

Supplementary Information

Study of the scale-up, formulation, ageing and ammonia adsorption capacity of MIL-100(Fe), CuBTC and CPO-27(Ni) for use in respiratory protection filters

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Rietveld refinement fit

Phase identification was completed using Bruker AXS Diffrac Plus, Eva V19 (1996-2013), Bruker AXS Diffrac Eva V4.0 (2010-2014) software and the ICDD PDF Files: PDF-4+ 2013, COD (REV30738 2011.11.2) database. Crystallite size and lattice parameter measurements were completed using Bruker-AXS Topas 4.2 (1999-2009).

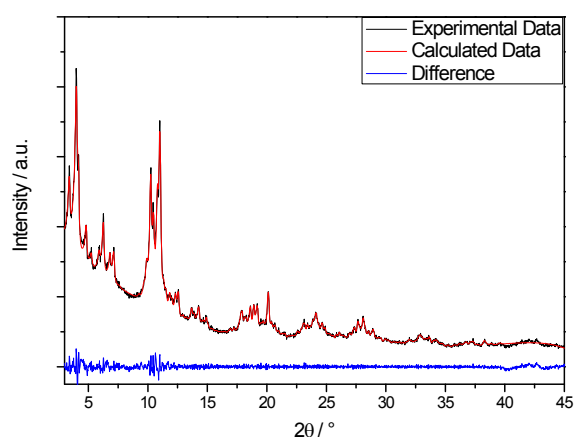


Figure 1. The Rietveld fitting profile of the XRD pattern of MIL-100(Fe) as-synthesised

