Electronic Supplementary Material (ESI) for RSC Advances.

SUPPLEMENTARY INFORMATION

Synthesis, structure and characterization of a layered coordination polymer based on Zn(II) and 6-(methylmercapto)purine

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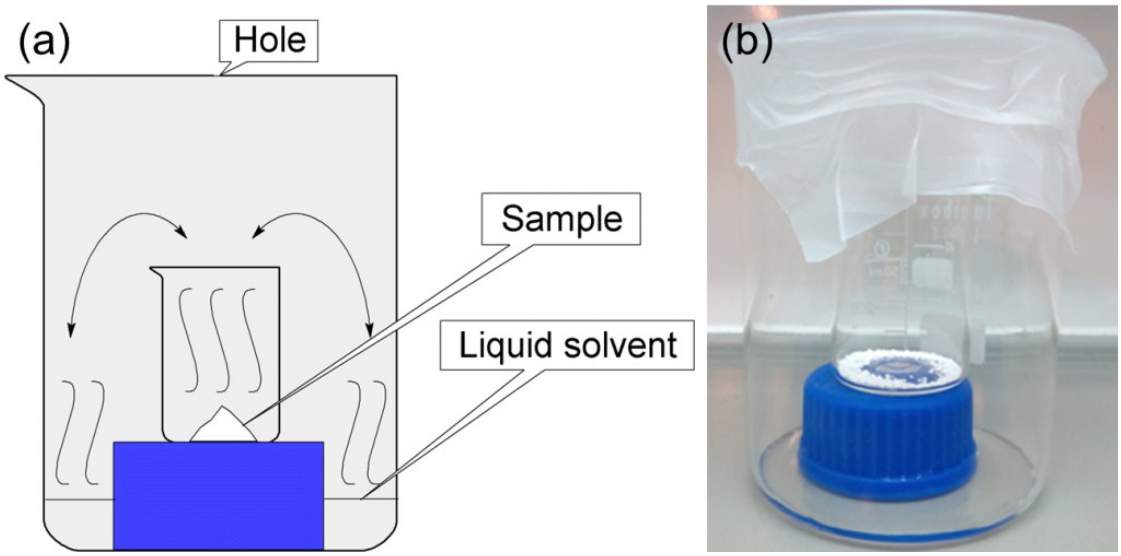

Fig. S1 Set-up for the solvent exchange in vapour phase. (a) Schematic illustration and (b) photograph.

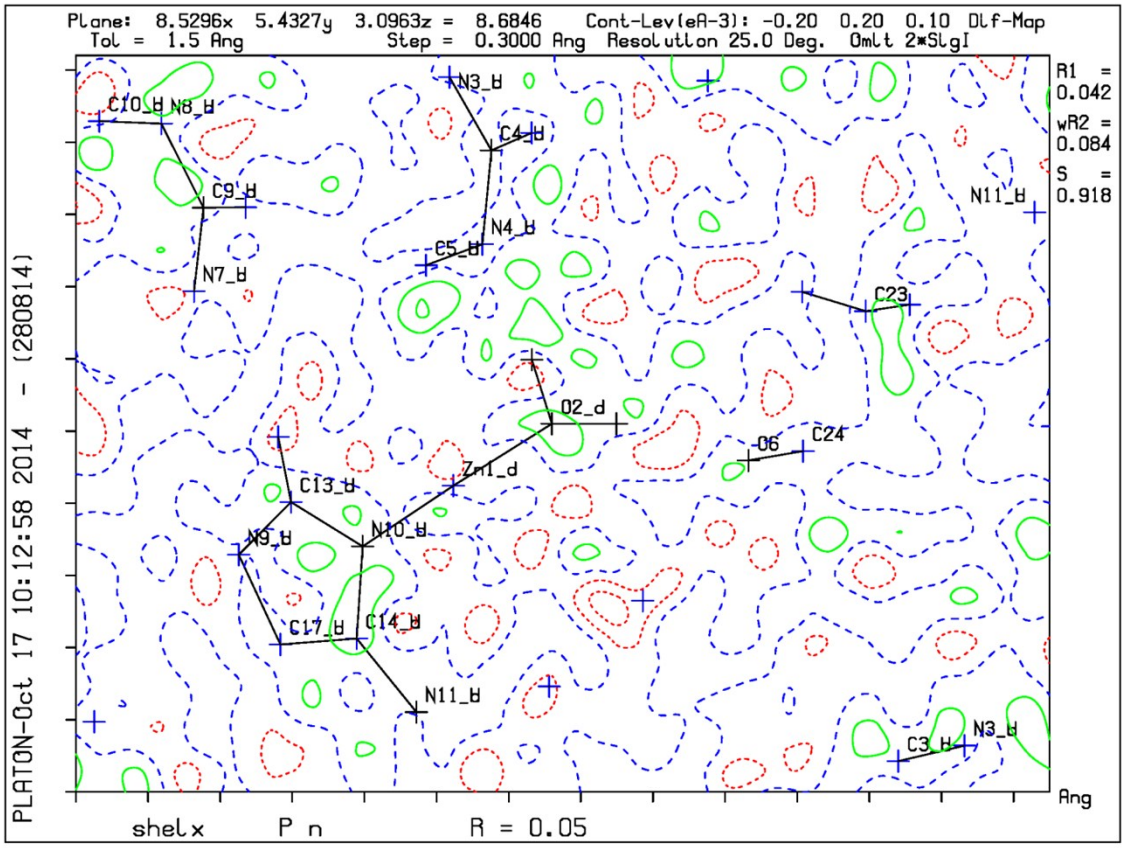

Fig. S2 Difference electron density map of structure **1**.

