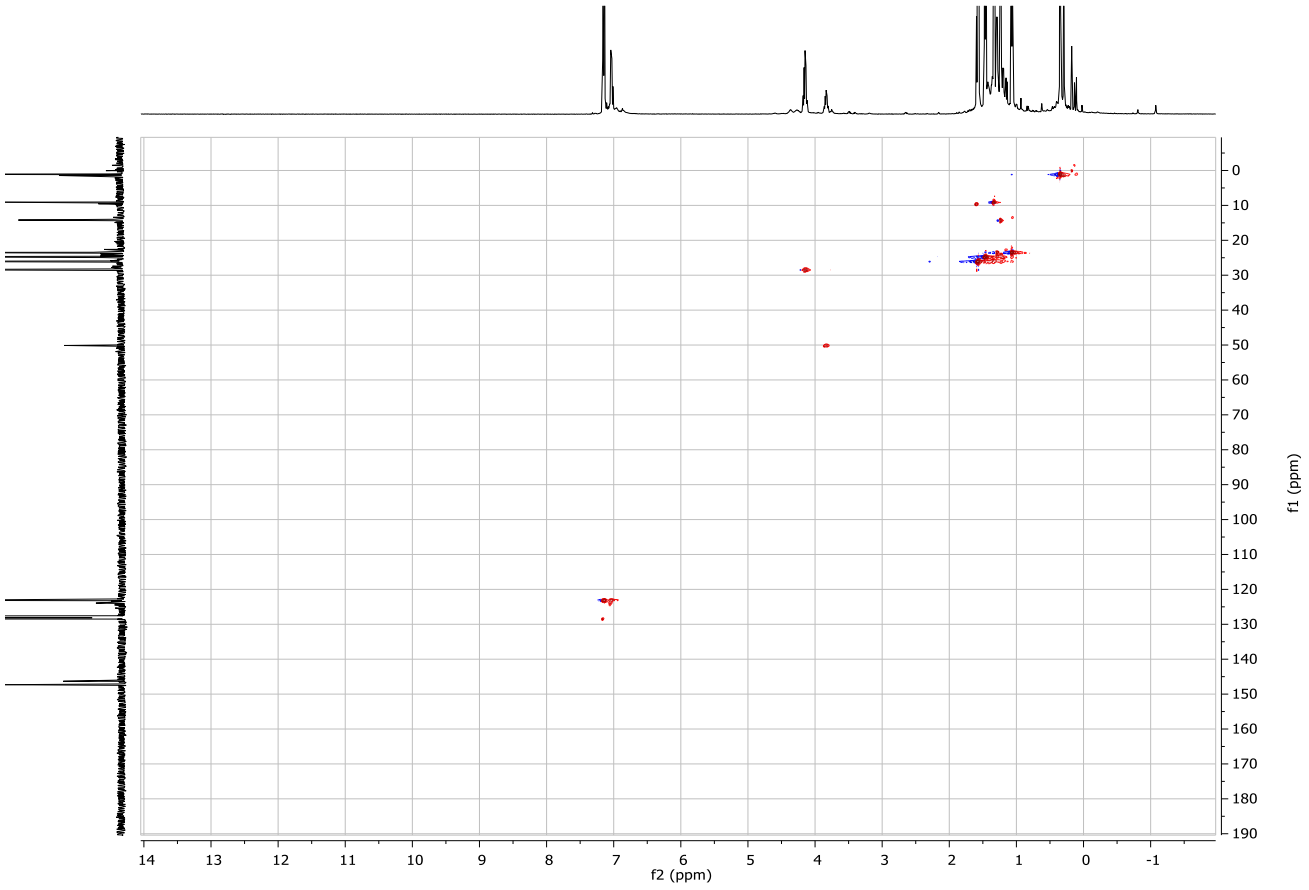
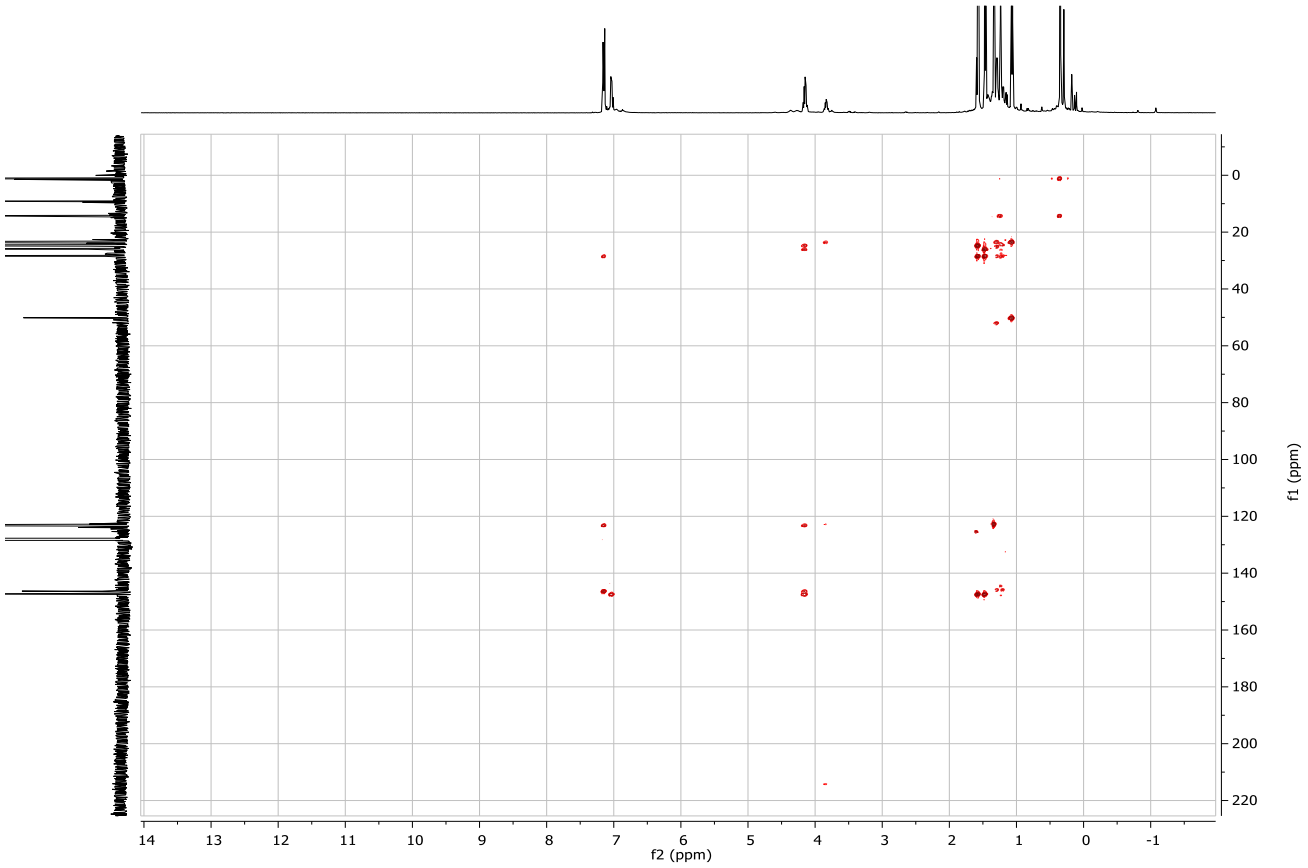


Figure S22. ^{1}H-^{13}C HMBC NMR spectrum of **17**.



*Isolation of {SiN^{Dipp}}Al-Ag{^{cy}CAAC}(**18**)*

Inside a J-Young's tube, ^{cy}CAACAgCl (23.5mg, 0.05mmol) was added to the C_6D_6 solution of [{SiN^{Dipp}}AlK]$_2$ (**3**) (28mg, 0.05mmol) to afford a pale-yellow reaction mixture. compound **18** was then identified by X-ray crystallography as a colourless crystal picked from the mix of crystalline and amorpous obtained from slow evaporation of the benzene solution of the crude reaction mixture.

*Synthesis of {SiN^{Dipp}}Al-C(N^{i}Pr)$_2$-Ag{NHC^{iPr}} (**19**)*

Inside a J Young's tube, {SiN^{Dipp}}Al- Ag{ NHC^{iPr}} (**16**, 40.5mg, 0.05mmol) was dissolved in 0.4mL of C_6D_6, *N,N'*-diisopropylcarbodiimide (7.8µL, 0.05mmol) was then added *via* a micropipette. ^{1}H NMR suggested a slow conversion of the starting materials into a new species within 30 min. Total transformation was observed after the reaction mixture was left at room temperature for 4 hours, cleanly forming a new single species. The benzene solution was then put under vacuum to remove all volatiles and giving **19** as white solid. Colourless crystals suitable for X-ray crystallography were obtained by slow evaporation of a methylcyclohexane solution at room temperature. Yield 34 mg, 73%. No meaningful result for elemental analysis was obtained after several attempts. ^{1}H NMR (500 MHz, 298 K, Benzene-d_6) δ 7.26-7.24 (m, 4H, *m*-C$_6$*H*$_3$), 7.16 – 7.11 (m, 2H, *p*-C$_6$*H*$_3$), 4.56 – 4.48 (m, 1H, NC*H*Me$_2$ on carbodiimide), 4.41 – 4.27 (m, 4H, C*H*Me$_2$ on SiN^{Dipp}), 4.06 (sept, *J* = 6.9 Hz, 2H, NC*H*Me$_2$ on NHC^{iPr}), 3.51 – 3.42 (m, 1H, NC*H*Me$_2$ on carbodiimide), 1.63 (d, *J* = 6.8 Hz, 6H, CH*Me$_2$* on SiN^{Dipp}), 1.56 (m, 6H, CH*Me$_2$* on SiN^{Dipp}), 1.53-1.48 (m, 12H, CH*Me$_2$* on SiN^{Dipp}), 1.40-1.35 (br, 4H, SiC*H*$_2$), 1.34 (s, 6H, NC*Me*), 1.09 (d, *J* = 6.9 Hz, 12H, NCH*Me$_2$* on NHC^{iPr}), 1.01 – 0.91 (m, 6H, NCH*Me$_2$* on carbodiimide) 0.91-0.77 (m, 6H, NCH*Me$_2$* on carbodiimide), 0.52 – 0.31 (br, 12H, Si*Me$_2$*). ^{13}C{^{1}H} NMR (126 MHz, 298 K, Benzene-d_6) δ 200.0 (*C*N$_2$ on carbodiimide) 148.6 (*i*-*C*$_6$H$_3$), 147.0 (*o*-*C*$_6$H$_3$), 146.5 (*o*-*C*$_6$H$_3$), 123.9 (*m*-*C*$_6$H$_3$), 123.6 (*p*-*C*$_6$H$_3$), 122.6 (N*C*Me), 57.8 (N*C*HMe$_2$ on carbodiimide), 52.0 (N*C*HMe$_2$ on NHC^{iPr}), 42.5 (N*C*HMe$_2$ on carbodiimide), 28.2 (NCH*Me$_2$* on carbodiimide), 28.1 (*C*HMe$_2$ on SiN^{Dipp}), 27.6 (*C*HMe$_2$ on SiN^{Dipp}), 26.5 (CH*Me$_2$* on SiN^{Dipp}), 26.4 (CH*Me$_2$* on SiN^{Dipp}), 26.1 (CH*Me$_2$* on SiN^{Dipp}), 25.9 (NCH*Me$_2$* on carbodiimide), 23.2 (NCH*Me$_2$* on NHC^{iPr}), 15.2 (Si*C*H$_2$) , 9.0 (NC*Me*), 2.0 (Si*Me$_2$*); ^{13}C resonance correlated to Ag-$C_{carbene}$ was not observed.

Figure S23. ^{1}H NMR spectrum of **19**. (500 MHz, 298 K, Benzene-d_6)

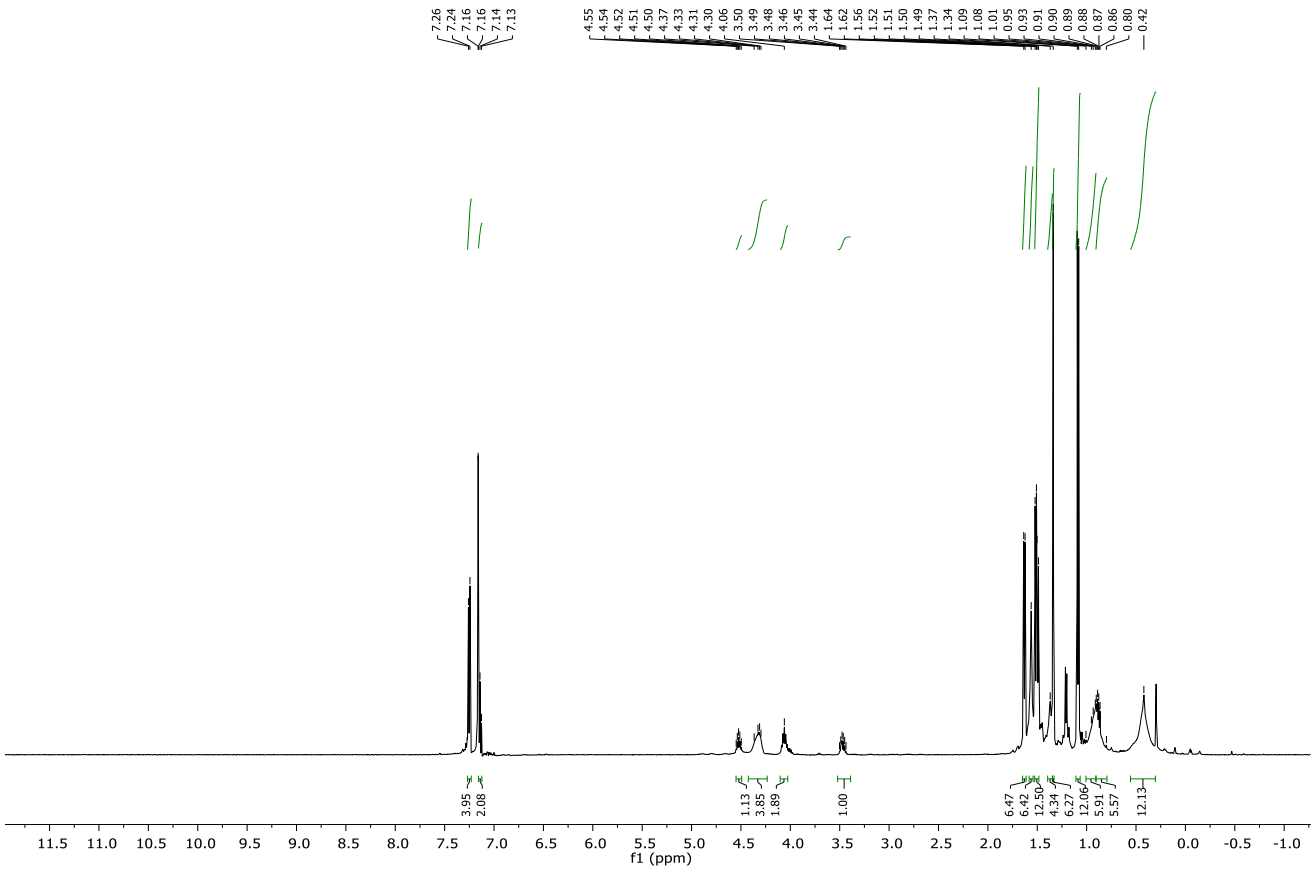


Figure S24. ^{13}C NMR spectrum of **19**. (126 MHz, 298 K, Benzene-d_6)

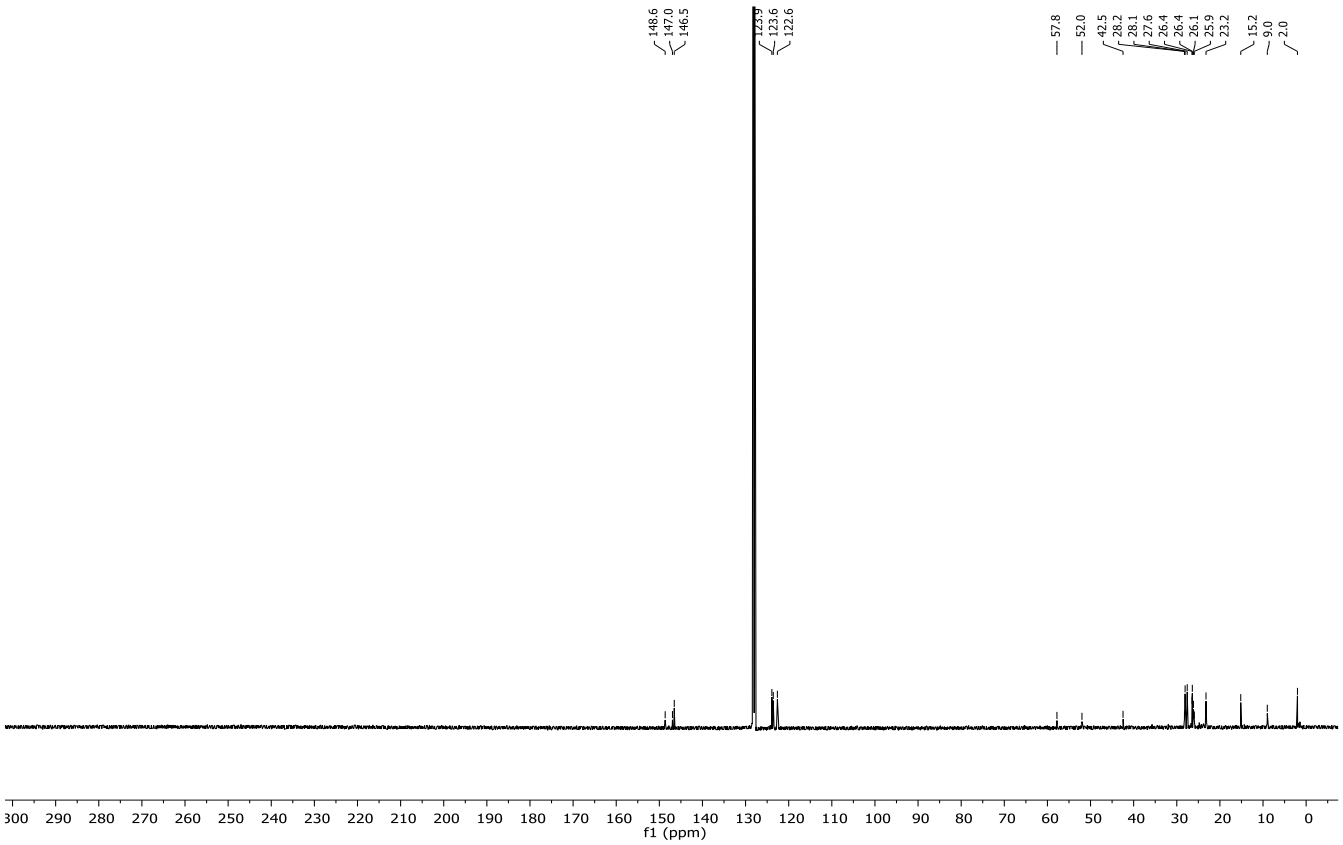


Figure S25. ^{1}H-^{1}H COSY NMR spectrum of **19**.

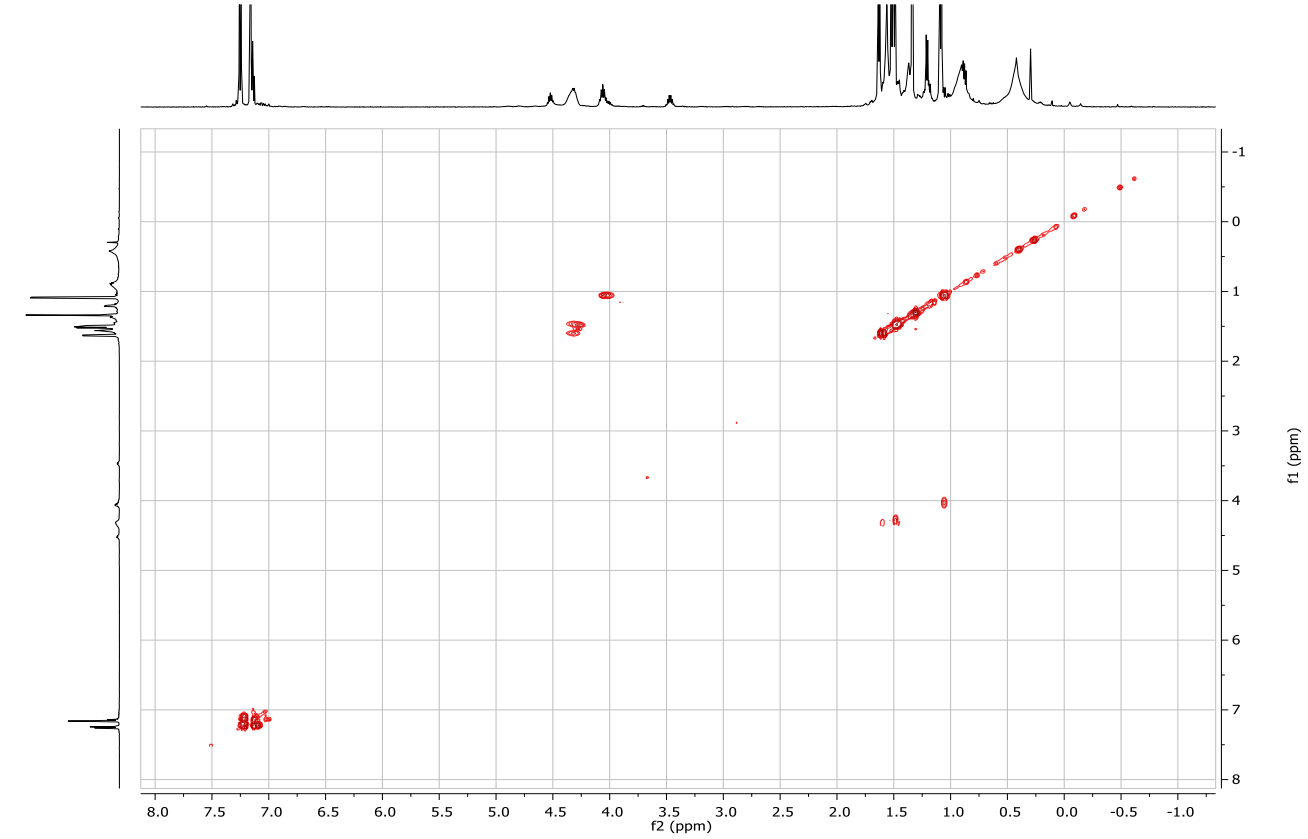


Figure S26. ^{1}H-^{13}C HSQC NMR spectrum of **19**.

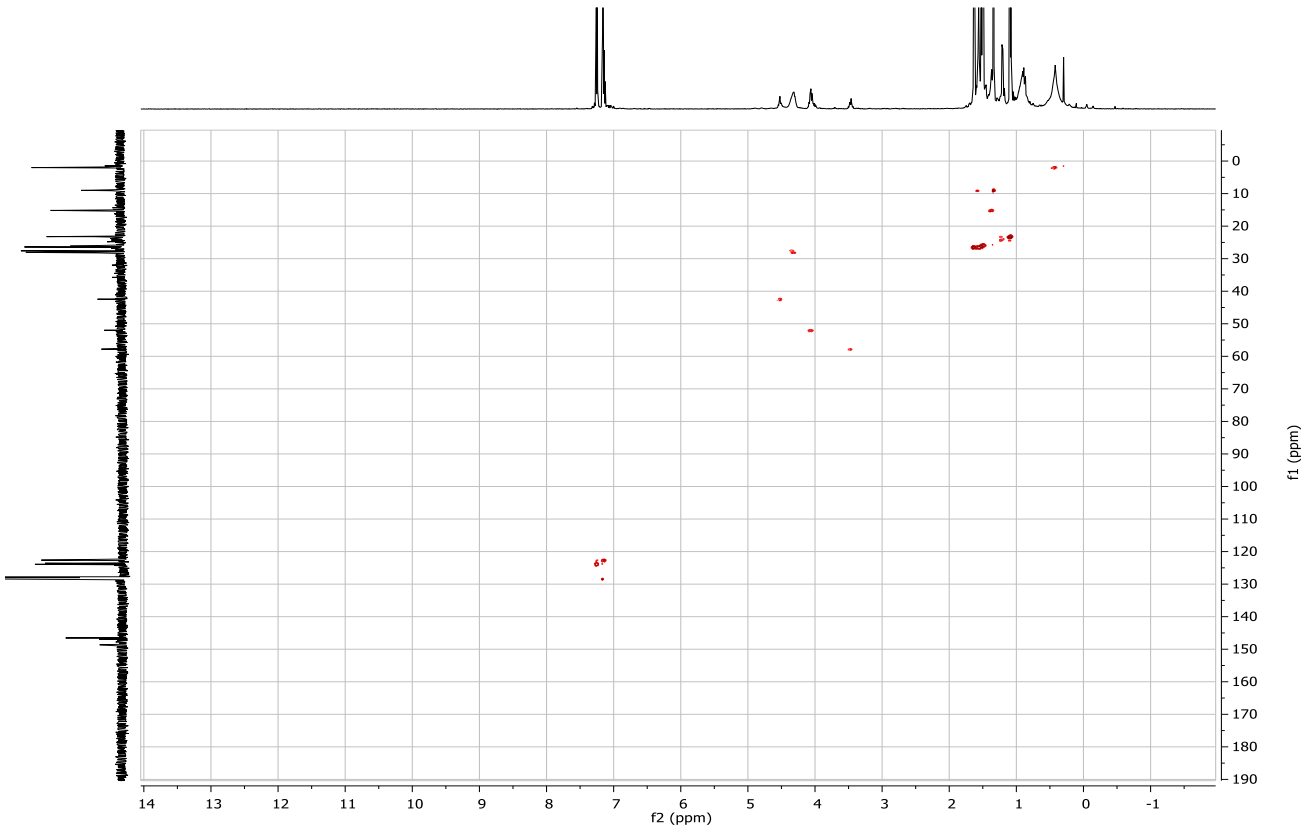
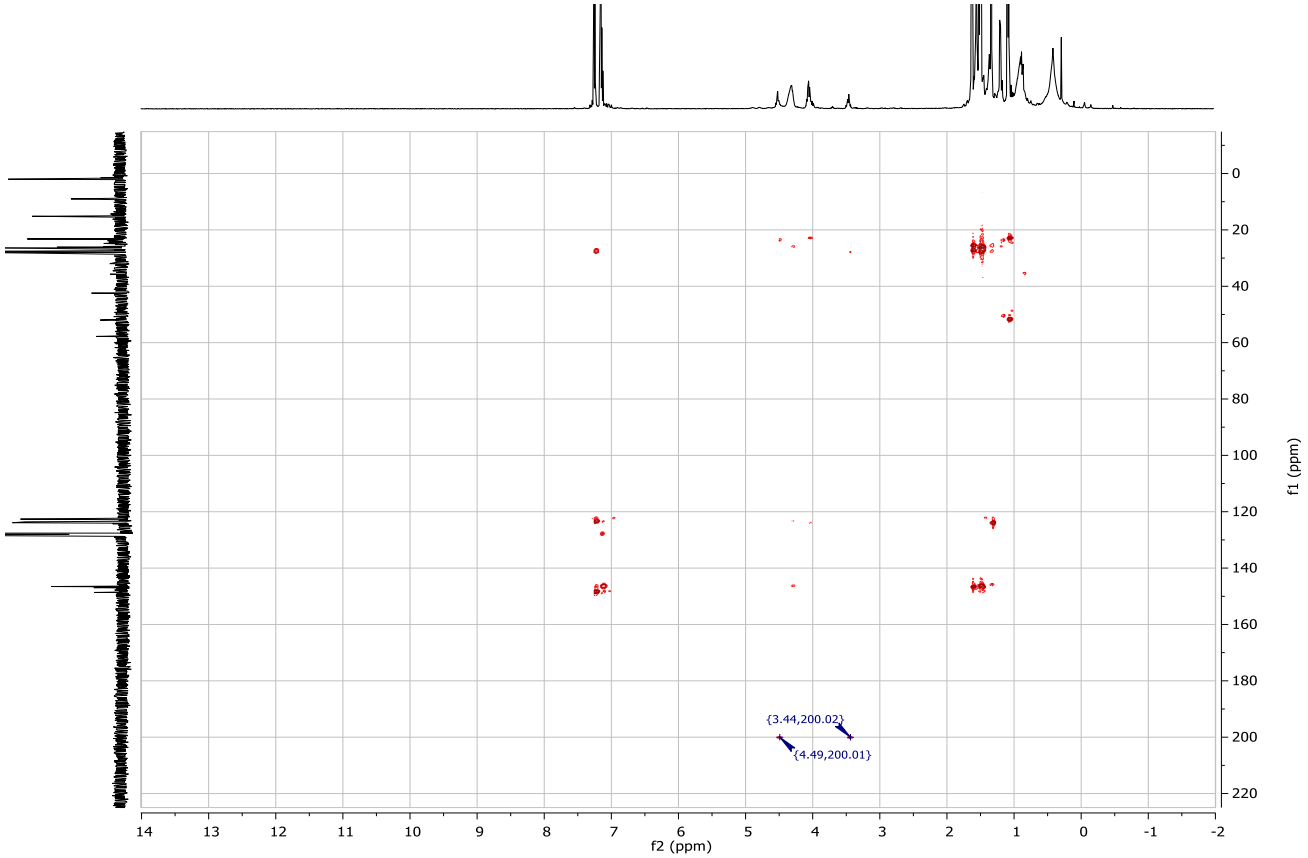


Figure S27. ^{1}H-^{13}C HMBC NMR spectrum of **19**.



*Synthesis of {SiN^{Dipp}}Al-(N^{i}Pr)$_2$C-Au{NHC^{iPr}} (**20**)*

Inside a J Young's tube, {SiN^{Dipp}}Al-Au{NHC^{iPr}} (**17**, 45.0mg, 0.05mmol) was dissolved in 0.4mL of C_6D_6, *N,N'*-diisopropylcarbodiimide (7.8μL, 0.05mmol) was then added *via* a micropipette. Total transformation was observed after the reaction mixture was left at room temperature for an hour, cleanly forming a new single species. The benzene solution was then put under vacuum to remove all volatiles and giving **20** as off white solid. Colourless crystals suitable for X-ray crystallography were obtained by slow evaporation of a methylcyclohexane solution at room temperature. Yield 38 mg, 74 %. Anal Calc'd for $C_{48}H_{84}AlAuN_6Si_2$ (**20**, 1025.36) C, 56.23; H, 8.26; N, 8.20 %. Found: C, 56.05; H, 8.00; N, 8.25 %. ^{1}H NMR (500 MHz, 298 K, Benzene-d_6) δ 7.31-7.24 (m, 4H, *m*-C_6H_3), 7.18-7.14 (m, 2H, *p*-C_6H_3, overlapping with C_6D_6), 4.61- 4.34 (m, 4H, C*H*Me$_2$ on SiN^{Dipp}), 4.34- 4.22 (m, 2H, C*H*Me$_2$ on carbodiimide) 4.04 (sept, *J* = 6.8 Hz, 2H, C*H*Me$_2$ on NHC^{iPr}), 1.67 – 1.60 (m, 12H, CH*Me*$_2$ on SiN^{Dipp}), 1.60-1.58 (m, 4H, SiC*H*$_2$) 1.54-1.45 (m, 12H, CH*Me*$_2$ on SiN^{Dipp}), 1.33 (s, 6H, NC*Me*), 1.22 (d, *J* = 6.8 Hz, 12H, CH*Me*$_2$ on NHC^{iPr}), 0.87 (d$_{app}$, 12H, CH*Me*$_2$ on carbodiimide) 0.85-0.73 (br, 6H, Si*Me*$_2$), 0.28 - −0.24 (br, 6H, Si*Me*$_2$). ^{13}C{^{1}H} NMR (126 MHz, 298 K, Benzene-d_6) δ 220.5 (Au*C* on NHC^{iPr}), 157.9, 149.5 (*i*- and *o*- C_6H_3), 124.2 (N*C*Me), 123.8 (*m*-C_6H_3), 122.7 (*p*-C_6H_3), 51.6 (*C*HMe$_2$ on carbodiimide), 51.2 (*C*HMe$_2$ on NHC^{iPr}), 35.7 (*C*HMe$_2$ on SiN^{Dipp}), 26.8 (CH*Me*$_2$ on SiN^{Dipp}), 26.7 (CH*Me*$_2$ on SiN^{Dipp}), 23.1 (CH*Me*$_2$ on carbodiimide), 22.9 (CH*Me*$_2$ on NHC^{iPr}), 15.1 (Si*C*H$_2$), 9.1 (NC*Me*), 1.4 (Si*Me*$_2$). ^{13}C resonance correlated to the Au*C* on carbodiimide not observed.

Figure S28. ^{1}H NMR spectrum of **20**. (500 MHz, 298 K, Benzene-d_6)

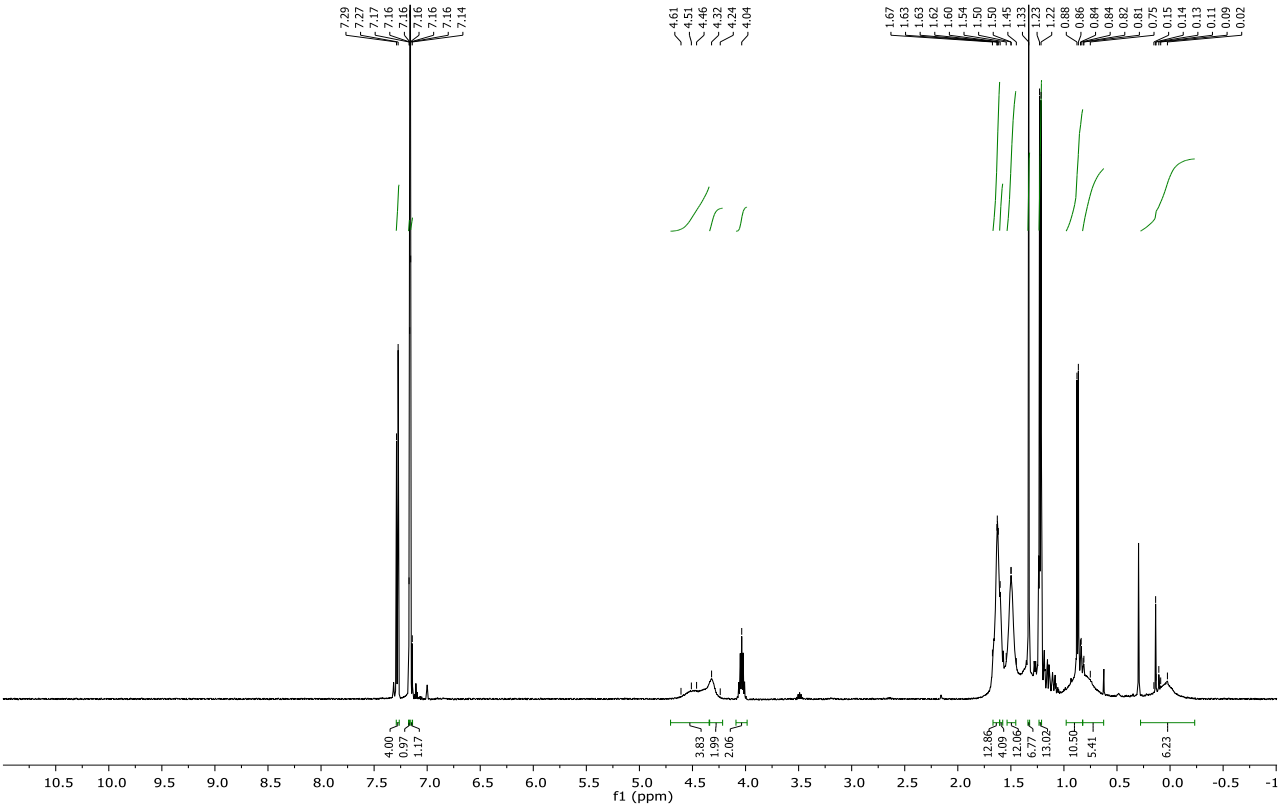


Figure S29. ^{13}C{^{1}H} NMR spectrum of **20**. (126 MHz, 298 K, Benzene-d_6)

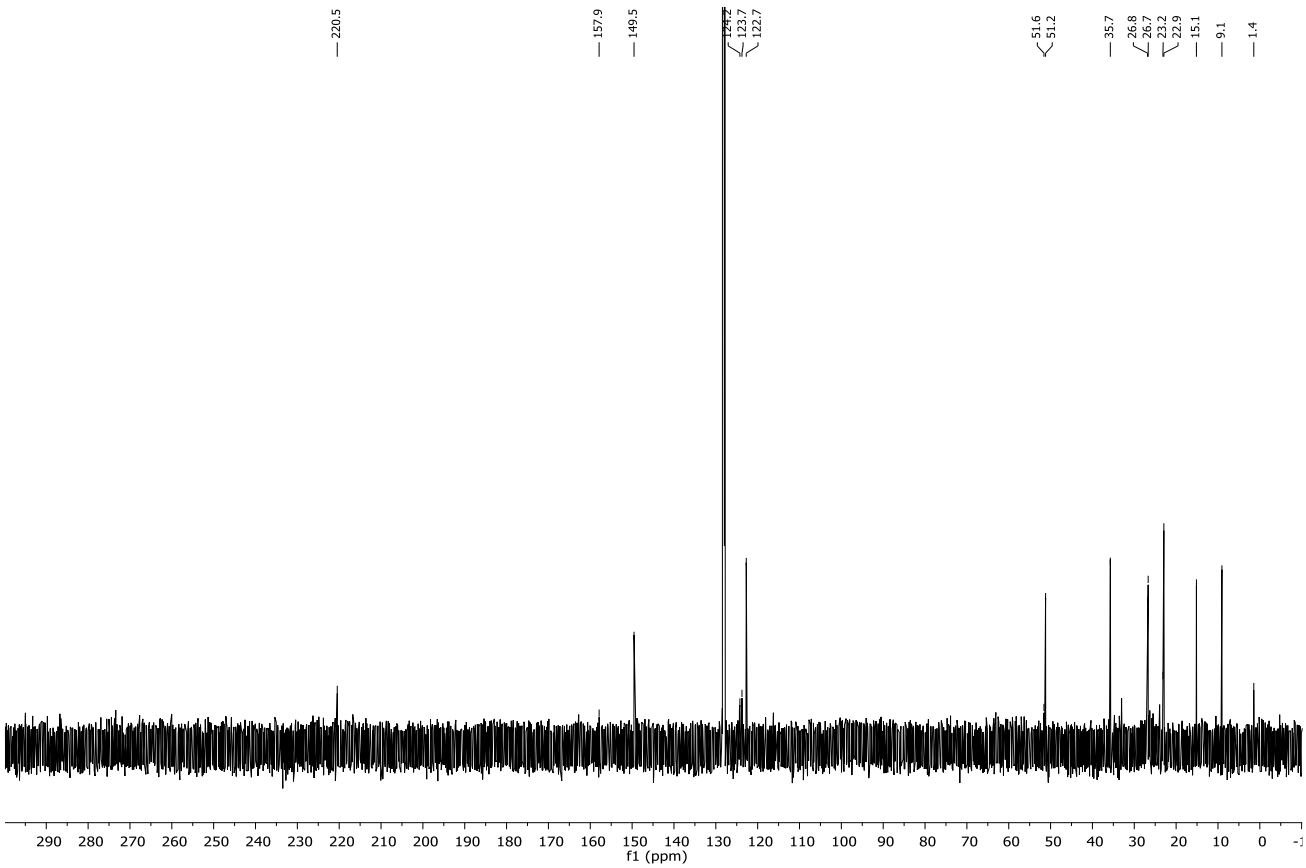


Figure S30. ^{1}H-^{1}H COSY NMR spectrum of **20**.

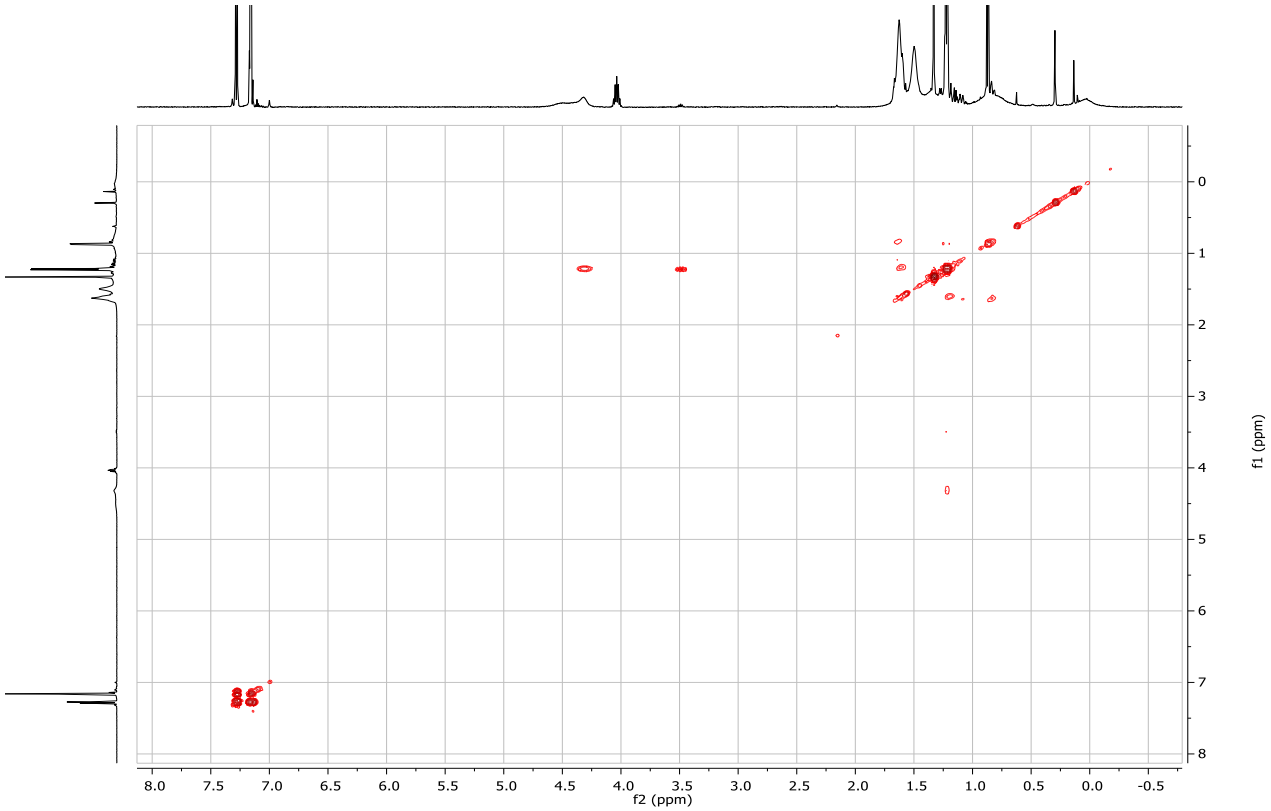


Figure S31. ^{1}H-^{13}C HSQC NMR spectrum of **20**.

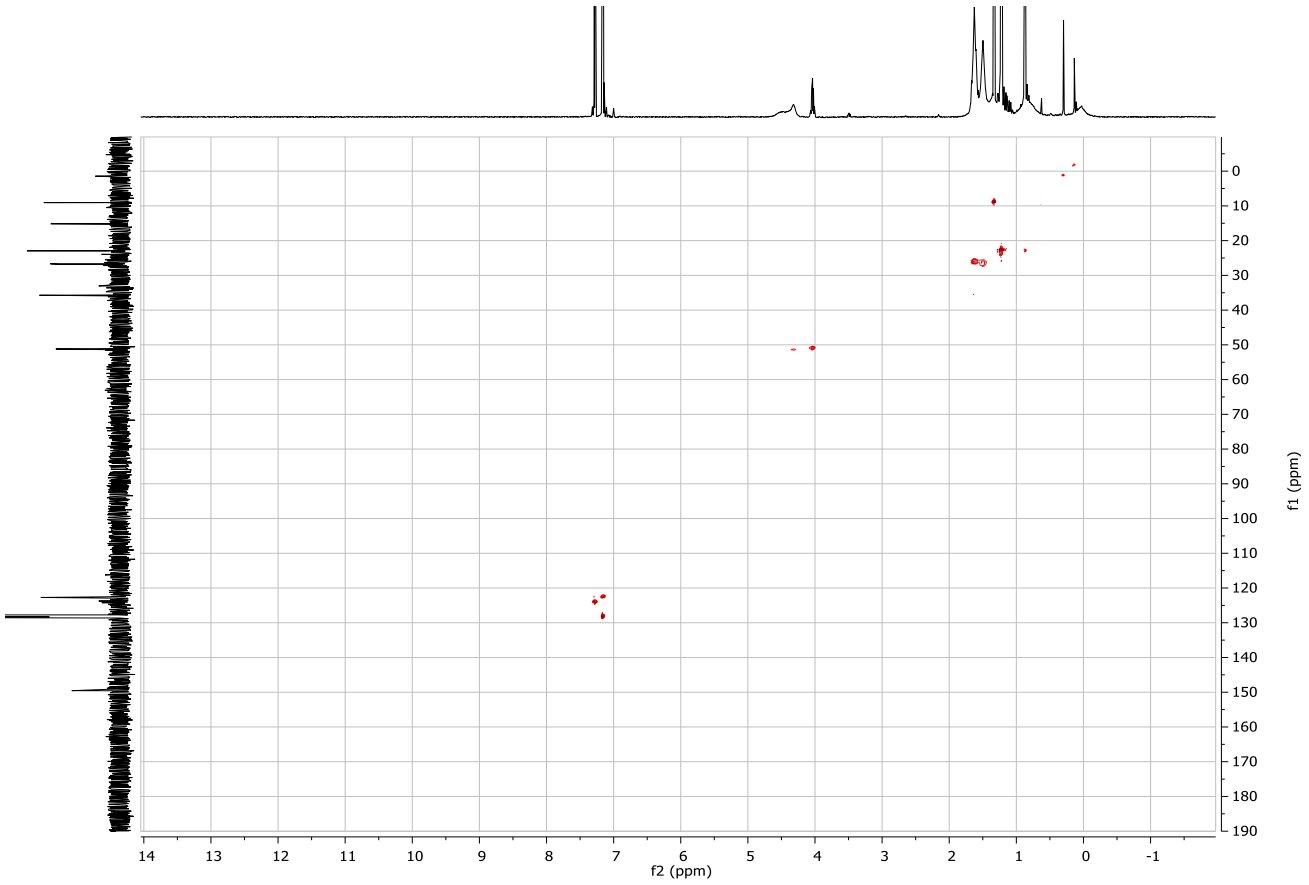
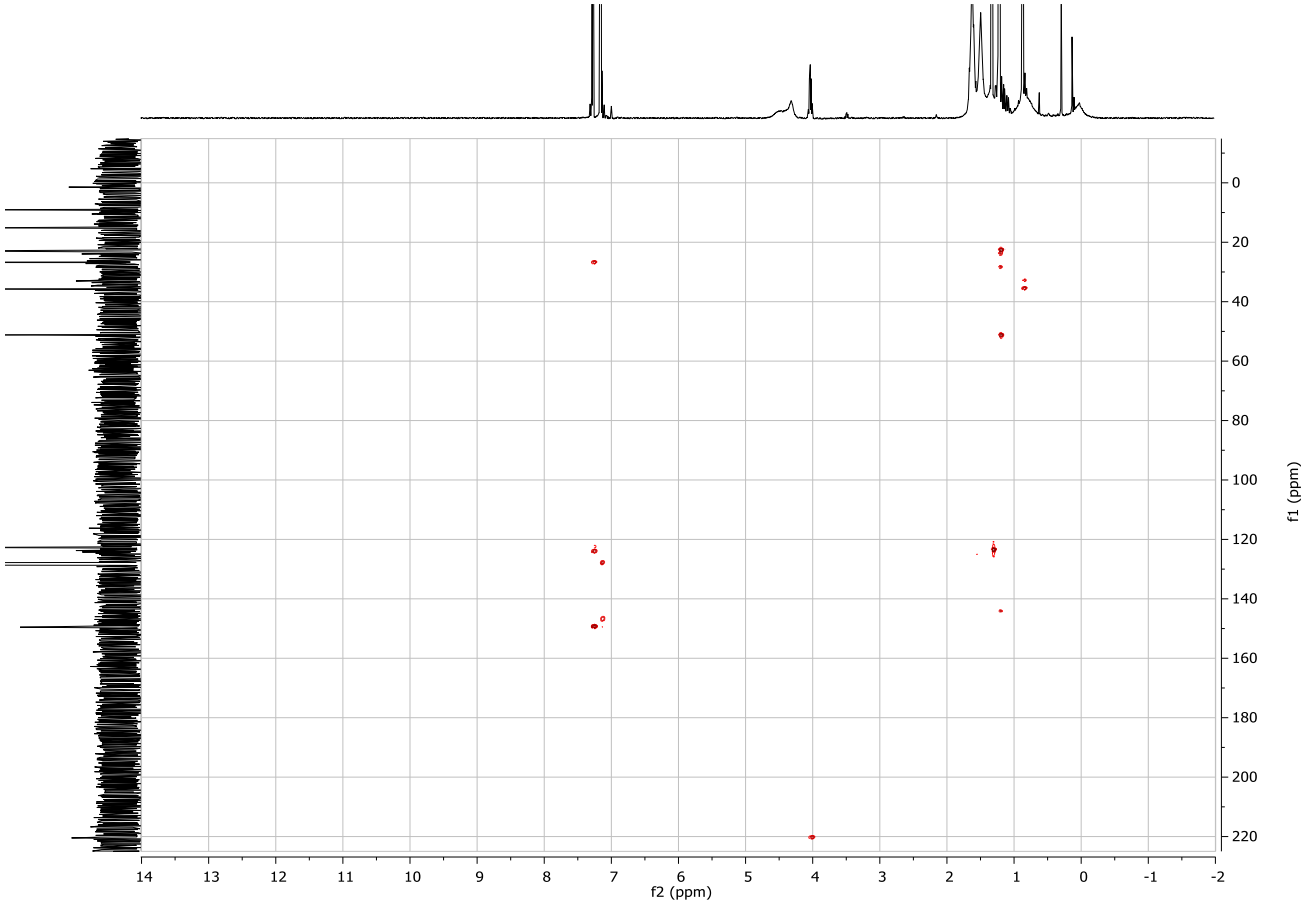


Figure S32. ^{1}H-^{13}C HMBC NMR spectrum of **20**.



*Synthesis of {SiN^{Dipp}}Al-O$_2$C-Ag{NHC^{iPr}} (**21**)*

{SiN^{Dipp}}Al-Ag{NHC^{iPr}} (**16**, 25mg, 0.031mmol) was dissolved in 0.4mL of C_6D_6 inside a J Young's tube. The solution was then degassed by three cycles of freeze-pump-thaw before the tube was charged with 2 atm of $^{13}CO_2$. Full Conversion of the starting material was determined by ^{1}H and ^{13}C NMR spectra within 30 minutes of the addition of the CO_2 to the solution. The benzene solution was then put under reduced pressure to remove all volatiles and giving **21** as an off-white waxy solid. Yield 19 mg, 71%. No meaningful result was obtained for elemental analysis after multiple attempts. ^{1}H NMR (500 MHz, 298 K, Benzene-d_6) δ 7.18 (d, J = 7.6 Hz, 4H, m-C$_6$H$_3$), 7.07 (t, J = 7.6 Hz, 2H, p-C$_6$H$_3$), 4.22 (sept, J = 6.9 Hz, 4H, C*H*Me$_2$ on SiN^{Dipp}), 3.63 (sept, J = 6.8 Hz, 2H, C*H*Me$_2$ on NHC^{iPr}), 1.60 (d, J = 6.9 Hz, 12H, CH*Me*$_2$ on SiN^{Dipp}), 1.47 (d, J = 6.9 Hz, 12H, CH*Me*$_2$ on SiN^{Dipp}), 1.30 (s, 4H, SiC*H*$_2$), 1.24 (s, 6H, NC*Me*), 0.99 (d, J = 6.8 Hz, 12H, CH*Me*$_2$ on NHC^{iPr}), 0.39 (s, br, 12H, Si*Me*$_2$). ^{13}C{^{1}H} NMR (126 MHz, 298 K, Benzene-d_6) δ 240.4 (2xd, $J_{109Ag-C}$ = 252.6, $J_{107Ag-C}$ = 218.9 Hz, Ag*C*O$_2$), 154.5 (*i*-*C*$_6$H$_3$), 146.8 (*o*-*C*$_6$H$_3$), 123.8 (*m*-*C*$_6$H$_3$), 123.6 (*p*-*C*$_6$H$_3$), 123.1 (N*C*Me), 50.3 (N*C*HMe$_2$ on NHC^{iPr}), 27.9 (*C*HMe$_2$ on SiN^{Dipp}), 25.5 (CH*Me*$_2$ on SiN^{Dipp}), 25.5 (CH*Me*$_2$ on SiN^{Dipp}), 23.9 (NCH*Me*$_2$ on NHC^{iPr}), 14.5 (Si*C*H$_2$), 8.7 (NC*Me*), 0.6 (Si*Me*$_2$). ^{13}C resonance correlated to Ag*C*$_{carbene}$ was not observed.

Figure S33. ^{1}H NMR spectrum of **21**. (500 MHz, 298 K, Benzene-d_6)

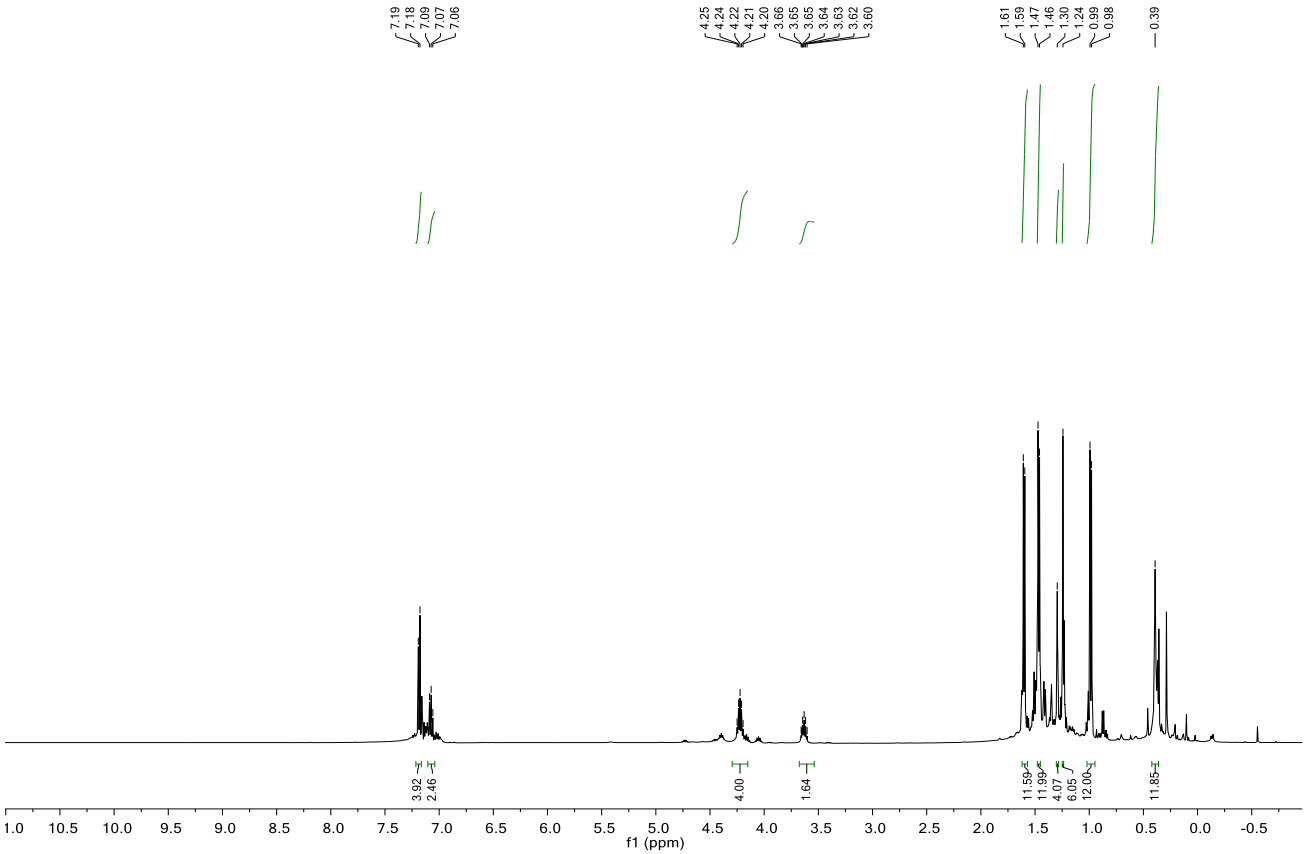
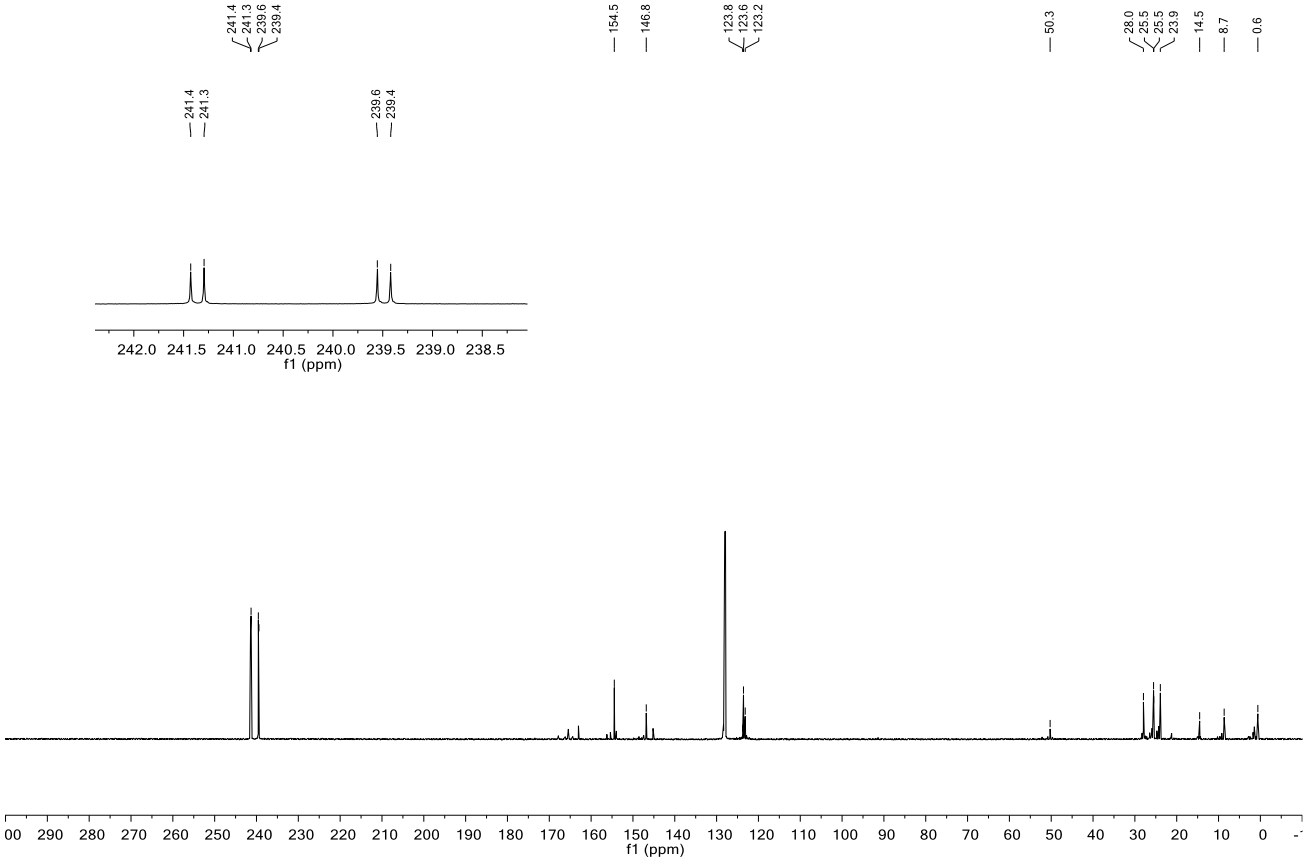


Figure S34. ^{13}C{^{1}H} NMR spectrum of **21**. (126 MHz, 298 K, Benzene-d_6)



*Synthesis of {SiN^{Dipp}}Al-O$_2$C-Au{NHC^{iPr}} (**22**)*

{SiN^{Dipp}}Al-Au{NHC^{iPr}} (**17**, 25mg, 0.028mmol) was dissolved in 0.4mL of C_6D_6 inside a J Young's tube. The solution was then degassed by three cycles of freeze-pump-thaw before the tube was charged with 2 atm of $^{13}CO_2$. Full Conversion of the starting material was determined by ^{1}H and ^{13}C NMR spectra within 30 minutes of the addition of the CO_2 to the solution. The benzene solution was then put under reduced pressure to remove all volatiles and giving **22** as an off-white waxy solid. Yield 20 mg, 78%. Anal Calc'd for $C_{42}H_{70}AlAuN_4Si_2O_2$ (**22**, 943.17) C, 53.49; H, 7.48; N, 5.94 %. Found: C, 52.95; H, 8.07; N, 5.38 %. ^{1}H NMR (500 MHz, 298 K, Benzene-d_6) δ 7.20-7.19 (m, 4H, *m*-C$_6$*H*$_3$), 7.11 – 7.08 (m, 2H, *p*-C$_6$*H*$_3$), 4.21 (sept, *J* = 6.8 Hz, 4H, C*H*Me$_2$ on N^{Dipp}), 3.92 (sept, *J* = 7.2 Hz, 2H, C*H*Me$_2$ on NHC), 1.62 (d, *J* = 6.8 Hz, 12H, CH*Me*$_2$ on N^{Dipp}), 1.47 (d, *J* = 6.8 Hz, 12H, CH*Me*$_2$ on N^{Dipp}), 1.29 (s, 4H, SiC*H*$_2$), 1.20 (s, 6H, NC*Me*), 1.09 (d, *J* = 7.2 Hz, 12H, CH*Me*$_2$ on NHC), 0.39 (s, br, 12H, Si*Me*$_2$). ^{13}C{^{1}H} NMR (126 MHz, 298 K, Benzene-d_6) δ 239.1 (Au*C*O$_2$), 146.8 (*i*-*C*$_6$H$_3$), 144.8 (*o*-*C*$_6$H$_3$), 124.8 (*m*-*C*$_6$H$_3$), 123.6 (*p*-*C*$_6$H$_3$), 123.3 (N*C*Me), 51.1 (N*C*HMe$_2$ on NHC), 28.0 (*C*HMe$_2$ on N^{Dipp}), 25.5 (CH*Me*$_2$ on N^{Dipp}), 23.9 (CH*Me*$_2$ on N$^{Dipp)}$, 23.2 (NCH*Me*$_2$ on NHC), 14.4 (Si*C*H$_2$), 8.9 (N*C*Me), 0.5 (Si*Me*$_2$). ^{13}C resonance correlated to Au*C*$_{carbene}$ was not observed.

Figure S35. ^{1}H NMR spectrum of **22**. (500 MHz, 298 K, Benzene-d_6)

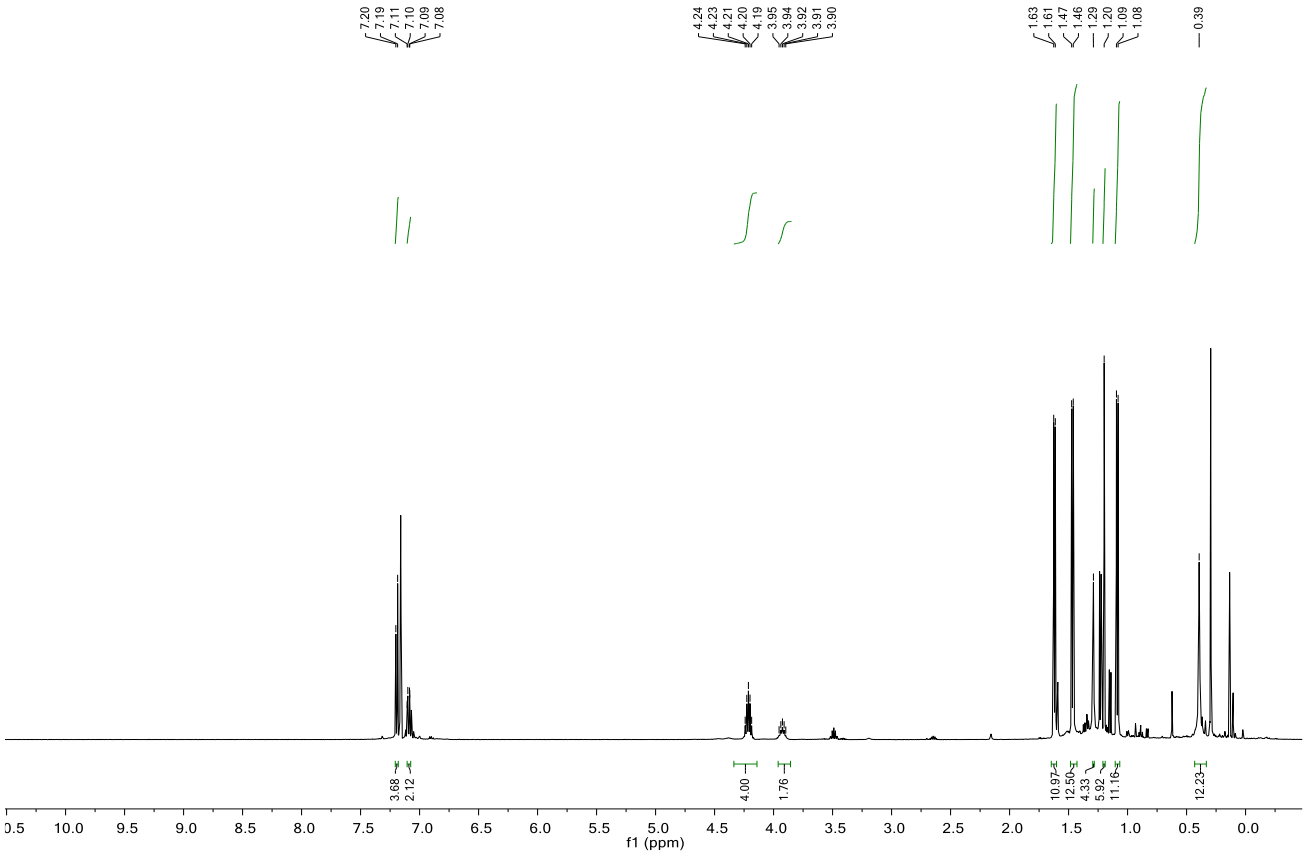
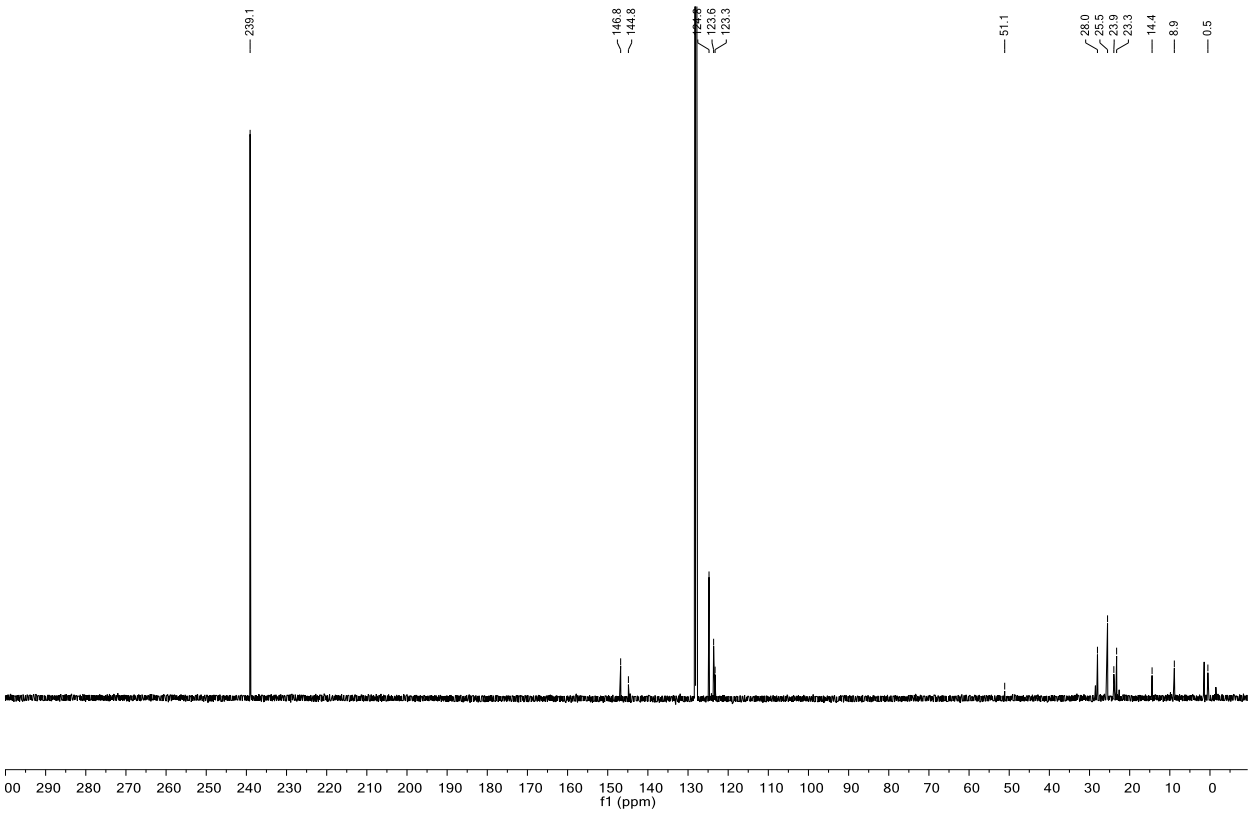


Figure S36. ^{13}C{^{1}H} NMR spectrum of **22**. (126 MHz, 298 K, Benzene-d_6)



*Synthesis of {SiN^{Dipp}}Al-Cu{P^{t}Bu$_3$}(**23**)*

Hexane (25 mL) was cannula transferred into a Schlenk flask charged with the mixture of tritertbutylphophine (P^{t}Bu$_3$, 0.200 g, 1.00 mmol), CuCl (0.100 g, 1.00 mmol), and [{SiN^{Dipp}}AlK]$_2$ (**3**, 0.560 g, 1.00 mmol). The resulting pale-yellow reaction mixture was left stirring overnight before filtering. The colourless filtrate was then collected, and all volatiles were removed *in vacuo* yielding **23** as a white solid. Yield 0.620 g, 78.7%. Colourless crystals suitable for X-ray crystallography were obtained by slow evaporation of a hexane solution at room temperature. Anal Calc'd for $C_{42}H_{77}AlCuN_2PSi_2$ (**23**, 787.76) C, 64.04; H, 9.85; N, 3.56 %. Found: C, 63.85; H, 9.96; N, 3.69 %. ^{1}H NMR (500 MHz, 298 K, Benzene-*d*$_6$) δ 6.94 (d, *J* = 7.9 Hz, 4H, *m*-C$_6$*H*$_3$), 6.82 (t, *J* = 7.9 Hz, 2H, *p*-C$_6$*H*$_3$), 3.85 (sept, *J* = 6.9 Hz, 4H, C*H*Me$_2$), 1.29 (d, *J* = 6.9 Hz, 12H, CH*Me*$_2$), 1.24 (d, *J* = 6.9 Hz, 12H, CH*Me*$_2$), 1.01 (s, 4H, SiC*H*$_2$), 0.69 (d, $^3J_{PH}$ = 12.1 Hz, 27H, PC*Me*$_3$), 0.19 (s, 12H, Si*Me*$_2$). ^{13}C{^{1}H} NMR (126 MHz, 298 K, Benzene-*d*$_6$) δ 146.7, 145.7 (*i*- and *o*- *C*$_6$H$_3$), 123.2 (*m*-*C*$_6$H$_3$), 122.7 (p-C$_6$H$_3$), 32.7 (d, $^1J_{PC}$ = 13.2Hz, PCMe$_3$), 32.2 (d, $^2J_{PC}$ = 6.4 Hz, PCMe3), 28.6 (*C*HMe$_2$), 26.0 (CH*Me*$_2$), 24.3 (CH*Me*$_2$), 14.4 (Si*C*H$_2$), 1.6 (Si*Me*$_2$). ^{31}P NMR (202 MHz, 298 K, Benzene-d6) δ 43.9.

