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Crystal and Electronic Structure of Apatite $Me_{10}(PO_4)_6F_2$; Me = Ca, Ba, Pb.

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Apatite is a mineral that we can find in the sedimentary rocks as well as in igneous one. It has the general chemical formula $Me_{10}(XO_4)_6Y_2$, where Me generally represents a bivalent cation, XO_4 a trivalent anion and Y monovalent anion. It is characterized by the ability to accept substitution on all sites from a large array of elements and exhibit a high resistance to temperature and to irradiation damage [1], [2], [3]. In Oklo mining, the apatite retain actinides (Pu, Am…) fission products (Sr, Cs, Ba…) for two thousand million years. In order to study this last apatite ability, we synthesized the reference apatite, fluorapatite $Ca_{10}(PO_4)_6F_2$ (apatite de refe), Ba-apatite and Pb-apatite by the substitution of Ca by pollutant elements Ba and Pb respectively. The characterization of these apatites is done by X-Ray diffraction, IR, TD/TG. The identification, calculation of crystal lattice parameters and positions of atoms by Rietveld refinements of X-ray diffraction patterns [4], [5] allow us to calculate the full potential electronic structure based on LCAO (Linear Combination Atomic Orbital) [6], [7], [8]. DOS modification and the charge transfer are estimated that is compared to experimental analysis by Multipurpose Electron Spectrometer.

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Structural Characterization of Two Novel Chiral Y(III)-MOFs.

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Materials known as coordination polymers or metal organic frameworks (MOF's), building from organic and inorganic units, represent one of the most active and attractive research fields in the materials science. A huge development in the last decades is taken place, due to the unique properties of these materials, considerable structural diversity, and improved properties as gas storage, catalysis, magnetism, luminescence proprieties etc. Those properties provide many possibilities to construct attractive multifunctional materials. Nowadays, there is considerable interest in chiral coordination polymers, owing to their potential application in asymmetric catalysis and chiral separation.[1]
Herein, we report the full structural study of two novel chiral Y(III) coordination polymers which have been synthesized via the hydrothermal route, by using a mixed-ligand system containing both chiral and achiral ligands. The crystal structure of these compounds was determined by single-crystal X-ray diffraction. They are extended in the 2D space, the 3D stability of the frameworks is provided through strong hydrogen bond interactions.

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