Electronic Supplementary Material (ESI) for CrystEngComm

Supporting information for:

Using hinged ligands to engineer structurally flexible copper(II) MOFs

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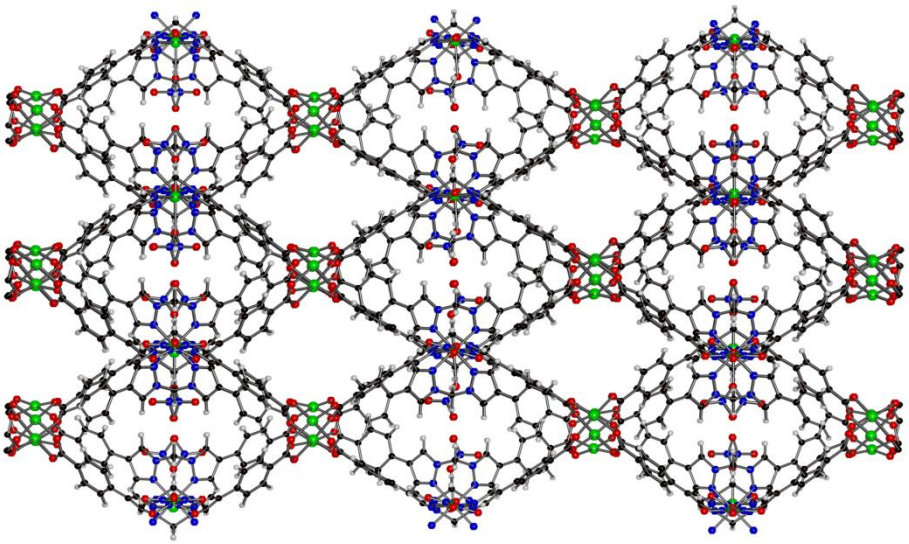

Figure SI 1. A view of hkl = 202 of the crystal structure of **1** with paddlewheel solvents removed.

Table SI 1. Comparison of the bond angles of the copper(I) centres in **2**.

Tetrahedral Cu(I)	θ_1	θ_2	θ_3	θ_4
Cu1	94.97	104.56	90.93	114.47
Cu2	94.22	111.38	94.41	104.99
[Cu(**bpy**)$_2$]ClO$_4$ [1]	81.50	109.70	81.50	127.10

Note: The major difference lies in the larger bite angles that the six-membered chelating ring of the di-pyrazolyl donors in ligand **bcpdmpm** can provide with respect to the five-membered chelating ring in **bpy**.

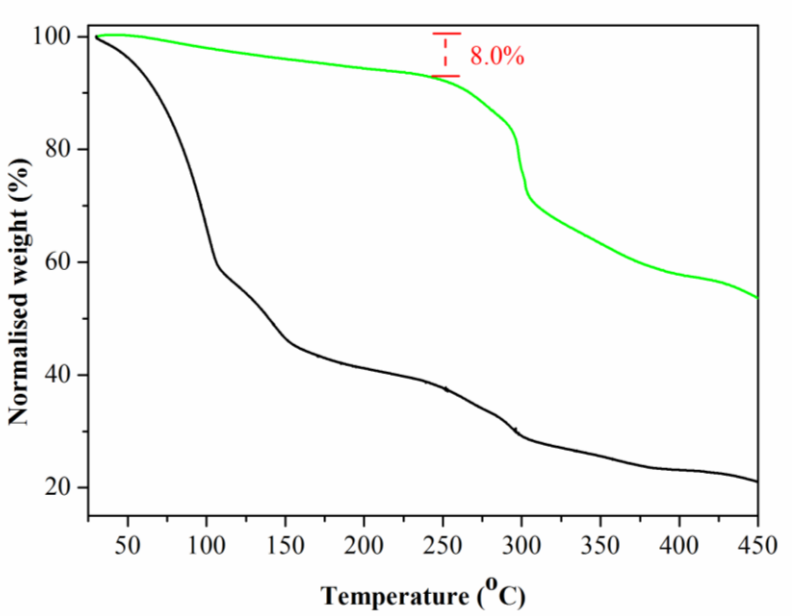

Figure SI 2. TGA trace of **1** (black) and **1**^{ac} (green). The % weight loss is shown for **1**^{ac} before decomposition at ~250°C.

