

**Electronic Supporting information**

**Synthesis, structure and properties of coordination polymers formed  
from bridging 4-hydroxybenzoic acid anions<sup>†</sup>**

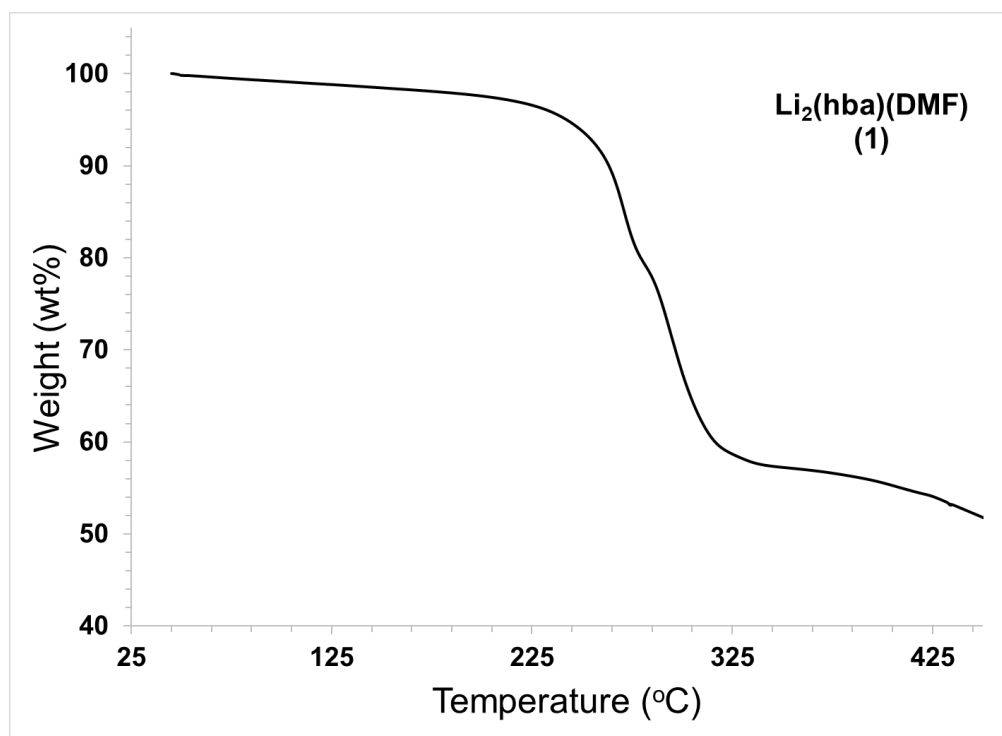
