

Supporting Information for Organometallics
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Table 1. Crystal data and structure refinement for 1.

Identification code	1
Empirical formula	C7 H7 Cl Cu N
Formula weight	204.13
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 7.9377(11) Å alpha = 90 deg. b = 9.4600(12) Å beta = 109.494(11) deg. c = 10.7491(12) Å gamma = 90 deg.
Volume	760.89(17) Å ³
Z, Calculated density	4, 1.782 Mg/m ³
Absorption coefficient	3.134 mm ⁻¹
F(000)	408
Crystal size	0.35 x 0.15 x 0.15 mm
Theta range for data collection	2.72 to 27.50 deg.
Limiting indices	-10<=h<=9, 0<=k<=12, 0<=l<=13
Reflections collected / unique	1737 / 1737 [R(int) = 0.0000]
Completeness to theta = 27.50	100.0 %
Absorption correction	Empirical used psi-scan
Max. and min. transmission	0.7608 and 0.6593
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1737 / 0 / 91
Goodness-of-fit on F ²	1.021
Final R indices [I>2sigma(I)]	R1 = 0.0282, wR2 = 0.0664
R indices (all data)	R1 = 0.0444, wR2 = 0.0708
Largest diff. peak and hole	0.282 and -0.392 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	1497(1)	1178(1)	735(1)	36(1)
Cl(1)	-1060(1)	756(1)	1162(1)	41(1)
N(1)	3399(3)	88(2)	2103(2)	34(1)
C(1)	809(4)	2928(3)	-407(3)	49(1)
C(2)	2611(4)	2751(3)	-71(3)	40(1)
C(3)	6032(4)	-1457(3)	4026(3)	33(1)
C(4)	4265(4)	-1451(3)	3969(3)	37(1)
C(5)	3007(4)	-669(3)	3017(3)	47(1)
C(6)	5100(4)	57(3)	2143(3)	42(1)
C(7)	6430(4)	-677(3)	3064(3)	40(1)

Table 3. Bond lengths [Å] and angles [deg] for 1.

Cu(1)-N(1)	2.006(2)
Cu(1)-C(1)	2.025(3)
Cu(1)-C(2)	2.064(3)
Cu(1)-Cl(1)	2.2599(8)
Cu(1)-Cl(1)#1	2.6751(8)
Cl(1)-Cu(1)#1	2.6751(8)
N(1)-C(5)	1.334(3)
N(1)-C(6)	1.337(3)
C(1)-C(2)	1.364(4)
C(2)-C(3)#2	1.475(4)
C(3)-C(4)	1.383(4)
C(3)-C(7)	1.391(4)
C(3)-C(2)#3	1.475(4)
C(4)-C(5)	1.381(4)
C(6)-C(7)	1.371(4)
N(1)-Cu(1)-C(1)	148.16(11)
N(1)-Cu(1)-C(2)	110.78(10)
C(1)-Cu(1)-C(2)	38.97(11)
N(1)-Cu(1)-Cl(1)	105.56(7)
C(1)-Cu(1)-Cl(1)	100.88(10)
C(2)-Cu(1)-Cl(1)	138.78(9)
N(1)-Cu(1)-Cl(1)#1	94.66(7)
C(1)-Cu(1)-Cl(1)#1	99.01(10)
C(2)-Cu(1)-Cl(1)#1	97.91(8)
Cl(1)-Cu(1)-Cl(1)#1	97.87(3)
Cu(1)-Cl(1)-Cu(1)#1	82.13(3)
C(5)-N(1)-C(6)	116.5(2)
C(5)-N(1)-Cu(1)	120.80(18)
C(6)-N(1)-Cu(1)	122.72(19)
C(2)-C(1)-Cu(1)	72.08(17)
C(1)-C(2)-C(3)#2	125.1(3)
C(1)-C(2)-Cu(1)	68.95(17)
C(3)#2-C(2)-Cu(1)	110.66(18)
C(4)-C(3)-C(7)	116.3(2)
C(4)-C(3)-C(2)#3	120.6(3)
C(7)-C(3)-C(2)#3	123.1(3)
C(5)-C(4)-C(3)	120.5(3)

