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\textsuperscript{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$_{\text{MeOHv.}}$

**Fig. S16** PXRD patterns of product 1 soaked in H$_2$O after 1 (1$_{\text{H}_2\text{O-1d}}$) and 3 d (1$_{\text{H}_2\text{O-3d}}$).
**Fig. S17** FTIR spectra detail for comparison of 1, 3_DEFv, 3_DEFi, 1_DEFv_DMv and 1_DEFv_DMFI 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\textsubscript{2} at 273 K on 2\_MeOHv. Error bars show standard errors of mean for 4 measurements on the same sample.

**Fig. S20** N\textsubscript{2} sorption of compound 2\_MeOHv. Filled and open squares for adsorption and desorption, respectively.

**References**