# Investigating carbon dioxide sorption properties of two isostructural Co(II) and Zn(II) mixed-ligand metal-organic frameworks containing imide based ligands

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Metal–organic frameworks (MOFs) are porous materials composed of metal ions or clusters coordinated to organic ligands.¹ Due to their tunable structures and porosity, MOFs have attracted attention for a variety of applications, including gas storage, separation, sequestration, drug delivery, and catalysis.²⁻⁵ Flexible MOFs or soft porous crystals, can undergo dynamic structural transformations in response to external stimuli.⁶ This structural flexibility can enhance their performance, particularly in selective gas adsorption and sensing applications.⁶ In this study, we present the synthesis, characterization, and carbon dioxide sorption studies of two isostructural, flexible MOFs: {[Co(OBZ)(L1)₀.₅]·2DMF}n (1) and {[Zn(OBZ)(L1)₀.₅]·2DMF}n (2). Where L1 is 2,7-bis(pyridin-3-ylmethyl)benzo[lmn][3,8]phenanthroline-1,3,6,8(2H,7H)-tetraone and H₂OBZ is 4,4′-oxybis(benzoic acid). The two MOFs were synthesized using the solvothermal method and characterized using single-crystal X-ray diffraction (SCXRD), powder X-ray diffraction (PXRD), and thermogravimetric analysis (TGA). Carbon dioxide sorption experiments were conducted up to 20 bar at 298 K. SCXRD analysis revealed that both MOFs are three-dimensional structures with 12% potential solvent-accessible volume. PXRD shows a structural change upon activation, which indicates structural flexibility. The CO₂ sorption isotherms of the two MOFs differ significantly. MOF 1 displays a type IV isotherm with pronounced hysteresis upon desorption. The MOF adsorbs 0.6 mmol g-1 CO₂ up to 15 bar after which the structure opens and adsorbs and additional 1.3 mmol g-1, resulting in a total of 1.9 mmol g-1 at 20 bar. In contrast, MOF 2 shows a typical type I isotherm, reaching a maximum CO₂ uptake of 1.2 mmol g-1 at 20 bar.

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