Electronic Supplementary Material (ESI) for CrystEngComm

Electronic Supplementary Information:

Crystallisation of solvothermally synthesized ZIF-8 investigated at the bulk, single crystal and surface level

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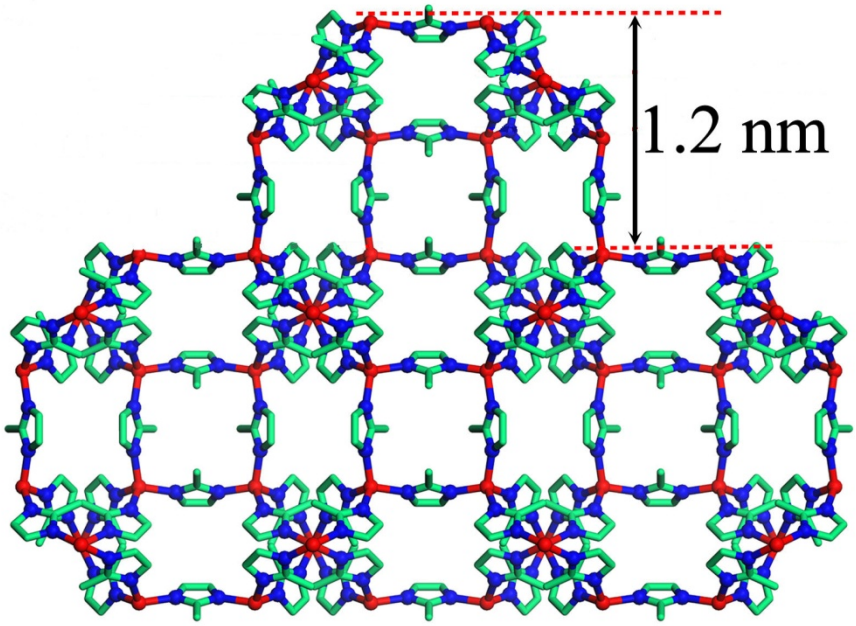

Figure S1. The crystallographic structure of ZIF-8 viewed along the [100] direction highlighting the d_{110} crystallographic spacing of 1.20 nm. H atoms and non-framework species have been omitted for clarity