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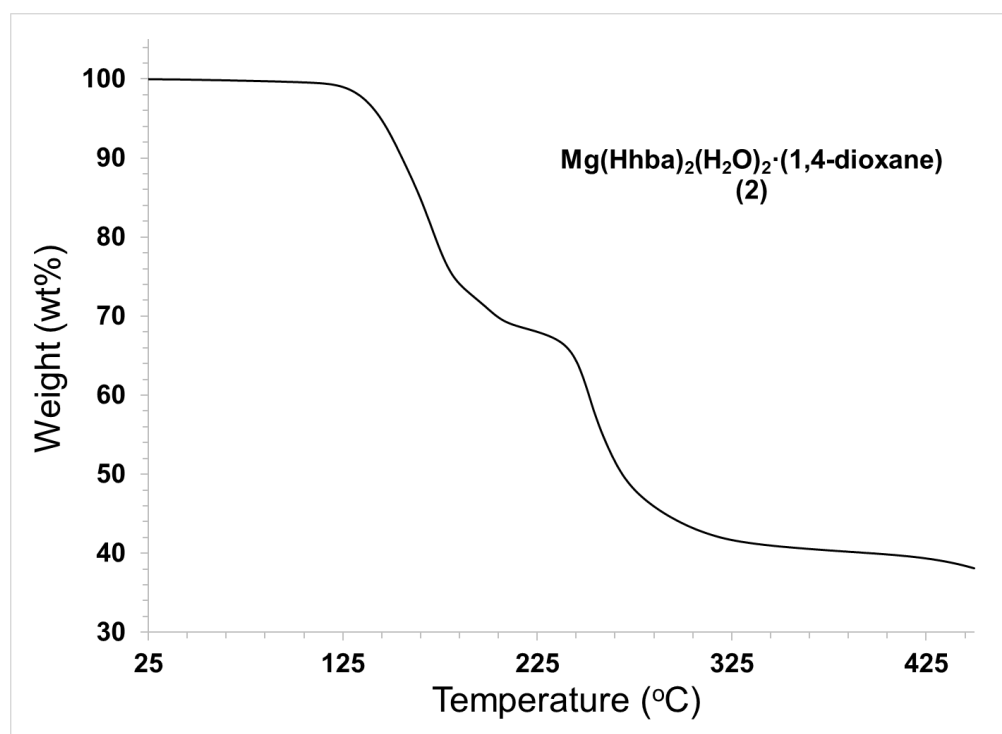
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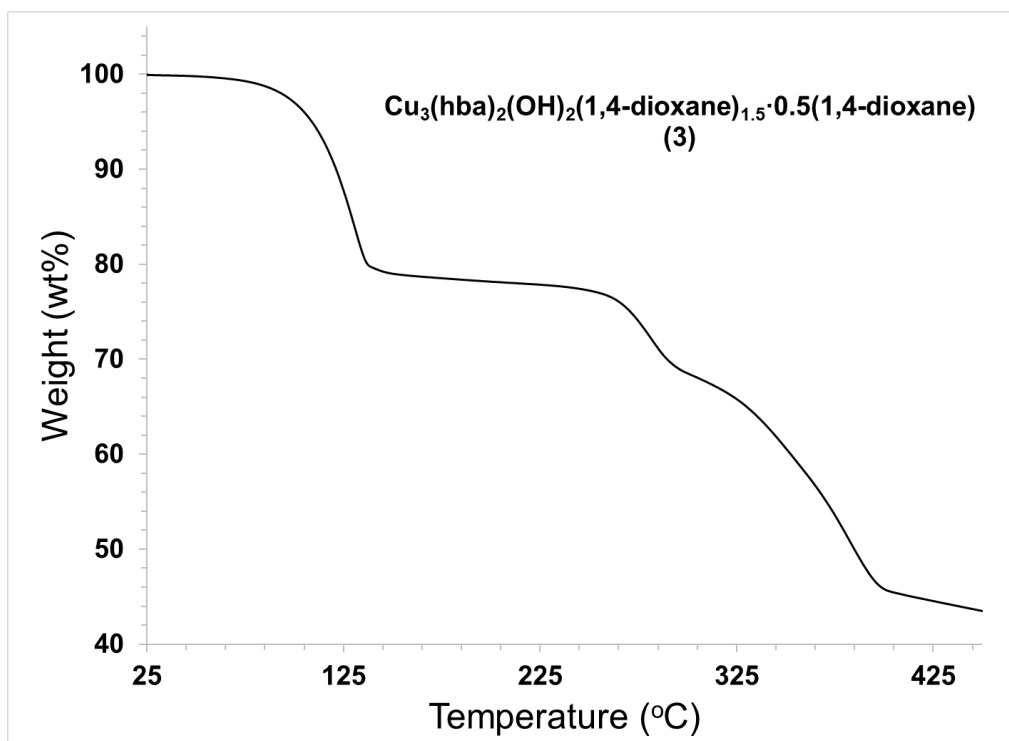
## 1. Experimental details relating to thermogravimetric analyses