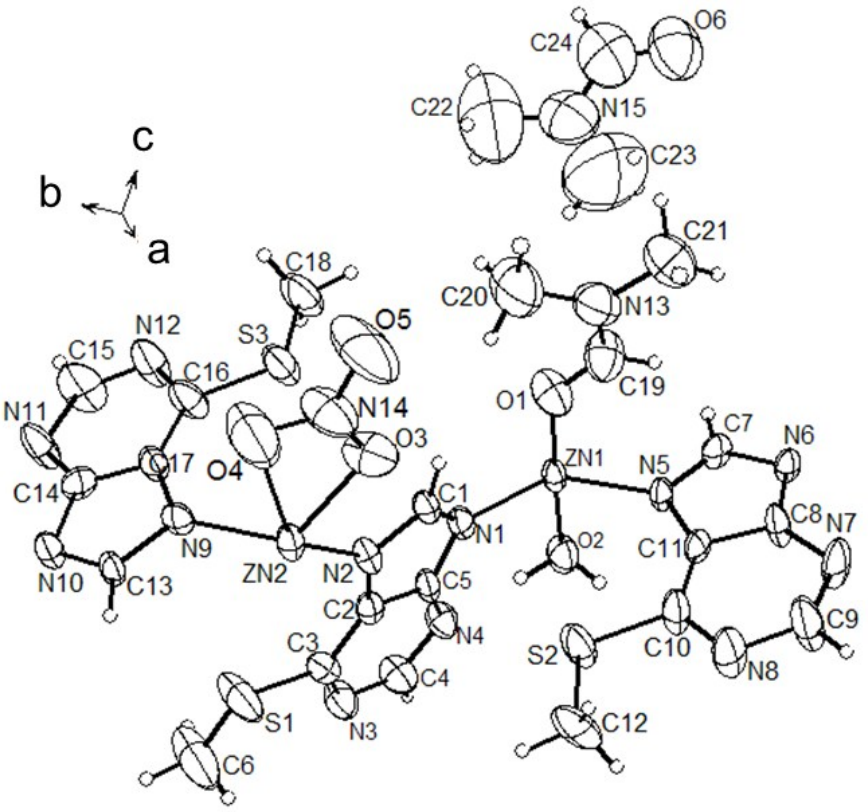

Fig. S3 ORTEP view of **1**.

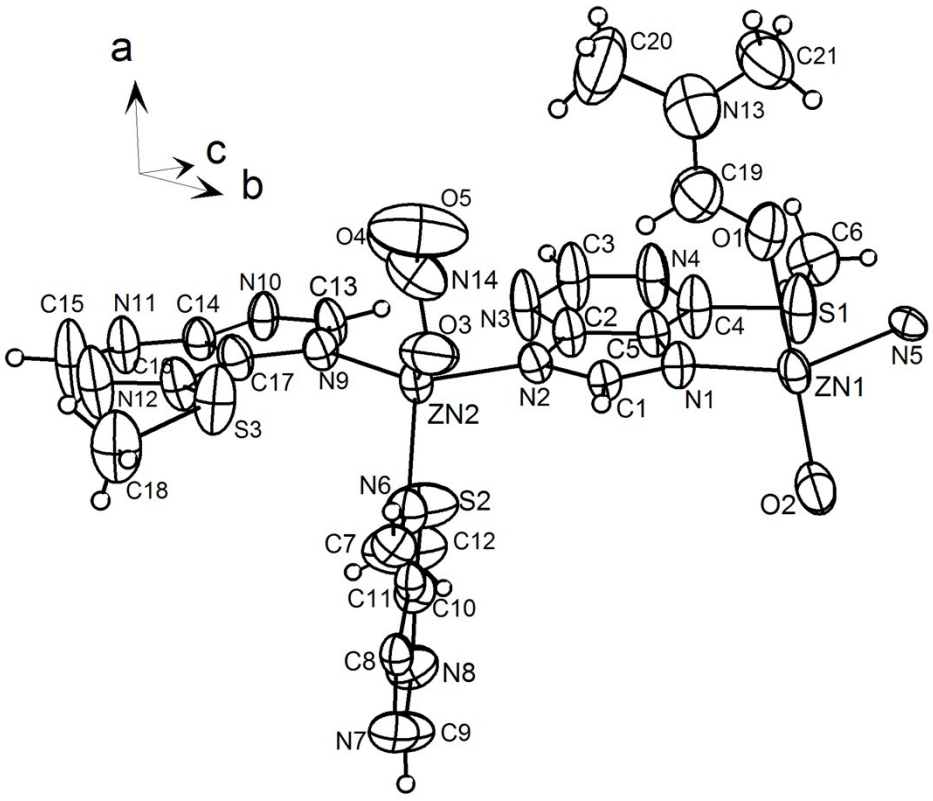

Fig. S4 ORTEP view of **1'**.