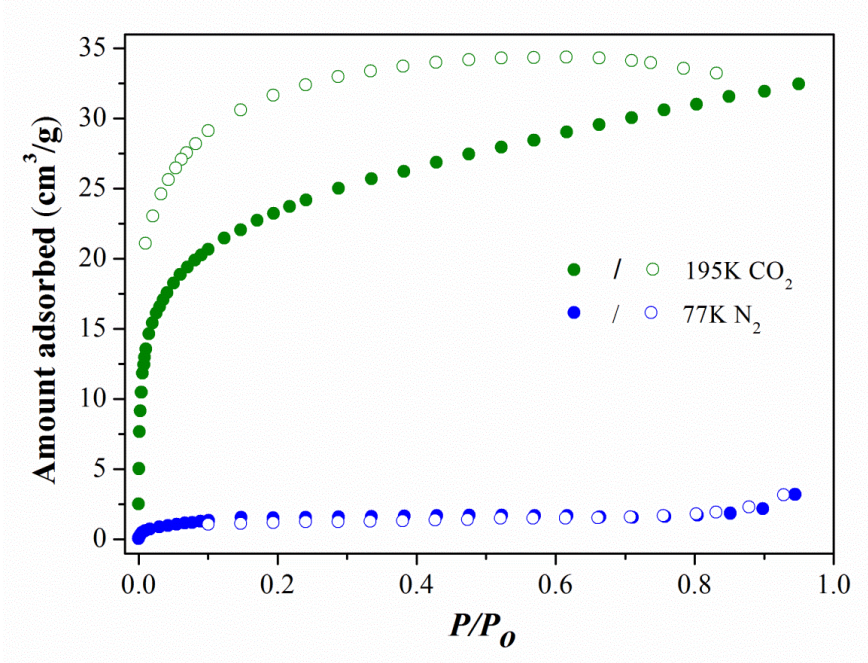

Figure SI 3. N_2 and CO_2 isotherms of **1**^{ac} measured at 77 K and 195 K respectively.

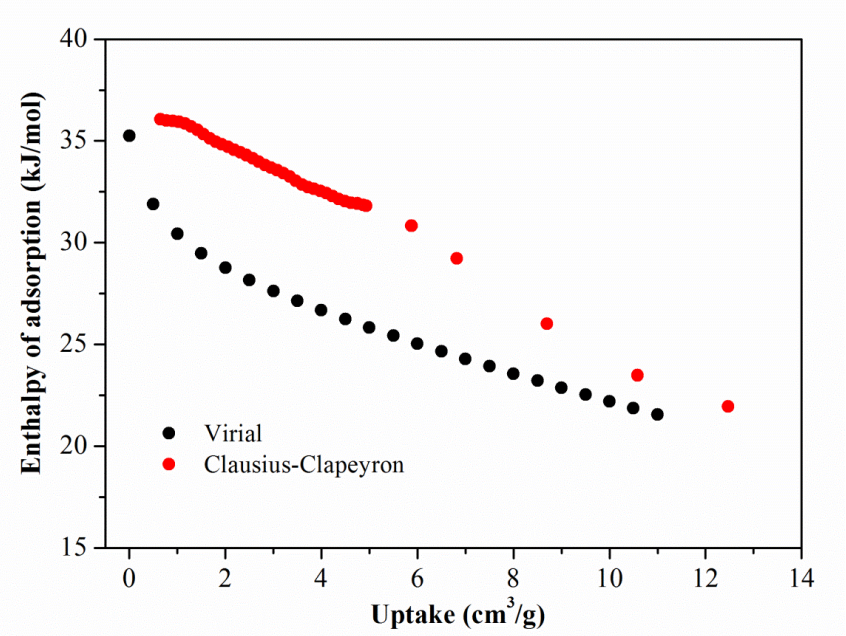

Figure SI 4. Enthalpy of adsorption of CO_2 for **1**^{ac}, calculated from the 293 and 273 K isotherms *via* the Virial and Clausius-Clapeyron equations.

