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SUPPLEMENTARY MATERIAL TO

Reactions of 2-acetylpyridine-aminoguanidine with Cu(II) under different reaction conditions

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TABLE OF CONTENTS:

{[Cu(L)(μ-Cl)]NO_3·0.25H_2O}$_n$ ***(1)***

Anal. Calcd. for $C_8H_{11.5}N_6O_{3.25}ClCu$: C, 28.02; H, 3.36; N, 24.52 %. Found: C, 27.63; H, 3.68; N, 24.01 %. Conductivity, Λ = 110 S cm^2 mol^{-1} (in MeOH), Λ = 76 S cm^2 mol^{-1} (in DMF). Selected IR bands [wavenumber, cm^{-1}]: 3320 (s), 3182 (s), 1680 (s), 1650 (s), 1603 (m), 1545 (m), 1385 (vs), 1331 (m), 1200 (m), 1156 (w), 1112 (w), 1048 (w), 822 (w), 779 (m), 647 (w).

[Cu(L–H)Cl] ***(2)***

Anal. Calcd. for $C_8H_{10}N_6ClCu$: C, 34.93; H, 3.63; N, 25.45. Found: C, 35.02; H, 3.68; N, 25.63 %. Conductivity, Λ = 5 S cm^2 mol^{-1} (in DMF). Selected IR bands [wavenumber, cm^{-1}]: 3376 (m), 3206 (s), 3122 (m), 1643 (m), 1595 (s), 1516 (s), 1489 (s), 1430 (s), 1366 (m), 1263 (m), 1171 (s), 1086 (m), 1025 (w), 887 (w), 796 (m), 640 (s).

[Cu(L)ClNO_3]·H_2O ***(3)***

Anal. Calcd. for $C_8H_{13}N_6O_4ClCu$: C, 26.28; H, 3.65; N, 23.60. Found: C, 26.97; H, 3.68; N, 23.21 %. Conductivity, Λ = 114 S cm^2 mol^{-1} (in DMF). Selected IR bands [wavenumber, cm^{-1}]: 3538 (m), 3368 (s), 3152 (s), 1647 (vs), 1623 (m), 1601 (s), 1545 (s), 1425 (vs), 1299 (vs), 1267 (s), 1015 (s), 905 (w), 724 (w), 703 (w), 645 (m).

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1. X-RAY DATA TABLE

Table S-I. Crystal data, data collection, and refinement details for **1**, **2,** and **3**

Chemical formula	$C_8H_{11.5}N_6O_{3.25}ClCu$ (**1**)	$C_8H_{10}N_6ClCu$ (**2**)	$C_8H_{13}N_6O_4ClCu$ (**3**)
CCDC No.	2279826	2279827	2279828
Temperature, K	295(2)	295(2)	295(2)
Formula weight, g mol^{-1}	342.72	275.20	356.23
Crystal system	monoclinic	triclinic	triclinic
Space group	$P2_1/c$	$P\bar{1}$	$P\bar{1}$
a / Å	15.2534(5)	6.9461(3)	8.8689(2)
b / Å	12.6235(5)	8.8077(4)	9.1112(2)
c / Å	6.9614(3)	9.3443(3)	9.1228(2)
α / °	90	65.659(4)	99.739(2)
β / °	91.933(4)	87.263(3)	91.368(2)
γ / °	90	87.946(3)	112.718(2)
V / Å^3	1339.67(9)	520.19(4)	666.95 (3)
Crystal size, mm^3	0.50×0.21×0.12	0.56 × 0.11 × 0.05	0.48 × 0.41 × 0.23
Reflections collected	11936	12706	25579
Unique reflections	3229	2124	4613
Observed reflections [$I \geq 2\sigma(I)$]	2544	1961	4005
R_{int}	0.030	0.029	0.025
R [$I > 2\sigma(I)$]	0.037	0.021	0.027
R (all data)	0.087	0.056	0.073
Goodness-of-fit, S	1.05	1.09	1.08
$\Delta\rho_{max}$, $\Delta\rho_{min}$, e Å^{-3}	0.29 / −0.25	0.23 / −0.19	0.36 / –0.28

