

## NEW MULTIFUNCTIONAL DIVALENT METAL-COORDINATED SULFOPHOSPHONATES: STRUCTURES AND PROTON CONDUCTIVITIES

M. Bazaga-García\*<sup>1</sup>, R.M.P. Colodrero<sup>1</sup>, I.R. Salcedo<sup>1</sup>, P. Olivera-Pastor<sup>1</sup>, A. Cabeza<sup>1</sup> and K.D. Demadis<sup>2</sup>

<sup>1</sup>Departamento de Química Inorgánica, Universidad de Málaga, SPAIN

*m.bazaga@uma.es\**, *colodrero@uma.es*, *inesrs@uma.es*, *poliverap@uma.es*, *aurelio@uma.es*

<sup>2</sup>Department of Chemistry, University of Crete, GREECE

*demadis@uoc.gr*

**Abstract:** Metal phosphonate-based coordination polymers are structurally versatile multifunctional compounds that may contain a number of acidic groups such as P-OH; SO<sub>3</sub>H, COOH, N<sup>+</sup>-H... These features result in formation of extended H-bond networks and confer proton conducting properties.

In this work, the crystal structures resulting from the combination of the amino-sulfophosphonate ligand (H<sub>2</sub>O<sub>3</sub>PCH<sub>2</sub>)<sub>2</sub>-N-(CH<sub>2</sub>)<sub>2</sub>-SO<sub>3</sub>H with different divalent metal ion, are reported. Optimal synthesis conditions were implemented by microwave methodology and high through-put screening. For copper derivatives, single-crystal data were employed. While for Mn(II) derivative the crystal structure was solved *ab initio* from synchrotron X-ray powder diffraction data. The arrangement of the sulfonic groups determines a wide variety of metal-ligand coordination modes and the creation of efficient hydrogen bonding networks for proton transport, as has been observed for other lanthanide derivatives<sup>1</sup>. For copper derivatives the presence of an auxiliary ligand (1,10-phenanthroline, 2,2'-bipyridine or 4,4'-bipyridine) were required to obtain a crystalline compound. As a consequence of this structural variability, different H bond networks can be generated leading to a wide range of proton conductivity values.

**Key words:** coordination polymers, sulfophosphonates, proton-conductivity

**Acknowledgments:** ALBA synchrotron is thanked for providing synchrotron beamtime at BL04-MSPD beamline. This research was supported by MAT2016-77648R and PID2019-110249RB-I00 research grant (Spain) and University of Malaga under Plan Propio de Investigación.

### References:

1. Bazaga-García, M., Salcedo, I. R., Colodrero, R.M. P., Xanthopoulos, K., Villemin, D., Stock, N., López-González, M., del Río, C., Losilla, E.R., Cabeza, A., Demadis, K.D., Olivera-Pastor, P. Layered Lanthanide Sulfophosphonates and Their Proton Conduction Properties in Membrane Electrode Assemblies (2019). *Chemistry of Materials*, 31 (23), 9625-9634.