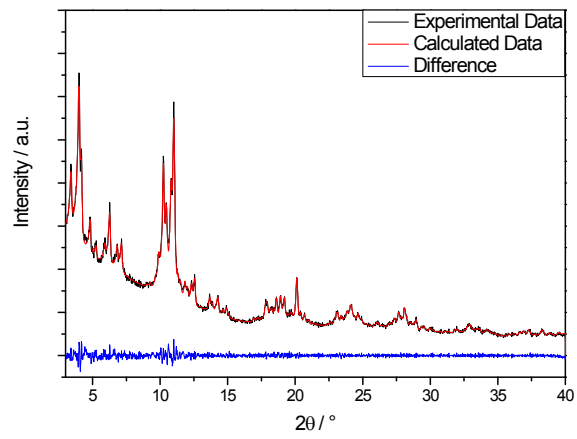


Figure 2. The Rietveld fitting profile of the XRD pattern of MIL-100(Fe)_1

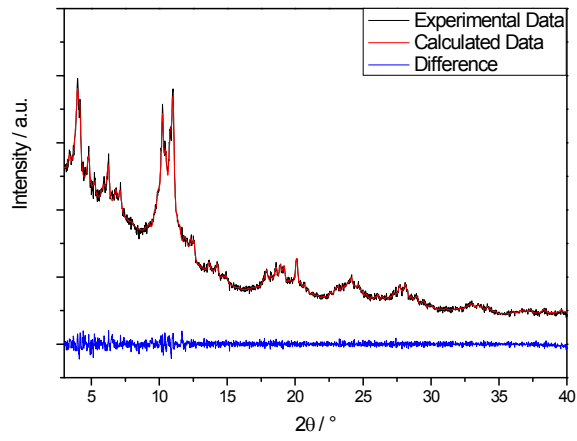


Figure 3. The Rietveld fitting profile of the XRD pattern of MIL-100(Fe)_2

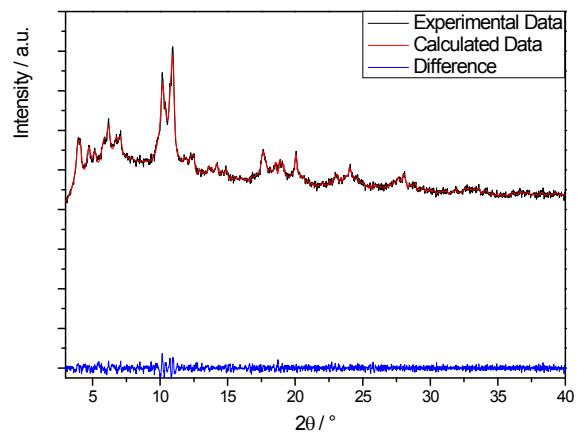


Figure 4. The Rietveld fitting profile of the XRD pattern of MIL-100(Fe)_3

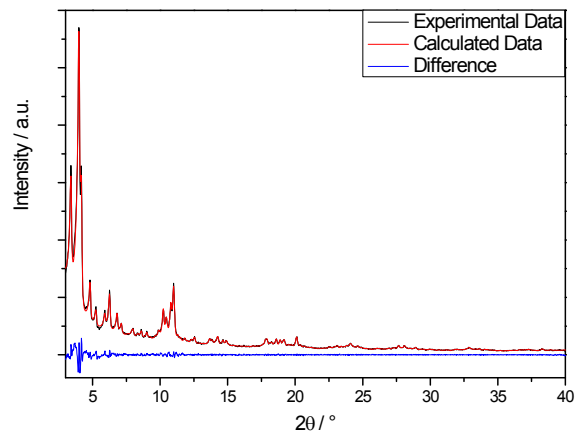


Figure 5. The Rietveld fitting profile of the XRD pattern of MIL-100(Fe)_4

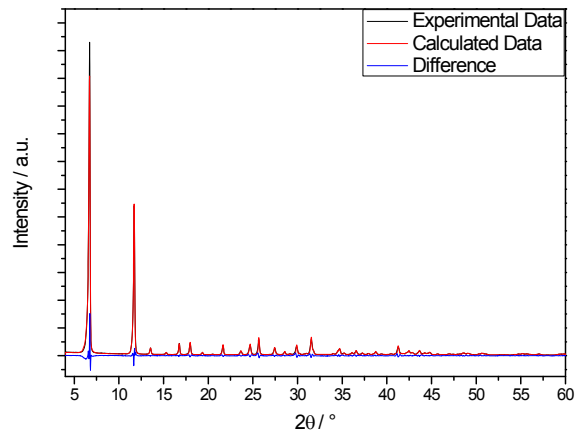


Figure 6. The Rietveld fitting profile of the XRD pattern of CPO-27(Ni) as-synthesised