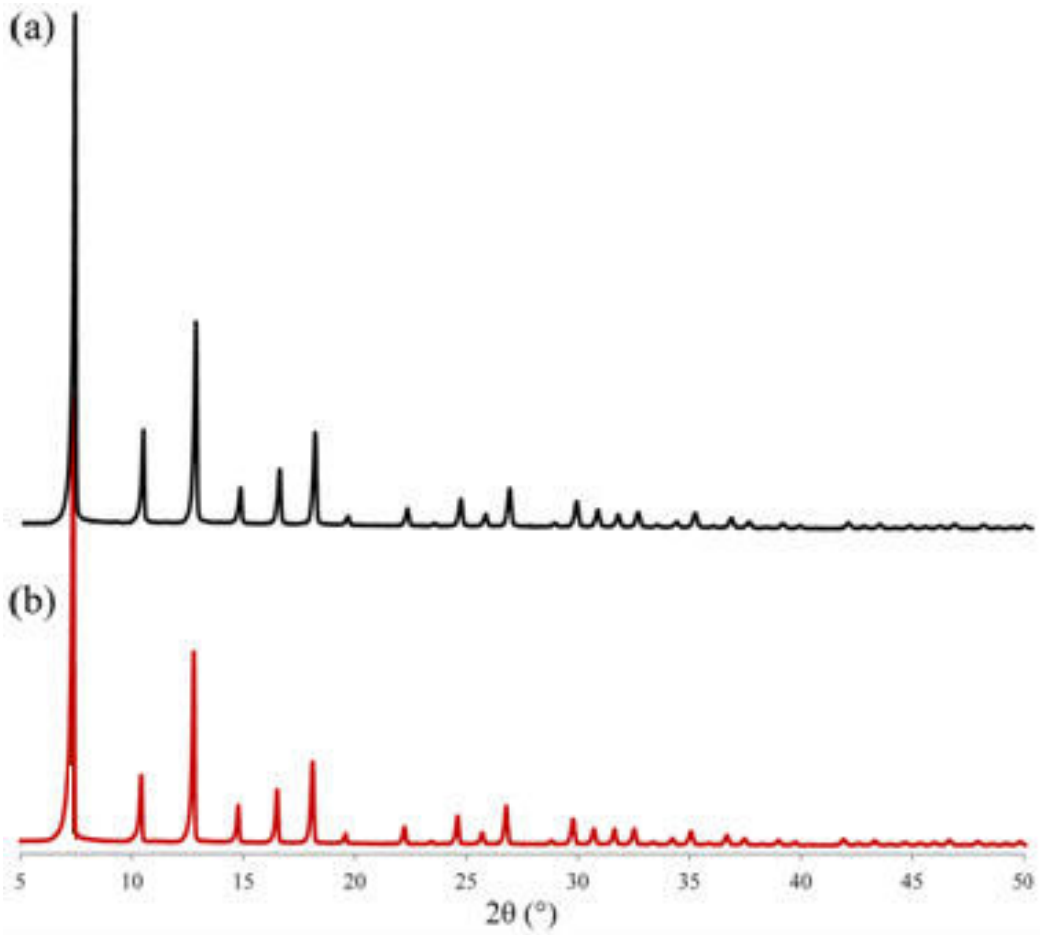

Figure S2. Representative powder X-ray patterns of ZIF-8 prepared for (a) 2 days and (b) 1 month at 100 °C.

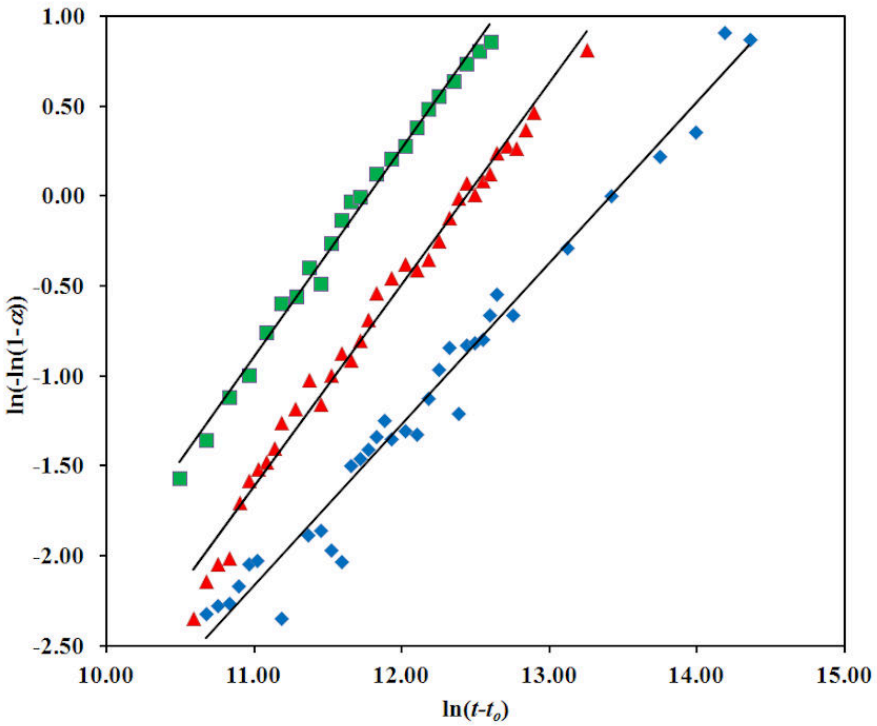

Figure S3. Sharp Hancock plots for the crystallisation of ZIF-8 at temperatures 100 (◆), 110(▲), and 120 °C (■).