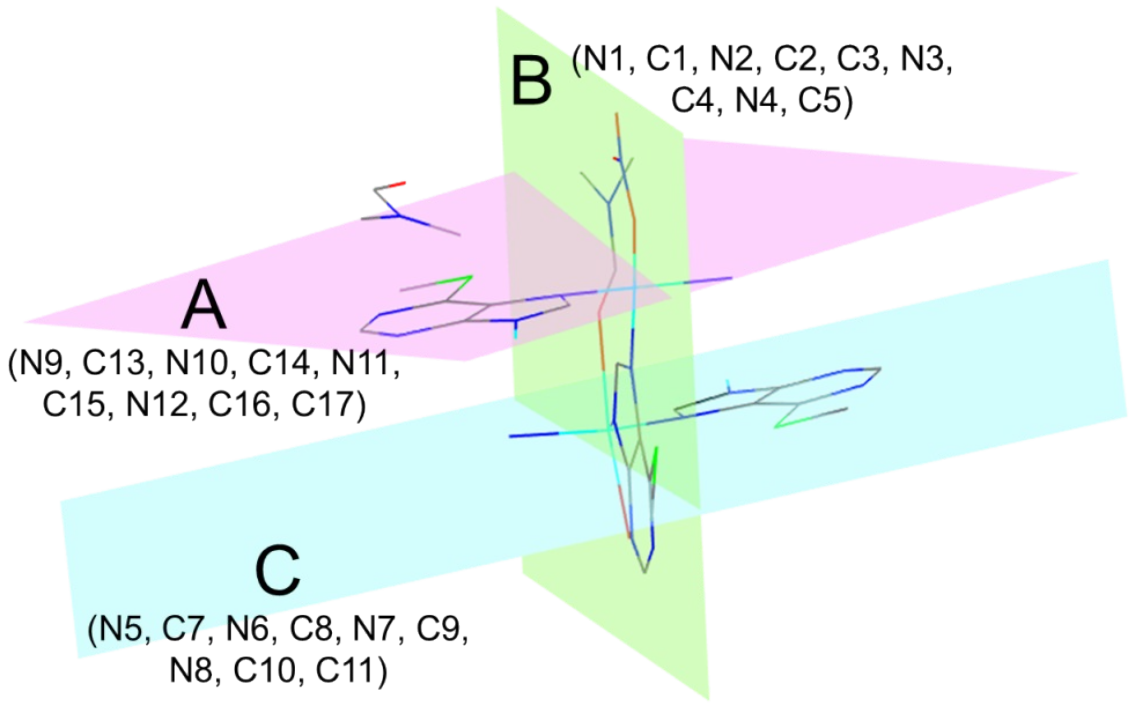

Fig. S5 Structure **1**. Calculated least squares planes. A (pink): defined by N9, C13, N10, C14, N11, C15, N12, C16, and C17 atoms. B (green): defined by N1, C1, N2, C2, C3, N3, C4, N4, and C5 atoms. C (red): defined by N5, C7, N6, C8, N7, C9, N8, C10, and C11 atoms. Dihedral angles: AB, 83.01°; AC, 3.95°; BC, 79.85°. Zn, N, C, O, and S atoms are represented in blue, dark blue, grey, red and green, respectively. H atoms omitted for clarity.

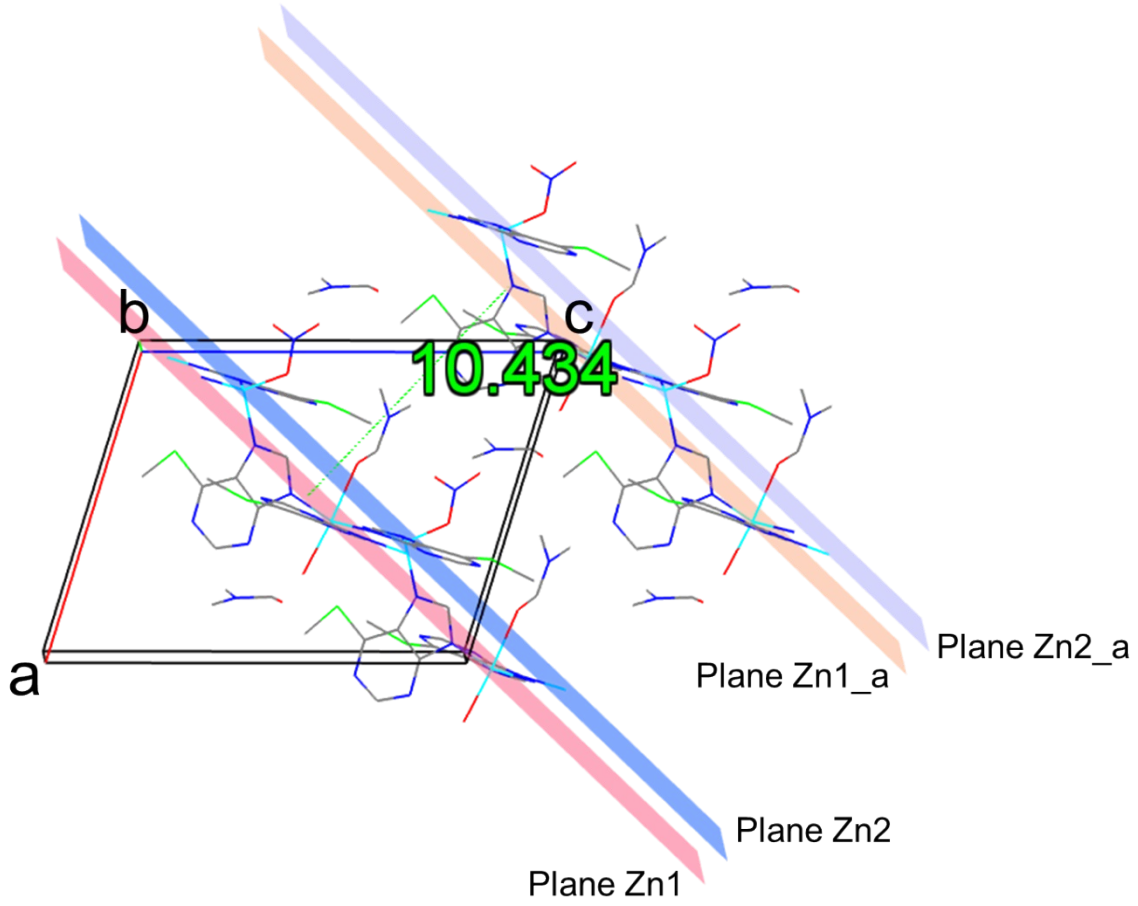

Fig. S6 Structure **1**. Distance between layers (defined by the distance in ångströms (Å) between two planes of the same kind of Zn atoms). Zn, N, C, O, and S atoms are represented in blue, dark blue, grey, red and green, respectively. H atoms omitted for clarity.