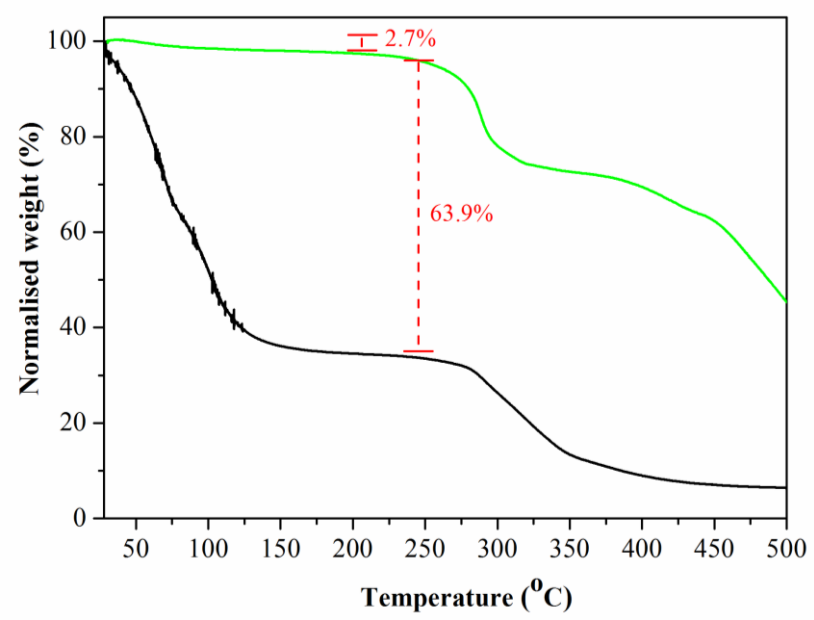

Figure SI 5. TGA trace of **2** (black) and **2**^{ac} (green). The % weight loss is shown for both forms of the material before decomposition at 260°C. We attribute the fluctuations (or 'noise') in the desolvation phase of the TGA trace of **2** to be due to movement of the crystals in the sample pan during desolvation. This occurs as a result of a large loss of pore solvent (60% by weight) and a dramatic change in the structure. This phenomenon was also observed when crystals were heated on a microscope slide.

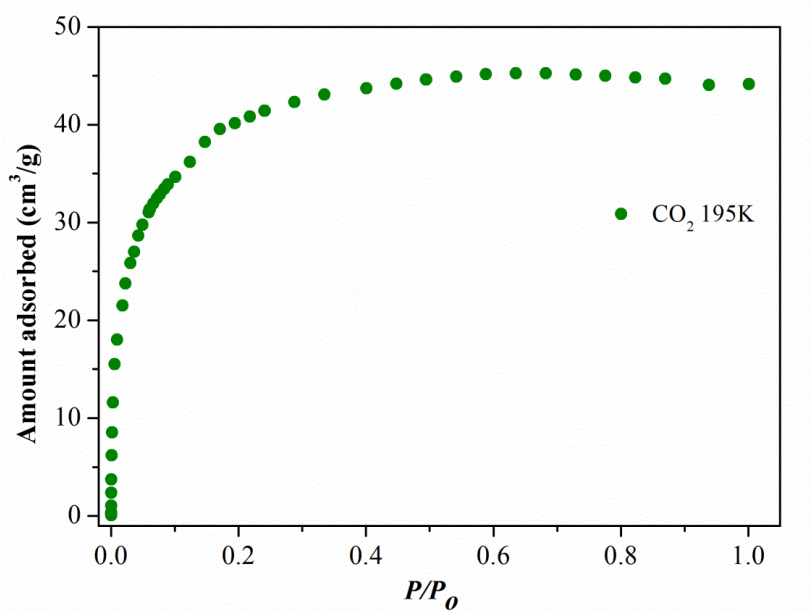

Figure SI 6. CO_2 isotherm of **2**^{ac} measured at 195 K.