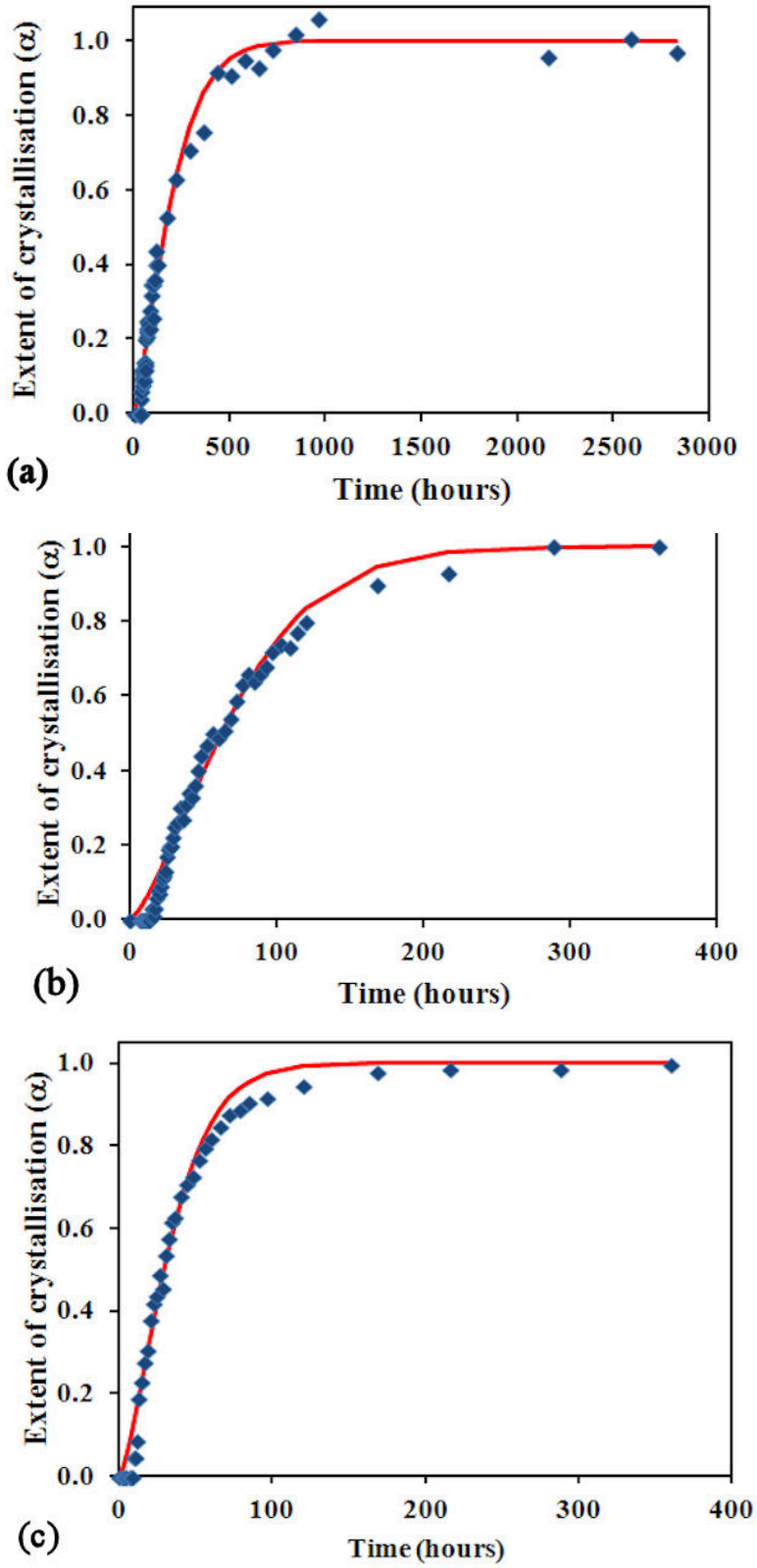

Figure S4. Fits (red lines) to the observed crystallisation curves (blue points) of ZIF-8 using using Khanna and Taylor's modified form of the Avrami equation derived from the Avrami-Erofe'ev model at temperatures of (a) 100, (b) 110, and (c) 120 °C.