Figure S37. ^{1}H NMR spectrum of **23**. (500 MHz, 298 K, Benzene-d_6) *free P^{t}Bu$_3$ impurity $^{+}$ grease

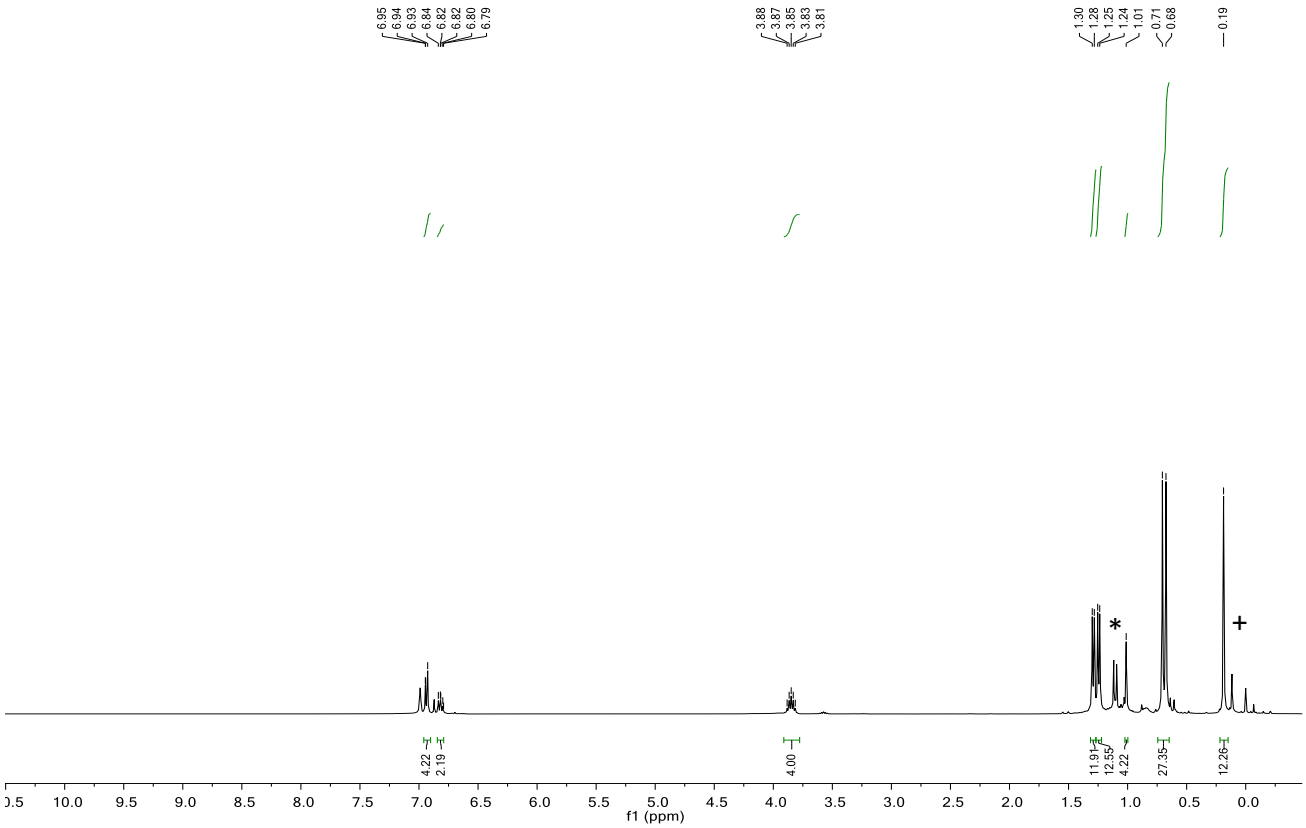


Figure S38. ^{13}C{^{1}H} NMR spectrum of **23**. (126 MHz, 298 K, Benzene-d_6) *free P^{t}Bu$_3$ impurity

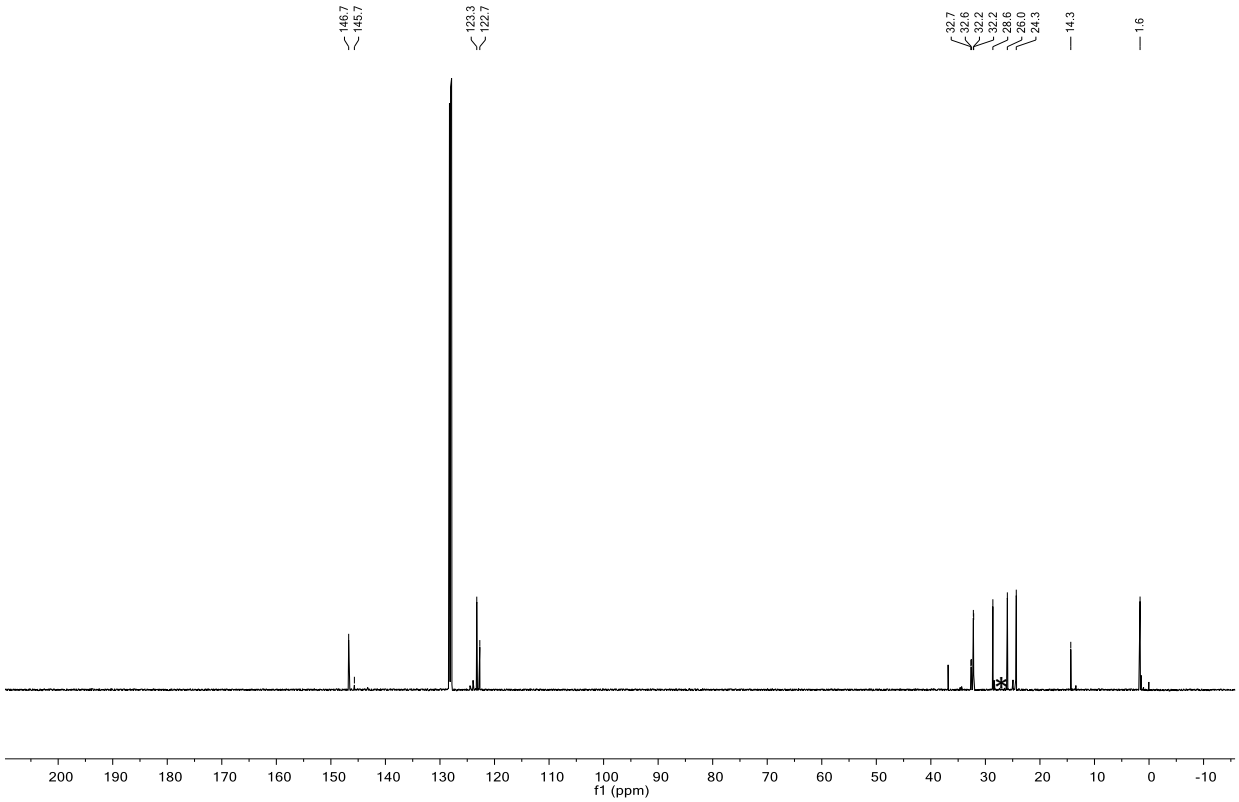


Figure S39. $^{31}P\{^{1}H\}$ NMR spectrum of **23** (202 MHz, 298 K, Benzene-d_6) *free P^{t}Bu$_3$ impurity

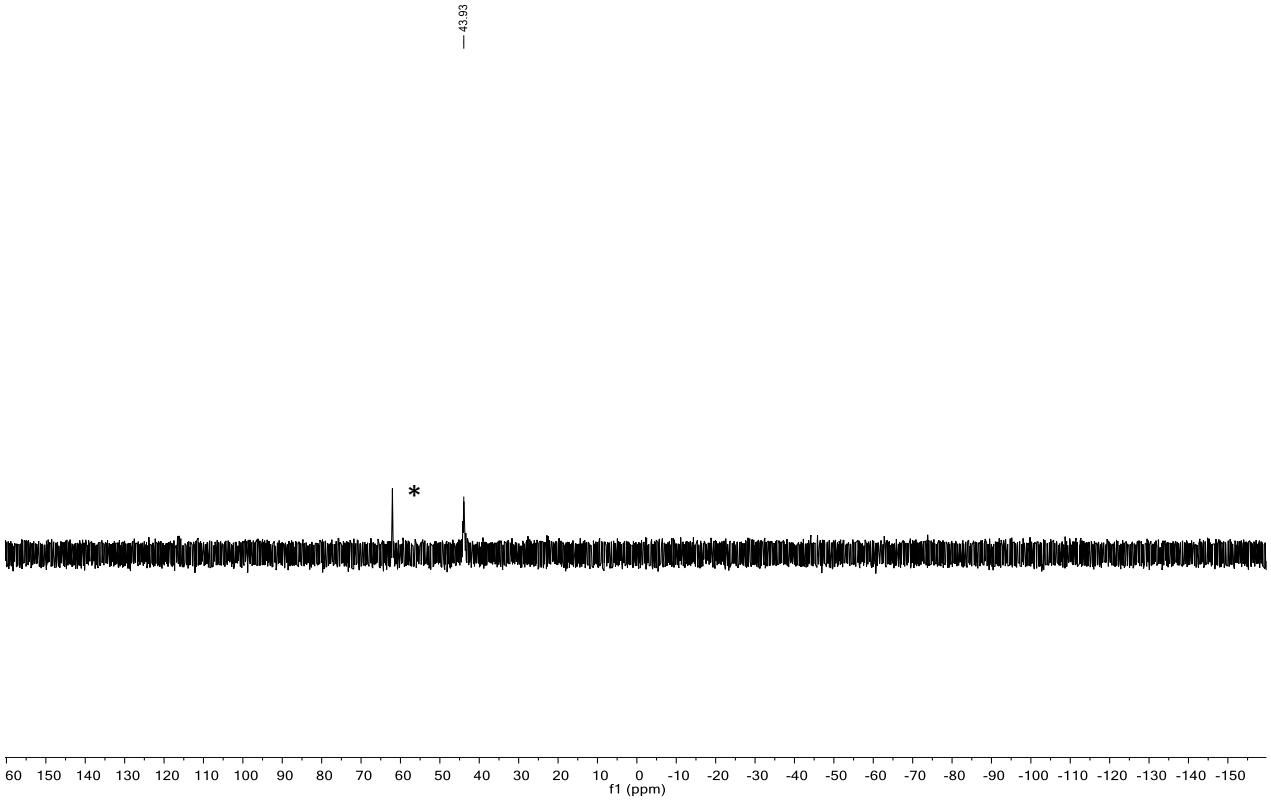


Figure S40. ^{1}H-^{1}H COSY NMR spectrum of **23**.

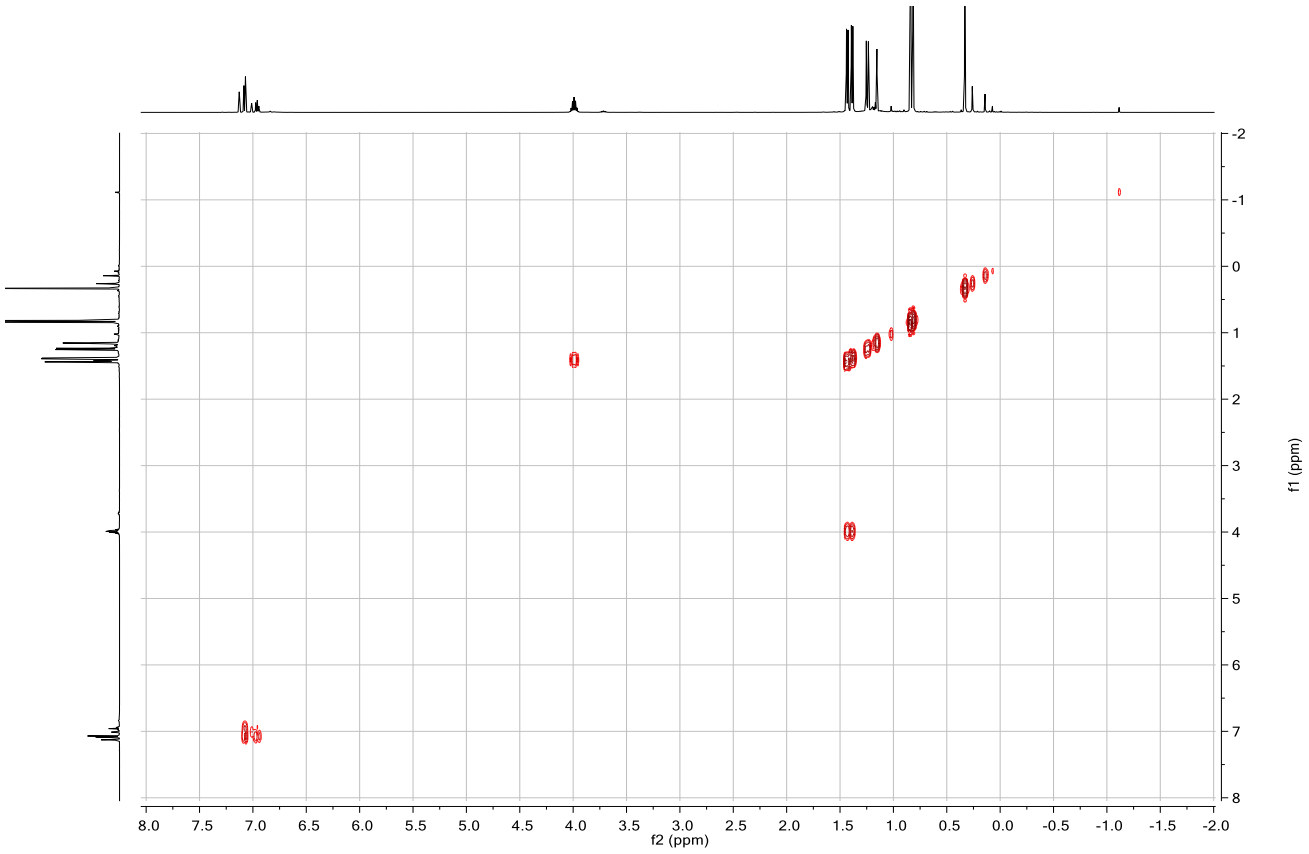


Figure S41. ^{1}H-^{13}C HSQC NMR spectrum of **23**.

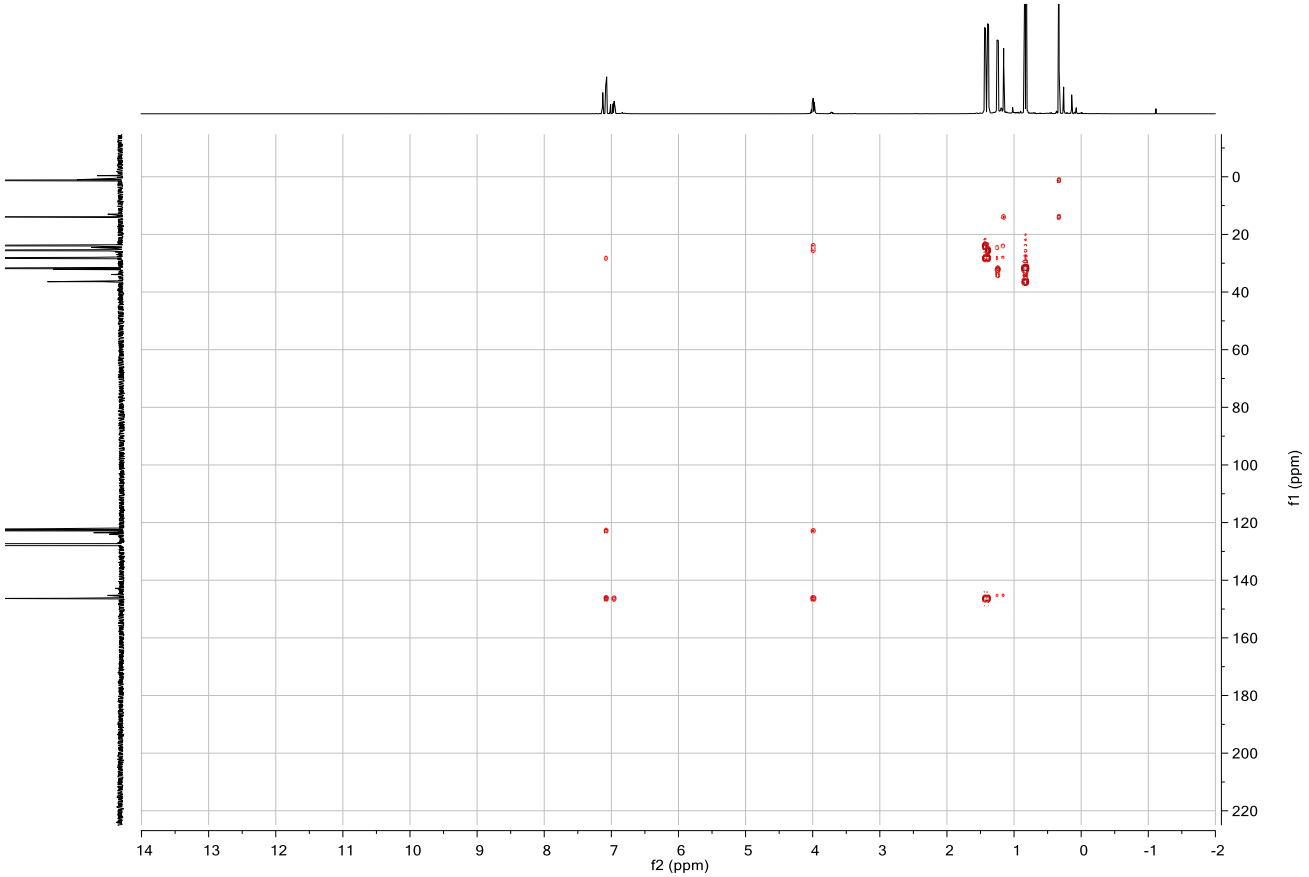
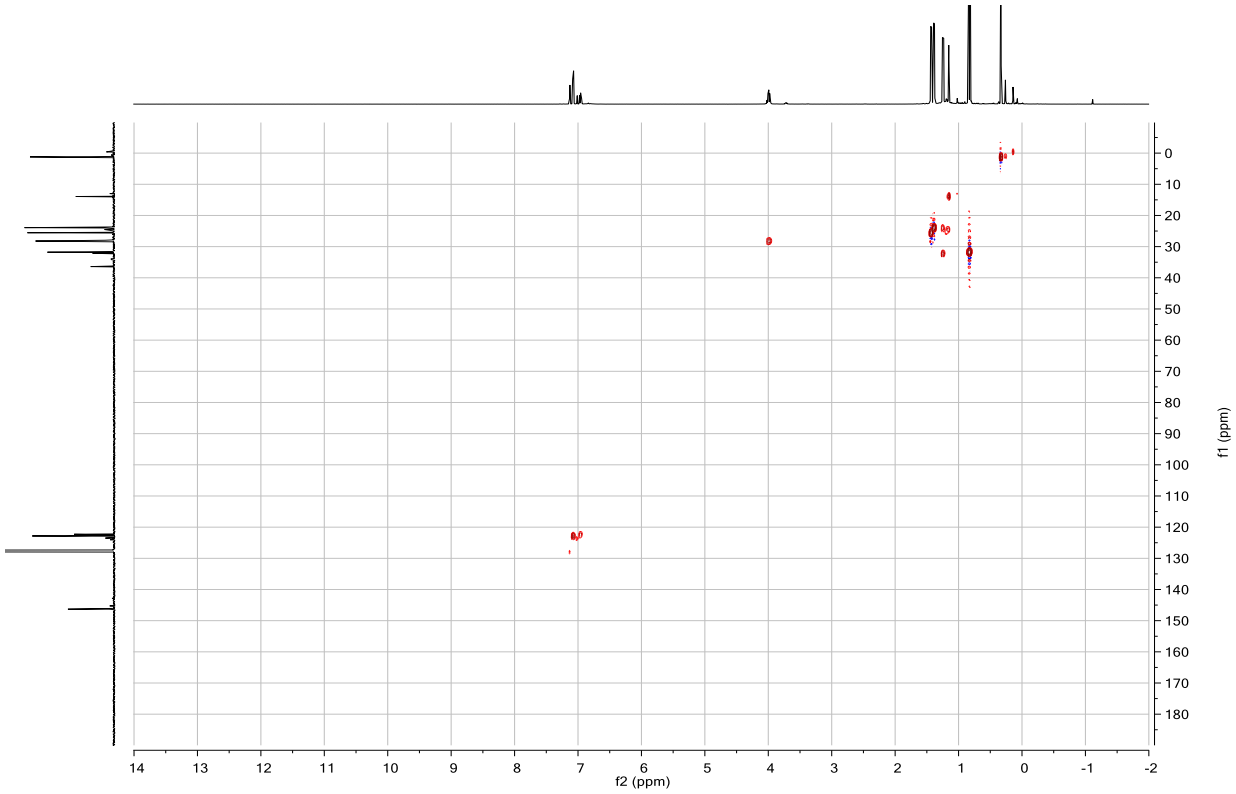


Figure S42. ^{1}H-^{13}C HMBC NMR spectrum of **23**.



*Synthesis of {SiN^{Dipp}}Al-(N^{i}Pr)$_2$C-Cu{P^{t}Bu$_3$}(**24**)*

Inside a J Young's tube, {SiN^{Dipp}}Al-Cu{P^{t}Bu$_3$} (**23**, 38.5mg, 0.05mmol) was dissolved in 0.4mL of C_6D_6, N,N'-diisopropylcarbodiimide (7.8μL, 0.05mmol) was then added via a micropipette. Total transformation was observed after the reaction mixture was left at room temperature for overnight. The benzene solution was then put under vacuum to remove all volatiles and giving **24** as waxy white solid. Colourless crystals suitable for X-ray crystallography were obtained by slow evaporation of a hexane solution at room temperature. Yield 35mg, 77%. Anal Calc'd for $C_{49}H_{91}AlCuN_4PSi_2$ (**24**,913.97) C, 64.39; H, 10.04; N, 6.13 %. Found: C, 64.01; H, 9.93; N, 6.24 %. ^{1}H NMR (500 MHz, 298 K, Benzene-d_6) δ 7.24 (d, J = 7.6 Hz, 4H, *m*-C$_6$*H*$_3$), 7.13 (t, J = 7.6 Hz, 2H, *p*-C$_6$*H*$_3$), 4.62-4.07 (m, 4H, C*H*Me$_2$), 3.68-3.60 (m, 2H, NC*H*Me$_2$), 1.65 – 1.32 (m, 30H, CH*Me*$_2$ on SiN^{Dipp} and CN$^{iPr}{}_2$), 1.30 – 1.21 (m, 4H, SiC*H*$_2$), 0.97 (d, $^3J_{PH}$ = 12.5 Hz, 27H, PC*Me*$_3$), 0.64 – -0.16 (m, 12H, SiMe$_2$). ^{13}C NMR (126 MHz, Benzene-d_6) δ 218.0 (Cu*C*N$^{iPr}{}_2$), 149.1, 147.1 (*i*- and *o*-*C*$_6$H$_3$), 123.8 (*m*-*C*$_6$H$_3$), 122.2 (p-*C*$_6$H$_3$), 51.8 (N*C*HMe$_2$), 36.4 (d, $^1J_{PC}$ = 9.6Hz, P*C*Me$_3$) 31.6 (d, $^2J_{PC}$ = 5.5Hz, PC*Me*$_3$), 26.4 (*C*HMe$_2$), 25.8, 22.6 (CH*Me*$_2$ on N^{Dipp} and CN$^{iPr}{}_2$), 14.7 (Si*C*H$_2$), 1.0 (Si*Me*$_2$). ^{31}P NMR (202 MHz, Benzene-d_6) δ 59.8.

Figure S43. ^{1}H NMR spectrum of **24**. (500 MHz, 298 K, Benzene-d_6)

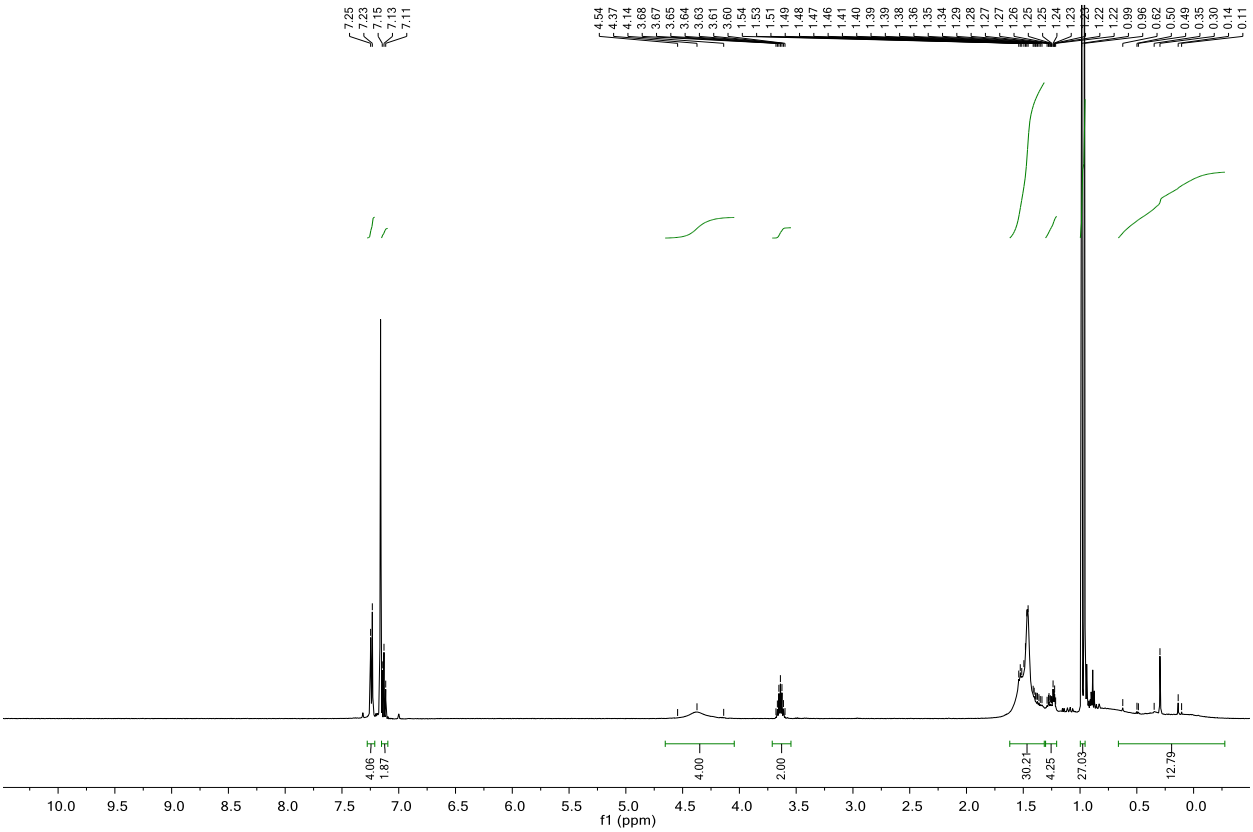


Figure S44. ^{13}C{^{1}H} NMR spectrum of **24**. (126 MHz, 298 K, Benzene-d_6)

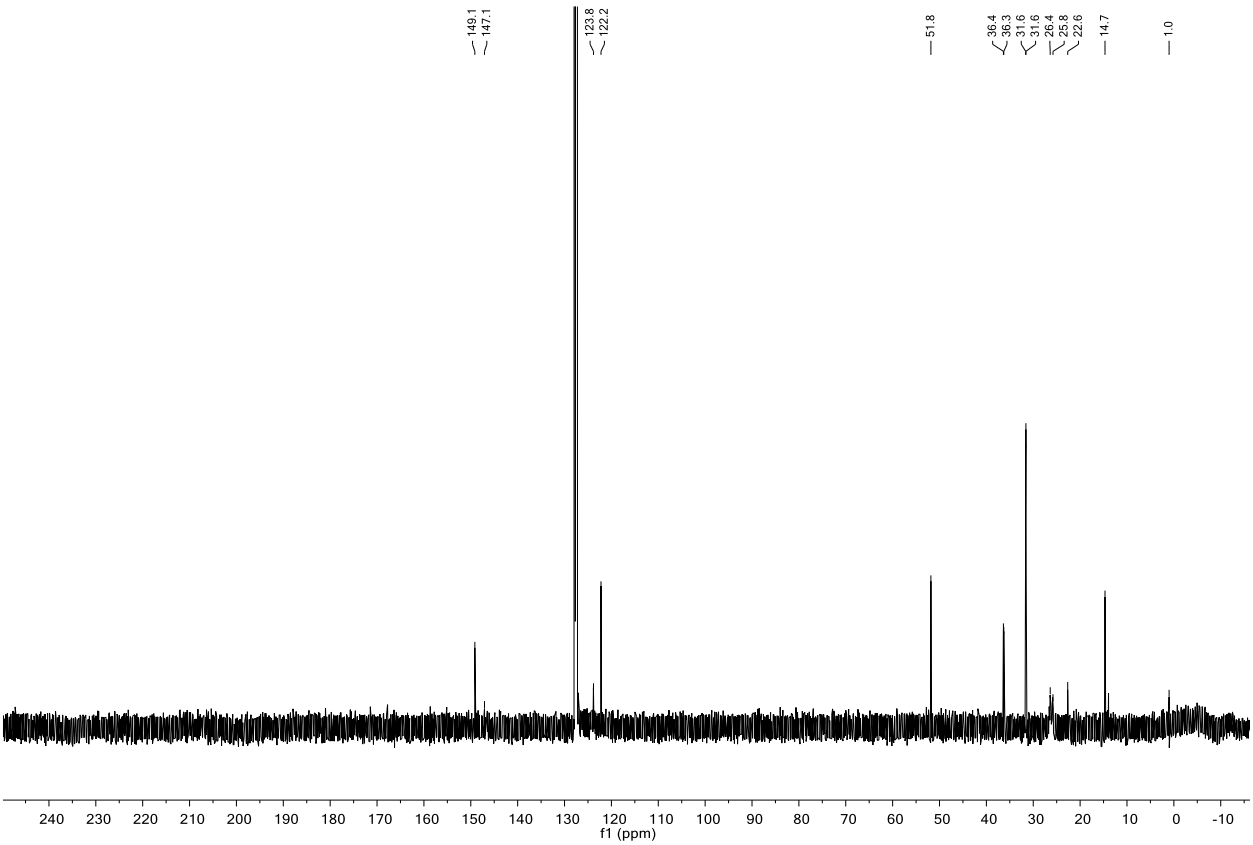


Figure S45. ^{31}P NMR spectrum of **24.** (202 MHz, 298K, Benzene-d_6)

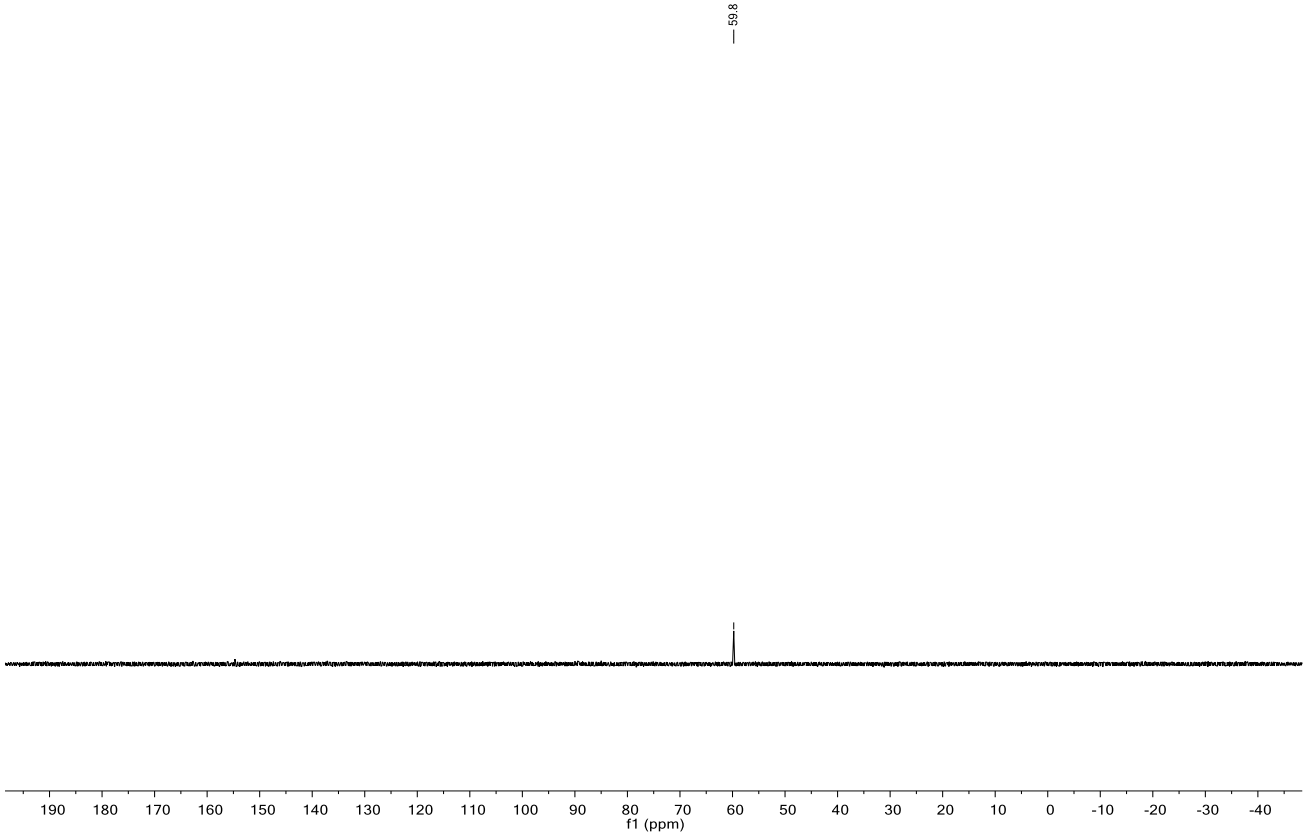


Figure S46. ^{1}H-^{1}H COSY NMR spectrum of **24**.

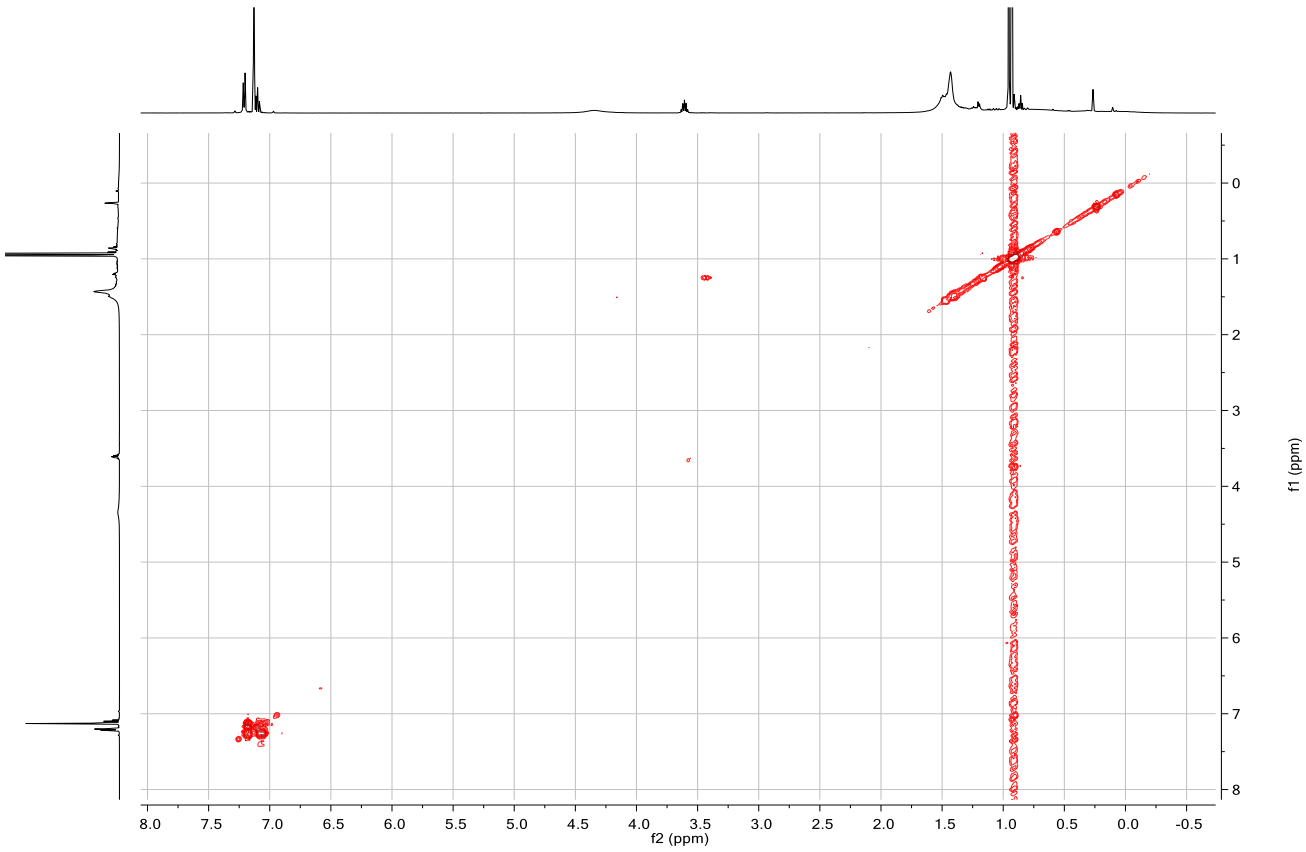


Figure S47. ^{1}H-^{13}C HSQC NMR spectrum of **24**.

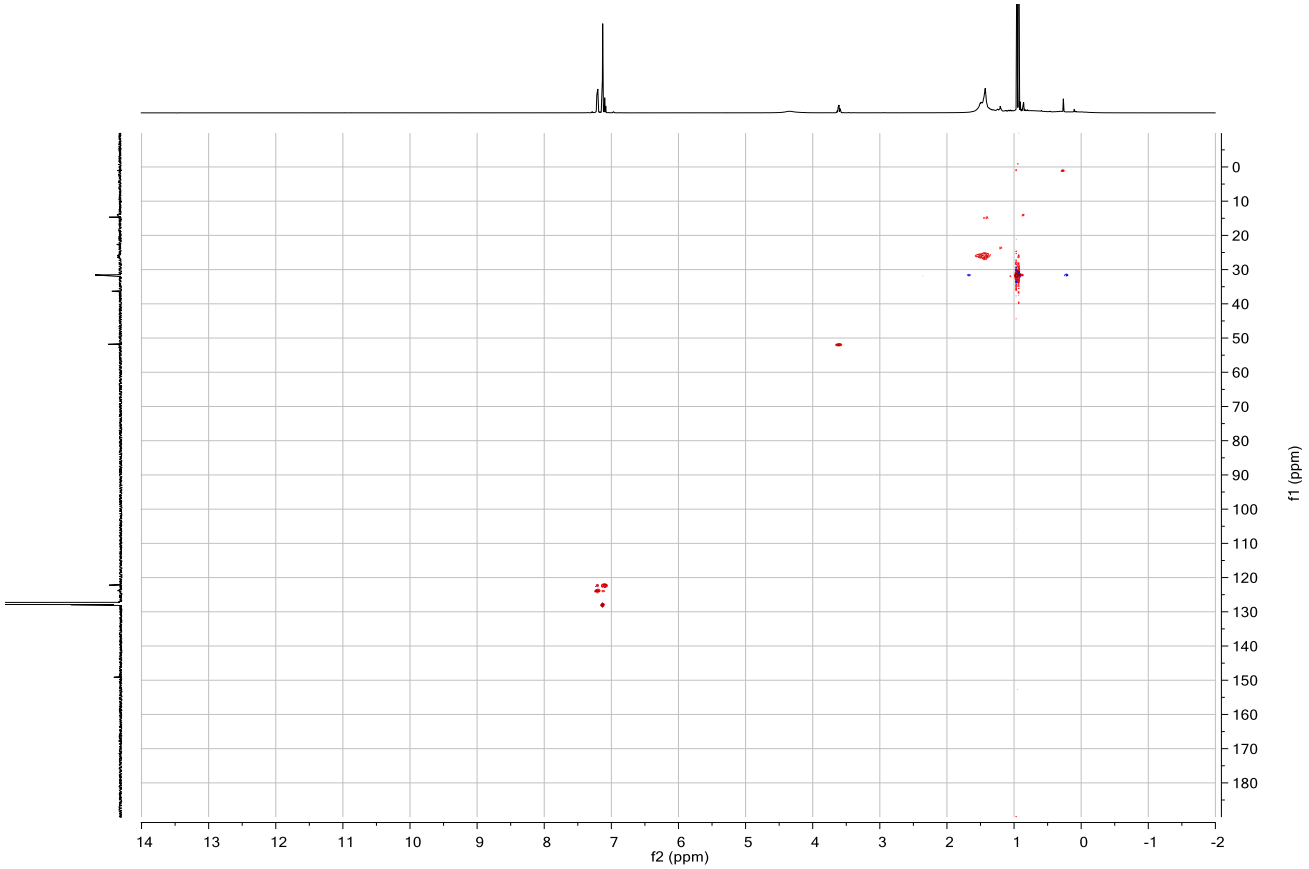
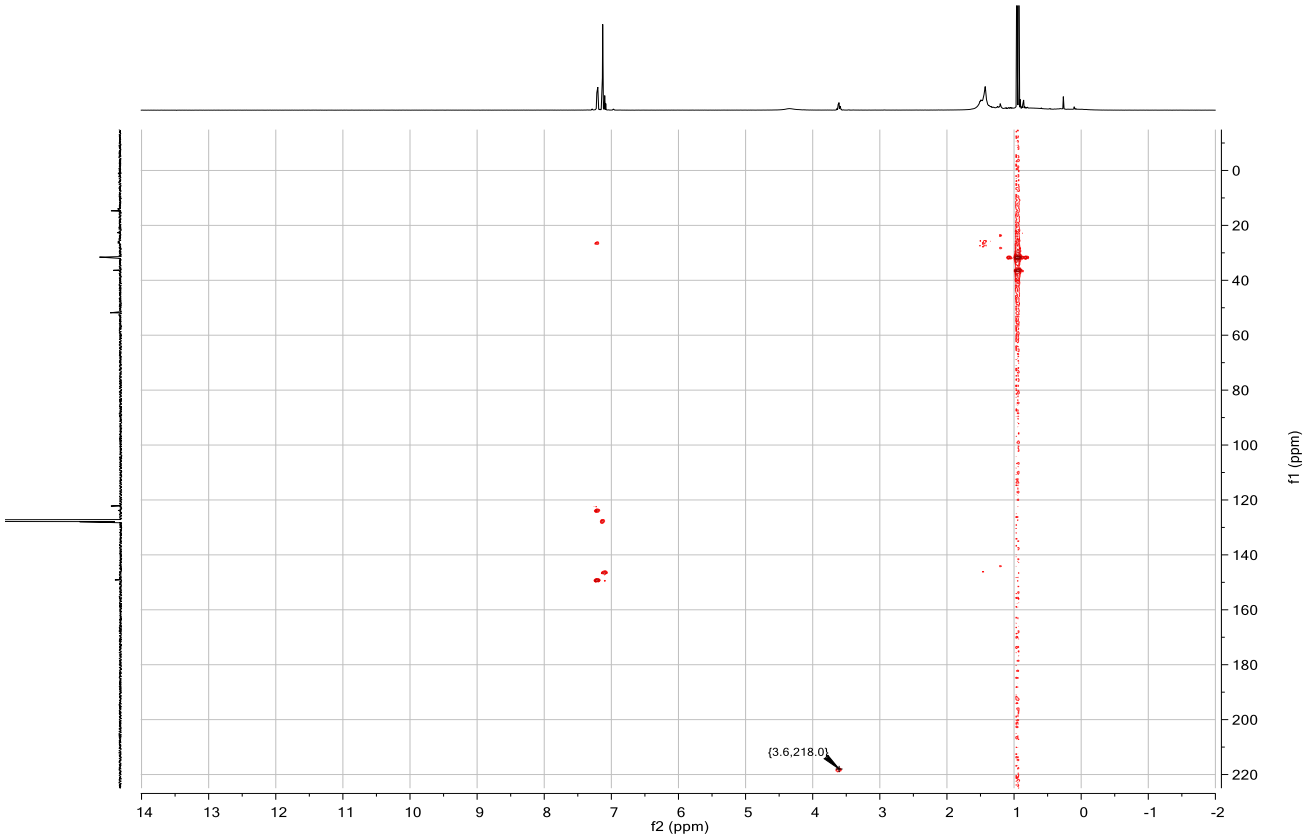


Figure S48. ^{1}H-^{13}C HMBC NMR spectrum of **24**.



*Synthesis of {SiN^{Dipp}}Al-O_2C-Cu{P^{t}Bu$_3$}(**25**)*

{SiN^{Dipp}}Al-Cu{P^{t}Bu$_3$} (**23**, 25mg, 0.032mmol) was dissolved in 0.4mL of C_6D_6 inside a J Young's tube. The solution was then degassed by three cycles of freeze-pump-thaw before the tube was charged with 2 atm of $^{13}CO_2$. Full Conversion of the starting material was determined by ^{1}H and ^{13}C NMR spectra within 30 minutes of the addition of the CO_2 to the solution. The benzene solution was then put under reduced pressure to remove all volatiles and giving **25** as an off-white solid. Yield 20 mg, 77 %. No meaningful result was obtained for elemental analysis after multiple attempts. ^{1}H NMR (500 MHz, 298 K, Benzene-d_6) δ 7.14-7.10 (m, 4H, *m*-C_6H_3), 7.04-6.98 (m, 2H, *p*-C_6H_3), 4.15 (sept, J = 6.9 Hz, 4H, C*H*Me2), 1.53 (d, J = 6.9 Hz, 12H, CH*Me*$_2$), 1.44 (d, J = 6.9 Hz, 12H, CH*Me*$_2$), 1.27 (s, 4H, SiC*H*$_2$), 0.80 (d, $^3J_{PH}$ = 12.9 Hz, 27H, C*Me*$_3$), 0.37 (s, 12H, Si*Me*$_2$). ^{13}C{^{1}H} NMR (126 MHz, 298 K, Benzene-d_6) δ 233.1 (d, $^2J_{PC}$ = 73.9Hz, Cu*C*O2) 146.8 (*o*-C_6H_3), 145.0 (*i*-C_6H_3), 123.5 (*m*-C_6H_3), 123.2 (*p*-C_6H_3), 36.4 (*C*Me$_3$), 31.9 (C*Me*$_3$), 27.9 (*C*HMe$_2$), 25.4 (CH*Me*$_2$), 25.4 (CH*Me*$_2$), 14.4 (Si*C*H$_2$), 0.5 (Si*Me*$_2$). ^{31}P{^{1}H} NMR (202 MHz, Benzene-d_6) δ 59.8.

Figure S49. ^{1}H NMR spectrum of **25**. (500 MHz, 298 K, Benzene-d_6)

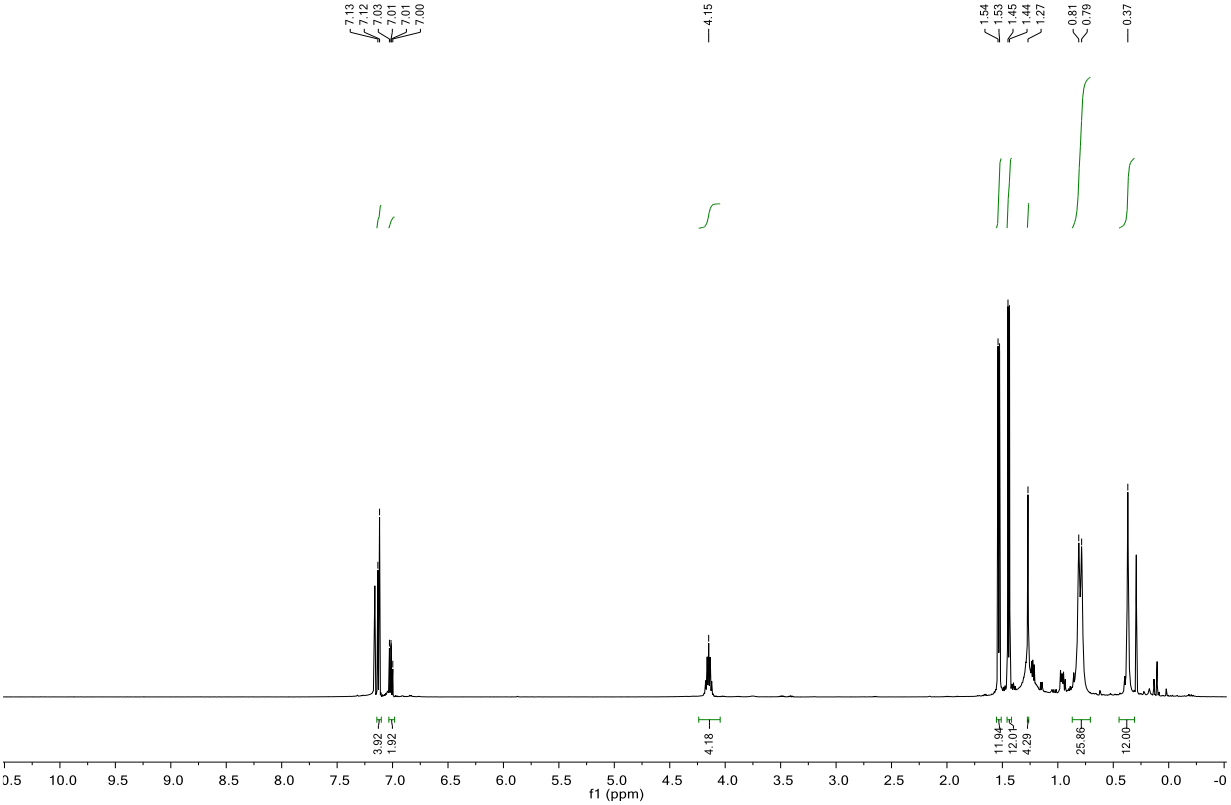


Figure S50. ^{13}C{^{1}H} NMR spectrum of **25**. (126 MHz, 298 K, Benzene-d_6)

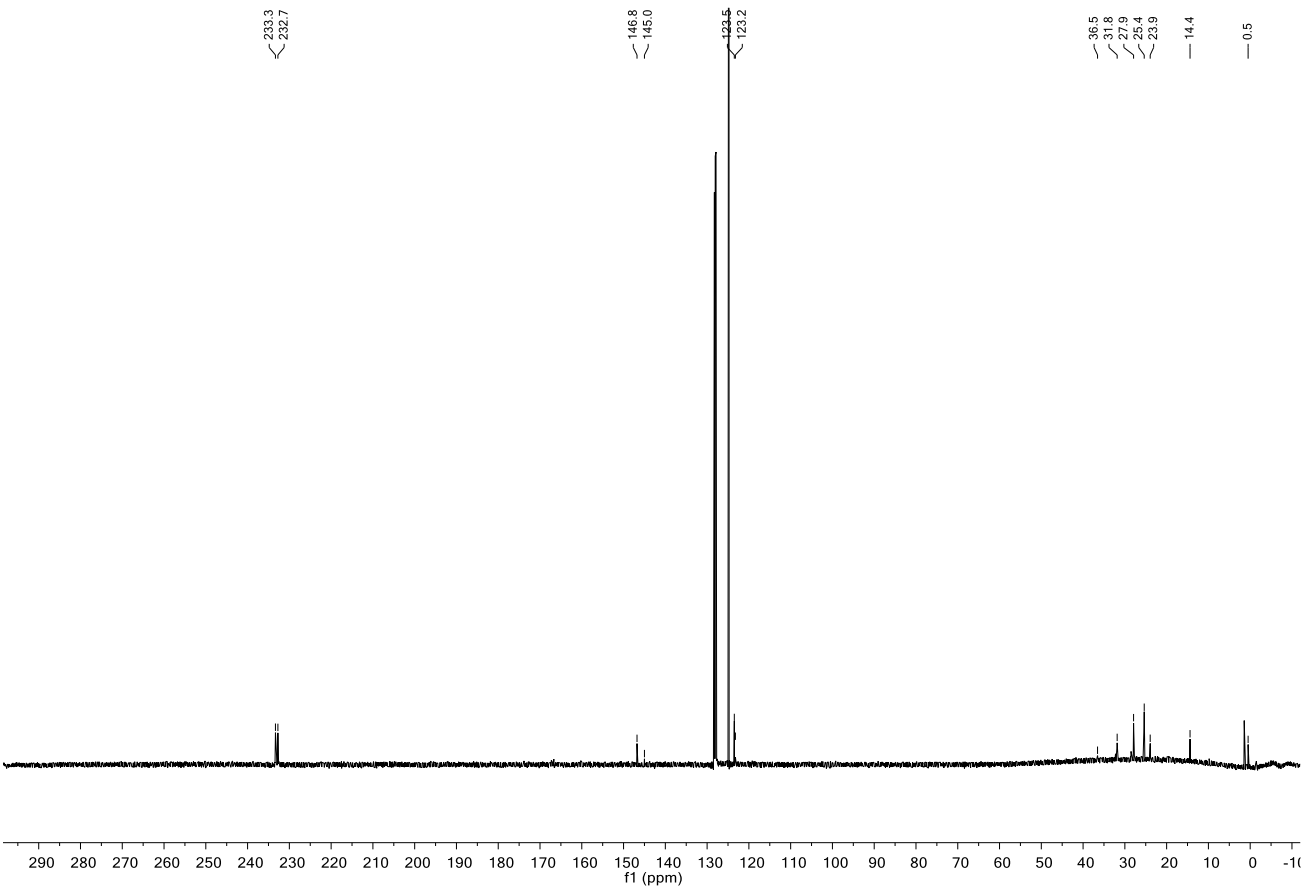
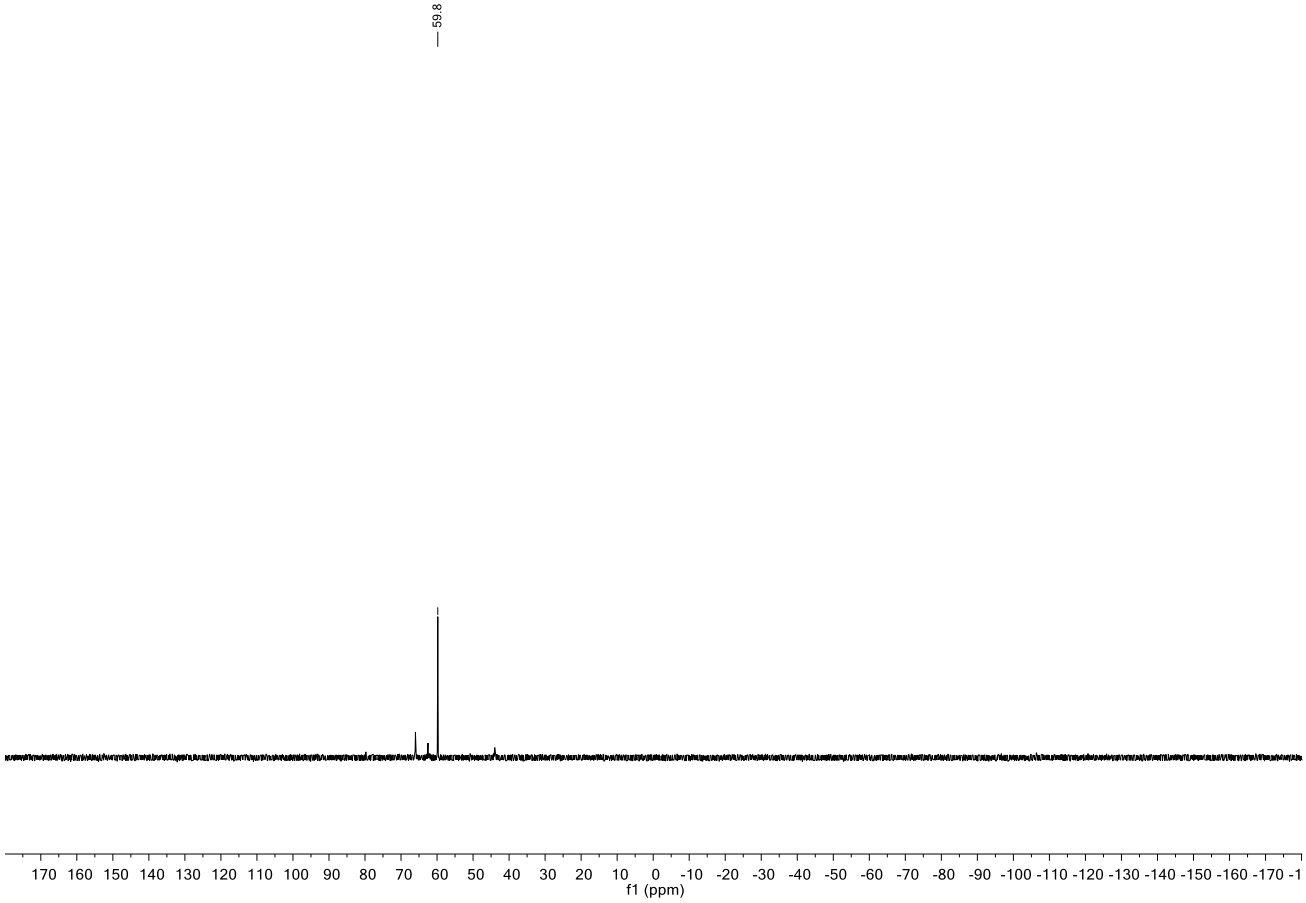


Figure S51. $^{31}P\{^{1}H\}$ NMR spectrum of **25.** (202 MHz, 298 K, Benzene-d_6)



*{SiN^{Dipp}}Al-O$_2$C-Cu{P^{t}Bu$_3$} (**25**) thermal stability test*

The d_6-benzene solution of **25** was kept at room temperature for three days, no significant change was observed by ^{1}H or ^{13}C NMR spectrum. The sample was then kept at 60 ^{o}C overnight, then monitored by NMR spectra. Further transformation was observed, especially with the disappearance of ^{13}C resonance at 233.1 (Cu*C*O2) ppm and the emergence of new sharp ^{13}C resonance at 166.7, 168.4, 176.7 ppm; as well as in in ^{31}P NMR spectrum, the diminishing of the peak at 59.8 ppm and the new peak at 62.1 ppm.

Figure S52. ^{1}H NMR spectrum of **25** after kept at 60°C overnight. (500 MHz, 298 K, Benzene-d_6)

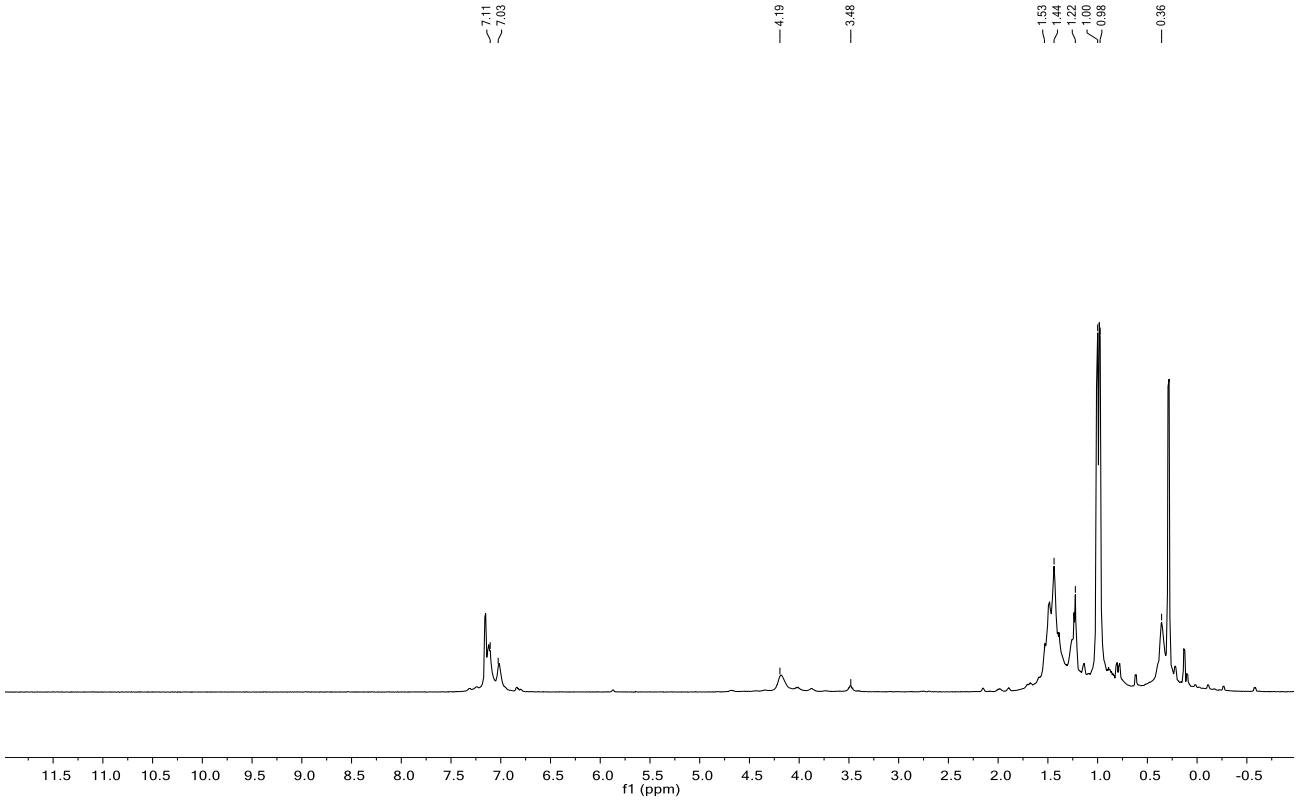


Figure S53. ^{13}C{^{1}H} NMR spectrum of **25** after kept at 60°C overnight. (126 MHz, 298 K, Benzene-d_6)

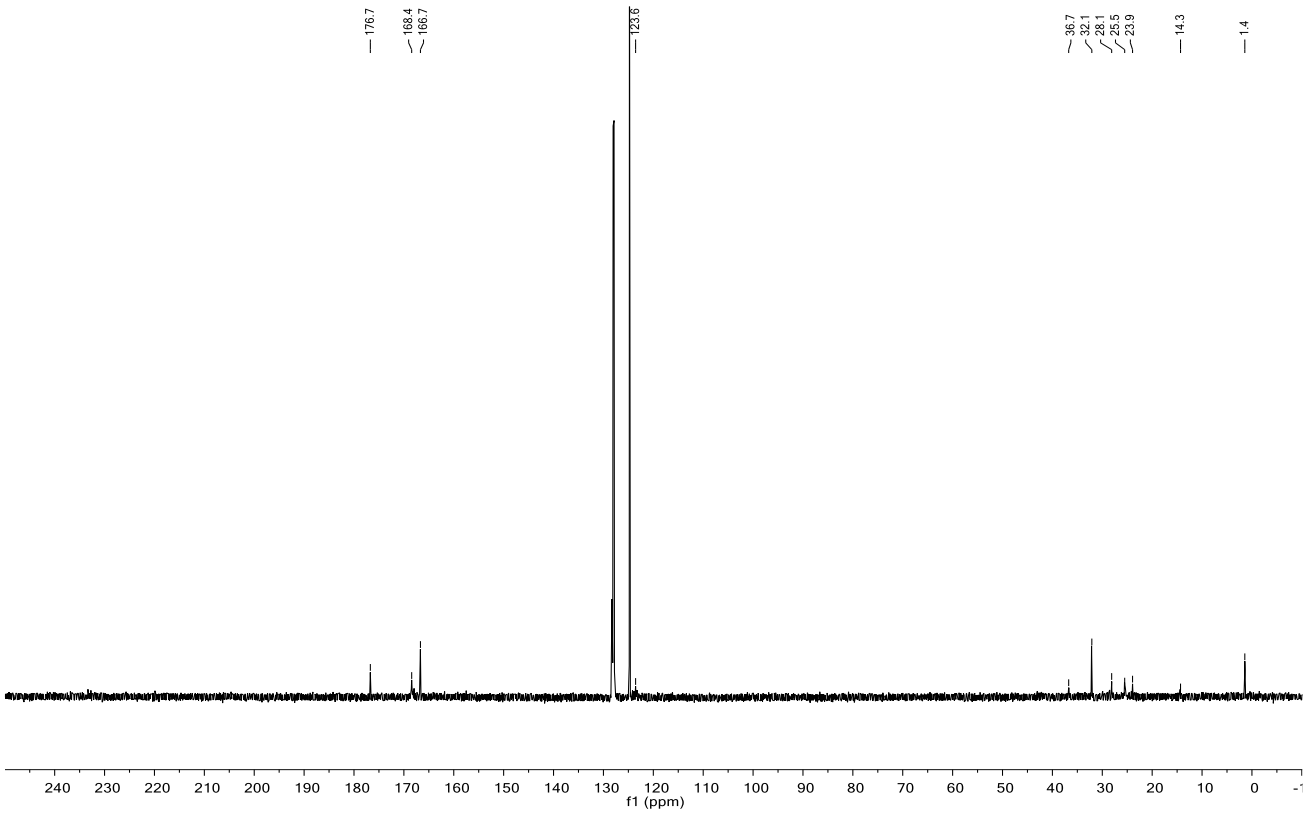
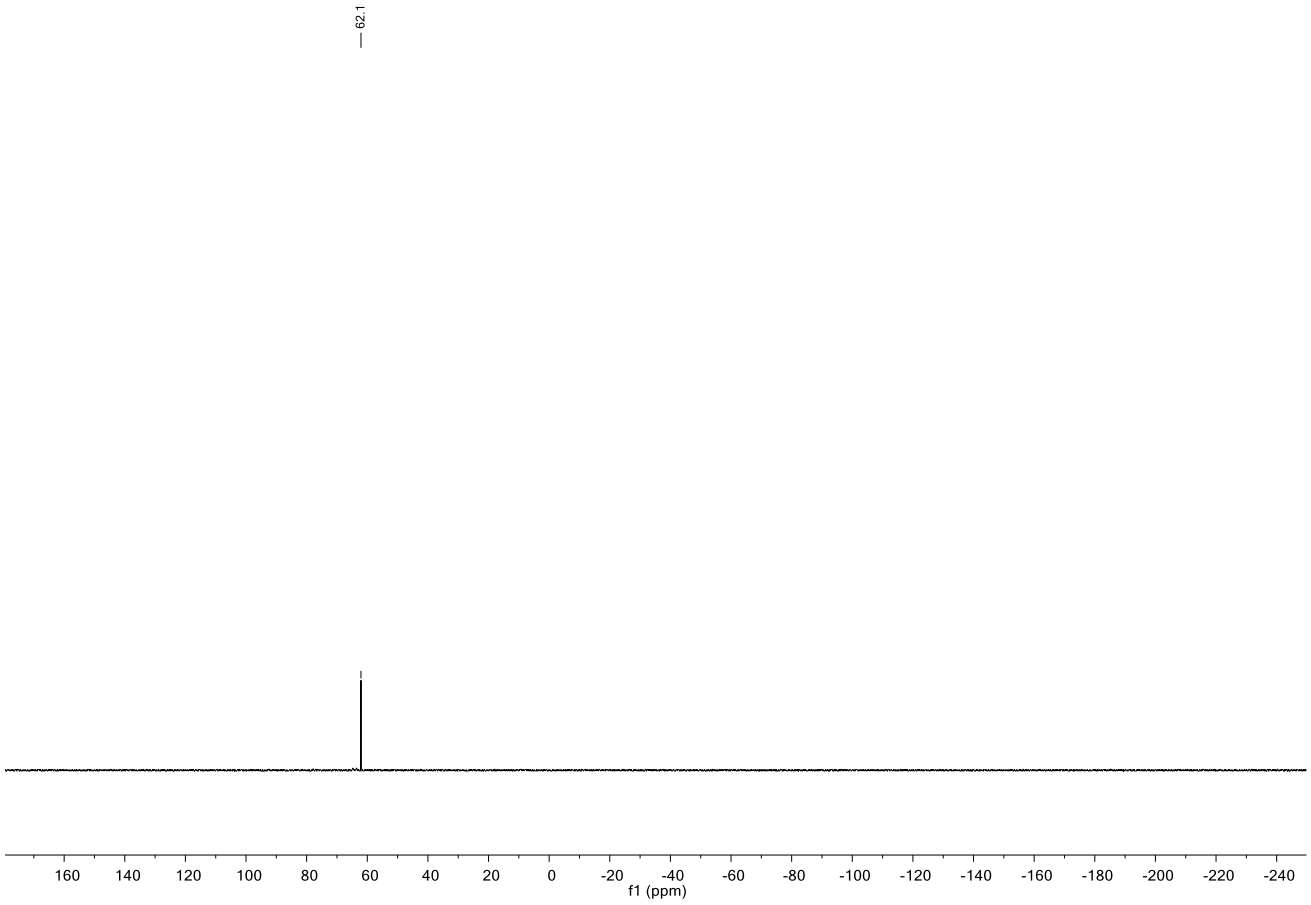


Figure S54. $^{31}P\{^{1}H\}$ NMR spectrum of **25** after kept at 60°C overnight. (202 MHz, 298 K, Benzene-d_6)



Single Crystal X-ray Diffraction Analysis:

Single Crystal X–ray diffraction data for compounds **17 – 20**, **2**3 and **24** were collected on a SuperNova, EosS2 diffractometer using CuKα (λ = 1.54184 Å) radiation throughout. The crystals were maintained at 150 K during data collection. Using Olex2,[5] the structures were solved with the olex2.solve[6] structure solution program or ShelXT and refined with the ShelXL[7] refinement package using Least Squares minimization.

It was clear from the diffraction data collected for compound **17** that the sample was twinned. This was addressed at the point of data reduction where, raw data were integrated as arising from two components. There was evidence of a very minor third component, but the intensity of diffraction from same was so low that this was ultimately ignored. The esds associated with the metric parameters are larger than one might wish for in this structure, but the characterisation is unequivocal.

The asymmetric unit of **19** comprises two molecules of the silver/aluminium containing complex. Disorder was present in both of the NHC rings. In particular, N3, N4, N9, N10, C35-C38 and C83-C86 were each disordered over two sites in a 55:45 ratio. Distance and ADP restraints were used in disordered regions to assist convergence. Residual electron density maxima are located at chemically insignificant distances from the silver centres.

The structure of **20** contains two crystallographically independent molecules of the gold complex and three regions of solvent. Disorder in the main feature was confined to the isopropyl group attached to N3 wherein all three carbons were treated for 63:37 disorder. The solvent of recrystallisation was methylcyclohexane, and three fractional occupancy moieties of same were evident in the asymmetric unit. However, in addition to having 50% site-occupancies approximately, disorder was prevalent in each of these solvent regions. In order to avoid over parameterisation of the model, given the paucity of electron density at each site due to this disorder, solvent was ultimately addressed using the solvent mask algorithm available in Olex-2. However, an allowance has been made for 1.5 molecules of methylcyclohexane per asymmetric unit in the formula, as presented.

65:35 disorder was evident for all phosphine carbons in the structure of **24**. This was modelled with the inclusion of distance and ADP restraints, with respect to fractional occupancy atoms, to assist convergence.

Table S1: Crystal data and structure refinement for compounds **17** - **19**.

Compound	**17**	**18**	**19**
Empirical formula	$C_{48}H_{84}AlAuN_4Si_2$	$C_{53}H_{85}AgAlN_3Si_2$	$C_{96}H_{168}Ag_2Al_2N_{12}Si_4$
Formula weight	997.31	955.26	1872.47
Crystal system	monoclinic	orthorhombic	orthorhombic
Space group	$P2_1/n$	$Pbca$	$Pna2_1$
a/Å	9.9421(2)	17.8026(3)	24.3646(2)
b/Å	18.8454(5)	20.9308(3)	10.9273(1)
c/Å	27.7494(9)	28.5781(4)	39.1524(3)
α/°	90	90	90
β/°	96.781(3)	90	90
γ/°	90	90	90
Volume/Å^3	5162.8(3)	10648.8(3)	10423.91(15)
Z	4	8	4
ρ_{calc} g/cm^3	1.283	1.192	1.193
μ/mm^{-1}	6.208	3.884	3.973
F(000)	2080.0	4096.0	4016.0
Crystal size/mm^3	0.135 × 0.080 × 0.060	0.182 × 0.106 × 0.044	0.171 × 0.09 × 0.054
2θ range /°	7.95 to 146.308	7.216 to 146.282	7.6 to 142.748
Index ranges	$-12 \le h \le 12$, $-23 \le k \le 23$, $-34 \le l \le 34$	$-21 \le h \le 21$, $-12 \le k \le 25$, $-35 \le l \le 35$	$-29 \le h \le 29$, $-13 \le k \le 13$, $-48 \le l \le 42$
Reflections collected	14179	38287	121205
Independent reflections	14179 [R_{int} = 0.0790, R_{sigma} = 0.0721]	10516 [R_{int} = 0.0470, R_{sigma} = 0.0436]	15006 [R_{int} = 0.0531, R_{sigma} = 0.0364]
Data/restraints/parameters	14179/0/525	10516/0/559	15006/115/1201
Goodness-of-fit on F^2	0.898	1.023	1.045
Final R indexes [I>=2σ (I)]	R_1 = 0.0662, wR_2 = 0.1585	R_1 = 0.0374, wR_2 = 0.0946	R_1 = 0.0571, wR_2 = 0.1422
Final R indexes [all data]	R_1 = 0.0988, wR_2 = 0.1739	R_1 = 0.0450, wR_2 = 0.1008	R_1 = 0.0591, wR_2 = 0.1454
Largest diff. peak/hole / e Å^{-3}	1.83/-1.09	0.60/-0.98	2.82/-0.85
Flack parameter	-	-	0.035(7)

Table S2: Crystal data and structure refinement for compounds **20, 23 - 24**.