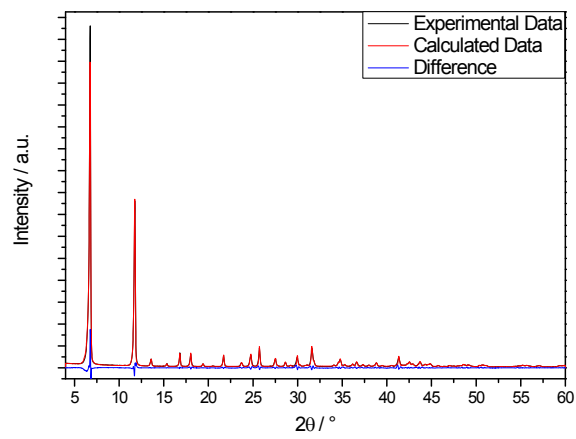


Figure 7. The Rietveld fitting profile of the XRD pattern of CPO-27(Ni)_1

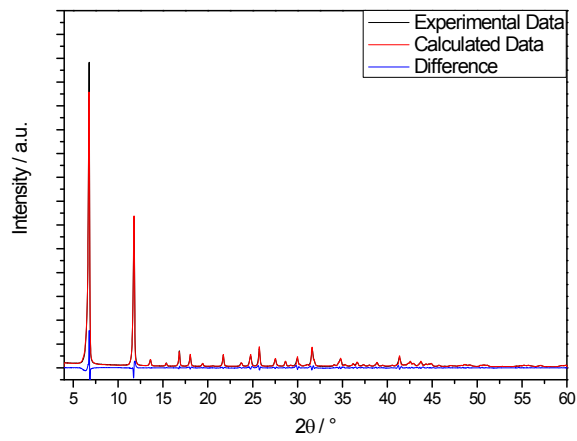


Figure 8. The Rietveld fitting profile of the XRD pattern of CPO-27(Ni)₂

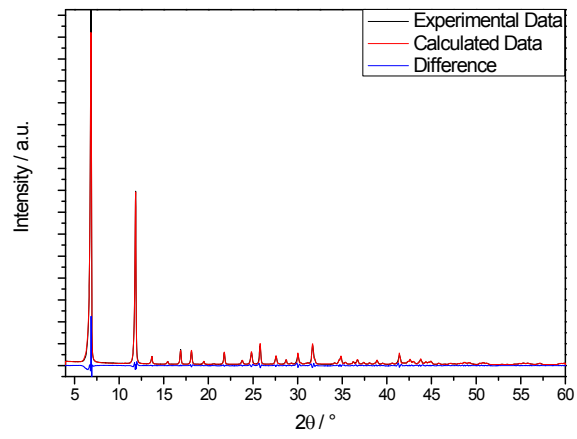


Figure 9. The Rietveld fitting profile of the XRD pattern of CPO-27(Ni)₃

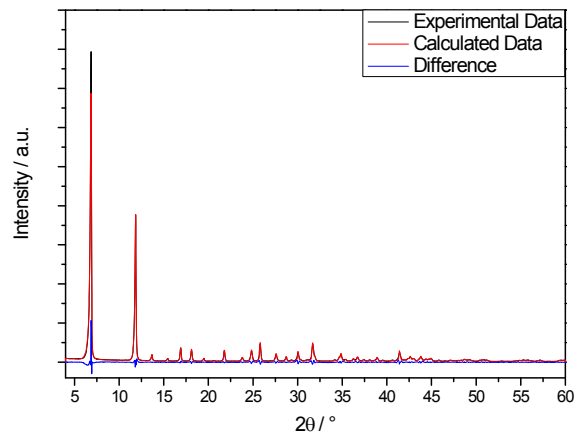


Figure 10. The Rietveld fitting profile of the XRD pattern of CPO-27(Ni)₄

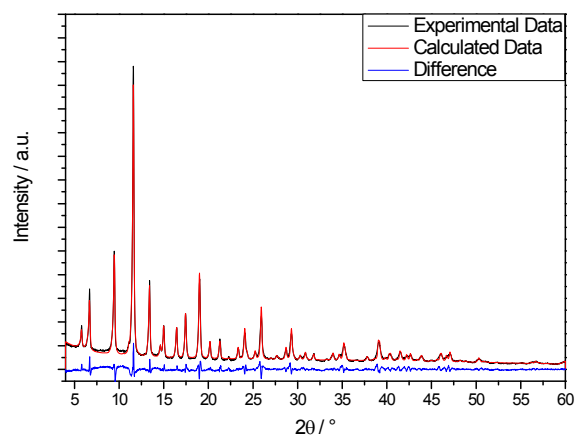


Figure 11. The Rietveld fitting profile of the XRD pattern of Cu-BTC as-synthesised

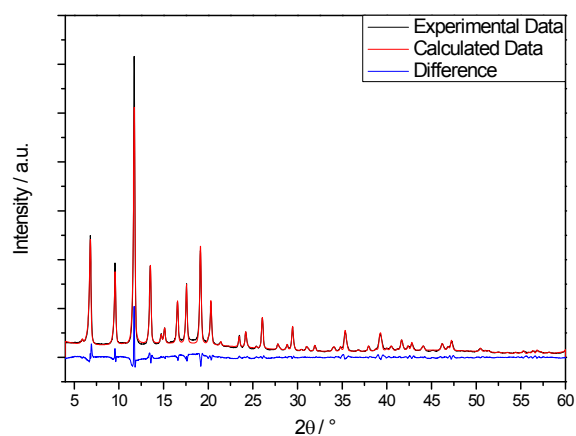


Figure 12. The Rietveld fitting profile of the XRD pattern of Cu-BTC_1

Nitrogen isotherms

Nitrogen isotherm measurements were collected on a Quantachrome Autosorb-iQ-MP at 77 K, 2-station model with each station having 1 Torr, 10 Torr and 1000 Torr transducers. MOF samples were degassed using a two-step programme ramp to 90°C for 2 hours followed by ramp to 150°C for 13 hours. All the BET surface areas were calculated using the Rouquerol method.