2. ADDITIONAL FIGURES

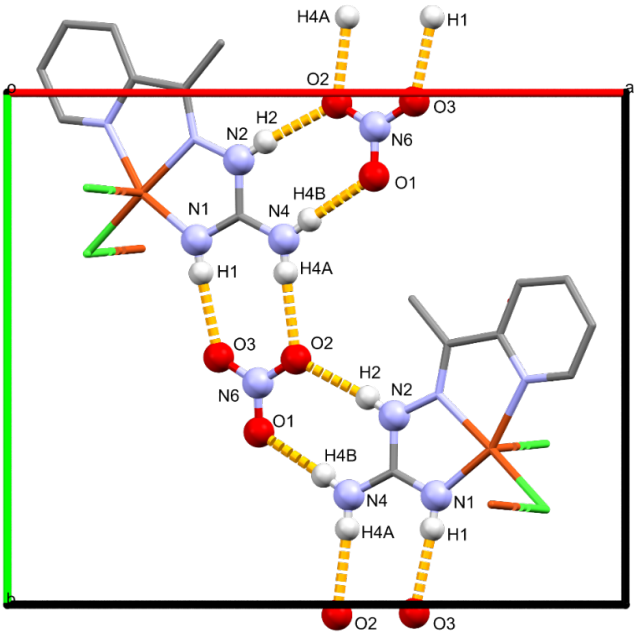

Figure S-1. Hydrogen bonding in **1**

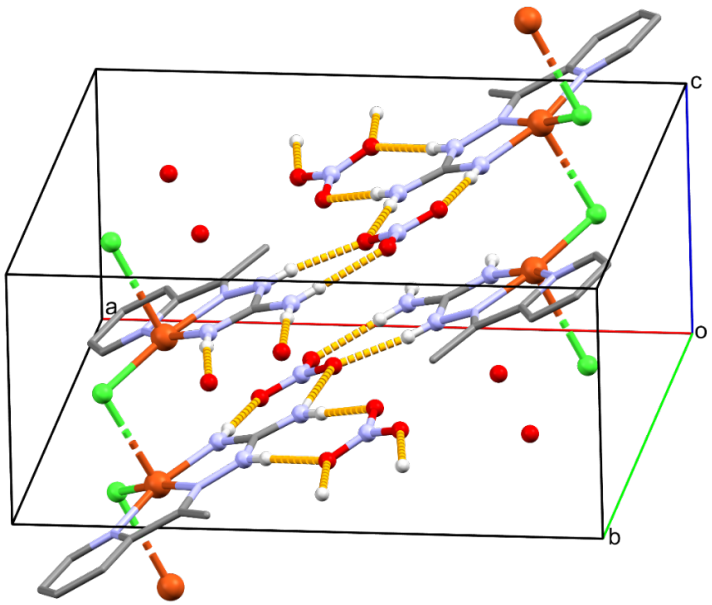

Fig. S-2. Crystal packing of **1** showing the hydrogen bonds that connect two monoperiodic polymer chains

