Supplementary data for article:

Milenković, M. R.; Papastavrou, A. T.; Radanović, D. D.; Pevec, A.; Jagličić, Z.; Zlatar, M.; Gruden, M.; Vougioukalakis, G. C.; Turel, I.; Anđelković, K. K.; et al. Highly-Efficient N-Arylation of Imidazole Catalyzed by Cu(II) Complexes with Quaternary Ammonium-Functionalized 2-Acetylpyridine Acylhydrazone. *Polyhedron* **2019**, *165*, 22–30. https://doi.org/10.1016/j.poly.2019.03.001

Supplementary material

Highly-efficient *N*-arylation of imidazole catalyzed by Cu(II) complexes with quaternary ammonium-functionalized 2-acetylpyridine acylhydrazone

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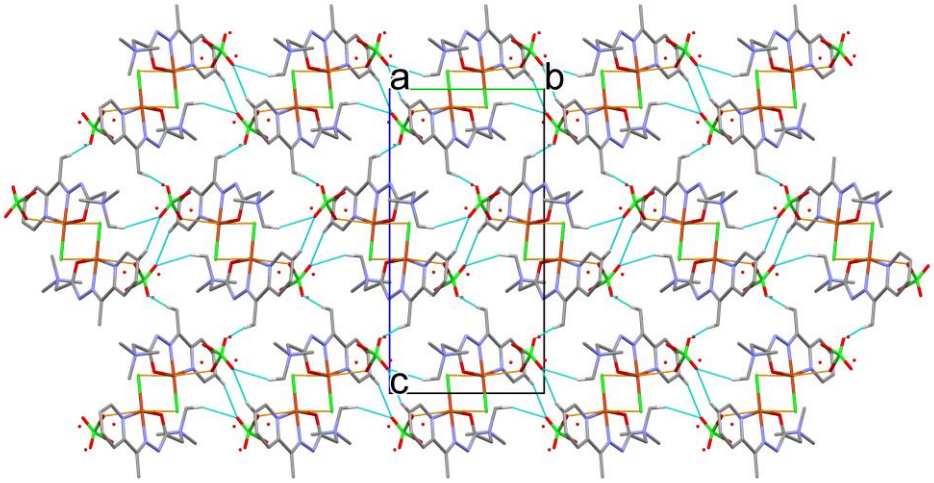
Table S1. Hydrogen-bond parameters for complexes **1** and **2**.

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)	Symm. operation on A
Complex **1**					
C2-H2···O2	0.93	2.54	3.440(7)	162	-x,1-y,1-z
C7-H7A···O4A	0.96	2.52	3.470(14)	172	-x,-1/2+y,3/2-z
Intra C7-H7C···N3	0.96	2.51	2.897(4)	104	
C10-H10A···O3B	0.96	2.51	3.395(8)	153	1-x,-1/2+y,3/2-z
Intra C11-H11A···O1	0.96	2.31	2.982(4)	126	
C11-H11B···O2	0.96	2.47	3.375(7)	158	x,-1+y,z
C12-H12A···Cl1	0.96	2.77	3.672(3)	156	1-x,-y,1-z
C12-H12C···O3A	0.96	2.52	3.405(10)	154	1-x,-1/2+y,3/2-z
Complex **2**					
C11-H11B···N7	0.96	2.39	3.278(4)	153	1-x,-y,1-z
C10-H10B···N7	0.96	2.62	3.446(4)	145	1-x,-y,1-z
C12-H12C···O3	0.96	2.58	3.504(4)	161	3/2-x,-1/2-y,1-z
Intra C12-H12A···O1	0.96	2.48	3.071(3)	120	
Intra C10-H10C···O1	0.96	2.34	2.989(3)	124	
Intra C7-H7A···N3	0.96	2.47	2.877(3)	105	

(a)



(b)

