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Title: A robust and water-stable two-fold interpenetrated metal-organic framework containing both rigid tetrapodal carboxylate and rigid bifunctional nitrogen linkers exhibiting selective CO2 capture† Authors: Gupta, Vijay (/jspui/browse?type=author&value=Gupta%2C+Vijay) Mandal, S.K. (/jspui/browse?type=author&value=Mandal%2C+S.K.) Microporous Keywords: Metal-organic framework Self-assembly 2019 Issue Date: Publisher: American Chemical Society Citation: Dalton Transactions, 48(2), pp.415-425. Abstract: A microporous metal-organic framework, {[Co2(4,4'-bpy)(L)]·H2O·0.5(DMF)}n (1), was obtained from the self-assembly of cobalt(II) nitrate hexahydrate, rigid tetrapodal carboxylic acid 4,4',4",4"'silanetetrayltetrabenzoic acid (H4L) and a rigid bifunctional linker 4'4'-bipyridine (4,4'-bpy) under solvothermal conditions. It was characterized by Fourier transform infrared spectroscopy, thermogravimetric analysis, elemental analysis, and powder and single crystal X-ray diffraction. Its single crystal structure reveals the presence of a Co(II)-paddle wheel core as the SBU, which is extended to form a doubly interpenetrated 3D framework with a (4.6)-connected sqc422-type uninodal net topology with the Schläfli point symbol {42·510·72·8}{42·54}. There are two types of open channels in this framework (rhombic and trigonal), which run along all three axes. Its thermal and chemical stabilities were established based on thermogravimetric analysis and in situ variable temperature powder X-ray diffraction. The activated framework (lattice solvent free) of 1 exhibits modest uptake of CO2 (53.8 and 36.4 cm3 g-1 at 273 and 298 K at 1 bar pressure, respectively),

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with moderately high selectivities for CO2/N2 and CO2/CH4 gas separation under ambient

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conditions (298 and 273 K under 1 bar pressure).

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