Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

For

N-Heterocyclic carbene copper(I) catalysed *N*-methylation of amines using CO_2

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Contents

1. General information

All reactions were carried out under argon atmosphere using standard Schlenk and glovebox techniques. Chemicals were used as received unless otherwise noted. Dry toluene was obtained from a PureSolv SPS-400-5 solvent purification system. ^{1}H, and ^{13}C-{^{1}H} Nuclear Magnetic Resonance (NMR) spectra were recorded on a Bruker-400 MHz or 300 MHz spectrometers using the residual solvent peak as reference ($CDCl_3$: δ_H = 7.26 ppm, δ_C = 77.16 ppm, CD_2Cl_2: δ_H = 5.32 ppm, δ_C = 53.84 ppm, C_7D_8: δ_H = 2.08 ppm) at 298K.

Elemental analyses were performed at London Metropolitan University 166-220, Holloway Road, London, N7 8DB.

HMRS analyses were carried out by the EPSRC National Mass Spectrometry Service Centre at Swansea University.

2. Synthesis of [Cu(OH)(IPr*)] (3)

In a glovebox, a round bottom flask was charged with [Cu(Cl)(IPr*)] (250 mg, 0.25 mmol), CsOH (74 mg, 2 equiv.) and THF (12.5 mL). The reaction mixture was stirred at room temperature during 15 hours. The solution was concentrated and pentane (10 mL) was added. The white precipitate was filtered and washed with pentane (3 x 5 mL) in order to give the desired compound as a colorless solid in 89% isolated yield (215 mg, 0.22 mmol).

^{1}H NMR (300 MHz, C_7D_8, 298 K): δ = 1.74 (s, 6H, CH_3), 5.58 (s, 2H, H^4 and H^5), 5.60 (s, 4H, CHPh$_2$), 6.97-7.01 (m, 28H, CH_{Ar}), 7.17 (m, 8H, CH_{Ar}), 7.41 (m, 8H, CH_{Ar}).

^{13}C-{^{1}H} NMR (75 MHz, C_7D_8, 298 K): δ = 21.1 (s, CH$_3$), 51.7 (s, CHPh$_2$), 123.2 (s, C^4 and C^5), 126.8 (s, CH Ar), 127.0 (s, CH Ar), 128.3 (s, CH Ar), 128.6 (s, CH Ar), 128.7 (s, CH Ar), 129.1 (s, CH Ar), 129.9 (s, CH Ar), 130.3 (s, C^{IV} Ar), 130.6 (s, C^{IV} Ar), 141.7 (s, C^{IV} Ar), 143.5 (s, C^{IV} Ar), 143.7 (s, C^{IV} Ar). C^2 has not been observed.

Elem. Anal.: Calcd. for $C_{25}H_{33}CuN_2O$: C, 83.40; H, 5.78, N, 2.82. **Found**: C, 83.46, H, 5.65, N, 2.74

3. Synthesis of [Cu(O^{t}Bu)(IMes)] (4)[1]

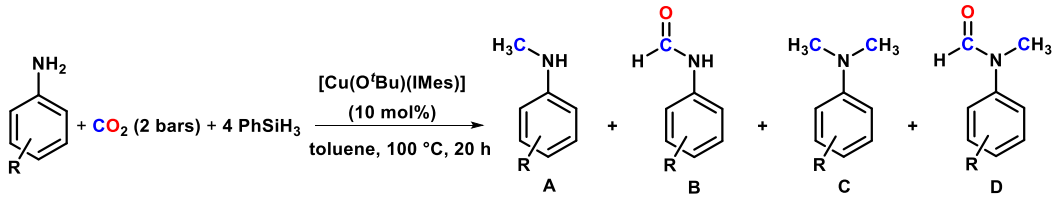
In a glovebox, a round bottom flask was charged with [Cu(Cl)(IMes)] (4.0 g, 9.8 mmol, 1 equiv.), and NaO^{t}Bu (953 mg, 9.8 mmol, 1 equiv.) and THF (80 mL). The reaction mixture was stirred at room temperature for 3 hours and then filtered through a plug of celite. Removal of the solvent under reduced pressure afforded the desired compound in 91% yield (4.0 g, 8.96 mmol) as a tan microcrystalline powder.

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 1.32 (s, 9H, C-C*H*$_3$), 1.97 (s, 12H,C*H*$_3$), 2.10 (s, 12H,C*H*$_3$), 6.26 (s, 2H, *H*^{4} and *5*^{4}), 6.72 (s, 4H, C*H* phenyl).

^{13}C-{^{1}H} NMR (75 MHz, $CDCl_3$, 298 K): δ = 17.8 (s, C-*C*H$_3$), 21.0 (s, *C*H$_3$), 35.0 (s, *C*H$_3$), 67.8 (s, *C*-CH$_3$), 121.6 (s, C^{IV} Ar), 129.5 (s, *C*H Ar), 134.9 (s, *C*^{4} and *C*^{5}), 136.1 (s, C^{IV} Ar), 139.0 (s, C^{IV} Ar), 181.4 (s, *C*^{2}).

Elem. Anal.: Calcd. for $C_{25}H_{33}CuN_2O$: C, 68.07; H, 7.54, N, 6.35. **Found:** C, 67.82, H, 7.69, N, 6.35

4. General procedure for methylation

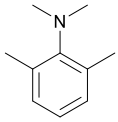


Under an argon atmosphere, a 3 mL vial was charged with [Cu(O^{t}Bu)(IMes)] **(4)** (11 mg, 10 mol%), KO^{t}Bu (2.8 mg, 10 mol%) and toluene (2 mL). The amine substrate (0.25 mmol, 1 equiv.) and $PhSiH_3$ (123 µL, 1.0 mol, 4 equiv.) were added and the vial was sealed with a septum cap. The septum cap was pierced with a syringe needle and placed into a six-slot steal autoclave. The autoclave was sealed, purged twice with CO_2 and heated at 100 °C (oil bath) under CO_2 atmosphere (2 bars) for 20 hours. After this time the reaction mixture was allowed to cool and the gas was carefully released. The reaction mixture was analysed by gas chromatography (GC).

In the case of isolated products, dichloromethane (5 mL) was added to the crude and the mixture was extracted with HCl 1M (3 x 10 mL). The aqueous layer was neutralized by addition of K_2CO_3 (pH = 12) and extracted with diethyl ether (3 x 10 mL). The ether layer was dried over Na_2SO_4. Removal of the solvent afforded the desired compounds.

5. Characterisation of *N*-methylated compounds

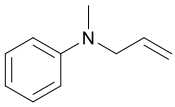
***N, N*-dimethyl-2,6-xylidine (6b)[2]**



^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 2.33 (s, 6H, C*H*$_3$), 2.85 (s, 3H, N-C*H*$_3$), 6.97 (t, $^{3}J_{H\text{-}H}$ = 6.8 Hz, 1H, C*H* phenyl), 7.00 (d, $^{3}J_{H\text{-}H}$ = 7.2 Hz, 2H, C*H* phenyl).

^{13}C-{^{1}H} NMR (75 MHz, $CDCl_3$, 298 K): δ = 19.3 (S, *C*H$_3$), 42.6 (s, N-*C*H$_3$), 124.8 (s, *C*H Ar), 128.9 (s, *C*H Ar), 137.2 (s, C^{IV} Ar), 149.8 (s, C^{IV} Ar).

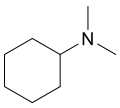
***N*-allyl-*N*-methylaniline (8b)[3]**



^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 2.94 (s, 3H, N-C*H*$_3$), 3.92 (d, $^{3}J_{H\text{-}H}$ = 5.2 Hz, 2H, C*H*$_2$ allyl), 5.16 (m, 2H, CH-C*H*$_2$), 5.85 (m, 1H, NCH$_2$-C*H*), 6.70-6.74 (m, 3H, C*H* phenyl), 7.21-7.26 (m, 2H, C*H* phenyl).

^{13}C-{^{1}H} NMR (75 MHz, $CDCl_3$, 298 K): δ = 38.1 (s, N-*C*H$_3$), 55.4 (s, *C*H$_2$ allyl), 112.6 (s, *C*H Ar), 116.3 (s, *C*H$_2$), 116.5 (s, *C*H Ar), 129.2 (s, *C*H Ar), 133.9 (s, CH$_2$-*C*H), 149.6 (s, C^{IV} Ar).

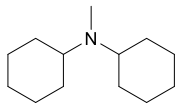
***N, N*-dimethylcyclohexylamine (9b)[4]**



^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 1.24 - 1.47 (m, 5H), 1.72 (m, 1H,), 1.93 (m, 2H, C*H*$_2$), 2.23 (m, 2H, C*H*$_2$), 2.71 (s, 6H, N-C*H*$_3$), 3.01 (m, 1H, C*H*).

^{13}C-{^{1}H} NMR (75 MHz, $CDCl_3$, 298 K): δ = 25.1 (s, *C*H$_2$), 25.2 (s, *C*H$_2$), 26.9 (s, *C*H$_2$), 39.5 (s, N-*C*H$_3$), 65.5 (s, *C*H$_2$).

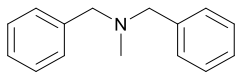
***N*-cyclohexyl-*N*-methylcyclohexylamine (10b)[5]**



^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 1.06 (m, 2H, C*H*$_2$), 1.08 (m, 8H, C*H*$_2$), 1.59 (m, 2H, C*H*$_2$), 1.77 (m, 8H, C*H*$_2$), 2.33 (s, 3H, N-C*H*$_3$), 2.49 (m, 2H, C*H*).

^{13}C-{^{1}H} NMR (75 MHz, $CDCl_3$, 298 K): δ = 26.3 (s, *C*H$_2$), 26.3 (s, *C*H$_2$), 30.5 (s, *C*H$_2$), 33.0 (s, N-*C*H$_3$), 59.6 (s, *C*H$_2$).

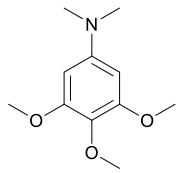
***N*-methyldibenzylamine (11b)[6]**



^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 2.12 (s, 3H, N-C*H*$_3$), 3.46 (s, 4H,C*H*$_2$ benzyl), 7.18 (t, $^{3}J_{H\text{-}H}$ = 7.8 Hz, 2H, C*H* phenyl), 7.25 (t, $^{3}J_{H\text{-}H}$ = 7.8 Hz, 4H, C*H* phenyl), 7.29 (d, $^{3}J_{H\text{-}H}$ = 7.8 Hz, 4H, C*H* phenyl).

^{13}C-{^{1}H} NMR (75 MHz, $CDCl_3$, 298 K): δ = 42.4 (s, N-*C*H$_3$), 62.0 (s, *C*H$_2$ benzyl), 127.1 (s, *C*H Ar), 128.4 (s, *C*H Ar), 129.1 (s, *C*H Ar), 139.5 (s, C^{IV} Ar).

3,4,5-trimethoxy-*N*,*N*-dimethylaniline (17d)

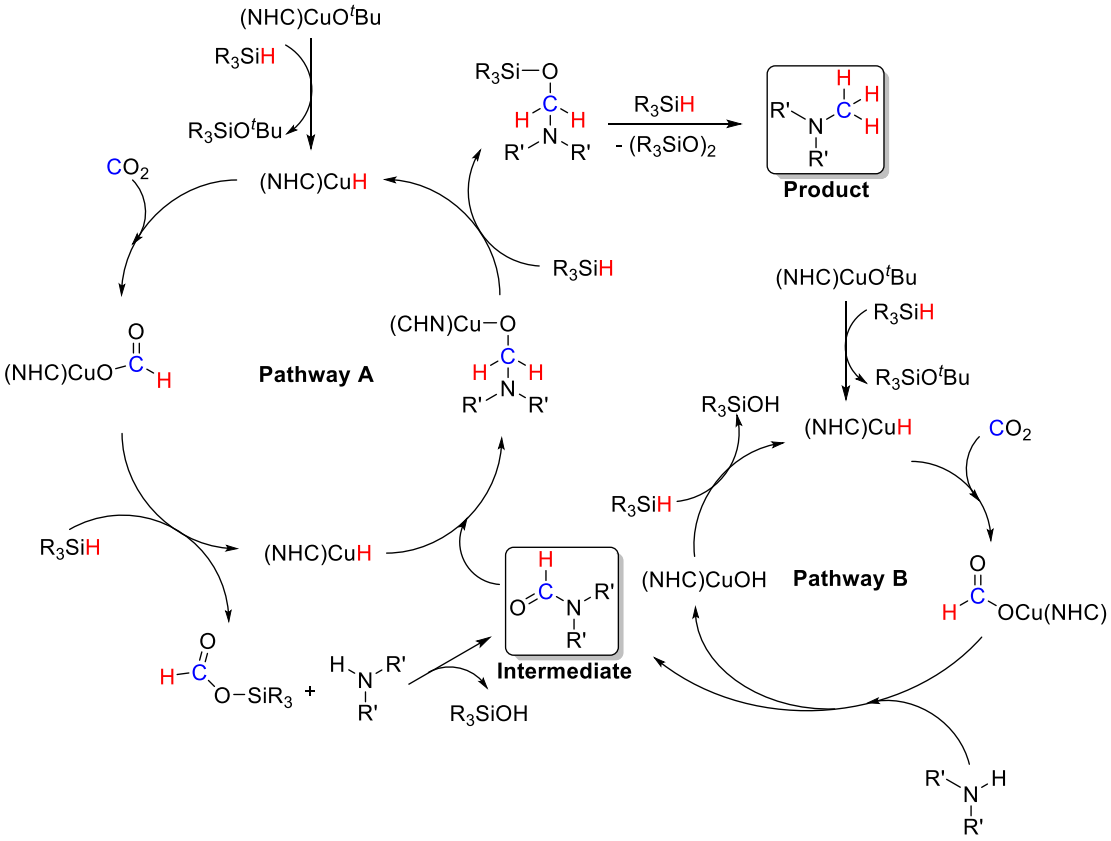


^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 2.93 (s, 6H, N-C*H*$_3$), 3.78 (s, 3H, O-C*H*$_3$), 3.86 (s, 6H, O-C*H*$_3$), 5.95 (s, 2H, C*H* phenyl).

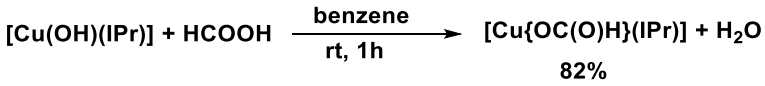
^{13}C-{^{1}H} NMR (75 MHz, $CDCl_3$, 298 K): δ = 41.3 (s, N-*C*H$_3$), 56.13 (s, O-*C*H$_3$), 61.2 (s, O-*C*H$_3$), 91.0 (s, *C*H Ar), 130.0 (s, C^{IV} Ar), 147.9 (s, C^{IV} Ar), 153.8 (s, C^{IV} Ar).

HMRS (APCI) m/z Calcd for $[C_{11}H_{17}O_3N + H]^+$ 212.1281. **Found** 212.1279.

6. Mechanistic studies



6.1. Synthesis of [Cu{OC(O)H}(IPr)] (19)[7]



Under an argon atmosphere, a vial was charged with [Cu(OH)(IPr)] **(1)** (200 mg, 0.21 mmol, 1 equiv.), formic acid (16 µL, 0.21 mmol, 1 equiv.) and benzene (2 mL). The mixture was stirred at room temperature for 1 hour, the solution was then concentrated under reduced pressure. The addition of pentane (10 mL) afforded a colorless solid collected by filtration (Yield = 82%). The spectroscopic data obtained matched the reported values.[7]

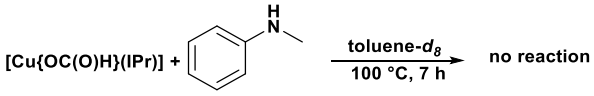
^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 1.22 (d, $^3J_{H\text{-}H}$ = 6.8 Hz, 12H, CH-C*H*$_3$), 1.29 (d, $^3J_{H\text{-}H}$ = 6.8 Hz, 12H, CH-C*H*$_3$), 2.56 (sept, $^3J_{H\text{-}H}$ = 7.0 Hz, 4H, C*H*-CH$_3$ isopropyl), 7.15 (s, 2H, H^4 and H^5), 7.29 (d, $^3J_{H\text{-}H}$ = 7.8 Hz, 4H, C*H* phenyl), 7.48 (t, $^3J_{H\text{-}H}$ = 7.9 Hz, 2H, C*H* phenyl), 8.11 (s, 1H, C(O)*H* formyl)

^{13}C-{^{1}H} NMR (75 MHz, $CDCl_3$, 298 K): δ = 24.0 (s, CH-*C*H$_3$), 24.8 (s, CH-*C*H$_3$) 28.8 (s, *C*H-CH$_3$), 123.3 (s, C^{IV} Ar), 124.3 (s, CH Ar), 130.6 (s, C^4 and C^5), 134.5 (s, C^{IV} Ar), 145.7 (s, CH Ar), 167.9 (s, O*C*(O)H), 180.4 (s, C^2).

6.2. General procedure for stoichiometric experiments

In a glovebox, a vial was charged with the reactants and toluene-d_8 (0.5 mL). The mixture was stirred at 100 ^{0}C for 7 hours. After which time the crude was filtered through cotton wool and recovered into a NMR tube and then analysed by ^{1}H NMR spectroscopy.

6.2.1. [Cu{OC(O)H}(IPr)] + *N*-methylaniline



The reaction between [Cu{OC(O)H}(IPr)] (50 mg, 0.1 mmol, 1 equiv.) and *N*-methylaniline (10.8 µL, 0.1 mmol, 1 equiv.) led to the decomposition of the organometallic species. Only the starting material was observed, no other product.

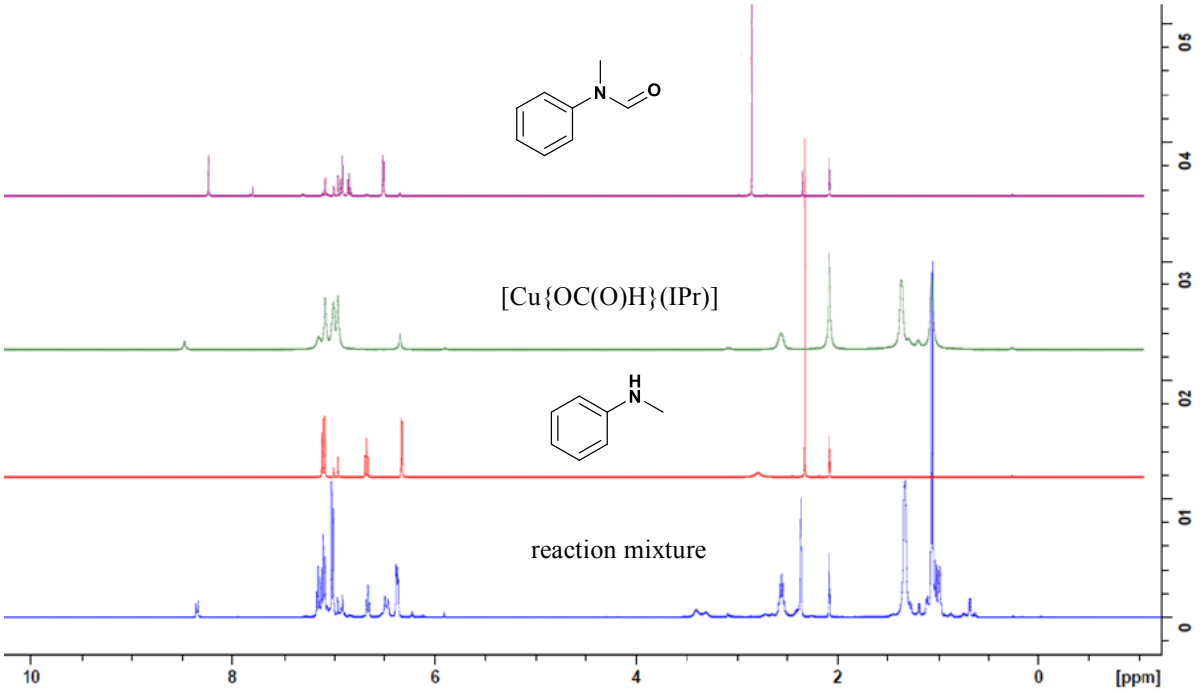
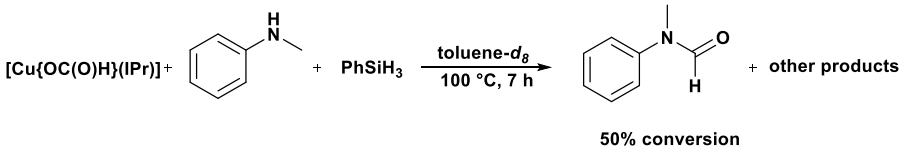


Figure S1. Comparison of the NMR spectra of *N*-methylformanilide (purple), [Cu{OC(O)H}(IPr)] (green), *N*-methylaniline (red) and [Cu{OC(O)H}(IPr)] + *N*-methylaniline (blue)

6.2.2 [Cu{OC(O)H}(IPr)] + *N*-methylaniline + $PhSiH_3$



The reaction between [Cu{OC(O)H}(IPr)] (50 mg, 0.1 mmol, 1 equiv.), *N*-methylaniline (10.8 µL, 0.1 mmol, 1 equiv.) and $PhSiH_3$ (12.3 µL, 0.1 mL, 1 equiv.) led to the conversion of 50% of the aniline into the formylated aniline. Decomposition of the organometallic species was also observed.

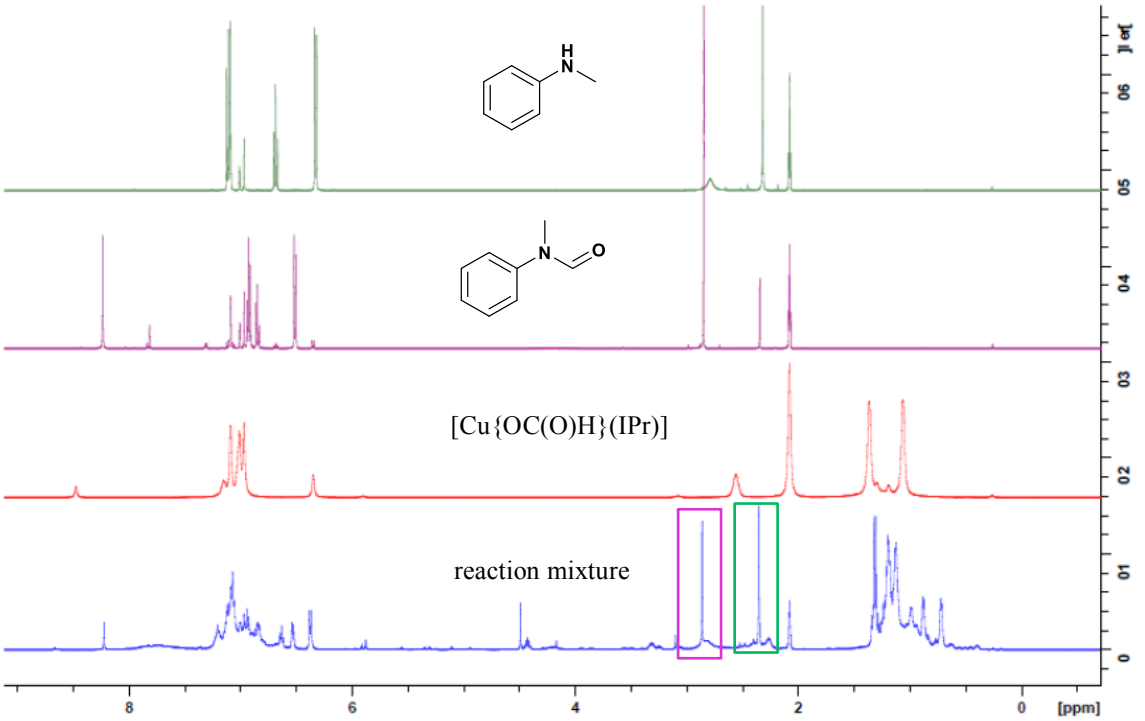
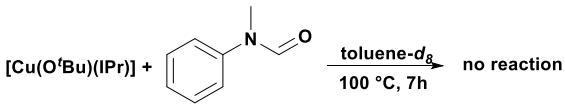


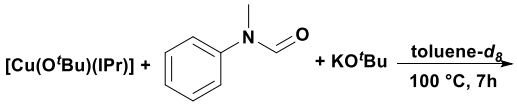
Figure S2. Comparison of the NMR spectra of *N*-methylaniline (green), *N*-methylformanilide (purple), [Cu{OC(O)H}(IPr)] (red) and [Cu{OC(O)H}(IPr)] + *N*-methylaniline + $PhSiH_3$ (blue).

6.2.3. [Cu(O^{t}Bu)(IPr)] + *N*-methylformanilide



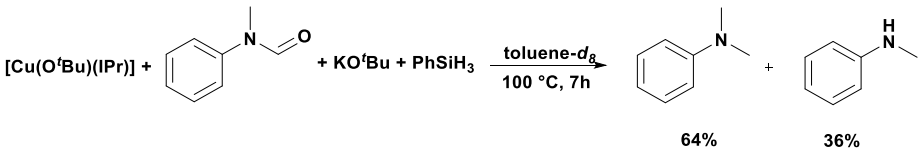
The reaction between [Cu(O^{t}Bu)(IPr)] (81 mg, 0.08 mmol, 1 equiv.) and *N*-methylformanilide (10.0 µL, 0.08 mmol, 1 equiv.) did not provide any product only the starting materials.

6.2.4 [Cu(O^{t}Bu)(IPr)] + *N*-methylformanilide



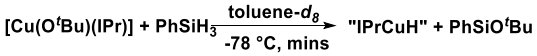
The reaction between [Cu(O^{t}Bu)(IPr)] (81 mg, 0.1 mmol, 1 equiv.), *N*-methylformanilide (10.0 µL, 0.1 mmol, 1 equiv.) and KO^{t}Bu (9.1 mg, 1equiv.) led to the full conversion of the anilide mainly towards *N*-methylaniline.

6.2.5. [Cu(O^{t}Bu)(IPr)] + *N*-methylformanilide



The reaction between [Cu(O^{t}Bu)(IPr)] (81 mg, 0.08 mmol, 1 equiv.), *N*-methylformanilide (10.0 µL, 0.08 mmol, 1 equiv.), KO^{t}Bu (9.1 mg, 0.08 mmol, 1equiv.) and $PhSiH_3$ (20.2 µL, 0.08 mmol, 1 equiv.) led to the full conversion of the anilide towards *N*-methylaniline (36%) and *N,N*-dimethylaniline (64%).

6.2.6. Formation of [Cu(H)(IPr)] (18)[8]



Under inert atmosphere, a NMR tube was charged with [Cu(O^{t}Bu)(IPr)] (20 mg, 0.04 mmol, 1 equiv.) and toluene-d_8 (0.6 mL). The suspension was cooled to -78 °C (acetone/dry ice bath) and $PhSiH_3$ (5 µL, 0.04 mmol, 1 equiv.) was added. The solution immediately turned light-orange. The frozen NMR tube was quickly warmed and placed in the NMR probe operating at 298K.