Compound	**20**	**23**	**24**
Empirical formula	$C_{106.5}H_{189}Al_2Au_2N_{12}Si_4$	$C_{42}H_{77}AlCuN_2PSi_2$	$C_{49}H_{91}AlCuN_4PSi_2$
Formula weight	2197.94	787.72	913.92
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/n$	$P2_1/n$
a/Å	14.9232(1)	12.4581(1)	20.4042(2)
b/Å	31.7335(1)	16.1906(1)	12.8489(1)
c/Å	26.0764(1)	23.0546(1)	21.4769(2)
α/°	90	90	90
β/°	91.103(1)	96.251(1)	106.300(1)
γ/°	90	90	90
Volume/Å^3	12346.6(1)	4622.56(5)	5404.31(9)
Z	4	4	4
ρ_{calc} g/cm^3	1.182	1.132	1.123
μ/mm^{-1}	5.245	1.876	1.678
F(000)	4608.0	1712.0	1992.0
Crystal size/mm^3	0.106 × 0.068 × 0.047	0.209 × 0.191 × 0.158	0.358 × 0.277 × 0.253
2θ range /°	7.32 to 147.01	7.716 to 146.316	7.044 to 144.248
Index ranges	-17 ≤ h ≤ 18, -39 ≤ k ≤ 35, -31 ≤ l ≤ 32	-15 ≤ h ≤ 11, -19 ≤ k ≤ 19, -28 ≤ l ≤ 28	-25 ≤ h ≤ 24, -12 ≤ k ≤ 15, -26 ≤ l ≤ 26
Reflections collected	172051	58911	71855
Independent reflections	24603 [R_{int} = 0.0529, R_{sigma} = 0.0320]	9195 [R_{int} = 0.0272, R_{sigma} = 0.0176]	10645 [R_{int} = 0.0485, R_{sigma} = 0.0307]
Data/restraints/parameters	24603/8/1118	9195/0/463	10645/126/665
Goodness-of-fit on F^2	1.026	1.018	1.021
Final R indexes [I>=2σ (I)]	R_1 = 0.0318, wR_2 = 0.0809	R_1 = 0.0271, wR_2 = 0.0712	R_1 = 0.0391, wR_2 = 0.1043
Final R indexes [all data]	R_1 = 0.0362, wR_2 = 0.0837	R_1 = 0.0286, wR_2 = 0.0724	R_1 = 0.0418, wR_2 = 0.1068
Largest diff. peak/hole / e Å^{-3}	0.97/-1.21	0.32/-0.28	0.48/-0.59

Computational Details

DFT calculations were run with Gaussian 09 (D.01).[8] The Cu, Ag, Au, Al, Si and P centres were described with the Stuttgart RECPs and associated basis sets,[9] and the 6-31G** basis set was used for all other atoms (BS1).[10, 11] A polarization function was also added to Al (ζd = 0.190), Si (ζd = 0.284) and P (ζd = 0.387).[12] Initial BP86 optimizations[13, 14] 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, Ag and Au, for which cc-pVTZ-pp (BS2) was employed. Corrections for the effect of benzene (ε = 2.2706) solvent were employed using the polarizable continuum model and BS1.[15] Single-point dispersion corrections to the BP86 results employed Grimme's D3 parameter set with Becke-Johnson damping as implemented in Gaussian.[16]

The Quantum Theory of Atoms in Molecules (QTAIM, AIMALL program)[17] and Natural Bonding Orbital (NBO7)[18] analyses were performed on the BP86-optmised geometries **7**, **16, 17**, **8, 23** and **4-Cu**. The QTAIM topological analyses used wavefunction files obtained with Gaussian 16 (C.01)[19] at the BP86/BS2 level, whilst NBO analyses were carried out with NBO 7 within Gaussian 16 (C.01) at the same methodology level as the QTAIM calculations. Contour plots were generated in the AIMStudio package, using critical point (CP) visualisation threshold values of 0.025 *e* bohr^{-3} (solid line BCP = strong) and 0.02 *e* bohr^{-3} (dashed line BCP = weak).

Functional testing of the energetics of CO extrusion were carried out with Gaussian 09 (D.01) at the DFA,C_6H_6/BS2//BP86/BS1 level, with B3LYP-D3BJ,[20, 21] M06,[22] PBE-D3BJ,[23] PBE0-D3BJ,[24, 25] TPSS-D3J and ωB97X-D.[26]

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:

$\mathbf{\Delta E_{BSI}}$	SCF energy computed with the BP86 functional with BS1
$\mathbf{\Delta H_{BSI}}$	Enthalpy at 0 K with BS1
$\mathbf{\Delta G_{BSI}}$	Free energy at 298.15 K and 1 atm with BS1
$\mathbf{\Delta G_{BSI/}}\boldsymbol{bnz}$	Free energy corrected for benzene solvent with BS1
$\mathbf{\Delta G_{BSI/}}\boldsymbol{bnz}\mathbf{+D3BJ}$	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 S3. Energies breakdown table (kcal/mol) of all stationary points in the free energy profiles in Figures 5 and S56, relative to the reactant L-M-Al complex ($\mathbf{I_{Cu}}$, $\mathbf{I_{Ag}}$, $\mathbf{I_{Au}}$, $\mathbf{I_{P,H}}$ and $\mathbf{I_{P,A}}$). In each case the final data used in the main article are highlighted in bold.

	ΔE_{BSI}	ΔH_{BSI}	ΔG_{BSI}	$\Delta G_{BSI/bnz}$	$\Delta G_{BSI/bnz+D3BJ}$	ΔE_{BS2}	ΔG_{bnz}
$\mathbf{I_{Cu}}$	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
$\mathbf{TS(I\text{-}II)_{Cu}}$	7.3	6.7	8.6	8.7	8.6	7.2	**8.5**
$\mathbf{II_{Cu}}$	0.1	0.2	-0.8	-0.7	1.7	-0.1	**1.5**
$\mathbf{TS(II\text{-}III)_{Cu}}$	7.9	8.3	20.2	20.9	10.9	11.8	**14.8**
$\mathbf{III_{Cu}}$	-13.3	-11.9	1.9	1.6	-9.1	-8.3	**-4.2**
$\mathbf{TS(III\text{-}IV)_{Cu}}$	-1.4	-1.1	11.8	11.2	8.1	4.6	**14.1**
$\mathbf{IV_{Cu}}$	-11.2	-10.2	0.3	-1.6	2.4	-6.9	**6.7**
$\mathbf{TS(IV\text{-}A)_{Cu}}$	-7.9	-7.6	2.3	0.1	7.5	-4.6	**10.8**
$\mathbf{A_{Cu}}$	-15.5	-14.5	-4.5	-5.6	-0.7	-11.2	**3.6**
$\mathbf{TS(III\text{-}S)_{Cu}}$	-9.4	-8.8	4.9	3.8	0.4	-5.3	**4.5**
$\mathbf{S_{Cu}}$	-40.0	-38.7	-28.9	-30.5	-23.4	-35.9	**-19.3**
$\mathbf{TS(S\text{-}E)_{Cu}}$	-0.8	-1.0	10.0	9.7	8.2	0.1	**9.1**
$\mathbf{E_{Cu}}$	-12.5	-12.0	-2.6	-2.1	-7.0	-13.5	**-7.9**
$\mathbf{III_{Cu,N}}$	-3.0	-1.1	21.6	23.1	-10.4	0.1	**-7.3**
$\mathbf{TS(III\text{-}IV)_{Cu,N}}$	-0.1	1.1	23.9	25.4	-5.2	2.9	**-2.2**
$\mathbf{IV_{Cu,N}}$	-11.0	-9.3	10.5	11.3	-12.6	-8.5	**-10.1**
$\mathbf{TS(IV\text{-}A)_{Cu,N}}$	9.1	9.8	29.4	29.7	8.9	11.3	**11.1**
$\mathbf{INT(IV\text{-}A)_{Cu,N}}$	-16.0	-14.5	4.3	4.1	-16.8	-14.2	**-14.9**
$\mathbf{TS\_A\_S_{Cu,N}}$	37.6	37.3	54.2	55.0	32.3	38.6	**33.3**
$\mathbf{A_{Cu,N}}$	-23.3	-22.0	-5.3	-5.4	-25.6	-21.7	**-24.0**
$\mathbf{S_{Cu,N}}$	-36.4	-34.9	-16.9	-16.8	-42.3	-34.1	**-40.0**
$\mathbf{I_{P,H}}$	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
$\mathbf{TS(I\text{-}II)_{P,H}}$	7.4	7.4	20.1	20.7	7.5	12.0	**12.1**
$\mathbf{III_{P,H}}$	-12.4	-11.6	2.3	1.9	-9.6	-7.4	**-4.6**
$\mathbf{S_{P,H}}$	-40.0	-39.3	-28.8	-30.3	-26.4	-36.1	**-22.5**
$\mathbf{TS(S\text{-}E)_{P,H}}$	-4.1	-5.0	5.6	5.3	1.2	-3.4	**1.9**
$\mathbf{E_{P,H}}$	-18.9	-19.0	-10.1	-9.6	-18.0	-19.5	**-18.6**
$\mathbf{I_{P,A}}$	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
$\mathbf{TS(I\text{-}II)_{P,A}}$	3.3	3.4	14.6	15.2	2.4	7.3	**6.4**
$\mathbf{II_{P,A}}$	-18.3	-17.1	-3.8	-4.4	-15.9	-13.3	**-10.9**
$\mathbf{S_{P,A}}$	-43.9	-43.0	-32.9	-34.7	-29.9	-39.9	**-25.9**
$\mathbf{TS(S\text{-}E)_{P,A}}$	-7.2	-7.9	2.0	1.8	-1.5	-7.0	**-1.3**
$\mathbf{E_{P,A}}$	-19.7	-19.6	-9.3	-9.0	-15.0	-21.3	**-16.6**
$\mathbf{I_{Ag}}$	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
$\mathbf{TS(I\text{-}II)_{Ag}}$	8.5	7.9	9.9	9.9	10.1	8.2	**9.9**
$\mathbf{II_{Ag}}$	0.2	0.3	-0.5	-0.5	1.7	0.0	**1.6**
$\mathbf{TS(II\text{-}III)_{Ag}}$	9.1	9.5	21.2	21.8	11.3	13.5	**15.7**
$\mathbf{III_{Ag}}$	-5.4	-4.2	9.8	9.1	-2.6	0.3	**3.1**
$\mathbf{TS(III\text{-}IV)_{Ag}}$	9.0	9.2	22.6	21.0	17.1	15.1	**23.2**
$\mathbf{IV_{Ag}}$	0.2	1.1	11.5	8.8	10.8	4.9	**15.5**
$\mathbf{A_{Ag}}$	-5.8	-4.8	5.0	3.2	7.4	-1.1	**12.1**
$\mathbf{TS(III\text{-}S)_{Ag}}$	-1.5	-1.1	12.5	11.0	6.5	3.1	**11.1**
$\mathbf{S_{Ag}}$	-32.0	-30.8	-20.5	-22.4	-16.5	-26.9	**-11.4**
$\mathbf{III_{Ag,N}}$	7.9	9.6	31.8	33.1	-1.3	11.8	**2.6**

$TS(III\text{-}IV)_{Ag,N}$	13.0	13.9	35.9	37.2	6.1	16.8	**9.9**
$IV_{Ag,N}$	-0.7	0.9	21.4	21.8	-2.7	2.1	**0.2**
$A_{Ag,N}$	-12.3	-11.0	5.9	5.4	-15.4	-10.5	**-13.6**
$S_{Ag,N}$	-28.9	-27.2	-7.6	-7.7	-33.9	-26.6	**-31.6**
I_{Au}	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
$TS(I\text{-}II)_{Au}$	9.2	8.6	10.1	10.1	10.6	8.8	**10.2**
II_{Au}	0.0	0.1	-0.9	-0.9	1.4	-0.2	**1.1**
$TS(II\text{-}III)_{Au}$	9.3	9.7	21.1	21.7	11.3	14.0	**15.9**
III_{Au}	-4.8	-3.6	10.0	9.1	-2.7	0.1	**2.3**
$TS(III\text{-}IV)_{Au}$	23.5	23.7	36.9	35.8	31.3	28.9	**36.8**
IV_{Au}	9.1	10.1	20.9	18.8	22.3	12.9	**26.0**
A_{Au}	3.9	4.9	14.1	12.4	19.1	7.6	**22.8**
$TS(III\text{-}S)_{Au}$	-1.8	-1.2	12.7	11.2	5.8	2.6	**10.2**
S_{Au}	-32.1	-30.8	-20.8	-22.4	-15.3	-27.6	**-10.8**
$III_{Au,N}$	9.4	11.2	32.9	34.1	-0.6	12.5	**2.5**
$TS(III\text{-}IV)_{Au,N}$	26.2	27.2	48.8	50.2	19.2	28.8	**21.8**
$IV_{Au,N}$	4.6	6.3	26.7	27.4	3.7	6.6	**5.7**
$A_{Au,N}$	-6.8	-5.4	11.7	11.4	-8.5	-5.8	**-7.5**
$S_{Au,N}$	-28.1	-26.3	-6.6	-6.6	-34.3	-25.9	**-32.1**

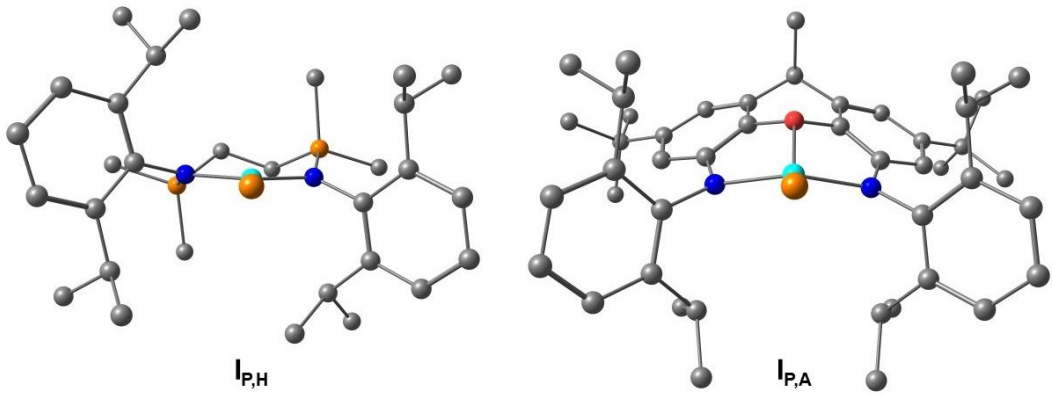


Figure S55. Comparison of the optimised structures of $\mathbf{I_{P,H}}$ (**23**) and $\mathbf{I_{P,A}}$ (**4-Cu**). All hydrogen atoms and $_{atoms}$ part of the *t*-Bu_3P ligand have been omitted for clarity.

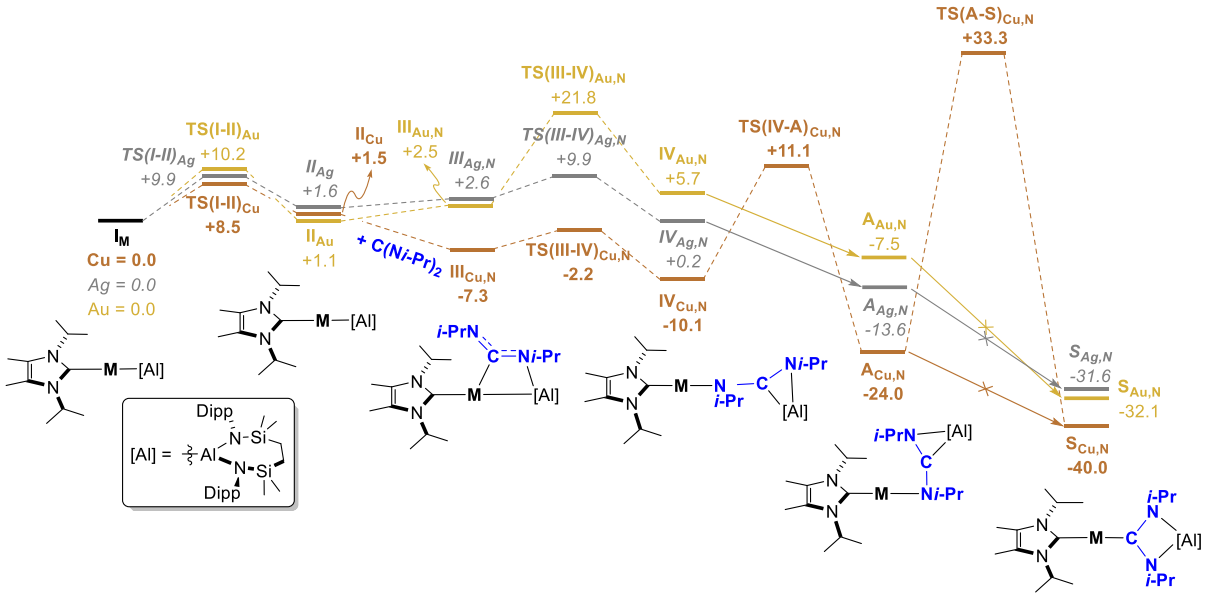


Figure S56. Computed free energy profile (in kcal mol^{-1}) of addition and activation of *i*-PrN=C=N*i*-*Pr* to form asymmetric group 11 metal alumanyl adducts "$\mathbf{A_{M,N}}$", where M = Cu (copper brown, bold), Ag (silver, italics) and Au (gold), whereby three separate energy profiles are presented for each coinage metal complex.

Discussion of $\mathbf{I_{Cu}}$ profile

From $\mathbf{II_{Cu}}$ (+1.5 kcal/mol) addition of *i*-PrN=C=N*i*-Pr takes place exergonically to form $\mathbf{III_{Cu,N}}$ (-7.3 kcal/mol). Note that in the other two complexes ($\mathbf{I_{Ag}}$, $\mathbf{I_{Au}}$) this process is marginally endergonic (where $\mathbf{III_{Ag,N}}$ = +2.6 kcal/mol, $\mathbf{III_{Au,N}}$ = +2.5 kcal/mol). From $\mathbf{III_{Cu,N}}$ Cu–Al bond cleavage can facilely take place via $\mathbf{TS(III\text{-}IV)_{Cu,N}}$ and a barrier of +5.1 kcal/mol to form the asymmetric adduct $\mathbf{IV_{Cu,N}}$ (-10.1 kcal/mol), and subsequent rate-limiting conformational rearrangement via $\mathbf{TS(IV\text{-}A)_{Cu,N}}$ can ultimately yield $\mathbf{A_{Cu,N}}$ (-24.0 kcal/mol). (*Note:* an intermediate species $\mathbf{INT(IV\text{-}A)_{Cu,N}}$, not shown in Figure S56 was optimised following IRC analysis of $\mathbf{TS(IV\text{-}A)_{Cu,N}}$ at (-14.9 kcal/mol), but comparison of this intermediate with $\mathbf{A_{Cu,N}}$ indicates that the barrier for arrangement of $\mathbf{INT(IV\text{-}A)_{Cu,N}}$ to $\mathbf{A_{Cu,N}}$ to be sufficiently small). Subsequent characterisation of an isomerisation process to form $\mathbf{S_{Cu,N}}$ from $\mathbf{A_{Cu,N}}$ identified that this process, via $\mathbf{TS(A\text{-}S)_{Cu,N}}$ (+33.3 kcal/mol) is extremely high in energy and kinetically inaccessible, which is consistent with the experimental observation that upon formation of $\mathbf{A_{Cu,N}}$, it is not amenable to onwards reactivity in this fashion.

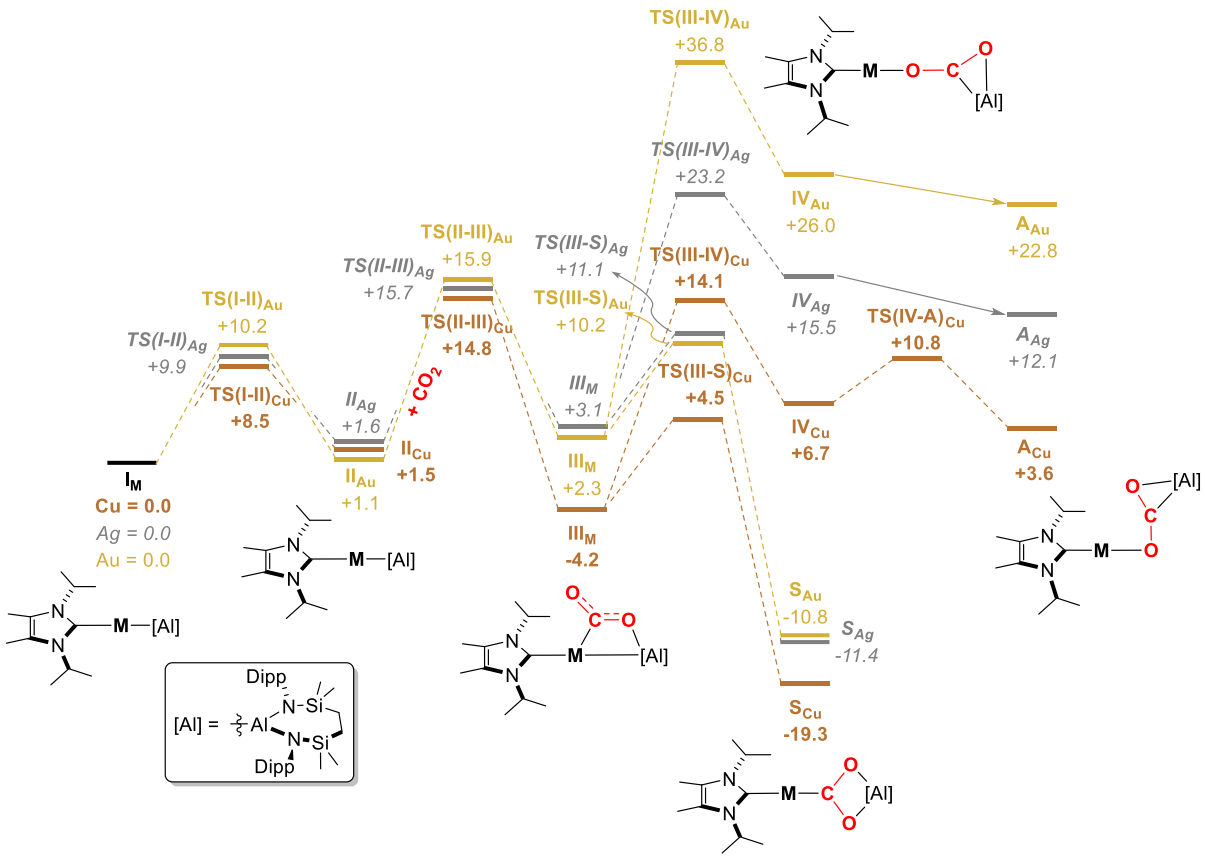


Figure S57. Computed free energy profile (in kcal mol^{-1}) of addition and activation of CO_2 to form asymmetric group 11 metal alumanyl adducts "$\mathbf{S_M}$" and "$\mathbf{A_M}$", where M = Cu (copper brown, bold), Ag (silver, italics) and Au (gold), whereby three separate energy profiles are presented for each coinage metal complex.

QTAIM contour plots & tabulated data

Combined Data

Table S4. BCP data for **7**, **16**, **17**, **8**, **23** and **4-Cu**.

Complex	BCP	ρ(r)	$\nabla^2\rho(r)$	ε	G(r)	V(r)	H(r)	DI(A|B)
7	Cu1 - Al4	0.061284	-0.04545	0.170355	0.019122	-0.04961	-0.03048	0.751638
	Cu1 - C89	0.105188	0.274515	0.060812	0.107578	-0.14653	-0.03895	0.734047
16	Ag1 - Al4	0.059934	-0.028136	0.161714	0.02156	-0.050153	-0.028594	0.719295
	Ag1 - C89	0.086395	0.214371	0.048192	0.078145	-0.102725	-0.02458	0.66521
17	Au1 - Al4	0.066345	0.048872	0.133499	0.041654	-0.07109	-0.029436	0.618397
	Au1 - C89	0.104615	0.209146	0.054995	0.089063	-0.125921	-0.036858	0.798752
8	Cu1 - Al4	0.058889	-0.061269	0.143801	0.012991	-0.041299	-0.028308	0.761956
	Cu1 - C88	0.10646	0.271683	0.067283	0.108037	-0.148154	-0.040117	0.811884
23	Cu1 - Al5	0.059877	-0.04149	0.168807	0.019073	-0.04852	-0.029444	0.724994
	Cu1 - P2	0.072261	0.118634	0.007243	0.051507	-0.07336	-0.021848	0.687771
4-Cu	Al2 - O3	0.03616	0.158888	0.295319	0.041933	-0.044145	-0.002211	0.134022
	Al2 - Cu154	0.059838	-0.043735	0.189032	0.018657	-0.048248	-0.029591	0.723444
	P1 - Cu154	0.072499	0.119147	0.007212	0.051765	-0.073742	-0.021978	0.687923

Table S5. Selected QTAIM and NBO atomic data for **7**, **16**, **17**, **8**, **23** and **4-Cu**.

Complex	Atom	Vol(r)	Loc(r)	$q(A)_{AIM}$	$q(A)_{NBO7}$
7	Cu1	181.8075	93.50836	-0.32294	0.03823
	Al4	84.03675	91.76677	1.817361	1.40023
	C89	71.95786	67.66834	0.621562	-0.01461
16	Ag1	233.5177	93.72572	-0.42795	0.05719
	Al4	79.29488	91.9187	1.874219	1.35352
	C89	72.72383	67.86935	0.66966	0.02113
17	Au1	256.123771	93.25664	-0.71988	-0.13943
	Al4	63.168608	92.60946	2.080411	1.50958
	C89	67.446312	66.71655	0.702368	0.02579
8	Cu1	191.3187	93.5677	-0.21193	0.12232
	Al4	93.73914	91.63562	1.734758	1.38051
	C88	72.01144	68.22331	0.325452	0.01333
23	Cu1	209.43012	94.13948	-0.40276	0.00099
	Al5	81.482699	91.83595	1.851329	1.40033
	P2	104.694774	85.84415	0.667465	0.83863
4-Cu	Cu154	210.7553	94.16081	-0.4057	0.11432
	Al2	80.69499	92.08756	1.887043	1.18243
	O3	86.2118	85.69318	-1.11682	-0.59587
	P1	104.4814	85.83918	0.667953	0.85494

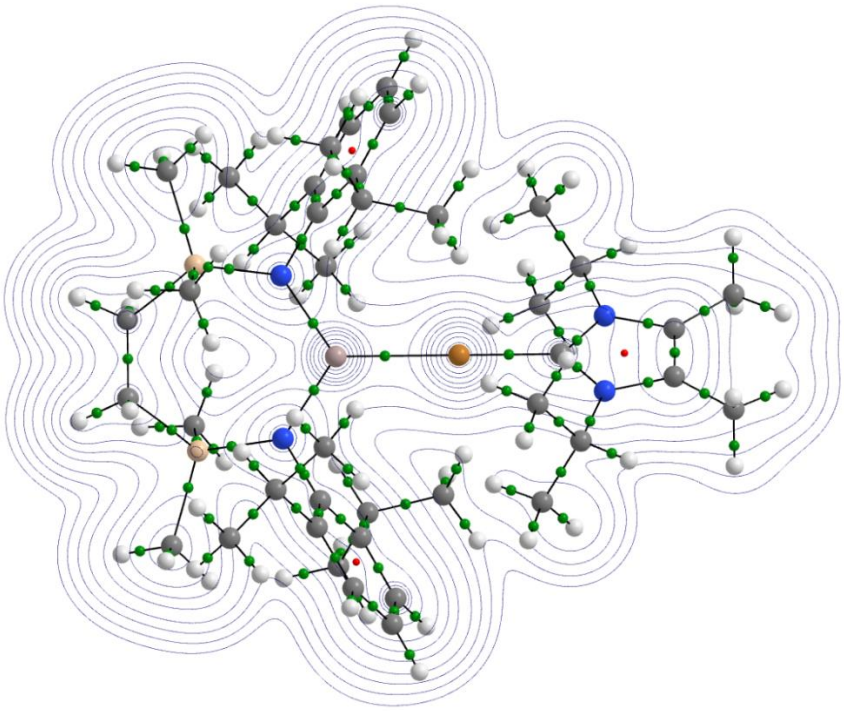


Figure S58. Contour plot of **7**.

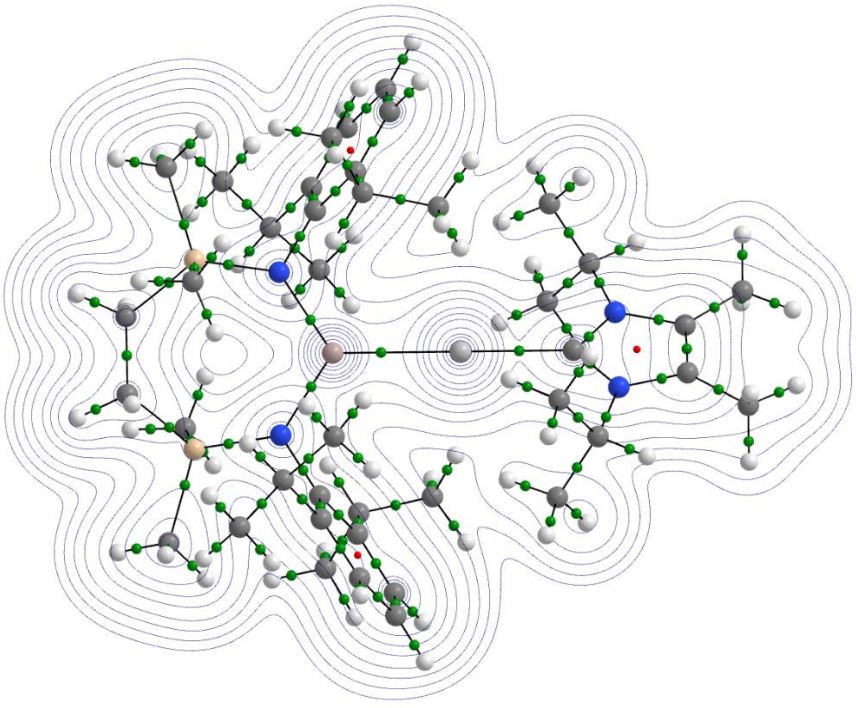


Figure S59. Contour plot of **16**.

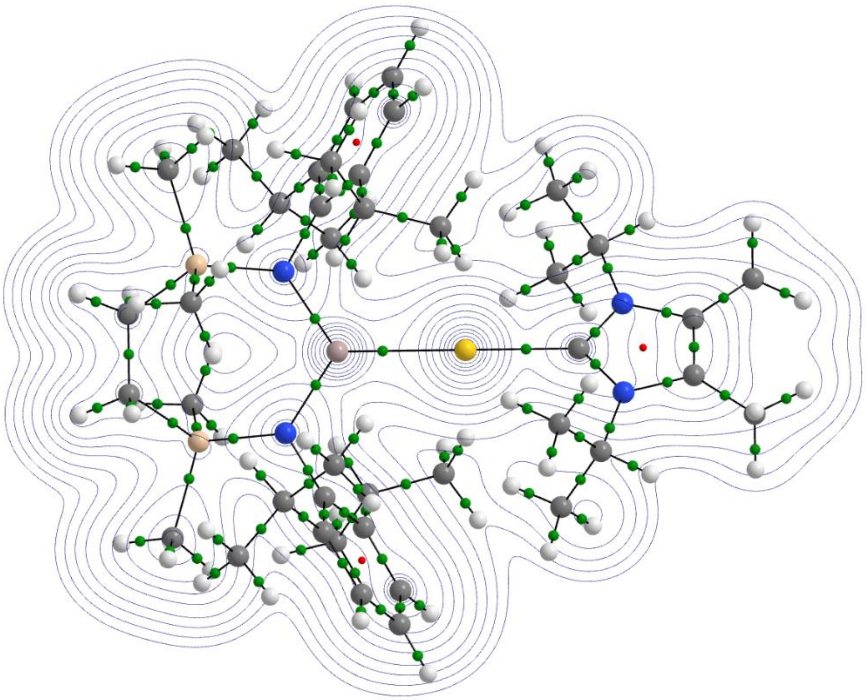


Figure S60. Contour plot of **17**.

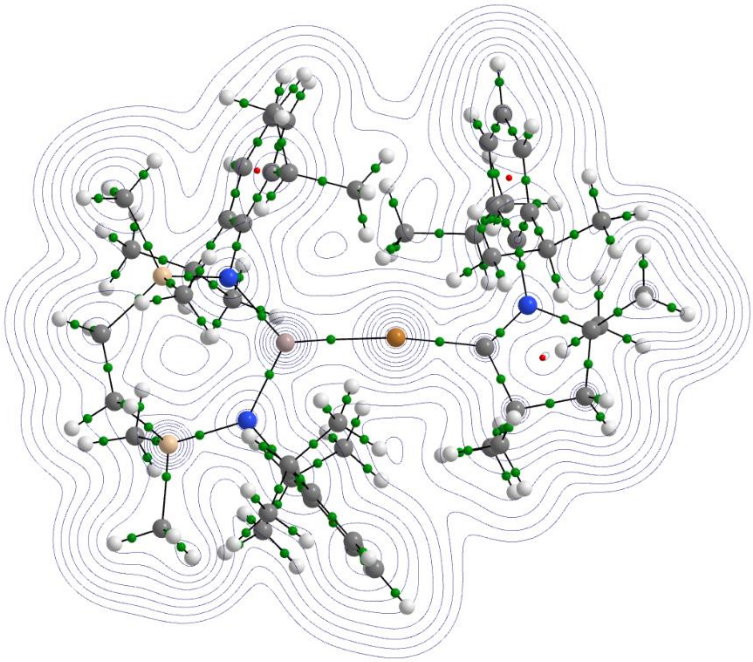


Figure S61. Contour plot of **8**.

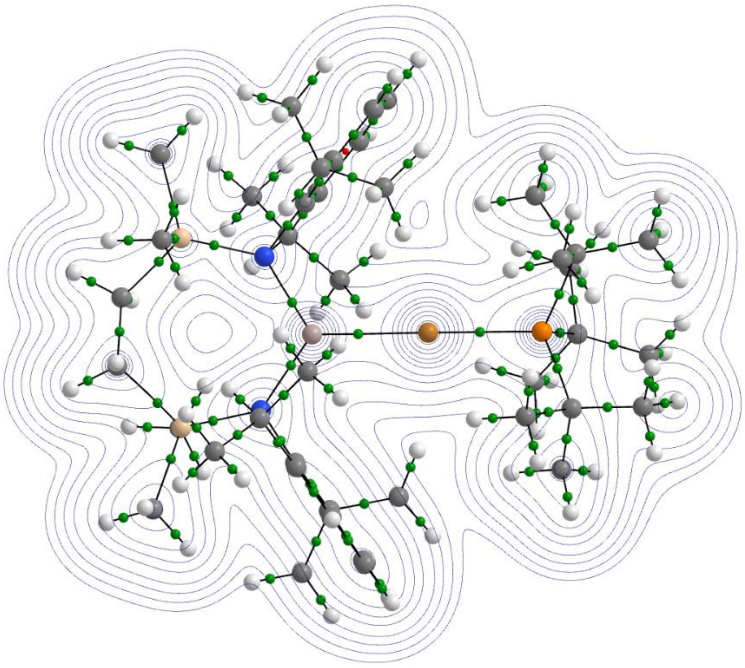


Figure S62. Contour plot of **23**.

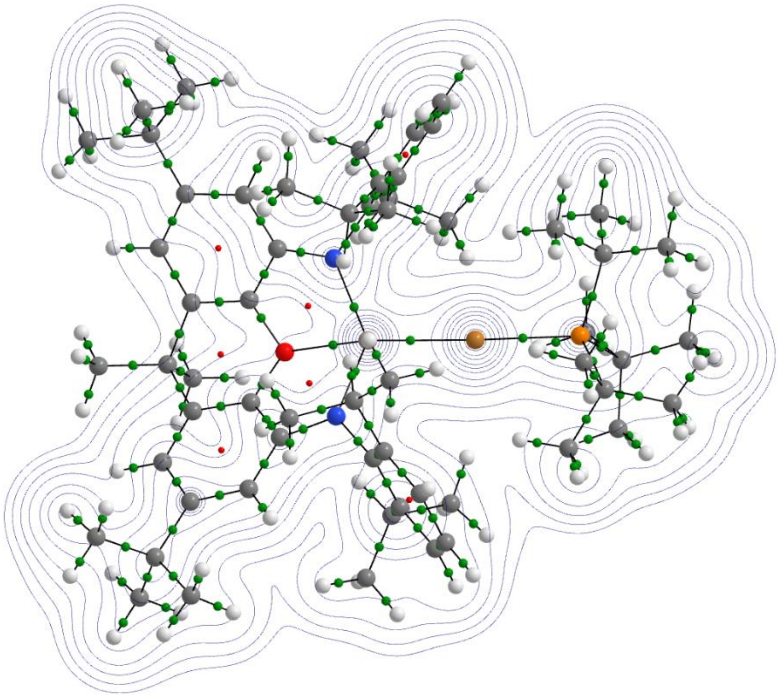


Figure S63. Contour plot of **4-Cu**.

NBO data

Table S6. L-M-Al bonding NLMO compositions

Complex	**Atom**	**Contribution to M-Al NLMO in % (*s, p, d* character)**			
		overall	***s orbital***	***p orbital***	***d* orbital**
7	Cu	45.49	94.74	0.81	4.45
	Al	51.00	88.15	11.77	0.08
16	Ag	43.24	95.02	0.67	4.30
	Al	53.09	83.80	16.11	0.09
17	Au	55.47	91.02	0.48	8.48
	Al	41.83	83.36	15.51	0.13
8	Cu	42.72	94.72	0.92	4.35
	Al	53.17	88.58	11.35	0.07
23	Cu	45.88	96.32	1.13	2.55
	Al	51.26	84.27	15.64	0.09
4-Cu	Cu	39.93	96.49	0.75	2.76
	Al	57.73	75.05	25.85	0.10

Functional testing of CO extrusion

Table S7. Computed single-point energies of CO extrusion intermediates (in Hartrees) for functional testing, computed at the DFA,C_6H_6/BS2//BP86/BS1 level.

	B3LYP-D3BJ	M06	PBE-D3BJ	PBE0-D3BJ	TPSS-D3BJ	wB97XD
S_{Cu}	-3032.1416000	-3030.2661120	-3028.8441563	-3029.0740846	-3032.3276633	-3031.1726794
$TS(S\text{-}E)_{Cu}$	-3032.0907935	-3030.2119610	-3028.7943387	-3029.0151039	-3032.2806477	-3031.1162654
E_{Cu}	-3032.1147104	-3030.2343053	-3028.8182445	-3029.0383125	-3032.3079802	-3031.1415873
$S_{P,H}$	-3306.3426145	-3304.4446490	-3302.8907805	-3303.1753041	-3306.5107728	-3305.3686093
$TS(S\text{-}E)_{P,H}$	-3306.2965362	-3304.3947216	-3302.8454562	-3303.1215560	-3306.4686713	-3305.3171757
$E_{P,H}$	-3306.3255973	-3304.4227393	-3302.8740111	-3303.1485807	-3306.5000847	-3305.3465865
$S_{P,A}$	-3457.7310962	-3455.2900036	-3453.6819892	-3453.9680998	-3458.0154536	-3456.5006396
$TS(S\text{-}E)_{P,A}$	-3457.6853587	-3455.2377642	-3453.6360840	-3453.9145483	-3457.9731106	-3456.4494710
$E_{P,A}$	-3457.7089940	-3455.2595342	-3453.6601092	-3453.9357016	-3457.9990674	-3456.4726795

Table S8. Computed free energies (kcal/mol) of CO extrusion intermediates (relative to $\mathbf{S_{L,[Al]}}$) for functional testing, computed at the DFA,C_6H_6/BS2//BP86/BS1 level. In bold are the kinetically favoured system for CO extrusion between $\mathbf{S_{P,H}}$ and $\mathbf{S_{P,A}}$.

	B3LYP-D3BJ	M06	PBE-D3BJ	PBE0-D3BJ	TPSS-D3BJ	wB97XD
S_{Cu}	0.0	0.0	0.0	0.0	0.0	0.0
$TS(S\text{-}E)_{Cu}$	+31.6	+33.7	+31.0	+36.7	+29.2	+35.1
E_{Cu}	+15.7	+18.8	+15.1	+21.3	+11.2	+18.4
$S_{P,H}$	0.0	0.0	0.0	0.0	0.0	0.0
$TS(S\text{-}E)_{P,H}$	+27.3	**+29.7**	**+26.8**	+32.1	+24.8	+30.7
$E_{P,H}$	+8.3	+11.3	+8.1	+14.3	+4.3	+11.4
$S_{P,A}$	0.0	0.0	0.0	0.0	0.0	0.0
$TS(S\text{-}E)_{P,A}$	**+26.9**	+31.0	+27.0	**+31.8**	**+24.8**	**+30.3**
$E_{P,A}$	+13.3	+18.5	+13.1	+19.7	+9.7	+16.9

Cartesian Coordinates and Energies

***i*-PrNCN*i*-Pr**
SCF (BP86) Energy = -384.663990790
Enthalpy 0K = -384.454365
Enthalpy 298K = -384.453420
Free Energy 298K = -384.504973
Lowest Frequency = 23.8218 cm^{-1}
Second Frequency = 27.2199 cm^{-1}
SCF (BP86-D3BJ) Energy = -384.692047877
SCF (C6H6) Energy = -384.665684967
SCF (BS2) Energy = -384.763019620

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

CO_2
SCF (BP86) Energy = -188.586707744
Enthalpy 0K = -188.572827
Enthalpy 298K = -188.571883
Free Energy 298K = -188.596251
Lowest Frequency = 616.1687 cm^{-1}
Second Frequency = 616.1687 cm^{-1}
SCF (BP86-D3BJ) Energy = -188.588114567
SCF (C6H6) Energy = -188.587597052
SCF (BS2) Energy = -188.654543408

C	0.00000	0.00000	0.00000
O	0.00000	0.00000	1.18174
O	0.00000	0.00000	-1.18174

I_{Cu}
SCF (BP86) Energy = -2031.04455884
Enthalpy 0K = -2029.975499
Enthalpy 298K = -2029.974554
Free Energy 298K = -2030.140763
Lowest Frequency = 15.1376 cm^{-1}
Second Frequency = 22.0369 cm^{-1}
SCF (BP86-D3BJ) Energy = -2031.36231088
SCF (C6H6) Energy = -2031.04865160
SCF (BS2) Energy = -2843.16767231

Cu	-1.54060	-0.00147	0.00124
Si	3.53486	1.66071	-1.05141
Si	3.53763	-1.65639	1.05041
Al	0.84199	0.00031	0.00018
N	1.88145	1.53821	-0.35909
N	1.88377	-1.53620	0.35879
N	-4.35625	-0.83633	-0.68704
N	-4.35724	0.83114	0.68863
C	1.16842	2.78268	-0.19774
C	0.40241	3.34893	-1.26742
C	-0.26336	4.57532	-1.06738
H	-0.84055	5.00682	-1.89418
C	-0.20275	5.25432	0.15441
H	-0.72110	6.21068	0.28539
C	0.53450	4.69578	1.20574
H	0.58561	5.22235	2.16590
C	1.22452	3.47826	1.05366
C	0.27720	2.67011	-2.63250
H	0.85909	1.73406	-2.58129
C	-1.18630	2.28891	-2.94652
H	-1.59277	1.62444	-2.16143
H	-1.25248	1.76114	-3.91514
H	-1.83438	3.18206	-3.00603
C	0.86406	3.53768	-3.76915
H	0.31024	4.48739	-3.87818
H	0.80377	3.00581	-4.73568
H	1.92168	3.79093	-3.58481
C	2.00331	2.90916	2.23972
H	2.65849	2.11904	1.83321
C	1.04435	2.23934	3.25041
H	0.33568	2.97782	3.66705
H	1.60132	1.78813	4.09129
H	0.44965	1.44431	2.76491
C	2.89754	3.95058	2.94458
H	3.57870	4.44775	2.23326
H	3.51169	3.46385	3.72262
H	2.30464	4.73755	3.44409
C	4.05766	3.49146	-1.14487
H	3.33079	4.10589	-1.69993
H	5.03462	3.57234	-1.65315
H	4.16165	3.93257	-0.13930
C	3.62221	0.91437	-2.80835
H	3.22323	-0.11361	-2.83363
H	4.66988	0.87532	-3.15715
H	3.04879	1.51514	-3.53331
C	4.86591	0.77550	-0.00177
H	5.82673	1.15008	-0.41349
H	4.82304	1.16834	1.03209
C	4.86705	-0.76926	0.00029
H	5.82855	-1.14241	0.41173
H	4.82445	-1.16218	-1.03355
C	3.62453	-0.91000	2.80735
H	3.22380	0.11730	2.83288
H	4.67222	-0.86923	3.15585
H	3.05233	-1.51181	3.53243
C	4.06301	-3.48641	1.14372
H	3.33785	-4.10150	1.70030
H	5.04090	-3.56577	1.65045
H	4.16589	-3.92792	0.13822
C	1.17246	-2.78165	0.19753
C	0.40768	-3.34914	1.26744
C	-0.25648	-4.57641	1.06747
H	-0.83273	-5.00885	1.89444
C	-0.19544	-5.25512	-0.15446
H	-0.71252	-6.21217	-0.28538
C	0.54060	-4.69538	-1.20601
H	0.59206	-5.22172	-2.16628
C	1.22898	-3.47693	-1.05400
C	0.28208	-2.67069	2.63267
H	0.86280	-1.73392	2.58141
C	-1.18179	-2.29131	2.94716
H	-1.58928	-1.62720	2.16229
H	-1.24833	-1.76376	3.91588
H	-1.82877	-3.18524	3.00672
C	0.87032	-3.53772	3.76901
H	0.31776	-4.48817	3.87797
H	0.80959	-3.00612	4.73566
H	1.92823	-3.78956	3.58436

C 2.00647 -2.90652 -2.24029
H 2.66075 -2.11559 -1.83388
C 1.04613 -2.23779 -3.25039
H 0.33830 -2.97716 -3.66687
H 1.60209 -1.78563 -4.09143
H 0.45053 -1.44370 -2.76446
C 2.90181 -3.94655 -2.94577
H 3.58403 -4.44288 -2.23489
H 3.51489 -3.45881 -3.72402
H 2.30978 -4.73426 -3.44515
C -3.50887 -0.00252 0.00133
C -3.89494 -1.93352 -1.57951
H -4.81943 -2.38603 -1.97675
C -3.08126 -1.37386 -2.75569
H -3.65015 -0.60939 -3.31029
H -2.81764 -2.18975 -3.44898
H -2.14468 -0.91615 -2.38945
C -3.12681 -2.99824 -0.78422
H -2.19190 -2.58191 -0.36969
H -2.85538 -3.83973 -1.44191
H -3.73363 -3.38761 0.04992
C -5.70228 -0.53458 -0.43888
C -6.85209 -1.27482 -1.04863
H -6.85455 -1.21146 -2.15179
H -7.80330 -0.84723 -0.69565
H -6.85368 -2.34565 -0.77624
C -5.70291 0.52960 0.43827
C -6.85359 1.26975 1.04652
H -6.85794 1.20571 2.14963
H -7.80430 0.84261 0.69165
H -6.85445 2.34074 0.77477
C -3.89719 1.92874 1.58124
H -4.82216 2.37898 1.97995
C -3.13232 2.99554 0.78553
H -2.19707 2.58136 0.36968
H -2.86188 3.83731 1.44327
H -3.74102 3.38402 -0.04767
C -3.08085 1.37025 2.75610
H -3.64737 0.60421 3.31095
H -2.81825 2.18639 3.44947
H -2.14365 0.91483 2.38856

TS(I-II)$_{Cu}$
SCF (BP86) Energy = -2031.03293630
Enthalpy 0K = -2029.964878
Enthalpy 298K = -2029.963933
Free Energy 298K = -2030.127085
Lowest Frequency = -60.8913 cm^{-1}
Second Frequency = 15.4374 cm^{-1}
SCF (BP86-D3BJ) Energy = -2031.35080856
SCF (C6H6) Energy = -2031.03687790
SCF (BS2) Energy = -2843.15626333

Cu 1.40889 -0.48014 -0.18763
Si -2.83992 2.46784 1.34578
Si -4.02913 -0.64457 -0.75965
Al -0.87889 0.12316 0.02140
N -1.37900 1.89005 0.48110
N -2.34448 -1.02944 -0.27186
N 3.98152 -1.85735 0.41923
N 4.38468 0.04380 -0.55777
C -0.33336 2.85001 0.22626
C 0.69530 3.10983 1.18935
C 1.71346 4.03577 0.88185
H 2.49085 4.23652 1.62932
C 1.74759 4.71269 -0.34276
H 2.54238 5.43604 -0.55684
C 0.74083 4.46333 -1.28372
H 0.75616 4.99574 -2.24207
C -0.29997 3.55177 -1.02279
C 0.72580 2.42756 2.55808
H -0.11422 1.71259 2.57932
C 2.02512 1.62217 2.77562
H 2.15360 0.86932 1.97583
H 1.99836 1.09586 3.74683
H 2.91533 2.27738 2.77637
C 0.52355 3.44063 3.70853
H 1.34205 4.18220 3.73801
H 0.50742 2.92358 4.68483
H -0.42293 3.99661 3.60203
C -1.36213 3.31098 -2.09582
H -2.18011 2.75409 -1.60655
C -0.80724 2.41781 -3.22910
H 0.03995 2.91046 -3.73985
H -1.58375 2.20698 -3.98622
H -0.44214 1.45260 -2.83421
C -1.95291 4.61567 -2.67082
H -2.34324 5.26994 -1.87294
H -2.78241 4.38830 -3.36338
H -1.20363 5.19472 -3.23974
C -2.79942 4.36905 1.47724
H -1.85984 4.73828 1.91879
H -3.63523 4.71772 2.10892
H -2.90578 4.84114 0.48602
C -2.94846 1.72890 3.10508
H -2.85020 0.63008 3.08772
H -3.92273 1.97058 3.56666
H -2.15727 2.12581 3.76223
C -4.47303 2.02218 0.45567
H -5.23788 2.63808 0.97410
H -4.43550 2.41906 -0.57683
C -4.91126 0.54011 0.45549
H -5.98241 0.46758 0.17222
H -4.85365 0.11449 1.47547
C -4.10314 0.17275 -2.48535
H -3.42333 1.03839 -2.55506
H -5.12656 0.53237 -2.69551
H -3.82654 -0.53694 -3.28233
C -5.06095 -2.24592 -0.81469
H -4.60403 -3.00885 -1.46558
H -6.07033 -2.02396 -1.20357
H -5.17473 -2.69158 0.18765
C -1.98267 -2.42662 -0.24866
C -1.49478 -3.08924 -1.42033
C -1.14627 -4.45326 -1.34735
H -0.77809 -4.95611 -2.24984
C -1.26121 -5.17840 -0.15629
H -0.99189 -6.24001 -0.12378
C -1.73381 -4.53018 0.99176
H -1.82899 -5.09415 1.92695
C -2.10243 -3.17188 0.96878
C -1.33949 -2.36941 -2.76132
H -1.67355 -1.32909 -2.60902
C 0.13517 -2.31730 -3.21862
H 0.75831 -1.79899 -2.46562
H 0.22743 -1.77285 -4.17584
H 0.55053 -3.33050 -3.36674
C -2.22625 -2.99866 -3.85989
H -1.92650 -4.04017 -4.07419
H -2.14148 -2.42879 -4.80256
H -3.28924 -3.01491 -3.56493
C -2.60134 -2.50905 2.25336
H -3.08299 -1.56275 1.95087
C -1.41647 -2.14573 3.17724
H -0.86856 -3.05362 3.48805
H -1.76480 -1.62791 4.08917
H -0.69776 -1.48516 2.65871
C -3.64554 -3.35213 3.01459
H -4.49007 -3.63615 2.36404
H -4.04900 -2.78110 3.86930
H -3.21115 -4.28244 3.42225
C 3.35580 -0.80618 -0.19897
C 3.27210 -3.02478 1.01025
H 4.06604 -3.76030 1.22505

C	2.59500	-2.62764	2.33189
H	3.31894	-2.19123	3.04042
H	2.13436	-3.51294	2.80063
H	1.80058	-1.88517	2.13918
C	2.29105	-3.65054	0.01199
H	1.45918	-2.95875	-0.21363
H	1.85281	-4.56481	0.44372
H	2.79485	-3.91090	-0.93328
C	5.36245	-1.66556	0.49745
C	6.29704	-2.65199	1.12778
H	6.04256	-2.85257	2.18383
H	7.32894	-2.27014	1.10669
H	6.29961	-3.62116	0.59634
C	5.62735	-0.45434	-0.10868
C	6.97076	0.20836	-0.19657
H	7.35109	0.29919	-1.22724
H	7.70061	-0.39256	0.36792
H	6.96985	1.21559	0.25428
C	4.11899	1.35822	-1.24205
H	3.89984	2.09214	-0.44362
C	2.89082	1.26641	-2.15916
H	3.04679	0.51771	-2.95460
H	2.72326	2.25363	-2.61875
H	1.96393	1.00938	-1.61029
C	5.30731	1.86550	-2.07913
H	6.16537	2.19973	-1.48179
H	4.96177	2.73562	-2.65992
H	5.64484	1.09937	-2.79819

II_{Cu}

SCF (BP86) Energy = -2031.04433624
Enthalpy 0K = -2029.975119
Enthalpy 298K = -2029.974175
Free Energy 298K = -2030.142050
Lowest Frequency = 12.0406 cm^{-1}
Second Frequency = 15.4502 cm^{-1}
SCF (BP86-D3BJ) Energy = -2031.35818912
SCF (C6H6) Energy = -2031.04833466
SCF (BS2) Energy = -2843.16780753

Cu	-1.43371	-0.31723	-0.13702
Si	3.83707	-1.08834	1.04855
Si	3.26027	2.21440	-1.02908
Al	0.90858	0.06851	-0.05576
N	2.18898	-1.25574	0.35625
N	1.64969	1.77879	-0.37036
N	-4.26366	0.35902	0.47938
N	-4.18637	-1.50643	-0.62082
C	1.67663	-2.59847	0.22346
C	1.00366	-3.24994	1.30659
C	0.52019	-4.56233	1.13044
H	0.01206	-5.05754	1.96680
C	0.67474	-5.24611	-0.08049
H	0.29788	-6.26873	-0.19347
C	1.32322	-4.60654	-1.14405
H	1.44695	-5.13676	-2.09552
C	1.83179	-3.30017	-1.01573
C	0.78574	-2.57014	2.65964
H	1.24449	-1.56912	2.59420
C	-0.71562	-2.36999	2.96418
H	-1.19512	-1.76317	2.17336
H	-0.85120	-1.84980	3.92980
H	-1.24929	-3.33577	3.02491
C	1.47423	-3.33692	3.81141
H	1.04269	-4.34572	3.94041
H	1.34864	-2.79816	4.76775
H	2.55511	-3.46086	3.62889
C	2.51662	-2.64421	-2.21514
H	3.05449	-1.76214	-1.82549
C	1.46703	-2.13418	-3.22955
H	0.87372	-2.97364	-3.63516
H	1.94978	-1.61585	-4.07769
H	0.76167	-1.43058	-2.75023
C	3.54643	-3.55929	-2.91001
H	4.29433	-3.94345	-2.19572
H	4.08167	-3.00322	-3.69975
H	3.06864	-4.43026	-3.39317
C	4.67281	-2.79936	1.12878
H	4.06638	-3.53083	1.68704
H	5.65265	-2.71252	1.63042
H	4.84375	-3.21298	0.12075
C	3.80009	-0.35284	2.81231
H	3.21456	0.58120	2.85066
H	4.82552	-0.11952	3.15132
H	3.35873	-1.05612	3.53748
C	4.98165	0.03355	0.00512
H	5.99612	-0.17105	0.40746
H	5.00254	-0.34532	-1.03454
C	4.71039	1.55497	0.02855
H	5.59673	2.09867	-0.36108
H	4.58560	1.91472	1.06777
C	3.50592	1.52676	-2.79529
H	3.28357	0.44702	-2.84293
H	4.55186	1.66750	-3.12226
H	2.85440	2.03581	-3.52448
C	3.44172	4.11112	-1.07571
H	2.61544	4.59575	-1.62030
H	4.38818	4.38421	-1.57450
H	3.46043	4.53695	-0.05832
C	0.69627	2.84741	-0.20131
C	-0.14730	3.27514	-1.27752
C	-1.06225	4.32567	-1.06377
H	-1.69640	4.65425	-1.89612
C	-1.17633	4.96101	0.17814
H	-1.88338	5.78660	0.31762
C	-0.36389	4.53417	1.23611
H	-0.44725	5.02712	2.21187
C	0.57223	3.49559	1.07053
C	-0.09621	2.62856	-2.66279
H	0.66405	1.83051	-2.61732
C	-1.44129	1.96442	-3.03134
H	-1.72242	1.20977	-2.27260
H	-1.37193	1.46049	-4.01232
H	-2.25733	2.70732	-3.09295
C	0.32804	3.63321	-3.75809
H	-0.40456	4.45420	-3.85774
H	0.39949	3.13147	-4.73981
H	1.30769	4.08905	-3.53639
C	1.42096	3.06241	2.26567
H	2.22391	2.42131	1.86204
C	0.58754	2.20186	3.24308
H	-0.25379	2.78506	3.65982
H	1.20500	1.84513	4.08703
H	0.16051	1.31994	2.73165
C	2.08330	4.24345	3.00570
H	2.67430	4.87156	2.31778
H	2.75971	3.87066	3.79496
H	1.33903	4.89584	3.49659
C	-3.38595	-0.51357	-0.11711
C	-3.75847	1.57742	1.16957
H	-2.68585	1.58591	0.89635
C	-4.38956	2.86912	0.62889
H	-4.38096	2.87957	-0.47278
H	-3.78858	3.72586	0.97362
H	-5.42418	3.01574	0.98016
C	-3.85577	1.44344	2.69753
H	-4.90030	1.44118	3.05301
H	-3.34394	2.29769	3.17064
H	-3.36670	0.51714	3.03921
C	-5.59069	-0.08267	0.36314
C	-6.79689	0.63367	0.88979
H	-6.69102	0.90950	1.95223
H	-7.68114	-0.01783	0.80910
H	-7.01694	1.55776	0.32703

C -5.53792 -1.27017 -0.34057
C -6.64731 -2.18096 -0.76694
H -6.72321 -2.26321 -1.86640
H -7.61244 -1.79639 -0.40294
H -6.52775 -3.20263 -0.36385
C -3.66708 -2.67847 -1.37451
H -4.56304 -3.25100 -1.66948
C -2.78908 -3.56094 -0.47567
H -1.87892 -3.02061 -0.16251
H -2.47154 -4.46194 -1.02537
H -3.33511 -3.87653 0.42879
C -2.93572 -2.22415 -2.64719
H -3.58223 -1.59079 -3.27686
H -2.62582 -3.10473 -3.23407
H -2.03041 -1.64819 -2.38471

TS(II-III)$_{Cu}$
SCF (BP86) Energy = -2219.61870797
Enthalpy 0K = -2218.534156
Enthalpy 298K = -2218.533211
Free Energy 298K = -2218.704789
Lowest Frequency = -151.1878 cm^{-1}
Second Frequency = 16.3587 cm^{-1}
SCF (BP86-D3BJ) Energy = -2219.95391095
SCF (C6H6) Energy = -2219.62253892
SCF (BS2) Energy = -3031.80340508

Cu 1.43359 0.23446 0.48342
Si -3.58081 1.42941 -1.21899
Si -3.51598 -1.98286 0.77727
Al -0.92485 -0.01266 0.18562
N -1.97292 1.44446 -0.40045
N -1.81638 -1.67710 0.26353
N 4.03077 -0.80348 -0.51161
N 4.33151 1.22147 0.20216
O -0.86466 0.20158 3.08254
O 1.40596 0.83735 3.12190
C -1.33411 2.74248 -0.36110
C -1.47057 3.58757 0.78988
C -0.91238 4.88183 0.76608
H -1.03901 5.52964 1.64110
C -0.20644 5.36085 -0.34220
H 0.21014 6.37416 -0.34127
C -0.03744 4.52287 -1.44954
H 0.52551 4.88569 -2.31805
C -0.58422 3.22508 -1.48439
C -2.19827 3.14155 2.06207
H -2.35066 2.05196 1.98284
C -1.36553 3.42225 3.33466
H -0.32607 3.06905 3.23575
H -1.81963 2.92253 4.20754
H -1.32310 4.50258 3.56199
C -3.59081 3.79634 2.21712
H -3.51277 4.89848 2.21053
H -4.05304 3.49714 3.17490
H -4.27724 3.50144 1.40828
C -0.34826 2.38019 -2.73894
H -0.91161 1.44103 -2.60944
C 1.14222 2.00479 -2.89862
H 1.77223 2.90533 -3.01884
H 1.29120 1.37094 -3.79165
H 1.50560 1.44801 -2.01559
C -0.86350 3.07395 -4.02021
H -1.92839 3.34900 -3.93714
H -0.74896 2.40856 -4.89456
H -0.29973 3.99933 -4.23501
C -4.19836 3.21075 -1.51034
H -4.37246 3.77781 -0.58360
H -5.15122 3.16639 -2.06742
H -3.47982 3.78736 -2.11570
C -3.57263 0.63642 -2.95986
H -3.02658 1.26024 -3.68576
H -4.61589 0.55029 -3.31535
H -3.13183 -0.37185 -2.97957
C -4.88284 0.48437 -0.18852
H -4.83538 0.82982 0.86135
H -5.86059 0.84255 -0.57227
C -4.82583 -1.05901 -0.26778
H -4.74282 -1.39246 -1.31961
H -5.78461 -1.48683 0.09454
C -3.81829 -1.46526 2.58923
H -3.25141 -2.09053 3.29766
H -4.89130 -1.56359 2.83347
H -3.52643 -0.41730 2.76707
C -3.91857 -3.83434 0.56949
H -3.91096 -4.12479 -0.49473
H -4.92749 -4.03895 0.96869
H -3.20385 -4.48808 1.09345
C -1.00982 -2.84676 -0.00516
C -0.35601 -3.57134 1.04509
C 0.38831 -4.72762 0.73320
H 0.86944 -5.28160 1.54831
C 0.52275 -5.18836 -0.58123
H 1.09581 -6.09673 -0.79831
C -0.10204 -4.47606 -1.61196
H -0.01280 -4.83228 -2.64513
C -0.87017 -3.32519 -1.35004
C -0.42606 -3.14008 2.51003
H -1.03183 -2.22133 2.54947
C 0.97690 -2.80102 3.06271
H 1.62997 -3.69225 3.08143
H 0.90838 -2.41861 4.09689
H 1.47490 -2.03477 2.44262
C -1.10401 -4.20161 3.40626
H -2.12766 -4.43110 3.06697
H -1.16488 -3.84399 4.44967
H -0.53545 -5.14890 3.41321
C -1.53883 -2.60828 -2.51964
H -2.24328 -1.88827 -2.07069
C -0.50640 -1.80446 -3.34152
H 0.03679 -1.08301 -2.70478
H -0.99806 -1.24096 -4.15452
H 0.24276 -2.47618 -3.79839
C -2.34639 -3.55418 -3.43369
H -1.69605 -4.26789 -3.97041
H -2.89356 -2.97386 -4.19757
H -3.08248 -4.14130 -2.85893
C 3.37316 0.24444 0.08975
C 3.33565 -2.09698 -0.75557
H 2.29054 -1.87317 -0.46651
C 3.33496 -2.50150 -2.23685
H 3.01028 -1.66364 -2.87473
H 2.61974 -3.32940 -2.37030
H 4.32230 -2.84966 -2.58232
C 3.85390 -3.20314 0.17663
H 3.84953 -2.86337 1.22476
H 4.87492 -3.53043 -0.08332
H 3.18478 -4.07506 0.09751
C 5.37466 -0.49509 -0.76667
C 6.36412 -1.39246 -1.44571
H 6.41229 -2.39273 -0.98494
H 7.37153 -0.95286 -1.37779
H 6.13791 -1.53042 -2.51755
C 5.56380 0.79270 -0.30785
C 6.79270 1.64778 -0.33442
H 7.08085 1.99924 0.67217
H 6.66653 2.54029 -0.97426
H 7.64228 1.07595 -0.73810
C 4.15805 2.52764 0.89328
H 4.93798 3.18118 0.46379
C 2.79722 3.16197 0.59591
H 2.63067 3.28244 -0.48493
H 2.74813 4.15753 1.06638
H 1.96486 2.56062 1.00254

C 4.42385 2.36629 2.40086
H 3.65896 1.71794 2.85460
H 4.38526 3.35096 2.89641
H 5.41721 1.92512 2.58984
C 0.28261 0.48934 2.89190

III$_{Cu}$
SCF (BP86) Energy = -2219.65240636
Enthalpy 0K = -2218.566407
Enthalpy 298K = -2218.565463
Free Energy 298K = -2218.733986
Lowest Frequency = 13.1394 cm^{-1}
Second Frequency = 20.5553 cm^{-1}
SCF (BP86-D3BJ) Energy = -2219.98860471
SCF (C6H6) Energy = -2219.65792566
SCF (BS2) Energy = -3031.83544960

Cu 1.46245 -0.25837 -0.82682
Si -3.43954 -1.39852 1.36783
Si -3.54285 2.01260 -0.71684
Al -1.16759 -0.06438 -0.54568
N -1.89771 -1.47722 0.43215
N -1.81740 1.67015 -0.30925
N   3.89792 0.82795 0.55632
N   4.26097 -1.14147 -0.28310
O -1.11106 -0.47084 -2.37228
O   0.99307 -0.85909 -3.17769
C -1.21937 -2.75826 0.40336
C -1.41154 -3.68256 -0.67842
C -0.74599 -4.92575 -0.64313
H -0.90078 -5.62782 -1.47044
C   0.08506 -5.29464 0.41855
H   0.57817 -6.27298 0.42585
C   0.26675 -4.39725 1.47599
H   0.90957 -4.67930 2.31873
C -0.36376 -3.13809 1.49052
C -2.33962 -3.42017 -1.86997
H -2.72509 -2.39205 -1.77066
C -1.60310 -3.52780 -3.22573
H -0.73318 -2.85818 -3.28411
H -2.28813 -3.26010 -4.04925
H -1.25732 -4.56133 -3.40966
C -3.54448 -4.39149 -1.87903
H -3.21097 -5.43603 -2.01460
H -4.22536 -4.14943 -2.71428
H -4.12248 -4.34966 -0.94293
C -0.11817 -2.23007 2.69764
H -0.73188 -1.32578 2.55426
C   1.35558 -1.77727 2.78801
H   2.03460 -2.63902 2.92394
H   1.50220 -1.09901 3.64832
H   1.66417 -1.24522 1.87103
C -0.54986 -2.90306 4.02057
H -1.59681 -3.24771 3.98107
H -0.45057 -2.19945 4.86648
H   0.07710 -3.78360 4.24861
C -4.10921 -3.15662 1.67622
H -4.62420 -3.56726 0.79363
H -4.84265 -3.11406 2.50070
H -3.31428 -3.86335 1.96352
C -3.31486 -0.60951 3.10465
H -2.79008 -1.26918 3.81396
H -4.33977 -0.45748 3.49037
H -2.80940 0.36724 3.11002
C -4.79055 -0.43519 0.41258
H -4.82145 -0.80409 -0.63045
H -5.73473 -0.79587 0.87194
C -4.75681 1.11160 0.45471
H -4.58418 1.46947 1.48758
H -5.75258 1.51303 0.17123
C -3.95407 1.44274 -2.49010
H -3.42661 2.05300 -3.24109
H -5.03905 1.53281 -2.67763
H -3.66562 0.39296 -2.66542
C -3.89332 3.87480 -0.54177
H -3.81486 4.20389 0.50750
H -4.92102 4.08367 -0.88717
H -3.20024 4.49190 -1.13468
C -0.97685 2.81956 -0.07673
C -0.33865 3.51009 -1.16003
C   0.39867 4.68230 -0.89337
H   0.86347 5.21504 -1.73155
C   0.54221 5.18809 0.40360
H   1.10485 6.11116 0.58295
C -0.05834 4.50163 1.46592
H   0.03965 4.89245 2.48601
C -0.81843 3.33547 1.25155
C -0.43369 3.04153 -2.61400
H -1.00707 2.10041 -2.62322
C   0.96289 2.74913 -3.20912
H   1.57075 3.66916 -3.28392
H   0.87138 2.32108 -4.22206
H   1.51943 2.02351 -2.59107
C -1.18016 4.06007 -3.50674
H -2.20266 4.25424 -3.14267
H -1.25439 3.68225 -4.54182
H -0.65022 5.02891 -3.54277
C -1.46543 2.65083 2.45199
H -2.13070 1.87725 2.03458
C -0.41000 1.94158 3.32946
H   0.17161 1.20992 2.74252
H -0.88919 1.40227 4.16601
H   0.29925 2.66966 3.76274
C -2.32136 3.60857 3.30853
H -1.70582 4.38269 3.80077
H -2.84241 3.04910 4.10556
H -3.08342 4.12615 2.70207
C   3.28386 -0.19006 -0.12919
C   3.20006 2.11942 0.80657
H   2.15546 1.90516 0.51464
C   3.20483 2.52426 2.28739
H   2.88898 1.68714 2.93042
H   2.48473 3.34738 2.42071
H   4.19066 2.88144 2.62582
C   3.73415 3.21960 -0.12447
H   3.70532 2.88860 -1.17495
H   4.76840 3.51186 0.12433
H   3.09136 4.10884 -0.02988
C   5.23937 0.52505 0.82900
C   6.19378 1.39077 1.59402
H   6.23181 2.42234 1.20761
H   7.21104 0.97642 1.51774
H   5.94046 1.44554 2.66710
C   5.46651 -0.72658 0.29181
C   6.71485 -1.55365 0.29145
H   7.04930 -1.80427 -0.73078
H   6.58790 -2.50217 0.84378
H   7.53295 -1.00098 0.77788
C   4.12159 -2.40139 -1.06932
H   5.01336 -2.99356 -0.80238
C   2.88490 -3.20028 -0.64784
H   2.88698 -3.41282 0.43185
H   2.86506 -4.15842 -1.19174
H   1.94669 -2.66938 -0.88746
C   4.16110 -2.09960 -2.57717
H   3.26498 -1.53659 -2.88676
H   4.18197 -3.04690 -3.14186
H   5.06143 -1.52004 -2.84349
C   0.19859 -0.55095 -2.27602

TS(III-IV)$_{Cu}$
SCF (BP86) Energy = -2219.63352751
Enthalpy 0K = -2218.549121
Enthalpy 298K = -2218.548175

Free Energy 298K = -2218.718141
Lowest Frequency = -150.2391 cm^{-1}
Second Frequency = -9.7014 cm^{-1}
SCF (BP86-D3BJ) Energy = -2219.95768034
SCF (C6H6) Energy = -2219.63952310
SCF (BS2) Energy = -3031.81488535

