

Supplementary material for the article:

Vojinović-Ješić, L. S.; Radanović, M. M.; Rodić, M. V.; Živković-Radovanović, V.; Jovanović, L. S.; Leovac, V. M. Syntheses and Characterization of 2-Acetylpyridine-Aminoguanidine and Its Copper(II) Complexes: Crystallographic and Antimicrobial Study. *Polyhedron* **2016**, *117*, 526–534. <https://doi.org/10.1016/j.poly.2016.06.032>

SUPPLEMENTARY MATERIAL

Syntheses and characterization of 2-acetylpyridine-aminoguanidine and its copper(II) complexes: Crystallographical and antimicrobial study

Ljiljana S. Vojinović-Ješić^a, Mirjana M. Radanović^a, Marko V. Rodić^a, Vukosava Živković-Radovanović^b, Ljiljana S. Jovanović^a, Vukadin M. Leovac^{a1}

^a Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia

^b Faculty of Chemistry, University of Belgrade, P.O. Box 51, 11158 Belgrade, Serbia

¹ Corresponding author. E-mail address: vukadin.leovac@dh.uns.ac.rs (V.M. Leovac)

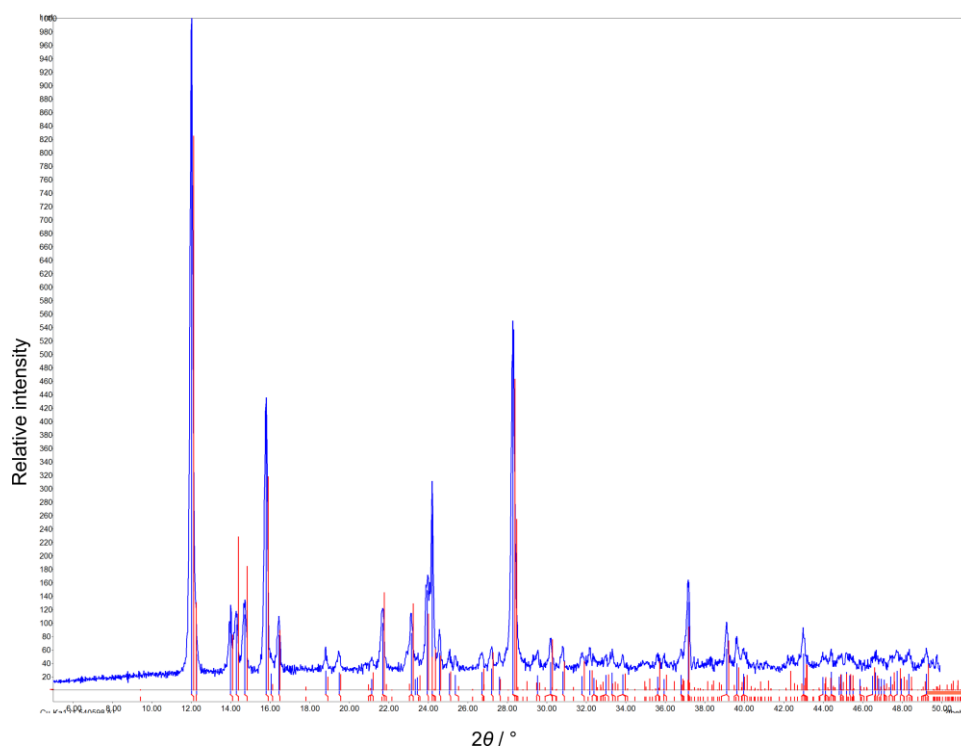


Fig. S1. Match between experimental powder diffraction pattern (blue line) of the batch sample (obtained by reaction of CuCl_2 and HL) with calculated peak positions for polymorph **1** (red lines).

