Supplementary information to accompany ‘Copper coordination polymers constructed from thiazole-5-carboxylic acid: synthesis, crystal structures, and structural transformation’

Fig. S1 PXRD patterns showing the phase transformation of 2a to 3:

(i) Simulated pattern of pristine [Cu(5-tza)₂]·1.5H₂O (CCDC 964607)
(ii) Pattern reported by Rossin et al. to be dehydrated form of [Cu(5-tza)₂]·1.5H₂O
(iii) (this work) pattern of 2a left in air for 12 hours
(iv) Simulated pattern of 3

The pattern of the dehydrated form of [Cu(5-tza)₂]·1.5H₂O does not match the pattern of the pristine form well and there has clearly been a structural change. The similarity in powder diffraction patterns between (ii) and (iii) is clear and the assignment of (ii) & (iii) as dominated by a phase resembling 3
Fig. S2 Diagram showing the structural transformation of 2 to 2a and 3 with conditions used in the experiments.
Fig. S3 IR spectrum of ligand (L)
Fig. S4 IR spectrum of 1
Fig. S5 IR spectrum of 2
Fig. S6 IR spectrum of 3
Fig. S7 The thermogravimetric profile of 3 recorded in air.