

# Supporting Information

## A novel T4(1)6(1) water tape encapsulated in a (3,3)-connected 2D copper metal-organic framework

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**Table S1. Selected bond lengths [Å] and angles [°] for 1.**

Cu(1)-N(1)	2.014(5)	Cu(1)-N(8)#1	1.991(5)
Cu(1)-O(1)	2.011(4)	Cu(1)-O(2)	1.970(5)
Cu(1)-N(6)#2	2.198(5)		
N(8)#1-Cu(1)-N(1)	94.1(2)	O(1)-Cu(1)-N(1)	156.5(2)
O(2)-Cu(1)-N(1)	95.8(2)	N(8)#1-Cu(1)-O(1)	97.3(2)
O(2)-Cu(1)-N(8)#1	154.9(2)	O(2)-Cu(1)-O(1)	66.12(19)
N(1)-Cu(1)-N(6)#2	99.6(2)	N(8)#1-Cu(1)-N(6)#2	101.9(2)
O(1)-Cu(1)-N(6)#2	98.0(2)	O(2)-Cu(1)-N(6)#2	99.1(2)

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

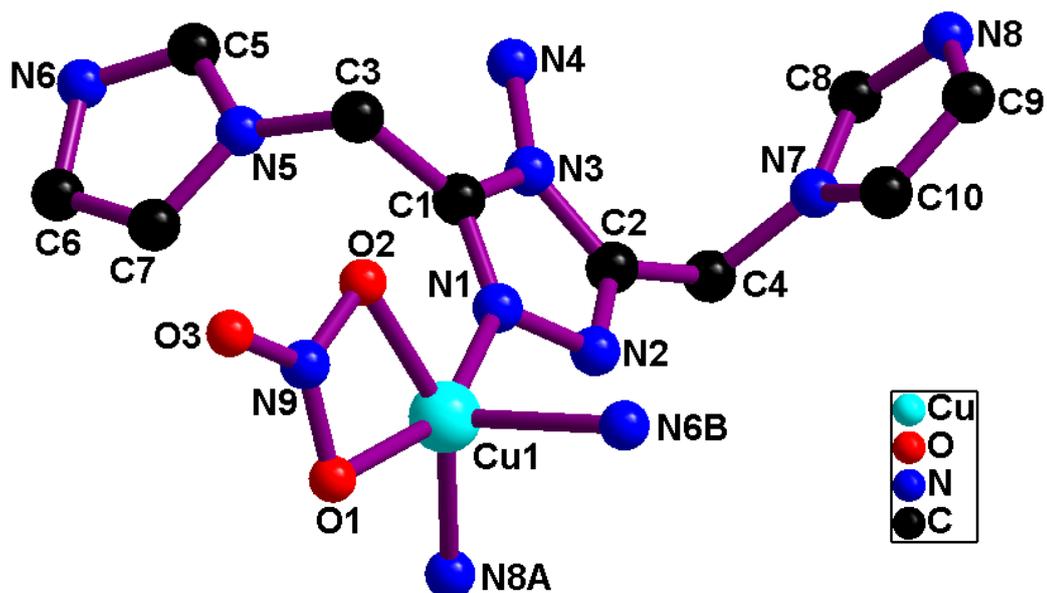
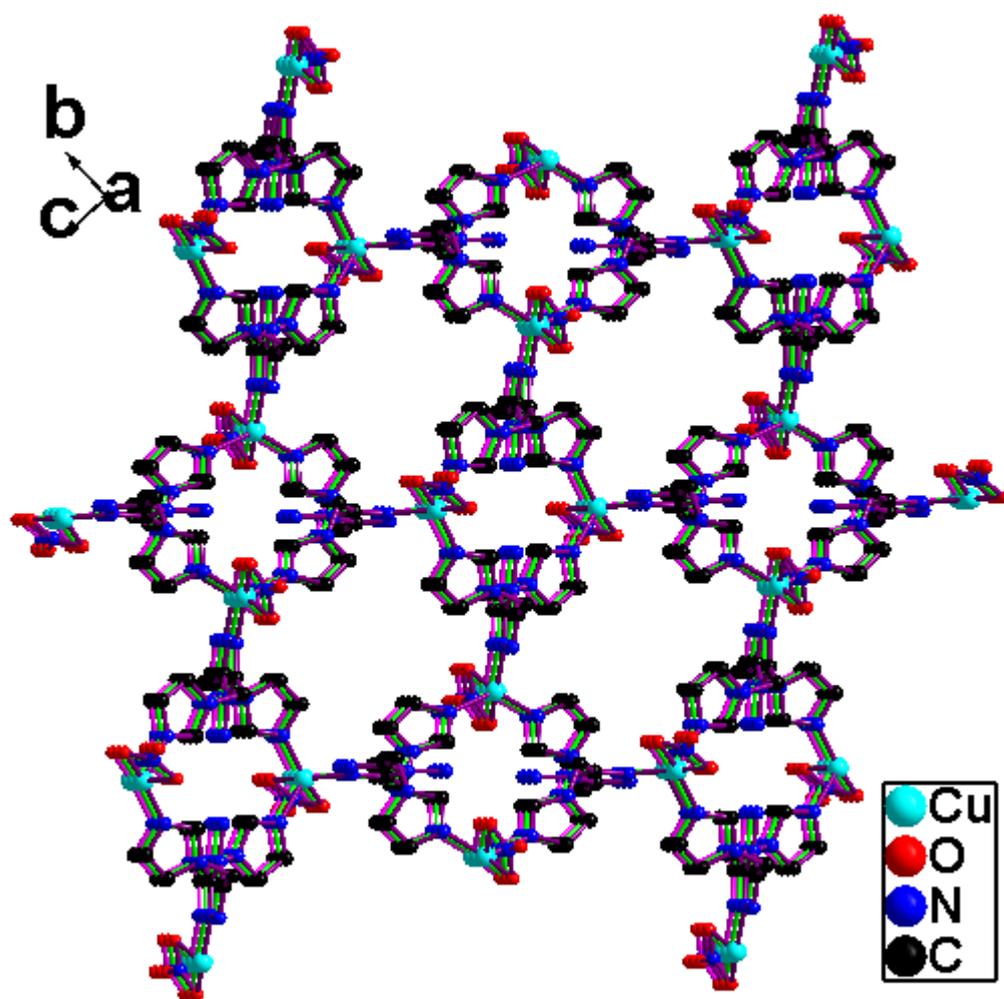
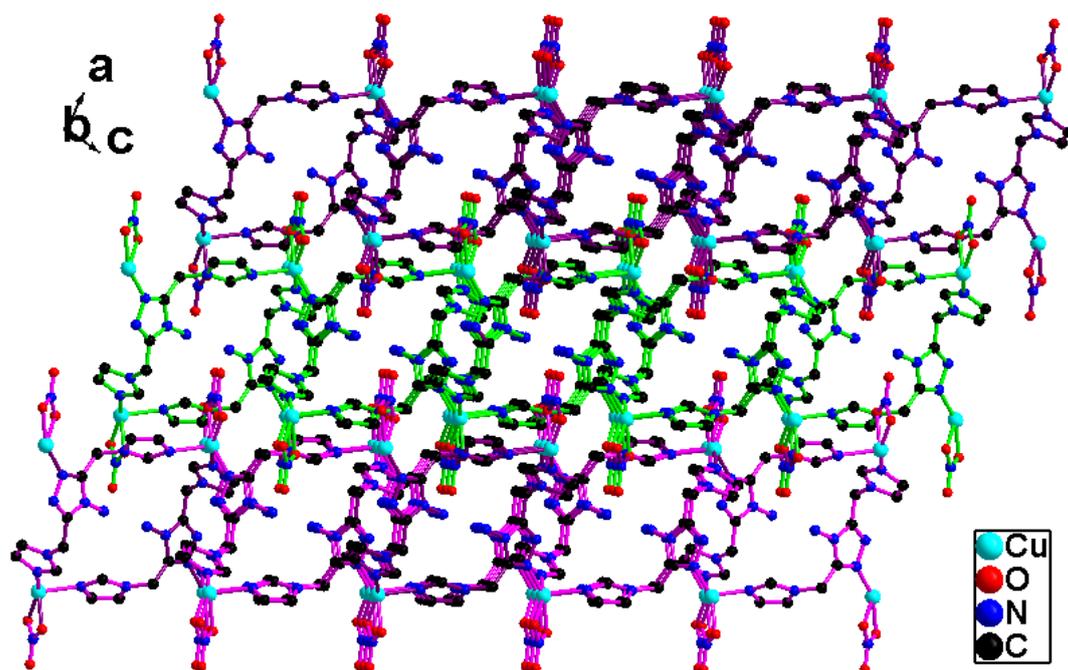