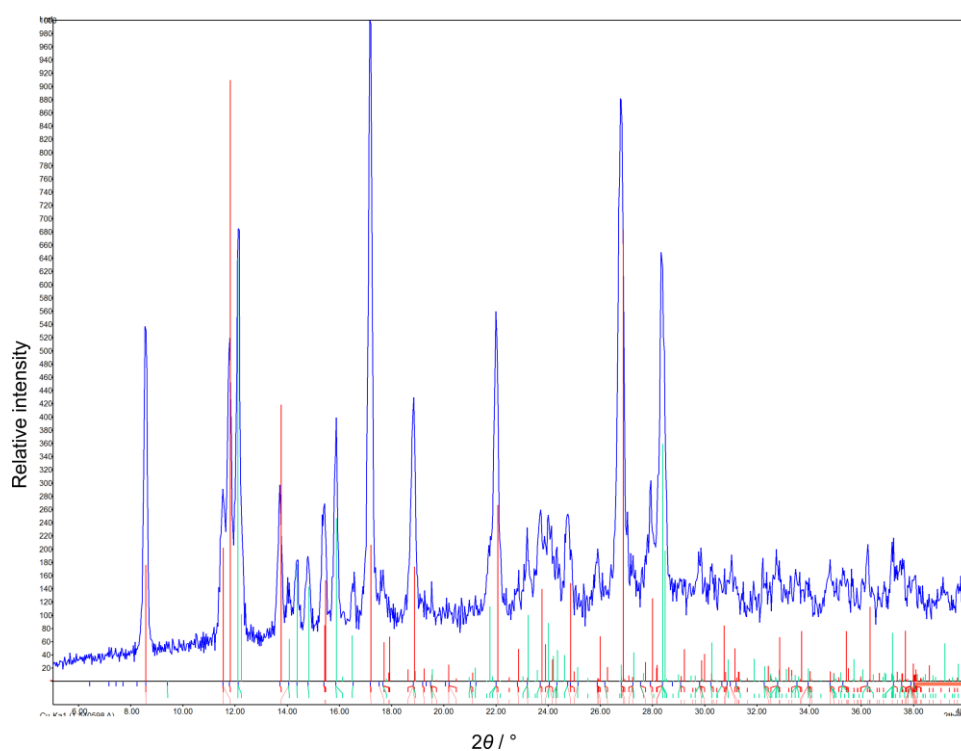


Fig. S2. Match between experimental powder diffraction pattern (blue line) of the batch sample (obtained by reaction of $\text{Cu}(\text{OAc})_2$ and HL) with calculated peak positions for polymorph **1** (green lines) and **1a** (red lines).

