Study of the mechanochemical formation and resulting properties of an archetypal MOF: $Cu_3(BTC)_2$ (BTC = 1,3,5-benzenetricarboxylate)

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Supplementary information: XRPD patterns, adsorption and desorption isotherms TGA-DSC.

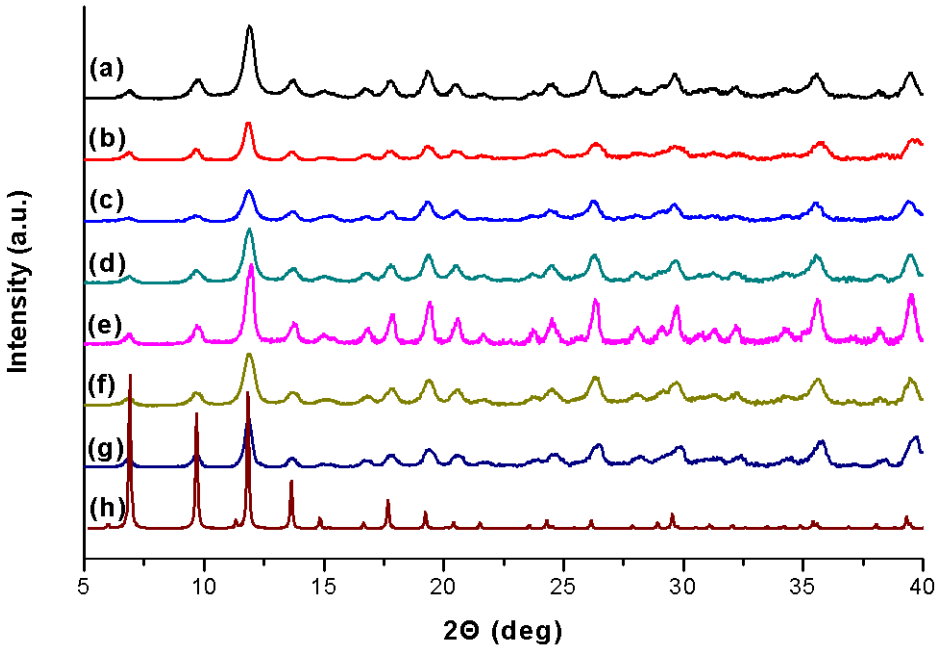

Figure S1. Comparison of experimental and simulated XRPD patterns for $Cu_3(BTC)_2$ synthesised by (a) 5 minutes grinding then washing with EtOH; (b) 5 minutes grinding with added MeOH (100 µL) then washed with EtOH; (c) 15 minutes grinding with no washing; (d) 15 minutes and washing with EtOH; (e) 15 minutes grinding with added MeOH (100 µL) and washing with EtOH; (f) 25 minutes and washing with EtOH; (g) 25 minutes grinding with added MeOH (100 µL) and washing with EtOH; (h) simulated for FIQCEN (CCDC code).