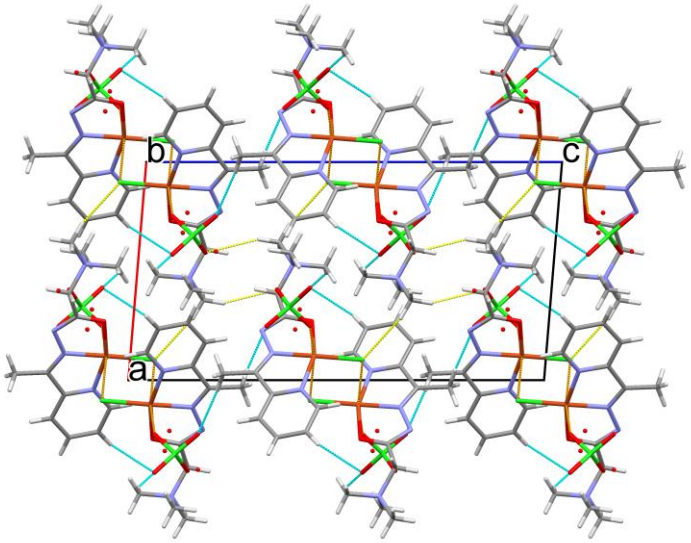


Fig. S1. Packing diagram of **1**: (a) A view of (100) layer showing centrosymmetric dimeric units $[Cu_2\mathbf{L}_2Cl_2](ClO_4)_2$ connected by means of C-H···O hydrogen bonds (dashed blue lines). Long contacts Cu···$O_{perchlorate}$ and Cu···Cl are represented as dashed orange lines. Hydrogen atoms have been omitted for the sake of clarity, except those involved in hydrogen bonding. (b) Side view of (100) layers showing intermolecular C_{Me}-H···Cl and C_{Me}-H···$O_{perchlorate}$ hydrogen bonds (dashed yellow lines) operating between neighboring layers.

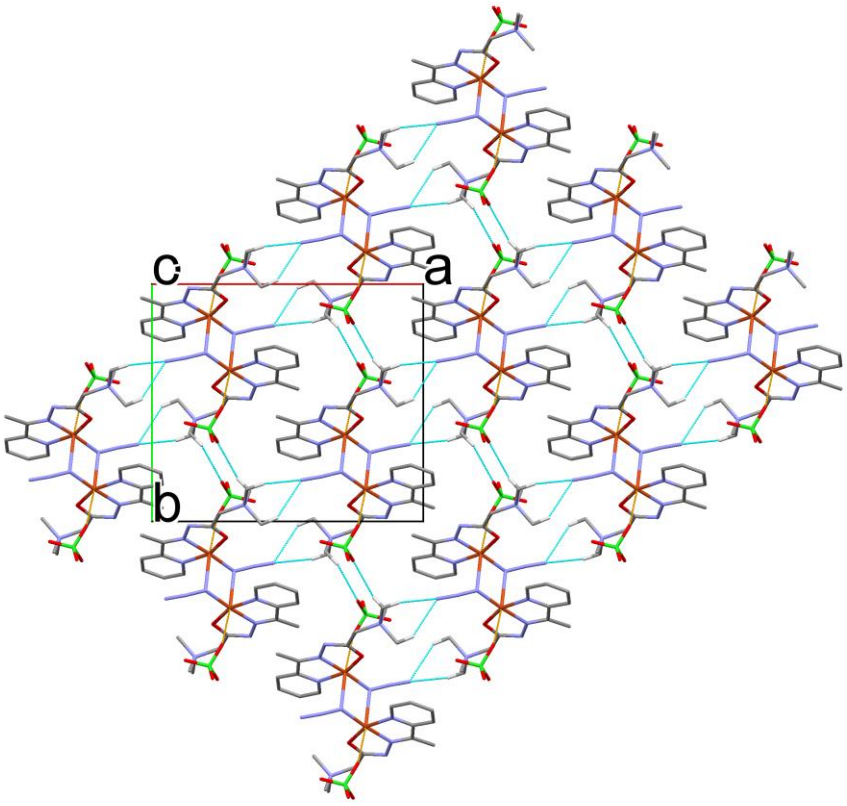


Fig. S2. Crystal packing of **2** showing dinuclear units $[Cu_2\mathbf{L}_2(N_3)_2]^{2+}$ connected by intermolecular C_{Me}-H···N_{azide} hydrogen bonds into 1D chains extending parallel with the [1 -1 0] direction. The perchlorate anions are involved in the intermolecular C-H···O hydrogen bonding and form long non-bonding contacts (represented as dashed orange lines) with Cu(II) ions. ~~from the neighboring chains~~ Hydrogen atoms have been omitted for the sake of clarity, except those involved in hydrogen bonding.

Table S2
Influence of the exchange-correlation functional and basis set on the calculated exchange coupling constant J (cm^{-1}).

		BP86	OLYP	OPBE	PW91	B3LYP	B3LYP*	TPSSH
$[Cu_2\mathbf{L}_2(N_3)_2]^{2+}$	def2-tzvp	5.36	4.75	5.61	5.22	3.58	3.55	2.06
	def2-tzvpp	5.91	4.74	5.32	5.82	3.81	2.67	1.74
$[Cu_2\mathbf{L}_2(N_3)_2](ClO_4)_2$	def2-tzvp	7.73	6.20	7.90	7.66	2.98	3.57	2.30
	def2-tzvpp	6.92	7.38	6.92	6.72	4.75	3.30	1.21