STRUCTURE-PROPERTIES CORRELATIONS IN DIVALENT METAL PHOSPHONATES

Rosario M. P. Colodrero[a], Montse Bazaga-García[a], Pascual Olivera-Pastor[a], Enrique R. Losilla[a], Inés R. Salcedo[a], Miguel Ángel G. Aranda[b], Aurelio Cabeza[a].

[a] *Departamento Química Inorgánica, Campus de Teatinos s/n, Universidad de Málaga, 29071 Málaga, SPAIN.*
[b] *CELL ALBA Synchrotron radiation facility, Ctra. BP1413 km 3.3, 08290 Cerdanyola del Vallès, Barcelona, SPAIN.*
colodrero@uma.es

Crystalline metal phosphonates may offer acidic sites, structural flexibility and guest molecules (H_2O, heterocyclics, 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, $[Mg_5(O_3PCHOHCOO)_2(HO_3PCHOHCOO)_2{\cdot}8H_2O]$, and zinc, $[Zn_6K(O_3PCHOHCOO)_4(OH){\cdot}6.5H_2O]$, prepared under hydrothermal conditions. Both solids present three-dimensional frameworks and their crystal structures were solved by *ab initio* x-ray powder diffraction methods. Their thermal stability, crystal structures and proton conductivity properties will be reported and discussed.

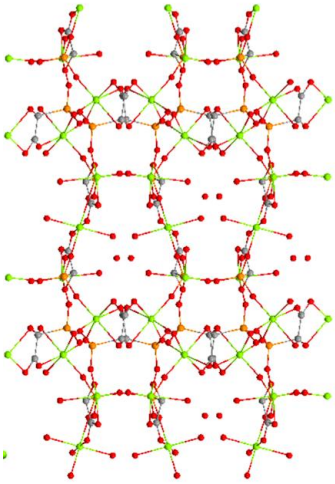

Figure 1. Crystal structure of $Mg_5(O_3PCHOHCOO)_2(HO_3PCHOHCOO)_2{\cdot}8H_2O$. Mg: green balls; P: orange balls; O: red balls; C: grey balls.

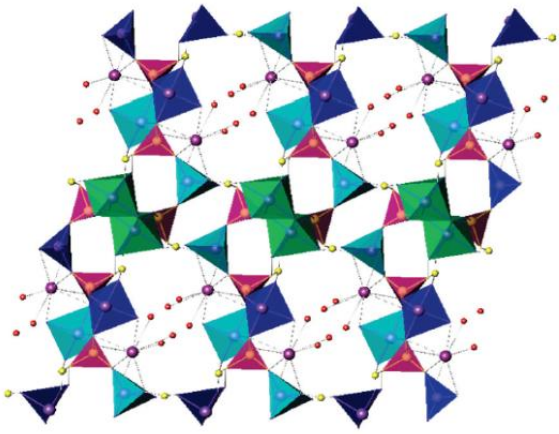

Figure 2. Polyhedra view of $Zn_6K[(O_3PCHOHCOO)_4(HO)]{\cdot}6.5(H_2O)$ framework. $Zn(1)O_6$, navy-blue octahedra; $Zn(2)O_4$, sky-blue tetrahedra; $Zn(3)O_5$, purple polyhedra; CPO3, green tetrahedra; O red balls; K, purple balls and C, yellow balls

References

[1] Ikawa, H. In *Proton Conductors*; Colomban, P., Ed.; Cambridge University Press: Cambridge, 1992; p. 511–515.

[2] Shimizu, G. K. H., Taylor, J. M. and Dawson, K.W. Metal Organophosphonate Proton Conductors. In *Metal Phosphonate Chemistry: From Synthesis to Applications*; Clearfield, A., Demadis, K.D., Eds.; RSC: Cambridge, 2012; Ch. 15; p 493–524.