

Electronic Supporting Information (ESI)

Dynamic porous coordination polymer based on 2D stacked layers exhibiting high sorption selectivity for CO₂

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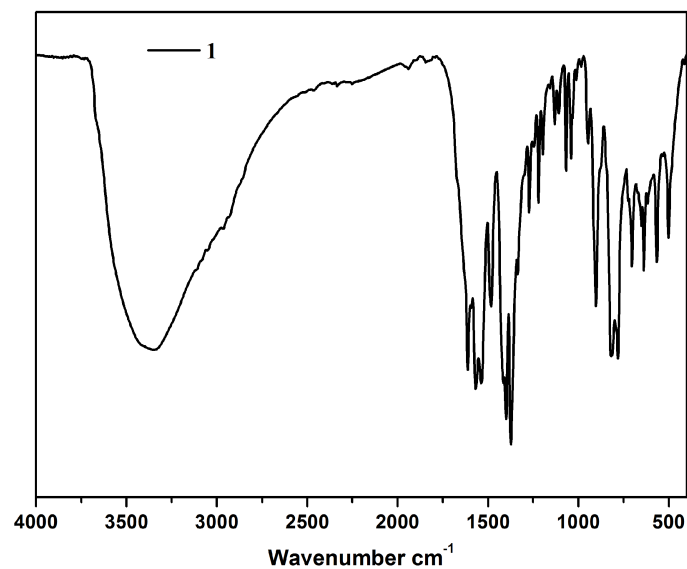


Figure. S1 IR spectrum for $\{[\text{Ni}(\text{dcpy})(\text{bipy})_{0.5}(\text{H}_2\text{O})] \cdot 1.5\text{H}_2\text{O}\}$ (**1**)

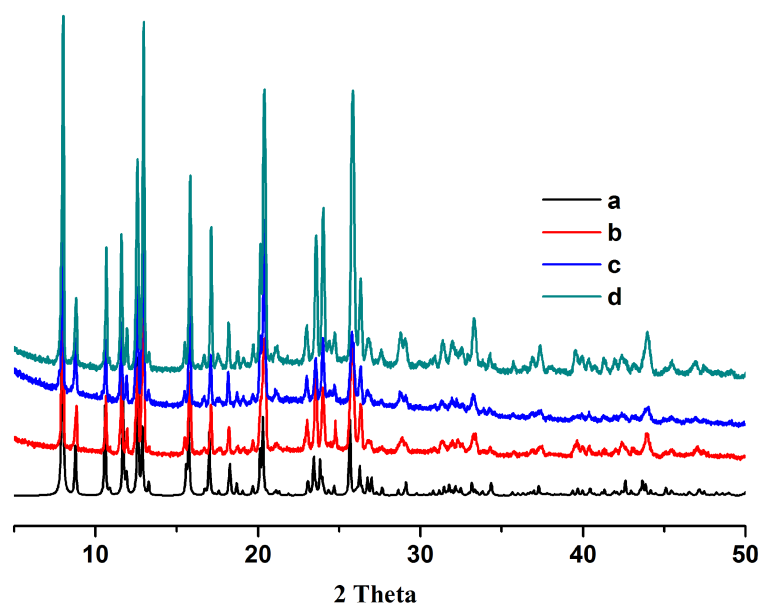


Figure. S2 PXRD patterns for **1** obtained under different synthesis methods; a) simulated from the single crystal data; b) as-synthesized **1** via conventional solvothermal; c) as-synthesized **1** via conventional hydrothermal; d) as-synthesized **1** via rapid microwave method.

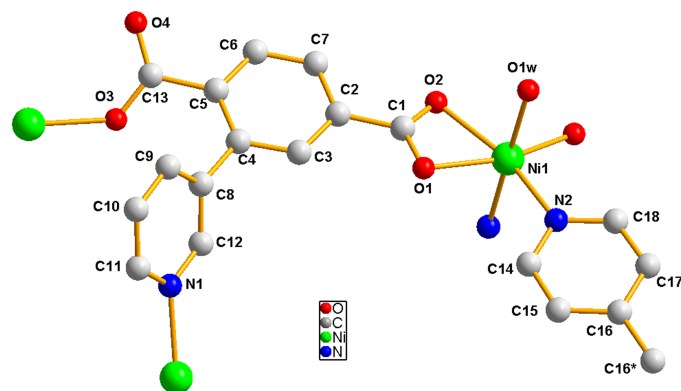


Figure. S3 The ball-and-stick drawing of the asymmetric unit in **1**, the hydrogen atoms and solvent molecules are omitted, and the atoms in the asymmetric unit are labeled. Symmetry codes: *: $1/2-x, 1/2-y, -z$.

