Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting information

Improvements to the production of ZIF-94; a case study in MOF scale-up.

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Determination of solid content.

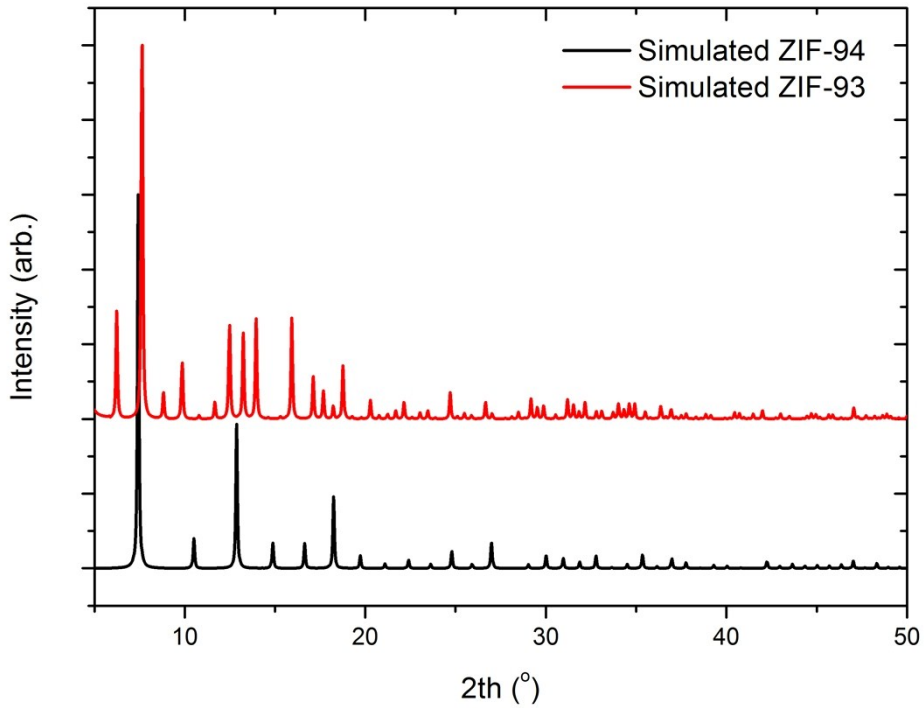
The solid content of the reaction was determined using the density of methanol (0.78 g mL-1) and THF (0.889 g mL-1). The final figure rounded to the closest whole number.

The below equation was used:

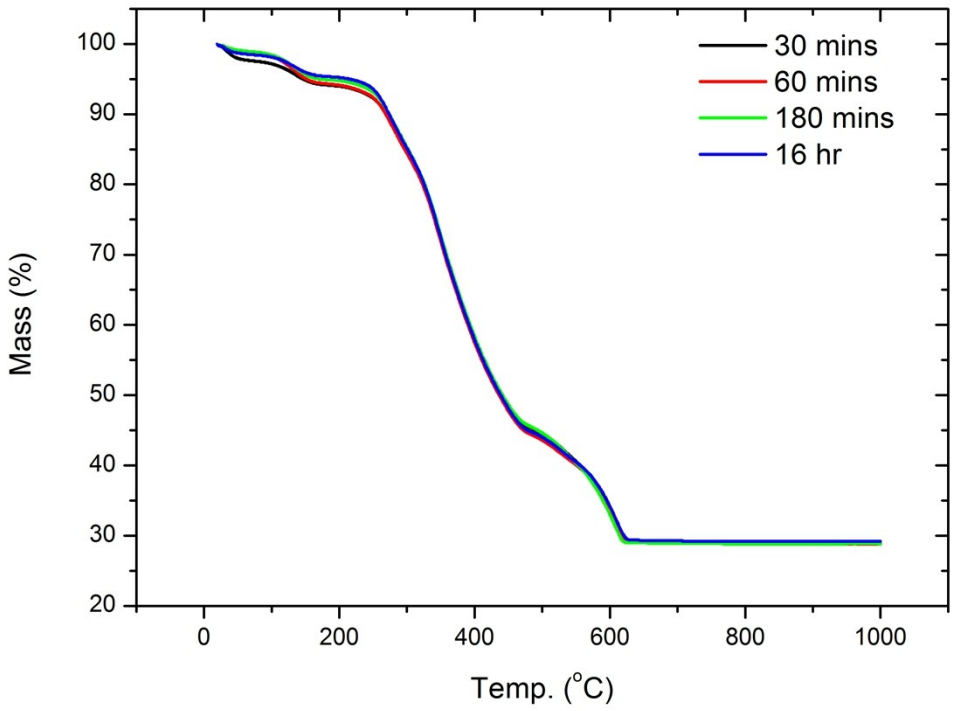
$$Solid\ Content\ (wt\%) = \frac{Total\ solids\ (g)}{((THF\ Vol.\ (mL)\ x\ 0.889) + (MeOH\ Vol.\ (mL) * 0.79)}\ x\ 100$$