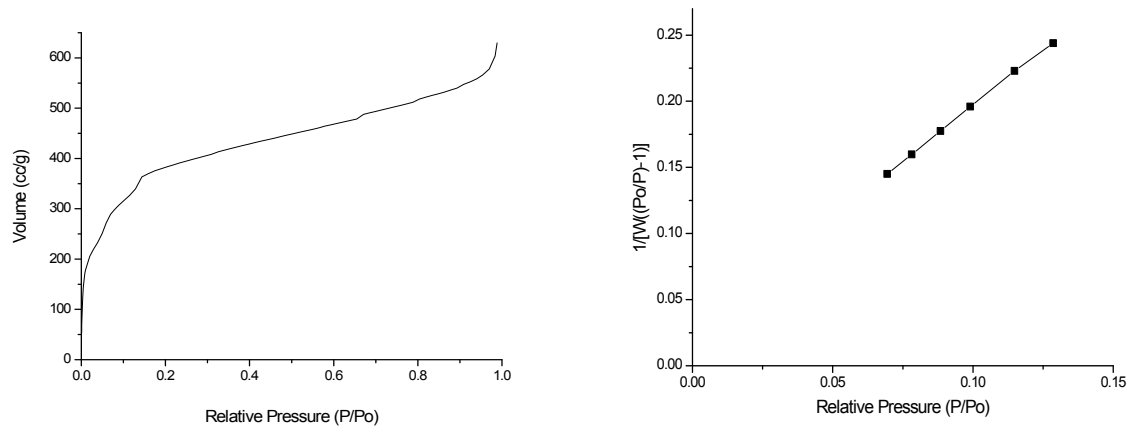


Figure 13. Nitrogen adsorption isotherm and multipoint BET plot for MIL-100(Fe) as-synthesised

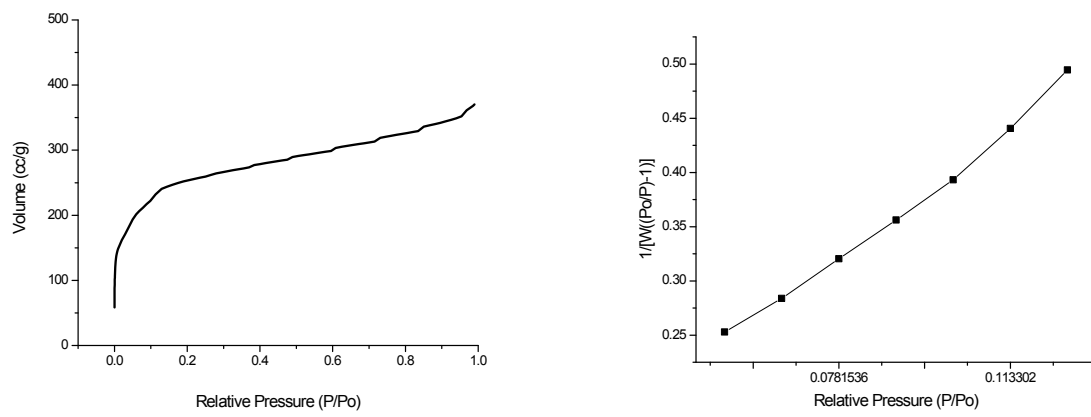


Figure 14. Nitrogen adsorption isotherm and multipoint BET plot for MIL-100(Fe)_1

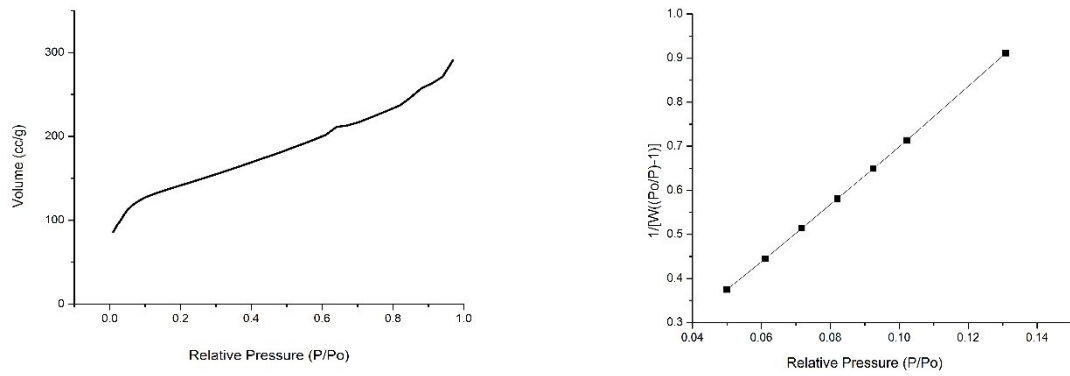


Figure 15. Nitrogen adsorption isotherm and multipoint BET plot for MIL-100(Fe)_2

