Supporting Information for:

M(II) (M = Mn, Co, Ni) Variants of the MIL-53-Type Structure

with Pyridine-N-Oxide as a Co-Ligand

Alexis S. Munn, Guy J. Clarkson, Franck Millange, Yves Dumont and Richard I. Walton



S1: IR Spectroscopy

Figure S1: IR spectrum of Co(BDC)(PNO) compared to MIL-53(Cr) [Cr(BDC)(OH)]. Assigments of bands in Co(BDC)(PNO) were made by reference to the literature. S. Kida, J. V. Quagliano, J. A. Walmsley and S. Y. Tyree, *Spectrochim. Acta*, 1963, **19**, 189-199 and L. C. Nathan, J. E. Armstrong and R. O. Ragsdale, *Inorg. Chim. Acta*, 1979, **35**, 293-296.



Figure S2: IR spectra of Co(BDC)(PNO), Mn(BDC)(PNO) and Ni(BDC)(PNO).



Figure S3: IR spectra of mixed-metal (Co,Mn,Ni)(BDC)(PNO) materials.

S2: Thermodiffraction



Figure S4: Thermodiffraction measured during heating of (a)Co(bdc)(PNO), (b) Ni(bdc)(PNO) and (c) Mn(bdc)(PNO) showing the rigidity of the framework until it begins to decompose.



S3. Space-Filling Representations of Crystal Structures





Figure S6: Space filling representation of Co(bdc)(PNO) at 298 K