A worked example for entry 9 is shown below

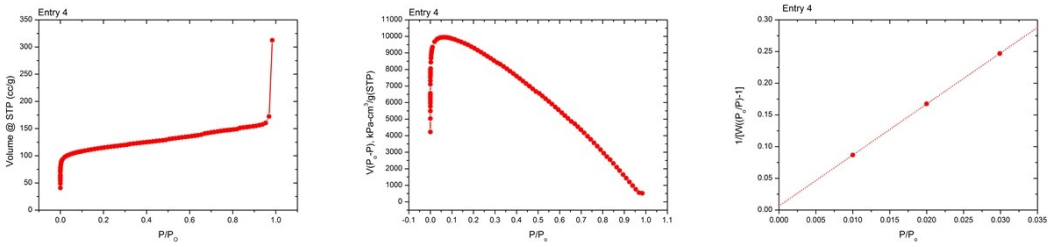
$$\frac{5.28}{((50\ x\ 0.889) + (20 * 0.79)}\ x\ 100 = \ 8.76\ \%\ \therefore 9\ wt\%$$



S 1: Simulated XRD patterns for ZIF-94 and ZIF-93

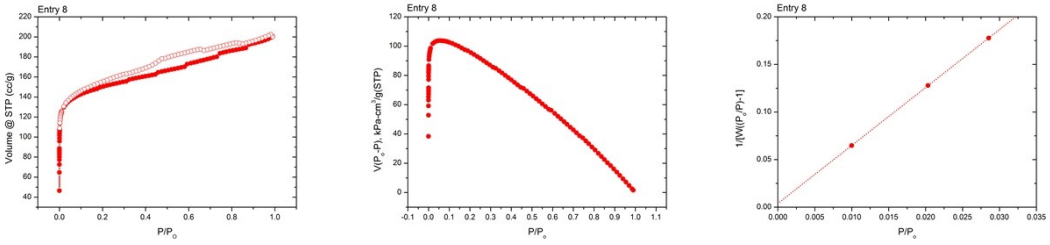


S 2 TGA traces for ZIF-94 samples produced at various reaction times



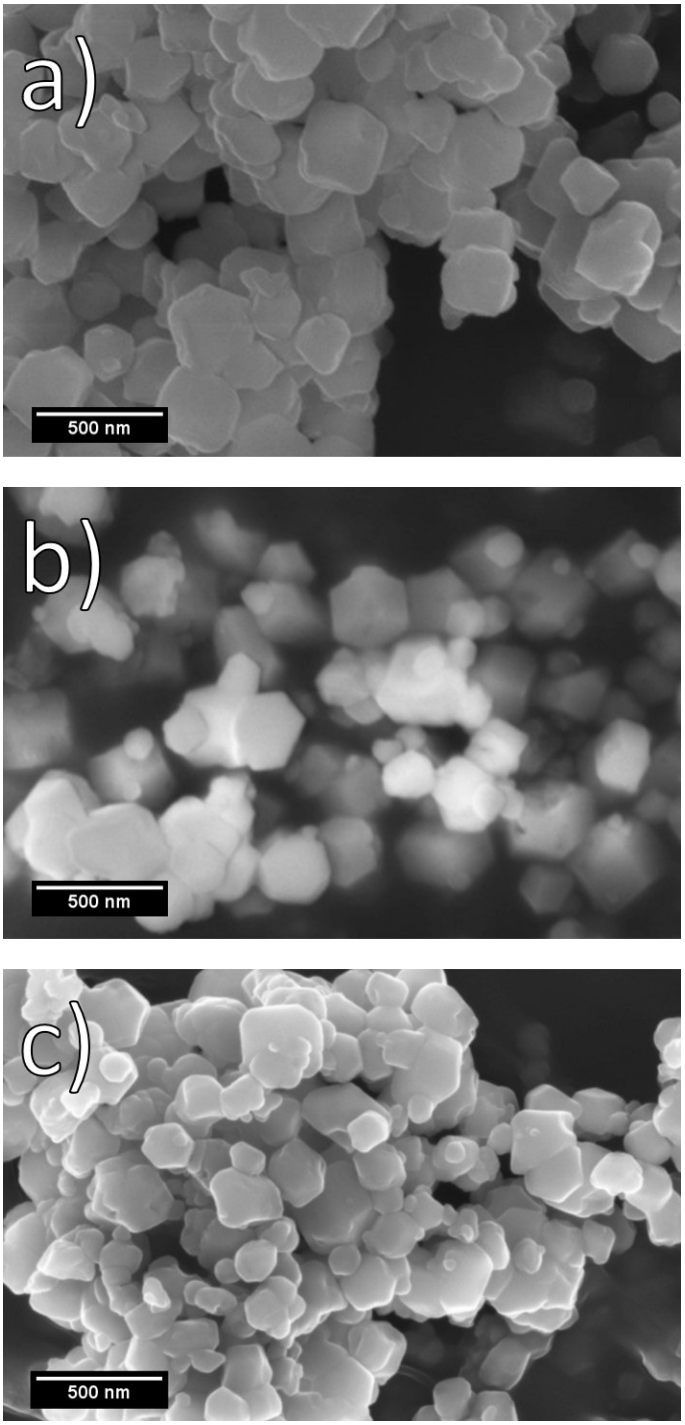
a) b) c)

