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Pore engineering through the supramolecular modification of Mo-based metallocycles: from 0D discrete cavities to 1D open channels

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The synthesis of novel crystalline discrete molecular materials combined with interesting supramolecular architectures providing porosity still consists one of the challenges in synthetic coordination chemistry. The forming cavities, resulting from the *coordination driven self-assembly* of the clusters, play a crucial role in the *host-guest recognition properties* with diverse applications in catalysis, adsorption, drug delivery *etc.*¹ Moreover, any crystal-packing modification can significantly differentiate the physical properties of the solid-state material.² Although network materials are representative examples of crystalline porous materials, discrete molecular compounds have shown a tendency to a more close-packing supramolecular assemblies. To this end, research efforts have been devoted to the development of new coordination clusters displaying permanent porosity.³

Herein we present the syntheses of two structurally similar Mo-based metallocycles with different supramolecular structures. The replacement of the terminally bound pyridines of the initial cluster by the 1,3-di(4-pyridyl)propane forced the metallocycles to reorient their positions yielding a crystal-packing architecture with well-defined channels within the compounds (see Figure). Fully chemical and physical characterization of both complexes is also discussed.

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Topological analysis and properties of new imidazole-based systems as potential candidates for biological applications

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Transition metal complexes based on imidazole have shown significant interest in biological systems, especially carboxylate mixed-ligands systems of copper(II), which display a variety of pharmacological effects, including antitumor, superoxide dismutase and catecholase activities [1]. Despite the considerable number of the reported imidazole systems built of different carboxylate ligands and metallic centers, namely; copper, cobalt, nickel, manganese, cadmium and ruthenium, the crystallographic information about imidazole-based copper(II) complexes containing citrate mixed-ligands is rather rare, except for only two hexacoordinated complexes of cobalt and nickel [2]. In order to contribute to the well-understanding of these systems, the one-pot synthesis, the crystal structure, the properties and the topological nets of two copper(II) potential candidates for biological applications involving imidazole and citrate mixed-ligands were reported [3].

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