EMBEDDED WATER MOTIFS IN CRYSTAL HOST OF 1,2,4,5-BENZENETETRACARBOXYLATE MOF`S

Oscar Fabelo,[a] María Milagros Laz[b], Laura Cañadillas-Delgado[a] Jorge Pasán,[a] Fernando S. Delgado[a] and Catalina Ruiz-Pérez[a]

[a]Laboratorio de Rayos X y Materiales Moleculares, Departamento de Física Fundamental II, Universidad de La Laguna, 38204 La Laguna, Tenerife, Spain
[b]Laboratorio de Rayos X y Materiales Moleculares, Departamento de Edafología y Geología, Universidad de La Laguna, 38204 La Laguna, Tenerife, Spain
caruiz@ull.es

A common feature of metal-organic frameworks (MOFs) is the high trend to crystallize as hydrates. These crystallization water molecules are presented as isolated entities tightly H-bonded to the MOF or as aggregates which fill the empty voids or channels generated in the crystal packing. The release of the water molecules in the latter case, can lead to the formation of porous anhydrous compounds with several potential applications in areas such as chemical separation, catalysis and sorption. Moreover, oligomeric and polymeric arrays of water molecules have been extensively studied both theoretically and experimentally because they can provide not only insights into the supramolecular architecture[1] or water condensed phase properties[2] but also clues on many biological processes.[3] For example, water chains appear to be important in the control of proton translocation through membranes by functioning as proton wires,[4] and a close behavior has been observed in the solid-state hydrated phase of an abiological imidazole derivative.[5] Because it is impossible for water clusters in solution and in the solid state to be fully discrete, the precise structural data and cooperative association of the water clusters and crystal hosts may be helpful in improving our understanding of the contribution of water clusters to the stability and function of the biological assemblies, as well as anomalous properties of water.

The presence of crystallization water molecules within the structure can play an important role in the stabilization of supramolecular architectures since the number of donor/acceptor can differ significantly from those of the anhydrous compounds (see Figure 1). Therefore, the hydrogen bonding interactions of the donor/acceptor groups of the organic molecules with the water molecules can be crucial in the overall covalent structure, but in the same way, the arrangement of water molecules vary significantly giving rise to different cluster patterns. So often it might be difficult to decide whether the metal-organic framework directs pattern of the water cluster or water templates the overall crystal structure,[6] but it also could be regarded as the cocrystallization of a complex entity and water.

Acknowledgements:
This work is financed by the Ministerio de Educación y Ciencia [Project MAT2004-03112]

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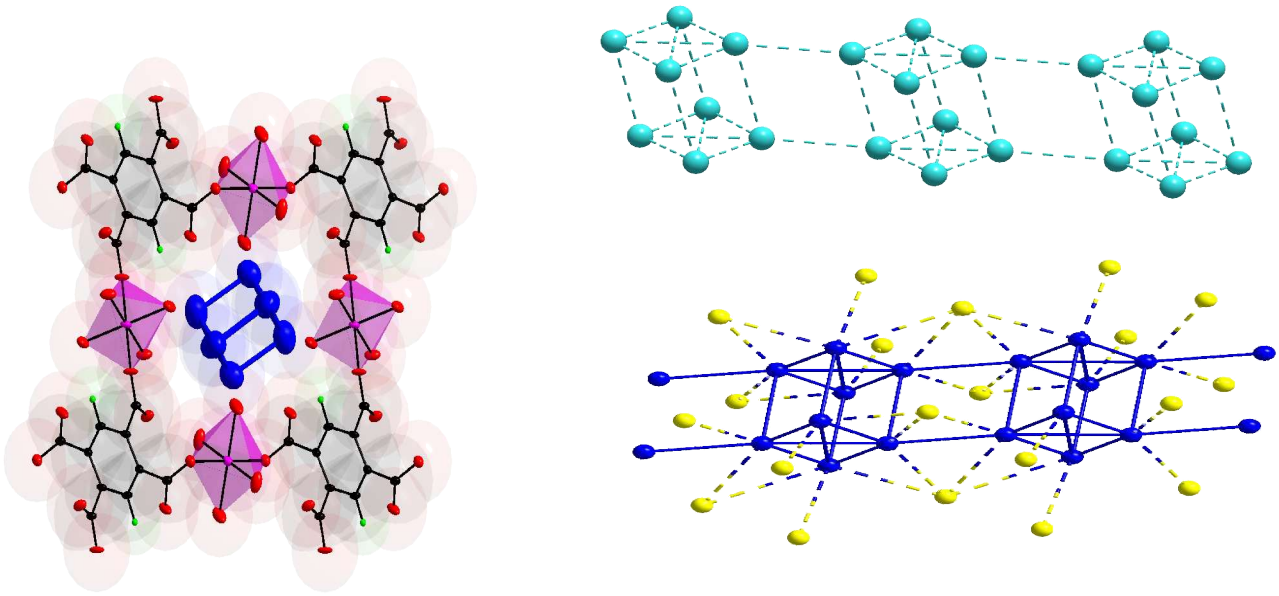

(a) **(b)**

Figure 1. (a) Perspective view of a host showing the Co atoms coordination environment. **(b)** Perspective drawing of a fragment of the one-dimensional water chain showing their immediate environment.