

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

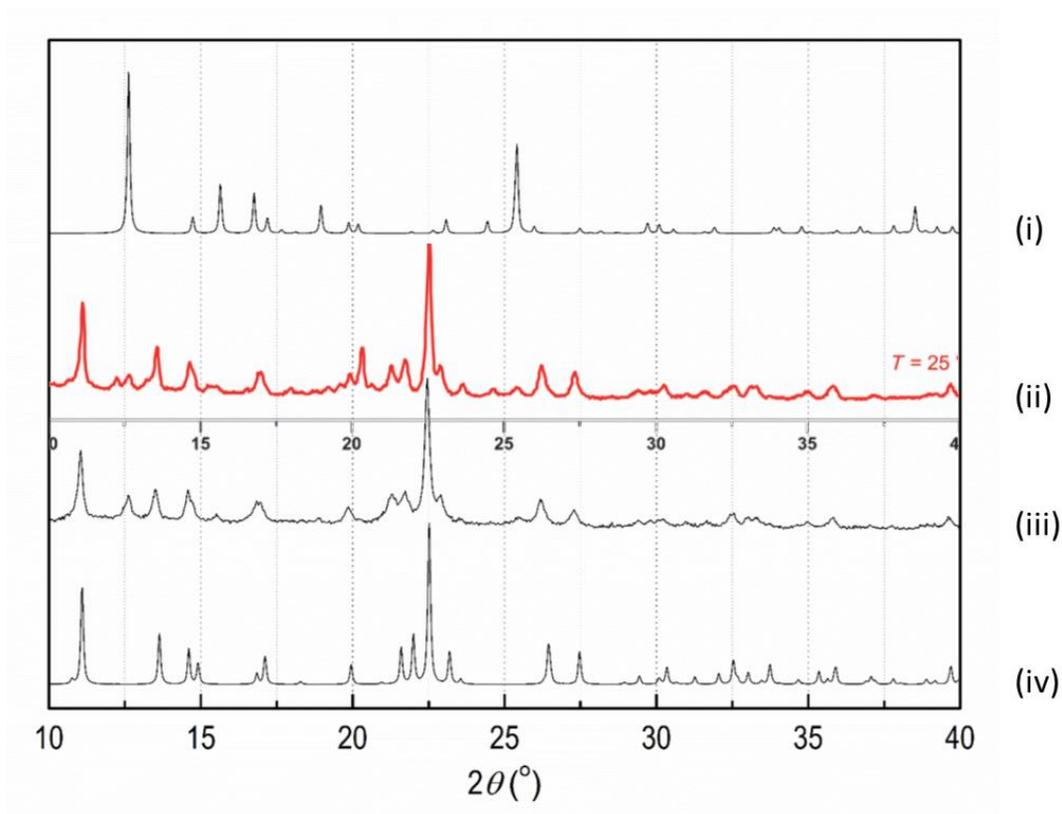


Fig. S1 PXRD patterns showing the phase transformation of **2a** to **3**:

- (i) Simulated pattern of pristine $[\text{Cu}(5\text{-tza})_2] \cdot 1.5\text{H}_2\text{O}$ (CCDC 964607)
- (ii) Pattern reported by Rossin *et al.* to be dehydrated form of $[\text{Cu}(5\text{-tza})_2] \cdot 1.5\text{H}_2\text{O}$
- (iii) (this work) pattern of **2a** left in air for 12 hours
- (iv) Simulated pattern of **3**

The pattern of the dehydrated form of $[\text{Cu}(5\text{-tza})_2] \cdot 1.5\text{H}_2\text{O}$ 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**