Cu	-2.03190	0.36345	-0.98805
Si	3.57067	1.35562	1.59732
Si	3.77463	-2.11516	-0.37686
Al	1.45760	0.04177	-0.51090
N	2.16614	1.44776	0.47324
N	2.02892	-1.70144	-0.21573
N	-4.72110	1.19055	-0.26833
N	-4.29271	-0.80858	0.47518
O	1.23589	0.44378	-2.33504
O	-0.98885	0.74894	-2.65776
C	1.52655	2.73548	0.27999
C	1.87361	3.57814	-0.82737
C	1.20516	4.80927	-0.98592
H	1.47319	5.44813	-1.83517
C	0.22350	5.24126	-0.08908
H	-0.27514	6.20612	-0.23292
C	-0.09989	4.42849	1.00244
H	-0.85547	4.76584	1.72227
C	0.53083	3.18593	1.20735
C	2.97099	3.23471	-1.84040
H	3.33689	2.22181	-1.59779
C	2.45302	3.22304	-3.29714
H	1.62700	2.50936	-3.42694
H	3.26725	2.93181	-3.98463
H	2.10707	4.22587	-3.60625
C	4.16242	4.21692	-1.73269
H	3.85564	5.24110	-2.01124
H	4.97354	3.91534	-2.41909
H	4.57453	4.26356	-0.71238
C	0.14378	2.37856	2.44811
H	0.73365	1.44749	2.42635
C	-1.34723	1.97981	2.45181
H	-2.00308	2.86837	2.49268
H	-1.57950	1.35531	3.33346
H	-1.61364	1.40745	1.54480
C	0.49231	3.14049	3.74782
H	1.55613	3.42989	3.77908
H	0.27835	2.51881	4.63589
H	-0.10285	4.06674	3.83968
C	4.25968	3.10173	1.92227
H	4.90414	3.44844	1.09885
H	4.87198	3.08199	2.84085
H	3.45941	3.84639	2.06116
C	3.17969	0.61591	3.31606
H	2.58492	1.30656	3.93490
H	4.13210	0.43128	3.84605
H	2.63938	-0.34143	3.25952
C	4.98969	0.30545	0.85767
H	5.18172	0.64303	-0.17872
H	5.88136	0.62879	1.43466
C	4.86413	-1.23558	0.92622
H	4.53694	-1.55531	1.93390
H	5.86498	-1.69654	0.78785
C	4.43111	-1.59097	-2.09042
H	3.99459	-2.20214	-2.89672
H	5.52944	-1.70007	-2.13498
H	4.19159	-0.53681	-2.31365
C	4.02225	-3.98324	-0.11363
H	3.82558	-4.26573	0.93405
H	5.06781	-4.25120	-0.34556
H	3.36220	-4.59230	-0.75061
C	1.08997	-2.79420	-0.11213
C	0.56577	-3.44765	-1.27580
C	-0.30866	-4.54244	-1.11436
H	-0.69269	-5.04633	-2.00905
C	-0.68334	-5.01120	0.14968
H	-1.34535	-5.87905	0.24793
C	-0.17879	-4.36799	1.28674
H	-0.45201	-4.73700	2.28280
C	0.70150	-3.27402	1.18124
C	0.93825	-3.03477	-2.70244
H	1.54723	-2.11864	-2.63503
C	-0.30528	-2.70712	-3.56038
H	-0.93825	-3.59986	-3.71451
H	0.00436	-2.34388	-4.55562
H	-0.92523	-1.92240	-3.09911
C	1.78210	-4.12320	-3.40775
H	2.70940	-4.35136	-2.85673
H	2.06307	-3.79427	-4.42407
H	1.21458	-5.06602	-3.50739
C	1.22397	-2.62377	2.45996
H	2.01945	-1.92787	2.14514
C	0.12127	-1.79224	3.15293
H	-0.29321	-1.02926	2.47125
H	0.51699	-1.27324	4.04419
H	-0.71175	-2.43854	3.48278
C	1.83850	-3.63712	3.44912
H	1.08048	-4.33261	3.85189
H	2.28783	-3.10993	4.30924
H	2.62589	-4.24443	2.97182
C	-3.72320	0.24848	-0.19334
C	-4.61443	2.47783	-1.01041
H	-5.55484	3.00899	-0.78639
C	-3.44965	3.33486	-0.49842
H	-3.52691	3.50886	0.58644
H	-3.45696	4.31015	-1.01240
H	-2.47598	2.85662	-0.70140
C	-4.54388	2.22486	-2.52661
H	-5.39651	1.61461	-2.86874
H	-3.60879	1.70328	-2.79138
H	-4.56635	3.18683	-3.06549
C	-5.89759	0.72906	0.33522
C	-7.15578	1.53598	0.42362
H	-7.01368	2.46972	0.99724
H	-7.93918	0.95656	0.93541
H	-7.54882	1.81175	-0.57133
C	-5.63033	-0.54077	0.80510
C	-6.54386	-1.46713	1.54823
H	-6.26003	-1.57702	2.60946
H	-6.56977	-2.47624	1.10431
H	-7.57188	-1.07358	1.52187
C	-3.55144	-2.08615	0.65175
H	-2.51466	-1.81171	0.38279
C	-3.54466	-2.58315	2.10438
H	-3.27732	-1.77288	2.80170
H	-2.78230	-3.37385	2.19227
H	-4.51101	-3.01388	2.41174
C	-4.03261	-3.14850	-0.34972
H	-5.05521	-3.49844	-0.12676
H	-3.35372	-4.01547	-0.30641
H	-4.01409	-2.75007	-1.37697
C	-0.01232	0.46385	-1.89642

IV_{Cu}
SCF (BP86) Energy = -2219.64915385
Enthalpy 0K = -2218.563655
Enthalpy 298K = -2218.562710
Free Energy 298K = -2218.736614
Lowest Frequency = 6.8496 cm^{-1}
Second Frequency = 12.6118 cm^{-1}
SCF (BP86-D3BJ) Energy = -2219.96202696
SCF (C6H6) Energy = -2219.65704470
SCF (BS2) Energy = -3031.83326421

Cu	2.78703	-0.75484	-0.83334
Si	-3.99392	-0.85254	1.84283
Si	-3.60220	2.65757	0.03050

```
Al -1.68077  0.06960 -0.27949
N  -2.82838 -1.15072  0.51170
N  -1.98109  1.88684 -0.05977
N   5.52114 -1.61498 -0.24661
N   5.15837  0.45482  0.31186
O  -1.05622 -0.51107 -1.99049
O   1.12609 -0.87765 -1.63108
C  -2.71374 -2.50931  0.02169
C  -3.48123 -2.93764 -1.10709
C  -3.36371 -4.26736 -1.55534
H  -3.95347 -4.58875 -2.42196
C  -2.51453 -5.18295 -0.92492
H  -2.44181 -6.21418 -1.28749
C  -1.75505 -4.76039  0.17087
H  -1.08121 -5.47056  0.66548
C  -1.83254 -3.44034  0.65678
C  -4.41612 -1.99486 -1.86669
H  -4.38972 -1.02557 -1.33758
C  -3.92632 -1.76230 -3.31504
H  -2.88981 -1.39025 -3.32945
H  -4.57344 -1.02876 -3.82945
H  -3.95977 -2.70018 -3.89852
C  -5.87969 -2.49080 -1.86712
H  -5.97752 -3.45730 -2.39308
H  -6.53331 -1.76578 -2.38419
H  -6.26804 -2.62992 -0.84405
C  -0.95572 -3.05221  1.84896
H  -1.15058 -1.98711  2.06092
C   0.54818 -3.19252  1.52065
H   0.81544 -4.24264  1.30355
H   1.16430 -2.85923  2.37568
H   0.81621 -2.58423  0.64025
C  -1.30500 -3.86493  3.11635
H  -2.36563 -3.74876  3.39607
H  -0.68816 -3.53829  3.97313
H  -1.11958 -4.94356  2.96539
C  -5.04682 -2.41253  2.12616
H  -5.70657 -2.62168  1.26847
H  -5.68224 -2.27043  3.01787
H  -4.42332 -3.30648  2.28750
C  -3.12788 -0.42473  3.49089
H  -2.57443 -1.28974  3.89192
H  -3.87655 -0.12413  4.24591
H  -2.41467  0.40817  3.37777
C  -5.20016  0.57913  1.44715
H  -5.67512  0.37504  0.46865
H  -6.01391  0.46348  2.19353
C  -4.65352  2.02528  1.49970
H  -4.08885  2.19570  2.43647
H  -5.50181  2.74095  1.54213
C  -4.60703  2.33821 -1.56007
H  -4.15450  2.83573 -2.43314
H  -5.63901  2.71675 -1.44946
H  -4.67185  1.26023 -1.78817
C  -3.39113  4.53190  0.29212
H  -2.93758  4.74961  1.27374
H  -4.37864  5.02433  0.25821
H  -2.75120  4.99331 -0.47661
C  -0.83229  2.75917 -0.12550
C  -0.35223  3.27229 -1.37333
C   0.74059  4.16367 -1.37556
H   1.09236  4.56574 -2.33296
C   1.37215  4.55947 -0.19158
H   2.19571  5.28269 -0.21558
C   0.91846  4.03849  1.02771
H   1.40018  4.35238  1.96141
C  -0.16773  3.14498  1.08402
C  -0.98913  2.90926 -2.71680
H  -1.76651  2.15343 -2.51641
C   0.03105  2.28010 -3.69275
H   0.82904  2.99641 -3.96094
H  -0.47320  1.98089 -4.62832
H   0.49956  1.38169 -3.26242
C  -1.66605  4.13445 -3.37496
H  -2.43286  4.58364 -2.72168
H  -2.15328  3.84447 -4.32301
H  -0.92699  4.92207 -3.60839
C  -0.59776  2.57466  2.43449
H  -1.61498  2.17067  2.29258
C   0.31674  1.39159  2.83082
H   0.31828  0.60978  2.05023
H  -0.01342  0.93047  3.77889
H   1.35918  1.73402  2.96381
C  -0.65727  3.62228  3.56471
H   0.34353  4.00882  3.82892
H  -1.08105  3.17251  4.47973
H  -1.28556  4.48511  3.28559
C   4.54569 -0.65178 -0.22164
C   5.31444 -3.00186 -0.74680
H   6.30060 -3.48646 -0.65273
C   4.31246 -3.76024  0.13768
H   4.62882 -3.75642  1.19364
H   4.23450 -4.80689 -0.20019
H   3.31024 -3.30309  0.07495
C   4.91601 -3.00084 -2.23150
H   5.65081 -2.45125 -2.84243
H   3.92640 -2.53204 -2.37377
H   4.85877 -4.03803 -2.60125
C   6.72907 -1.12298  0.26269
C   7.97681 -1.94283  0.37423
H   7.84654 -2.81482  1.04008
H   8.79122 -1.33292  0.79360
H   8.32021 -2.31858 -0.60628
C   6.50241  0.19353  0.61464
C   7.45908  1.17262  1.22351
H   7.21802  1.39402  2.27778
H   7.48191  2.13069  0.67843
H   8.47929  0.75949  1.19949
C   4.42435  1.74592  0.43062
H   3.38379  1.46048  0.18845
C   4.43360  2.30672  1.85976
H   4.16954  1.52809  2.59380
H   3.67578  3.10432  1.92262
H   5.40551  2.74460  2.13921
C   4.88713  2.75873 -0.62805
H   5.90350  3.13974 -0.43075
H   4.19403  3.61566 -0.62619
H   4.86861  2.30762 -1.63331
C  -0.01712 -0.51264 -1.16979
```

TS(IV-A)$_{Cu}$

SCF (BP86) Energy = -2219.64383775
Enthalpy 0K = -2218.559528
Enthalpy 298K = -2218.558584
Free Energy 298K = -2218.733297
Lowest Frequency = -57.1257 cm^{-1}
Second Frequency = 5.7700 cm^{-1}
SCF (BP86-D3BJ) Energy = -2219.95123059
SCF (C6H6) Energy = -2219.65231738
SCF (BS2) Energy = -3031.82957902

```
Cu  2.98583  0.66929 -0.52091
Si -3.43716 -2.20772  1.68637
Si -4.86186  0.90682 -0.35522
Al -1.76971 -0.08594 -0.14730
N  -2.10175 -1.76166  0.57405
N  -3.10140  1.19867 -0.18886
N   5.63670 -0.48537 -0.86799
N   5.63404  1.15928  0.55555
O  -0.59445 -0.12549 -1.67746
O   1.21227  0.95147 -0.85682
C  -1.11681 -2.77042  0.25503
C  -1.24729 -3.55286 -0.93647
C  -0.28179 -4.53616 -1.22583
```

H	-0.39017	-5.13286	-2.13938
C	0.80458	-4.77174	-0.37591
H	1.53666	-5.55201	-0.61268
C	0.93857	-3.99979	0.78356
H	1.78676	-4.17866	1.45578
C	0.00365	-2.99920	1.11641
C	-2.39845	-3.35110	-1.92339
H	-3.05421	-2.57338	-1.49321
C	-1.88748	-2.84194	-3.29132
H	-1.30323	-1.91497	-3.17840
H	-2.73545	-2.64396	-3.97165
H	-1.24196	-3.59597	-3.77760
C	-3.24397	-4.63159	-2.10624
H	-2.64810	-5.44868	-2.55110
H	-4.09622	-4.43866	-2.78184
H	-3.64555	-4.99918	-1.14689
C	0.22448	-2.19637	2.40003
H	-0.59201	-1.45745	2.46295
C	1.55588	-1.41233	2.37195
H	2.42436	-2.09271	2.30659
H	1.67017	-0.81115	3.29211
H	1.59270	-0.72596	1.50830
C	0.16140	-3.09249	3.65830
H	-0.79516	-3.63741	3.72437
H	0.27358	-2.48680	4.57564
H	0.97063	-3.84484	3.65560
C	-3.43739	-4.09371	1.94876
H	-3.73048	-4.63090	1.03177
H	-4.16088	-4.35547	2.74062
H	-2.44717	-4.47108	2.25052
C	-3.27788	-1.36829	3.39562
H	-2.42610	-1.76896	3.96911
H	-4.19394	-1.54199	3.98868
H	-3.14060	-0.27754	3.30688
C	-5.15435	-1.73470	0.98995
H	-5.25133	-2.15560	-0.02898
H	-5.86468	-2.31865	1.61242
C	-5.55674	-0.24064	1.01004
H	-5.33626	0.21053	1.99638
H	-6.65749	-0.15216	0.89271
C	-5.28567	0.08894	-2.02851
H	-5.10676	0.77299	-2.87377
H	-6.34835	-0.21230	-2.05440
H	-4.67919	-0.81736	-2.19997
C	-5.79009	2.56104	-0.19505
H	-5.69695	2.97062	0.82493
H	-6.86362	2.41059	-0.40400
H	-5.40740	3.32282	-0.89264
C	-2.62406	2.56600	-0.22113
C	-2.35542	3.23374	-1.45790
C	-1.90021	4.56772	-1.43236
H	-1.70058	5.07621	-2.38297
C	-1.69254	5.25328	-0.23162
H	-1.33752	6.28982	-0.23767
C	-1.94311	4.59548	0.97795
H	-1.77688	5.12424	1.92383
C	-2.41011	3.26834	1.00784
C	-2.54203	2.56157	-2.82026
H	-2.81471	1.50994	-2.63062
C	-1.23961	2.56075	-3.65284
H	-0.91529	3.58827	-3.89797
H	-1.39929	2.02759	-4.60708
H	-0.42244	2.05626	-3.11513
C	-3.68654	3.21984	-3.62578
H	-4.64334	3.19872	-3.07726
H	-3.83387	2.69943	-4.58935
H	-3.45789	4.27725	-3.85056
C	-2.63636	2.59357	2.36027
H	-3.20108	1.66668	2.15785
C	-1.28598	2.18856	2.99679
H	-0.70703	1.53559	2.31984
H	-1.44000	1.65219	3.95069
H	-0.66835	3.08144	3.20342
C	-3.46847	3.44901	3.33849
H	-2.93650	4.36932	3.63901
H	-3.68189	2.88025	4.26093
H	-4.43126	3.75198	2.89294
C	4.81167	0.43024	-0.26937
C	5.17660	-1.50584	-1.85217
H	6.08972	-2.05662	-2.13356
C	4.19294	-2.49181	-1.20328
H	4.63165	-2.96353	-0.30884
H	3.92991	-3.28429	-1.92267
H	3.25913	-1.98559	-0.90477
C	4.60532	-0.83824	-3.11359
H	5.32897	-0.13494	-3.55773
H	3.67827	-0.28546	-2.88117
H	4.36198	-1.61008	-3.86232
C	6.95757	-0.33708	-0.42881
C	8.08774	-1.20000	-0.89736
H	7.93651	-2.26332	-0.63851
H	9.02784	-0.88047	-0.42277
H	8.23460	-1.13925	-1.99051
C	6.96044	0.70899	0.47367
C	8.11508	1.26329	1.25111
H	8.05530	1.01669	2.32564
H	8.19391	2.35954	1.16435
H	9.05669	0.83882	0.87011
C	5.09627	2.29918	1.34745
H	4.00624	2.21542	1.17705
C	5.35065	2.14482	2.85459
H	5.04743	1.14566	3.20655
H	4.74954	2.89327	3.39674
H	6.40557	2.31177	3.12547
C	5.55695	3.65180	0.78062
H	6.63684	3.82254	0.92506
H	5.02001	4.46529	1.29606
H	5.33179	3.72080	-0.29580
C	0.05126	0.44575	-0.67376

A_{Cu}

SCF (BP86) Energy = -2219.65595776
Enthalpy 0K = -2218.570426
Enthalpy 298K = -2218.569482
Free Energy 298K = -2218.744187
Lowest Frequency = 9.0803 cm^{-1}
Second Frequency = 10.6532 cm^{-1}
SCF (BP86-D3BJ) Energy = -2219.96727440
SCF (C6H6) Energy = -2219.66269536
SCF (BS2) Energy = -3031.84001718

Cu	-2.86512	0.23896	-0.88656
Si	4.22211	-1.86937	-0.45325
Si	4.03310	1.66209	1.40520
Al	1.63208	0.06107	-0.13000
N	2.47220	-1.58938	-0.16704
N	2.53781	1.57557	0.41875
N	-5.07048	-1.16266	0.40876
N	-5.65972	0.81424	-0.27880
O	-0.25017	-0.06607	0.34300
O	-1.17002	0.51997	-1.65862
C	1.60021	-2.73777	-0.06264
C	1.28145	-3.27350	1.22587
C	0.42850	-4.38966	1.32111
H	0.19395	-4.79672	2.31208
C	-0.11093	-4.99729	0.18083
H	-0.75646	-5.87826	0.27257
C	0.19971	-4.47292	-1.07891
H	-0.21551	-4.94669	-1.97650
C	1.04098	-3.35175	-1.22878
C	1.83030	-2.65662	2.51278
H	2.56327	-1.88976	2.20665
C	0.71412	-1.94807	3.31481
H	0.20222	-1.18775	2.70235

H	1.12912	-1.45373	4.21173
H	-0.04644	-2.67419	3.65558
C	2.56633	-3.68528	3.39900
H	1.88068	-4.46547	3.77541
H	3.01209	-3.18790	4.27863
H	3.37524	-4.19328	2.84717
C	1.33427	-2.85033	-2.64526
H	1.94354	-1.93587	-2.54562
C	0.04906	-2.47236	-3.41638
H	-0.61594	-3.34523	-3.54682
H	0.30532	-2.10008	-4.42433
H	-0.51427	-1.68037	-2.89843
C	2.15019	-3.88551	-3.45512
H	3.09832	-4.14569	-2.95563
H	2.39003	-3.49204	-4.45924
H	1.58034	-4.82213	-3.59237
C	4.60455	-3.72311	-0.25082
H	4.51155	-4.03662	0.80247
H	5.64058	-3.92592	-0.57373
H	3.92894	-4.35802	-0.84553
C	4.74967	-1.30021	-2.19805
H	4.31195	-1.93658	-2.98433
H	5.84886	-1.34304	-2.30079
H	4.43783	-0.26058	-2.39802
C	5.33284	-0.94412	0.79979
H	5.03097	-1.23967	1.82279
H	6.33346	-1.40256	0.65173
C	5.44760	0.59450	0.68451
H	5.61822	0.89836	-0.36597
H	6.34814	0.94046	1.23431
C	3.74354	1.07324	3.19912
H	3.10906	1.77850	3.76036
H	4.70627	0.98594	3.73417
H	3.25392	0.08495	3.23024
C	4.65889	3.45924	1.43801
H	5.00043	3.78292	0.44070
H	5.51196	3.54490	2.13352
H	3.87761	4.16423	1.76412
C	1.90587	2.81698	0.02145
C	0.98988	3.48752	0.89224
C	0.39854	4.69517	0.47070
H	-0.29799	5.20810	1.14490
C	0.67588	5.25106	-0.78257
H	0.20510	6.19129	-1.09033
C	1.56210	4.58798	-1.63840
H	1.77795	5.01337	-2.62556
C	2.18746	3.38422	-1.26214
C	0.61851	2.94159	2.27278
H	1.14979	1.98290	2.39573
C	-0.89502	2.65003	2.38943
H	-1.49336	3.57012	2.26047
H	-1.13060	2.23675	3.38695
H	-1.21128	1.91612	1.63063
C	1.07125	3.89115	3.40571
H	2.15648	4.08598	3.36904
H	0.83513	3.45881	4.39482
H	0.55828	4.86746	3.33913
C	3.12803	2.70582	-2.25882
H	3.59045	1.85347	-1.73002
C	2.34422	2.14422	-3.46823
H	1.54714	1.45527	-3.14265
H	3.01853	1.60166	-4.15532
H	1.86604	2.95927	-4.04081
C	4.26575	3.63692	-2.73205
H	3.87622	4.49986	-3.30104
H	4.95984	3.09173	-3.39608
H	4.84682	4.03479	-1.88275
C	-4.59398	-0.05140	-0.23449
C	-4.24806	-2.37438	0.69316
H	-4.94370	-3.07872	1.17987
C	-3.74380	-3.01171	-0.61066
H	-4.57896	-3.26393	-1.28527
H	-3.17832	-3.92912	-0.38078
H	-3.06044	-2.32499	-1.14051
C	-3.10960	-2.04809	1.67202
H	-3.50081	-1.60984	2.60545
H	-2.38671	-1.34173	1.22667
H	-2.55927	-2.97087	1.91834
C	-6.41235	-0.99988	0.77057
C	-7.20920	-2.04649	1.48552
H	-7.30392	-2.97530	0.89477
H	-8.22816	-1.67859	1.67967
H	-6.76490	-2.31448	2.46059
C	-6.79122	0.25595	0.33609
C	-8.13258	0.91380	0.44910
H	-8.64010	1.00537	-0.52723
H	-8.07244	1.92288	0.88952
H	-8.78570	0.31356	1.10119
C	-5.50978	2.16816	-0.87724
H	-4.48597	2.13177	-1.29519
C	-6.48607	2.41023	-2.03853
H	-6.45746	1.57654	-2.75880
H	-6.19111	3.33024	-2.56975
H	-7.52457	2.54676	-1.69611
C	-5.53892	3.27214	0.19202
H	-6.53669	3.39246	0.64591
H	-5.26702	4.23510	-0.27127
H	-4.81168	3.05910	0.99155
C	-0.14325	0.30511	-0.93236

TS(III-S)$_{Cu}$

SCF (BP86) Energy = -2219.64619075
Enthalpy 0K = -2218.561456
Enthalpy 298K = -2218.560511
Free Energy 298K = -2218.729162
Lowest Frequency = -50.7251 cm^{-1}
Second Frequency = 14.9841 cm^{-1}
SCF (BP86-D3BJ) Energy = -2219.97072098
SCF (C6H6) Energy = -2219.65301778
SCF (BS2) Energy = -3031.83061770

Cu	1.93063	-0.39169	-0.72878
Si	-3.56631	-1.32424	1.65298
Si	-3.80634	2.12619	-0.35039
Al	-1.46941	-0.01441	-0.46150
N	-2.16302	-1.40800	0.51369
N	-2.05607	1.71408	-0.21511
N	4.34711	0.80863	0.55520
N	4.75229	-1.16397	-0.25571
O	-0.78245	-0.43056	-2.04125
O	1.07056	-1.19989	-3.02496
C	-1.58895	-2.72001	0.26427
C	-1.94854	-3.47056	-0.90038
C	-1.37386	-4.74306	-1.09225
H	-1.65011	-5.31702	-1.98386
C	-0.46679	-5.29061	-0.17992
H	-0.03879	-6.28425	-0.35165
C	-0.11574	-4.55241	0.95523
H	0.59359	-4.97518	1.67671
C	-0.65746	-3.27528	1.19812
C	-2.94366	-2.97235	-1.95345
H	-3.20563	-1.93029	-1.69485
C	-2.34281	-2.97054	-3.37771
H	-1.41773	-2.37681	-3.42471
H	-3.06825	-2.53968	-4.09099
H	-2.12076	-3.99735	-3.71970
C	-4.25092	-3.79962	-1.93665
H	-4.05121	-4.85847	-2.17977
H	-4.96191	-3.41297	-2.68828
H	-4.74756	-3.77385	-0.95288
C	-0.22988	-2.53579	2.46863
H	-0.77558	-1.57838	2.48756
C	1.27664	-2.19963	2.46588
H	1.89426	-3.11536	2.44568

H	1.54951	-1.63070	3.37322
H	1.54817	-1.59083	1.58296
C	-0.59553	-3.32411	3.74723
H	-1.67253	-3.55758	3.79242
H	-0.33254	-2.74478	4.65060
H	-0.04848	-4.28233	3.79868
C	-4.23904	-3.07815	1.95420
H	-4.76274	-3.47910	1.07196
H	-4.95979	-3.04664	2.79016
H	-3.43967	-3.78902	2.21678
C	-3.14668	-0.58533	3.36272
H	-2.54852	-1.27907	3.97469
H	-4.08819	-0.38727	3.90662
H	-2.59688	0.36594	3.29052
C	-4.99649	-0.27773	0.93131
H	-5.20993	-0.62380	-0.09788
H	-5.87668	-0.59516	1.52866
C	-4.86832	1.26400	0.98482
H	-4.51998	1.59265	1.98245
H	-5.87146	1.72426	0.86304
C	-4.48674	1.57464	-2.04553
H	-4.03971	2.15325	-2.86981
H	-5.58224	1.71030	-2.08712
H	-4.28019	0.50779	-2.24311
C	-4.03316	3.99969	-0.12332
H	-3.78672	4.30976	0.90576
H	-5.08628	4.26869	-0.31616
H	-3.39828	4.58417	-0.80746
C	-1.10800	2.80742	-0.16127
C	-0.59800	3.41842	-1.35116
C	0.27503	4.51971	-1.23265
H	0.65090	4.99476	-2.14613
C	0.66339	5.02529	0.01264
H	1.32486	5.89670	0.07666
C	0.18082	4.41235	1.17588
H	0.47396	4.80667	2.15606
C	-0.70048	3.31617	1.11399
C	-0.97154	2.94503	-2.75776
H	-1.57832	2.03100	-2.65078
C	0.27417	2.57384	-3.59301
H	0.91308	3.45515	-3.78376
H	-0.03145	2.16520	-4.57156
H	0.88340	1.80757	-3.08874
C	-1.81501	4.00207	-3.50897
H	-2.74014	4.25814	-2.96564
H	-2.09966	3.62848	-4.50861
H	-1.24608	4.93817	-3.65334
C	-1.19491	2.68684	2.41508
H	-2.02927	2.02068	2.13779
C	-0.09432	1.81145	3.05642
H	0.25785	1.03203	2.35726
H	-0.46571	1.30846	3.96711
H	0.77830	2.42499	3.34288
C	-1.72802	3.71908	3.43100
H	-0.92790	4.38002	3.80936
H	-2.16582	3.20545	4.30501
H	-2.50716	4.36120	2.98660
C	3.74123	-0.25603	-0.06441
C	3.59334	2.06743	0.80192
H	2.54740	1.77314	0.59694
C	3.67775	2.54335	2.25913
H	3.44972	1.72440	2.96046
H	2.93059	3.33992	2.40783
H	4.66451	2.96305	2.51266
C	3.98250	3.15246	-0.21498
H	3.90817	2.76262	-1.24286
H	5.00712	3.52902	-0.05390
H	3.28447	4.00000	-0.12157
C	5.71819	0.57965	0.74487
C	6.67410	1.51992	1.41373
H	6.63407	2.53571	0.98649
H	7.70474	1.15381	1.28635
H	6.48798	1.60708	2.49864
C	5.97153	-0.67593	0.22890
C	7.25604	-1.44344	0.17111
H	7.54516	-1.69731	-0.86427
H	7.20558	-2.38675	0.74438
H	8.07283	-0.84435	0.60187
C	4.60758	-2.45110	-0.99543
H	5.57085	-2.96746	-0.84488
C	3.49902	-3.32453	-0.39467
H	3.67063	-3.50805	0.67824
H	3.47340	-4.29416	-0.91860
H	2.50754	-2.85392	-0.51426
C	4.41226	-2.19662	-2.50015
H	3.42813	-1.73826	-2.70340
H	4.45607	-3.15643	-3.04239
H	5.20509	-1.54036	-2.89751
C	0.55324	-0.70596	-2.01166

S_{Cu}

SCF (BP86) Energy = -2219.69501398
Enthalpy 0K = -2218.609133
Enthalpy 298K = -2218.608189
Free Energy 298K = -2218.783086
Lowest Frequency = 5.2966 cm^{-1}
Second Frequency = 10.1637 cm^{-1}
SCF (BP86-D3BJ) Energy = -2220.00288130
SCF (C6H6) Energy = -2219.70253794
SCF (BS2) Energy = -3031.87939786

Cu	2.65331	-0.16598	-0.08707
Si	-4.16667	-1.50642	1.16516
Si	-4.05427	1.82104	-1.02515
Al	-1.55442	0.02393	-0.00076
N	-2.52880	-1.48426	0.43251
N	-2.38888	1.62656	-0.38606
N	5.38112	0.64757	0.64091
N	5.42326	-1.01691	-0.75196
O	0.06467	0.28920	0.99679
O	-0.02053	-0.39745	-1.08098
C	-1.84656	-2.74767	0.24550
C	-1.93285	-3.42648	-1.01189
C	-1.27363	-4.65878	-1.18064
H	-1.34496	-5.17112	-2.14755
C	-0.53646	-5.24291	-0.14475
H	-0.03916	-6.20825	-0.29133
C	-0.44441	-4.57577	1.08117
H	0.13398	-5.02628	1.89673
C	-1.07794	-3.33572	1.30039
C	-2.70180	-2.84348	-2.19800
H	-3.19849	-1.92707	-1.83362
C	-1.74289	-2.44022	-3.34273
H	-0.97001	-1.74045	-2.98621
H	-2.30013	-1.96045	-4.16773
H	-1.23088	-3.32731	-3.75823
C	-3.79842	-3.79780	-2.72024
H	-3.36599	-4.73085	-3.12378
H	-4.37057	-3.32013	-3.53545
H	-4.50845	-4.07912	-1.92419
C	-0.91741	-2.67641	2.67279
H	-1.41022	-1.69103	2.62071
C	0.56591	-2.43567	3.03459
H	1.12370	-3.38624	3.11436
H	0.64285	-1.92272	4.01007
H	1.05906	-1.80342	2.27921
C	-1.60491	-3.50189	3.78546
H	-2.67771	-3.65489	3.58096
H	-1.51291	-2.99321	4.76208
H	-1.14174	-4.50012	3.88489
C	-4.78869	-3.30253	1.27454
H	-4.99014	-3.71942	0.27380
H	-5.73041	-3.33386	1.84999
H	-4.06229	-3.96726	1.76840

C	-4.17091	-0.74183	2.91518
H	-3.61468	-1.36779	3.63189
H	-5.20627	-0.63987	3.28716
H	-3.71385	0.26237	2.92430
C	-5.45146	-0.54553	0.12176
H	-5.44427	-0.95676	-0.90584
H	-6.42741	-0.85779	0.54988
C	-5.37158	0.99934	0.09368
H	-5.26303	1.40521	1.11770
H	-6.33240	1.41265	-0.27947
C	-4.23476	1.06071	-2.76773
H	-3.66258	1.63001	-3.51839
H	-5.29473	1.05966	-3.07945
H	-3.87797	0.01707	-2.79762
C	-4.49084	3.67213	-1.10982
H	-4.59199	4.10734	-0.10176
H	-5.45458	3.80129	-1.63275
H	-3.72765	4.25774	-1.64640
C	-1.57305	2.81317	-0.23552
C	-0.81258	3.33083	-1.33247
C	-0.04947	4.50182	-1.14916
H	0.52176	4.89970	-1.99656
C	-0.00495	5.16653	0.08075
H	0.59038	6.07890	0.19869
C	-0.73284	4.64861	1.15760
H	-0.69781	5.15862	2.12782
C	-1.51703	3.48692	1.02632
C	-0.79399	2.66649	-2.71155
H	-1.37982	1.73527	-2.63293
C	0.63651	2.27969	-3.15080
H	1.28058	3.17032	-3.26514
H	0.61011	1.76143	-4.12610
H	1.10407	1.60268	-2.41839
C	-1.45269	3.56190	-3.78681
H	-2.49250	3.82085	-3.52624
H	-1.46374	3.05093	-4.76648
H	-0.89738	4.50899	-3.91152
C	-2.26714	2.97290	2.25546
H	-2.85799	2.10118	1.92330
C	-1.28682	2.49309	3.35128
H	-0.59433	1.73121	2.95875
H	-1.83861	2.06155	4.20601
H	-0.68312	3.33520	3.73626
C	-3.25057	4.01780	2.82772
H	-2.72020	4.91397	3.19671
H	-3.81413	3.59417	3.67807
H	-3.97809	4.35265	2.06916
C	4.56520	-0.19322	-0.07393
C	4.79579	1.72738	1.48423
H	3.71091	1.51800	1.42401
C	5.21568	1.61577	2.95762
H	5.06119	0.59235	3.33609
H	4.59303	2.29821	3.55921
H	6.26802	1.89956	3.12082
C	5.03710	3.11873	0.87776
H	4.70514	3.14915	-0.17234
H	6.09711	3.42001	0.92174
H	4.45474	3.86619	1.44124
C	6.73509	0.36008	0.41217
C	7.89363	1.06835	1.04538
H	7.83295	2.16292	0.92813
H	8.83251	0.74195	0.57197
H	7.97846	0.85254	2.12479
C	6.75791	-0.70121	-0.47326
C	7.92363	-1.43280	-1.06270
H	7.93191	-1.38493	-2.16628
H	7.93719	-2.49918	-0.77397
H	8.86627	-0.98828	-0.70902
C	4.97313	-2.10657	-1.66151
H	5.90220	-2.57331	-2.02975
C	4.16451	-3.16249	-0.89117
H	4.73386	-3.55657	-0.03334
H	3.91343	-4.00154	-1.56076
H	3.21958	-2.73254	-0.51462
C	4.20160	-1.53292	-2.86093
H	3.25895	-1.06379	-2.52825
H	3.95013	-2.34367	-3.56456
H	4.79787	-0.77604	-3.39666
C	0.75524	-0.08929	-0.06108

TS(S-E)$_{Cu}$

SCF (BP86) Energy = -2219.63255726
Enthalpy 0K = -2218.548927
Enthalpy 298K = -2218.547983
Free Energy 298K = -2218.721122
Lowest Frequency = -186.5620 cm^{-1}
Second Frequency = 8.3311 cm^{-1}
SCF (BP86-D3BJ) Energy = -2219.95402622
SCF (C6H6) Energy = -2219.63803473
SCF (BS2) Energy = -3031.82201944

Cu	2.48199	-0.29072	-0.98686
Si	-3.33873	-1.75167	1.88328
Al	-1.34290	-0.04120	-0.04760
Si	-4.16835	1.55536	-0.41396
N	-2.11433	-1.61048	0.57523
N	-2.39610	1.48576	-0.10648
O	0.31297	-1.30717	-2.85963
N	4.54151	1.42152	0.29467
O	0.30506	0.02671	-0.53947
N	5.24496	-0.60030	-0.07077
C	1.08125	-0.89868	-2.07308
C	4.13985	0.20905	-0.19946
C	6.32552	0.09775	0.48972
C	-0.40503	-3.45188	0.65646
C	-1.53053	-2.82533	0.03457
C	5.87435	1.38291	0.71914
C	-1.23324	3.45693	-1.14706
C	-1.69257	2.74779	0.00675
C	-2.07355	-3.40413	-1.15800
C	-1.41275	2.92267	-2.56773
H	-2.02325	2.00783	-2.49657
C	0.21067	-2.93902	1.95854
H	-0.37835	-2.06334	2.27635
C	-1.45282	3.30811	1.30351
C	0.13591	-4.00490	3.07653
H	-0.89355	-4.37369	3.22204
H	0.49326	-3.59093	4.03647
H	0.76605	-4.88047	2.83811
C	-2.62855	-1.66648	3.65598
H	-2.06614	-2.56882	3.94216
H	-3.46678	-1.55569	4.36818
H	-1.96572	-0.79432	3.78633
C	3.66701	2.62691	0.34470
H	4.26953	3.39211	0.86320
C	-4.25741	-3.40992	1.71005
H	-4.94357	-3.40369	0.84731
H	-4.85704	-3.59819	2.61772
H	-3.55937	-4.25296	1.58056
C	0.16366	-4.59654	0.06263
H	1.02948	-5.06802	0.54300
C	-4.62198	-0.33627	1.80001
H	-5.47527	-0.72765	2.39172
H	-4.25380	0.53227	2.37804
C	-0.05415	2.52371	-3.18648
H	0.60599	3.40332	-3.29648
H	-0.19603	2.08165	-4.18879
H	0.45088	1.78408	-2.54519
C	-4.85778	3.17053	0.32312
H	-4.80234	3.17000	1.42462
H	-5.91838	3.28449	0.03823
H	-4.30982	4.05457	-0.04091
C	-1.87699	2.58255	2.58027
H	-2.60260	1.80850	2.27785

C	7.67110	-0.48407	0.79987
H	7.63625	-1.19939	1.64041
H	8.36602	0.32101	1.08509
H	8.11575	-1.00665	-0.06338
C	-0.34887	-5.14459	-1.11733
H	0.11116	-6.03235	-1.56492
C	-0.56090	4.68483	-0.98039
H	-0.21332	5.22186	-1.87082
C	-4.64841	1.48778	-2.26083
H	-4.38907	2.40583	-2.81065
H	-5.74177	1.34689	-2.34202
H	-4.16556	0.63601	-2.76968
C	6.58988	2.55732	1.31115
H	6.62089	3.41860	0.62024
H	7.63097	2.28679	1.54474
H	6.12246	2.90090	2.25155
C	1.66884	-2.46804	1.76750
H	2.31664	-3.29956	1.43496
H	2.08043	-2.07958	2.71713
H	1.71877	-1.66369	1.01219
C	-1.46456	-4.54669	-1.71165
H	-1.87797	-4.97497	-2.63199
C	-0.77690	4.53836	1.41600
H	-0.60273	4.96161	2.41191
C	-5.08850	0.08497	0.38955
H	-6.14409	0.42634	0.41405
H	-5.08528	-0.77362	-0.30770
C	-0.33173	5.23411	0.28552
H	0.18130	6.19660	0.39065
C	3.35638	3.12643	-1.07490
H	2.78635	2.36540	-1.63453
H	4.27966	3.35475	-1.63384
H	2.73659	4.03611	-1.02059
C	-3.30009	-2.82374	-1.86475
H	-3.70816	-2.04202	-1.20176
C	-0.67010	1.85943	3.22180
H	-0.20536	1.14337	2.51997
H	-0.97383	1.30584	4.12854
H	0.11113	2.58400	3.51383
C	-2.56493	3.50200	3.61112
H	-1.86661	4.24571	4.03472
H	-2.95414	2.90628	4.45549
H	-3.40785	4.05396	3.16256
C	-2.14997	3.92680	-3.48189
H	-3.11135	4.25043	-3.04779
H	-2.35228	3.47466	-4.46890
H	-1.54577	4.83533	-3.65518
C	-2.92846	-2.15382	-3.20703
H	-2.49846	-2.88986	-3.90966
H	-2.17488	-1.36069	-3.07645
H	-3.82388	-1.71641	-3.68466
C	2.40073	2.35629	1.16801
H	1.81794	3.28730	1.26270
H	2.65838	1.99628	2.17823
H	1.75111	1.60842	0.67761
C	-4.40382	-3.88164	-2.09106
H	-5.31368	-3.40650	-2.49906
H	-4.67425	-4.39800	-1.15530
H	-4.08594	-4.65224	-2.81575
C	5.22155	-1.99922	-0.57474
H	4.15910	-2.13504	-0.85210
C	5.56599	-3.02872	0.51206
H	6.63507	-3.02124	0.77944
H	5.32833	-4.03826	0.13748
H	4.97074	-2.85468	1.42272
C	6.05965	-2.15284	-1.85453
H	5.75228	-1.41153	-2.60965
H	5.90165	-3.15931	-2.27669
H	7.14038	-2.03685	-1.66739

E_{Cu}

SCF (BP86) Energy = -2219.65120583

Enthalpy 0K = -2218.566535
Enthalpy 298K = -2218.565591
Free Energy 298K = -2218.741088
Lowest Frequency = 9.2641 cm^{-1}
Second Frequency = 14.9714 cm^{-1}
SCF (BP86-D3BJ) Energy = -2219.97805876
SCF (C6H6) Energy = -2219.65550997
SCF (BS2) Energy = -3031.84368962

Cu	1.91959	-0.33279	1.04204
Si	-2.86120	2.79438	-1.37679
Al	-1.29464	0.20585	-0.04038
Si	-4.44039	-0.48928	0.64853
N	-1.51714	1.99171	-0.50078
N	-2.76378	-0.91011	0.16795
O	2.41612	0.27594	3.91686
N	3.86534	-2.10054	-0.50316
O	0.27068	-0.43870	0.10315
N	4.72554	-0.16493	-0.04117
C	2.10398	0.11387	2.80592
C	3.56947	-0.89963	0.08567
C	5.73279	-0.89697	-0.69191
C	0.69246	3.07318	-1.00017
C	-0.38978	2.81072	-0.10381
C	5.17978	-2.12554	-0.98769
C	-2.15327	-3.21800	0.95179
C	-2.47058	-2.30504	-0.10130
C	-0.34514	3.35067	1.22240
C	-2.09266	-2.78559	2.41686
H	-2.50586	-1.76635	2.47008
C	0.72964	2.50752	-2.41997
H	-0.26805	2.08837	-2.62387
C	-2.48375	-2.77988	-1.45257
C	1.02523	3.58871	-3.48228
H	0.34036	4.44970	-3.39724
H	0.92389	3.16793	-4.49822
H	2.05538	3.97827	-3.39307
C	-2.60285	3.00430	-3.25871
H	-1.80372	3.71900	-3.51051
H	-3.54171	3.38853	-3.69815
H	-2.37350	2.04494	-3.75315
C	2.90837	-3.23681	-0.62540
H	3.49181	-4.04485	-1.09886
C	-3.14531	4.53418	-0.65167
H	-3.57764	4.49056	0.36193
H	-3.84423	5.09873	-1.29324
H	-2.20388	5.10472	-0.59212
C	1.78113	3.84895	-0.55280
H	2.60692	4.05119	-1.24479
C	-4.46695	1.78392	-1.20256
H	-5.24953	2.45795	-1.60602
H	-4.44200	0.92876	-1.90508
C	-0.63282	-2.70717	2.91602
H	-0.14530	-3.69811	2.87737
H	-0.59544	-2.35287	3.96226
H	-0.05501	-2.01091	2.28487
C	-5.66376	-1.60664	-0.29157
H	-5.67939	-1.37729	-1.37018
H	-6.68542	-1.46152	0.10072
H	-5.40409	-2.67188	-0.17802
C	-2.78763	-1.84553	-2.62450
H	-3.26627	-0.94699	-2.19769
C	7.11100	-0.39941	-1.00658
H	7.11355	0.36421	-1.80409
H	7.73559	-1.23726	-1.35392
H	7.61367	0.03652	-0.12679
C	1.83054	4.36815	0.74600
H	2.68162	4.97796	1.06981
C	-1.84705	-4.55642	0.63416
H	-1.59895	-5.25035	1.44583
C	-4.82811	-0.65509	2.51320
H	-4.84942	-1.69889	2.86321

H -5.82769 -0.22191 2.70122
H -4.10445 -0.09987 3.13434
C 5.78378 -3.29999 -1.69352
H 5.80029 -4.20608 -1.06155
H 6.82482 -3.07698 -1.97363
H 5.24231 -3.55200 -2.62298
C 1.73821 1.34224 -2.53336
H 2.76868 1.69550 -2.34393
H 1.71652 0.90752 -3.54951
H 1.50045 0.55392 -1.79940
C 0.76856 4.11340 1.62267
H 0.79992 4.52290 2.63846
C -2.16840 -4.12632 -1.71717
H -2.17663 -4.48261 -2.75355
C -4.82162 1.33160 0.23329
H -5.91202 1.42014 0.41415
H -4.35596 1.98701 0.99451
C -1.85042 -5.01837 -0.68633
H -1.61503 -6.06483 -0.91004
C 2.46200 -3.71834 0.76250
H 1.89193 -2.93018 1.28184
H 3.32567 -4.00042 1.38823
H 1.79848 -4.59204 0.65620
C -1.46571 3.07580 2.22643
H -2.34736 2.76815 1.63837
C -1.48048 -1.39030 -3.31526
H -0.77802 -0.92471 -2.59992
H -1.68894 -0.66209 -4.11981
H -0.95582 -2.25276 -3.76430
C -3.76193 -2.45178 -3.65602
H -3.31743 -3.30911 -4.19212
H -4.03006 -1.69840 -4.41766
H -4.69138 -2.80189 -3.17662
C -2.93204 -3.69662 3.33925
H -3.97132 -3.79724 2.98240
H -2.95822 -3.28845 4.36506
H -2.50704 -4.71421 3.40400
C -1.09746 1.89162 3.15005
H -0.21882 2.13756 3.77238
H -0.83714 0.98491 2.57112
H -1.93416 1.63787 3.82551
C 1.73050 -2.86768 -1.53853
H 1.07312 -3.74428 -1.66426
H 2.09168 -2.55618 -2.53355
H 1.13197 -2.04990 -1.09582
C -1.86343 4.30945 3.06245
H -2.74741 4.08019 3.68317
H -2.10993 5.17045 2.41890
H -1.05875 4.62255 3.75125
C 4.83515 1.19420 0.55054
H 3.78784 1.44517 0.79690
C 5.34042 2.24996 -0.44545
H 6.42399 2.17627 -0.62976
H 5.14260 3.25125 -0.02937
H 4.80971 2.17335 -1.40779
C 5.64670 1.16824 1.85691
H 5.23195 0.43013 2.56146
H 5.61019 2.16105 2.33584
H 6.70730 0.92176 1.67916

III$_{Cu,N}$
SCF (BP86) Energy = -2415.71340402
Enthalpy 0K = -2414.430660
Enthalpy 298K = -2414.429716
Free Energy 298K = -2414.611371
Lowest Frequency = 23.7273 cm^{-1}
Second Frequency = 26.4390 cm^{-1}
SCF (BP86-D3BJ) Energy = -2416.11252107
SCF (C6H6) Energy = -2415.71680398
SCF (BS2) Energy = -3227.93059301

Cu 1.48513 -0.07033 0.66760
Si -3.08494 2.00324 -1.58878
Si -3.93698 -1.44567 0.35222
Al -1.14293 0.31421 0.37506
N -1.45434 1.72872 -0.86942
N -2.15813 -1.28853 0.09875
N 3.50965 -1.72198 -0.79668
N 4.24657 0.27950 -0.39478
N -1.01276 0.79059 2.24800
N 1.40929 0.47837 2.79988
C -0.48292 2.73462 -1.26365
C -0.28636 3.92876 -0.48612
C 0.59336 4.93246 -0.93797
H 0.71899 5.83502 -0.32873
C 1.29106 4.81689 -2.14242
H 1.95721 5.61632 -2.48496
C 1.11943 3.65508 -2.89779
H 1.66546 3.54512 -3.84188
C 0.25824 2.61472 -2.48874
C -0.98705 4.18015 0.84748
H -1.72938 3.37394 0.97059
C 0.02366 4.09877 2.01378
H 0.53574 3.12506 2.03870
H -0.48273 4.25089 2.98471
H 0.79261 4.88647 1.91633
C -1.71655 5.54253 0.91221
H -1.00064 6.38370 0.92944
H -2.31448 5.61123 1.83896
H -2.39066 5.69784 0.05630
C 0.19756 1.38792 -3.39990
H -0.59824 0.72817 -3.01612
C 1.53642 0.61647 -3.34710
H 2.37612 1.27337 -3.63877
H 1.52728 -0.23854 -4.04582
H 1.73673 0.23983 -2.33027
C -0.12300 1.75277 -4.86839
H -1.00185 2.41210 -4.95290
H -0.31970 0.84023 -5.45850
H 0.72463 2.27308 -5.34931
C -3.47248 3.86601 -1.73921
H -3.73519 4.30400 -0.76292
H -4.34472 3.98889 -2.40576
H -2.63662 4.44374 -2.16439
C -3.35340 1.32034 -3.35402
H -2.81099 1.91911 -4.10205
H -4.43024 1.39438 -3.59316
H -3.05472 0.26854 -3.47857
C -4.50149 1.28682 -0.51277
H -4.32068 1.51765 0.55545
H -5.35341 1.94047 -0.79302
C -4.89869 -0.19500 -0.71724
H -4.81734 -0.47669 -1.78304
H -5.96521 -0.34357 -0.45059
C -4.55082 -1.14543 2.13873
H -4.05850 -1.81557 2.86122
H -5.63360 -1.36643 2.16612
H -4.42195 -0.11019 2.48750
C -4.54847 -3.21440 -0.02342
H -4.24201 -3.60555 -1.00352
H -5.65256 -3.21256 0.01922
H -4.18672 -3.92537 0.73762
C -1.55713 -2.57265 -0.18859
C -1.12298 -3.44075 0.86859
C -0.68933 -4.74817 0.56696
H -0.38523 -5.40714 1.38932
C -0.67757 -5.23732 -0.74358
H -0.37107 -6.26822 -0.95288
C -1.07265 -4.38537 -1.78158
H -1.06790 -4.75739 -2.81333
C -1.49271 -3.06263 -1.53731
C -1.16409 -3.02785 2.34050
H -1.53963 -1.99149 2.37565
C 0.24167 -3.04790 2.98005

H 0.68198 -4.06117 2.95505
H 0.18702 -2.73933 4.03983
H 0.92872 -2.35703 2.46396
C -2.12045 -3.92135 3.16486
H -3.13765 -3.93994 2.74025
H -2.19153 -3.55571 4.20498
H -1.76080 -4.96525 3.20571
C -1.88161 -2.20155 -2.74011
H -2.04873 -1.18216 -2.35154
C -0.74473 -2.14355 -3.78270
H 0.20510 -1.83397 -3.32153
H -0.99058 -1.42240 -4.58220
H -0.58393 -3.12479 -4.26458
C -3.17774 -2.67464 -3.43908
H -3.08497 -3.72242 -3.77783
H -3.38219 -2.05480 -4.33051
H -4.05708 -2.61082 -2.77999
C 3.13342 -0.51613 -0.25220
C 2.60177 -2.89964 -0.77955
H 1.62018 -2.46319 -0.51838
C 2.47517 -3.57229 -2.15504
H 2.33887 -2.82522 -2.95342
H 1.58467 -4.21943 -2.14147
H 3.34642 -4.19989 -2.40110
C 2.99977 -3.88474 0.33142
H 3.05839 -3.37287 1.30519
H 3.97217 -4.36594 0.12862
H 2.23354 -4.67341 0.40204
C 4.83362 -1.68941 -1.25978
C 5.56442 -2.82199 -1.91513
H 5.48951 -3.75897 -1.33895
H 6.63431 -2.57279 -1.99331
H 5.19831 -3.02820 -2.93572
C 5.29684 -0.41655 -1.00535
C 6.62802 0.19568 -1.31488
H 7.12791 0.59524 -0.41485
H 6.54676 1.02192 -2.04453
H 7.29697 -0.56008 -1.75406
C 4.43233 1.64607 0.16504
H 5.22872 2.09674 -0.45280
C 3.18361 2.51721 0.03035
H 2.81567 2.55957 -1.00551
H 3.42785 3.54343 0.35053
H 2.36658 2.15500 0.67726
C 4.92307 1.54262 1.61958
H 4.13601 1.08232 2.23914
H 5.14274 2.54794 2.01695
H 5.83887 0.93231 1.69835
C 0.30500 0.50064 2.10259
C 1.63430 0.65968 4.24844
H 0.69749 0.47949 4.81132
C -1.57185 1.24251 3.54694
H -0.79241 1.85493 4.04239
C 2.11216 2.09015 4.56483
H 3.04102 2.31773 4.01451
H 1.35733 2.84022 4.27835
H 2.31618 2.20001 5.64494
C 2.67059 -0.37734 4.71798
H 3.62990 -0.22912 4.19208
H 2.85324 -0.28476 5.80306
H 2.32345 -1.40159 4.50771
C -1.91131 0.06173 4.47992
H -1.05280 -0.61935 4.59718
H -2.19407 0.43355 5.48121
H -2.75512 -0.52330 4.08320
C -2.79894 2.14352 3.34580
H -3.23215 2.41852 4.32288
H -2.54160 3.07003 2.81239
H -3.58179 1.62584 2.76746

TS(III-IV)$_{Cu,N}$
SCF (BP86) Energy = -2415.70873615
Enthalpy 0K = -2414.427238
Enthalpy 298K = -2414.426294
Free Energy 298K = -2414.607670
Lowest Frequency = -109.2456 cm^{-1}
Second Frequency = 21.0041 cm^{-1}
SCF (BP86-D3BJ) Energy = -2416.10340527
SCF (C6H6) Energy = -2415.71203388
SCF (BS2) Energy = -3227.92606068

Cu 1.76064 -0.08011 0.92263
Si -3.04399 2.02405 -1.72054
Si -4.02635 -1.42755 0.16317
Al -1.28955 0.33415 0.36861
N -1.45814 1.72478 -0.91395
N -2.23725 -1.28151 -0.00212
N 3.65280 -1.70042 -0.64858
N 4.40531 0.30731 -0.28902
N -1.29600 0.80617 2.24176
N 1.11336 0.35842 2.72914
C -0.45505 2.72349 -1.24087
C -0.29783 3.91322 -0.44889
C 0.61054 4.91395 -0.84766
H 0.70628 5.81423 -0.22978
C 1.37479 4.79790 -2.01104
H 2.06184 5.59578 -2.31357
C 1.24415 3.63732 -2.77651
H 1.84430 3.52606 -3.68695
C 0.35668 2.60010 -2.41945
C -1.06095 4.15729 0.85149
H -1.81354 3.35520 0.93661
C -0.09885 4.05338 2.05599
H 0.41164 3.07875 2.07692
H -0.64250 4.18471 3.00950
H 0.67392 4.84162 2.00450
C -1.78261 5.52411 0.89910
H -1.06239 6.36022 0.94951
H -2.41457 5.59022 1.80314
H -2.42316 5.69032 0.01970
C 0.34660 1.37088 -3.32898
H -0.47621 0.71728 -2.99448
C 1.67575 0.59357 -3.18746
H 2.53442 1.24371 -3.43561
H 1.70453 -0.26835 -3.87713
H 1.81776 0.22708 -2.15713
C 0.12155 1.73160 -4.81593
H -0.75068 2.38970 -4.95876
H -0.03589 0.81737 -5.41501
H 0.99807 2.25127 -5.24262
C -3.40442 3.89141 -1.87370
H -3.71900 4.32232 -0.90969
H -4.23500 4.03043 -2.58849
H -2.53921 4.46414 -2.24326
C -3.21945 1.35748 -3.50266
H -2.62458 1.95237 -4.21312
H -4.27912 1.45053 -3.80374
H -2.93052 0.30183 -3.61672
C -4.51714 1.31002 -0.72037
H -4.38398 1.53146 0.35720
H -5.34871 1.97446 -1.03420
C -4.91952 -0.16688 -0.95410
H -4.78401 -0.44450 -2.01544
H -6.00037 -0.30389 -0.74553
C -4.69655 -1.09243 1.92065
H -4.26241 -1.78122 2.66261
H -5.79041 -1.25007 1.91627
H -4.51404 -0.06269 2.26231
C -4.63351 -3.19119 -0.23580
H -4.29974 -3.57651 -1.20949
H -5.73827 -3.18605 -0.22570
H -4.29563 -3.90798 0.53047
C -1.61712 -2.56153 -0.26780
C -1.23314 -3.43633 0.80324

C	-0.77154	-4.73687	0.51354
H	-0.50467	-5.40041	1.34500
C	-0.68700	-5.21453	-0.79829
H	-0.35948	-6.24048	-0.99983
C	-1.03703	-4.35763	-1.84787
H	-0.97446	-4.72021	-2.88091
C	-1.48063	-3.04056	-1.61485
C	-1.35282	-3.04074	2.27566
H	-1.71499	-1.99940	2.30556
C	0.01420	-3.09385	2.99211
H	0.42792	-4.11854	2.99746
H	-0.09160	-2.77792	4.04591
H	0.74643	-2.42496	2.51099
C	-2.36711	-3.93011	3.03269
H	-3.36297	-3.91690	2.56036
H	-2.48057	-3.58566	4.07630
H	-2.03130	-4.98216	3.06595
C	-1.81363	-2.17426	-2.83036
H	-1.99254	-1.15501	-2.44662
C	-0.63409	-2.12083	-3.82493
H	0.30089	-1.83205	-3.32156
H	-0.83644	-1.38720	-4.62518
H	-0.46800	-3.09852	-4.31205
C	-3.08161	-2.63995	-3.58367
H	-2.97885	-3.68773	-3.91945
H	-3.24649	-2.01811	-4.48196
H	-3.98715	-2.57339	-2.96142
C	3.29917	-0.49052	-0.09058
C	2.73353	-2.86660	-0.59904
H	1.76330	-2.41133	-0.32683
C	2.56873	-3.55686	-1.96143
H	2.42756	-2.81845	-2.76712
H	1.66912	-4.19066	-1.92280
H	3.42596	-4.20027	-2.21611
C	3.13213	-3.84259	0.51982
H	3.21177	-3.31708	1.48506
H	4.09517	-4.33972	0.30993
H	2.35719	-4.62104	0.61209
C	4.95808	-1.66846	-1.16518
C	5.66204	-2.80867	-1.83616
H	5.60898	-3.73836	-1.24519
H	6.72835	-2.56202	-1.95929
H	5.25617	-3.02833	-2.83890
C	5.43017	-0.39412	-0.93916
C	6.74528	0.21843	-1.30988
H	7.28580	0.62161	-0.43490
H	6.63078	1.04258	-2.03774
H	7.39471	-0.53786	-1.77673
C	4.60763	1.67060	0.26811
H	5.38618	2.12454	-0.36994
C	3.35485	2.54421	0.17157
H	2.95589	2.58571	-0.85298
H	3.60839	3.57079	0.48440
H	2.55584	2.17785	0.83979
C	5.14434	1.56980	1.70759
H	4.38740	1.09691	2.35499
H	5.36554	2.57548	2.10304
H	6.06769	0.96797	1.75600
C	-0.00180	0.45696	2.02844
C	1.37468	0.53599	4.17118
H	0.44679	0.36037	4.74928
C	-1.83123	1.25166	3.55401
H	-1.02838	1.82512	4.05843
C	1.87691	1.95849	4.48531
H	2.78145	2.18328	3.89403
H	1.11841	2.72028	4.24468
H	2.13245	2.05232	5.55577
C	2.41439	-0.50986	4.61046
H	3.35105	-0.37717	4.04078
H	2.64349	-0.40697	5.68551
H	2.04887	-1.53230	4.42628
C	-2.21429	0.06588	4.46250
H	-1.37838	-0.64374	4.57522
H	-2.49426	0.42867	5.46779
H	-3.07230	-0.48543	4.04765
C	-3.02533	2.19953	3.36675
H	-3.41801	2.51517	4.34878
H	-2.74271	3.10131	2.80355
H	-3.84666	1.70322	2.82318

$IV_{Cu,N}$

SCF (BP86) Energy = -2415.72601978
Enthalpy 0K = -2414.443752
Enthalpy 298K = -2414.442808
Free Energy 298K = -2414.628996
Lowest Frequency = 9.6389 cm^{-1}
Second Frequency = 20.9427 cm^{-1}
SCF (BP86-D3BJ) Energy = -2416.10990053
SCF (C6H6) Energy = -2415.73061383
SCF (BS2) Energy = -3227.94419156

Cu	2.52412	0.39326	0.94643
Si	-3.69186	1.42112	-1.83366
Si	-4.06204	-1.95496	0.35426
Al	-1.64251	0.19507	0.39948
N	-2.16304	1.48125	-0.89355
N	-2.32006	-1.56841	0.15116
N	4.35855	-1.32340	-0.53109
N	5.12211	0.70824	-0.44949
N	-1.40830	0.79451	2.22788
N	1.08388	0.78772	2.10538
C	-1.28414	2.57962	-1.24916
C	-1.39721	3.87024	-0.62845
C	-0.56528	4.92675	-1.05128
H	-0.66941	5.90489	-0.56759
C	0.38401	4.76432	-2.06293
H	1.01136	5.60391	-2.38219
C	0.51603	3.50635	-2.65593
H	1.26358	3.36018	-3.44429
C	-0.29313	2.41770	-2.27456
C	-2.34237	4.16596	0.53732
H	-2.99340	3.28274	0.66197
C	-1.51885	4.35403	1.83229
H	-0.91886	3.45564	2.04126
H	-2.17350	4.55207	2.69976
H	-0.82947	5.21142	1.73101
C	-3.22868	5.41428	0.32018
H	-2.62624	6.34021	0.31560
H	-3.95868	5.50975	1.14385
H	-3.78526	5.37462	-0.62822
C	-0.02193	1.07407	-2.94931
H	-0.85165	0.39762	-2.68334
C	1.28693	0.47225	-2.39195
H	2.14250	1.13939	-2.60009
H	1.50851	-0.50872	-2.84958
H	1.23451	0.33839	-1.29531
C	0.05239	1.16922	-4.48904
H	-0.84460	1.64981	-4.91308
H	0.14328	0.16268	-4.93248
H	0.92970	1.75203	-4.82229
C	-4.40205	3.16633	-2.13500
H	-4.86316	3.58205	-1.22480
H	-5.18770	3.10002	-2.90853
H	-3.63696	3.87468	-2.49095
C	-3.53301	0.68181	-3.59043
H	-2.92079	1.33515	-4.23395
H	-4.53908	0.62286	-4.04425
H	-3.09335	-0.32691	-3.61503
C	-5.08936	0.48340	-0.91654
H	-5.15127	0.86503	0.12164
H	-5.99649	0.88823	-1.41209
C	-5.13608	-1.06351	-0.95057
H	-4.87832	-1.43644	-1.95889
H	-6.17331	-1.41099	-0.76239

C	-4.75389	-1.40593	2.04789
H	-4.13768	-1.77820	2.88239
H	-5.77525	-1.80866	2.17287
H	-4.82129	-0.31022	2.13535
C	-4.38305	-3.83342	0.26181
H	-3.90970	-4.32725	-0.59914
H	-5.47302	-4.00263	0.20238
H	-4.01654	-4.34067	1.16921
C	-1.48379	-2.73238	-0.03702
C	-0.88504	-3.40562	1.07984
C	-0.17745	-4.60809	0.87691
H	0.24844	-5.12311	1.74654
C	-0.03963	-5.17976	-0.39222
H	0.48713	-6.13167	-0.52340
C	-0.60100	-4.51675	-1.48910
H	-0.50166	-4.95412	-2.48976
C	-1.30670	-3.30577	-1.34306
C	-1.01898	-2.90058	2.51682
H	-1.52707	-1.92287	2.47341
C	0.36234	-2.69152	3.17516
H	0.92912	-3.63785	3.24236
H	0.24355	-2.31123	4.20560
H	0.96380	-1.96187	2.60899
C	-1.87417	-3.85271	3.38516
H	-2.88610	-3.99033	2.97033
H	-1.97917	-3.45341	4.41012
H	-1.40838	-4.85169	3.46320
C	-1.87410	-2.65850	-2.60674
H	-2.24665	-1.66454	-2.30490
C	-0.79234	-2.46876	-3.69284
H	0.09281	-1.94771	-3.29651
H	-1.19253	-1.87852	-4.53605
H	-0.45618	-3.43765	-4.10392
C	-3.05212	-3.45410	-3.21707
H	-2.73426	-4.47557	-3.49446
H	-3.41786	-2.95846	-4.13445
H	-3.90169	-3.54501	-2.52338
C	4.05215	-0.06481	-0.07012
C	3.43563	-2.46890	-0.29370
H	2.52429	-1.97408	0.08999
C	3.06200	-3.21132	-1.58457
H	2.79823	-2.50282	-2.38627
H	2.17835	-3.83957	-1.38594
H	3.87072	-3.86859	-1.94338
C	3.96213	-3.39964	0.80976
H	4.18698	-2.83133	1.72680
H	4.87140	-3.94297	0.50070
H	3.18614	-4.14595	1.04637
C	5.60578	-1.34553	-1.17161
C	6.24047	-2.54875	-1.79993
H	6.24754	-3.41960	-1.12376
H	7.28817	-2.32504	-2.05476
H	5.73238	-2.85442	-2.73094
C	6.08923	-0.05379	-1.11771
C	7.36740	0.51299	-1.65337
H	7.97780	0.99004	-0.86582
H	7.19367	1.26627	-2.44331
H	7.97635	-0.28835	-2.09890
C	5.28428	2.15121	-0.12721
H	6.13171	2.48700	-0.74878
C	4.04786	2.96693	-0.52806
H	3.81046	2.83767	-1.59571
H	4.23641	4.03691	-0.33918
H	3.16016	2.66460	0.05502
C	5.66555	2.32947	1.35214
H	4.84421	1.98544	2.00269
H	5.85806	3.39355	1.56868
H	6.57155	1.75345	1.60493
C	-0.17344	0.61294	1.66585
C	1.43065	1.29880	3.46286
H	0.55551	1.20995	4.12522
C	-1.83031	1.26345	3.57166
H	-1.16695	2.09371	3.88677
C	1.83748	2.78263	3.40240
H	2.71111	2.91282	2.73826
H	1.02147	3.40620	3.00435
H	2.10852	3.16057	4.40487
C	2.55741	0.44869	4.07661
H	3.45751	0.47583	3.43274
H	2.83900	0.83002	5.07425
H	2.24992	-0.60460	4.17770
C	-1.75676	0.14172	4.62749
H	-0.74239	-0.27961	4.71626
H	-2.05918	0.52256	5.61945
H	-2.44008	-0.68024	4.35440
C	-3.26189	1.81939	3.51027
H	-3.53110	2.28958	4.47215
H	-3.36731	2.57158	2.71492
H	-3.98459	1.00992	3.32008

TS(IV-A)$_{Cu,N}$

SCF (BP86) Energy = -2415.69402965
Enthalpy 0K = -2414.413252
Enthalpy 298K = -2414.412308
Free Energy 298K = -2414.598944
Lowest Frequency = -58.4940 cm^{-1}
Second Frequency = 9.6406 cm^{-1}
SCF (BP86-D3BJ) Energy = -2416.07297025
SCF (C6H6) Energy = -2415.69927449
SCF (BS2) Energy = -3227.91262383

Cu	-2.73720	-0.99697	-0.31013
Si	2.52678	3.36566	0.36052
Si	4.85836	0.35779	-0.85155
Al	1.66924	0.25244	-0.40226
N	1.32558	2.08255	-0.03236
N	3.42250	-0.40552	-0.08728
N	-5.13404	-0.78438	1.35588
N	-5.58350	-0.26543	-0.70287
N	0.77459	-0.54244	-1.99608
N	-1.06754	-1.64060	-0.86685
C	-0.04794	2.47397	0.22132
C	-0.82186	3.16587	-0.77244
C	-2.12269	3.60992	-0.46037
H	-2.69203	4.15247	-1.22436
C	-2.70129	3.38546	0.79195
H	-3.70772	3.75523	1.01795
C	-1.96631	2.68330	1.75130
H	-2.40870	2.49758	2.73704
C	-0.65791	2.22604	1.49747
C	-0.32937	3.41347	-2.20086
H	0.72768	3.09578	-2.24234
C	-1.14436	2.55207	-3.19300
H	-1.11584	1.48662	-2.91879
H	-0.76237	2.66166	-4.22358
H	-2.20182	2.87100	-3.19566
C	-0.42955	4.89068	-2.64928
H	-1.48372	5.20685	-2.74788
H	0.03919	5.01957	-3.64120
H	0.05854	5.58095	-1.94633
C	0.04526	1.44925	2.61123
H	1.10167	1.33180	2.31370
C	-0.57185	0.03916	2.75617
H	-1.62695	0.12091	3.07387
H	-0.03982	-0.55238	3.52284
H	-0.54378	-0.51531	1.80266
C	0.01115	2.18275	3.97047
H	0.39169	3.21450	3.89219
H	0.62732	1.64510	4.71155
H	-1.01443	2.23824	4.37783
C	1.86081	5.11544	-0.00789
H	1.92073	5.35486	-1.08133
H	2.49272	5.84377	0.53077
H	0.82092	5.25931	0.32542

C	3.03214	3.46189	2.20228
H	2.18825	3.80607	2.82253
H	3.84064	4.20873	2.30471
H	3.39685	2.51286	2.62179
C	4.11943	3.21650	-0.68336
H	3.83845	3.11957	-1.74986
H	4.56222	4.23109	-0.59819
C	5.16697	2.15663	-0.28397
H	5.33206	2.16245	0.80989
H	6.15213	2.41321	-0.72857
C	4.62484	0.45653	-2.74493
H	4.53759	-0.54275	-3.20125
H	5.48206	0.97425	-3.21165
H	3.71505	1.02287	-3.00619
C	6.47292	-0.58478	-0.44121
H	7.04095	-0.05049	0.33930
H	7.11620	-0.63470	-1.33714
H	6.30070	-1.61147	-0.08508
C	3.67530	-1.60002	0.69472
C	3.74870	-2.89727	0.08176
C	4.08096	-4.01990	0.86801
H	4.14779	-5.00150	0.38644
C	4.33217	-3.91870	2.23890
H	4.58942	-4.80691	2.82617
C	4.25244	-2.66180	2.84224
H	4.45679	-2.56497	3.91492
C	3.93574	-1.50605	2.10220
C	3.51804	-3.13005	-1.41458
H	2.98603	-2.24298	-1.80230
C	2.65583	-4.38387	-1.68649
H	3.21374	-5.31374	-1.47626
H	2.35752	-4.42597	-2.74813
H	1.74399	-4.39757	-1.06906
C	4.84841	-3.27919	-2.19230
H	5.49066	-2.39070	-2.10476
H	4.65299	-3.45433	-3.26620
H	5.42232	-4.14348	-1.81155
C	3.94484	-0.16945	2.83852
H	3.52216	0.57378	2.14119
C	3.08380	-0.18482	4.11927
H	2.05952	-0.53493	3.91426
H	3.02310	0.82840	4.55475
H	3.51434	-0.84562	4.89275
C	5.38567	0.26899	3.19108
H	5.85136	-0.44828	3.89078
H	5.38778	1.26204	3.67614
H	6.02708	0.32228	2.29717
C	-4.54471	-0.62707	0.12051
C	-4.34078	-1.25133	2.52286
H	-3.30363	-1.20574	2.13975
C	-4.44576	-0.30673	3.72948
H	-4.27352	0.73848	3.42588
H	-3.67121	-0.57923	4.46530
H	-5.42029	-0.37287	4.23940
C	-4.65272	-2.71738	2.86571
H	-4.52858	-3.35843	1.97802
H	-5.67688	-2.85105	3.25316
H	-3.95429	-3.06865	3.64357
C	-6.51331	-0.53363	1.30520
C	-7.45375	-0.58749	2.47083
H	-7.36166	-1.52461	3.04443
H	-8.49296	-0.52743	2.11174
H	-7.30079	0.24988	3.17414
C	-6.79542	-0.20349	-0.00464
C	-8.09953	0.17532	-0.63548
H	-8.37773	-0.50142	-1.46314
H	-8.08723	1.20524	-1.03602
H	-8.90681	0.12766	0.11117
C	-5.45953	-0.04201	-2.16776
H	-6.44096	0.35364	-2.47922
C	-4.39130	1.01170	-2.48206
H	-4.57821	1.94990	-1.93596
H	-4.38856	1.22412	-3.56430
H	-3.38926	0.64829	-2.19740
C	-5.21219	-1.37220	-2.89897
H	-4.23687	-1.79406	-2.60263
H	-5.20344	-1.20556	-3.98928
H	-5.99822	-2.11000	-2.66599
C	0.09755	-0.88696	-0.89585
C	-0.87704	-3.10973	-0.77213
H	0.00296	-3.38723	-1.38566
C	0.37361	-0.78403	-3.41265
H	-0.71723	-0.59402	-3.46508
C	-2.08934	-3.85385	-1.35282
H	-3.00492	-3.59436	-0.78680
H	-2.25426	-3.57895	-2.40853
H	-1.94936	-4.94785	-1.29051
C	-0.58470	-3.57680	0.67093
H	-1.45580	-3.36653	1.31827
H	-0.37529	-4.66244	0.71014
H	0.28736	-3.04502	1.08462
C	0.61992	-2.22509	-3.88976
H	0.02448	-2.95623	-3.32494
H	0.34616	-2.31227	-4.95663
H	1.68632	-2.48919	-3.79353
C	1.13329	0.19680	-4.31734
H	0.72390	0.17422	-5.34238
H	1.06787	1.22908	-3.94207
H	2.20009	-0.07860	-4.37154

