

FLEXIBLE METAL ORGANIC FRAMEWORK {[Ni(dp bz)][Ni(CN)₄]}_n, dp bz=1,4-bis(4-pyridyl)benzene) WITH AN UNUSUAL Ni-N BOND

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To mitigate global warming as a major result of fossil fuel burning, CO₂ capture and storage (CCS) technology is critical. Effective sorbent materials are needed for carbon capture because coal-fired electrical power plants, the largest emitters of the greenhouse gas, will continue to produce much of our nation's electricity for at least several decades. Within the family of pillared layer metal organic frameworks (MOFs), the Ni-based Hofmann compounds [Ni'(L)Ni(CN)₄]_n (L=pillar ligand), have been shown to be especially diverse. To understand the CO₂ sorption mechanism of these MOFs, and enable the design of more efficient sorbent materials, detailed knowledge of the crystal structure is necessary. A selected flexible MOF, [Ni'(L)Ni(CN)₄]_n (L= 1,4-Bis(4-pyridyl)benzene, or dpbz)) that shows a reversible structural transition between low porosity and high porosity phases during the sorption of CO₂ has been synthesized and analyzed using synchrotron single crystal diffraction, powder X-ray diffraction, and adsorption/desorption isotherm measurements. The structure consists of an unusual 5-fold pseudo square-pyramid environment for Ni and a significantly long Ni-N distance of 2.369(4) Å. DFT calculations have been conducted to understand the charge distribution in this unusual Hoffmann compound.