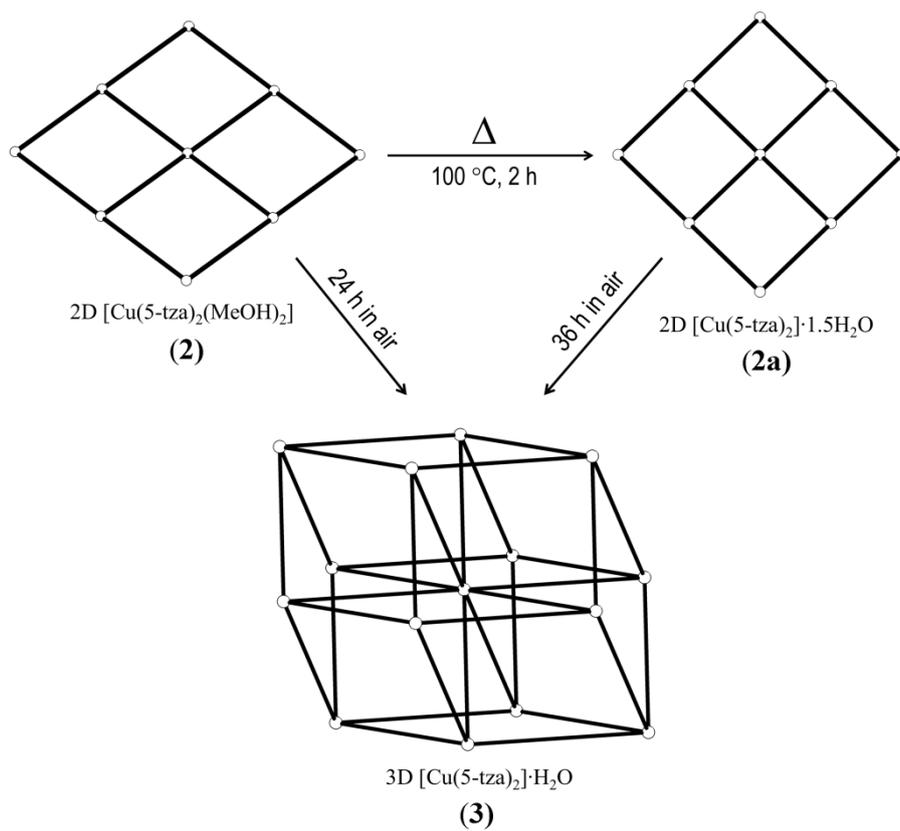


Fig. S2 Diagram showing the structural transformation of **2** to **2a** and **3** with conditions used in the experiments.