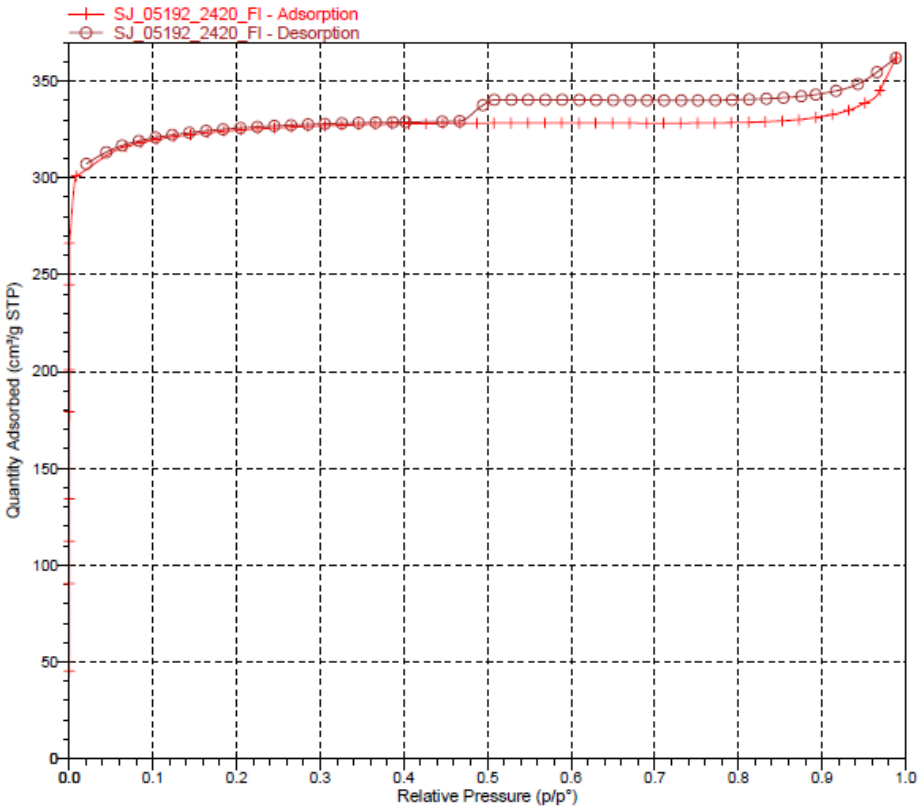

Figure S2. Adsorption and desorption N_2 isotherms for $Cu_3(BTC)_2$ prepared by neat grinding for 5 minutes followed by washing with EtOH.

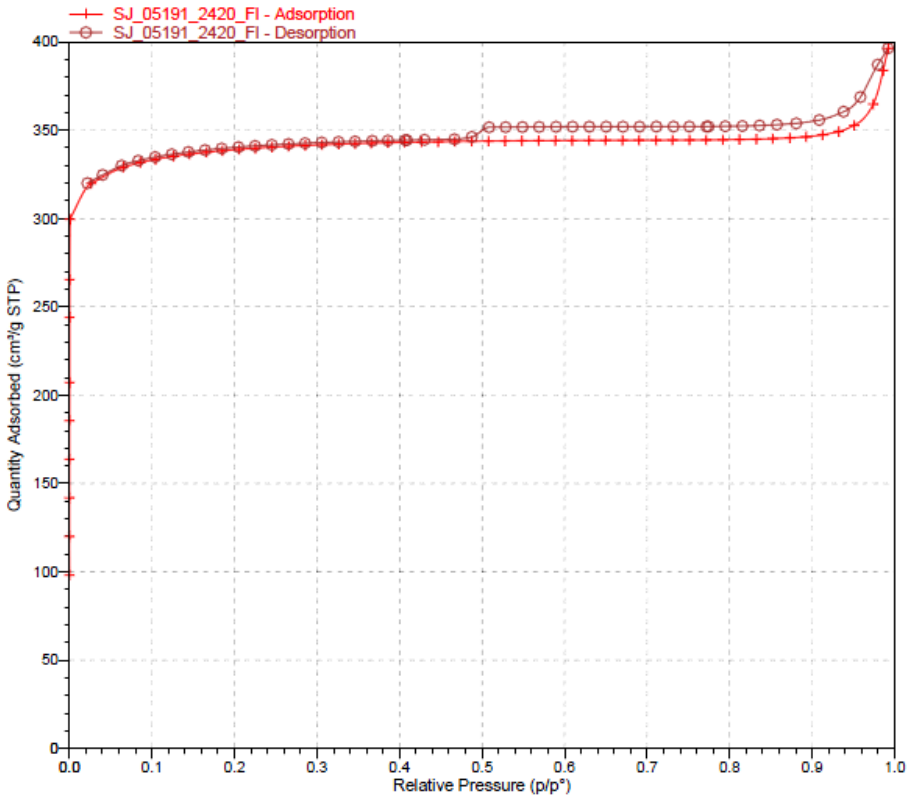

Figure S3. N_2 adsorption and desorption isotherms for $Cu_3(BTC)_2$ prepared by liquid-assisted grinding for 5 minutes with added MeOH (100 µL) followed by washing with EtOH.