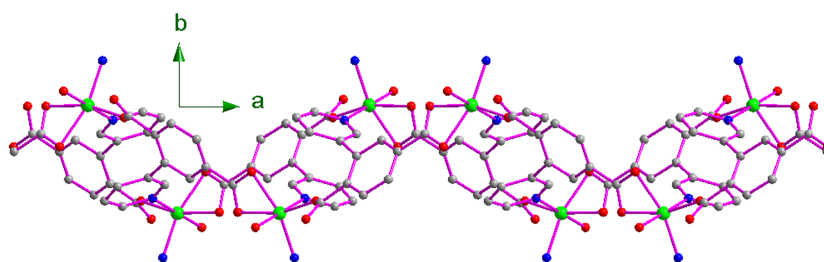
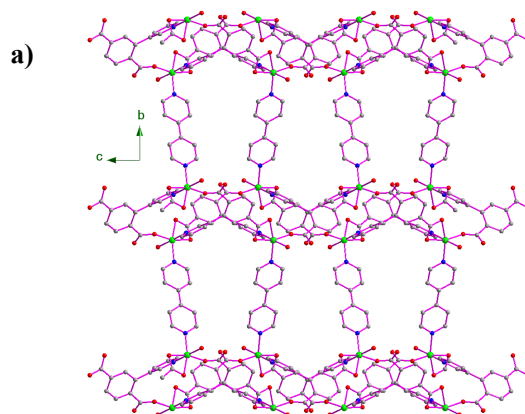


Figure. S4 View of the 1D chain structure linked by Ni^{2+} centers and dcpy^{2-} ligands in **1** along the crystallographic c -axis.



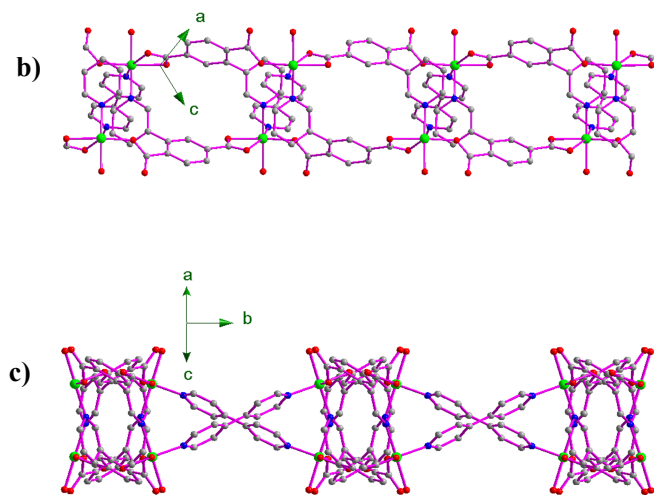


Figure. S5 View of the 2D layer of **1**: a) along the crystallographic *a*-axis; b) along the crystallographic *b*-axis; c) along the crystallographic (101)-axis.

