Supplemental documents

Experimental

General Considerations: All manipulations involving the synthesis and handling of copper(I) compounds were performed in a nitrogen filled drybox. All manipulations involving the synthesis of the pyrrole and the pyrrolidine were preformed in air. The chemicals: CuCl, 2.5M BuLi in hexanes, tert-butyl amine, and diethyl sulfate were purchased from Aldrich Chemical Company and used as received. All solvents used in manipulation of copper(I) compounds were ACS grade and purified from an Mbraun Solvent Purifier System. All other solvents were ACS grade and used as received. Nuclear Magnetic Resonance was done on 300 MHz Avance 3 and 400 MHz Bruker AMX. Canadian Microanalytical Service Ltd. performed combustion analysis. Thermogravimetric analysis was performed on a TA Instruments Q50 apparatus located in an MBraun Labmaster 130 Dry box under a nitrogen atmosphere. 5, 5-dimethyl-2-pyrrolidone was prepared by literature procedures.[i] Tert-butyl ammonium chloride was prepared by addition of $HCl_{(aq)}$ to tert-butyl amine in ethanol followed by solvent removal.

5-ethoxy-3, 4-dihydro-2,2-dimethyl-2H-pyrrole: Similar to the literature preparation for 5-ethoxy-3, 4-dihydro-2H-pyrrole:[ii] 5, 5-dimethyl-2-pyrrolidone (9.82 g, 86.8 mmol) and diethyl sulfate (13.38 g, 86.8 mmol) were added to a pressure vessel and heated for 24 h at 60 °C. Et_2O (30 ml) was added and the biphasic mixture was cool in an ice bath. A 25 ml aqueous solution of Na_2CO_3 (9.20 g, 86.8 mmol) was added drop wise. The top organic layer was separated and extraction continued with 3 x 40 ml of Et_2O. The combined extractions were dried over $MgSO_4$. The majority of Et_2O was removed on a roto-vap followed by condensation of the remaining volatiles into a cold trap under reduced pressure thereby transferring remaining Et_2O and product to the cold trap. A solution of the intended product (11.45 g, 93.4%) in 10.65 g of Et_2O was obtained and used without additional purification. ^1H NMR (400 MHz, $CDCl_3$): δ 4.16 (q, 2H, $COCH_2CH_3$), δ 2.53 (t, 2H, $NC(CH_3)_2CH_2CH_2C$), δ 1.80 (t, 2H, $NC(CH_3)_2CH_2CH_2C$), δ 1.30 (t, 3H, $COCH_2CH_3$), δ 1.23 (s, 6H, $NC(CH_3)_2CH_2CH_2C$). ^{13}C NMR (400 MHz, $CDCl_3$): δ 170.05 (NCO), δ 67.36 (NC(CH_3)_2), δ 63.67 (OCH_2CH_3), δ 36.73 (NC(CH_3)_2CH_2CH_2C), δ 31.58 (NC(CH_3)_2CH_2CH_2C), δ 29.84 (NC(CH_3)_2CH_2CH_2C), δ 14.41 (OCH_2CH_3). HRMS (EI) m/z calcd for $C_8H_{15}NO$ M^+ 141.1154, found 141.1164.