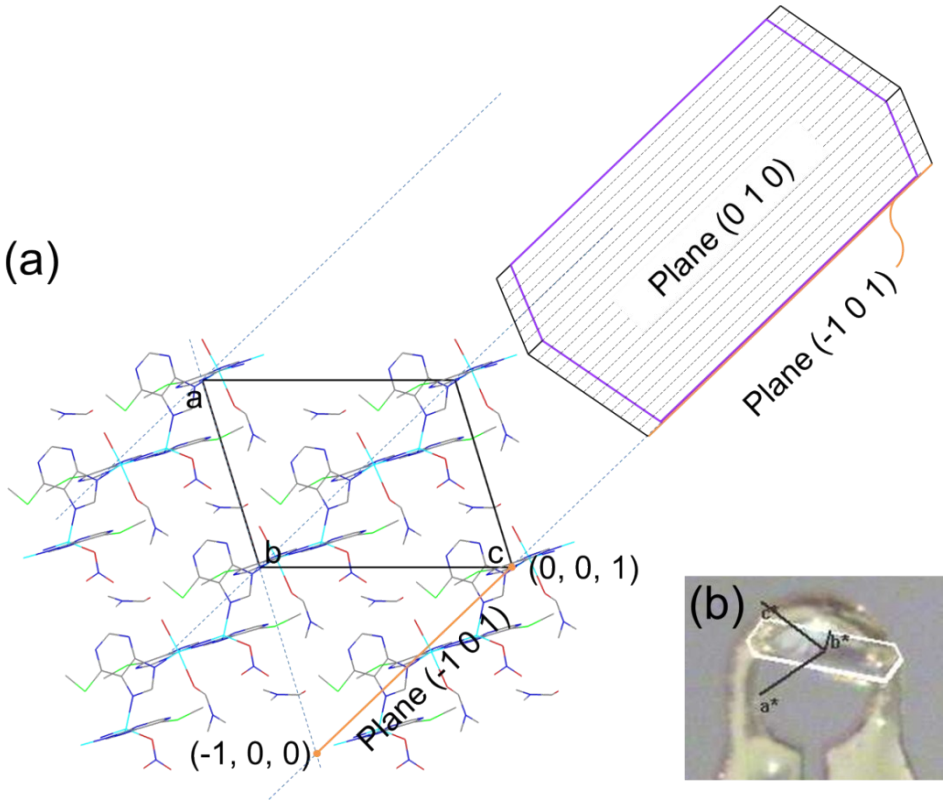

Fig. S7. (a) Correspondence between the crystal structure and shape of **1**. Zn, N, C, O, and S atoms are represented in blue, dark blue, grey, red and green, respectively. H atoms omitted for clarity. (b) Optical image of a single crystal (type II) of **1** where the polyhedron edges and the reciprocal cell axes are drawn using CrysAlis software.[1]

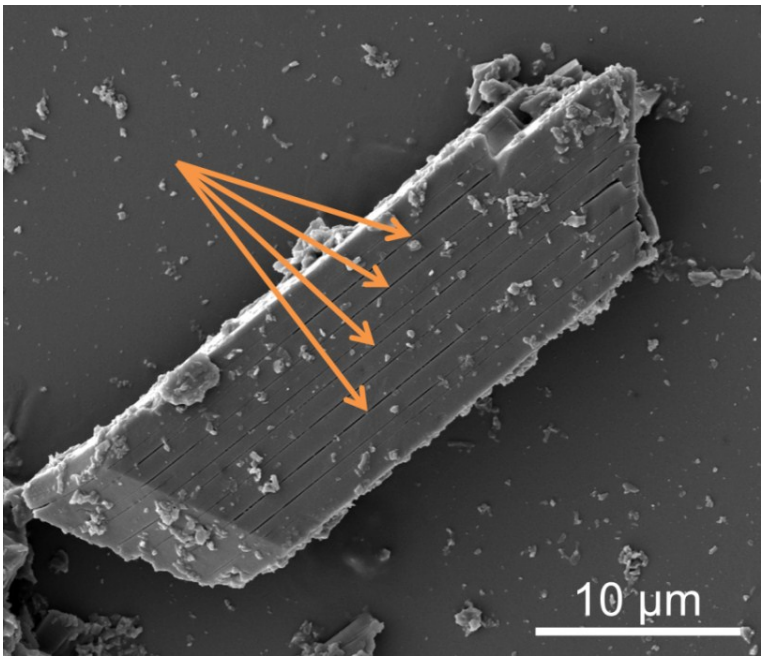

Fig. S8 SEM image of **1** where marks are observed.

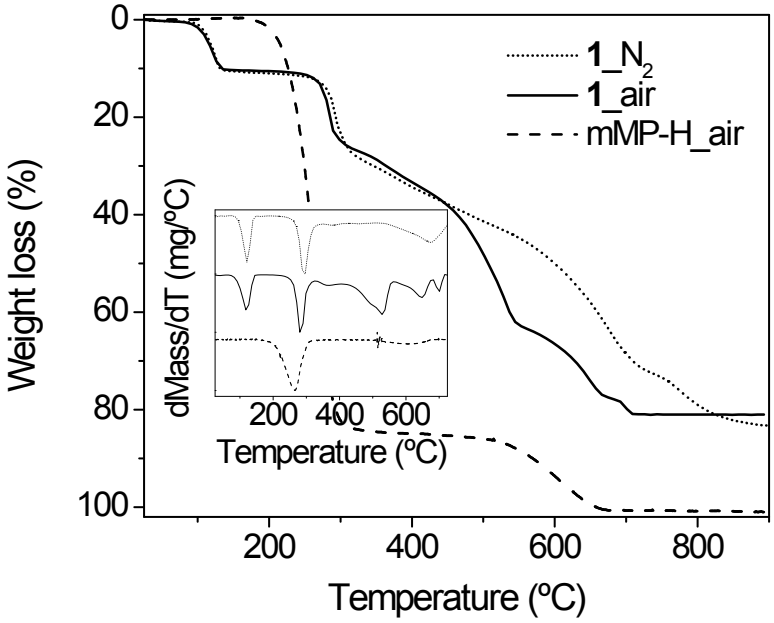

Fig. S9 TGA and DTG (inset) characterization of **1** under air and nitrogen conditions and mMP-H under air atmosphere.