**Figure S1.** Thermogravimetric trace measured on a freshly prepared sample of  $\text{Li}_2(\text{hba})(\text{DMF})$ , (1).

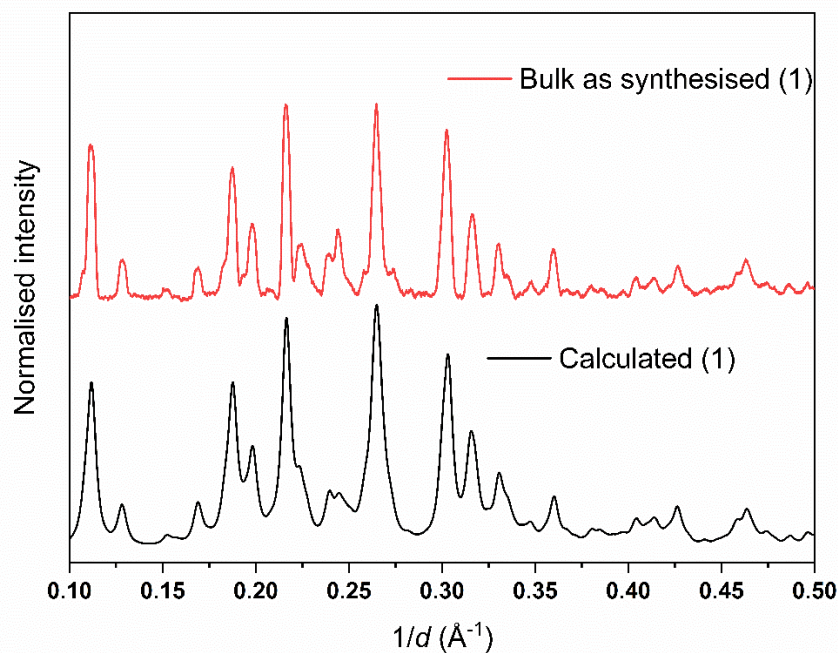


**Figure S2.** Thermogravimetric trace measured on a freshly prepared sample of  $\text{Mg}(\text{Hhba})_2(\text{H}_2\text{O})_2 \cdot (1,4\text{-dioxane})$ , (2)

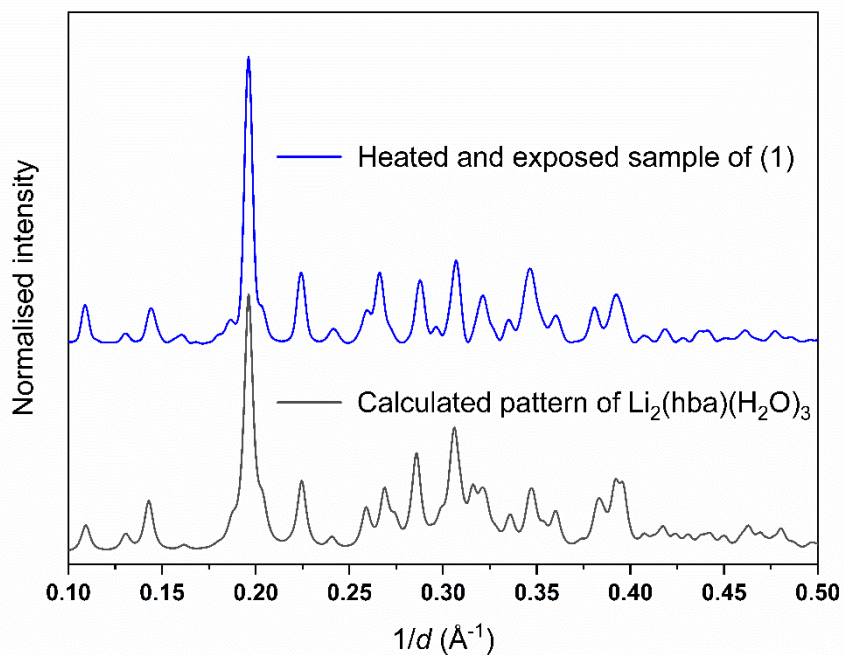


**Figure S3.** Thermogravimetric trace measured on a freshly prepared sample of  $\text{Cu}_3(\text{hba})_2(\text{OH})_2(1,4\text{-dioxane})_{1.5} \cdot 0.5(1,4\text{-dioxane})$ , (3).

