CO_2-induced spin-state conversion in a porous molecular crystal consisting of a cobalt(II) complex

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Porous molecular crystals (PMCs) that are composed by molecular assembly of discrete metal complexes have attracted much attention due to the potential to be a new type of guest adsorbable materials through the flexible pseudo-framework structure. Spin-crossover (SCO) phenomenon represents a stimulus-driven spin-state change between the low-spin (LS) and high-spin (HS) states of a metal center and is quite sensitive to structural changes. Thus, SCO behaviors in PMCs are expected to be controlled by structural changes through guest adsorption.[1]

In this research, we designed a neutral mononuclear cobalt(II) complex of type [Co(COO-terpy)$_2$] (**1**). **1** was found to form cavities generated via π–π stacking motifs and hydrogen bond networks in the molecular assemblies (**Figure (a)**), initially resulted in crystals with four water molecules in the cavity (**1·4H$_2$O**). Desolvated **1** maintained the cavity and it was found to show selective CO_2 gas adsorption. Unlike **1** showing gradual SCO behavior and was in the HS state at 290 K (near room temperature), the CO_2-accommodated form **1⊃CO$_2$** varied the SCO behavior based on the CO_2 pressure, and was stabilized in the LS state under 110 kPa CO_2 pressure at 290 K (**Figure (b)**). This provided a reversible spin-state conversion by introducing/evacuating CO_2 gas into/from **1** at 290 K.[2]

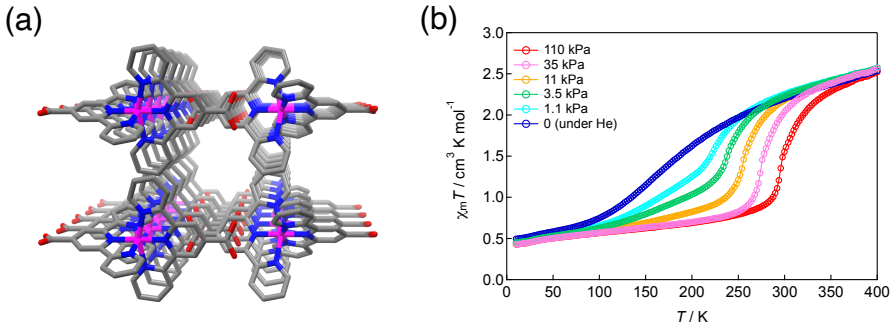

Figure (a) The porous assembly structure in the crystal packing of **1**. **(b)** Magnetic behaviors of **1⊃CO$_2$** at various pressures (0–110 kPa) of CO_2 for the cooling process.

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