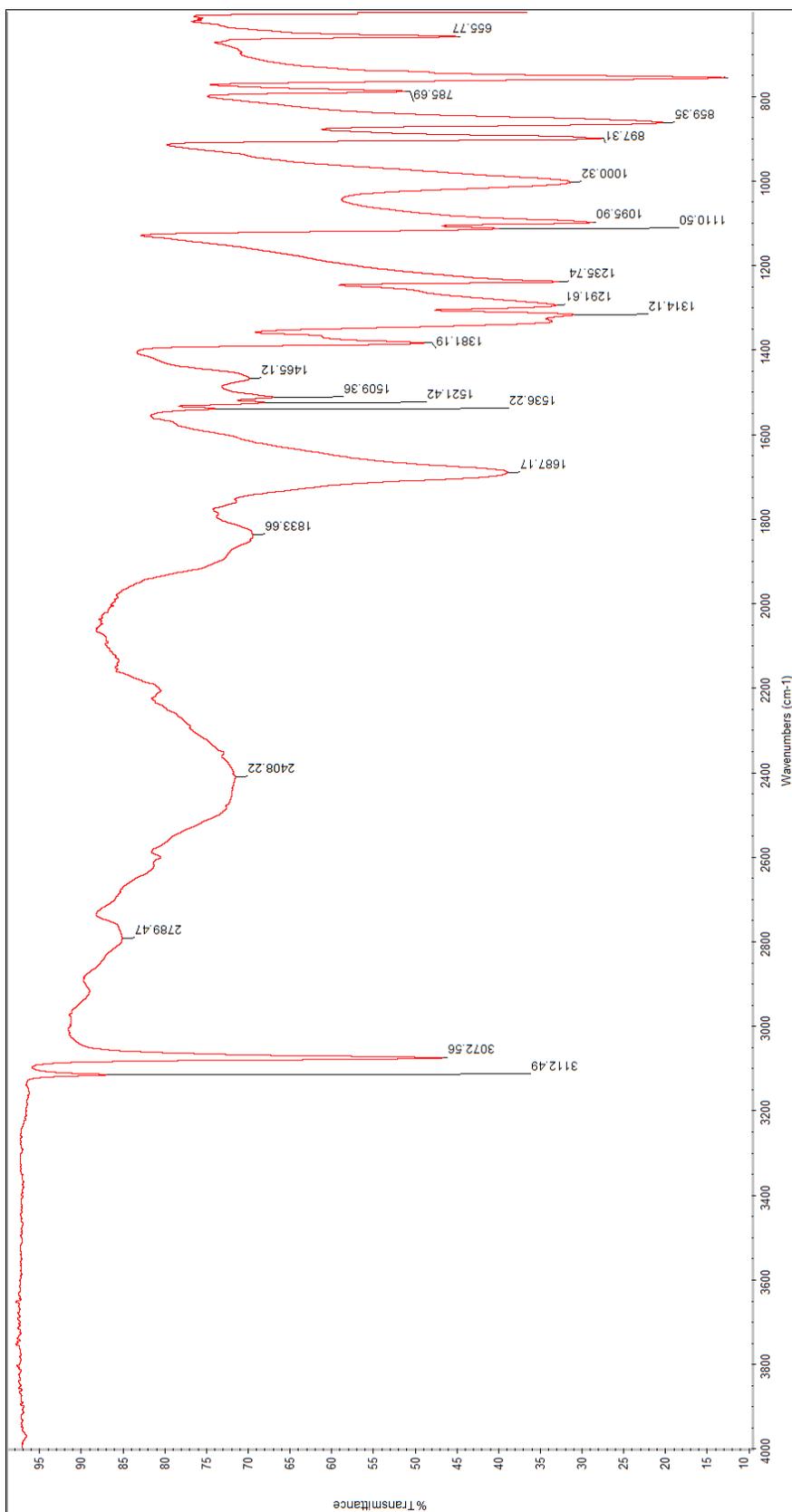


Fig. S3 IR spectrum of ligand (L)