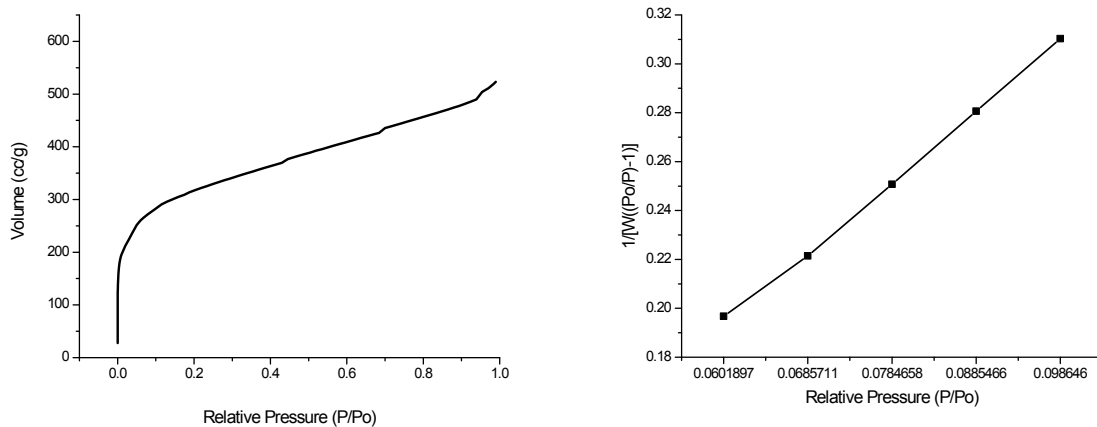


Figure 16. Nitrogen adsorption isotherm and multipoint BET plot for MIL-100(Fe)₃

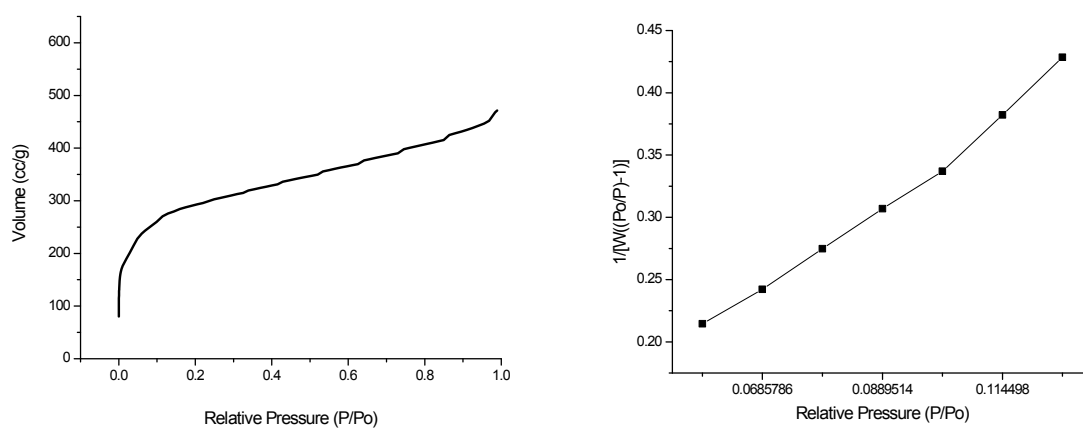


Figure 17. Nitrogen adsorption isotherm and multipoint BET plot for MIL-100(Fe)₄

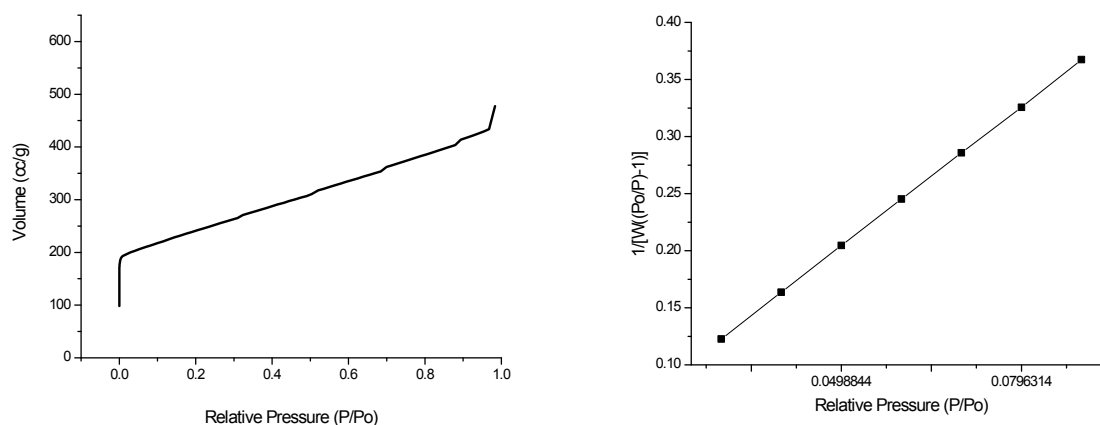


Figure 18. Nitrogen adsorption isotherm and multipoint BET plot for CPO-27(Ni) as-synthesised

