

## Poster Presentation

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### *Desconstruction of Two compounds of p-sulfobenzoic ligand by Reticular Chemistry*

C. Franco<sup>1</sup>, R. Aglio<sup>1</sup>, C. Corrêa<sup>1</sup>, R. Diniz<sup>1</sup>

<sup>1</sup>Universidade Federal de Juiz de Fora, Department of Chemistry, Juiz de Fora, Brazil

The p-sulfobenzoic (4-psb) acid may be used as precursors for different Metal Organic frameworks (MOFs) since they can display different coordination site on the metal with two different functional groups (carboxylate and sulfonate). Details of the crystal packing can be studied using the Reticular Chemistry like a power tool for the deconstruction process of crystal structure of this compounds formed [1]. Two crystal structures Zn-psb and Mn-psb with 4-psb ligand and Zn+2 and Mn+2 ions, respectively, were synthesized. Single crystal-data were collected using an Oxford GEMINI A-Ultra diffractometer with MoK $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) at room temperature (298 K). These structures were refined by SHELXL-97 program [2]. Both compounds crystallized in the triclinic system and space group P-1. Zn-psb structure shows a coordinated Zn atom with a slightly distorted octahedral geometry formed by four oxygen atoms from water molecules with averaged distances at 2.08 (2)  $\text{\AA}$  and two oxygen atoms with distances at 2.12 (2)  $\text{\AA}$  derived from the ligand. Mn-psb structure has coordinated Mn atom with a slightly distorted octahedral geometry formed by four oxygen atoms from sulfonate group coordinated with averaged distances at 2.19 (3)  $\text{\AA}$  and two oxygen atoms from water molecules with distances at 2.17 (2)  $\text{\AA}$ . Despite the structural similarities of the structures, a simple modification of the metal in the reaction leads to a tendency for different network. Thus, Zn-psb structure consists of a network-connected system binodal (3,8). This network is deposited in Reticular Chemistry Structural Resource as a network type tfz-d system with tiling of transitivity [2222] and signature  $3[4^2.6^2] + 2[6^3]$ . However, the Mn-psb structure leads to formation of a regular network with pcu topologic type presenting tiling with transitivity [1111] and signature  $[4^6]$ . The system of cavities formed into networks are blocked by ligands in the crystal structure.

[1] O'KEEFFE, M. Peskov, Maxim A. Ramsden, Stuart J. Yaghi, Omar M. *Accounts of Chemical Research*, 2008, v. 41, n. 12, p. 1782-1789, [2] Sheldrick, G. M. *Germany, University of Goettingen*, 1997

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