

Poster Presentation

MS43.P12

Crystallographic Study of a coordination polymer based on Zn²⁺ ion

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Several studies have aimed to better understand coordination polymers, which are structures based on a connection between a metal ion and an organic ligand that extends infinitely, forming a macro-structure¹. The interest in this type of structure is mainly due to its properties, such as its pore-forming ability, presenting many potential applications² like selective separations, catalysis and gas storage. It is interesting to study the structure of coordination polymers to focus in some particular future application. In these way, a coordination polymer was synthesized by simple mixture with isonicotinylhydrazine (INH) and 1,2,4,5-benzenetetracarboxylic acid (BTC) ligands and zinc metallic ion. Yellow single crystals were formed in solution and one was separated, measured and solved by single crystal X-ray diffraction. The crystal-data for the structure were collected using an Oxford GEMINI A-Ultra diffractometer with MoK α radiation ($\lambda = 0.71073 \text{ \AA}$) at room temperature and solved using SHELXL-97 program³. The compound crystallized in monoclinic crystalline system in space group P21/c, cell parameters: $a=9.2502(6) \text{ \AA}$, $b= 15.0004(6) \text{ \AA}$, $c=9.2947(4) \text{ \AA}$, $\beta= 108.459^\circ(6)$, $V=1223,35 \text{ \AA}^3$ and $Z=4$. The final statistical parameters of the structure refinement were $R=0.0326$, $wR=0.0835$ and $S=1,053$. In this compound the BTC and INH ligands are coordinated like a bridge to two zinc ions. The BTC forms chelates by two carboxylate groups and INH coordinates by pyridine ring and by chelate at hydrazide group. This polymer extends in only one direction along a axis forming a 1D network. There is only one metallic zinc ion crystallographically independent on structure, it is in a distorted octahedral geometry with oxygen and nitrogen atoms of ligands and one coordinated water molecule in its coordination sphere. The 1D network formed by coordination polymers stabilizes the crystalline arrangement by hydrogen bonds between carboxylate and hydrazide groups and coordinated water molecules.

[1] J.W. Steed, J.L. Atwood, *Supramolecular Chemistry, 2th ed.*, John Wiley & Sons Ltd, West Sussex, 2009., [2] M. Schröder, M. Banerjee, N.R. Champness, A.I. Cooper, S. Das, R.A. Fischer, J.-X. Jiang, K. Kim, S. Kitagawa, W. Lin, X. Lin, L. Ma, V. Mugnaini, N. Roques, F. Schröder, M. Schröder, T. Uemura, J. Veciana, M. Yoon, *Functional Metal-Organic Frameworks: Ga*, [3] G.M. Sheldrick, *Acta Crystallogr. Sect. A*, 64 (2008) 112-122.

Keywords: Coordination polymer, Zinc, X-ray diffraction