The ^{1}H NMR is consistent with data reported in the literature.[8]

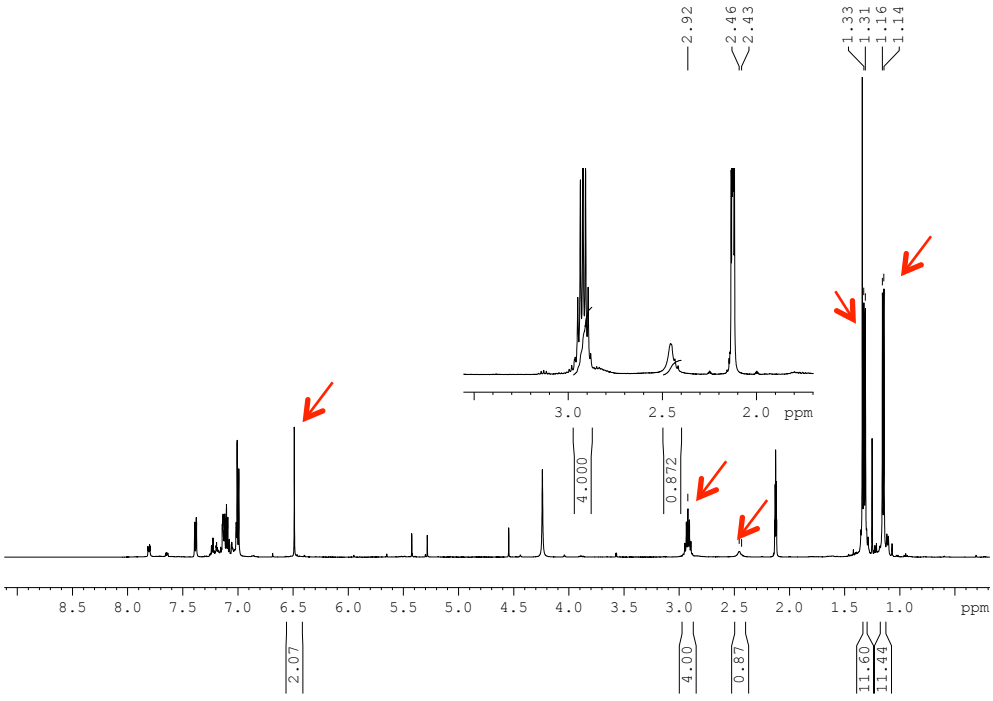
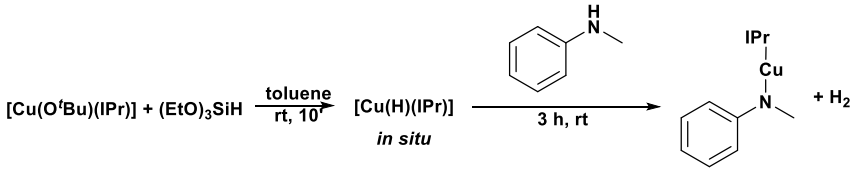


Figure S3. ^{1}H NMR of [Cu(H)(IPr)][8]. The red arrows indicate the signals belonging to the product.

6.2.7. Reaction of [Cu(H)(IPr)] with *N*-methylaniline



In a glovebox a vial was charged with [Cu(O^{t}Bu)(IPr)] (250 mg, 0.5 mmol, 1 equiv.) and toluene (2 mL). The suspension stirred and triethoxysilane (90 µL, 0.5 mmol, 1 equiv.) was added. The solution immediately turned orange (formation of Cu-H). The mixture was stirred for 10 minutes at room temperature then *N*-methylaniline (54 µL, 0.5 mmol, 1 equiv.) was added. The mixture was stirred at room temperature for 3 h. Evolution of gas was observed. The solvent was removed under reduced pressure. The mixture obtained was dissolved in CH_2Cl_2 (1 mL) hexane was added affording a grey solid (200 mg) recovered by filtration and analysed by NMR (Figure S4).

Although the spectrum suggested the formation of the desired compound, the structure was not confirmed by X-Ray diffraction on single crystal.

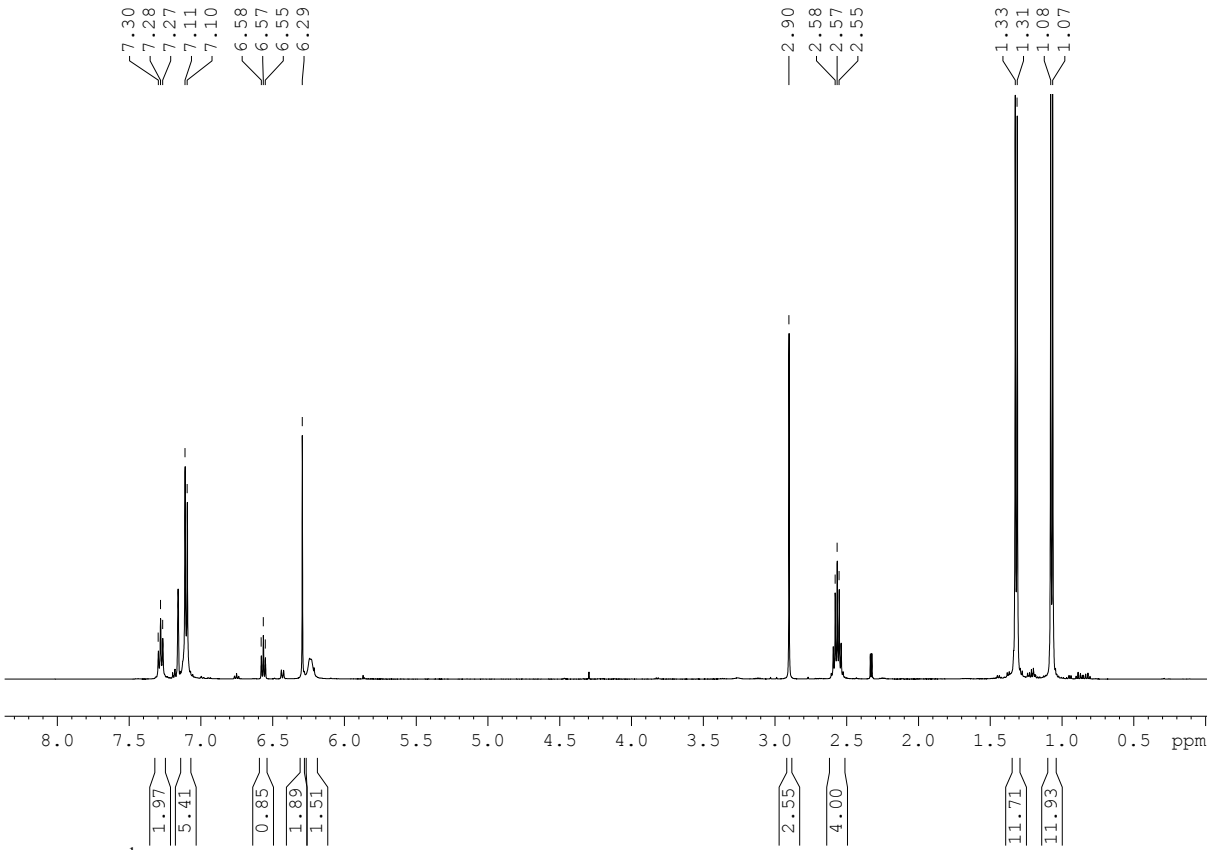
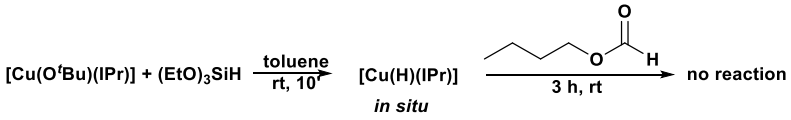


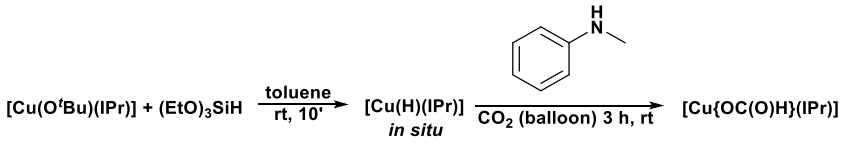
Figure S4. ^{1}H NMR of the product isolated from the reaction of [Cu(H)(IPr)] with *N*-methylaniline.

6.2.8. Reaction of [Cu(H)(IPr)] with butyl formate



In a glovebox a vial was charged with [Cu(O^{t}Bu)(IPr)] (200 mg, 0.4 mmol, 1 equiv.) and toluene (3 mL). The suspension stirred and triethoxysilane (72 µL, 0.4 mmol, 1 equiv.) was added. The solution immediately turned orange (formation of Cu-H). The mixture was stirred for 10 minutes at room temperature then butyl formate (46 µL, 0.4 mmol, 1 equiv.) was added. The mixture was stirred at room temperature for 3 h. The solvent was then removed under reduced pressure. The mixture obtained was dissolved in CH_2Cl_2 (1 mL), hexane was added affording a grey solid (90 mg) recovered by filtration and analysed by ^{1}H NMR. Only decomposition of the starting material was observed.

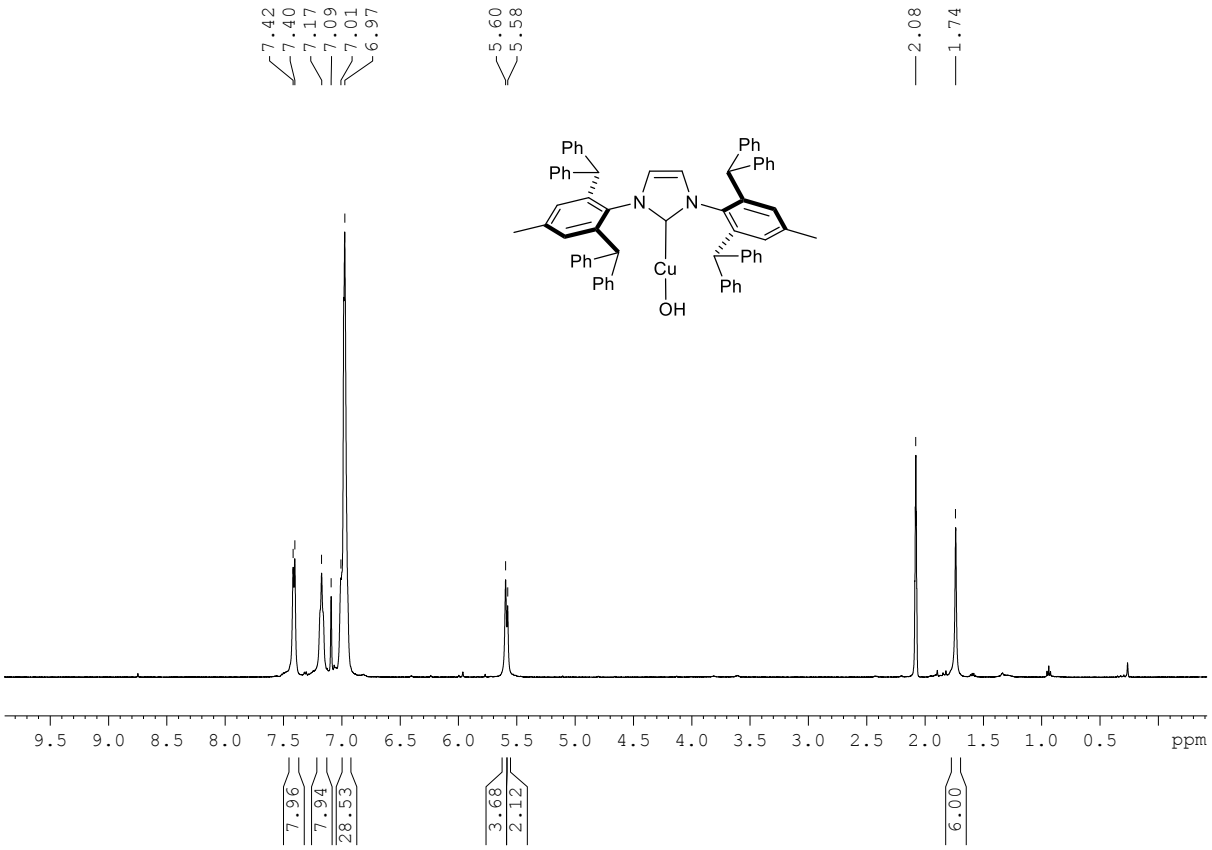
6.2.9. Reaction of [Cu(H)(IPr)] *N*-methylaniline under CO_2 atmosphere

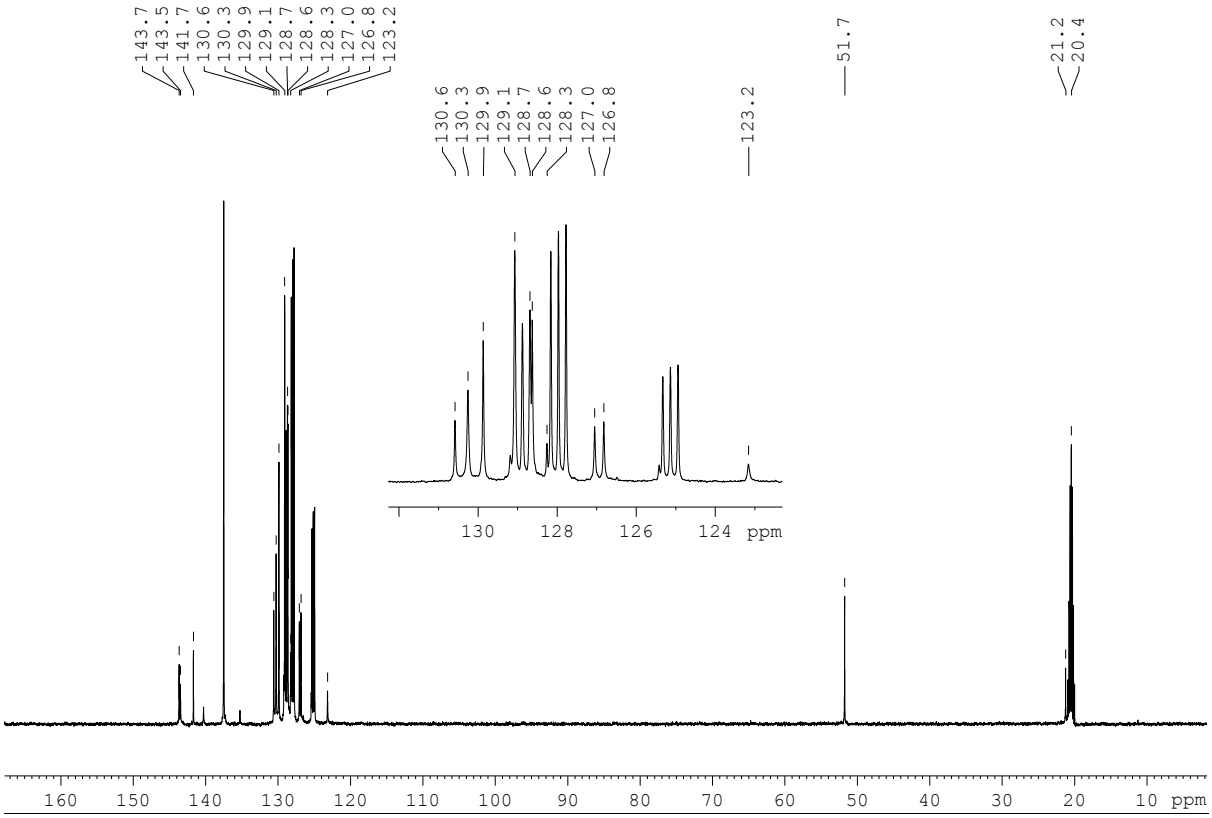


In a glovebox a Schlenk tube was charged with [Cu(O^{t}Bu)(IPr)] (200 mg, 0.4 mmol, 1 equiv.) and toluene (3 mL). Outside the glovebox the mixture was frozen by mean of liquid N_2 then evacuated and purged with CO_2 three times. The mixture was then allowed to reach room temperature. Under CO_2 atmosphere, *N*-methylaniline (47 µL, 0.4 mmol, 1 equiv.) was added. The mixture was stirred at room temperature for 10 minutes. Triethoxysilane (72 µL, 0.4 mmol, 1 equiv.) was added and the mixture was stirred for 3 hours at room temperature under CO_2 atmosphere (balloon connected to the Schlenk inlet). In the glovebox the mixture was filtered on celite and the solvent removed under reduced pressure. The mixture obtained was dissolved in CH_2Cl_2 (1 mL), hexane was added affording a grey solid (80 mg) recovered by filtration and analysed by NMR. The date matched the reported values for [Cu{OC(O)H}(IPr)].[7]

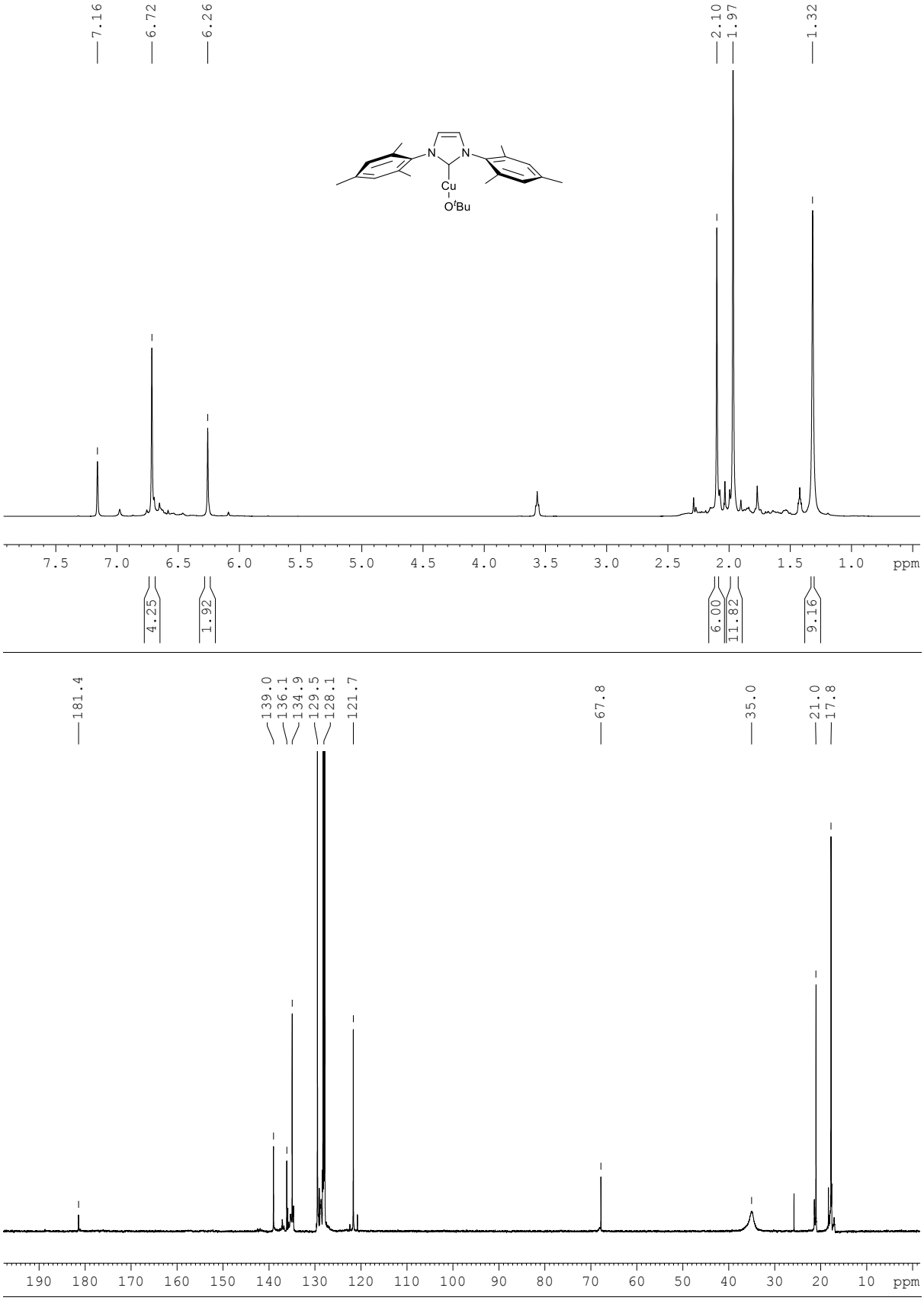
7. ^{1}H and ^{13}C-{1H} NMR spectra

[Cu(OH)(IPr*)](**3**), ^{1}H NMR, C_7D_8, 298K.

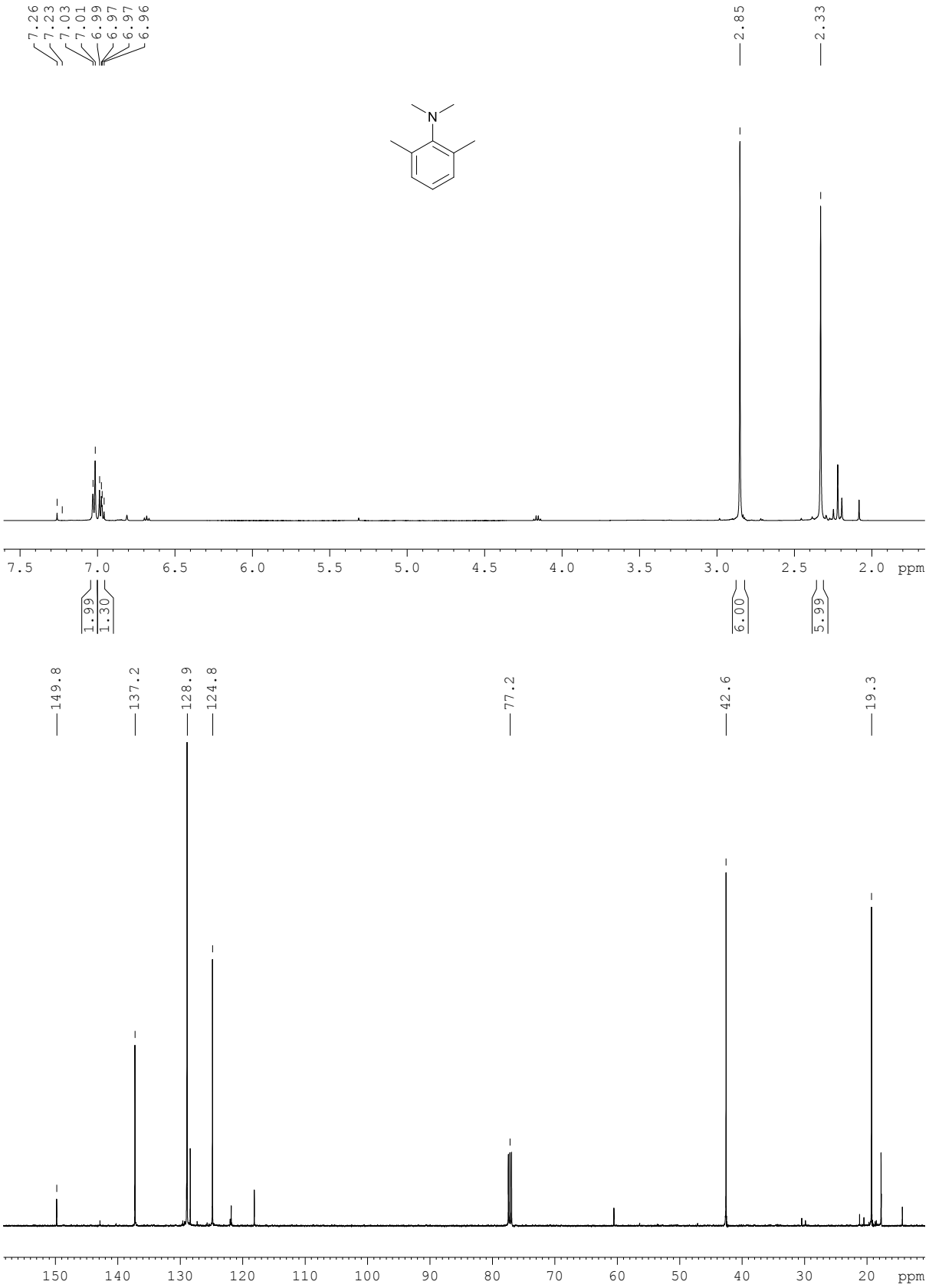




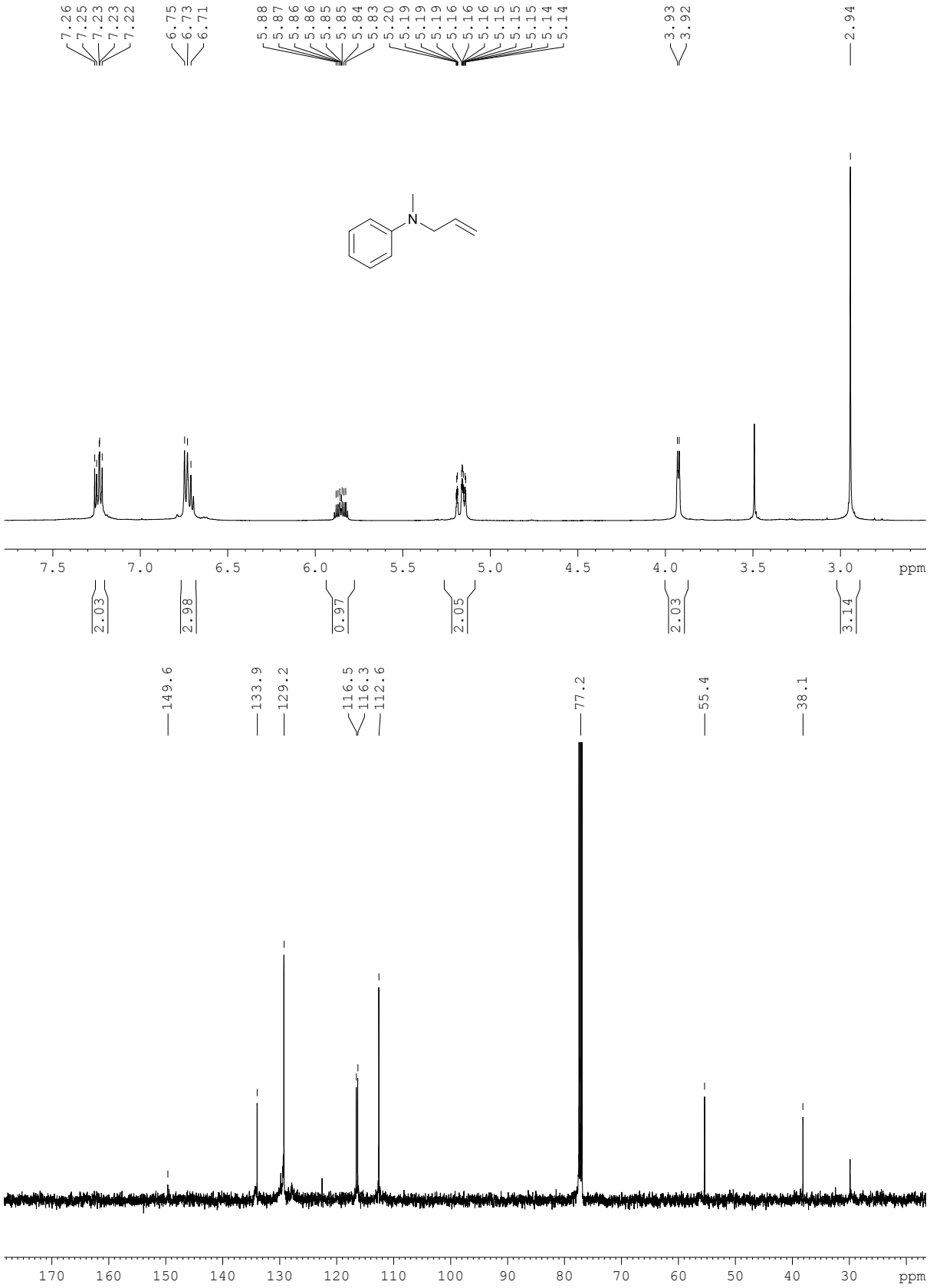
[Cu(OtBu)(IMes)](**4**), ^{1}H NMR, C_6D_6, 298K and ^{13}C-{^{1}H} NMR, C_6D_6, 298 K