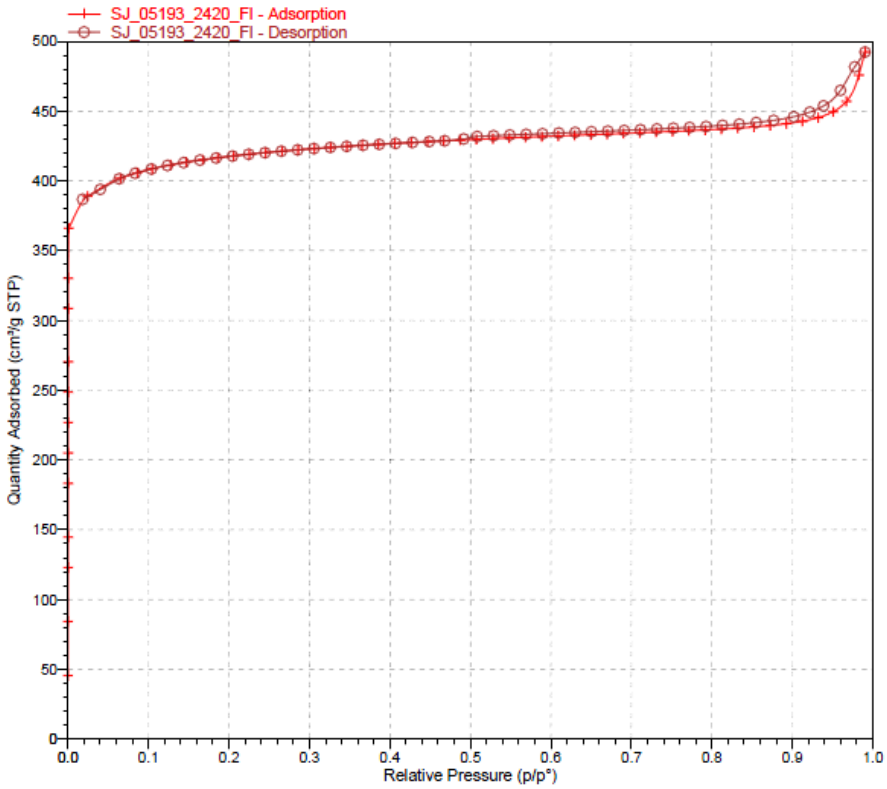

Figure S4. N_2 adsorption and desorption isotherms for $Cu_3(BTC)_2$ prepared by liquid-assisted grinding for 15 minutes with added MeOH (100 µL) followed by washing with EtOH.