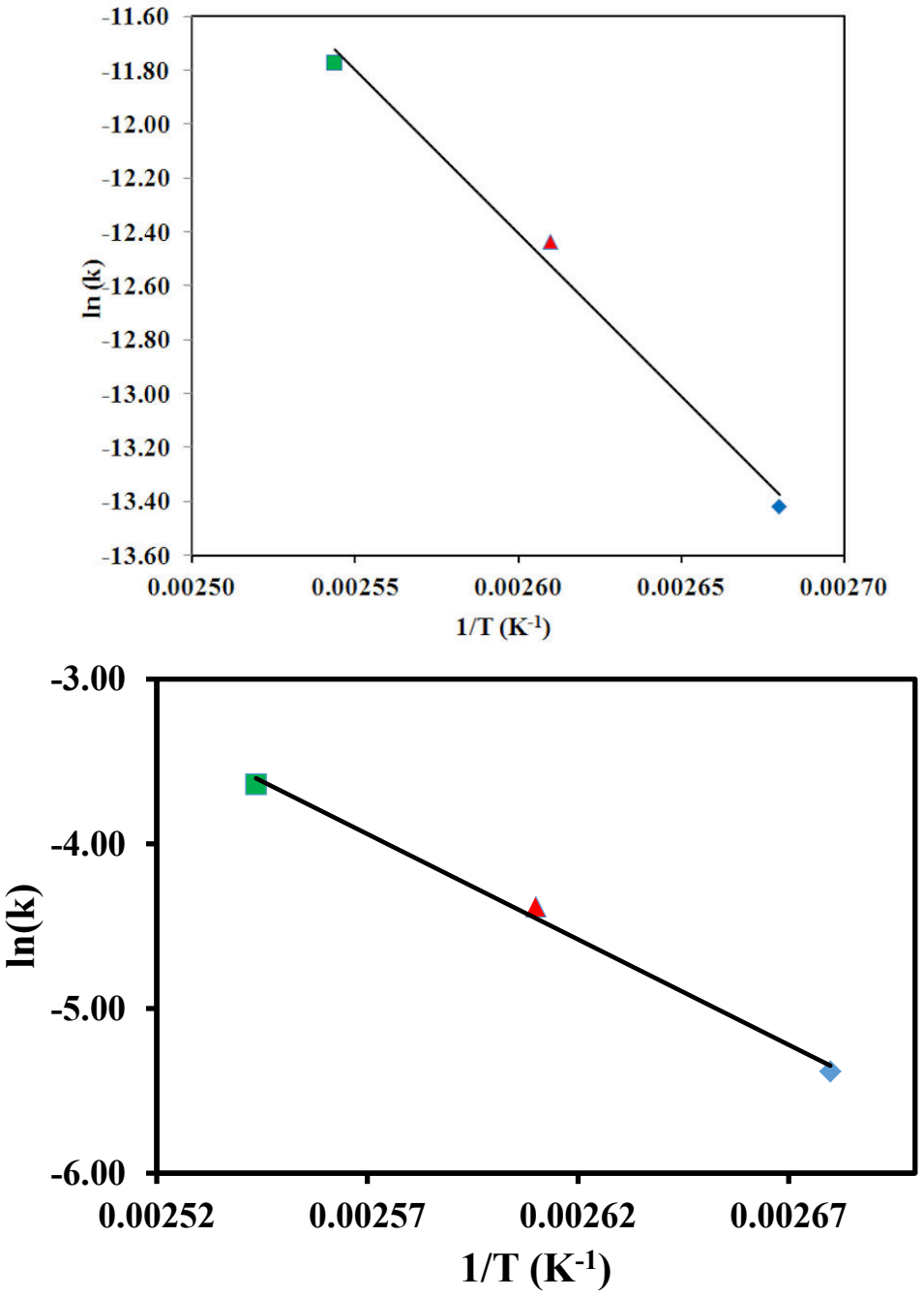

Figure S5. Arrhenius plots used to determine the overall activation energy for crystallisation from the results of the SH analyses of the crystallisation data using the AE model (top) and nonlinear least squares fitting using Khanna and Taylor's modified form of the Avrami equation (bottom).