Tertbutyl-imino-2,2-dimethylpyrrolidine: In a pressure vessel, 5-ethoxy-3,4-dihydro-2,2-dimethyl-2H-pyrrole (11.45 g, 81.1 mmol) in 10.65 g of Et_2O, tert-butyl ammonium chloride (8.89 g, 81.1 mmol), and tert butyl amine (11.86g, 162.2 mmol) were dissolved in 80 mL of ethanol. The pressure vessel was heated to 130 °C for 2 days with stirring. The vessels was removed from heat and cooled to room temperature. Volatiles were stripped under reduced pressure. The solid residue was dissolved in 80 mL of H_2O and made basic with 40 mL of 6 M NaOH. The aqueous solution was extracted with 3 x 60 mL of Et_2O. The combined Et_2O extractions were dried over Na_2SO_4 and then the solution was concentrated under reduced pressure to obtain 11.43 g of a light yellow liquid, 83.8%. ^1H NMR (400 MHz, $CDCl_3$): δ 2.46 (t, 2H, $NC(CH_3)_2CH_2CH_2C$), δ 1.65 (t, 2H, $NC(CH_3)_2CH_2CH_2C$), δ 1.34 (s, (H, $NC(CH_3)_3$), δ 1.19 (s, 6H, $NC(CH_3)_2CH_2CH_2C$) ^{13}C NMR (400 MHz, $CDCl_3$): δ 161.57 (NCO), δ 69.03 (NC(CH_3)_2), δ 50.81 (NC(CH_3)_3), δ 36.60 (NC(CH_3)_2CH_2CH_2C), δ 34.62 (NC(CH_3)_2CH_2CH_2C), δ 29.85 (NC(CH_3)_2), δ 29.30 (NC(CH_3)_3). HRMS (EI) m/z calcd for $C_{10}H_{20}N_2$ M^+ 168.1626, found 168.1618.

Copper(I) tertbutyl-imino-2,2-dimethylpyrrolidinate (1): Tertbutyl-imino-2,2-dimethylpyrrolidine (5.103 g, 13.07 mmol) was dissolved in 170 mL of toluene and the solution was cooled on an ice bath. 12.13 ml of 2.5 M BuLi was added dropwise. The solution warmed to r.t as it stirred overnight. CuCl (3.26 g, 32.9 mmol) was added and stirring continued for 18 h. The cloudy, light brown solution was filtered and the filter cake was extracted with 4 x 20 of THF. Volatiles were stripped from the combined toluene and THF solutions to afford an off-white solid. The solid was sublimed at 130°C at 40 mtorr

and 5.795 g, 82.7 %, of a white solid was obtained. Mp >270°C. ^{1}H NMR (300 MHz, C$_6$D$_6$): δ 2.428 (t, 2H, NC(CH$_3$)$_2$CH$_2$CH_2C), δ 1.581 (t, 2H, NC(CH$_3$)$_2$CH_2CH$_2$C), δ 1.328 (s, 9H, NC(CH_3)$_3$), δ 1.196 (s, 6H, NC(CH_3)$_2$CH$_2$CH$_2$C). ^{13}C NMR (300 MHz, C$_6$D$_6$): δ 177.617 (NC(CH$_3$)$_2$CH$_2$CH$_2$$C$), δ 61.176 (N$C$(CH$_3$)$_3$), δ 53.332 (N$C$(CH$_3$)$_2CH_2CH_2$C), δ 38.095 (NC(CH$_3$)$_2$$CH_2CH_2$C), δ 33.215 (NC($CH_3$)$_3$), δ 31.931 (NC(CH$_3$)$_2CH_2$$CH_2$C), δ 30.940 (NC($CH_3$)$_2CH_2CH_2$C). Combustion analysis, found (calculated): C, 52.44(52.04); H, 8.36(8.30); N, 12.27(12.14).

Crystallography: X-ray structural analysis for **1** : Crystals were selected and mounted on plastic mesh using viscous oil flash-cooled to the data collection temperature. Data were collected on a Bruker-AXS APEX CCD diffractometer with graphite-monochromated Mo-Kα radiation (λ=0.71073 Å). Unit cell parameters were obtained from 60 data frames, 0.3° ω, from three different sections of the Ewald sphere. The systematic absences in the data and the unit cell parameters were uniquely consistent to P2$_1$/c. The data-sets were treated with SADABS absorption corrections based on redundant multiscan data.[iii] The structures were solved using direct methods and refined with full-matrix, least-squares procedures on F2. The compound molecules each located on an inversion point. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were treated as idealized contributions. Atomic scattering factors are contained in the SHELXTL 6.12 program library.

