Supplementary materials for UK3122

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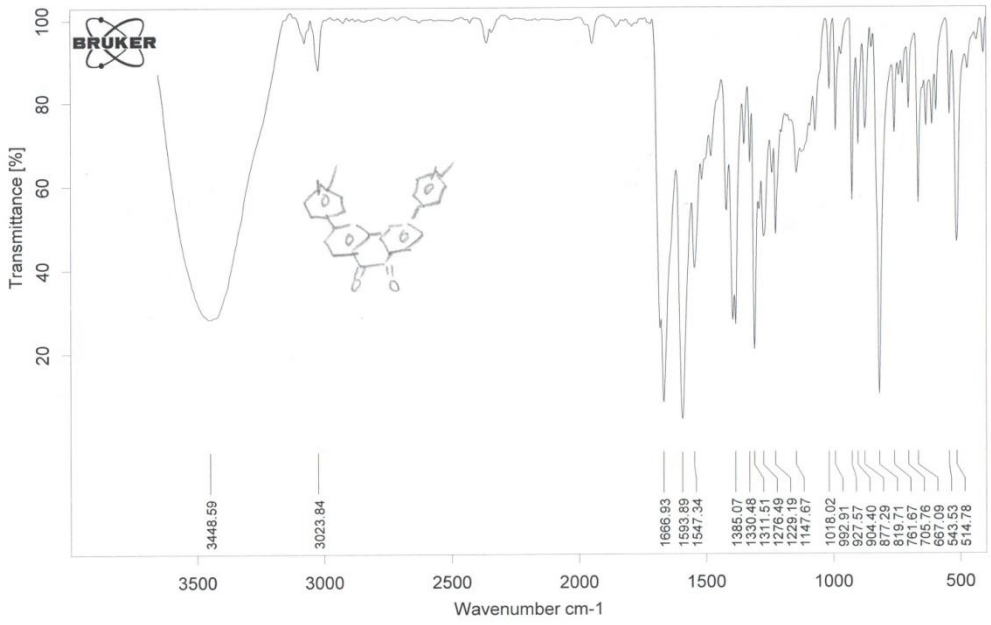
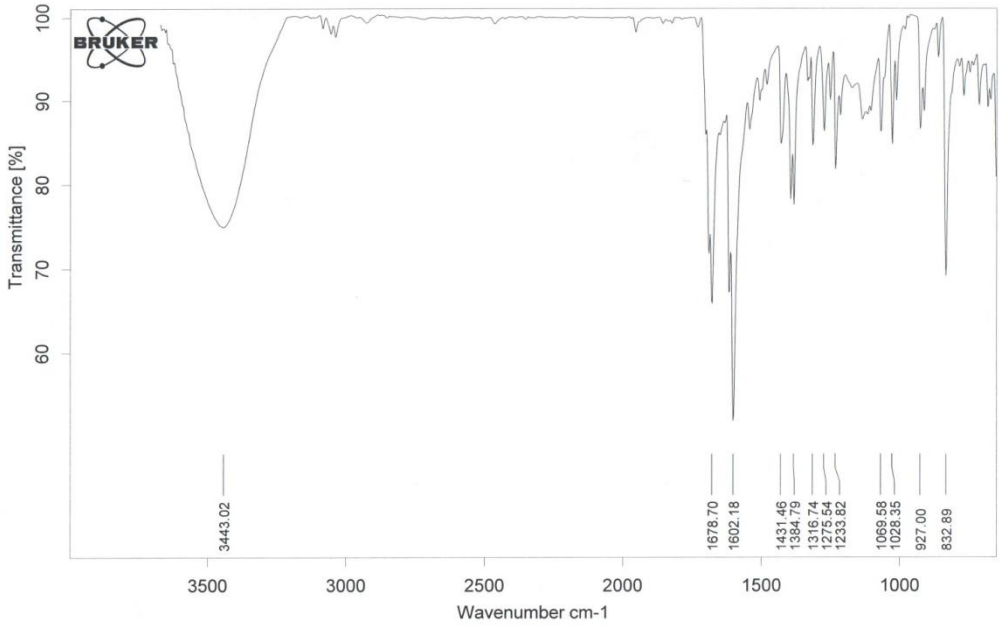
IR Spectroscopy analysis and spectra

The IR spectra of **L**, **1-2** are similar (see Fig. S1a-c in the Supporting Information). The absorption bands in the region 3600–3200 cm^{-1} indicate the presence of -OH groups and/or lattice water molecules. The bands at around 3050 and 3020 cm^{-1} can be ascribed to C–H stretching vibrations of the pyridine and benzene ring. The feature at around 1600 and 1580 cm^{-1} is associated with the presence of pyridine ring and benzene ring. For **L** and **1**, the bands at 1667 and 1678 cm^{-1} indicate the presence of carbonyl groups. For **2**, the characteristic peaks for carbonyl stretch disappeared, and the new peaks at 1031 cm^{-1} can be ascribed to C–O stretching vibrations, which further indicate the presence of –OH. These findings are consistent with the crystal structures. The bands at around 810 cm^{-1} can be ascribed to the stretching vibrations para-substituted benzene respectively.

