

Supporting Information for

Packing polymorphism of two-dimensional coordination polymer cuprous 3-amino-1,2,4-triazolate

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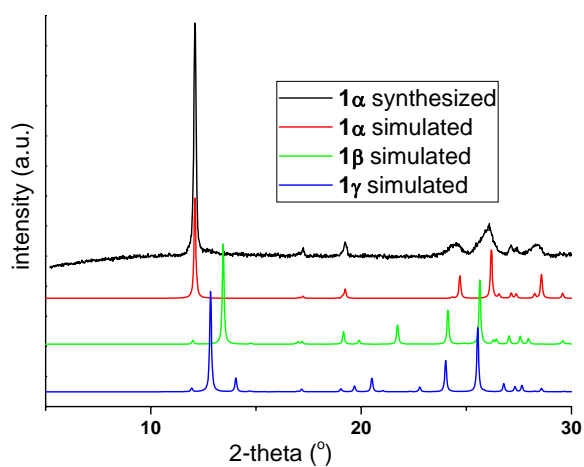


Fig. S1 Simulated and experimental XRPD patterns of **1** prepared by rapid solution mixing method.

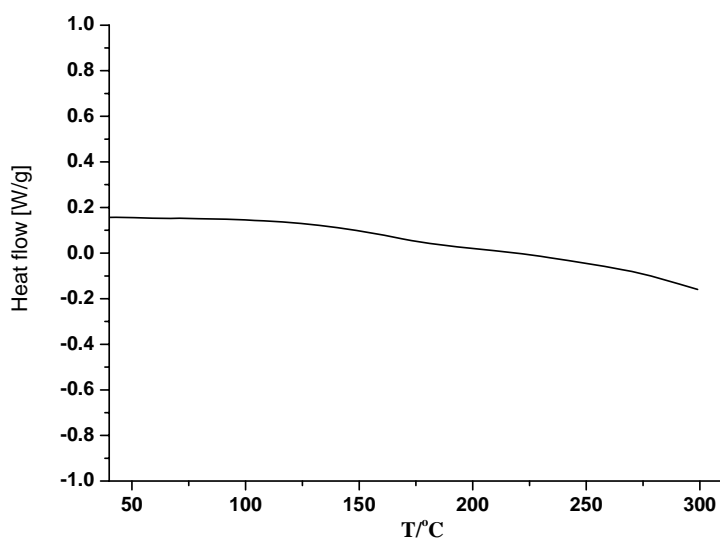


Fig. S2 DSC curve of **1** showing no phase transition.

Table S1. Selected bond lengths (Å) and angles (°) for **1 α** , **1 β** , and **1 γ** .

1α			
Cu1-N1	1.960(7)	N1-Cu1-N2	115.4(3)
Cu1-N2	1.970(7)	N1-Cu1-N3	121.9(3)
Cu1-N3	1.958(7)	N2-Cu1-N3	121.6(3)
1β			
Cu1-N1	1.942(4)	N1-Cu1-N6	114.4(2)
Cu1-N6	1.973(4)	N1-Cu1-N3	122.0(2)
Cu1-N3	1.959(4)	N3-Cu1-N6	123.4(2)
Cu2-N5	1.955(4)	N2-Cu2-N5	114.3(2)
Cu2-N2	1.989(4)	N5-Cu2-N7	122.7(2)
Cu2-N7	1.949(4)	N2-Cu2-N7	119.6(2)
1γ			
Cu1-N1	1.980(3)	N1-Cu1-N6	113.9(1)
Cu1-N6	1.989(3)	N1-Cu1-N3	122.0(1)
Cu1-N3	1.977(3)	N3-Cu1-N6	123.9(1)
Cu2-N5	1.965(4)	N2-Cu2-N5	114.0(1)
Cu2-N2	1.988(3)	N5-Cu2-N7	123.8(1)
Cu2-N7	1.964(3)	N2-Cu2-N7	118.8(1)

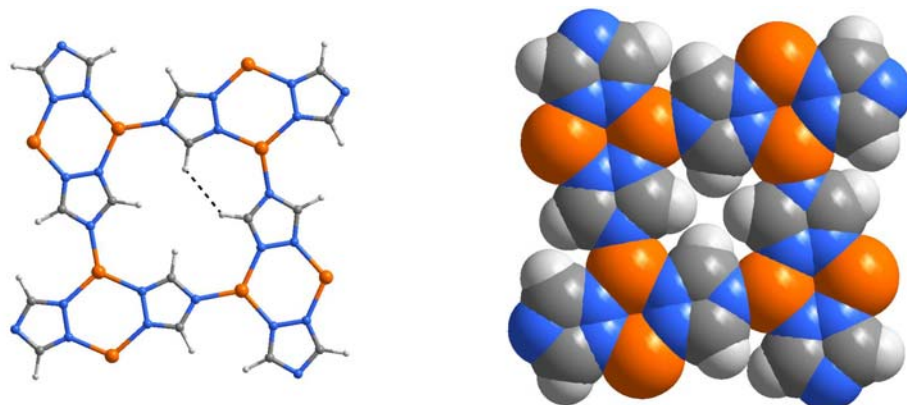


Fig. S3 Ball-and-stick (left, dash line = 2.5 Å) and space-filling (right) presentations of interaction between adjacent hydrogen atoms in [Cu(tz)].

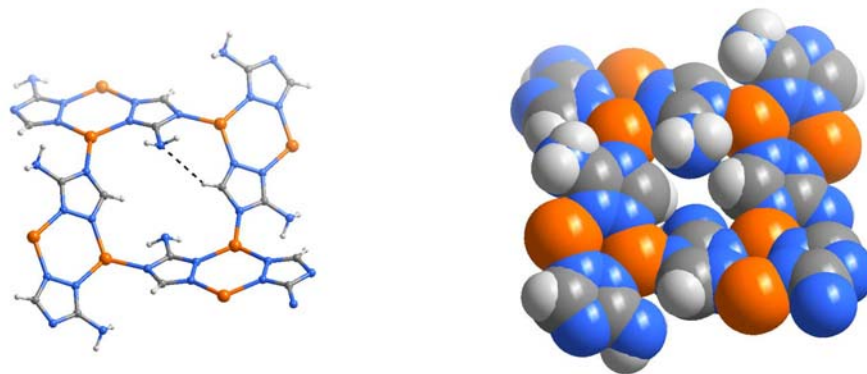


Fig. S4 Ball-and-stick (left, dash line = 2.7 Å) and space-filling (right) presentations of interaction between adjacent hydrogen atoms and amino groups in **1**.