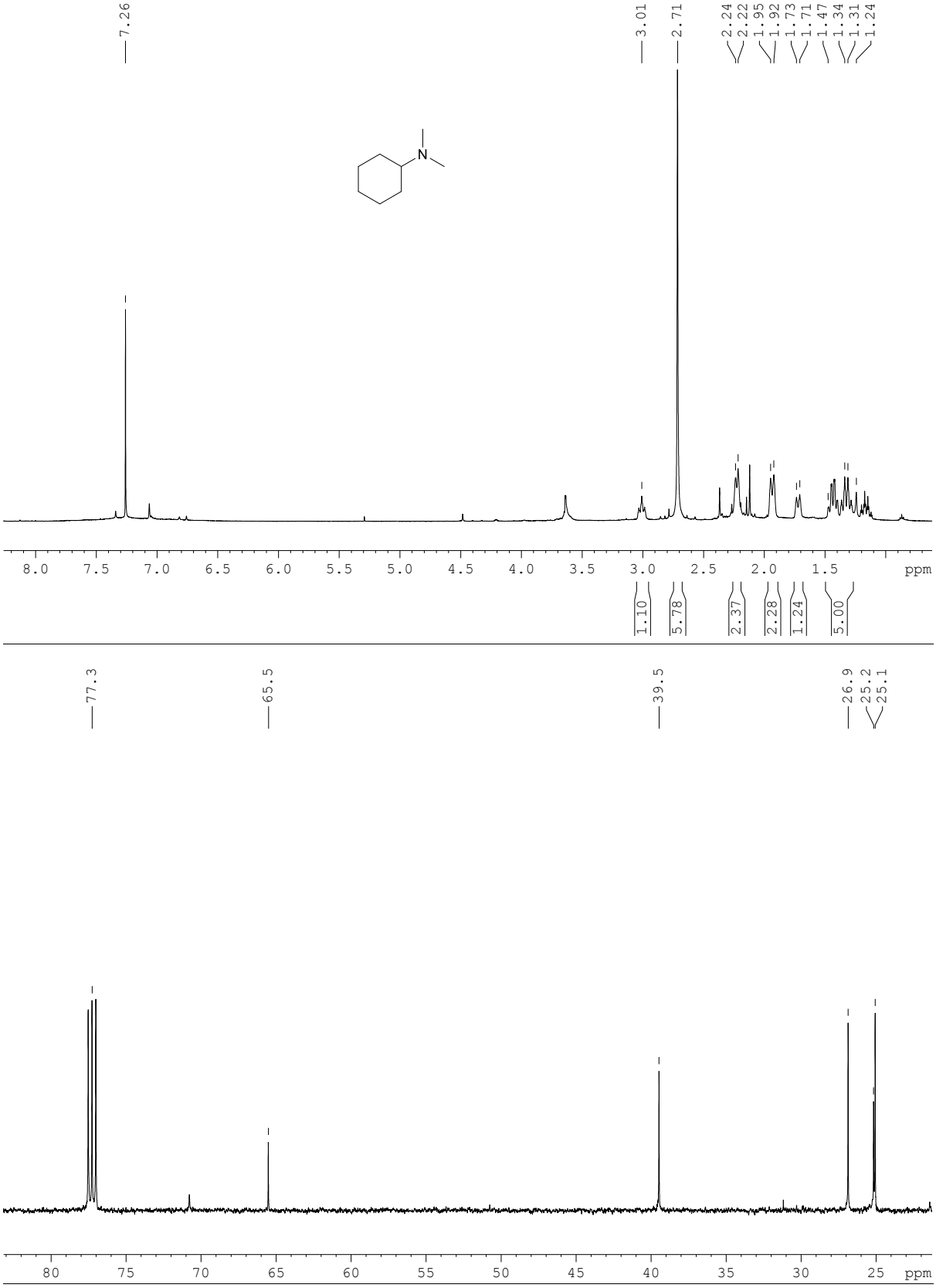
N, *N*-dimethy-2,6-xylidine (**6b**), ^{1}H NMR, $CDCl_3$, 298K and ^{13}C-{^{1}H} NMR, $CDCl_3$, 298 K



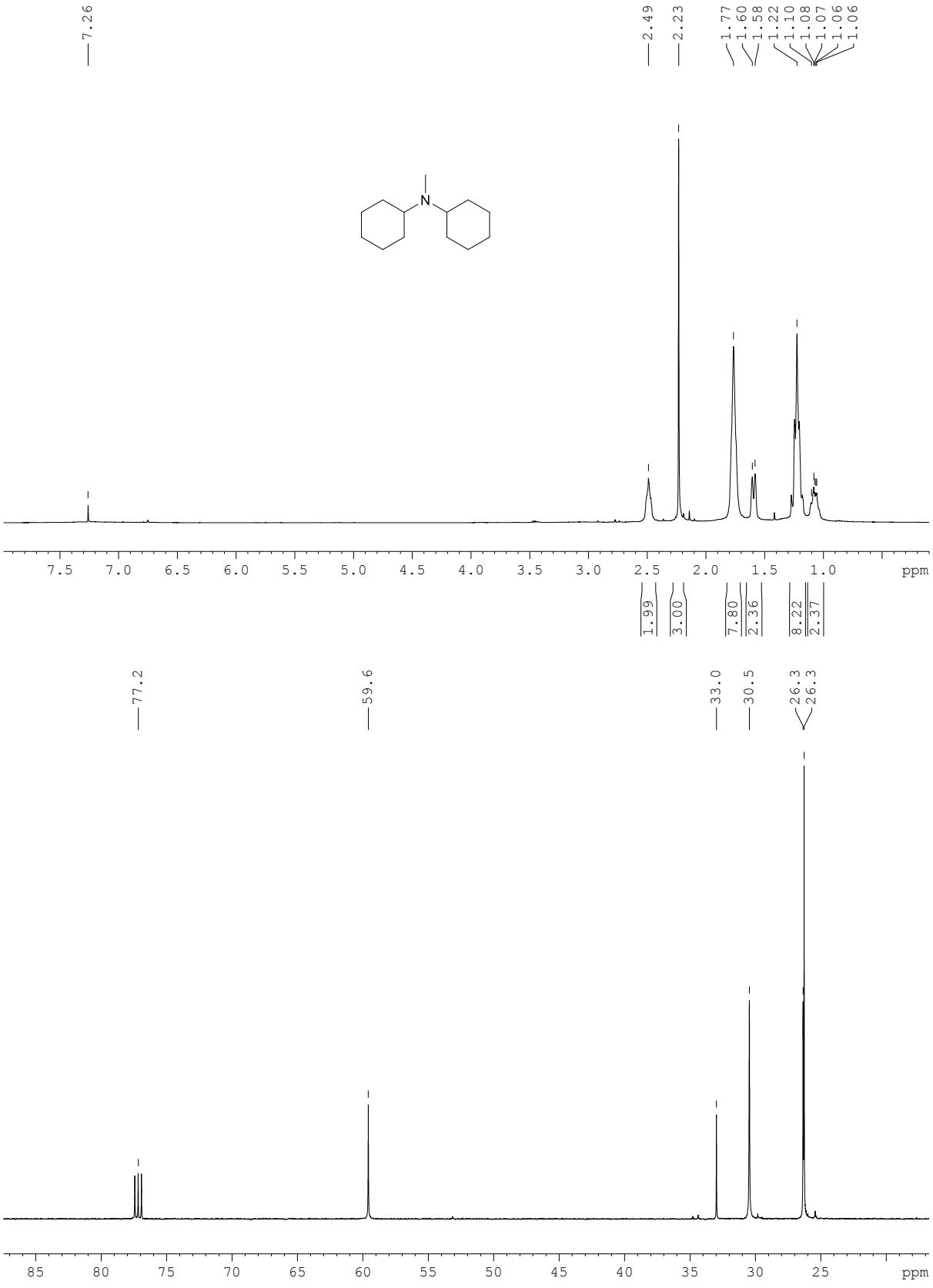
N-allyl-N-methylaniline (**8b**), ^{1}H NMR, $CDCl_3$, 298K and ^{13}C-{^{1}H} NMR, $CDCl_3$, 298 K



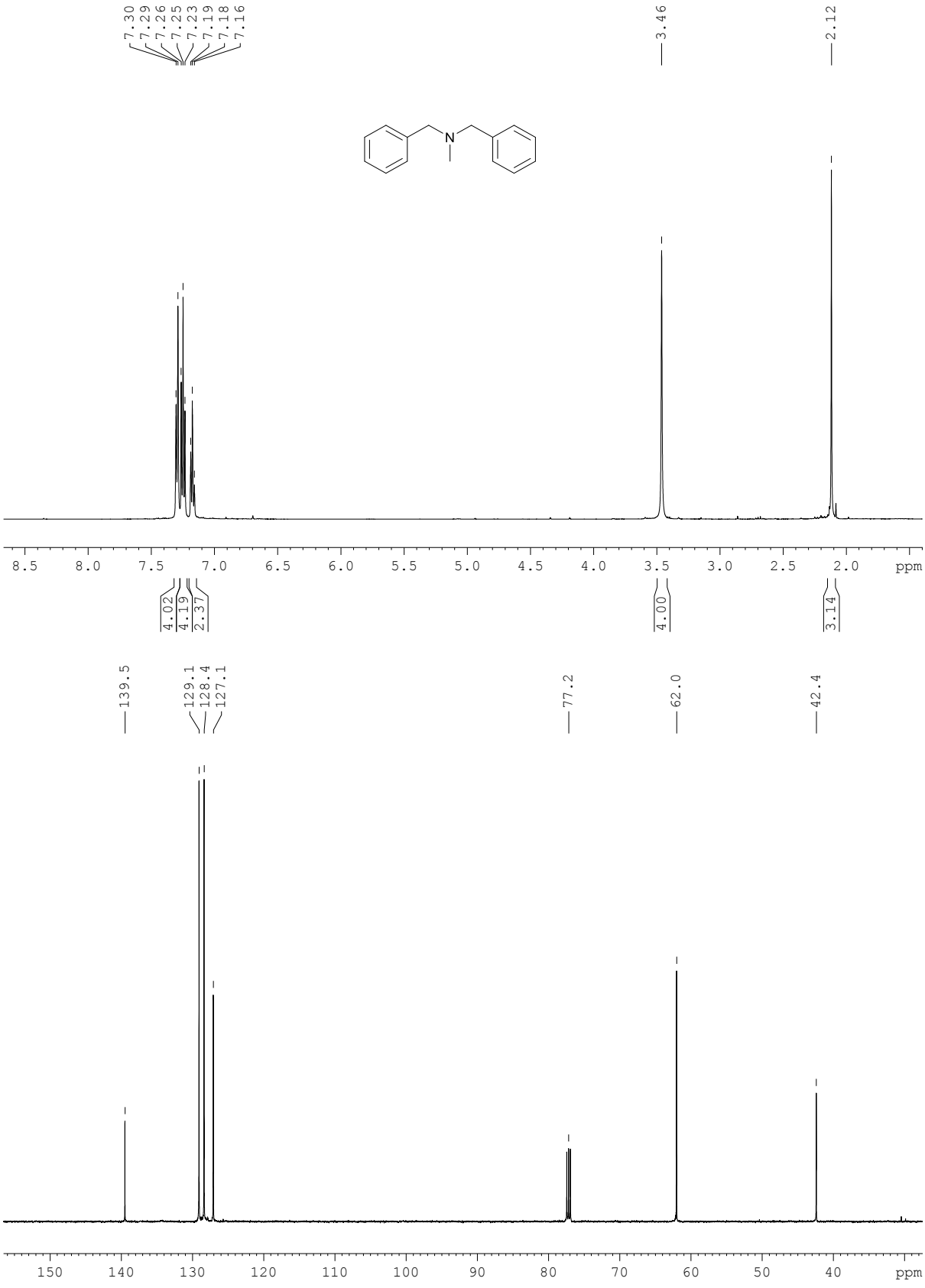
N, *N*-dimethylcyclohexylamine (**9b**), ^{1}H NMR, $CDCl_3$, 298K and ^{13}C-{^{1}H} NMR, $CDCl_3$, 298 K



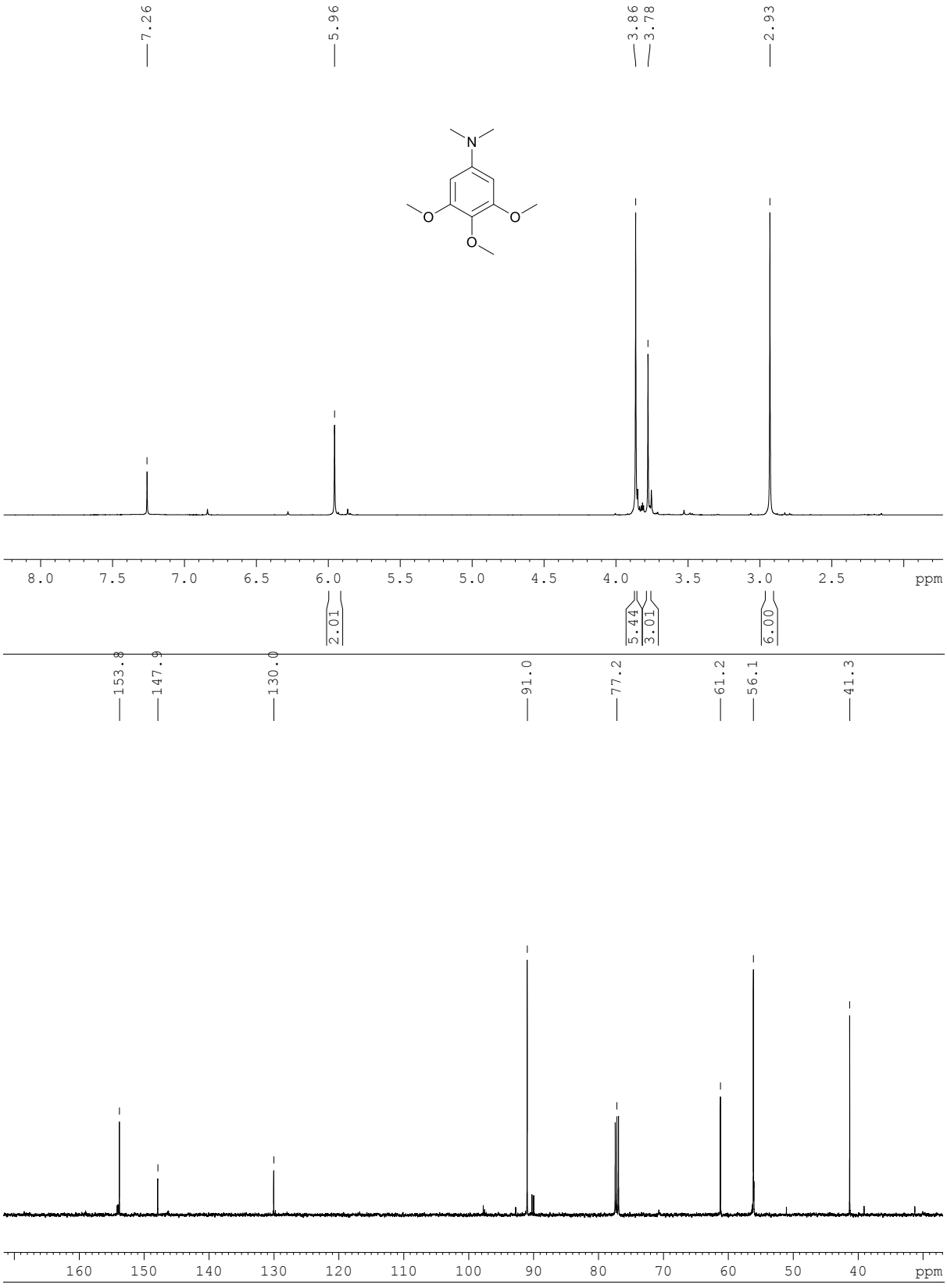
N-cyclohexyl-*N*-methylcyclohexylamine (**10b**), ^{1}H NMR, $CDCl_3$, 298K and ^{13}C-{^{1}H} NMR, $CDCl_3$, 298 K



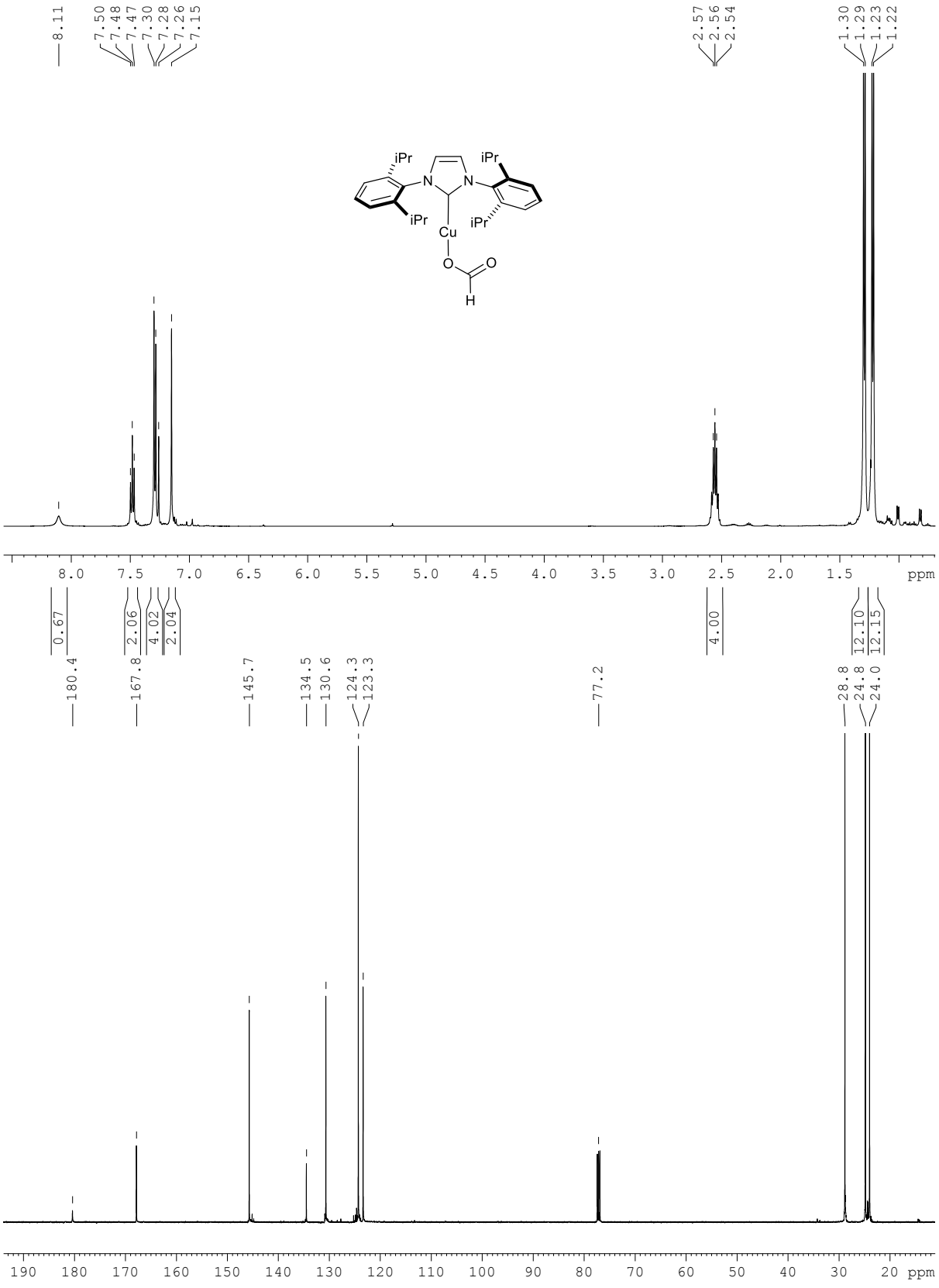
N-methyldibenzylamine (**11b**), ^{1}H NMR, $CDCl_3$, 298K and ^{13}C-{^{1}H} NMR, $CDCl_3$, 298 K



3,4,5-trimethoxy-*N*,*N*-dimethylaniline (**17d**), ^{1}H NMR, $CDCl_3$, 298K and ^{13}C-{^{1}H} NMR, $CDCl_3$, 298 K



[Cu(OC(O)H)IPr)](**19**), ^{1}H NMR, $CDCl_3$, 298K and ^{13}C-{^{1}H} NMR, $CDCl_3$, 298 K



8. Computational details

8.1 Geometry optimisations and calculations of thermochemical corrections.

All geometry optimisation were performed using the PBE GGA functional as implemented in PRIRODA 13 DFT code.[9] All electron basis sets (L1)[10] comparable in quality to the correlation consistent valence double-ζ plus polarization (cc-PVDZ) basis sets of Dunning were used. All stationary geometries were characterised by analytically calculated Hessian matrix. Possible relativistic effects (for copper) were taken into account via the Dyall Hamiltonian.[11]

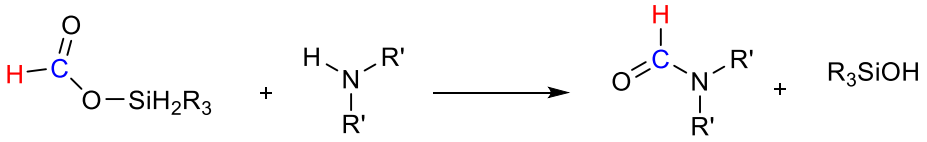
The default, adaptively generated PRIRODA grid, corresponding to an accuracy of the exchange-correlation energy per atom (1×10^{-8} hartree) was decreased by a factor of 100 for more accurate evaluation of the exchange-correlation energy. Default values were used for the Self-Consistent-Field (SCF) convergence and the maximum gradient for geometry optimisation criterion (1×10^{-4} au), whereas the maximum displacement geometry convergence criterion was decreased to 0.0018 au.

Translational, rotational, and vibrational partition functions for thermal corrections to arrive at total Gibbs free energies were computed within the ideal-gas, rigid-rotor, and harmonic oscillator approximations. The temperature used in the calculations of thermochemical corrections was set to 298.15 K in all the cases.

Single-point (SP) energy evaluations. The energies were re-evaluated at optimised geometries by means PBE GGA functional as implemented in Gaussian 09 code.[12] The effects from dispersion were included via DFT-D3(BJ)[13] correction term. All electron def2-tzvpp basis sets of Ahlrichs groups were used with corresponding density-fitting basis sets.[14] The default value for the SP SCF convergence was adopted. The "Integral(grid=ultrafine)" option was used for evaluation of the exchange-correlation term.

Solvent effects. Electrostatic and non-electrostatic solvent effects were estimated by means of SMD[15] solvation model as implemented in Gaussian 09 code. The internal program values for toluene (dielectric constant, etc.) were adopted. A standard state corresponding to 1M ideal dilute solution was used.

8.2 Mechanism of the first organic transformation (Formylation of *N*-methylaniline)



Following the literature[16] we have considered the two mechanisms for the organic transformation above: concerted mechanism and stepwise addition/elimination, see Figure S5. The free energy barrier for the concerted mechanism was found to be 33.3 kcal/mol. The stepwise addition/elimination mechanism turned out to be not much easier. Thus, the first and the second free energy barriers associated the addition/elimination mechanism were calculated to be 41.1 and 30.1 kcal/mol correspondingly relative to the energy of infinitely separated reactants. This indicates non-catalysed process of aminolysis of esters as relatively difficult process which is in line with previous observations.[16]

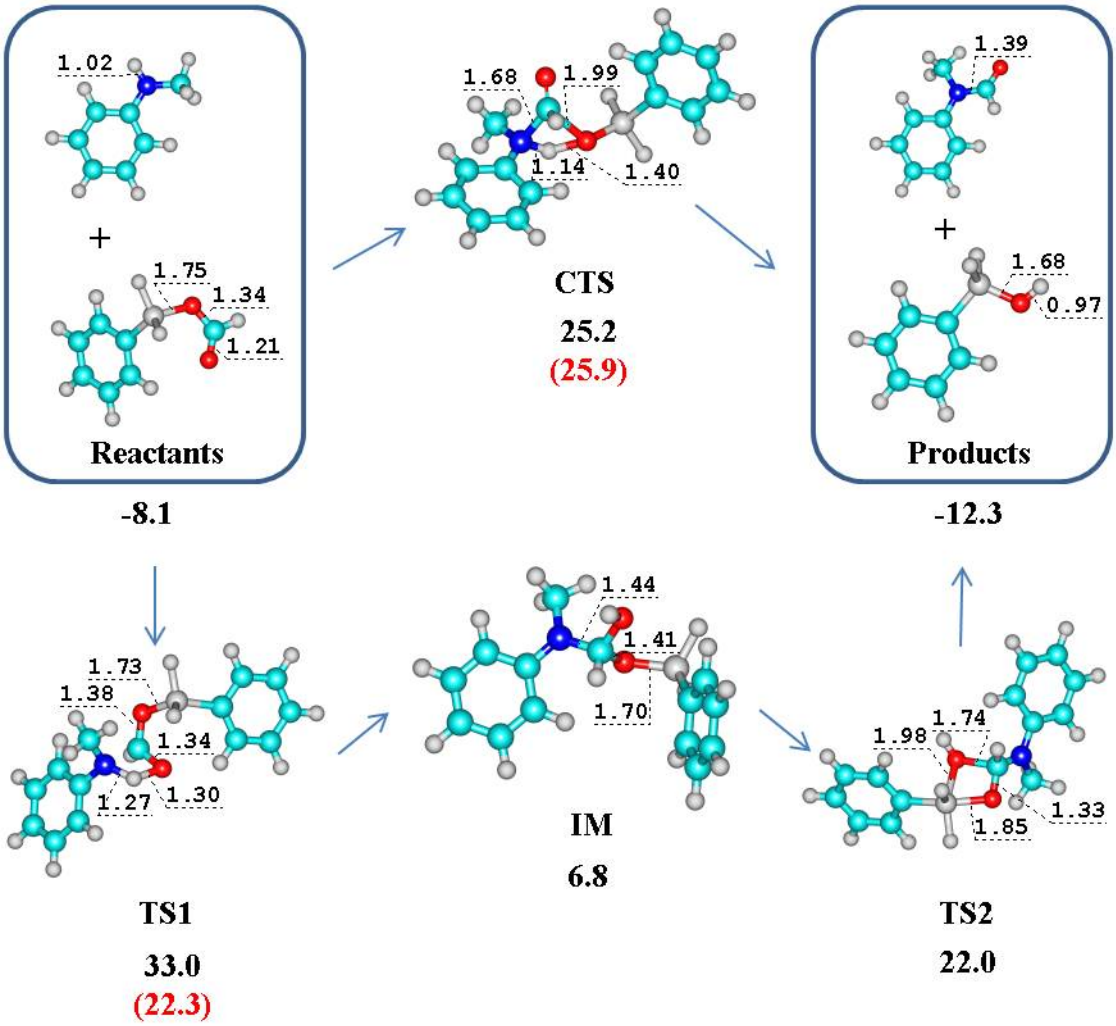


Figure S5. PBE/L1 optimised structures along the addition/elimination and concerted mechanisms for the first organic transformation. All the distances are in Angstroms. All the relative Gibbs free energies are in kcal/mol. The values in red are obtained for catalytic assistance of another amine molecule. Colour coding: H (gray), O (red), Si (gray), C (cyan), N (blue).

We also checked the possible catalytic effect of the second amine molecule on the aminolysis process as suggested in ref.16. Perhaps surprisingly, but when assisted with the second amine molecule the transition state (Figure S6) for concerted mechanism turned out to be 34.0 kcal/mol, i.e. 0.7 kcal/mol higher comparing non-catalytic process. On the other hand, the second amine molecule significantly reduced the barrier for the rate-limiting first transformation in the addition/elimination mechanism (Figure S7) which became 30.4 kcal/mol instead of 41.1 kcal/mol. That probably means that the second amine molecule acting as catalyst significantly the hydrogen addition process and does not affect the COH transfer in concerted mechanism. Eventually, we estimate the overall free energy barrier associated with the organic transformation above to be 30.4 kcal/mol.

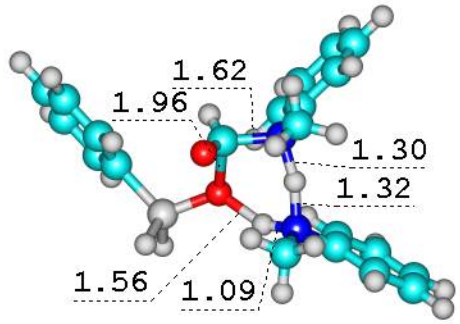


Figure S6. PBE/L1 optimised structure of the concerted transition state with second amine molecule assisting transformation. All the distances are in Angstroms. Color coding: H (gray), O (red), Si (gray), C (cyan), N (blue).

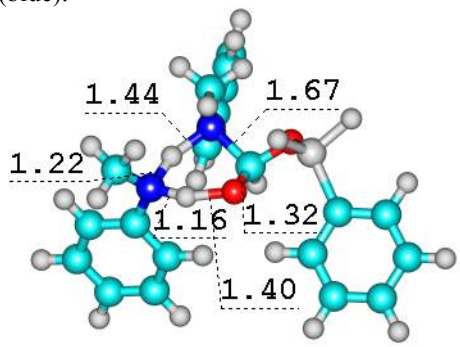
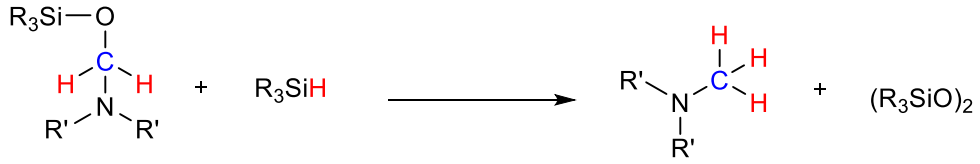


Figure S7. PBE/L1 optimised structure of the first (rate-limiting) transition state along addition/elimination pathway with second amine molecule assisting transformation. All the distances are in Angstroms. Color coding: H (gray), O (red), Si (gray), C (cyan), N (blue).