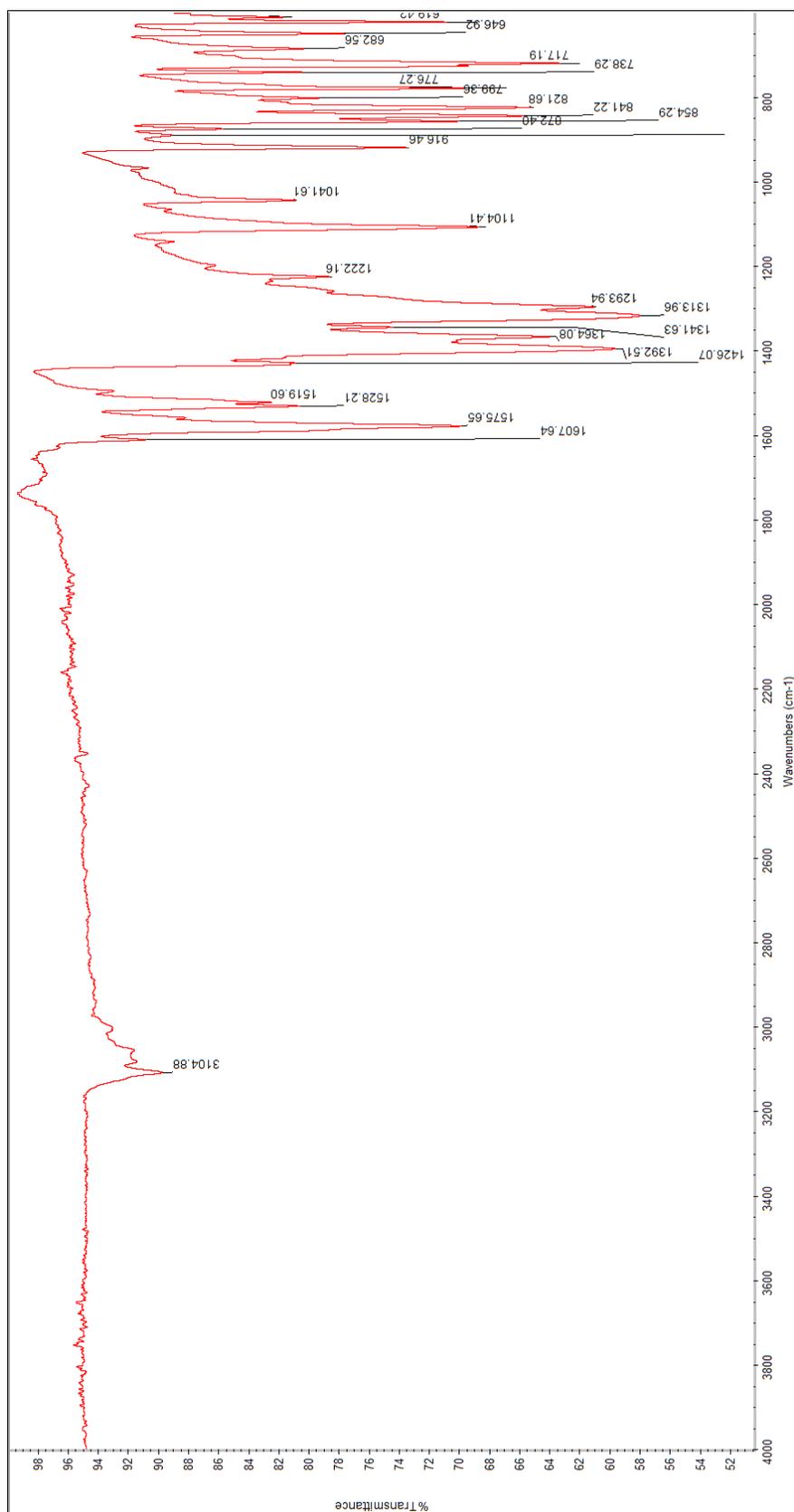


Fig. S4 IR spectrum of **1**

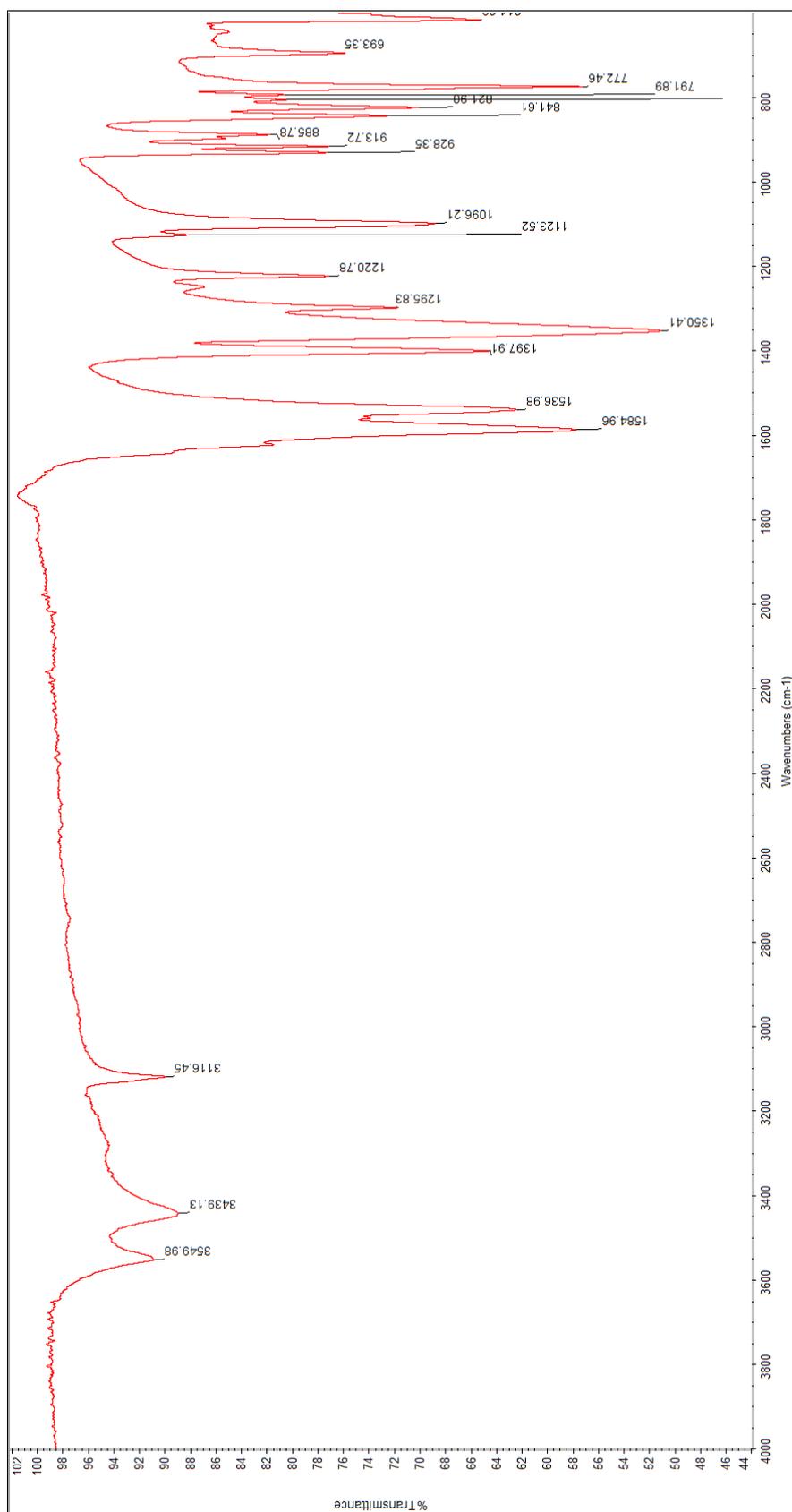


