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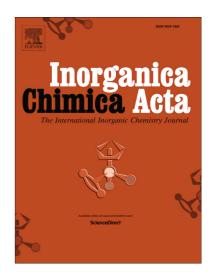
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Urea-based flexible dicarboxylate linkers for three-dimensionalmetal-organic frameworks

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Dedicated to Prof. Ionel Haiduc on the occasion of his 80th birthday.

Keywords: MOFs, metal-organic frameworks; urea function; 4,4'-(carbonylbis(azanediyl))dibenzoic acid; interpenetration, four-fold; diamondoiddiatopology; hydrogen bonding

Abstract

The frameworks $(MOFs)3D-[Mn_2(L1)_2(DMF)]\cdot 2DMF(1)$, 3Dmetal-organic $[Cd_2(L2)_2(DMF)_3](3)$, $[Zn_2(L2)_2(DMF)_3](4)$ and $3D-[Mn_2(L2)_2(DMF)_3]$ (5) are the first examples of three-dimensional metal-organic networks constructed from a single ditopic dicarboxylate linker (i.e., without bridging co-ligands) with an urea group in the 4,4'-(carbonylbis(azanediyl))dibenzoate; L2²⁻ linker (carbonylbis(azanediyl))bis(3-methylbenzoate), DMF = dimethylformamide). From Cd²⁺ and L1²⁻ a 1D coordination polymer 1D-[Cd(L1)(DMF)₃] (2) is formed. The urea group is engaged in hydrogen bonding with the C(4)[R¹₂(6)] motif to an oxygen atom of a DMF solvent (in 1) or a metal-coordinated carboxylate group (in 3-5). Network1has infinite channels with parallelepiped cross sections and 30% solventfilled volume. The 3D frameworks 3-5 are of diamond (6,6), dia topology with a single framework having large voids with 17.6 Å and 19.7 Å nodal separation. Thus, four symmetry-related nets interpenetrate, organized via H-bonds in the C(4)[R¹₂(6)] motif, still leaving about 50% solvent-filled void volume in the four-fold interpenetrated structure.

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