

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 (H₂O, 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, [Mg₅(O₃PCHOHCOO)₂(HO₃PCHOHCOO)₂·8H₂O], and zinc, [Zn₆K(O₃PCHOHCOO)₄(OH)·6.5H₂O], 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.

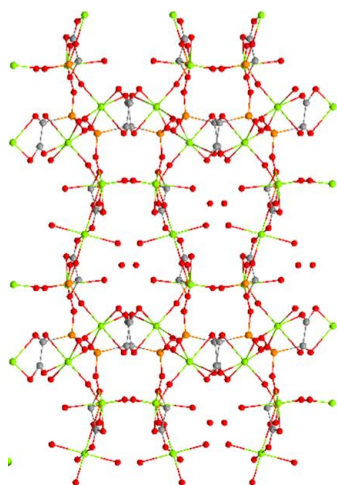


Figure 1. Crystal structure of Mg₅(O₃PCHOHCOO)₂(HO₃PCHOHCOO)₂·8H₂O. Mg: green balls; P: orange balls; O: red balls; C: grey balls.

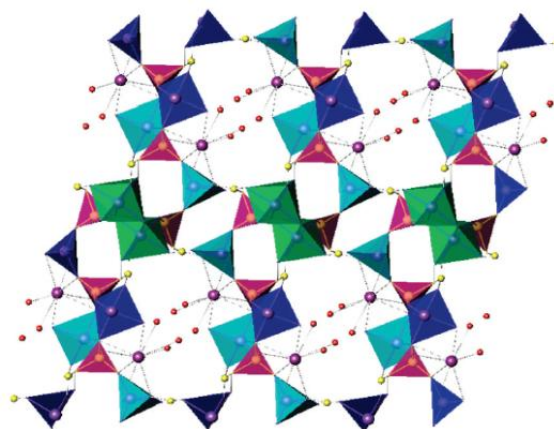


Figure 2. Polyhedra view of Zn₆K[(O₃PCHOHCOO)₄(OH)]·6.5(H₂O) framework. Zn(1)O₆, navy-blue octahedra; Zn(2)O₄, sky-blue tetrahedra; Zn(3)O₅, purple polyhedra; CPO₃, green tetrahedra; O red balls; K, purple balls and C, yellow balls

References

- [1] Ikawa, H. In *Proton Conductors*; Colombari, 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.