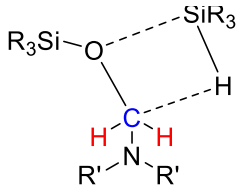
8.3 Mechanism of the second organic transformation (reduction with hydrosilanes)



The above transformation, the reduction of R_3-Si-O-CH_2-NR'$_2$ with phenylsilane, is not trivial and can occur via several mechanisms.

8.3.1 Non-catalysed mechanism

First, the concerted mechanism with the only one transition state in which simultaneous breaking of Si – H and C – O and formation Si – O and C – H bonds occur as in σ-bond metathesis (Scheme S1) may be proposed. However, all our attempts to locate this transition state were not successful indicating that transformation occurs via another probably more complex mechanism.



Scheme S1. Putative structure for transition state for reduction with hydrosylanol in σ-bond metathesis fashion.

After detailed scan of the potential energy surface (PES) along rupture of Si – H and C – O bond the transition state leading to the reactants and products has been located, see Figure S8. The structure has one imaginary frequency (*i*174 cm^{-1}) which corresponds to formation/breaking of C – O bond and moving hydride to/apart from CH_2 group. To understand the mechanism the intrinsic reaction coordinate (IRC) calculations were performed, see Figure S8.

The reaction starts from weak complex of hydrosilane denoted as "**R**" (reactants) in Figure S8. Since silanes are known to be not intrinsically nucleophilic they interact only with very electrophilic functional groups that have carbocationic character. Perhaps the only possibility to form carbocation in R_3-Si-O-CH_2-N(R')$_2$ is to elongate C – O bond and form $^{+}CH_2$–N(R')$_2$ cation and $^{-}$O–Si–R_3 counter anion. Indeed, this structure termed "**CC**" (carbocation) is formed on IRC profile. In this structure the C – O and Si – O bond get longer comparing to their initial values in the starting complex by 0.16 Å and 0.13 Å respectively while Si – O distance from upcoming hydrosylanol gets 1.92 Å which is much shorter comparing to its initial value in the weak complex. Then, in the transition state structure (TS) the C – O bond is completely broken while both Si – O distances are significantly shorter than in CC structure. The CH_2 group has a planar structure and essentially the double bond is formed with N atom indicating that the carbocataion is stabilized by nitrogen lone pair. Finally, the transition state beaks down to the products ("**P**") via hydride transfer from Si to CH_2 group.

The reaction barrier estimated with the transition state above was estimated to be 35.4 kcal/mol. This indicates that the final organic transformation if non-catalysed (see below) is the rate-limiting step in the catalytic cycle and is probably responsible for the harsh experimental conditions.

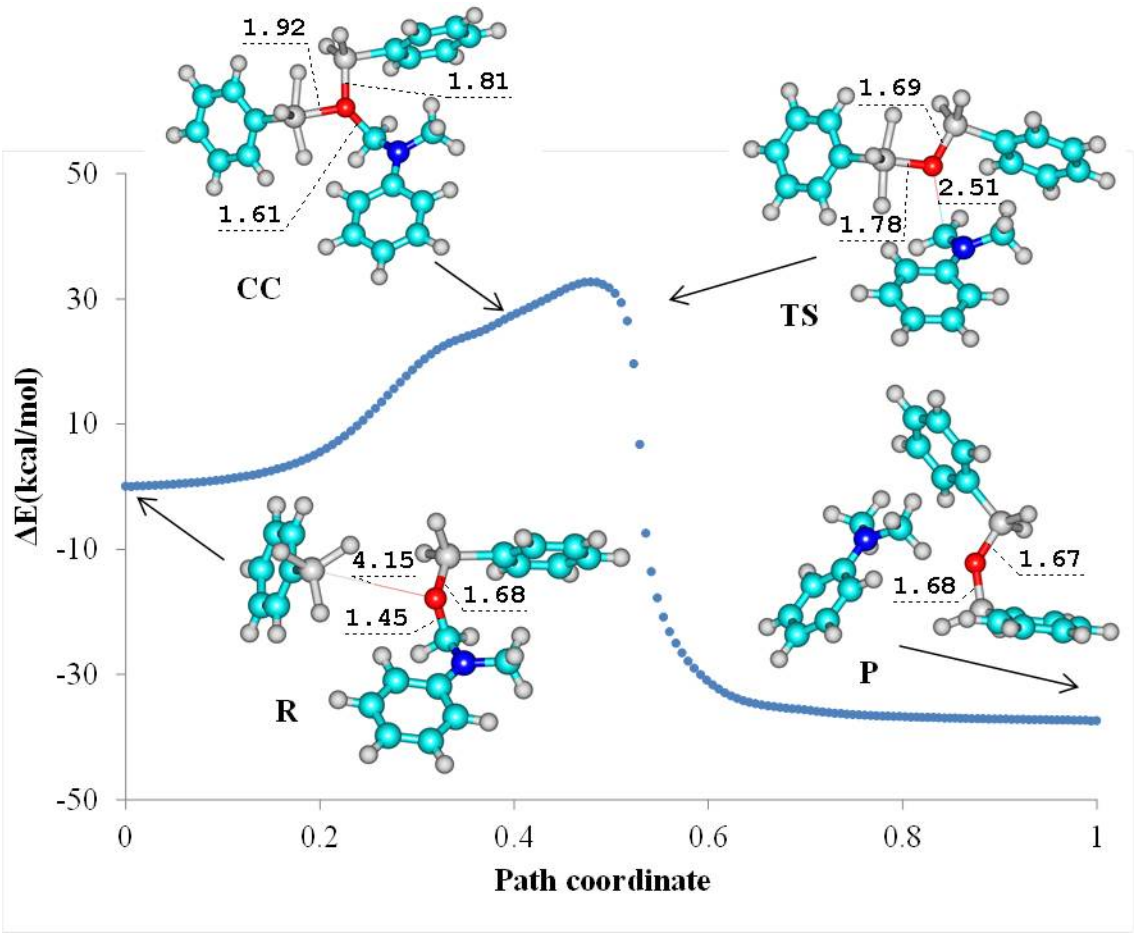


Figure S8. Intrinsic reaction coordinate (IRC) profile of the second organic transformation (hydrosilane reduction). The path coordinate is the normalize reaction coordinate, and is equal to zero (unity) for the weakly bound long-distance complex of initial hydrosilane and R_3-Si-O-CH_2-N(R')$_2$ (the weakly bound, long- distance complex of $(R_3SiO)_2$ and N(Ph)$(CH_3)_2$). Color coding: H (gray), O (red), Si (gray), C (cyan), N (blue).

8.3.2 Catalysis by [Cu(H)(NHC)]

In fact the above transformation, the reduction of $R_3SiO\text{-}CH_2\text{-}NR'_2$ can also be done with [Cu(H)(NHC)] forming $CH_3\text{-}NR'_2$ and [Cu($OSiR_3$)(NHC)]. The latter can be further reduced by hydrosilane to form [Cu(H)(NHC)] again and R_3SiOH.

The found transition states for this process both for NHC=IMes (*i*130 cm^{-1}) and IPr (*i*139 cm^{-1}) are given in Figure S9. The imaginary frequency corresponds to breaking of CH_2-O bond in $R_3SiO\text{-}CH_2N(R')_2$ and formation Cu-$OSiR_3$ bond and $CH_2\text{-}NR_2$' carbocation. The associated Gibbs free energy barriers are 26.4 and 28.6 kcal/mol for IMes and IPr NHC ligands, correspondingly.

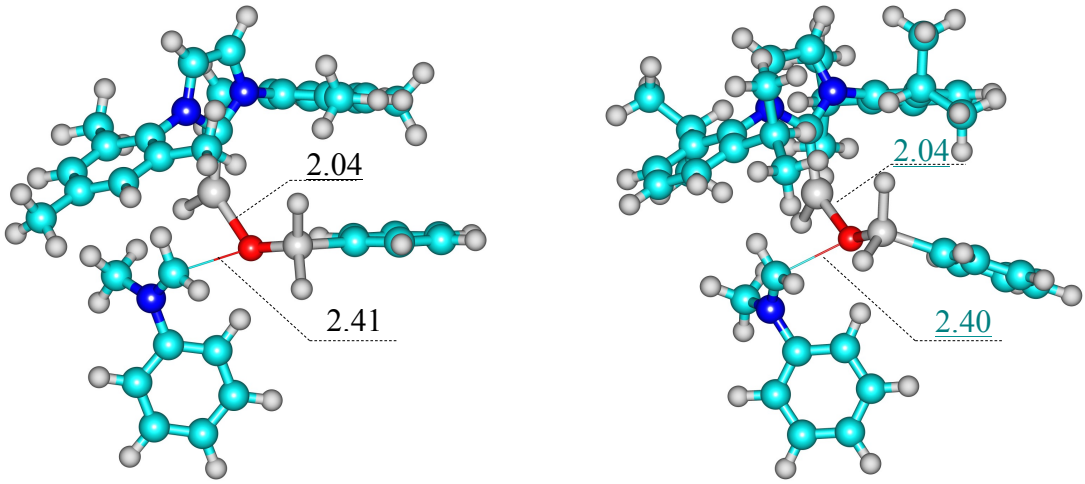


Figure S9. PBE/L1 optimised structure of the transition states for reduction of $R_3SiO\text{-}CH_2NR'_2$ with [Cu(H)(NHC)] (NHC=IMes (left) and NHC=IPr (right)). All the distances are in Angstroms. Color coding: H (gray), O (red), Si (gray), C (cyan), N (blue).

8.4 Energies (a.u.) and Cartesian coordinates (Å) of the individual compounds investigated in the present work

IMesCu-O-tBu

Multiplicity: 1
E (PBE/L1, Priroda)= -2811.56644850 (a.u.)
Thermal correction to Gibbs free energy= 0.438354634115 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -2796.561855

(a.u.)
DFT-D3(BJ) correction to PBE= -0.08491190 (a.u.)

Cu	0.73143783	-0.40735622	-0.38189259
N	-1.63477685	0.89132123	0.64701400
N	-0.26925498	0.37133889	2.23629924
C	-0.41254539	0.30004790	0.86985090
C	1.96768390	0.72078085	3.17279347
C	-1.94138723	2.21932359	-1.38936773
C	-2.21737944	1.05035929	-0.66137862
C	0.85815871	-1.46154579	3.40761454
C	-2.22569019	1.31317951	1.83421160
C	-3.04498704	0.03285288	-1.16358659
C	3.08046596	-1.10251857	4.36501849
C	-1.36534221	0.98510552	2.83590164
C	3.05758303	0.21215606	3.88659439
C	1.97311816	-1.92082401	4.11616535
C	-3.60901620	0.21808617	-2.43011896
C	-3.36410332	1.36822255	-3.18863552
C	-2.53033860	2.35503399	-2.65076902
C	0.87552467	-0.13366895	2.95102695
C	-3.95433791	1.52386733	-4.56816356
H	-3.27336399	1.10819002	-5.33058032
H	-4.91381298	0.99156985	-4.65587574
H	-4.12065258	2.58348669	-4.81561510
C	-3.28622648	-1.23325426	-0.38360830
H	-4.01346303	-1.87476885	-0.90167947
H	-2.34428852	-1.79837596	-0.27059530
H	-3.66337491	-1.02637891	0.63072979
C	-1.01159188	3.27428240	-0.84889710
H	-1.31791579	3.61953239	0.15154700
H	0.01157472	2.87004268	-0.75345947
H	-0.97811357	4.14285050	-1.52215405
C	-0.30478161	-2.37333966	3.11397854
H	-0.38309413	-2.55613739	2.02790556
H	-0.17415035	-3.34187575	3.61764430
H	-1.26280614	-1.93713199	3.43923116
C	1.98241486	2.12638973	2.63058289
H	1.99050051	2.11067516	1.52656986
H	1.09207191	2.69671492	2.94022991
H	2.87766534	2.66443829	2.97387101
C	4.28601848	-1.63655155	5.09780348
H	4.00378028	-2.42287693	5.81454029
H	5.00674671	-2.07793694	4.38798194
H	4.80855691	-0.83759174	5.64580871
H	-3.19375911	1.80304015	1.85270587
H	-1.42737684	1.12902719	3.90966098
H	-4.25621357	-0.56589772	-2.83662968
H	-2.32488713	3.26005190	-3.23171126
H	1.97567049	-2.95355488	4.47969477
H	3.91710688	0.86534661	4.06894283
O	1.91026452	-1.11936623	-1.51705698
C	1.76148785	-1.19318387	-2.92185637
C	0.51827982	-2.02685192	-3.29425070
H	0.41488340	-2.15399877	-4.38628851
H	0.58838564	-3.02255498	-2.82619920
H	-0.38934477	-1.52950599	-2.90884808
C	1.63588235	0.21796274	-3.53163119
H	1.58250709	0.19079242	-4.63426792
H	0.72446098	0.70786785	-3.14561652
H	2.50491190	0.82724240	-3.23329568
C	3.02808974	-1.88179192	-3.46903903
H	3.12645977	-2.88360665	-3.02120828
H	2.99902033	-1.98447377	-4.56675710

R3Si-O-tBu

Multiplicity: 1
E (PBE/L1, Priroda)= -755.68052256 (a.u.)
Thermal correction to Gibbs free energy= 0.185570977817 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -754.8892456 (a.u.)
DFT-D3(BJ) correction to PBE= -0.03031877 (a.u.)

O	-0.42949998	0.32405886	-0.74972825
C	-1.38994482	0.26387314	-1.83688543
C	-2.49868570	-0.72749814	-1.46090411
H	-3.27486497	-0.75922597	-2.24236271
H	-2.08934506	-1.74300268	-1.33994273
H	-2.96819737	-0.42626147	-0.51182218
C	-1.95255134	1.68398147	-1.95990225
H	-2.71645928	1.73313373	-2.75165429
H	-2.41238246	1.99145537	-1.00821791
H	-1.14583145	2.39260860	-2.20264912
C	-0.69961811	-0.15501993	-3.14106210
H	-0.27303240	-1.16898233	-3.05417949
H	-1.41968789	-0.16356206	-3.97495310
H	0.11320395	0.54574386	-3.38822267
Si	0.79666203	-0.76028137	-0.39594483
H	0.33029133	-2.19224320	-0.48503592
H	1.96814222	-0.62388779	-1.33303960
C	1.34143647	-0.35176009	1.36097729
C	0.63268657	0.56898205	2.15060682
C	2.47161071	-0.98034966	1.91248441
C	1.04177718	0.85199472	3.45601913
C	2.88051443	-0.70106824	3.21762078
C	2.16405011	0.21606433	3.99148960
H	-0.24415617	1.06745190	1.72731738
H	3.04636352	-1.69710183	1.31431862
H	0.48170142	1.57184565	4.05938425
H	3.76177793	-1.19761019	3.63283507

R3Si-H

Multiplicity: 1
E (PBE/L1, Priroda)= -523.27400467 (a.u.)
Thermal correction to Gibbs free energy= 0.0781874681285 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -522.5723243 (a.u.)
DFT-D3(BJ) correction to PBE= -0.01539031 (a.u.)

H	0.15141727	-2.34248694	-2.34264544
Si	0.74551590	-2.16618597	-0.97520644
H	0.30125588	-3.31776488	-0.11668376
H	2.24358644	-2.20819887	-1.06906119
C	0.18581414	-0.51376828	-0.24459760
C	-1.00671587	0.09767270	-0.67088545
C	0.94297306	0.12723857	0.75277360
C	-1.43415175	1.30437947	-0.11264981
C	0.51883664	1.33436457	1.31125943
C	-0.67190827	1.92405711	0.87993989
H	-1.61126013	-0.37371818	-1.45265841
H	1.88147414	-0.31981709	1.09729460
H	-2.36394174	1.76518470	-0.45707666
H	1.12106988	1.81893034	2.08454257

IMesCu-H

Multiplicity: 1
E (PBE/L1, Priroda)= -2579.16168343 (a.u.)

Thermal correction to Gibbs free energy= 0.332882776645 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -2564.25505058 (a.u.)
DFT-D3(BJ) correction to PBE= -0.06865992 (a.u.)

Cu	1.23796084	-0.80755639	-1.32381076
N	-1.16017201	0.56207755	-0.28363808
N	0.19741893	0.04400118	1.30444451
C	0.05527196	-0.03529556	-0.05864080
C	2.42898710	0.39374824	2.25563140
C	-1.48179640	1.89339604	-2.31618733
C	-1.74774814	0.72047281	-1.59138804
C	1.32171901	-1.79111303	2.47768988
C	-1.75108459	0.99566674	0.89935594
C	-2.57500595	-0.29822704	-2.09090514
C	3.53456184	-1.42871796	3.45589183
C	-0.89284281	0.66784001	1.90354918
C	3.51337497	-0.11361548	2.97864156
C	2.43133167	-2.24892107	3.19552641
C	-3.15335228	-0.10768536	-3.35001677
C	-2.92167584	1.04791672	-4.10399906
C	-2.08516929	2.03427308	-3.57001922
C	1.34047537	-0.46247361	2.02378497
C	-3.52776122	1.20939273	-5.47589693
H	-2.85352291	0.80042264	-6.24816638
H	-4.48613848	0.67394619	-5.55649634
H	-3.70048486	2.26975692	-5.71581127
C	-2.80260288	-1.57085146	-1.31751678
H	-3.53480789	-2.21017110	-1.83131756
H	-1.85792772	-2.13476776	-1.22316833
H	-3.16727693	-1.37377024	-0.29669924
C	-0.54905421	2.94899768	-1.78166481
H	-0.84383719	3.28967726	-0.77623811
H	0.47682855	2.54882991	-1.70208152
H	-0.52694888	3.82065856	-2.45141204
C	0.16497104	-2.70629928	2.17126286
H	0.09963600	-2.88888988	1.08420315
H	0.29375685	-3.67484108	2.67543245
H	-0.79804434	-2.27410148	2.48694263
C	2.44787578	1.79964672	1.71425848
H	2.46610400	1.78479167	0.61044717
H	1.55546641	2.37050096	2.01677808
H	3.34018055	2.33747796	2.06551580
C	4.73407116	-1.96096837	4.19980195
H	4.44662215	-2.74881076	4.91281580
H	5.46288742	-2.40001775	3.49672680
H	5.24950501	-1.16157766	4.75391673
H	-2.71648359	1.49126614	0.91430503
H	-0.95378539	0.81790810	2.97667383
H	-3.80111339	-0.89223009	-3.75445726
H	-1.88880452	2.94302915	-4.14822354
H	2.43279111	-3.28228238	3.55725261
H	4.36997879	0.54106644	3.16925336

CO2

Multiplicity: 1
E (PBE/L1, Priroda)= -188.58479636 (a.u.)
Thermal correction to Gibbs free energy= -0.00995314890362 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -188.479212351 (a.u.)
DFT-D3(BJ) correction to PBE= -0.00093617 (a.u.)

C	0.00000002	-0.00000000	0.00000002
O	0.55254426	-0.12699402	1.02421690

IMesCu-O-COH

Multiplicity: 1
E (PBE/L1, Priroda)= -2767.78149513 (a.u.)
Thermal correction to Gibbs free energy= 0.34755290668 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -2752.77100793 (a.u.)
DFT-D3(BJ) correction to PBE= -0.07382069 (a.u.)

Cu	1.01863780	-0.68401337	-1.11425747
N	-1.39850275	0.52853311	-0.08560024
N	-0.04087190	-0.02815085	1.49708578
C	-0.20647898	-0.11004074	0.13881058
C	2.29765512	0.22431604	2.19575970
C	-1.47977569	1.76459149	-2.20354461
C	-1.96814262	0.72220326	-1.39702183
C	1.01569078	-1.77547922	2.84894675
C	-1.95378790	0.99934036	1.09955117
C	-2.99525688	-0.13912753	-1.81827136
C	3.33949228	-1.52033964	3.56449599
C	-1.09723714	0.64848909	2.09786876
C	3.39456373	-0.29416276	2.89465161
C	2.14205329	-2.24455963	3.53114704
C	-3.54588068	0.07447585	-3.08533400
C	-3.09541872	1.10214106	-3.92215987
C	-2.06738198	1.93160254	-3.46336811
C	1.11567115	-0.53610885	2.19437483
C	-3.68154210	1.28866467	-5.29956008
H	-3.12414006	0.69249337	-6.04258965
H	-4.73273282	0.96395802	-5.33588957
H	-3.63141098	2.34151488	-5.61657202
C	-3.46761979	-1.27968522	-0.95246712
H	-4.26845950	-1.83942406	-1.45649975
H	-2.63970049	-1.97764030	-0.74125656
H	-3.85190093	-0.93120022	0.01981154
C	-0.34925854	2.65583845	-1.76071999
H	-0.45640154	2.96177055	-0.70829471
H	0.62478397	2.13656336	-1.85287574
H	-0.30867973	3.56020037	-2.38497681
C	-0.24963381	-2.59358219	2.79187578
H	-0.50176036	-2.84966937	1.74879151
H	-0.12835059	-3.52965833	3.35557405
H	-1.11360469	-2.05123394	3.20886299
C	2.40846243	1.53186598	1.45630018
H	2.53312737	1.36272698	0.36880484
H	1.51060656	2.15537477	1.58886883
H	3.28219304	2.09774134	1.81087618
C	4.55178853	-2.06612684	4.27732986
H	4.26436627	-2.70032346	5.12994899
H	5.15853721	-2.68448039	3.59343753
H	5.19656022	-1.25505983	4.64871969
H	-2.89199264	1.54409098	1.11878156
H	-1.13346044	0.82439610	3.16796279
H	-4.34788235	-0.58698559	-3.42886641
H	-1.70356262	2.74034440	-4.10529183
H	2.08145378	-3.20860061	4.04662318
H	4.32324439	0.28528998	2.91153150
O	2.32917716	-1.08333828	-2.37932834
C	3.05334883	-0.02840190	-2.62936553
O	2.94009381	1.09565648	-2.13631357

IMesCu-O-H

Multiplicity: 1
E (PBE/L1, Priroda)= -2654.43624214 (a.u.)
Thermal correction to Gibbs free energy= 0.338427619837 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -2639.48409349 (a.u.)
DFT-D3(BJ) correction to PBE= -0.06980824 (a.u.)

Cu	1.17972533	-0.71593368	-1.21975628
N	-1.20961372	0.58466080	-0.21836719
N	0.14666057	0.06241367	1.37753119
C	0.01152813	-0.00723757	0.00987528
C	2.37601258	0.42074539	2.32868217
C	-1.52848164	1.92381772	-2.24512353
C	-1.79234176	0.74672925	-1.52602849
C	1.27780767	-1.76879307	2.54825809
C	-1.80676913	1.00532856	0.96674246
C	-2.61504163	-0.27214414	-2.03317044
C	3.49130870	-1.40016724	3.52208744
C	-0.95187441	0.67606948	1.97238016
C	3.46399666	-0.08398994	3.04807139

C	2.39068475	-2.22415278	3.26256179
C	-3.18968571	-0.07846531	-3.29365142
C	-2.95946360	1.08149554	-4.04170733
C	-2.12751524	2.06816557	-3.50080300
C	1.29012960	-0.43906217	2.09693165
C	-3.56464102	1.24866479	-5.41356797
H	-2.88994332	0.84559735	-6.18860110
H	-4.52195059	0.71178708	-5.49743729
H	-3.73977313	2.30990934	-5.64778849
C	-2.84211023	-1.54670416	-1.26287358
H	-3.56356475	-2.19182915	-1.78463758
H	-1.89366786	-2.10198238	-1.15576320
H	-3.21985162	-1.35143223	-0.24644865
C	-0.60184407	2.97917931	-1.69997579
H	-0.91454759	3.32582641	-0.70193431
H	0.42025060	2.57421974	-1.59766107
H	-0.56401998	3.84728368	-2.37367831
C	0.12292127	-2.68669175	2.24227021
H	0.05285547	-2.86334781	1.15463815
H	0.25738958	-3.65737269	2.74085233
H	-0.83993142	-2.25906261	2.56470748
C	2.38721771	1.82739863	1.78915648
H	2.39421417	1.81324067	0.68516447
H	1.49635934	2.39564411	2.10131345
H	3.28198952	2.36641531	2.13227014
C	4.69526928	-1.92989085	4.26061089
H	4.41319745	-2.72081205	4.97238805
H	5.42322334	-2.36415520	3.55369617
H	5.20954418	-1.13006889	4.81519820
H	-2.77577403	1.49352210	0.98069138
H	-1.01980338	0.81818304	3.04603247
H	-3.83543010	-0.86239397	-3.70272704
H	-1.93314371	2.98069015	-4.07386526
H	2.39726334	-3.25847911	3.62153041
H	4.31897480	0.57320009	3.23740148
O	2.36580674	-1.42211495	-2.34479209

R2-N-CH3

Multiplicity: 1
E (PBE/L1, Priroda)= -365.99103426 (a.u.)
Thermal correction to Gibbs free energy= 0.134738972463 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -365.875134596 (a.u.)
DFT-D3(BJ) correction to PBE= -0.02035142 (a.u.)

C	1.51392941	-0.23931128	-1.97191926
C	0.25912245	-0.36329612	-1.37998082
C	2.59057228	0.31606574	-1.27733878
H	-0.55189358	-0.81108329	-1.95518523
H	3.57171594	0.40869763	-1.74775332
C	0.03342334	0.08081274	-0.05412075
C	2.38406621	0.74298626	0.03607404
H	3.21132510	1.17340705	0.60757220
C	1.13683668	0.62751895	0.64558982
H	1.02176720	0.96525193	1.67603249
H	1.64848609	-0.59088951	-2.99881303
N	-1.22000457	-0.00944027	0.53318417
C	-1.36586353	0.26578726	1.95191336
H	-2.42572557	0.16966852	2.22513111
H	-0.77919191	-0.42500723	2.59079938
H	-1.05570027	1.29780279	2.19075188
C	-2.27038774	-0.75736798	-0.13553484
H	-2.49385524	-0.32897137	-1.12787581
H	-2.02003107	-1.82881359	-0.27305375

R2-N-COH

Multiplicity: 1
E (PBE/L1, Priroda)= -440.04449058 (a.u.)
Thermal correction to Gibbs free energy= 0.116682655533 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -439.885100802 (a.u.)
DFT-D3(BJ) correction to PBE= -0.02024009 (a.u.)

C	0.80950967	0.54622814	-2.16133698
C	-0.23554146	0.33779600	-1.26209565
C	2.13608133	0.36584032	-1.76480670
H	-1.26795935	0.46469048	-1.59325467
H	2.95164686	0.52810624	-2.47307980
C	0.03395978	-0.04784846	0.06150024
C	2.40873953	-0.00500696	-0.44649348
H	3.44278717	-0.12317279	-0.11273365
C	1.37264959	-0.19491414	0.46703263
H	1.60401491	-0.42261608	1.50953404
H	0.58008942	0.84669283	-3.18689967
N	-1.02527501	-0.26587759	0.97545353
C	-2.25907859	0.51254534	0.87861731
H	-2.89006087	0.18253376	0.03628220
H	-2.81054681	0.34202310	1.81395520
H	-2.02301199	1.58018002	0.76096898
C	-0.96703722	-1.27508883	1.92406980
O	-1.82772676	-1.50058310	2.75372744

R2-N-H

Multiplicity: 1
E (PBE/L1, Priroda)= -326.71769609 (a.u.)
Thermal correction to Gibbs free energy= 0.109909484957 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -326.615313608 (a.u.)
DFT-D3(BJ) correction to PBE= -0.01647508 (a.u.)

C	0.98218804	-0.35301303	-2.07646507
C	-0.25608871	-0.43362322	-1.45031495
C	2.10384829	0.12322221	-1.38772999
H	-1.12612947	-0.80362950	-2.00316945
H	3.07493042	0.18696820	-1.88313704
C	-0.41375635	-0.03965295	-0.10269842
C	1.95686129	0.51203275	-0.05582286
H	2.82069908	0.88401430	0.50231994
C	0.72109393	0.43289164	0.58827242
H	0.63835144	0.73860811	1.63300652
H	1.07325884	-0.66669008	-3.12012553
N	-1.66497949	-0.09680005	0.48873082
H	-2.33197229	-0.69980476	0.01298979
C	-1.84508669	0.02281260	1.92217607
H	-2.90291760	-0.15880541	2.16054322
H	-1.22892046	-0.69141000	2.50518859

R3Si-O-COH

Multiplicity: 1
E (PBE/L1, Priroda)= -711.87700923 (a.u.)
Thermal correction to Gibbs free energy= 0.0921511664967 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -711.074922619 (a.u.)
DFT-D3(BJ) correction to PBE= -0.01980638 (a.u.)