S 3: N_2 isotherm, b) Rouquerol plot and c) three-point BET plot for entry 4.

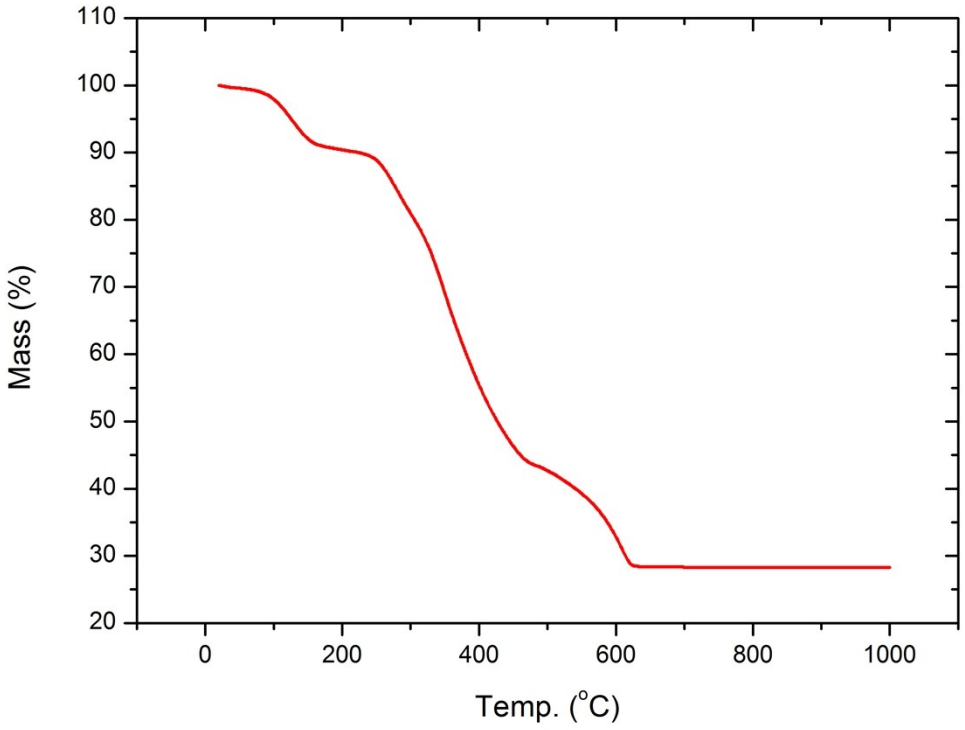


a) b) c)

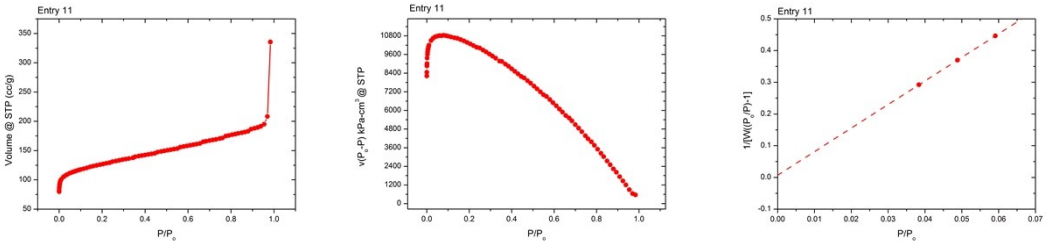
S 4 N_2 isotherm, b) Rouquerol plot and c) three-point BET plot for entry 8.



S 5: SEM micrographs for entries a) 4, b) 5 and c) 6.