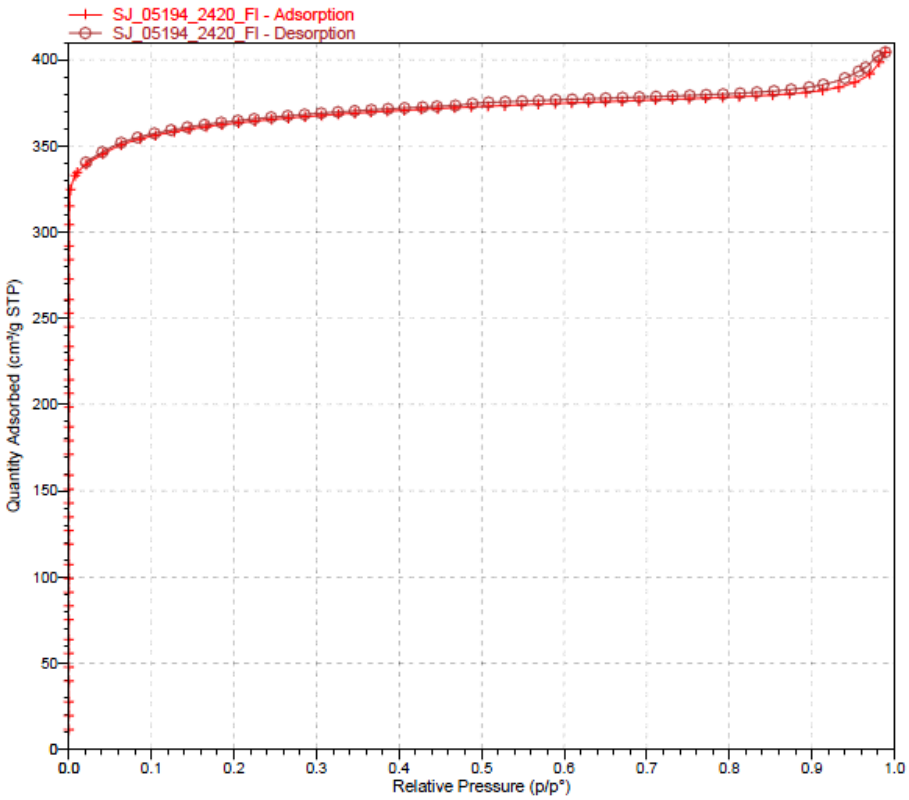

Figure S5. N_2 adsorption and desorption isotherms for the $Cu_3(BTC)_2$ prepared by neat grinding for 15 minutes followed by washing with EtOH.

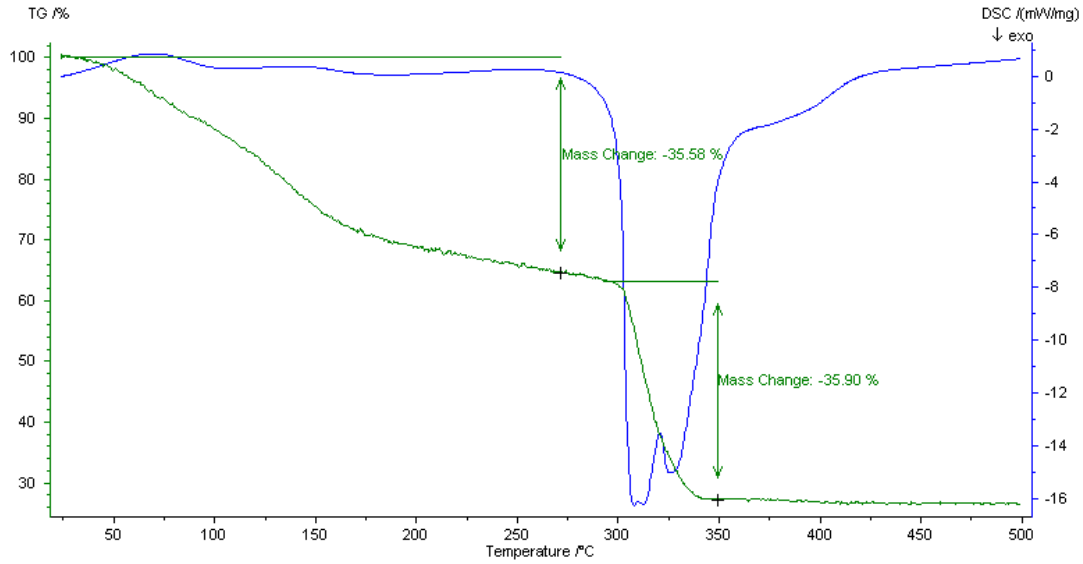

Figure S6. TGA-DSC mechanochemically-prepared $Cu_3(BTC)_2$ without LAG and without subsequent washing.