(a)



(b)



(c)

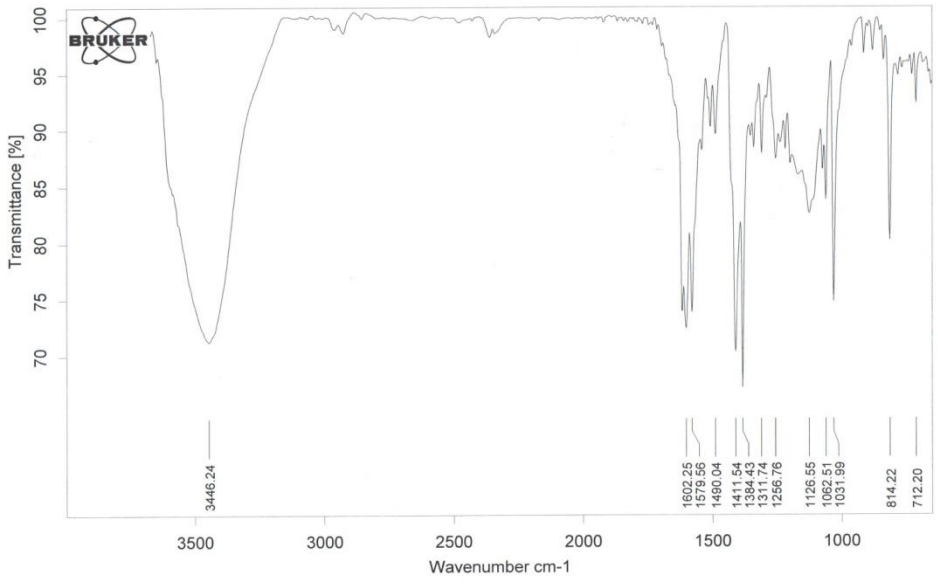


Fig. S1. IR spectra of **L** and **1-2**.

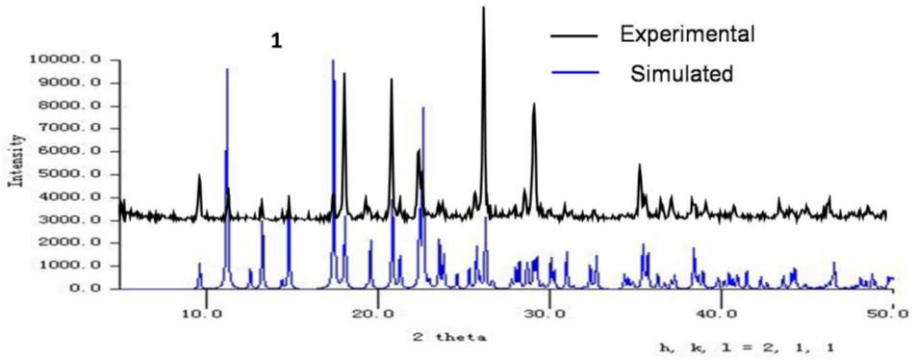


Fig. S2. Experimental and simulated PXRD patterns of **1**.

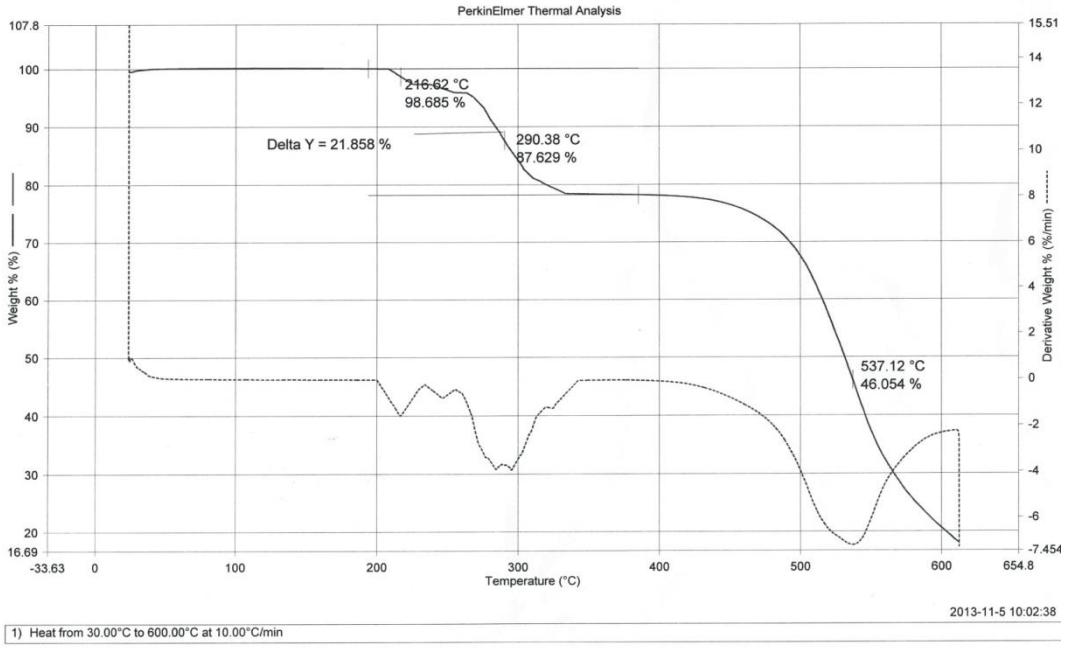


Fig. S3. TGA curves of **1**.