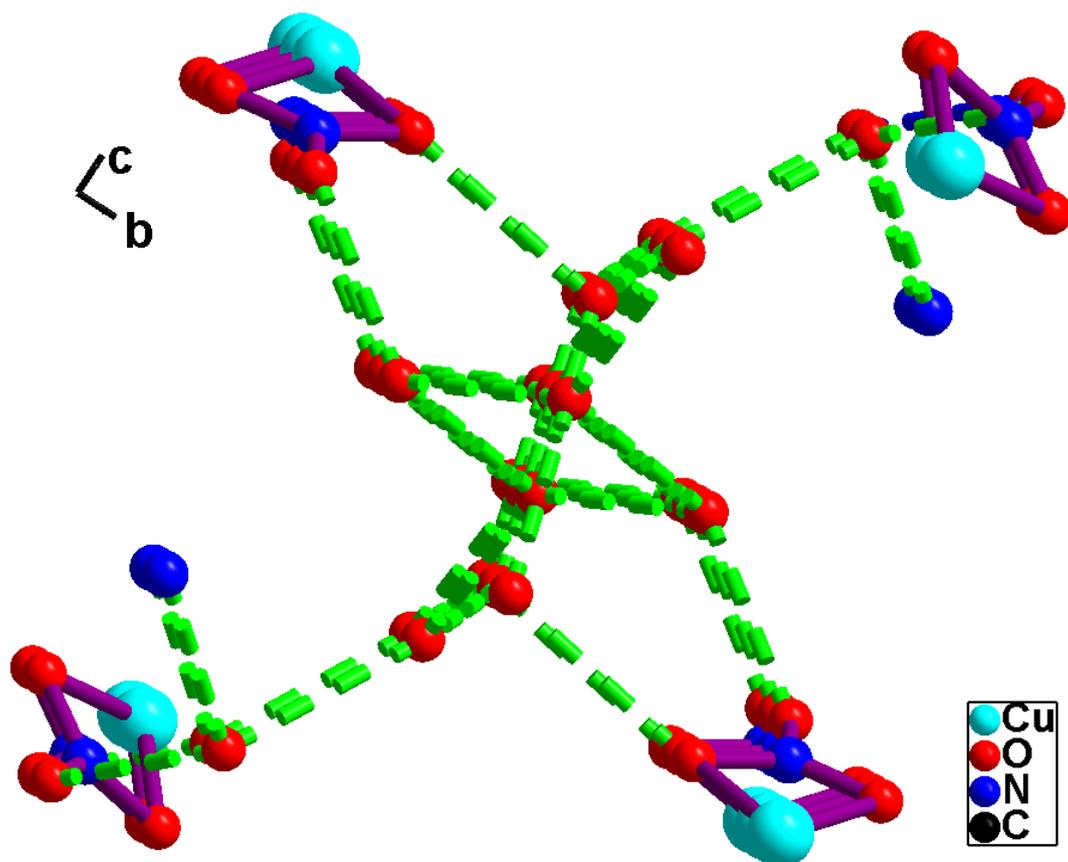
Figure S1. The coordination environment of the copper atom in 1.