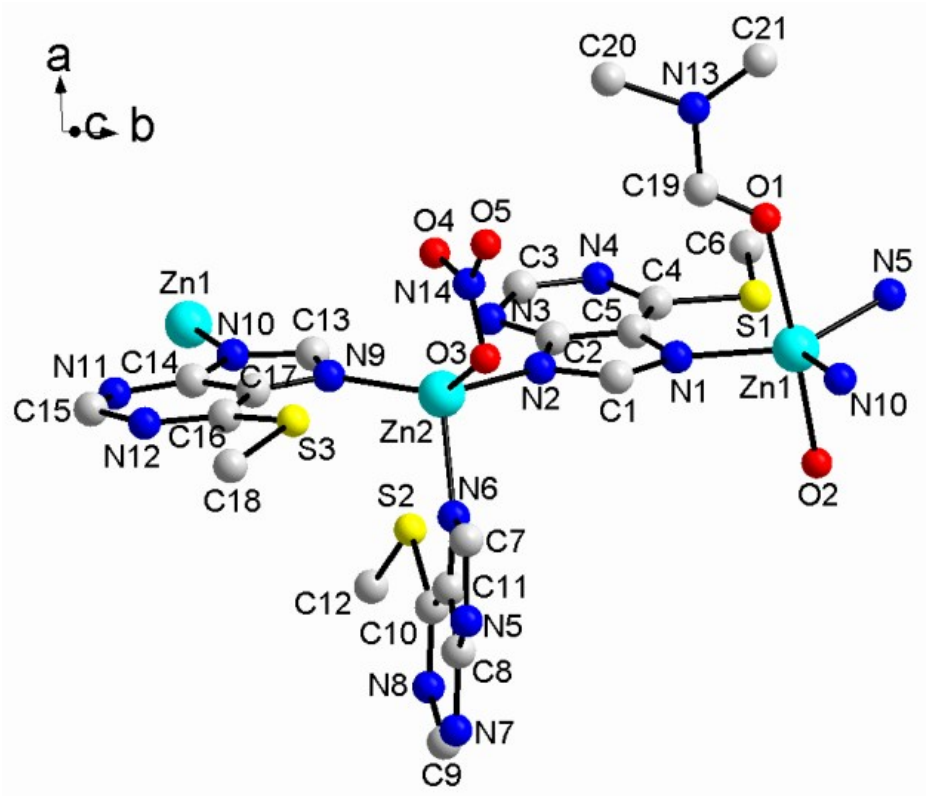

Fig. S10 Crystal structure of **1'** displaying the asymmetric unit. Zn, N, C, O, and S atoms coloured in blue, dark blue, grey, red and green, respectively. H atoms are omitted for clarity.

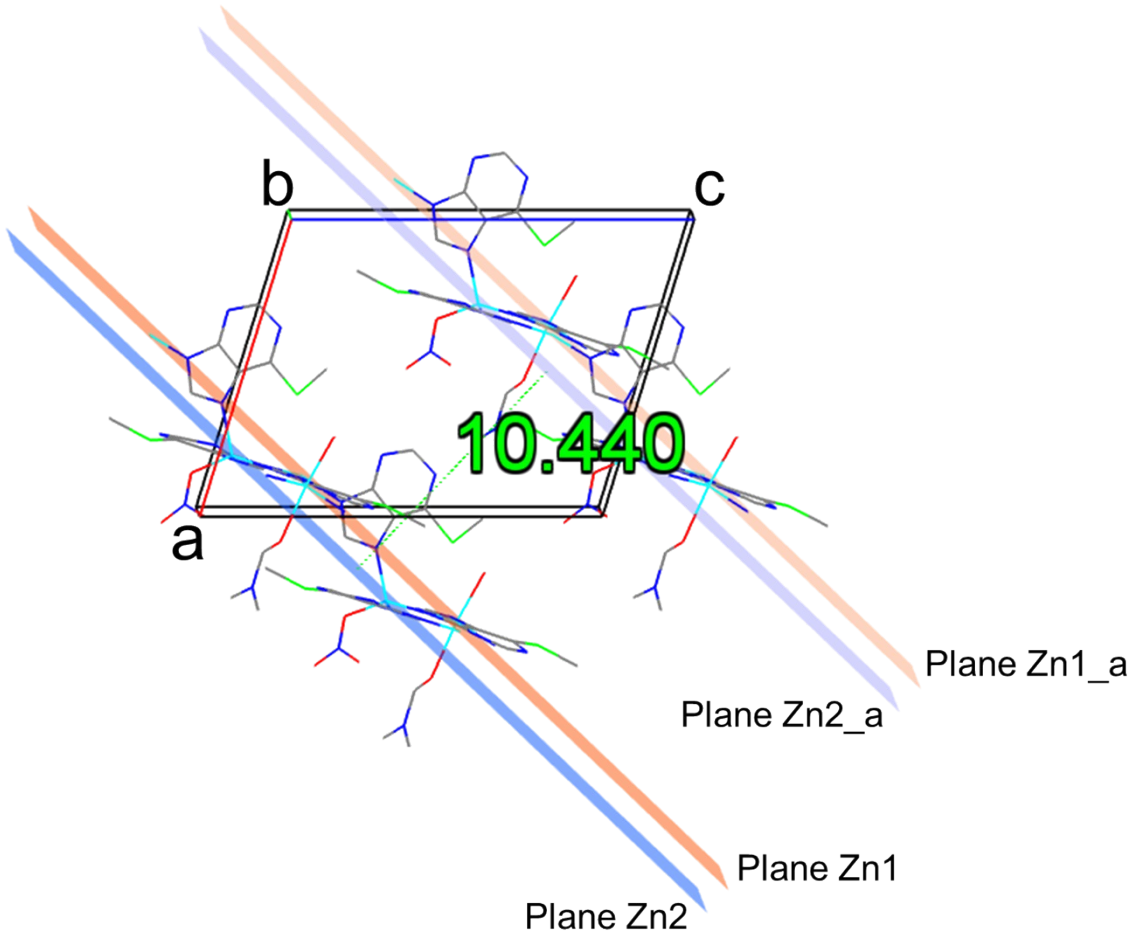

Fig. S11 Structure **1'**. Distance between layers (defined by the distance in ångströms (Å) between two planes of the same type of Zn atoms). Zn, N, C, O, and S atoms are represented in blue, dark blue, grey, red and green, respectively. H atoms omitted for clarity

