Carbon dioxide gate sorption properties of one-dimensional Cu complexes with paddlewheel dimer units

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In recent decades, with an increasing demand for global energy and concomitant usage of fossil fuels, the concentration of CO_2 in the atmosphere has increased gradually. As this gas is one of the leading greenhouse gas, CO_2 separation and conversion have been considered a research topic with high priority. Polymeric metal complexes such as metal-organic frameworks/coordination polymers have attracted significant attention as CO_2 separation materials due to their high surface area, tunable pore structures, and high flexibility.[1] Previously, our group found CO_2 gate sorption, concomitant gas adsorption and structural change, in the one-dimensional Cu complexes $[Cu_2(2\text{-tc})_4(L)]$ (2-tc = 2-thiophenecarboxylate, L = pyrazine (pyz) and aminopyrazine) in the mild condition. In this work, we synthesized a series of their derivatives to investigate the effect of functional groups of the pyz ligand on CO_2 gate sorption properties.

The one-dimensional Cu complexes, $[Cu_2(2\text{-tc})_4(2,3\text{-dmpyz})]$, $[Cu_2(2\text{-tc})_4(2,5\text{-dmpyz})]$, and $[Cu_2(2\text{-tc})_4(2\text{-epyz})]$ (2,3-dmpyz = 2,3-dimethylpyrazine, 2,5-dmpyz = 2,5-dimethylpyrazine, 2-epyz = 2-ethylpyrazine), were prepared and structurally characterized. They exhibited one-dimensional structures, in which paddlewheel Cu(II) dimers were bridged by pyz derivatives. $[Cu_2(2\text{-tc})_4(2,5\text{-dmpyz})]$ and $[Cu_2(2\text{-tc})_4(2\text{-epyz})]$ showed CO_2 gate sorption at 195 K, while $[Cu_2(2\text{-tc})_4(2,3\text{-dmpyz})]$ was unable to show CO_2 gate sorption (Figure 1).

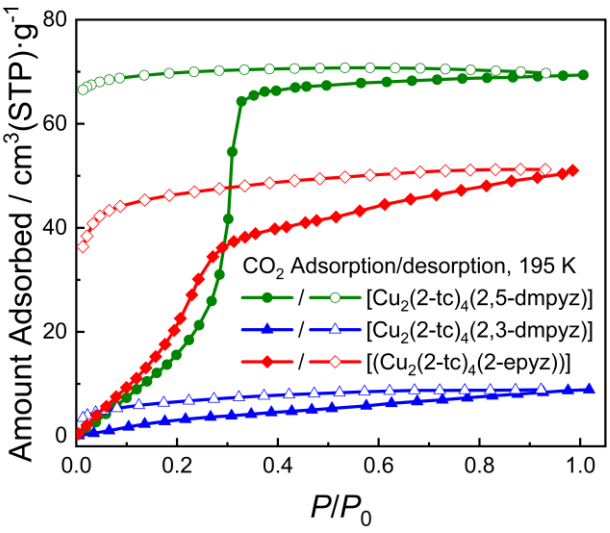

Figure 1. Adsorption/desorption isotherms of CO_2 195 K.

1) W. Kosaka, et al., *Inorg. Chem.* **2022**, *61*, 12698.