STRUCTURE-PROPERTIES CORRELATIONS IN DIVALENT METAL PHOSPHONATES

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Crystalline metal phosphonates may offer acidic sites, structural flexibility and guest molecules (H\textsubscript{2}O, heterocycles, etc.) which can act as proton carriers. In addition, some frameworks are also amenable for post-synthesis modifications in order to enhance desired properties [1,2].

In this work, we present the synthesis and characterization of two hydroxyphosphonoacetates hybrids based on magnesium, \([\text{Mg}_5(\text{O}_3\text{PCHOHCOO})_2(\text{HO}_3\text{PCHOHCOO})_2\cdot 8\text{H}_2\text{O}]\), and zinc, \([\text{Zn}_6\text{K}(\text{O}_3\text{PCHOHCOO})_4(\text{OH})\cdot 6.5\text{H}_2\text{O}]\), prepared under hydrothermal conditions. Both solids present three-dimensional frameworks and their crystal structures were solved by \textit{ab initio} x-ray powder diffraction methods. Their thermal stability, crystal structures and proton conductivity properties will be reported and discussed.

\textbf{Figure 1.} Crystal structure of \([\text{Mg}_5(\text{O}_3\text{PCHOHCOO})_2(\text{HO}_3\text{PCHOHCOO})_2\cdot 8\text{H}_2\text{O}]\). Mg: green balls; P: orange balls; O: red balls; C: grey balls.

\textbf{Figure 2.} Polyhedra view of \([\text{Zn}_6\text{K}(\text{O}_3\text{PCHOHCOO})_4(\text{OH})\cdot 6.5\text{H}_2\text{O}]\) framework. Zn(1)O\textsubscript{6}, navy-blue octahedra; Zn(2)O\textsubscript{4}, sky-blue tetrahedra; Zn(3)O\textsubscript{5}, purple polyhedra; CPO\textsubscript{3}, green tetrahedra; O red balls; K, purple balls and C, yellow balls.

\textbf{References}