O	-0.29651805	0.85564403	-2.77752253
Si	-0.19820606	-0.64856859	-1.89333641
H	-1.46353386	-1.40463988	-2.14469896
H	0.97136293	-1.29677001	-2.56142286
C	0.17581931	-0.42945001	-0.06715388
C	-0.81810198	-0.06193280	0.86064186
C	1.48022926	-0.67181899	0.40328368
C	-0.51268194	0.05805373	2.21647191
C	1.78488072	-0.55000788	1.76052763
C	0.78763296	-0.18599816	2.66759609
H	-1.83277872	0.14492177	0.50964131
H	2.26819078	-0.96087600	-0.29990267
H	-1.29316969	0.34369088	2.92661949
H	2.80272864	-0.74045153	2.11097955
H	1.02405776	-0.09170746	3.73089403
C	-1.34997923	1.65391696	-2.53256519
O	-2.22343455	1.43430903	-1.72534282

R3Si-OH

Multiplicity: 1

E (PBE/L1, Priroda)= -598.55204301 (a.u.)
Thermal correction to Gibbs free energy= 0.0859798890872 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -597.811952836 (a.u.)
DFT-D3(BJ) correction to PBE= -0.01659244 (a.u.)

O	-1.90092898	0.48499808	-2.37525740
Si	-0.56105606	-0.49984401	-2.11224149
H	-0.90742174	-1.95671832	-2.27914165
H	0.54468751	-0.19178746	-3.08851903
C	-0.01633374	-0.14419002	-0.34734370
C	-0.69003210	0.80439627	0.44066081
C	1.07698319	-0.82908523	0.21153761
C	-0.27990570	1.06133467	1.75113295
C	1.48816626	-0.57295921	1.52040827
C	0.80891630	0.37405982	2.29190735
H	-1.54256651	1.34318946	0.01698839
H	1.61805640	-1.57586348	-0.38104826
H	-0.81241761	1.80268437	2.35327976
H	2.34034895	-1.11329683	1.94141495
H	1.12971955	0.57542900	3.31755020

R3-Si-O-Si-R3

Multiplicity: 1
E (PBE/L1, Priroda)= -1120.68757265 (a.u.)
Thermal correction to Gibbs free energy= 0.167831304182 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -1119.24488814 (a.u.)
DFT-D3(BJ) correction to PBE= -0.03698662 (a.u.)

O	-1.92910931	1.66292822	-0.44414134
Si	-1.51376256	0.84950164	-1.85160897
C	-1.22019760	-0.99178253	-1.56665310
C	-2.30211456	-1.88424983	-1.44338188
C	0.08443452	-1.50801971	-1.45767177
C	-2.08860511	-3.24444624	-1.21445665
C	0.30147666	-2.86888531	-1.23039580
C	-0.78538981	-3.73777208	-1.10770554
H	-3.32808935	-1.51078322	-1.53123540
H	0.94328633	-0.83538754	-1.55208133
H	-2.94022993	-3.92391299	-1.12228003
H	1.32182319	-3.25382159	-1.15149702
H	-0.61696100	-4.80370706	-0.93212253
Si	-1.46253027	1.71497561	1.16659966
H	-2.04316151	0.53819000	1.89603227
H	-2.01877175	3.00020213	1.70086313
C	0.41129049	1.68888136	1.38089031
C	1.08309371	0.50255605	1.72973282
C	1.17658079	2.85356888	1.18068494
C	2.47234401	0.47935217	1.87186228
C	2.56517336	2.83330824	1.32036466
C	3.21425008	1.64492706	1.66621916
H	0.51074583	-0.41639245	1.89381035
H	0.67891018	3.79255170	0.91526000
H	2.97808128	-0.45013184	2.14717737
H	3.14411919	3.74748214	1.16367054
H	4.30153722	1.62894168	1.78009892
H	-2.67434774	1.04259138	-2.78026416

IPrCu-H

Multiplicity: 1
E (PBE/L1, Priroda)= -2814.84863553 (a.u.)
Thermal correction to Gibbs free energy= 0.493752231005 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -2799.86394673 (a.u.)
DFT-D3(BJ) correction to PBE= -0.09937892 (a.u.)

Cu	1.27673057	-0.79209503	-1.42699244
N	-1.11871956	0.52498379	-0.30560171
N	0.28145083	-0.00302004	1.24173894
C	0.10679371	-0.06634736	-0.11902323
C	2.53458692	0.36181199	2.14264829
C	-1.49252960	1.87623639	-2.31946658
C	-1.74712308	0.69443947	-1.59624507
C	1.44045159	-1.84526948	2.37541526
C	-1.68245641	0.93970986	0.89653508
C	-2.59484794	-0.32515355	-2.07213291
C	3.66084278	-1.46224362	3.29164587
C	-0.79706085	0.60599118	1.87493245
C	3.64127723	-0.14751923	2.83365189
C	2.57381689	-2.30103453	3.06064552
C	-3.20640901	-0.12487071	-3.31613961
C	-2.98134368	1.03681486	-4.04998446
C	-2.13067942	2.02293611	-3.55760669
C	1.44649918	-0.50802528	1.93243528
C	-2.80550789	-1.62983513	-1.31602367
H	-2.37341110	-1.50856670	-0.30934947
C	-0.52025456	2.94014931	-1.82855501
H	-0.25606481	2.69855171	-0.78616028
C	0.28917308	-2.79724194	2.08133535
H	-0.54635375	-2.20040986	1.68074537
C	2.56009117	1.78285076	1.59647937
H	1.54562646	2.02384014	1.23927904
H	-2.65019468	1.42848917	0.94050017
H	-0.83112028	0.74255165	2.95082274
H	-3.86478425	-0.89826653	-3.71937894
H	-1.95044637	2.92413950	-4.14890137
H	2.60619654	-3.33503428	3.41283538
H	4.50580913	0.49751295	3.00894785
H	2.20844422	-1.36882199	-2.46908615
H	-3.46780695	1.17135220	-5.01959763
H	4.53557170	-1.83943322	3.82781172
C	-4.29469040	-1.97570943	-1.14219679
H	-4.78407033	-2.16723969	-2.11078585
H	-4.39892426	-2.88909578	-0.53432643
H	-4.84218704	-1.16242674	-0.64002506
C	-2.04026018	-2.77192050	-2.01243813
H	-0.96551607	-2.53253547	-2.09343985
H	-2.14751308	-3.70940966	-1.44254686
H	-2.42753052	-2.94169658	-3.03059509
C	0.77866000	2.89101669	-2.65624058
H	1.50566288	3.62580140	-2.27323653
H	1.23672009	1.88767328	-2.60833857
H	0.58017222	3.12339082	-3.71551615
C	-1.13889000	4.34904747	-1.83524130
H	-1.38367473	4.68124019	-2.85704718
H	-2.06202487	4.38698422	-1.23543882
H	-0.42374979	5.07472282	-1.41494352
C	-0.21786338	-3.51471705	3.34461744
H	-1.09018454	-4.14059803	3.09562518
H	0.55143044	-4.17714567	3.77324098
H	-0.51950201	-2.79605565	4.12302233
C	0.70240661	-3.80353020	0.98984928
H	1.54163246	-4.43188653	1.33093652
H	-0.14255006	-4.46505366	0.73774526
H	1.02198423	-3.27861917	0.07262995
C	2.93109049	2.82008263	2.67072766
H	2.25089147	2.76601452	3.53547351
H	3.96001756	2.67613510	3.03803415
H	2.87147840	3.83587134	2.24733856
C	3.50756299	1.86452143	0.38380860
H	4.54388506	1.62932074	0.67741787
H	3.20563287	1.14745503	-0.39948378

IPrCu-O-COH

Multiplicity: 1
E (PBE/L1, Priroda)= -3003.46711578 (a.u.)
Thermal correction to Gibbs free energy= 0.505245569862 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -2988.37948055 (a.u.)
DFT-D3(BJ) correction to PBE= -0.10374867 (a.u.)

Cu	1.19404064	-0.60847777	-1.27426365
N	-1.18692154	0.65908861	-0.20735606
N	0.20996246	0.13732207	1.35113530
C	0.05152723	0.10357710	-0.01066113
C	2.45681667	0.49284639	2.27069843

C	-1.56841154	1.99556444	-2.22934719
C	-1.80016449	0.80757137	-1.50812198
C	1.37810113	-1.73083331	2.42897959
C	-1.77896480	1.02460781	0.99582601
C	-2.59739304	-0.24525342	-1.99877749
C	3.60258427	-1.36390901	3.34476758
C	-0.89700106	0.69529871	1.97984918
C	3.57112570	-0.03281796	2.93611066
C	2.51961513	-2.20095310	3.09152386
C	-3.17958380	-0.07163404	-3.26125934
C	-2.97445848	1.09261110	-3.99618417
C	-2.17575955	2.11295149	-3.48559722
C	1.37481682	-0.37832357	2.03480899
C	-2.83129847	-1.53600503	-1.22509910
H	-2.29329658	-1.45719439	-0.26649202
C	-0.66000990	3.10276359	-1.71152815
H	-0.39745631	2.86221170	-0.66846150
C	0.21379727	-2.67450806	2.15839757
H	-0.56867371	-2.10321670	1.63310172
C	2.46350509	1.93718876	1.78792563
H	1.45091485	2.17463080	1.42296166
H	-2.76328195	1.47896394	1.03716747
H	-0.95193910	0.80245674	3.05804915
H	-3.79949779	-0.87041641	-3.67613214
H	-2.01334135	3.01797657	-4.07640404
H	2.55913389	-3.24644378	3.40751547
H	4.43199935	0.61178267	3.13060259
O	2.35773089	-1.29866015	-2.54933672
H	-3.43670736	1.20393338	-4.98045304
H	4.48356027	-1.75416922	3.86094410
C	-4.32623902	-1.72892913	-0.90516915
H	-4.92117229	-1.84485611	-1.82570066
H	-4.46711570	-2.63854616	-0.29904084
H	-4.73441150	-0.87286880	-0.34426558
C	-2.25574667	-2.75223963	-1.97451571
H	-1.16623125	-2.66700039	-2.12117242
H	-2.44672827	-3.67086727	-1.39577518
H	-2.73114095	-2.87333044	-2.96196505
C	0.65159954	3.14068832	-2.51900975
H	1.32773479	3.91297703	-2.11715528
H	1.16826250	2.16714404	-2.47310845
H	0.45745774	3.37187388	-3.57915982
C	-1.35719823	4.47481123	-1.70984848
H	-1.61067218	4.80259315	-2.73089572
H	-2.28726767	4.45275445	-1.12022477
H	-0.68958523	5.23566887	-1.27386962
C	-0.39454524	-3.19607627	3.47463117
H	-1.26686615	-3.83431307	3.25947623
H	0.33266051	-3.80208761	4.03919341
H	-0.72264807	-2.36935265	4.12497705
C	0.63168470	-3.83344755	1.23408720
H	1.43950959	-4.43288838	1.68540084
H	-0.22776035	-4.50251360	1.06395749
H	0.97468750	-3.47071467	0.25093431
C	2.79330622	2.92890247	2.91751107
H	2.09622921	2.82163617	3.76350940
H	3.81628489	2.78330411	3.30027153
H	2.72464652	3.96281956	2.54209055
C	3.43080229	2.09880755	0.59946927
H	4.46631534	1.86718245	0.89794960
H	3.15550382	1.41958067	-0.22501570
H	3.40523858	3.13386728	0.22123519
C	2.14355234	-2.56522705	-2.78374643
O	1.29519434	-3.29100412	-2.26831136

IPrCu-OH

Multiplicity: 1
E (PBE/L1, Priroda)= -2890.12294355 (a.u.)
Thermal correction to Gibbs free energy= 0.498190017848 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -2875.09271079 (a.u.)
DFT-D3(BJ) correction to PBE= -0.10043642 (a.u.)

Cu	1.19553778	-0.75737017	-1.36362747
N	-1.15221596	0.55438802	-0.27917342
N	0.24762174	0.01560248	1.27291266
C	0.07228221	-0.04612757	-0.09112104
C	2.50906482	0.37100890	2.15344294
C	-1.51414513	1.89542999	-2.30147855
C	-1.77772322	0.72059530	-1.56983109
C	1.40623857	-1.83005273	2.39903562
C	-1.71089401	0.97256985	0.92437657
C	-2.62695783	-0.29907731	-2.04356535
C	3.64442078	-1.46297760	3.27804076
C	-0.82848182	0.63335470	1.90273989
C	3.62406710	-0.14635638	2.82506783
C	2.54800315	-2.29440558	3.06437286
C	-3.23690785	-0.10224311	-3.28889901
C	-3.00677486	1.05494585	-4.02826476
C	-2.15078663	2.03887845	-3.54075060
C	1.41270697	-0.49208400	1.95732944
C	-2.85318679	-1.59581472	-1.27846317
H	-2.37344751	-1.49105718	-0.29182955
C	-0.54251320	2.96140744	-1.81401412
H	-0.24527189	2.69895397	-0.78572166
C	0.23735175	-2.77016055	2.13718847
H	-0.59040478	-2.16898995	1.72736461
C	2.52764420	1.80002101	1.62798801
H	1.51691454	2.03340650	1.25586809
H	-2.67534774	1.46749902	0.96879212
H	-0.86366462	0.76922104	2.97855593
H	-3.89785012	-0.87544503	-3.68878520
H	-1.96425819	2.93569118	-4.13700659
H	2.57884139	-3.32893848	3.41563707
H	4.49427365	0.49421966	2.98941233
O	2.21160956	-1.41833990	-2.67008761
H	-3.49182435	1.18668152	-4.99896497
H	4.52629258	-1.84684301	3.79763550
C	-4.34767142	-1.87799578	-1.04192544
H	-4.88500944	-2.03883040	-1.99058049
H	-4.46678844	-2.79039796	-0.43514422
H	-4.83612805	-1.04476689	-0.51226868
C	-2.16576867	-2.77002888	-2.00153178
H	-1.08606614	-2.57904323	-2.12187461
H	-2.29344874	-3.70085213	-1.42472270
H	-2.59872239	-2.92629069	-3.00329958
C	0.73429171	2.95504604	-2.67654933
H	1.45474359	3.69884813	-2.29827619
H	1.21503219	1.96239210	-2.65786498
H	0.50520208	3.20307642	-3.72603472
C	-1.18594754	4.35887077	-1.77077081
H	-1.47229179	4.70494817	-2.77711452
H	-2.08839727	4.36791872	-1.13911024
H	-0.47014157	5.08980645	-1.36054274
C	-0.26899485	-3.44267394	3.42551141
H	-1.15213956	-4.06329848	3.20283760
H	0.49548320	-4.10216264	3.86729457
H	-0.55342734	-2.69674416	4.18448026
C	0.61868575	-3.81358009	1.06964569
H	1.45683440	-4.44262950	1.41229346
H	-0.23881106	-4.47189908	0.85409710
H	0.92105800	-3.31751637	0.13146185
C	2.86438982	2.82068361	2.72965162
H	2.16460928	2.74367442	3.57689267
H	3.88520791	2.67664585	3.11908871
H	2.80537716	3.84404201	2.32481785
C	3.49471581	1.91925854	0.43445720
H	4.52856054	1.68495306	0.73761360
H	3.20576479	1.22309350	-0.37139358
H	3.47947230	2.94480574	0.03057944

IPrCu-O-tBu

Multiplicity: 1
E (PBE/L1, Priroda)= -3047.25218010 (a.u.)
Thermal correction to Gibbs free energy= 0.598111932687 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3032.16950148 (a.u.)
DFT-D3(BJ) correction to PBE= -0.11598214 (a.u.)

Cu	0.83387314	-0.52155684	-0.70447883
N	-1.51548960	0.77890224	0.43122639
N	-0.06365985	0.24300438	1.93615151

C	-0.27957725	0.18952995	0.57689034
C	2.21175098	0.61619325	2.77213107
C	-1.96009713	2.14248411	-1.55765041
C	-2.17880551	0.95048080	-0.83892735
C	1.14770163	-1.60561106	3.00139144
C	-2.04195094	1.17998231	1.65515329
C	-3.01775516	-0.08051243	-1.30629030
C	3.39115415	-1.21419003	3.85598434
C	-1.12687548	0.84189208	2.60340006
C	3.34432370	0.10739445	3.42005075
C	2.30612228	-2.06045478	3.64400349
C	-3.63654393	0.10704456	-2.54881328
C	-3.43213694	1.27031149	-3.28648493
C	-2.60479994	2.27636695	-2.79387227
C	1.12471650	-0.26032761	2.58348653
C	-3.24045718	-1.37020813	-0.52755052
H	-2.75286257	-1.25655947	0.45422359
C	-1.04095538	3.24561050	-1.04995832
H	-0.74017225	2.98450773	-0.02243368
C	-0.00677573	-2.56356513	2.74148161
H	-0.83365848	-1.98123369	2.30369815
C	2.20489283	2.04923959	2.25756138
H	1.19137527	2.26651996	1.88327455
H	-3.01035875	1.66288328	1.73284749
H	-1.13033724	0.96898136	3.68087756
H	-4.28731276	-0.67620196	-2.94589704
H	-2.45109470	3.18468621	-3.38203076
H	2.35944128	-3.10016579	3.97691109
H	4.20805445	0.75837392	3.57745366
O	2.02391371	-1.29327643	-1.78553065
C	2.04146658	-1.34025701	-3.19893255
C	0.65800275	-1.71105959	-3.76684470
H	0.67170075	-1.79465444	-4.86790024
H	0.33065509	-2.67601742	-3.34521170
H	-0.08157566	-0.94206994	-3.48176264
C	2.48296318	0.02382282	-3.76605690
H	2.57787287	0.00422020	-4.86562930
H	1.74470250	0.79603174	-3.49051394
H	3.45477404	0.30780369	-3.33063464
C	3.06819336	-2.42026469	-3.59647264
H	2.76195595	-3.39325064	-3.17970943
H	3.16065946	-2.51591587	-4.69127383
H	4.05440964	-2.16414213	-3.17764916
H	-3.92277819	1.39413238	-4.25539104
H	4.28595616	-1.59085473	4.35826448
C	-4.73529650	-1.63874814	-0.27610707
H	-5.28135509	-1.80498859	-1.21880559
H	-4.85610571	-2.54362362	0.34142156
H	-5.21336934	-0.79627785	0.24837483
C	-2.56738660	-2.55903905	-1.23846379
H	-1.48556950	-2.38054331	-1.35403232
H	-2.70842103	-3.48285004	-0.65357896
H	-2.99762521	-2.71861505	-2.24077436
C	0.24211730	3.31712921	-1.89847665
H	0.91724495	4.09597108	-1.50739836
H	0.77530604	2.35228676	-1.87663043
H	0.01128851	3.55921981	-2.94884733
C	-1.75344153	4.60901329	-0.99357205
H	-2.04462246	4.95622041	-1.99812195
H	-2.66316161	4.56272471	-0.37423158
H	-1.08008359	5.36765875	-0.56259326
C	-0.52572374	-3.20851478	4.03927217
H	-1.39127597	-3.85446196	3.81924296
H	0.24493279	-3.83628597	4.51524630
H	-0.84052990	-2.44641638	4.76973755
C	0.40207466	-3.62932687	1.70674068
H	1.23178193	-4.25014703	2.08269160
H	-0.44978821	-4.29345042	1.48638960
H	0.72862078	-3.15654916	0.76516189
C	2.51934495	3.06732134	3.36817249
H	1.81439887	2.97605530	4.20968983
H	3.53902974	2.93330464	3.76411790
H	2.45071897	4.09259904	2.96956801
C	3.17450849	2.19450720	1.06894141
H	4.21237272	1.98607717	1.37659704
H	2.91019092	1.49156692	0.26104312

TS_IMesCu-O-tBu_R3Si-H

Multiplicity: 1
E (PBE/L1, Priroda)= -3334.84137983 (a.u.)
Thermal correction to Gibbs free energy= 0.54324722718 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3319.13392011 (a.u.)
DFT-D3(BJ) correction to PBE= -0.11467417 (a.u.)

Cu	0.57995325	-0.09841680	0.03390651
N	-1.45910433	1.91942055	0.22080689
N	0.42424789	2.70544843	0.92524921
C	-0.13722923	1.57609939	0.37875185
C	2.68350402	3.45795792	0.35319602
C	-2.69396436	0.99937426	-1.68660172
C	-2.44078209	1.00363751	-0.30664093
C	2.27052392	2.31449200	2.49105586
C	-1.70906238	3.21542891	0.65846672
C	-3.07915525	0.11651352	0.57781154
C	4.52212646	3.08799052	1.92413721
C	-0.52281966	3.71204455	1.10322236
C	4.03174468	3.57630211	0.70852718
C	3.62768207	2.45730117	2.79666609
C	-3.98027372	-0.80363190	0.03735770
C	-4.25698915	-0.84949134	-1.33454335
C	-3.61363758	0.06382295	-2.17551932
C	1.81908313	2.82856445	1.26356176
C	-5.20830309	-1.88300495	-1.88346721
H	-4.82598618	-2.89825927	-1.68624273
H	-6.19815484	-1.80716275	-1.40431544
H	-5.34237607	-1.76917548	-2.96948979
C	-2.77520958	0.13020718	2.05275833
H	-3.40370278	-0.59987041	2.58100066
H	-1.71959944	-0.13870711	2.22856935
H	-2.94063648	1.12660641	2.49417356
C	-1.97540069	1.94144950	-2.61876228
H	-2.12584632	2.99560847	-2.33435225
H	-0.88777126	1.75494465	-2.60116495
H	-2.33068223	1.80901663	-3.65081541
C	1.33451726	1.60624263	3.43519191
H	0.99508345	0.65068947	2.99664457
H	1.83713407	1.38906712	4.38851931
H	0.43253483	2.20425629	3.64148432
C	2.18769031	3.96280352	-0.97776947
H	1.76458300	3.13787446	-1.57533325
H	1.39211904	4.71641620	-0.86156163
H	3.01028779	4.41604782	-1.54919362
C	5.97504597	3.25092571	2.29641265
H	6.11250665	4.11123057	2.97388117
H	6.35540953	2.35850147	2.81728084
H	6.59881565	3.42417301	1.40664888
H	-2.69954717	3.65656876	0.61710383
H	-0.26436817	4.67500189	1.53125407
H	-4.45897084	-1.52407840	0.70799605
H	-3.81866684	0.04025772	-3.25070126
H	3.99581168	2.05776595	3.74723951
H	4.71972167	4.05912838	0.00696679
O	1.47709366	-1.53272769	-0.94690044
C	2.10276042	-1.52197068	-2.26285771
C	1.02310024	-1.56621765	-3.35373221
H	1.47701025	-1.49152598	-4.35591555
H	0.44992658	-2.50255153	-3.29304378
H	0.32488613	-0.72246559	-3.22057989
C	2.88938817	-0.21045142	-2.34931055
H	3.37437200	-0.10709072	-3.33364183
H	2.20646514	0.64428781	-2.19901669
H	3.66002486	-0.17365327	-1.56270724
C	3.05514392	-2.72095453	-2.36861720
H	2.49968498	-3.66723965	-2.29100009
H	3.58866745	-2.70467821	-3.33314275
H	3.79732831	-2.68551132	-1.55564113
H	0.33431211	-1.57468020	0.93677531
Si	0.55585976	-2.89894045	-0.03164348
H	0.36255241	-3.64676364	-1.34834667
H	1.67744902	-3.57383856	0.71448925
C	-1.06688277	-3.64265541	0.75598272
C	-1.90052551	-4.49105397	0.00967510
C	-1.43554342	-3.38326176	2.08682915
C	-3.05144210	-5.06249597	0.56393952

C	-2.57202853	-3.95923267	2.65877447
C	-3.38931359	-4.79898494	1.89356183
H	-1.63448045	-4.70966658	-1.03171547
H	-0.81249045	-2.71067989	2.69046465
H	-3.68434024	-5.72029595	-0.04038836
H	-2.82639790	-3.75502315	3.70383524

TS_IPrCu-O-tBu_R3Si-H

Multiplicity: 1
E (PBE/L1, Priroda)= -3570.52423618 (a.u.)
Thermal correction to Gibbs free energy= 0.70410154258 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3554.74000275 (a.u.)
DFT-D3(BJ) correction to PBE= -0.14337878 (a.u.)

Cu	0.17533519	-0.70515605	-0.32988753
N	-1.44370492	1.69548327	-0.63972666
N	-0.69285460	1.50057357	1.37693896
C	-0.72641397	0.83853355	0.16845836
C	1.25090431	1.43727851	2.87303506
C	-0.85248260	1.63250015	-3.02716583
C	-1.80502937	1.41385548	-2.00949236
C	-0.77137467	0.11111068	3.40147287
C	-1.82543890	2.84671117	0.04285677
C	-3.11177331	0.95492841	-2.27514223
C	1.14128026	0.10571761	4.90516476
C	-1.35491734	2.72320972	1.31190420
C	1.82863176	0.97315145	4.06257427
C	-0.14292489	-0.32232979	4.57477844
C	-3.45597348	0.72287772	-3.61320872
C	-2.53742693	0.93047795	-4.63779370
C	-1.25128967	1.37749604	-4.34524260
C	-0.05225642	0.99674925	2.56988145
C	-4.14469807	0.73156692	-1.17677728
H	-3.63158830	0.83468078	-0.20702298
C	0.53824305	2.18046347	-2.73338354
H	0.76142430	1.96661759	-1.67520162
C	-2.19298827	-0.32827922	3.07289545
H	-2.31900383	-0.23685080	1.98097026
C	2.02028122	2.39817315	1.97681743
H	1.46273044	2.49144726	1.03059047
H	-2.39453654	3.63632561	-0.43575573
H	-1.42237237	3.38605532	2.16778673
H	-4.46185479	0.36915900	-3.85365319
H	-0.53894704	1.53418506	-5.15806911
H	-0.66824293	-1.00861211	5.24243152
H	2.83888491	1.29495320	4.32665828
O	0.49130890	-2.62252713	-0.65939608
C	-0.32011233	-3.82260910	-0.47658282
C	0.10649401	-4.52273765	0.82105060
H	-0.52621962	-5.40446739	1.01621489
H	1.15492421	-4.84782502	0.75380369
H	0.01340538	-3.82729761	1.67131405
C	-1.77128364	-3.34703276	-0.38000850
H	-2.44891228	-4.19477302	-0.18798036
H	-1.87829763	-2.61409897	0.43743797
H	-2.06922064	-2.85851163	-1.32206530
C	-0.15379004	-4.74631843	-1.69154191
H	0.88456972	-5.09722558	-1.77851033
H	-0.81498544	-5.62341458	-1.59647358
H	-0.41747830	-4.20684355	-2.61501293
H	1.78012610	-0.86152508	-0.94697070
Si	2.25187519	-2.44046734	-1.22093257
H	2.54621368	-3.88218415	-0.80667856
H	2.13660002	-2.44704206	-2.72587004
C	4.07559611	-1.85137418	-0.87958204
C	5.04636049	-2.77455094	-0.45842095
C	4.49590917	-0.53217653	-1.11609322
C	6.38475023	-2.40401427	-0.29255368
C	5.83143743	-0.15172587	-0.96695872
C	6.78155377	-1.08994978	-0.55076255
H	4.74131671	-3.80932739	-0.26163072
H	3.75337152	0.21379784	-1.42603296
H	7.12142013	-3.14193800	0.03998624
H	6.13602092	0.88002761	-1.16895272
H	7.82694176	-0.79486474	-0.42304285
H	-2.82497729	0.74052331	-5.67513157
H	1.61168445	-0.24596965	5.82700460
C	-5.25489916	1.79893242	-1.24078174
H	-5.80723202	1.73546502	-2.19261924
H	-5.97504137	1.65195679	-0.41925841
H	-4.84335289	2.81725305	-1.15900766
C	-4.74546797	-0.68437252	-1.22638623
H	-5.44657236	-0.82422834	-0.38747330
H	-5.30562338	-0.85698249	-2.15949181
H	-3.95864600	-1.44971558	-1.15109790
C	0.56046670	3.71043578	-2.92996010
H	1.55703153	4.11172238	-2.68336392
H	0.33536728	3.97224500	-3.97713989
H	-0.18030598	4.21180459	-2.28708336
C	1.63723781	1.50214374	-3.56587884
H	2.62400834	1.87616895	-3.24917808
H	1.62625065	0.41045216	-3.42373977
H	1.53639187	1.71940255	-4.64184055
C	-3.21924632	0.60109207	3.75347012
H	-4.24554242	0.29632914	3.49025982
H	-3.11757091	0.55238428	4.85020289
H	-3.08377096	1.64903886	3.44450420
C	-2.46948085	-1.79467939	3.44120091
H	-1.71818313	-2.46762005	3.00031332
H	-2.47493997	-1.95087824	4.53226989
H	-3.46138262	-2.09138137	3.06448642
C	2.10283632	3.79737496	2.61908793
H	1.10261268	4.21134362	2.82356503
H	2.65370055	3.75926915	3.57325324
H	2.63259353	4.49350438	1.94849562
C	3.42168365	1.86712980	1.63176975
H	4.06000259	1.78635597	2.52648283
H	3.37010589	0.87654628	1.15565274

TS_IMesCu-H_CO2

Multiplicity: 1
E (PBE/L1, Priroda)= -2767.74113587 (a.u.)
Thermal correction to Gibbs free energy= 0.339573878123 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -2752.73081268 (a.u.)
DFT-D3(BJ) correction to PBE= -0.07357647 (a.u.)