INT(IV-A)$_{Cu,N}$

SCF (BP86) Energy = -2415.73408297
Enthalpy 0K = -2414.451965
Enthalpy 298K = -2414.451021
Free Energy 298K = -2414.638846
Lowest Frequency = 11.0816 cm^{-1}
Second Frequency = 16.9222 cm^{-1}
SCF (BP86-D3BJ) Energy = -2416.11317826
SCF (C6H6) Energy = -2415.74022221
SCF (BS2) Energy = -3227.95325549

Cu	-3.14590	-0.41417	0.50266
Si	3.69393	2.25010	-1.46521
Si	3.56420	-1.74213	-2.21687
Al	1.61150	0.01464	-0.39122
N	2.30127	1.77218	-0.43917
N	2.84659	-1.40562	-0.61167
N	-5.76132	0.70361	-0.08245
N	-5.93957	-1.44004	0.21843
N	-0.17752	-0.28516	-1.12607
N	-1.32726	-0.31500	1.02079
C	1.72654	2.82367	0.37593
C	0.67238	3.66657	-0.11704
C	0.19132	4.72739	0.67707
H	-0.60505	5.36652	0.27747
C	0.69408	4.98268	1.95505
H	0.30894	5.81575	2.55319
C	1.69050	4.14279	2.45736
H	2.07815	4.31616	3.46763
C	2.21673	3.07586	1.70169
C	-0.03010	3.43906	-1.45644
H	0.50544	2.62217	-1.97133
C	-1.48858	2.98655	-1.20455
H	-1.52282	2.08588	-0.57090
H	-2.00720	2.77212	-2.15654
H	-2.05111	3.78705	-0.68914
C	-0.04420	4.68607	-2.37028
H	-0.65691	5.49596	-1.93482
H	-0.48670	4.43672	-3.35171
H	0.96460	5.08972	-2.54229
C	3.26943	2.19847	2.37975
H	3.68855	1.53005	1.60903
C	2.60740	1.32293	3.46978
H	2.09692	1.95208	4.22074

H	3.35432	0.70749	4.00145
H	1.85621	0.64368	3.03418
C	4.42646	3.01821	2.99369
H	4.87751	3.70580	2.25923
H	5.21851	2.34561	3.36508
H	4.08654	3.62599	3.85111
C	3.43567	3.98093	-2.22680
H	2.71286	3.95568	-3.05831
H	4.39781	4.34420	-2.62936
H	3.08326	4.71332	-1.48260
C	5.36845	2.38420	-0.55471
H	5.35439	3.21577	0.16902
H	6.16055	2.60350	-1.29367
H	5.65499	1.46947	-0.01401
C	3.92048	1.07986	-2.96855
H	2.94069	0.95181	-3.47000
H	4.50127	1.72139	-3.66421
C	4.64673	-0.27827	-2.80155
H	5.51532	-0.17433	-2.12507
H	5.06874	-0.59795	-3.77734
C	2.22081	-1.95832	-3.55688
H	1.57059	-2.81957	-3.32963
H	2.69198	-2.13528	-4.54064
H	1.58104	-1.06659	-3.64630
C	4.60342	-3.35006	-2.22148
H	4.77552	-3.74940	-1.21012
H	5.58628	-3.17632	-2.69295
H	4.09136	-4.13060	-2.80966
C	3.10926	-2.35208	0.45037
C	2.22868	-3.45852	0.68772
C	2.52669	-4.38255	1.70919
H	1.84803	-5.22793	1.87328
C	3.67222	-4.26339	2.50040
H	3.88713	-4.99556	3.28646
C	4.54521	-3.19836	2.26096
H	5.45469	-3.10407	2.86513
C	4.29193	-2.24261	1.25729
C	1.00280	-3.73478	-0.18446
H	0.85470	-2.85349	-0.83076
C	-0.28325	-3.93581	0.64546
H	-0.19059	-4.78038	1.35149
H	-1.13556	-4.16288	-0.02031
H	-0.53100	-3.02800	1.21803
C	1.24341	-4.96445	-1.09244
H	2.14725	-4.84200	-1.71125
H	0.38344	-5.12859	-1.76750
H	1.37747	-5.88153	-0.49058
C	5.32646	-1.13827	1.04193
H	4.83562	-0.37145	0.41777
C	5.78897	-0.48033	2.35966
H	4.93652	-0.17253	2.98398
H	6.40358	0.41235	2.14719
H	6.41419	-1.16556	2.95970
C	6.57327	-1.65266	0.28324
H	7.07873	-2.44583	0.86361
H	7.29990	-0.83401	0.12987
H	6.32041	-2.07234	-0.70165
C	-5.01526	-0.42427	0.17946
C	-5.11943	2.04538	-0.14033
H	-4.04145	1.80049	-0.09199
C	-5.37918	2.76812	-1.47077
H	-5.18559	2.10191	-2.32706
H	-4.69260	3.62669	-1.54856
H	-6.40701	3.15747	-1.54963
C	-5.46171	2.89299	1.09535
H	-5.23493	2.34101	2.02169
H	-6.52171	3.19675	1.11857
H	-4.85249	3.81184	1.08654
C	-7.12500	0.40175	-0.20717
C	-8.21315	1.38813	-0.50483
H	-8.19258	2.25669	0.17379
H	-9.19499	0.90497	-0.38397
H	-8.16082	1.77157	-1.53871
C	-7.23428	-0.96145	-0.02275
C	-8.44914	-1.83620	-0.05407
H	-8.62509	-2.34355	0.91173
H	-8.38426	-2.61625	-0.83361
H	-9.34262	-1.23195	-0.27249
C	-5.62603	-2.88544	0.38433
H	-6.59212	-3.35546	0.63541
C	-5.12290	-3.47874	-0.94202
H	-5.84611	-3.30831	-1.75714
H	-4.97119	-4.56590	-0.83638
H	-4.16294	-3.02043	-1.22904
C	-4.66295	-3.13646	1.55058
H	-3.66722	-2.70379	1.34933
H	-4.54277	-4.22305	1.69555
H	-5.04540	-2.69844	2.48668
C	-0.24633	-0.23802	0.23025
C	-1.06851	-0.06895	2.46489
H	0.01415	-0.23084	2.62673
C	-1.31716	-0.44951	-2.04345
H	-2.20436	0.05193	-1.57996
C	-1.84017	-1.06068	3.34994
H	-2.93212	-0.92674	3.22932
H	-1.59047	-2.10368	3.09349
H	-1.59740	-0.89934	4.41501
C	-1.40146	1.38570	2.84017
H	-2.47453	1.58860	2.65876
H	-1.19364	1.57838	3.90795
H	-0.80915	2.09331	2.23786
C	-1.67049	-1.93722	-2.23169
H	-1.89392	-2.41274	-1.26239
H	-2.54864	-2.05106	-2.89326
H	-0.82367	-2.47655	-2.68862
C	-1.04346	0.21641	-3.40002
H	-1.95006	0.19504	-4.03035
H	-0.72771	1.26354	-3.27937
H	-0.24834	-0.32074	-3.94413

TS_A_S$_{Cu,N}$

SCF (BP86) Energy = -2415.64865920
Enthalpy 0K = -2414.369505
Enthalpy 298K = -2414.368561
Free Energy 298K = -2414.559438
Lowest Frequency = -725.5661 cm^{-1}
Second Frequency = 9.9042 cm^{-1}
SCF (BP86-D3BJ) Energy = -2416.03066919
SCF (C6H6) Energy = -2415.65308541
SCF (BS2) Energy = -3227.86918918

Cu	3.10980	0.51980	0.46921
Si	-3.95255	-1.74838	1.18919
Si	-4.28300	1.40626	-1.06203
Al	-1.59055	-0.08520	-0.24764
N	-2.45127	-1.69012	0.18342
N	-2.64526	1.46542	-0.30100
N	5.63966	-0.89118	0.34501
N	5.79543	1.04870	-0.63267
N	0.08463	-0.19319	-1.03181
N	1.35782	0.81619	1.05264
C	-1.88919	-2.98972	-0.12578
C	-2.34802	-3.73884	-1.26123
C	-1.84990	-5.03777	-1.48586
H	-2.21588	-5.60179	-2.35178
C	-0.91237	-5.62505	-0.63185
H	-0.54473	-6.63964	-0.81941
C	-0.45264	-4.89215	0.46549
H	0.28208	-5.34505	1.14141
C	-0.91447	-3.58882	0.73736
C	-3.37175	-3.19585	-2.26067
H	-3.56248	-2.14697	-1.97851
C	-2.84072	-3.22767	-3.71309
H	-1.84377	-2.76881	-3.80007

H	-3.52942	-2.68924	-4.38808
H	-2.75962	-4.26397	-4.08686
C	-4.71906	-3.95425	-2.21046
H	-4.57720	-5.02534	-2.44058
H	-5.42105	-3.54286	-2.95781
H	-5.20181	-3.88606	-1.22315
C	-0.34688	-2.88435	1.97216
H	-0.73521	-1.84936	1.97329
C	1.19611	-2.81283	1.92577
H	1.64461	-3.82248	1.91752
H	1.58657	-2.28269	2.81138
H	1.54095	-2.27278	1.02904
C	-0.79776	-3.56481	3.28577
H	-1.89552	-3.59372	3.37938
H	-0.39676	-3.02377	4.16148
H	-0.43236	-4.60613	3.33908
C	-4.41495	-3.55140	1.60228
H	-4.68678	-4.15285	0.72187
H	-5.28169	-3.53859	2.28742
H	-3.58992	-4.07451	2.11151
C	-3.67319	-0.88374	2.86709
H	-3.26525	-1.60580	3.59481
H	-4.61501	-0.48355	3.28167
H	-2.95568	-0.05276	2.78996
C	-5.45959	-1.01509	0.25881
H	-5.51612	-1.54683	-0.71005
H	-6.34270	-1.36935	0.83117
C	-5.57524	0.50923	0.03173
H	-5.59651	1.03741	1.00345
H	-6.55461	0.73737	-0.43924
C	-4.18219	0.58212	-2.78020
H	-3.67270	1.25569	-3.49005
H	-5.19321	0.37539	-3.17418
H	-3.62927	-0.37066	-2.77122
C	-4.95211	3.16569	-1.35391
H	-5.07775	3.74020	-0.42371
H	-5.93724	3.09205	-1.84810
H	-4.28650	3.74919	-2.00962
C	-2.19484	2.79971	0.04831
C	-1.39257	3.56387	-0.86093
C	-1.03630	4.88837	-0.53551
H	-0.43079	5.46230	-1.24687
C	-1.44626	5.49047	0.65724
H	-1.16457	6.52352	0.88776
C	-2.22466	4.74750	1.54880
H	-2.55384	5.20896	2.48736
C	-2.60897	3.41986	1.27508
C	-0.90890	3.01444	-2.20306
H	-1.22346	1.95858	-2.25436
C	0.63142	3.05744	-2.30970
H	1.00688	4.09642	-2.29938
H	0.96930	2.59631	-3.25525
H	1.10374	2.51622	-1.47359
C	-1.54232	3.75772	-3.40191
H	-2.64275	3.68963	-3.39306
H	-1.18491	3.33053	-4.35631
H	-1.27550	4.82970	-3.39641
C	-3.47614	2.71228	2.31898
H	-3.67127	1.69796	1.93709
C	-2.75564	2.58158	3.68069
H	-1.79793	2.04506	3.58636
H	-3.38552	2.02925	4.40017
H	-2.54198	3.57332	4.11778
C	-4.83796	3.41375	2.53363
H	-4.70422	4.44088	2.91714
H	-5.44330	2.86059	3.27404
H	-5.42388	3.48105	1.60280
C	4.89714	0.23092	0.02251
C	5.03443	-1.98966	1.13581
H	3.96754	-1.69953	1.17532
C	5.12543	-3.35231	0.43091
H	4.77966	-3.27904	-0.61282
H	4.47583	-4.07310	0.95461
H	6.14732	-3.76519	0.43712
C	5.56348	-2.00999	2.57991
H	5.45300	-1.01640	3.04357
H	6.62420	-2.30774	2.63451
H	4.98378	-2.73526	3.17516
C	6.96999	-0.77031	-0.08863
C	8.03542	-1.81053	0.07905
H	8.13544	-2.15025	1.12370
H	9.01009	-1.39520	-0.22118
H	7.85453	-2.70431	-0.54420
C	7.06421	0.45605	-0.71095
C	8.24037	1.10337	-1.37366
H	8.50768	2.06874	-0.90650
H	8.06681	1.29159	-2.44901
H	9.12260	0.44943	-1.29748
C	5.45812	2.37897	-1.19689
H	6.40855	2.77135	-1.59669
C	4.46495	2.23999	-2.36155
H	4.86449	1.57572	-3.14601
H	4.26404	3.22809	-2.80800
H	3.51028	1.81748	-2.00489
C	4.96499	3.33870	-0.10240
H	4.03065	2.96251	0.35132
H	4.77085	4.33370	-0.53676
H	5.71546	3.44476	0.69845
C	0.84153	0.25385	-0.01175
C	0.78074	-0.70591	-2.27265
H	1.70799	-0.10237	-2.33988
C	1.17036	-2.17997	-2.11944
H	1.80926	-2.30798	-1.22890
H	1.74019	-2.52630	-3.00017
H	0.28081	-2.82218	-2.00403
C	-0.09623	-0.45553	-3.50239
H	-1.09284	-0.91086	-3.37333
H	0.35974	-0.90424	-4.40118
H	-0.23830	0.62073	-3.68920
C	0.63106	1.41091	2.20896
H	-0.45237	1.27546	1.97478
C	0.98232	0.66796	3.50525
H	0.64149	-0.37947	3.46986
H	0.51596	1.15528	4.37889
H	2.07729	0.67286	3.65148
C	0.96214	2.90625	2.30558
H	2.04764	3.03878	2.46109
H	0.43292	3.37087	3.15431
H	0.66726	3.43550	1.38556

$A_{Cu,N}$

SCF (BP86) Energy = -2415.74569463
Enthalpy 0K = -2414.464005
Enthalpy 298K = -2414.463061
Free Energy 298K = -2414.654138
Lowest Frequency = 7.9095 cm^{-1}
Second Frequency = 12.8536 cm^{-1}
SCF (BP86-D3BJ) Energy = -2416.12376326
SCF (C6H6) Energy = -2415.75165274
SCF (BS2) Energy = -3227.96520377

Cu	-3.07534	-0.47795	0.46937
Si	4.28287	1.93391	0.67753
Si	4.35456	-1.46284	-1.25979
Al	1.70735	0.05170	-0.09408
N	2.61226	1.70109	0.04679
N	2.80288	-1.45473	-0.35478
N	-5.64204	0.87557	0.26990
N	-5.79795	-1.12876	-0.55134
N	-0.06474	0.19100	-0.83489
N	-1.29934	-0.59150	1.10418
C	1.86960	2.92521	-0.15765
C	1.86570	3.57433	-1.43872
C	1.20989	4.81268	-1.58910

H	1.22832	5.30795	-2.56641
C	0.53905	5.42550	-0.52537
H	0.04193	6.39207	-0.66326
C	0.51267	4.78055	0.71414
H	-0.01504	5.24999	1.55331
C	1.16048	3.54642	0.92257
C	2.55489	2.97133	-2.66567
H	2.69805	1.89804	-2.44662
C	1.71323	3.10373	-3.95582
H	0.66297	2.81039	-3.80143
H	2.13671	2.46922	-4.75427
H	1.71446	4.14096	-4.33664
C	3.94734	3.59009	-2.93195
H	3.86109	4.68003	-3.09257
H	4.40046	3.15067	-3.83902
H	4.64296	3.42737	-2.09593
C	1.08275	2.93324	2.32318
H	1.61859	1.96893	2.28929
C	-0.37704	2.64685	2.74045
H	-0.96999	3.57852	2.78929
H	-0.40462	2.18476	3.74393
H	-0.86555	1.95783	2.03302
C	1.76078	3.82574	3.38891
H	2.81634	4.03097	3.14691
H	1.72701	3.33951	4.38047
H	1.24716	4.79986	3.47941
C	4.72286	3.79098	0.74990
H	4.79575	4.26863	-0.23892
H	5.70175	3.89688	1.25098
H	3.98166	4.36161	1.33167
C	4.49744	1.30327	2.46840
H	3.99009	1.97403	3.18142
H	5.57033	1.28312	2.73247
H	4.09669	0.29035	2.62085
C	5.61473	1.09927	-0.41772
H	5.48102	1.46308	-1.45379
H	6.57055	1.54822	-0.07394
C	5.73205	-0.44117	-0.40689
H	5.84018	-0.81513	0.62926
H	6.66744	-0.74575	-0.92217
C	4.11899	-0.79459	-3.03204
H	3.42773	-1.43397	-3.60614
H	5.08519	-0.77181	-3.56729
H	3.71279	0.23032	-3.03835
C	5.03526	-3.23912	-1.38879
H	5.31646	-3.64276	-0.40251
H	5.93843	-3.23529	-2.02437
H	4.30839	-3.93869	-1.83058
C	2.36563	-2.74852	0.12272
C	1.52796	-3.59140	-0.67827
C	1.19714	-4.88338	-0.22061
H	0.57200	-5.52515	-0.85292
C	1.64489	-5.36829	1.01177
H	1.37803	-6.37699	1.34545
C	2.43482	-4.53726	1.81184
H	2.78345	-4.89970	2.78639
C	2.80579	-3.24483	1.39417
C	0.96095	-3.15231	-2.02963
H	1.23455	-2.09202	-2.16850
C	-0.58133	-3.25443	-2.04054
H	-0.91736	-4.29786	-1.90347
H	-0.98988	-2.90654	-3.00648
H	-1.02136	-2.64655	-1.23236
C	1.55304	-3.96132	-3.20653
H	2.64906	-3.85820	-3.26402
H	1.13011	-3.61779	-4.16804
H	1.32482	-5.03789	-3.10706
C	3.66934	-2.40900	2.33609
H	3.90480	-1.47835	1.79454
C	2.89636	-2.03414	3.62101
H	1.96792	-1.48837	3.38283
H	3.51168	-1.39488	4.27943
H	2.61652	-2.93572	4.19490
C	5.00469	-3.09615	2.69771
H	4.84160	-4.03331	3.25935
H	5.61987	-2.43362	3.33247
H	5.59242	-3.34587	1.79849
C	-4.90451	-0.26090	0.02499
C	-5.03169	2.04336	0.96266
H	-3.96598	1.75202	1.02793
C	-5.12004	3.33525	0.13662
H	-4.76496	3.17006	-0.89305
H	-4.47356	4.09970	0.59802
H	-6.14185	3.74629	0.10016
C	-5.56263	2.19346	2.39758
H	-5.45490	1.24859	2.95396
H	-6.62173	2.49951	2.42636
H	-4.97970	2.96870	2.92191
C	-6.97306	0.72325	-0.14649
C	-8.04067	1.77065	-0.05344
H	-8.13243	2.19191	0.96121
H	-9.01608	1.33004	-0.31138
H	-7.86606	2.61044	-0.74850
C	-7.06805	-0.55025	-0.67085
C	-8.24672	-1.25159	-1.27167
H	-8.51285	-2.17149	-0.72056
H	-8.07475	-1.53168	-2.32647
H	-9.12786	-0.59250	-1.25039
C	-5.45784	-2.49860	-1.02245
H	-6.42022	-2.93766	-1.33465
C	-4.52946	-2.44096	-2.24559
H	-4.96744	-1.82788	-3.05069
H	-4.35930	-3.45818	-2.63537
H	-3.55244	-2.01018	-1.97059
C	-4.88702	-3.35269	0.11900
H	-3.92028	-2.94526	0.46385
H	-4.72025	-4.38333	-0.23564
H	-5.57735	-3.38419	0.97797
C	-0.17772	-0.27140	0.43997
C	-1.16684	0.48931	-1.76019
H	-2.01742	-0.19802	-1.51763
C	-1.66077	1.93609	-1.56379
H	-1.98939	2.09845	-0.52318
H	-2.50860	2.15698	-2.23815
H	-0.84859	2.65336	-1.76853
C	-0.73562	0.22754	-3.20895
H	0.14742	0.83699	-3.46001
H	-1.54403	0.48838	-3.91459
H	-0.46854	-0.82914	-3.36127
C	-1.08801	-1.19722	2.44564
H	-0.09502	-0.85655	2.79939
C	-2.15220	-0.71430	3.44502
H	-2.16195	0.38561	3.51737
H	-1.95872	-1.12902	4.45021
H	-3.16060	-1.04768	3.13207
C	-1.06677	-2.73276	2.36068
H	-2.04285	-3.10963	2.00114
H	-0.87366	-3.18240	3.35119
H	-0.28571	-3.07726	1.66500

$S_{Cu,N}$

SCF (BP86) Energy = -2415.76651891
Enthalpy 0K = -2414.484465
Enthalpy 298K = -2414.483521
Free Energy 298K = -2414.672601
Lowest Frequency = 11.2447 cm^{-1}
Second Frequency = 15.8784 cm^{-1}
SCF (BP86-D3BJ) Energy = -2416.15303370
SCF (C6H6) Energy = -2415.77222331
SCF (BS2) Energy = -3227.98497605

Cu	2.90200	-0.20795	0.07333
Si	-3.94367	1.63084	-1.20911
Si	-4.13879	-1.57213	0.95104

Al	-1.44585	0.00376	0.01834
N	-2.44638	1.59770	-0.20898
N	-2.52583	-1.55089	0.15642
N	5.58276	0.81470	-0.56111
N	5.75233	-0.94923	0.68996
N	0.19766	0.28765	1.07518
N	0.15257	-0.44009	-1.01440
C	-1.99314	2.90890	0.20227
C	-2.55200	3.55825	1.35672
C	-2.15039	4.86691	1.69138
H	-2.59165	5.34487	2.57420
C	-1.21730	5.57085	0.92608
H	-0.92594	6.59150	1.19694
C	-0.66698	4.94427	-0.19494
H	0.05953	5.49050	-0.80832
C	-1.02623	3.63463	-0.57130
C	-3.58496	2.89351	2.26867
H	-3.74254	1.87590	1.87703
C	-3.08051	2.78413	3.72605
H	-2.09238	2.30139	3.78312
H	-3.78684	2.19696	4.33939
H	-2.98633	3.78118	4.19258
C	-4.94750	3.62529	2.26670
H	-4.84281	4.66298	2.63104
H	-5.66243	3.11022	2.93337
H	-5.39687	3.66944	1.26201
C	-0.36595	3.06454	-1.82947
H	-0.65719	2.00280	-1.90875
C	1.17525	3.12360	-1.73814
H	1.53594	4.16169	-1.62504
H	1.63158	2.71161	-2.65520
H	1.53837	2.53508	-0.87913
C	-0.84006	3.79103	-3.11002
H	-1.93203	3.71951	-3.24056
H	-0.36315	3.35452	-4.00647
H	-0.57865	4.86426	-3.08022
C	-4.49333	3.42334	-1.56975
H	-4.80774	3.97569	-0.67114
H	-5.34923	3.39344	-2.26792
H	-3.69001	4.00868	-2.04474
C	-3.61078	0.85031	-2.92118
H	-3.14153	1.60028	-3.58121
H	-4.54445	0.51256	-3.40478
H	-2.92878	-0.01127	-2.86595
C	-5.44356	0.81263	-0.33701
H	-5.56000	1.34180	0.62768
H	-6.32481	1.12134	-0.93839
C	-5.48964	-0.71359	-0.10510
H	-5.50269	-1.24156	-1.07740
H	-6.45200	-0.98427	0.37852
C	-4.03896	-0.80703	2.69764
H	-3.57889	-1.53015	3.39284
H	-5.04303	-0.55797	3.08478
H	-3.43159	0.11017	2.72442
C	-4.75772	-3.35890	1.21101
H	-4.90414	-3.91113	0.27035
H	-5.72692	-3.32358	1.74012
H	-4.05945	-3.94839	1.82604
C	-2.03112	-2.85432	-0.23439
C	-1.18388	-3.61340	0.64224
C	-0.76047	-4.90447	0.26738
H	-0.12592	-5.47383	0.95711
C	-1.13430	-5.48061	-0.94997
H	-0.79514	-6.48621	-1.22156
C	-1.95785	-4.74814	-1.80873
H	-2.26702	-5.19189	-2.76274
C	-2.42021	-3.45810	-1.48004
C	-0.72496	-3.09466	2.00693
H	-1.05667	-2.04563	2.08520
C	0.81353	-3.11734	2.14070
H	1.21240	-4.14522	2.06953
H	1.12349	-2.71438	3.12201
H	1.28635	-2.50622	1.35444
C	-1.35883	-3.88676	3.17436
H	-2.45951	-3.83701	3.15516
H	-1.01985	-3.48478	4.14643
H	-1.07309	-4.95344	3.13553
C	-3.35812	-2.77996	-2.48332
H	-3.58564	-1.78001	-2.08147
C	-2.71437	-2.60662	-3.87825
H	-1.77660	-2.02904	-3.83472
H	-3.40420	-2.07592	-4.55783
H	-2.47993	-3.58322	-4.33798
C	-4.69316	-3.54485	-2.64975
H	-4.52290	-4.56289	-3.04337
H	-5.35262	-3.01865	-3.36329
H	-5.23872	-3.64377	-1.69814
C	4.82807	-0.14048	0.07851
C	4.92695	1.92629	-1.30211
H	3.85816	1.64196	-1.26824
C	5.07349	3.26715	-0.56517
H	4.74359	3.17424	0.48193
H	4.43912	4.02247	-1.05734
H	6.10993	3.64396	-0.57580
C	5.35301	1.98595	-2.77680
H	5.27434	0.99460	-3.25176
H	6.38153	2.35998	-2.90602
H	4.68193	2.67553	-3.31472
C	6.95531	0.61192	-0.35268
C	8.05720	1.45113	-0.92448
H	8.15692	1.32564	-2.01686
H	9.01818	1.15974	-0.47300
H	7.91639	2.52603	-0.72420
C	7.05968	-0.51205	0.44246
C	8.28023	-1.19858	0.97264
H	8.37185	-2.23554	0.60231
H	8.29404	-1.23522	2.07670
H	9.18454	-0.65882	0.65290
C	5.40838	-2.13633	1.51806
H	6.37852	-2.54262	1.84991
C	4.60413	-1.72171	2.75957
H	5.14318	-0.96196	3.34936
H	4.42491	-2.60095	3.40020
H	3.62552	-1.30471	2.46480
C	4.69643	-3.20596	0.67660
H	3.71379	-2.84119	0.33321
H	4.53223	-4.11110	1.28434
H	5.29415	-3.48196	-0.20770
C	0.97123	-0.13712	0.03362
C	0.81226	0.77326	2.31304
H	1.83779	0.33813	2.35059
C	0.97016	2.30654	2.33183
H	1.57305	2.64296	1.47201
H	1.47499	2.63426	3.25920
H	-0.00793	2.81156	2.26963
C	0.04159	0.27824	3.54776
H	-1.01359	0.59616	3.50217
H	0.47858	0.69212	4.47322
H	0.05658	-0.82018	3.61903
C	0.60584	-1.11104	-2.23891
H	-0.32069	-1.40296	-2.76356
C	1.39222	-0.17806	-3.18133
H	0.80097	0.71410	-3.44234
H	1.66276	-0.70268	-4.11534
H	2.32686	0.15749	-2.69409
C	1.39687	-2.40614	-1.97066
H	2.36519	-2.17096	-1.48719
H	1.61286	-2.93145	-2.91796
H	0.83147	-3.08465	-1.31300

$I_{P,H}$
SCF (BP86) Energy = -1970.41065264
Enthalpy 0K = -1969.267413
Enthalpy 298K = -1969.266469

Free Energy 298K = -1969.436687
Lowest Frequency = 11.9835 cm^{-1}
Second Frequency = 19.1143 cm^{-1}
SCF (BP86-D3BJ) Energy = -1970.75455904
SCF (C6H6) Energy = -1970.41366312
SCF (BS2) Energy = -3117.34318072

Cu	1.31793	0.06953	0.02060
P	3.66004	0.18200	-0.02279
Si	-3.84557	1.63328	0.90485
Si	-3.66603	-2.11026	-0.39938
Al	-1.07164	-0.02959	0.05892
N	-2.20803	1.47316	0.18191
N	-1.96227	-1.69275	-0.00423
C	-1.57963	2.68283	-0.29713
C	-1.59995	2.98975	-1.69573
C	-0.94570	4.14633	-2.16308
H	-0.95994	4.36953	-3.23643
C	-0.29123	5.02076	-1.28825
H	0.20486	5.92023	-1.66911
C	-0.28923	4.73452	0.08184
H	0.21437	5.42022	0.77413
C	-0.91934	3.58497	0.59764
C	-2.31484	2.08834	-2.70307
H	-2.89524	1.35645	-2.11384
C	-3.30610	2.86414	-3.59761
H	-4.03655	3.42930	-2.99430
H	-3.86467	2.16775	-4.24776
H	-2.78963	3.58487	-4.25631
C	-1.30266	1.29981	-3.56485
H	-0.67174	1.98468	-4.15991
H	-1.82124	0.62061	-4.26516
H	-0.62794	0.69425	-2.93254
C	-0.86099	3.33458	2.10488
H	-1.43983	2.41776	2.30033
C	-1.48805	4.48597	2.92201
H	-1.46958	4.25011	4.00120
H	-2.53613	4.67020	2.63252
H	-0.93406	5.43128	2.78159
C	0.58277	3.06308	2.57527
H	1.23508	3.93845	2.40198
H	1.00657	2.20276	2.02810
H	0.60959	2.83215	3.65564
C	-4.53933	3.36723	0.52877
H	-3.85397	4.17249	0.83690
H	-5.49734	3.50932	1.05897
H	-4.72905	3.49095	-0.55094
C	-3.83481	1.35290	2.79836
H	-3.25482	0.45448	3.07182
H	-4.86741	1.20564	3.16290
H	-3.40679	2.20833	3.34573
C	-5.11154	0.38572	0.20683
H	-6.08484	0.76291	0.58536
H	-5.16678	0.49589	-0.89266
C	-4.93344	-1.09651	0.60575
H	-5.88761	-1.64362	0.45486
H	-4.71146	-1.19412	1.68524
C	-4.10298	-1.81376	-2.23938
H	-3.74151	-0.83395	-2.59532
H	-5.20051	-1.83025	-2.36720
H	-3.67992	-2.58898	-2.89853
C	-3.98016	-3.94560	0.00554
H	-3.25346	-4.61207	-0.48608
H	-4.99165	-4.23276	-0.33159
H	-3.91989	-4.13299	1.09088
C	-1.06001	-2.79907	0.21619
C	-0.74828	-3.21279	1.55128
C	0.16508	-4.26563	1.75584
H	0.40163	-4.57422	2.78111
C	0.76354	-4.93482	0.68200
H	1.46303	-5.75881	0.86078
C	0.44592	-4.54353	-0.62407
H	0.90606	-5.06861	-1.46988
C	-0.45221	-3.48913	-0.88183
C	-1.37967	-2.53675	2.76955
H	-2.16727	-1.86492	2.38473
C	-0.34897	-1.66691	3.52493
H	0.47873	-2.28562	3.91668
H	-0.81810	-1.14732	4.37985
H	0.09169	-0.90601	2.85461
C	-2.04699	-3.54495	3.73052
H	-2.78898	-4.17188	3.20786
H	-2.56374	-3.01319	4.54893
H	-1.30747	-4.22180	4.19430
C	-0.74589	-3.11557	-2.33610
H	-1.50794	-2.32043	-2.31494
C	0.49520	-2.52925	-3.04212
H	0.85499	-1.63231	-2.50673
H	0.25392	-2.23713	-4.07993
H	1.32325	-3.25956	-3.08002
C	-1.31481	-4.30464	-3.14206
H	-0.58085	-5.12573	-3.22817
H	-1.57716	-3.98833	-4.16753
H	-2.22152	-4.71988	-2.67068
C	4.15942	1.93170	-0.75867
C	3.17365	2.22503	-1.91921
H	3.29089	1.54499	-2.77413
H	3.35533	3.25286	-2.28587
H	2.12381	2.17312	-1.58003
C	5.61431	2.05073	-1.25957
H	6.35235	1.85208	-0.46656
H	5.78518	3.08382	-1.61802
H	5.82862	1.37868	-2.10500
C	3.90763	3.02482	0.30532
H	2.88065	2.98464	0.70313
H	4.03173	4.01175	-0.17843
H	4.61901	2.98446	1.14470
C	4.41413	-1.22448	-1.16531
C	4.09324	-0.89750	-2.64280
H	3.01953	-0.70307	-2.80011
H	4.36130	-1.77641	-3.25842
H	4.66840	-0.04300	-3.03123
C	5.93494	-1.44977	-1.02402
H	6.52392	-0.54864	-1.25542
H	6.24531	-2.23854	-1.73578
H	6.21771	-1.79737	-0.01814
C	3.66194	-2.53710	-0.83037
H	3.91241	-2.94174	0.15893
H	3.94200	-3.30341	-1.57782
H	2.56760	-2.41150	-0.87481
C	4.42928	-0.00489	1.77465
C	3.51330	0.77563	2.74865
H	3.49873	1.85841	2.56599
H	3.87890	0.61783	3.78117
H	2.47457	0.40681	2.70017
C	5.88513	0.48793	1.92209
H	6.58091	-0.03320	1.24642
H	6.22436	0.29458	2.95781
H	5.98511	1.57103	1.74928
C	4.35225	-1.48655	2.21249
H	3.33942	-1.90426	2.08568
H	4.60058	-1.54143	3.28909
H	5.07049	-2.13115	1.68328

TS(I-II)$_{P,H}$
SCF (BP86) Energy = -2158.98551772
Enthalpy 0K = -2157.827492
Enthalpy 298K = -2157.826547
Free Energy 298K = -2158.000976
Lowest Frequency = -174.1223 cm^{-1}
Second Frequency = 18.2355 cm^{-1}
SCF (BP86-D3BJ) Energy = -2159.35179657
SCF (C6H6) Energy = -2158.98845697
SCF (BS2) Energy = -3305.97857852

Cu	-1.35011	-0.44878	-0.09939
P	-3.73756	-0.65673	-0.00738
Si	3.64671	-0.86423	1.72664
Si	3.20122	2.61174	-0.00328
Al	1.01726	0.10308	0.03644
N	2.41831	-1.11129	0.43473
N	1.53699	1.91492	0.06254
C	2.30952	-2.43439	-0.13670
C	3.00063	-2.76393	-1.35133
C	2.85395	-4.05152	-1.90385
H	3.38558	-4.29395	-2.83090
C	2.06119	-5.02989	-1.29423
H	1.96061	-6.02391	-1.74327
C	1.41507	-4.72365	-0.09287
H	0.81314	-5.49304	0.40572
C	1.52919	-3.45210	0.50406
C	3.96240	-1.78651	-2.02981
H	3.75363	-0.79206	-1.60001
C	5.43087	-2.14749	-1.69962
H	5.61305	-2.16857	-0.61398
H	6.12430	-1.41524	-2.15107
H	5.68623	-3.14557	-2.09897
C	3.79372	-1.70243	-3.56222
H	4.08225	-2.64606	-4.05880
H	4.44744	-0.91148	-3.97050
H	2.75754	-1.46816	-3.84983
C	0.83355	-3.22468	1.84683
H	1.03474	-2.18260	2.14617
C	1.38155	-4.15748	2.95157
H	0.89175	-3.94251	3.91839
H	2.46865	-4.03625	3.08557
H	1.19201	-5.21901	2.71205
C	-0.69439	-3.37772	1.72877
H	-0.97875	-4.38940	1.38763
H	-1.09199	-2.64349	0.99948
H	-1.18424	-3.19554	2.70245
C	4.67131	-2.45295	2.01833
H	4.16975	-3.35849	1.64309
H	4.84750	-2.58156	3.10065
H	5.65849	-2.39146	1.53066
C	2.82364	-0.39785	3.38839
H	2.09667	0.42395	3.28191
H	3.59303	-0.06938	4.11059
H	2.29605	-1.25907	3.83155
C	4.88474	0.52642	1.30234
H	5.72173	0.38974	2.01908
H	5.31653	0.31719	0.30530
C	4.36070	1.97565	1.37934
H	5.21438	2.68527	1.34575
H	3.87274	2.16234	2.35533
C	4.06501	2.28386	-1.67344
H	4.03634	1.21768	-1.95070
H	5.12580	2.58663	-1.61180
H	3.59971	2.85559	-2.49261
C	3.11074	4.49701	0.27346
H	2.38224	4.99641	-0.38377
H	4.10471	4.93922	0.08337
H	2.83267	4.73304	1.31442
C	0.46298	2.88308	0.07834
C	-0.08305	3.32795	1.32663
C	-1.14656	4.25126	1.33268
H	-1.56176	4.58045	2.29245
C	-1.66273	4.78013	0.14363
H	-2.47912	5.51030	0.16777
C	-1.10328	4.37981	-1.07454
H	-1.48765	4.80786	-2.00820
C	-0.05358	3.44098	-1.13682
C	0.47940	2.84065	2.66268
H	1.43323	2.33508	2.43223
C	-0.45046	1.79929	3.32230
H	-1.43476	2.24284	3.55679
H	-0.01755	1.41638	4.26402
H	-0.62161	0.94098	2.64673
C	0.78025	3.99232	3.64627
H	1.42943	4.75796	3.18929
H	1.28934	3.60394	4.54592
H	-0.14163	4.49731	3.98573
C	0.51806	3.08723	-2.51286
H	1.28531	2.31198	-2.35541
C	-0.54687	2.50361	-3.46702
H	-1.04058	1.61860	-3.03332
H	-0.08463	2.20414	-4.42424
H	-1.33633	3.24170	-3.69623
C	1.19236	4.30808	-3.18253
H	0.46085	5.11383	-3.37275
H	1.63352	4.02302	-4.15452
H	1.99481	4.73066	-2.55628
C	-4.43387	-2.45930	-0.39611
C	-3.53389	-3.06120	-1.50316
H	-3.58534	-2.51510	-2.45437
H	-3.86060	-4.10048	-1.69743
H	-2.47698	-3.09286	-1.19287
C	-5.91179	-2.49935	-0.84287
H	-6.59321	-2.07184	-0.09055
H	-6.20698	-3.55557	-0.99207
H	-6.08367	-1.98167	-1.79872
C	-4.28054	-3.37802	0.83828
H	-3.25049	-3.39154	1.22470
H	-4.52640	-4.41077	0.52711
H	-4.96515	-3.11917	1.66024
C	-4.46158	0.58448	-1.34470
C	-4.22272	-0.01226	-2.75254
H	-3.17280	-0.31238	-2.90312
H	-4.45668	0.76636	-3.50241
H	-4.86827	-0.87616	-2.97309
C	-5.95429	0.94737	-1.19281
H	-6.61919	0.07171	-1.23989
H	-6.23922	1.62278	-2.02207
H	-6.16042	1.48859	-0.25591
C	-3.61396	1.87684	-1.26463
H	-3.80398	2.47395	-0.36355
H	-3.85357	2.51332	-2.13680
H	-2.53165	1.66456	-1.29495
C	-4.38357	-0.11506	1.76310
C	-3.48065	-0.81749	2.80789
H	-3.60218	-1.90909	2.82417
H	-3.74189	-0.43928	3.81425
H	-2.41475	-0.59379	2.63178
C	-5.86578	-0.43514	2.05567
H	-6.55128	0.04885	1.34297
H	-6.11855	-0.05607	3.06433
H	-6.07832	-1.51523	2.05637
C	-4.16415	1.40556	1.93962
H	-3.13854	1.71842	1.68315
H	-4.33205	1.65782	3.00368
H	-4.87309	2.00789	1.35089
O	1.11579	-0.29769	-2.46695
C	0.05704	-0.86617	-2.47002
O	-0.88911	-1.49554	-2.82187

$III_{P,H}$

SCF (BP86) Energy = -2159.01708011
Enthalpy 0K = -2157.857753
Enthalpy 298K = -2157.856808
Free Energy 298K = -2158.029246
Lowest Frequency = 17.2869 cm^{-1}
Second Frequency = 23.9284 cm^{-1}
SCF (BP86-D3BJ) Energy = -2159.38062580
SCF (C6H6) Energy = -2159.02168851
SCF (BS2) Energy = -3306.00945026

Cu	-1.45900	-0.50599	-0.37288
P	-3.77134	-0.70158	0.00323

Si	3.64000	-0.86606	1.76119
Si	3.17326	2.72360	0.18018
Al	1.29925	0.14517	-0.30414
N	2.45668	-1.11259	0.42024
N	1.54581	1.94342	0.09091
C	2.46906	-2.42403	-0.20191
C	3.21331	-2.66122	-1.40128
C	3.19807	-3.94850	-1.97388
H	3.76860	-4.12466	-2.89294
C	2.47949	-5.00251	-1.40149
H	2.48084	-5.99369	-1.86756
C	1.76483	-4.77370	-0.22117
H	1.20628	-5.59755	0.23887
C	1.75139	-3.50800	0.39575
C	4.05916	-1.58272	-2.08164
H	3.86121	-0.63532	-1.54991
C	5.57119	-1.88307	-1.95158
H	5.88868	-1.95946	-0.89822
H	6.16744	-1.08509	-2.42918
H	5.82995	-2.83583	-2.44699
C	3.68361	-1.38311	-3.56684
H	3.90518	-2.28546	-4.16426
H	4.27079	-0.55317	-3.99942
H	2.61447	-1.14648	-3.67444
C	0.95266	-3.33681	1.68854
H	1.15966	-2.32305	2.06825
C	1.34753	-4.35294	2.78355
H	0.78699	-4.15349	3.71441
H	2.42337	-4.30465	3.01973
H	1.12117	-5.39007	2.47932
C	-0.56271	-3.41715	1.41763
H	-0.84184	-4.39037	0.97560
H	-0.87323	-2.62262	0.70833
H	-1.13560	-3.28471	2.35354
C	4.71768	-2.42143	1.96200
H	4.11833	-3.33145	2.11844
H	5.37620	-2.28885	2.83853
H	5.35612	-2.59815	1.08164
C	2.78879	-0.51831	3.43335
H	2.04789	0.29331	3.35890
H	3.54434	-0.21506	4.18027
H	2.27433	-1.41267	3.82201
C	4.83779	0.58283	1.41377
H	5.67246	0.42657	2.12874
H	5.28383	0.43617	0.41178
C	4.28685	2.01808	1.56567
H	5.13092	2.73866	1.60814
H	3.76319	2.13467	2.53381
C	4.12542	2.54074	-1.46287
H	4.17954	1.49083	-1.79658
H	5.16152	2.90523	-1.34370
H	3.65316	3.12146	-2.27145
C	2.96366	4.57278	0.58279
H	2.25332	5.07979	-0.08828
H	3.94289	5.07449	0.48946
H	2.60773	4.71954	1.61606
C	0.41183	2.84088	0.12176
C	-0.18162	3.18247	1.38055
C	-1.28184	4.06033	1.41515
H	-1.73035	4.31755	2.38165
C	-1.79215	4.63621	0.24505
H	-2.63725	5.33188	0.29108
C	-1.19188	4.32956	-0.98034
H	-1.57357	4.79529	-1.89644
C	-0.09927	3.44238	-1.07387
C	0.36939	2.62618	2.69406
H	1.36954	2.22016	2.46493
C	-0.49347	1.45474	3.20908
H	-1.51827	1.79441	3.44091
H	-0.06715	1.01428	4.12824
H	-0.56495	0.65632	2.44746
C	0.53082	3.69825	3.79273
H	1.12064	4.55989	3.43742
H	1.04485	3.27014	4.67117
H	-0.44346	4.08349	4.14268
C	0.52388	3.21089	-2.45412
H	1.30199	2.43845	-2.34005
C	-0.49581	2.69312	-3.49258
H	-0.96474	1.74946	-3.17465
H	0.00768	2.50368	-4.45651
H	-1.29774	3.43057	-3.67725
C	1.19501	4.49917	-2.98823
H	0.45172	5.30309	-3.13636
H	1.67690	4.30740	-3.96351
H	1.96432	4.88341	-2.29835
C	-4.39334	-2.51779	-0.42983
C	-3.49722	-3.05137	-1.57470
H	-3.55576	-2.45806	-2.49579
H	-3.81691	-4.08303	-1.81523
H	-2.43699	-3.08968	-1.27650
C	-5.87941	-2.59387	-0.84559
H	-6.55901	-2.22120	-0.06298
H	-6.13795	-3.65427	-1.02724
H	-6.09131	-2.04855	-1.77731
C	-4.18228	-3.46546	0.77343
H	-3.14671	-3.44641	1.14471
H	-4.38827	-4.49748	0.43300
H	-4.86579	-3.26177	1.61201
C	-4.54472	0.54886	-1.29954
C	-4.34065	-0.01310	-2.72734
H	-3.29049	-0.28945	-2.91880
H	-4.61365	0.78234	-3.44572
H	-4.98421	-0.87837	-2.94827
C	-6.03848	0.87597	-1.08631
H	-6.68336	-0.01543	-1.11784
H	-6.36798	1.54898	-1.90030
H	-6.22535	1.40601	-0.13892
C	-3.71660	1.85363	-1.22167
H	-3.82382	2.39536	-0.27311
H	-4.05343	2.53104	-2.02845
H	-2.64041	1.66872	-1.37944
C	-4.39581	-0.23168	1.79729
C	-3.46269	-0.94051	2.81010
H	-3.56976	-2.03373	2.80493
H	-3.71377	-0.58848	3.82828
H	-2.40410	-0.69730	2.62375
C	-5.86424	-0.60579	2.09776
H	-6.57342	-0.12999	1.40340
H	-6.11617	-0.25593	3.11684
H	-6.04064	-1.69232	2.07911
C	-4.22010	1.28986	2.00980
H	-3.20772	1.64029	1.75069
H	-4.38443	1.51062	3.08128
H	-4.95185	1.88508	1.44233
O	1.01200	-0.22908	-2.08646
C	-0.25326	-0.56399	-1.90691
O	-1.01599	-0.97663	-2.79042

$S_{P,H}$

SCF (BP86) Energy = -2159.06112397
Enthalpy 0K = -2157.901976
Enthalpy 298K = -2157.901031
Free Energy 298K = -2158.078758
Lowest Frequency = 7.3330 cm^{-1}
Second Frequency = 9.9777 cm^{-1}
SCF (BP86-D3BJ) Energy = -2159.40024716
SCF (C6H6) Energy = -2159.06749147
SCF (BS2) Energy = -3306.05519267

Cu	2.50232	-0.01512	-0.07998
P	4.74930	-0.01091	-0.01479
Al	-1.72058	0.00191	-0.00973
Si	-4.29315	1.84034	-0.74250
Si	-4.26122	-1.80429	0.88491

N	-2.61511	1.61086	-0.14842
O	-0.10933	0.16483	1.03310
O	-0.16146	-0.17937	-1.12893
N	-2.62403	-1.59663	0.17878
C	-1.82978	2.78464	0.17266
C	-1.09880	3.48315	-0.84076
C	0.59384	-0.01086	-0.06562
C	-1.88177	-2.78163	-0.19810
C	-1.91761	-3.24622	-1.55162
C	-1.77077	3.25770	1.52253
C	-0.99775	4.39491	1.82416
H	-0.95587	4.74879	2.86116
C	-1.10223	-3.50177	0.76271
C	-1.10702	3.05329	-2.31010
H	-1.68209	2.11428	-2.37251
C	-0.34666	4.62131	-0.48577
H	0.20371	5.15758	-1.26819
C	-1.19587	-4.40157	-1.90660
H	-1.22827	-4.74944	-2.94599
C	-0.28855	5.08283	0.83344
H	0.30023	5.97159	1.08641
C	-2.70357	-2.51601	-2.64110
H	-3.23398	-1.68412	-2.14501
C	-2.51051	2.55782	2.66346
H	-3.09766	1.74135	2.20729
C	-0.44513	-5.11439	-0.96546
H	0.10200	-6.01725	-1.25869
C	-0.99634	-3.07416	2.22889
H	-1.54137	-2.12089	2.33134
C	-0.40497	-4.65746	0.35597
H	0.18190	-5.21111	1.09884
C	-4.46516	1.36726	-2.58481
H	-3.93976	2.08218	-3.23878
H	-5.52970	1.35860	-2.88042
H	-4.05492	0.36357	-2.78944
C	-5.56369	0.79163	0.23039
H	-5.46094	1.02599	1.30720
H	-6.54371	1.22172	-0.06575
C	-5.58178	-0.73862	0.00097
H	-5.55701	-0.97392	-1.08024
H	-6.54461	-1.15571	0.36447
C	0.31435	2.76164	-2.84208
H	0.95277	3.66289	-2.80845
H	0.26857	2.42554	-3.89343
H	0.79590	1.96568	-2.25205
C	5.41729	-1.72107	-0.69477
C	5.43398	1.45906	-1.11097
C	-4.29802	-1.32624	2.73352
H	-3.73104	-2.04206	3.35075
H	-5.33824	-1.30877	3.10541
H	-3.86712	-0.32461	2.90333
C	-1.80170	4.10498	-3.20657
H	-2.83568	4.30547	-2.87960
H	-1.83622	3.76127	-4.25613
H	-1.25731	5.06629	-3.18861
C	-4.80091	3.66142	-0.52066
H	-4.92948	3.91534	0.54462
H	-5.76362	3.84241	-1.02984
H	-4.05554	4.35661	-0.93847
C	-1.76044	-1.91089	-3.70717
H	-1.21933	-2.70557	-4.25226
H	-1.01110	-1.24783	-3.24582
H	-2.33548	-1.33011	-4.45095
C	-1.52367	1.92724	3.67373
H	-0.92279	2.70675	4.17655
H	-0.82798	1.23574	3.17213
H	-2.07039	1.37193	4.45728
C	-4.80666	-3.61810	0.69736
H	-4.99920	-3.87097	-0.35851
H	-5.74118	-3.78478	1.26102
H	-4.04856	-4.32360	1.07262
C	0.46672	-2.81907	2.65727
H	0.50378	-2.47596	3.70679
H	0.92840	-2.04112	2.02835
H	1.07594	-3.73813	2.58545
C	-1.65021	-4.10861	3.17461
H	-1.13359	-5.08360	3.11723
H	-2.71027	-4.28184	2.92488
H	-1.59864	-3.76553	4.22370
C	-3.49768	3.49947	3.38867
H	-4.05948	2.94847	4.16382
H	-4.22617	3.94470	2.69023
H	-2.97001	4.32989	3.89096
C	-3.76467	-3.41997	-3.30715
H	-4.35249	-2.84722	-4.04641
H	-4.46518	-3.84164	-2.56668
H	-3.29739	-4.26668	-3.84112
C	5.29854	0.23242	1.84903
C	5.26232	-1.75352	-2.23357
H	4.23241	-1.51768	-2.55076
H	5.48456	-2.77994	-2.57955
H	5.95931	-1.07909	-2.75424
C	5.16817	2.79959	-0.38623
H	4.11011	2.90977	-0.09453
H	5.40292	3.62195	-1.08715
H	5.79982	2.94354	0.50371
C	6.88394	-2.02954	-0.32656
H	7.58393	-1.26689	-0.70278
H	7.17175	-2.99548	-0.78248
H	7.03468	-2.12899	0.75974
C	4.48432	-2.82983	-0.14318
H	4.54656	-2.95409	0.94605
H	4.77402	-3.79318	-0.60304
H	3.42909	-2.63829	-0.40574
C	4.36440	1.30441	2.46817
H	4.50670	2.30778	2.04529
H	4.57614	1.36956	3.55183
H	3.30084	1.03179	2.35041
C	4.59110	1.49598	-2.41168
H	4.73713	0.61805	-3.05483
H	4.88775	2.38690	-2.99618
H	3.51273	1.58438	-2.19231
C	5.03129	-1.07567	2.63036
H	3.99138	-1.42374	2.51095
H	5.18717	-0.87183	3.70591
H	5.71471	-1.89313	2.35405
C	6.93513	1.35755	-1.45511
H	7.57362	1.33140	-0.55806
H	7.22821	2.24754	-2.04313
H	7.16916	0.47443	-2.07008
C	6.77407	0.64334	2.03831
H	7.47638	-0.09350	1.61769
H	6.98724	0.72163	3.12098
H	6.99905	1.62582	1.59465

$TS(S-E)_{P,H}$

SCF (BP86) Energy = -2159.00385018
Enthalpy 0K = -2157.847208
Enthalpy 298K = -2157.846264
Free Energy 298K = -2158.024037
Lowest Frequency = -207.6444 cm^{-1}
Second Frequency = 12.7026 cm^{-1}
SCF (BP86-D3BJ) Energy = -2159.35566603
SCF (C6H6) Energy = -2159.00827403
SCF (BS2) Energy = -3306.00307793

Cu	-2.22983	0.86518	-0.73461
P	-4.29197	0.54152	0.01621
Al	1.47671	-0.11335	-0.02197
Si	3.48845	-2.65178	-0.41293
Si	4.25844	0.73965	1.42630
N	1.87472	-1.91839	-0.08296
O	-0.14254	0.41957	-0.29588
O	0.07858	1.75759	-2.54734

N	2.84473	1.06801	0.36137
C	0.75242	-2.82490	0.03327
C	0.01128	-3.23644	-1.11764
C	-0.74508	1.41757	-1.77983
C	2.65279	2.43726	-0.07934
C	3.23728	2.87945	-1.30739
C	0.38277	-3.33348	1.31860
C	-0.70860	-4.21615	1.42719
H	-0.98741	-4.60228	2.41419
C	1.88911	3.35862	0.70294
C	0.34602	-2.74836	-2.52769
H	1.16914	-2.01944	-2.43249
C	-1.06713	-4.13003	-0.95726
H	-1.62475	-4.45265	-1.84469
C	3.02902	4.20625	-1.73023
H	3.47099	4.53785	-2.67706
C	-1.43428	-4.62146	0.30052
H	-2.27011	-5.32265	0.40102
C	4.07873	1.95482	-2.18975
H	4.19908	1.00855	-1.63389
C	1.13349	-2.91465	2.58308
H	2.09097	-2.47748	2.25038
C	2.27301	5.10657	-0.97243
H	2.12330	6.13506	-1.31841
C	1.25584	2.97388	2.04154
H	1.48889	1.90966	2.21845
C	1.71402	4.67611	0.23551
H	1.12614	5.37951	0.83731
C	4.10276	-2.20737	-2.16279
H	3.48386	-2.68248	-2.94139
H	5.14391	-2.54874	-2.30357
H	4.08237	-1.11831	-2.33658
C	4.83544	-2.10814	0.83254
H	4.48084	-2.33754	1.85569
H	5.66524	-2.82324	0.65018
C	5.37331	-0.66073	0.75385
H	5.66398	-0.40788	-0.28351
H	6.30913	-0.57886	1.34539
C	-0.84878	-2.02337	-3.18489
H	-1.69800	-2.71104	-3.34884
H	-0.56096	-1.60974	-4.16759
H	-1.19570	-1.19121	-2.54974
C	-5.19951	2.28055	0.00526
C	-5.22476	-0.69028	-1.19127
C	3.70268	0.24280	3.18358
H	3.21334	1.08412	3.70175
H	4.57477	-0.06490	3.78808
H	2.99371	-0.60153	3.16896
C	0.83268	-3.90233	-3.43465
H	1.71389	-4.41326	-3.01182
H	1.10546	-3.52251	-4.43544
H	0.04278	-4.66269	-3.57073
C	3.35183	-4.54403	-0.25685
H	3.13829	-4.84805	0.78150
H	4.30918	-5.00625	-0.55492
H	2.55640	-4.96210	-0.89393
C	3.36438	1.63320	-3.52254
H	3.22880	2.54773	-4.12727
H	2.36376	1.20593	-3.35321
H	3.95862	0.91989	-4.12180
C	0.35942	-1.80992	3.33861
H	-0.62084	-2.18581	3.68207
H	0.16831	-0.93618	2.69005
H	0.92077	-1.46318	4.22463
C	5.33216	2.30320	1.56460
H	5.83380	2.54244	0.61312
H	6.11257	2.14192	2.32885
H	4.74091	3.18524	1.85781
C	-0.28242	3.10975	2.01057
H	-0.71491	2.80601	2.98179
H	-0.70150	2.46561	1.21951
H	-0.59339	4.15236	1.81896
C	1.84910	3.79010	3.21297
H	1.64058	4.86861	3.09673
H	2.94370	3.67107	3.28174
H	1.40972	3.46819	4.17437
C	1.45596	-4.09244	3.52614
H	2.09158	-3.75014	4.36158
H	1.99050	-4.90037	2.99842
H	0.54448	-4.53029	3.97062
C	5.48821	2.52351	-2.46830
H	6.08872	1.79913	-3.04681
H	6.03272	2.75071	-1.53647
H	5.43949	3.45578	-3.05855
C	-4.30226	-0.19436	1.83063
C	-5.48781	2.69346	-1.45700
H	-4.57954	2.64398	-2.08116
H	-5.83470	3.74361	-1.45816
H	-6.27883	2.09119	-1.92958
C	-4.73209	-2.13275	-0.92855
H	-3.63304	-2.21625	-0.96431
H	-5.13884	-2.78382	-1.72488
H	-5.08458	-2.53969	0.03135
C	-6.51227	2.33162	0.81534
H	-7.25745	1.60252	0.46072
H	-6.95922	3.33814	0.70900
H	-6.35189	2.16385	1.89189
C	-4.19642	3.32524	0.55686
H	-3.94941	3.18010	1.61697
H	-4.64368	4.33199	0.45474
H	-3.25429	3.31547	-0.01931
C	-3.19749	-1.27895	1.87865
H	-3.42442	-2.17180	1.28166
H	-3.07807	-1.60861	2.92771
H	-2.22549	-0.88560	1.53579
C	-4.80056	-0.34272	-2.64084
H	-5.14259	0.64667	-2.97295
H	-5.24161	-1.09321	-3.32371
H	-3.70427	-0.38087	-2.75912
C	-3.86903	0.91023	2.82295
H	-2.91790	1.38251	2.52488
H	-3.70632	0.44062	3.81088
H	-4.62969	1.69444	2.95962
C	-6.76385	-0.65512	-1.07451
H	-7.11724	-0.89368	-0.05917
H	-7.19079	-1.41264	-1.75861
H	-7.18851	0.31787	-1.36739
C	-5.65058	-0.78662	2.29236
H	-6.46762	-0.04804	2.27608
H	-5.54620	-1.13950	3.33580
H	-5.95912	-1.65547	1.68998

$E_{P,H}$

SCF (BP86) Energy = -2159.02752545
Enthalpy 0K = -2157.869523
Enthalpy 298K = -2157.868579
Free Energy 298K = -2158.049022
Lowest Frequency = 6.1781 cm^{-1}
Second Frequency = 15.0510 cm^{-1}
SCF (BP86-D3BJ) Energy = -2159.38620210
SCF (C6H6) Energy = -2159.03070066
SCF (BS2) Energy = -3306.02879797

Cu	1.77426	-0.71786	-0.63264
P	3.91357	-0.02589	0.14753
Al	-1.36447	0.06439	0.14827
Si	-3.85667	2.05313	-0.67909
Si	-4.09381	-1.50725	1.04733
N	-2.17613	1.70210	-0.13685
O	0.33468	0.00999	0.32411
O	2.01632	-2.60992	-2.92367
N	-2.44596	-1.42758	0.33238
C	-1.30409	2.84617	0.03268
C	-0.58143	3.38943	-1.07297

