'Auto–Click' Functionalization for Diversified Copper(I) and Gold(I) NHCs

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Supporting information

NMR survey of a 'auto–click' reaction

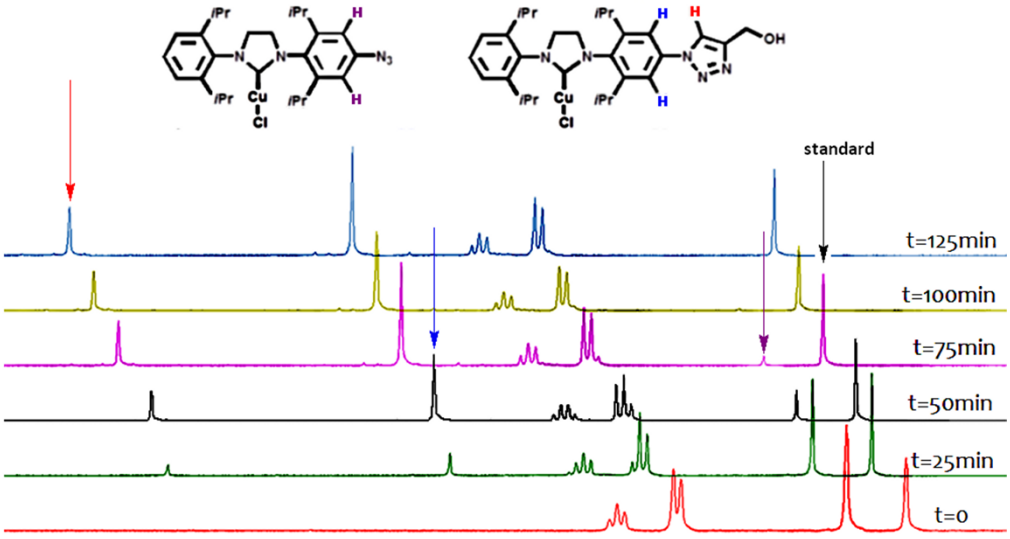

Figure S1. ^{1}H NMR (CD_3CN, 70°C) profile of the reaction vs time (1,4–dimethoxybenzene as internal standard).

X-ray cristallography

X-ray diffraction data was collected by using a Kappa X8 APPEX II Bruker diffractometer with graphite-monochromated MoKα radiation (λ = 0.71073 Å). The crystal was mounted on a CryoLoop (Hampton Research) with Paratone-N (Hampton Research) as cryoprotectant and then flashfrozen in a nitrogen gas stream at 100 K. The temperature of the crystal was maintained at the selected value (100 K) by a 700 series Cryostream cooling device with an accuracy of ±1 K. The data were corrected for Lorentz polarization, and absorption effects. The structures were solved by direct methods using SHELXS-97[i] and refined against F^2 by full-matrix least-squares techniques using SHELXL-97[ii] with anisotropic displacement parameters for all non-hydrogen atoms. Hydrogen atoms were located on a difference Fourier map and introduced into the calculations as a riding model with isotropic thermal parameters. All calculations were performed by using WINGX.[iii]The crystal data collection and

refinement parameters are given in Table S1. CCDC 977560 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/Community/Requestastructure.

Table S1. Crystallographic data and structure refinement details for compound **7c**.

Compound	**7c**
Empirical Formula	C_{38} H_{43} Cl Cu N_5 O_2, 2(C_2 H_6 O S)
M_r	857.05
Crystal size, mm^3	0.18 x 0.10 x 0.04
Crystal system	triclinic
Space group	*P -1*
a, Å	10.6132(3)
b, Å	17.8260(5)
c, Å	23.1406(6)
α, °	92.0760(10)
β, °	94.6390(10)
γ, °	90.1870(10)
Cell volume, $Å^3$	4360.7(2)
Z ; Z'	4 ; 2
T, K	100(1)
F_{000}	1808
μ, mm^{-1}	0.703
θ range, °	0.88 – 30.61
Reflection collected	82 883
Reflections unique	25 773
R_{int}	0.0421
GOF	1.026
Refl. obs. (I>2σ(I))	18 361
Parameters	1022
wR_2 (all data)	0.1334
R value (I>2σ(I))	0.0509
Largest diff. peak and hole (e-.$Å^{-3}$)	-1.446 ; 2.410

[i] G. M. Sheldrick, SHELXS-97, Program for Crystal Structure Solution, University of Göttingen, Göttingen, Germany, **1997**.

[ii] G. M. Sheldrick, SHELXL-97, Program for the refinement of crystal structures from diffraction data, University of Göttingen, Göttingen, Germany, **1997**.

[iii] L. J. Farrugia, L. J. *J. Appl. Cryst*., **1999**, *32*, 837.