Cu	1.08385516	-0.71428378	-1.08331690
N	-1.35242349	0.60191343	-0.15746397
N	-0.06384587	0.06456539	1.48589964
C	-0.16355878	-0.01864457	0.12215008
C	2.19869059	0.33819417	2.39289080
C	-1.45001251	1.85964903	-2.26107869
C	-1.87667146	0.76464338	-1.49181278
C	0.94393216	-1.74059319	2.79922295
C	-1.97387509	1.05881090	1.00093807
C	-2.79855212	-0.17981664	-1.97313230
C	3.19017944	-1.46043636	3.72522627
C	-1.16049284	0.71961733	2.03826929
C	3.25423923	-0.18917321	3.14522476
C	2.02820078	-2.21867776	3.54130955
C	-3.30690528	0.00624377	-3.26227007
C	-2.91610115	1.08595219	-4.06253487
C	-1.99057947	1.99787291	-3.54442320
C	1.05013832	-0.45587237	2.24086918
C	-3.45196198	1.24178230	-5.46388553
H	-2.80683472	0.71273275	-6.18641931
H	-4.46512090	0.82130526	-5.55507544
H	-3.48579986	2.30007241	-5.76448085
C	-3.19936159	-1.37482018	-1.14673486
H	-3.94857761	-1.97819821	-1.67894266
H	-2.32326872	-2.01429288	-0.94260755
H	-3.62089653	-1.08126294	-0.17189174
C	-0.42028178	2.83317149	-1.74925678
H	-0.63966177	3.16271004	-0.72165779
H	0.58066040	2.36535496	-1.73882313
H	-0.37362945	3.71973993	-2.39785395
C	-0.27903144	-2.59282850	2.57634448
H	-0.40482821	-2.81400340	1.50238343
H	-0.18799669	-3.54674666	3.11522000
H	-1.20013503	-2.09130799	2.91432714

C	2.31664143	1.69205502	1.74234501
H	2.45411401	1.58465725	0.65128371
H	1.41598931	2.30547268	1.90118994
H	3.18460795	2.23610027	2.14172211
C	4.35977804	-2.01579197	4.49906415
H	4.02797601	-2.72027773	5.27702151
H	5.04466195	-2.56160731	3.82738153
H	4.93914172	-1.21315830	4.98030727
H	-2.92396953	1.58243563	0.97565811
H	-1.25306691	0.88563405	3.10661856
H	-4.02655253	-0.72025370	-3.65340426
H	-1.67218294	2.84683451	-4.15791341
H	1.96253364	-3.21797580	3.98376723
H	4.15672274	0.41630408	3.27714547
H	1.99950820	-1.52603898	-2.06652080
C	3.02855873	-0.40808632	-2.50826815
O	2.78236600	0.66026386	-1.96622852

TS_IPrCu-H_CO2

Multiplicity: 1
E (PBE/L1, Priroda)= -3003.42705458 (a.u.)
Thermal correction to Gibbs free energy= 0.49928177588 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -2988.33840354 (a.u.)
DFT-D3(BJ) correction to PBE= -0.10370086 (a.u.)

Cu	1.12291309	-0.97896464	-1.19130119
N	-1.18727232	0.57538718	-0.29556679
N	0.12708365	0.08896130	1.34313676
C	-0.00910525	-0.06761900	-0.01276012
C	2.36328075	0.41381721	2.29851328
C	-1.40867852	1.80970105	-2.40419435
C	-1.74374725	0.68454414	-1.62508826
C	1.17117003	-1.73338763	2.61246459
C	-1.76600643	1.11022377	0.85046799
C	-2.59633680	-0.33912368	-2.08454975
C	3.38424264	-1.39558725	3.56433696
C	-0.93628650	0.80315501	1.88494053
C	3.42959339	-0.10501506	3.04430690
C	2.26825611	-2.19973645	3.34757517
C	-3.12401719	-0.20417198	-3.37482526
C	-2.81709310	0.89938668	-4.16667018
C	-1.96858122	1.89270348	-3.68561420
C	1.24596447	-0.42186812	2.10232801
C	-2.92373727	-1.57133445	-1.25178397
H	-2.48455104	-1.42751743	-0.25126139
C	-0.47159720	2.90470706	-1.91186909
H	-0.14448667	2.63601840	-0.89448387
C	-0.02341169	-2.64464746	2.36421721
H	-0.79829508	-2.05144266	1.85209826
C	2.44886029	1.82397882	1.72959744
H	1.51629367	2.02145320	1.17679077
H	-2.70434616	1.65394056	0.81996051
H	-0.99954568	1.02302058	2.94545827
H	-3.78352728	-0.98274384	-3.76657400
H	-1.72740921	2.75035409	-4.31878050
H	2.24774083	-3.21478910	3.75234560
H	4.31402552	0.51459056	3.21311656
H	1.82357454	-2.06578976	-2.07618687
C	2.99298078	-1.17889304	-2.74981785
O	2.93305078	-0.02408230	-2.35910438
O	3.53968783	-1.98964898	-3.42846869
H	4.22970570	-1.78095634	4.14010077
H	-3.23947268	0.98322856	-5.17135285
C	2.55833745	2.87371715	2.85175551
H	1.71036210	2.80647673	3.55184640
H	3.48645018	2.74377783	3.43182869
H	2.57130084	3.88808208	2.42088601
C	3.61082821	1.95195504	0.72709463
H	4.58173610	1.76214824	1.21337980
H	3.49849961	1.24317815	-0.10856578
H	3.63700908	2.97219373	0.31049541
C	0.79071606	2.99540629	-2.78930957
H	1.46411226	3.77615127	-2.39930961
H	1.34111969	2.04131940	-2.79871334
H	0.53718269	3.25863517	-3.82930566
C	-1.19431985	4.26253125	-1.82721343
H	-1.52923875	4.60002523	-2.82153951
H	-2.07913901	4.20899919	-1.17304252
H	-0.51271109	5.02941780	-1.42466425
C	-0.63054690	-3.16785753	3.67864766
H	-1.52474377	-3.77548678	3.46443437
H	0.08083264	-3.80596304	4.22739714
H	-0.92605775	-2.34066905	4.34335639
C	0.36478974	-3.80100321	1.42350181
H	1.15163115	-4.43053739	1.87037878
H	-0.51099224	-4.43935403	1.22183190
H	0.74038043	-3.41207812	0.46152798
C	-4.44134088	-1.75711358	-1.07171405
H	-4.94317202	-1.94601040	-2.03444701
H	-4.63956957	-2.62237973	-0.41848636
H	-4.90500695	-0.86745374	-0.61682608
C	-2.27120063	-2.82586450	-1.86262118
H	-1.17649971	-2.70341276	-1.92857462
H	-2.48485783	-3.70931226	-1.23890117

TS_R3Si-O-COH_R2N-H (concerted, non-catalysed)

Multiplicity: 1
E (PBE/L1, Priroda)= -1038.54936767 (a.u.)
Thermal correction to Gibbs free energy= 0.21911939061703214 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -1037.64384324 (a.u.)
DFT-D3(BJ) correction to PBE= -0.04368110 (a.u.)

O	1.39418783	-1.61192228	-0.49245561
Si	-1.64361675	-1.45822146	1.20236863
H	-3.09771633	-1.12706919	1.42798851
H	-1.55508511	-2.89335512	0.73869437
C	-0.76445778	-1.32361760	2.87574675
C	-1.43107098	-0.81254879	4.00359720
C	0.57577823	-1.73005275	3.02634285
C	-0.78718705	-0.71185492	5.23979488
C	1.22365476	-1.62764747	4.25875708
C	0.54217187	-1.11950636	5.36846319
H	-2.47347080	-0.48843289	3.91366675
H	1.12262394	-2.12709627	2.16413565
H	-1.32396787	-0.31332410	6.10541673
H	2.26470052	-1.94825413	4.35669029
H	1.04861961	-1.04197453	6.33453259
C	0.84373002	-0.56185379	-0.63010461
O	-1.01577923	-0.41158608	0.07285911
H	1.09208116	0.43639036	-0.23611371
C	-0.09360025	3.41883547	-2.24465302
C	-0.30030007	2.11246308	-1.80339636
C	0.57706894	3.66163503	-3.44576176
H	-0.83559613	1.90129344	-0.87267295
H	0.73284380	4.68623063	-3.79124732
C	0.17258006	1.03691275	-2.57074619
C	1.04411905	2.58731841	-4.20509654
H	1.56841784	2.76842813	-5.14660732
C	0.85071125	1.27424388	-3.77156655
H	1.22529036	0.44475814	-4.37389494
H	-0.46763759	4.25293854	-1.64601763
N	-0.02602523	-0.28895707	-2.04677189
H	-0.90848942	-0.35380045	-1.32648741
C	0.09246971	-1.43636330	-2.95954764
H	-0.21227756	-2.33563136	-2.40867148
H	-0.56709176	-1.28609197	-3.82555969
H	1.13232094	-1.57228600	-3.29168198

TS_R3Si-O-COH_R2N-H (concerted, catalysed)

Multiplicity: 1
E (PBE/L1, Priroda)= -1365.27978396 (a.u.)
Thermal correction to Gibbs free energy= 0.3505566356 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -1364.2642759 (a.u.)
DFT-D3(BJ) correction to PBE= -0.07234808 (a.u.)

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O  0.911738270  -2.567690100 0.407918440
Si  -1.376816310 -1.161165140 2.304256030
H  -2.532759000 -0.281379860 2.714581870
H -1.894468870 -2.570647840  2.146584140
C  -0.139865570  -1.155357030  3.744925530
C  -0.219984150  -0.181938580  4.757543690
C   0.883365420  -2.119597280  3.834624160
C   0.685332390  -0.168225920  5.821824690
C   1.792428340  -2.107004320  4.894664860
C   1.693944860  -1.131852180  5.891119470
H  -1.009287570   0.576561400  4.715085760
H    0.973046660 -2.883566350  3.054691490
H 0.603245300  0.595319090  6.600657550
H 2.580519130 -2.863615220  4.946889820
H 2.403344050 -1.124336610  6.723296960
C 0.985360180 -1.359985390  0.399129790
O   -0.738621980 -0.563414530  0.888116900
H 1.496335300 -0.710536400  1.131079000
C   -2.762179470  2.627193460 -2.411864500
C   -2.160597230  1.578275360 -1.721751610
C   -3.292241350  2.424905940 -3.689852110
H   -1.750992790  1.733322680 -0.720517590
H   -3.765279920  3.249409120 -4.228034930
C   -2.078894780  0.304543890 -2.305576210
C   -3.216483340  1.157883710 -4.267423250
H   -3.631892260  0.983409980 -5.263255270
C   -2.614965620  0.098347960 -3.583072580
H   -2.570533300 -0.887090400 -4.050392690
H   -2.821506090  3.612567560 -1.943041680
N   -1.418641060 -0.738892770 -1.577948530
H   -1.457633710 -0.612357530 -0.495024540
C   -1.748627550 -2.137118250 -1.919050500
H   -1.273264250 -2.779566470 -1.163190320
H   -2.838404330 -2.301832400 -1.907055550
H   -1.356811590 -2.409066420 -2.911083720
H 2.883837020 -1.601430900 -1.812229600
H 1.392731550 -2.584220820 -1.773267920
C 1.795152670 -1.584236890 -1.979289560
H 1.583936420 -1.294306360 -3.018927940
N 1.121783300 -0.650656010 -1.048074030
H   -0.114228710 -0.615645940 -1.452598440
C 1.681385130  0.682891180 -0.983935580
C 2.678313330  1.114962300 -1.870591940
H 3.068699000  0.451484310 -2.642699290
H 3.951976180  2.738829270 -2.481519660
C 3.178955750  2.415793780 -1.779656200
H 3.101980420  4.309660840 -0.738338730
C 2.703527040  3.294699470 -0.806768880
C 1.710550920  2.862944180  0.075341680
H 1.325583150  3.540469800  0.841880480
C 1.195210090  1.570514140 -0.009005910
H 0.402698930  1.222744510  0.660826970
```

TS_R3Si-O-COH_R2N-H (TS1, addition/elimination, non-catalysed)

Multiplicity: 1
E (PBE/L1, Priroda)= -1038.53845857 (a.u.)
Thermal correction to Gibbs free energy= 0.22039998725140234 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -1037.63284778 (a.u.)

DFT-D3(BJ) correction to PBE= -0.04344349 (a.u.)

```
 O     0.74502604  -0.72758028  -0.05456223
Si    -1.44483058  -1.36165293   1.37860056
 H    -2.86852797  -1.26401690   1.84596766
 H    -1.33533190  -2.55457801   0.47572219
 C    -0.38685726  -1.50313805   2.93405840
 C    -1.04808503  -1.64363113   4.16920013
 C     1.02108481  -1.51496906   2.92280346
 C    -0.32862011  -1.80055695   5.35616344
 C     1.73901704  -1.66633510   4.11003289
 C     1.06728923  -1.81259517   5.32705481
 H    -2.14264664  -1.62775118   4.20367450
 H     1.53753122  -1.38478853   1.96773855
 H    -0.85915811  -1.90892232   6.30620166
 H     2.83239396  -1.67024043   4.08685467
 H     1.63314894  -1.93222187   6.25515916
 C    -0.13595648   0.27914031  -0.17834335
O    -1.31882386   0.12602933   0.50819591
 H     0.21911931   1.32732558  -0.09375601
 C     0.06082997   3.41348901  -3.42425487
 C    -0.45514251   2.37372201  -2.65003493
 C     1.19863073   3.20964603  -4.20926696
 H    -1.34285855   2.53436884  -2.03228573
 H     1.60013259   4.02614239  -4.81417597
 C     0.17003557   1.11960512  -2.66004154
 C     1.82360353   1.96094692  -4.21379414
 H     2.71661074   1.79620710  -4.82166944
 C     1.31380747   0.91748800  -3.43921150
 H     1.79875180  -0.06209564  -3.43196636
 H    -0.42789006   4.39091004  -3.41111261
 N    -0.32179025   0.04322776  -1.83984330
 H     0.51022823  -0.77082966  -1.33475994
 C    -1.64410264  -0.47324806  -2.23490982
 H    -1.86235924  -1.38064626  -1.65344732
 H    -2.43597080   0.26881136  -2.04486280
 H    -1.62828916  -0.72726227  -3.30512919
```

TS_R3Si-O-COH_R2N-H (addition/elimination, TS1, catalysed)

Multiplicity: 1
E (PBE/L1, Priroda)= -1365.28780191 (a.u.)
Thermal correction to Gibbs free energy= 0.35335208439571647 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -1364.27225986 (a.u.)

DFT-D3(BJ) correction to PBE= -0.07297746 (a.u.)

```
O  1.429805610  0.715623160  0.429783320
Si   1.258620050  2.440585010  2.299220940
H  2.697171510  2.624707960  1.929406220
H  0.788137770  3.655466240  3.051157570
C  1.047266270  1.009340820  3.529859720
C  0.150924500  1.145666180  4.605462470
C  1.788928730 -0.183362910  3.436316920
C   -0.013884150  0.123974200  5.545263390
C  1.638740370 -1.201078270  4.380122890
C  0.731398460 -1.051492630  5.434077780
H   -0.426138330  2.070695890  4.711336160
H  2.489648810 -0.307560860  2.605631100
H   -0.719840420  0.248957140  6.371145660
H  2.233309950 -2.115695170  4.298001940
H  0.610950810 -1.849541930  6.171903080
C  0.466605400  1.522646880  0.017156690
O  0.196871020  2.530066300  0.954906850
H  0.579631400  1.992779620 -0.985295850
C  1.106357250 -3.088311150 -3.864562460
C  0.617118300 -2.847919290 -2.579171740
C  2.028776820 -2.217349800 -4.447562890
H   -0.110060680 -3.533710500 -2.139071040
H  2.407646790 -2.410674010 -5.453805770
C  1.057198100 -1.727171200 -1.864370450
C  2.469535440 -1.101866480 -3.730782630
H  3.201637730 -0.420452610 -4.171550530
C  1.992776810 -0.855882080 -2.443524750
H  2.347205990 -0.000770680 -1.859881870
H  0.758115110 -3.965791860 -4.415291940
N  0.556308580 -1.412088430 -0.554125680
H  1.178960580 -0.586165470 -0.049504800
C  0.232909800 -2.541714510  0.339495230
H  0.150005020 -2.155272660  1.365884440
H   -0.720487160 -3.019886490  0.064840660
H  1.033822750 -3.296865540  0.308477390
C   -1.989037380  1.715501800 -3.643678390
C   -1.249705620  1.191947330 -2.584939700
```

```
C   -3.255999140  2.261328200 -3.422845510
H   -0.275785170  0.734927090 -2.780075340
H   -3.837806550  2.664226010 -4.255128640
C   -1.759142800  1.215556480 -1.272591000
C   -3.771820900  2.277475990 -2.126742280
H   -4.762395300  2.699185960 -1.936729350
C   -3.033021530  1.765817820 -1.057955070
H   -3.455548030  1.802619340 -0.053219820
H   -1.573400080  1.682968990 -4.654076880
N   -0.954201920  0.673993640 -0.222184110
C   -1.634136180  0.472315210  1.066984730
H   -2.469550940 -0.234782530  0.944575470
H   -0.903560390  0.054779140  1.775396670
H   -2.005291390  1.417040420  1.493799830
H   -0.325571680 -0.584785740 -0.561538640
```

TS_R3Si-O-COH_R2N-H (addition/elimination, intermediate, catalysed)

Multiplicity: 1
E (PBE/L1, Priroda)= -1038.58043815 (a.u.)
Thermal correction to Gibbs free energy= 0.22359096124426311 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -1037.67825308 (a.u.)

DFT-D3(BJ) correction to PBE= -0.04296655 (a.u.)

```
O     0.40334707  -2.15170485  -0.54540277
Si    -1.84282724  -1.70189368   1.22400500
H    -3.20577221  -1.16321190   1.53425682
H    -1.89551809  -3.18420565   1.01234995
 C    -0.65583315  -1.30867121   2.63814505
C    -0.78459411  -0.11186486   3.36823560
 C     0.38727027  -2.18867730   2.98166561
 C     0.09907421   0.19665754   4.40434970
 C     1.27109436  -1.88445873   4.01909606
 C     1.12822378  -0.69040539   4.73041493
 H    -1.59266997   0.58728269   3.12707719
 H     0.50547386  -3.12574248   2.42824310
 H    -0.01680298   1.12956922   4.96258322
 H     2.07371955  -2.58118216   4.27607429
 H     1.81914127  -0.45155756   5.54339889
 C    -0.10477387  -0.82375352  -0.66346596
 O    -1.43651483  -0.87004202  -0.20196394
 H     0.49239170  -0.13263389  -0.03757108
 C     0.26935874   3.33943589  -1.59101476
 C     0.02709159   1.99936635  -1.29358790
 C     0.61111348   3.74131409  -2.88384518
 H    -0.31034649   1.73207056  -0.29087162
 H     0.78783063   4.79472560  -3.11151032
 C     0.15404002   1.00662136  -2.29066009
 C     0.69938760   2.77118437  -3.88434871
 H     0.95181277   3.06153754  -4.90793923
 C     0.47682551   1.42561104  -3.59963305
 H     0.56800528   0.68802010  -4.39885254
 H     0.15983587   4.08428110  -0.79799720
 N    -0.02977947  -0.35250183  -2.01776474
 H     1.37170929  -2.09544588  -0.65722606
 C    -0.50116527  -1.25002490  -3.06933267
 H    -0.82724316  -2.18582835  -2.59743965
 H    -1.34933410  -0.80703257  -3.61755010
 H     0.29642808  -1.49683875  -3.79191784
```

TS_R3Si-O-COH_R2N-H (addition/elimination, TS2)

Multiplicity: 1
E (PBE/L1, Priroda)= -1038.55889774 (a.u.)
Thermal correction to Gibbs free energy= 0.2242899031 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -1037.65443585 (a.u.)

DFT-D3(BJ) correction to PBE= -0.0433769 (a.u.)

```
O     0.045091280 -0.059646520  0.763767630
Si   -0.818735100 -1.777609940  1.004486350
H    -1.505755180 -3.105949210  0.713796870
H    -1.737285250 -1.175795760  2.034153540
C     0.797518120 -2.537543990  1.713732530
C     1.664678350 -1.843477320  2.582201190
C     1.127716420 -3.865710200  1.390730040
C     2.808264580 -2.451205920  3.105910240
C     2.280371080 -4.474292090  1.894407250
C     3.122468720 -3.767345420  2.755728860
H     1.426150720 -0.813865580  2.871202750
H     0.457001430 -4.431286780  0.734552710
H     3.456136180 -1.898988550  3.792942080
H     2.519691350 -5.505990450  1.620625570
H     4.020611430 -4.242999570  3.159416320
C    -0.772747510 -0.152385010 -1.046087550
O    -1.281486540 -1.317033920 -0.736913570
H     0.197811950 -0.071115630 -1.557971450
C     0.574993680  3.934605840 -1.341944480
C     0.024067710  2.715592820 -0.940987410
C     0.073103260  4.599927800 -2.461827550
H     0.372943410  2.189225560 -0.048623430
H     0.503299880  5.555731340 -2.770430050
C    -1.023866010  2.156105330 -1.679606880
C    -0.983817870  4.042263990 -3.187488430
H    -1.376753280  4.557532920 -4.067316550
C    -1.532465360  2.819709960 -2.802292490
H    -2.344078600  2.368655160 -3.378985710
H     1.393918870  4.372267150 -0.765649640
N    -1.588192590  0.899051440 -1.277524930
H     1.006648740 -0.222429080  0.680975980
C    -2.969631540  0.881846860 -0.779630290
H    -3.308142350 -0.160892490 -0.743165610
H    -3.022123230  1.323224560  0.229658590
H    -3.607406780  1.459822720 -1.461842490
```

TS_IMesCu-O-COH_R2N-H

Multiplicity: 1
E (PBE/L1, Priroda)= -3094.44371275 (a.u.)
Thermal correction to Gibbs free energy= 0.47466168408975012 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3079.32425292 (a.u.)
DFT-D3(BJ) correction to PBE= -0.09896498 (a.u.)