Fig. S5 IR spectrum of 2

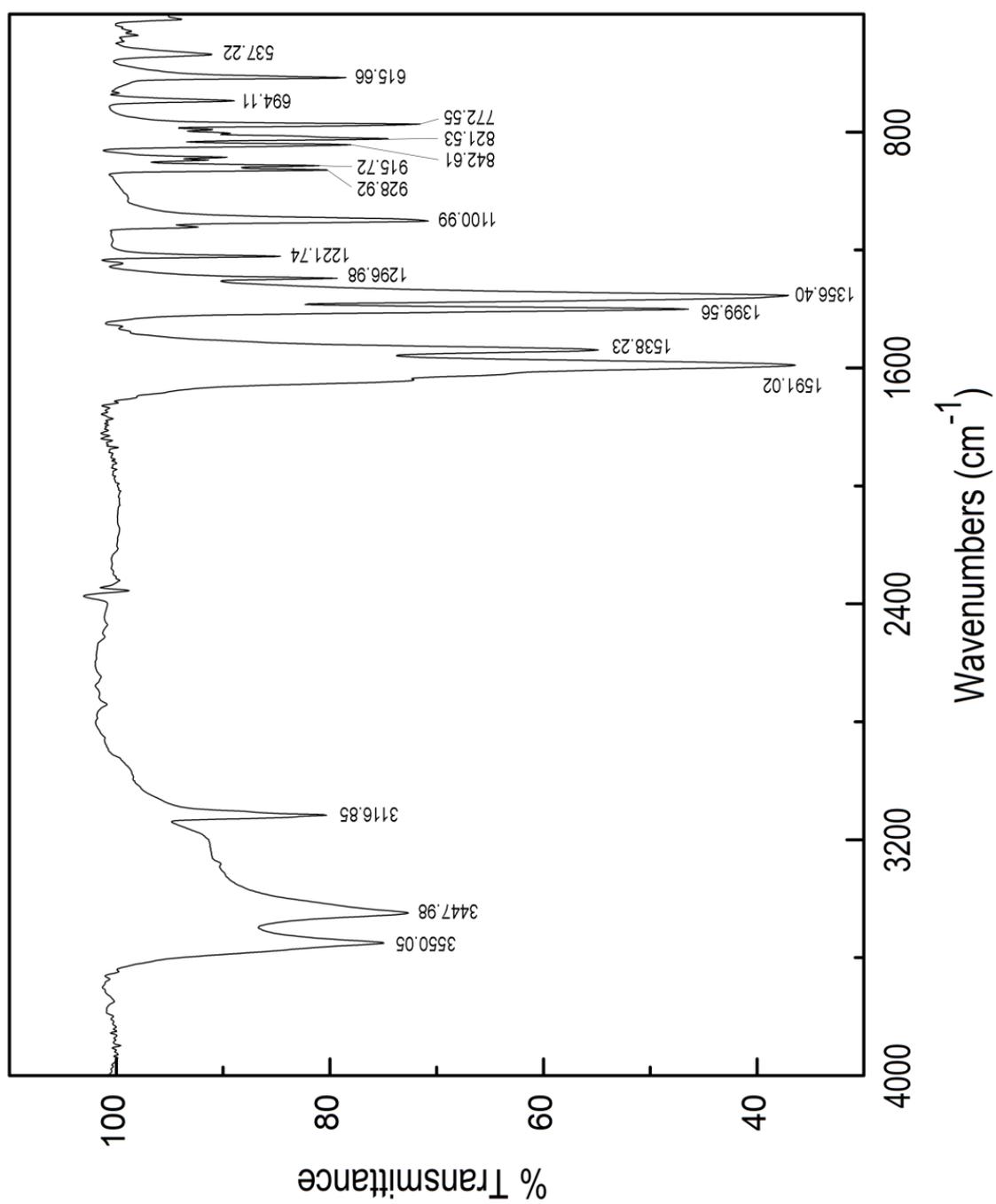


Fig. S6 IR spectrum of 3