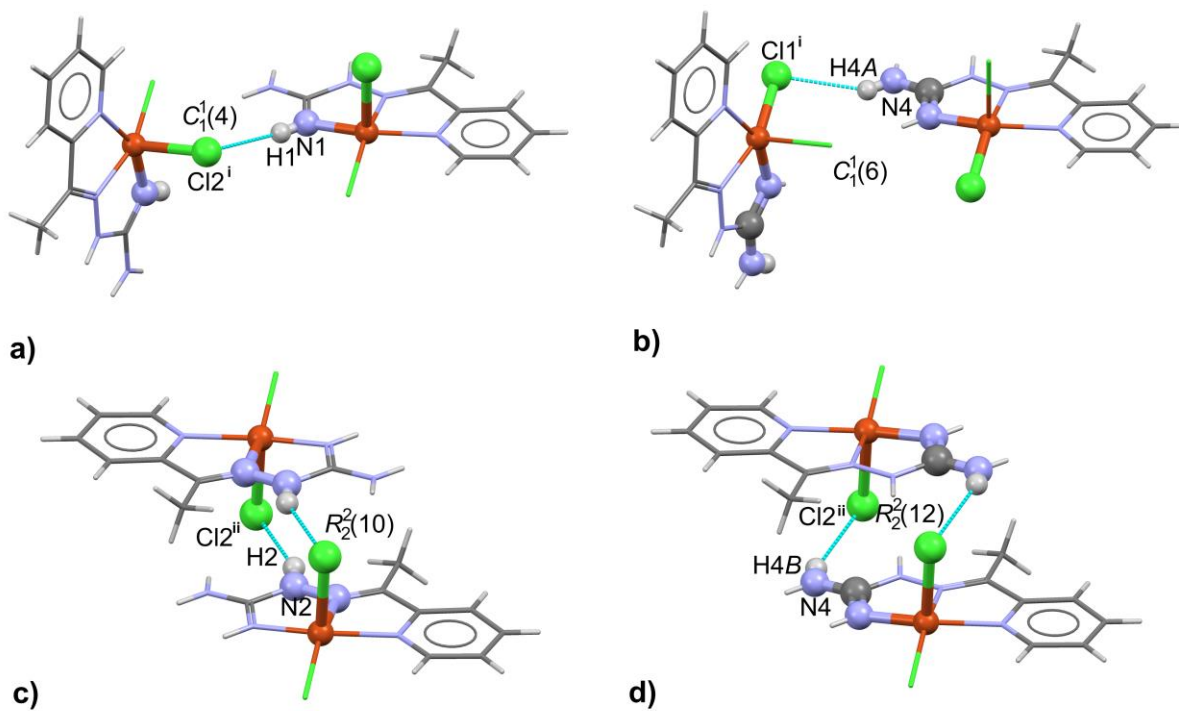


Fig. S3. Depictions of hydrogen bonds and corresponding motifs in crystal structure of the **1**. Symmetry codes: (i) $-x+2, y+1/2, -z+3/2$; (ii) $-x+2, -y+1, -z+1$.