```
Cu  -0.59934303  -0.26646967   0.02067953
 N  -2.04167540   1.99118794  -1.06998727
 N  -0.76812036   2.57284599   0.57176618
 C  -1.19377667   1.47385218  -0.12630888
 C   1.55529538   2.48916462   1.35081033
 C  -2.01748587   0.81874552  -3.22542637
 C  -2.71646340   1.19297621  -2.06525225
 C  -0.29773688   2.48693226   2.97428003
 C  -2.13603952   3.37462484  -0.96366859
 C  -4.05269310   0.82285925  -1.83721461
 C   2.01853005   2.41791854   3.75538081
 C  -1.33269378   3.74168184   0.07252249
 C   2.45144762   2.44456977   2.42545575
 C   0.64209056   2.44170989   4.00851359
 C  -4.69421720   0.06347730  -2.82004481
 C  -4.04043019  -0.32950845  -3.99376002
 C  -2.70920739   0.05818736  -4.17578562
 C   0.18360447   2.51409368   1.65483435
 C  -4.74474109  -1.17949799  -5.02173957
 H  -4.60204601  -2.25159208  -4.80190691
 H  -5.82804876  -0.98454574  -5.02949899
 H  -4.35030567  -0.99434174  -6.03243134
 C  -4.76532780   1.19915180  -0.56296630
 H  -5.80025922   0.82860040  -0.57684919
 H  -4.25522354   0.76226996   0.31253453
 H  -4.79266353   2.29005958  -0.40981925
```

C	-0.57183559	1.18413505	-3.43980888
H	-0.36502349	2.22759069	-3.15550922
H	0.09147901	0.54036107	-2.83152611
H	-0.29645232	1.04917664	-4.49574562
C	-1.77599251	2.47333196	3.26971401
H	-2.25143191	1.57554762	2.83901569
H	-1.95218459	2.46777436	4.35484609
H	-2.29107654	3.34842840	2.84163202
C	2.05485069	2.47240714	-0.07033678
H	1.89474858	1.47894620	-0.53031714
H	1.53365643	3.21315181	-0.69688877
H	3.13258252	2.68860935	-0.09925044
C	3.01031539	2.33080818	4.88847249
H	2.62106516	2.80946595	5.80002473
H	3.22694081	1.27684766	5.13365791
H	3.96436461	2.81117664	4.62313153
H	-2.75346170	3.96209329	-1.63526743
H	-1.10446990	4.71562356	0.49291052
H	-5.73571548	-0.23326020	-2.65908501
H	-2.18366233	-0.23960721	-5.08877687
H	0.28496434	2.41990331	5.04320275
H	3.52470196	2.42818035	2.20997710
O	0.04590062	-2.04580275	0.05382286
C	1.25161774	-2.00542422	-0.85594028
O	1.54890861	-0.91745325	-1.34753839
H	1.34021787	-2.98024705	-1.37599616
C	4.58720658	-5.44555329	0.73296248
C	4.12624454	-4.13272321	0.84063128
C	3.71287899	-6.49379140	0.43967784
H	4.83732019	-3.33554332	1.06554123
H	4.08066796	-7.51924529	0.35661872
C	2.75666401	-3.82655008	0.66617223
C	2.35431625	-6.20695879	0.26366337
H	1.64951663	-7.01446202	0.04428254
C	1.88078508	-4.90412122	0.37875601
H	0.81190099	-4.69727901	0.26888929
H	5.65229643	-5.64934975	0.87942124
N	2.22796563	-2.54097822	0.74479965
H	0.76803854	-2.32507237	0.83914154
C	3.12611925	-1.46411790	1.11662753
H	3.95170627	-1.32051007	0.39111277
H	2.55229937	-0.52384482	1.15251993
H	3.56659567	-1.63061707	2.11664412

TS_IPrCu-O-COH_R2N-H

Multiplicity: 1
E (PBE/L1, Priroda)= -3330.13295684 (a.u.)
Thermal correction to Gibbs free energy= 0.63254477944926057 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3314.93761762 (a.u.)
DFT-D3(BJ) correction to PBE= -0.13004622 (a.u.)

Cu	0.25130491	-0.42707279	-0.73971756
N	-1.57876444	1.77201005	-1.15429504
N	-0.30844776	2.12093974	0.55415081
C	-0.56069299	1.20387663	-0.43323092
C	2.01524722	2.30756934	1.32402058
C	-1.66361889	1.41328534	-3.58002548
C	-2.19451899	1.14470626	-2.30273517
C	0.27094277	1.38225624	2.81932351
C	-1.94688595	3.00539761	-0.63098358
C	-3.29425828	0.28969421	-2.09194130
C	2.57825276	1.56125668	3.56988924
C	-1.14443085	3.22616161	0.44694135
C	2.95334707	2.10537053	2.34433391
C	1.25264307	1.20482439	3.80262231
C	-3.87246993	-0.29879439	-3.22424485
C	-3.37515106	-0.04913733	-4.50021944
C	-2.28142199	0.79526789	-4.67423884
C	0.68280609	1.93540118	1.59036626
C	-3.85691717	-0.00930524	-0.70863788
H	-3.24366930	0.53249300	0.02957953
C	-0.44151291	2.29742808	-3.79029069
H	-0.19733598	2.77041993	-2.82510978
C	-1.16551344	0.95425042	3.09132644
H	-1.77915742	1.25836818	2.22789691
C	2.45719982	2.88206045	-0.01525259
H	1.55615040	3.02766264	-0.63305414
H	-2.73844917	3.60287108	-1.07080879
H	-1.09007945	4.05643464	1.14312571
H	-4.72543833	-0.97045913	-3.09881750
H	-1.89310237	0.97477542	-5.67992233
H	0.97206988	0.76928016	4.76486993
H	3.99810795	2.37548362	2.17103976
O	-0.41072300	-2.89151728	0.25371340
C	0.71573047	-3.01655871	-0.49771014
O	1.13066208	-2.02300849	-1.18748517
H	1.01396495	-4.02244342	-0.83934253
C	4.14378776	-6.08443644	1.89833737
C	3.60823861	-4.79811556	1.82411417
C	3.36174708	-7.20886205	1.62567070
H	4.24873394	-3.94163180	2.04409032
H	3.78813226	-8.21295797	1.68662240
C	2.25031085	-4.59036189	1.47530585
C	2.01635775	-7.02379950	1.28289030
H	1.38167762	-7.89084773	1.07639851
C	1.46899674	-5.74807743	1.21349689
H	0.40910380	-5.61746942	0.97218945
H	5.19533699	-6.20802001	2.17570507
N	1.64727572	-3.35037980	1.36053489
H	0.16365914	-3.17300648	1.14257051
C	2.44240382	-2.18553924	1.68471502
H	3.36173065	-2.09788951	1.06853537
H	1.83971177	-1.27738613	1.49652703
H	2.74680555	-2.16126878	2.74952582
H	-3.84107248	-0.52223827	-5.36843840
H	3.32806742	1.40834640	4.35023866
C	3.13734614	4.25387292	0.14668636
H	2.47782146	4.97182106	0.65924085
H	4.07040402	4.17624654	0.72770900
H	3.39462713	4.66589730	-0.84257779
C	3.36898339	1.88855077	-0.75936880
H	4.29052653	1.68864267	-0.18895685
H	2.85328144	0.92649727	-0.91978619
H	3.65623676	2.29553149	-1.74254936
C	-1.74176878	1.65303864	4.33675081
H	-2.79819985	1.36980432	4.47137676
H	-1.20015047	1.36037495	5.25062534
H	-1.68640240	2.74958634	4.24694201
C	-1.26830097	-0.57821328	3.21073681
H	-2.31431926	-0.87371020	3.39414592
H	-0.92852795	-1.07438790	2.28736252
H	-0.65657229	-0.95482198	4.04655640
C	-0.70733162	3.42454341	-4.80421441
H	0.17783999	4.07635073	-4.88279061
H	-0.91478396	3.02489698	-5.80987134
H	-1.56649960	4.04374513	-4.50169155
C	0.77307904	1.44513351	-4.20530678
H	0.98924102	0.67330997	-3.44745047
H	0.59034464	0.93515556	-5.16517350
H	1.66650582	2.08054381	-4.31902002
C	-5.30514834	0.50081025	-0.57802325
H	-5.97703413	-0.02139823	-1.27845162
H	-5.67858638	0.32003331	0.44299129
H	-5.37418308	1.58067805	-0.78539468
C	-3.75781240	-1.50884749	-0.37183795
H	-4.16664593	-1.69212433	0.63537636
H	-4.33760607	-2.11825236	-1.08436376
H	-2.71323865	-1.86061613	-0.38383739

TS_IMesCu-O-COH_R3Si-H

Multiplicity: 1
E (PBE/L1, Priroda)= -3291.04168509 (a.u.)
Thermal correction to Gibbs free energy= 0.448298221571 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3275.32681972 (a.u.)
DFT-D3(BJ) correction to PBE= -0.09667278 (a.u.)

Cu	-0.20028144	-0.33160491	-0.39204312
N	0.14352086	2.52454861	-0.87134701
N	1.28832026	1.85872055	0.83127797
C	0.41651859	1.40791135	-0.12529071

C	3.12297351	0.39242986	1.52837497
C	-0.12612847	2.22181288	-3.28758836
C	-0.70215812	2.51376140	-2.03948514
C	1.22917303	0.81257450	3.04635833
C	0.82463304	3.63850794	-0.38946816
C	-2.06980754	2.79488221	-1.88669207
C	3.06264192	-0.64682523	3.74518734
C	1.54721174	3.21830028	0.68458951
C	3.68762429	-0.42667743	2.51309504
C	1.83714199	-0.01764087	3.99295565
C	-2.86822343	2.78425227	-3.03450424
C	-2.33940950	2.50043833	-4.29901106
C	-0.97168479	2.22593958	-4.40318516
C	1.89278095	1.00410263	1.82331308
C	-3.22997151	2.45964455	-5.51594399
H	-3.64549229	1.44723222	-5.65896372
H	-4.07819566	3.15403623	-5.41563984
H	-2.67285127	2.72026641	-6.42872007
C	-2.66440774	3.07053519	-0.52944692
H	-3.73255449	3.31527084	-0.61805450
H	-2.56544934	2.18655791	0.12419726
H	-2.15794985	3.90660002	-0.02065210
C	1.33728005	1.89218932	-3.42795888
H	1.97277562	2.62522327	-2.90612536
H	1.56839852	0.89866947	-3.00182190
H	1.62554950	1.87876589	-4.48898584
C	-0.10629071	1.45488140	3.31979972
H	-0.87142446	1.06495545	2.62590629
H	-0.43341836	1.24402584	4.34794165
H	-0.07216672	2.54770742	3.18238404
C	3.80260154	0.58150981	0.19667879
H	3.24485513	0.07689772	-0.61269400
H	3.87957212	1.64600801	-0.07603766
H	4.81683841	0.15769353	0.22163009
C	3.67764978	-1.56705157	4.77010156
H	3.42793699	-1.25015665	5.79430773
H	3.30207034	-2.59674005	4.64133466
H	4.77350418	-1.59929172	4.67307866
H	0.73340343	4.61400165	-0.85570491
H	2.21727701	3.75092469	1.35139036
H	-3.93645196	3.00236067	-2.93452585
H	-0.54180230	2.00514267	-5.38552884
H	1.33433153	-0.17807700	4.95209865
H	4.64789634	-0.90926480	2.30441780
O	0.48181909	-1.92672349	-1.56417251
C	1.62878376	-2.22533256	-2.17633799
O	2.47019531	-1.40733009	-2.48643972
H	1.73062796	-3.31676017	-2.37238880
H	-1.21719295	-1.58619202	-0.09785386
Si	-0.89416576	-3.05618925	-0.86513088
H	-1.92001568	-2.92343516	-1.95383417
H	-0.01904724	-4.25092942	-1.23002671
C	-1.73885689	-3.88946450	0.65692325
C	-1.63680968	-5.28282392	0.80760471
C	-2.51360309	-3.18283308	1.58935464
C	-2.30696529	-5.95160934	1.83538092
C	-3.18797336	-3.84213498	2.61947796
C	-3.08666148	-5.23082560	2.74334857
H	-1.01850723	-5.85227710	0.10374149
H	-2.58531565	-2.09134088	1.50603554
H	-2.21625997	-7.03753240	1.93309990
H	-3.79074175	-3.27263136	3.33331726

TS_IPrCu-O-COH_R3Si-H

Multiplicity: 1
E (PBE/L1, Priroda)= -3526.72453352 (a.u.)
Thermal correction to Gibbs free energy= 0.606880736869 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3510.93344497 (a.u.)
DFT-D3(BJ) correction to PBE= -0.12769273 (a.u.)

Cu	-0.18215770	-0.88813984	-0.45563612
N	0.03850609	1.98687855	-0.83829885
N	1.12185836	1.35186082	0.91681264
C	0.38128217	0.85944150	-0.13097577
C	3.09701406	0.14423584	1.72297241
C	-0.01063567	1.91314269	-3.28789585
C	-0.71728221	1.96045301	-2.06901297
C	1.00832570	0.14482449	3.05320473
C	0.54426292	3.13851331	-0.24455429
C	-2.12478077	1.98569033	-2.00140358
C	2.98102657	-1.03612018	3.84752302
C	1.22653260	2.73818389	0.86227597
C	3.69133680	-0.64550418	2.71577470
C	1.65520873	-0.64385691	4.01298547
C	-2.82724635	1.96238621	-3.21289862
C	-2.15762511	1.91389065	-4.43277710
C	-0.76604619	1.88959356	-4.46738872
C	1.75363738	0.52451454	1.91875178
C	-2.88355457	2.04742960	-0.68265222
H	-2.14451883	1.98450416	0.13226345
C	1.51096068	1.89883444	-3.36048794
H	1.89849442	1.90848950	-2.32909879
C	-0.43227990	0.58709777	3.27156153
H	-0.78755466	1.04213763	2.33292905
C	3.91051017	0.58200373	0.51145948
H	3.23040966	1.10603052	-0.17928253
H	0.37435024	4.12383541	-0.66540255
H	1.77630676	3.30182376	1.60846481
H	-3.92001404	1.97966984	-3.19726164
H	-0.25027309	1.84864360	-5.43022144
H	1.10759458	-0.95664553	4.90541343
H	4.73093464	-0.96042056	2.59519531
O	0.37780498	-2.68414223	-1.39423952
C	1.43603953	-3.20589105	-2.03952780
O	2.43506913	-2.58219173	-2.31335147
H	1.28028706	-4.27872941	-2.28771333
H	-1.40924461	-1.96649107	-0.23186644
Si	-1.27246624	-3.48906822	-1.01603751
H	-2.20108323	-3.08008041	-2.12693246
H	-0.69982205	-4.82387410	-1.49712702
C	-2.24866012	-4.21868408	0.47113377
C	-2.21888979	-5.60523135	0.69543030
C	-3.05796069	-3.43362856	1.30851288
C	-2.97968769	-6.19088252	1.71134309
C	-3.83029430	-4.01130370	2.31757509
C	-3.78984261	-5.39398086	2.52300077
H	-1.58877364	-6.23388091	0.05644047
H	-3.08159848	-2.34739658	1.16324045
H	-2.93936817	-7.27230450	1.87148714
H	-4.46220755	-3.38300518	2.95228611
H	-4.38552326	-5.84821515	3.31967263
C	-0.51105136	1.65786370	4.37773703
H	-1.55160050	1.99843012	4.50587136
H	-0.16419332	1.25341514	5.34282828
H	0.11090725	2.53421761	4.13543790
C	-1.36021640	-0.59981339	3.57956853
H	-1.31325153	-1.35626239	2.78089890
H	-1.09845672	-1.08852615	4.53205659
H	-2.40209321	-0.24936455	3.66123869
C	-3.83873790	0.85113154	-0.52490982
H	-4.62299143	0.85271853	-1.29930209
H	-3.28619341	-0.09978114	-0.59458998
H	-4.33604520	0.89232413	0.45798874
C	-3.63312137	3.38580623	-0.53742974
H	-4.39602661	3.50198048	-1.32449967
H	-4.14444913	3.43131622	0.43799630
H	-2.94385272	4.24236786	-0.60600659
C	5.01275152	1.57531819	0.93050203
H	5.73553376	1.09929220	1.61323407
H	5.56533351	1.92505316	0.04328895
H	4.59288939	2.45474087	1.44473494
C	4.50150649	-0.61402161	-0.25532759
H	5.17614200	-1.20992683	0.38091596
H	3.71174450	-1.27229693	-0.64779421
H	5.09045977	-0.24947794	-1.11285689
C	2.04049880	3.16026273	-4.07001219
H	3.14261023	3.16141726	-4.06585939
H	1.70840029	3.19712775	-5.12034868
H	1.69180063	4.07998578	-3.57360573
C	2.03741550	0.61762358	-4.03216857
H	3.13787467	0.64778675	-4.08485999
H	1.75520035	-0.28079716	-3.46218611
H	1.65407211	0.51601068	-5.06074171
H	3.46518951	-1.65362709	4.60852187

TS_IMesCu-H_R2N-COH

Multiplicity: 1
E (PBE/L1, Priroda)= -3019.19377069 (a.u.)
Thermal correction to Gibbs free energy= 0.469666146099 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3004.12333523 (a.u.)
DFT-D3(BJ) correction to PBE= -0.09765014 (a.u.)

Cu	-0.28116766	-0.25162198	-0.38859276
N	-2.17729713	1.60042711	0.82267672
N	-0.66919944	0.94626225	2.22395658
C	-1.06174825	0.80080671	0.91363344
C	1.72666412	0.89880565	2.72752885
C	-2.73621243	2.91095394	-1.16822964
C	-2.94543916	1.76374945	-0.38406340
C	0.29286668	-0.99390885	3.36967039
C	-2.46391842	2.21928157	2.03831558
C	-3.87655301	0.77358901	-0.73985847
C	2.68296007	-1.02831979	3.89293696
C	-1.51463711	1.80770314	2.92052809
C	2.81740456	0.22820799	3.29182930
C	1.41528366	-1.62114984	3.92067962
C	-4.62082114	0.97211526	-1.90824746
C	-4.45437041	2.10543564	-2.71097984
C	-3.50808940	3.06137927	-2.32452855
C	0.47123008	0.27198821	2.78697631
C	-5.24871433	2.27509896	-3.98245698
H	-4.71611636	1.82391081	-4.83745020
H	-6.23116620	1.78406586	-3.90917646
H	-5.40842512	3.33881560	-4.21653500
C	-4.04815042	-0.47745321	0.08135784
H	-4.94110494	-1.03180070	-0.24203498
H	-3.16900329	-1.13599679	-0.04086547
H	-4.14274996	-0.25230718	1.15528058
C	-1.68683979	3.92840199	-0.79953015
H	-1.86675255	4.36819658	0.19477311
H	-0.68880554	3.45850784	-0.76977988
H	-1.66349041	4.74313843	-1.53745865
C	-1.05311348	-1.67121300	3.36719885
H	-1.36051368	-1.90882238	2.33367244
H	-1.01573819	-2.60875994	3.94038895
H	-1.83681396	-1.02882935	3.79958742
C	1.89892734	2.22979725	2.04349638
H	1.66283599	2.13625720	0.96861983
H	1.22413781	2.99525228	2.45928610
H	2.93416046	2.58639960	2.14327281
C	3.88113860	-1.74346640	4.46740066
H	3.60251081	-2.35216747	5.34139056
H	4.32586580	-2.42326036	3.72035939
H	4.66248656	-1.03197849	4.77495114
H	-3.31438816	2.88214985	2.15916853
H	-1.36221357	2.04032028	3.96936304
H	-5.35415880	0.21221429	-2.19732893
H	-3.35781533	3.95095846	-2.94502467
H	1.29251273	-2.60629955	4.38271560
H	3.80260740	0.70484849	3.25702673
H	0.85911025	-0.31484870	-1.52504095
C	5.01613909	-1.73805620	-3.13334172
C	4.03461507	-1.90282220	-2.15452414
C	4.71352779	-1.90669300	-4.48463814
H	4.29014382	-1.74203867	-1.10602505
H	5.48444558	-1.77513694	-5.24741265
C	2.71958523	-2.26001801	-2.50922751
C	3.41012831	-2.26204706	-4.84623819
H	3.15843713	-2.42182634	-5.89826311
C	2.42851092	-2.44868133	-3.87733322
H	1.43218774	-2.78428953	-4.17320239
H	6.03017267	-1.46279235	-2.83008657
N	1.71654779	-2.46091850	-1.54366101
C	2.09638613	-2.60201785	-0.14668816
H	2.40227554	-1.63284502	0.30500354
H	1.21290201	-2.96694462	0.39564850
H	2.91513101	-3.32969381	-0.05236291
C	0.44585445	-1.81792547	-1.74056066
O	-0.55420358	-2.17022288	-0.97738058

TS_IPrCu-H_R2N-COH

Multiplicity: 1
E (PBE/L1, Priroda)= -3254.88063634 (a.u.)
Thermal correction to Gibbs free energy= 0.631236613972 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3239.73150343 (a.u.)
DFT-D3(BJ) correction to PBE= -0.12894892 (a.u.)

Cu	-0.09965608	-0.62010263	-0.53600305
N	-1.71525808	1.58071256	0.47868406
N	-0.14789999	1.02787367	1.85829425
C	-0.66933417	0.69867943	0.62743728
C	2.27157688	0.82732523	2.20493863
C	-2.24529594	2.47490742	-1.74217608
C	-2.57341509	1.60748542	-0.68053313
C	0.72318507	-0.80909154	3.22915089
C	-1.83391156	2.42618781	1.57934515
C	-3.69823269	0.75879838	-0.70903507
C	3.12632579	-1.00578828	3.55691201
C	-0.84690741	2.07843007	2.44807990
C	3.34188286	0.12914694	2.77885073
C	1.83136480	-1.46800236	3.77749368
C	-4.51476643	0.81033052	-1.84635410
C	-4.22156124	1.66456292	-2.90588264
C	-3.09720420	2.48472093	-2.85376998
C	0.97224222	0.33779230	2.44823156
C	-4.03780104	-0.19573558	0.42778987
H	-3.27509051	-0.06551894	1.21215715
C	-0.99773336	3.34813939	-1.72880062
H	-0.53589195	3.25756881	-0.73243842
C	-0.68121197	-1.34015039	3.48427735
H	-1.38987771	-0.66875756	2.97360713
C	2.53630653	2.04982539	1.33621906
H	1.56059442	2.47052841	1.04479028
H	-2.60449929	3.18762966	1.63783279
H	-0.57750149	2.47331775	3.42198364
H	-5.39436652	0.16363256	-1.90104447
H	-2.86944602	3.14279839	-3.69633926
H	1.67310713	-2.36176043	4.38673476
H	4.36272360	0.48091969	2.60771179
H	0.87970712	-0.92364951	-1.78169950
C	4.68950356	-2.76462277	-3.75748487
C	3.86896638	-2.73361511	-2.62852952
C	4.17766727	-3.12895086	-5.00298556
H	4.28707697	-2.42328892	-1.66966740
H	4.82315267	-3.15041369	-5.88405231
C	2.50926497	-3.08633245	-2.72044038
C	2.82814631	-3.48173659	-5.10312008
H	2.41382339	-3.79319570	-6.06584064
C	2.00568756	-3.47377040	-3.98019669
H	0.96980005	-3.80958983	-4.06442221
H	5.74298847	-2.48863615	-3.65832961
N	1.66305035	-3.08998051	-1.59500152
C	2.25332498	-3.04447129	-0.26623443
H	2.64316340	-2.03396757	-0.01477603
H	1.46257857	-3.29271069	0.45501006
H	3.06436258	-3.78251210	-0.19186815
C	0.39834012	-2.42191392	-1.70023880
O	-0.48443377	-2.59901885	-0.75211510
H	0.06250061	-2.41197121	-2.75449865
C	3.30553053	3.13958965	2.10530426
H	2.76971844	3.44167484	3.01916283
H	4.30943120	2.79338598	2.40049833
H	3.43385412	4.03067172	1.46945667
C	3.26741845	1.65318789	0.03983955
H	4.25085987	1.20462069	0.25753011
H	2.67009386	0.92585878	-0.53482029
H	3.43120935	2.54208089	-0.59135601
C	-1.01974059	-1.32235642	4.98708117
H	-2.05686202	-1.66068514	5.14434303
H	-0.35782738	-1.99591164	5.55559953
H	-0.91817219	-0.31079146	5.41142893
C	-0.86795061	-2.74579535	2.88324083
H	-0.17526332	-3.47108724	3.34162285
H	-1.89530984	-3.09978649	3.07007013

H	-0.70026689	-2.73997581	1.79351525
C	-3.97045761	-1.66245544	-0.03752853
H	-2.96570950	-1.91851400	-0.41265955
H	-4.20297765	-2.33420478	0.80528073
H	-4.70300865	-1.86085886	-0.83747661
C	-5.40879055	0.13613881	1.04689413
H	-6.22232038	0.00313346	0.31512352
H	-5.61113862	-0.53446346	1.89794373
H	-5.44658257	1.17577998	1.40950777
C	-1.32976885	4.83399720	-1.95559806
H	-1.76159268	5.00475905	-2.95510035
H	-2.04909745	5.20473108	-1.20816719
H	-0.41223316	5.44033870	-1.88252093
C	0.02942783	2.83641535	-2.75686333
H	0.94405344	3.45089171	-2.72018876
H	0.30398964	1.78986194	-2.54242486
H	-0.37531157	2.88627344	-3.78121353
H	-4.87258579	1.68752669	-3.78381806

IMesCu-O-CH2-NR2

Multiplicity: 1
E (PBE/L1, Priroda)= -3019.23539853 (a.u.)
Thermal correction to Gibbs free energy= 0.475478072412 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3004.16127158 (a.u.)
DFT-D3(BJ) correction to PBE= -0.10117341 (a.u.)

Cu	-0.09444094	0.08334605	-1.25165461
N	-1.37422509	2.18124619	0.25085241
N	0.41856554	1.50124205	1.24212900
C	-0.33484735	1.29094453	0.11208082
C	2.86255239	1.37373274	1.18126664
C	-2.32922448	3.26395236	-1.72936734
C	-2.44806847	2.31476409	-0.70128533
C	1.56062096	-0.42120208	2.25035322
C	-1.26848444	2.91449778	1.42817317
C	-3.58188116	1.49741699	-0.56199694
C	4.00823937	-0.50488757	2.24833544
C	-0.13874591	2.48587662	2.05293175
C	4.03570984	0.70190203	1.53931332
C	2.76511072	-1.05173637	2.58434451
C	-4.61825358	1.66133955	-1.48680207
C	-4.54426180	2.59716076	-2.52435187
C	-3.39440168	3.38781933	-2.62714407
C	1.63725237	0.79863371	1.55848396
C	-5.66113311	2.72427494	-3.53025263
H	-5.49608186	2.04062600	-4.38086879
H	-6.63394966	2.46754204	-3.08375199
H	-5.72264277	3.74634270	-3.93434003
C	-3.66770411	0.45704337	0.52417564
H	-4.65840786	-0.01947490	0.52585386
H	-2.90646540	-0.32742857	0.36690892
H	-3.48599416	0.88812194	1.52173203
C	-1.08343167	4.09761699	-1.88369034
H	-0.83649199	4.64518456	-0.96002802
H	-0.21739633	3.45546678	-2.12144524
H	-1.20427725	4.82647803	-2.69795398
C	0.23771342	-1.05682826	2.58560124
H	-0.24252589	-1.44522237	1.66994666
H	0.37778499	-1.90499927	3.26982896
H	-0.45768777	-0.33759472	3.04610245
C	2.91283943	2.65374310	0.38689178
H	2.41889477	2.52170803	-0.59132347
H	2.39343841	3.47817659	0.90164881
H	3.95437076	2.95841529	0.21000456
C	5.28908039	-1.19182259	2.65402479
H	5.62008877	-0.84797203	3.64922745
H	5.15642238	-2.28306630	2.70949081
H	6.10140097	-0.97647594	1.94301671
H	-2.00316379	3.66235581	1.70805983
H	0.31785651	2.78131542	2.99181964
H	-5.50981856	1.03294960	-1.39276599
H	-3.31848548	4.12337563	-3.43453485
H	2.72226298	-2.00776787	3.11536389
H	4.99912467	1.13409501	1.24919861
O	-0.05012815	-1.07370715	-2.62325353
C	0.78449855	-2.17552422	-2.72422590
H	0.20016407	-3.05386805	-3.07743741
H	1.58862517	-1.99996127	-3.47264817
N	1.48271789	-2.59418662	-1.49976436
C	2.89663418	-2.29596531	-1.36004841
H	3.12253902	-1.88009273	-0.36265192
H	3.54432758	-3.18197074	-1.52216361
H	3.16321869	-1.53304218	-2.10582008
C	0.84244840	-3.38253490	-0.56224197
C	-0.56601561	-3.55749552	-0.59564948
C	1.55608529	-4.03634333	0.47191972
C	-1.20538825	-4.36183110	0.34304769
C	0.89487537	-4.83337537	1.40628283
C	-0.48931890	-5.01024270	1.35573830
H	-1.15084818	-3.02187242	-1.34660495
H	2.64082700	-3.93431218	0.53263406
H	-2.29255612	-4.47422908	0.28700343
H	1.48115128	-5.33361631	2.18330106

IPrCu-O-CH2-NR2

Multiplicity: 1
E (PBE/L1, Priroda)= -3254.92064745 (a.u.)
Thermal correction to Gibbs free energy= 0.63521481387 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3239.76961873 (a.u.)
DFT-D3(BJ) correction to PBE= -0.13120770 (a.u.)

Cu	-0.02407517	-0.24951933	-1.23113436
N	-1.31264205	1.93004892	0.14731051
N	0.43940530	1.26925390	1.22066169
C	-0.29288813	1.00783825	0.08599671
C	2.87466323	0.98245398	1.15976065
C	-2.17290983	2.87774666	-1.94625282
C	-2.36490745	2.03103639	-0.83679859
C	1.46133632	-0.59345127	2.44453825
C	-1.21324477	2.73218807	1.27860736
C	-3.54009866	1.27725937	-0.64455520
C	3.87932936	-0.85835317	2.39216098
C	-0.10918058	2.31529058	1.95562072
C	4.00179285	0.25826324	1.56801442
C	2.62358104	-1.27810045	2.82338331
C	-4.54858166	1.40227192	-1.60834518
C	-4.39150848	2.23832775	-2.71072065
C	-3.21535151	2.96444582	-2.87761586
C	1.61813813	0.53329249	1.61306353
C	-3.71558590	0.31999819	0.52669730
H	-2.87247903	0.47748138	1.21886501
C	-0.87884899	3.64691528	-2.17467082
H	-0.24146859	3.50155103	-1.28737034
C	0.10088563	-1.05939453	2.94578926
H	-0.66683311	-0.45522568	2.43608085
C	3.02583712	2.18350522	0.23512217
H	2.04954986	2.69274131	0.18628282
H	-1.93240481	3.51595225	1.49196935
H	0.33592637	2.65962344	2.88308214
H	-5.47097595	0.82727839	-1.49459042
H	-3.09808797	3.60815042	-3.75313721
H	2.53853841	-2.15941415	3.46389233
H	4.99261921	0.57426319	1.23173245
O	0.04748461	-1.41509633	-2.59470876
C	1.05541919	-2.33791499	-2.83489950