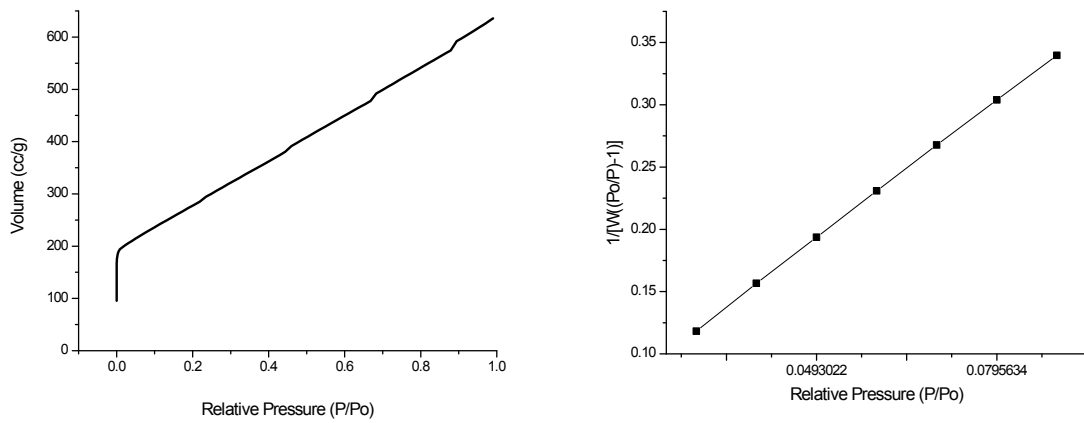


Figure 19. Nitrogen adsorption isotherm and multipoint BET plot for CPO-27(Ni)_1

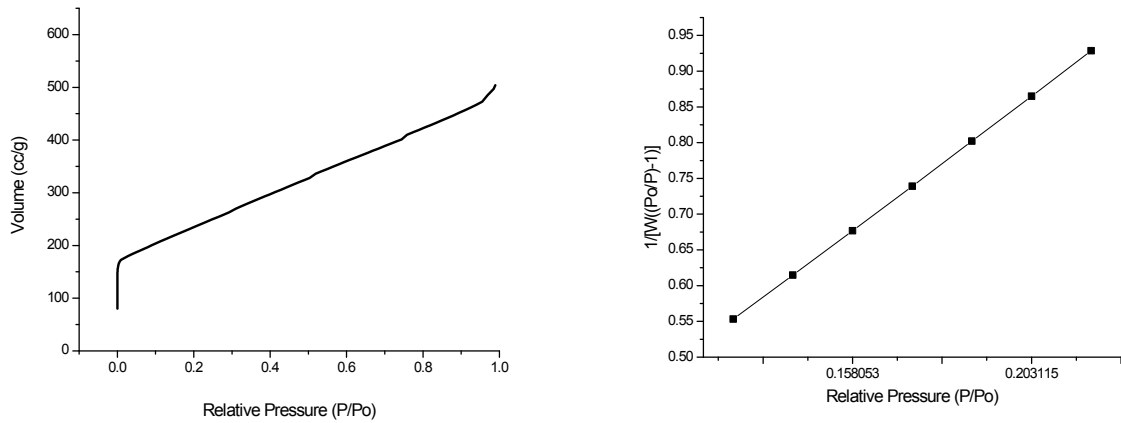


Figure 20. Nitrogen adsorption isotherm and multipoint BET plot for CPO-27(Ni)_2

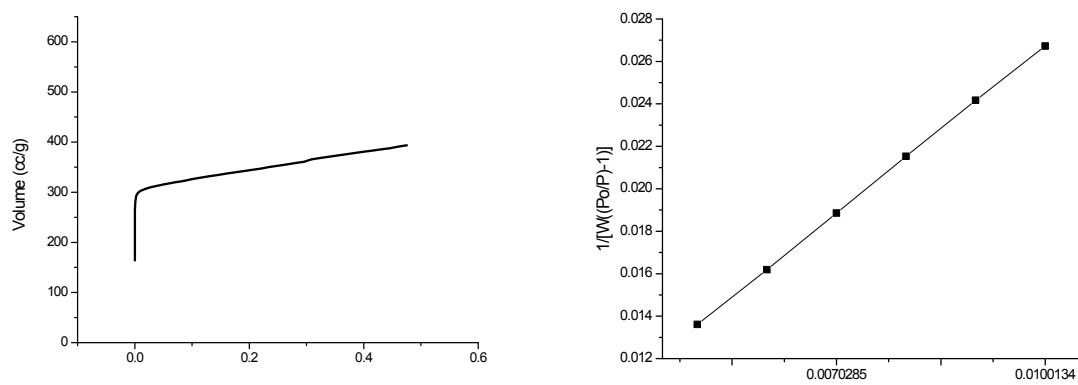


Figure 21. Nitrogen adsorption isotherm and multipoint BET plot for CPO-27(Ni)_3

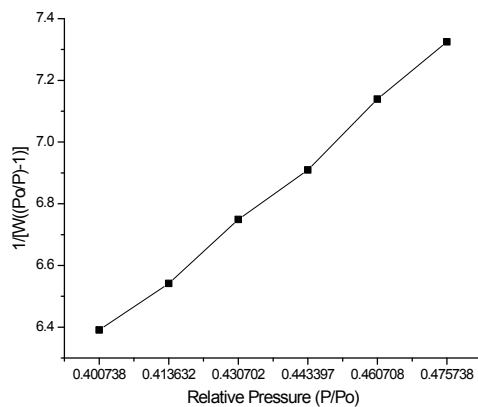