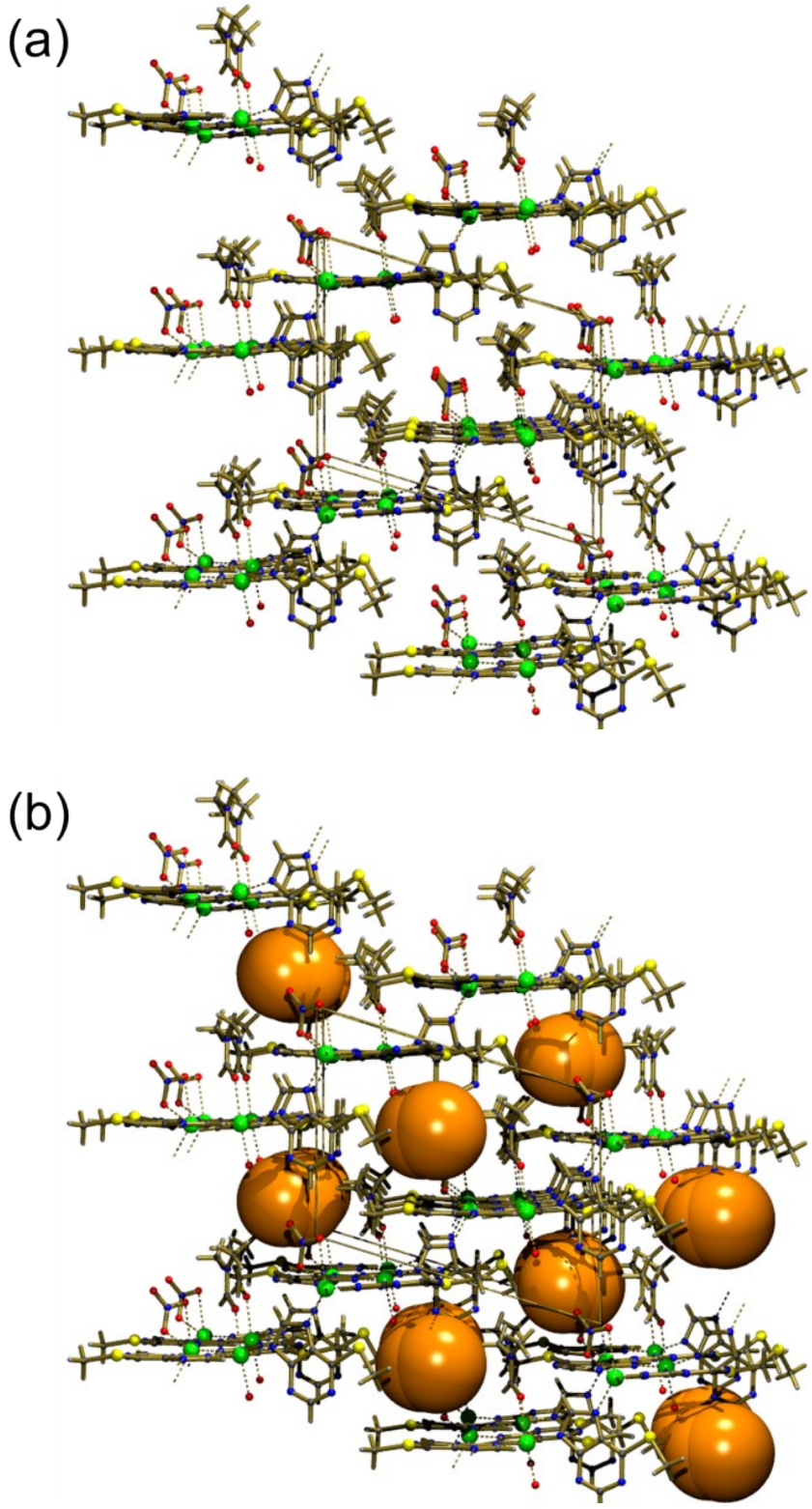

Fig. S12 Solvent accessible void volume of compound **1'** determined by PLATON/SQUEEZE[55] (view along the *b* axis). Empty cavities in (a) are represented by orange spheres in (b). Zn, N, C, O, H, and S atoms are depicted in green, dark blue, grey, red, light grey, and yellow, respectively. H atoms omitted for clarity.

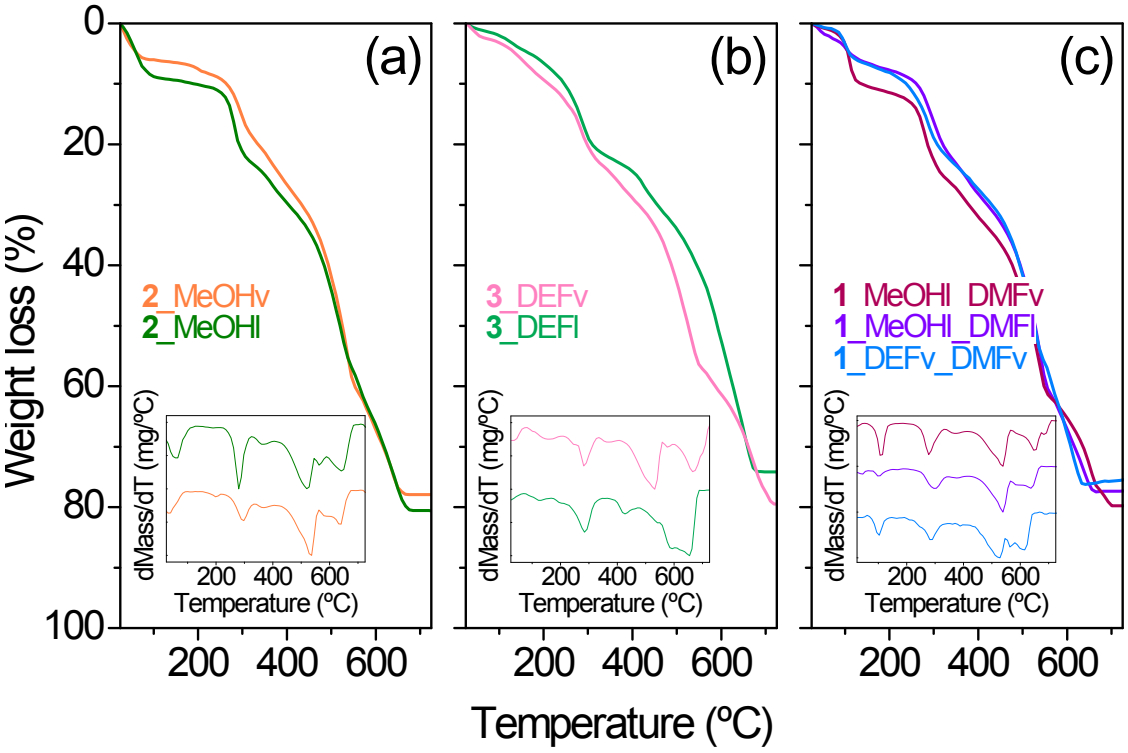

Fig. S13 TGA and DTG (insets) characterization under air flow of products obtained after: exchange of DMF for (a) MeOH and (b) DEF, and (c) framework recovery.