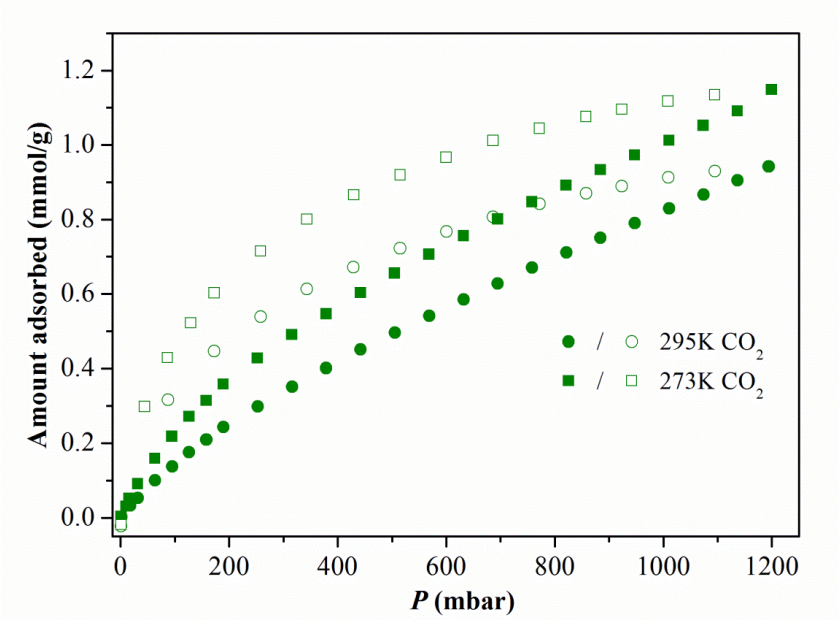

Figure S7. 293 K and 273 K CO_2 isotherms of **2**^{ac}.

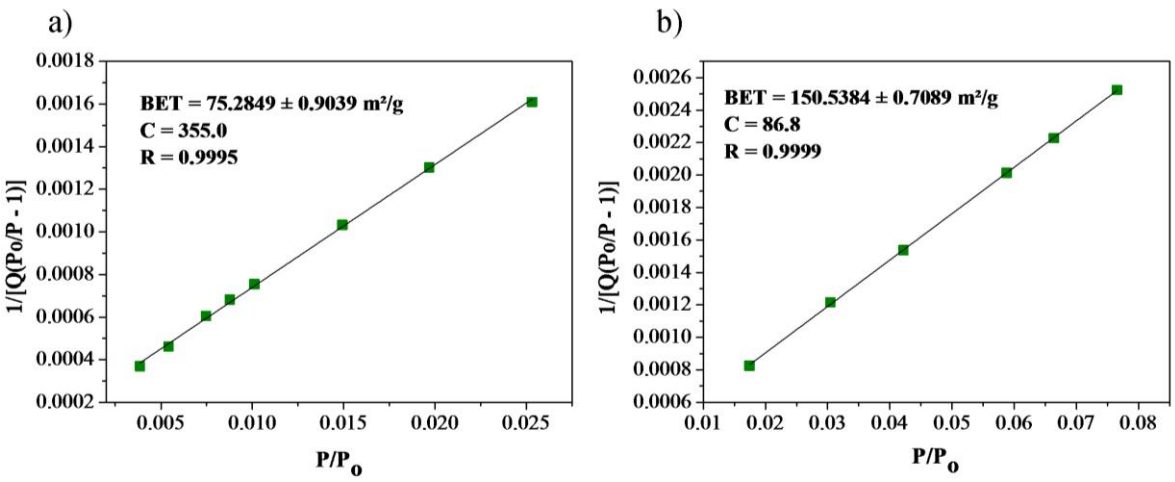

Figure SI 8. Derivation of the BET surface area from the CO_2 adsorption isotherm at 195 K for a) **1**; b) **2**.

References

1. M. Munakata, S. Kitagawa, A. Asahara and H. Masuda, *Bull. Chem. Soc. Jpn*, **1987**, *60*, 1927-1929.