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C   1.83900 -1.88002 -2.03469
C  -1.81337 -2.67552 -0.04138
C  -1.88529 -3.12659 -1.39695
C  -1.16805  3.44921  1.32215
C  -0.31433  4.55753  1.47814
H  -0.20940  5.01640  2.46773
C  -1.11279 -3.46635  0.92104
C  -0.67832  2.79335 -2.47784
H  -1.40385  1.96426 -2.42725
C   0.25668  4.50321 -0.86671
H   0.80814  4.91938 -1.71853
C  -1.22860 -4.31675 -1.76520
H  -1.27735 -4.65445 -2.80664
C   0.39649  5.09039  0.39570
H   1.04894  5.95936  0.53479
C  -2.64419 -2.33120 -2.45967
H  -3.27804 -1.60752 -1.91761
C  -1.90175  2.88591  2.53995
H  -2.71594  2.24851  2.15171
C  -0.52257 -5.08041 -0.82803
H  -0.02165 -6.00616 -1.13150
C  -1.01117 -3.05560  2.38983
H  -1.63942 -2.15902  2.51746
C  -0.47651 -4.65230  0.50376
H   0.06557 -5.25321  1.24371
C  -4.15811  1.54692 -2.49620
H  -3.61152  2.19650 -3.19896
H  -5.23407  1.62420 -2.73524
H  -3.84809  0.50609 -2.68844
C  -5.18436  1.15909  0.36594
H  -5.02938  1.40308  1.43422
H  -6.12736  1.67438  0.08680
C  -5.34767 -0.36554  0.16669
H  -5.37414 -0.62069 -0.90972
H  -6.33131 -0.69120  0.56568
C   0.66973  2.19548 -2.93735
H   1.44618  2.97646 -3.02701
H   0.56823  1.71006 -3.92486
H   1.02347  1.44057 -2.21199
C   4.94507 -1.65338  0.54167
C   4.88665  1.01344 -1.20735
C  -4.09244 -0.99295  2.88808
H  -3.62298 -1.75744  3.52859
H  -5.12793 -0.84605  3.24412
H  -3.55020 -0.04448  3.04583
C  -1.19516  3.81799 -3.51256
H  -2.17317  4.23534 -3.21856
H  -1.30848  3.34666 -4.50527
H  -0.49547  4.66513 -3.62652
C  -4.18195  3.92040 -0.50851
H  -4.14381  4.24324  0.54517
H  -5.18691  4.15591 -0.90043
H  -3.44676  4.52258 -1.06591
C  -1.67179 -1.52108 -3.34783
H  -0.98815 -2.19260 -3.89690
H  -1.04645 -0.83723 -2.74450
H  -2.22087 -0.91243 -4.08841
C  -0.96170  1.97997  3.37047
H  -0.13479  2.57224  3.80231
H  -0.50330  1.19095  2.74773
H  -1.50593  1.49929  4.20341
C  -4.75054 -3.28519  0.88703
H  -4.88212 -3.57031 -0.17017
H  -5.73221 -3.36454  1.38572
H  -4.07205 -4.02177  1.34600
C   0.43312 -2.64887  2.75341
H   0.49202 -2.30982  3.80371
H   0.76188 -1.82703  2.09508
H   1.12925 -3.49870  2.63355
C  -1.53555 -4.14696  3.34876
H  -0.92649 -5.06668  3.29209
H  -2.57870 -4.42588  3.12186
H  -1.49763 -3.79199  4.39412
C  -2.53966  3.97073  3.43204
H  -3.14144  3.50330  4.23117
H  -3.20015  4.63767  2.85214
H  -1.77917  4.60108  3.92638
C  -3.56912 -3.20869 -3.32951
H  -4.17226 -2.57716 -4.00532
H  -4.26053 -3.80441 -2.70985
H  -2.99890 -3.91096 -3.96298
C   3.76998  1.05569  1.77608
C   5.39799 -2.32282 -0.77712
H   4.55604 -2.49143 -1.46765
H   5.82418 -3.31412 -0.53329
H   6.17996 -1.75734 -1.30649
C   4.32076  2.45185 -1.25842
H   3.22363  2.46590 -1.35730
H   4.74204  2.95653 -2.14836
H   4.60034  3.05466 -0.38141
C   6.18159 -1.44622  1.44277
H   6.91015 -0.74446  1.00801
H   6.69622 -2.41735  1.57384
H   5.91423 -1.08580  2.44800
C   3.97085 -2.64922  1.21999
H   3.60920 -2.30787  2.19900
H   4.49586 -3.61108  1.37442
H   3.08920 -2.84886  0.58612
C   2.61965  2.06773  1.54356
H   2.86779  2.85371  0.81794
H   2.40932  2.57464  2.50407
H   1.69529  1.56228  1.21115
C   4.58907  0.38221 -2.59025
H   4.94316 -0.65324 -2.68769
H   5.09819  0.98136 -3.36877
H   3.50885  0.39916 -2.81145
C   3.31531  0.14324  2.93869
H   2.40195 -0.41756  2.68375
H   3.07209  0.78780  3.80383
H   4.09332 -0.56194  3.27096
C   6.41381  1.09253 -0.98999
H   6.67888  1.52723 -0.01386
H   6.85159  1.74360 -1.77067
H   6.90820  0.11255 -1.07577
C   5.05625  1.79940  2.19585
H   5.90536  1.12290  2.38192
H   4.85495  2.34254  3.13883
H   5.37024  2.55271  1.45645
```

$I_{P,A}$

SCF (BP86) Energy = -2692.79918540
Enthalpy 0K = -2691.405628
Enthalpy 298K = -2691.404684
Free Energy 298K = -2691.596381
Lowest Frequency = 14.4745 cm^{-1}
Second Frequency = 15.5302 cm^{-1}
SCF (BP86-D3BJ) Energy = -2693.21033140
SCF (C6H6) Energy = -2692.80284619
SCF (BS2) Energy = -3268.63692961

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P   4.61535 -0.04016 -0.55761
Al -0.09710 -0.00705 -0.13332
O  -2.05753  0.00726 -1.00768
N  -0.75925  1.80545  0.28809
N  -0.79249 -1.80210  0.31037
C  -2.79602  1.18476 -0.76277
C  -2.06202  2.16312 -0.06707
C  -2.74896  3.37504  0.18349
H  -2.21324  4.17977  0.69568
C  -4.10729  3.53911 -0.18121
C  -4.79242  2.47699 -0.81070
H  -5.84847  2.58439 -1.06198
C  -4.13787  1.26168 -1.11408
C  -4.77437  0.02674 -1.78851
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C	-4.15911	-1.21603	-1.10917
C	-4.82804	-2.41674	-0.79875
H	-5.88725	-2.51675	-1.04999
C	-4.15910	-3.48820	-0.15790
C	-2.80484	-3.34251	0.21147
H	-2.27946	-4.14577	0.73194
C	-2.09912	-2.13924	-0.05083
C	-2.81374	-1.15802	-0.75635
C	-4.94652	-4.78631	0.14108
C	-6.15497	-4.45838	1.05819
H	-5.81590	-4.03112	2.01743
H	-6.73342	-5.37460	1.27513
H	-6.84019	-3.73151	0.59114
C	-5.46365	-5.39308	-1.19039
H	-6.12254	-4.69286	-1.73052
H	-6.03892	-6.31647	-0.99635
H	-4.62366	-5.64676	-1.85974
C	-4.08423	-5.85296	0.85130
H	-3.21607	-6.15481	0.24028
H	-4.69065	-6.75650	1.03685
H	-3.71061	-5.49669	1.82657
C	-4.38366	0.02039	-3.29810
H	-3.28954	0.01025	-3.42820
H	-4.78142	0.91983	-3.79919
H	-4.79769	-0.87345	-3.79602
C	-6.31038	0.03942	-1.67196
H	-6.74373	-0.84396	-2.16959
H	-6.72992	0.92683	-2.17412
H	-6.63991	0.04467	-0.62005
C	-4.81369	4.87414	0.15674
C	-4.80862	5.08516	1.69442
H	-3.78338	5.11820	2.09868
H	-5.34499	4.26707	2.20519
H	-5.30536	6.03730	1.95520
C	-4.06327	6.05019	-0.52164
H	-4.05578	5.93276	-1.61906
H	-3.01647	6.11877	-0.18172
H	-4.55592	7.01029	-0.28350
C	-6.28127	4.90442	-0.32527
H	-6.73470	5.87828	-0.07146
H	-6.88957	4.12031	0.15790
H	-6.35678	4.77617	-1.41905
C	0.12122	2.87891	0.65338
C	0.49208	3.07451	2.01743
C	1.35094	4.14446	2.34015
H	1.63473	4.30842	3.38471
C	1.84331	5.00851	1.35418
H	2.50418	5.83821	1.62863
C	1.48127	4.80633	0.01719
H	1.86816	5.48165	-0.75507
C	0.62407	3.75369	-0.35866
C	0.26061	3.58610	-1.83650
H	-0.46310	2.75854	-1.91117
C	1.49269	3.18852	-2.67739
H	2.27203	3.97164	-2.64865
H	1.21083	3.03430	-3.73451
H	1.93056	2.24755	-2.29823
C	-0.41685	4.84813	-2.41470
H	-1.32412	5.10731	-1.84559
H	-0.71031	4.67910	-3.46581
H	0.26059	5.72056	-2.39557
C	-0.07634	2.18590	3.12526
H	-0.28615	1.19922	2.67241
C	0.89661	1.96865	4.30043
H	1.87750	1.59907	3.95699
H	0.47882	1.22900	5.00439
H	1.06506	2.89637	4.87605
C	-1.42524	2.74246	3.64087
H	-1.28624	3.74503	4.08463
H	-1.84772	2.08200	4.41893
H	-2.16291	2.82714	2.82702
C	0.06200	-2.88743	0.70017
C	0.52054	-3.81530	-0.28469
C	1.33803	-4.88834	0.12035
H	1.68968	-5.60537	-0.63067
C	1.71337	-5.05260	1.45877
H	2.34563	-5.89658	1.75600
C	1.27475	-4.12953	2.41640
H	1.57217	-4.26228	3.46141
C	0.44827	-3.04350	2.06539
C	-0.07704	-2.09353	3.14326
H	-0.19106	-1.09948	2.67113
C	-1.48188	-2.52964	3.62449
H	-2.19745	-2.57889	2.78854
H	-1.87546	-1.81886	4.37281
H	-1.43526	-3.52833	4.09534
C	0.87229	-1.93527	4.34624
H	0.94173	-2.86244	4.94293
H	0.49638	-1.14872	5.02209
H	1.89245	-1.65670	4.03185
C	0.16775	-3.67083	-1.76751
H	-0.55767	-2.84710	-1.86233
C	-0.50054	-4.94046	-2.33865
H	0.17792	-5.81165	-2.30936
H	-0.78957	-4.78146	-3.39243
H	-1.41026	-5.19661	-1.77101
C	1.41146	-3.27734	-2.59547
H	1.83100	-2.32385	-2.22418
H	1.14746	-3.14720	-3.66042
H	2.19864	-4.05028	-2.53227
C	5.34107	-0.23241	-2.37363
C	6.82331	0.16840	-2.53489
H	7.49287	-0.42872	-1.89601
H	7.00230	1.23294	-2.31905
H	7.12900	-0.00408	-3.58471
C	5.16942	-1.69154	-2.85580
H	4.13197	-2.04676	-2.74451
H	5.84126	-2.39802	-2.34476
H	5.41722	-1.73010	-3.93338
C	4.45416	0.63542	-3.30166
H	4.78086	0.48622	-4.34841
H	4.51609	1.71084	-3.08656
H	3.39403	0.33557	-3.23327
C	5.25814	-1.53152	0.54043
C	4.38179	-2.75921	0.19011
H	4.53489	-3.12811	-0.83292
H	3.30724	-2.54384	0.31937
H	4.63668	-3.58492	0.88009
C	4.97943	-1.21760	2.02919
H	5.17223	-2.13397	2.61766
H	3.92622	-0.93499	2.19616
H	5.62908	-0.42732	2.43565
C	6.75093	-1.88459	0.37052
H	7.41810	-1.04453	0.61891
H	6.99074	-2.22300	-0.64966
H	7.00089	-2.71866	1.05380
C	5.27370	1.64232	0.21171
C	6.74245	1.62149	0.68632
H	7.44832	1.38069	-0.12398
H	6.91045	0.91133	1.51116
H	7.00770	2.62613	1.06759
C	5.09431	2.78350	-0.81620
H	5.31349	3.74131	-0.30854
H	4.05809	2.84379	-1.18638
H	5.77872	2.70832	-1.67520
C	4.34148	1.98672	1.40076
H	4.61630	2.98571	1.78730
H	4.42031	1.27724	2.23585
H	3.28386	2.03543	1.08843
Cu	2.27312	-0.03198	-0.49795

TS(I-II)$_{P,A}$

SCF (BP86) Energy = -2881.38067951

Enthalpy 0K = -2879.972160

Enthalpy 298K = -2879.971216
Free Energy 298K = -2880.169396
Lowest Frequency = -145.5530 cm^{-1}
Second Frequency = 9.8776 cm^{-1}
SCF (BP86-D3BJ) Energy = -2881.81364980
SCF (C6H6) Energy = -2881.38424136
SCF (BS2) Energy = -3457.27980629

P	4.55999	-0.01868	-0.30968
Al	-0.13676	-0.01255	-0.22800
O	-2.09422	0.00580	-0.98133
N	-0.74066	1.79788	0.25861
N	-0.77649	-1.80609	0.27732
C	-2.80690	1.20153	-0.75108
C	-2.04270	2.17653	-0.08573
C	-2.70444	3.40393	0.15761
H	-2.14835	4.20814	0.64809
C	-4.06717	3.58460	-0.18495
C	-4.78491	2.52017	-0.77172
H	-5.84495	2.63880	-0.99968
C	-4.15743	1.28766	-1.06172
C	-4.83391	0.03977	-1.66881
C	-4.21310	-1.18628	-0.96400
C	-4.88788	-2.36086	-0.57690
H	-5.95930	-2.44914	-0.77504
C	-4.20990	-3.41927	0.07533
C	-2.83360	-3.29263	0.36335
H	-2.29966	-4.08757	0.88761
C	-2.11537	-2.12134	0.00948
C	-2.85230	-1.14355	-0.67486
C	-5.00943	-4.68233	0.47540
C	-6.15520	-4.28183	1.44281
H	-5.75175	-3.82091	2.36069
H	-6.74194	-5.17169	1.73427
H	-6.84848	-3.55885	0.98159
C	-5.61625	-5.33328	-0.79598
H	-6.28779	-4.64050	-1.33005
H	-6.20194	-6.23107	-0.52762
H	-4.82264	-5.63959	-1.49903
C	-4.13361	-5.73916	1.18400
H	-3.30925	-6.09089	0.53994
H	-4.75019	-6.61710	1.44393
H	-3.69700	-5.35053	2.12003
C	-4.49414	-0.03004	-3.18915
H	-3.40570	-0.05798	-3.35605
H	-4.89952	0.85447	-3.71027
H	-4.93628	-0.93667	-3.63735
C	-6.36449	0.08058	-1.50013
H	-6.82694	-0.81434	-1.94852
H	-6.78836	0.95444	-2.02191
H	-6.65792	0.13134	-0.43870
C	-4.74096	4.94309	0.12578
C	-4.69727	5.20733	1.65433
H	-3.66290	5.23878	2.03487
H	-5.23524	4.41719	2.20588
H	-5.17274	6.17619	1.89196
C	-3.98471	6.08062	-0.60955
H	-4.00306	5.92481	-1.70201
H	-2.92968	6.14102	-0.29458
H	-4.45475	7.05741	-0.39483
C	-6.21858	4.98540	-0.32386
H	-6.64796	5.97548	-0.09202
H	-6.82982	4.22913	0.19842
H	-6.32172	4.82337	-1.41083
C	0.10552	2.84964	0.75382
C	0.28854	3.02380	2.15871
C	1.09791	4.08555	2.61121
H	1.23549	4.23274	3.68779
C	1.71819	4.96422	1.71528
H	2.33735	5.78721	2.08915
C	1.52949	4.79105	0.33915
H	2.00401	5.48698	-0.36264
C	0.72641	3.74908	-0.16574
C	0.52046	3.63931	-1.67750
H	-0.10787	2.75315	-1.86350
C	1.85512	3.41982	-2.41905
H	2.54216	4.27590	-2.29113
H	1.68279	3.29093	-3.50247
H	2.36597	2.51584	-2.04246
C	-0.22069	4.87101	-2.24499
H	-1.20110	5.00271	-1.76014
H	-0.39052	4.75141	-3.32956
H	0.36325	5.79735	-2.09727
C	-0.42338	2.13134	3.17681
H	-0.71398	1.20494	2.64916
C	0.47076	1.74260	4.37150
H	1.41265	1.27227	4.04319
H	-0.06181	1.02975	5.02456
H	0.72849	2.61581	4.99684
C	-1.72562	2.79771	3.68251
H	-1.50158	3.74878	4.19899
H	-2.24702	2.13764	4.39837
H	-2.41565	3.01262	2.85129
C	0.06136	-2.91220	0.65427
C	0.42218	-3.89593	-0.31934
C	1.18936	-5.00553	0.08825
H	1.45636	-5.76853	-0.65211
C	1.61764	-5.15058	1.41146
H	2.20885	-6.02346	1.70972
C	1.28233	-4.17099	2.35462
H	1.62137	-4.28905	3.38816
C	0.50371	-3.04934	2.00607
C	0.09344	-2.03643	3.07917
H	0.10631	-1.03501	2.60575
C	-1.35356	-2.29182	3.56533
H	-2.07537	-2.26160	2.73502
H	-1.65196	-1.53226	4.30977
H	-1.42594	-3.28407	4.04622
C	1.04642	-1.99531	4.28982
H	0.98635	-2.92130	4.88927
H	0.77034	-1.16308	4.95759
H	2.09844	-1.85530	3.98852
C	-0.00162	-3.80506	-1.78867
H	-0.54124	-2.85265	-1.92368
C	-0.96307	-4.95094	-2.18116
H	-0.47254	-5.93572	-2.07934
H	-1.28032	-4.84284	-3.23335
H	-1.86635	-4.94841	-1.55066
C	1.21818	-3.79047	-2.73791
H	1.89972	-2.95555	-2.50959
H	0.88623	-3.68278	-3.78580
H	1.79571	-4.72957	-2.66976
C	5.69726	0.22916	-1.89616
C	7.17368	0.56242	-1.58921
H	7.66636	-0.20603	-0.97407
H	7.29134	1.53465	-1.08560
H	7.72856	0.62584	-2.54484
C	5.64078	-1.04572	-2.77071
H	4.60459	-1.34457	-2.99521
H	6.17272	-1.89984	-2.32457
H	6.13605	-0.82357	-3.73472
C	5.07975	1.36406	-2.75046
H	5.68422	1.47453	-3.67096
H	5.07167	2.33921	-2.24550
H	4.05110	1.11908	-3.05638
C	4.97635	-1.76386	0.48191
C	4.21484	-2.82449	-0.35003
H	4.57313	-2.91190	-1.38462
H	3.13176	-2.61241	-0.37424
H	4.33930	-3.81151	0.13218
C	4.37776	-1.82784	1.90587
H	4.44793	-2.87138	2.26407
H	3.30855	-1.55819	1.91018
H	4.91311	-1.19503	2.63043

C	6.47490	-2.12636	0.55200
H	7.06194	-1.39929	1.13472
H	6.93453	-2.22163	-0.44399
H	6.57857	-3.10920	1.05003
C	4.98694	1.38580	0.99308
C	6.31414	1.19186	1.75824
H	7.18813	1.14379	1.09038
H	6.31231	0.28868	2.38822
H	6.46259	2.05541	2.43430
C	5.01766	2.75729	0.27954
H	5.08406	3.54573	1.05190
H	4.09470	2.94665	-0.29268
H	5.88617	2.87974	-0.38582
C	3.80970	1.44862	1.99769
H	3.97115	2.30529	2.67801
H	3.71814	0.54560	2.61672
H	2.84690	1.61358	1.48417
Cu	2.22486	-0.01550	-0.72003
C	1.03036	-0.05705	-3.04532
O	-0.11341	0.26042	-3.20335
O	2.14895	-0.39022	-3.33487

$II_{P,A}$

SCF (BP86) Energy = -2881.41502890
Enthalpy 0K = -2880.004826
Enthalpy 298K = -2880.003882
Free Energy 298K = -2880.198706
Lowest Frequency = 15.5124 cm^{-1}
Second Frequency = 18.9508 cm^{-1}
SCF (BP86-D3BJ) Energy = -2881.84581709
SCF (C6H6) Energy = -2881.42057691
SCF (BS2) Energy = -3457.31262663

P	4.67105	0.03516	-0.01930
Al	-0.39816	0.00634	-0.70499
O	-2.38031	-0.01748	-1.06778
N	-0.83588	1.78912	-0.08280
N	-0.79001	-1.77279	-0.04045
C	-3.05496	1.16181	-0.70303
C	-2.18890	2.15100	-0.20329
C	-2.81488	3.37797	0.12266
H	-2.19346	4.20430	0.47940
C	-4.22024	3.53843	0.01515
C	-5.02080	2.45087	-0.39748
H	-6.10550	2.55813	-0.43755
C	-4.43920	1.21673	-0.76586
C	-5.18964	-0.05033	-1.24002
C	-4.41521	-1.27969	-0.70805
C	-4.96802	-2.50090	-0.27428
H	-6.05295	-2.63350	-0.29134
C	-4.14316	-3.55682	0.18502
C	-2.74348	-3.37614	0.25479
H	-2.10178	-4.16976	0.64141
C	-2.14164	-2.15190	-0.13657
C	-3.02836	-1.19777	-0.65836
C	-4.80824	-4.88462	0.62100
C	-5.79960	-4.60929	1.78302
H	-5.27489	-4.18348	2.65542
H	-6.28954	-5.54728	2.10094
H	-6.59152	-3.90037	1.48915
C	-5.58180	-5.49025	-0.58048
H	-6.36312	-4.80604	-0.95129
H	-6.07284	-6.43531	-0.28590
H	-4.89896	-5.70585	-1.42012
C	-3.78182	-5.93184	1.10658
H	-3.05786	-6.19615	0.31673
H	-4.30769	-6.85726	1.39898
H	-3.21762	-5.57805	1.98655
C	-5.16936	-0.08718	-2.79898
H	-4.13793	-0.08619	-3.18638
H	-5.69140	0.79510	-3.20778
H	-5.67407	-0.99770	-3.16547
C	-6.65279	-0.05331	-0.75630
H	-7.17816	-0.95288	-1.11723
H	-7.19646	0.81657	-1.16011
H	-6.71910	-0.02714	0.34373
C	-4.84201	4.91532	0.35579
C	-4.49588	5.31067	1.81504
H	-3.40762	5.38831	1.97372
H	-4.89012	4.56809	2.53000
H	-4.93918	6.29223	2.06198
C	-4.27133	5.98701	-0.61070
H	-4.51065	5.73963	-1.65921
H	-3.17506	6.07029	-0.52648
H	-4.70309	6.97888	-0.38485
C	-6.38093	4.91793	0.21603
H	-6.77277	5.91937	0.46466
H	-6.85778	4.19545	0.90100
H	-6.70104	4.68258	-0.81367
C	0.05306	2.82412	0.37942
C	0.25779	3.01820	1.77973
C	1.11001	4.05961	2.20008
H	1.26560	4.22303	3.27236
C	1.74465	4.90002	1.27820
H	2.39715	5.70822	1.62690
C	1.52270	4.71472	-0.09181
H	2.00006	5.38955	-0.81095
C	0.67557	3.69343	-0.56844
C	0.38566	3.60348	-2.06892
H	-0.09882	2.63125	-2.25700
C	1.65991	3.66412	-2.93578
H	2.16174	4.64624	-2.86718
H	1.40254	3.50052	-3.99611
H	2.38304	2.88743	-2.64343
C	-0.60274	4.71284	-2.50372
H	-1.55368	4.64611	-1.95163
H	-0.82720	4.62451	-3.58133
H	-0.17198	5.71562	-2.32876
C	-0.47110	2.18186	2.83570
H	-0.92100	1.31744	2.31581
C	0.46933	1.64413	3.93362
H	1.27706	1.02284	3.51629
H	-0.10190	1.02712	4.64889
H	0.93463	2.46117	4.51307
C	-1.61999	2.98526	3.49096
H	-1.22810	3.87758	4.01203
H	-2.14743	2.36395	4.23640
H	-2.35639	3.31750	2.74394
C	0.11979	-2.83586	0.30768
C	0.53400	-3.76173	-0.69893
C	1.34171	-4.85440	-0.32278
H	1.65108	-5.57473	-1.08852
C	1.74566	-5.04005	1.00265
H	2.36397	-5.90199	1.27716
C	1.35106	-4.11783	1.98011
H	1.67131	-4.27006	3.01527
C	0.53686	-3.01116	1.66414
C	0.07401	-2.06450	2.77760
H	-0.02350	-1.05762	2.32860
C	-1.31920	-2.46129	3.32437
H	-2.08573	-2.47271	2.53561
H	-1.64027	-1.75168	4.10762
H	-1.27973	-3.46877	3.77705
C	1.06296	-1.97029	3.95731
H	1.11661	-2.91716	4.52343
H	0.72952	-1.19453	4.66545
H	2.08499	-1.71438	3.63115
C	0.10053	-3.64153	-2.16258
H	-0.43527	-2.68529	-2.27788
C	-0.87171	-4.77927	-2.55517
H	-0.38416	-5.76756	-2.47189
H	-1.20225	-4.65561	-3.60139
H	-1.76685	-4.78256	-1.91234
C	1.30784	-3.61397	-3.12680

H	1.99268	-2.78232	-2.89745
H	0.95846	-3.47934	-4.16498
H	1.88188	-4.55736	-3.08966
C	5.74927	0.53461	-1.58491
C	7.21402	0.89267	-1.25134
H	7.75323	0.07278	-0.75218
H	7.29911	1.79402	-0.62448
H	7.74565	1.10802	-2.19737
C	5.72795	-0.61298	-2.62236
H	4.69752	-0.90368	-2.88424
H	6.29467	-1.50093	-2.30328
H	6.20602	-0.23997	-3.54745
C	5.05454	1.73511	-2.27342
H	5.65327	2.01975	-3.15936
H	4.96807	2.62509	-1.63599
H	4.05251	1.44802	-2.63091
C	5.15801	-1.78314	0.51932
C	4.41915	-2.74760	-0.44116
H	4.75030	-2.66733	-1.48490
H	3.32721	-2.58998	-0.41222
H	4.60459	-3.78580	-0.10949
C	4.59924	-2.06880	1.93081
H	4.74174	-3.14351	2.14724
H	3.51579	-1.87466	1.98536
H	5.11016	-1.50477	2.72638
C	6.67187	-2.08678	0.51038
H	7.24377	-1.42241	1.17697
H	7.11156	-2.02730	-0.49706
H	6.82483	-3.12268	0.86774
C	5.05383	1.27874	1.44143
C	6.39390	1.03007	2.16688
H	7.26107	1.10404	1.49263
H	6.42977	0.05028	2.66782
H	6.51991	1.79924	2.95213
C	5.02761	2.73239	0.91439
H	5.08491	3.41186	1.78503
H	4.08890	2.96777	0.38583
H	5.87931	2.97168	0.25977
C	3.87986	1.16323	2.44239
H	4.03029	1.89973	3.25368
H	3.79586	0.17133	2.90759
H	2.92029	1.40231	1.95380
Cu	2.44534	0.03588	-0.68184
C	1.33348	-0.02295	-2.27471
O	0.03227	-0.01580	-2.50007
O	2.21148	-0.06663	-3.15108

$S_{P,A}$

SCF (BP86) Energy = -2881.45587901
Enthalpy 0K = -2880.046112
Enthalpy 298K = -2880.045168
Free Energy 298K = -2880.245067
Lowest Frequency = 5.6688 cm^{-1}
Second Frequency = 9.9661 cm^{-1}
SCF (BP86-D3BJ) Energy = -2881.86081190
SCF (C6H6) Energy = -2881.46331606
SCF (BS2) Energy = -3457.35499786

P	5.73791	-0.01470	-0.49496
Al	-0.70285	0.00212	0.06446
O	-2.44889	-0.00413	-1.01136
N	-1.27810	1.81579	0.35206
N	-1.28613	-1.80430	0.39227
C	-3.21109	1.17535	-0.87254
C	-2.53519	2.17346	-0.14472
C	-3.23643	3.39169	0.00405
H	-2.74836	4.21104	0.53999
C	-4.55359	3.54427	-0.49592
C	-5.18445	2.46308	-1.14938
H	-6.20979	2.56794	-1.50654
C	-4.51253	1.23464	-1.34912
C	-5.08292	-0.01300	-2.06177
C	-4.50374	-1.25981	-1.35522
C	-5.16253	-2.49068	-1.15715
H	-6.18792	-2.61058	-1.51649
C	-4.52422	-3.57036	-0.49922
C	-3.21698	-3.40656	0.01005
H	-2.72198	-4.21661	0.54931
C	-2.52784	-2.17528	-0.13147
C	-3.20181	-1.18987	-0.87269
C	-5.29403	-4.90309	-0.33724
C	-6.59249	-4.65437	0.47571
H	-6.35802	-4.26640	1.48177
H	-7.15934	-5.59560	0.59374
H	-7.25374	-3.92383	-0.01942
C	-5.66482	-5.45744	-1.73860
H	-6.29345	-4.75061	-2.30548
H	-6.22483	-6.40531	-1.64280
H	-4.75830	-5.65372	-2.33657
C	-4.46746	-5.98000	0.39979
H	-3.53593	-6.22426	-0.13924
H	-5.05837	-6.90886	0.48161
H	-4.19999	-5.66499	1.42300
C	-4.59235	-0.00731	-3.54203
H	-3.49180	-0.00424	-3.59760
H	-4.96574	0.89024	-4.06481
H	-4.96103	-0.90363	-4.07029
C	-6.62407	-0.01929	-2.04531
H	-7.01396	-0.90471	-2.57405
H	-7.02144	0.86535	-2.56966
H	-7.02045	-0.02352	-1.01678
C	-5.27327	4.89891	-0.28958
C	-5.39054	5.20085	1.22805
H	-4.40126	5.26110	1.71124
H	-5.96962	4.41464	1.74228
H	-5.90274	6.16650	1.39062
C	-4.45782	6.02816	-0.97314
H	-4.36832	5.84766	-2.05830
H	-3.43864	6.10468	-0.55945
H	-4.95439	7.00472	-0.82787
C	-6.69739	4.90891	-0.88870
H	-7.16245	5.89605	-0.72219
H	-7.34773	4.15214	-0.41668
H	-6.68645	4.72549	-1.97715
C	-0.45172	2.88343	0.85285
C	-0.38753	3.14847	2.25027
C	0.40370	4.22306	2.70307
H	0.44849	4.43791	3.77676
C	1.12358	5.02495	1.81068
H	1.72548	5.86193	2.18205
C	1.06562	4.74993	0.43916
H	1.62933	5.37742	-0.26112
C	0.29153	3.68646	-0.06504
C	0.25670	3.44669	-1.57619
H	-0.28299	2.50115	-1.74930
C	1.67157	3.27834	-2.17240
H	2.27414	4.19853	-2.06576
H	1.60538	3.04691	-3.25012
H	2.20976	2.44983	-1.68017
C	-0.50862	4.57418	-2.30725
H	-1.54051	4.66364	-1.93080
H	-0.55636	4.37066	-3.39190
H	-0.00799	5.54982	-2.16949
C	-1.17023	2.31937	3.26726
H	-1.57477	1.44338	2.72946
C	-0.26739	1.80286	4.40715
H	0.57529	1.21350	4.01034
H	-0.84552	1.16132	5.09429
H	0.14836	2.63146	5.00781
C	-2.37123	3.11241	3.83259
H	-2.03222	4.01955	4.36492
H	-2.94419	2.49587	4.54791
H	-3.05662	3.42557	3.02792
C	-0.46451	-2.85582	0.93328

C	0.27699	-3.69491	0.04814
C	1.04777	-4.74096	0.59347
H	1.60950	-5.39714	-0.08161
C	1.10739	-4.95837	1.97410
H	1.70848	-5.78008	2.37935
C	0.39299	-4.11712	2.83569
H	0.44730	-4.28736	3.91577
C	-0.39842	-3.06119	2.34272
C	-1.19380	-2.18746	3.31433
H	-1.35260	-1.21271	2.81747
C	-2.59074	-2.79233	3.59473
H	-3.17123	-2.91811	2.66685
H	-3.16762	-2.14033	4.27481
H	-2.49408	-3.78291	4.07535
C	-0.45261	-1.92703	4.64086
H	-0.35809	-2.84518	5.24794
H	-1.01432	-1.19901	5.25043
H	0.55910	-1.52376	4.46986
C	0.25056	-3.51060	-1.47123
H	-0.29519	-2.57662	-1.68354
C	-0.49749	-4.67070	-2.16857
H	0.00962	-5.63634	-1.99028
H	-0.53517	-4.50704	-3.26031
H	-1.53294	-4.75464	-1.80038
C	1.66953	-3.35190	-2.06131
H	2.19672	-2.50208	-1.59442
H	1.61048	-3.16057	-3.14735
H	2.27836	-4.26241	-1.91536
C	6.33354	-0.46930	-2.30293
C	7.80973	-0.13054	-2.60062
H	8.50662	-0.64357	-1.91923
H	8.01463	0.95047	-2.55235
H	8.05179	-0.45920	-3.62885
C	6.10115	-1.97841	-2.55102
H	5.06238	-2.27887	-2.33353
H	6.78537	-2.62206	-1.97720
H	6.28467	-2.18312	-3.62212
C	5.40430	0.28014	-3.29248
H	5.64305	-0.05288	-4.31993
H	5.52384	1.37144	-3.26467
H	4.34186	0.04790	-3.10173
C	6.39798	-1.34265	0.78270
C	5.48939	-2.59294	0.65812
H	5.58656	-3.11173	-0.30478
H	4.42518	-2.33734	0.80365
H	5.77158	-3.31127	1.45045
C	6.19660	-0.80619	2.21960
H	6.41503	-1.62758	2.92687
H	5.15576	-0.48792	2.39927
H	6.87260	0.02542	2.47062
C	7.87666	-1.74167	0.59220
H	8.56108	-0.88263	0.67337
H	8.05976	-2.23756	-0.37407
H	8.15698	-2.46285	1.38287
C	6.38820	1.76562	-0.00410
C	7.87962	1.81992	0.38942
H	8.54365	1.47378	-0.41836
H	8.10013	1.23030	1.29308
H	8.15198	2.86839	0.61392
C	6.13822	2.74050	-1.17885
H	6.35631	3.76574	-0.82665
H	5.08673	2.72611	-1.51166
H	6.78965	2.55144	-2.04586
C	5.50922	2.26898	1.17019
H	5.78371	3.31799	1.38848
H	5.64396	1.69508	2.09656
H	4.43612	2.25160	0.91114
Cu	3.49105	-0.00947	-0.40652
C	1.59072	-0.00563	-0.22658
O	1.01647	0.01037	0.95348
O	0.72503	-0.01801	-1.22101

$TS(S-E)_{P,A}$

SCF (BP86) Energy = -2881.39731620
Enthalpy 0K = -2879.990049
Enthalpy 298K = -2879.989105
Free Energy 298K = -2880.189370
Lowest Frequency = -214.8819 cm^{-1}
Second Frequency = 5.2396 cm^{-1}
SCF (BP86-D3BJ) Energy = -2881.81499226
SCF (C6H6) Energy = -2881.40233751
SCF (BS2) Energy = -3457.30259026

P	5.13862	-0.07189	-0.33731
Al	-0.46603	-0.00762	-0.21495
O	-2.29976	0.04926	-1.08641
N	-0.97311	1.77750	0.30135
N	-1.07782	-1.76719	0.27710
C	-3.02017	1.23394	-0.78788
C	-2.27119	2.16866	-0.05021
C	-2.94687	3.37376	0.25402
H	-2.40365	4.15067	0.79982
C	-4.30448	3.56504	-0.10221
C	-5.00291	2.53788	-0.77494
H	-6.05835	2.66710	-1.01810
C	-4.36141	1.33051	-1.13178
C	-5.00693	0.12427	-1.85231
C	-4.41139	-1.14878	-1.20946
C	-5.09490	-2.34709	-0.92329
H	-6.15268	-2.43375	-1.18471
C	-4.43960	-3.43444	-0.29399
C	-3.09128	-3.30396	0.10453
H	-2.58209	-4.11749	0.62501
C	-2.37305	-2.10293	-0.12929
C	-3.06852	-1.11954	-0.85015
C	-5.23642	-4.73613	-0.03824
C	-6.45590	-4.42671	0.87054
H	-6.12875	-4.02675	1.84559
H	-7.04088	-5.34577	1.05508
H	-7.13193	-3.68493	0.41357
C	-5.73730	-5.30505	-1.39261
H	-6.38695	-4.58878	-1.92267
H	-6.31775	-6.23120	-1.23034
H	-4.88921	-5.54383	-2.05704
C	-4.38771	-5.82552	0.65368
H	-3.51100	-6.11103	0.04730
H	-4.99939	-6.73224	0.80246
H	-4.02923	-5.50101	1.64569
C	-4.60699	0.16479	-3.35891
H	-3.51294	0.14483	-3.48582
H	-4.99159	1.08556	-3.83033
H	-5.03041	-0.70597	-3.88848
C	-6.54301	0.15065	-1.74206
H	-6.98306	-0.71027	-2.27196
H	-6.94935	1.05950	-2.21581
H	-6.87830	0.12353	-0.69229
C	-4.99508	4.89283	0.29226
C	-4.97431	5.04639	1.83657
H	-3.94569	5.05531	2.23325
H	-5.51457	4.21545	2.32192
H	-5.45955	5.99294	2.13594
C	-4.23857	6.08514	-0.35020
H	-4.24695	6.01046	-1.45130
H	-3.18638	6.12782	-0.02351
H	-4.71668	7.04061	-0.06832
C	-6.46670	4.95436	-0.17424
H	-6.90863	5.92139	0.12201
H	-7.07780	4.15732	0.28368
H	-6.55377	4.87066	-1.27146
C	-0.06433	2.82494	0.69137
C	0.28587	2.99579	2.06358
C	1.14308	4.05725	2.41665
H	1.41392	4.20298	3.46674
C	1.64897	4.93860	1.45336

H	2.30263	5.76553	1.75225
C	1.31601	4.75169	0.10785
H	1.72024	5.43441	-0.64827
C	0.47258	3.69978	-0.30151
C	0.16800	3.54264	-1.79282
H	-0.38248	2.59583	-1.92339
C	1.45873	3.44420	-2.63486
H	2.03971	4.38331	-2.60365
H	1.21169	3.24085	-3.69127
H	2.10435	2.62711	-2.27250
C	-0.72585	4.68966	-2.31876
H	-1.67972	4.73995	-1.77014
H	-0.95339	4.54094	-3.38914
H	-0.21820	5.66589	-2.21613
C	-0.27853	2.07496	3.14839
H	-0.39006	1.06982	2.69801
C	0.64351	1.94150	4.37641
H	1.67060	1.65697	4.08982
H	0.25372	1.17061	5.06087
H	0.70012	2.88245	4.95216
C	-1.68858	2.52877	3.59599
H	-1.64357	3.53800	4.04380
H	-2.09625	1.83882	4.35625
H	-2.39292	2.56106	2.75025
C	-0.26752	-2.82847	0.81781
C	0.42701	-3.70963	-0.06519
C	1.18822	-4.75816	0.48810
H	1.71578	-5.44519	-0.18310
C	1.27623	-4.94623	1.87243
H	1.86930	-5.77180	2.28132
C	0.59352	-4.07677	2.72993
H	0.65593	-4.23139	3.81254
C	-0.18544	-3.01417	2.22902
C	-0.95824	-2.12658	3.20605
H	-1.25282	-1.21463	2.65557
C	-2.25930	-2.81750	3.68088
H	-2.91868	-3.05848	2.83183
H	-2.81792	-2.16134	4.37189
H	-2.02950	-3.75675	4.21589
C	-0.11115	-1.70029	4.42250
H	0.14576	-2.55937	5.06722
H	-0.67744	-0.98869	5.04803
H	0.83079	-1.21649	4.11485
C	0.34042	-3.57765	-1.58644
H	-0.11851	-2.59980	-1.80821
C	-0.56318	-4.67760	-2.19352
H	-0.14712	-5.68258	-1.99761
H	-0.64209	-4.55204	-3.28790
H	-1.58031	-4.63979	-1.77111
C	1.72856	-3.59860	-2.25960
H	2.38164	-2.81339	-1.84029
H	1.62978	-3.41321	-3.34312
H	2.23456	-4.57275	-2.13510
C	6.28302	1.33886	-1.07431
C	7.46733	1.74606	-0.17177
H	8.13943	0.90268	0.05173
H	7.13880	2.18652	0.78255
H	8.06663	2.51590	-0.69374
C	6.82479	0.88905	-2.45113
H	6.01331	0.55265	-3.11846
H	7.58114	0.09234	-2.37996
H	7.31215	1.75745	-2.93240
C	5.38021	2.56752	-1.34896
H	5.98714	3.34597	-1.84894
H	4.95183	3.01306	-0.44152
H	4.54801	2.30438	-2.02464
C	6.03395	-1.80535	-0.53147
C	5.86900	-2.26027	-2.00370
H	6.41785	-1.63274	-2.71871
H	4.80774	-2.26997	-2.30496
H	6.25965	-3.29099	-2.09851
C	5.29739	-2.85384	0.33476
H	5.70459	-3.85210	0.08782
H	4.21416	-2.88070	0.12999
H	5.44739	-2.70168	1.41432
C	7.53016	-1.79935	-0.15111
H	7.70177	-1.47806	0.88808
H	8.13236	-1.15798	-0.81374
H	7.92765	-2.82731	-0.24865
C	4.79684	0.28082	1.56013
C	5.97020	-0.04341	2.50835
H	6.88455	0.51960	2.26276
H	6.21919	-1.11632	2.52163
H	5.68067	0.23219	3.54004
C	4.40161	1.76654	1.72736
H	4.05039	1.91383	2.76536
H	3.56865	2.05330	1.06427
H	5.24199	2.46072	1.57147
C	3.54545	-0.54537	1.95428
H	3.25390	-0.25793	2.98252
H	3.71705	-1.63013	1.95778
H	2.69265	-0.33444	1.28467
Cu	3.20326	-0.09036	-1.41523
C	1.70075	-0.10893	-2.58097
O	1.16464	-0.04612	-0.77923
O	0.82267	-0.13723	-3.36627

$E_{P,A}$

SCF (BP86) Energy = -2881.41731184
Enthalpy 0K = -2880.008764
Enthalpy 298K = -2880.007820
Free Energy 298K = -2880.207458
Lowest Frequency = 12.6741 cm^{-1}
Second Frequency = 14.4994 cm^{-1}
SCF (BP86-D3BJ) Energy = -2881.83942324
SCF (C6H6) Energy = -2881.42144881
SCF (BS2) Energy = -3457.32535258

P	4.83787	0.03978	-0.30533
Al	-0.37593	0.04024	-0.05196
O	-2.17462	-0.03017	-1.06320
N	-1.06109	1.78716	0.39601
N	-0.92915	-1.75664	0.39445
C	-2.99160	1.10220	-0.81631
C	-2.35668	2.08692	-0.03769
C	-3.12884	3.24499	0.21659
H	-2.67400	4.05595	0.79291
C	-4.47135	3.34387	-0.22304
C	-5.05482	2.27203	-0.93455
H	-6.09929	2.32915	-1.24381
C	-4.31226	1.11057	-1.24456
C	-4.83049	-0.13734	-1.99517
C	-4.19502	-1.36341	-1.30219
C	-4.82020	-2.59815	-1.03910
H	-5.85304	-2.75275	-1.36178
C	-4.14088	-3.63386	-0.35126
C	-2.82903	-3.41541	0.12233
H	-2.30517	-4.18755	0.68931
C	-2.17209	-2.17496	-0.08772
C	-2.88057	-1.24344	-0.86285
C	-4.87508	-4.97495	-0.11222
C	-6.16128	-4.71897	0.71796
H	-5.91486	-4.27953	1.69969
H	-6.70189	-5.66684	0.89176
H	-6.85130	-4.02837	0.20513
C	-5.26277	-5.59931	-1.47913
H	-5.91943	-4.93249	-2.06244
H	-5.79876	-6.55382	-1.32878
H	-4.36517	-5.80263	-2.08809
C	-4.00779	-5.99835	0.65347
H	-3.08238	-6.24606	0.10549
H	-4.57467	-6.93565	0.78963
H	-3.72659	-5.63181	1.65562
C	-4.33853	-0.07827	-3.47349

H	-3.23942	-0.02646	-3.52913
H	-4.75100	0.81275	-3.97742
H	-4.66865	-0.97772	-4.02127
C	-6.36889	-0.21169	-1.98434
H	-6.71676	-1.10206	-2.53387
H	-6.80243	0.66663	-2.49050
H	-6.76844	-0.25630	-0.95797
C	-5.27773	4.61681	0.13068
C	-5.37885	4.74775	1.67402
H	-4.38394	4.81891	2.14378
H	-5.89439	3.87472	2.10979
H	-5.94767	5.65477	1.94761
C	-4.56181	5.86813	-0.44179
H	-4.48158	5.80898	-1.54095
H	-3.54354	5.98117	-0.03413
H	-5.12663	6.78354	-0.18888
C	-6.71230	4.58516	-0.44217
H	-7.23846	5.51774	-0.17439
H	-7.30056	3.74505	-0.03420
H	-6.71303	4.50621	-1.54321
C	-0.23568	2.89716	0.79431
C	0.10540	3.08027	2.16672
C	0.91949	4.17406	2.52199
H	1.18911	4.32518	3.57156
C	1.38682	5.07906	1.56080
H	2.01291	5.92668	1.86056
C	1.04495	4.89311	0.21713
H	1.41234	5.59939	-0.53660
C	0.24037	3.81183	-0.19255
C	-0.07877	3.65956	-1.68215
H	-0.72799	2.77711	-1.80126
C	1.19957	3.39672	-2.50719
H	1.90864	4.24101	-2.43886
H	0.94989	3.25279	-3.57380
H	1.70689	2.48722	-2.14252
C	-0.84704	4.87993	-2.23631
H	-1.78687	5.04241	-1.68457
H	-1.09804	4.72581	-3.30067
H	-0.24486	5.80345	-2.16697
C	-0.43271	2.13632	3.24434
H	-0.45986	1.12070	2.80480
C	0.44591	2.07591	4.50850
H	1.49845	1.84912	4.26758
H	0.07544	1.29163	5.18891
H	0.42226	3.02630	5.07111
C	-1.88677	2.50044	3.62931
H	-1.92642	3.51509	4.06512
H	-2.27908	1.79304	4.38159
H	-2.55639	2.47661	2.75548
C	-0.06973	-2.77239	0.94307
C	0.63562	-3.65146	0.06761
C	1.45988	-4.64770	0.62682
H	1.99710	-5.33250	-0.03974
C	1.60103	-4.78394	2.01258
H	2.24555	-5.56618	2.42850
C	0.90365	-3.91908	2.86414
H	1.00892	-4.03530	3.94763
C	0.05869	-2.91202	2.35635
C	-0.74627	-2.03696	3.31898
H	-0.97713	-1.09486	2.78820
C	-2.09972	-2.70156	3.67033
H	-2.70224	-2.89228	2.76811
H	-2.68757	-2.05330	4.34436
H	-1.93506	-3.66606	4.18405
C	0.01759	-1.68231	4.60989
H	0.18433	-2.56836	5.24797
H	-0.56920	-0.96543	5.20942
H	0.99972	-1.22942	4.39451
C	0.50937	-3.56675	-1.45489
H	-0.09106	-2.67189	-1.68929
C	-0.22544	-4.79837	-2.03383
H	0.33419	-5.72885	-1.82936
H	-0.33398	-4.70520	-3.12901
H	-1.23278	-4.90089	-1.59914
C	1.88112	-3.39272	-2.13918
H	2.39303	-2.49019	-1.75620
H	1.75766	-3.28032	-3.23101
H	2.54207	-4.26085	-1.96680
C	5.85312	1.59967	-0.94342
C	6.98439	2.07579	-0.00660
H	7.73501	1.29339	0.18508
H	6.60521	2.43472	0.96247
H	7.50854	2.92620	-0.48330
C	6.45460	1.30168	-2.33699
H	5.69341	0.93886	-3.04711
H	7.28400	0.57849	-2.30851
H	6.86144	2.24506	-2.74726
C	4.83548	2.74863	-1.15362
H	5.37175	3.62665	-1.56153
H	4.32662	3.06628	-0.23403
H	4.05920	2.46519	-1.88429
C	5.92242	-1.57098	-0.60476
C	5.79226	-1.96292	-2.09752
H	6.20213	-1.21232	-2.78698
H	4.74047	-2.14499	-2.37248
H	6.34896	-2.90446	-2.26446
C	5.32749	-2.74575	0.20662
H	5.82822	-3.67762	-0.11752
H	4.24641	-2.87355	0.03336
H	5.49799	-2.64669	1.28923
C	7.41505	-1.42251	-0.23636
H	7.56261	-1.13811	0.81680
H	7.93837	-0.68738	-0.86735
H	7.91913	-2.39591	-0.38933
C	4.51344	0.23535	1.61682
C	5.74156	0.00975	2.52416
H	6.57723	0.69098	2.30089
H	6.11643	-1.02503	2.47517
H	5.44009	0.19099	3.57344
C	3.93784	1.64877	1.86740
H	3.60664	1.69992	2.92139
H	3.05297	1.84680	1.24004
H	4.67610	2.45351	1.72689
C	3.38729	-0.75937	1.99629
H	3.09205	-0.55031	3.04257
H	3.69535	-1.81275	1.95600
H	2.50226	-0.61861	1.35047
Cu	2.77822	0.00740	-1.48188
C	2.88238	-0.01002	-3.29770
O	1.29672	0.11204	-0.35629
O	3.04944	-0.01811	-4.45022

I_{Ag}

SCF (BP86) Energy = -1980.65898404
Enthalpy 0K = -1979.589925
Enthalpy 298K = -1979.588981
Free Energy 298K = -1979.756815
Lowest Frequency = 14.4813 cm^{-1}
Second Frequency = 14.6261 cm^{-1}
SCF (BP86-D3BJ) Energy = -1980.97621804
SCF (C6H6) Energy = -1980.66337131
SCF (BS2) Energy = -2792.75258057

Ag	-1.47245	0.00043	-0.00031
Si	3.69735	1.68141	-1.02813
Si	3.69701	-1.68145	1.02902
Al	1.01352	-0.00010	0.00016
N	2.03758	1.54478	-0.35498
N	2.03746	-1.54484	0.35522
N	-4.50990	-0.84977	-0.66636
N	-4.51008	0.85012	0.66538
C	1.30726	2.77884	-0.18523
C	0.55179	3.35390	-1.25779
C	-0.14141	4.56257	-1.04392

H	-0.71050	5.00153	-1.87239
C	-0.11770	5.21545	0.19337
H	-0.65722	6.15856	0.33476
C	0.61186	4.64938	1.24573
H	0.63520	5.15595	2.21775
C	1.32849	3.44883	1.08081
C	0.46990	2.70703	-2.64180
H	1.04947	1.76942	-2.59400
C	-0.98144	2.33549	-3.01811
H	-1.41682	1.65557	-2.26329
H	-1.01082	1.82860	-3.99965
H	-1.62625	3.23044	-3.08397
C	1.09433	3.60275	-3.73619
H	0.54444	4.55568	-3.83696
H	1.06448	3.09671	-4.71793
H	2.14560	3.84991	-3.51218
C	2.09713	2.87324	2.27063
H	2.75712	2.08575	1.86668
C	1.13058	2.19977	3.27187
H	0.42292	2.93790	3.69086
H	1.68247	1.74110	4.11212
H	0.53443	1.41109	2.77786
C	2.98502	3.91373	2.98541
H	3.67509	4.40939	2.28166
H	3.58942	3.42702	3.77111
H	2.38699	4.70208	3.47649
C	4.22134	3.51332	-1.07517
H	3.49657	4.14269	-1.61593
H	5.19992	3.60717	-1.57804
H	4.32259	3.92759	-0.05793
C	3.80391	0.96673	-2.79735
H	3.39729	-0.05767	-2.84620
H	4.85615	0.92488	-3.13173
H	3.24586	1.58390	-3.52034
C	5.01595	0.77201	0.01612
H	5.98049	1.15405	-0.37979
H	4.96521	1.14296	1.05764
C	5.01567	-0.77273	-0.01571
H	5.98035	-1.15518	0.37941
H	4.96395	-1.14360	-1.05722
C	3.80307	-0.96601	2.79792
H	3.39866	0.05930	2.84579
H	4.85506	-0.92626	3.13336
H	3.24295	-1.58160	3.52064
C	4.22090	-3.51336	1.07709
H	3.49555	-4.14280	1.61698
H	5.19885	-3.60691	1.58126
H	4.32364	-3.92774	0.06004
C	1.30726	-2.77899	0.18530
C	0.55137	-3.35394	1.25760
C	-0.14159	-4.56275	1.04359
H	-0.71101	-5.00164	1.87187
C	-0.11720	-5.21581	-0.19357
H	-0.65652	-6.15902	-0.33509
C	0.61277	-4.64981	-1.24569
H	0.63662	-5.15654	-2.21762
C	1.32914	-3.44913	-1.08065
C	0.46874	-2.70691	2.64150
H	1.04809	-1.76915	2.59382
C	-0.98285	-2.33567	3.01713
H	-1.41793	-1.65576	2.26214
H	-1.01279	-1.82886	3.99869
H	-1.62755	-3.23073	3.08262
C	1.09296	-3.60235	3.73622
H	0.54338	-4.55548	3.83677
H	1.06246	-3.09628	4.71793
H	2.14443	-3.84911	3.51272
C	2.09811	-2.87349	-2.27021
H	2.75791	-2.08594	-1.86608
C	1.13178	-2.20010	-3.27173
H	0.42413	-2.93824	-3.69073
H	1.68386	-1.74158	-4.11195
H	0.53558	-1.41129	-2.77794
C	2.98625	-3.91392	-2.98476
H	3.67585	-4.40987	-2.28076
H	3.59116	-3.42708	-3.77000
H	2.38838	-4.70204	-3.47641
C	-3.66537	0.00047	-0.00076
C	-4.05724	-1.96791	-1.53997
H	-4.98780	-2.43205	-1.90804
C	-3.27155	-1.43782	-2.74911
H	-3.85551	-0.68798	-3.30823
H	-3.02814	-2.27176	-3.42825
H	-2.32528	-0.97229	-2.42250
C	-3.27583	-3.01678	-0.73559
H	-2.32933	-2.59895	-0.35155
H	-3.02596	-3.87445	-1.38107
H	-3.86725	-3.38322	0.11983
C	-5.85746	-0.54285	-0.42511
C	-7.00828	-1.29752	-1.01536
H	-7.01211	-1.26181	-2.11969
H	-7.95874	-0.86022	-0.67234
H	-7.01102	-2.36106	-0.71588
C	-5.85757	0.54215	0.42513
C	-7.00856	1.29604	1.01605
H	-7.01170	1.26038	2.12039
H	-7.95892	0.85808	0.67362
H	-7.01220	2.35956	0.71653
C	-4.05764	1.96836	1.53896
H	-4.98828	2.43281	1.90643
C	-3.27552	3.01688	0.73484
H	-2.32896	2.59874	0.35130
H	-3.02568	3.87453	1.38037
H	-3.86644	3.38343	-0.12089
C	-3.27273	1.43823	2.74860
H	-3.85728	0.68877	3.30764
H	-3.02923	2.27219	3.42768
H	-2.32653	0.97218	2.42250

TS(I-II)$_{Ag}$

SCF (BP86) Energy = -1980.64548523
Enthalpy 0K = -1979.577262
Enthalpy 298K = -1979.576318
Free Energy 298K = -1979.741061
Lowest Frequency = -59.0677 cm^{-1}
Second Frequency = 12.1966 cm^{-1}
SCF (BP86-D3BJ) Energy = -1980.96229533
SCF (C6H6) Energy = -1980.64987732
SCF (BS2) Energy = -2792.73949398

Ag	1.35510	-0.43713	-0.22668
Si	-3.05344	2.45706	1.29555
Si	-4.16591	-0.75040	-0.73366
Al	-1.04588	0.13126	0.01726
N	-1.56842	1.88991	0.46368
N	-2.46854	-1.07413	-0.24616
N	4.18074	-1.74497	0.40114
N	4.53728	0.18918	-0.52179
C	-0.53612	2.86450	0.20372
C	0.46273	3.17588	1.18250
C	1.46639	4.11593	0.87106
H	2.22077	4.35685	1.63008
C	1.51678	4.75396	-0.37357
H	2.30004	5.48889	-0.59086
C	0.54144	4.45056	-1.33127
H	0.57041	4.95112	-2.30631
C	-0.48613	3.52517	-1.06661
C	0.47878	2.53226	2.57028
H	-0.34069	1.79383	2.59150
C	1.79482	1.77134	2.84360
H	1.96543	0.99989	2.07075
H	1.75726	1.27343	3.82938
H	2.66554	2.45205	2.84703
C	0.22037	3.57070	3.68646

H	1.01875	4.33395	3.71516
H	0.19260	3.08072	4.67639
H	-0.73676	4.09896	3.54104
C	-1.51566	3.22911	-2.15770
H	-2.32907	2.65980	-1.67495
C	-0.90906	2.32892	-3.25864
H	-0.06648	2.83641	-3.76242
H	-1.66259	2.07766	-4.02669
H	-0.52179	1.38518	-2.83368
C	-2.13031	4.50397	-2.77362
H	-2.56083	5.16113	-1.99909
H	-2.93422	4.23842	-3.48262
H	-1.38373	5.09453	-3.33414
C	-3.05990	4.36169	1.36770
H	-2.13350	4.76708	1.80523
H	-3.90971	4.71002	1.98063
H	-3.16809	4.79930	0.36092
C	-3.16918	1.76784	3.07433
H	-3.04252	0.67182	3.09137
H	-4.15691	1.99722	3.51304
H	-2.39972	2.20441	3.73187
C	-4.66309	1.94425	0.39972
H	-5.44742	2.56006	0.88831
H	-4.62193	2.30731	-0.64500
C	-5.06940	0.45358	0.44585
H	-6.13858	0.34980	0.16462
H	-5.00435	0.06054	1.47839
C	-4.27205	0.01007	-2.48366
H	-3.60994	0.88659	-2.58584
H	-5.30407	0.34385	-2.69429
H	-3.98891	-0.71698	-3.26224
C	-5.15479	-2.37912	-0.71694
H	-4.68006	-3.15874	-1.33422
H	-6.17178	-2.20298	-1.10926
H	-5.25136	-2.78068	0.30575
C	-2.05460	-2.45645	-0.18299
C	-1.56534	-3.14215	-1.34069
C	-1.15553	-4.48594	-1.22443
H	-0.78737	-5.00746	-2.11627
C	-1.21096	-5.16875	-0.00448
H	-0.89384	-6.21551	0.06153
C	-1.68769	-4.49841	1.12864
H	-1.73767	-5.02937	2.08646
C	-2.11659	-3.15912	1.06345
C	-1.47767	-2.47267	-2.71375
H	-1.82339	-1.43258	-2.58823
C	-0.02666	-2.41525	-3.24050
H	0.62143	-1.86227	-2.53588
H	0.01170	-1.90239	-4.21860
H	0.39801	-3.42634	-3.37561
C	-2.39844	-3.16183	-3.74692
H	-2.08924	-4.20707	-3.92691
H	-2.36142	-2.63296	-4.71625
H	-3.44826	-3.18163	-3.40876
C	-2.61773	-2.47387	2.33545
H	-3.12414	-1.54686	2.01425
C	-1.43350	-2.06266	3.24023
H	-0.86423	-2.95070	3.56954
H	-1.78638	-1.52977	4.14169
H	-0.73232	-1.40066	2.69995
C	-3.63706	-3.32189	3.12501
H	-4.48230	-3.63563	2.48918
H	-4.04320	-2.74212	3.97260
H	-3.17962	-4.23519	3.54561
C	3.54293	-0.73131	-0.26195
C	3.52001	-2.98525	0.89694
H	4.35323	-3.65778	1.16256
C	2.70122	-2.69820	2.16577
H	3.32150	-2.22506	2.94552
H	2.28912	-3.63873	2.56731
H	1.85755	-2.02456	1.93192
C	2.69362	-3.66667	-0.20173
H	1.81672	-3.05811	-0.48006
H	2.32252	-4.63648	0.16816
H	3.30085	-3.84130	-1.10523
C	5.53357	-1.46080	0.60722
C	6.47519	-2.38669	1.31452
H	6.13295	-2.63079	2.33590
H	7.47031	-1.92522	1.40394
H	6.60926	-3.34005	0.77139
C	5.76698	-0.22667	0.03739
C	7.05897	0.53520	0.09127
H	7.55804	0.63040	-0.88723
H	7.75484	0.00666	0.76143
H	6.92669	1.54941	0.50506
C	4.26995	1.48002	-1.25229
H	3.97514	2.22248	-0.48679
C	3.11464	1.33316	-2.25475
H	3.34191	0.55767	-3.00610
H	2.97677	2.29902	-2.76689
H	2.15415	1.08353	-1.77254
C	5.49929	2.00459	-2.01891
H	6.29816	2.39206	-1.37417
H	5.16922	2.83973	-2.65707
H	5.91649	1.22587	-2.68038

II_{Ag}

SCF (BP86) Energy = -1980.65869698
Enthalpy 0K = -1979.589454
Enthalpy 298K = -1979.588509
Free Energy 298K = -1979.757555
Lowest Frequency = 11.3936 cm^{-1}
Second Frequency = 13.3361 cm^{-1}
SCF (BP86-D3BJ) Energy = -1980.97233857
SCF (C6H6) Energy = -1980.66317581
SCF (BS2) Energy = -2792.75257409

Ag	1.39043	-0.27016	0.09854
Si	-3.47087	2.14505	1.00897
Si	-3.95724	-1.21223	-1.02207
Al	-1.06767	0.06314	0.03782
N	-1.84666	1.75270	0.35538
N	-2.29671	-1.31260	-0.34628
N	4.39950	-1.40511	0.55821
N	4.41714	0.50563	-0.46016
C	-0.92123	2.84472	0.17339
C	-0.09051	3.30847	1.24480
C	0.80496	4.37227	1.01399
H	1.42940	4.72873	1.84217
C	0.91205	4.98600	-0.23930
H	1.60473	5.82140	-0.39224
C	0.10822	4.52740	-1.29024
H	0.18392	5.00496	-2.27429
C	-0.80937	3.47512	-1.10830
C	-0.13967	2.69419	2.64517
H	-0.86066	1.86006	2.60548
C	1.22526	2.10656	3.06739
H	1.56454	1.34659	2.33968
H	1.15096	1.62673	4.06007
H	2.00253	2.88952	3.13229
C	-0.63535	3.70859	3.70150
H	0.05730	4.56474	3.79091
H	-0.70565	3.23269	4.69614
H	-1.62928	4.11282	3.44625
C	-1.65193	3.01352	-2.29761
H	-2.43167	2.34727	-1.88918
C	-0.80014	2.18254	-3.28482
H	0.01703	2.79370	-3.70935
H	-1.41481	1.80777	-4.12304
H	-0.33839	1.31470	-2.77987
C	-2.35709	4.17522	-3.02942
H	-2.96492	4.78079	-2.33596
H	-3.02475	3.78395	-3.81723
H	-1.63657	4.85376	-3.52021

C	-3.71699	4.03501	1.02123
H	-2.90122	4.55945	1.54415
H	-4.66587	4.28570	1.52715
H	-3.76424	4.43845	-0.00436
C	-3.69425	1.47723	2.78561
H	-3.43596	0.40629	2.84938
H	-4.74492	1.58734	3.10922
H	-3.06151	2.01806	3.50824
C	-4.89906	1.42014	-0.03568
H	-5.80105	1.94320	0.34631
H	-4.78744	1.76563	-1.08120
C	-5.12422	-0.10827	0.01521
H	-6.13576	-0.34943	-0.37412
H	-5.12451	-0.47069	1.06091
C	-3.96404	-0.50424	-2.79740
H	-3.41011	0.44803	-2.85633
H	-5.00031	-0.30939	-3.12765
H	-3.50791	-1.20294	-3.51763
C	-4.73664	-2.95086	-1.05653
H	-4.10972	-3.67623	-1.59970
H	-5.72214	-2.90974	-1.55283
H	-4.88711	-3.34341	-0.03683
C	-1.73111	-2.63262	-0.19378
C	-1.05059	-3.28171	-1.27375
C	-0.50715	-4.56698	-1.07425
H	0.00553	-5.06145	-1.90826
C	-0.60901	-5.22576	0.15596
H	-0.18564	-6.22788	0.28677
C	-1.26710	-4.58892	1.21493
H	-1.35135	-5.09987	2.18122
C	-1.83497	-3.30946	1.06429
C	-0.89251	-2.63313	-2.65050
H	-1.36392	-1.63733	-2.59359
C	0.59183	-2.42080	-3.02259
H	1.09644	-1.79109	-2.26706
H	0.67835	-1.91994	-4.00391
H	1.13562	-3.38058	-3.08730
C	-1.61235	-3.44212	-3.75379
H	-1.17040	-4.44826	-3.86775
H	-1.52919	-2.93060	-4.72959
H	-2.68393	-3.57575	-3.52892
C	-2.52996	-2.65928	2.26120
H	-3.09012	-1.79333	1.86694
C	-1.49122	-2.11910	3.27142
H	-0.87943	-2.94217	3.68322
H	-1.98625	-1.60676	4.11616
H	-0.80137	-1.40325	2.78820
C	-3.53668	-3.59488	2.96334
H	-4.27915	-3.99739	2.25351
H	-4.08054	-3.04901	3.75439
H	-3.03702	-4.45400	3.44554
C	3.56963	-0.42496	0.08556
C	3.92525	-2.63181	1.25560
H	4.84447	-3.18117	1.52087
C	3.18380	-2.27214	2.55265
H	3.80798	-1.64285	3.20859
H	2.91985	-3.19378	3.09749
H	2.25148	-1.72587	2.32740
C	3.08436	-3.50974	0.31687
H	2.14662	-3.00177	0.03427
H	2.81716	-4.45082	0.82488
H	3.64044	-3.75410	-0.60347
C	5.74585	-1.10372	0.31121
C	6.88553	-1.98665	0.71647
H	6.94677	-2.11642	1.81217
H	7.83927	-1.54555	0.38828
H	6.81688	-2.99250	0.26472
C	5.76060	0.11365	-0.34013
C	6.94491	0.90131	-0.81207
H	6.85140	1.21185	-1.86597
H	7.85526	0.28657	-0.73369
H	7.11104	1.81211	-0.21063
C	3.88035	1.73201	-1.11242
H	2.80139	1.68358	-0.87501
C	4.02824	1.67216	-2.64116
H	5.08087	1.73408	-2.96538
H	3.49037	2.52279	-3.09135
H	3.59291	0.74117	-3.03857
C	4.43571	3.02408	-0.49423
H	4.39350	2.98309	0.60605
H	3.80794	3.86891	-0.82077
H	5.47269	3.23312	-0.80434

TS(II-III)$_{Ag}$

SCF (BP86) Energy = -2169.23116833
Enthalpy 0K = -2168.146672
Enthalpy 298K = -2168.145727
Free Energy 298K = -2168.319315
Lowest Frequency = -189.8566 cm^{-1}
Second Frequency = 9.6639 cm^{-1}
SCF (BP86-D3BJ) Energy = -2169.56663609
SCF (C6H6) Energy = -2169.23541627
SCF (BS2) Energy = -2981.38560288

Ag	1.36802	-0.36868	-0.30004
Si	-3.87615	-0.93822	1.25288
Si	-3.35640	2.43018	-0.76976
Al	-1.09628	0.09899	-0.20068
N	-2.32344	-1.21578	0.38116
N	-1.71335	1.87951	-0.28044
N	4.33806	0.45413	0.44220
N	4.39587	-1.61513	-0.19677
O	-1.22820	-0.24539	-2.66285
O	0.87788	-1.15825	-3.19912
C	-1.83688	-2.57927	0.34736
C	-2.11022	-3.42664	-0.77888
C	-1.64223	-4.75651	-0.77435
H	-1.86668	-5.39872	-1.63379
C	-0.90820	-5.27849	0.29509
H	-0.56047	-6.31730	0.27779
C	-0.63543	-4.45404	1.39125
H	-0.06781	-4.85628	2.23910
C	-1.08564	-3.11999	1.44467
C	-2.91285	-2.96132	-1.99807
H	-3.02767	-1.86824	-1.91173
C	-2.19529	-3.27765	-3.33180
H	-1.13670	-2.97380	-3.32421
H	-2.69750	-2.76264	-4.16914
H	-2.21975	-4.35963	-3.55439
C	-4.32636	-3.58788	-2.04012
H	-4.26755	-4.69055	-2.07756
H	-4.87254	-3.24935	-2.93882
H	-4.92413	-3.31566	-1.15757
C	-0.77907	-2.31771	2.71190
H	-1.20880	-1.31150	2.57372
C	0.73686	-2.14305	2.94828
H	1.24198	-3.11692	3.08160
H	0.92028	-1.54380	3.85845
H	1.21170	-1.62555	2.09421
C	-1.43903	-2.95520	3.95704
H	-2.52517	-3.08968	3.82119
H	-1.27932	-2.32427	4.84985
H	-1.00890	-3.94971	4.17265
C	-4.78230	-2.58726	1.57925
H	-5.36938	-2.93413	0.71445
H	-5.48512	-2.43974	2.41836
H	-4.08659	-3.39543	1.85697
C	-3.67931	-0.14495	2.98331
H	-3.26341	-0.85903	3.71208
H	-4.67777	0.15782	3.34920
H	-3.04034	0.75107	2.98418
C	-5.04663	0.20110	0.26045
H	-5.09400	-0.15368	-0.78643
H	-6.05224	-0.00345	0.68374

C	-4.75782	1.71921	0.32144
H	-4.58827	2.04089	1.36665
H	-5.65479	2.28316	-0.01158
C	-3.77631	1.94674	-2.56844
H	-3.11227	2.44168	-3.29547
H	-4.81454	2.24438	-2.80134
H	-3.69434	0.85951	-2.72975
C	-3.47211	4.32416	-0.58896
H	-3.39303	4.63057	0.46768
H	-4.44844	4.67195	-0.96980
H	-2.68054	4.85183	-1.14397
C	-0.73269	2.91520	-0.04237
C	0.01136	3.50702	-1.11555
C	0.92982	4.54028	-0.83857
H	1.47961	4.99582	-1.67100
C	1.15171	5.00220	0.46359
H	1.85800	5.81836	0.65349
C	0.44010	4.41559	1.51679
H	0.59848	4.77400	2.54093
C	-0.50047	3.39246	1.28954
C	-0.14333	3.06130	-2.57025
H	-0.87951	2.24196	-2.58069
C	1.18708	2.51055	-3.13344
H	1.95884	3.29971	-3.18678
H	1.04689	2.11483	-4.15543
H	1.58213	1.69801	-2.49846
C	-0.67407	4.19301	-3.47981
H	-1.64926	4.57374	-3.13376
H	-0.79975	3.83019	-4.51566
H	0.02513	5.04785	-3.51055
C	-1.25052	2.81149	2.48474
H	-2.04989	2.17917	2.06319
C	-0.32853	1.90529	3.33180
H	0.10830	1.09650	2.71907
H	-0.88511	1.44236	4.16632
H	0.50663	2.48652	3.76316
C	-1.91518	3.88954	3.36731
H	-1.16886	4.53031	3.87013
H	-2.52470	3.41609	4.15722
H	-2.57426	4.54732	2.77585
C	3.54028	-0.55796	-0.03129
C	3.76799	1.79032	0.77042
H	2.71861	1.70229	0.43276
C	3.74609	2.05338	2.28410
H	3.27350	1.21462	2.81985
H	3.15107	2.96121	2.47599
H	4.75453	2.21532	2.70096
C	4.42383	2.92211	-0.03466
H	4.48510	2.66116	-1.10371
H	5.43395	3.17230	0.32902
H	3.79655	3.82320	0.05863
C	5.67379	0.04222	0.57171
C	6.80983	0.89421	1.05071
H	7.07675	1.68494	0.32815
H	7.70490	0.27000	1.19844
H	6.59181	1.38398	2.01404
C	5.70821	-1.27409	0.15820
C	6.86597	-2.22037	0.07463
H	7.04293	-2.57609	-0.95624
H	6.72676	-3.11013	0.71491
H	7.78736	-1.71895	0.40829
C	4.02484	-2.93044	-0.78940
H	4.88481	-3.58742	-0.57399
C	2.78880	-3.53630	-0.11448
H	2.92588	-3.61295	0.97585
H	2.61026	-4.54687	-0.51693
H	1.88183	-2.93616	-0.30356
C	3.87340	-2.80435	-2.31433
H	3.02273	-2.15227	-2.56694
H	3.69020	-3.79836	-2.75593
H	4.78566	-2.38578	-2.77220
C	-0.09963	-0.67164	-2.71897

III_{Ag}

SCF (BP86) Energy = -2169.25428771
Enthalpy 0K = -2168.168520
Enthalpy 298K = -2168.167576
Free Energy 298K = -2168.337474
Lowest Frequency = 14.4938 cm^{-1}
Second Frequency = 20.7326 cm^{-1}
SCF (BP86-D3BJ) Energy = -2169.59157143
SCF (C6H6) Energy = -2169.26067834
SCF (BS2) Energy = -2981.40661968

Ag	1.38363	-0.32457	-0.77976
Si	-3.60809	-1.15070	1.49698
Si	-3.53464	2.25740	-0.60642
Al	-1.32526	0.00400	-0.51770
N	-2.12370	-1.34916	0.49113
N	-1.82450	1.78488	-0.27646
N	4.08589	0.65699	0.58964
N	4.33632	-1.32443	-0.26057
O	-1.35729	-0.43236	-2.33297
O	0.61867	-1.07363	-3.27455
C	-1.52763	-2.66942	0.41923
C	-1.82451	-3.56568	-0.66280
C	-1.20664	-4.83329	-0.69083
H	-1.43827	-5.51189	-1.51959
C	-0.32660	-5.25423	0.31031
H	0.13004	-6.24923	0.26777
C	-0.05495	-4.39039	1.37614
H	0.61830	-4.71730	2.17783
C	-0.63531	-3.10929	1.45312
C	-2.82717	-3.25202	-1.77928
H	-3.14479	-2.20345	-1.65481
C	-2.21861	-3.40540	-3.19258
H	-1.31611	-2.79324	-3.33038
H	-2.95588	-3.09532	-3.95394
H	-1.95746	-4.45872	-3.40195
C	-4.07991	-4.15601	-1.67719
H	-3.81483	-5.21619	-1.84018
H	-4.81921	-3.87612	-2.44862
H	-4.56710	-4.08667	-0.69257
C	-0.31440	-2.25345	2.68068
H	-0.85532	-1.30017	2.56281
C	1.18906	-1.92049	2.79292
H	1.79878	-2.83467	2.91222
H	1.37843	-1.27772	3.67180
H	1.54884	-1.39005	1.89375
C	-0.80334	-2.93231	3.98142
H	-1.87504	-3.18782	3.93148
H	-0.64692	-2.26997	4.85186
H	-0.25152	-3.86971	4.17457
C	-4.40425	-2.85047	1.83451
H	-5.05707	-3.16928	1.00649
H	-5.02914	-2.77804	2.74195
H	-3.65451	-3.64088	1.99907
C	-3.33961	-0.37085	3.22202
H	-2.83885	-1.06824	3.91220
H	-4.32989	-0.13296	3.65233
H	-2.75583	0.56106	3.19661
C	-4.91956	-0.07900	0.60351
H	-5.03466	-0.44867	-0.43339
H	-5.86582	-0.35769	1.11311
C	-4.75652	1.46006	0.63078
H	-4.50099	1.80605	1.65052
H	-5.72977	1.94080	0.39679
C	-4.06858	1.70965	-2.35380
H	-3.51224	2.25474	-3.13361
H	-5.14576	1.90476	-2.50251
H	-3.89415	0.63398	-2.52373
C	-3.73255	4.14244	-0.43383
H	-3.58042	4.47135	0.60738
H	-4.75586	4.42867	-0.73382

H	-3.02220	4.70033	-1.06386
C	-0.88129	2.86019	-0.08696
C	-0.23239	3.48911	-1.20082
C	0.61436	4.59355	-0.97327
H	1.08767	5.08143	-1.83360
C	0.85563	5.08877	0.31326
H	1.50018	5.96248	0.46235
C	0.24557	4.45865	1.40471
H	0.42092	4.84174	2.41737
C	-0.62013	3.36149	1.23018
C	-0.42873	3.02436	-2.64571
H	-1.06642	2.12557	-2.62131
C	0.91393	2.63272	-3.30469
H	1.57887	3.50801	-3.41989
H	0.74353	2.20391	-4.30715
H	1.44911	1.87682	-2.70395
C	-1.14308	4.09094	-3.50811
H	-2.13076	4.35856	-3.09751
H	-1.29291	3.71738	-4.53655
H	-0.54753	5.01932	-3.57382
C	-1.26597	2.73422	2.46212
H	-2.00572	2.01142	2.08012
C	-0.22979	1.95194	3.29969
H	0.26950	1.17581	2.69417
H	-0.71121	1.45454	4.16063
H	0.54968	2.62725	3.69625
C	-2.00968	3.75922	3.34537
H	-1.31723	4.48940	3.80123
H	-2.53449	3.24616	4.17069
H	-2.75787	4.32723	2.76738
C	3.41042	-0.33184	-0.07596
C	3.45107	1.97691	0.86207
H	2.39194	1.80866	0.59597
C	3.50821	2.37392	2.34392
H	3.16783	1.54956	2.99102
H	2.83066	3.22921	2.49698
H	4.51655	2.68384	2.66197
C	4.00531	3.05841	-0.07898