Surface Exposure Experiments: The exposure experiments were performed in a home-built reactor. The reaction chamber consisted of a stainless steel ring support covered in 200 stainless steel mesh with a plug of glass wool to prevent loss of silica powder. The system had one inlet from a heated bubbler and one inlet for He (purity of 99.999%). All fittings used in this system were either CF or VCR to ensure a high-vacuum seal. The system was leak checked using a gas thermal conductivity/ leak detector (Gow-Mac Instrument Co.) and an overpressure of He. For the exposure experiments, typically about 1g of high surface area SiO$_2$ powder (EP10X; PQ Corporation; 300m2/g S.A.; 1.8cm3/g P.V.; 24nm P.S.; 100μm P.D.) was used. The powder was pre-treated in the reactor at 350˚C for 16h under vacuum before exposure to the precursor. The reactor and lines were heated to temperature and allowed to equilibrate for 1-2h before introduction of the precursor. The precursor (typically 0.6-0.8g) was then vaporized and transported to the substrate with the system under 10^{-4} Torr vacuum. The substrate was exposed to volatilized precursor for 17h before the system was cooled to room temperature for handling. Both precursor and substrate were handled in inert atmosphere.

Characterization of Surface Species: Solid-state NMR experiments were performed at 4.7T on a Bruker Avance III console. All spectra were obtained using a Bruker 7mm ^{1}H/X/Y probe. ^{13}C (ν$_0$ = 50.3MHz) cross-polarization magic angle spinning (CP/MAS) experiments were collected at a spinning rate of 4.5kHz using a 3.4μs 90° proton pulse with a contact time of 2ms where the contact pulse was ramped on the ^{1}H channel. A relaxation delay of 2s was sufficient to prevent saturation and typically total acquisition times were 16-30h. Glycine was used as an external secondary reference for the ^{13}C chemical shift scale. Spectra were treated with 40Hz line broadening during processing. All spectra were obtained with high power proton decoupling during acquisition.
Samples were prepared for High Resolution NMR (HR-NMR) by adding a small amount, typically 40-50mg, of modified silica powder to 2mL of D$_2$O, agitating, and allowed to sit for 15min. The D$_2$O solution was then decanted and studied via HR-NMR. d$_4$-TSP was used as an internal reference.

i   Moffett, R. B. Organic Synthesis, **1952**, *32*, 59; Osby, J. O.; Ganem, B. *Tetrahedron Lett.* **1985**, *26*, 6413.

ii   Beckmann, U, Eichberger, E.; Lindner, M.; Bongartz. M.; Kunz, P. C. *Eur. J. Org. Chem.* **2008**, *24*, 4139.

iii   G. M. Sheldrick, Acta Cryst. 2008, A64, 112.

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Cu N1 C1 C2 165.66(13) 3_756 . . . ?
C4 N1 C1 C6 -138.11(17) . . . . ?
Cu N1 C1 C6 45.7(2) 3_756 . . . ?
N1 C1 C2 C3 28.5(2) . . . . ?
C5 C1 C2 C3 -90.35(19) . . . . ?
C6 C1 C2 C3 147.16(17) . . . . ?
C1 C2 C3 C4 -28.4(2) . . . . ?
C8 N2 C4 N1 -176.00(15) . . . . ?
Cu N2 C4 N1 1.9(2) . . . . ?
C8 N2 C4 C3 5.8(3) . . . . ?
Cu N2 C4 C3 -176.26(14) . . . . ?
C1 N1 C4 N2 -178.92(14) . . . . ?
Cu N1 C4 N2 -2.8(2) 3_756 . . . ?
C1 N1 C4 C3 -0.4(2) . . . . ?
Cu N1 C4 C3 175.70(12) 3_756 . . . ?
C2 C3 C4 N2 -162.95(18) . . . . ?
C2 C3 C4 N1 18.7(2) . . . . ?
C4 N2 C8 C11 -177.58(18) . . . . ?
Cu N2 C8 C11 4.5(2) . . . . ?
C4 N2 C8 C10 64.9(2) . . . . ?
Cu N2 C8 C10 -113.04(16) . . . . ?
C4 N2 C8 C9 -60.3(2) . . . . ?
Cu N2 C8 C9 121.77(16) . . . . ?

_diffrn_measured_fraction_theta_max     0.997
_diffrn_reflns_theta_full               25.00
_diffrn_measured_fraction_theta_full    0.998
_refine_diff_density_max     0.712
_refine_diff_density_min    -0.515
_refine_diff_density_rms     0.079
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