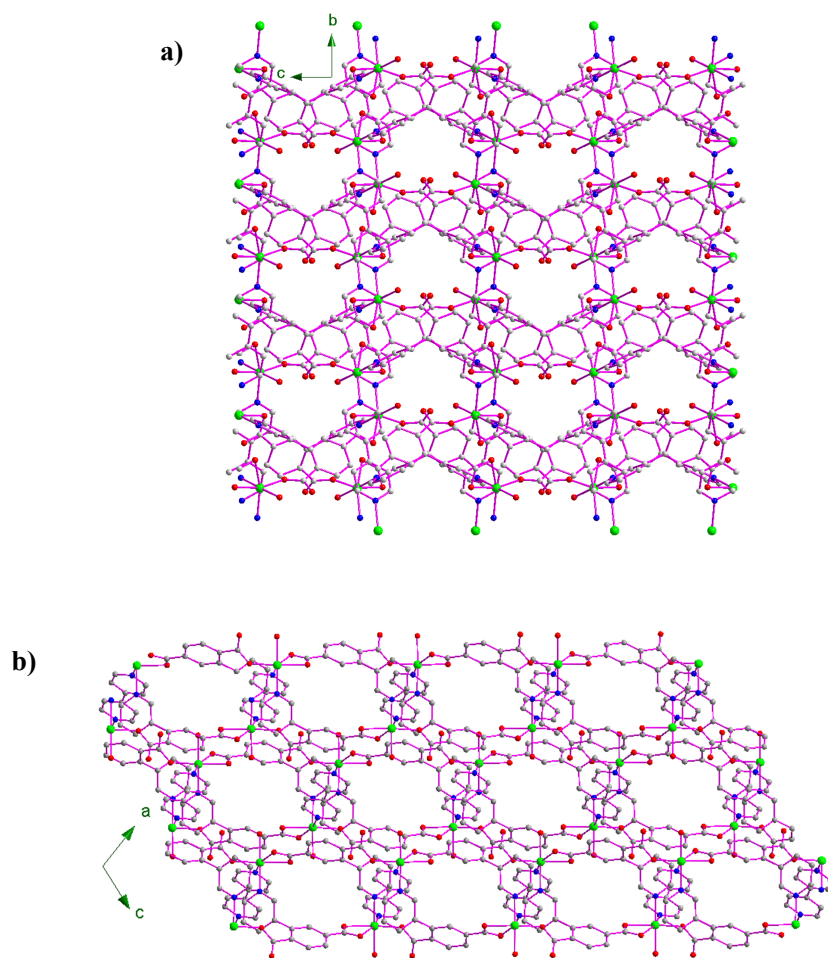


Figure. S6 View of the 2D stacked layers of **1**: a) along the crystallographic *a*-axis; b) along the crystallographic *b*-axis.

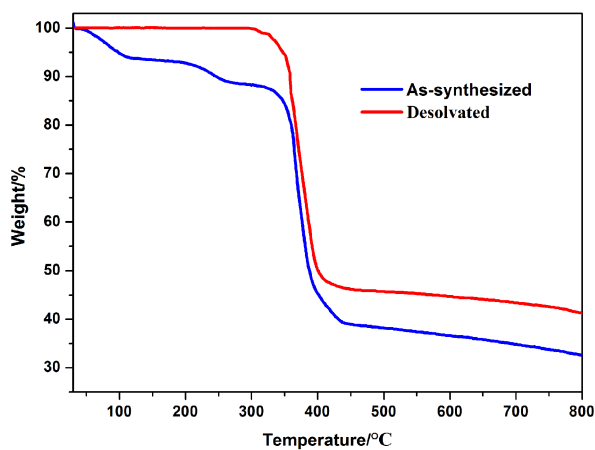


Figure. S7 TGA plots of the as-synthesized and desolvated samples of **1**.

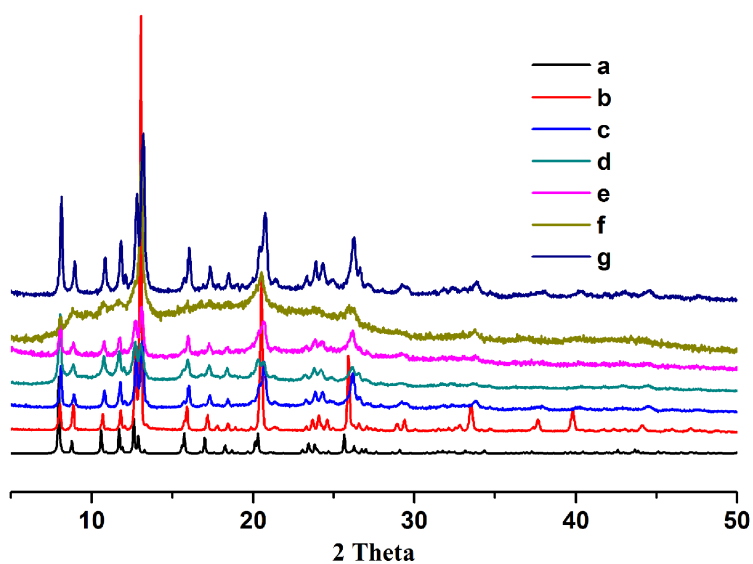


Figure. S8 PXRD patterns for **1** in different state; a) simulated from the single crystal data; b) synthesized powder samples; c) dehydrated samples **1a**; d) dehydrated samples **1b**; e) dehydrated samples **1c**; f) dehydrated samples **1d**; g) rehydrated samples.