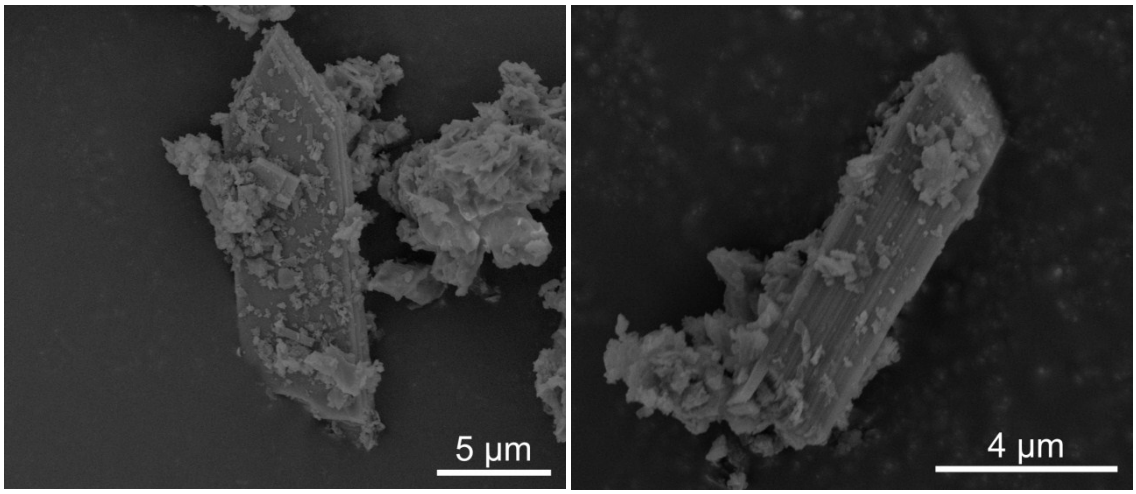

Fig. S14 SEM images of **2**_MeOHl.

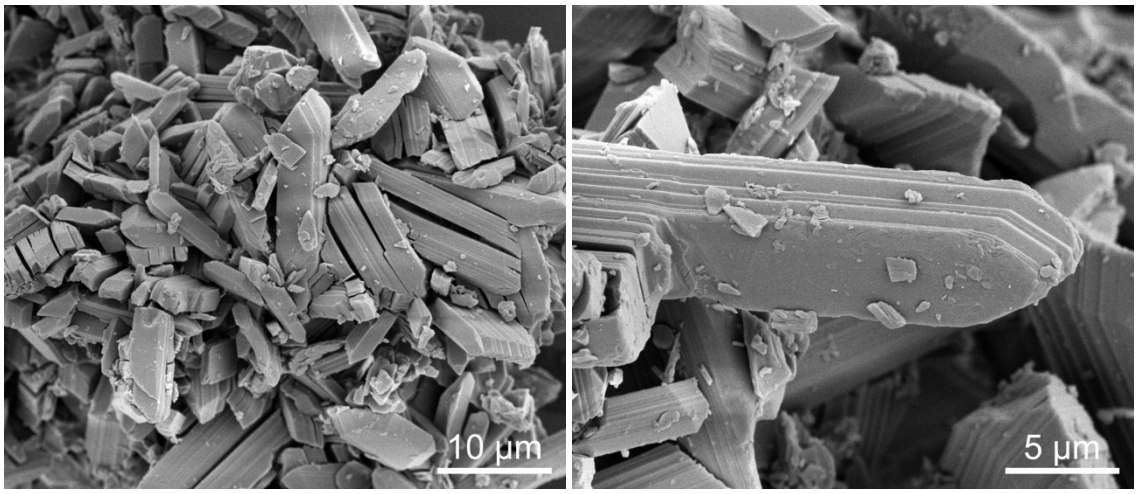

Fig. S15 SEM images of **2**_MeOHv.

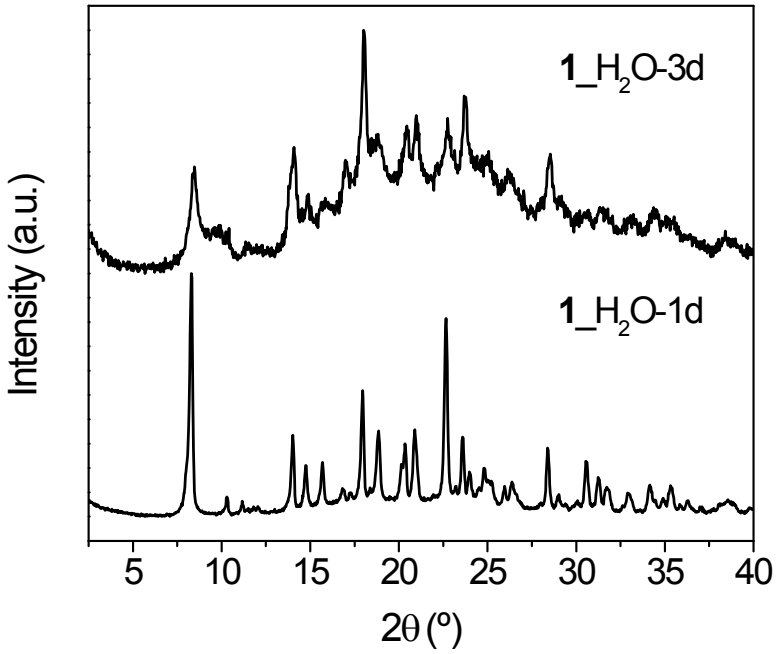

Fig. S16 PXRD patterns of product **1** soaked in H_2O after 1 (**1**_H_2O-1d) and 3 d (**1**_H_2O-3d).

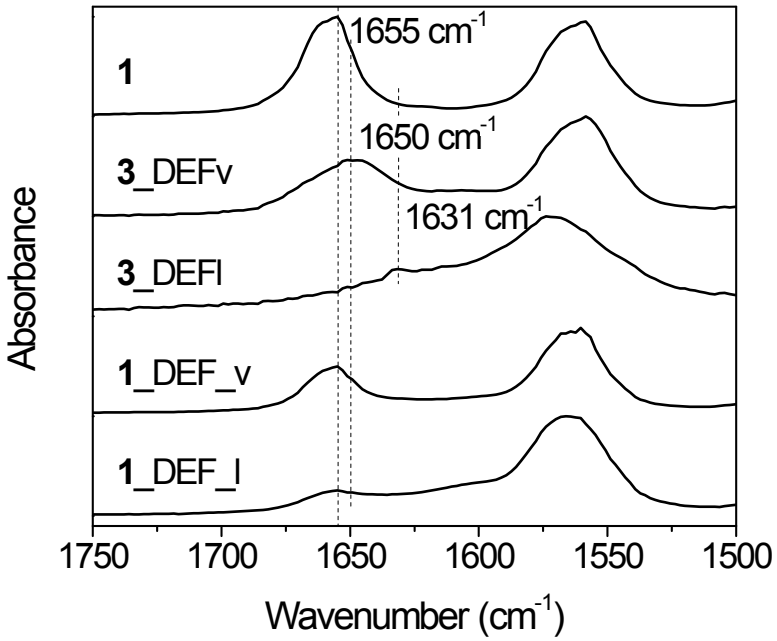

Fig. S17 FTIR spectra detail for comparison of **1**, **3**_DEFv, **3**_DEFl, **1**_DEFv_DMFv and **1**_DEFv_DMFl between 1500 and 1750 cm^{-1} showing the displacement of C=O band towards smaller wavenumbers.