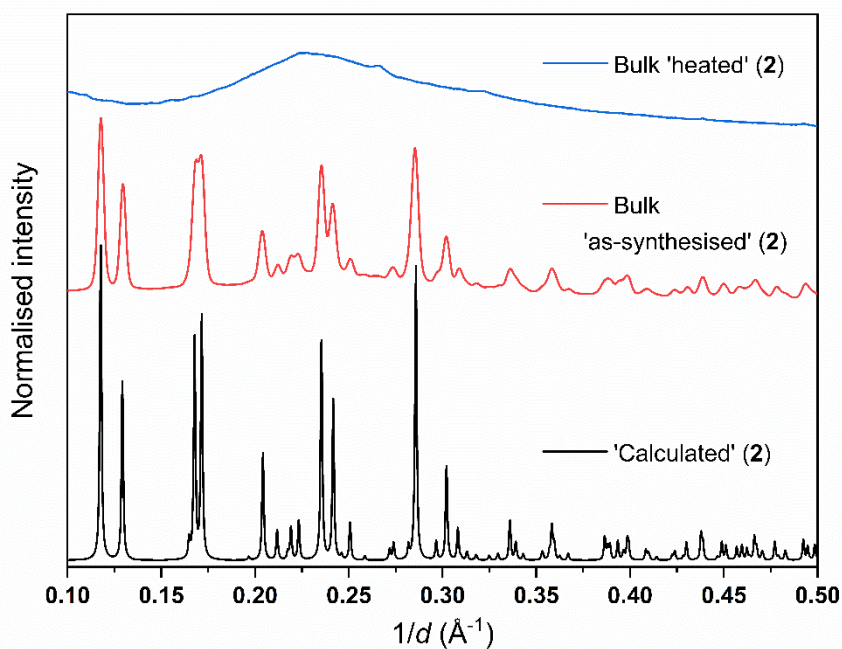
## 2. Powder X-ray diffraction data



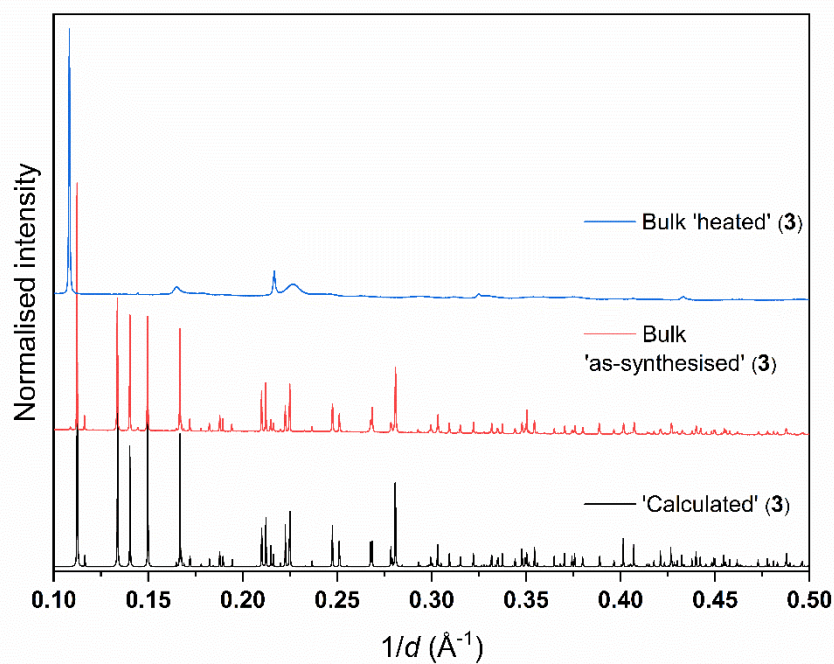
**Figure S4.** Experimental and calculated powder X-ray diffraction patterns for  $\text{Li}_2(\text{hba})(\text{DMF})$ , (**1**). The experimental powder diffraction pattern was measured at 300 K with  $\text{CuK}\alpha$  radiation ( $\lambda = 1.54184 \text{ \AA}$ ). The red trace is obtained from a bulk sample of freshly prepared **1** and the black trace is the powder pattern calculated from single crystal X-ray data.



**Figure S5.** Experimental and calculated powder X-ray diffraction patterns for  $\text{Li}_2(\text{hba})(\text{H}_2\text{O})_3$ . The blue trace represents the powder diffraction pattern obtained upon heating a sample of **1** to 573 K and exposing the sample to the atmosphere; the powder pattern was measured at 300 K with  $\text{CuK}\alpha$  radiation ( $\lambda = 1.54184 \text{ \AA}$ ). The black trace represents the calculated powder diffraction pattern based upon the  $\text{Li}_2(\text{hba})(\text{H}_2\text{O})_3$  structure determined by single crystal X-ray diffraction.<sup>3</sup>



**Figure S6** Experimental and calculated powder X-ray diffraction patterns for  $\text{Mg}(\text{Hhba})_2(\text{H}_2\text{O})_2 \cdot (1,4\text{-dioxane})$ , (**2**). The red trace corresponds to a bulk sample of freshly prepared **2** and the blue trace corresponds to a sample of **2** heated to 130 °C under vacuum. The black trace is the pattern calculated from the single crystal structure determination of **2**. Experimental powder diffraction patterns were measured at 130 K with  $\text{CuK}\alpha$  radiation ( $\lambda = 1.54184 \text{ \AA}$ ).