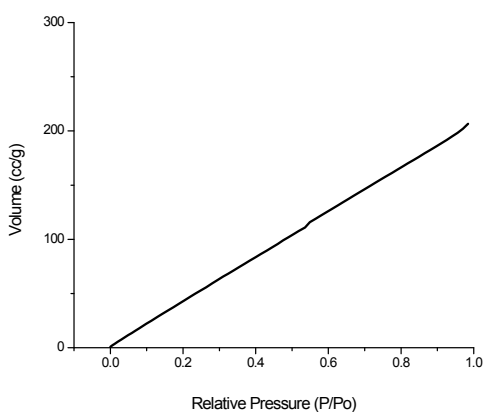


Figure 22. Nitrogen adsorption isotherm and multipoint BET plot for CPO-27(Ni)₄

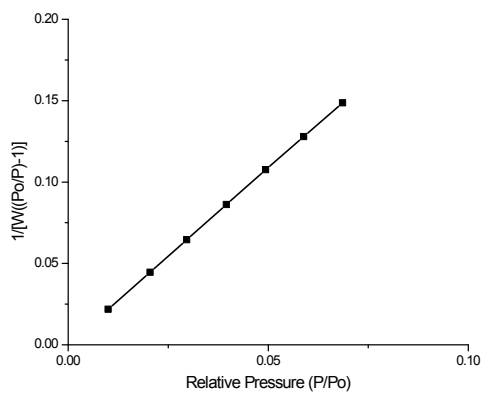
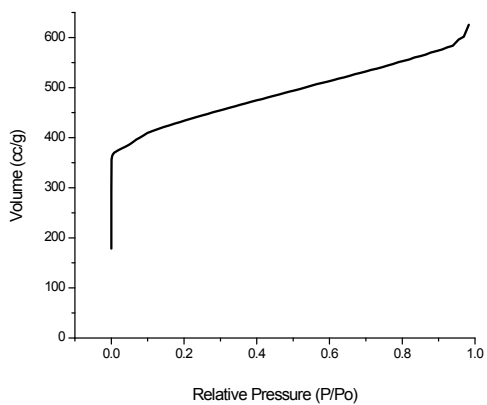


Figure 23. Nitrogen adsorption isotherm and multipoint BET plot for Cu-BTC as-synthesised

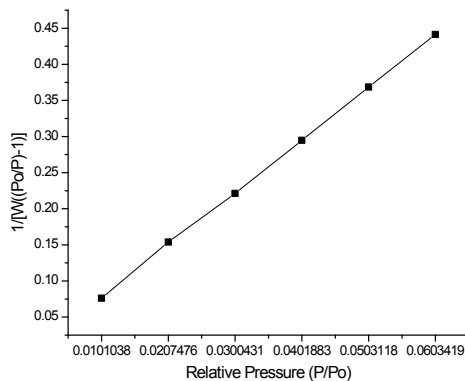
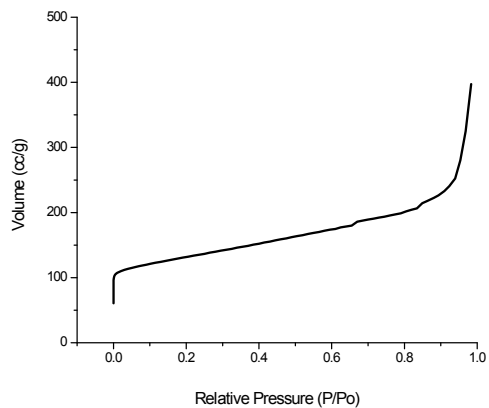