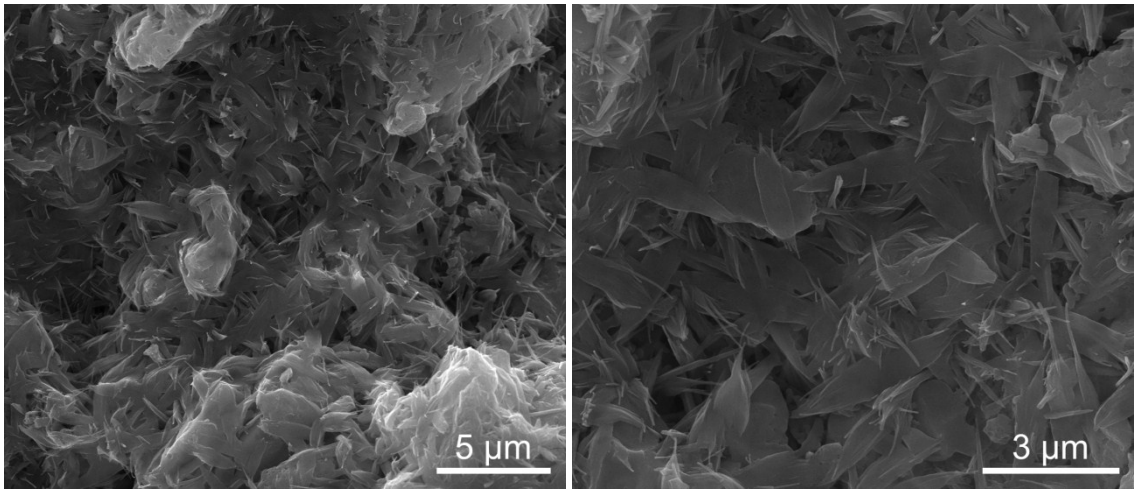

Fig. S18 SEM images of **3**_DEFv.

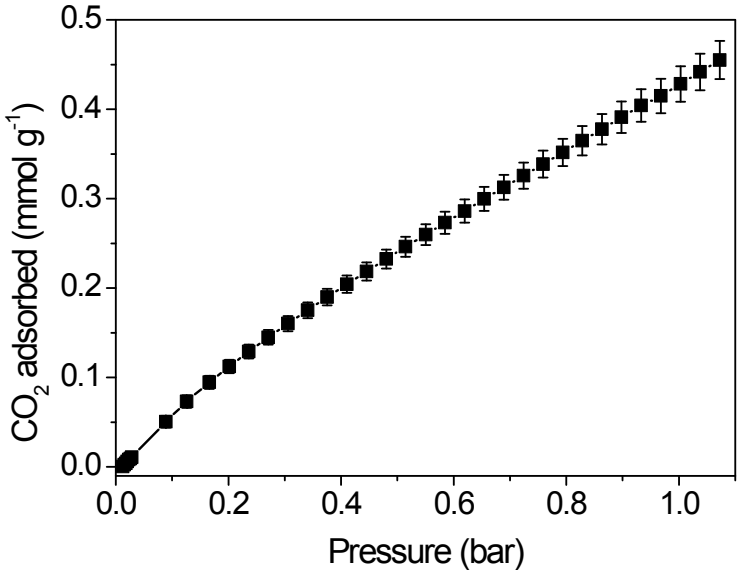

Fig. S19 Adsorption isotherm of CO_2 at 273 K on **2**_MeOHv. Error bars show standard errors of mean for 4 measurements on the same sample.

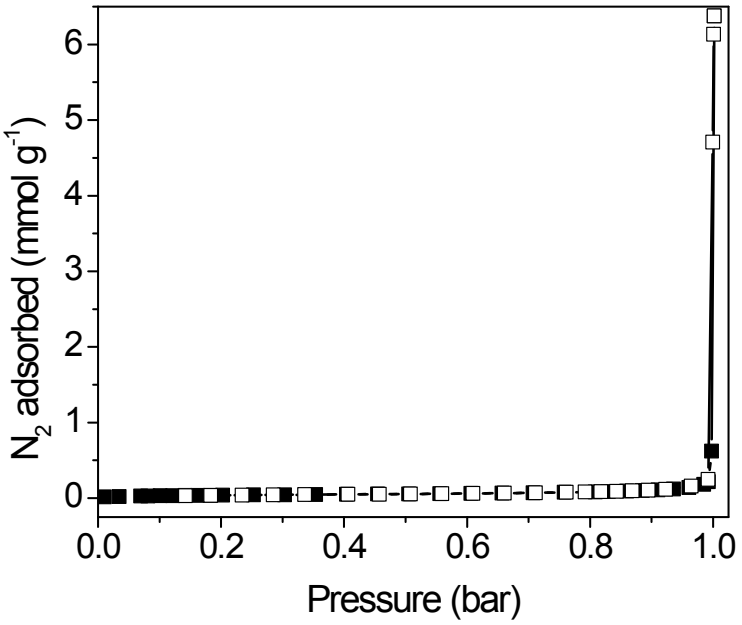

Fig. S20 N_2 sorption of compound **2**_MeOHv. Filled and open squares for adsorption and desorption, respectively.

References

1 *CrisAlisPro Software*, Version 1.171.37.31 (release 14-01-2014 CrysAlis171 .NET), Agilent Technologies UK Ltd: Oxford, UK, 2014.