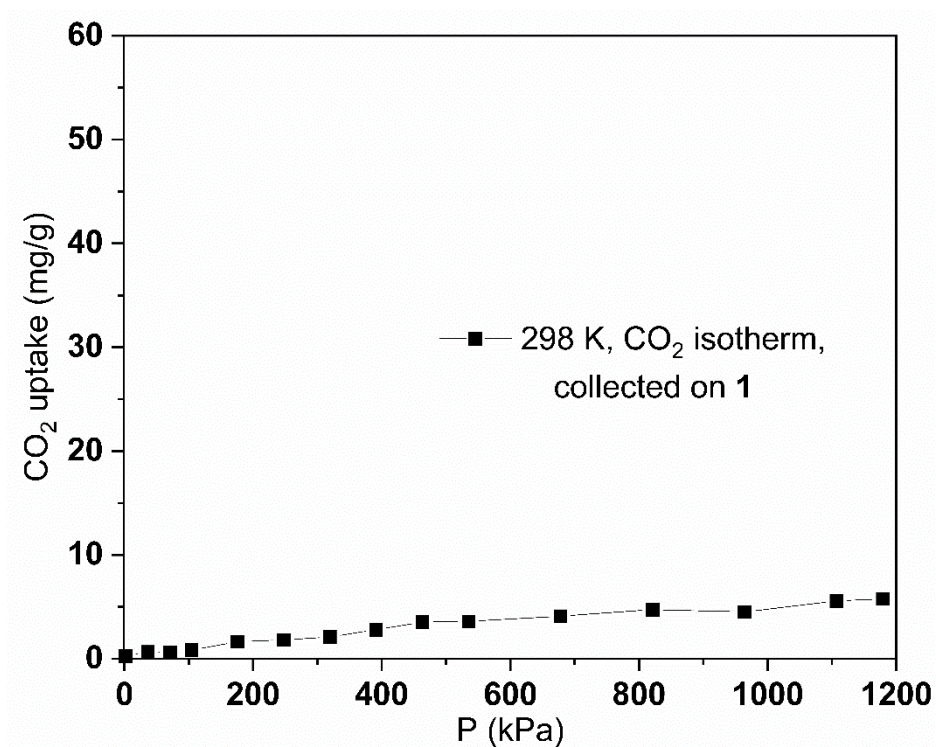


**Figure S7.** Powder X-ray diffraction data for  $\text{Cu}_3(\text{hba})_2(\text{OH})_2 \cdot (1,4\text{-dioxane})_{1.5} \cdot 0.5(1,4\text{-dioxane})$ , (**3**). The black trace is the pattern calculated from single crystal X-ray data, the red trace is obtained from a bulk sample of freshly prepared **3** and the blue trace is obtained from a sample of **3** heated to 180 °C under vacuum. Experimental powder diffraction patterns were measured using synchrotron radiation ( $\lambda = 0.7745$  Å) at 300 K.

### 3. Gas sorption experimental details

Compound 1:

A freshly isolated sample of **1** was heated to 300 °C under dynamic vacuum and the evacuation pressure monitored. When the evacuation pressure stabilized, the solid was weighed and then re-heated at 300 °C under dynamic vacuum until the evacuation pressure stabilized. CO<sub>2</sub> uptake measurements were conducted on a residue of mass 0.1437 g.



**Figure S8.** 298 K, CO<sub>2</sub> uptake data collected on a sample of **1** that had been heated to 300 °C.

Compound 2:

For CO<sub>2</sub> uptake experiments, a sample of **2** was heated at 130 °C under vacuum. Uptake measurements were conducted on a residue of mass 0.2303 g. CH<sub>4</sub> uptake experiments were collected on a sample of **2** heated at 100 °C under vacuum. The mass of the residue was 0.3010 g.