H	0.63101204	-3.18648480	-3.41475466
H	1.87526335	-1.90164079	-3.44726030
N	1.71962566	-2.90988056	-1.65477274
C	3.09290344	-2.54055530	-1.36753195
H	3.22872482	-2.29090193	-0.30044663
H	3.82013170	-3.33587542	-1.63192462
H	3.33910867	-1.64250159	-1.95204562
C	1.11913146	-3.93886886	-0.95119755
C	-0.25234292	-4.24659472	-1.14508942
C	1.83700578	-4.71499941	-0.00941972
C	-0.85099194	-5.29156076	-0.44853052
C	1.21554238	-5.75401491	0.68335002
C	-0.13012216	-6.05976675	0.47289373
H	-0.84537913	-3.62296224	-1.81746208
H	2.89394729	-4.51352240	0.17211274

H	-1.91126564	-5.50041521	-0.62092717
H	1.80369035	-6.33903844	1.39692910
H	-0.61033147	-6.87547291	1.01815592
H	4.77255353	-1.40878635	2.69932896
H	-5.19137997	2.31915900	-3.45130019
C	-5.01328164	0.58929662	1.30927675
H	-5.90638717	0.40418100	0.69084511
H	-5.07072277	-0.08086846	2.18225757
H	-5.05900881	1.62956401	1.66862926
C	-3.64502940	-1.14069818	0.04099292
H	-2.68849483	-1.33827178	-0.47152365
H	-3.72911815	-1.83224779	0.89503049
H	-4.46241255	-1.36283531	-0.66456434
C	-1.12449618	5.15844069	-2.33055375
H	-1.73005431	5.37982746	-3.22428311
H	-1.64862424	5.57328234	-1.45501443
H	-0.16373379	5.68725879	-2.44055571
C	-0.11849090	3.07217825	-3.38511384
H	0.83863974	3.60202658	-3.52134759
H	0.09307263	1.99921091	-3.24073449
H	-0.70541669	3.18224413	-4.31170507
C	-0.03449758	-0.81264923	4.46153012
H	-1.03637323	-1.11551982	4.80709571
H	0.70925839	-1.39958768	5.02503426
H	0.11138463	0.24977076	4.71463599
C	-0.17070837	-2.53239813	2.59564802
H	0.54456638	-3.20881851	3.09020716
H	-1.18157846	-2.81437112	2.93225891
H	-0.10615981	-2.71015528	1.51132226
C	4.05308690	3.20068643	0.76275944
H	3.80076448	3.53599663	1.78108844
H	5.07029392	2.77760309	0.78694386
H	4.07851595	4.08411049	0.10435896
C	3.37435605	1.72448151	-1.19363102
H	4.33360295	1.18135685	-1.21131705
H	2.58882318	1.05681342	-1.58759002

R3Si-O-CH2-NR2

Multiplicity: 1
E (PBE/L1, Priroda)= -963.34709994 (a.u.)
Thermal correction to Gibbs free energy= 0.222587965324 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -962.486778855 (a.u.)
DFT-D3(BJ) correction to PBE= -0.04369376 (a.u.)

O	-1.13077169	1.79184485	-0.45609264
C	-0.54114021	0.94234702	-1.44899704
H	-1.22563566	0.98346209	-2.31561120
H	0.43988034	1.35046078	-1.74680373
N	-0.33314717	-0.42457777	-1.03182824
C	1.02703613	-0.94915024	-1.02108611
H	1.18047702	-1.61435060	-0.15542380
H	1.27608090	-1.51227366	-1.94173656
H	1.72799708	-0.11020985	-0.91748450
C	-1.41085728	-1.31930975	-1.07921969
C	-2.74075126	-0.84216184	-1.11124307
C	-1.20725366	-2.71514086	-1.08669126
C	-3.81068174	-1.73116230	-1.17202545
C	-2.29188226	-3.59119564	-1.13838584
C	-3.60127205	-3.11267426	-1.18752636
H	-2.93275595	0.23089485	-1.04994871
H	-0.19721945	-3.12570832	-1.06257487
H	-4.82850486	-1.33189810	-1.19284790
H	-2.10148465	-4.66796111	-1.14650100
H	-4.44595630	-3.80378821	-1.22925659
Si	-0.71895184	1.66162946	1.17816545
H	-1.21151557	0.39610416	1.81750640
H	-1.42443173	2.84600415	1.76532484
C	1.14733717	1.77418174	1.46001308
C	1.82167810	0.82350794	2.24698433
C	1.90053555	2.81564400	0.88459055
C	3.20005662	0.91068184	2.45800154
C	3.27915727	2.90188977	1.08679173
C	3.93039150	1.94914078	1.87576685
H	1.25832101	0.00117604	2.70093147
H	1.39993566	3.57260901	0.27067066
H	3.70696608	0.16509615	3.07678631
H	3.84885200	3.71713457	0.63230265

TS_R3Si-O-CH2-NR2_H-SiR3

Multiplicity: 1
E (PBE/L1, Priroda)= -1486.56808109 (a.u.)
Thermal correction to Gibbs free energy= 0.3203665221825599 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -1485.01259326 (a.u.)

DFT-D3(BJ) correction to PBE= -0.06577968 (a.u.)

O	-0.33718703	0.61919886	-0.89318253
C	0.50165270	-1.19052461	0.62913227
H	-0.34439889	-1.32790629	1.29683991
H	0.43151511	-1.44710460	-0.42183178
N	1.67006175	-0.83752321	1.11646607
C	2.81970384	-0.70482074	0.19969507
H	3.34637489	0.23288536	0.42235640
H	3.50628448	-1.55508382	0.32369429
H	2.44495501	-0.67870346	-0.83150725
C	1.85994884	-0.48702082	2.49838743
C	0.79459525	0.04481790	3.23513594
C	3.11416054	-0.67498371	3.09402965
C	0.98963653	0.37194001	4.57549840
C	3.28932559	-0.35132025	4.43913805
C	2.22985348	0.16842729	5.18538377
H	-0.15898183	0.25639726	2.73459072
H	3.94899813	-1.08576042	2.52423335
H	0.16233534	0.80508253	5.14275237
H	4.26482311	-0.50939952	4.90469830
H	2.37368806	0.42328740	6.23782817
Si	-0.16607373	1.07313746	-2.51691795
H	0.39719903	2.44467366	-2.75840099
H	-1.37855313	0.81860370	-3.36436778
C	1.18392985	-0.13140118	-3.14069835
C	2.48448040	0.31460565	-3.44066059
C	0.91915458	-1.50813504	-3.28691001
C	3.48329726	-0.57341270	-3.85302928
C	1.91214062	-2.40269261	-3.69475855
C	3.19988879	-1.93590441	-3.97563970
H	2.71864341	1.38136814	-3.35091068
H	-0.09094093	-1.88769105	-3.09035570
H	4.48540673	-0.20065719	-4.08475729
H	1.68021365	-3.46606255	-3.80519732
H	3.97758128	-2.63233910	-4.30094172
H	-1.72963452	2.32874218	-1.39782033
Si	-1.57851910	1.53480021	-0.01177933
H	-1.25891976	0.55779731	1.20913076
H	-1.16540726	2.78374604	0.74972217
C	-3.46724125	1.15011684	0.06460755
C	-4.01331505	0.38796334	1.11177702
C	-4.35186707	1.64784251	-0.90822864
C	-5.38612512	0.14433585	1.19830636
C	-5.72592902	1.40692222	-0.83300138
C	-6.24707888	0.65444892	0.22282797
H	-3.33970560	-0.01949967	1.87442903
H	-3.94500245	2.23650754	-1.73751043
H	-5.78823126	-0.44776029	2.02610927
H	-6.39465658	1.80605021	-1.60160037
H	-7.32207980	0.46200886	0.28323766

TS_R3Si-O-CH2-NR2_H-SiR3 (ImesCu-H assisted)

Multiplicity: 1
E (PBE/L1, Priroda)= -3542.47546533 (a.u.)
Thermal correction to Gibbs free energy= 0.5738005163 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3526.69862308 (a.u.)

DFT-D3(BJ) correction to PBE= -0.12887837 (a.u.)

O	0.565253900	-1.415596860	0.191146610
C	-1.420320450	-2.382014760	-0.774252370
H	-1.180899170	-2.994645330	0.088339770
H	-2.027800670	-1.480276490	-0.674776980
N	-1.210697740	-2.873736910	-1.976891990
C	-1.550576440	-2.074143000	-3.160895870
H	-0.870190440	-1.181535950	-3.137929450
H	-1.402838380	-2.677957210	-4.063065550
H	-2.591588310	-1.729633000	-3.088791810
C	-0.355470800	-4.021225220	-2.150548060
C	-0.742666510	-5.056161520	-3.008103510
C	0.858435980	-4.064588110	-1.458596730
C	0.097040000	-6.158948980	-3.161933000
C	1.685228290	-5.177184680	-1.621419810
C	1.309515100	-6.222303750	-2.468668960
H	-1.699611740	-5.008647560	-3.533820960
H	1.123695150	-3.203943700	-0.827004020
H	-0.201736510	-6.976670910	-3.822155190
H	2.638919310	-5.217032700	-1.089139650
H	1.964167440	-7.088168110	-2.594657650
Si	0.967720750	-1.521750610	1.779540670
H	0.755359200	-2.932362290	2.304143630
H	0.139240970	-0.639523510	2.700928310
C	2.796278510	-1.089713640	2.085665940
C	3.370524810	-1.207629020	3.363711520
C	3.610787230	-0.649815250	1.029232960
C	4.714729430	-0.898159810	3.582037030
C	4.958148260	-0.343048020	1.241492730
C	5.512666930	-0.466575010	2.517542350
H	2.757637970	-1.549488620	4.206566360
H	3.174813960	-0.544229940	0.029887170
H	5.144775420	-0.997220460	4.583161950
H	5.577881570	-0.006043960	0.405058570
H	6.567324520	-0.229700520	2.684861010
Cu	-0.107102010	0.254924520	-0.758090690
N	-2.207373510	1.979540460	0.398942630
N	-0.274373400	2.913107570	0.582938820
C	-0.864630020	1.729961790	0.188711470
C	1.765614240	3.485873990	-0.650529790
C	-3.738662250	0.925258580	-1.196361370
C	-3.241719610	1.023550670	0.115735490
C	1.869292440	3.028432580	1.764290270
C	-2.433745570	3.264644110	0.891491890
C	-3.726197690	0.213006840	1.158562040
C	3.903518240	3.603461030	0.535866360
C	-1.213591150	3.851948160	1.006176010
C	3.148449300	3.709247350	-0.635143610
C	3.245676690	3.263893810	1.724187340
C	-4.736898510	-0.707660170	0.858005540
C	-5.265687620	-0.831792470	-0.432643950
C	-4.749718510	-0.012553170	-1.443688160
C	1.146585690	3.146763620	0.563225800
C	-6.383551770	-1.805185170	-0.717276660
H	-6.275820530	-2.724683450	-0.121111320
H	-7.362065690	-1.362219850	-0.463595480
H	-6.412709060	-2.082743350	-1.781979640
C	-3.152728310	0.309763640	2.548583700
H	-3.661110290	-0.390956680	3.226587270
H	-2.074540260	0.074485880	2.545656830
H	-3.256833470	1.326802030	2.959588870
C	-3.170896900	1.771884460	-2.303387130
H	-3.207841690	2.844027100	-2.051870400
H	-2.105624380	1.511965870	-2.461281710
H	-3.724243150	1.611745590	-3.240293890
C	1.194149940	2.622346180	3.049233080
H	0.714907200	1.635040320	2.941968170
H	1.929235630	2.559534800	3.864259500
H	0.408127320	3.336492580	3.344582720
C	0.981256690	3.573089680	-1.932316450
H	0.611481590	2.568256630	-2.216601390
H	0.099525130	4.225891160	-1.826403440
H	1.611229940	3.961738900	-2.745775050
C	5.396287720	3.823135250	0.525965660
H	5.693159200	4.583936090	1.266442430
H	5.926571160	2.891112110	0.784137160
H	5.745993690	4.152957060	-0.463847960
H	-3.430741990	3.637281660	1.103491350
H	-0.926934070	4.844406800	1.338678380
H	-5.118876780	-1.348622810	1.659793280
H	-5.150002530	-0.096812730	-2.459994920
H	3.823165040	3.156002060	2.647960230
H	3.647214650	3.970755740	-1.574209200
H	0.077031660	0.056638580	-2.299325110

TS_R3Si-O-CH2-NR2_H-SiR3 (IPrCu-H assisted)

Multiplicity: 1
E (PBE/L1, Priroda)= -3778.15669619 (a.u.)
Thermal correction to Gibbs free energy= 0.7329296277 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3762.30411974 (a.u.)

DFT-D3(BJ) correction to PBE= -0.15773263 (a.u.)

O	0.795958540	-1.728402830	0.253757150
C	-0.928117900	-2.884011170	-0.956765010
H	-0.772458440	-3.455585120	-0.047061710
H	-1.601538050	-2.024952960	-0.975945640
N	-0.520426340	-3.390519860	-2.101145420
C	-0.765114440	-2.658717600	-3.350668820
H	-0.235514990	-1.675761550	-3.237086690
H	-0.375379700	-3.239070180	-4.194156080
H	-1.840787440	-2.471130900	-3.473425330
C	0.426302070	-4.477810600	-2.119316980
C	0.219049820	-5.569496910	-2.968775450
C	1.548047740	-4.405788460	-1.289659640
C	1.146641590	-6.611147300	-2.970992940
C	2.465301550	-5.457325970	-1.300339800
C	2.267623560	-6.558480690	-2.136803320
H	-0.667664270	-5.612245300	-3.606230180
H	1.677025010	-3.506379730	-0.673540200
H	0.987937780	-7.472926180	-3.623680790
H	3.346335180	-5.402558990	-0.655922670
H	2.990482320	-7.377925360	-2.144185680
Si	1.055300400	-2.069365550	1.836649890
H	0.321086700	-3.338934080	2.249502790
H	0.582523160	-1.006765930	2.808483690
C	2.900391210	-2.394104680	2.183666390
C	3.334980530	-2.971101010	3.389969250
C	3.870821470	-2.051520560	1.225711950
C	4.691179230	-3.197336690	3.634824270
C	5.230014900	-2.276228150	1.465327780
C	5.642307780	-2.849562180	2.670613090
H	2.600343310	-3.253322040	4.153635220
H	3.547108510	-1.598996020	0.281830430
H	5.009937930	-3.648307060	4.579205270
H	5.970861220	-2.000519060	0.708936610
H	6.704768940	-3.026217340	2.860365380
Cu	0.077159020	-0.086637830	-0.710265030
N	-2.071888310	1.647902010	0.334044740
N	-0.161930000	2.647511530	0.432253840
C	-0.721351170	1.419329780	0.129540510
C	1.712650740	3.423889320	-0.942338510
C	-3.688512530	0.667225030	-1.222855380
C	-3.086837360	0.665718270	0.052380710
C	2.086896590	2.791961510	1.419744340
C	-2.330971410	2.965290850	0.710276180
C	-3.444063150	-0.260025690	1.058302290
C	3.922567150	3.620374540	0.053610680
C	-1.127859660	3.593336750	0.771462450
C	3.070640750	3.756507420	-1.037591490
C	3.434673990	3.139660970	1.266898210
C	-4.430504690	-1.204327920	0.747042890
C	-5.037370850	-1.227427160	-0.508272110
C	-4.670183390	-0.300917200	-1.479460250
C	1.242870110	2.951739410	0.299777440
C	-2.812296800	-0.209822130	2.443913510
H	-1.786918270	0.176666420	2.317613760
C	-3.317510030	1.672899510	-2.305234290
H	-2.544301190	2.338840370	-1.891222940
C	1.559642030	2.291847170	2.759008370
H	0.670981470	1.673688360	2.547141230
C	0.806020520	3.596924850	-2.153730200
H	-0.187627150	3.204554700	-1.885205820
H	-3.336893660	3.329676080	0.890708410

H	-0.870184410	4.618325700	1.016348000
H	-4.729128670	-1.935751820	1.501022610
H	-5.154410420	-0.322870000	-2.459698900
H	4.116118680	3.025091100	2.112423420
H	3.463649520	4.126340570	-1.988311820
H	0.326082600	-0.374246780	-2.231972060
H	-5.806422220	-1.973319990	-0.727191140
H	4.979032040	3.885127280	-0.041654350
C	-3.587328650	0.765118390	3.355408140
H	-4.627065730	0.423863000	3.491344090
H	-3.110000500	0.817363770	4.347642820
H	-3.611008430	1.781989330	2.935716050
C	-2.702741440	-1.585720830	3.116406520
H	-3.691150430	-1.996231080	3.381689200
H	-2.181847220	-2.311965940	2.473607490
H	-2.124340700	-1.493262750	4.049046240
C	2.566397510	1.405573800	3.508900690
H	2.081238840	0.964373230	4.394068070
H	2.931336840	0.581240870	2.878085500
H	3.434771200	1.983638550	3.865842580
C	1.124292140	3.473805090	3.650268800
H	0.342929430	4.081923040	3.169484880
H	0.725459070	3.101745010	4.608473090
H	1.983560020	4.129658840	3.868210210
C	0.648940520	5.086221140	-2.516790820
H	0.249170780	5.667653290	-1.670467850
H	1.616190190	5.530400410	-2.804464390
H	-0.040969340	5.199118560	-3.369339530
C	1.302331550	2.772154800	-3.354001430
H	1.324811200	1.701069660	-3.093820360
H	0.617912040	2.905436250	-4.208500400
H	2.308725960	3.086612910	-3.676417650
C	-4.527390210	2.542691500	-2.695656010
H	-4.224889800	3.298166240	-3.439068390
H	-5.332566720	1.936236350	-3.142088500
H	-4.945253810	3.067189280	-1.821564050
C	-2.701404830	0.977193890	-3.532099470
H	-1.778274790	0.448283290	-3.240472510
H	-3.406587400	0.260151110	-3.985486620
H	-2.442395990	1.725744020	-4.299242460

TS_IMesCu-O-CH2-NR2_R3Si-H

Multiplicity: 1
E (PBE/L1, Priroda)= -3542.51028606 (a.u.)
Thermal correction to Gibbs free energy= 0.580770652728 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3526.73555969 (a.u.)
DFT-D3(BJ) correction to PBE= -0.12933514 (a.u.)

Cu	0.74621456	0.59818935	-0.19572730
N	-0.30500545	-0.26673813	2.34011888
N	1.84940537	-0.40641721	2.34466779
C	0.78887520	-0.08790290	1.52868421
C	3.90870760	0.82778669	1.83896794
C	-2.18749776	1.27456621	2.05276061
C	-1.65651659	-0.01818578	1.89905002
C	3.84197131	-1.61933452	1.60260517
C	0.06368914	-0.67721781	3.61615171
C	-2.37959939	-1.06284404	1.30417175
C	5.89981395	-0.39296718	1.10549792
C	1.42131393	-0.76481534	3.62149819
C	5.24632855	0.80098455	1.43047636
C	5.18171825	-1.58999428	1.20013089
C	-3.67262515	-0.77691609	0.84870948
C	-4.23492608	0.49717904	0.96735790
C	-3.48017438	1.50615173	1.57854613
C	3.22436771	-0.39722614	1.91792329
C	-5.60757942	0.80031560	0.42064465
H	-5.53345915	1.49969925	-0.42901986
H	-6.11118748	-0.11367533	0.07211571
H	-6.24493568	1.27671488	1.18320692
C	-1.78025864	-2.43242848	1.12029915
H	-2.52779172	-3.13070989	0.71908691
H	-0.94435994	-2.39720370	0.40134983
H	-1.38788036	-2.83868208	2.06654857
C	-1.37697084	2.38398641	2.67075357
H	-1.02603289	2.12210291	3.68240104
H	-0.48341866	2.59446942	2.05795285
H	-1.97310454	3.30498519	2.73552595
C	3.08868381	-2.92317080	1.68147938
H	2.13982995	-2.86735810	1.12339381
H	3.69257135	-3.74254266	1.26574284
H	2.83192326	-3.18508157	2.72128465
C	3.22683278	2.13039045	2.16528099
H	2.46248308	2.36816982	1.40295089
H	2.70792257	2.08651740	3.13609112
H	3.95563053	2.95302601	2.19203999
C	7.33391846	-0.38423929	0.63724050
H	7.91476516	0.40224288	1.14331038
H	7.82299183	-1.35206085	0.82514127
H	7.38928710	-0.18766237	-0.44734816
H	-0.66919601	-0.86418646	4.39409674
H	2.11864098	-1.03935956	4.40601112
H	-4.24517164	-1.57651265	0.36842856
H	-3.89812249	2.51396351	1.66355709
H	5.67668504	-2.53454620	0.95149877
H	5.79386134	1.74701888	1.36761773
O	0.78550022	0.54687848	-2.17761012
C	0.94400855	-0.45399051	-3.19539242
H	0.18125704	-0.27168663	-3.97387878
H	1.94198901	-0.32819677	-3.65054246
N	0.84857802	-1.79824069	-2.70424091
C	2.07314782	-2.49017608	-2.33518791
H	2.00041663	-2.92359977	-1.32249545
H	2.33001219	-3.30273358	-3.04269238
H	2.89660395	-1.76330978	-2.32328945
C	-0.37404653	-2.45804034	-2.62068730
C	-1.59767551	-1.77106807	-2.80348978
C	-0.43345385	-3.84438947	-2.34841978
C	-2.80932446	-2.45333396	-2.74736618
C	-1.65819474	-4.50959096	-2.28983799
C	-2.85860366	-3.82775171	-2.49298363
H	-1.60250375	-0.69141213	-2.96683587
H	0.48497205	-4.41389350	-2.19965889
H	-3.73508923	-1.88994660	-2.89447549
H	-1.66588966	-5.58456933	-2.08804944
H	-3.81439732	-4.35491738	-2.45271355
H	0.89877673	3.12241215	-2.87987600
Si	-0.12989798	2.14725188	-2.36622123
H	-0.79523380	1.56025908	-3.62559274
H	0.35342192	2.18476346	-0.76038043
C	-1.68112092	3.19790464	-1.86409846
C	-1.64915296	4.09976775	-0.78740291
C	-2.86873283	3.11712135	-2.60868155
C	-2.74469828	4.90854594	-0.47967342
C	-3.98079007	3.90752222	-2.29838510
C	-3.91942840	4.80950568	-1.23357712
H	-0.73984099	4.16825523	-0.17754891
H	-2.91647741	2.42207142	-3.45527076
H	-2.68793364	5.61901442	0.35116631
H	-4.89572989	3.82560661	-2.89345725

TS_IMesCu-OH_R3Si-H

Multiplicity: 1
E (PBE/L1, Priroda)= -3177.71285872 (a.u.)
Thermal correction to Gibbs free energy= 0.44177731387 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3162.05800878 (a.u.)
DFT-D3(BJ) correction to PBE= -0.09657931 (a.u.)

Cu	1.07265553	-0.32149496	-0.47448727
N	-1.02594658	1.63251260	-0.19629959
N	0.84772417	2.43264889	0.51698468
C	0.30263904	1.31117091	-0.05838413
C	3.12142342	3.10092998	-0.10234483
C	-2.27400322	0.76947293	-2.12120651
C	-1.99625440	0.71799540	-0.74692776
C	2.67597542	2.15985248	2.12603670
C	-1.29542438	2.91152868	0.27842416
C	-2.60036114	-0.22017177	0.10842782
C	4.94211102	2.84837884	1.51183525
C	-0.11485954	3.41708591	0.72880617

C	4.46737335	3.23498930	0.25352275
C	4.03210459	2.31553667	2.43158036
C	-3.49516854	-1.13181145	-0.45632731
C	-3.79914069	-1.11999341	-1.82316939
C	-3.18710238	-0.15945997	-2.63437180
C	2.24266925	2.56482128	0.85297774
C	-4.74699770	-2.14193736	-2.39865468
H	-4.36907850	-3.16083710	-2.21296866
H	-5.74173079	-2.07048185	-1.92860053
H	-4.87022847	-2.00968587	-3.48388869
C	-2.26656374	-0.26930962	1.57627358
H	-2.88069698	-1.02563842	2.08408836
H	-1.20634448	-0.54031980	1.71896679
H	-2.42779499	0.70563269	2.06448721
C	-1.58540804	1.76125115	-3.02399389
H	-1.74878821	2.80047165	-2.69546415
H	-0.49469649	1.59216450	-3.02937774
H	-1.95376334	1.66456074	-4.05547901
C	1.72123598	1.55223792	3.12092868
H	1.33608107	0.58720741	2.74786970
H	2.22568562	1.37246889	4.08104145
H	0.84846429	2.19999934	3.30136193
C	2.63825116	3.49212682	-1.47492815
H	2.26866325	2.60633103	-2.02013104
H	1.80587543	4.21257635	-1.42771278
H	3.45402776	3.94181130	-2.05892638
C	6.40571401	2.96996535	1.85594068
H	6.55164787	3.13172293	2.93488468
H	6.94640533	2.04720394	1.58328631
H	6.87753061	3.80274218	1.31239212
H	-2.29366677	3.33615011	0.25421354
H	0.13094254	4.37413529	1.17715847
H	-3.94584015	-1.89224188	0.18906068
H	-3.41135065	-0.13982658	-3.70582792
H	4.38639818	2.00662725	3.42034832
H	5.16560991	3.65296435	-0.47892912
O	2.04881263	-1.69562636	-1.46976219
H	0.83082310	-1.87705776	0.40522174
Si	1.00438532	-3.07724918	-0.69647727
H	0.72839664	-3.55737490	-2.12737550
H	2.11132221	-3.89966614	-0.09570476
C	-0.61055874	-3.90473002	0.02016496
C	-1.45834510	-4.65466687	-0.81088453
C	-0.95763545	-3.81015570	1.37862832
C	-2.60041719	-5.29106878	-0.31205097
C	-2.08890393	-4.44795094	1.89295312
C	-2.91885955	-5.18928871	1.04448975
H	-1.21136905	-4.74159539	-1.87611384
H	-0.32225614	-3.21959012	2.05121254
H	-3.24212554	-5.87315557	-0.98144501
H	-2.32816495	-4.37001533	2.95839603
H	-3.80822103	-5.68733537	1.44134798

TS_IPrCu-OH_R3Si-H

Multiplicity: 1
E (PBE/L1, Priroda)= -3413.39544397 (a.u.)
Thermal correction to Gibbs free energy= 0.598928799082 (a.u.)
E (PBE/def2-tzvpp, G09, SMD)= -3397.66480326 (a.u.)
DFT-D3(BJ) correction to PBE= -0.12549014 (a.u.)

Cu	0.03846356	-0.83145153	-0.86424606
N	-1.74457977	1.46141412	-0.74990531
N	-0.77703181	1.11778290	1.14633912
C	-0.85802246	0.61414348	-0.12935733
C	1.35463293	1.12192649	2.35827034
C	-1.38689183	1.99132031	-3.11800366
C	-2.14681843	1.33216649	-2.13137750
C	-0.43199685	-0.47222946	2.98487354
C	-2.19651054	2.45458640	0.11162960
C	-3.28261945	0.55490457	-2.43269016
C	1.67622400	-0.43740392	4.19753675
C	-1.58643803	2.23611818	1.30861176
C	2.14441498	0.59362796	3.38747103
C	0.40451368	-0.96635236	3.99355558
C	-3.65063612	0.44927747	-3.78000406
C	-2.92000208	1.08953110	-4.77780488
C	-1.80066073	1.84969464	-4.44879542
C	0.06831983	0.57417630	2.18564107
C	-4.07033565	-0.19004965	-1.36336431
H	-3.69374133	0.13592218	-0.38025760
C	-0.13564472	2.79344207	-2.78627501
H	-0.08218209	2.89469146	-1.69008600
C	-1.80549044	-1.08994964	2.76039876
H	-2.33219605	-0.47543666	2.01205748
C	1.90963980	2.22119691	1.46209346
H	1.12327028	2.49767969	0.74126412
H	-2.90246676	3.21480963	-0.20579036
H	-1.64985243	2.76585269	2.25328536
H	-4.52367541	-0.14987574	-4.05089602
H	-1.23102320	2.34172060	-5.24109914
H	0.05361762	-1.78502028	4.62665370
H	3.15020178	0.99082102	3.54627590
O	0.61561382	-2.33647478	-1.90687901
H	1.72317024	-1.53524775	-0.21217144
Si	2.38957301	-2.52577956	-1.30991584
H	2.44078880	-3.80931671	-2.15411765
H	3.16605387	-1.51456378	-2.12478422
C	3.64426648	-3.17346065	0.02555321
C	4.49354850	-4.25230345	-0.27397438
C	3.77467541	-2.57534039	1.28891400
C	5.45722591	-4.69685219	0.63510554
C	4.73112303	-3.01453028	2.20883952
C	5.57926620	-4.07614581	1.88181615
H	4.39120829	-4.75428306	-1.24392720
H	3.10388890	-1.75063262	1.55835901
H	6.11144647	-5.53529704	0.37615134
H	4.81316202	-2.53260352	3.18849684
H	6.32637805	-4.42641288	2.59992171
H	-3.22462826	0.99289885	-5.82315294
H	2.31259666	-0.84003627	4.98961985
C	-5.57396351	0.13379479	-1.41535069
H	-6.03162044	-0.20999224	-2.35696933
H	-6.09654065	-0.37400513	-0.58856175
H	-5.75570026	1.21636365	-1.32542769
C	-3.81820515	-1.70615667	-1.47156564
H	-4.35573949	-2.24265815	-0.67276194
H	-4.16609263	-2.09732823	-2.44180341
H	-2.74193429	-1.92885489	-1.37719727
C	-0.17862402	4.21252728	-3.38056513
H	0.71114532	4.77911903	-3.06180172
H	-0.18011265	4.19242600	-4.48229743
H	-1.07453603	4.76115421	-3.04959670
C	1.12508717	2.03311413	-3.23988815
H	2.03225820	2.59519840	-2.96505759
H	1.17782891	1.03957489	-2.76274786
H	1.12848609	1.88666464	-4.33245381
C	-2.65774516	-1.09223190	4.04219907
H	-3.66230375	-1.49033140	3.82522012
H	-2.21182695	-1.72704939	4.82468022
H	-2.76991386	-0.07627359	4.45258922
C	-1.66671280	-2.50850949	2.17630089
H	-1.10017722	-2.48790239	1.22967745
H	-1.13403707	-3.17513245	2.87372049
H	-2.66106316	-2.94072269	1.97759441
C	2.26865151	3.48354466	2.26777052
H	1.39850711	3.87022614	2.82194271
H	3.07003852	3.27966076	2.99627915
H	2.62666555	4.27570269	1.59018493
C	3.11596140	1.71073276	0.65137695
H	3.95164526	1.42765694	1.31174951
H	2.84477044	0.82644315	0.05286370
H	3.47495260	2.49938879	-0.03001558

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