N(1)-C(5)-C(4)	123.0(3)
N(1)-C(6)-C(7)	124.1(3)
C(6)-C(7)-C(3)	119.7(3)

Symmetry transformations used to generate equivalent atoms:
 #1 -x, -y, -z #2 -x+1, y+1/2, -z+1/2
 #3 -x+1, y-1/2, -z+1/2

Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^{-3}$) for 1.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cu(1)	28(1)	33(1)	42(1)	5(1)	6(1)	-2(1)
Cl(1)	31(1)	48(1)	47(1)	-7(1)	16(1)	0(1)
N(1)	30(1)	34(1)	36(1)	4(1)	8(1)	3(1)
C(1)	49(2)	38(2)	43(2)	11(1)	-6(1)	-7(1)
C(2)	49(2)	37(2)	31(1)	3(1)	9(1)	-12(1)
C(3)	39(2)	26(1)	32(1)	-4(1)	10(1)	2(1)
C(4)	41(2)	33(2)	37(2)	3(1)	15(1)	0(1)
C(5)	28(1)	38(2)	43(2)	0(1)	10(1)	-2(1)
C(6)	36(2)	44(2)	48(2)	14(1)	18(1)	5(1)
C(7)	29(1)	44(2)	48(2)	8(1)	15(1)	8(1)

Table 5. Hydrogen coordinates ($\times 10^{-4}$) and isotropic displacement parameters ($\text{Å}^2 \times 10^{-3}$) for 1.

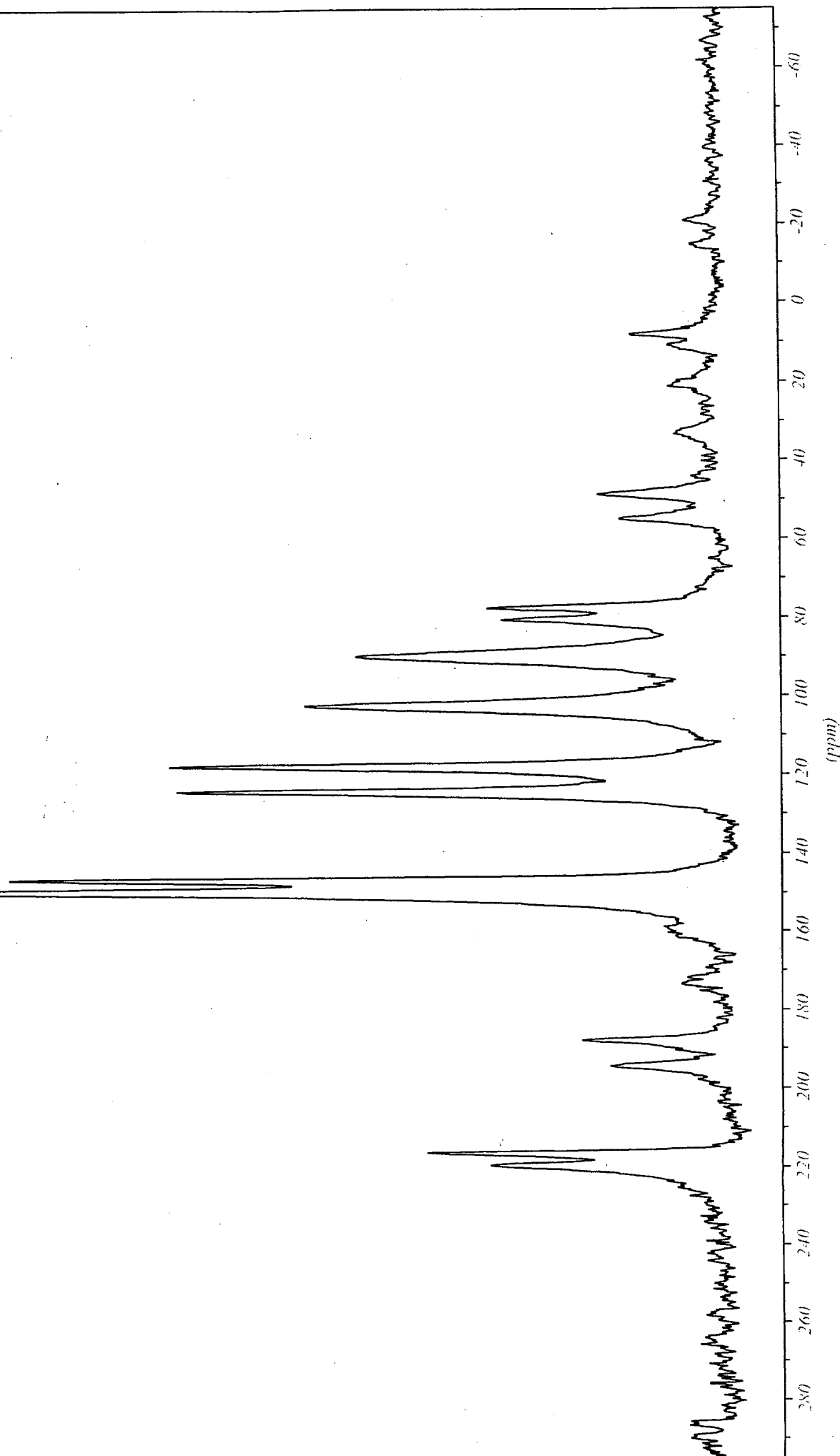
	x	y	z	U(eq)
H(1A)	110	2776	-1328	58
H(1B)	412	3735	-21	58
H(2A)	3008	2438	-797	48
H(4A)	3921	-1976	4575	44
H(5A)	1834	-671	3013	44
H(6A)	5400	566	1507	50
H(7A)	7592	-654	3044	48