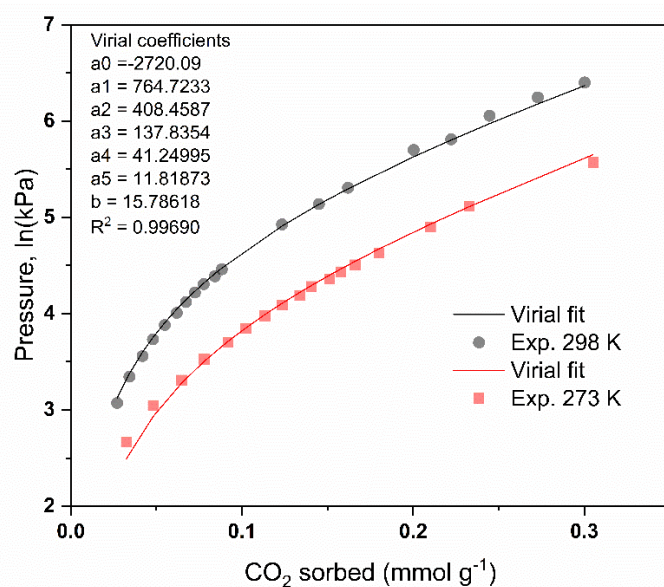


### Compound 3

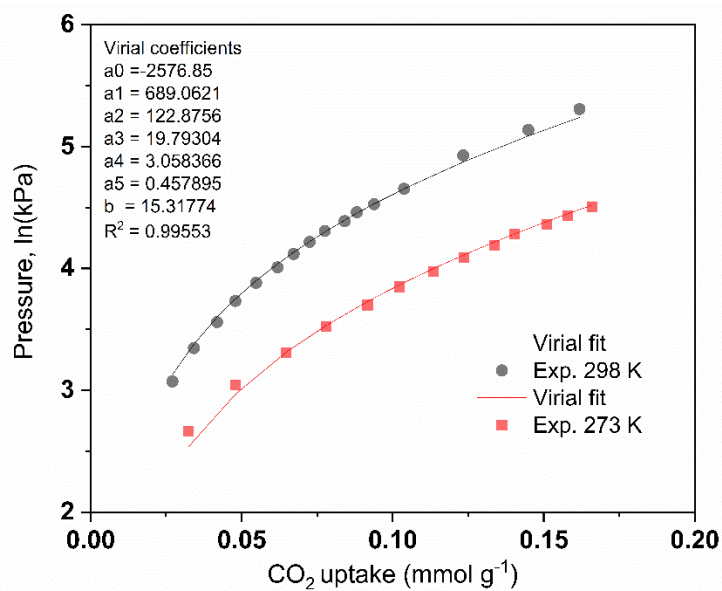
For CO<sub>2</sub> uptake experiments, a sample of **3** was heated at 180 °C under vacuum. Uptake measurements were conducted on a residue of mass 0.1553 g. CH<sub>4</sub> measurements were conducted on a freshly prepared sample that was heated at 100 °C for 1 hour; the mass of the resultant residue was 0.5821 g.

### Isosteric enthalpies of CO<sub>2</sub> sorption

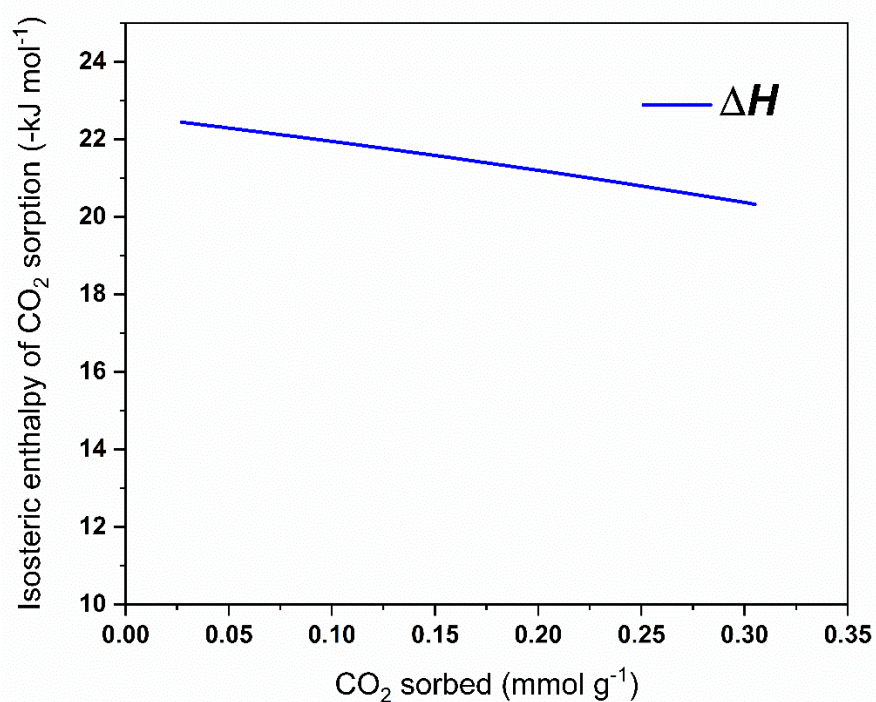
The isosteric enthalpy of CO<sub>2</sub> sorption for **2** and **3** were estimated using ‘virial analysis’.<sup>1,2</sup> For the virial fit, 273 and 298 K CO<sub>2</sub> isotherm measurements were used. Plots showing the fit of  $\ln(P)$  vs  $n$  where  $P$  = pressure in kPa and  $n$  = CO<sub>2</sub> sorbed in mmol per gram of sorbent, along with the optimized virial coefficients and  $R^2$  values are presented in Figures S9 (**2**) and S10 (**3**). Plots showing the isosteric heat of CO<sub>2</sub> sorption ( $\Delta H_{\text{ads}}$ , kJmol<sup>-1</sup>) vs amount sorbed (mmol CO<sub>2</sub> per gram of adsorbent) are presented in Figures S11 (**2**) and S12 (**3**).