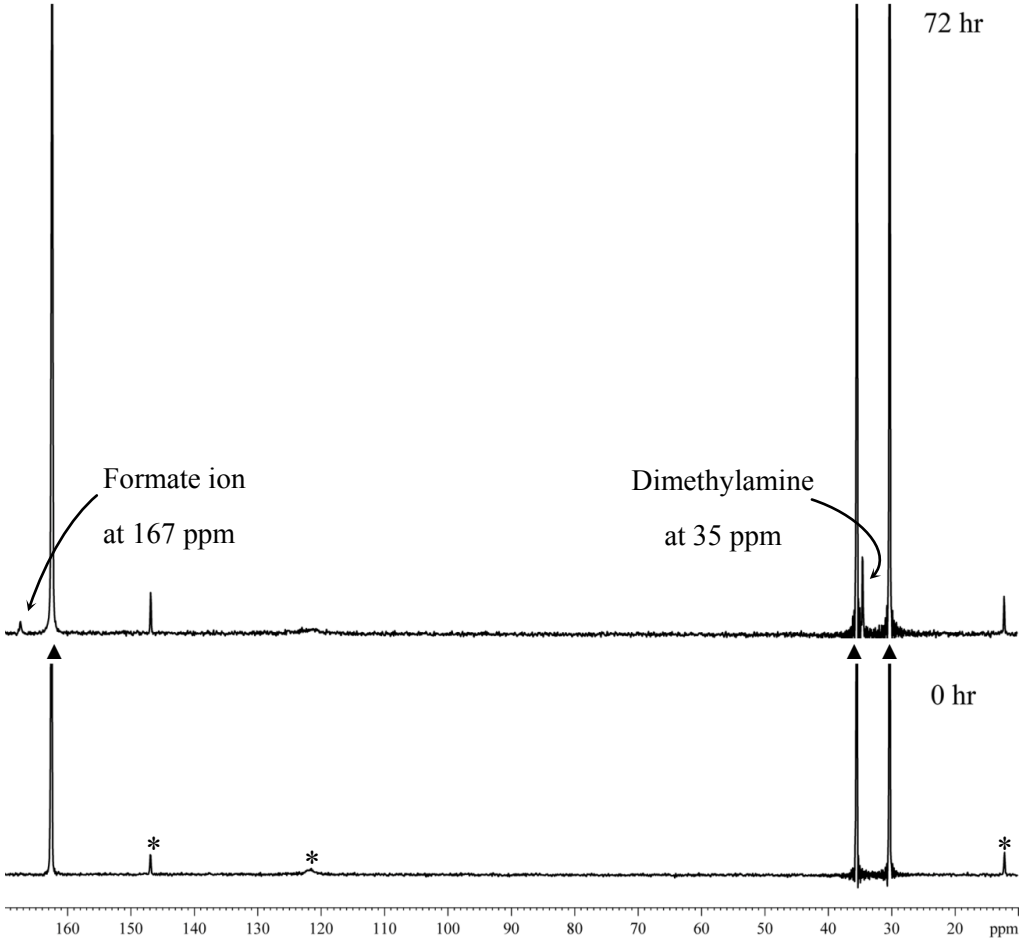

Figure S6. ^{13}C HPDEC NMR spectra of the mother solutions of the ZIF-8 reaction mixture extracted after heating at 100 °C for 0 hour and 72 hours, respectively. Partial decomposition of the DMF during the synthesis is evidenced through the presence of the formate ions and dimethylamine in the spectrum of the sample heated for 72 hours. The characteristic peaks for $meIm^-$ are marked as * while peaks for DMF are marked with ▲.