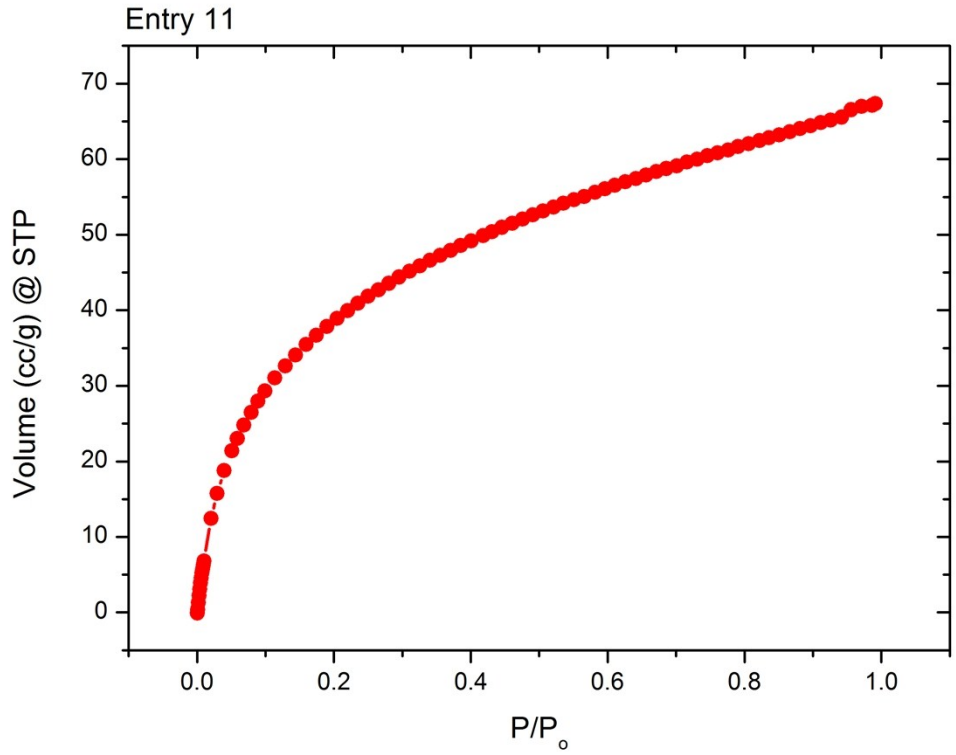


S 6: TGA of ZIF-94 produced at large scale (entry 11)

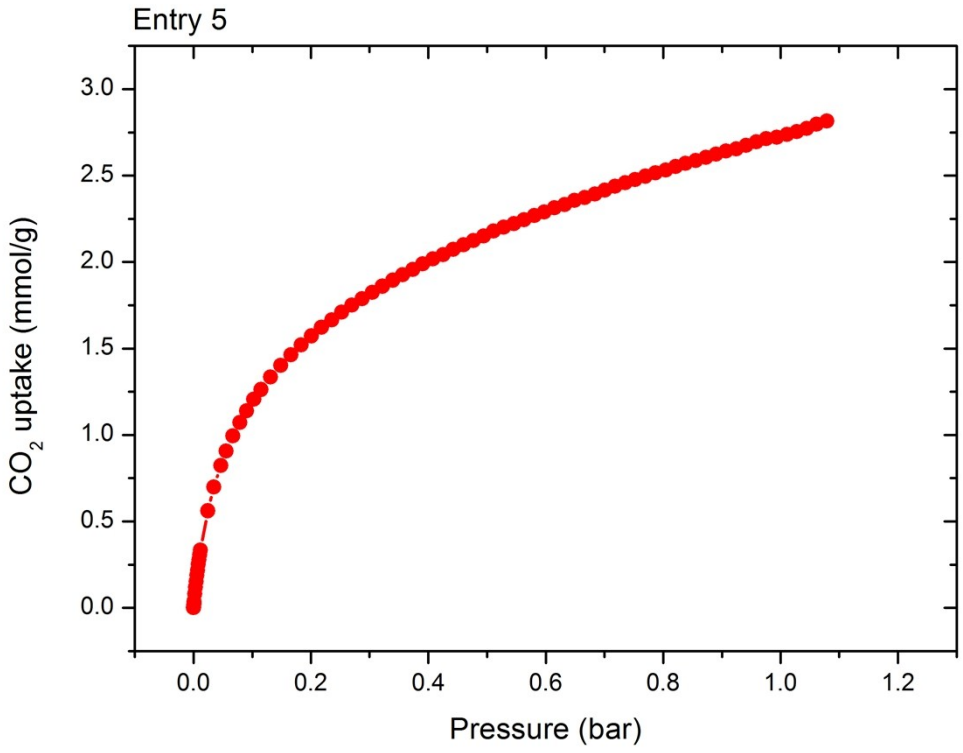


a) b) c)

S 7 a) N_2 isotherm, b) Rouquerol plot and c) three-point BET plot for entry 11.



S 8 CO_2 uptake isotherm for Entry 11



S9 CO_2 uptake isotherm for Entry 5