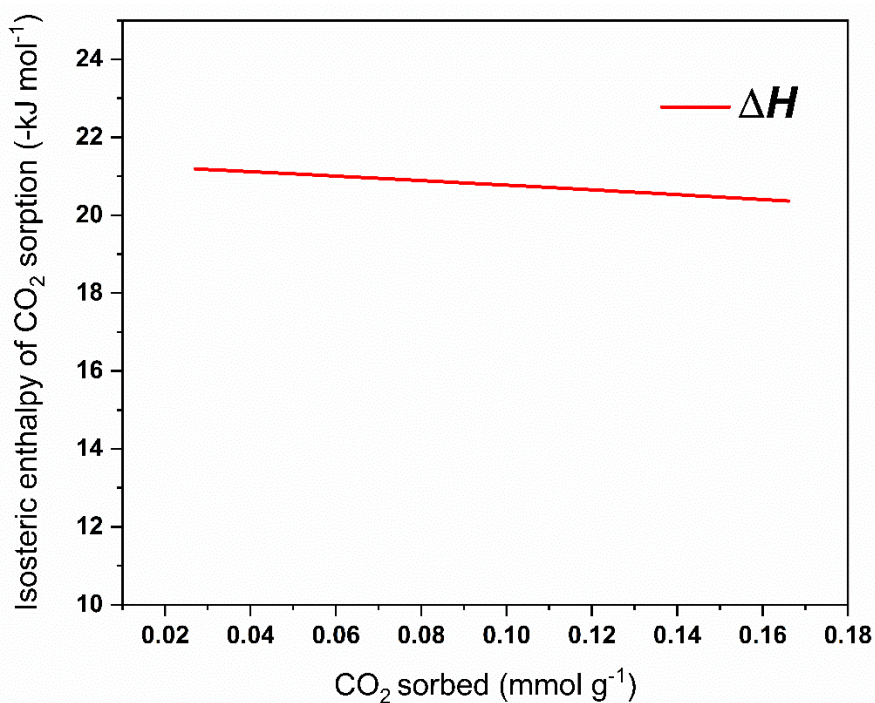
**Figure S9:** Virial fit of 273 and 298 K  $\ln(P)$  vs CO<sub>2</sub> uptake data for **2**.



**Figure S10:** Virial fit of 273 and 298 K  $\ln(P)$  vs CO<sub>2</sub> uptake data for **3**



**Figure S11.** CO<sub>2</sub> sorption enthalpies ( $\Delta H_{\text{ads}}$ ) vs quantity of CO<sub>2</sub> adsorbed for **2**



**Figure S12.** CO<sub>2</sub> sorption enthalpies ( $\Delta H_{\text{ads}}$ ) vs quantity of CO<sub>2</sub> adsorbed for **3**

## References

1. Czepirski, L., Jagiello, J., *Chem. Eng. Sci.* 1989, **44**, 797–801.
2. Nuhnen, A., Janiak, C., *Dalton Trans*, 2020, **49**, 10295-10307.
3. B. F. Abrahams, C. J. Commons, T. A. Hudson, R. Sanchez Arlt, K. F. White, M. Chang, J. J. Jackowski, M. Lee, S. X. Lee, H. D. Liu, B. M. Mei, J. E. Meng, L. Poon, X. Xu and Z. Yu, *Acta Cryst. Sect. C*, 2021, **77**, 340-353.