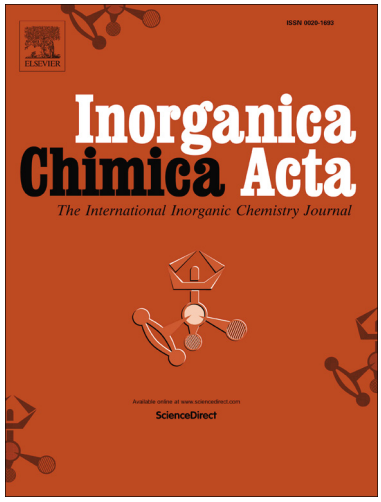

Urea-based flexible dicarboxylate linkers for three-dimensionalmetal-organic frameworks

Sebastian Glomb, Gamall Makhloufi, Irina Gruber, Christoph Janiak

PII: S0020-1693(17)31028-9
DOI: http://dx.doi.org/10.1016/j.ica.2017.09.029
Reference: ICA 17888

To appear in: *Inorganica Chimica Acta*

Received Date: 30 June 2017
Revised Date: 7 September 2017
Accepted Date: 11 September 2017

Please cite this article as: S. Glomb, G. Makhloufi, I. Gruber, C. Janiak, Urea-based flexible dicarboxylate linkers for three-dimensionalmetal-organic frameworks, *Inorganica Chimica Acta* (2017), doi: http://dx.doi.org/10.1016/j.ica.2017.09.029

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

Sebastian Glomb, Gamall Makhloufi, Irina Gruber, Christoph Janiak*

Institut für Anorganische Chemie und Strukturchemie, Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany. Email: janiak@uni-duesseldorf.de

* Corresponding author:
C. Janiak Tel.: +49 211 81 12286; fax: +49 211 81 12287. E-mail address: janiak@hhu.de

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; diamondoid**dia**topology; hydrogen bonding

Abstract

The metal-organic frameworks (MOFs)3D-$[Mn_2(L1)_2(DMF)]\cdot 2$ DMF(**1**), 3D-$[Cd_2(L2)_2(DMF)_3]$(**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 linker axis($L1^{2-}$ = 4,4'-(carbonylbis(azanediyl))dibenzoate; $L2^{2-}$ = 4,4'-(carbonylbis(azanediyl))bis(3-methylbenzoate), DMF = dimethylformamide). From Cd^{2+} and $L1^{2-}$ a 1D coordination polymer 1D-$[Cd(L1)(DMF)_3]$ (**2**) is formed.The urea group is engaged in hydrogen bonding with the C(4)[R^1_2(6)] motif to an oxygen atom of a DMF solvent (in **1**) or a metal-coordinated carboxylate group (in **3-5**). Network**1**has infinite channels with parallelepiped cross sections and 30% solvent-filled 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)[R^1_2(6)] motif, still leaving about 50% solvent-filled void volume in the four-fold interpenetrated structure.