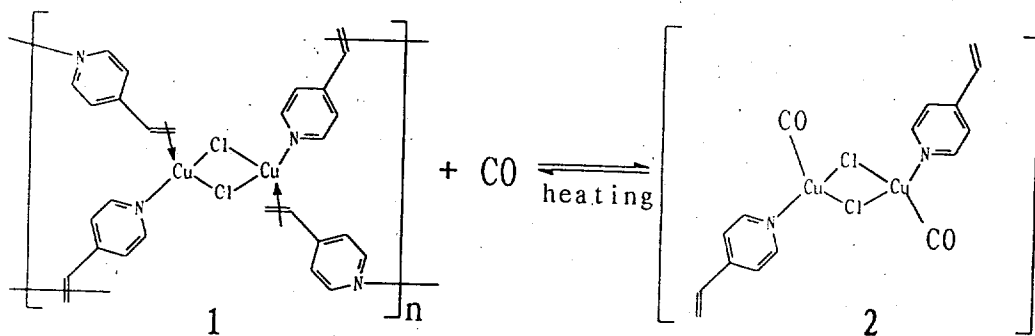
OM010665P

¹³C CP-MAS

MASr=7kHz, O1=11052.11Hz, O2=2300Hz, d1=50s



Preparation of 2: We consider that **1** can react with CO (atmosphere of CO) to give an unstable intermediate, $\text{CuCl}(\text{CO})(4\text{-VPY})$ (**2**) while **2** loses CO easily to convert into **1** when **2** was heated to ca. 90 °C. The converted **1** has the same formula, IR spectrum and solid state ^{13}C NMR as originally synthesized **1**. The proposed equation is given below.



Elemental analysis for **2** ($\text{C}_8\text{H}_7\text{NOClCu}$): Found: C, 41.44; H, 3.10; N, 6.13; Calc.: C, 41.38; H, 3.02; N, 6.03. IR (KBr, cm^{-1}): 3435(w), 3354(w), 2112(m, ν_{CO}), 1618(s), 1547(w), 1504(w), 1416(m), 1423(m), 1225(m), 1206(w), 1069(w), 1023(w), 988(w), 935(w) 841(s), 583(w).