Figure 24. Nitrogen adsorption isotherm and multipoint BET plot for Cu-BTC₁

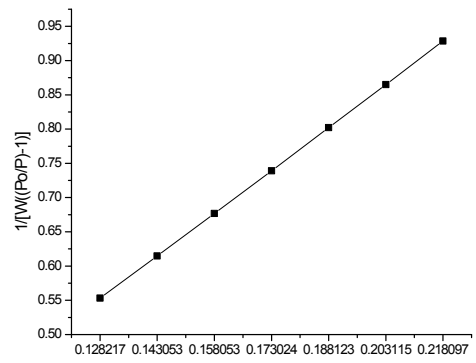
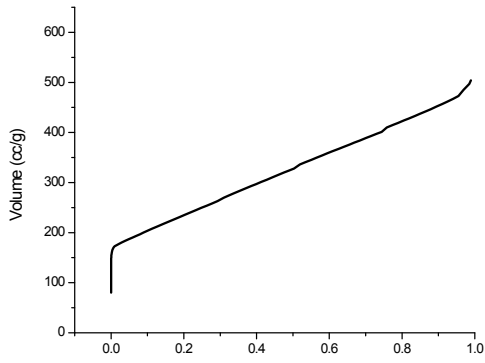


Figure 25. Nitrogen adsorption isotherm and multipoint BET plot for Cu-BTC_2

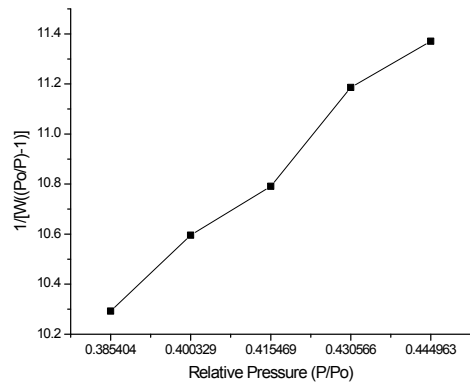
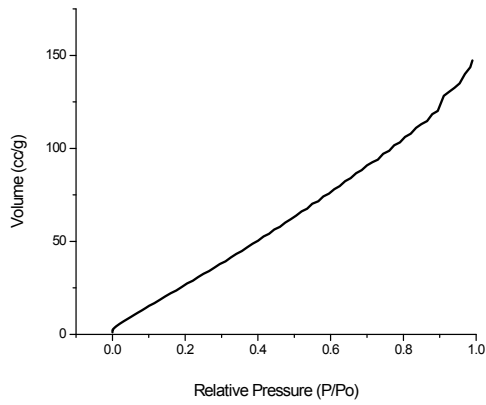


Figure 26. Nitrogen adsorption isotherm and multipoint BET plot for Cu-BTC_3

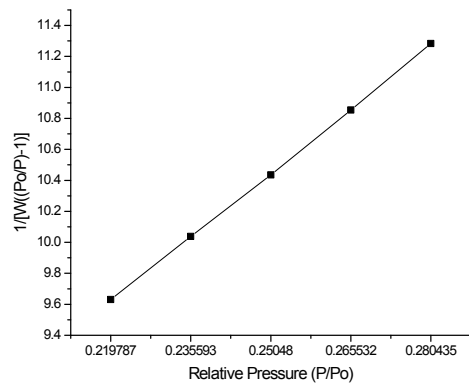
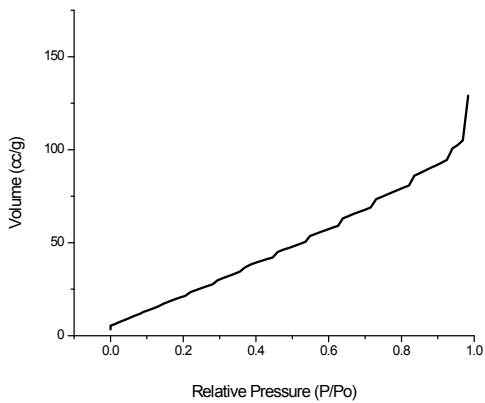


Figure 27. Nitrogen adsorption isotherm and multipoint BET plot for Cu-BTC_4