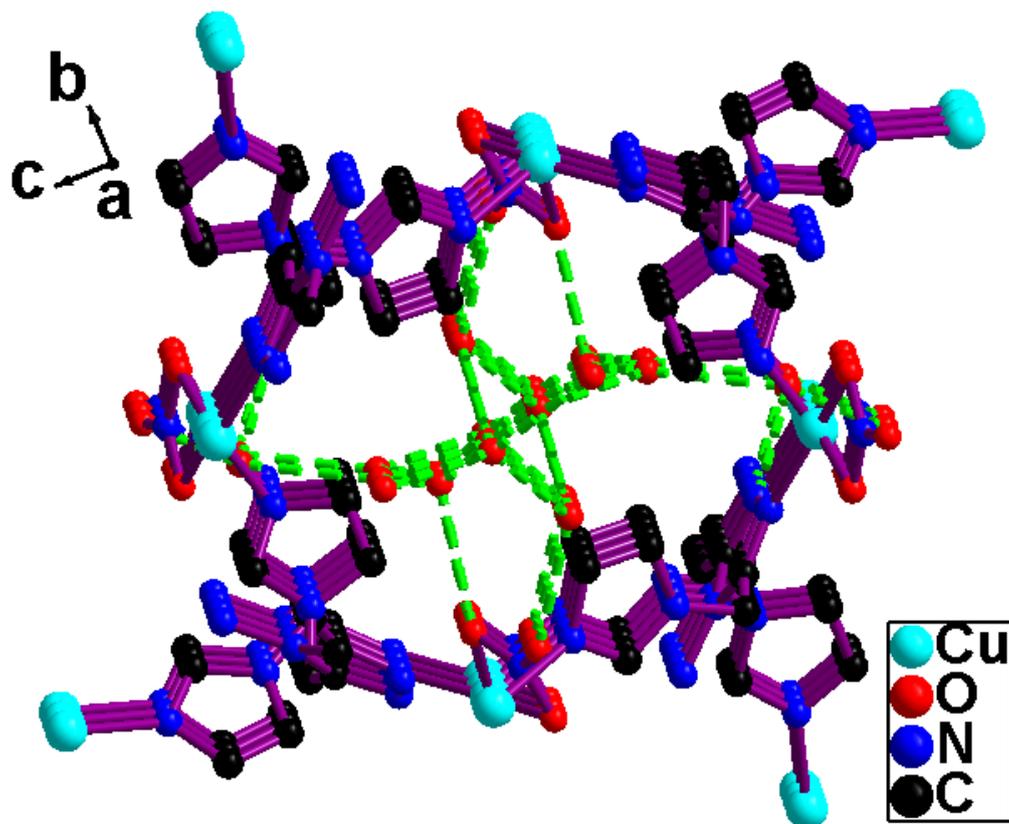
**Figure S2.** The parallel packed of the 2D network in **1**.



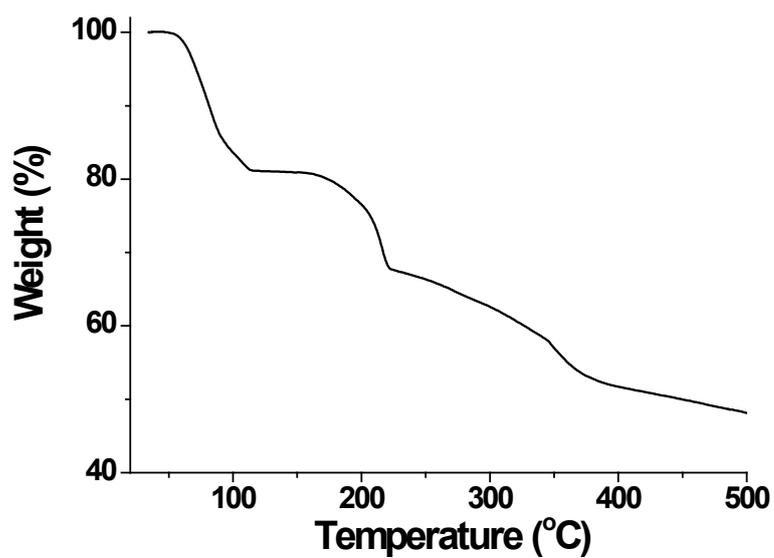
**Figure S3.** Viewing the packed of the 2D network in **1** along the *b* direction.



**Figure S4.** Viewing the hydrogen bond interactions between tape water and the nitrate/triazole nitrogen atoms along the *a* direction.



**Figure S5** A water tape joins the adjacent 2D network via the hydrogen bond interactions, viewing along the *a* direction.



**Figure S6.** TG curve of **1**.