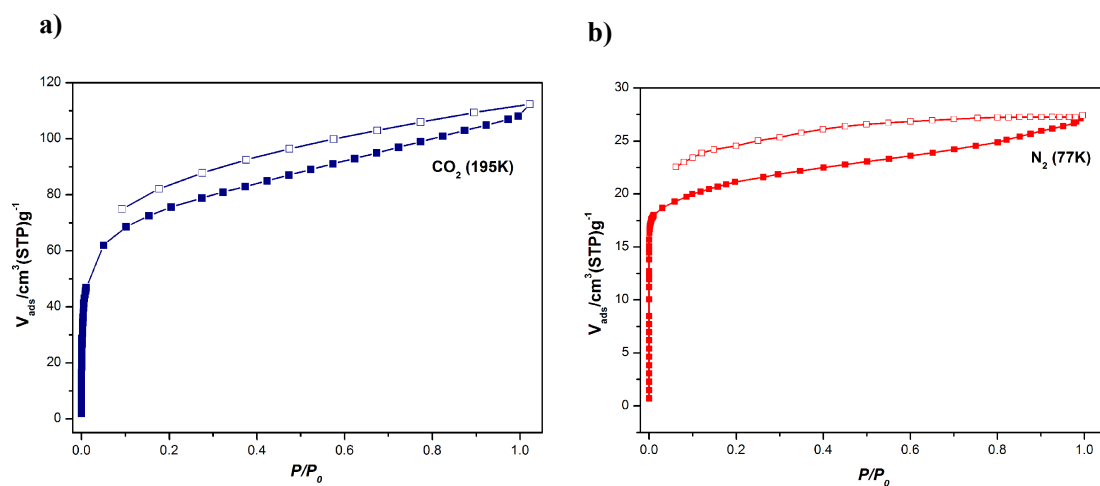


Figure. S9 Sorption isotherms of CO₂ measured at 195 K a) and N₂ measured at 77 K b).

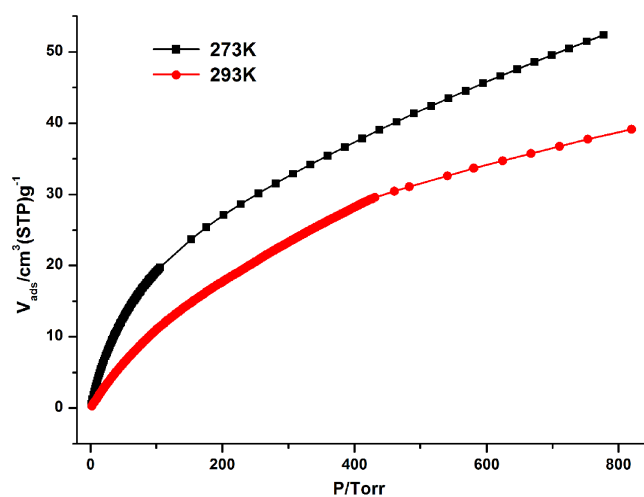


Figure. S10 Sorption isotherms of CO₂ measured at 273 K and 293 K.

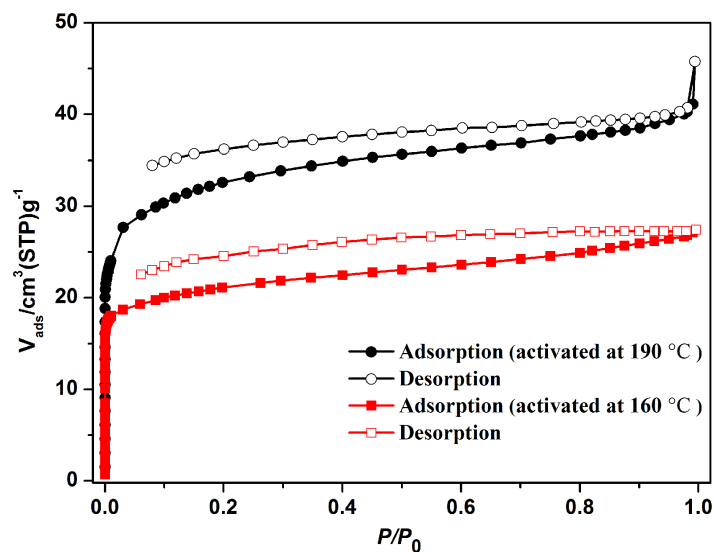


Figure. S11 Sorption isotherms of N_2 measured at 77K at different activation temperatures.

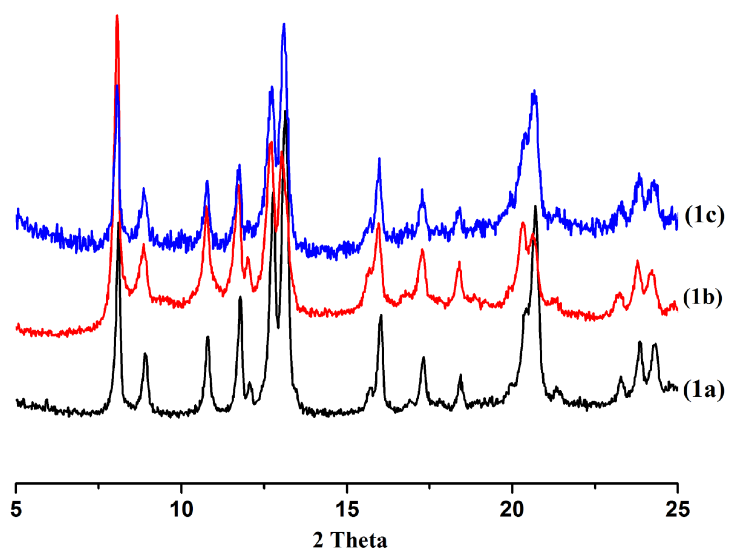


Figure. S12 PXRD patterns for **1a**, **1b** and **1c** at low angles ($2\theta = 5\text{--}25^\circ$).