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The quest for ordered porosity in zirconium phosphonates: blood, sweat and tears (and powder X-ray diffraction)

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The chemistry of metal phosphonates has a long history, started in 1978 when the first examples of zirconium phosphonates were reported [1]. From the structural point of view, metal phosphonates often adopt dense layered or pillared-layered arrangements, with the organic moieties residing in the interlayer region, hardly accessible to potential guest species. In fact, most metal phosphonates are non-porous materials. When porosity is present, it is usually the result of a disordered assembly of the structure and lacks the specificity desirable for many applications, such as gas sorption/separation and catalysis [2].
The advent of metal-organic frameworks (MOFs), a class of porous and crystalline organic-inorganic materials, has sparked huge research interest, thanks to their high surface areas and well-defined pore size distribution. Most MOFs are based on carboxylate or N-heterocyclic linkers, and phosphonate-based MOFs only represent a rather small fraction of the thousands of MOF structures reported over the last 20 years [2]. Yet, the exceptional stability and insolubility of metal phosphonates are attractive features for practical employment.
This contribution is concerned with the challenging development of zirconium phosphonates possessing ordered porosity, starting from the design and synthesis of suitable polyphosphonic linkers to escape the ubiquitous dense layered motif, through the identification of the synthetic conditions to obtain sufficiently (micro)crystalline products, and ending with the ab initio determination of crystal structures from powder X-ray diffraction data [3].

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