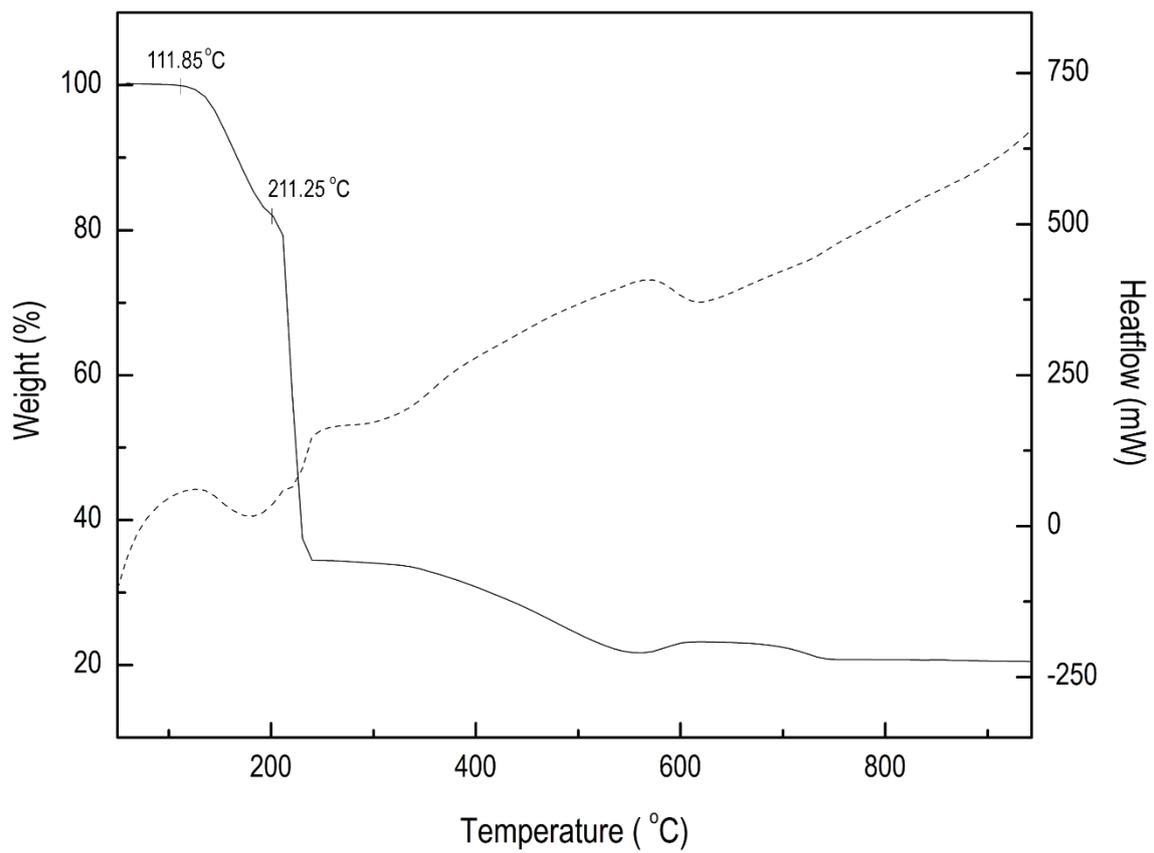


Fig. S7 The thermogravimetric profile of **3** recorded in air.