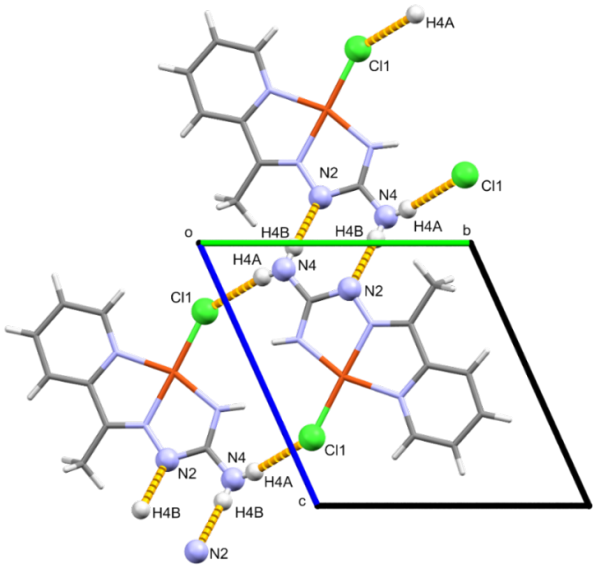

Fig. S-3. Hydrogen bonding in **2**

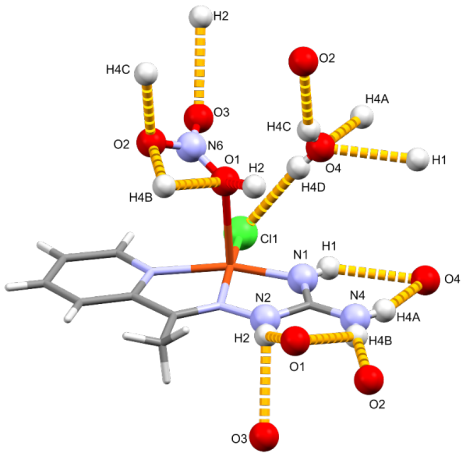

Fig. S-4. Hydrogen bonding in **3**

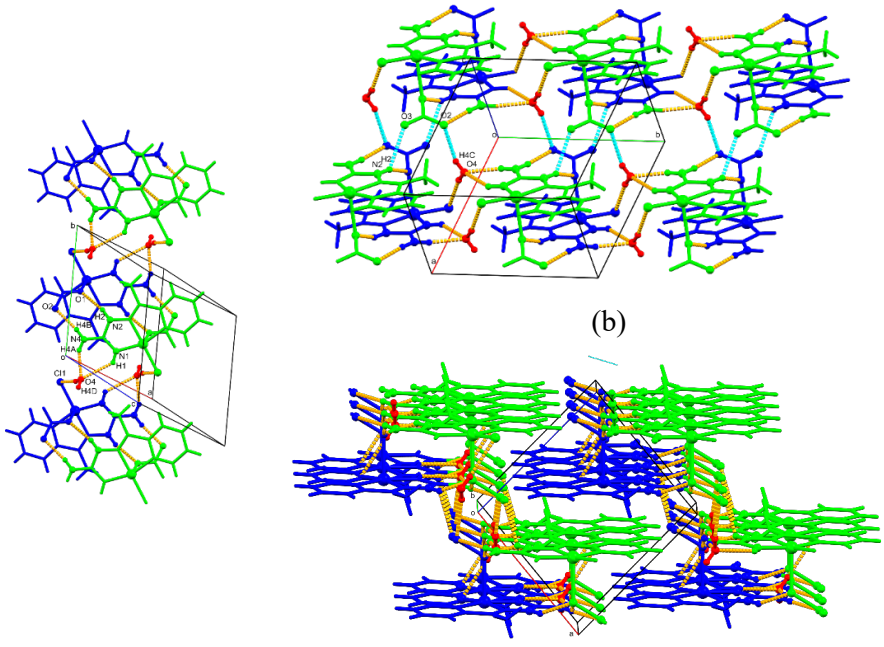

Fig. S-5. Hydrogen bonds responsible for dimer and chain formation (a), interconnecting the chains (b) and crystal packing of **3**

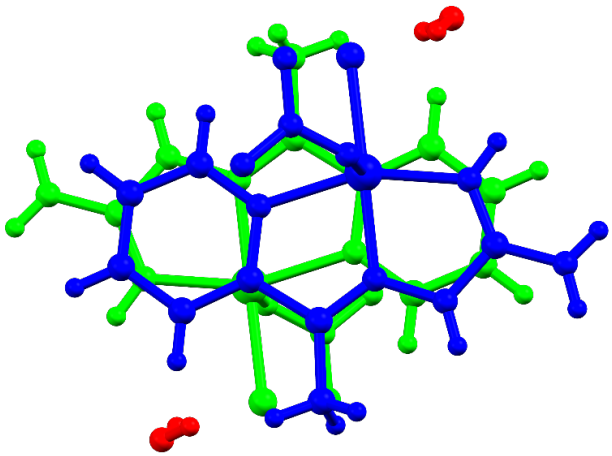

Fig. S-6. Stacking of py ring and aminoguanidine mettalocycle Ж

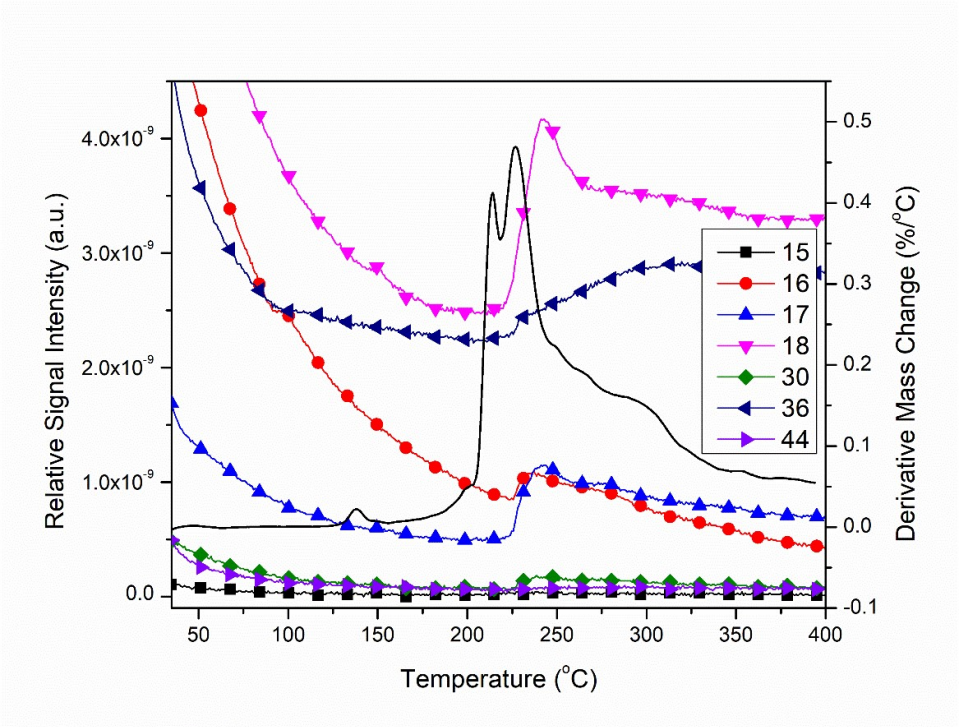

Fig. S-7. Fragments of complex **2** in argon