FLEXIBLE METAL ORGANIC FRAMEWORK
{[Ni(4,4'azopyridine)][Ni(CN)$_4$]}$_n$ or (Ni-AzoPyr)

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As a result of fossil fuel burning, CO_2 capture and storage (CCS) technology is critical for mitigating global warming. 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. Therefore, effective sorbent materials are needed for carbon capture. 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 structural diverse. To understand the CO_2 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=4,4'azopyridine ($C_{10}N_4H_8$), nicknamed AzoPyr) that shows a reversible structural transition between low porosity and high porosity phases during the sorption of CO_2 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 2.436(11) Å. DFT calculations have been conducted to understand the bonding characteristics in this unusual Hoffmann compound.