H	3.94659	2.72791	-1.12844
H	5.05258	3.31796	0.15076
H	3.39302	3.96803	0.02552
C	5.42113	0.29445	0.82369
C	6.43440	1.11919	1.55776
H	6.51016	2.14540	1.16256
H	7.42920	0.65785	1.45865
H	6.21186	1.19263	2.63654
C	5.57675	-0.96557	0.28108
C	6.78758	-1.84624	0.24555
H	7.09511	-2.09380	-0.78598
H	6.62917	-2.79713	0.78525
H	7.63670	-1.33720	0.72646
C	4.10486	-2.58849	-1.02095
H	5.03459	-3.16482	-0.88144
C	2.95061	-3.40624	-0.42873
H	3.10506	-3.60080	0.64439
H	2.88028	-4.37299	-0.95328
H	1.97965	-2.89604	-0.54728
C	3.93330	-2.30248	-2.52236
H	2.98993	-1.76945	-2.72946
H	3.90650	-3.25663	-3.07506
H	4.77360	-1.70250	-2.91063
C	-0.06002	-0.64799	-2.33780

TS(III-IV)$_{Ag}$

SCF (BP86) Energy = -2169.23140354
Enthalpy 0K = -2168.147155
Enthalpy 298K = -2168.146211
Free Energy 298K = -2168.317124
Lowest Frequency = -127.9488 cm^{-1}
Second Frequency = 9.3822 cm^{-1}
SCF (BP86-D3BJ) Energy = -2169.55623532
SCF (C6H6) Energy = -2169.23919031
SCF (BS2) Energy = -2981.38306973

Ag	1.98376	-0.47388	-0.91759
Si	-3.81318	-1.09998	1.66924
Si	-3.76264	2.36439	-0.32040
Al	-1.64585	0.01818	-0.50554
N	-2.45653	-1.31466	0.50745
N	-2.05522	1.80616	-0.19596
N	4.85990	-1.33291	-0.17382
N	4.47719	0.68939	0.52528
O	-1.50808	-0.41117	-2.33189
O	0.66601	-0.96702	-2.66726
C	-1.92790	-2.64902	0.29581
C	-2.37335	-3.45869	-0.80078
C	-1.79766	-4.73162	-0.98980
H	-2.13895	-5.34362	-1.83248
C	-0.81571	-5.23673	-0.13255
H	-0.38892	-6.23164	-0.30076
C	-0.40029	-4.45788	0.95255
H	0.35285	-4.85385	1.64467
C	-0.93701	-3.17696	1.18696
C	-3.48224	-3.03440	-1.76947
H	-3.76482	-1.99866	-1.51206
C	-3.02456	-3.05471	-3.24601
H	-2.15595	-2.40051	-3.40737
H	-3.84392	-2.70486	-3.89936
H	-2.76323	-4.07843	-3.56945
C	-4.73445	-3.93070	-1.61206
H	-4.51325	-4.97176	-1.90876
H	-5.55220	-3.56798	-2.26004
H	-5.10211	-3.95588	-0.57419
C	-0.46070	-2.41271	2.42368
H	-0.97359	-1.43687	2.41970
C	1.05731	-2.13664	2.40293
H	1.64055	-3.07496	2.41106
H	1.35835	-1.54850	3.28882
H	1.35064	-1.56813	1.50085
C	-0.84507	-3.15625	3.72417
H	-1.92792	-3.35999	3.77212
H	-0.56647	-2.56256	4.61354
H	-0.32467	-4.12817	3.79628
C	-4.65183	-2.77695	2.01180
H	-5.37411	-3.04112	1.22281
H	-5.20512	-2.71785	2.96540
H	-3.92184	-3.59873	2.09058
C	-3.30863	-0.40745	3.37925
H	-2.76335	-1.15344	3.97927
H	-4.22536	-0.13964	3.93609
H	-2.68449	0.49695	3.31235
C	-5.15391	0.07716	0.97603
H	-5.41543	-0.24602	-0.04969
H	-6.04893	-0.16020	1.58866
C	-4.88546	1.60059	1.02691
H	-4.49397	1.89431	2.01958
H	-5.84399	2.15101	0.91938
C	-4.50309	1.87014	-2.00825
H	-4.03117	2.42464	-2.83547
H	-5.58795	2.07696	-2.03234
H	-4.36399	0.79487	-2.21535
C	-3.84557	4.25141	-0.08845
H	-3.60352	4.53594	0.94912
H	-4.86928	4.60328	-0.30531
H	-3.14988	4.79045	-0.75025
C	-1.02565	2.81402	-0.11564
C	-0.47199	3.41782	-1.29294
C	0.48828	4.44150	-1.15491
H	0.89252	4.91055	-2.05966
C	0.92193	4.88604	0.09925
H	1.64681	5.70423	0.17988
C	0.39375	4.28633	1.24930
H	0.71415	4.63696	2.23813
C	-0.57044	3.26325	1.16711

C	-0.89890	3.02272	-2.70904
H	-1.58316	2.16326	-2.62186
C	0.30154	2.57666	-3.57475
H	1.00624	3.40965	-3.75119
H	-0.04900	2.22248	-4.55956
H	0.85740	1.75017	-3.10411
C	-1.65569	4.16959	-3.42005
H	-2.55486	4.48060	-2.86288
H	-1.97442	3.85268	-4.42897
H	-1.01309	5.06075	-3.53805
C	-1.11240	2.65915	2.46018
H	-1.94541	2.00041	2.16286
C	-0.04710	1.78516	3.15961
H	0.32071	0.98830	2.49023
H	-0.46127	1.30516	4.06430
H	0.82158	2.39323	3.47050
C	-1.66600	3.71908	3.43686
H	-0.87078	4.38683	3.81416
H	-2.12715	3.23088	4.31365
H	-2.43129	4.35247	2.95766
C	3.88557	-0.37211	-0.10833
C	4.71786	-2.65470	-0.85064
H	5.67666	-3.16491	-0.66063
C	3.60036	-3.50069	-0.22460
H	3.73789	-3.60035	0.86422
H	3.61066	-4.50793	-0.67304
H	2.60640	-3.06027	-0.40975
C	4.55692	-2.48066	-2.37034
H	5.37932	-1.87878	-2.79154
H	3.60107	-1.98673	-2.61315
H	4.56426	-3.46979	-2.85774
C	6.05186	-0.88077	0.40926
C	7.29680	-1.70743	0.50488
H	7.14446	-2.62586	1.09988
H	8.09337	-1.12995	0.99811
H	7.67770	-2.00995	-0.48690
C	5.81275	0.40449	0.85106
C	6.74934	1.33057	1.56546
H	6.47727	1.46647	2.62660
H	6.78808	2.32940	1.10043
H	7.77013	0.91891	1.53791
C	3.76226	1.98552	0.68931
H	2.72126	1.73164	0.41939
C	3.76043	2.49134	2.13881
H	3.47376	1.69115	2.84019
H	3.01291	3.29692	2.21852
H	4.73356	2.90522	2.44789
C	4.26718	3.02896	-0.31985
H	5.29240	3.36876	-0.09432
H	3.59938	3.90494	-0.28998
H	4.24903	2.62042	-1.34317
C	-0.25901	-0.55596	-1.90734

IV_{Ag}

SCF (BP86) Energy = -2169.24530840
Enthalpy 0K = -2168.160061
Enthalpy 298K = -2168.159116
Free Energy 298K = -2168.33474300
Lowest Frequency = 5.7237 cm^{-1}
Second Frequency = 10.8992 cm^{-1}
SCF (BP86-D3BJ) Energy = -2169.56081799
SCF (C6H6) Energy = -2169.25481690
SCF (BS2) Energy = -2981.39926312

Ag	2.69005	-0.73011	-0.84938
Si	-4.05016	-0.83746	1.97828
Si	-3.67972	2.72474	0.27282
Al	-1.86716	0.08846	-0.27382
N	-3.01198	-1.11927	0.54356
N	-2.10001	1.90673	0.02087
N	5.57313	-1.58633	-0.09850
N	5.23341	0.51709	0.32972
O	-1.34702	-0.45836	-2.02539
O	0.84820	-0.86345	-1.78966
C	-3.00310	-2.45546	-0.01603
C	-3.88024	-2.79151	-1.09484
C	-3.86481	-4.10023	-1.61401
H	-4.53742	-4.34989	-2.44311
C	-3.01343	-5.08413	-1.10025
H	-3.02063	-6.09769	-1.51591
C	-2.14784	-4.75241	-0.05296
H	-1.47175	-5.51653	0.34960
C	-2.11986	-3.45628	0.49846
C	-4.82426	-1.76847	-1.72811
H	-4.72205	-0.83701	-1.14339
C	-4.41989	-1.46189	-3.18906
H	-3.37158	-1.12921	-3.25039
H	-5.06775	-0.67361	-3.61386
H	-4.52837	-2.35933	-3.82466
C	-6.30409	-2.20708	-1.65767
H	-6.48016	-3.13000	-2.23862
H	-6.95982	-1.42333	-2.07718
H	-6.62633	-2.40196	-0.62070
C	-1.12979	-3.16894	1.62874
H	-1.24290	-2.10404	1.89494
C	0.33249	-3.38157	1.17458
H	0.52124	-4.43680	0.90583
H	1.03148	-3.11206	1.98768
H	0.56426	-2.76071	0.29302
C	-1.42577	-4.01354	2.88889
H	-2.45125	-3.84799	3.25970
H	-0.72320	-3.76113	3.70384
H	-1.32013	-5.09351	2.68112
C	-5.14663	-2.36413	2.28083
H	-5.88747	-2.49802	1.47565
H	-5.69562	-2.24053	3.23082
H	-4.55676	-3.29254	2.34275
C	-3.02894	-0.51957	3.56132
H	-2.48171	-1.42344	3.87585
H	-3.69478	-0.22205	4.39137
H	-2.29146	0.28752	3.41904
C	-5.22789	0.65421	1.75266
H	-5.79996	0.50763	0.81665
H	-5.97259	0.53682	2.56782
C	-4.62291	2.07664	1.80707
H	-3.97066	2.18985	2.69439
H	-5.43525	2.82016	1.95135
C	-4.82423	2.49719	-1.23690
H	-4.42532	3.01019	-2.12708
H	-5.82825	2.90827	-1.02836
H	-4.94859	1.43144	-1.49496
C	-3.38441	4.58222	0.57280
H	-2.84499	4.75422	1.51937
H	-4.35430	5.10594	0.63520
H	-2.79440	5.04798	-0.23245
C	-0.93147	2.74468	-0.10766
C	-0.53234	3.28314	-1.37326
C	0.58610	4.13984	-1.43467
H	0.87621	4.56063	-2.40460
C	1.31869	4.47984	-0.29228
H	2.16019	5.17941	-0.35946
C	0.94319	3.93406	0.94249
H	1.50238	4.20521	1.84609
C	-0.16204	3.06986	1.05661
C	-1.28426	2.98477	-2.67239
H	-2.06969	2.24887	-2.43297
C	-0.36589	2.35428	-3.74382
H	0.43593	3.05095	-4.04978
H	-0.95092	2.10618	-4.64679
H	0.09848	1.42525	-3.37919
C	-1.96738	4.25227	-3.23749
H	-2.66368	4.70513	-2.51171
H	-2.53809	4.00921	-4.15154
H	-1.22179	5.02233	-3.50621

C	-0.49950	2.46524	2.41844
H	-1.52851	2.07412	2.33926
C	0.42917	1.26371	2.71492
H	0.37122	0.50835	1.91078
H	0.15909	0.77458	3.66812
H	1.48126	1.59513	2.78875
C	-0.46626	3.48158	3.57801
H	0.55422	3.85726	3.77430
H	-0.82142	3.00910	4.51069
H	-1.10885	4.35413	3.37114
C	4.61428	-0.61144	-0.14003
C	5.36493	-3.00307	-0.51356
H	6.33976	-3.48871	-0.34201
C	4.32060	-3.69367	0.37695
H	4.59139	-3.61565	1.44270
H	4.25592	-4.76159	0.11066
H	3.32242	-3.24500	0.23927
C	5.03764	-3.10272	-2.01220
H	5.80518	-2.59971	-2.62314
H	4.05957	-2.64311	-2.23604
H	4.99317	-4.16320	-2.31065
C	6.78515	-1.07911	0.38859
C	8.02222	-1.90506	0.56031
H	7.87978	-2.72732	1.28431
H	8.84254	-1.27746	0.94014
H	8.36407	-2.35072	-0.39083
C	6.57301	0.25832	0.65819
C	7.54036	1.25944	1.21248
H	7.30869	1.53382	2.25624
H	7.56672	2.18903	0.62071
H	8.55721	0.83763	1.20166
C	4.52046	1.82574	0.38095
H	3.47289	1.54820	0.16507
C	4.55401	2.46454	1.77673
H	4.29028	1.73129	2.55626
H	3.80500	3.27205	1.80458
H	5.53279	2.90762	2.02051
C	4.99129	2.76859	-0.73717
H	6.01894	3.13536	-0.57517
H	4.31939	3.64152	-0.77227
H	4.94683	2.26527	-1.71652
C	-0.26171	-0.49878	-1.26096

A_{Ag}

SCF (BP86) Energy = -2169.25485896
Enthalpy 0K = -2168.169510
Enthalpy 298K = -2168.168565
Free Energy 298K = -2168.345109
Lowest Frequency = 6.6710 cm^{-1}
Second Frequency = 10.2469 cm^{-1}
SCF (BP86-D3BJ) Energy = -2169.56675456
SCF (C6H6) Energy = -2169.26300048
SCF (BS2) Energy = -2981.40886137

Ag	2.75840	-0.61337	-0.87792
Si	-4.17881	2.16753	-0.49526
Si	-4.27600	-1.22067	1.61129
Al	-1.79632	-0.00937	-0.14265
N	-2.45612	1.71786	-0.26491
N	-2.83542	-1.37000	0.55402
N	5.82168	-0.96012	-0.35406
N	4.98640	0.72074	0.74003
O	0.10782	-0.05428	0.22607
O	0.84995	-0.87555	-1.76477
C	-1.46635	2.77116	-0.27568
C	-1.03458	3.35392	0.95800
C	-0.07332	4.38269	0.94094
H	0.24490	4.82952	1.89074
C	0.46902	4.85636	-0.25994
H	1.20049	5.67249	-0.25709
C	0.05159	4.28228	-1.46609
H	0.47186	4.64910	-2.41010
C	-0.90242	3.24557	-1.50336
C	-1.57551	2.87660	2.30579
H	-2.38938	2.16436	2.08367
C	-0.49088	2.11666	3.10400
H	-0.07783	1.27934	2.51750
H	-0.90419	1.71467	4.04661
H	0.34405	2.79212	3.36820
C	-2.17016	4.02364	3.15153
H	-1.39930	4.75981	3.44208
H	-2.61372	3.62768	4.08234
H	-2.95723	4.56757	2.60249
C	-1.30628	2.68139	-2.86801
H	-1.99568	1.84058	-2.68003
C	-0.09856	2.12698	-3.65777
H	0.63916	2.91975	-3.87816
H	-0.43483	1.71166	-4.62456
H	0.41099	1.32300	-3.10419
C	-2.05392	3.73516	-3.71871
H	-2.95012	4.12075	-3.20461
H	-2.37393	3.30047	-4.68267
H	-1.40324	4.59946	-3.94341
C	-4.35340	4.06206	-0.41927
H	-4.17633	4.43880	0.60205
H	-5.37745	4.35155	-0.71317
H	-3.64578	4.57657	-1.08839
C	-4.85010	1.53715	-2.16782
H	-4.39206	2.07124	-3.01621
H	-5.94346	1.68497	-2.22512
H	-4.65251	0.46016	-2.30554
C	-5.31928	1.46490	0.87128
H	-4.93636	1.79741	1.85517
H	-6.27040	2.02067	0.73030
C	-5.60558	-0.05550	0.87959
H	-5.86510	-0.41174	-0.13566
H	-6.50658	-0.25930	1.49571
C	-3.82806	-0.54543	3.34123
H	-3.23671	-1.27385	3.91972
H	-4.74523	-0.32253	3.91557
H	-3.24082	0.38637	3.27599
C	-5.08828	-2.93061	1.80860
H	-5.51161	-3.28609	0.85443
H	-5.90979	-2.87146	2.54376
H	-4.37121	-3.69183	2.15522
C	-2.36792	-2.69995	0.21949
C	-1.47929	-3.40771	1.08901
C	-1.04977	-4.70078	0.72924
H	-0.37318	-5.24130	1.40207
C	-1.46169	-5.30706	-0.46208
H	-1.11485	-6.31308	-0.72264
C	-2.32120	-4.60912	-1.31744
H	-2.64122	-5.07475	-2.25697
C	-2.78780	-3.31939	-1.00054
C	-0.96803	-2.81389	2.40348
H	-1.37794	-1.79266	2.47922
C	0.57320	-2.69651	2.42239
H	1.05500	-3.68741	2.33898
H	0.91130	-2.24088	3.37100
H	0.92679	-2.06388	1.59210
C	-1.45985	-3.62176	3.62649
H	-2.56056	-3.68844	3.65863
H	-1.11855	-3.15298	4.56718
H	-1.06703	-4.65428	3.60838
C	-3.70719	-2.60841	-1.99424
H	-4.05274	-1.68258	-1.50096
C	-2.93453	-2.20435	-3.27190
H	-2.05670	-1.58281	-3.02819
H	-3.58545	-1.63798	-3.96237
H	-2.56985	-3.09780	-3.80995
C	-4.95638	-3.44223	-2.35376
H	-4.68761	-4.37137	-2.88718
H	-5.62720	-2.86622	-3.01569
H	-5.52752	-3.72942	-1.45451

C 4.65297 -0.28917 -0.12388
C 5.94774 -2.15420 -1.23595
H 7.01111 -2.43922 -1.17229
C 5.10237 -3.32433 -0.70792
H 5.35748 -3.56080 0.33810
H 5.28439 -4.22066 -1.32378
H 4.02613 -3.08538 -0.75603
C 5.62937 -1.79830 -2.69714
H 6.25755 -0.96425 -3.05100
H 4.57082 -1.50637 -2.80694
H 5.81474 -2.67363 -3.34153
C 6.88404 -0.37874 0.35165
C 8.28971 -0.89266 0.30842
H 8.37261 -1.92100 0.70404
H 8.94155 -0.25504 0.92471
H 8.70471 -0.89291 -0.71536
C 6.35574 0.69173 1.04605
C 7.05860 1.64017 1.96880
H 6.78949 1.47327 3.02629
H 6.83996 2.69404 1.73118
H 8.14784 1.50500 1.88187
C 3.96522 1.70821 1.19858
H 3.02096 1.28609 0.80840
C 3.84936 1.76739 2.72858
H 3.76244 0.75653 3.15874
H 2.93506 2.32448 2.98956
H 4.70001 2.28473 3.20102
C 4.16766 3.08218 0.54117
H 5.05223 3.61282 0.93266
H 3.28056 3.70688 0.73630
H 4.27254 2.97944 -0.55096
C -0.10442 -0.50546 -1.01455

TS(III-S)$_{Ag}$
SCF (BP86) Energy = -2169.24812559
Enthalpy 0K = -2168.163568
Enthalpy 298K = -2168.162624
Free Energy 298K = -2168.333135
Lowest Frequency = -47.7498 cm^{-1}
Second Frequency = 13.9928 cm^{-1}
SCF (BP86-D3BJ) Energy = -2169.57399851
SCF (C6H6) Energy = -2169.25580125
SCF (BS2) Energy = -2981.40215584

Ag 1.85288 -0.47263 -0.76877
Si -3.72476 -1.08493 1.74950
Si -3.77400 2.32714 -0.32053
Al -1.60258 0.03679 -0.44542
N -2.36967 -1.28995 0.56759
N -2.04999 1.80704 -0.20454
N 4.45625 0.70583 0.61400
N 4.83205 -1.27398 -0.18974
O -1.01305 -0.45939 -2.04178
O 0.67774 -1.47915 -3.09099
C -1.91940 -2.64821 0.30779
C -2.38357 -3.37028 -0.83778
C -1.92837 -4.68865 -1.03977
H -2.28441 -5.24036 -1.91691
C -1.03997 -5.30844 -0.15591
H -0.70506 -6.33585 -0.33535
C -0.58726 -4.59851 0.96093
H 0.10721 -5.07850 1.66077
C -1.00796 -3.27839 1.21359
C -3.36922 -2.79386 -1.85934
H -3.52016 -1.72804 -1.60928
C -2.83060 -2.86917 -3.30621
H -1.84913 -2.38028 -3.39762
H -3.53442 -2.36880 -3.99535
H -2.73470 -3.91678 -3.64387
C -4.74747 -3.49159 -1.77559
H -4.65804 -4.56926 -2.00083
H -5.44703 -3.05379 -2.50976
H -5.20120 -3.39868 -0.77530
C -0.47736 -2.57809 2.46764
H -0.92478 -1.57091 2.49352
C 1.05491 -2.39515 2.42740
H 1.57685 -3.36768 2.38221
H 1.40694 -1.86631 3.33187
H 1.36179 -1.80553 1.54370
C -0.88691 -3.32169 3.75999
H -1.98013 -3.44618 3.83471
H -0.54368 -2.76892 4.65307
H -0.43709 -4.32965 3.80198
C -4.52095 -2.77697 2.10287
H -5.12388 -3.13863 1.25487
H -5.19009 -2.68075 2.97604
H -3.77022 -3.55035 2.32934
C -3.18925 -0.35937 3.43222
H -2.62198 -1.08966 4.03103
H -4.09231 -0.08549 4.00751
H -2.57282 0.54680 3.32781
C -5.10008 0.05325 1.05969
H -5.38068 -0.29988 0.04916
H -5.97583 -0.18400 1.69940
C -4.85897 1.58227 1.06630
H -4.45715 1.90986 2.04406
H -5.82942 2.11135 0.96038
C -4.51641 1.76194 -1.98460
H -4.03785 2.27463 -2.83467
H -5.59947 1.97622 -2.02072
H -4.39152 0.67612 -2.14378
C -3.87728 4.21831 -0.16082
H -3.58148 4.55159 0.84767
H -4.91739 4.54465 -0.33511
H -3.22885 4.73606 -0.88489
C -1.03846 2.84267 -0.17746
C -0.50094 3.39680 -1.38305
C 0.42982 4.45261 -1.29439
H 0.82540 4.88547 -2.22044
C 0.85012 4.96669 -0.06304
H 1.55516 5.80475 -0.02231
C 0.34233 4.40670 1.11583
H 0.66117 4.80702 2.08560
C -0.59624 3.35763 1.08359
C -0.90070 2.90687 -2.77649
H -1.55575 2.02999 -2.64650
C 0.32617 2.44599 -3.59482
H 1.00083 3.29030 -3.82613
H 0.00334 2.00299 -4.55260
H 0.90466 1.68244 -3.05022
C -1.68634 3.98457 -3.55967
H -2.60067 4.29869 -3.02853
H -1.98418 3.59975 -4.55113
H -1.07165 4.88789 -3.72403
C -1.11401 2.78861 2.40318
H -1.96961 2.14180 2.14606
C -0.04408 1.90139 3.07932
H 0.28389 1.08674 2.40966
H -0.43415 1.44452 4.00641
H 0.84718 2.49628 3.34745
C -1.61522 3.87272 3.38109
H -0.79506 4.52325 3.73366
H -2.06657 3.40483 4.27374
H -2.37592 4.52100 2.91430
C 3.84066 -0.34388 -0.01638
C 3.72925 1.98213 0.85601
H 2.68110 1.71832 0.62669
C 3.79491 2.44190 2.31939
H 3.53063 1.62275 3.00769
H 3.06499 3.25559 2.46025
H 4.78599 2.83419 2.59836
C 4.16772 3.06583 -0.14205
H 4.11001 2.68616 -1.17483
H 5.19556 3.41980 0.04683

H	3.48566	3.92728	-0.05860
C	5.81825	0.44477	0.83349
C	6.78234	1.36249	1.52196
H	6.77341	2.37944	1.09608
H	7.80668	0.97346	1.41317
H	6.57789	1.45185	2.60329
C	6.05322	-0.81591	0.32283
C	7.32114	-1.61239	0.29331
H	7.63372	-1.86514	-0.73557
H	7.23467	-2.55797	0.85830
H	8.13888	-1.03459	0.75052
C	4.67189	-2.57158	-0.90947
H	5.64967	-3.06930	-0.79824
C	3.60858	-3.46082	-0.25031
H	3.81289	-3.59986	0.82384
H	3.60658	-4.44936	-0.73882
H	2.59995	-3.02847	-0.36250
C	4.41106	-2.34557	-2.40860
H	3.41555	-1.90213	-2.58259
H	4.44295	-3.31395	-2.93565
H	5.17624	-1.68539	-2.85027
C	0.28797	-0.86315	-2.09612

S_{Ag}

SCF (BP86) Energy = -2169.29660773
Enthalpy 0K = -2168.210819
Enthalpy 298K = -2168.209875
Free Energy 298K = -2168.385725
Lowest Frequency = 4.5068 cm^{-1}
Second Frequency = 8.9182 cm^{-1}
SCF (BP86-D3BJ) Energy = -2169.60586205
SCF (C6H6) Energy = -2169.30484550
SCF (BS2) Energy = -2981.45001543

Ag	2.62057	-0.10366	-0.03670
Si	-4.36431	-1.54402	1.14662
Si	-4.27412	1.78854	-1.04020
Al	-1.76312	0.02353	0.01179
N	-2.71866	-1.49941	0.43210
N	-2.61129	1.61439	-0.38792
N	5.55556	0.65469	0.66613
N	5.55858	-0.96354	-0.77944
O	-0.15829	0.31019	1.03426
O	-0.20226	-0.37255	-1.04427
C	-2.01678	-2.75299	0.25004
C	-2.07563	-3.42744	-1.01121
C	-1.39813	-4.65049	-1.17499
H	-1.44857	-5.15983	-2.14478
C	-0.66874	-5.22926	-0.13061
H	-0.15712	-6.18763	-0.27347
C	-0.60317	-4.56590	1.09910
H	-0.03085	-5.01217	1.92118
C	-1.25572	-3.33494	1.31379
C	-2.83500	-2.85051	-2.20645
H	-3.34359	-1.93807	-1.84846
C	-1.86661	-2.44045	-3.34075
H	-1.10181	-1.73599	-2.97598
H	-2.41820	-1.96362	-4.17121
H	-1.34459	-3.32381	-3.75158
C	-3.91802	-3.81398	-2.74043
H	-3.47335	-4.74441	-3.13664
H	-4.48381	-3.34222	-3.56349
H	-4.63549	-4.09924	-1.95252
C	-1.12273	-2.67882	2.69071
H	-1.62429	-1.69805	2.63463
C	0.35251	-2.42513	3.07609
H	0.91664	-3.37100	3.16656
H	0.40922	-1.91015	4.05189
H	0.85337	-1.79085	2.32781
C	-1.81850	-3.51492	3.79025
H	-2.88687	-3.67702	3.57024
H	-1.74486	-3.00939	4.77005
H	-1.34740	-4.50918	3.89226
C	-4.96490	-3.34804	1.24503
H	-5.15536	-3.76261	0.24114
H	-5.90962	-3.39350	1.81456
H	-4.23338	-4.00615	1.74010
C	-4.39732	-0.78085	2.89692
H	-3.84343	-1.40112	3.62027
H	-5.43807	-0.68948	3.25642
H	-3.95084	0.22808	2.91173
C	-5.64954	-0.59708	0.09126
H	-5.62606	-1.00554	-0.93720
H	-6.62593	-0.92283	0.50818
C	-5.58875	0.94881	0.06818
H	-5.49217	1.35331	1.09393
H	-6.55193	1.35125	-0.31065
C	-4.43434	1.02653	-2.78409
H	-3.86592	1.60317	-3.53192
H	-5.49268	1.01202	-3.10104
H	-4.06441	-0.01257	-2.81233
C	-4.73292	3.63406	-1.12764
H	-5.69232	3.75177	-1.66113
H	-3.97117	4.22981	-1.65499
H	-4.85080	4.06662	-0.12028
C	-1.80866	2.81029	-0.23578
C	-1.04885	3.33360	-1.33050
C	-0.29772	4.51210	-1.14568
H	0.27312	4.91442	-1.99119
C	-0.26458	5.17864	0.08363
H	0.32185	6.09655	0.20294
C	-0.99238	4.65555	1.15804
H	-0.96610	5.16728	2.12758
C	-1.76499	3.48626	1.02532
C	-1.01890	2.66818	-2.70890
H	-1.59511	1.73086	-2.63123
C	0.41682	2.29605	-3.14409
H	1.05107	3.19352	-3.25956
H	0.39794	1.77501	-4.11815
H	0.89048	1.62674	-2.40879
C	-1.68381	3.55577	-3.78681
H	-2.72698	3.80437	-3.52961
H	-1.68663	3.04399	-4.76612
H	-1.13779	4.50835	-3.91066
C	-2.51682	2.96882	2.25215
H	-3.09208	2.08594	1.92192
C	-1.53910	2.51233	3.36018
H	-0.83057	1.75942	2.97926
H	-2.09210	2.07743	4.21242
H	-0.95296	3.36650	3.74550
C	-3.52062	4.00315	2.80840
H	-3.00641	4.91032	3.17335
H	-4.08383	3.57809	3.65828
H	-4.24760	4.32053	2.04187
C	4.72163	-0.15681	-0.05931
C	5.00500	1.71679	1.55465
H	3.91818	1.51517	1.52854
C	5.47437	1.57020	3.01009
H	5.33378	0.53763	3.36879
H	4.87024	2.23626	3.64786
H	6.53055	1.85282	3.14686
C	5.23279	3.12020	0.97068
H	4.85591	3.17757	-0.06310
H	6.29634	3.41181	0.97469
H	4.68270	3.85931	1.57618
C	6.90383	0.36617	0.40185
C	8.08044	1.04470	1.03484
H	8.01792	2.14340	0.97076
H	9.00506	0.74129	0.51987
H	8.19591	0.77836	2.10003
C	6.90201	-0.66541	-0.51664
C	8.05242	-1.38448	-1.15035
H	8.04132	-1.30246	-2.25184
H	8.06650	-2.45919	-0.89456

H	9.00347	-0.95517	-0.80035
C	5.09882	-2.02616	-1.71855
H	6.02691	-2.47590	-2.10904
C	4.30773	-3.11510	-0.97660
H	4.89030	-3.53135	-0.13824
H	4.06259	-3.93394	-1.67296
H	3.36134	-2.71169	-0.57718
C	4.31948	-1.42157	-2.89745
H	3.37391	-0.96909	-2.55223
H	4.07450	-2.21350	-3.62445
H	4.91028	-0.64545	-3.41142
C	0.54849	-0.05220	-0.01333

$III_{Ag,N}$

SCF (BP86) Energy = -2365.31044474
Enthalpy 0K = -2364.028007
Enthalpy 298K = -2364.027063
Free Energy 298K = -2364.211086
Lowest Frequency = 18.4764 cm^{-1}
Second Frequency = 25.2979 cm^{-1}
SCF (BP86-D3BJ) Energy = -2365.71064649
SCF (C6H6) Energy = -2365.31440605
SCF (BS2) Energy = -3177.49682734

Ag	-1.39893	-0.15982	0.58450
Si	3.39348	-1.40848	-1.82688
Si	3.77019	2.03198	0.29247
Al	1.32365	-0.18385	0.32744
N	1.78063	-1.45225	-1.02352
N	2.03351	1.58168	0.10936
N	-3.89471	1.33170	-0.69959
N	-4.36318	-0.75302	-0.32330
N	1.30384	-0.78988	2.15375
N	-1.04859	-0.98501	2.95628
C	0.94648	-2.57308	-1.42581
C	0.96222	-3.81555	-0.70078
C	0.19497	-4.90904	-1.14883
H	0.22886	-5.84404	-0.57767
C	-0.58691	-4.84016	-2.30374
H	-1.16239	-5.70735	-2.64586
C	-0.61101	-3.63883	-3.01423
H	-1.21920	-3.56774	-3.92359
C	0.12807	-2.50900	-2.60538
C	1.77893	-4.03193	0.57038
H	2.38925	-3.12476	0.71054
C	0.84820	-4.19231	1.79325
H	0.17070	-3.33200	1.90128
H	1.43665	-4.29499	2.72364
H	0.22979	-5.10285	1.69410
C	2.71985	-5.25709	0.49117
H	2.14880	-6.20251	0.47045
H	3.37307	-5.29533	1.38174
H	3.36010	-5.23663	-0.40364
C	-0.01350	-1.26140	-3.47895
H	0.67976	-0.49908	-3.08648
C	-1.45170	-0.69992	-3.39839
H	-2.18787	-1.46631	-3.70222
H	-1.57556	0.16319	-4.07547
H	-1.69941	-0.38099	-2.37197
C	0.33767	-1.54150	-4.95969
H	1.30139	-2.06450	-5.06822
H	0.39112	-0.59780	-5.53107
H	-0.43146	-2.17106	-5.44198
C	4.06316	-3.17167	-2.11631
H	4.45170	-3.61409	-1.18503
H	4.89933	-3.11901	-2.83607
H	3.30140	-3.85121	-2.53051
C	3.47146	-0.57952	-3.54803
H	3.00950	-1.20974	-4.32331
H	4.53587	-0.45355	-3.81937
H	2.99743	0.41266	-3.58859
C	4.72351	-0.52849	-0.75929
H	4.63526	-0.84651	0.29794
H	5.65597	-1.01609	-1.11222
C	4.86863	1.00812	-0.88319
H	4.69687	1.33102	-1.92627
H	5.90915	1.31116	-0.64609
C	4.52351	1.77041	2.03184
H	3.95432	2.30054	2.81186
H	5.54421	2.19505	2.02153
H	4.61500	0.71584	2.33100
C	4.04816	3.89519	-0.01543
H	3.60831	4.27740	-0.94695
H	5.13682	4.08194	-0.04367
H	3.62967	4.49268	0.81151
C	1.19942	2.75034	-0.07515
C	0.67103	3.47020	1.04825
C	0.00605	4.69662	0.84382
H	-0.36628	5.24731	1.71612
C	-0.15642	5.24411	-0.43304
H	-0.64241	6.21704	-0.56697
C	0.32214	4.52719	-1.53570
H	0.20054	4.94526	-2.54232
C	0.97751	3.28816	-1.38851
C	0.84025	2.98855	2.48943
H	1.37973	2.02762	2.44959
C	-0.52399	2.74142	3.17112
H	-1.12130	3.66965	3.22608
H	-0.37780	2.38214	4.20569
H	-1.11218	1.98043	2.63124
C	1.67172	3.98019	3.33643
H	2.65328	4.19061	2.88069
H	1.84531	3.57423	4.34911
H	1.14850	4.94635	3.45300
C	1.43827	2.57029	-2.65802
H	1.77699	1.56804	-2.34372
C	0.27639	2.39892	-3.65990
H	-0.60034	1.93781	-3.18077
H	0.58586	1.75693	-4.50355
H	-0.04010	3.36796	-4.08608
C	2.61254	3.27954	-3.37249
H	2.34731	4.32134	-3.62858
H	2.86083	2.75920	-4.31497
H	3.52415	3.30591	-2.75636
C	-3.34070	0.15859	-0.25398
C	-3.12601	2.60685	-0.69859
H	-2.08640	2.28000	-0.51591
C	-3.16588	3.32596	-2.05529
H	-2.97379	2.62513	-2.88376
H	-2.36965	4.08671	-2.06344
H	-4.12453	3.83734	-2.23711
C	-3.55315	3.50572	0.47295
H	-3.49326	2.95703	1.42660
H	-4.58077	3.88913	0.35149
H	-2.86794	4.36651	0.52912
C	-5.24705	1.16534	-1.03616
C	-6.15499	2.23021	-1.57296
H	-6.12917	3.15016	-0.96617
H	-7.19419	1.86594	-1.56767
H	-5.90896	2.50922	-2.61219
C	-5.54075	-0.16089	-0.79624
C	-6.82752	-0.90262	-0.98928
H	-7.19331	-1.35928	-0.05248
H	-6.73823	-1.70739	-1.74120
H	-7.60854	-0.21289	-1.34405
C	-4.30024	-2.16954	0.14021
H	-5.23845	-2.61919	-0.22598
C	-3.13803	-2.93650	-0.49863
H	-3.16642	-2.87371	-1.59704
H	-3.20183	-3.99849	-0.21061
H	-2.15654	-2.55912	-0.16442
C	-4.29652	-2.23096	1.67616
H	-3.36966	-1.79133	2.08515
H	-4.35583	-3.28318	2.00276

H -5.16159 -1.69014 2.09693
C -0.06068 -0.74149 2.15104
C -1.07837 -1.32425 4.39187
H -0.11450 -1.09173 4.88544
C 2.04930 -1.20468 3.37066
H 1.44998 -1.99219 3.86807
C -1.36678 -2.82446 4.59201
H -2.31561 -3.10010 4.10022
H -0.56799 -3.44967 4.16186
H -1.45252 -3.06267 5.66726
C -2.16805 -0.46986 5.06672
H -3.15247 -0.68053 4.61359
H -2.22661 -0.68957 6.14747
H -1.95934 0.60460 4.93865
C 2.22757 -0.03850 4.36506
H 1.26642 0.45323 4.58602
H 2.65322 -0.40474 5.31673
H 2.91059 0.72252 3.95740
C 3.40750 -1.82745 3.01785
H 3.97685 -2.04204 3.93860
H 3.29436 -2.76802 2.45963
H 4.01309 -1.13995 2.40490

TS(III-IV)$_{Ag,N}$
SCF (BP86) Energy = -2365.30228943
Enthalpy 0K = -2364.021233
Enthalpy 298K = -2364.020289
Free Energy 298K = -2364.204566
Lowest Frequency = -103.4212 cm^{-1}
Second Frequency = 17.1636 cm^{-1}
SCF (BP86-D3BJ) Energy = -2365.69718986
SCF (C6H6) Energy = -2365.30632513
SCF (BS2) Energy = -3177.48884309

Ag 1.68936 0.17875 0.83397
Si -3.35223 1.48165 -1.95354
Si -3.87653 -2.01199 0.04273
Al -1.49412 0.19216 0.31403
N -1.79215 1.48147 -1.05092
N -2.13080 -1.57363 -0.03494
N 4.03169 -1.32096 -0.56844
N 4.55644 0.75632 -0.20878
N -1.67502 0.72698 2.15543
N 0.74713 0.76391 2.77046
C -0.92970 2.61202 -1.34847
C -0.99873 3.82919 -0.58538
C -0.19846 4.93351 -0.93953
H -0.27243 5.84948 -0.34199
C 0.66722 4.89945 -2.03486
H 1.26730 5.77552 -2.30437
C 0.74194 3.72252 -2.78191
H 1.41440 3.67921 -3.64671
C -0.02786 2.58351 -2.46644
C -1.90085 4.00539 0.63425
H -2.52393 3.09799 0.70674
C -1.04602 4.11477 1.91600
H -0.38444 3.24308 2.02859
H -1.68652 4.19080 2.81375
H -0.41319 5.02023 1.88543
C -2.82762 5.23997 0.53862
H -2.25115 6.18100 0.58835
H -3.53636 5.25168 1.38637
H -3.40937 5.25650 -0.39543
C 0.16955 1.36428 -3.36850
H -0.55196 0.59384 -3.04926
C 1.59695 0.79302 -3.20837
H 2.35395 1.56228 -3.44696
H 1.76150 -0.05428 -3.89665
H 1.78010 0.44999 -2.17594
C -0.08074 1.69405 -4.85933
H -1.03792 2.21715 -5.01539
H -0.08981 0.77047 -5.46504
H 0.71591 2.34267 -5.26588
C -3.98835 3.25817 -2.23457
H -4.43482 3.67726 -1.31870
H -4.77513 3.23372 -3.00938
H -3.19587 3.94245 -2.57725
C -3.32734 0.70265 -3.69897
H -2.80406 1.34737 -4.42182
H -4.37250 0.60277 -4.04551
H -2.86638 -0.29572 -3.73696
C -4.74523 0.58454 -0.98407
H -4.70504 0.86755 0.08656
H -5.65425 1.09409 -1.36575
C -4.89893 -0.94636 -1.16466
H -4.67073 -1.23941 -2.20577
H -5.95412 -1.24424 -0.99604
C -4.69418 -1.74864 1.74960
H -4.18670 -2.32201 2.54148
H -5.73988 -2.10255 1.69700
H -4.71968 -0.69232 2.05624
C -4.15681 -3.86301 -0.32345
H -3.69202 -4.21814 -1.25397
H -5.24493 -4.04253 -0.38936
H -3.76463 -4.48832 0.49542
C -1.28480 -2.73486 -0.20155
C -0.82903 -3.49083 0.93014
C -0.13478 -4.70176 0.73007
H 0.18466 -5.27858 1.60637
C 0.11935 -5.20380 -0.55036
H 0.62648 -6.16598 -0.68354
C -0.29767 -4.45691 -1.65800
H -0.10666 -4.84053 -2.66748
C -0.97458 -3.22928 -1.51380
C -1.10677 -3.06675 2.37260
H -1.64216 -2.10326 2.33325
C 0.20326 -2.85315 3.16220
H 0.78592 -3.78909 3.23883
H -0.01823 -2.51907 4.19197
H 0.83714 -2.08642 2.68683
C -1.99800 -4.09019 3.11496
H -2.94767 -4.27306 2.58573
H -2.23809 -3.72944 4.13121
H -1.48695 -5.06396 3.22174
C -1.36227 -2.47451 -2.78563
H -1.71857 -1.48155 -2.46107
C -0.14659 -2.27636 -3.71628
H 0.70569 -1.84010 -3.17362
H -0.40585 -1.60240 -4.55185
H 0.18709 -3.23189 -4.15956
C -2.49514 -3.16200 -3.58340
H -2.21541 -4.19663 -3.85274
H -2.69159 -2.61572 -4.52348
H -3.43933 -3.20451 -3.01919
C 3.51888 -0.13615 -0.09999
C 3.22441 -2.57082 -0.56276
H 2.19680 -2.20596 -0.38257
C 3.23744 -3.29640 -1.91650
H 3.07861 -2.59098 -2.74817
H 2.40822 -4.02114 -1.92495
H 4.17310 -3.85038 -2.09331
C 3.61595 -3.48095 0.61242
H 3.57131 -2.92769 1.56445
H 4.63109 -3.89803 0.49511
H 2.90307 -4.31961 0.66770
C 5.37589 -1.18084 -0.95090
C 6.24432 -2.26873 -1.50619
H 6.21103 -3.18464 -0.89317
H 7.29190 -1.92980 -1.52796
H 5.96643 -2.54757 -2.53741
C 5.70442 0.13873 -0.72515
C 6.99575 0.85630 -0.97050
H 7.40792 1.30867 -0.05079
H 6.89178 1.66089 -1.72099

H	7.74911	0.15152	-1.35434
C	4.53475	2.17133	0.25701
H	5.46738	2.60687	-0.13932
C	3.36248	2.96107	-0.33620
H	3.34687	2.89760	-1.43478
H	3.45625	4.02182	-0.05091
H	2.38987	2.59781	0.03624
C	4.58528	2.23293	1.79276
H	3.66904	1.79597	2.22413
H	4.65976	3.28290	2.12240
H	5.45620	1.68212	2.18665
C	-0.32551	0.61140	2.01511
C	0.85620	1.03692	4.21890
H	-0.07749	0.75250	4.74210
C	-2.36390	1.13483	3.40706
H	-1.70978	1.86679	3.92047
C	1.12935	2.52827	4.49435
H	2.02931	2.85724	3.94575
H	0.28842	3.16327	4.17415
H	1.29994	2.70000	5.57223
C	1.99760	0.17446	4.78843
H	2.94880	0.42543	4.28632
H	2.11978	0.34980	5.87183
H	1.80219	-0.89728	4.62668
C	-2.59262	-0.05639	4.35962
H	-1.65439	-0.59871	4.56111
H	-2.99917	0.29611	5.32461
H	-3.31051	-0.77095	3.92755
C	-3.69178	1.84275	3.09830
H	-4.19973	2.12525	4.03666
H	-3.53682	2.75509	2.50346
H	-4.37326	1.18251	2.53619

$IV_{Ag,N}$

SCF (BP86) Energy = -2365.32414109
Enthalpy 0K = -2364.041977
Enthalpy 298K = -2364.041033
Free Energy 298K = -2364.227648
Lowest Frequency = 13.8757 cm^{-1}
Second Frequency = 19.7187 cm^{-1}
SCF (BP86-D3BJ) Energy = -2365.70845507
SCF (C6H6) Energy = -2365.32957014
SCF (BS2) Energy = -3177.51220290

Ag	-2.48448	-0.56941	0.87695
Si	3.93527	-1.03068	-1.96218
Si	4.04406	2.23216	0.41665
Al	1.82776	-0.13299	0.37385
N	2.44157	-1.28870	-0.99967
N	2.34170	1.69442	0.22122
N	-4.50470	1.24851	-0.59242
N	-5.31425	-0.76158	-0.46770
N	1.66720	-0.87040	2.15772
N	-0.81466	-1.09024	2.03458
C	1.66969	-2.45560	-1.38497
C	1.91986	-3.74974	-0.81346
C	1.19114	-4.86861	-1.26490
H	1.40074	-5.84809	-0.81953
C	0.21339	-4.76592	-2.25720
H	-0.33305	-5.65186	-2.59906
C	-0.05312	-3.50702	-2.80081
H	-0.82540	-3.40828	-3.57253
C	0.65036	-2.35712	-2.39047
C	2.90847	-3.98985	0.32849
H	3.45201	-3.04249	0.49187
C	2.13273	-4.34175	1.61897
H	1.40648	-3.55242	1.86372
H	2.81817	-4.46995	2.47577
H	1.57840	-5.28892	1.49101
C	3.93221	-5.11247	0.04025
H	3.43971	-6.09974	-0.01657
H	4.67450	-5.16929	0.85655
H	4.47314	-4.95631	-0.90502
C	0.23715	-1.02596	-3.01695
H	0.98886	-0.27451	-2.72218
C	-1.13075	-0.58659	-2.44869
H	-1.90757	-1.33961	-2.67257
H	-1.45986	0.37452	-2.88365
H	-1.08946	-0.47228	-1.34950
C	0.17589	-1.07302	-4.55966
H	1.11768	-1.44438	-4.99590
H	-0.01668	-0.06560	-4.96789
H	-0.63651	-1.73075	-4.91727
C	4.79759	-2.68124	-2.37853
H	5.33041	-3.09268	-1.50625
H	5.54382	-2.50118	-3.17267
H	4.09136	-3.44339	-2.74477
C	3.67437	-0.20846	-3.66961
H	3.12947	-0.88435	-4.34915
H	4.66291	-0.01308	-4.12386
H	3.12788	0.74593	-3.63027
C	5.26191	-0.01961	-1.01759
H	5.38441	-0.45324	-0.00558
H	6.19019	-0.30808	-1.55377
C	5.16509	1.52410	-0.95883
H	4.84986	1.93023	-1.93761
H	6.16999	1.95562	-0.76894
C	4.82541	1.65603	2.06197
H	4.17541	1.87505	2.92464
H	5.78356	2.18487	2.21448
H	5.04420	0.57660	2.06368
C	4.18207	4.13523	0.42629
H	3.64617	4.62510	-0.39964
H	5.24930	4.41233	0.35988
H	3.78640	4.55608	1.36522
C	1.39742	2.78283	0.11196
C	0.76045	3.33367	1.27376
C	-0.05394	4.47811	1.15083
H	-0.50638	4.90320	2.05491
C	-0.26657	5.10562	-0.08122
H	-0.87527	6.01437	-0.14914
C	0.32864	4.55720	-1.22299
H	0.17392	5.04045	-2.19536
C	1.14223	3.40834	-1.15662
C	0.96332	2.75863	2.67580
H	1.54707	1.82942	2.56623
C	-0.38267	2.40005	3.34333
H	-1.02061	3.29203	3.48045
H	-0.20962	1.96765	4.34487
H	-0.93882	1.66110	2.74356
C	1.75853	3.72500	3.58450
H	2.74937	3.96245	3.16388
H	1.91244	3.27957	4.58404
H	1.21903	4.67910	3.72496
C	1.73844	2.88428	-2.46316
H	2.22314	1.92378	-2.21863
C	0.64919	2.62581	-3.52741
H	-0.15739	1.98862	-3.13295
H	1.08351	2.12577	-4.41122
H	0.19270	3.56925	-3.87747
C	2.80660	3.82858	-3.06284
H	2.37421	4.82033	-3.28828
H	3.20003	3.41439	-4.00867
H	3.65903	3.98203	-2.38352
C	-4.21158	-0.01465	-0.14574
C	-3.54871	2.37726	-0.40364
H	-2.63436	1.86940	-0.04761
C	-3.20689	3.09136	-1.71903
H	-2.97842	2.36532	-2.51613
H	-2.30908	3.70941	-1.55545
H	-4.01596	3.75533	-2.06406
C	-4.01172	3.33392	0.70582
H	-4.22627	2.78136	1.63498
H	-4.91112	3.90559	0.42024

H	-3.20209	4.05344 0.91034
C	-5.77915	1.30025 -1.17733
C	-6.41275	2.51756 -1.77928
H	-6.36427	3.39038 -1.10783
H	-7.47705	2.32009 -1.98126
H	-5.94343	2.80620 -2.73565
C	-6.29118	0.02126 -1.09804
C	-7.60650	-0.51328 -1.57405
H	-8.20036	-0.95836 -0.75575
H	-7.48780	-1.28244 -2.35854
H	-8.20697	0.30077 -2.00779
C	-5.48089	-2.21056 -0.16804
H	-6.43751	-2.48610 -0.64235
C	-4.37047	-3.05189 -0.81504
H	-4.31905	-2.87253 -1.90127
H	-4.57453	-4.12265 -0.64771
H	-3.38441	-2.81614 -0.38034
C	-5.61040	-2.44253 1.34592
H	-4.67627	-2.16242 1.86120
H	-5.81188	-3.50801 1.54645
H	-6.43371	-1.84511 1.77182
C	0.41283	-0.75462 1.61569
C	-1.10314	-1.82210 3.29766
H	-0.18526	-1.89725 3.90077
C	2.14166	-1.37947 3.46836
H	1.62559	-2.33369 3.69592
C	-1.57805	-3.25305 2.98377
H	-2.50012	-3.22292 2.37397
H	-0.81710	-3.80721 2.41153
H	-1.79778	-3.81143 3.91164
C	-2.15009	-1.06744 4.13579
H	-3.08757	-0.94389 3.55945
H	-2.38838	-1.61981 5.06207
H	-1.79235	-0.06136 4.40900
C	1.86126	-0.38374 4.61156
H	0.78851	-0.14911 4.70188
H	2.20557	-0.79477 5.57747
H	2.40014	0.56203 4.43114
C	3.64522	-1.68689 3.39999
H	3.97576	-2.18990 4.32544
H	3.88116	-2.34110 2.54684
H	4.22712	-0.75753 3.29650

$A_{Ag,N}$

SCF (BP86) Energy = -2365.34260426
Enthalpy 0K = -2364.060944
Enthalpy 298K = -2364.060000
Free Energy 298K = -2364.252394
Lowest Frequency = 8.5166 cm^{-1}
Second Frequency = 11.6306 cm^{-1}
SCF (BP86-D3BJ) Energy = -2365.72104556
SCF (C6H6) Energy = -2365.34951141
SCF (BS2) Energy = -3177.53230737

Ag	3.08432	-0.33157 0.47735
Si	-4.45293	-1.62053 -1.30750
Si	-4.60736	1.74379 0.67286
Al	-1.91394	0.04226 -0.09679
N	-2.91345	-1.52594 -0.38756
N	-2.92306	1.63149 0.04636
N	-0.14741	0.29092 -0.80796
N	1.09854	-0.45260 1.14749
C	-2.39556	-2.79510 0.07406
C	-1.49514	-3.56650 -0.73113
C	-1.07893	-4.83900 -0.28897
H	-0.40568	-5.42643 -0.92478
C	-1.50330	-5.37254 0.93167
H	-1.17005	-6.36522 1.25353
C	-2.35771	-4.61108 1.73482
H	-2.69044	-5.01245 2.69964
C	-2.81378	-3.34115 1.33256
C	-0.95269	-3.07029 -2.07274
H	-1.30160	-2.03088 -2.19945
C	0.59303	-3.05918 -2.07591
H	0.98248	-2.43025 -1.25800
H	0.97925	-2.66894 -3.03489
H	1.00338	-4.07713 -1.94924
C	-1.47758	-3.90482 -3.26366
H	-1.07502	-3.51918 -4.21794
H	-2.57784	-3.88083 -3.32742
H	-1.17241	-4.96322 -3.17602
C	-3.74687	-2.58510 2.27611
H	-4.03561	-1.66027 1.75066
C	-3.02408	-2.18874 3.58346
H	-3.69320	-1.60781 4.24341
H	-2.13084	-1.57601 3.37548
H	-2.69373	-3.08208 4.14322
C	-5.03867	-3.36863 2.59849
H	-4.82131	-4.30701 3.13940
H	-5.59513	-3.63374 1.68398
H	-5.70620	-2.76494 3.23903
C	-5.01204	-3.43552 -1.47652
H	-4.23941	-4.07389 -1.93307
H	-5.91353	-3.47890 -2.11302
H	-5.26450	-3.87948 -0.49992
C	-4.24864	-0.90410 -3.06467
H	-3.91742	0.14727 -3.04684
H	-5.20873	-0.94046 -3.61007
H	-3.50760	-1.48115 -3.64269
C	-5.90056	-0.70778 -0.44815
H	-6.81174	-1.06332 -0.97400
H	-5.98956	-1.10442 0.58134
C	-5.88153	0.83690 -0.43477
H	-6.86374	1.21867 -0.08396
H	-5.77329	1.22344 -1.46543
C	-5.17530	3.56533 0.76248
H	-4.46857	4.18501 1.33678
H	-6.15244	3.59920 1.27689
H	-5.29603	4.03980 -0.22334
C	-4.78352	1.07561 2.45494
H	-4.28022	0.10883 2.60377
H	-5.85182	0.93999 2.70291
H	-4.35918	1.78765 3.18200
C	-2.25693	2.90367 -0.12928
C	-1.60910	3.55524 0.97154
C	-1.03812	4.83095 0.79063
H	-0.55643	5.32141 1.64522
C	-1.08154	5.48861 -0.44150
H	-0.64415	6.48630 -0.55849
C	-1.69063	4.84743 -1.52543
H	-1.72060	5.35274 -2.49714
C	-2.26948	3.56833 -1.40247
C	-1.51282	2.92935 2.36508
H	-1.98606	1.93370 2.31155
C	-0.04316	2.72858 2.79699
H	0.49073	3.69401 2.86621
H	0.49510	2.08245 2.08547
H	0.00076	2.25433 3.79416
C	-2.25866	3.76320 3.43296
H	-2.20950	3.26487 4.41785
H	-3.32121	3.90873 3.17824
H	-1.80581	4.76480 3.54549
C	-2.89660	2.93945 -2.64949
H	-2.94554	1.85203 -2.45943
C	-2.06650	3.18003 -3.93167
H	-2.42368	2.52455 -4.74539
H	-0.99300	2.98729 -3.77815
H	-2.16796	4.21988 -4.29125
C	-4.33724	3.43974 -2.90793
H	-5.01720	3.19925 -2.07805
H	-4.74879	2.98266 -3.82607
H	-4.34510	4.53636 -3.04438
C	5.09924	-0.12745 -0.01810
C	5.25550	2.22991 0.78265

C	5.16823	3.37249	-0.24146
H	6.15728	3.78317	-0.50369
H	4.57123	4.19533	0.18522
H	4.66972	3.03431	-1.16364
C	5.92811	2.63723	2.10280
H	6.00230	1.77872	2.78986
H	5.31543	3.41251	2.59177
H	6.93474	3.05998	1.95344
C	5.60764	-2.41484	-0.98272
C	4.57626	-2.40829	-2.12116
H	3.61300	-1.99615	-1.77703
H	4.40241	-3.43959	-2.46994
H	4.92869	-1.80596	-2.97479
C	5.16109	-3.24962	0.22749
H	5.92655	-3.24353	1.02103
H	4.98936	-4.29303	-0.08487
H	4.21985	-2.85637	0.64827
C	-0.01842	-0.17932	0.46499
C	0.92654	0.65788	-1.74250
H	1.80256	-0.00980	-1.55294
C	1.37827	2.11238	-1.50348
H	0.53695	2.80837	-1.65931
H	2.19798	2.38705	-2.19317
H	1.73273	2.24650	-0.46726
C	0.46580	0.43654	-3.18873
H	-0.44536	1.02135	-3.39249
H	0.23391	-0.62304	-3.37580
H	1.24488	0.75401	-3.90432
C	0.90249	-1.08885	2.47378
H	-0.13092	-0.84993	2.79261
C	1.87695	-0.51778	3.51762
H	2.92400	-0.75359	3.24422
H	1.68288	-0.95813	4.51171
H	1.78221	0.57733	3.59608
C	1.03458	-2.61835	2.37478
H	0.30444	-3.03085	1.66096
H	0.87184	-3.09647	3.35734
H	2.05035	-2.88972	2.02776
H	8.01265	2.78992	-0.56584
N	5.85552	0.99871	0.19630
N	5.96733	-1.02719	-0.57536
H	4.22370	1.90685	1.01490
H	6.54664	-2.84422	-1.36959
C	7.18200	0.80985	-0.22376
C	8.28372	1.82006	-0.11774
H	9.17421	1.45365	-0.65137
H	8.58340	2.00707	0.92808
C	7.24961	-0.47883	-0.71349
C	8.41465	-1.22353	-1.28847
H	8.67695	-2.11623	-0.69269
H	9.30319	-0.57444	-1.30803
H	8.22902	-1.55538	-2.32558

$S_{Ag,N}$

SCF (BP86) Energy = -2365.36903722
Enthalpy 0K = -2364.086667
Enthalpy 298K = -2364.085722
Free Energy 298K = -2364.273848
Lowest Frequency = 8.7334 cm^{-1}
Second Frequency = 12.6452 cm^{-1}
SCF (BP86-D3BJ) Energy = -2365.75597657
SCF (C6H6) Energy = -2365.37540051
SCF (BS2) Energy = -3177.55803299

Ag	-2.87950	-0.28375	-0.04550
Si	3.97263	1.81246	1.29317
Al	1.62580	0.03549	0.00471
Si	4.22631	-1.05159	-1.45068
N	2.48311	1.69824	0.28944
N	2.87471	-1.34732	-0.29922
N	0.01819	0.27364	-1.07464
N	-5.85788	-1.37713	-0.13298
N	0.01301	-0.52669	0.99094
N	-5.80933	0.75809	0.24187
C	-0.77434	-0.17338	-0.06315
C	-4.99608	-0.32444	0.01747
C	-7.16519	0.39215	0.22886
C	0.93996	3.60525	0.83772
C	1.85778	2.95670	-0.05570
C	-7.19220	-0.96745	-0.00845
C	1.88137	-3.61395	-0.75136
C	2.65955	-2.72986	0.06821
C	2.17346	3.62299	-1.29035
C	-0.55494	-1.15748	2.18469
H	-1.63773	-0.89428	2.19924
C	1.16320	-3.16422	-2.02622
H	1.31505	-2.07606	-2.13114
C	0.51192	3.00063	2.17606
H	0.98921	2.00950	2.25579
C	3.27001	-3.27465	1.24970
C	-0.48255	0.89731	-2.30628
H	0.42552	1.19236	-2.86187
C	0.97860	3.86230	3.37282
H	2.06862	4.02676	3.36043
H	0.71739	3.37555	4.32990
H	0.49520	4.85586	3.36281
C	3.69507	1.24040	3.09790
H	3.07398	1.95486	3.66226
H	4.66856	1.15972	3.61551
H	3.20875	0.25364	3.15567
C	-5.43502	-2.78381	-0.38095
H	-6.37723	-3.35182	-0.45605
C	4.54776	3.62724	1.43748
H	4.92346	4.04798	0.49223
H	5.36784	3.67480	2.17632
H	3.73611	4.28502	1.78840
C	0.40391	4.86586	0.50440
H	-0.28524	5.34933	1.20739
C	5.42864	0.75792	0.60166
H	6.33478	1.36251	0.81468
H	5.53193	-0.14210	1.23286
C	-0.45257	-2.69491	2.13360
H	-0.96120	-3.08913	1.23817
H	-0.92009	-3.14662	3.02777
H	0.59923	-3.02315	2.08665
C	-0.35846	-3.42119	-1.93719
H	-0.57679	-4.49144	-1.77206
H	-0.85883	-3.12228	-2.87524
H	-0.80838	-2.84499	-1.11236
C	5.26892	-2.63223	-1.68849
H	5.86287	-2.89755	-0.79988
H	5.97210	-2.46377	-2.52395
H	4.64433	-3.50473	-1.93901
C	4.08800	-2.42832	2.22552
H	3.96524	-1.37974	1.90992
C	-8.32168	1.31636	0.46141
H	-8.38224	1.65841	1.50932
H	-9.26420	0.79499	0.23328
H	-8.28242	2.21202	-0.17994
C	0.73582	5.51849	-0.68562
H	0.31690	6.50298	-0.92103
C	-1.26139	-0.07989	-3.20953
H	-2.17923	-0.43289	-2.70314
H	-0.64851	-0.96014	-3.45899
H	-1.56057	0.41654	-4.14998
C	1.76464	-4.97442	-0.40116
H	1.17630	-5.63729	-1.04693
C	-1.29710	2.18140	-2.04766
H	-1.55459	2.67630	-3.00130
H	-0.73032	2.89050	-1.42443
H	-2.24168	1.93575	-1.52602
C	0.08144	-0.60281	3.46848
H	1.16964	-0.78175	3.47551
H	-0.34544	-1.09715	4.35859

H -0.08295 0.48158 3.56203
C 3.58706 -0.59015 -3.19675
H 3.20291 -1.47429 -3.73128
H 4.40637 -0.16102 -3.80192
H 2.77571 0.15559 -3.16090
C -8.36146 -1.89642 -0.11909
H -8.40213 -2.40345 -1.09969
H -9.30075 -1.33461 -0.00317
H -8.35121 -2.67790 0.66185
C -1.01897 2.79635 2.24587
H -1.55600 3.75653 2.14114
H -1.30989 2.36181 3.21967
H -1.36470 2.11537 1.45056
C 1.61304 4.88512 -1.57008
H 1.87782 5.38316 -2.51011
C 3.12373 -4.64351 1.55010
H 3.60908 -5.04171 2.44893
C 5.40547 0.36610 -0.89233
H 6.41425 0.02243 -1.20267
H 5.20169 1.25221 -1.51807
C 2.38283 -5.50279 0.73455
H 2.28624 -6.56558 0.98189
C -4.68792 -2.91020 -1.71745
H -3.72857 -2.36613 -1.68294
H -5.28791 -2.50709 -2.54997
H -4.47274 -3.97176 -1.92328
C 3.11212 3.02793 -2.34199
H 3.30064 1.98464 -2.04196
C 3.58595 -2.56421 3.68146
H 2.50039 -2.39281 3.76033
H 4.09809 -1.83671 4.33568
H 3.79039 -3.57057 4.08883
C 5.59585 -2.76866 2.18158
H 5.76737 -3.83022 2.43543
H 6.15541 -2.15528 2.91076
H 6.03191 -2.58932 1.18618
C 1.73655 -3.86085 -3.28291
H 2.82354 -3.70476 -3.37996
H 1.25251 -3.47573 -4.19865
H 1.56254 -4.95145 -3.24912
C -5.23801 2.12147 0.42417
H -4.14989 1.92722 0.44737
C 2.49607 3.02515 -3.76038
H 2.40595 4.04849 -4.16663
H 1.48988 2.57611 -3.77658
H 3.13697 2.45360 -4.45426
C -5.52641 3.02709 -0.78388
H -5.21489 2.53880 -1.72116
H -6.59274 3.29605 -0.86518
C -4.63138 -3.33374 0.80774
H -4.40244 -4.39942 0.64148
H -5.19736 -3.24071 1.74937
H -3.67814 -2.78918 0.91971
C 4.47211 3.76308 -2.40048
H 5.11336 3.33306 -3.19102
H 5.02192 3.69597 -1.44906
H 4.32904 4.83428 -2.63046
C -5.63001 2.74850 1.77090
H -6.68420 3.06786 1.80001
H -5.00983 3.64362 1.94178
H -5.44860 2.04642 2.60078
H -4.95498 3.96423 -0.68017

I_{Au}
SCF (BP86) Energy = -1969.49198123
Enthalpy 0K = -1968.422567
Enthalpy 298K = -1968.421622
Free Energy 298K = -1968.588167
Lowest Frequency = 15.9356 cm^{-1}
Second Frequency = 16.1510 cm^{-1}
SCF (BP86-D3BJ) Energy = -1969.81400010
SCF (C6H6) Energy = -1969.49626748
SCF (BS2) Energy = -2781.60167060

Au 1.34687 -0.00008 0.00010
Si -3.77146 -1.68474 -1.02449
Si -3.77144 1.68541 1.02403
Al -1.10164 0.00002 0.00006
N -2.10928 -1.54386 -0.35455
N -2.10907 1.54404 0.35464
N 4.35385 0.84886 -0.67121
N 4.35390 -0.84913 0.67109
C -1.38258 -2.78103 -0.17828
C -0.63844 -3.36832 -1.25103
C 0.04396 -4.58227 -1.03298
H 0.60614 -5.03076 -1.86095
C 0.01919 -5.22754 0.20825
H 0.55079 -6.17460 0.35299
C -0.70004 -4.64867 1.26072
H -0.72382 -5.14945 2.23562
C -1.40603 -3.44239 1.09173
C -0.55346 -2.72782 -2.63770
H -1.13331 -1.79017 -2.59592
C 0.89959 -2.35719 -3.00894
H 1.33042 -1.67529 -2.25329
H 0.93268 -1.85416 -3.99239
H 1.54343 -3.25327 -3.06987
C -1.17489 -3.62759 -3.73036
H -0.62487 -4.58088 -3.82651
H -1.14144 -3.12492 -4.71369
H -2.22710 -3.87392 -3.50936
C -2.16458 -2.85149 2.28058
H -2.82835 -2.06922 1.87255
C -1.18919 -2.16529 3.26470
H -0.48051 -2.89925 3.68907
H -1.73369 -1.69308 4.10226
H -0.59310 -1.38590 2.75633
C -3.04684 -3.88157 3.01694
H -3.74162 -4.38795 2.32556
H -3.64585 -3.38327 3.79947
H -2.44512 -4.66209 3.51586
C -4.29124 -3.51735 -1.05965
H -3.56835 -4.14818 -1.60103
H -5.27222 -3.61449 -1.55713
H -4.38678 -3.92662 -0.03987
C -3.88109 -0.97861 -2.79650
H -3.47727 0.04661 -2.85136
H -4.93396 -0.94093 -3.12936
H -3.32265 -1.59816 -3.51707
C -5.08833 -0.77192 0.01858
H -6.05323 -1.15563 -0.37472
H -5.03625 -1.13912 1.06134
C -5.08830 0.77265 -0.01912
H -6.05318 1.15641 0.37422
H -5.03624 1.13985 -1.06188
C -3.88166 0.97967 2.79616
H -3.47841 -0.04575 2.85125
H -4.93456 0.94266 3.12899
H -3.32290 1.59905 3.51663
C -4.29074 3.51816 1.05879
H -3.56824 4.14867 1.60105
H -5.27222 3.61555 1.55523
H -4.38504 3.92761 0.03897
C -1.38211 2.78108 0.17847
C -0.63789 3.36816 1.25129
C 0.04479 4.58196 1.03333
H 0.60702 5.03030 1.86135
C 0.02021 5.22730 -0.20787
H 0.55202 6.17425 -0.35253
C -0.69911 4.64866 -1.26040
H -0.72275 5.14950 -2.23527
C -1.40536 3.44252 -1.09151
C -0.55315 2.72758 2.63794
H -1.13325 1.79009 2.59610

C	0.89979	2.35654	3.00920
H	1.33045	1.67457	2.25352
H	0.93273	1.85347	3.99264
H	1.54387	3.25245	3.07018
C	-1.17439	3.62749	3.73059
H	-0.62406	4.58059	3.82686
H	-1.14121	3.12475	4.71389
H	-2.22649	3.87419	3.50950
C	-2.16396	2.85178	-2.28040
H	-2.82841	2.07009	-1.87232
C	-1.18874	2.16453	-3.26395
H	-0.47937	2.89784	-3.68830
H	-1.73327	1.69243	-4.10154
H	-0.59337	1.38488	-2.75512
C	-3.04527	3.88218	-3.01744
H	-3.73982	4.38942	-2.32646
H	-3.64449	3.38394	-3.79985
H	-2.44286	4.66199	-3.51662
C	3.51126	-0.00010	0.00002
C	3.90764	1.96658	-1.54974
H	4.84255	2.42051	-1.91939
C	3.11867	1.43684	-2.75669
H	3.70025	0.68508	-3.31588
H	2.87781	2.27120	-3.43626
H	2.17299	0.97437	-2.42408
C	3.13611	3.02524	-0.74888
H	2.19083	2.61192	-0.35728
H	2.88840	3.87925	-1.40007
H	3.73491	3.39537	0.09993
C	5.70032	0.54037	-0.42751
C	6.85210	1.29123	-1.02066
H	6.85654	1.25018	-2.12477
H	7.80171	0.85443	-0.67478
H	6.85559	2.35610	-0.72611
C	5.70035	-0.54073	0.42718
C	6.85216	-1.29166	1.02018
H	6.85678	-1.25055	2.12430
H	7.80176	-0.85498	0.67413
H	6.85550	-2.35656	0.72569
C	3.90773	-1.96686	1.54963
H	4.84267	-2.42080	1.91921
C	3.13617	-3.02551	0.74880
H	2.19077	-2.61225	0.35742
H	2.88869	-3.87962	1.39994
H	3.73484	-3.39547	-0.10017
C	3.11885	-1.43715	2.75664
H	3.70053	-0.68551	3.31590
H	2.87791	-2.27155	3.43613
H	2.17321	-0.97455	2.42410

TS(I-II)$_{Au}$

SCF (BP86) Energy = -1969.47736011
Enthalpy 0K = -1968.408874
Enthalpy 298K = -1968.407930
Free Energy 298K = -1968.572007
Lowest Frequency = -58.6604 cm^{-1}
Second Frequency = 12.9604 cm^{-1}
SCF (BP86-D3BJ) Energy = -1969.79862283
SCF (C6H6) Energy = -1969.48168770
SCF (BS2) Energy = -2781.58760099

Au	1.24117	-0.37778	-0.19963
Si	-4.22116	-0.76965	-0.73255
Si	-3.15559	2.45590	1.29628
Al	-1.12925	0.15492	0.03223
N	-2.51948	-1.07043	-0.23996
N	-1.65871	1.90127	0.47473
N	4.39916	0.24871	-0.50794
N	4.03731	-1.66902	0.45733
C	-2.09119	-2.44978	-0.17344
C	-1.59733	-3.13237	-1.33003
C	-1.17897	-4.47319	-1.21123
H	-0.80513	-4.99310	-2.10155
C	-1.23135	-5.15431	0.00981
H	-0.90667	-6.19859	0.07777
C	-1.71419	-4.48617	1.14165
H	-1.76222	-5.01653	2.09979
C	-2.15212	-3.14994	1.07391
C	-1.51048	-2.46261	-2.70291
H	-1.87486	-1.42847	-2.58149
C	-0.05569	-2.38046	-3.21627
H	0.57585	-1.81618	-2.50526
H	-0.01818	-1.86852	-4.19495
H	0.38597	-3.38490	-3.34705
C	-2.41181	-3.16729	-3.74268
H	-2.08334	-4.20685	-3.92121
H	-2.37622	-2.63737	-4.71146
H	-3.46391	-3.20553	-3.41286
C	-2.66212	-2.46510	2.34274
H	-3.18794	-1.55049	2.01700
C	-1.48313	-2.02374	3.24020
H	-0.89717	-2.89838	3.57569
H	-1.84296	-1.48906	4.13781
H	-0.79388	-1.35498	2.69330
C	-3.66189	-3.32587	3.14331
H	-4.50213	-3.66334	2.51301
H	-4.07765	-2.74585	3.98600
H	-3.18484	-4.22509	3.57226
C	-5.18417	-2.41289	-0.71026
H	-4.70106	-3.18472	-1.33073
H	-6.20577	-2.25168	-1.09682
H	-5.26860	-2.81619	0.31276
C	-4.33410	-0.01760	-2.48528
H	-3.68377	0.86727	-2.59103
H	-5.37027	0.30166	-2.69795
H	-4.04087	-0.74428	-3.26039
C	-5.14233	0.42566	0.44170
H	-6.20904	0.30823	0.15656
H	-5.07667	0.03539	1.47524
C	-4.75419	1.92115	0.39391
H	-5.54819	2.52816	0.87780
H	-4.71309	2.28258	-0.65135
C	-3.27267	1.77379	3.07728
H	-3.13368	0.67935	3.10082
H	-4.26548	1.99389	3.50920
H	-2.51201	2.22262	3.73675
C	-3.18010	4.35996	1.35613
H	-2.26292	4.77631	1.80248
H	-4.04061	4.70355	1.95657
H	-3.27981	4.79029	0.34540
C	-0.63940	2.89135	0.21163
C	0.34397	3.22992	1.19580
C	1.33213	4.18554	0.88325
H	2.07712	4.44587	1.64502
C	1.38019	4.81276	-0.36695
H	2.15214	5.55915	-0.58556
C	0.41774	4.48358	-1.32902
H	0.44489	4.97595	-2.30820
C	-0.59459	3.54176	-1.06348
C	0.36316	2.59588	2.58777
H	-0.45205	1.85309	2.61412
C	1.68359	1.84286	2.86219
H	1.85333	1.06906	2.09143
H	1.65110	1.35119	3.85135
H	2.55016	2.52891	2.85939
C	0.09882	3.63893	3.69809
H	0.89275	4.40687	3.72335
H	0.07436	3.15366	4.69041
H	-0.86148	4.16113	3.55073
C	-1.61142	3.21770	-2.15861
H	-2.42041	2.64228	-1.67554
C	-0.98342	2.31461	-3.24521
H	-0.14764	2.83124	-3.75086
H	-1.72826	2.04075	-4.01399

H	-0.58005	1.38329	-2.80845
C	-2.24082	4.47588	-2.79369
H	-2.68678	5.13545	-2.03002
H	-3.03547	4.19000	-3.50524
H	-1.49917	5.07102	-3.35583
C	3.40410	-0.66908	-0.23362
C	4.16650	1.51492	-1.29247
H	3.91444	2.30158	-0.55643
C	5.40668	1.94809	-2.10055
H	6.22495	2.35038	-1.49046
H	5.09862	2.74905	-2.79135
H	5.79087	1.11271	-2.71093
C	2.99412	1.37534	-2.27462
H	3.19046	0.57654	-3.01019
H	2.87942	2.33229	-2.80897
H	2.03609	1.16033	-1.77071
C	5.62029	-0.14977	0.08075
C	6.90203	0.62817	0.14847
H	7.44724	0.67065	-0.80913
H	7.56924	0.14911	0.88206
H	6.73986	1.66332	0.49368
C	5.38497	-1.37135	0.67461
C	6.32256	-2.27290	1.41763
H	5.96181	-2.50362	2.43564
H	7.30963	-1.79675	1.51866
H	6.48018	-3.23362	0.89415
C	3.38623	-2.90995	0.96673
H	4.22745	-3.56622	1.24739
C	2.57857	-3.61859	-0.12832
H	1.70204	-3.01931	-0.42660
H	2.21205	-4.58437	0.25641
H	3.19885	-3.80622	-1.02043
C	2.55612	-2.61502	2.22603
H	3.16767	-2.13017	3.00567
H	2.14816	-3.55479	2.63365
H	1.71239	-1.94846	1.97389

II_{Au}

SCF (BP86) Energy = -1969.49191552
Enthalpy 0K = -1968.422359
Enthalpy 298K = -1968.421415
Free Energy 298K = -1968.589666
Lowest Frequency = 12.7854 cm^{-1}
Second Frequency = 13.7277 cm^{-1}
SCF (BP86-D3BJ) Energy = -1969.81027942
SCF (C6H6) Energy = -1969.49618756
SCF (BS2) Energy = -2781.60195959

Au	1.27083	-0.23897	0.08329
Si	-4.03392	-1.19294	-1.01900
Si	-3.53675	2.17536	0.99669
Al	-1.15352	0.08169	0.03274
N	-2.36987	-1.29291	-0.34833
N	-1.91162	1.76993	0.35024
N	4.27794	0.51983	-0.47163
N	4.23785	-1.38962	0.55789
C	-1.80989	-2.61640	-0.19119
C	-1.14489	-3.27616	-1.27327
C	-0.61290	-4.56567	-1.07134
H	-0.10993	-5.06858	-1.90612
C	-0.71244	-5.21715	0.16296
H	-0.29757	-6.22253	0.29576
C	-1.35621	-4.56900	1.22388
H	-1.43813	-5.07447	2.19316
C	-1.91251	-3.28473	1.07096
C	-0.98676	-2.63279	-2.65231
H	-1.46234	-1.63878	-2.60086
C	0.49849	-2.41502	-3.01817
H	0.99568	-1.78075	-2.26127
H	0.58701	-1.91807	-4.00137
H	1.04538	-3.37349	-3.07709
C	-1.70057	-3.44786	-3.75485
H	-1.25407	-4.45224	-3.86613
H	-1.61694	-2.93816	-4.73152
H	-2.77231	-3.58577	-3.53266
C	-2.59202	-2.61998	2.26881
H	-3.15683	-1.75817	1.87190
C	-1.53975	-2.06902	3.25922
H	-0.92668	-2.88880	3.67543
H	-2.02294	-1.54289	4.10230
H	-0.85117	-1.36361	2.75941
C	-3.59084	-3.54531	2.99531
H	-4.34225	-3.95640	2.29993
H	-4.12451	-2.98841	3.78556
H	-3.08617	-4.39832	3.48301
C	-4.81336	-2.93100	-1.03703
H	-4.19256	-3.65875	-1.58391
H	-5.80396	-2.89100	-1.52307
H	-4.95301	-3.31912	-0.01415
C	-4.04614	-0.49673	-2.79865
H	-3.48893	0.45300	-2.86742