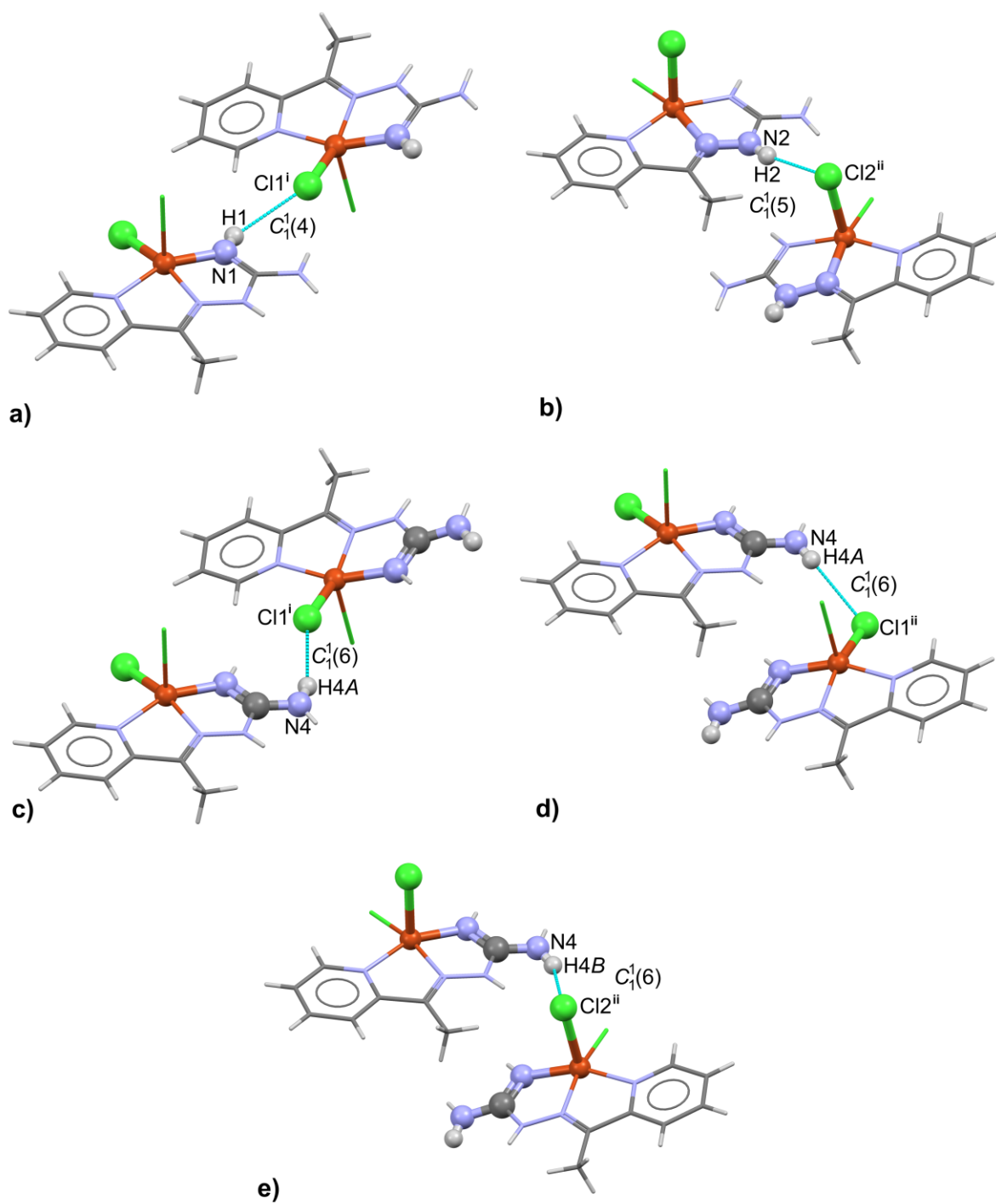


Fig. S4. Depictions of hydrogen bonds and corresponding motifs in crystal structure of the **1a**. Symmetry codes: (i) $-x+1, y+1/2, -z+1/2$; (ii) $x, -y+3/2, z+1/2$.

Table S1. Hydrogen-bond geometry of the form **1** (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>	Graph set descriptor
N1—H1...Cl2 ⁱ	0.83(2)	2.48(2)	3.2904(18)	168(2)	<i>C</i> ₁ ¹ (4)
N2—H2...Cl2 ⁱⁱ	0.85(2)	2.36(2)	3.1574(18)	155(2)	<i>R</i> ₂ ² (10)
N4—H4B...Cl2 ⁱⁱ	0.84(2)	2.55(2)	3.276(2)	145(2)	<i>R</i> ₂ ² (12)
N4—H4A...Cl1 ⁱ	0.82(2)	2.69(2)	3.426(2)	151(2)	<i>C</i> ₁ ¹ (6)

Symmetry codes: (i) $-x+2, y+1/2, -z+3/2$; (ii) $-x+2, -y+1, -z+1$.

Table S2. Hydrogen-bond geometry of the form **1a** (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>	Graph set descriptor
N1—H1...Cl1 ⁱ	0.82(2)	2.85(2)	3.5601(17)	146(2)	<i>C</i> ₁ ¹ (4)
N2—H2...Cl2 ⁱⁱ	0.83(2)	2.27(2)	3.0778(16)	165(2)	<i>C</i> ₁ ¹ (5)
N4—H4A...Cl1 ⁱ	0.88(2)	2.42(2)	3.2394(18)	155(2)	<i>C</i> ₁ ¹ (6)
N4—H4B...Cl1 ⁱⁱ	0.82(2)	2.85(2)	3.483(2)	136(2)	<i>C</i> ₁ ¹ (6)
N4—H4B...Cl2 ⁱⁱ	0.82(2)	2.79(2)	3.4506(19)	139(2)	<i>C</i> ₁ ¹ (6)

Symmetry codes: (i) $-x+1, y+1/2, -z+1/2$; (ii) $x, -y+3/2, z+1/2$.