

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...C11	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	

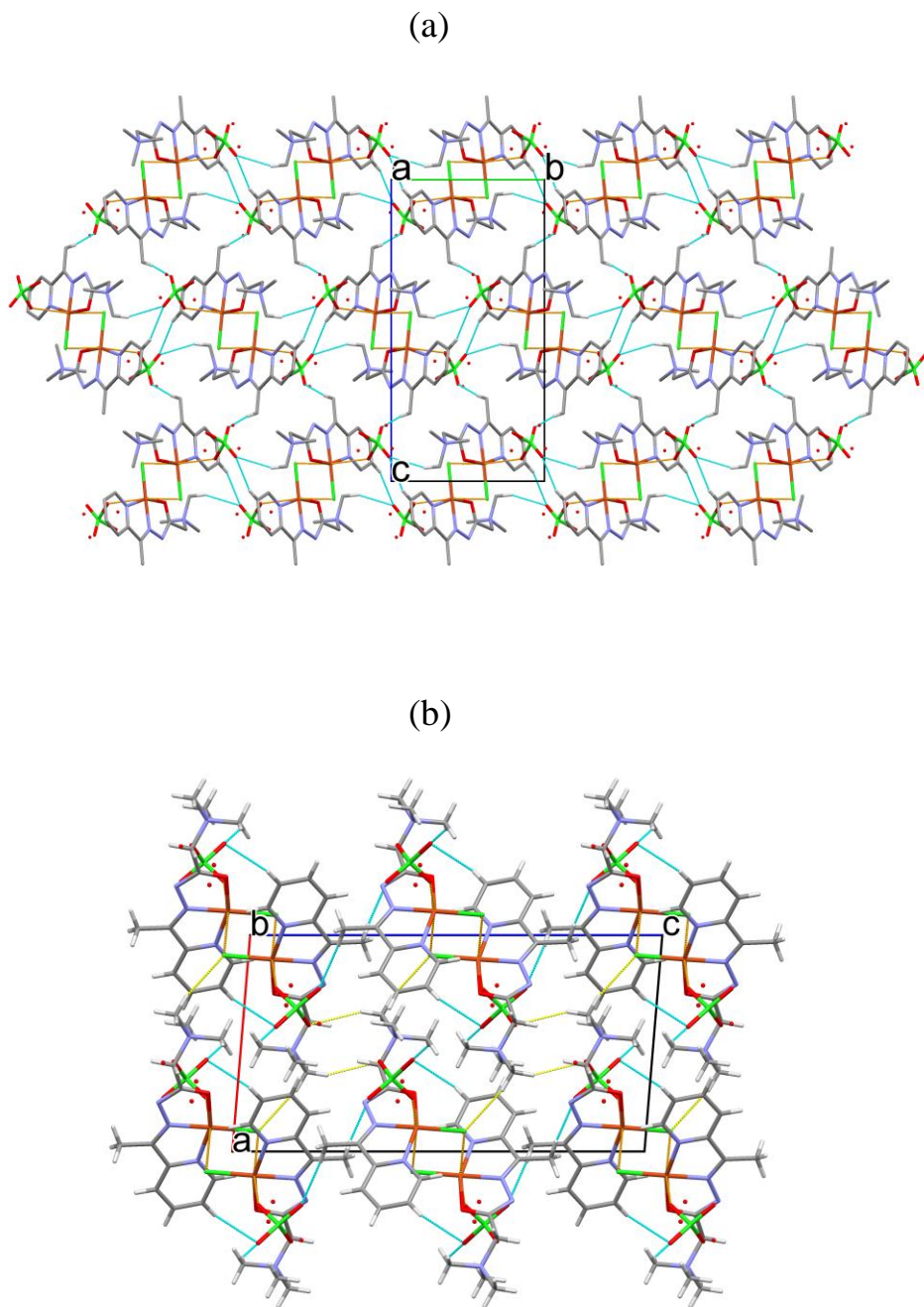


Fig. S1. Packing diagram of **1**: (a) A view of (100) layer showing centrosymmetric dimeric units $[\text{Cu}_2\text{L}_2\text{Cl}_2](\text{ClO}_4)_2$ connected by means of $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds (dashed blue lines). Long contacts $\text{Cu}\cdots\text{O}_{\text{perchlorate}}$ and $\text{Cu}\cdots\text{Cl}$ 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 $\text{C}_{\text{Me}}-\text{H}\cdots\text{Cl}$ and $\text{C}_{\text{Me}}-\text{H}\cdots\text{O}_{\text{perchlorate}}$ hydrogen bonds (dashed yellow lines) operating between neighboring layers.

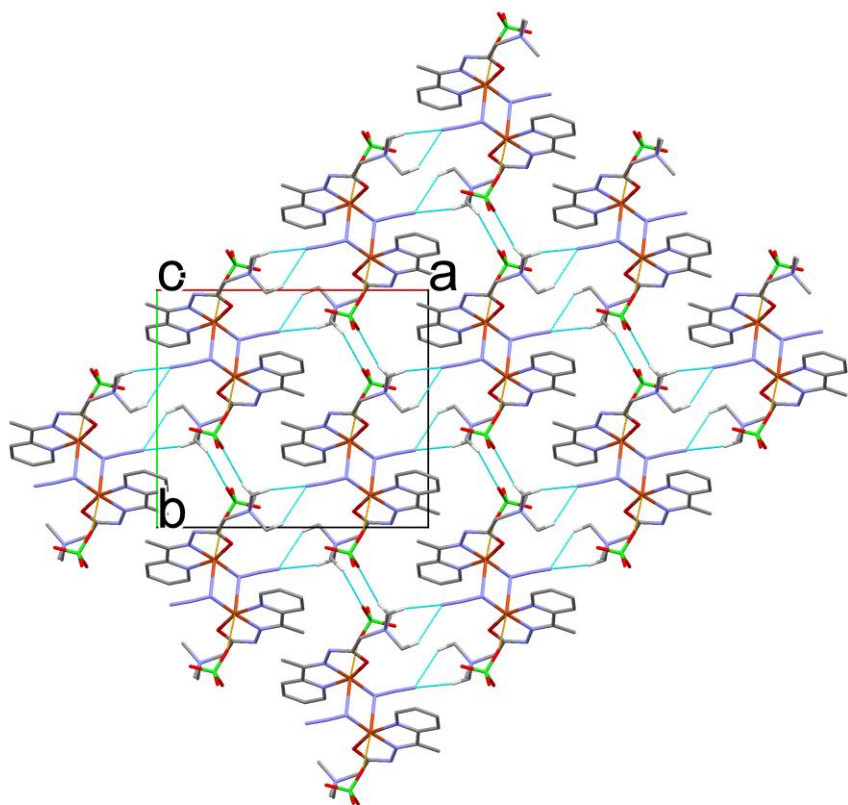


Fig. S2. Crystal packing of **2** showing dinuclear units $[\text{Cu}_2\text{L}_2(\text{N}_3)_2]^{2+}$ connected by intermolecular $\text{C}_{\text{Me}}\text{-H}\cdots\text{N}_{\text{azide}}$ hydrogen bonds into 1D chains extending parallel with the $[1 -1 0]$ direction. The perchlorate anions are involved in the intermolecular $\text{C-H}\cdots\text{O}$ 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 S2Influence 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 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 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
