## In situ Control of Guest Exchange in Single Crystal X-ray Diffraction

Joseph J. Bevitt, Cameron J. Kepert, School of Chemistry, The University of Sydney. E-mail: bevitt\_j@chem.usyd.edu.au

By variation of template, with novel *in-situ* variable temperature Single Crystal X-ray Diffraction techniques we demonstrate the reversible nature of guest uptake by a coordination polymer, confirming their analogy with zeolites. Our work also demonstrates the subtle changes imposed on the host framework due to various guests (including 1-propanol, carbon dioxide, dinitrogen and argon) *and their occupancies*, quantifying the extent of host-guest interactions. Host distortions include asymmetric layer shifts of up to 0.7 Å, framework 'scissoring', ligand torsion angle changes, changes in nitrate binding and host symmetry. We present our techniques and demonstrate their applicability to the study of dynamic structures.



**Figure:** Reversible exchange of guests into the evacuated framework is achieved through repeated heating and cooling of sample under guest atmospheres.

Keywords: guest exchange, in-situ experiments, gas sorption