H	-5.08341	-0.29989	-3.12446
H	-3.59685	-1.20223	-3.51647
C	-5.19409	-0.07975	0.01559
H	-6.20721	-0.32054	-0.36979
H	-5.19285	-0.43576	1.06347
C	-4.96470	1.44767	-0.04583
H	-5.86562	1.97583	0.33154
H	-4.85081	1.78578	-1.09348
C	-3.76815	1.52387	2.77804
H	-3.51267	0.45292	2.85296
H	-4.81999	1.63910	3.09592
H	-3.13745	2.06993	3.49843
C	-3.76989	4.06619	0.98900
H	-2.95742	4.58956	1.51796
H	-4.72358	4.32726	1.48031
H	-3.80073	4.46054	-0.04071
C	-0.98294	2.86035	0.16243
C	-0.16331	3.33666	1.23581
C	0.72990	4.40133	1.00128
H	1.34762	4.76729	1.83027
C	0.84423	5.00286	-0.25732
H	1.53538	5.83895	-0.41328
C	0.05073	4.53097	-1.31017
H	0.13278	4.99881	-2.29829
C	-0.86461	3.47729	-1.12467
C	-0.21717	2.73145	2.63980
H	-0.94591	1.90396	2.60602
C	1.14344	2.13206	3.05998
H	1.47079	1.36629	2.33269
H	1.06778	1.65829	4.05552
H	1.92755	2.90876	3.11879
C	-0.70188	3.75539	3.69179
H	-0.00100	4.60516	3.77742
H	-0.77510	3.28421	4.68844
H	-1.69240	4.16829	3.43662
C	-1.69504	2.99812	-2.31558
H	-2.48176	2.34122	-1.90521
C	-0.83380	2.14808	-3.27836
H	-0.01372	2.75202	-3.70746
H	-1.44043	1.75616	-4.11457
H	-0.37382	1.29132	-2.75334
C	-2.38897	4.14832	-3.07564
H	-3.00284	4.76764	-2.39985
H	-3.04893	3.74464	-3.86365
H	-1.66142	4.81613	-3.57069
C	3.42149	-0.40263	0.07462
C	3.75616	1.74880	-1.13263
H	2.67713	1.71455	-0.89291
C	4.33129	3.03715	-0.52518
H	4.29194	3.00493	0.57549
H	3.71294	3.88743	-0.85550
H	5.36972	3.23142	-0.84020
C	3.90243	1.67337	-2.66070

H	4.95571	1.71420	-2.98657
H	3.37887	2.52947	-3.11743
H	3.44998	0.74705	-3.04954
C	5.61600	0.11449	-0.34255
C	6.80948	0.88847	-0.81387
H	6.71917	1.20058	-1.86752
H	7.71241	0.26288	-0.73595
H	6.98612	1.79699	-0.21197
C	5.58725	-1.09919	0.31470
C	6.71789	-1.98912	0.72959
H	6.77384	-2.11275	1.82627
H	7.67626	-1.55746	0.40243
H	6.64268	-2.99702	0.28356
C	3.75451	-2.61140	1.25894
H	4.67153	-3.16073	1.53164
C	2.91734	-3.49058	0.31845
H	1.98893	-2.97358	0.02207
H	2.63662	-4.42469	0.83197
H	3.48240	-3.74818	-0.59289
C	3.00738	-2.24316	2.55021
H	3.63154	-1.61562	3.20798
H	2.73658	-3.16238	3.09583
H	2.08015	-1.69247	2.31445

TS(II-III)$_{Au}$

SCF (BP86) Energy = -2158.06381130
Enthalpy 0K = -2156.979017
Enthalpy 298K = -2156.978073
Free Energy 298K = -2157.150832
Lowest Frequency = -196.7411 cm^{-1}
Second Frequency = 7.2823 cm^{-1}
SCF (BP86-D3BJ) Energy = -2158.40386691
SCF (C6H6) Energy = -2158.06791473
SCF (BS2) Energy = -2970.23395978

Au	1.25042	-0.31578	-0.30314
Si	-3.97590	-0.96837	1.14783
Si	-3.41978	2.44877	-0.81068
Al	-1.18628	0.10411	-0.24056
N	-2.37930	-1.22894	0.35483
N	-1.79309	1.88593	-0.28467
N	4.24790	-1.56722	-0.16076
N	4.19945	0.50919	0.46857
O	-1.31283	-0.22770	-2.54258
O	0.79445	-0.90953	-3.34692
C	-1.85818	-2.58101	0.37873
C	-2.06827	-3.46963	-0.72927
C	-1.56575	-4.78550	-0.66796
H	-1.74155	-5.45800	-1.51572
C	-0.86125	-5.25710	0.44359
H	-0.48687	-6.28639	0.47106
C	-0.65404	-4.39408	1.52420
H	-0.10991	-4.75565	2.40498
C	-1.13810	-3.07096	1.51953
C	-2.83958	-3.06952	-1.99090
H	-3.04680	-1.98908	-1.91729
C	-2.02463	-3.32914	-3.28024
H	-1.00107	-2.92712	-3.22110
H	-2.52600	-2.87466	-4.15270
H	-1.93320	-4.41120	-3.48393
C	-4.19148	-3.81222	-2.10762
H	-4.03703	-4.90427	-2.17309
H	-4.72960	-3.49510	-3.01885
H	-4.84364	-3.62141	-1.24236
C	-0.89398	-2.22402	2.77065
H	-1.35605	-1.23846	2.59403
C	0.60950	-1.98988	3.03510
H	1.14245	-2.94225	3.20935
H	0.75152	-1.35819	3.93060
H	1.08463	-1.48384	2.17429
C	-1.56178	-2.85111	4.01669
H	-2.63639	-3.03923	3.85433
H	-1.45658	-2.18565	4.89228
H	-1.09504	-3.81779	4.27793
C	-4.89065	-2.62552	1.39598
H	-5.45081	-2.93437	0.49920
H	-5.62066	-2.50538	2.21585
H	-4.20727	-3.44626	1.66690
C	-3.88703	-0.19510	2.89615
H	-3.50023	-0.91103	3.63880
H	-4.91015	0.08506	3.20816
H	-3.26590	0.71224	2.94483
C	-5.10336	0.17241	0.10705
H	-5.08650	-0.16514	-0.94658
H	-6.12668	-0.05923	0.46970
C	-4.85030	1.69465	0.20983
H	-4.72847	1.99847	1.26692
H	-5.74464	2.24718	-0.14821
C	-3.78110	2.01908	-2.63636
H	-3.09244	2.53297	-3.32635
H	-4.81018	2.32755	-2.89435
H	-3.69796	0.93664	-2.82697
C	-3.55064	4.33581	-0.57880
H	-3.50544	4.61156	0.48812
H	-4.51733	4.68895	-0.97882
H	-2.74611	4.88387	-1.09396
C	-0.82641	2.92064	0.01129
C	-0.05488	3.54502	-1.02314
C	0.83833	4.58498	-0.69377
H	1.40817	5.06656	-1.49762
C	1.01023	5.02158	0.62465
H	1.69769	5.84322	0.85542
C	0.27428	4.40073	1.64065
H	0.39491	4.73718	2.67736
C	-0.64283	3.36943	1.36028
C	-0.15166	3.12817	-2.49149
H	-0.87465	2.29810	-2.54308
C	1.20761	2.61311	-3.01920
H	1.96475	3.41802	-3.02782
H	1.11115	2.23926	-4.05434
H	1.59354	1.79262	-2.38855
C	-0.67183	4.26973	-3.39486
H	-1.66448	4.62701	-3.07441
H	-0.75569	3.92757	-4.44196
H	0.01341	5.13621	-3.38345
C	-1.41810	2.74879	2.51850
H	-2.18016	2.09718	2.05931
C	-0.49967	1.86193	3.38924
H	-0.00753	1.08116	2.78322
H	-1.07423	1.36439	4.19106
H	0.29376	2.46516	3.86675
C	-2.14976	3.79373	3.38799
H	-1.44309	4.45352	3.92246
H	-2.76979	3.29145	4.15157
H	-2.81020	4.43572	2.78092
C	3.40148	-0.50063	-0.00844
C	3.86485	-2.88908	-0.73229
H	4.75343	-3.52532	-0.58207
C	2.69319	-3.51992	0.02989
H	2.91661	-3.60356	1.10575
H	2.49786	-4.52991	-0.36603
H	1.76975	-2.92595	-0.08415
C	3.60328	-2.76430	-2.24156
H	4.47612	-2.33661	-2.76331
H	2.73173	-2.11912	-2.43380
H	3.39901	-3.76063	-2.66831
C	5.55763	-1.23349	0.20899
C	6.71032	-2.18727	0.14264
H	6.55401	-3.07814	0.77714
H	7.62851	-1.69248	0.49452
H	6.90387	-2.54001	-0.88631
C	5.52904	0.08541	0.61524
C	6.66664	0.93187	1.10017
H	6.43665	1.44085	2.05053

H	6.95579	1.70667	0.36890
H	7.55119	0.29974	1.27502
C	3.63506	1.85060	0.78949
H	2.59140	1.77119	0.43251
C	3.58927	2.10744	2.30360
H	3.09810	1.27136	2.82651
H	2.99916	3.01995	2.48818
H	4.59159	2.25723	2.73970
C	4.31722	2.97773	0.00032
H	5.32355	3.21664	0.38161
H	3.69762	3.88469	0.08778
H	4.39321	2.72129	-1.06888
C	-0.16176	-0.54902	-2.74014

III$_{Au}$

SCF (BP86) Energy = -2158.08634539
Enthalpy 0K = -2157.000114
Enthalpy 298K = -2156.999170
Free Energy 298K = -2157.168523
Lowest Frequency = 12.3741 cm^{-1}
Second Frequency = 20.2579 cm^{-1}
SCF (BP86-D3BJ) Energy = -2158.42855885
SCF (C6H6) Energy = -2158.09292396
SCF (BS2) Energy = -2970.25598638

Au	1.31054	-0.24659	-0.83375
Si	-3.58900	-1.33856	1.51497
Si	-3.70962	2.04297	-0.61700
Al	-1.35349	-0.05080	-0.47077
N	-2.07349	-1.44496	0.53917
N	-1.97760	1.69266	-0.24211
N	3.82024	0.88716	0.73698
N	4.23227	-1.07983	-0.09664
O	-1.35448	-0.48882	-2.28164
O	0.57227	-0.95803	-3.39983
C	-1.40151	-2.72976	0.49474
C	-1.62489	-3.65490	-0.58058
C	-0.94072	-4.88845	-0.57446
H	-1.11617	-5.58994	-1.39798
C	-0.06627	-5.24932	0.45472
H	0.44177	-6.21990	0.43874
C	0.13364	-4.35759	1.51353
H	0.80324	-4.63723	2.33597
C	-0.51321	-3.10734	1.55598
C	-2.61794	-3.41217	-1.72322
H	-2.99748	-2.38203	-1.62067
C	-1.97085	-3.54839	-3.12088
H	-1.10730	-2.88160	-3.25353
H	-2.71020	-3.29848	-3.90203
H	-1.63851	-4.58591	-3.30695
C	-3.81931	-4.38511	-1.63758
H	-3.49113	-5.43018	-1.78240
H	-4.55570	-4.15568	-2.42816
H	-4.33170	-4.33338	-0.66485
C	-0.26211	-2.21427	2.77316
H	-0.86539	-1.30198	2.63653
C	1.21415	-1.77632	2.88440
H	1.88439	-2.64457	3.02179
H	1.35543	-1.10735	3.75289
H	1.53547	-1.23941	1.97550
C	-0.71237	-2.90233	4.08255
H	-1.76397	-3.23083	4.03108
H	-0.60754	-2.21533	4.94151
H	-0.09963	-3.79623	4.29708
C	-4.27248	-3.08542	1.85993
H	-4.88301	-3.46090	1.02364
H	-4.92152	-3.04195	2.75220
H	-3.47460	-3.81991	2.05424
C	-3.41026	-0.52877	3.23762
H	-2.87881	-1.18643	3.94374
H	-4.42366	-0.35622	3.64469
H	-2.89078	0.44026	3.21755
C	-4.95517	-0.37167	0.58509
H	-5.02202	-0.75734	-0.45022
H	-5.88931	-0.71341	1.07844
C	-4.90299	1.17502	0.60011
H	-4.69884	1.54770	1.62198
H	-5.90156	1.58303	0.33663
C	-4.16484	1.44354	-2.36924
H	-3.63724	2.02497	-3.14268
H	-5.25082	1.55398	-2.53944
H	-3.90308	0.38402	-2.52723
C	-4.04140	3.91106	-0.46967
H	-3.94828	4.25772	0.57264
H	-5.07135	4.12248	-0.80675
H	-3.35045	4.51216	-1.08106
C	-1.12293	2.83749	-0.03936
C	-0.49402	3.50526	-1.14240
C	0.26044	4.67251	-0.90349
H	0.71828	5.18810	-1.75603
C	0.42810	5.19608	0.38354
H	1.00204	6.11634	0.54060
C	-0.16557	4.53303	1.46442
H	-0.05097	4.93940	2.47677
C	-0.94087	3.37184	1.27852
C	-0.62171	3.02230	-2.58943
H	-1.19028	2.07809	-2.57592
C	0.75974	2.73349	-3.22056
H	1.35993	3.65605	-3.32148
H	0.64160	2.29607	-4.22674
H	1.33565	2.01616	-2.60971
C	-1.39714	4.02937	-3.47087
H	-2.41170	4.22028	-3.08390
H	-1.49401	3.64338	-4.50104
H	-0.87374	5.00088	-3.52627
C	-1.58171	2.71658	2.49884
H	-2.25061	1.93428	2.10418
C	-0.52448	2.02816	3.39066
H	0.05598	1.28200	2.82128
H	-1.00240	1.50995	4.24117
H	0.18502	2.76642	3.80583
C	-2.43177	3.69681	3.33592
H	-1.81212	4.48282	3.80359
H	-2.94800	3.15862	4.15058
H	-3.19740	4.19950	2.72163
C	3.24464	-0.13799	0.03476
C	3.10403	2.17608	0.95864
H	2.06698	1.94672	0.65529
C	3.08518	2.60468	2.43241
H	2.77445	1.77458	3.08692
H	2.34891	3.41700	2.54090
H	4.05931	2.98642	2.77738
C	3.64279	3.26491	0.01718
H	3.62891	2.91738	-1.02826
H	4.67179	3.56874	0.27436
H	2.99161	4.15024	0.08967
C	5.15599	0.59677	1.04997
C	6.07772	1.47560	1.83966
H	6.11286	2.50647	1.45121
H	7.10186	1.07440	1.79228
H	5.79333	1.52920	2.90478
C	5.41387	-0.65172	0.51947
C	6.67218	-1.46269	0.56089
H	7.06080	-1.68522	-0.44872
H	6.53220	-2.42436	1.08614
H	7.45713	-0.90983	1.09881
C	4.12685	-2.35188	-0.87415
H	5.08803	-2.85984	-0.69059
C	3.00740	-3.25549	-0.34409
H	3.12574	-3.45228	0.73299
H	3.03223	-4.21844	-0.87974
H	2.01050	-2.81062	-0.50294
C	4.01447	-2.06708	-2.38142
H	3.05079	-1.59361	-2.63553

H 4.07733 -3.01749 -2.93738
H 4.83233 -1.41139 -2.72481
C -0.04862 -0.60978 -2.39455

TS(III-IV)$_{Au}$
SCF (BP86) Energy = -2158.04127066
Enthalpy 0K = -2156.956671
Enthalpy 298K = -2156.955726
Free Energy 298K = -2157.125691
Lowest Frequency = -213.1480 cm^{-1}
Second Frequency = 12.5000 cm^{-1}
SCF (BP86-D3BJ) Energy = -2158.37171877
SCF (C6H6) Energy = -2158.04819867
SCF (BS2) Energy = -2970.21014990

Au -1.87807 0.29318 -0.96539
Si 3.81002 1.44148 1.56938
Si 4.05960 -2.02459 -0.43611
Al 1.71414 0.07320 -0.49796
N 2.34542 1.49247 0.52125
N 2.31057 -1.66146 -0.19366
N -4.63212 0.98289 0.05100
N -4.05966 -1.03778 0.65486
O 1.60565 0.46601 -2.34067
O -0.59570 0.77775 -2.78728
C 1.62822 2.74831 0.40025
C 1.86880 3.64355 -0.69510
C 1.12977 4.84197 -0.77467
H 1.31797 5.52060 -1.61434
C 0.17821 5.19351 0.18683
H -0.37515 6.13544 0.10370
C -0.04284 4.32976 1.26444
H -0.77422 4.60310 2.03462
C 0.66131 3.11677 1.39268
C 2.92219 3.39778 -1.78091
H 3.34504 2.39281 -1.61214
C 2.32457 3.43456 -3.20682
H 1.50265 2.71481 -3.32700
H 3.10405 3.18530 -3.94845
H 1.94720 4.44303 -3.45512
C 4.07335 4.42882 -1.69108
H 3.70557 5.44932 -1.90100
H 4.85553 4.19816 -2.43610
H 4.54136 4.44672 -0.69460
C 0.37864 2.25225 2.62281
H 1.01610 1.35631 2.54352
C -1.08808 1.77333 2.67990
H -1.78550 2.62473 2.78131
H -1.24563 1.11014 3.54985
H -1.36403 1.21955 1.76516
C 0.74493 2.99370 3.92936
H 1.78865 3.34997 3.91843
H 0.61552 2.33244 4.80507
H 0.09877 3.87678 4.08212
C 4.46017 3.20724 1.87150
H 5.07679 3.56579 1.03196
H 5.09364 3.20836 2.77580
H 3.64381 3.93120 2.02573
C 3.54717 0.68560 3.30610
H 2.96889 1.35596 3.96153
H 4.53699 0.53597 3.77534
H 3.03900 -0.29041 3.28433
C 5.22271 0.44440 0.74581
H 5.34370 0.79063 -0.29856
H 6.13028 0.80614 1.27317
C 5.17023 -1.10143 0.81813
H 4.90238 -1.43450 1.83889
H 6.18384 -1.51623 0.63463
C 4.62385 -1.48567 -2.17729
H 4.15360 -2.09901 -2.96285
H 5.71968 -1.58574 -2.27487
H 4.36346 -0.43418 -2.38725
C 4.37802 -3.88427 -0.19181
H 4.24088 -4.17979 0.86148
H 5.41906 -4.11734 -0.47596
H 3.70753 -4.50984 -0.80151
C 1.41588 -2.78348 -0.03303
C 0.85617 -3.46431 -1.16432
C 0.04111 -4.59603 -0.95381
H -0.36677 -5.12089 -1.82569
C -0.24332 -5.07585 0.32963
H -0.85898 -5.97221 0.46570
C 0.29122 -4.40358 1.43558
H 0.08693 -4.77723 2.44647
C 1.11386 -3.27108 1.28032
C 1.12356 -3.03674 -2.60947
H 1.70291 -2.09983 -2.57782
C -0.18624 -2.75402 -3.38077
H -0.78411 -3.67409 -3.51369
H 0.03901 -2.35463 -4.38465
H -0.81274 -2.01165 -2.85995
C 1.96029 -4.09004 -3.37370
H 2.93032 -4.28166 -2.88576
H 2.16047 -3.74818 -4.40469
H 1.42534 -5.05461 -3.44002
C 1.66593 -2.59084 2.53010
H 2.37569 -1.82663 2.17227
C 0.54745 -1.86721 3.31291
H 0.02095 -1.13662 2.67525
H 0.96075 -1.32538 4.18238
H -0.20071 -2.58699 3.69135
C 2.43157 -3.55957 3.45721
H 1.76580 -4.32916 3.88728
H 2.88372 -3.00845 4.30082
H 3.24008 -4.08320 2.92011
C -3.60534 0.07482 -0.00725
C -4.64794 2.32703 -0.59844
H -5.61498 2.76056 -0.29455
C -3.53416 3.23711 -0.06273
H -3.57627 3.31408 1.03562
H -3.65431 4.24703 -0.48856
H -2.53530 2.86525 -0.34508
C -4.63988 2.20159 -2.13148
H -5.46185 1.55570 -2.48274
H -3.68514 1.77937 -2.48683
H -4.76567 3.20055 -2.58121
C -5.72630 0.44074 0.74015
C -7.00048 1.18709 0.98757
H -6.84052 2.09874 1.59090
H -7.70487 0.55000 1.54343
H -7.50071 1.48867 0.04999
C -5.36970 -0.83683 1.11749
C -6.17743 -1.83656 1.88747
H -5.80530 -1.97523 2.91729
H -6.19153 -2.82591 1.40140
H -7.22106 -1.49308 1.95735
C -3.24960 -2.28674 0.73339
H -2.25002 -1.95602 0.39845
C -3.11418 -2.82150 2.16587
H -2.84492 -2.01667 2.86874
H -2.30062 -3.56441 2.17462
H -4.02904 -3.31919 2.52491
C -3.75602 -3.33899 -0.26545
H -4.74592 -3.73916 0.01338
H -3.04055 -4.17684 -0.29073
H -3.82079 -2.91295 -1.27963
C 0.33628 0.49025 -1.97569

IV$_{Au}$
SCF (BP86) Energy = -2158.06411364
Enthalpy 0K = -2156.978398
Enthalpy 298K = -2156.977454
Free Energy 298K = -2157.151156
Lowest Frequency = 7.0177 cm^{-1}

Second Frequency = 14.4979 cm^{-1}
SCF (BP86-D3BJ) Energy = -2158.38206549
SCF (C6H6) Energy = -2158.07256546
SCF (BS2) Energy = -2970.23563061

Au 2.55547 -0.61714 -0.78882
Si -4.22744 -0.88231 1.96459
Si -3.97439 2.63790 0.14706
Al -2.02286 0.08637 -0.24711
N -3.11389 -1.15687 0.58440
N -2.34428 1.89660 -0.01201
N 5.37800 -1.38841 0.02442
N 4.93248 0.69117 0.51409
O -1.46025 -0.48634 -1.98284
O 0.73803 -0.80176 -1.74545
C -3.00878 -2.51078 0.07827
C -3.81600 -2.93479 -1.02405
C -3.70878 -4.26058 -1.48630
H -4.32920 -4.57881 -2.33243
C -2.83158 -5.17600 -0.89541
H -2.76690 -6.20401 -1.26838
C -2.03330 -4.75722 0.17389
H -1.33733 -5.46723 0.63696
C -2.09915 -3.44126 0.67255
C -4.78508 -1.99262 -1.74042
H -4.73635 -1.02345 -1.21262
C -4.36300 -1.75855 -3.20964
H -3.32861 -1.38571 -3.27194
H -5.03359 -1.02464 -3.69245
H -4.42313 -2.69541 -3.79252
C -6.24654 -2.49056 -1.67366
H -6.36564 -3.45905 -2.19147
H -6.92397 -1.76834 -2.16330
H -6.58849 -2.62676 -0.63377
C -1.18018 -3.05856 1.83454
H -1.36786 -1.99496 2.06016
C 0.31115 -3.19567 1.45263
H 0.57099 -4.24349 1.21630
H 0.95591 -2.87015 2.28935
H 0.55220 -2.57881 0.57066
C -1.48257 -3.87945 3.10889
H -2.53185 -3.76538 3.42916
H -0.83405 -3.55829 3.94409
H -1.30285 -4.95698 2.94392
C -5.24358 -2.45946 2.28479
H -5.93123 -2.67801 1.45173
H -5.84778 -2.32778 3.19953
H -4.60144 -3.34415 2.42152
C -3.29769 -0.44462 3.57455
H -2.71231 -1.30109 3.94750
H -4.01706 -0.15870 4.36299
H -2.60443 0.40053 3.43230
C -5.47507 0.52900 1.62682
H -5.99126 0.31732 0.67104
H -6.25135 0.39810 2.40974
C -4.95274 1.98471 1.65697
H -4.35212 2.16491 2.56929
H -5.81112 2.68507 1.73607
C -5.03601 2.30762 -1.40371
H -4.62504 2.81526 -2.29145
H -6.06831 2.67045 -1.25137
H -5.09385 1.22988 -1.63420
C -3.78647 4.51518 0.40539
H -3.30283 4.73975 1.37094
H -4.78321 4.98992 0.40716
H -3.18239 4.98900 -0.38450
C -1.21500 2.79103 -0.11951
C -0.78876 3.30956 -1.38435
C 0.28954 4.21743 -1.42698
H 0.60164 4.62155 -2.39709
C 0.95568 4.62656 -0.26687
H 1.76759 5.36114 -0.32212
C 0.55131 4.10431 0.96892
H 1.05765 4.43111 1.88510
C -0.51705 3.19288 1.06544
C -1.47092 2.93821 -2.70312
H -2.22606 2.16778 -2.47499
C -0.47965 2.33252 -3.72265
H 0.29106 3.06599 -4.02217
H -1.01652 2.02498 -4.63710
H 0.02648 1.44381 -3.31561
C -2.19629 4.15327 -3.32795
H -2.94450 4.58578 -2.64261
H -2.71550 3.85797 -4.25719
H -1.48154 4.95522 -3.58691
C -0.89170 2.62242 2.43231
H -1.90251 2.19259 2.32468
C 0.06346 1.46558 2.80988
H 0.06678 0.68040 2.03299
H -0.22943 1.00099 3.76851
H 1.09941 1.83640 2.91413
C -0.94304 3.67752 3.55606
H 0.05508 4.09274 3.78465
H -1.32512 3.22460 4.48777
H -1.60260 4.52119 3.29088
C 4.38595 -0.44518 -0.02573
C 5.25828 -2.79754 -0.45133
H 6.24649 -3.23954 -0.24296
C 4.20711 -3.57228 0.35830
H 4.42127 -3.52371 1.43863
H 4.21328 -4.63069 0.04931
H 3.19662 -3.16656 0.18470
C 5.01833 -2.85781 -1.96853
H 5.79492 -2.30036 -2.51786
H 4.03367 -2.43356 -2.22860
H 5.04181 -3.90858 -2.30192
C 6.54248 -0.84827 0.58705
C 7.80347 -1.62973 0.78911
H 7.66139 -2.48466 1.47426
H 8.57651 -0.98420 1.23250
H 8.20965 -2.02338 -0.15966
C 6.26434 0.46814 0.89391
C 7.16412 1.48493 1.52734
H 6.87549 1.71049 2.56853
H 7.17782 2.43620 0.97070
H 8.19676 1.10407 1.54730
C 4.16931 1.97255 0.57288
H 3.14249 1.66247 0.30894
C 4.12830 2.57345 1.98495
H 3.86441 1.81045 2.73530
H 3.34716 3.35040 2.00395
H 5.07869 3.04782 2.27729
C 4.64896 2.95934 -0.50246
H 5.65897 3.35218 -0.29573
H 3.95130 3.81185 -0.53762
H 4.65168 2.48159 -1.49540
C -0.38680 -0.45945 -1.21244

A_{Au}
SCF (BP86) Energy = -2158.07245010
Enthalpy 0K = -2156.986662
Enthalpy 298K = -2156.985718
Free Energy 298K = -2157.161986
Lowest Frequency = 6.9232 cm^{-1}
Second Frequency = 8.8722 cm^{-1}
SCF (BP86-D3BJ) Energy = -2158.38523880
SCF (C6H6) Energy = -2158.08022216
SCF (BS2) Energy = -2970.24414385

Au 2.66717 -0.49471 -0.72008
Si -4.43602 2.09678 -0.59598
Si -4.52956 -1.27077 1.54932
Al -2.01066 0.00115 -0.09025
N -2.71308 1.70232 -0.27962

N	-3.03537	-1.38734	0.56449
N	5.67000	-0.83810	-0.26209
N	4.84081	0.83457	0.86712
O	-0.12853	0.03216	0.39298
O	0.76059	-0.78911	-1.54301
C	-1.75225	2.78347	-0.27028
C	-1.38420	3.39709	0.96894
C	-0.45141	4.45181	0.97047
H	-0.18050	4.92078	1.92423
C	0.12396	4.92077	-0.21645
H	0.83422	5.75519	-0.19938
C	-0.23072	4.31610	-1.42755
H	0.21687	4.67803	-2.36080
C	-1.15401	3.25271	-1.48333
C	-1.96046	2.92669	2.30455
H	-2.73582	2.17739	2.06681
C	-0.87986	2.23084	3.16470
H	-0.41006	1.39726	2.61727
H	-1.31624	1.83535	4.09965
H	-0.08342	2.94492	3.44509
C	-2.63499	4.06738	3.09752
H	-1.90670	4.84195	3.39783
H	-3.09781	3.67549	4.02066
H	-3.42178	4.56458	2.50542
C	-1.48548	2.65269	-2.85206
H	-2.15897	1.79651	-2.67627
C	-0.23083	2.11802	-3.57974
H	0.48929	2.92864	-3.79297
H	-0.51519	1.66684	-4.54712
H	0.28338	1.34731	-2.98480
C	-2.22530	3.66875	-3.75384
H	-3.15266	4.03850	-3.28538
H	-2.49216	3.20747	-4.72165
H	-1.58958	4.54669	-3.96812
C	-4.66758	3.98579	-0.55197
H	-4.53907	4.37936	0.47023
H	-5.68759	4.24237	-0.88743
H	-3.94992	4.51197	-1.20102
C	-5.01222	1.42729	-2.28873
H	-4.52798	1.96030	-3.12310
H	-6.10493	1.54781	-2.39854
H	-4.78349	0.35348	-2.40080
C	-5.61577	1.37449	0.72615
H	-5.28924	1.73004	1.72215
H	-6.57590	1.89867	0.53449
C	-5.85605	-0.15392	0.74054
H	-6.05690	-0.52923	-0.28111
H	-6.77870	-0.37809	1.31624
C	-4.18422	-0.56278	3.28955
H	-3.59488	-1.26404	3.90261
H	-5.13373	-0.36638	3.81928
H	-3.62741	0.38859	3.24051
C	-5.29956	-3.00212	1.72799
H	-5.67063	-3.37838	0.76009
H	-6.15384	-2.95997	2.42603
H	-4.57707	-3.73905	2.11359
C	-2.50934	-2.70492	0.26883
C	-1.63951	-3.37291	1.18726
C	-1.15159	-4.65467	0.86304
H	-0.48910	-5.16486	1.57246
C	-1.48779	-5.28688	-0.33848
H	-1.09603	-6.28329	-0.57070
C	-2.32941	-4.62744	-1.24092
H	-2.59025	-5.11359	-2.18830
C	-2.85218	-3.35073	-0.96143
C	-1.21042	-2.74949	2.51737
H	-1.65130	-1.73924	2.55973
C	0.32424	-2.59016	2.61281
H	0.83533	-3.56887	2.56986
H	0.60038	-2.11292	3.57073
H	0.70605	-1.96064	1.79306
C	-1.74187	-3.55686	3.72421
H	-2.84064	-3.65331	3.70226
H	-1.46074	-3.06862	4.67485
H	-1.32108	-4.57835	3.73826
C	-3.74672	-2.68031	-2.00475
H	-4.15070	-1.76530	-1.53637
C	-2.92598	-2.25404	-3.24462
H	-2.08613	-1.59742	-2.96170
H	-3.56166	-1.71721	-3.97190
H	-2.49970	-3.13574	-3.75606
C	-4.94444	-3.56192	-2.42070
H	-4.61539	-4.48212	-2.93552
H	-5.60291	-3.01383	-3.11777
H	-5.54792	-3.86723	-1.54894
C	4.50450	-0.16772	-0.00699
C	5.79906	-2.02434	-1.15634
H	6.86720	-2.29278	-1.10373
C	4.97795	-3.21136	-0.62741
H	5.25185	-3.45364	0.41265
H	5.16823	-4.09849	-1.25405
H	3.89837	-2.98655	-0.66034
C	5.46435	-1.66226	-2.61235
H	6.07992	-0.81831	-2.96518
H	4.40114	-1.38447	-2.71042
H	5.65904	-2.53166	-3.26205
C	6.73566	-0.25955	0.44147
C	8.14219	-0.76848	0.37782
H	8.23197	-1.80175	0.75866
H	8.79716	-0.13692	0.99685
H	8.54755	-0.75312	-0.64965
C	6.21351	0.80082	1.15454
C	6.92463	1.73873	2.08143
H	6.66974	1.55566	3.13974
H	6.69917	2.79492	1.86152
H	8.01293	1.60869	1.97817
C	3.82491	1.81827	1.34897
H	2.87664	1.39872	0.96654
C	3.73115	1.86298	2.88092
H	3.64788	0.84821	3.30248
H	2.82122	2.41883	3.15943
H	4.58816	2.37490	3.34772
C	4.02006	3.19667	0.69887
H	4.91623	3.72015	1.07328
H	3.14184	3.82461	0.92119
H	4.09700	3.10252	-0.39621
C	-0.24797	-0.44005	-0.84017

TS(III-S)$_{Au}$

SCF (BP86) Energy = -2158.08153390
Enthalpy 0K = -2156.996334
Enthalpy 298K = -2156.995390
Free Energy 298K = -2157.164183
Lowest Frequency = -42.1007 cm^{-1}
Second Frequency = 16.0925 cm^{-1}
SCF (BP86-D3BJ) Energy = -2158.41357735
SCF (C6H6) Energy = -2158.08908477
SCF (BS2) Energy = -2970.25200568

Au	1.70184	-0.41925	-0.83008
Si	-3.73034	-1.20360	1.74160
Si	-3.91399	2.10994	-0.45440
Al	-1.61288	-0.01171	-0.42092
N	-2.32576	-1.35815	0.60873
N	-2.16282	1.73582	-0.21177
N	4.06692	0.93855	0.74386
N	4.61050	-1.05269	0.05871
O	-1.07895	-0.50936	-2.04143
O	0.58939	-1.43496	-3.21103
C	-1.77793	-2.69180	0.41475
C	-2.15912	-3.48988	-0.71150
C	-1.60036	-4.77649	-0.85093
H	-1.89118	-5.38591	-1.71374
C	-0.69305	-5.29491	0.07786

H -0.27768 -6.29995 -0.05392
C -0.32913 -4.51460 1.18030
H 0.37529 -4.91685 1.91817
C -0.85318 -3.22134 1.37070
C -3.17097 -3.03600 -1.76929
H -3.39986 -1.97325 -1.57373
C -2.61971 -3.14554 -3.20912
H -1.67707 -2.59174 -3.33130
H -3.35636 -2.73539 -3.92300
H -2.44679 -4.19947 -3.49243
C -4.49494 -3.82987 -1.66159
H -4.32377 -4.90659 -1.83929
H -5.21806 -3.47729 -2.41845
H -4.96336 -3.72855 -0.66937
C -0.42251 -2.44252 2.61672
H -0.94581 -1.47283 2.59217
C 1.09166 -2.14262 2.62340
H 1.68551 -3.07382 2.65369
H 1.36392 -1.54410 3.51194
H 1.38869 -1.58005 1.72025
C -0.82341 -3.17349 3.91889
H -1.90603 -3.37971 3.95922
H -0.55720 -2.56727 4.80354
H -0.30007 -4.14178 4.01227
C -4.42660 -2.93086 2.13589
H -5.01610 -3.34417 1.30245
H -5.09314 -2.85203 3.01283
H -3.63229 -3.65600 2.37314
C -3.30418 -0.39522 3.41747
H -2.73581 -1.08031 4.06670
H -4.24435 -0.14277 3.94082
H -2.72221 0.53233 3.30985
C -5.15346 -0.18730 0.96368
H -5.37271 -0.59966 -0.03962
H -6.03352 -0.45901 1.58358
C -5.01935 1.35373 0.91068
H -4.69252 1.75095 1.89060
H -6.01741 1.80677 0.73302
C -4.49973 1.39771 -2.12410
H -4.01604 1.91273 -2.96992
H -5.59318 1.51095 -2.23285
H -4.27000 0.32192 -2.22266
C -4.17929 3.99158 -0.41606
H -3.98965 4.40497 0.58808
H -5.22652 4.21626 -0.68371
H -3.52236 4.52217 -1.12279
C -1.25080 2.85740 -0.14423
C -0.66857 3.42043 -1.32546
C 0.14997 4.56294 -1.20726
H 0.57732 5.00041 -2.11692
C 0.41897 5.15659 0.03089
H 1.04049 6.05699 0.09297
C -0.13218 4.59132 1.18736
H 0.06587 5.05281 2.16228
C -0.96423 3.45686 1.12476
C -0.90569 2.85108 -2.72622
H -1.48538 1.92029 -2.61664
C 0.42227 2.48535 -3.42702
H 1.03193 3.38308 -3.63681
H 0.22259 1.98264 -4.38878
H 1.02421 1.79840 -2.80834
C -1.72085 3.82240 -3.61177
H -2.70416 4.05801 -3.17108
H -1.89304 3.38037 -4.60902
H -1.18517 4.77763 -3.75818
C -1.53936 2.89576 2.42368
H -2.27425 2.12875 2.12798
C -0.44484 2.20020 3.26452
H 0.05686 1.40177 2.69072
H -0.87401 1.74673 4.17584
H 0.32688 2.92324 3.58356
C -2.27305 3.95771 3.27103
H -1.58286 4.73541 3.64387
H -2.74345 3.48768 4.15271
H -3.06369 4.46540 2.69340
C 3.56495 -0.16562 0.10597
C 3.26705 2.19063 0.85585
H 2.25045 1.86364 0.57356
C 3.21181 2.74354 2.28657
H 2.94875 1.95586 3.01100
H 2.42736 3.51641 2.32362
H 4.15802 3.21313 2.59918
C 3.73165 3.22853 -0.17826
H 3.74404 2.78856 -1.18837
H 4.73739 3.62275 0.04738
H 3.02254 4.07193 -0.18212
C 5.41367 0.75444 1.09300
C 6.26810 1.74716 1.82089
H 6.24798 2.74393 1.35009
H 7.31522 1.40684 1.81783
H 5.96434 1.86983 2.87510
C 5.75435 -0.51068 0.65938
C 7.05653 -1.24055 0.77916
H 7.47753 -1.51230 -0.20524
H 6.96271 -2.16878 1.37099
H 7.79773 -0.60505 1.28726
C 4.59365 -2.37748 -0.63028
H 5.58015 -2.81412 -0.40207
C 3.51925 -3.31148 -0.05777
H 3.62520 -3.42028 1.03361
H 3.62130 -4.30699 -0.52087
H 2.50459 -2.93770 -0.27656
C 4.48362 -2.20428 -2.15489
H 3.49537 -1.80432 -2.43987
H 4.60696 -3.18448 -2.64511
H 5.26421 -1.52487 -2.53640
C 0.22445 -0.85777 -2.18526

S_{Au}

SCF (BP86) Energy = -2158.12979348
Enthalpy 0K = -2157.043510
Enthalpy 298K = -2157.042565
Free Energy 298K = -2157.217498
Lowest Frequency = 4.9341 cm^{-1}
Second Frequency = 9.8781 cm^{-1}
SCF (BP86-D3BJ) Energy = -2158.44191750
SCF (C6H6) Energy = -2158.13752887
SCF (BS2) Energy = -2970.30012847

Au 2.42546 -0.10886 -0.05760
Si -4.50100 -1.54078 1.17085
Si -4.42950 1.78189 -1.03362
Al -1.91454 0.02542 0.01039
N -2.85994 -1.49727 0.44415
N -2.76205 1.61366 -0.38965
N 5.30373 0.65291 0.72013
N 5.34598 -0.89450 -0.80874
O -0.29927 0.31733 1.02061
O -0.35840 -0.37753 -1.05555
C -2.15800 -2.75137 0.26108
C -2.22960 -3.43218 -0.99594
C -1.55186 -4.65497 -1.16056
H -1.61130 -5.16918 -2.12724
C -0.81052 -5.22706 -0.12102
H -0.29810 -6.18484 -0.26467
C -0.73330 -4.55764 1.10466
H -0.15141 -4.99868 1.92274
C -1.38555 -3.32661 1.32011
C -3.00245 -2.86266 -2.18613
H -3.51048 -1.95022 -1.82732
C -2.04641 -2.45472 -3.33162
H -1.28037 -1.74594 -2.97812
H -2.60751 -1.98399 -4.15916
H -1.52496 -3.33816 -3.74285

C	-4.08758	-3.83162	-2.70574
H	-3.64381	-4.76203	-3.10290
H	-4.66292	-3.36474	-3.52493
H	-4.79636	-4.11629	-1.90979
C	-1.24037	-2.66416	2.69275
H	-1.73974	-1.68229	2.63588
C	0.23822	-2.41379	3.06745
H	0.79793	-3.36158	3.16471
H	0.30229	-1.88993	4.03805
H	0.74074	-1.79030	2.31118
C	-1.93111	-3.49328	3.80084
H	-3.00157	-3.65300	3.58936
H	-1.84867	-2.98393	4.77795
H	-1.46229	-4.48854	3.90341
C	-5.09742	-3.34511	1.28251
H	-5.29486	-3.76519	0.28231
H	-6.03764	-3.38913	1.85953
H	-4.36099	-3.99935	1.77540
C	-4.52109	-0.76876	2.91722
H	-3.95504	-1.38121	3.63779
H	-5.55869	-0.68315	3.28707
H	-4.08208	0.24354	2.92225
C	-5.79446	-0.60061	0.11936
H	-5.77807	-1.01497	-0.90687
H	-6.76754	-0.92483	0.54504
C	-5.73583	0.94527	0.08689
H	-5.63380	1.35576	1.10972
H	-6.70195	1.34405	-0.28829
C	-4.59544	1.01098	-2.77273
H	-4.02677	1.58224	-3.52449
H	-5.65438	0.99760	-3.08764
H	-4.22837	-0.02925	-2.79632
C	-4.89106	3.62616	-1.12704
H	-5.00454	4.06323	-0.12115
H	-5.85330	3.73991	-1.65624
H	-4.13288	4.22049	-1.66107
C	-1.96142	2.81234	-0.24410
C	-1.20550	3.33236	-1.34289
C	-0.45726	4.51375	-1.16483
H	0.11120	4.91345	-2.01309
C	-0.42344	5.18580	0.06141
H	0.16133	6.10538	0.17552
C	-1.14774	4.66588	1.13965
H	-1.12067	5.18200	2.10681
C	-1.91762	3.49404	1.01377
C	-1.17655	2.66087	-2.71834
H	-1.74718	1.72062	-2.63475
C	0.25975	2.29608	-3.15790
H	0.88565	3.19765	-3.28606
H	0.23934	1.76580	-4.12688
H	0.74562	1.63863	-2.41982
C	-1.85101	3.53991	-3.79744
H	-2.89499	3.78265	-3.53794
H	-1.85346	3.02439	-4.77477
H	-1.31157	4.49552	-3.92649
C	-2.66584	2.98032	2.24438
H	-3.24261	2.09672	1.91873
C	-1.68462	2.52663	3.35052
H	-0.97768	1.77186	2.97034
H	-2.23483	2.09521	4.20630
H	-1.09621	3.38159	3.73049
C	-3.66743	4.01637	2.80141
H	-3.15176	4.92396	3.16313
H	-4.22839	3.59329	3.65375
H	-4.39644	4.33263	2.03637
C	4.49214	-0.13294	-0.05810
C	4.72962	1.66419	1.65410
H	3.64637	1.44854	1.60739
C	5.18995	1.45372	3.10433
H	5.06061	0.40336	3.41192
H	4.57001	2.07943	3.76729
H	6.24046	1.74466	3.26545
C	4.94335	3.09589	1.13778
H	4.57011	3.19690	0.10612
H	6.00284	3.40146	1.16158
H	4.37997	3.79815	1.77414
C	6.65722	0.39298	0.45769
C	7.81673	1.05388	1.13877
H	7.73785	2.15328	1.13213
H	8.75093	0.79163	0.61868
H	7.92471	0.73297	2.18955
C	6.68055	-0.59128	-0.51092
C	7.84928	-1.26274	-1.16284
H	7.85333	-1.12454	-2.25873
H	7.87367	-2.34880	-0.96181
H	8.78905	-0.83998	-0.77648
C	4.91881	-1.91693	-1.80722
H	5.86243	-2.32864	-2.20231
C	4.13806	-3.05663	-1.13352
H	4.71720	-3.50496	-0.30934
H	3.92058	-3.84283	-1.87532
H	3.17924	-2.68941	-0.72916
C	4.14897	-1.26829	-2.96876
H	3.19175	-0.84777	-2.61585
H	3.93049	-2.02925	-3.73623
H	4.73630	-0.46028	-3.43556
C	0.39388	-0.05391	-0.03008

III$_{Au,N}$

SCF (BP86) Energy = -2354.14103361
Enthalpy 0K = -2352.858126
Enthalpy 298K = -2352.857182
Free Energy 298K = -2353.040720
Lowest Frequency = 19.3299 cm^{-1}
Second Frequency = 25.5126 cm^{-1}
SCF (BP86-D3BJ) Energy = -2354.54642653
SCF (C6H6) Energy = -2354.14510527
SCF (BS2) Energy = -3166.34475727

Au	1.32509	0.08953	0.58100
Si	-3.37984	1.56852	-1.83781
Si	-3.94629	-1.77836	0.38190
Al	-1.32600	0.25137	0.29796
N	-1.74960	1.51722	-1.06764
N	-2.18482	-1.45614	0.15820
N	3.61687	-1.57583	-0.82948
N	4.23260	0.48418	-0.50277
N	-1.19080	0.90763	2.11583
N	1.11506	0.99591	3.04524
C	-0.85873	2.57208	-1.52714
C	-0.77172	3.83240	-0.83897
C	0.04172	4.86459	-1.34710
H	0.08561	5.81500	-0.80270
C	0.77165	4.71753	-2.52836
H	1.38331	5.53889	-2.91757
C	0.69801	3.49726	-3.20230
H	1.26674	3.36360	-4.12989
C	-0.08931	2.42547	-2.73202
C	-1.52651	4.13296	0.45286
H	-2.19237	3.27373	0.63325
C	-0.54766	4.25473	1.64236
H	0.06702	3.34927	1.75647
H	-1.09813	4.42471	2.58611
H	0.13208	5.11433	1.49937
C	-2.38409	5.41810	0.37580
H	-1.75138	6.32193	0.31977
H	-3.00598	5.51716	1.28397
H	-3.05111	5.42509	-0.49950
C	-0.04295	1.14236	-3.56317
H	-0.78106	0.44289	-3.13737
C	1.35532	0.48992	-3.46875
H	2.13778	1.19434	-3.80523
H	1.41751	-0.40473	-4.11300
H	1.58548	0.19651	-2.43123

C	-0.38736	1.38862	-5.05123
H	-1.31122	1.97611	-5.17500
H	-0.51556	0.42893	-5.58260
H	0.42105	1.93874	-5.56539
C	-3.93647	3.36905	-2.13698
H	-4.26456	3.85005	-1.20145
H	-4.79669	3.36259	-2.82979
H	-3.14415	3.98929	-2.58527
C	-3.54555	0.72733	-3.54727
H	-3.06094	1.31948	-4.33852
H	-4.62132	0.66725	-3.79522
H	-3.13666	-0.29359	-3.58717
C	-4.75650	0.79848	-0.74564
H	-4.65554	1.14576	0.30081
H	-5.65722	1.32767	-1.12094
C	-4.99152	-0.72959	-0.81931
H	-4.84381	-1.09546	-1.85201
H	-6.04665	-0.96371	-0.56911
C	-4.65804	-1.42005	2.12229
H	-4.11381	-1.96948	2.90710
H	-5.70252	-1.78262	2.13119
H	-4.68296	-0.35706	2.40254
C	-4.35577	-3.62859	0.14920
H	-3.97088	-4.07391	-0.77834
H	-5.45495	-3.74101	0.15846
H	-3.95359	-4.22302	0.98645
C	-1.45164	-2.69224	-0.02117
C	-0.93375	-3.41748	1.10334
C	-0.37261	-4.69681	0.91241
H	-0.00705	-5.24855	1.78688
C	-0.30569	-5.29263	-0.35152
H	0.10059	-6.30301	-0.47293
C	-0.77674	-4.57480	-1.45688
H	-0.73038	-5.03041	-2.45358
C	-1.33035	-3.28559	-1.32375
C	-1.00948	-2.88316	2.53384
H	-1.47224	-1.88378	2.48233
C	0.39406	-2.72627	3.15971
H	0.91723	-3.69758	3.22668
H	0.31564	-2.32235	4.18500
H	1.01874	-2.03221	2.57232
C	-1.88644	-3.77961	3.43913
H	-2.89831	-3.92167	3.02482
H	-1.98876	-3.33260	4.44419
H	-1.43904	-4.78179	3.56718
C	-1.79099	-2.57290	-2.59630
H	-2.08218	-1.55257	-2.29342
C	-0.64150	-2.46525	-3.62090
H	0.25517	-2.01696	-3.16755
H	-0.94408	-1.83894	-4.47886
H	-0.36077	-3.45626	-4.02101
C	-3.00592	-3.24562	-3.27691
H	-2.78356	-4.29656	-3.53633
H	-3.26001	-2.72003	-4.21493
H	-3.90242	-3.23974	-2.63832
C	3.16232	-0.36547	-0.37214
C	2.77771	-2.80501	-0.76148
H	1.76862	-2.41499	-0.53871
C	2.71774	-3.55766	-2.09911
H	2.54052	-2.86710	-2.93928
H	1.87261	-4.26220	-2.05643
H	3.63197	-4.13790	-2.30172
C	3.21265	-3.69769	0.41179
H	3.21798	-3.12772	1.35461
H	4.21543	-4.13139	0.25595
H	2.49123	-4.52374	0.51522
C	4.95531	-1.49364	-1.23935
C	5.76683	-2.61660	-1.81080
H	5.72016	-3.52672	-1.19070
H	6.82431	-2.31510	-1.86765
H	5.44631	-2.89061	-2.83069
C	5.34216	-0.18588	-1.03092
C	6.66076	0.47091	-1.30132
H	7.10897	0.90364	-0.38935
H	6.57983	1.27866	-2.05077
H	7.37336	-0.26858	-1.69720
C	4.29368	1.90460	-0.04483
H	5.24754	2.27773	-0.45350
C	3.16993	2.75760	-0.64105
H	3.15494	2.69797	-1.73984
H	3.32561	3.81042	-0.35417
H	2.17668	2.45023	-0.27225
C	4.36576	1.97303	1.48948
H	3.42880	1.61312	1.95010
H	4.52492	3.01937	1.80114
H	5.20459	1.36798	1.87446
C	0.16936	0.77712	2.19173
C	1.13349	1.41461	4.45301
H	0.13494	1.32050	4.92392
C	-1.93907	1.39306	3.30384
H	-1.31467	2.17058	3.78618
C	1.57614	2.88620	4.57000
H	2.56975	3.02332	4.10948
H	0.86887	3.55940	4.05938
H	1.64074	3.18870	5.63036
C	2.10173	0.49518	5.22197
H	3.11672	0.56903	4.79428
H	2.14882	0.77841	6.28837
H	1.78138	-0.55722	5.15316
C	-2.17764	0.26807	4.33295
H	-1.24050	-0.25797	4.57670
H	-2.59368	0.68185	5.26932
H	-2.89024	-0.47462	3.94313
C	-3.26307	2.06523	2.91483
H	-3.84992	2.29817	3.81992
H	-3.10146	3.00292	2.36396
H	-3.87594	1.40252	2.28288

TS(III-IV)$_{Au,N}$

SCF (BP86) Energy = -2354.11417240
Enthalpy 0K = -2352.832691
Enthalpy 298K = -2352.831746
Free Energy 298K = -2353.015404
Lowest Frequency = -156.3615 cm^{-1}
Second Frequency = 16.4531 cm^{-1}
SCF (BP86-D3BJ) Energy = -2354.51360756
SCF (C6H6) Energy = -2354.11790113
SCF (BS2) Energy = -3166.31872245

Au	1.65371	0.04388	0.83709
Si	-3.32095	1.75866	-1.90853
Si	-4.10769	-1.70871	0.04396
Al	-1.52805	0.27111	0.28677
N	-1.74090	1.60065	-1.05213
N	-2.32993	-1.42504	-0.05980
N	3.70954	-1.54196	-0.73944
N	4.38527	0.50619	-0.39261
N	-1.67137	0.81294	2.13945
N	0.71683	0.54910	2.80823
C	-0.80450	2.66474	-1.37380
C	-0.74807	3.87280	-0.59595
C	0.10451	4.92546	-0.98385
H	0.12544	5.83696	-0.37539
C	0.90363	4.84694	-2.12652
H	1.54446	5.68476	-2.42252
C	0.86335	3.67405	-2.88286
H	1.48841	3.59383	-3.77988
C	0.03875	2.58431	-2.53372
C	-1.56664	4.08930	0.67484
H	-2.25674	3.23337	0.76219
C	-0.63905	4.09345	1.90996
H	-0.04623	3.16821	1.96836
H	-1.22435	4.19611	2.84223
H	0.06359	4.94535	1.86604

C	-2.39371	5.39606	0.66020
H	-1.74186	6.28691	0.70187
H	-3.05413	5.43996	1.54518
H	-3.02027	5.48540	-0.24024
C	0.12623	1.35238	-3.43554
H	-0.65050	0.64289	-3.10526
C	1.50544	0.67122	-3.27947
H	2.31830	1.37934	-3.52375
H	1.60049	-0.18835	-3.96594
H	1.66091	0.32019	-2.24579
C	-0.10934	1.69054	-4.92644
H	-1.02073	2.29061	-5.08010
H	-0.20181	0.76546	-5.52265
H	0.73532	2.26464	-5.34776
C	-3.80897	3.59020	-2.12464
H	-4.18136	4.02199	-1.18178
H	-4.62516	3.65231	-2.86626
H	-2.97483	4.21323	-2.48435
C	-3.40739	1.02866	-3.67262
H	-2.84961	1.64674	-4.39295
H	-4.46579	1.02747	-3.99212
H	-3.03422	-0.00371	-3.74857
C	-4.76585	0.96435	-0.92691
H	-4.68163	1.22201	0.14744
H	-5.63364	1.55841	-1.28138
C	-5.05416	-0.54337	-1.13200
H	-4.86856	-0.83610	-2.18161
H	-6.12816	-0.75287	-0.94979
C	-4.87383	-1.39451	1.76577
H	-4.40239	-2.01387	2.54501
H	-5.94500	-1.66382	1.72583
H	-4.81133	-0.34196	2.07983
C	-4.55732	-3.52318	-0.33572
H	-4.14052	-3.90738	-1.27724
H	-5.65812	-3.60321	-0.38586
H	-4.21054	-4.19110	0.46984
C	-1.60133	-2.65746	-0.27156
C	-1.18460	-3.47093	0.83452
C	-0.61156	-4.73688	0.59538
H	-0.32033	-5.35539	1.45284
C	-0.44477	-5.23842	-0.69954
H	-0.03128	-6.23996	-0.86241
C	-0.82626	-4.43865	-1.78278
H	-0.70180	-4.82085	-2.80313
C	-1.38119	-3.15621	-1.59994
C	-1.38449	-3.04967	2.29080
H	-1.81852	-2.03554	2.28088
C	-0.04418	-2.99129	3.05564
H	0.43662	-3.98522	3.10391
H	-0.21103	-2.65774	4.09591
H	0.65844	-2.28654	2.58146
C	-2.36277	-3.99059	3.03306
H	-3.33795	-4.05968	2.52379
H	-2.54056	-3.63118	4.06255
H	-1.95504	-5.01492	3.10567
C	-1.73665	-2.34818	-2.84863
H	-2.00777	-1.33720	-2.49871
C	-0.52766	-2.22554	-3.80061
H	0.36195	-1.85483	-3.26961
H	-0.75397	-1.52676	-4.62531
H	-0.26952	-3.19787	-4.25754
C	-2.93522	-2.92940	-3.63463
H	-2.74044	-3.97453	-3.93625
H	-3.11114	-2.34556	-4.55603
H	-3.86713	-2.91634	-3.04897
C	3.31294	-0.33669	-0.20570
C	2.83874	-2.74687	-0.67887
H	1.84275	-2.32560	-0.45129
C	2.74623	-3.48886	-2.02058
H	2.60331	-2.78624	-2.85744
H	1.86773	-4.15198	-1.98393
H	3.63142	-4.11167	-2.22539
C	3.24504	-3.66322	0.48644
H	3.26470	-3.10060	1.43375
H	4.23721	-4.12015	0.32622
H	2.50362	-4.47325	0.58139
C	5.02215	-1.46337	-1.23384
C	5.78012	-2.58913	-1.86902
H	5.75697	-3.50537	-1.25561
H	6.83681	-2.30184	-1.98456
H	5.39644	-2.84883	-2.87072
C	5.44284	-0.16989	-1.01980
C	6.74585	0.47864	-1.37168
H	7.27116	0.87996	-0.48642
H	6.61977	1.30871	-2.09034
H	7.41472	-0.25773	-1.84258
C	4.51017	1.89943	0.12073
H	5.43707	2.27678	-0.34256
C	3.36160	2.80321	-0.34014
H	3.25084	2.79247	-1.43488
H	3.56726	3.83914	-0.02332
H	2.39745	2.49634	0.09844
C	4.70273	1.89597	1.64701
H	3.80118	1.50196	2.14478
H	4.87946	2.92498	2.00270
H	5.56550	1.27382	1.93978
C	-0.34732	0.54456	2.03084
C	0.89213	0.81737	4.24932
H	-0.05897	0.63701	4.78787
C	-2.31384	1.26402	3.40315
H	-1.58719	1.92195	3.91988
C	1.32529	2.27382	4.50391
H	2.24823	2.49954	3.94172
H	0.55170	2.99031	4.18609
H	1.52667	2.43613	5.57776
C	1.94665	-0.15903	4.79976
H	2.90461	-0.01818	4.26877
H	2.11582	0.01417	5.87687
H	1.63134	-1.20438	4.65704
C	-2.64243	0.08504	4.34116
H	-1.75948	-0.55191	4.51361
H	-2.99160	0.46026	5.31986
H	-3.43672	-0.54682	3.91506
C	-3.56908	2.10080	3.11718
H	-4.03889	2.41612	4.06485
H	-3.33108	3.00352	2.53490
H	-4.31635	1.51869	2.55232

$IV_{Au,N}$

SCF (BP86) Energy = -2354.14869572
Enthalpy 0K = -2352.865897
Enthalpy 298K = -2352.864953
Free Energy 298K = -2353.050522
Lowest Frequency = 16.0840 cm^{-1}
Second Frequency = 20.2332 cm^{-1}
SCF (BP86-D3BJ) Energy = -2354.53649672
SCF (C6H6) Energy = -2354.15369109
SCF (BS2) Energy = -3166.35422203

Au	2.37229	0.45221	0.80552
Si	-4.05831	1.11917	-1.93546
Si	-4.23850	-2.12794	0.46491
Al	-1.93650	0.15492	0.34791
N	-2.52482	1.32499	-1.02241
N	-2.52252	-1.65109	0.22961
N	4.22203	-1.40107	-0.74231
N	5.09493	0.59103	-0.62254
N	-1.72237	0.89567	2.13047
N	0.75983	1.02075	1.98073
C	-1.72586	2.46783	-1.42803
C	-1.91282	3.76626	-0.84167
C	-1.16078	4.86272	-1.30948
H	-1.32197	5.84546	-0.85132
C	-0.22097	4.73425	-2.33467

H	0.34490	5.60317	-2.68832
C	-0.01863	3.47158	-2.89608
H	0.72214	3.35211	-3.69532
C	-0.74653	2.34267	-2.46969
C	-2.85998	4.03661	0.32838
H	-3.42770	3.10666	0.50848
C	-2.03909	4.36734	1.59616
H	-1.32853	3.55852	1.82237
H	-2.69651	4.51624	2.47139
H	-1.46172	5.29812	1.45142
C	-3.85702	5.18965	0.06683
H	-3.33652	6.16156	-0.00287
H	-4.57610	5.26822	0.90191
H	-4.42615	5.05075	-0.86437
C	-0.40551	1.00823	-3.13198
H	-1.14929	0.26964	-2.78837
C	0.99331	0.53621	-2.67610
H	1.76528	1.27458	-2.95896
H	1.26443	-0.42582	-3.14787
H	1.04368	0.41359	-1.57904
C	-0.45803	1.07229	-4.67501
H	-1.41868	1.47252	-5.03808
H	-0.32045	0.06578	-5.10753
H	0.34259	1.71519	-5.08270
C	-4.85932	2.80056	-2.34961
H	-5.35278	3.24315	-1.46947
H	-5.63205	2.64358	-3.12303
H	-4.13129	3.52862	-2.74163
C	-3.89702	0.25739	-3.63541
H	-3.36883	0.90471	-4.35432
H	-4.91123	0.07960	-4.03749
H	-3.37418	-0.71025	-3.60267
C	-5.39366	0.17799	-0.93226
H	-5.45400	0.61676	0.08322
H	-6.32832	0.51032	-1.43050
C	-5.36614	-1.36882	-0.87689
H	-5.09818	-1.78718	-1.86461
H	-6.38324	-1.75502	-0.65726
C	-4.96219	-1.53724	2.13182
H	-4.29471	-1.76713	2.97795
H	-5.92567	-2.04793	2.31020
H	-5.16152	-0.45406	2.13687
C	-4.44609	-4.02428	0.46641
H	-3.98548	-4.52501	-0.39754
H	-5.52550	-4.25900	0.46767
H	-4.00618	-4.47101	1.37309
C	-1.62392	-2.77732	0.10845
C	-0.99267	-3.35234	1.26135
C	-0.23210	-4.53221	1.12825
H	0.21757	-4.97427	2.02550
C	-0.06941	-5.17192	-0.10506
H	0.49719	-6.10689	-0.18019
C	-0.65772	-4.59982	-1.23873
H	-0.54060	-5.09141	-2.21220
C	-1.41681	-3.41492	-1.16240
C	-1.14549	-2.76483	2.66457
H	-1.69062	-1.81168	2.56161
C	0.22616	-2.46306	3.30753
H	0.82337	-3.38279	3.44430
H	0.08898	-2.01449	4.30762
H	0.80862	-1.75820	2.69215
C	-1.96542	-3.69300	3.59111
H	-2.97257	-3.89046	3.18894
H	-2.08304	-3.23766	4.59115
H	-1.46391	-4.66822	3.72696
C	-2.00509	-2.86270	-2.46072
H	-2.44726	-1.88408	-2.20785
C	-0.91543	-2.64353	-3.53316
H	-0.08212	-2.03911	-3.14290
H	-1.33695	-2.12406	-4.41197
H	-0.49864	-3.60293	-3.88928
C	-3.11687	-3.75971	-3.05319
H	-2.72959	-4.76889	-3.28309
H	-3.49956	-3.32779	-3.99546
H	-3.97006	-3.87692	-2.36746
C	3.98568	-0.13466	-0.26769
C	3.24770	-2.51049	-0.52736
H	2.35504	-1.98455	-0.14483
C	2.85751	-3.21685	-1.83314
H	2.62385	-2.48650	-2.62473
H	1.95055	-3.81409	-1.64523
H	3.64140	-3.89967	-2.19862
C	3.72577	-3.47522	0.56851
H	3.96800	-2.92657	1.49304
H	4.61143	-4.05696	0.26062
H	2.91237	-4.18511	0.79102
C	5.47148	-1.47605	-1.37531
C	6.04930	-2.70209	-2.01430
H	5.99809	-3.58227	-1.35278
H	7.11148	-2.53137	-2.24873
H	5.54058	-2.96406	-2.95806
C	6.02153	-0.21351	-1.29988
C	7.33225	0.28893	-1.82109
H	7.97153	0.70449	-1.02172
H	7.20583	1.07203	-2.59042
H	7.88961	-0.53668	-2.28900
C	5.32351	2.03112	-0.31725
H	6.27299	2.27204	-0.82340
C	4.22669	2.92065	-0.92177
H	4.13708	2.75501	-2.00773
H	4.47952	3.98052	-0.75126
H	3.24681	2.71559	-0.45926
C	5.51839	2.24458	1.19238
H	4.59636	1.98538	1.73889
H	5.75989	3.30185	1.39228
H	6.34030	1.61967	1.58010
C	-0.48612	0.72796	1.57130
C	1.08887	1.75009	3.23860
H	0.16919	1.86808	3.82972
C	-2.16219	1.42434	3.44651
H	-1.61136	2.36082	3.66465
C	1.62487	3.15734	2.91716
H	2.54784	3.08569	2.31422
H	0.89046	3.73997	2.33861
H	1.86038	3.70952	3.84466
C	2.09357	0.95505	4.09098
H	3.03171	0.79151	3.52874
H	2.33710	1.50236	5.01880
H	1.69042	-0.03408	4.36249
C	-1.90167	0.42078	4.58738
H	-0.83710	0.14748	4.66399
H	-2.21786	0.84604	5.55660
H	-2.47689	-0.50501	4.41656
C	-3.65456	1.78425	3.39630
H	-3.95464	2.29787	4.32619
H	-3.87820	2.44754	2.54697
H	-4.27025	0.87627	3.30024

$A_{Au,N}$

SCF (BP86) Energy = -2354.16684065
Enthalpy 0K = -2352.884520
Enthalpy 298K = -2352.883576
Free Energy 298K = -2353.074473
Lowest Frequency = 9.4963 cm^{-1}
Second Frequency = 12.4068 cm^{-1}
SCF (BP86-D3BJ) Energy = -2354.54864678
SCF (C6H6) Energy = -2354.17328871
SCF (BS2) Energy = -3166.37398540

Au	-2.91477	-0.30723	-0.44044
Si	4.63845	-1.60047	1.28506
Si	4.75082	1.73670	-0.74296
Al	2.07615	0.05241	0.11244
N	3.07928	-1.51386	0.39632

N	3.08242	1.63764	-0.07147
N	0.31946	0.31706	0.84821
N	-0.94884	-0.48894	-1.08194
C	2.55344	-2.78944	-0.03973
C	1.66909	-3.55077	0.79248
C	1.24635	-4.82959	0.37523
H	0.58548	-5.40878	1.03117
C	1.64923	-5.37950	-0.84538
H	1.31114	-6.37668	-1.14759
C	2.48869	-4.62873	-1.67377
H	2.80565	-5.04375	-2.63812
C	2.95083	-3.35299	-1.29741
C	1.15265	-3.03897	2.13858
H	1.50430	-1.99849	2.24737
C	-0.39259	-3.02775	2.17262
H	-0.79980	-2.40483	1.35901
H	-0.75959	-2.63092	3.13639
H	-0.80535	-4.04651	2.06186
C	1.70133	-3.85996	3.32831
H	1.31816	-3.46271	4.28575
H	2.80266	-3.83614	3.36974
H	1.39380	-4.91903	3.25944
C	3.87200	-2.61360	-2.26604
H	4.16490	-1.67808	-1.76229
C	3.13750	-2.24529	-3.57502
H	3.80129	-1.67971	-4.25337
H	2.24675	-1.62678	-3.37400
H	2.80143	-3.15014	-4.11236
C	5.16164	-3.40179	-2.58668
H	4.93921	-4.35160	-3.10506
H	5.72945	-3.64683	-1.67369
H	5.82052	-2.81074	-3.24764
C	5.19787	-3.41414	1.46655
H	4.43469	-4.04316	1.95113
H	6.11345	-3.44936	2.08318
H	5.42710	-3.87480	0.49212
C	4.47361	-0.86791	3.03966
H	4.14054	0.18276	3.02304
H	5.44653	-0.89941	3.56217
H	3.74760	-1.44193	3.63946
C	6.06815	-0.70106	0.38277
H	6.98989	-1.04947	0.89477
H	6.13539	-1.11348	-0.64216
C	6.05055	0.84323	0.34561
H	7.02477	1.21779	-0.03395
H	5.96713	1.24592	1.37245
C	5.32068	3.55491	-0.87355
H	4.60485	4.16628	-1.44548
H	6.28831	3.57777	-1.40627
H	5.46026	4.04619	0.10144
C	4.87114	1.04498	-2.52030
H	4.35383	0.08204	-2.64340
H	5.93013	0.89574	-2.79835
H	4.43228	1.75334	-3.24243
C	2.43424	2.91735	0.11894
C	1.75194	3.56601	-0.96244
C	1.20293	4.84997	-0.77214
H	0.69464	5.33832	-1.61237
C	1.30103	5.51877	0.45081
H	0.87973	6.52253	0.57449
C	1.94380	4.88066	1.51670
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C	2.50288	3.59378	1.38401
C	1.59531	2.92920	-2.34550
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C	0.10794	2.75010	-2.72262
H	-0.41282	3.72349	-2.77684
H	-0.41578	2.11543	-1.99031
H	0.02055	2.27371	-3.71580
C	2.31535	3.74127	-3.44739
H	2.22143	3.23595	-4.42541
H	3.38885	3.86998	-3.23306
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C	3.16976	2.97095	2.61312
H	3.22362	1.88429	2.42121
C	2.37094	3.20378	3.91652
H	2.75825	2.55531	4.72209
H	1.29666	2.99601	3.79170
H	2.46767	4.24598	4.27045
C	4.61185	3.48548	2.83263
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C	-4.86310	-0.06775	0.07396
C	-5.00363	2.29643	-0.72848
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$S_{Au,N}$

SCF (BP86) Energy = -2354.20072914
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Second Frequency = 15.9411 cm^{-1}
SCF (BP86-D3BJ) Energy = -2354.59488379
SCF (C6H6) Energy = -2354.20672469
SCF (BS2) Energy = -3166.40603146

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Al	1.74493	0.00271	0.01455
Si	4.22698	-1.40074	-1.38351
N	2.76874	1.57949	0.22027
N	2.85094	-1.50813	-0.22546
N	0.16568	0.34161	-1.08446
N	-5.66283	-1.07332	-0.35333
N	0.07800	-0.35447	1.01527
N	-5.68051	0.93463	0.46676
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C	-4.83099	-0.04229	0.00867
C	-7.01997	0.52573	0.39176
C	1.43817	3.66172	0.67963
C	2.27921	2.88141	-0.18271
C	-7.00871	-0.74918	-0.12887
C	1.64998	-3.68921	-0.58343
C	2.50550	-2.84673	0.20219
C	2.66298	3.45657	-1.44337
C	-0.53446	-0.88399	2.23823
H	-1.58911	-0.53009	2.24860
C	0.98578	-3.23101	-1.88404
H	1.23694	-2.16639	-2.03108
C	0.95052	3.16229	2.04046
H	1.32793	2.13359	2.16673
C	3.05999	-3.39416	1.40979
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H	2.59622	4.08085	3.19250
H	1.18314	3.60920	4.17736
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$CAAC_{Cu}$
SCF (BP86) Energy = -2325.83210865
Enthalpy 0K = -2324.588619
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SCF (BP86-D3BJ) Energy = -2326.21387528
SCF (C6H6) Energy = -2325.83592901
SCF (BS2) Energy = -3138.01898184

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```

References

1. R. J. Schwamm, M. P. Coles, M. S. Hill, M. F. Mahon, C. L. McMullin, N. A. Rajabi, A. S. S. Wilson, *Angew. Chem. Int. Ed.* **2020**, *59*, 3928.
2. N. Kuhn, T. Kratz, *Synthesis* **1993**, *6*, 561.
3. R. Hamze, S. Shi, S. C. Kapper, D. S. M. Ravinson, L. Estergreen, M. -C. Jung, A. C. Tadle, R. Haiges, P. I. Djurovich, J. L. Peltier, R. Jazzar, G. Bertrand, S. E. Bradforth, M. E. Thompson, *J. Am. Chem. Soc*., **2019***, 141*, 8616
4. B. R. Dible and M. S. Sigman, *J. Am. Chem. Soc.* **2003**, *125*, 872–873.
5. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Cryst.* **2009**, *42*, 339-341.
6. L. J. Bourhis, O. V. Dolomanov, R. J. Gildea, J. A. K. Howard, H. Puschmann, *Acta Cryst. a-Foundation and Advances*, **2015**, *71*, 59-75.
7. G. M. Sheldrick, *Acta Cryst. Sect. C-Structural Chemistry*, **2015**, *71*, 3-8.
8. Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.
9. Andrae, D.; Häußermann, U.; Dolg, M.; Stoll, H.; Preuß, H., Energy-adjusted ab initio pseudopotentials for the second and third row transition elements. *Theoretica chimica acta*

1990, *77* (2), 123-141.

10. Hehre, W. J.; Ditchfield, R.; Pople, J. A., Self—Consistent Molecular Orbital Methods. XII. Further Extensions of Gaussian—Type Basis Sets for Use in Molecular Orbital Studies of Organic Molecules. *J. Chem. Phys.* **1972,** *56* (5), 2257-2261.
11. Hariharan, P. C.; Pople, J. A., The influence of polarization functions on molecular orbital hydrogenation energies. *Theoretica chimica acta* **1973,** *28* (3), 213-222.
12. Höllwarth, A.; Böhme, M.; Dapprich, S.; Ehlers, A. W.; Gobbi, A.; Jonas, V.; Köhler, K. F.; Stegmann, R.; Veldkamp, A.; Frenking, G., A set of d-polarization functions for pseudo-potential basis sets of the main group elements Al-Bi and f-type polarization functions for Zn, Cd, Hg. *Chem. Phys. Lett.* **1993,** *208* (3), 237-240.
13. Becke, A. D., Density-functional exchange-energy approximation with correct asymptotic behavior. *Phys. Rev. A* **1988,** *38* (6), 3098-3100.
14. Perdew, J. P., Density-functional approximation for the correlation energy of the inhomogeneous electron gas. *Phys. Rev. B* **1986,** *33* (12), 8822-8824.
15. Cancès, E.; Mennucci, B.; Tomasi, J., A new integral equation formalism for the polarizable continuum model: Theoretical background and applications to isotropic and anisotropic dielectrics. *J. Chem. Phys.* **1997,** *107* (8), 3032-3041.
16. Grimme, S.; Ehrlich, S.; Goerigk, L., Effect of the damping function in dispersion corrected density functional theory. *J. Comp. Chem.* **2011,** *32* (7), 1456-1465.
17. Keith, T. A. AIMAll Version 19.10.12; TK Gristmill Software: Overland Park KS, USA, , 2019.
18. NBO 7.0. E. D. Glendening, J, K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, P. Karafiloglou, C. R. Landis, and F. Weinhold, Theoretical Chemistry Institute, University of Wisconsin, Madison, 2018.
19. Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li,

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

20. Becke, A. D., Density-functional thermochemistry. III. The role of exact exchange. *The J. Chem. Phys.* **1993,** *98* (7), 5648-5652.
21. Lee, C.; Yang, W.; Parr, R. G., Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B* **1988,** *37* (2), 785-789.
22. Zhao, Y.; Truhlar, D. G., The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theoretical Chemistry Accounts* **2008,** *120* (1), 215-241.
23. Perdew, J. P.; Burke, K.; Ernzerhof, M., Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **1996,** *77* (18), 3865-3868.
24. Adamo, C.; Barone, V., Toward reliable density functional methods without adjustable parameters: The PBE0 model. *J. Chem. Phys.* **1999,** *110* (13), 6158-6170.
25. Tao, J.; Perdew, J. P.; Staroverov, V. N.; Scuseria, G. E., Climbing the Density Functional Ladder: Nonempirical Meta--Generalized Gradient Approximation Designed for Molecules and Solids. *Phys. Rev. Lett.* **2003,** *91* (14), 146401.

26. Chai, J.-D.; Head-Gordon, M., Long-range corrected hybrid density functionals with damped atom-atom dispersion corrections. *Phys. Chem. Chem. Phys.* **2008,** *10* (44), 6615-6620.